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Special issue :

Proceedings of
National Conference on Molecular Docking (Series I):
Phytochemicals against Herpes
10-12 June 2019

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Botany and Zoology Departments
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THE VISION

Objective

The distressing threat of viral diseases to human beings raises a serious concern worldwide. New viral diseases have been reported continuously with severe health issues, and the lack of effective antiviral treatment makes them more severe. Nowadays, the development of effective treatment and antivirals against virus has become difficult, due to the ability of viruses to mutate their genome and become resistant to drugs. Moreover, the antiviral drugs also exhibit adverse side effects, which directly and indirectly affect the human health. This leads towards the development of plant-based drugs and herbal treatments with minimal side effects.

Being partnered with the DASSAULT SYSTEMES, we employed *in silico* molecular docking approaches using Discovery Studio suite and performed virtual screenings to identify phytochemicals against HSV. Post graduate students of biological sciences actively participated and have presented their work in the conference.

Introduction

Herpes simplex virus (HSV) infections are among the infections most frequently encountered by humans (Whitley et al., 2001). Two types of HSV infections have been identified-HSV-1, which usually causes orolabial disease, and HSV-2, which is associated more frequently with genital and newborn infections (Whitley and Gnann 1992; El-Toumy 2018). Usually, HSV causes mild and self-limited disease of the mouth and lips or at genital sites. However, on occasion, the disease can be life-threatening. Such is the case with neonatal HSV infection and HSV infections of the central nervous system. Some of the viral diseases can be cured by approved antiviral drugs, but for others still do not have any vaccines or drugs available. Most of the approved antiviral drugs are somehow directly or indirectly associated with side effects, which eventually raise the need for the development of antivirals based on natural phytochemicals (Lakeman et al., 1995; Perry et al., 1996). Globally, the development of antivirals is shifting towards the plant-derived products as they are less toxic and has less chance to develop resistance (Balfour 1998). Phytochemicals have been exploited traditionally for the cure of many diseases, and also have been reported to inhibit viral replication/transcription (Anand et al., 2003; Aati 2020). Most of them inhibit the viruses either during the viral entry inside the host cell or during their replication. Moreover, 50% of the drugs derived from plants are being used in the Western nations (DeLano 2002). Plants have a variety of phytochemicals like flavonoids, terpenoids, lignins, alkaloids, and coumarins that are having antioxidant activity, and help to inhibit viral genome (Dallakyan et al., 2015; Alamri 2020).

Viral Protein Structure and Phytochemical dataset collection

The 3D structure of the viral protein was accessed from Protein Data Bank with accessions 1AT3, 1KIM and 3M1C (Figure 1). Phytochemicals present in different plants (Figure 2) were obtained and consequently both the protein and the ligands were used for *in silico* analysis.

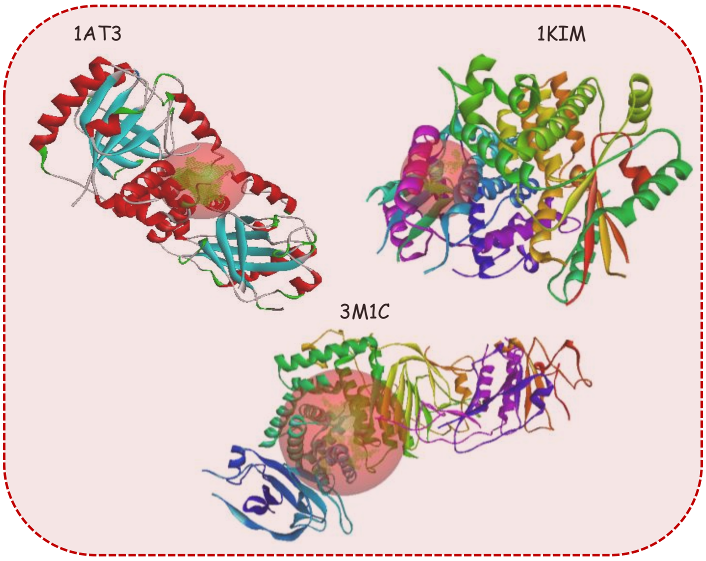

Figure 1. Different enzymes present in Herpes virus

Molecular docking

For the *in silico* molecular docking, BIOVIA's Discovery Studio docking suite was used for molecular docking. The catalytic pocket of the viral proteins were specified and targeted for binding of the ligand(s). -CDOCKER Energy and -CDOCKER Interaction Energy signify the affinity of the ligands with the protein receptors. Basically, high positive values of the CDOCKER Energy, CDOCKER Interaction Energy and a diminutive difference between the -CDOCKER Energy and -CDOCKER Interaction Energy are considered to be the most favourable. Discovery Studio is a software suite for performing computational analysis of data relevant to Life Sciences research. The product itself comprises several distinct, but tightly integrated, functional layers. It consists of a set of products that enable researchers to capture, access, and analyze scientific data. By using common underlying technologies and data models, the software allows the full range of methodologies used in modern research to be seamlessly combined to solve diverse computational problems. The Discovery Studio Visualizer is a powerful desktop application for viewing and editing molecular structures, sequences, and other data relevant to Life Sciences research. It provides a convenient interface for everyday data analysis tasks. The Visualizer supports a wide variety of industry-standard formats. A set of integrated analysis functions are provided that allows you to compute basic properties of molecules and sequences. The Visualizer also provides access to the Discovery Script Perl Application Programming Interface (API), which enables to create new analysis tools and to automate common tasks.

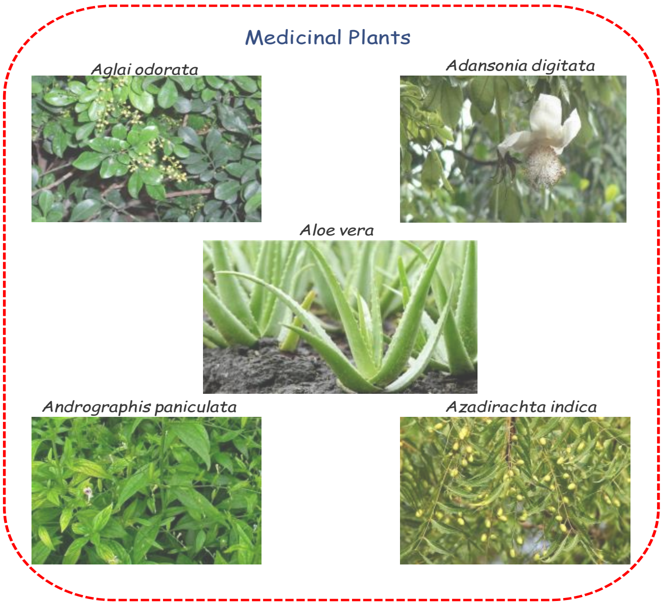

Figure 2. Plants that can fight against Herpes virus

Conclusion

A substantial number of plant extracts and phytochemicals have been explored for antiviral property. Herbal preparations owing to their holistic approach strengthen the body's immune system, which in turn may help the body fight against invading infectious viruses. Herbal antiviral compounds, which are accessible and do not require laborious pharmaceutical synthesis are emerging as interesting alternatives in today's world of growing resistance to antiviral drug therapy. Many promising herbal treatments exist for viral diseases with proof of their efficacy and safety in advanced clinical trials. However, a lot of work still remains to be done to determine optimal treatments, doses, and formulae for those herbal preparations. Although, herbal plant preparations are widely used in several parts of the world, individually or in combination, data about the interactions of these medicinal plants in living system is non-existent. Therefore, the traditional medicine practice should be clubbed with scientific research facilitating modern drug discovery from phytochemicals. Scientific data pertaining to detailed pharmacokinetic and pharmacodynamics of medicinal plants and their preparations should be made available to researchers and policy makers so that larger randomized multicenter clinical trials may be designed and conducted. By adopting such approaches, the idea of incorporating and implementing a particular herbal formulation in routine therapy may be transformed into reality.

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Activity of Pandanus amaryllifolius against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Sk Imran[1], Debashish Tripathy[2]

[1]180705180024@cutm.ac.in

[2]debashish.tripathy@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Pandanus amaryllifolius against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Ellagic acid helped to prevent Herpes.

Introduction: Pandanus amaryllifolius is known for its medicinal activities. The leaves are used in the perfume industry and traditional medicine to treat diseases like cough, asthma, herpes and diarrhea.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Pandanales
Family	Pandanaceae
Genus	Pandanus
Species	amaryllifolius

Major phytochemicals present in the plant are:

a. Ellagic acid
b. Gallic acid
c. Peonidin
d. Limonene

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Ellagic acid	-12.34	-15.39	Positive
Gallic acid	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Limonene	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ellagic acid helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Pandanus amaryllifolius can prevent Herpes due to the presence of Ellagic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Adansonia digitata against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Aishwarya Dash[1], Debashish Tripathy[2]

[1]adash8116@gmail.com

[2]debashish.tripathy@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Adansonia digitata against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Capsaicin helped to prevent Herpes.

Introduction: Adansonia digitata is known for its medicinal activities. The various parts of the plant (leaves, bark and seeds) are used to cure tuberculosis, fever, microbial infections, diarrhea and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Malvales
Family	Bombacaceae
Genus	Adansonia
Species	digitata

Major phytochemicals present in the plant are:

a. Resveratrol
b. Phenyl isothiocyanate
c. Capsaicin
d. Peonidin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Resveratrol	Not Applicable	Not Applicable	Failed
Phenyl isothiocyanate	Not Applicable	Not Applicable	Failed
Capsaicin	-11.05	-18.36	Positive
Peonidin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Capsaicin helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Adansonia digitata can prevent Herpes due to the presence of Capsaicin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Aglai odorata against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Krishna Subedita Jena[1], Debashish Tripathy[2]

[1]180705180026@cutm.ac.in

[2]debashish.tripathy@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Aglai odorata against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Myricetin helped to prevent Herpes.

Introduction: Aglai odorata is known for its medicinal activities. Aglaia species are used in traditional medicine: leaves to treat wounds, fever, headache, asthma, jaundice, and as a tonic e.g. after childbirth; flowers against fever, asthma, jaundice and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Sapindales
Family	Meliaceae
Genus	Aglai
Species	odorata

Major phytochemicals present in the plant are:

a. Morphine
b. Myricetin
c. Peonidin
d. Benzyl isothiocyanate

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Morphine	Not Applicable	Not Applicable	Failed
Myricetin	-9.66	-12.81	Positive
Peonidin	Not Applicable	Not Applicable	Failed
Benzyl isothiocyanate	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Myricetin helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Aglai odorata can prevent Herpes due to the presence of Myricetin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Aloe vera against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Bijan Kumar Patra[1], Sujit Mishra[2]

[1]patramail1998@gmail.com

[2]sujit.mishra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Aloe vera against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Salicylic acid helped to prevent Herpes.

Introduction: Aloe vera is known for its medicinal activities. Aloe vera used to cure herpes, weak digestion, general weakness, anaemia, bloating, stomach ulcers and gum disease.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Liliopsida
Order	Liliales
Family	Aloeaceae
Genus	Aloe
Species	vera

Major phytochemicals present in the plant are:

a. Phytoene
b. Salicylic acid
c. Sitosterol
d. Lupeol

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Phytoene	Not Applicable	Not Applicable	Failed
Salicylic acid	-14.28	-18.22	Positive
Sitosterol	Not Applicable	Not Applicable	Failed
Lupeol	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Salicylic acid helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Aloe vera can prevent Herpes due to the presence of Salicylic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Andrographis paniculata against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Sasmita Patra[1], Sujit Mishra[2]

[1]mail2sasmita98@gmail.com

[2]sujit.mishra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Andrographis paniculata against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Genistein helped to prevent Herpes.

Introduction: Andrographis paniculata is known for its medicinal activities. A. paniculata has been used in Siddha and Ayurvedic medicine. It is promoted as a dietary supplement for cancer prevention and cure. In the traditional medicine of India, A. paniculata has also been used for jaundice therapy.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Lamiales
Family	Acanthaceae
Genus	Andrographis
Species	paniculata

Major phytochemicals present in the plant are:

a. Genistein
b. Daidzein
c. Theobromine
d. Quercetin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Genistein	-12.55	-15.45	Positive
Daidzein	Not Applicable	Not Applicable	Failed
Theobromine	Not Applicable	Not Applicable	Failed
Quercetin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Genistein helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Andrographis paniculata can prevent Herpes due to the presence of Genistein. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Atlantia sp. against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Biaisali Basabadutta Baliarsingh[1], Sujit Mishra[2]

[1]baisalibasabadutta@gmail.com

[2]sujit.mishra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Atlantia sp. against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Ellagic acid helped to prevent Herpes.

Introduction: Atlantia sp. is known for its medicinal activities. The flowers, fruit and roots are used to cure herpes, jaundice, fever, headache and asthma.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Sapindales
Family	Rutaceae
Genus	Atalantia
Species	racemosa

Major phytochemicals present in the plant are:

a. Allicin
b. Ajoene
c. Gallic acid
d. Ellagic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Allicin	Not Applicable	Not Applicable	Failed
Ajoene	Not Applicable	Not Applicable	Failed
Gallic acid	Not Applicable	Not Applicable	Failed
Ellagic acid	-11.84	-21.37	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ellagic acid helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Atlantia sp. can prevent Herpes due to the presence of Ellagic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Azadirachta indica against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Lopamudra Ojha[1], Sujit Mishra[2]

[1]lopamudraojha96@gmail.com

[2]sujit.mishra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Azadirachta indica against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Tocopherol helped to prevent Herpes.

Introduction: Azadirachta indica is known for its medicinal activities. Neem has an anti-inflammatory property which helps reduces acne, herpes, skin blemishes and malaria.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Sapindales
Family	Meliaceae
Genus	Azadirachta
Species	indica

Major phytochemicals present in the plant are:

a. Tocopherol
b. Isorhamnetin
c. Rutin
d. Azadirichtin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tocopherol	-11.51	-19.38	Positive
Isorhamnetin	Not Applicable	Not Applicable	Failed
Rutin	Not Applicable	Not Applicable	Failed
Azadirichtin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Tocopherol helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Azadirachta indica can prevent Herpes due to the presence of Tocopherol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Barleria lupulina against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Aditya Satapathy[1], Sujit Mishra[2]

[1]180705180031@cutm.ac.in

[2]sujit.mishra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Barleria lupulina against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Epicatechin helped to prevent Herpes.

Introduction: Barleria lupulina is known for its medicinal activities. The flowers are used internally for the treatment of migraine, internal abscesses, oedema, haemoptysis, herpes, urethral discharges, seminal disorders and reduce obesity.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Scrophulariales
Family	Acanthaceae
Genus	Barleria
Species	lupulina

Major phytochemicals present in the plant are:

a. Hesperidin
b. Epicatechin
c. Coumarin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Hesperidin	Not Applicable	Not Applicable	Failed
Epicatechin	-12.11	-19.08	Positive
Coumarin	Not Applicable	Not Applicable	Failed
Ferulic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Epicatechin helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Barleria lupulina can prevent Herpes due to the presence of Epicatechin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Bauhinia racemosa against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Prachipadma Sahoo[1], Sujit Mishra[2]

[1]prachipadmasahoo@gmail.com

[2]sujit.mishra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Bauhinia racemosa against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Tannic acid helped to prevent Herpes.

Introduction: Bauhinia racemosa is known for its medicinal activities. Bauhinia racemosa leaves have been used in the treatment of asthma traditionally because of their antihistaminic action it also used to cure herpes and urethral discharges.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Equisetopsida
Order	Fabales
Family	Fabaceae
Genus	Bauhinia
Species	racemosa

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Digoxin
c. Rosmarinic acid
d. Tannic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Digoxin	Not Applicable	Not Applicable	Failed
Rosmarinic acid	Not Applicable	Not Applicable	Failed
Tannic acid	-9.67	-16.18	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Tannic acid helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Bauhinia racemosa can prevent Herpes due to the presence of Tannic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Bauhinia variegate against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Nibedita Patra[1], Sujit Mishra[2]

[1]180705180033@cutm.ac.in

[2]sujit.mishra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Bauhinia variegate against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Lycopene helped to prevent Herpes.

Introduction: Bauhinia variegate is known for its medicinal activities. The bark decoction is used for diarrhoea control, as an astringent alternative and for treating scrofula, herpes, skin diseases and ulcers.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Equisetopsida
Order	Fabales
Family	Fabaceae
Genus	Bauhinia
Species	variegata

Major phytochemicals present in the plant are:

a. Cryptoxanthin
b. Carotene
c. Lutein
d. Lycopene

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Cryptoxanthin	Not Applicable	Not Applicable	Failed
Carotene	Not Applicable	Not Applicable	Failed
Lutein	Not Applicable	Not Applicable	Failed
Lycopene	-9.63	-17.95	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Lycopene helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Bauhinia variegate can prevent Herpes due to the presence of Lycopene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Bidens pilosa against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Priyanka Dash[1], Sujit Mishra[2]

[1]priyankadash240197@gmail.com

[2]sujit.mishra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Bidens pilosa against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Apigenin helped to prevent Herpes.

Introduction: Bidens pilosa is known for its medicinal activities. Roots, leaves and seed have been reported to possess antibacterial, antidysenteric, anti-inflammatory, antimicrobial, herpes, antimalarial, diuretic, hepato-protective and hypotensive activities.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Asterales
Family	Asteraceae
Genus	Bidens
Species	pilosa

Major phytochemicals present in the plant are:

a. Eugenol
b. Apigenin
c. Luteolin
d. Carnosic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Eugenol	Not Applicable	Not Applicable	Failed
Apigenin	-12.18	-19.37	Positive
Luteolin	Not Applicable	Not Applicable	Failed
Carnosic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Apigenin helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Bidens pilosa can prevent Herpes due to the presence of Apigenin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Cedrus libani against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Diksha Mohanta[1], Sujit Mishra[2]

[1]mohantadiksha58@gmail.com

[2]sujit.mishra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Cedrus libani against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Eugenol helped to prevent Herpes.

Introduction: Cedrus libani is known for its medicinal activities. It is traditionally used to treat diseases like arteriosclerosis, water retention, herpes, lymphatic damage, etc.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Pinopsida
Order	Pinales
Family	Pinaceae
Genus	Cedrus
Species	libani

Major phytochemicals present in the plant are:

a. Luteolin
b. Carnosic acid
c. Eugenol
d. Salicylic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Luteolin	Not Applicable	Not Applicable	Failed
Carnosic acid	Not Applicable	Not Applicable	Failed
Eugenol	-14.09	-19.22	Positive
Salicylic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Eugenol helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Cedrus libani can prevent Herpes due to the presence of Eugenol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Cissus quadrangularis against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Barsha Nayak[1], Sujit Mishra[2]

[1]barshanayak73@gmail.com

[2]sujit.mishra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Cissus quadrangularis against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Naringin helped to prevent Herpes.

Introduction: Cissus quadrangularis is known for its medicinal activities. The roots and stems are most useful for healing of fracture of the bones. The stem is bitter; it is given internally and applied topically in broken bones, used in complaints of the back and spine. A paste of stem is useful for muscular pains and herpes. The plant has been documented in Ayurveda for the treatment of osteoarthritis, rheumatoid arthritis and osteoporosis.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Vitales
Family	Vitacea
Genus	Cissus
Species	quadrangularis

Major phytochemicals present in the plant are:

a. Lupeol
b. Ferulic acid
c. Hesperidin
d. Naringin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lupeol	Not Applicable	Not Applicable	Failed
Ferulic acid	Not Applicable	Not Applicable	Failed
Hesperidin	Not Applicable	Not Applicable	Failed
Naringin	-11.84	-19.14	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Naringin helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Cissus quadrangularis can prevent Herpes due to the presence of Naringin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Conyza aegyptica against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Ashima Mishra[1], Pankaj Meher[2]

[1]ashimamishra4040@gmail.com

[2]pankaj.meher@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Conyza aegyptica against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Limonene helped to prevent Herpes.

Introduction: Conyza aegyptica is known for its medicinal activities. The whole plants used to treat herpes, wound, skin diseases and toothache.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Dicotyledonae
Order	Asterales
Family	Asteraceae
Genus	Conyza
Species	aegyptiaca

Major phytochemicals present in the plant are:

a. Theobromine
b. Epicatechin
c. Catechin
d. Limonene

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	Not Applicable	Not Applicable	Failed
Epicatechin	-16.33	-22.34	Positive
Catechin	Not Applicable	Not Applicable	Failed
Limonene	-11.88	-18.91	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Limonene helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Conyza aegyptica can prevent Herpes due to the presence of Limonene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Cyperus rotundus against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Manoranjan Behera[1], Pankaj Meher[2]

[1]180705180038@cutm.ac.in

[2]pankaj.meher@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Cyperus rotundus against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Ellagic acid and Pelargonidin helped to prevent Herpes.

Introduction: Cyperus rotundus is known for its medicinal activities. It is a medicinal herb traditionally used to treat various clinical conditions at home such as diarrhea, diabetes, pyresis, herpes, inflammation, malaria, and stomach and bowel disorders.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Poales
Family	Cyperaceae
Genus	Cyperus
Species	rotundus

Major phytochemicals present in the plant are:

a. Ellagic acid
b. Gallic acid
c. Pelargonidin
d. Limonene

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Ellagic acid	-16.81	-20.37	Positive
Gallic acid	Not Applicable	Not Applicable	Failed
Pelargonidin	-11.04	-18.46	Positive
Limonene	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ellagic acid and Pelargonidin helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Cyperus rotundus can prevent Herpes due to the presence of Ellagic acid and Pelargonidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Euphorbia peplus against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Lopita Mishra[1], Pankaj Meher[2]

[1]180705180039@cutm.ac.in

[2]pankaj.meher@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Euphorbia peplus against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Lutein and Digoxin helped to prevent Herpes.

Introduction: Euphorbia peplus is known for its medicinal activities. The plant is administered in the form of herbal tea as diuretic, laxative and emollient. It is also used for the treatment of asthma and bronchitis, as it relaxes the smooth muscles of bronchi. It is recommended against dry cough, herpes, runny nose and liver diseases.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Malpighiales
Family	Euphorbiaceae
Genus	Euphorbia
Species	peplus

Major phytochemicals present in the plant are:

a. Lutein
b. Digoxin
c. Tannic acid
d. Theobromine

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lutein	-12.34	-14.39	Positive
Digoxin	-9.67	-15.01	Positive
Tannic acid	Not Applicable	Not Applicable	Failed
Theobromine	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Lutein and Digoxin helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Euphorbia peplus can prevent Herpes due to the presence of Lutein and Digoxin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Glycyrrhiza glabra against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Sujata Prusty[1], Pankaj Meher[2]

[1]sujataprusty898@gmail.com

[2]pankaj.meher@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Glycyrrhiza glabra against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Tangeretin helped to prevent Herpes.

Introduction: Glycyrrhiza glabra is known for its medicinal activities. Traditionally used to treat many diseases, such as respiratory disorders, hyperdipsia, epilepsy, fever, sexual debility, paralysis, stomach ulcers, rheumatism, skin diseases, hemorrhagic diseases, and jaundice.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Fabales
Family	Fabaceae
Genus	Glycyrrhiza
Species	glabra

Major phytochemicals present in the plant are:

a. Pelletierine
b. Alliin
c. Tangeretin
d. Campesterol

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	Not Applicable	Not Applicable	Failed
Alliin	Not Applicable	Not Applicable	Failed
Tangeretin	-12.08	-18.39	Positive
Campesterol	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Tangeretin helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Glycyrrhiza glabra can prevent Herpes due to the presence of Tangeretin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Heliotropium marifolium against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Biren Pattanaik[1], Pankaj Meher[2]

[1]birenpattanaik51@gmai9l.com

[2]pankaj.meher@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Heliotropium marifolium against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Linamarin helped to prevent Herpes.

Introduction: Heliotropium marifolium is known for its medicinal activities. Heliotropium marifolium is used against syphilis, asthma, herpes, UTI and wound.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Boraginales
Family	Boraginaceae
Genus	Heliotropium
Species	marifolium

Major phytochemicals present in the plant are:

a. Campesterol
b. Linamarin
c. Naringin
d. Pelargonidin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Campesterol	Not Applicable	Not Applicable	Failed
Linamarin	-14.89	-19.42	Positive
Naringin	Not Applicable	Not Applicable	Failed
Pelargonidin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Linamarin helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Heliotropium marifolium can prevent Herpes due to the presence of Linamarin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Holoptelea integrifolia against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Tejaswini Pradhan[1], Pankaj Meher[2]

[1]pradhantejaswini12@gmail.com

[2]pankaj.meher@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Holoptelea integrifolia against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Malvidin helped to prevent Herpes.

Introduction: Holoptelea integrifolia is known for its medicinal activities. The plant Holoptelea integrifolia is used traditionally for the treatment of inflammation, gastritis, dyspepsia, colic, intestinal worms, vomiting, wound healing, leprosy, diabetes, hemorrhoids, herpes, dysmenorrhea, and rheumatism.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Rosales
Family	Ulmaceae
Genus	Holoptelea
Species	integrifolia

Major phytochemicals present in the plant are:

a. Naringin
b. Limonene
c. Glutathione
d. Malvidin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Naringin	Not Applicable	Not Applicable	Failed
Limonene	Not Applicable	Not Applicable	Failed
Glutathione	Not Applicable	Not Applicable	Failed
Malvidin	-16.33	-19.84	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Malvidin helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Holoptelea integrifolia can prevent Herpes due to the presence of Malvidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Houttuynia cordata against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Krishna Kalyani Lar[1], Pankaj Meher[2]

[1]krishnakar6410@gmail.com

[2]pankaj.meher@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Houttuynia cordata against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Tangeretin and Limonene helped to prevent Herpes.

Introduction: Houttuynia cordata is known for its medicinal activities. It is used as a fresh herbal garnish. In northeastern India, it is commonly used in salads and as a garnish over side dishes. The tender roots can also be ground into chutneys along with dry meat or fish, chilies, and tamarind. It is taken raw as salad and cooked along with fish as fish curry. In Japan and Korea, its dried leaves may be used as a tea. Houttuynia cordata was used in traditional Chinese medicine.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Piperales
Family	Saururaceae
Genus	Houttuynia
Species	cordata

Major phytochemicals present in the plant are:

a. Tangeretin
b. Salicylic acid
c. Limonene
d. Naringin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tangeretin	-12.38	-15.67	Positive
Salicylic acid	Not Applicable	Not Applicable	Failed
Limonene	-11.44	-16.82	Positive
Naringin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Tangeretin and Limonene helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Houttuynia cordata can prevent Herpes due to the presence of Tangeretin and Limonene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Hypericum hookerianum against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Bijayalaxmi Sahu[1], Pankaj Meher[2]

[1]bijayalaxmisahu4444@gmail.com

[2]pankaj.meher@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Hypericum hookerianum against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Salicylic acid and Astaxanthin helped to prevent Herpes.

Introduction: Hypericum hookerianum is known for its medicinal activities. It was recommended in the first century by Greek physicians as a diuretic, wound-healer, and treatment for menstrual disorders. It has been used as an anti-inflammatory, anti-bacterial, disinfectant, and a remedy for disorders of the respiratory tract and gall bladder and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Malpighiales
Family	Hypericaceae
Genus	Hypericum
Species	hookerianum

Major phytochemicals present in the plant are:

a. Malvidin
b. Salicylic acid
c. Ursolic acid
d. Astaxanthin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Malvidin	Not Applicable	Not Applicable	Failed
Salicylic acid	-12.37	-17.08	Positive
Ursolic acid	Not Applicable	Not Applicable	Failed
Astaxanthin	-11.38	-17.22	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Salicylic acid and Astaxanthin helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Hypericum hookerianum can prevent Herpes due to the presence of Salicylic acid and Astaxanthin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Hypericum mysorense against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Subhakant Khandual[1], Pankaj Meher[2]

[1]18070518045@cutm.ac.in

[2]pankaj.meher@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Hypericum mysorense against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Ursolic acid and Astaxanthin helped to prevent Herpes.

Introduction: Hypericum mysorense is known for its medicinal activities. Hypericum mysorense has been used to treat wounds and herpes as part of the Ayurvedic system of traditional medicine.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Equisetopsida
Order	Malpighiales
Family	Hypericaceae
Genus	Hypericum
Species	mysorense

Major phytochemicals present in the plant are:

a. Ursolic acid
b. Astaxanthin
c. Sitosterol
d. Astaxanthin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Ursolic acid	-15.02	-18.34	Positive
Astaxanthin	Not Applicable	Not Applicable	Failed
Sitosterol	Not Applicable	Not Applicable	Failed
Astaxanthin	-11.84	-19.63	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ursolic acid and Astaxanthin helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Hypericum mysorense can prevent Herpes due to the presence of Ursolic acid and Astaxanthin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Lippia alba against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Banaja Prakashini Samantaray[1], Pankaj Meher[2]

[1]banajaprakashini@gmail.com

[2]pankaj.meher@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Lippia alba against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Caffeine and Ascorbic acid helped to prevent Herpes.

Introduction: Lippia alba is known for its medicinal activities. A tea made from the leaves is used to treat intestinal and respiratory disturbances, including influenza and herpes. A well-sugared infusion is drunk to bring relief of heart problems and to soothe tachycardia.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Equisetopsida
Order	Lamiales
Family	Verbenaceae
Genus	Lippia
Species	alba

Major phytochemicals present in the plant are:

a. Pelargonidin
b. Caffeine
c. Curcumin
d. Ascorbic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelargonidin	Not Applicable	Not Applicable	Failed
Caffeine	-14.22	-16.33	Positive
Curcumin	Not Applicable	Not Applicable	Failed
Ascorbic acid	-11.37	-14.95	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Caffeine and Ascorbic acid helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Lippia alba can prevent Herpes due to the presence of Caffeine and Ascorbic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Melia azaderach against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Ashish Champathy[1], Shantanu Bhattacharya[2]

[1]180705180048@cutm.ac.in

[2]shantanu.bhattacharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Melia azaderach against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Zingiberene helped to prevent Herpes.

Introduction: Melia azaderach is known for its medicinal activities. The leaf juice is anthelmintic, antilithic, diuretic, herpes and emmenagogue.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Sapindales
Family	Meliaceae
Genus	Melia
Species	azedarach

Major phytochemicals present in the plant are:

a. Zingiberene
b. Ursolic acid
c. Astaxanthin
d. Digoxin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Zingiberene	-9.66	-12.84	Positive
Ursolic acid	Not Applicable	Not Applicable	Failed
Astaxanthin	Not Applicable	Not Applicable	Failed
Digoxin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Zingiberene helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Melia azaderach can prevent Herpes due to the presence of Zingiberene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Mentha piperata against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Pratyasa Pradhan[1], Shantanu Bhattacharya[2]

[1]pratyasapradhan@gmail.com

[2]shantanu.bhattacharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Mentha piperata against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Sulforaphane and Tannic acid helped to prevent Herpes.

Introduction: Mentha piperata is known for its medicinal activities. It is used for treatment of a variety of conditions, including irritable bowel syndrome (IBS), nausea, herpes and other digestive issues, as well as the common cold and headaches.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Lamiales
Family	Lamiaceae
Genus	Mentha
Species	piperata

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Carotene
c. Digoxin
d. Tannic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	-10.95	-15.66	Positive
Carotene	Not Applicable	Not Applicable	Failed
Digoxin	Not Applicable	Not Applicable	Failed
Tannic acid	-14.38	-19.33	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Sulforaphane and Tannic acid helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Mentha piperata can prevent Herpes due to the presence of Sulforaphane and Tannic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Momordia charantia against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Bibhuprasad Mishra[1], Shantanu Bhattacharya[2]

[1]180705180050@cutm.ac.in

[2]shantanu.bhattacharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Momordia charantia against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Curcumin helped to prevent Herpes.

Introduction: Momordia charantia is known for its medicinal activities. Juice of the leaves is used to treat piles and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Cucurbitales
Family	Cucurbitaceae
Genus	Momordia
Species	charantia

Major phytochemicals present in the plant are:

a. Curcumin
b. Ascorbic acid
c. Sulforaphane
d. Digoxin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Curcumin	-15.84	-17.92	Positive
Ascorbic acid	Not Applicable	Not Applicable	Failed
Sulforaphane	Not Applicable	Not Applicable	Failed
Digoxin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Curcumin helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Momordia charantia can prevent Herpes due to the presence of Curcumin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Moringa oleifera against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Madhuchhanda Samantaray[1], Shantanu Bhattacharya[2]

[1]madhuchhandasamantaraymadhu17@gmail.com

[2]shantanu.bhattacharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Moringa oleifera against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Lycopene helped to prevent Herpes.

Introduction: Moringa oleifera is known for its medicinal activities. Various parts of this plant such as the leaves, roots, seed, bark, fruit, flowers and immature pods act as cardiac and circulatory stimulants, possess antitumor, antipyretic, antiepileptic, antiinflammatory, herpes, antiulcer, antispasmodic, diuretic, antihypertensive, cholesterol lowering.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Brassicales
Family	Moringaceae
Genus	Moringa
Species	oleifera

Major phytochemicals present in the plant are:

a. Isorhamnetin
b. Rosmarinic acid
c. Lutein
d. Lycopene

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Isorhamnetin	Not Applicable	Not Applicable	Failed
Rosmarinic acid	Not Applicable	Not Applicable	Failed
Lutein	Not Applicable	Not Applicable	Failed
Lycopene	-13.11	-17.29	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Lycopene helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Moringa oleifera can prevent Herpes due to the presence of Lycopene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Myrica rubra against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Sushree Sangita Das[1], Shantanu Bhattacharya[2]

[1]180705180052@cutm.ac.in

[2]shantanu.bhattacharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Myrica rubra against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Mangiferin helped to prevent Herpes.

Introduction: Myrica rubra is known for its medicinal activities. The stem bark is used as a wash in the treatment of arsenic poisoning, skin diseases, wounds and ulcers. The fruit is carminative, herpes, pectoral and stomachic.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Fagales
Family	Myricaceae
Genus	Myrica
Species	rubra

Major phytochemicals present in the plant are:

a. Theobromine
b. Tannic acid
c. Mangiferin
d. Digoxin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	Not Applicable	Not Applicable	Failed
Tannic acid	Not Applicable	Not Applicable	Failed
Mangiferin	-18.32	-24.39	Positive
Digoxin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Mangiferin helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Myrica rubra can prevent Herpes due to the presence of Mangiferin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Neerium indicum against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Subham Nanda[1], Shantanu Bhattacharya[2]

[1]subhamnanda97@gmail.com

[2]shantanu.bhattacharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Neerium indicum against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Curcumin helped to prevent Herpes.

Introduction: Neerium indicum is known for its medicinal activities. Nerium indicum has many medicinal properties like bitter, acrid, astringent, anthelmintic, aphrodisiac, stomachic, febrifuge, diuretic, emetic, expectorant, cardio tonic, anticancer etc which is used in the treatment of cardiac asthma, renal and vesicle calculi, chronic stomach, skin related problems, snake bites joint pains, leprosy, cancer, ulcers etc. Leaves and flowers are also used to treat malaria. Leaves and bark is treated as insecticide, rat poison and parasitic.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Gentianales
Family	Apocynaceae
Genus	Nerium
Species	indicum

Major phytochemicals present in the plant are:

a. Myricetin
b. Peonidin
c. Curcumin
d. Ascorbic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Myricetin	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Curcumin	-14.58	-19.63	Positive
Ascorbic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Curcumin helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Neerium indicum can prevent Herpes due to the presence of Curcumin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Peganum harmala against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Saloni Mohanty[1], Dojalisa Sahu[2]

[1]saloni.mohanty10@gmail.com

[2]dojalisa.sahu@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Peganum harmala against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Quercetin helped to prevent Herpes.

Introduction: Peganum harmala is known for its medicinal activities. It has been used as an analgesic, emmenagogue, and abortifacient agent. Leaf was used to cure herpes. In a certain region of India the root was applied to kill body lice.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Sapindales
Family	Nitrariaceae
Genus	Peganum
Species	harmala

Major phytochemicals present in the plant are:

a. Genistein
b. Myricetin
c. Theobromine
d. Quercetin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Genistein	Not Applicable	Not Applicable	Failed
Myricetin	Not Applicable	Not Applicable	Failed
Theobromine	Not Applicable	Not Applicable	Failed
Quercetin	-8.67	-15.94	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Quercetin helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Peganum harmala can prevent Herpes due to the presence of Quercetin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Phyllanthus emblica against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Subhasmita Mishra[1], Dojalisa Sahu[2]

[1]subhasmitasm86@gmail.com

[2]dojalisa.sahu@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Phyllanthus emblica against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Malvidin helped to prevent Herpes.

Introduction: Phyllanthus emblica is known for its medicinal activities. Seeds of the fruits are used in treatment of asthma, herpes and bronchitis. The leaves are used as fodder. Alcoholic extract of the fruit is anti–viral.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Malpighiales
Family	Phyllanthaceae
Genus	Phyllanthus
Species	emblica

Major phytochemicals present in the plant are:

a. Malvidin
b. Myricetin
c. Ursolic acid
d. Ascorbic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Malvidin	-13.87	-16.78	Positive
Myricetin	Not Applicable	Not Applicable	Failed
Ursolic acid	Not Applicable	Not Applicable	Failed
Ascorbic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Malvidin helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Phyllanthus emblica can prevent Herpes due to the presence of Malvidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Phyllanthus urinaria against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Rojalin Mallik[1], Dojalisa Sahu[2]

[1]180705180056@cutm.ac.in

[2]dojalisa.sahu@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Phyllanthus urinaria against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Ursolic acid helped to prevent Herpes.

Introduction: Phyllanthus urinaria is known for its medicinal activities. It is used in folk medicine as a cure to treat jaundice, herpes, diabetes, malaria, and liver diseases.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Malpighiales
Family	Phyllanthaceae
Genus	Phyllanthus
Species	urinaria

Major phytochemicals present in the plant are:

a. Tangeretin
b. Ursolic acid
c. Limonene
d. Naringin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tangeretin	Not Applicable	Not Applicable	Failed
Ursolic acid	-15.67	-18.97	Positive
Limonene	Not Applicable	Not Applicable	Failed
Naringin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ursolic acid helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Phyllanthus urinaria can prevent Herpes due to the presence of Ursolic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Pinus massoniana against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Elina Sahoo[1], Dojalisa Sahu[2]

[1]180705180057@cutm.ac.in

[2]dojalisa.sahu@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Pinus massoniana against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Genistein helped to prevent Herpes.

Introduction: Pinus massoniana is known for its medicinal activities. The chopped or decocted leaves are used in the treatment of rheumatism, herpes and intestinal parasites.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Pinopsida
Order	Pinales
Family	Pinaceae
Genus	Pinus
Species	massoniana

Major phytochemicals present in the plant are:

a. Genistein
b. Daidzein
c. Peonidin
d. Quercetin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Genistein	-11.12	-17.82	Positive
Daidzein	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Quercetin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Genistein helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Pinus massoniana can prevent Herpes due to the presence of Genistein. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Plantago major against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Kumarika Mishra[1], Gyanranjan Mahalik[2]

[1]180705180058@cutm.ac.in

[2]gyanranjan.mahalik@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Plantago major against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Daidzein and Gallic acid helped to prevent Herpes.

Introduction: Plantago major is known for its medicinal activities. Plantago major is used in wound healing and the leaves were used as a remedy of wounds and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Lamiales
Family	Plantaginaceae
Genus	Plantago
Species	major

Major phytochemicals present in the plant are:

a. Genistein
b. Daidzein
c. Gallic acid
d. Ellagic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Genistein	Not Applicable	Not Applicable	Failed
Daidzein	-13.67	-19.33	Positive
Gallic acid	-11.27	-18.82	Positive
Ellagic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Daidzein and Gallic acid helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Plantago major can prevent Herpes due to the presence of Daidzein and Gallic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Portulaca oleracea against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Subhsmruti Satapathy[1], Gyanranjan Mahalik[2]

[1]180705180059@cutm.ac.in

[2]gyanranjan.mahalik@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Portulaca oleracea against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Ajoene helped to prevent Herpes.

Introduction: Portulaca oleracea is known for its medicinal activities. Portulaca oleracea has been used as a folk medicine in many countries, acting as a febrifuge, antiseptic, herpes and vermifuge.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Caryophyllales
Family	Portulacaceae
Genus	Portulaca
Species	oleracea

Major phytochemicals present in the plant are:

a. Allicin
b. Ajoene
c. Theobromine
d. Quercetin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Allicin	Not Applicable	Not Applicable	Failed
Ajoene	-12.41	-19.37	Positive
Theobromine	Not Applicable	Not Applicable	Failed
Quercetin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ajoene helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Portulaca oleracea can prevent Herpes due to the presence of Ajoene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Salvia officinalis against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Krutanjali rout[1], Gyanranjan Mahalik[2]

[1]180705180060@cutm.ac.in

[2]gyanranjan.mahalik@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Salvia officinalis against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Coumarin helped to prevent Herpes.

Introduction: Salvia officinalis is known for its medicinal activities. S. officinalis has been used for the treatment of different kinds of disorders including seizure, ulcers, gout, rheumatism, herpes, inflammation, dizziness, tremor, paralysis, diarrhea, and hyperglycemia.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Lamiales
Family	Lamiaceae
Genus	Salvia
Species	officinalis

Major phytochemicals present in the plant are:

a. Tocopherol
b. Epicatechin
c. Coumarin
d. Proanthocyanidins

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tocopherol	Not Applicable	Not Applicable	Failed
Epicatechin	Not Applicable	Not Applicable	Failed
Coumarin	-12.39	-18.47	Positive
Proanthocyanidins	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Coumarin helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Salvia officinalis can prevent Herpes due to the presence of Coumarin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Santalum album against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Debasis Prusty[1], Gyanranjan Mahalik[2]

[1]debasisdp1996@gmail.com

[2]gyanranjan.mahalik@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Santalum album against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Rutin and Ferulic acid helped to prevent Herpes.

Introduction: Santalum album is known for its medicinal activities. Sandalwood oil has been widely used in folk medicine for treatment of common colds, bronchitis, skin disorders, heart ailments, general weakness, fever, herpes, infection of the urinary tract, inflammation of the mouth and pharynx, liver and gallbladder complaints and other maladies.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Santalales
Family	Santalaceae
Genus	Santalum
Species	album

Major phytochemicals present in the plant are:

a. Hesperidin
b. Isorhamnetin
c. Rutin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Hesperidin	Not Applicable	Not Applicable	Failed
Isorhamnetin	Not Applicable	Not Applicable	Failed
Rutin	-9.37	-14.58	Positive
Ferulic acid	-12.47	-18.37	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Rutin and Ferulic acid helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Santalum album can prevent Herpes due to the presence of Rutin and Ferulic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Scinaia hatei against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Bhagyashree Bhargavi Tanaya[1], Gyanranjan Mahalik[2]

[1]bbhargavitanaya@gmail.com

[2]gyanranjan.mahalik@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Scinaia hatei against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Tangeretin helped to prevent Herpes.

Introduction: Scinaia hatei is known for its medicinal activities. It helps to treat herpes, dengue, myalgia, pancreatitis, cardiac arrhythmia, and hepatitis.

The plant is classified as follows:

Kingdom	Plantae
Division	Rhodophyta
Class	Florideophyceae
Order	Nemalionales
Family	Chaetangiaceae
Genus	Scinaia
Species	hatei

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Alliin
c. Tangeretin
d. Tannic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Alliin	Not Applicable	Not Applicable	Failed
Tangeretin	-12.14	-21.84	Positive
Tannic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Tangeretin helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Scinaia hatei can prevent Herpes due to the presence of Tangeretin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Scoparia dulcis against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Sonali Suchismita Behera[1], Gyanranjan Mahalik[2]

[1]lizasonali98@gmail.com

[2]gyanranjan.mahalik@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Scoparia dulcis against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Digoxin helped to prevent Herpes.

Introduction: Scoparia dulcis is known for its medicinal activities. It is considered a weed in many areas but used as medicinal herb for a wide range of uses including treatment for digestive problems, pulmonary conditions, fever, skin disorders, hypertension, hemorrhoids, diarrhea, dysentery, insect bites, anemia, albuminuria, diabetes, herpes, etc.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Lamiales
Family	Plantaginaceae
Genus	Scoparia
Species	dulcis

Major phytochemicals present in the plant are:

a. Pelletierine
b. Digoxin
c. Rosmarinic acid
d. Campesterol

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	Not Applicable	Not Applicable	Failed
Digoxin	-14.66	-18.84	Positive
Rosmarinic acid	Not Applicable	Not Applicable	Failed
Campesterol	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Digoxin helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Scoparia dulcis can prevent Herpes due to the presence of Digoxin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Solanum torvum against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Sukanya Singh[1], Gyanranjan Mahalik[2]

[1]180705180064@cutm.ac.in

[2]gyanranjan.mahalik@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Solanum torvum against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Malvidin helped to prevent Herpes.

Introduction: Solanum torvum is known for its medicinal activities. Fruit and leaf decoction is used to treat cough, herpes and to treat liver and spleen enlargement.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Solanales
Family	Solanaceae
Genus	Solanum
Species	torvum

Major phytochemicals present in the plant are:

a. Campesterol
b. Linamarin
c. Glutathione
d. Malvidin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Campesterol	Not Applicable	Not Applicable	Failed
Linamarin	Not Applicable	Not Applicable	Failed
Glutathione	Not Applicable	Not Applicable	Failed
Malvidin	-11.84	-16.38	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Malvidin helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Solanum torvum can prevent Herpes due to the presence of Malvidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Sorghum bicolor against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Dushmanta Meher[1], Gyanranjan Mahalik[2]

[1]180705180065@cutm.ac.in

[2]gyanranjan.mahalik@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Sorghum bicolor against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Limonene helped to prevent Herpes.

Introduction: Sorghum bicolor is known for its medicinal activities. Seed extracts are drunk to treat hepatitis and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Poales
Family	Poaceae
Genus	Sorghum
Species	bicolor

Major phytochemicals present in the plant are:

a. Naringin
b. Limonene
c. Naringin
d. Pelargonidin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Naringin	Not Applicable	Not Applicable	Failed
Limonene	-12.5	-17.28	Positive
Naringin	Not Applicable	Not Applicable	Failed
Pelargonidin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Limonene helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Sorghum bicolor can prevent Herpes due to the presence of Limonene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Strobilanthus cusia against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Chinmayee Naik[1], Gyanranjan Mahalik[2]

[1]chinmayeenaik75@gmail.com

[2]gyanranjan.mahalik@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Strobilanthus cusia against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Tangeretin and Epicatechin helped to prevent Herpes.

Introduction: Strobilanthus cusia is known for its medicinal activities. It is used for influenza, herpes, epidemic cerebrospinal meningitis, encephalitis B, viral pneumonia and mumps.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Lamiales
Family	Acanthaceae
Genus	Strobilanthus
Species	cusia

Major phytochemicals present in the plant are:

a. Tangeretin
b. Salicylic acid
c. Epicatechin
d. Catechin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tangeretin	-14.22	-18.08	Positive
Salicylic acid	Not Applicable	Not Applicable	Failed
Epicatechin	-12.44	-15.75	Positive
Catechin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Tangeretin and Epicatechin helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Strobilanthus cusia can prevent Herpes due to the presence of Tangeretin and Epicatechin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Swertia chirata against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Seema Suvadarshini[1], Gyanranjan Mahalik[2]

[1]seema.subha1997@gmail.com

[2]gyanranjan.mahalik@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Swertia chirata against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that -12.08 helped to prevent Herpes.

Introduction: Swertia chirata is known for its medicinal activities. People use the parts that grow above the ground to make medicine. Chirata is used for fever, constipation, herpes, upset stomach, loss of appetite, intestinal worms, skin diseases, and cancer.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Gentianales
Family	Gentianaceae
Genus	Swertia
Species	chirayita

Major phytochemicals present in the plant are:

a. Theobromine
b. Limonene
c. Naringin
d. Limonene

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	-12.08	-12.19	Positive
Limonene	Not Applicable	Not Applicable	Failed
Naringin	Not Applicable	Not Applicable	Failed
Limonene	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that -12.08 helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Swertia chirata can prevent Herpes due to the presence of -12.08. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Syzygium aromaticum against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Soumyasmita Pradhan[1], Atia Arzoo[2]

[1]soumyasmitapradhan1997@gmail.com

[2]atia.arzoo@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Syzygium aromaticum against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Pelargonidin helped to prevent Herpes.

Introduction: Syzygium aromaticum is known for its medicinal activities. Traditionally, cloves have been used for centuries in the treatment of vomiting; flatulence; nausea; liver, herpes, bowel and stomach disorders; and as a stimulant for the nerves.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Myrtales
Family	Myrtaceae
Genus	Syzygium
Species	aromaticum

Major phytochemicals present in the plant are:

a. Lutein
b. Digoxin
c. Pelargonidin
d. Limonene

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lutein	Not Applicable	Not Applicable	Failed
Digoxin	Not Applicable	Not Applicable	Failed
Pelargonidin	-12.39	-15.97	Positive
Limonene	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Pelargonidin helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Syzygium aromaticum can prevent Herpes due to the presence of Pelargonidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Syzygium jambos against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Satabdee Panda[1], Atia Arzoo[2]

[1]satabdee1998@gmail.com

[2]atia.arzoo@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Syzygium jambos against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Tannic acid helped to prevent Herpes.

Introduction: Syzygium jambos is known for its medicinal activities. A decoction of the leaves is used as a diuretic, herpes, a remedy for sore eyes and for rheumatism. The seeds are used to treat diarrhoea, dysentery, diabetes and catarrh. A decoction of bark is administered to relieve asthma and bronchitis.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Myrtales
Family	Myrtaceae
Genus	Syzygium
Species	jambos

Major phytochemicals present in the plant are:

a. Ellagic acid
b. Gallic acid
c. Tannic acid
d. Theobromine

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Ellagic acid	Not Applicable	Not Applicable	Failed
Gallic acid	Not Applicable	Not Applicable	Failed
Tannic acid	-13.28	-17.21	Positive
Theobromine	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Tannic acid helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Syzygium jambos can prevent Herpes due to the presence of Tannic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Taracetium vulgare against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Binita Pradhan[1], Atia Arzoo[2]

[1]pbinita1996@gmail.com

[2]atia.arzoo@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Taracetium vulgare against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Alliin helped to prevent Herpes.

Introduction: Taracetium vulgare is known for its medicinal activities. In larger doses the plant can procure an abortion, though these doses can be poisonous. Externally, tansy is used as a poultice on swellings, herpes and some eruptive skin diseases.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Asterales
Family	Asteraceae
Genus	Taracetum
Species	vulgare

Major phytochemicals present in the plant are:

a. Pelletierine
b. Alliin
c. Theobromine
d. Quercetin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	Not Applicable	Not Applicable	Failed
Alliin	-10.18	-19.74	Positive
Theobromine	Not Applicable	Not Applicable	Failed
Quercetin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Alliin helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Taracetium vulgare can prevent Herpes due to the presence of Alliin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Usnea complanta against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Soumya Sucharita Sahu[1], Atia Arzoo[2]

[1]soumyasucharitasahu7@gmail.com

[2]atia.arzoo@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Usnea complanta against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Genistein helped to prevent Herpes.

Introduction: Usnea complanta is known for its medicinal activities. It can sometimes be used as a bioindicator, because it tends to only grow in those regions where the air is clean, and of high quality. It is also used to cure herpes.

The plant is classified as follows:

Kingdom	Fungi
Division	Ascomycota
Class	Lecanoromycetes
Order	Lecanorales
Family	Asteraceae
Genus	Usnea
Species	complanta

Major phytochemicals present in the plant are:

a. Genistein
b. Daidzein
c. Tangeretin
d. Campesterol

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Genistein	-13.64	-23.11	Positive
Daidzein	Not Applicable	Not Applicable	Failed
Tangeretin	Not Applicable	Not Applicable	Failed
Campesterol	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Genistein helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Usnea complanta can prevent Herpes due to the presence of Genistein. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Ventilago denticulate against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Rituparnna Mohanty[1], Atia Arzoo[2]

[1]rituparnnamohanty06@gmail.com

[2]atia.arzoo@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Ventilago denticulate against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Ferulic acid helped to prevent Herpes.

Introduction: Ventilago denticulate is known for its medicinal activities. Stem bark is powdered and mixed with sesame oil, externally applied to skin diseases and sprains. Root bark—used for atonic dyspepsia, mild fever, herpes and debility. Sap is used for the treatment of deafness.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Rosales
Family	Rhamnaceae
Genus	Ventilago
Species	denticulate

Major phytochemicals present in the plant are:

a. Allicin
b. Hesperidin
c. Ferulic acid
d. Epicatechin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Allicin	Not Applicable	Not Applicable	Failed
Hesperidin	Not Applicable	Not Applicable	Failed
Ferulic acid	-16.84	-19.77	Positive
Epicatechin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ferulic acid helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Ventilago denticulate can prevent Herpes due to the presence of Ferulic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Withania somnifera against Herpes through deactivation of Herpes Simplex virus type 1 DNA polymerase (2GV9)

Subhasmita Das[1], Atia Arzoo[2]

[1]subhasmitadas478@gmail.com

[2]atia.arzoo@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Withania somnifera against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. It was found that Tannic acid helped to prevent Herpes.

Introduction: Withania somnifera is known for its medicinal activities. The medicinal plants are widely used by the traditional medical practitioners for curing various diseases like diarrhea, dysentery, insect bites, anemia, albuminuria, diabetes, herpes, etc.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Solanales
Family	Solanaceae
Genus	Withania
Species	somnifera

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Tannic acid
c. Rosmarinic acid
d. Cryptoxanthin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Tannic acid	-11.67	-19.38	Positive
Rosmarinic acid	Not Applicable	Not Applicable	Failed
Cryptoxanthin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Tannic acid helped deactivate the Herpes Simplex virus type 1 DNA polymerase (2GV9) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Withania somnifera can prevent Herpes due to the presence of Tannic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Pandanus amaryllifolius against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Rabinarayan Kar[1], Atia Arzoo[2]

[1]rabinarayankar07@gmail.com

[2]atia.arzoo@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Pandanus amaryllifolius against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Limonene helped to prevent Herpes.

Introduction: Pandanus amaryllifolius is known for its medicinal activities. The leaves are used in the perfume industry and traditional medicine to treat diseases like cough, asthma, herpes and diarrhea.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Pandanales
Family	Pandanaceae
Genus	Pandanus
Species	amaryllifolius

Major phytochemicals present in the plant are:

a. Ellagic acid
b. Gallic acid
c. Peonidin
d. Limonene

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Ellagic acid	Not Applicable	Not Applicable	Failed
Gallic acid	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Limonene	-15.99	-19.18	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Limonene helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Pandanus amaryllifolius can prevent Herpes due to the presence of Limonene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Adansonia digitata against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Sachidananda Behera[1], Atia Arzoo[2]

[1]sai.sachin.725@gmail.com

[2]atia.arzoo@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Adansonia digitata against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Resveratrol and Peonidin helped to prevent Herpes.

Introduction: Adansonia digitata is known for its medicinal activities. The various parts of the plant (leaves, bark and seeds) are used to cure tuberculosis, fever, microbial infections, diarrhea and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Malvales
Family	Bombacaceae
Genus	Adansonia
Species	digitata

Major phytochemicals present in the plant are:

a. Resveratrol
b. Phenyl isothiocyanate
c. Capsaicin
d. Peonidin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Resveratrol	-10.56	-12.37	Positive
Phenyl isothiocyanate	Not Applicable	Not Applicable	Failed
Capsaicin	Not Applicable	Not Applicable	Failed
Peonidin	-8.37	-15.34	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Resveratrol and Peonidin helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Adansonia digitata can prevent Herpes due to the presence of Resveratrol and Peonidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Aglai odorata against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Arya Lopamudra[1], Atia Arzoo[2]

[1]aryalopamudra@gmail.com

[2]atia.arzoo@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Aglai odorata against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Myricetin and Benzyl isothiocyanate helped to prevent Herpes.

Introduction: Aglai odorata is known for its medicinal activities. Aglaia species are used in traditional medicine: leaves to treat wounds, fever, headache, asthma, jaundice, and as a tonic e.g. after childbirth; flowers against fever, asthma, jaundice and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Sapindales
Family	Meliaceae
Genus	Aglai
Species	odorata

Major phytochemicals present in the plant are:

a. Morphine
b. Myricetin
c. Peonidin
d. Benzyl isothiocyanate

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Morphine	Not Applicable	Not Applicable	Failed
Myricetin	-15.37	-21.52	Positive
Peonidin	Not Applicable	Not Applicable	Failed
Benzyl isothiocyanate	-12.07	-15.45	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Myricetin and Benzyl isothiocyanate helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Aglai odorata can prevent Herpes due to the presence of Myricetin and Benzyl isothiocyanate. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Aloe vera against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Sunita Sasmal[1], Atia Arzoo[2]

[1]sunitasasmal1995@gmail.com

[2]atia.arzoo@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Aloe vera against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Phytoene helped to prevent Herpes.

Introduction: Aloe vera is known for its medicinal activities. Aloe vera used to cure herpes, weak digestion, general weakness, anaemia, bloating, stomach ulcers and gum disease.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Liliopsida
Order	Liliales
Family	Aloeaceae
Genus	Aloe
Species	vera

Major phytochemicals present in the plant are:

a. Phytoene
b. Salicylic acid
c. Sitosterol
d. Lupeol

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Phytoene	-18.37	-21.77	Positive
Salicylic acid	Not Applicable	Not Applicable	Failed
Sitosterol	Not Applicable	Not Applicable	Failed
Lupeol	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Phytoene helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Aloe vera can prevent Herpes due to the presence of Phytoene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Andrographis paniculata against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Gopesh Chandra Sahoo[1], Jyoti Prakash Rath[2]

[1]gcs.b.p143@gmail.com

[2]jyotiprakash.rath@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Andrographis paniculata against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Genistein and Daidzein helped to prevent Herpes.

Introduction: Andrographis paniculata is known for its medicinal activities. A. paniculata has been used in Siddha and Ayurvedic medicine. It is promoted as a dietary supplement for cancer prevention and cure. In the traditional medicine of India, A. paniculata has also been used for jaundice therapy.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Lamiales
Family	Acanthaceae
Genus	Andrographis
Species	paniculata

Major phytochemicals present in the plant are:

a. Genistein
b. Daidzein
c. Theobromine
d. Quercetin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Genistein	-8.91	-10.83	Positive
Daidzein	-12.32	-14.88	Positive
Theobromine	Not Applicable	Not Applicable	Failed
Quercetin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Genistein and Daidzein helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Andrographis paniculata can prevent Herpes due to the presence of Genistein and Daidzein. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Atlantia sp. against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Subhrasweta Das[1], Jyoti Prakash Rath[2]

[1]dassubhrasweta17@gmail.com

[2]jyotiprakash.rath@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Atlantia sp. against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Gallic acid helped to prevent Herpes.

Introduction: Atlantia sp. is known for its medicinal activities. The flowers, fruit and roots are used to cure herpes, jaundice, fever, headache and asthma.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Sapindales
Family	Rutaceae
Genus	Atalantia
Species	racemosa

Major phytochemicals present in the plant are:

a. Allicin
b. Ajoene
c. Gallic acid
d. Ellagic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Allicin	Not Applicable	Not Applicable	Failed
Ajoene	Not Applicable	Not Applicable	Failed
Gallic acid	-12.97	-21.87	Positive
Ellagic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Gallic acid helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Atlantia sp. can prevent Herpes due to the presence of Gallic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Azadirachta indica against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Sidharth Ray[1], Jyoti Prakash Rath[2]

[1]sray999999999@gmail.com

[2]jyotiprakash.rath@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Azadirachta indica against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Tocopherol and Isorhamnetin helped to prevent Herpes.

Introduction: Azadirachta indica is known for its medicinal activities. Neem has an anti-inflammatory property which helps reduces acne, herpes, skin blemishes and malaria.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Sapindales
Family	Meliaceae
Genus	Azadirachta
Species	indica

Major phytochemicals present in the plant are:

a. Tocopherol
b. Isorhamnetin
c. Rutin
d. Azadirichtin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tocopherol	-11.3	-18.33	Positive
Isorhamnetin	-15.38	-21.88	Positive
Rutin	Not Applicable	Not Applicable	Failed
Azadirichtin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Tocopherol and Isorhamnetin helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Azadirachta indica can prevent Herpes due to the presence of Tocopherol and Isorhamnetin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Barleria lupulina against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Gitisnigdha Sahoo[1], Jyoti Prakash Rath[2]

[1]geetsahoo1996@gmail.com

[2]jyotiprakash.rath@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Barleria lupulina against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Coumarin helped to prevent Herpes.

Introduction: Barleria lupulina is known for its medicinal activities. The flowers are used internally for the treatment of migraine, internal abscesses, oedema, haemoptysis, herpes, urethral discharges, seminal disorders and reduce obesity.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Scrophulariales
Family	Acanthaceae
Genus	Barleria
Species	lupulina

Major phytochemicals present in the plant are:

a. Hesperidin
b. Epicatechin
c. Coumarin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Hesperidin	Not Applicable	Not Applicable	Failed
Epicatechin	Not Applicable	Not Applicable	Failed
Coumarin	-14.91	-21.33	Positive
Ferulic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Coumarin helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Barleria lupulina can prevent Herpes due to the presence of Coumarin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Bauhinia racemosa against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Subhadra Manjari Parida[1], Jyoti Prakash Rath[2]

[1]subhadramp1998@gmail.com

[2]jyotiprakash.rath@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Bauhinia racemosa against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Sulforaphane and Digoxin helped to prevent Herpes.

Introduction: Bauhinia racemosa is known for its medicinal activities. Bauhinia racemosa leaves have been used in the treatment of asthma traditionally because of their antihistaminic action it also used to cure herpes and urethral discharges.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Equisetopsida
Order	Fabales
Family	Fabaceae
Genus	Bauhinia
Species	racemosa

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Digoxin
c. Rosmarinic acid
d. Tannic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	-12.3	-15.33	Positive
Digoxin	-9.38	-14.88	Positive
Rosmarinic acid	Not Applicable	Not Applicable	Failed
Tannic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Sulforaphane and Digoxin helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Bauhinia racemosa can prevent Herpes due to the presence of Sulforaphane and Digoxin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Bauhinia variegate against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Sanchayita Nayak[1], Jyoti Prakash Rath[2]

[1]sanchayitanayak7761@gmail.com

[2]jyotiprakash.rath@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Bauhinia variegate against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Cryptoxanthin helped to prevent Herpes.

Introduction: Bauhinia variegate is known for its medicinal activities. The bark decoction is used for diarrhoea control, as an astringent alternative and for treating scrofula, herpes, skin diseases and ulcers.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Equisetopsida
Order	Fabales
Family	Fabaceae
Genus	Bauhinia
Species	variegata

Major phytochemicals present in the plant are:

a. Cryptoxanthin
b. Carotene
c. Lutein
d. Lycopene

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Cryptoxanthin	-10.59	-18.37	Positive
Carotene	Not Applicable	Not Applicable	Failed
Lutein	Not Applicable	Not Applicable	Failed
Lycopene	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Cryptoxanthin helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Bauhinia variegate can prevent Herpes due to the presence of Cryptoxanthin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Bidens pilosa against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Sutapa Mohanty[1], Jyoti Prakash Rath[2]

[1]sutapagudu12@gmail.com

[2]jyotiprakash.rath@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Bidens pilosa against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Apigenin and Carnosic acid helped to prevent Herpes.

Introduction: Bidens pilosa is known for its medicinal activities. Roots, leaves and seed have been reported to possess antibacterial, antidysenteric, anti-inflammatory, antimicrobial, herpes, antimalarial, diuretic, hepato-protective and hypotensive activities.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Asterales
Family	Asteraceae
Genus	Bidens
Species	pilosa

Major phytochemicals present in the plant are:

a. Eugenol
b. Apigenin
c. Luteolin
d. Carnosic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Eugenol	Not Applicable	Not Applicable	Failed
Apigenin	-15.98	-21.66	Positive
Luteolin	Not Applicable	Not Applicable	Failed
Carnosic acid	-12.47	-15.88	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Apigenin and Carnosic acid helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Bidens pilosa can prevent Herpes due to the presence of Apigenin and Carnosic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Cedrus libani against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Soumyashree Rath[1], Jyoti Prakash Rath[2]

[1]soumyashree.rath998@gmail.com

[2]jyotiprakash.rath@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Cedrus libani against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Eugenol helped to prevent Herpes.

Introduction: Cedrus libani is known for its medicinal activities. It is traditionally used to treat diseases like arteriosclerosis, water retention, herpes, lymphatic damage, etc.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Pinopsida
Order	Pinales
Family	Pinaceae
Genus	Cedrus
Species	libani

Major phytochemicals present in the plant are:

a. Luteolin
b. Carnosic acid
c. Eugenol
d. Salicylic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Luteolin	Not Applicable	Not Applicable	Failed
Carnosic acid	Not Applicable	Not Applicable	Failed
Eugenol	-18.34	-21.39	Positive
Salicylic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Eugenol helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Cedrus libani can prevent Herpes due to the presence of Eugenol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Cissus quadrangularis against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Swagat Rath[1], Jyoti Prakash Rath[2]

[1]swagatrath1998@gmail.com

[2]jyotiprakash.rath@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Cissus quadrangularis against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Lupeol and Ferulic acid helped to prevent Herpes.

Introduction: Cissus quadrangularis is known for its medicinal activities. The roots and stems are most useful for healing of fracture of the bones. The stem is bitter; it is given internally and applied topically in broken bones, used in complaints of the back and spine. A paste of stem is useful for muscular pains and herpes. The plant has been documented in Ayurveda for the treatment of osteoarthritis, rheumatoid arthritis and osteoporosis.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Vitales
Family	Vitacea
Genus	Cissus
Species	quadrangularis

Major phytochemicals present in the plant are:

a. Lupeol
b. Ferulic acid
c. Hesperidin
d. Naringin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lupeol	-8.78	-10.58	Positive
Ferulic acid	-12.79	-14.17	Positive
Hesperidin	Not Applicable	Not Applicable	Failed
Naringin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Lupeol and Ferulic acid helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Cissus quadrangularis can prevent Herpes due to the presence of Lupeol and Ferulic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Conyza aegyptica against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Samita Padhi[1], Jyoti Prakash Rath[2]

[1]samita.padhi.1997@gmail.com

[2]jyotiprakash.rath@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Conyza aegyptica against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Epicatechin and Limonene helped to prevent Herpes.

Introduction: Conyza aegyptica is known for its medicinal activities. The whole plants used to treat herpes, wound, skin diseases and toothache.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Dicotyledonae
Order	Asterales
Family	Asteraceae
Genus	Conyza
Species	aegyptiaca

Major phytochemicals present in the plant are:

a. Theobromine
b. Epicatechin
c. Catechin
d. Limonene

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	Not Applicable	Not Applicable	Failed
Epicatechin	-19.98	-21.41	Positive
Catechin	Not Applicable	Not Applicable	Failed
Limonene	-9.47	-15.28	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Epicatechin and Limonene helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Conyza aegyptica can prevent Herpes due to the presence of Epicatechin and Limonene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Cyperus rotundus against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Lopamudra Kar[1], Suchismita Acharya[2]

[1]lopamudrakar69@gmail.com

[2]suchismita.acharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Cyperus rotundus against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Pelargonidin helped to prevent Herpes.

Introduction: Cyperus rotundus is known for its medicinal activities. It is a medicinal herb traditionally used to treat various clinical conditions at home such as diarrhea, diabetes, pyresis, herpes, inflammation, malaria, and stomach and bowel disorders.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Poales
Family	Cyperaceae
Genus	Cyperus
Species	rotundus

Major phytochemicals present in the plant are:

a. Ellagic acid
b. Gallic acid
c. Pelargonidin
d. Limonene

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Ellagic acid	Not Applicable	Not Applicable	Failed
Gallic acid	Not Applicable	Not Applicable	Failed
Pelargonidin	-11.91	-18.33	Positive
Limonene	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Pelargonidin helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Cyperus rotundus can prevent Herpes due to the presence of Pelargonidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Euphorbia peplus against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Sudipta Bharata Nandini[1], Suchismita Acharya[2]

[1]sudeeptanandinee136@gmail.com

[2]suchismita.acharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Euphorbia peplus against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Lutein and Theobromine helped to prevent Herpes.

Introduction: Euphorbia peplus is known for its medicinal activities. The plant is administered in the form of herbal tea as diuretic, laxative and emollient. It is also used for the treatment of asthma and bronchitis, as it relaxes the smooth muscles of bronchi. It is recommended against dry cough, herpes, runny nose and liver diseases.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Malpighiales
Family	Euphorbiaceae
Genus	Euphorbia
Species	peplus

Major phytochemicals present in the plant are:

a. Lutein
b. Digoxin
c. Tannic acid
d. Theobromine

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lutein	-11.56	-18.37	Positive
Digoxin	Not Applicable	Not Applicable	Failed
Tannic acid	Not Applicable	Not Applicable	Failed
Theobromine	-10.37	-19.34	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Lutein and Theobromine helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Euphorbia peplus can prevent Herpes due to the presence of Lutein and Theobromine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Glycyrrhiza glabra against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Jibanjyoti Bidyasagar[1], Suchismita Acharya[2]

[1]jibanjyotionline@gmail.com

[2]suchismita.acharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Glycyrrhiza glabra against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Alliin and Campesterol helped to prevent Herpes.

Introduction: Glycyrrhiza glabra is known for its medicinal activities. Traditionally used to treat many diseases, such as respiratory disorders, hyperdipsia, epilepsy, fever, sexual debility, paralysis, stomach ulcers, rheumatism, skin diseases, hemorrhagic diseases, and jaundice.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Fabales
Family	Fabaceae
Genus	Glycyrrhiza
Species	glabra

Major phytochemicals present in the plant are:

a. Pelletierine
b. Alliin
c. Tangeretin
d. Campesterol

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	Not Applicable	Not Applicable	Failed
Alliin	-15.96	-21.01	Positive
Tangeretin	Not Applicable	Not Applicable	Failed
Campesterol	-12.18	-15.87	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Alliin and Campesterol helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Glycyrrhiza glabra can prevent Herpes due to the presence of Alliin and Campesterol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Heliotropium marifolium against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Subhashree Sahu[1], Suchismita Acharya[2]

[1]cutiesubha.2020@gmail.com

[2]suchismita.acharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Heliotropium marifolium against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Campesterol helped to prevent Herpes.

Introduction: Heliotropium marifolium is known for its medicinal activities. Heliotropium marifolium is used against syphilis, asthma, herpes, UTI and wound.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Boraginales
Family	Boraginaceae
Genus	Heliotropium
Species	marifolium

Major phytochemicals present in the plant are:

a. Campesterol
b. Linamarin
c. Naringin
d. Pelargonidin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Campesterol	-18.3	-20.75	Positive
Linamarin	Not Applicable	Not Applicable	Failed
Naringin	Not Applicable	Not Applicable	Failed
Pelargonidin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Campesterol helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Heliotropium marifolium can prevent Herpes due to the presence of Campesterol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Holoptelea integrifolia against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Debesh kumar Hota[1], Suchismita Acharya[2]

[1]deb.hota04@gmail.com

[2]suchismita.acharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Holoptelea integrifolia against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Naringin and Limonene helped to prevent Herpes.

Introduction: Holoptelea integrifolia is known for its medicinal activities. The plant Holoptelea integrifolia is used traditionally for the treatment of inflammation, gastritis, dyspepsia, colic, intestinal worms, vomiting, wound healing, leprosy, diabetes, hemorrhoids, herpes, dysmenorrhea, and rheumatism.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Rosales
Family	Ulmaceae
Genus	Holoptelea
Species	integrifolia

Major phytochemicals present in the plant are:

a. Naringin
b. Limonene
c. Glutathione
d. Malvidin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Naringin	-12.91	-14.83	Positive
Limonene	-16.32	-19.88	Positive
Glutathione	Not Applicable	Not Applicable	Failed
Malvidin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Naringin and Limonene helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Holoptelea integrifolia can prevent Herpes due to the presence of Naringin and Limonene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Houttuynia cordata against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Biswajit Jena[1], Suchismita Acharya[2]

[1]jaganjena2015@gmail.com

[2]suchismita.acharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Houttuynia cordata against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Limonene helped to prevent Herpes.

Introduction: Houttuynia cordata is known for its medicinal activities. It is used as a fresh herbal garnish. In northeastern India, it is commonly used in salads and as a garnish over side dishes. The tender roots can also be ground into chutneys along with dry meat or fish, chilies, and tamarind. It is taken raw as salad and cooked along with fish as fish curry. In Japan and Korea, its dried leaves may be used as a tea. Houttuynia cordata was used in traditional Chinese medicine.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Piperales
Family	Saururaceae
Genus	Houttuynia
Species	cordata

Major phytochemicals present in the plant are:

a. Tangeretin
b. Salicylic acid
c. Limonene
d. Naringin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tangeretin	Not Applicable	Not Applicable	Failed
Salicylic acid	Not Applicable	Not Applicable	Failed
Limonene	-11.99	-19.87	Positive
Naringin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Limonene helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Houttuynia cordata can prevent Herpes due to the presence of Limonene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Hypericum hookerianum against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Sonali Priyadarshini[1], Suchismita Acharya[2]

[1]sonalipriyadarshini98@gmail.com

[2]suchismita.acharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Hypericum hookerianum against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Malvidin and Salicylic acid helped to prevent Herpes.

Introduction: Hypericum hookerianum is known for its medicinal activities. It was recommended in the first century by Greek physicians as a diuretic, wound-healer, and treatment for menstrual disorders. It has been used as an anti-inflammatory, anti-bacterial, disinfectant, and a remedy for disorders of the respiratory tract and gall bladder and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Malpighiales
Family	Hypericaceae
Genus	Hypericum
Species	hookerianum

Major phytochemicals present in the plant are:

a. Malvidin
b. Salicylic acid
c. Ursolic acid
d. Astaxanthin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Malvidin	-18.35	-21.33	Positive
Salicylic acid	-12.38	-17.88	Positive
Ursolic acid	Not Applicable	Not Applicable	Failed
Astaxanthin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Malvidin and Salicylic acid helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Hypericum hookerianum can prevent Herpes due to the presence of Malvidin and Salicylic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Hypericum mysorense against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Upendra Kumar Nayak[1], Suchismita Acharya[2]

[1]nayakupendra629@gmail.com

[2]suchismita.acharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Hypericum mysorense against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Sitosterol helped to prevent Herpes.

Introduction: Hypericum mysorense is known for its medicinal activities. Hypericum mysorense has been used to treat wounds and herpes as part of the Ayurvedic system of traditional medicine.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Equisetopsida
Order	Malpighiales
Family	Hypericaceae
Genus	Hypericum
Species	mysorense

Major phytochemicals present in the plant are:

a. Ursolic acid
b. Astaxanthin
c. Sitosterol
d. Astaxanthin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Ursolic acid	Not Applicable	Not Applicable	Failed
Astaxanthin	Not Applicable	Not Applicable	Failed
Sitosterol	-17.91	-19.33	Positive
Astaxanthin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Sitosterol helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Hypericum mysorense can prevent Herpes due to the presence of Sitosterol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Lippia alba against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Jagannath Dash[1], Suchismita Acharya[2]

[1]jagannathdash5002@gmail.com

[2]suchismita.acharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Lippia alba against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Pelargonidin and Caffeine helped to prevent Herpes.

Introduction: Lippia alba is known for its medicinal activities. A tea made from the leaves is used to treat intestinal and respiratory disturbances, including influenza and herpes. A well-sugared infusion is drunk to bring relief of heart problems and to soothe tachycardia.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Equisetopsida
Order	Lamiales
Family	Verbenaceae
Genus	Lippia
Species	alba

Major phytochemicals present in the plant are:

a. Pelargonidin
b. Caffeine
c. Curcumin
d. Ascorbic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelargonidin	-17.39	-18.33	Positive
Caffeine	-10.38	-15.88	Positive
Curcumin	Not Applicable	Not Applicable	Failed
Ascorbic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Pelargonidin and Caffeine helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Lippia alba can prevent Herpes due to the presence of Pelargonidin and Caffeine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Melia azaderach against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Sujnyani Jena[1], Suchismita Acharya[2]

[1]suggu.crazy123@gmail.com

[2]suchismita.acharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Melia azaderach against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Zingiberene helped to prevent Herpes.

Introduction: Melia azaderach is known for its medicinal activities. The leaf juice is anthelmintic, antilithic, diuretic, herpes and emmenagogue.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Sapindales
Family	Meliaceae
Genus	Melia
Species	azedarach

Major phytochemicals present in the plant are:

a. Zingiberene
b. Ursolic acid
c. Astaxanthin
d. Digoxin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Zingiberene	-18.59	-21.37	Positive
Ursolic acid	Not Applicable	Not Applicable	Failed
Astaxanthin	Not Applicable	Not Applicable	Failed
Digoxin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Zingiberene helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Melia azaderach can prevent Herpes due to the presence of Zingiberene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Mentha piperata against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Debadatta Nayak[1], Yashaswi Nayak[2]

[1]debadattanayak21@gmail.com

[2]yashaswi.nayak@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Mentha piperata against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Carotene and Tannic acid helped to prevent Herpes.

Introduction: Mentha piperata is known for its medicinal activities. It is used for treatment of a variety of conditions, including irritable bowel syndrome (IBS), nausea, herpes and other digestive issues, as well as the common cold and headaches.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Lamiales
Family	Lamiaceae
Genus	Mentha
Species	piperata

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Carotene
c. Digoxin
d. Tannic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Carotene	-19.98	-28.66	Positive
Digoxin	Not Applicable	Not Applicable	Failed
Tannic acid	-12.47	-15.88	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Carotene and Tannic acid helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Mentha piperata can prevent Herpes due to the presence of Carotene and Tannic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Momordia charantia against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Sanjeeb Kumar Dash[1], Yashaswi Nayak[2]

[1]das.sanjeeb97@gmail.com

[2]yashaswi.nayak@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Momordia charantia against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Sulforaphane helped to prevent Herpes.

Introduction: Momordia charantia is known for its medicinal activities. Juice of the leaves is used to treat piles and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Cucurbitales
Family	Cucurbitaceae
Genus	Momordia
Species	charantia

Major phytochemicals present in the plant are:

a. Curcumin
b. Ascorbic acid
c. Sulforaphane
d. Digoxin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Curcumin	Not Applicable	Not Applicable	Failed
Ascorbic acid	Not Applicable	Not Applicable	Failed
Sulforaphane	-8.34	-11.39	Positive
Digoxin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Sulforaphane helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Momordia charantia can prevent Herpes due to the presence of Sulforaphane. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Moringa oleifera against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Ipsita Aparajita Mohapatra[1], Yashaswi Nayak[2]

[1]ipsitaaparajitamohapatra7@gmail.com

[2]yashaswi.nayak@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Moringa oleifera against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Isorhamnetin Lycopene helped to prevent Herpes.

Introduction: Moringa oleifera is known for its medicinal activities. Various parts of this plant such as the leaves, roots, seed, bark, fruit, flowers and immature pods act as cardiac and circulatory stimulants, possess antitumor, antipyretic, antiepileptic, antiinflammatory, herpes, antiulcer, antispasmodic, diuretic, antihypertensive, cholesterol lowering.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Brassicales
Family	Moringaceae
Genus	Moringa
Species	oleifera

Major phytochemicals present in the plant are:

a. Isorhamnetin
b. Rosmarinic acid
c. Lutein
d. Lycopene

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Isorhamnetin	-12.56	-17.37	Positive
Rosmarinic acid	Not Applicable	Not Applicable	Failed
Lutein	Not Applicable	Not Applicable	Failed
Lycopene	-15.37	-18.34	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Isorhamnetin Lycopene helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Moringa oleifera can prevent Herpes due to the presence of Isorhamnetin Lycopene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Myrica rubra against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Prativa Routray[1], Yashaswi Nayak[2]

[1]180705180104@cutm.ac.in

[2]yashaswi.nayak@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Myrica rubra against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Tannic acid and Digoxin helped to prevent Herpes.

Introduction: Myrica rubra is known for its medicinal activities. The stem bark is used as a wash in the treatment of arsenic poisoning, skin diseases, wounds and ulcers. The fruit is carminative, herpes, pectoral and stomachic.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Fagales
Family	Myricaceae
Genus	Myrica
Species	rubra

Major phytochemicals present in the plant are:

a. Theobromine
b. Tannic acid
c. Mangiferin
d. Digoxin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	Not Applicable	Not Applicable	Failed
Tannic acid	-19.96	-21.78	Positive
Mangiferin	Not Applicable	Not Applicable	Failed
Digoxin	-11.18	-13.87	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Tannic acid and Digoxin helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Myrica rubra can prevent Herpes due to the presence of Tannic acid and Digoxin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Neerium indicum against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Elora Barik[1], Yashaswi Nayak[2]

[1]elora.barik1996@gmail.com

[2]yashaswi.nayak@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Neerium indicum against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Myricetin helped to prevent Herpes.

Introduction: Neerium indicum is known for its medicinal activities. Nerium indicum has many medicinal properties like bitter, acrid, astringent, anthelmintic, aphrodisiac, stomachic, febrifuge, diuretic, emetic, expectorant, cardio tonic, anticancer etc which is used in the treatment of cardiac asthma, renal and vesicle calculi, chronic stomach, skin related problems, snake bites joint pains, leprosy, cancer, ulcers etc. Leaves and flowers are also used to treat malaria. Leaves and bark is treated as insecticide, rat poison and parasitic.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Gentianales
Family	Apocynaceae
Genus	Nerium
Species	indicum

Major phytochemicals present in the plant are:

a. Myricetin
b. Peonidin
c. Curcumin
d. Ascorbic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Myricetin	-14.3	-19.75	Positive
Peonidin	Not Applicable	Not Applicable	Failed
Curcumin	Not Applicable	Not Applicable	Failed
Ascorbic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Myricetin helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Neerium indicum can prevent Herpes due to the presence of Myricetin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Peganum harmala against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Pratyasha Moharana[1], Yashaswi Nayak[2]

[1]pratyashamoharana24@gmail.com

[2]yashaswi.nayak@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Peganum harmala against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Myricetin and Theobromine helped to prevent Herpes.

Introduction: Peganum harmala is known for its medicinal activities. It has been used as an analgesic, emmenagogue, and abortifacient agent. Leaf was used to cure herpes. In a certain region of India the root was applied to kill body lice.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Sapindales
Family	Nitrariaceae
Genus	Peganum
Species	harmala

Major phytochemicals present in the plant are:

a. Genistein
b. Myricetin
c. Theobromine
d. Quercetin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Genistein	Not Applicable	Not Applicable	Failed
Myricetin	-14.35	-19.33	Positive
Theobromine	-11.38	-16.88	Positive
Quercetin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Myricetin and Theobromine helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Peganum harmala can prevent Herpes due to the presence of Myricetin and Theobromine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Phyllanthus emblica against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Shibashis Mishra[1], Yashaswi Nayak[2]

[1]shibashis.jajpur@gmail.com

[2]yashaswi.nayak@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Phyllanthus emblica against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Ursolic acid helped to prevent Herpes.

Introduction: Phyllanthus emblica is known for its medicinal activities. Seeds of the fruits are used in treatment of asthma, herpes and bronchitis. The leaves are used as fodder. Alcoholic extract of the fruit is anti–viral.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Malpighiales
Family	Phyllanthaceae
Genus	Phyllanthus
Species	emblica

Major phytochemicals present in the plant are:

a. Malvidin
b. Myricetin
c. Ursolic acid
d. Ascorbic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Malvidin	Not Applicable	Not Applicable	Failed
Myricetin	Not Applicable	Not Applicable	Failed
Ursolic acid	-17.08	-19.75	Positive
Ascorbic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ursolic acid helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Phyllanthus emblica can prevent Herpes due to the presence of Ursolic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Phyllanthus urinaria against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Priyadarshini Pradhan[1], Pratibharani Deep[2]

[1]180705180108@cutm.ac.in

[2]pratibharani.deep@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Phyllanthus urinaria against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Tangeretin and Ursolic acid helped to prevent Herpes.

Introduction: Phyllanthus urinaria is known for its medicinal activities. It is used in folk medicine as a cure to treat jaundice, herpes, diabetes, malaria, and liver diseases.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Malpighiales
Family	Phyllanthaceae
Genus	Phyllanthus
Species	urinaria

Major phytochemicals present in the plant are:

a. Tangeretin
b. Ursolic acid
c. Limonene
d. Naringin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tangeretin	-14.39	-17.33	Positive
Ursolic acid	-12.38	-16.88	Positive
Limonene	Not Applicable	Not Applicable	Failed
Naringin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Tangeretin and Ursolic acid helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Phyllanthus urinaria can prevent Herpes due to the presence of Tangeretin and Ursolic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Pinus massoniana against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Abhilash Pattnaik[1], Pratibharani Deep[2]

[1]pattnaikabhilash9@gmail.com

[2]pratibharani.deep@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Pinus massoniana against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Quercetin helped to prevent Herpes.

Introduction: Pinus massoniana is known for its medicinal activities. The chopped or decocted leaves are used in the treatment of rheumatism, herpes and intestinal parasites.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Pinopsida
Order	Pinales
Family	Pinaceae
Genus	Pinus
Species	massoniana

Major phytochemicals present in the plant are:

a. Genistein
b. Daidzein
c. Peonidin
d. Quercetin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Genistein	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Quercetin	-12.48	-15.82	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Quercetin helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Pinus massoniana can prevent Herpes due to the presence of Quercetin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Plantago major against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Minati Rani Muni[1], Pratibharani Deep[2]

[1]myselfminatirani@gmail.com

[2]pratibharani.deep@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Plantago major against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Genistein helped to prevent Herpes.

Introduction: Plantago major is known for its medicinal activities. Plantago major is used in wound healing and the leaves were used as a remedy of wounds and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Lamiales
Family	Plantaginaceae
Genus	Plantago
Species	major

Major phytochemicals present in the plant are:

a. Genistein
b. Daidzein
c. Gallic acid
d. Ellagic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Genistein	-11.37	-15.37	Positive
Daidzein	Not Applicable	Not Applicable	Failed
Gallic acid	Not Applicable	Not Applicable	Failed
Ellagic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Genistein helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Plantago major can prevent Herpes due to the presence of Genistein. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Portulaca oleracea against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Nibedita Pradhan[1], Pratibharani Deep[2]

[1]180705180111@cutm.ac.in

[2]pratibharani.deep@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Portulaca oleracea against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Allicin and Ajoene helped to prevent Herpes.

Introduction: Portulaca oleracea is known for its medicinal activities. Portulaca oleracea has been used as a folk medicine in many countries, acting as a febrifuge, antiseptic, herpes and vermifuge.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Caryophyllales
Family	Portulacaceae
Genus	Portulaca
Species	oleracea

Major phytochemicals present in the plant are:

a. Allicin
b. Ajoene
c. Theobromine
d. Quercetin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Allicin	-12.37	-15.82	Positive
Ajoene	-14.38	-18.67	Positive
Theobromine	Not Applicable	Not Applicable	Failed
Quercetin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Allicin and Ajoene helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Portulaca oleracea can prevent Herpes due to the presence of Allicin and Ajoene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Salvia officinalis against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Selina Swain[1], Pratibharani Deep[2]

[1]swainselina996@gmail.com

[2]pratibharani.deep@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Salvia officinalis against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Coumarin helped to prevent Herpes.

Introduction: Salvia officinalis is known for its medicinal activities. S. officinalis has been used for the treatment of different kinds of disorders including seizure, ulcers, gout, rheumatism, herpes, inflammation, dizziness, tremor, paralysis, diarrhea, and hyperglycemia.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Lamiales
Family	Lamiaceae
Genus	Salvia
Species	officinalis

Major phytochemicals present in the plant are:

a. Tocopherol
b. Epicatechin
c. Coumarin
d. Proanthocyanidins

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tocopherol	Not Applicable	Not Applicable	Failed
Epicatechin	Not Applicable	Not Applicable	Failed
Coumarin	-16.97	-21.67	Positive
Proanthocyanidins	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Coumarin helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Salvia officinalis can prevent Herpes due to the presence of Coumarin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Santalum album against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Sarthak Siddhant Mishra[1], Pratibharani Deep[2]

[1]mishra.sarthaksiddhant@gmail.com

[2]pratibharani.deep@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Santalum album against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Hesperidin and Isorhamnetin helped to prevent Herpes.

Introduction: Santalum album is known for its medicinal activities. Sandalwood oil has been widely used in folk medicine for treatment of common colds, bronchitis, skin disorders, heart ailments, general weakness, fever, herpes, infection of the urinary tract, inflammation of the mouth and pharynx, liver and gallbladder complaints and other maladies.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Santalales
Family	Santalaceae
Genus	Santalum
Species	album

Major phytochemicals present in the plant are:

a. Hesperidin
b. Isorhamnetin
c. Rutin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Hesperidin	-14.37	-18.94	Positive
Isorhamnetin	-15.67	-21.39	Positive
Rutin	Not Applicable	Not Applicable	Failed
Ferulic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Hesperidin and Isorhamnetin helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Santalum album can prevent Herpes due to the presence of Hesperidin and Isorhamnetin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Scinaia hatei against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Manisha Panda[1], Pratibharani Deep[2]

[1]manishapanda07697@gmail.com

[2]pratibharani.deep@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Scinaia hatei against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Tangeretin helped to prevent Herpes.

Introduction: Scinaia hatei is known for its medicinal activities. It helps to treat herpes, dengue, myalgia, pancreatitis, cardiac arrhythmia, and hepatitis.

The plant is classified as follows:

Kingdom	Plantae
Division	Rhodophyta
Class	Florideophyceae
Order	Nemalionales
Family	Chaetangiaceae
Genus	Scinaia
Species	hatei

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Alliin
c. Tangeretin
d. Tannic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Alliin	Not Applicable	Not Applicable	Failed
Tangeretin	-14.67	-18.33	Positive
Tannic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Tangeretin helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Scinaia hatei can prevent Herpes due to the presence of Tangeretin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Scoparia dulcis against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Ashok Kumar Sahoo[1], Pratibharani Deep[2]

[1]ashoksahuk4note@gmail.com

[2]pratibharani.deep@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Scoparia dulcis against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Pelletierine and Digoxin helped to prevent Herpes.

Introduction: Scoparia dulcis is known for its medicinal activities. It is considered a weed in many areas but used as medicinal herb for a wide range of uses including treatment for digestive problems, pulmonary conditions, fever, skin disorders, hypertension, hemorrhoids, diarrhea, dysentery, insect bites, anemia, albuminuria, diabetes, herpes, etc.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Lamiales
Family	Plantaginaceae
Genus	Scoparia
Species	dulcis

Major phytochemicals present in the plant are:

a. Pelletierine
b. Digoxin
c. Rosmarinic acid
d. Campesterol

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	-14.37	-15.33	Positive
Digoxin	-9.96	-14.84	Positive
Rosmarinic acid	Not Applicable	Not Applicable	Failed
Campesterol	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Pelletierine and Digoxin helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Scoparia dulcis can prevent Herpes due to the presence of Pelletierine and Digoxin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Solanum torvum against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Subhasmita Rout[1], Pratibharani Deep[2]

[1]routsonali220@gmail.com

[2]pratibharani.deep@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Solanum torvum against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Campesterol helped to prevent Herpes.

Introduction: Solanum torvum is known for its medicinal activities. Fruit and leaf decoction is used to treat cough, herpes and to treat liver and spleen enlargement.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Solanales
Family	Solanaceae
Genus	Solanum
Species	torvum

Major phytochemicals present in the plant are:

a. Campesterol
b. Linamarin
c. Glutathione
d. Malvidin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Campesterol	-12.82	-18.88	Positive
Linamarin	Not Applicable	Not Applicable	Failed
Glutathione	Not Applicable	Not Applicable	Failed
Malvidin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Campesterol helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Solanum torvum can prevent Herpes due to the presence of Campesterol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Sorghum bicolor against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Leepsa Priyadarshini[1], Pratibharani Deep[2]

[1]lovelyleepsa@gmail.com

[2]pratibharani.deep@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Sorghum bicolor against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Limonene and Pelargonidin helped to prevent Herpes.

Introduction: Sorghum bicolor is known for its medicinal activities. Seed extracts are drunk to treat hepatitis and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Poales
Family	Poaceae
Genus	Sorghum
Species	bicolor

Major phytochemicals present in the plant are:

a. Naringin
b. Limonene
c. Naringin
d. Pelargonidin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Naringin	Not Applicable	Not Applicable	Failed
Limonene	-14.28	-20.92	Positive
Naringin	Not Applicable	Not Applicable	Failed
Pelargonidin	-12.54	-15.25	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Limonene and Pelargonidin helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Sorghum bicolor can prevent Herpes due to the presence of Limonene and Pelargonidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Strobilanthus cusia against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Bidyashree Tripathy[1], Gagan Kumar Panigrahi[2]

[1]tripathybidyashree9@gmail.com

[2]gagan.panigrahi@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Strobilanthus cusia against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Epicatechin helped to prevent Herpes.

Introduction: Strobilanthus cusia is known for its medicinal activities. It is used for influenza, herpes, epidemic cerebrospinal meningitis, encephalitis B, viral pneumonia and mumps.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Lamiales
Family	Acanthaceae
Genus	Strobilanthus
Species	cusia

Major phytochemicals present in the plant are:

a. Tangeretin
b. Salicylic acid
c. Epicatechin
d. Catechin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tangeretin	Not Applicable	Not Applicable	Failed
Salicylic acid	Not Applicable	Not Applicable	Failed
Epicatechin	-18.82	-21.84	Positive
Catechin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Epicatechin helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Strobilanthus cusia can prevent Herpes due to the presence of Epicatechin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Swertia chirata against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Sutapa Nayak[1], Gagan Kumar Panigrahi[2]

[1]ppupuli33@gmail.com

[2]gagan.panigrahi@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Swertia chirata against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Theobromine and Limoene helped to prevent Herpes.

Introduction: Swertia chirata is known for its medicinal activities. People use the parts that grow above the ground to make medicine. Chirata is used for fever, constipation, herpes, upset stomach, loss of appetite, intestinal worms, skin diseases, and cancer.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Gentianales
Family	Gentianaceae
Genus	Swertia
Species	chirayita

Major phytochemicals present in the plant are:

a. Theobromine
b. Limonene
c. Naringin
d. Limonene

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	-8.72	-10.55	Positive
Limonene	-12.73	-14.82	Positive
Naringin	Not Applicable	Not Applicable	Failed
Limonene	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Theobromine and Limoene helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Swertia chirata can prevent Herpes due to the presence of Theobromine and Limoene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Syzygium aromaticum against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Archana Pati[1], Gagan Kumar Panigrahi[2]

[1]patiarchana10@gmail.com

[2]gagan.panigrahi@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Syzygium aromaticum against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Digoxin and Limonene helped to prevent Herpes.

Introduction: Syzygium aromaticum is known for its medicinal activities. Traditionally, cloves have been used for centuries in the treatment of vomiting; flatulence; nausea; liver, herpes, bowel and stomach disorders; and as a stimulant for the nerves.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Myrtales
Family	Myrtaceae
Genus	Syzygium
Species	aromaticum

Major phytochemicals present in the plant are:

a. Lutein
b. Digoxin
c. Pelargonidin
d. Limonene

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lutein	Not Applicable	Not Applicable	Failed
Digoxin	-19.72	-21.39	Positive
Pelargonidin	Not Applicable	Not Applicable	Failed
Limonene	-9.54	-15.37	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Digoxin and Limonene helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Syzygium aromaticum can prevent Herpes due to the presence of Digoxin and Limonene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Syzygium jambos against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Leenarani Nayak[1], Gagan Kumar Panigrahi[2]

[1]leenaraninayak23@gmail.com

[2]gagan.panigrahi@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Syzygium jambos against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Tannic acid helped to prevent Herpes.

Introduction: Syzygium jambos is known for its medicinal activities. A decoction of the leaves is used as a diuretic, herpes, a remedy for sore eyes and for rheumatism. The seeds are used to treat diarrhoea, dysentery, diabetes and catarrh. A decoction of bark is administered to relieve asthma and bronchitis.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Myrtales
Family	Myrtaceae
Genus	Syzygium
Species	jambos

Major phytochemicals present in the plant are:

a. Ellagic acid
b. Gallic acid
c. Tannic acid
d. Theobromine

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Ellagic acid	Not Applicable	Not Applicable	Failed
Gallic acid	Not Applicable	Not Applicable	Failed
Tannic acid	-11.71	-18.28	Positive
Theobromine	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Tannic acid helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Syzygium jambos can prevent Herpes due to the presence of Tannic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Taracetium vulgare against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Suinita Panda[1], Gagan Kumar Panigrahi[2]

[1]pandasunita160@gmail.com

[2]gagan.panigrahi@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Taracetium vulgare against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Pelletierine and Quercetin helped to prevent Herpes.

Introduction: Taracetium vulgare is known for its medicinal activities. In larger doses the plant can procure an abortion, though these doses can be poisonous. Externally, tansy is used as a poultice on swellings, herpes and some eruptive skin diseases.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Asterales
Family	Asteraceae
Genus	Taracetum
Species	vulgare

Major phytochemicals present in the plant are:

a. Pelletierine
b. Alliin
c. Theobromine
d. Quercetin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	-11.42	-18.84	Positive
Alliin	Not Applicable	Not Applicable	Failed
Theobromine	Not Applicable	Not Applicable	Failed
Quercetin	-10.32	-19.08	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Pelletierine and Quercetin helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Taracetium vulgare can prevent Herpes due to the presence of Pelletierine and Quercetin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Usnea complanta against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Nabakrushna Behera[1], Gagan Kumar Panigrahi[2]

[1]nabakrushnabehera06@gmail.com

[2]gagan.panigrahi@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Usnea complanta against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Daidzein and Campesterol helped to prevent Herpes.

Introduction: Usnea complanta is known for its medicinal activities. It can sometimes be used as a bioindicator, because it tends to only grow in those regions where the air is clean, and of high quality. It is also used to cure herpes.

The plant is classified as follows:

Kingdom	Fungi
Division	Ascomycota
Class	Lecanoromycetes
Order	Lecanorales
Family	Asteraceae
Genus	Usnea
Species	complanta

Major phytochemicals present in the plant are:

a. Genistein
b. Daidzein
c. Tangeretin
d. Campesterol

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Genistein	Not Applicable	Not Applicable	Failed
Daidzein	-15.18	-21.07	Positive
Tangeretin	Not Applicable	Not Applicable	Failed
Campesterol	-12.78	-15.38	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Daidzein and Campesterol helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Usnea complanta can prevent Herpes due to the presence of Daidzein and Campesterol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Ventilago denticulate against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Nishivijita Nayak[1], Gagan Kumar Panigrahi[2]

[1]nishivijitanayak@gmail.com

[2]gagan.panigrahi@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Ventilago denticulate against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Allicin helped to prevent Herpes.

Introduction: Ventilago denticulate is known for its medicinal activities. Stem bark is powdered and mixed with sesame oil, externally applied to skin diseases and sprains. Root bark—used for atonic dyspepsia, mild fever, herpes and debility. Sap is used for the treatment of deafness.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Rosales
Family	Rhamnaceae
Genus	Ventilago
Species	denticulate

Major phytochemicals present in the plant are:

a. Allicin
b. Hesperidin
c. Ferulic acid
d. Epicatechin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Allicin	-18.19	-20.37	Positive
Hesperidin	Not Applicable	Not Applicable	Failed
Ferulic acid	Not Applicable	Not Applicable	Failed
Epicatechin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Allicin helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Ventilago denticulate can prevent Herpes due to the presence of Allicin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Withania somnifera against Herpes through deactivation of Herpes Simplex virus Type II Protease (1AT3)

Suraj Kumar Sahu[1], Gagan Kumar Panigrahi[2]

[1]ssuraj2437@gmail.com

[2]gagan.panigrahi@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Withania somnifera against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes Simplex virus Type II Protease (1AT3) enzyme. It was found that Rosmarinic acid helped to prevent Herpes.

Introduction: Withania somnifera is known for its medicinal activities. The medicinal plants are widely used by the traditional medical practitioners for curing various diseases like diarrhea, dysentery, insect bites, anemia, albuminuria, diabetes, herpes, etc.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Solanales
Family	Solanaceae
Genus	Withania
Species	somnifera

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Tannic acid
c. Rosmarinic acid
d. Cryptoxanthin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes Simplex virus Type II Protease (1AT3) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes Simplex virus Type II Protease (1AT3) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Tannic acid	Not Applicable	Not Applicable	Failed
Rosmarinic acid	-18.34	-19.48	Positive
Cryptoxanthin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Rosmarinic acid helped deactivate the Herpes Simplex virus Type II Protease (1AT3) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Withania somnifera can prevent Herpes due to the presence of Rosmarinic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Pandanus amaryllifolius against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Jogesh Kumar Nayak[1], Gagan Kumar Panigrahi[2]

[1]jogeshnayak1998@gmail.com

[2]gagan.panigrahi@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Pandanus amaryllifolius against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Limonene helped to prevent Herpes.

Introduction: Pandanus amaryllifolius is known for its medicinal activities. The leaves are used in the perfume industry and traditional medicine to treat diseases like cough, asthma, herpes and diarrhea.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Pandanales
Family	Pandanaceae
Genus	Pandanus
Species	amaryllifolius

Major phytochemicals present in the plant are:

a. Ellagic acid
b. Gallic acid
c. Peonidin
d. Limonene

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Ellagic acid	Not Applicable	Not Applicable	Failed
Gallic acid	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Limonene	-11.84	-17.08	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Limonene helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Pandanus amaryllifolius can prevent Herpes due to the presence of Limonene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Adansonia digitata against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Pratishruti Gouda[1], Gagan Kumar Panigrahi[2]

[1]pratishrutigouda260@gmail.com

[2]gagan.panigrahi@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Adansonia digitata against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Peonidin helped to prevent Herpes.

Introduction: Adansonia digitata is known for its medicinal activities. The various parts of the plant (leaves, bark and seeds) are used to cure tuberculosis, fever, microbial infections, diarrhea and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Malvales
Family	Bombacaceae
Genus	Adansonia
Species	digitata

Major phytochemicals present in the plant are:

a. Resveratrol
b. Phenyl isothiocyanate
c. Capsaicin
d. Peonidin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Resveratrol	Not Applicable	Not Applicable	Failed
Phenyl isothiocyanate	Not Applicable	Not Applicable	Failed
Capsaicin	Not Applicable	Not Applicable	Failed
Peonidin	-12.37	-17.57	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Peonidin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Adansonia digitata can prevent Herpes due to the presence of Peonidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Aglai odorata against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Swati Maitri Kar[1], Siba Prasad Parida[2]

[1]swatimaitrikar909@gmail.com

[2]siba.parida@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Aglai odorata against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Myricetin and Peonidin helped to prevent Herpes.

Introduction: Aglai odorata is known for its medicinal activities. Aglaia species are used in traditional medicine: leaves to treat wounds, fever, headache, asthma, jaundice, and as a tonic e.g. after childbirth; flowers against fever, asthma, jaundice and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Sapindales
Family	Meliaceae
Genus	Aglai
Species	odorata

Major phytochemicals present in the plant are:

a. Morphine
b. Myricetin
c. Peonidin
d. Benzyl isothiocyanate

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Morphine	Not Applicable	Not Applicable	Failed
Myricetin	-11.27	-24.37	Positive
Peonidin	-12.57	-18.64	Positive
Benzyl isothiocyanate	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Myricetin and Peonidin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Aglai odorata can prevent Herpes due to the presence of Myricetin and Peonidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Aloe vera against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Karishma Sultana[1], Siba Prasad Parida[2]

[1]karishmacharmy@gmail.com

[2]siba.parida@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Aloe vera against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Lupeol helped to prevent Herpes.

Introduction: Aloe vera is known for its medicinal activities. Aloe vera used to cure herpes, weak digestion, general weakness, anaemia, bloating, stomach ulcers and gum disease.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Liliopsida
Order	Liliales
Family	Aloeaceae
Genus	Aloe
Species	vera

Major phytochemicals present in the plant are:

a. Phytoene
b. Salicylic acid
c. Sitosterol
d. Lupeol

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Phytoene	Not Applicable	Not Applicable	Failed
Salicylic acid	Not Applicable	Not Applicable	Failed
Sitosterol	Not Applicable	Not Applicable	Failed
Lupeol	-9.47	-11.57	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Lupeol helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Aloe vera can prevent Herpes due to the presence of Lupeol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Andrographis paniculata against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Padmaja Biswal[1], Siba Prasad Parida[2]

[1]biswalpadmaja972@gmail.com

[2]siba.parida@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Andrographis paniculata against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Genistein and Theobromine helped to prevent Herpes.

Introduction: Andrographis paniculata is known for its medicinal activities. A. paniculata has been used in Siddha and Ayurvedic medicine. It is promoted as a dietary supplement for cancer prevention and cure. In the traditional medicine of India, A. paniculata has also been used for jaundice therapy.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Lamiales
Family	Acanthaceae
Genus	Andrographis
Species	paniculata

Major phytochemicals present in the plant are:

a. Genistein
b. Daidzein
c. Theobromine
d. Quercetin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Genistein	-12.15	-19.37	Positive
Daidzein	Not Applicable	Not Applicable	Failed
Theobromine	-11.27	-14.27	Positive
Quercetin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Genistein and Theobromine helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Andrographis paniculata can prevent Herpes due to the presence of Genistein and Theobromine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Atlantia sp. against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Smruti Ranjan Behera[1], Siba Prasad Parida[2]

[1]smrutiranjansrb7@gmail.com

[2]siba.parida@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Atlantia sp. against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Ajoene helped to prevent Herpes.

Introduction: Atlantia sp. is known for its medicinal activities. The flowers, fruit and roots are used to cure herpes, jaundice, fever, headache and asthma.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Sapindales
Family	Rutaceae
Genus	Atalantia
Species	racemosa

Major phytochemicals present in the plant are:

a. Allicin
b. Ajoene
c. Gallic acid
d. Ellagic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Allicin	Not Applicable	Not Applicable	Failed
Ajoene	-12.33	-19.67	Positive
Gallic acid	Not Applicable	Not Applicable	Failed
Ellagic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ajoene helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Atlantia sp. can prevent Herpes due to the presence of Ajoene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Azadirachta indica against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Swetapadma Mishra[1], Siba Prasad Parida[2]

[1]swetapadmamishra8888@gmail.com

[2]siba.parida@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Azadirachta indica against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Rutin helped to prevent Herpes.

Introduction: Azadirachta indica is known for its medicinal activities. Neem has an anti-inflammatory property which helps reduces acne, herpes, skin blemishes and malaria.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Sapindales
Family	Meliaceae
Genus	Azadirachta
Species	indica

Major phytochemicals present in the plant are:

a. Tocopherol
b. Isorhamnetin
c. Rutin
d. Azadirichtin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tocopherol	Not Applicable	Not Applicable	Failed
Isorhamnetin	Not Applicable	Not Applicable	Failed
Rutin	-9.67	-12.67	Positive
Azadirichtin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Rutin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Azadirachta indica can prevent Herpes due to the presence of Rutin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Barleria lupulina against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Pooja Pradhan[1], Siba Prasad Parida[2]

[1]poojapradhan23453@gmail.com

[2]siba.parida@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Barleria lupulina against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Epicatechin helped to prevent Herpes.

Introduction: Barleria lupulina is known for its medicinal activities. The flowers are used internally for the treatment of migraine, internal abscesses, oedema, haemoptysis, herpes, urethral discharges, seminal disorders and reduce obesity.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Scrophulariales
Family	Acanthaceae
Genus	Barleria
Species	lupulina

Major phytochemicals present in the plant are:

a. Hesperidin
b. Epicatechin
c. Coumarin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Hesperidin	Not Applicable	Not Applicable	Failed
Epicatechin	-14.28	-19.17	Positive
Coumarin	Not Applicable	Not Applicable	Failed
Ferulic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Epicatechin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Barleria lupulina can prevent Herpes due to the presence of Epicatechin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Bauhinia racemosa against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Sushree Elora[1], Siba Prasad Parida[2]

[1]sushreeelora340@gmail.com

[2]siba.parida@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Bauhinia racemosa against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Digoxin and Tannic acid helped to prevent Herpes.

Introduction: Bauhinia racemosa is known for its medicinal activities. Bauhinia racemosa leaves have been used in the treatment of asthma traditionally because of their antihistaminic action it also used to cure herpes and urethral discharges.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Equisetopsida
Order	Fabales
Family	Fabaceae
Genus	Bauhinia
Species	racemosa

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Digoxin
c. Rosmarinic acid
d. Tannic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Digoxin	-12.24	-17.59	Positive
Rosmarinic acid	Not Applicable	Not Applicable	Failed
Tannic acid	-11.34	-15.38	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Digoxin and Tannic acid helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Bauhinia racemosa can prevent Herpes due to the presence of Digoxin and Tannic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Bauhinia variegate against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Rutuparna parida[1], Siba Prasad Parida[2]

[1]rutuparnaparidalikun1998@gmail.com

[2]siba.parida@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Bauhinia variegate against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Cryptoxanthin helped to prevent Herpes.

Introduction: Bauhinia variegate is known for its medicinal activities. The bark decoction is used for diarrhoea control, as an astringent alternative and for treating scrofula, herpes, skin diseases and ulcers.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Equisetopsida
Order	Fabales
Family	Fabaceae
Genus	Bauhinia
Species	variegata

Major phytochemicals present in the plant are:

a. Cryptoxanthin
b. Carotene
c. Lutein
d. Lycopene

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Cryptoxanthin	-11.57	-18.12	Positive
Carotene	Not Applicable	Not Applicable	Failed
Lutein	Not Applicable	Not Applicable	Failed
Lycopene	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Cryptoxanthin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Bauhinia variegate can prevent Herpes due to the presence of Cryptoxanthin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Bidens pilosa against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Ashutosh Dash[1], Siba Prasad Parida[2]

[1]kunudash3@gmail.com

[2]siba.parida@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Bidens pilosa against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Eugenol and Apigenin helped to prevent Herpes.

Introduction: Bidens pilosa is known for its medicinal activities. Roots, leaves and seed have been reported to possess antibacterial, antidysenteric, anti-inflammatory, antimicrobial, herpes, antimalarial, diuretic, hepato-protective and hypotensive activities.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Asterales
Family	Asteraceae
Genus	Bidens
Species	pilosa

Major phytochemicals present in the plant are:

a. Eugenol
b. Apigenin
c. Luteolin
d. Carnosic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Eugenol	-9.67	-15.64	Positive
Apigenin	-11.27	-14.87	Positive
Luteolin	Not Applicable	Not Applicable	Failed
Carnosic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Eugenol and Apigenin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Bidens pilosa can prevent Herpes due to the presence of Eugenol and Apigenin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Cedrus libani against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Aryaratna Mangaldeep[1], Siba Prasad Parida[2]

[1]aryaratnamangaldeep@gmail.com

[2]siba.parida@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Cedrus libani against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Carnosic acid helped to prevent Herpes.

Introduction: Cedrus libani is known for its medicinal activities. It is traditionally used to treat diseases like arteriosclerosis, water retention, herpes, lymphatic damage, etc.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Pinopsida
Order	Pinales
Family	Pinaceae
Genus	Cedrus
Species	libani

Major phytochemicals present in the plant are:

a. Luteolin
b. Carnosic acid
c. Eugenol
d. Salicylic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Luteolin	Not Applicable	Not Applicable	Failed
Carnosic acid	-9.17	-14.85	Positive
Eugenol	Not Applicable	Not Applicable	Failed
Salicylic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Carnosic acid helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Cedrus libani can prevent Herpes due to the presence of Carnosic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Cissus quadrangularis against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Anwesha Aparamita Nayak[1], Shantanu Bhattacharya[2]

[1]anweshanayak426@gmail.com

[2]shantanu.bhattacharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Cissus quadrangularis against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Ferulic acid helped to prevent Herpes.

Introduction: Cissus quadrangularis is known for its medicinal activities. The roots and stems are most useful for healing of fracture of the bones. The stem is bitter; it is given internally and applied topically in broken bones, used in complaints of the back and spine. A paste of stem is useful for muscular pains and herpes. The plant has been documented in Ayurveda for the treatment of osteoarthritis, rheumatoid arthritis and osteoporosis.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Vitales
Family	Vitacea
Genus	Cissus
Species	quadrangularis

Major phytochemicals present in the plant are:

a. Lupeol
b. Ferulic acid
c. Hesperidin
d. Naringin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lupeol	Not Applicable	Not Applicable	Failed
Ferulic acid	-12.57	-18.17	Positive
Hesperidin	Not Applicable	Not Applicable	Failed
Naringin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ferulic acid helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Cissus quadrangularis can prevent Herpes due to the presence of Ferulic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Conyza aegyptica against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Pooja Gadtia[1], Shantanu Bhattacharya[2]

[1]poojagadtia@gmail.com

[2]shantanu.bhattacharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Conyza aegyptica against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Epicatechin helped to prevent Herpes.

Introduction: Conyza aegyptica is known for its medicinal activities. The whole plants used to treat herpes, wound, skin diseases and toothache.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Dicotyledonae
Order	Asterales
Family	Asteraceae
Genus	Conyza
Species	aegyptiaca

Major phytochemicals present in the plant are:

a. Theobromine
b. Epicatechin
c. Catechin
d. Limonene

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	Not Applicable	Not Applicable	Failed
Epicatechin	-14.87	-19.63	Positive
Catechin	Not Applicable	Not Applicable	Failed
Limonene	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Epicatechin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Conyza aegyptica can prevent Herpes due to the presence of Epicatechin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Cyperus rotundus against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Prachiprava Das[1], Shantanu Bhattacharya[2]

[1]prachipravadas4@gmail.com

[2]shantanu.bhattacharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Cyperus rotundus against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Pelargonidin helped to prevent Herpes.

Introduction: Cyperus rotundus is known for its medicinal activities. It is a medicinal herb traditionally used to treat various clinical conditions at home such as diarrhea, diabetes, pyresis, herpes, inflammation, malaria, and stomach and bowel disorders.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Poales
Family	Cyperaceae
Genus	Cyperus
Species	rotundus

Major phytochemicals present in the plant are:

a. Ellagic acid
b. Gallic acid
c. Pelargonidin
d. Limonene

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Ellagic acid	Not Applicable	Not Applicable	Failed
Gallic acid	Not Applicable	Not Applicable	Failed
Pelargonidin	-13.67	-15.87	Positive
Limonene	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Pelargonidin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Cyperus rotundus can prevent Herpes due to the presence of Pelargonidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Euphorbia peplus against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Mukesh Kumar Biswal[1], Shantanu Bhattacharya[2]

[1]argainmukesh@gmail.com

[2]shantanu.bhattacharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Euphorbia peplus against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Digoxin helped to prevent Herpes.

Introduction: Euphorbia peplus is known for its medicinal activities. The plant is administered in the form of herbal tea as diuretic, laxative and emollient. It is also used for the treatment of asthma and bronchitis, as it relaxes the smooth muscles of bronchi. It is recommended against dry cough, herpes, runny nose and liver diseases.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Malpighiales
Family	Euphorbiaceae
Genus	Euphorbia
Species	peplus

Major phytochemicals present in the plant are:

a. Lutein
b. Digoxin
c. Tannic acid
d. Theobromine

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lutein	Not Applicable	Not Applicable	Failed
Digoxin	-12.57	-15.89	Positive
Tannic acid	Not Applicable	Not Applicable	Failed
Theobromine	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Digoxin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Euphorbia peplus can prevent Herpes due to the presence of Digoxin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Glycyrrhiza glabra against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Kshyanaprava Rout[1], Shantanu Bhattacharya[2]

[1]kshyanapravarout901@gmail.com

[2]shantanu.bhattacharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Glycyrrhiza glabra against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Pelletierine helped to prevent Herpes.

Introduction: Glycyrrhiza glabra is known for its medicinal activities. Traditionally used to treat many diseases, such as respiratory disorders, hyperdipsia, epilepsy, fever, sexual debility, paralysis, stomach ulcers, rheumatism, skin diseases, hemorrhagic diseases, and jaundice.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Fabales
Family	Fabaceae
Genus	Glycyrrhiza
Species	glabra

Major phytochemicals present in the plant are:

a. Pelletierine
b. Alliin
c. Tangeretin
d. Campesterol

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	-11.84	-19.67	Positive
Alliin	Not Applicable	Not Applicable	Failed
Tangeretin	Not Applicable	Not Applicable	Failed
Campesterol	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Pelletierine helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Glycyrrhiza glabra can prevent Herpes due to the presence of Pelletierine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Heliotropium marifolium against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Priyadarshini Nanda[1], Shantanu Bhattacharya[2]

[1]priyadrshini19763@gmail.com

[2]shantanu.bhattacharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Heliotropium marifolium against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Pelargonidin helped to prevent Herpes.

Introduction: Heliotropium marifolium is known for its medicinal activities. Heliotropium marifolium is used against syphilis, asthma, herpes, UTI and wound.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Boraginales
Family	Boraginaceae
Genus	Heliotropium
Species	marifolium

Major phytochemicals present in the plant are:

a. Campesterol
b. Linamarin
c. Naringin
d. Pelargonidin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Campesterol	Not Applicable	Not Applicable	Failed
Linamarin	Not Applicable	Not Applicable	Failed
Naringin	Not Applicable	Not Applicable	Failed
Pelargonidin	-12.67	-22.57	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Pelargonidin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Heliotropium marifolium can prevent Herpes due to the presence of Pelargonidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Holoptelea integrifolia against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Deepanjali Dhal[1], Shantanu Bhattacharya[2]

[1]deepalopa121@gmail.com

[2]shantanu.bhattacharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Holoptelea integrifolia against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Limonene helped to prevent Herpes.

Introduction: Holoptelea integrifolia is known for its medicinal activities. The plant Holoptelea integrifolia is used traditionally for the treatment of inflammation, gastritis, dyspepsia, colic, intestinal worms, vomiting, wound healing, leprosy, diabetes, hemorrhoids, herpes, dysmenorrhea, and rheumatism.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Rosales
Family	Ulmaceae
Genus	Holoptelea
Species	integrifolia

Major phytochemicals present in the plant are:

a. Naringin
b. Limonene
c. Glutathione
d. Malvidin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Naringin	Not Applicable	Not Applicable	Failed
Limonene	-12.57	-18.94	Positive
Glutathione	Not Applicable	Not Applicable	Failed
Malvidin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Limonene helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Holoptelea integrifolia can prevent Herpes due to the presence of Limonene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Houttuynia cordata against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Niharika Mohanta[1], Shantanu Bhattacharya[2]

[1]niharikamohanta75@gmail.com

[2]shantanu.bhattacharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Houttuynia cordata against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Limonene helped to prevent Herpes.

Introduction: Houttuynia cordata is known for its medicinal activities. It is used as a fresh herbal garnish. In northeastern India, it is commonly used in salads and as a garnish over side dishes. The tender roots can also be ground into chutneys along with dry meat or fish, chilies, and tamarind. It is taken raw as salad and cooked along with fish as fish curry. In Japan and Korea, its dried leaves may be used as a tea. Houttuynia cordata was used in traditional Chinese medicine.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Piperales
Family	Saururaceae
Genus	Houttuynia
Species	cordata

Major phytochemicals present in the plant are:

a. Tangeretin
b. Salicylic acid
c. Limonene
d. Naringin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tangeretin	Not Applicable	Not Applicable	Failed
Salicylic acid	Not Applicable	Not Applicable	Failed
Limonene	-12.57	-15.67	Positive
Naringin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Limonene helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Houttuynia cordata can prevent Herpes due to the presence of Limonene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Hypericum hookerianum against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Sangita Khuntia[1], Shantanu Bhattacharya[2]

[1]sangitakhuntia1998@gmail.com

[2]shantanu.bhattacharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Hypericum hookerianum against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Malvidin helped to prevent Herpes.

Introduction: Hypericum hookerianum is known for its medicinal activities. It was recommended in the first century by Greek physicians as a diuretic, wound-healer, and treatment for menstrual disorders. It has been used as an anti-inflammatory, anti-bacterial, disinfectant, and a remedy for disorders of the respiratory tract and gall bladder and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Malpighiales
Family	Hypericaceae
Genus	Hypericum
Species	hookerianum

Major phytochemicals present in the plant are:

a. Malvidin
b. Salicylic acid
c. Ursolic acid
d. Astaxanthin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Malvidin	-9.67	-17.54	Positive
Salicylic acid	Not Applicable	Not Applicable	Failed
Ursolic acid	Not Applicable	Not Applicable	Failed
Astaxanthin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Malvidin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Hypericum hookerianum can prevent Herpes due to the presence of Malvidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Hypericum mysorense against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Jhili Meher[1], Shantanu Bhattacharya[2]

[1]meherjhili35@gmail.com

[2]shantanu.bhattacharya@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Hypericum mysorense against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Ursolic acid and Astaxanthin helped to prevent Herpes.

Introduction: Hypericum mysorense is known for its medicinal activities. Hypericum mysorense has been used to treat wounds and herpes as part of the Ayurvedic system of traditional medicine.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Equisetopsida
Order	Malpighiales
Family	Hypericaceae
Genus	Hypericum
Species	mysorense

Major phytochemicals present in the plant are:

a. Ursolic acid
b. Astaxanthin
c. Sitosterol
d. Astaxanthin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Ursolic acid	-9.64	-17.31	Positive
Astaxanthin	-12.97	-15.44	Positive
Sitosterol	Not Applicable	Not Applicable	Failed
Astaxanthin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ursolic acid and Astaxanthin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Hypericum mysorense can prevent Herpes due to the presence of Ursolic acid and Astaxanthin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Lippia alba against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Subhashree Pattanayak[1], Rukmini Mishra[2]

[1]subhashreepattanayak7001@gmail.com

[2]rukmini.mishra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Lippia alba against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Pelargonidin and Ascorbic acid helped to prevent Herpes.

Introduction: Lippia alba is known for its medicinal activities. A tea made from the leaves is used to treat intestinal and respiratory disturbances, including influenza and herpes. A well-sugared infusion is drunk to bring relief of heart problems and to soothe tachycardia.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Equisetopsida
Order	Lamiales
Family	Verbenaceae
Genus	Lippia
Species	alba

Major phytochemicals present in the plant are:

a. Pelargonidin
b. Caffeine
c. Curcumin
d. Ascorbic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelargonidin	-11.94	-16.37	Positive
Caffeine	Not Applicable	Not Applicable	Failed
Curcumin	Not Applicable	Not Applicable	Failed
Ascorbic acid	-12.37	-13.18	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Pelargonidin and Ascorbic acid helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Lippia alba can prevent Herpes due to the presence of Pelargonidin and Ascorbic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Melia azaderach against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Bapujee Palai[1], Rukmini Mishra[2]

[1]bapujeepalai@gmail.com

[2]rukmini.mishra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Melia azaderach against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Digoxin helped to prevent Herpes.

Introduction: Melia azaderach is known for its medicinal activities. The leaf juice is anthelmintic, antilithic, diuretic, herpes and emmenagogue.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Sapindales
Family	Meliaceae
Genus	Melia
Species	azedarach

Major phytochemicals present in the plant are:

a. Zingiberene
b. Ursolic acid
c. Astaxanthin
d. Digoxin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Zingiberene	Not Applicable	Not Applicable	Failed
Ursolic acid	Not Applicable	Not Applicable	Failed
Astaxanthin	Not Applicable	Not Applicable	Failed
Digoxin	-6.36	-15.89	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Digoxin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Melia azaderach can prevent Herpes due to the presence of Digoxin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Mentha piperata against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Saswotika Nayak[1], Rukmini Mishra[2]

[1]nayaksaswotika@gmail.com

[2]rukmini.mishra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Mentha piperata against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Digoxin helped to prevent Herpes.

Introduction: Mentha piperata is known for its medicinal activities. It is used for treatment of a variety of conditions, including irritable bowel syndrome (IBS), nausea, herpes and other digestive issues, as well as the common cold and headaches.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Lamiales
Family	Lamiaceae
Genus	Mentha
Species	piperata

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Carotene
c. Digoxin
d. Tannic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Carotene	Not Applicable	Not Applicable	Failed
Digoxin	-9.64	-12.08	Positive
Tannic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Digoxin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Mentha piperata can prevent Herpes due to the presence of Digoxin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Momordia charantia against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Babita Das[1], Rukmini Mishra[2]

[1]babaitamani145@gmail.com

[2]rukmini.mishra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Momordia charantia against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Sulforaphane helped to prevent Herpes.

Introduction: Momordia charantia is known for its medicinal activities. Juice of the leaves is used to treat piles and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Cucurbitales
Family	Cucurbitaceae
Genus	Momordia
Species	charantia

Major phytochemicals present in the plant are:

a. Curcumin
b. Ascorbic acid
c. Sulforaphane
d. Digoxin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Curcumin	Not Applicable	Not Applicable	Failed
Ascorbic acid	Not Applicable	Not Applicable	Failed
Sulforaphane	-15.47	-18.59	Positive
Digoxin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Sulforaphane helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Momordia charantia can prevent Herpes due to the presence of Sulforaphane. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Moringa oleifera against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Shuvashree Suvasmita Tripathy[1], Rukmini Mishra[2]

[1]luckytripathy65@gmail.com

[2]rukmini.mishra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Moringa oleifera against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Rosmarinic acid helped to prevent Herpes.

Introduction: Moringa oleifera is known for its medicinal activities. Various parts of this plant such as the leaves, roots, seed, bark, fruit, flowers and immature pods act as cardiac and circulatory stimulants, possess antitumor, antipyretic, antiepileptic, antiinflammatory, herpes, antiulcer, antispasmodic, diuretic, antihypertensive, cholesterol lowering.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Brassicales
Family	Moringaceae
Genus	Moringa
Species	oleifera

Major phytochemicals present in the plant are:

a. Isorhamnetin
b. Rosmarinic acid
c. Lutein
d. Lycopene

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Isorhamnetin	Not Applicable	Not Applicable	Failed
Rosmarinic acid	-13.48	-16.87	Positive
Lutein	Not Applicable	Not Applicable	Failed
Lycopene	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Rosmarinic acid helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Moringa oleifera can prevent Herpes due to the presence of Rosmarinic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Myrica rubra against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Pratyasha Mohanty[1], Rukmini Mishra[2]

[1]pratyasha008@gmail.com

[2]rukmini.mishra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Myrica rubra against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Tannic acid helped to prevent Herpes.

Introduction: Myrica rubra is known for its medicinal activities. The stem bark is used as a wash in the treatment of arsenic poisoning, skin diseases, wounds and ulcers. The fruit is carminative, herpes, pectoral and stomachic.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Fagales
Family	Myricaceae
Genus	Myrica
Species	rubra

Major phytochemicals present in the plant are:

a. Theobromine
b. Tannic acid
c. Mangiferin
d. Digoxin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	Not Applicable	Not Applicable	Failed
Tannic acid	-11.44	-18.37	Positive
Mangiferin	Not Applicable	Not Applicable	Failed
Digoxin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Tannic acid helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Myrica rubra can prevent Herpes due to the presence of Tannic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Neerium indicum against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Sunanya Das[1], Rukmini Mishra[2]

[1]dsunanya2016@gmail.com

[2]rukmini.mishra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Neerium indicum against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Peonidin helped to prevent Herpes.

Introduction: Neerium indicum is known for its medicinal activities. Nerium indicum has many medicinal properties like bitter, acrid, astringent, anthelmintic, aphrodisiac, stomachic, febrifuge, diuretic, emetic, expectorant, cardio tonic, anticancer etc which is used in the treatment of cardiac asthma, renal and vesicle calculi, chronic stomach, skin related problems, snake bites joint pains, leprosy, cancer, ulcers etc. Leaves and flowers are also used to treat malaria. Leaves and bark is treated as insecticide, rat poison and parasitic.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Gentianales
Family	Apocynaceae
Genus	Nerium
Species	indicum

Major phytochemicals present in the plant are:

a. Myricetin
b. Peonidin
c. Curcumin
d. Ascorbic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Myricetin	Not Applicable	Not Applicable	Failed
Peonidin	-14.06	-18.47	Positive
Curcumin	Not Applicable	Not Applicable	Failed
Ascorbic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Peonidin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Neerium indicum can prevent Herpes due to the presence of Peonidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Peganum harmala against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Sonu Priya Sahu[1], Rukmini Mishra[2]

[1]sonupriyasahu111@gmail.com

[2]rukmini.mishra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Peganum harmala against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Myricetin helped to prevent Herpes.

Introduction: Peganum harmala is known for its medicinal activities. It has been used as an analgesic, emmenagogue, and abortifacient agent. Leaf was used to cure herpes. In a certain region of India the root was applied to kill body lice.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Sapindales
Family	Nitrariaceae
Genus	Peganum
Species	harmala

Major phytochemicals present in the plant are:

a. Genistein
b. Myricetin
c. Theobromine
d. Quercetin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Genistein	Not Applicable	Not Applicable	Failed
Myricetin	-12.84	-16.91	Positive
Theobromine	Not Applicable	Not Applicable	Failed
Quercetin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Myricetin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Peganum harmala can prevent Herpes due to the presence of Myricetin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Phyllanthus emblica against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Somali Biswal[1], Rukmini Mishra[2]

[1]somalibiswal.jsp@gmail.com

[2]rukmini.mishra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Phyllanthus emblica against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Ursolic acid helped to prevent Herpes.

Introduction: Phyllanthus emblica is known for its medicinal activities. Seeds of the fruits are used in treatment of asthma, herpes and bronchitis. The leaves are used as fodder. Alcoholic extract of the fruit is anti–viral.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Malpighiales
Family	Phyllanthaceae
Genus	Phyllanthus
Species	emblica

Major phytochemicals present in the plant are:

a. Malvidin
b. Myricetin
c. Ursolic acid
d. Ascorbic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Malvidin	Not Applicable	Not Applicable	Failed
Myricetin	Not Applicable	Not Applicable	Failed
Ursolic acid	-12.77	-18.74	Positive
Ascorbic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ursolic acid helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Phyllanthus emblica can prevent Herpes due to the presence of Ursolic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Phyllanthus urinaria against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Archita Sahoo[1], Rukmini Mishra[2]

[1]architashoo1997@gmail.com

[2]rukmini.mishra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Phyllanthus urinaria against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Naringin helped to prevent Herpes.

Introduction: Phyllanthus urinaria is known for its medicinal activities. It is used in folk medicine as a cure to treat jaundice, herpes, diabetes, malaria, and liver diseases.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Malpighiales
Family	Phyllanthaceae
Genus	Phyllanthus
Species	urinaria

Major phytochemicals present in the plant are:

a. Tangeretin
b. Ursolic acid
c. Limonene
d. Naringin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tangeretin	Not Applicable	Not Applicable	Failed
Ursolic acid	Not Applicable	Not Applicable	Failed
Limonene	Not Applicable	Not Applicable	Failed
Naringin	-14.98	-18.82	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Naringin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Phyllanthus urinaria can prevent Herpes due to the presence of Naringin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Pinus massoniana against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Asutosh Sarangi[1], Preetha Bhadra[2]

[1]asutoshsarangi087@gmail.com

[2]preeta.bhadra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Pinus massoniana against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Quercetin helped to prevent Herpes.

Introduction: Pinus massoniana is known for its medicinal activities. The chopped or decocted leaves are used in the treatment of rheumatism, herpes and intestinal parasites.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Pinopsida
Order	Pinales
Family	Pinaceae
Genus	Pinus
Species	massoniana

Major phytochemicals present in the plant are:

a. Genistein
b. Daidzein
c. Peonidin
d. Quercetin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Genistein	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Quercetin	-15.66	-18.01	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Quercetin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Pinus massoniana can prevent Herpes due to the presence of Quercetin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Plantago major against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Kabyashree Diptimayee Swain[1], Preetha Bhadra[2]

[1]kabyashreeswain20@gmail.com

[2]preeta.bhadra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Plantago major against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Gallic acid helped to prevent Herpes.

Introduction: Plantago major is known for its medicinal activities. Plantago major is used in wound healing and the leaves were used as a remedy of wounds and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Lamiales
Family	Plantaginaceae
Genus	Plantago
Species	major

Major phytochemicals present in the plant are:

a. Genistein
b. Daidzein
c. Gallic acid
d. Ellagic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Genistein	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Failed
Gallic acid	-11.57	-17.94	Positive
Ellagic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Gallic acid helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Plantago major can prevent Herpes due to the presence of Gallic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Portulaca oleracea against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Priyanka Payal[1], Preetha Bhadra[2]

[1]payalpriyanka98@gmail.com

[2]preeta.bhadra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Portulaca oleracea against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Ajoene helped to prevent Herpes.

Introduction: Portulaca oleracea is known for its medicinal activities. Portulaca oleracea has been used as a folk medicine in many countries, acting as a febrifuge, antiseptic, herpes and vermifuge.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Caryophyllales
Family	Portulacaceae
Genus	Portulaca
Species	oleracea

Major phytochemicals present in the plant are:

a. Allicin
b. Ajoene
c. Theobromine
d. Quercetin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Allicin	Not Applicable	Not Applicable	Failed
Ajoene	-9.67	-15.67	Positive
Theobromine	Not Applicable	Not Applicable	Failed
Quercetin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ajoene helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Portulaca oleracea can prevent Herpes due to the presence of Ajoene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Salvia officinalis against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Prangya Paramita Behera[1], Preetha Bhadra[2]

[1]prangyaparamitabehera6@gmail.com

[2]preeta.bhadra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Salvia officinalis against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Coumarin helped to prevent Herpes.

Introduction: Salvia officinalis is known for its medicinal activities. S. officinalis has been used for the treatment of different kinds of disorders including seizure, ulcers, gout, rheumatism, herpes, inflammation, dizziness, tremor, paralysis, diarrhea, and hyperglycemia.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Lamiales
Family	Lamiaceae
Genus	Salvia
Species	officinalis

Major phytochemicals present in the plant are:

a. Tocopherol
b. Epicatechin
c. Coumarin
d. Proanthocyanidins

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tocopherol	Not Applicable	Not Applicable	Failed
Epicatechin	Not Applicable	Not Applicable	Failed
Coumarin	-12.11	-18.57	Positive
Proanthocyanidins	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Coumarin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Salvia officinalis can prevent Herpes due to the presence of Coumarin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Santalum album against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Debasmita Rautaray[1], Preetha Bhadra[2]

[1]debasmitaroutray123@gmai.com

[2]preeta.bhadra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Santalum album against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Ferulic acid helped to prevent Herpes.

Introduction: Santalum album is known for its medicinal activities. Sandalwood oil has been widely used in folk medicine for treatment of common colds, bronchitis, skin disorders, heart ailments, general weakness, fever, herpes, infection of the urinary tract, inflammation of the mouth and pharynx, liver and gallbladder complaints and other maladies.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Santalales
Family	Santalaceae
Genus	Santalum
Species	album

Major phytochemicals present in the plant are:

a. Hesperidin
b. Isorhamnetin
c. Rutin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Hesperidin	Not Applicable	Not Applicable	Failed
Isorhamnetin	Not Applicable	Not Applicable	Failed
Rutin	Not Applicable	Not Applicable	Failed
Ferulic acid	-6.87	-15.78	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ferulic acid helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Santalum album can prevent Herpes due to the presence of Ferulic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Scinaia hatei against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Aischarya Mohanty[1], Preetha Bhadra[2]

[1]aischaryamohanty98@gmail.com

[2]preeta.bhadra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Scinaia hatei against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Alliin helped to prevent Herpes.

Introduction: Scinaia hatei is known for its medicinal activities. It helps to treat herpes, dengue, myalgia, pancreatitis, cardiac arrhythmia, and hepatitis.

The plant is classified as follows:

Kingdom	Plantae
Division	Rhodophyta
Class	Florideophyceae
Order	Nemalionales
Family	Chaetangiaceae
Genus	Scinaia
Species	hatei

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Alliin
c. Tangeretin
d. Tannic acid

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Alliin	-11.88	-14.57	Positive
Tangeretin	Not Applicable	Not Applicable	Failed
Tannic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Alliin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Scinaia hatei can prevent Herpes due to the presence of Alliin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Scoparia dulcis against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Anusaya Panda[1], Preetha Bhadra[2]

[1]anusayapanda801@gmail.com

[2]preeta.bhadra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Scoparia dulcis against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Campesterol helped to prevent Herpes.

Introduction: Scoparia dulcis is known for its medicinal activities. It is considered a weed in many areas but used as medicinal herb for a wide range of uses including treatment for digestive problems, pulmonary conditions, fever, skin disorders, hypertension, hemorrhoids, diarrhea, dysentery, insect bites, anemia, albuminuria, diabetes, herpes, etc.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Lamiales
Family	Plantaginaceae
Genus	Scoparia
Species	dulcis

Major phytochemicals present in the plant are:

a. Pelletierine
b. Digoxin
c. Rosmarinic acid
d. Campesterol

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	Not Applicable	Not Applicable	Failed
Digoxin	Not Applicable	Not Applicable	Failed
Rosmarinic acid	Not Applicable	Not Applicable	Failed
Campesterol	-11.44	-19.63	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Campesterol helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Scoparia dulcis can prevent Herpes due to the presence of Campesterol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Solanum torvum against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Jiten Kumar Sutar[1], Preetha Bhadra[2]

[1]jitensutar1997@gmail.com

[2]preeta.bhadra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Solanum torvum against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Linamarin helped to prevent Herpes.

Introduction: Solanum torvum is known for its medicinal activities. Fruit and leaf decoction is used to treat cough, herpes and to treat liver and spleen enlargement.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Solanales
Family	Solanaceae
Genus	Solanum
Species	torvum

Major phytochemicals present in the plant are:

a. Campesterol
b. Linamarin
c. Glutathione
d. Malvidin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Campesterol	Not Applicable	Not Applicable	Failed
Linamarin	-12.54	-16.77	Positive
Glutathione	Not Applicable	Not Applicable	Failed
Malvidin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Linamarin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Solanum torvum can prevent Herpes due to the presence of Linamarin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Sorghum bicolor against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Sasmita Mallick[1], Preetha Bhadra[2]

[1]sasmitamallickds@gmail.com

[2]preeta.bhadra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Sorghum bicolor against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Pelargonidin helped to prevent Herpes.

Introduction: Sorghum bicolor is known for its medicinal activities. Seed extracts are drunk to treat hepatitis and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Poales
Family	Poaceae
Genus	Sorghum
Species	bicolor

Major phytochemicals present in the plant are:

a. Naringin
b. Limonene
c. Naringin
d. Pelargonidin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Naringin	Not Applicable	Not Applicable	Failed
Limonene	Not Applicable	Not Applicable	Failed
Naringin	Not Applicable	Not Applicable	Failed
Pelargonidin	-19.37	-22.37	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Pelargonidin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Sorghum bicolor can prevent Herpes due to the presence of Pelargonidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Strobilanthus cusia against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Akshaya Kumar Sahoo[1], Preetha Bhadra[2]

[1]sakshayakumar128@gmail.com

[2]preeta.bhadra@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Strobilanthus cusia against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Tangeretin and Catechin helped to prevent Herpes.

Introduction: Strobilanthus cusia is known for its medicinal activities. It is used for influenza, herpes, epidemic cerebrospinal meningitis, encephalitis B, viral pneumonia and mumps.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Lamiales
Family	Acanthaceae
Genus	Strobilanthus
Species	cusia

Major phytochemicals present in the plant are:

a. Tangeretin
b. Salicylic acid
c. Epicatechin
d. Catechin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tangeretin	-14.47	-18.79	Positive
Salicylic acid	Not Applicable	Not Applicable	Failed
Epicatechin	Not Applicable	Not Applicable	Failed
Catechin	-14.28	-18.94	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Tangeretin and Catechin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Strobilanthus cusia can prevent Herpes due to the presence of Tangeretin and Catechin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Swertia chirata against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Pooja Mohanty[1], Ranjan Kumar Sahoo[2]

[1]poojamohanty39@gmail.com

[2]ranjan.sahoo@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Swertia chirata against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Naringin helped to prevent Herpes.

Introduction: Swertia chirata is known for its medicinal activities. People use the parts that grow above the ground to make medicine. Chirata is used for fever, constipation, herpes, upset stomach, loss of appetite, intestinal worms, skin diseases, and cancer.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Gentianales
Family	Gentianaceae
Genus	Swertia
Species	chirayita

Major phytochemicals present in the plant are:

a. Theobromine
b. Limonene
c. Naringin
d. Limonene

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	Not Applicable	Not Applicable	Failed
Limonene	Not Applicable	Not Applicable	Failed
Naringin	-15.37	-17.58	Positive
Limonene	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Naringin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Swertia chirata can prevent Herpes due to the presence of Naringin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Syzygium aromaticum against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Smitanjali Nayak[1], Ranjan Kumar Sahoo[2]

[1]smitanjali64@gmail.com

[2]ranjan.sahoo@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Syzygium aromaticum against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Pelargonidin helped to prevent Herpes.

Introduction: Syzygium aromaticum is known for its medicinal activities. Traditionally, cloves have been used for centuries in the treatment of vomiting; flatulence; nausea; liver, herpes, bowel and stomach disorders; and as a stimulant for the nerves.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Myrtales
Family	Myrtaceae
Genus	Syzygium
Species	aromaticum

Major phytochemicals present in the plant are:

a. Lutein
b. Digoxin
c. Pelargonidin
d. Limonene

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lutein	Not Applicable	Not Applicable	Failed
Digoxin	Not Applicable	Not Applicable	Failed
Pelargonidin	-13.69	-18.37	Positive
Limonene	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Pelargonidin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Syzygium aromaticum can prevent Herpes due to the presence of Pelargonidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Syzygium jambos against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Monalisha Giri[1], Ranjan Kumar Sahoo[2]

[1]monalishagiri880@gmail.com

[2]ranjan.sahoo@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Syzygium jambos against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Tannic acid helped to prevent Herpes.

Introduction: Syzygium jambos is known for its medicinal activities. A decoction of the leaves is used as a diuretic, herpes, a remedy for sore eyes and for rheumatism. The seeds are used to treat diarrhoea, dysentery, diabetes and catarrh. A decoction of bark is administered to relieve asthma and bronchitis.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Myrtales
Family	Myrtaceae
Genus	Syzygium
Species	jambos

Major phytochemicals present in the plant are:

a. Ellagic acid
b. Gallic acid
c. Tannic acid
d. Theobromine

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Ellagic acid	Not Applicable	Not Applicable	Failed
Gallic acid	Not Applicable	Not Applicable	Failed
Tannic acid	-12.14	-17.87	Positive
Theobromine	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Tannic acid helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Syzygium jambos can prevent Herpes due to the presence of Tannic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Taracetium vulgare against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Soumya Ranjan Nayak[1], Ranjan Kumar Sahoo[2]

[1]soumyaranjann04@gmail.com

[2]ranjan.sahoo@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Taracetium vulgare against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Alliin and Quercetin helped to prevent Herpes.

Introduction: Taracetium vulgare is known for its medicinal activities. In larger doses the plant can procure an abortion, though these doses can be poisonous. Externally, tansy is used as a poultice on swellings, herpes and some eruptive skin diseases.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Asterales
Family	Asteraceae
Genus	Taracetum
Species	vulgare

Major phytochemicals present in the plant are:

a. Pelletierine
b. Alliin
c. Theobromine
d. Quercetin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	Not Applicable	Not Applicable	Failed
Alliin	-10.78	-12.38	Positive
Theobromine	Not Applicable	Not Applicable	Failed
Quercetin	-15.78	-21.57	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Alliin and Quercetin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Taracetium vulgare can prevent Herpes due to the presence of Alliin and Quercetin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Usnea complanta against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Bhagyalaxmi Santi[1], Ranjan Kumar Sahoo[2]

[1]bhagyalaxmisanti123@gmail.com

[2]ranjan.sahoo@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Usnea complanta against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Campesterol helped to prevent Herpes.

Introduction: Usnea complanta is known for its medicinal activities. It can sometimes be used as a bioindicator, because it tends to only grow in those regions where the air is clean, and of high quality. It is also used to cure herpes.

The plant is classified as follows:

Kingdom	Fungi
Division	Ascomycota
Class	Lecanoromycetes
Order	Lecanorales
Family	Asteraceae
Genus	Usnea
Species	complanta

Major phytochemicals present in the plant are:

a. Genistein
b. Daidzein
c. Tangeretin
d. Campesterol

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Genistein	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Failed
Tangeretin	Not Applicable	Not Applicable	Failed
Campesterol	-13.87	-21.57	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Campesterol helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Usnea complanta can prevent Herpes due to the presence of Campesterol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Ventilago denticulate against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Rajashree Mishra[1], Ranjan Kumar Sahoo[2]

[1]rajashree.mishra015@gmail.com

[2]ranjan.sahoo@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Ventilago denticulate against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Hesperidin helped to prevent Herpes.

Introduction: Ventilago denticulate is known for its medicinal activities. Stem bark is powdered and mixed with sesame oil, externally applied to skin diseases and sprains. Root bark—used for atonic dyspepsia, mild fever, herpes and debility. Sap is used for the treatment of deafness.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Rosales
Family	Rhamnaceae
Genus	Ventilago
Species	denticulate

Major phytochemicals present in the plant are:

a. Allicin
b. Hesperidin
c. Ferulic acid
d. Epicatechin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Allicin	Not Applicable	Not Applicable	Failed
Hesperidin	-6.33	-14.39	Positive
Ferulic acid	Not Applicable	Not Applicable	Failed
Epicatechin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Hesperidin helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Ventilago denticulate can prevent Herpes due to the presence of Hesperidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Withania somnifera against Herpes through deactivation of Herpes virus fusion regulator complex gH-Gl (3M1C)

Chinmayee Rath[1], Ranjan Kumar Sahoo[2]

[1]chinmayee984@gmail.com

[2]ranjan.sahoo@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Withania somnifera against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. It was found that Rosmarinic acid helped to prevent Herpes.

Introduction: Withania somnifera is known for its medicinal activities. The medicinal plants are widely used by the traditional medical practitioners for curing various diseases like diarrhea, dysentery, insect bites, anemia, albuminuria, diabetes, herpes, etc.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Solanales
Family	Solanaceae
Genus	Withania
Species	somnifera

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Tannic acid
c. Rosmarinic acid
d. Cryptoxanthin

One of the major enzymes required for the survival of the organism causing Herpes is Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Tannic acid	Not Applicable	Not Applicable	Failed
Rosmarinic acid	-11.05	-18.36	Positive
Cryptoxanthin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Rosmarinic acid helped deactivate the Herpes virus fusion regulator complex gH-Gl (3M1C) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Withania somnifera can prevent Herpes due to the presence of Rosmarinic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Pandanus amaryllifolius against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Pratibha Karmee[1], Ranjan Kumar Sahoo[2]

[1]pratibha.karmee@gmail.com

[2]ranjan.sahoo@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Pandanus amaryllifolius against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Limonene helped to prevent Herpes.

Introduction: Pandanus amaryllifolius is known for its medicinal activities. The leaves are used in the perfume industry and traditional medicine to treat diseases like cough, asthma, herpes and diarrhea.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Pandanales
Family	Pandanaceae
Genus	Pandanus
Species	amaryllifolius

Major phytochemicals present in the plant are:

a. Ellagic acid
b. Gallic acid
c. Peonidin
d. Limonene

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Ellagic acid	Not Applicable	Not Applicable	Failed
Gallic acid	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Limonene	-11.38	-14.92	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Limonene helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Pandanus amaryllifolius can prevent Herpes due to the presence of Limonene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Adansonia digitata against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Hrudaya Ballava Dash[1], Ranjan Kumar Sahoo[2]

[1]hrudayaballava1997@gmail.com

[2]ranjan.sahoo@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Adansonia digitata against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Peonidin helped to prevent Herpes.

Introduction: Adansonia digitata is known for its medicinal activities. The various parts of the plant (leaves, bark and seeds) are used to cure tuberculosis, fever, microbial infections, diarrhea and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Malvales
Family	Bombacaceae
Genus	Adansonia
Species	digitata

Major phytochemicals present in the plant are:

a. Resveratrol
b. Phenyl isothiocyanate
c. Capsaicin
d. Peonidin

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Resveratrol	Not Applicable	Not Applicable	Failed
Phenyl isothiocyanate	Not Applicable	Not Applicable	Failed
Capsaicin	Not Applicable	Not Applicable	Failed
Peonidin	-12.37	-17.34	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Peonidin helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Adansonia digitata can prevent Herpes due to the presence of Peonidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Aglai odorata against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Ananya Pani[1], Ranjan Kumar Sahoo[2]

[1]ananyapani16@gmail.com

[2]ranjan.sahoo@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Aglai odorata against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Myricetin helped to prevent Herpes.

Introduction: Aglai odorata is known for its medicinal activities. Aglaia species are used in traditional medicine: leaves to treat wounds, fever, headache, asthma, jaundice, and as a tonic e.g. after childbirth; flowers against fever, asthma, jaundice and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Sapindales
Family	Meliaceae
Genus	Aglai
Species	odorata

Major phytochemicals present in the plant are:

a. Morphine
b. Myricetin
c. Peonidin
d. Benzyl isothiocyanate

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Morphine	Not Applicable	Not Applicable	Failed
Myricetin	-18.37	-22.52	Positive
Peonidin	Not Applicable	Not Applicable	Failed
Benzyl isothiocyanate	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Myricetin helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Aglai odorata can prevent Herpes due to the presence of Myricetin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Aloe vera against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Shubhranshee Sanshlishta Sahu[1], Debanjana Saha[2]

[1]sonushubhra98@gmail.com

[2]deepanjana.saha@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Aloe vera against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Sitosterol helped to prevent Herpes.

Introduction: Aloe vera is known for its medicinal activities. Aloe vera used to cure herpes, weak digestion, general weakness, anaemia, bloating, stomach ulcers and gum disease.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Liliopsida
Order	Liliales
Family	Aloeaceae
Genus	Aloe
Species	vera

Major phytochemicals present in the plant are:

a. Phytoene
b. Salicylic acid
c. Sitosterol
d. Lupeol

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Phytoene	Not Applicable	Not Applicable	Failed
Salicylic acid	Not Applicable	Not Applicable	Failed
Sitosterol	-18.88	-22.87	Positive
Lupeol	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Sitosterol helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Aloe vera can prevent Herpes due to the presence of Sitosterol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Andrographis paniculata against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Subhashree Subhasmita[1], Debanjana Saha[2]

[1]subhasmitashine@gmail.com

[2]deepanjana.saha@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Andrographis paniculata against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Genistein helped to prevent Herpes.

Introduction: Andrographis paniculata is known for its medicinal activities. A. paniculata has been used in Siddha and Ayurvedic medicine. It is promoted as a dietary supplement for cancer prevention and cure. In the traditional medicine of India, A. paniculata has also been used for jaundice therapy.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Lamiales
Family	Acanthaceae
Genus	Andrographis
Species	paniculata

Major phytochemicals present in the plant are:

a. Genistein
b. Daidzein
c. Theobromine
d. Quercetin

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Genistein	-12.37	-15.67	Positive
Daidzein	Not Applicable	Not Applicable	Failed
Theobromine	Not Applicable	Not Applicable	Failed
Quercetin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Genistein helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Andrographis paniculata can prevent Herpes due to the presence of Genistein. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Atlantia sp. against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Subhadarshini Satapathy[1], Debanjana Saha[2]

[1]subhadarshini.satapathy@gmail.com

[2]deepanjana.saha@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Atlantia sp. against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Ajoene helped to prevent Herpes.

Introduction: Atlantia sp. is known for its medicinal activities. The flowers, fruit and roots are used to cure herpes, jaundice, fever, headache and asthma.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Sapindales
Family	Rutaceae
Genus	Atalantia
Species	racemosa

Major phytochemicals present in the plant are:

a. Allicin
b. Ajoene
c. Gallic acid
d. Ellagic acid

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Allicin	Not Applicable	Not Applicable	Failed
Ajoene	-12.86	-19.81	Positive
Gallic acid	Not Applicable	Not Applicable	Failed
Ellagic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ajoene helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Atlantia sp. can prevent Herpes due to the presence of Ajoene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Azadirachta indica against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Sonalika Pasayat[1], Debanjana Saha[2]

[1]sonalikapasayat1997@gmail.com

[2]deepanjana.saha@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Azadirachta indica against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Isorhamnetin helped to prevent Herpes.

Introduction: Azadirachta indica is known for its medicinal activities. Neem has an anti-inflammatory property which helps reduces acne, herpes, skin blemishes and malaria.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Sapindales
Family	Meliaceae
Genus	Azadirachta
Species	indica

Major phytochemicals present in the plant are:

a. Tocopherol
b. Isorhamnetin
c. Rutin
d. Azadirichtin

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tocopherol	Not Applicable	Not Applicable	Failed
Isorhamnetin	-15.48	-21.38	Positive
Rutin	Not Applicable	Not Applicable	Failed
Azadirichtin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Isorhamnetin helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Azadirachta indica can prevent Herpes due to the presence of Isorhamnetin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Barleria lupulina against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Sharbani Bahali[1], Debanjana Saha[2]

[1]bahalisharbani@gmail.com

[2]deepanjana.saha@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Barleria lupulina against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Coumarin helped to prevent Herpes.

Introduction: Barleria lupulina is known for its medicinal activities. The flowers are used internally for the treatment of migraine, internal abscesses, oedema, haemoptysis, herpes, urethral discharges, seminal disorders and reduce obesity.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Scrophulariales
Family	Acanthaceae
Genus	Barleria
Species	lupulina

Major phytochemicals present in the plant are:

a. Hesperidin
b. Epicatechin
c. Coumarin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Hesperidin	Not Applicable	Not Applicable	Failed
Epicatechin	Not Applicable	Not Applicable	Failed
Coumarin	-12.97	-19.67	Positive
Ferulic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Coumarin helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Barleria lupulina can prevent Herpes due to the presence of Coumarin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Bauhinia racemosa against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Meenakshee Mohanty[1], Debanjana Saha[2]

[1]meenakshimohanty100@gmail.com

[2]deepanjana.saha@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Bauhinia racemosa against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Sulforaphane helped to prevent Herpes.

Introduction: Bauhinia racemosa is known for its medicinal activities. Bauhinia racemosa leaves have been used in the treatment of asthma traditionally because of their antihistaminic action it also used to cure herpes and urethral discharges.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Equisetopsida
Order	Fabales
Family	Fabaceae
Genus	Bauhinia
Species	racemosa

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Digoxin
c. Rosmarinic acid
d. Tannic acid

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	-14.37	-15.89	Positive
Digoxin	Not Applicable	Not Applicable	Failed
Rosmarinic acid	Not Applicable	Not Applicable	Failed
Tannic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Sulforaphane helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Bauhinia racemosa can prevent Herpes due to the presence of Sulforaphane. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Bauhinia variegate against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Shubham Pradhan[1], Debanjana Saha[2]

[1]shubham9668518446@gmail.com

[2]deepanjana.saha@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Bauhinia variegate against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Lutein helped to prevent Herpes.

Introduction: Bauhinia variegate is known for its medicinal activities. The bark decoction is used for diarrhoea control, as an astringent alternative and for treating scrofula, herpes, skin diseases and ulcers.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Equisetopsida
Order	Fabales
Family	Fabaceae
Genus	Bauhinia
Species	variegata

Major phytochemicals present in the plant are:

a. Cryptoxanthin
b. Carotene
c. Lutein
d. Lycopene

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Cryptoxanthin	Not Applicable	Not Applicable	Failed
Carotene	Not Applicable	Not Applicable	Failed
Lutein	-10.12	-18.07	Positive
Lycopene	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Lutein helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Bauhinia variegate can prevent Herpes due to the presence of Lutein. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Bidens pilosa against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Piyush Pradhan[1], Debanjana Saha[2]

[1]pradhanpiyush97@gmail.com

[2]deepanjana.saha@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Bidens pilosa against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Carnosic acid helped to prevent Herpes.

Introduction: Bidens pilosa is known for its medicinal activities. Roots, leaves and seed have been reported to possess antibacterial, antidysenteric, anti-inflammatory, antimicrobial, herpes, antimalarial, diuretic, hepato-protective and hypotensive activities.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Asterales
Family	Asteraceae
Genus	Bidens
Species	pilosa

Major phytochemicals present in the plant are:

a. Eugenol
b. Apigenin
c. Luteolin
d. Carnosic acid

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Eugenol	Not Applicable	Not Applicable	Failed
Apigenin	Not Applicable	Not Applicable	Failed
Luteolin	Not Applicable	Not Applicable	Failed
Carnosic acid	-12.27	-15.47	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Carnosic acid helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Bidens pilosa can prevent Herpes due to the presence of Carnosic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Cedrus libani against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Punya Prateek Majhi[1], Debanjana Saha[2]

[1]somprateek283@gmail.com

[2]deepanjana.saha@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Cedrus libani against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Luteolin helped to prevent Herpes.

Introduction: Cedrus libani is known for its medicinal activities. It is traditionally used to treat diseases like arteriosclerosis, water retention, herpes, lymphatic damage, etc.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Pinopsida
Order	Pinales
Family	Pinaceae
Genus	Cedrus
Species	libani

Major phytochemicals present in the plant are:

a. Luteolin
b. Carnosic acid
c. Eugenol
d. Salicylic acid

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Luteolin	-14.37	-19.31	Positive
Carnosic acid	Not Applicable	Not Applicable	Failed
Eugenol	Not Applicable	Not Applicable	Failed
Salicylic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Luteolin helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Cedrus libani can prevent Herpes due to the presence of Luteolin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Cissus quadrangularis against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Chinmayee Chitralekha Pradhan[1], Debanjana Saha[2]

[1]pradhanchinmayee96@gmail.com

[2]deepanjana.saha@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Cissus quadrangularis against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Ferulic acid helped to prevent Herpes.

Introduction: Cissus quadrangularis is known for its medicinal activities. The roots and stems are most useful for healing of fracture of the bones. The stem is bitter; it is given internally and applied topically in broken bones, used in complaints of the back and spine. A paste of stem is useful for muscular pains and herpes. The plant has been documented in Ayurveda for the treatment of osteoarthritis, rheumatoid arthritis and osteoporosis.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Vitales
Family	Vitacea
Genus	Cissus
Species	quadrangularis

Major phytochemicals present in the plant are:

a. Lupeol
b. Ferulic acid
c. Hesperidin
d. Naringin

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lupeol	Not Applicable	Not Applicable	Failed
Ferulic acid	-12.58	-14.49	Positive
Hesperidin	Not Applicable	Not Applicable	Failed
Naringin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ferulic acid helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Cissus quadrangularis can prevent Herpes due to the presence of Ferulic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Conyza aegyptica against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Debasmita Das[1], Pradipta Banerjee[2]

[1]smitadeba98@gmail.com

[2]pradipta.banerjee@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Conyza aegyptica against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Epicatechin helped to prevent Herpes.

Introduction: Conyza aegyptica is known for its medicinal activities. The whole plants used to treat herpes, wound, skin diseases and toothache.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Dicotyledonae
Order	Asterales
Family	Asteraceae
Genus	Conyza
Species	aegyptiaca

Major phytochemicals present in the plant are:

a. Theobromine
b. Epicatechin
c. Catechin
d. Limonene

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	Not Applicable	Not Applicable	Failed
Epicatechin	-17.27	-20.29	Positive
Catechin	Not Applicable	Not Applicable	Failed
Limonene	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Epicatechin helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Conyza aegyptica can prevent Herpes due to the presence of Epicatechin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Cyperus rotundus against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Prabhashini Behera[1], Pradipta Banerjee[2]

[1]prabhashini999@gmail.com

[2]pradipta.banerjee@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Cyperus rotundus against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Pelargonidin helped to prevent Herpes.

Introduction: Cyperus rotundus is known for its medicinal activities. It is a medicinal herb traditionally used to treat various clinical conditions at home such as diarrhea, diabetes, pyresis, herpes, inflammation, malaria, and stomach and bowel disorders.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Poales
Family	Cyperaceae
Genus	Cyperus
Species	rotundus

Major phytochemicals present in the plant are:

a. Ellagic acid
b. Gallic acid
c. Pelargonidin
d. Limonene

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Ellagic acid	Not Applicable	Not Applicable	Failed
Gallic acid	Not Applicable	Not Applicable	Failed
Pelargonidin	-11.48	-18.61	Positive
Limonene	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Pelargonidin helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Cyperus rotundus can prevent Herpes due to the presence of Pelargonidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Euphorbia peplus against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Swetanginee Gouda[1], Pradipta Banerjee[2]

[1]swetasona14@gmail.com

[2]pradipta.banerjee@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Euphorbia peplus against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Lutein and Theobromine helped to prevent Herpes.

Introduction: Euphorbia peplus is known for its medicinal activities. The plant is administered in the form of herbal tea as diuretic, laxative and emollient. It is also used for the treatment of asthma and bronchitis, as it relaxes the smooth muscles of bronchi. It is recommended against dry cough, herpes, runny nose and liver diseases.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Malpighiales
Family	Euphorbiaceae
Genus	Euphorbia
Species	peplus

Major phytochemicals present in the plant are:

a. Lutein
b. Digoxin
c. Tannic acid
d. Theobromine

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lutein	-11.79	-18.09	Positive
Digoxin	Not Applicable	Not Applicable	Failed
Tannic acid	Not Applicable	Not Applicable	Failed
Theobromine	-10.58	-18.91	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Lutein and Theobromine helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Euphorbia peplus can prevent Herpes due to the presence of Lutein and Theobromine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Glycyrrhiza glabra against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Purnotoya Nayak[1], Pradipta Banerjee[2]

[1]purnopoyanayak1998@gmail.com

[2]pradipta.banerjee@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Glycyrrhiza glabra against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Campesterol helped to prevent Herpes.

Introduction: Glycyrrhiza glabra is known for its medicinal activities. Traditionally used to treat many diseases, such as respiratory disorders, hyperdipsia, epilepsy, fever, sexual debility, paralysis, stomach ulcers, rheumatism, skin diseases, hemorrhagic diseases, and jaundice.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Fabales
Family	Fabaceae
Genus	Glycyrrhiza
Species	glabra

Major phytochemicals present in the plant are:

a. Pelletierine
b. Alliin
c. Tangeretin
d. Campesterol

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	Not Applicable	Not Applicable	Failed
Alliin	Not Applicable	Not Applicable	Failed
Tangeretin	Not Applicable	Not Applicable	Failed
Campesterol	-12.38	-15.91	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Campesterol helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Glycyrrhiza glabra can prevent Herpes due to the presence of Campesterol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Heliotropium marifolium against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Shibani Sahoo[1], Pradipta Banerjee[2]

[1]shibanisahoo777@gmail.com

[2]pradipta.banerjee@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Heliotropium marifolium against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Pelargonidin helped to prevent Herpes.

Introduction: Heliotropium marifolium is known for its medicinal activities. Heliotropium marifolium is used against syphilis, asthma, herpes, UTI and wound.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Boraginales
Family	Boraginaceae
Genus	Heliotropium
Species	marifolium

Major phytochemicals present in the plant are:

a. Campesterol
b. Linamarin
c. Naringin
d. Pelargonidin

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Campesterol	Not Applicable	Not Applicable	Failed
Linamarin	Not Applicable	Not Applicable	Failed
Naringin	Not Applicable	Not Applicable	Failed
Pelargonidin	-9.67	-12.84	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Pelargonidin helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Heliotropium marifolium can prevent Herpes due to the presence of Pelargonidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Holoptelea integrifolia against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Sushree Susmita Palei[1], Pradipta Banerjee[2]

[1]susmitapalei123@gmail.com

[2]pradipta.banerjee@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Holoptelea integrifolia against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Limonene helped to prevent Herpes.

Introduction: Holoptelea integrifolia is known for its medicinal activities. The plant Holoptelea integrifolia is used traditionally for the treatment of inflammation, gastritis, dyspepsia, colic, intestinal worms, vomiting, wound healing, leprosy, diabetes, hemorrhoids, herpes, dysmenorrhea, and rheumatism.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Rosales
Family	Ulmaceae
Genus	Holoptelea
Species	integrifolia

Major phytochemicals present in the plant are:

a. Naringin
b. Limonene
c. Glutathione
d. Malvidin

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Naringin	Not Applicable	Not Applicable	Failed
Limonene	-16.48	-21.87	Positive
Glutathione	Not Applicable	Not Applicable	Failed
Malvidin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Limonene helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Holoptelea integrifolia can prevent Herpes due to the presence of Limonene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Houttuynia cordata against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

SatyajitMohanty[1], Pradipta Banerjee[2]

[1]1998satyajeetmohanty1@gmail.com

[2]pradipta.banerjee@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Houttuynia cordata against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Limonene helped to prevent Herpes.

Introduction: Houttuynia cordata is known for its medicinal activities. It is used as a fresh herbal garnish. In northeastern India, it is commonly used in salads and as a garnish over side dishes. The tender roots can also be ground into chutneys along with dry meat or fish, chilies, and tamarind. It is taken raw as salad and cooked along with fish as fish curry. In Japan and Korea, its dried leaves may be used as a tea. Houttuynia cordata was used in traditional Chinese medicine.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Piperales
Family	Saururaceae
Genus	Houttuynia
Species	cordata

Major phytochemicals present in the plant are:

a. Tangeretin
b. Salicylic acid
c. Limonene
d. Naringin

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tangeretin	Not Applicable	Not Applicable	Failed
Salicylic acid	Not Applicable	Not Applicable	Failed
Limonene	-11.78	-16.97	Positive
Naringin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Limonene helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Houttuynia cordata can prevent Herpes due to the presence of Limonene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Hypericum hookerianum against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Nibedita Jena[1], Pradipta Banerjee[2]

[1]nibeditajena2088@gmail.com

[2]pradipta.banerjee@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Hypericum hookerianum against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Salicylic acid helped to prevent Herpes.

Introduction: Hypericum hookerianum is known for its medicinal activities. It was recommended in the first century by Greek physicians as a diuretic, wound-healer, and treatment for menstrual disorders. It has been used as an anti-inflammatory, anti-bacterial, disinfectant, and a remedy for disorders of the respiratory tract and gall bladder and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Malpighiales
Family	Hypericaceae
Genus	Hypericum
Species	hookerianum

Major phytochemicals present in the plant are:

a. Malvidin
b. Salicylic acid
c. Ursolic acid
d. Astaxanthin

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Malvidin	Not Applicable	Not Applicable	Failed
Salicylic acid	-12.47	-17.67	Positive
Ursolic acid	Not Applicable	Not Applicable	Failed
Astaxanthin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Salicylic acid helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Hypericum hookerianum can prevent Herpes due to the presence of Salicylic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Hypericum mysorense against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Jyotiranjan Das[1], Pradipta Banerjee[2]

[1]dasjyotiranjan1998@gmail.com

[2]pradipta.banerjee@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Hypericum mysorense against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Ursolic acid helped to prevent Herpes.

Introduction: Hypericum mysorense is known for its medicinal activities. Hypericum mysorense has been used to treat wounds and herpes as part of the Ayurvedic system of traditional medicine.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Equisetopsida
Order	Malpighiales
Family	Hypericaceae
Genus	Hypericum
Species	mysorense

Major phytochemicals present in the plant are:

a. Ursolic acid
b. Astaxanthin
c. Sitosterol
d. Astaxanthin

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Ursolic acid	-12.67	-17.81	Positive
Astaxanthin	Not Applicable	Not Applicable	Failed
Sitosterol	Not Applicable	Not Applicable	Failed
Astaxanthin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ursolic acid helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Hypericum mysorense can prevent Herpes due to the presence of Ursolic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Lippia alba against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Subhashree[1], Pradipta Banerjee[2]

[1]subhashree777mohanty@gmail.com

[2]pradipta.banerjee@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Lippia alba against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Caffeine helped to prevent Herpes.

Introduction: Lippia alba is known for its medicinal activities. A tea made from the leaves is used to treat intestinal and respiratory disturbances, including influenza and herpes. A well-sugared infusion is drunk to bring relief of heart problems and to soothe tachycardia.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Equisetopsida
Order	Lamiales
Family	Verbenaceae
Genus	Lippia
Species	alba

Major phytochemicals present in the plant are:

a. Pelargonidin
b. Caffeine
c. Curcumin
d. Ascorbic acid

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelargonidin	Not Applicable	Not Applicable	Failed
Caffeine	-10.47	-15.24	Positive
Curcumin	Not Applicable	Not Applicable	Failed
Ascorbic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Caffeine helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Lippia alba can prevent Herpes due to the presence of Caffeine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Melia azaderach against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Manasi Mohapatra[1], Chinmaya Chidananda Behera[2]

[1]manasimohapatra2098@gmail.com

[2]chinmaya.pradhan@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Melia azaderach against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Astaxanthin helped to prevent Herpes.

Introduction: Melia azaderach is known for its medicinal activities. The leaf juice is anthelmintic, antilithic, diuretic, herpes and emmenagogue.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Sapindales
Family	Meliaceae
Genus	Melia
Species	azedarach

Major phytochemicals present in the plant are:

a. Zingiberene
b. Ursolic acid
c. Astaxanthin
d. Digoxin

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Zingiberene	Not Applicable	Not Applicable	Failed
Ursolic acid	Not Applicable	Not Applicable	Failed
Astaxanthin	-12.78	-17.58	Positive
Digoxin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Astaxanthin helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Melia azaderach can prevent Herpes due to the presence of Astaxanthin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Mentha piperata against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Soumyashree Nayak[1], Chinmaya Chidananda Behera[2]

[1]soumyashreenayak973@gmail.com

[2]chinmaya.pradhan@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Mentha piperata against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Sulforaphane helped to prevent Herpes.

Introduction: Mentha piperata is known for its medicinal activities. It is used for treatment of a variety of conditions, including irritable bowel syndrome (IBS), nausea, herpes and other digestive issues, as well as the common cold and headaches.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Lamiales
Family	Lamiaceae
Genus	Mentha
Species	piperata

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Carotene
c. Digoxin
d. Tannic acid

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	-11.34	-14.54	Positive
Carotene	Not Applicable	Not Applicable	Failed
Digoxin	Not Applicable	Not Applicable	Failed
Tannic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Sulforaphane helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Mentha piperata can prevent Herpes due to the presence of Sulforaphane. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Momordia charantia against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Soumyshree Behera[1], Chinmaya Chidananda Behera[2]

[1]soumyashreebehera30@gmail.com

[2]chinmaya.pradhan@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Momordia charantia against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Sulforaphane helped to prevent Herpes.

Introduction: Momordia charantia is known for its medicinal activities. Juice of the leaves is used to treat piles and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Cucurbitales
Family	Cucurbitaceae
Genus	Momordia
Species	charantia

Major phytochemicals present in the plant are:

a. Curcumin
b. Ascorbic acid
c. Sulforaphane
d. Digoxin

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Curcumin	Not Applicable	Not Applicable	Failed
Ascorbic acid	Not Applicable	Not Applicable	Failed
Sulforaphane	-15.93	-17.78	Positive
Digoxin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Sulforaphane helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Momordia charantia can prevent Herpes due to the presence of Sulforaphane. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Moringa oleifera against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Geetanjali Rana[1], Chinmaya Chidananda Behera[2]

[1]geetanjalirana20@gmail.com

[2]chinmaya.pradhan@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Moringa oleifera against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Lycopene helped to prevent Herpes.

Introduction: Moringa oleifera is known for its medicinal activities. Various parts of this plant such as the leaves, roots, seed, bark, fruit, flowers and immature pods act as cardiac and circulatory stimulants, possess antitumor, antipyretic, antiepileptic, antiinflammatory, herpes, antiulcer, antispasmodic, diuretic, antihypertensive, cholesterol lowering.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Brassicales
Family	Moringaceae
Genus	Moringa
Species	oleifera

Major phytochemicals present in the plant are:

a. Isorhamnetin
b. Rosmarinic acid
c. Lutein
d. Lycopene

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Isorhamnetin	Not Applicable	Not Applicable	Failed
Rosmarinic acid	Not Applicable	Not Applicable	Failed
Lutein	Not Applicable	Not Applicable	Failed
Lycopene	-15.28	-19.34	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Lycopene helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Moringa oleifera can prevent Herpes due to the presence of Lycopene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Myrica rubra against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Runki Priyadarsani Samal[1], Chinmaya Chidananda Behera[2]

[1]runkisamal2018@gmail.com

[2]chinmaya.pradhan@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Myrica rubra against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Theobromine helped to prevent Herpes.

Introduction: Myrica rubra is known for its medicinal activities. The stem bark is used as a wash in the treatment of arsenic poisoning, skin diseases, wounds and ulcers. The fruit is carminative, herpes, pectoral and stomachic.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Fagales
Family	Myricaceae
Genus	Myrica
Species	rubra

Major phytochemicals present in the plant are:

a. Theobromine
b. Tannic acid
c. Mangiferin
d. Digoxin

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	-19.04	-25.27	Positive
Tannic acid	Not Applicable	Not Applicable	Failed
Mangiferin	Not Applicable	Not Applicable	Failed
Digoxin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Theobromine helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Myrica rubra can prevent Herpes due to the presence of Theobromine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Neerium indicum against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

SwastiPrava Das[1], Chinmaya Chidananda Behera[2]

[1]swastipravadas@gmail.com

[2]chinmaya.pradhan@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Neerium indicum against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Myricetin helped to prevent Herpes.

Introduction: Neerium indicum is known for its medicinal activities. Nerium indicum has many medicinal properties like bitter, acrid, astringent, anthelmintic, aphrodisiac, stomachic, febrifuge, diuretic, emetic, expectorant, cardio tonic, anticancer etc which is used in the treatment of cardiac asthma, renal and vesicle calculi, chronic stomach, skin related problems, snake bites joint pains, leprosy, cancer, ulcers etc. Leaves and flowers are also used to treat malaria. Leaves and bark is treated as insecticide, rat poison and parasitic.

The plant is classified as follows:

Kingdom	Plantae
Division	Magnoliophyta
Class	Magnoliopsida
Order	Gentianales
Family	Apocynaceae
Genus	Nerium
Species	indicum

Major phytochemicals present in the plant are:

a. Myricetin
b. Peonidin
c. Curcumin
d. Ascorbic acid

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Myricetin	-12.21	-17.81	Positive
Peonidin	Not Applicable	Not Applicable	Failed
Curcumin	Not Applicable	Not Applicable	Failed
Ascorbic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Myricetin helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Neerium indicum can prevent Herpes due to the presence of Myricetin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Peganum harmala against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Dinesh Kumar Mohanty[1], Chinmaya Chidananda Behera[2]

[1]dineshkumarmohanty1998@gmail.com

[2]chinmaya.pradhan@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Peganum harmala against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Myricetin helped to prevent Herpes.

Introduction: Peganum harmala is known for its medicinal activities. It has been used as an analgesic, emmenagogue, and abortifacient agent. Leaf was used to cure herpes. In a certain region of India the root was applied to kill body lice.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Sapindales
Family	Nitrariaceae
Genus	Peganum
Species	harmala

Major phytochemicals present in the plant are:

a. Genistein
b. Myricetin
c. Theobromine
d. Quercetin

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Genistein	Not Applicable	Not Applicable	Failed
Myricetin	-14.21	-18.37	Positive
Theobromine	Not Applicable	Not Applicable	Failed
Quercetin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Myricetin helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Peganum harmala can prevent Herpes due to the presence of Myricetin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Phyllanthus emblica against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Sushanta Kumar Sethy[1], Chinmaya Chidananda Behera[2]

[1]sushantakumarsethy30@gmail.com

[2]chinmaya.pradhan@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Phyllanthus emblica against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Malvidin helped to prevent Herpes.

Introduction: Phyllanthus emblica is known for its medicinal activities. Seeds of the fruits are used in treatment of asthma, herpes and bronchitis. The leaves are used as fodder. Alcoholic extract of the fruit is anti–viral.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Malpighiales
Family	Phyllanthaceae
Genus	Phyllanthus
Species	emblica

Major phytochemicals present in the plant are:

a. Malvidin
b. Myricetin
c. Ursolic acid
d. Ascorbic acid

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Malvidin	-11.27	-18.82	Positive
Myricetin	Not Applicable	Not Applicable	Failed
Ursolic acid	Not Applicable	Not Applicable	Failed
Ascorbic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Malvidin helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Phyllanthus emblica can prevent Herpes due to the presence of Malvidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Phyllanthus urinaria against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Abinash Mohapatra[1], Chinmaya Chidananda Behera[2]

[1]mohapatraa098@gmail.com

[2]chinmaya.pradhan@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Phyllanthus urinaria against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Ursolic acid helped to prevent Herpes.

Introduction: Phyllanthus urinaria is known for its medicinal activities. It is used in folk medicine as a cure to treat jaundice, herpes, diabetes, malaria, and liver diseases.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Malpighiales
Family	Phyllanthaceae
Genus	Phyllanthus
Species	urinaria

Major phytochemicals present in the plant are:

a. Tangeretin
b. Ursolic acid
c. Limonene
d. Naringin

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tangeretin	Not Applicable	Not Applicable	Failed
Ursolic acid	-13.67	-19.33	Positive
Limonene	Not Applicable	Not Applicable	Failed
Naringin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ursolic acid helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Phyllanthus urinaria can prevent Herpes due to the presence of Ursolic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Pinus massoniana against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Rahnuma Neshan[1], Chinmaya Chidananda Behera[2]

[1]rahnumaneshan2015@gmail.com

[2]chinmaya.pradhan@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Pinus massoniana against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Genistein helped to prevent Herpes.

Introduction: Pinus massoniana is known for its medicinal activities. The chopped or decocted leaves are used in the treatment of rheumatism, herpes and intestinal parasites.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Pinopsida
Order	Pinales
Family	Pinaceae
Genus	Pinus
Species	massoniana

Major phytochemicals present in the plant are:

a. Genistein
b. Daidzein
c. Peonidin
d. Quercetin

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Genistein	-13.87	-16.78	Positive
Daidzein	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Quercetin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Genistein helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Pinus massoniana can prevent Herpes due to the presence of Genistein. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Plantago major against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Swatiprava Panda[1], Pratap Kumar Chhotaray[2]

[1]swatiprava.98@gmail.com

[2]pratap.chottaray@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Plantago major against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Gallic acid helped to prevent Herpes.

Introduction: Plantago major is known for its medicinal activities. Plantago major is used in wound healing and the leaves were used as a remedy of wounds and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Lamiales
Family	Plantaginaceae
Genus	Plantago
Species	major

Major phytochemicals present in the plant are:

a. Genistein
b. Daidzein
c. Gallic acid
d. Ellagic acid

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Genistein	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Failed
Gallic acid	-15.67	-18.97	Positive
Ellagic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Gallic acid helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Plantago major can prevent Herpes due to the presence of Gallic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Portulaca oleracea against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Bijayprava Sur[1], Pratap Kumar Chhotaray[2]

[1]bijayapravasurmusic@gmail.com

[2]pratap.chottaray@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Portulaca oleracea against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Ajoene helped to prevent Herpes.

Introduction: Portulaca oleracea is known for its medicinal activities. Portulaca oleracea has been used as a folk medicine in many countries, acting as a febrifuge, antiseptic, herpes and vermifuge.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Caryophyllales
Family	Portulacaceae
Genus	Portulaca
Species	oleracea

Major phytochemicals present in the plant are:

a. Allicin
b. Ajoene
c. Theobromine
d. Quercetin

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Allicin	Not Applicable	Not Applicable	Failed
Ajoene	-12.92	-17.99	Positive
Theobromine	Not Applicable	Not Applicable	Failed
Quercetin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ajoene helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Portulaca oleracea can prevent Herpes due to the presence of Ajoene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Salvia officinalis against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Prasityaditya Mohanty[1], Pratap Kumar Chhotaray[2]

[1]prasityadityamohanty1997@gmail.com

[2]pratap.chottaray@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Salvia officinalis against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Tocopherol helped to prevent Herpes.

Introduction: Salvia officinalis is known for its medicinal activities. S. officinalis has been used for the treatment of different kinds of disorders including seizure, ulcers, gout, rheumatism, herpes, inflammation, dizziness, tremor, paralysis, diarrhea, and hyperglycemia.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Lamiales
Family	Lamiaceae
Genus	Salvia
Species	officinalis

Major phytochemicals present in the plant are:

a. Tocopherol
b. Epicatechin
c. Coumarin
d. Proanthocyanidins

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tocopherol	-14.95	-23.66	Positive
Epicatechin	Not Applicable	Not Applicable	Failed
Coumarin	Not Applicable	Not Applicable	Failed
Proanthocyanidins	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Tocopherol helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Salvia officinalis can prevent Herpes due to the presence of Tocopherol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Santalum album against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Prerana Jena[1], Pratap Kumar Chhotaray[2]

[1]prenajena234@gmail.com

[2]pratap.chottaray@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Santalum album against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Isorhamnetin and Ferulic acid helped to prevent Herpes.

Introduction: Santalum album is known for its medicinal activities. Sandalwood oil has been widely used in folk medicine for treatment of common colds, bronchitis, skin disorders, heart ailments, general weakness, fever, herpes, infection of the urinary tract, inflammation of the mouth and pharynx, liver and gallbladder complaints and other maladies.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Santalales
Family	Santalaceae
Genus	Santalum
Species	album

Major phytochemicals present in the plant are:

a. Hesperidin
b. Isorhamnetin
c. Rutin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Hesperidin	Not Applicable	Not Applicable	Failed
Isorhamnetin	-7.38	-15.91	Positive
Rutin	Not Applicable	Not Applicable	Failed
Ferulic acid	-15.37	-23.34	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Isorhamnetin and Ferulic acid helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Santalum album can prevent Herpes due to the presence of Isorhamnetin and Ferulic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Scinaia hatei against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Soumyaranjan Behera[1], Pratap Kumar Chhotaray[2]

[1]soumya.babuji@gmail.com

[2]pratap.chottaray@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Scinaia hatei against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Sulforaphane helped to prevent Herpes.

Introduction: Scinaia hatei is known for its medicinal activities. It helps to treat herpes, dengue, myalgia, pancreatitis, cardiac arrhythmia, and hepatitis.

The plant is classified as follows:

Kingdom	Plantae
Division	Rhodophyta
Class	Florideophyceae
Order	Nemalionales
Family	Chaetangiaceae
Genus	Scinaia
Species	hatei

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Alliin
c. Tangeretin
d. Tannic acid

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	-12.78	-19.44	Positive
Alliin	Not Applicable	Not Applicable	Failed
Tangeretin	Not Applicable	Not Applicable	Failed
Tannic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Sulforaphane helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Scinaia hatei can prevent Herpes due to the presence of Sulforaphane. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Scoparia dulcis against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Swatee Swagatika[1], Pratap Kumar Chhotaray[2]

[1]swateeswagatika1998@gmail.com

[2]pratap.chottaray@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Scoparia dulcis against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Campesterol helped to prevent Herpes.

Introduction: Scoparia dulcis is known for its medicinal activities. It is considered a weed in many areas but used as medicinal herb for a wide range of uses including treatment for digestive problems, pulmonary conditions, fever, skin disorders, hypertension, hemorrhoids, diarrhea, dysentery, insect bites, anemia, albuminuria, diabetes, herpes, etc.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Lamiales
Family	Plantaginaceae
Genus	Scoparia
Species	dulcis

Major phytochemicals present in the plant are:

a. Pelletierine
b. Digoxin
c. Rosmarinic acid
d. Campesterol

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	Not Applicable	Not Applicable	Failed
Digoxin	Not Applicable	Not Applicable	Failed
Rosmarinic acid	Not Applicable	Not Applicable	Failed
Campesterol	-9.66	-13.84	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Campesterol helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Scoparia dulcis can prevent Herpes due to the presence of Campesterol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Solanum torvum against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

JangyasimniSahu[1], Pratap Kumar Chhotaray[2]

[1]sahujangyasini@gmail.com

[2]pratap.chottaray@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Solanum torvum against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Malvidin helped to prevent Herpes.

Introduction: Solanum torvum is known for its medicinal activities. Fruit and leaf decoction is used to treat cough, herpes and to treat liver and spleen enlargement.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Solanales
Family	Solanaceae
Genus	Solanum
Species	torvum

Major phytochemicals present in the plant are:

a. Campesterol
b. Linamarin
c. Glutathione
d. Malvidin

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Campesterol	Not Applicable	Not Applicable	Failed
Linamarin	Not Applicable	Not Applicable	Failed
Glutathione	Not Applicable	Not Applicable	Failed
Malvidin	-12.52	-16.92	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Malvidin helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Solanum torvum can prevent Herpes due to the presence of Malvidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Sorghum bicolor against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

ChintamaniBisoi[1], Pratap Kumar Chhotaray[2]

[1]bisoichintamani@gmail.com

[2]pratap.chottaray@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Sorghum bicolor against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Pelargonidin helped to prevent Herpes.

Introduction: Sorghum bicolor is known for its medicinal activities. Seed extracts are drunk to treat hepatitis and herpes.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Poales
Family	Poaceae
Genus	Sorghum
Species	bicolor

Major phytochemicals present in the plant are:

a. Naringin
b. Limonene
c. Naringin
d. Pelargonidin

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Naringin	Not Applicable	Not Applicable	Failed
Limonene	Not Applicable	Not Applicable	Failed
Naringin	Not Applicable	Not Applicable	Failed
Pelargonidin	-12.33	-15.88	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Pelargonidin helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Sorghum bicolor can prevent Herpes due to the presence of Pelargonidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Strobilanthus cusia against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

DebikaTripathy[1], Pratap Kumar Chhotaray[2]

[1]debikatripathy52@gmail.com

[2]pratap.chottaray@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Strobilanthus cusia against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Tangeretin helped to prevent Herpes.

Introduction: Strobilanthus cusia is known for its medicinal activities. It is used for influenza, herpes, epidemic cerebrospinal meningitis, encephalitis B, viral pneumonia and mumps.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Lamiales
Family	Acanthaceae
Genus	Strobilanthus
Species	cusia

Major phytochemicals present in the plant are:

a. Tangeretin
b. Salicylic acid
c. Epicatechin
d. Catechin

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tangeretin	-14.37	-19.64	Positive
Salicylic acid	Not Applicable	Not Applicable	Failed
Epicatechin	Not Applicable	Not Applicable	Failed
Catechin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Tangeretin helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Strobilanthus cusia can prevent Herpes due to the presence of Tangeretin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Swertia chirata against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

MonalisaNayak[1], Pratap Kumar Chhotaray[2]

[1]monalisanayak11798@gmail.com

[2]pratap.chottaray@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Swertia chirata against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Naringin helped to prevent Herpes.

Introduction: Swertia chirata is known for its medicinal activities. People use the parts that grow above the ground to make medicine. Chirata is used for fever, constipation, herpes, upset stomach, loss of appetite, intestinal worms, skin diseases, and cancer.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Gentianales
Family	Gentianaceae
Genus	Swertia
Species	chirayita

Major phytochemicals present in the plant are:

a. Theobromine
b. Limonene
c. Naringin
d. Limonene

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	Not Applicable	Not Applicable	Failed
Limonene	Not Applicable	Not Applicable	Failed
Naringin	-8.66	-12.57	Positive
Limonene	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Naringin helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Swertia chirata can prevent Herpes due to the presence of Naringin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Syzygium aromaticum against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

NibeditaNayak[1], Dojalisa Sahu[2]

[1]nibeditanayak1512@gmail.com

[2]dojalisa.sahu@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Syzygium aromaticum against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Digoxin and Pelargonidin helped to prevent Herpes.

Introduction: Syzygium aromaticum is known for its medicinal activities. Traditionally, cloves have been used for centuries in the treatment of vomiting; flatulence; nausea; liver, herpes, bowel and stomach disorders; and as a stimulant for the nerves.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Myrtales
Family	Myrtaceae
Genus	Syzygium
Species	aromaticum

Major phytochemicals present in the plant are:

a. Lutein
b. Digoxin
c. Pelargonidin
d. Limonene

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lutein	Not Applicable	Not Applicable	Failed
Digoxin	-14.35	-19.66	Positive
Pelargonidin	-8.11	-11.57	Positive
Limonene	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Digoxin and Pelargonidin helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Syzygium aromaticum can prevent Herpes due to the presence of Digoxin and Pelargonidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Syzygium jambos against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

Shatabdi Das[1], Dojalisa Sahu[2]

[1]shatabdidas19962gmail.com

[2]dojalisa.sahu@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Syzygium jambos against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Ellagic acid helped to prevent Herpes.

Introduction: Syzygium jambos is known for its medicinal activities. A decoction of the leaves is used as a diuretic, herpes, a remedy for sore eyes and for rheumatism. The seeds are used to treat diarrhoea, dysentery, diabetes and catarrh. A decoction of bark is administered to relieve asthma and bronchitis.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Myrtales
Family	Myrtaceae
Genus	Syzygium
Species	jambos

Major phytochemicals present in the plant are:

a. Ellagic acid
b. Gallic acid
c. Tannic acid
d. Theobromine

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Ellagic acid	-14.55	-18.32	Positive
Gallic acid	Not Applicable	Not Applicable	Failed
Tannic acid	Not Applicable	Not Applicable	Failed
Theobromine	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ellagic acid helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Syzygium jambos can prevent Herpes due to the presence of Ellagic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Taracetium vulgare against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

NiharikaSadangi[1], Dojalisa Sahu[2]

[1]chunmun1805@gmail.com

[2]dojalisa.sahu@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Taracetium vulgare against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Quercetin helped to prevent Herpes.

Introduction: Taracetium vulgare is known for its medicinal activities. In larger doses the plant can procure an abortion, though these doses can be poisonous. Externally, tansy is used as a poultice on swellings, herpes and some eruptive skin diseases.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Asterales
Family	Asteraceae
Genus	Taracetum
Species	vulgare

Major phytochemicals present in the plant are:

a. Pelletierine
b. Alliin
c. Theobromine
d. Quercetin

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	Not Applicable	Not Applicable	Failed
Alliin	Not Applicable	Not Applicable	Failed
Theobromine	Not Applicable	Not Applicable	Failed
Quercetin	-10.36	-14.17	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Quercetin helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Taracetium vulgare can prevent Herpes due to the presence of Quercetin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Usnea complanta against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

AtasiRoutray[1], Dojalisa Sahu[2]

[1]atasiroutray2018@gmai.com

[2]dojalisa.sahu@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Usnea complanta against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Genistein helped to prevent Herpes.

Introduction: Usnea complanta is known for its medicinal activities. It can sometimes be used as a bioindicator, because it tends to only grow in those regions where the air is clean, and of high quality. It is also used to cure herpes.

The plant is classified as follows:

Kingdom	Fungi
Division	Ascomycota
Class	Lecanoromycetes
Order	Lecanorales
Family	Asteraceae
Genus	Usnea
Species	complanta

Major phytochemicals present in the plant are:

a. Genistein
b. Daidzein
c. Tangeretin
d. Campesterol

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Genistein	-13.64	-23.11	Positive
Daidzein	Not Applicable	Not Applicable	Failed
Tangeretin	Not Applicable	Not Applicable	Failed
Campesterol	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Genistein helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Usnea complanta can prevent Herpes due to the presence of Genistein. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Ventilago denticulate against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

ArsiaTabish[1], Dojalisa Sahu[2]

[1]tabisharsia@gmail.com

[2]dojalisa.sahu@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Ventilago denticulate against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Ferulic acid helped to prevent Herpes.

Introduction: Ventilago denticulate is known for its medicinal activities. Stem bark is powdered and mixed with sesame oil, externally applied to skin diseases and sprains. Root bark—used for atonic dyspepsia, mild fever, herpes and debility. Sap is used for the treatment of deafness.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Rosales
Family	Rhamnaceae
Genus	Ventilago
Species	denticulate

Major phytochemicals present in the plant are:

a. Allicin
b. Hesperidin
c. Ferulic acid
d. Epicatechin

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Allicin	Not Applicable	Not Applicable	Failed
Hesperidin	Not Applicable	Not Applicable	Failed
Ferulic acid	-16.84	-19.77	Positive
Epicatechin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ferulic acid helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Ventilago denticulate can prevent Herpes due to the presence of Ferulic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Withania somnifera against Herpes through deactivation of Thymidine Kinase of Herpes Simplex virus (1KIM)

SwagatikaMohapatra[1], Dojalisa Sahu[2]

[1]basudev7489@gmail.com

[2]dojalisa.sahu@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Withania somnifera against Herpes. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. It was found that Tannic acid helped to prevent Herpes.

Introduction: Withania somnifera is known for its medicinal activities. The medicinal plants are widely used by the traditional medical practitioners for curing various diseases like diarrhea, dysentery, insect bites, anemia, albuminuria, diabetes, herpes, etc.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Solanales
Family	Solanaceae
Genus	Withania
Species	somnifera

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Tannic acid
c. Rosmarinic acid
d. Cryptoxanthin

One of the major enzymes required for the survival of the organism causing Herpes is Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

Methodology: Biovia Discovery Studio was used to do molecular docking. Sdf files of the phytochemicals and pdb codes of the enzyme were used for molecular docking. C-docking resulted in C-Docker energy and C-Docker interaction energy. High negative values of C-Docker energy and C-Docker interaction energy indicated strong interaction between the phytochemical and the enzyme.

Results and discussion: The result of molecular docking is presented in Table 1. “Positive” in the remarks column indicated that the phytochemical is capable of deactivating the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Tannic acid	-11.67	-19.38	Positive
Rosmarinic acid	Not Applicable	Not Applicable	Failed
Cryptoxanthin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Tannic acid helped deactivate the Thymidine Kinase of Herpes Simplex virus (1KIM) enzyme of the organism causing Herpes.

Conclusions: The molecular docking study showed that Withania somnifera can prevent Herpes due to the presence of Tannic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

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