ISSN 2395-6216 (PRINT VERSION)
ISSN 2395-6224 (ONLINE VERSION)
Volume 10 Number 2 Jun 2020

Centurion Journal of Multidisciplinary Research

Special issue :
Proceedings of
National Conference on Molecular Docking (Series III):
Phytochemicals against Covid-19
25-27 June 2020

Centurion
UNIVERSITY

Shaping Lives...
Empowering Communities...

centurion university of technology and management

Centurion Journal of Multidisciplinary Research
ISSN 2395-6216 (PRINT VERSION) ISSN 2395-6224 (ONLINE VERSION)

Centurion Journal of Multidisciplinary Research is published by Centurion University of Technology and Management, Odisha, bi-annually.

Annual Subscription: Rs 300 (within India) excluding postage charges. Outside India USD 30, excluding postage charges.
The designations employed and the presentation of material in the CJMR journal do not imply the expression of an opinion whatsoever on the part of Centurion University of Technology and Management concerning the legal status of any country, territory, city or area of its authorities, or concerning the delimitation of its frontiers or boundaries.

The authors are responsible for the choice and the presentation of the facts contained in the journal and for the opinions expressed therein, which are not necessarily those of Centurion University of Technology and Management.

Published by:
Registrar, Centurion University of Technology and Management
R. Sitapur, Parlakhemundi, Gajapati, Odisha
Pin – 761211

Printer:
Srimandira Publication
EPF Colony, E-Block, Saheed Nagar, Bhubaneswar, Odisha 751007

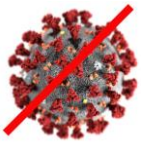
Volume 10 Number 2
June 2020

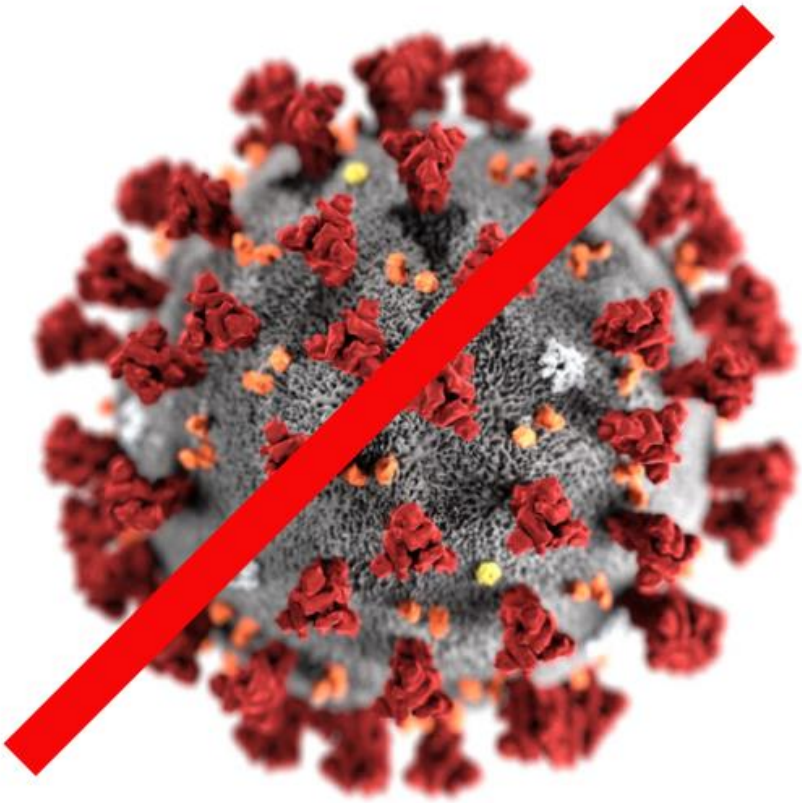
Centurion Journal of Multidisciplinary Research

Special issue : Proceedings of National Conference on Molecular Docking
(Series III): Phytochemicals against COVID-19
25-27 June 2020
organized by: Botany and Zoology Departments
Centurion University of Technology and management, Odisha, India

Centurion
UNIVERSITY
Shaping Lives...
Empowering Communities...

CENTURION UNIVERSITY PRESS, ODISHA, INDIA

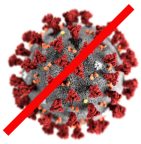




Proceedings of National Conference on Molecular Docking (Series III): Phytochemicals against COVID-19 25-27 June 2020

Organized by: Botany and Zoology Departments, Centurion University of Technology and Management, Odisha, India

Centurion Journal of Multidisciplinary Research
Special Issue: June 2020



Organizing Committee

Patrons

Dr Dipankar Bhattacharyay

Dr Yashaswi Nayak

Convener

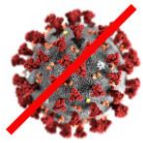
Dr Siba Prasad Parida, Dr Rukmini Mishra

Organizing Secretaries

Mrs Bhagyeswari Behera, Dr Sujit Kumar Mishra

Committee members

Dr Gyanaranjan Mahalik, Dr Sitaram Swain, Mr Srimay Pradhan, Mrs Sunita Satapathy, Dr Sagarika Parida, Mr Gagan Kumar Panigrahi, Dr Jyoti Prakash Rath, Mrs Namita Panda, Mr Debasis Tripathy, Dr Ashwini Rath



THE VISION

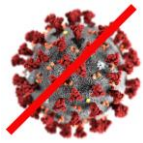
Objective

Coronavirus disease 2019 (COVID-19) has affected almost every country in the world by causing a global pandemic with a high mortality rate. The emerging 2019 Novel coronavirus (2019-nCoV) threatens public health. 2019-nCoV is also referred to as severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2). Lack of an effective vaccine and/or antiviral drugs against SARS-CoV-2, the causative agent, has severely hampered the response to this novel coronavirus. Natural products have long been used in traditional medicines to treat various diseases, and purified phytochemicals from medicinal plants provide a valuable scaffold for the discovery of new drug leads.

Being partnered with the DASSAULT SYSTEMES, *in silico* molecular docking approaches were explored using Discovery Studio suite and performed virtual screenings to identify phytochemicals against SARS-CoV-2. Post graduate students of biological sciences actively participated and have presented their work in the conference.

Introduction

The global threat of the 2019 novel coronavirus disease is rapidly escalating with unprecedented international health and economic burden in the recent history. The whole-genome of SARS-CoV-2 had been sequenced and revealed that SARS-CoV-2 pathogen is the fifth strain of β-coronaviruses, which include OC43, HKU1, SARS-CoV-1 and Middle East respiratory syndrome coronavirus (MERS CoV) (Wang et al., 2020). After the entry into the host cell through strong binding of β-coronaviruses' protein spikes with the human angiotensin-converting enzyme 2 (ACE2) receptor (Xu et al., 2020), β-coronaviruses generate large polyproteins (PP1a and PP1ab) upon genome translation of open reading frame (ORF) 1a and ORF1ab by the host cell machinery. These polyproteins, also known as replicase polyproteins, are proteolytically cleaved by essential cysteine proteases encoded by the virus, explicitly 3-chymotrypsin-like protease ($3CL^{pro}$; sometimes called main protease (M^{pro})) and papain-like proteases (PL^{pro}), to release 16 non-structural proteins (nsps) (Thiel et al., 2003; Ziebuhr, 2004). Among those nsps is the RNA-dependent RNA polymerase (RdRp or sometimes



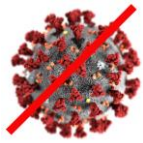
referred to as nsp12). RdRp catalyses the synthesis of a complementary RNA strand using the viral RNA and hence, it plays an essential role in directing the replication and transcription of SARS-CoV-2 genome (Chen et al., 2020; Lung et al., 2020; Zumla et al., 2016). The proteolysis of PP1a and PP1ab by $3CL^{pro}$ occurs at 11 distinct sites and generates various nsps that are important for the viral replication (Anand et al., 2003). For ages, phytochemicals have been found to be a fruitful source of molecules with diverse therapeutic potentials and still are considered a valuable resource for the discovery of novel drug leads in other word, herbal medicines and purified phytochemicals can be used to develop more efficient drugs based on the structure of natural compounds (Mani et al., 2020). Given the time of its emergence, few studies related to the development of naturally-derived inhibitors of three main druggable targets of SARS-CoV-2 (RdRp, $3CL^{pro}$ and PL^{pro}) have already been reported using computer modelling for screening purposes. For instance, in silico or biological screening of a series of biologically active natural compounds have been demonstrated to directly inhibit these important proteins in pervious HCoVs such as SARS-CoV, MERS CoV (Park et al., 2012; Shen et al., 2019) and the novel SARS-CoV-2 (Aanouz et al., 2020; Ul Qamar et al., 2020; Zhang et al., 2020).

Viral Protein Structure and Phytochemical dataset collection

The 3D structure of the viral protein was accessed from Protein Data Bank with accessions 6M03, 6LVN, 6M3M, 6VWW, 6VXS, 6W02, 6W4B, 6W6Y, 6W9C, 6W61 and 6Y2E (Figure 1). Phytochemical dataset present in different plants (Figure 2) was obtained and consequently both the protein and the ligands were used for *in silico* analysis.

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.

Conclusion

Antiviral therapies for the life-threatening viral diseases are generally expensive and have adverse side effects. In the realm of the therapeutics, there is an urgent need of effective, safe, and inexpensive antiviral therapies/drugs/inhibitors with minimal side effects to the mankind. Therefore, the approach using the phytochemical could be the better option in the development of antivirals. Synergistic studies employing phytochemicals in combination with either already FDA-approved drugs or inhibitors could be explored in the future for better and long-term efficacy of antiviral. Moreover, repurposing of already reported phytochemical as an inhibitor for viral diseases could be done in search of potential antivirals. Phytochemicals having antiviral activity can be nanoencapsulated for better delivery, prolonged action, and enhanced bioavailability. It is being difficult for the researchers worldwide to prepare any kind of vaccine because corona virus is a novel virus that means it’s contact was not traced anytime before in the history and it is a virus which finds humans as it’s suitable hosts and it also changes its structure to defy the action of various photochemical with which it is treated. It is our hope that in the future high quality clinically relevant studies will accumulate in the literature, which will shed light on the full potential of phytochemicals as novel antiviral agents in adequate delivery systems.

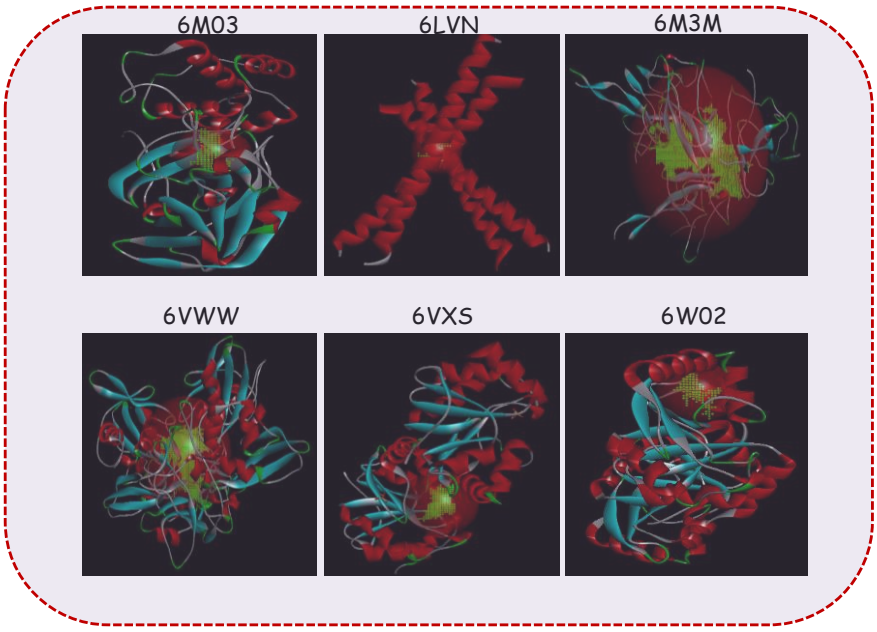


Figure 1. Different enzymes of Covid-19

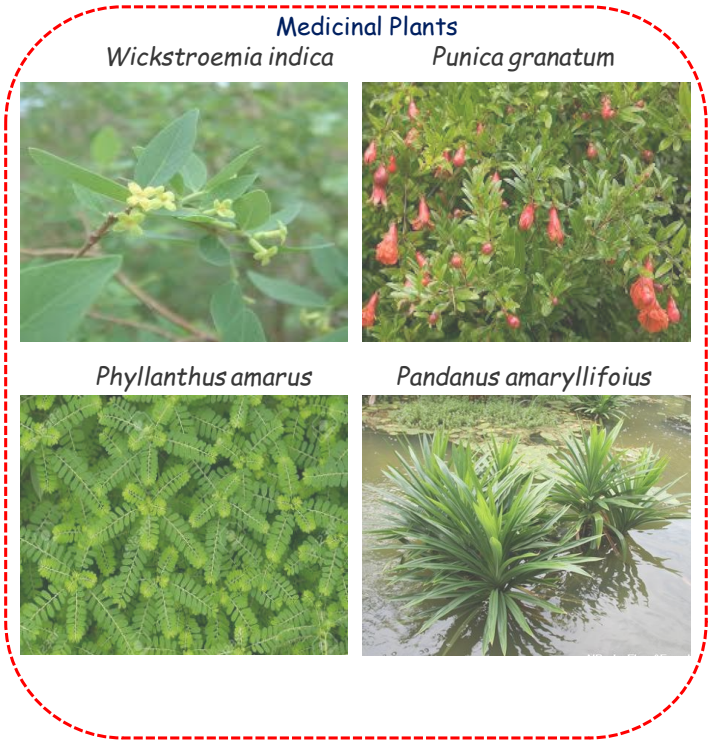
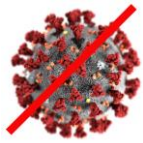


Figure 2. Some plants that can fight against Covid-19



References

Aanouz, I., Belhassan, A., El Khatabi, K., Lakhlifi, T., El Idrissi, M., Bouachrine, M., 2020. Moroccan medicinal plants as inhibitors of COVID-19: Computational investigations. J. Biomol. Struct. Dyn., 1–12

Anand, K., Ziebuhr, J., Wadhwani, P., Mesters, J.R., Hilgenfeld, R., 2003. Coronavirus main proteinase (3CLpro) structure: basis for design of anti-SARS drugs. Science 300 (5626), 1763–1767.

Chen, Y., Liu, Q., Guo, D., 2020. Emerging coronaviruses: genome structure, replication, and pathogenesis. J. Med. Virol. 92 (4), 418–423.

Lung, J., Lin, Y.S., Yang, Y.H., Chou, Y.L., Shu, L.H., Cheng, Y.C., Liu, H.T., Wu, C.Y., 2020. The potential chemical structure of anti-SARS-CoV-2 RNA-dependent RNA polymerase. J. Med. Virol. 92 (6), 693–697.

Mani, J.S., Johnson, J.B., Steel, J.C., Broszczak, D.A., Neilsen, P.M., Walsh, K.B., Naiker, M., 2020. Natural product-derived phytochemicals as potential agents against coronaviruses: A review. Virus Res. 284, 197989.

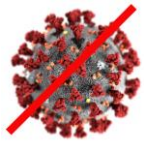
Park, J.-Y., Kim, J.H., Kim, Y.M., Jeong, H.J., Kim, D.W., Park, K. H., Kwon, H.-J., Park, S.-J., Lee, W.S., Ryu, Y.B., 2012. Tanshinones as selective and slow-binding inhibitors for SARS CoV cysteine proteases. Bioorg. Med. Chem. 20 (19), 5928–5935.

Shen, L., Niu, J., Wang, C., Huang, B., Wang, W., Zhu, N., Deng, Y., Wang, H., Ye, F., Cen, S., 2019. High-throughput screening and identification of potent broad-spectrum inhibitors of coronaviruses. J. Virol. 93 (12), e00023–00019.

Thiel, V., Ivanov, K.A., Putics, A., Hertzig, T., Schelle, B., Bayer, S., Weißbrich, B., Snijder, E.J., Rabenau, H., Doerr, H.W., 2003. Mechanisms and enzymes involved in SARS coronavirus genome expression. J. Gen. Virol. 84 (9), 2305–2315.

Ul Qamar, M.T., Alqahtani, S.M., Alamri, M.A., Chen, L.-L., 2020. Structural basis of SARS-CoV-2 3CLpro and anti-COVID-19 drug discovery from medicinal plants. J. Pharm. Anal.

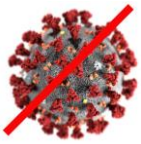
Xu, X., Chen, P., Wang, J., Feng, J., Zhou, H., Li, X., Zhong, W., Hao, P., 2020. Evolution of the novel coronavirus from the ongoing Wuhan outbreak and modeling of its spike protein for risk of human transmission. Sci. China Life Sci. 63 (3), 457–460.



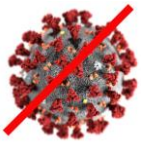
Zhang, D.H., Wu, K.L., Zhang, X., Deng, S.Q., Peng, B., 2020. In silico screening of Chinese herbal medicines with the potential to directly inhibit 2019 novel coronavirus. J. Integr. Med. 18 (2), 152–158.

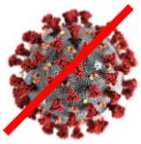
Ziebuhr, J., 2004. Molecular biology of severe acute respiratory syndrome coronavirus. Curr. Opin. Microbiol. 7 (4), 412–419.

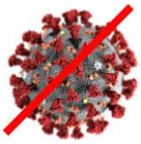
Zumla, A., Chan, J.F., Azhar, E.I., Hui, D.S., Yuen, K.-Y., 2016. Coronaviruses drug discovery and therapeutic options. Nat. Rev. Drug Discovery 15 (5), 327.

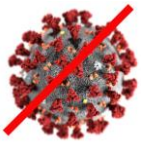


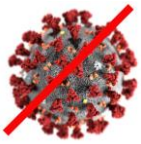
Index

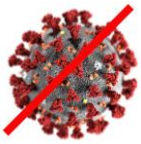


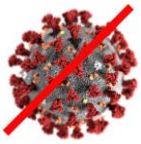


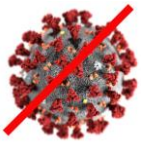












Activity of Alpinia officinarium against COVID 19 through deactivation of 2019-nCoV HR2 Domain (6LVN)

Zarifa Naaz[1], Yashaswi Nayak[2]

[1]190705180001@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 Alpinia officinarium against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate 2019-nCoV HR2 Domain (6LVN) enzyme. It was found that Luteolin helped to prevent COVID 19.

Introduction: Alpinia officinarium is known for its medicinal activities. In Asia the rhizomes are ground to powder for use in curries, drinks, and jellies. In India an extract is used in perfumes. Alpinia officinarum contains high concentrations of the flavonol galangin. Historically, the rhizomes were reputed to have stimulant and digestive effects.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Zingiberales
Family	Zingiberaceae
Genus	Alpinia
Species	officinarum

Major phytochemicals present in the plant are:

a. Resveratrol
b. Phenyl isothiocyanate
c. Luteolin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is 2019-nCoV HR2 Domain (6LVN) 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 2019-nCoV HR2 Domain (6LVN) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Resveratrol	Not Applicable	Not Applicable	Failed
Phenyl isothiocyanate	Not Applicable	Not Applicable	Failed
Luteolin	-12.38	-18.88	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 Luteolin helped deactivate the 2019-nCoV HR2 Domain (6LVN) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Alpinia officinarium can prevent COVID 19 due to the presence of Luteolin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Andrographis paniculata against COVID 19 through deactivation of 2019-nCoV HR2 Domain (6LVN)

Sipra Swain[1], Yashaswi Nayak[2]

[1]190705180002@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 Andrographis paniculata against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate 2019-nCoV HR2 Domain (6LVN) enzyme. It was found that Glutathione helped to prevent COVID 19.

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. Cryptoxanthin
b. Quercetin
c. Salicylic acid
d. Glutathione

One of the major enzymes required for the survival of the organism causing COVID 19 is 2019-nCoV HR2 Domain (6LVN) 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 2019-nCoV HR2 Domain (6LVN) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Cryptoxanthin	Not Applicable	Not Applicable	Failed
Quercetin	Not Applicable	Not Applicable	Failed
Salicylic acid	Not Applicable	Not Applicable	Failed
Glutathione	-11.32	-18.29	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Glutathione helped deactivate the 2019-nCoV HR2 Domain (6LVN) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Andrographis paniculata can prevent COVID 19 due to the presence of Glutathione. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Avicennia marina against COVID 19 through deactivation of 2019-nCoV HR2 Domain (6LVN)

Shivangi Mohapatra[1], Sitaram Swain[2]

[1]190705180003@cutm.ac.in

[2]Sitaram.swain@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Avicennia marina against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate 2019-nCoV HR2 Domain (6LVN) enzyme. It was found that Salicylic acid helped to prevent COVID 19.

Introduction: Avicennia marina is known for its medicinal activities. White mangrove is used in traditional medicine as several medically active components are present in the plant including iridoid glucosides, flavonoids and naphthoquinone derivatives. They have strong antiproliferative and moderate cytotoxic activities as well as antibacterial effects. The resin from the bark is used to treat snake bites and to remove the placenta after childbirth. Leaf and bark decoctions are used as an anodyne and are applied externally against scabies. The wood ash has been used to treat skin complaints. Aqueous, ethanol and butanol crude extracts of the aerial parts of the plant were tested for antimicrobial activity.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Lamiales
Family	Acanthaceae
Genus	Avicennia
Species	marina

Major phytochemicals present in the plant are:

a. Tangeretin
b. Salicylic acid
c. Pelletierine
d. Digoxin

One of the major enzymes required for the survival of the organism causing COVID 19 is 2019-nCoV HR2 Domain (6LVN) 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 2019-nCoV HR2 Domain (6LVN) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tangeretin	Not Applicable	Not Applicable	Failed
Salicylic acid	-14.66	-18.94	Positive
Pelletierine	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 Salicylic acid helped deactivate the 2019-nCoV HR2 Domain (6LVN) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Avicennia marina can prevent COVID 19 due to the presence of Salicylic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Barleria prionitis against COVID 19 through deactivation of 2019-nCoV HR2 Domain (6LVN)

Swatiswagatika Nayak[1], Sitaram Swain[2]

[1]190705180004@cutm.ac.in

[2]Sitaram.swain@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Barleria prionitis against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate 2019-nCoV HR2 Domain (6LVN) enzyme. It was found that Benzyl isothiocyanate helped to prevent COVID 19.

Introduction: Barleria prionitis is known for its medicinal activities. It is used for various medicinal purposes in ayurvedic medicine. The juice of the leaves is applied to feet to prevent maceration and cracking in the monsoon season. Its leaves are known to contain 6-Hydroxyflavone, one of the chemical compounds that is a noncompetitive inhibitor of the protein cytochrome P450 2C9.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Lamiales
Family	Acanthaceae
Genus	Barleria
Species	prionitis

Major phytochemicals present in the plant are:

a. Rosmarinic acid
b. Daidzein
c. Benzyl isothiocyanate
d. Quercetin

One of the major enzymes required for the survival of the organism causing COVID 19 is 2019-nCoV HR2 Domain (6LVN) 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 2019-nCoV HR2 Domain (6LVN) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Rosmarinic acid	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Failed
Benzyl isothiocyanate	-13.92	-15.78	Positive
Quercetin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Benzyl isothiocyanate helped deactivate the 2019-nCoV HR2 Domain (6LVN) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Barleria prionitis can prevent COVID 19 due to the presence of Benzyl isothiocyanate. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Berginia ligulata against COVID 19 through deactivation of 2019-nCoV HR2 Domain (6LVN)

Nitesh Sahoo[1], Gagan Kumar Panigrahi[2]

[1]190705180005@cutm.ac.in

[2]gagan.panigrahi@gmail.com

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Berginia ligulata against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate 2019-nCoV HR2 Domain (6LVN) enzyme. It was found that Ferulic acid helped to prevent COVID 19.

Introduction: Berginia ligulata is known for its medicinal activities. Ligulata possesses cooling, laxative, analgesic, abortifacient, aphrodisiac properties and used in treatment of vesicular calculi, urinary discharges, excessive uterine haemorrhage, diseases of the bladder, dysentery, menorrhagia, splenic enlargement and heart diseases.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Saxifragales
Family	Saxifragaceae
Genus	Bergenia
Species	ligulata

Major phytochemicals present in the plant are:

a. Pelargonidin
b. Ferulic acid
c. Rutin
d. Epicatechin

One of the major enzymes required for the survival of the organism causing COVID 19 is 2019-nCoV HR2 Domain (6LVN) 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 2019-nCoV HR2 Domain (6LVN) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelargonidin	Not Applicable	Not Applicable	Failed
Ferulic acid	-12.38	-16.84	Positive
Rutin	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 Ferulic acid helped deactivate the 2019-nCoV HR2 Domain (6LVN) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Berginia ligulata can prevent COVID 19 due to the presence of Ferulic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Caesalpinea sappan against COVID 19 through deactivation of 2019-nCoV HR2 Domain (6LVN)

Anwesha Naik[1], Gagan Kumar Panigrahi[2]

[1]190705180006@cutm.ac.in

[2]gagan.panigrahi@gmail.com

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Caesalpinea sappan against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate 2019-nCoV HR2 Domain (6LVN) enzyme. It was found that Phenyl isothiocyanate helped to prevent COVID 19.

Introduction: Caesalpinea sappan is known for its medicinal activities. This plant has antibacterial and anticoagulant properties. Slivers of heartwood are used for making herbal drinking water in various regions, such as Kerala, Karnataka and Central Java, where it is usually mixed with ginger, cinnamon, and cloves. The heartwood also contains juglone (5-hydroxy-1,4-naphthoquinone), which has antimicrobial activity.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Fabales
Family	Fabaceae
Genus	Caesalpinia
Species	sappan

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Phenyl isothiocyanate
c. Digoxin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is 2019-nCoV HR2 Domain (6LVN) 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 2019-nCoV HR2 Domain (6LVN) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Phenyl isothiocyanate	-11.94	-17.64	Positive
Digoxin	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 Phenyl isothiocyanate helped deactivate the 2019-nCoV HR2 Domain (6LVN) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Caesalpinea sappan can prevent COVID 19 due to the presence of Phenyl isothiocyanate. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Curcuma longa against COVID 19 through deactivation of 2019-nCoV HR2 Domain (6LVN)

Sourav Patra[1], Gagan Kumar Panigrahi[2]

[1]190705180007@cutm.ac.in

[2]gagan.panigrahi@gmail.com

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Curcuma longa against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate 2019-nCoV HR2 Domain (6LVN) enzyme. It was found that Pelletierine helped to prevent COVID 19.

Introduction: Curcuma longa is known for its medicinal activities. Turmeric is used widely as a spice in South Asian and Middle Eastern cooking. The golden yellow colour of turmeric is due to curcumin which contains an orange-coloured volatile oil. It is used to protect food products from sunlight. Curcumin reduces inflammation.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Zingiberales
Family	Zingiberaceae
Genus	Curcuma
Species	longa

Major phytochemicals present in the plant are:

a. Pelletierine
b. Isorhamnetin
c. Theobromine
d. Tannic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is 2019-nCoV HR2 Domain (6LVN) 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 2019-nCoV HR2 Domain (6LVN) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	-13.61	-18.57	Positive
Isorhamnetin	Not Applicable	Not Applicable	Failed
Theobromine	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 Pelletierine helped deactivate the 2019-nCoV HR2 Domain (6LVN) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Curcuma longa can prevent COVID 19 due to the presence of Pelletierine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Ephedra sinica against COVID 19 through deactivation of 2019-nCoV HR2 Domain (6LVN)

Mohitaksha Kar[1], Gagan Kumar Panigrahi[2]

[1]190705180008@cutm.ac.in

[2]gagan.panigrahi@gmail.com

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Ephedra sinica against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate 2019-nCoV HR2 Domain (6LVN) enzyme. It was found that Theobromine helped to prevent COVID 19.

Introduction: Ephedra sinica is known for its medicinal activities. Ephedra is used for weight loss and obesity and to enhance athletic performance. It is also used for allergies and hay fever; nasal congestion; and respiratory tract conditions such as bronchospasm, asthma, and bronchitis. It is also used for colds, flu, swine flu, fever, chills, headache, inability to sweat, joint and bone pain, and as a "water pill" to increase urine flow in people who retain fluids.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Gnetophyta
Order	Ephedrales
Family	Ephedraceae
Genus	Ephedra
Species	E. sinica

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Theobromine
c. Apigenin
d. Rosmarinic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is 2019-nCoV HR2 Domain (6LVN) 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 2019-nCoV HR2 Domain (6LVN) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Theobromine	-12.94	-19.61	Positive
Apigenin	Not Applicable	Not Applicable	Failed
Rosmarinic acid	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 2019-nCoV HR2 Domain (6LVN) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Ephedra sinica can prevent COVID 19 due to the presence of Theobromine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Gardenia sp. against COVID 19 through deactivation of 2019-nCoV HR2 Domain (6LVN)

Sashmita Sharma[1], Gagan Kumar Panigrahi[2]

[1]190705180009@cutm.ac.in

[2]gagan.panigrahi@gmail.com

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Gardenia sp. against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate 2019-nCoV HR2 Domain (6LVN) enzyme. It was found that Pelargonidin and Genistein helped to prevent COVID 19.

Introduction: Gardenia sp. is known for its medicinal activities. Gardenia plants are known for its strong sweet scent of their flowers. Gardenia jasminoides (syn. G. grandiflora, G. Florida) is cultivated as a house plant. Its fruit is used as a yellow dye and used on fabric and food. Its fruits are also used in traditional Chinese medicine for their clearing, calming, and cooling properties.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Gentianales
Family	Rubiaceae
Genus	Gardenieae
Species	Gardenia

Major phytochemicals present in the plant are:

a. Pelargonidin
b. Genistein
c. Genistein
d. Daidzein

One of the major enzymes required for the survival of the organism causing COVID 19 is 2019-nCoV HR2 Domain (6LVN) 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 2019-nCoV HR2 Domain (6LVN) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelargonidin	-12.39	-18.64	Positive
Genistein	-11.31	-15.94	Positive
Genistein	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Pelargonidin and Genistein helped deactivate the 2019-nCoV HR2 Domain (6LVN) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Gardenia sp. can prevent COVID 19 due to the presence of Pelargonidin and Genistein. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Glycyrrhiza glabra against COVID 19 through deactivation of 2019-nCoV HR2 Domain (6LVN)

Subhasmita Behera[1], Gagan Kumar Panigrahi[2]

[1]190705180010@cutm.ac.in

[2]gagan.panigrahi@gmail.com

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Glycyrrhiza glabra against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate 2019-nCoV HR2 Domain (6LVN) enzyme. It was found that Alliin helped to prevent COVID 19.

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. Alliin
b. Isorhamnetin
c. Sulforaphane
d. Ascorbic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is 2019-nCoV HR2 Domain (6LVN) 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 2019-nCoV HR2 Domain (6LVN) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Alliin	-12.64	-15.91	Positive
Isorhamnetin	Not Applicable	Not Applicable	Failed
Sulforaphane	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 Alliin helped deactivate the 2019-nCoV HR2 Domain (6LVN) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Glycyrrhiza glabra can prevent COVID 19 due to the presence of Alliin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Hottuynia cordata against COVID 19 through deactivation of 2019-nCoV HR2 Domain (6LVN)

Sanjib Kumar Mohanty[1], Gagan Kumar Panigrahi[2]

[1]190705180011@cutm.ac.in

[2]gagan.panigrahi@gmail.com

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Hottuynia cordata against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate 2019-nCoV HR2 Domain (6LVN) enzyme. It was found that Coumarin helped to prevent COVID 19.

Introduction: Hottuynia 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. Lupeol
b. Peonidin
c. Coumarin
d. Malvidin

One of the major enzymes required for the survival of the organism causing COVID 19 is 2019-nCoV HR2 Domain (6LVN) 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 2019-nCoV HR2 Domain (6LVN) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lupeol	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Coumarin	-11.61	-13.67	Positive
Malvidin	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 2019-nCoV HR2 Domain (6LVN) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Hottuynia cordata can prevent COVID 19 due to the presence of Coumarin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Neerium indicum against COVID 19 through deactivation of 2019-nCoV HR2 Domain (6LVN)

Monalisa Sahu[1], Srimay Pradhan[2]

[1]190705180012@cutm.ac.in

[2]srimay.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 COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate 2019-nCoV HR2 Domain (6LVN) enzyme. It was found that Caffeine helped to prevent COVID 19.

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. Theobromine
b. Daidzein
c. Caffeine
d. Limonene

One of the major enzymes required for the survival of the organism causing COVID 19 is 2019-nCoV HR2 Domain (6LVN) 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 2019-nCoV HR2 Domain (6LVN) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Failed
Caffeine	-14.37	-19.67	Positive
Limonene	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 2019-nCoV HR2 Domain (6LVN) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Neerium indicum can prevent COVID 19 due to the presence of Caffeine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Nigelia sativa against COVID 19 through deactivation of 2019-nCoV HR2 Domain (6LVN)

Soubhagini Sahoo[1], Srimay Pradhan[2]

[1]190705180013@cutm.ac.in

[2]srimay.pradhan@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Nigelia sativa against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate 2019-nCoV HR2 Domain (6LVN) enzyme. It was found that Kaempferol helped to prevent COVID 19.

Introduction: Nigelia sativa is known for its medicinal activities. Nigella sativa is used as a spice, natural seasoning, or flavoring. The seeds of N. sativa are used as a spice in many cuisines. They can be used as a seasoning in recipes with pod fruit, vegetables, salads, and poultry. The black seeds are used to flavour bread products, and are used as part of the spice mixture. Nigella is also used in tresse cheese, a braided string cheese called majdouleh or majdouli in the Middle East.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Ranunculales
Family	Ranunculaceae
Genus	Nigella
Species	sativa

Major phytochemicals present in the plant are:

a. Theobromine
b. Kaempferol
c. Limonene
d. Malvidin

One of the major enzymes required for the survival of the organism causing COVID 19 is 2019-nCoV HR2 Domain (6LVN) 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 2019-nCoV HR2 Domain (6LVN) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	Not Applicable	Not Applicable	Failed
Kaempferol	-11.32	-17.64	Positive
Limonene	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 Kaempferol helped deactivate the 2019-nCoV HR2 Domain (6LVN) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Nigelia sativa can prevent COVID 19 due to the presence of Kaempferol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Pandanus amaryllifoius against COVID 19 through deactivation of 2019-nCoV HR2 Domain (6LVN)

Shakti Swarupa Debata[1], Srimay Pradhan[2]

[1]190705180014@cutm.ac.in

[2]srimay.pradhan@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Pandanus amaryllifoius against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate 2019-nCoV HR2 Domain (6LVN) enzyme. It was found that Lutein helped to prevent COVID 19.

Introduction: Pandanus amaryllifoius is known for its medicinal activities. The leaves are used in the perfume industry and traditional medicine. P. amaryllifolius essence may substitute for vanilla essence. The leaves possess a pleasant aroma and can be used as natural air fresheners. The green juice acquired from its leaf is used extensively in Indonesian cuisine as green food colouring and flavouring agents that gave pleasant aroma for kue, a tapioca, flour or glutinous rice-based traditional cakes.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Pandanales
Family	Pandanaceae
Genus	Pandanus
Species	amaryllifolius

Major phytochemicals present in the plant are:

a. Lutein
b. Genistein
c. Gallic acid
d. Theobromine

One of the major enzymes required for the survival of the organism causing COVID 19 is 2019-nCoV HR2 Domain (6LVN) 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 2019-nCoV HR2 Domain (6LVN) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lutein	-12.61	-18.39	Positive
Genistein	Not Applicable	Not Applicable	Failed
Gallic acid	-12.61	-18.83	Positive
Theobromine	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 2019-nCoV HR2 Domain (6LVN) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Pandanus amaryllifoius can prevent COVID 19 due to the presence of Lutein. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Phyllanthus amarus against COVID 19 through deactivation of 2019-nCoV HR2 Domain (6LVN)

Saswati Samant[1], Srimay Pradhan[2]

[1]190705180015@cutm.ac.in

[2]srimay.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 amarus against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate 2019-nCoV HR2 Domain (6LVN) enzyme. It was found that Ellagic acid and Campesterol helped to prevent COVID 19.

Introduction: Phyllanthus amarus is known for its medicinal activities. P.amarus is an important plant of Indian Ayurvedic system of medicine which is used in the problems of stomach, genitourinary system, liver, kidney and spleen. It is bitter, astringent, stomachic, diuretic, febrifuge and antiseptic. The whole plant is used in gonorrhea, menorrhagia and other genital affections.

The plant is classified as follows:

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

Major phytochemicals present in the plant are:

a. Pelletierine
b. Daidzein
c. Ellagic acid
d. Campesterol

One of the major enzymes required for the survival of the organism causing COVID 19 is 2019-nCoV HR2 Domain (6LVN) 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 2019-nCoV HR2 Domain (6LVN) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Failed
Ellagic acid	-12.94	-19.75	Positive
Campesterol	-19.66	-24.61	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ellagic acid and Campesterol helped deactivate the 2019-nCoV HR2 Domain (6LVN) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Phyllanthus amarus can prevent COVID 19 due to the presence of Ellagic acid and Campesterol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Punica granatum against COVID 19 through deactivation of 2019-nCoV HR2 Domain (6LVN)

Swati Choudhury[1], Srimay Pradhan[2]

[1]190705180016@cutm.ac.in

[2]srimay.pradhan@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Punica granatum against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate 2019-nCoV HR2 Domain (6LVN) enzyme. It was found that Campesterol helped to prevent COVID 19.

Introduction: Punica granatum is known for its medicinal activities. Pomegranate seeds are used as a spice known as anar dana. Pomegranate is used mainly for juice. Pomegranate syrup or molasses is used in muhammara, a roasted red pepper, walnut, and garlic. Grenadine syrup originally consisted of thickened and sweetened pomegranate juice mainly used in cocktail mixing.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Myrtales
Family	Lythraceae
Genus	Punica
Species	granatum

Major phytochemicals present in the plant are:

a. Campesterol
b. Malvidin
c. Myricetin
d. Pelargonidin

One of the major enzymes required for the survival of the organism causing COVID 19 is 2019-nCoV HR2 Domain (6LVN) 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 2019-nCoV HR2 Domain (6LVN) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Campesterol	-17.59	-22.64	Positive
Malvidin	Not Applicable	Not Applicable	Failed
Myricetin	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 2019-nCoV HR2 Domain (6LVN) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Punica granatum can prevent COVID 19 due to the presence of Campesterol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Wickstroemia indica against COVID 19 through deactivation of 2019-nCoV HR2 Domain (6LVN)

Sushree Swati Rout[1], Bhagyeswari Behera[2]

[1]190705180017@cutm.ac.in

[2]bhayeswari.behera@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Wickstroemia indica against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate 2019-nCoV HR2 Domain (6LVN) enzyme. It was found that Naringin and Zingiberene helped to prevent COVID 19.

Introduction: Wickstroemia indica is known for its medicinal activities. It is used in traditional Chinese medicine. This plant has antipyretic, detoxicant, expectorant, vermifuge, and abortifacient properties used in clinical practice in China. An alcoholic extract of the plant was found to contain daphnoretin, chrysophanol, myricitrime and rutin. The extract of W. indica displays antimicrobial and anti-inflammatory activities in vitro.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Malvales
Family	Thymelaeaceae
Genus	Wikstroemia
Species	indica

Major phytochemicals present in the plant are:

a. Naringin
b. Daidzein
c. Peonidin
d. Zingiberene

One of the major enzymes required for the survival of the organism causing COVID 19 is 2019-nCoV HR2 Domain (6LVN) 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 2019-nCoV HR2 Domain (6LVN) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Naringin	-15.94	-17.83	Positive
Daidzein	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Zingiberene	-14.61	-19.37	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Naringin and Zingiberene helped deactivate the 2019-nCoV HR2 Domain (6LVN) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Wickstroemia indica can prevent COVID 19 due to the presence of Naringin and Zingiberene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Zizyphus spira-christi against COVID 19 through deactivation of 2019-nCoV HR2 Domain (6LVN)

Deepanwita Kar[1], Bhagyeswari Behera[2]

[1]190705180018@cutm.ac.in

[2]bhayeswari.behera@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Zizyphus spira-christi against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate 2019-nCoV HR2 Domain (6LVN) enzyme. It was found that Eugenol helped to prevent COVID 19.

Introduction: Zizyphus spira-christi is known for its medicinal activities. Fruits of Z. spina-christi is used as food. The wood is used as a source of fuel and it produces an excellent charcoal. Z. spina-christi fruits are eaten to treat diarrhoea and malaria and as an antispasmodic. The powder of the twigs is used externally to treat rheumatism and scorpion sting. Ash of wood mixed with vinegar is applied to heal snake bites and a tea made of fruit is used to treat measles. Fruits and crashed kernels are eaten to treat chest pains, respiratory problems and as a tonic.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Rosales
Family	Rhamnaceae
Genus	Ziziphus
Species	spina-christi

Major phytochemicals present in the plant are:

a. Eugenol
b. Daidzein
c. Peonidin
d. Myricetin

One of the major enzymes required for the survival of the organism causing COVID 19 is 2019-nCoV HR2 Domain (6LVN) 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 2019-nCoV HR2 Domain (6LVN) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Eugenol	-14.91	-24.08	Positive
Daidzein	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Myricetin	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 2019-nCoV HR2 Domain (6LVN) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Zizyphus spira-christi can prevent COVID 19 due to the presence of Eugenol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Alpinia officinarium against COVID 19 through deactivation of ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS)

Swagatika Parida[1], Bhagyeswari Behera[2]

[1]190705180019@cutm.ac.in

[2]bhayeswari.behera@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Alpinia officinarium against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme. It was found that Luteolin helped to prevent COVID 19.

Introduction: Alpinia officinarium is known for its medicinal activities. In Asia the rhizomes are ground to powder for use in curries, drinks, and jellies. In India an extract is used in perfumes. Alpinia officinarum contains high concentrations of the flavonol galangin. Historically, the rhizomes were reputed to have stimulant and digestive effects.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Zingiberales
Family	Zingiberaceae
Genus	Alpinia
Species	officinarum

Major phytochemicals present in the plant are:

a. Resveratrol
b. Phenyl isothiocyanate
c. Luteolin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) 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 ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Resveratrol	Not Applicable	Not Applicable	Failed
Phenyl isothiocyanate	Not Applicable	Not Applicable	Failed
Luteolin	-12.97	-19.84	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 Luteolin helped deactivate the ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Alpinia officinarium can prevent COVID 19 due to the presence of Luteolin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Andrographis paniculata against COVID 19 through deactivation of ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS)

Soumyakanta Sahoo[1], Bhagyeswari Behera[2]

[1]190705180020@cutm.ac.in

[2]bhayeswari.behera@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 COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme. It was found that Glutathione helped to prevent COVID 19.

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. Cryptoxanthin
b. Quercetin
c. Salicylic acid
d. Glutathione

One of the major enzymes required for the survival of the organism causing COVID 19 is ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) 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 ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Cryptoxanthin	Not Applicable	Not Applicable	Failed
Quercetin	Not Applicable	Not Applicable	Failed
Salicylic acid	Not Applicable	Not Applicable	Failed
Glutathione	-10.34	-15.61	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Glutathione helped deactivate the ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Andrographis paniculata can prevent COVID 19 due to the presence of Glutathione. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Avicennia marina against COVID 19 through deactivation of ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS)

Pragati Priyambada Badapanda[1], Bhagyeswari Behera[2]

[1]190705180021@cutm.ac.in

[2]bhayeswari.behera@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Avicennia marina against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme. It was found that Salicylic acid helped to prevent COVID 19.

Introduction: Avicennia marina is known for its medicinal activities. White mangrove is used in traditional medicine as several medically active components are present in the plant including iridoid glucosides, flavonoids and naphthoquinone derivatives. They have strong antiproliferative and moderate cytotoxic activities as well as antibacterial effects. The resin from the bark is used to treat snake bites and to remove the placenta after childbirth. Leaf and bark decoctions are used as an anodyne and are applied externally against scabies. The wood ash has been used to treat skin complaints. Aqueous, ethanol and butanol crude extracts of the aerial parts of the plant were tested for antimicrobial activity.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Lamiales
Family	Acanthaceae
Genus	Avicennia
Species	marina

Major phytochemicals present in the plant are:

a. Tangeretin
b. Salicylic acid
c. Pelletierine
d. Digoxin

One of the major enzymes required for the survival of the organism causing COVID 19 is ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) 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 ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tangeretin	Not Applicable	Not Applicable	Failed
Salicylic acid	-18.23	-21.61	Positive
Pelletierine	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 Salicylic acid helped deactivate the ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Avicennia marina can prevent COVID 19 due to the presence of Salicylic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Barleria prionitis against COVID 19 through deactivation of ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS)

Soumya Sephalika Nayak[1], Gyanranjan Mahalik[2]

[1]190705180022@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 Barleria prionitis against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme. It was found that Benzyl isothiocyanate helped to prevent COVID 19.

Introduction: Barleria prionitis is known for its medicinal activities. It is used for various medicinal purposes in ayurvedic medicine. The juice of the leaves is applied to feet to prevent maceration and cracking in the monsoon season. Its leaves are known to contain 6-Hydroxyflavone, one of the chemical compounds that is a noncompetitive inhibitor of the protein cytochrome P450 2C9.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Lamiales
Family	Acanthaceae
Genus	Barleria
Species	prionitis

Major phytochemicals present in the plant are:

a. Rosmarinic acid
b. Daidzein
c. Benzyl isothiocyanate
d. Quercetin

One of the major enzymes required for the survival of the organism causing COVID 19 is ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) 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 ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Rosmarinic acid	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Failed
Benzyl isothiocyanate	-13.57	-15.91	Positive
Quercetin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Benzyl isothiocyanate helped deactivate the ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Barleria prionitis can prevent COVID 19 due to the presence of Benzyl isothiocyanate. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Berginia ligulata against COVID 19 through deactivation of ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS)

Shubhashree Khadgaray[1], Gyanranjan Mahalik[2]

[1]190705180023@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 Berginia ligulata against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme. It was found that Ferulic acid helped to prevent COVID 19.

Introduction: Berginia ligulata is known for its medicinal activities. Ligulata possesses cooling, laxative, analgesic, abortifacient, aphrodisiac properties and used in treatment of vesicular calculi, urinary discharges, excessive uterine haemorrhage, diseases of the bladder, dysentery, menorrhagia, splenic enlargement and heart diseases.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Saxifragales
Family	Saxifragaceae
Genus	Bergenia
Species	ligulata

Major phytochemicals present in the plant are:

a. Pelargonidin
b. Ferulic acid
c. Rutin
d. Epicatechin

One of the major enzymes required for the survival of the organism causing COVID 19 is ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) 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 ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelargonidin	Not Applicable	Not Applicable	Failed
Ferulic acid	-12.54	-15.66	Positive
Rutin	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 Ferulic acid helped deactivate the ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Berginia ligulata can prevent COVID 19 due to the presence of Ferulic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Caesalpinea sappan against COVID 19 through deactivation of ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS)

Satyajit Mohanty[1], Gyanranjan Mahalik[2]

[1]190705180024@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 Caesalpinea sappan against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme. It was found that Phenyl isothiocyanate helped to prevent COVID 19.

Introduction: Caesalpinea sappan is known for its medicinal activities. This plant has antibacterial and anticoagulant properties. Slivers of heartwood are used for making herbal drinking water in various regions, such as Kerala, Karnataka and Central Java, where it is usually mixed with ginger, cinnamon, and cloves. The heartwood also contains juglone (5-hydroxy-1,4-naphthoquinone), which has antimicrobial activity.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Fabales
Family	Fabaceae
Genus	Caesalpinia
Species	sappan

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Phenyl isothiocyanate
c. Digoxin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) 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 ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Phenyl isothiocyanate	-15.64	-18.78	Positive
Digoxin	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 Phenyl isothiocyanate helped deactivate the ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Caesalpinea sappan can prevent COVID 19 due to the presence of Phenyl isothiocyanate. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Curcuma longa against COVID 19 through deactivation of ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS)

Sushantika Biswal[1], Gyanranjan Mahalik[2]

[1]190705180025@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 Curcuma longa against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme. It was found that Pelletierine helped to prevent COVID 19.

Introduction: Curcuma longa is known for its medicinal activities. Turmeric is used widely as a spice in South Asian and Middle Eastern cooking. The golden yellow colour of turmeric is due to curcumin which contains an orange-coloured volatile oil. It is used to protect food products from sunlight. Curcumin reduces inflammation.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Zingiberales
Family	Zingiberaceae
Genus	Curcuma
Species	longa

Major phytochemicals present in the plant are:

a. Pelletierine
b. Isorhamnetin
c. Theobromine
d. Tannic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) 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 ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	-12.61	-16.84	Positive
Isorhamnetin	Not Applicable	Not Applicable	Failed
Theobromine	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 Pelletierine helped deactivate the ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Curcuma longa can prevent COVID 19 due to the presence of Pelletierine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Ephedra sinica against COVID 19 through deactivation of ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS)

Bibhuprasad Sahu[1], Gyanranjan Mahalik[2]

[1]190705180026@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 Ephedra sinica against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme. It was found that Theobromine helped to prevent COVID 19.

Introduction: Ephedra sinica is known for its medicinal activities. Ephedra is used for weight loss and obesity and to enhance athletic performance. It is also used for allergies and hay fever; nasal congestion; and respiratory tract conditions such as bronchospasm, asthma, and bronchitis. It is also used for colds, flu, swine flu, fever, chills, headache, inability to sweat, joint and bone pain, and as a "water pill" to increase urine flow in people who retain fluids.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Gnetophyta
Order	Ephedrales
Family	Ephedraceae
Genus	Ephedra
Species	E. sinica

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Theobromine
c. Apigenin
d. Rosmarinic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) 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 ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Theobromine	-15.67	-19.34	Positive
Apigenin	Not Applicable	Not Applicable	Failed
Rosmarinic acid	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 ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Ephedra sinica can prevent COVID 19 due to the presence of Theobromine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Gardenia sp. against COVID 19 through deactivation of ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS)

Zizibisa Lenka[1], Kalpita Bhatta[2]

[1]190705180027@cutm.ac.in

[2]kalpita.bhatta@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Gardenia sp. against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme. It was found that Genistein helped to prevent COVID 19.

Introduction: Gardenia sp. is known for its medicinal activities. Gardenia plants are known for its strong sweet scent of their flowers. Gardenia jasminoides (syn. G. grandiflora, G. Florida) is cultivated as a house plant. Its fruit is used as a yellow dye and used on fabric and food. Its fruits are also used in traditional Chinese medicine for their clearing, calming, and cooling properties.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Gentianales
Family	Rubiaceae
Genus	Gardenieae
Species	Gardenia

Major phytochemicals present in the plant are:

a. Pelargonidin
b. Genistein
c. Genistein
d. Daidzein

One of the major enzymes required for the survival of the organism causing COVID 19 is ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) 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 ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelargonidin	Not Applicable	Not Applicable	Failed
Genistein	-12.27	-15.61	Positive
Genistein	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Genistein helped deactivate the ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Gardenia sp. can prevent COVID 19 due to the presence of Genistein. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Punica granatum against COVID 19 through deactivation of ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS)

Akankshya Abhilipsa Pradhan[1], Kalpita Bhatta[2]

[1]190705180028@cutm.ac.in

[2]kalpita.bhatta@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Punica granatum against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme. It was found that Campesterol helped to prevent COVID 19.

Introduction: Punica granatum is known for its medicinal activities. Pomegranate seeds are used as a spice known as anar dana. Pomegranate is used mainly for juice. Pomegranate syrup or molasses is used in muhammara, a roasted red pepper, walnut, and garlic. Grenadine syrup originally consisted of thickened and sweetened pomegranate juice mainly used in cocktail mixing.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Myrtales
Family	Lythraceae
Genus	Punica
Species	granatum

Major phytochemicals present in the plant are:

a. Campesterol
b. Malvidin
c. Myricetin
d. Pelargonidin

One of the major enzymes required for the survival of the organism causing COVID 19 is ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) 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 ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Campesterol	-18.61	-21.54	Positive
Malvidin	Not Applicable	Not Applicable	Failed
Myricetin	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 ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Punica granatum can prevent COVID 19 due to the presence of Campesterol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Wickstroemia indica against COVID 19 through deactivation of ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS)

Janmejaya Nayak[1], Kalpita Bhatta[2]

[1]190705180029@cutm.ac.in

[2]kalpita.bhatta@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Wickstroemia indica against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme. It was found that Naringin helped to prevent COVID 19.

Introduction: Wickstroemia indica is known for its medicinal activities. It is used in traditional Chinese medicine. This plant has antipyretic, detoxicant, expectorant, vermifuge, and abortifacient properties used in clinical practice in China. An alcoholic extract of the plant was found to contain daphnoretin, chrysophanol, myricitrime and rutin. The extract of W. indica displays antimicrobial and anti-inflammatory activities in vitro.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Malvales
Family	Thymelaeaceae
Genus	Wikstroemia
Species	indica

Major phytochemicals present in the plant are:

a. Naringin
b. Daidzein
c. Peonidin
d. Zingiberene

One of the major enzymes required for the survival of the organism causing COVID 19 is ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) 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 ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Naringin	-16.24	-21.63	Positive
Daidzein	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Zingiberene	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 ADP ribose phosphatase of NSP3 from SARS CoV-2 (6VXS) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Wickstroemia indica can prevent COVID 19 due to the presence of Naringin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Alpinia officinarium against COVID 19 through deactivation of COVID-19 main protease (6M03)

Neha Rani Lenka[1], Kalpita Bhatta[2]

[1]190705180030@cutm.ac.in

[2]kalpita.bhatta@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Alpinia officinarium against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate COVID-19 main protease (6M03) enzyme. It was found that Phenyl isothiocyanate and Luteolin helped to prevent COVID 19.

Introduction: Alpinia officinarium is known for its medicinal activities. In Asia the rhizomes are ground to powder for use in curries, drinks, and jellies. In India an extract is used in perfumes. Alpinia officinarum contains high concentrations of the flavonol galangin. Historically, the rhizomes were reputed to have stimulant and digestive effects.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Zingiberales
Family	Zingiberaceae
Genus	Alpinia
Species	officinarum

Major phytochemicals present in the plant are:

a. Resveratrol
b. Phenyl isothiocyanate
c. Luteolin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is COVID-19 main protease (6M03) 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 COVID-19 main protease (6M03) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Resveratrol	Not Applicable	Not Applicable	Failed
Phenyl isothiocyanate	-12.54	-15.66	Positive
Luteolin	-11.38	-18.36	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 Phenyl isothiocyanate and Luteolin helped deactivate the COVID-19 main protease (6M03) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Alpinia officinarium can prevent COVID 19 due to the presence of Phenyl isothiocyanate and Luteolin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Andrographis paniculata against COVID 19 through deactivation of COVID-19 main protease (6M03)

Dibyasa Samal[1], Kalpita Bhatta[2]

[1]190705180031@cutm.ac.in

[2]kalpita.bhatta@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 COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate COVID-19 main protease (6M03) enzyme. It was found that Quercetin helped to prevent COVID 19.

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. Cryptoxanthin
b. Quercetin
c. Salicylic acid
d. Glutathione

One of the major enzymes required for the survival of the organism causing COVID 19 is COVID-19 main protease (6M03) 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 COVID-19 main protease (6M03) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Cryptoxanthin	Not Applicable	Not Applicable	Failed
Quercetin	-12.41	-17.39	Positive
Salicylic acid	Not Applicable	Not Applicable	Failed
Glutathione	-11.67	-19.64	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Quercetin helped deactivate the COVID-19 main protease (6M03) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Andrographis paniculata can prevent COVID 19 due to the presence of Quercetin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Avicennia marina against COVID 19 through deactivation of COVID-19 main protease (6M03)

Subhashree Rout[1], Debanjana Saha[2]

[1]190705180032@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 Avicennia marina against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate COVID-19 main protease (6M03) enzyme. It was found that Salicylic acid helped to prevent COVID 19.

Introduction: Avicennia marina is known for its medicinal activities. White mangrove is used in traditional medicine as several medically active components are present in the plant including iridoid glucosides, flavonoids and naphthoquinone derivatives. They have strong antiproliferative and moderate cytotoxic activities as well as antibacterial effects. The resin from the bark is used to treat snake bites and to remove the placenta after childbirth. Leaf and bark decoctions are used as an anodyne and are applied externally against scabies. The wood ash has been used to treat skin complaints. Aqueous, ethanol and butanol crude extracts of the aerial parts of the plant were tested for antimicrobial activity.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Lamiales
Family	Acanthaceae
Genus	Avicennia
Species	marina

Major phytochemicals present in the plant are:

a. Tangeretin
b. Salicylic acid
c. Pelletierine
d. Digoxin

One of the major enzymes required for the survival of the organism causing COVID 19 is COVID-19 main protease (6M03) 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 COVID-19 main protease (6M03) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tangeretin	Not Applicable	Not Applicable	Failed
Salicylic acid	-18.64	-19.67	Positive
Pelletierine	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 Salicylic acid helped deactivate the COVID-19 main protease (6M03) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Avicennia marina can prevent COVID 19 due to the presence of Salicylic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Barleria prionitis against COVID 19 through deactivation of COVID-19 main protease (6M03)

Manisha Mandal[1], Debanjana Saha[2]

[1]190705180033@cutm.ac.in

[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 Barleria prionitis against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate COVID-19 main protease (6M03) enzyme. It was found that Rosmarinic acid and Benzyl isothiocyanate helped to prevent COVID 19.

Introduction: Barleria prionitis is known for its medicinal activities. It is used for various medicinal purposes in ayurvedic medicine. The juice of the leaves is applied to feet to prevent maceration and cracking in the monsoon season. Its leaves are known to contain 6-Hydroxyflavone, one of the chemical compounds that is a noncompetitive inhibitor of the protein cytochrome P450 2C9.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Lamiales
Family	Acanthaceae
Genus	Barleria
Species	prionitis

Major phytochemicals present in the plant are:

a. Rosmarinic acid
b. Daidzein
c. Benzyl isothiocyanate
d. Quercetin

One of the major enzymes required for the survival of the organism causing COVID 19 is COVID-19 main protease (6M03) 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 COVID-19 main protease (6M03) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Rosmarinic acid	-9.67	-15.45	Positive
Daidzein	Not Applicable	Not Applicable	Failed
Benzyl isothiocyanate	-13.92	-15.78	Positive
Quercetin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Rosmarinic acid and Benzyl isothiocyanate helped deactivate the COVID-19 main protease (6M03) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Barleria prionitis can prevent COVID 19 due to the presence of Rosmarinic acid and Benzyl isothiocyanate. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Berginia ligulata against COVID 19 through deactivation of COVID-19 main protease (6M03)

Soumya Bahalia[1], Debanjana Saha[2]

[1]190705180034@cutm.ac.in

[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 Berginia ligulata against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate COVID-19 main protease (6M03) enzyme. It was found that Ferulic acid helped to prevent COVID 19.

Introduction: Berginia ligulata is known for its medicinal activities. Ligulata possesses cooling, laxative, analgesic, abortifacient, aphrodisiac properties and used in treatment of vesicular calculi, urinary discharges, excessive uterine haemorrhage, diseases of the bladder, dysentery, menorrhagia, splenic enlargement and heart diseases.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Saxifragales
Family	Saxifragaceae
Genus	Bergenia
Species	ligulata

Major phytochemicals present in the plant are:

a. Pelargonidin
b. Ferulic acid
c. Rutin
d. Epicatechin

One of the major enzymes required for the survival of the organism causing COVID 19 is COVID-19 main protease (6M03) 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 COVID-19 main protease (6M03) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelargonidin	Not Applicable	Not Applicable	Failed
Ferulic acid	-15.64	-18.78	Positive
Rutin	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 Ferulic acid helped deactivate the COVID-19 main protease (6M03) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Berginia ligulata can prevent COVID 19 due to the presence of Ferulic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Caesalpinea sappan against COVID 19 through deactivation of COVID-19 main protease (6M03)

Mrutyunjay Pradhan[1], Debanjana Saha[2]

[1]190705180035@cutm.ac.in

[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 Caesalpinea sappan against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate COVID-19 main protease (6M03) enzyme. It was found that Phenyl isothiocyanate helped to prevent COVID 19.

Introduction: Caesalpinea sappan is known for its medicinal activities. This plant has antibacterial and anticoagulant properties. Slivers of heartwood are used for making herbal drinking water in various regions, such as Kerala, Karnataka and Central Java, where it is usually mixed with ginger, cinnamon, and cloves. The heartwood also contains juglone (5-hydroxy-1,4-naphthoquinone), which has antimicrobial activity.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Fabales
Family	Fabaceae
Genus	Caesalpinia
Species	sappan

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Phenyl isothiocyanate
c. Digoxin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is COVID-19 main protease (6M03) 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 COVID-19 main protease (6M03) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Phenyl isothiocyanate	-12.54	-15.66	Positive
Digoxin	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 Phenyl isothiocyanate helped deactivate the COVID-19 main protease (6M03) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Caesalpinea sappan can prevent COVID 19 due to the presence of Phenyl isothiocyanate. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Curcuma longa against COVID 19 through deactivation of COVID-19 main protease (6M03)

Iswar Ranjan Panigrahi[1], Debanjana Saha[2]

[1]190705180036@cutm.ac.in

[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 Curcuma longa against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate COVID-19 main protease (6M03) enzyme. It was found that Pelletierine helped to prevent COVID 19.

Introduction: Curcuma longa is known for its medicinal activities. Turmeric is used widely as a spice in South Asian and Middle Eastern cooking. The golden yellow colour of turmeric is due to curcumin which contains an orange-coloured volatile oil. It is used to protect food products from sunlight. Curcumin reduces inflammation.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Zingiberales
Family	Zingiberaceae
Genus	Curcuma
Species	longa

Major phytochemicals present in the plant are:

a. Pelletierine
b. Isorhamnetin
c. Theobromine
d. Tannic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is COVID-19 main protease (6M03) 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 COVID-19 main protease (6M03) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	-15.84	-19.34	Positive
Isorhamnetin	Not Applicable	Not Applicable	Failed
Theobromine	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 Pelletierine helped deactivate the COVID-19 main protease (6M03) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Curcuma longa can prevent COVID 19 due to the presence of Pelletierine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Ephedra sinica against COVID 19 through deactivation of COVID-19 main protease (6M03)

Subhashree Das[1], Ranjan Kumar Sahoo[2]

[1]190705180037@cutm.ac.in

[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 Ephedra sinica against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate COVID-19 main protease (6M03) enzyme. It was found that Theobromine helped to prevent COVID 19.

Introduction: Ephedra sinica is known for its medicinal activities. Ephedra is used for weight loss and obesity and to enhance athletic performance. It is also used for allergies and hay fever; nasal congestion; and respiratory tract conditions such as bronchospasm, asthma, and bronchitis. It is also used for colds, flu, swine flu, fever, chills, headache, inability to sweat, joint and bone pain, and as a "water pill" to increase urine flow in people who retain fluids.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Gnetophyta
Order	Ephedrales
Family	Ephedraceae
Genus	Ephedra
Species	E. sinica

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Theobromine
c. Apigenin
d. Rosmarinic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is COVID-19 main protease (6M03) 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 COVID-19 main protease (6M03) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Theobromine	-10.14	-18.51	Positive
Apigenin	Not Applicable	Not Applicable	Failed
Rosmarinic acid	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 COVID-19 main protease (6M03) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Ephedra sinica can prevent COVID 19 due to the presence of Theobromine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Gardenia sp. against COVID 19 through deactivation of COVID-19 main protease (6M03)

Kruttidipa Jena[1], Ranjan Kumar Sahoo[2]

[1]190705180038@cutm.ac.in

[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 Gardenia sp. against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate COVID-19 main protease (6M03) enzyme. It was found that Pelargonidin and Genistein helped to prevent COVID 19.

Introduction: Gardenia sp. is known for its medicinal activities. Gardenia plants are known for its strong sweet scent of their flowers. Gardenia jasminoides (syn. G. grandiflora, G. Florida) is cultivated as a house plant. Its fruit is used as a yellow dye and used on fabric and food. Its fruits are also used in traditional Chinese medicine for their clearing, calming, and cooling properties.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Gentianales
Family	Rubiaceae
Genus	Gardenieae
Species	Gardenia

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing COVID 19 is COVID-19 main protease (6M03) 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 COVID-19 main protease (6M03) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelargonidin	-15.52	-21.38	Positive
Genistein	-12.54	-15.69	Positive
Peonidin	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Pelargonidin and Genistein helped deactivate the COVID-19 main protease (6M03) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Gardenia sp. can prevent COVID 19 due to the presence of Pelargonidin and Genistein. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Glycyrrhiza glabra against COVID 19 through deactivation of COVID-19 main protease (6M03)

Nandita Parida[1], Ranjan Kumar Sahoo[2]

[1]190705180039@cutm.ac.in

[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 Glycyrrhiza glabra against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate COVID-19 main protease (6M03) enzyme. It was found that Allin and Sulforaphane helped to prevent COVID 19.

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. Alliin
b. Isorhamnetin
c. Sulforaphane
d. Ascorbic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is COVID-19 main protease (6M03) 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 COVID-19 main protease (6M03) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Alliin	-15.34	-16.78	Positive
Isorhamnetin	Not Applicable	Not Applicable	Failed
Sulforaphane	-18.01	-19.61	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 Allin and Sulforaphane helped deactivate the COVID-19 main protease (6M03) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Glycyrrhiza glabra can prevent COVID 19 due to the presence of Allin and Sulforaphane. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Hottuynia cordata against COVID 19 through deactivation of COVID-19 main protease (6M03)

Sasirekha Parida[1], Ranjan Kumar Sahoo[2]

[1]190705180040@cutm.ac.in

[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 Hottuynia cordata against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate COVID-19 main protease (6M03) enzyme. It was found that Coumarin helped to prevent COVID 19.

Introduction: Hottuynia 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. Lupeol
b. Peonidin
c. Coumarin
d. Malvidin

One of the major enzymes required for the survival of the organism causing COVID 19 is COVID-19 main protease (6M03) 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 COVID-19 main protease (6M03) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lupeol	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Coumarin	-12.85	-14.47	Positive
Malvidin	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 COVID-19 main protease (6M03) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Hottuynia cordata can prevent COVID 19 due to the presence of Coumarin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Neerium indicum against COVID 19 through deactivation of COVID-19 main protease (6M03)

Ankit Kumar Rath[1], Ranjan Kumar Sahoo[2]

[1]190705180041@cutm.ac.in

[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 Neerium indicum against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate COVID-19 main protease (6M03) enzyme. It was found that Caffeine helped to prevent COVID 19.

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. Theobromine
b. Daidzein
c. Caffeine
d. Limonene

One of the major enzymes required for the survival of the organism causing COVID 19 is COVID-19 main protease (6M03) 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 COVID-19 main protease (6M03) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Failed
Caffeine	-14.25	-18.34	Positive
Limonene	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 COVID-19 main protease (6M03) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Neerium indicum can prevent COVID 19 due to the presence of Caffeine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Nigelia sativa against COVID 19 through deactivation of COVID-19 main protease (6M03)

Amit Kumar Mohanta[1], Debanjana Saha[2]

[1]190705180042@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 Nigelia sativa against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate COVID-19 main protease (6M03) enzyme. It was found that Kaempferol helped to prevent COVID 19.

Introduction: Nigelia sativa is known for its medicinal activities. Nigella sativa is used as a spice, natural seasoning, or flavoring. The seeds of N. sativa are used as a spice in many cuisines. They can be used as a seasoning in recipes with pod fruit, vegetables, salads, and poultry. The black seeds are used to flavour bread products, and are used as part of the spice mixture. Nigella is also used in tresse cheese, a braided string cheese called majdouleh or majdouli in the Middle East.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Ranunculales
Family	Ranunculaceae
Genus	Nigella
Species	sativa

Major phytochemicals present in the plant are:

a. Theobromine
b. Kaempferol
c. Limonene
d. Malvidin

One of the major enzymes required for the survival of the organism causing COVID 19 is COVID-19 main protease (6M03) 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 COVID-19 main protease (6M03) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	Not Applicable	Not Applicable	Failed
Kaempferol	-10.84	-18.27	Positive
Limonene	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 Kaempferol helped deactivate the COVID-19 main protease (6M03) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Nigelia sativa can prevent COVID 19 due to the presence of Kaempferol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Pandanus amaryllifoius against COVID 19 through deactivation of COVID-19 main protease (6M03)

Abinash Sahu[1], Debanjana Saha[2]

[1]190705180043@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 Pandanus amaryllifoius against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate COVID-19 main protease (6M03) enzyme. It was found that Lutein and Gallic acid helped to prevent COVID 19.

Introduction: Pandanus amaryllifoius is known for its medicinal activities. The leaves are used in the perfume industry and traditional medicine. P. amaryllifolius essence may substitute for vanilla essence. The leaves possess a pleasant aroma and can be used as natural air fresheners. The green juice acquired from its leaf is used extensively in Indonesian cuisine as green food colouring and flavouring agents that gave pleasant aroma for kue, a tapioca, flour or glutinous rice-based traditional cakes.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Pandanales
Family	Pandanaceae
Genus	Pandanus
Species	amaryllifolius

Major phytochemicals present in the plant are:

a. Lutein
b. Genistein
c. Gallic acid
d. Theobromine

One of the major enzymes required for the survival of the organism causing COVID 19 is COVID-19 main protease (6M03) 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 COVID-19 main protease (6M03) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lutein	-11.21	-18.04	Positive
Genistein	Not Applicable	Not Applicable	Failed
Gallic acid	-12.37	-18.08	Positive
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 Gallic acid helped deactivate the COVID-19 main protease (6M03) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Pandanus amaryllifoius can prevent COVID 19 due to the presence of Lutein and Gallic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Phyllanthus amarus against COVID 19 through deactivation of COVID-19 main protease (6M03)

Smrutisoumya Das[1], Debanjana Saha[2]

[1]190705180044@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 Phyllanthus amarus against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate COVID-19 main protease (6M03) enzyme. It was found that Ellagic acid and Campesterol helped to prevent COVID 19.

Introduction: Phyllanthus amarus is known for its medicinal activities. P.amarus is an important plant of Indian Ayurvedic system of medicine which is used in the problems of stomach, genitourinary system, liver, kidney and spleen. It is bitter, astringent, stomachic, diuretic, febrifuge and antiseptic. The whole plant is used in gonorrhea, menorrhagia and other genital affections.

The plant is classified as follows:

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

Major phytochemicals present in the plant are:

a. Pelletierine
b. Daidzein
c. Ellagic acid
d. Campesterol

One of the major enzymes required for the survival of the organism causing COVID 19 is COVID-19 main protease (6M03) 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 COVID-19 main protease (6M03) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Failed
Ellagic acid	-12.54	-17.34	Positive
Campesterol	-17.58	-21.33	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ellagic acid and Campesterol helped deactivate the COVID-19 main protease (6M03) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Phyllanthus amarus can prevent COVID 19 due to the presence of Ellagic acid and Campesterol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Punica granatum against COVID 19 through deactivation of COVID-19 main protease (6M03)

Deeptimayi Dash[1], Debanjana Saha[2]

[1]190705180045@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 Punica granatum against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate COVID-19 main protease (6M03) enzyme. It was found that Campesterol helped to prevent COVID 19.

Introduction: Punica granatum is known for its medicinal activities. Pomegranate seeds are used as a spice known as anar dana. Pomegranate is used mainly for juice. Pomegranate syrup or molasses is used in muhammara, a roasted red pepper, walnut, and garlic. Grenadine syrup originally consisted of thickened and sweetened pomegranate juice mainly used in cocktail mixing.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Myrtales
Family	Lythraceae
Genus	Punica
Species	granatum

Major phytochemicals present in the plant are:

a. Campesterol
b. Malvidin
c. Myricetin
d. Pelargonidin

One of the major enzymes required for the survival of the organism causing COVID 19 is COVID-19 main protease (6M03) 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 COVID-19 main protease (6M03) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Campesterol	-17.58	-21.33	Positive
Malvidin	Not Applicable	Not Applicable	Failed
Myricetin	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 COVID-19 main protease (6M03) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Punica granatum can prevent COVID 19 due to the presence of Campesterol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Wickstroemia indica against COVID 19 through deactivation of COVID-19 main protease (6M03)

Sambit Kumar Rout[1], Debanjana Saha[2]

[1]190705180046@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 Wickstroemia indica against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate COVID-19 main protease (6M03) enzyme. It was found that Naringin and Zingiberene helped to prevent COVID 19.

Introduction: Wickstroemia indica is known for its medicinal activities. It is used in traditional Chinese medicine. This plant has antipyretic, detoxicant, expectorant, vermifuge, and abortifacient properties used in clinical practice in China. An alcoholic extract of the plant was found to contain daphnoretin, chrysophanol, myricitrime and rutin. The extract of W. indica displays antimicrobial and anti-inflammatory activities in vitro.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Malvales
Family	Thymelaeaceae
Genus	Wikstroemia
Species	indica

Major phytochemicals present in the plant are:

a. Naringin
b. Daidzein
c. Peonidin
d. Zingiberene

One of the major enzymes required for the survival of the organism causing COVID 19 is COVID-19 main protease (6M03) 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 COVID-19 main protease (6M03) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Naringin	-14.59	-19.64	Positive
Daidzein	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Zingiberene	-15.69	-18.11	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Naringin and Zingiberene helped deactivate the COVID-19 main protease (6M03) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Wickstroemia indica can prevent COVID 19 due to the presence of Naringin and Zingiberene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Zizyphus spira-christi against COVID 19 through deactivation of COVID-19 main protease (6M03)

Smrutirekha Sahoo[1], Pratibharani Deep[2]

[1]190705180047@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 Zizyphus spira-christi against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate COVID-19 main protease (6M03) enzyme. It was found that Eugenol and Zingiberene helped to prevent COVID 19.

Introduction: Zizyphus spira-christi is known for its medicinal activities. Fruits of Z. spina-christi is used as food. The wood is used as a source of fuel and it produces an excellent charcoal. Z. spina-christi fruits are eaten to treat diarrhoea and malaria and as an antispasmodic. The powder of the twigs is used externally to treat rheumatism and scorpion sting. Ash of wood mixed with vinegar is applied to heal snake bites and a tea made of fruit is used to treat measles. Fruits and crashed kernels are eaten to treat chest pains, respiratory problems and as a tonic.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Rosales
Family	Rhamnaceae
Genus	Ziziphus
Species	spina-christi

Major phytochemicals present in the plant are:

a. Eugenol
b. Daidzein
c. Peonidin
d. Zingiberene

One of the major enzymes required for the survival of the organism causing COVID 19 is COVID-19 main protease (6M03) 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 COVID-19 main protease (6M03) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Eugenol	-15.94	-21.94	Positive
Daidzein	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Zingiberene	-15.69	-18.11	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Eugenol and Zingiberene helped deactivate the COVID-19 main protease (6M03) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Zizyphus spira-christi can prevent COVID 19 due to the presence of Eugenol and Zingiberene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Alpinia officinarium against COVID 19 through deactivation of methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61)

Sweet Swapna Lenka[1], Pratibharani Deep[2]

[1]190705180048@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 Alpinia officinarium against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme. It was found that Phenyl isothiocyanate and Luteolin helped to prevent COVID 19.

Introduction: Alpinia officinarium is known for its medicinal activities. In Asia the rhizomes are ground to powder for use in curries, drinks, and jellies. In India an extract is used in perfumes. Alpinia officinarum contains high concentrations of the flavonol galangin. Historically, the rhizomes were reputed to have stimulant and digestive effects.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Zingiberales
Family	Zingiberaceae
Genus	Alpinia
Species	officinarum

Major phytochemicals present in the plant are:

a. Resveratrol
b. Phenyl isothiocyanate
c. Luteolin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) 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 methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Resveratrol	Not Applicable	Not Applicable	Failed
Phenyl isothiocyanate	-12.69	-15.91	Positive
Luteolin	-11.25	-18.61	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 Phenyl isothiocyanate and Luteolin helped deactivate the methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Alpinia officinarium can prevent COVID 19 due to the presence of Phenyl isothiocyanate and Luteolin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Andrographis paniculata against COVID 19 through deactivation of methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61)

Soumyasmruti Sahoo[1], Pratibharani Deep[2]

[1]190705180049@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 Andrographis paniculata against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme. It was found that Salicylic acid and Glutathione helped to prevent COVID 19.

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. Cryptoxanthin
b. Quercetin
c. Salicylic acid
d. Glutathione

One of the major enzymes required for the survival of the organism causing COVID 19 is methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) 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 methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Cryptoxanthin	Not Applicable	Not Applicable	Failed
Quercetin	-18.57	-19.91	Positive
Salicylic acid	Not Applicable	Not Applicable	Failed
Glutathione	-11.55	-19.69	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Salicylic acid and Glutathione helped deactivate the methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Andrographis paniculata can prevent COVID 19 due to the presence of Salicylic acid and Glutathione. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Avicennia marina against COVID 19 through deactivation of methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61)

Parichita Mahapatra[1], Pratibharani Deep[2]

[1]190705180050@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 Avicennia marina against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme. It was found that Salicylic acid helped to prevent COVID 19.

Introduction: Avicennia marina is known for its medicinal activities. White mangrove is used in traditional medicine as several medically active components are present in the plant including iridoid glucosides, flavonoids and naphthoquinone derivatives. They have strong antiproliferative and moderate cytotoxic activities as well as antibacterial effects. The resin from the bark is used to treat snake bites and to remove the placenta after childbirth. Leaf and bark decoctions are used as an anodyne and are applied externally against scabies. The wood ash has been used to treat skin complaints. Aqueous, ethanol and butanol crude extracts of the aerial parts of the plant were tested for antimicrobial activity.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Lamiales
Family	Acanthaceae
Genus	Avicennia
Species	marina

Major phytochemicals present in the plant are:

a. Tangeretin
b. Salicylic acid
c. Pelletierine
d. Digoxin

One of the major enzymes required for the survival of the organism causing COVID 19 is methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) 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 methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tangeretin	Not Applicable	Not Applicable	Failed
Salicylic acid	-18.57	-19.91	Positive
Pelletierine	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 Salicylic acid helped deactivate the methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Avicennia marina can prevent COVID 19 due to the presence of Salicylic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Barleria prionitis against COVID 19 through deactivation of methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61)

Punyasloka Mishra[1], Pratibharani Deep[2]

[1]190705180051@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 Barleria prionitis against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme. It was found that Benzyl isothiocyanate helped to prevent COVID 19.

Introduction: Barleria prionitis is known for its medicinal activities. It is used for various medicinal purposes in ayurvedic medicine. The juice of the leaves is applied to feet to prevent maceration and cracking in the monsoon season. Its leaves are known to contain 6-Hydroxyflavone, one of the chemical compounds that is a noncompetitive inhibitor of the protein cytochrome P450 2C9.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Lamiales
Family	Acanthaceae
Genus	Barleria
Species	prionitis

Major phytochemicals present in the plant are:

a. Rosmarinic acid
b. Daidzein
c. Benzyl isothiocyanate
d. Quercetin

One of the major enzymes required for the survival of the organism causing COVID 19 is methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) 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 methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Rosmarinic acid	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Failed
Benzyl isothiocyanate	-13.45	-15.64	Positive
Quercetin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Benzyl isothiocyanate helped deactivate the methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Barleria prionitis can prevent COVID 19 due to the presence of Benzyl isothiocyanate. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Berginia ligulata against COVID 19 through deactivation of methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61)

Sainivedita Rout[1], Pratibharani Deep[2]

[1]190705180052@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 Berginia ligulata against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme. It was found that Ferulic acid helped to prevent COVID 19.

Introduction: Berginia ligulata is known for its medicinal activities. Ligulata possesses cooling, laxative, analgesic, abortifacient, aphrodisiac properties and used in treatment of vesicular calculi, urinary discharges, excessive uterine haemorrhage, diseases of the bladder, dysentery, menorrhagia, splenic enlargement and heart diseases.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Saxifragales
Family	Saxifragaceae
Genus	Bergenia
Species	ligulata

Major phytochemicals present in the plant are:

a. Pelargonidin
b. Ferulic acid
c. Rutin
d. Epicatechin

One of the major enzymes required for the survival of the organism causing COVID 19 is methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) 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 methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelargonidin	Not Applicable	Not Applicable	Failed
Ferulic acid	-17.33	-22.34	Positive
Rutin	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 Ferulic acid helped deactivate the methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Berginia ligulata can prevent COVID 19 due to the presence of Ferulic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Caesalpinea sappan against COVID 19 through deactivation of methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61)

Rajib Lochan Kar[1], Pratibharani Deep[2]

[1]190705180053@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 Caesalpinea sappan against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme. It was found that Phenyl isothiocyanate helped to prevent COVID 19.

Introduction: Caesalpinea sappan is known for its medicinal activities. This plant has antibacterial and anticoagulant properties. Slivers of heartwood are used for making herbal drinking water in various regions, such as Kerala, Karnataka and Central Java, where it is usually mixed with ginger, cinnamon, and cloves. The heartwood also contains juglone (5-hydroxy-1,4-naphthoquinone), which has antimicrobial activity.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Fabales
Family	Fabaceae
Genus	Caesalpinia
Species	sappan

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Phenyl isothiocyanate
c. Digoxin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) 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 methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Phenyl isothiocyanate	-12.61	-15.84	Positive
Digoxin	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 Phenyl isothiocyanate helped deactivate the methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Caesalpinea sappan can prevent COVID 19 due to the presence of Phenyl isothiocyanate. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Curcuma longa against COVID 19 through deactivation of methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61)

Rudranarayan Sahoo[1], Pratibharani Deep[2]

[1]190705180054@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 Curcuma longa against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme. It was found that Pelletierine helped to prevent COVID 19.

Introduction: Curcuma longa is known for its medicinal activities. Turmeric is used widely as a spice in South Asian and Middle Eastern cooking. The golden yellow colour of turmeric is due to curcumin which contains an orange-coloured volatile oil. It is used to protect food products from sunlight. Curcumin reduces inflammation.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Zingiberales
Family	Zingiberaceae
Genus	Curcuma
Species	longa

Major phytochemicals present in the plant are:

a. Pelletierine
b. Isorhamnetin
c. Theobromine
d. Tannic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) 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 methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	-16.34	-22.39	Positive
Isorhamnetin	Not Applicable	Not Applicable	Failed
Theobromine	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 Pelletierine helped deactivate the methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Curcuma longa can prevent COVID 19 due to the presence of Pelletierine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Ephedra sinica against COVID 19 through deactivation of methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61)

Sadhana Shradhanjali Rout[1], Pratibharani Deep[2]

[1]190705180055@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 Ephedra sinica against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme. It was found that Theobromine helped to prevent COVID 19.

Introduction: Ephedra sinica is known for its medicinal activities. Ephedra is used for weight loss and obesity and to enhance athletic performance. It is also used for allergies and hay fever; nasal congestion; and respiratory tract conditions such as bronchospasm, asthma, and bronchitis. It is also used for colds, flu, swine flu, fever, chills, headache, inability to sweat, joint and bone pain, and as a "water pill" to increase urine flow in people who retain fluids.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Gnetophyta
Order	Ephedrales
Family	Ephedraceae
Genus	Ephedra
Species	E. sinica

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Theobromine
c. Apigenin
d. Rosmarinic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) 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 methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Theobromine	-12.65	-19.87	Positive
Apigenin	Not Applicable	Not Applicable	Failed
Rosmarinic acid	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 methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Ephedra sinica can prevent COVID 19 due to the presence of Theobromine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Gardenia sp. against COVID 19 through deactivation of methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61)

Snigdhanjali Das[1], Pratibharani Deep[2]

[1]190705180056@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 Gardenia sp. against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme. It was found that Genistein helped to prevent COVID 19.

Introduction: Gardenia sp. is known for its medicinal activities. Gardenia plants are known for its strong sweet scent of their flowers. Gardenia jasminoides (syn. G. grandiflora, G. Florida) is cultivated as a house plant. Its fruit is used as a yellow dye and used on fabric and food. Its fruits are also used in traditional Chinese medicine for their clearing, calming, and cooling properties.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Gentianales
Family	Rubiaceae
Genus	Gardenieae
Species	Gardenia

Major phytochemicals present in the plant are:

a. Pelargonidin
b. Genistein
c. Isorhamnetin
d. Daidzein

One of the major enzymes required for the survival of the organism causing COVID 19 is methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) 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 methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelargonidin	Not Applicable	Not Applicable	Failed
Genistein	-12.44	-17.64	Positive
Isorhamnetin	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Genistein helped deactivate the methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Gardenia sp. can prevent COVID 19 due to the presence of Genistein. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Glycyrrhiza glabra against COVID 19 through deactivation of methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61)

Siprarani Sahoo[1], Pradip Kumar Prusty[2]

[1]190705180057@cutm.ac.in

[2]pradip.prusty@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 COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme. It was found that Sulforaphane helped to prevent COVID 19.

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. Alliin
b. Isorhamnetin
c. Sulforaphane
d. Ascorbic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) 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 methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Alliin	Not Applicable	Not Applicable	Failed
Isorhamnetin	Not Applicable	Not Applicable	Failed
Sulforaphane	-19.61	-24.38	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 Sulforaphane helped deactivate the methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Glycyrrhiza glabra can prevent COVID 19 due to the presence of Sulforaphane. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Hottuynia cordata against COVID 19 through deactivation of methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61)

Snehashish Tripathy[1], Pradip Kumar Prusty[2]

[1]190705180058@cutm.ac.in

[2]pradip.prusty@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Hottuynia cordata against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme. It was found that Coumarin helped to prevent COVID 19.

Introduction: Hottuynia 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. Lupeol
b. Peonidin
c. Coumarin
d. Malvidin

One of the major enzymes required for the survival of the organism causing COVID 19 is methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) 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 methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lupeol	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Coumarin	-13.64	-19.31	Positive
Malvidin	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 methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Hottuynia cordata can prevent COVID 19 due to the presence of Coumarin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Punica granatum against COVID 19 through deactivation of methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61)

Laxmipriya Panda[1], Pradip Kumar Prusty[2]

[1]190705180059@cutm.ac.in

[2]pradip.prusty@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Punica granatum against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme. It was found that Campesterol helped to prevent COVID 19.

Introduction: Punica granatum is known for its medicinal activities. Pomegranate seeds are used as a spice known as anar dana. Pomegranate is used mainly for juice. Pomegranate syrup or molasses is used in muhammara, a roasted red pepper, walnut, and garlic. Grenadine syrup originally consisted of thickened and sweetened pomegranate juice mainly used in cocktail mixing.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Myrtales
Family	Lythraceae
Genus	Punica
Species	granatum

Major phytochemicals present in the plant are:

a. Campesterol
b. Malvidin
c. Myricetin
d. Pelargonidin

One of the major enzymes required for the survival of the organism causing COVID 19 is methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) 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 methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Campesterol	-17.58	-21.33	Positive
Malvidin	Not Applicable	Not Applicable	Failed
Myricetin	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 methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Punica granatum can prevent COVID 19 due to the presence of Campesterol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Wickstroemia indica against COVID 19 through deactivation of methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61)

Nikita Priyadarshini Dhall[1], Pradip Kumar Prusty[2]

[1]190705180060@cutm.ac.in

[2]pradip.prusty@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Wickstroemia indica against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme. It was found that Naringin helped to prevent COVID 19.

Introduction: Wickstroemia indica is known for its medicinal activities. It is used in traditional Chinese medicine. This plant has antipyretic, detoxicant, expectorant, vermifuge, and abortifacient properties used in clinical practice in China. An alcoholic extract of the plant was found to contain daphnoretin, chrysophanol, myricitrime and rutin. The extract of W. indica displays antimicrobial and anti-inflammatory activities in vitro.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Malvales
Family	Thymelaeaceae
Genus	Wikstroemia
Species	indica

Major phytochemicals present in the plant are:

a. Naringin
b. Daidzein
c. Peonidin
d. Zingiberene

One of the major enzymes required for the survival of the organism causing COVID 19 is methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) 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 methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Naringin	-14.59	-19.64	Positive
Daidzein	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Zingiberene	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 methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Wickstroemia indica can prevent COVID 19 due to the presence of Naringin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Zizyphus spira-christi against COVID 19 through deactivation of methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61)

Gurujyoti Rout[1], Pradip Kumar Prusty[2]

[1]190705180061@cutm.ac.in

[2]pradip.prusty@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Zizyphus spira-christi against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme. It was found that Eugenol helped to prevent COVID 19.

Introduction: Zizyphus spira-christi is known for its medicinal activities. Fruits of Z. spina-christi is used as food. The wood is used as a source of fuel and it produces an excellent charcoal. Z. spina-christi fruits are eaten to treat diarrhoea and malaria and as an antispasmodic. The powder of the twigs is used externally to treat rheumatism and scorpion sting. Ash of wood mixed with vinegar is applied to heal snake bites and a tea made of fruit is used to treat measles. Fruits and crashed kernels are eaten to treat chest pains, respiratory problems and as a tonic.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Rosales
Family	Rhamnaceae
Genus	Ziziphus
Species	spina-christi

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing COVID 19 is methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) 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 methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Eugenol	-15.84	-21.47	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 Eugenol helped deactivate the methyltransferase-stimulatory factor complex of NSP16 and NSP10 (6W61) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Zizyphus spira-christi can prevent COVID 19 due to the presence of Eugenol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Alpinia officinarium against COVID 19 through deactivation of NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW)

A S Ananya Das[1], Pradip Kumar Prusty[2]

[1]190705180062@cutm.ac.in

[2]pradip.prusty@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Alpinia officinarium against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme. It was found that Pheny isothiocyanate and Luteolin helped to prevent COVID 19.

Introduction: Alpinia officinarium is known for its medicinal activities. In Asia the rhizomes are ground to powder for use in curries, drinks, and jellies. In India an extract is used in perfumes. Alpinia officinarum contains high concentrations of the flavonol galangin. Historically, the rhizomes were reputed to have stimulant and digestive effects.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Zingiberales
Family	Zingiberaceae
Genus	Alpinia
Species	officinarum

Major phytochemicals present in the plant are:

a. Resveratrol
b. Phenyl isothiocyanate
c. Luteolin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) 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 NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Resveratrol	Not Applicable	Not Applicable	Failed
Phenyl isothiocyanate	-11.64	-17.94	Positive
Luteolin	-15.23	-19.28	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 Pheny isothiocyanate and Luteolin helped deactivate the NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Alpinia officinarium can prevent COVID 19 due to the presence of Pheny isothiocyanate and Luteolin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Andrographis paniculata against COVID 19 through deactivation of NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW)

Nitesh Kumar Meher[1], Pradip Kumar Prusty[2]

[1]190705180063@cutm.ac.in

[2]pradip.prusty@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 COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme. It was found that Quercetin and Glutathione helped to prevent COVID 19.

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. Cryptoxanthin
b. Quercetin
c. Salicylic acid
d. Glutathione

One of the major enzymes required for the survival of the organism causing COVID 19 is NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) 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 NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Cryptoxanthin	Not Applicable	Not Applicable	Failed
Quercetin	-11.92	-17.58	Positive
Salicylic acid	Not Applicable	Not Applicable	Failed
Glutathione	-15.64	-18.67	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Quercetin and Glutathione helped deactivate the NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Andrographis paniculata can prevent COVID 19 due to the presence of Quercetin and Glutathione. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Avicennia marina against COVID 19 through deactivation of NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW)

Amlan Mohanty[1], Pradip Kumar Prusty[2]

[1]190705180064@cutm.ac.in

[2]pradip.prusty@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Avicennia marina against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme. It was found that Salicylic acid helped to prevent COVID 19.

Introduction: Avicennia marina is known for its medicinal activities. White mangrove is used in traditional medicine as several medically active components are present in the plant including iridoid glucosides, flavonoids and naphthoquinone derivatives. They have strong antiproliferative and moderate cytotoxic activities as well as antibacterial effects. The resin from the bark is used to treat snake bites and to remove the placenta after childbirth. Leaf and bark decoctions are used as an anodyne and are applied externally against scabies. The wood ash has been used to treat skin complaints. Aqueous, ethanol and butanol crude extracts of the aerial parts of the plant were tested for antimicrobial activity.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Lamiales
Family	Acanthaceae
Genus	Avicennia
Species	marina

Major phytochemicals present in the plant are:

a. Tangeretin
b. Salicylic acid
c. Pelletierine
d. Digoxin

One of the major enzymes required for the survival of the organism causing COVID 19 is NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) 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 NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tangeretin	Not Applicable	Not Applicable	Failed
Salicylic acid	-17.94	-18.67	Positive
Pelletierine	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 Salicylic acid helped deactivate the NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Avicennia marina can prevent COVID 19 due to the presence of Salicylic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Barleria prionitis against COVID 19 through deactivation of NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW)

Swati Sucharita Panigrahi[1], Pradip Kumar Prusty[2]

[1]190705180065@cutm.ac.in

[2]pradip.prusty@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Barleria prionitis against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme. It was found that Rosmarinic acid helped to prevent COVID 19.

Introduction: Barleria prionitis is known for its medicinal activities. It is used for various medicinal purposes in ayurvedic medicine. The juice of the leaves is applied to feet to prevent maceration and cracking in the monsoon season. Its leaves are known to contain 6-Hydroxyflavone, one of the chemical compounds that is a noncompetitive inhibitor of the protein cytochrome P450 2C9.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Lamiales
Family	Acanthaceae
Genus	Barleria
Species	prionitis

Major phytochemicals present in the plant are:

a. Rosmarinic acid
b. Daidzein
c. Benzyl isothiocyanate
d. Quercetin

One of the major enzymes required for the survival of the organism causing COVID 19 is NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) 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 NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Rosmarinic acid	-10.94	-14.67	Positive
Daidzein	Not Applicable	Not Applicable	Failed
Benzyl isothiocyanate	-13.18	-19.67	Positive
Quercetin	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 NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Barleria prionitis can prevent COVID 19 due to the presence of Rosmarinic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Berginia ligulata against COVID 19 through deactivation of NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW)

Prasant Kumar Sahu[1], Pradip Kumar Prusty[2]

[1]190705180066@cutm.ac.in

[2]pradip.prusty@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Berginia ligulata against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme. It was found that Ferulic acid helped to prevent COVID 19.

Introduction: Berginia ligulata is known for its medicinal activities. Ligulata possesses cooling, laxative, analgesic, abortifacient, aphrodisiac properties and used in treatment of vesicular calculi, urinary discharges, excessive uterine haemorrhage, diseases of the bladder, dysentery, menorrhagia, splenic enlargement and heart diseases.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Saxifragales
Family	Saxifragaceae
Genus	Bergenia
Species	ligulata

Major phytochemicals present in the plant are:

a. Pelargonidin
b. Ferulic acid
c. Rutin
d. Epicatechin

One of the major enzymes required for the survival of the organism causing COVID 19 is NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) 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 NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelargonidin	Not Applicable	Not Applicable	Failed
Ferulic acid	-15.15	-19.67	Positive
Rutin	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 Ferulic acid helped deactivate the NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Berginia ligulata can prevent COVID 19 due to the presence of Ferulic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Caesalpinea sappan against COVID 19 through deactivation of NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW)

Janmajay Samal[1], Sunita Satapathy[2]

[1]190705180067@cutm.ac.in

[2]sunita.satapathy@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Caesalpinea sappan against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme. It was found that Phenyl isothiocyanate and Ferulic acid helped to prevent COVID 19.

Introduction: Caesalpinea sappan is known for its medicinal activities. This plant has antibacterial and anticoagulant properties. Slivers of heartwood are used for making herbal drinking water in various regions, such as Kerala, Karnataka and Central Java, where it is usually mixed with ginger, cinnamon, and cloves. The heartwood also contains juglone (5-hydroxy-1,4-naphthoquinone), which has antimicrobial activity.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Fabales
Family	Fabaceae
Genus	Caesalpinia
Species	sappan

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Phenyl isothiocyanate
c. Digoxin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) 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 NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Phenyl isothiocyanate	-11.94	-15.81	Positive
Digoxin	Not Applicable	Not Applicable	Failed
Ferulic acid	-15.15	-19.67	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Phenyl isothiocyanate and Ferulic acid helped deactivate the NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Caesalpinea sappan can prevent COVID 19 due to the presence of Phenyl isothiocyanate and Ferulic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Curcuma longa against COVID 19 through deactivation of NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW)

Sarmistha Pattnayak[1], Sunita Satapathy[2]

[1]190705180068@cutm.ac.in

[2]sunita.satapathy@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Curcuma longa against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme. It was found that Pelletierine helped to prevent COVID 19.

Introduction: Curcuma longa is known for its medicinal activities. Turmeric is used widely as a spice in South Asian and Middle Eastern cooking. The golden yellow colour of turmeric is due to curcumin which contains an orange-coloured volatile oil. It is used to protect food products from sunlight. Curcumin reduces inflammation.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Zingiberales
Family	Zingiberaceae
Genus	Curcuma
Species	longa

Major phytochemicals present in the plant are:

a. Pelletierine
b. Isorhamnetin
c. Theobromine
d. Tannic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) 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 NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	-12.67	-19.84	Positive
Isorhamnetin	Not Applicable	Not Applicable	Failed
Theobromine	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 Pelletierine helped deactivate the NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Curcuma longa can prevent COVID 19 due to the presence of Pelletierine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Punica granatum against COVID 19 through deactivation of NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW)

Radha Binodini Biswal[1], Sunita Satapathy[2]

[1]190705180069@cutm.ac.in

[2]sunita.satapathy@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Punica granatum against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme. It was found that Campesterol helped to prevent COVID 19.

Introduction: Punica granatum is known for its medicinal activities. Pomegranate seeds are used as a spice known as anar dana. Pomegranate is used mainly for juice. Pomegranate syrup or molasses is used in muhammara, a roasted red pepper, walnut, and garlic. Grenadine syrup originally consisted of thickened and sweetened pomegranate juice mainly used in cocktail mixing.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Myrtales
Family	Lythraceae
Genus	Punica
Species	granatum

Major phytochemicals present in the plant are:

a. Campesterol
b. Malvidin
c. Myricetin
d. Pelargonidin

One of the major enzymes required for the survival of the organism causing COVID 19 is NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) 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 NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Campesterol	-17.58	-21.33	Positive
Malvidin	Not Applicable	Not Applicable	Failed
Myricetin	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 NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Punica granatum can prevent COVID 19 due to the presence of Campesterol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Wickstroemia indica against COVID 19 through deactivation of NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW)

Pragyan Paramita Barik[1], Sunita Satapathy[2]

[1]190705180070@cutm.ac.in

[2]sunita.satapathy@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Wickstroemia indica against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme. It was found that Naringin helped to prevent COVID 19.

Introduction: Wickstroemia indica is known for its medicinal activities. It is used in traditional Chinese medicine. This plant has antipyretic, detoxicant, expectorant, vermifuge, and abortifacient properties used in clinical practice in China. An alcoholic extract of the plant was found to contain daphnoretin, chrysophanol, myricitrime and rutin. The extract of W. indica displays antimicrobial and anti-inflammatory activities in vitro.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Malvales
Family	Thymelaeaceae
Genus	Wikstroemia
Species	indica

Major phytochemicals present in the plant are:

a. Naringin
b. Daidzein
c. Peonidin
d. Zingiberene

One of the major enzymes required for the survival of the organism causing COVID 19 is NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) 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 NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Naringin	-14.59	-19.64	Positive
Daidzein	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Zingiberene	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 NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Wickstroemia indica can prevent COVID 19 due to the presence of Naringin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Zizyphus spira-christi against COVID 19 through deactivation of NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW)

Subhasmita Acharya[1], Sunita Satapathy[2]

[1]190705180071@cutm.ac.in

[2]sunita.satapathy@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Zizyphus spira-christi against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme. It was found that Eugenol and Quercetin helped to prevent COVID 19.

Introduction: Zizyphus spira-christi is known for its medicinal activities. Fruits of Z. spina-christi is used as food. The wood is used as a source of fuel and it produces an excellent charcoal. Z. spina-christi fruits are eaten to treat diarrhoea and malaria and as an antispasmodic. The powder of the twigs is used externally to treat rheumatism and scorpion sting. Ash of wood mixed with vinegar is applied to heal snake bites and a tea made of fruit is used to treat measles. Fruits and crashed kernels are eaten to treat chest pains, respiratory problems and as a tonic.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Rosales
Family	Rhamnaceae
Genus	Ziziphus
Species	spina-christi

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing COVID 19 is NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) 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 NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Eugenol	-15.94	-21.94	Positive
Daidzein	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Quercetin	-11.92	-17.58	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Eugenol and Quercetin helped deactivate the NSP15 Endo-ribonuclease from SARS CoV-2 (6VWW) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Zizyphus spira-christi can prevent COVID 19 due to the presence of Eugenol and Quercetin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Alpinia officinarium against COVID 19 through deactivation of Nsp9 RNA binding protein of SARS CoV-2 (6W4B)

Nabalipi Mohanta[1], Sunita Satapathy[2]

[1]190705180072@cutm.ac.in

[2]sunita.satapathy@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Alpinia officinarium against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme. It was found that Luteolin helped to prevent COVID 19.

Introduction: Alpinia officinarium is known for its medicinal activities. In Asia the rhizomes are ground to powder for use in curries, drinks, and jellies. In India an extract is used in perfumes. Alpinia officinarum contains high concentrations of the flavonol galangin. Historically, the rhizomes were reputed to have stimulant and digestive effects.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Zingiberales
Family	Zingiberaceae
Genus	Alpinia
Species	officinarum

Major phytochemicals present in the plant are:

a. Resveratrol
b. Phenyl isothiocyanate
c. Luteolin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is Nsp9 RNA binding protein of SARS CoV-2 (6W4B) 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 Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Resveratrol	Not Applicable	Not Applicable	Failed
Phenyl isothiocyanate	Not Applicable	Not Applicable	Failed
Luteolin	-11.22	-17.84	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 Luteolin helped deactivate the Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Alpinia officinarium can prevent COVID 19 due to the presence of Luteolin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Avicennia marina against COVID 19 through deactivation of Nsp9 RNA binding protein of SARS CoV-2 (6W4B)

Pravas Pattnayak[1], Sunita Satapathy[2]

[1]190705180073@cutm.ac.in

[2]sunita.satapathy@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Avicennia marina against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme. It was found that Salicylic acid helped to prevent COVID 19.

Introduction: Avicennia marina is known for its medicinal activities. White mangrove is used in traditional medicine as several medically active components are present in the plant including iridoid glucosides, flavonoids and naphthoquinone derivatives. They have strong antiproliferative and moderate cytotoxic activities as well as antibacterial effects. The resin from the bark is used to treat snake bites and to remove the placenta after childbirth. Leaf and bark decoctions are used as an anodyne and are applied externally against scabies. The wood ash has been used to treat skin complaints. Aqueous, ethanol and butanol crude extracts of the aerial parts of the plant were tested for antimicrobial activity.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Lamiales
Family	Acanthaceae
Genus	Avicennia
Species	marina

Major phytochemicals present in the plant are:

a. Tangeretin
b. Salicylic acid
c. Pelletierine
d. Digoxin

One of the major enzymes required for the survival of the organism causing COVID 19 is Nsp9 RNA binding protein of SARS CoV-2 (6W4B) 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 Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tangeretin	Not Applicable	Not Applicable	Failed
Salicylic acid	-17.67	-23.61	Positive
Pelletierine	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 Salicylic acid helped deactivate the Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Avicennia marina can prevent COVID 19 due to the presence of Salicylic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Barleria prionitis against COVID 19 through deactivation of Nsp9 RNA binding protein of SARS CoV-2 (6W4B)

Sucharita Nayak[1], Sunita Satapathy[2]

[1]190705180074@cutm.ac.in

[2]sunita.satapathy@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Barleria prionitis against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme. It was found that Benzyl isothiocyanate helped to prevent COVID 19.

Introduction: Barleria prionitis is known for its medicinal activities. It is used for various medicinal purposes in ayurvedic medicine. The juice of the leaves is applied to feet to prevent maceration and cracking in the monsoon season. Its leaves are known to contain 6-Hydroxyflavone, one of the chemical compounds that is a noncompetitive inhibitor of the protein cytochrome P450 2C9.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Lamiales
Family	Acanthaceae
Genus	Barleria
Species	prionitis

Major phytochemicals present in the plant are:

a. Rosmarinic acid
b. Daidzein
c. Benzyl isothiocyanate
d. Quercetin

One of the major enzymes required for the survival of the organism causing COVID 19 is Nsp9 RNA binding protein of SARS CoV-2 (6W4B) 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 Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Rosmarinic acid	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Failed
Benzyl isothiocyanate	-14.55	-18.67	Positive
Quercetin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Benzyl isothiocyanate helped deactivate the Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Barleria prionitis can prevent COVID 19 due to the presence of Benzyl isothiocyanate. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Berginia ligulata against COVID 19 through deactivation of Nsp9 RNA binding protein of SARS CoV-2 (6W4B)

Aparna Rani Behera[1], Sunita Satapathy[2]

[1]190705180075@cutm.ac.in

[2]sunita.satapathy@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Berginia ligulata against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme. It was found that Ferulic acid helped to prevent COVID 19.

Introduction: Berginia ligulata is known for its medicinal activities. Ligulata possesses cooling, laxative, analgesic, abortifacient, aphrodisiac properties and used in treatment of vesicular calculi, urinary discharges, excessive uterine haemorrhage, diseases of the bladder, dysentery, menorrhagia, splenic enlargement and heart diseases.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Saxifragales
Family	Saxifragaceae
Genus	Bergenia
Species	ligulata

Major phytochemicals present in the plant are:

a. Pelargonidin
b. Ferulic acid
c. Rutin
d. Epicatechin

One of the major enzymes required for the survival of the organism causing COVID 19 is Nsp9 RNA binding protein of SARS CoV-2 (6W4B) 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 Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelargonidin	Not Applicable	Not Applicable	Failed
Ferulic acid	-15.69	-24.61	Positive
Rutin	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 Ferulic acid helped deactivate the Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Berginia ligulata can prevent COVID 19 due to the presence of Ferulic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Caesalpinea sappan against COVID 19 through deactivation of Nsp9 RNA binding protein of SARS CoV-2 (6W4B)

Ipsita Nayak[1], Sunita Satapathy[2]

[1]190705180076@cutm.ac.in

[2]sunita.satapathy@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Caesalpinea sappan against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme. It was found that Phenyl isothiocyanate helped to prevent COVID 19.

Introduction: Caesalpinea sappan is known for its medicinal activities. This plant has antibacterial and anticoagulant properties. Slivers of heartwood are used for making herbal drinking water in various regions, such as Kerala, Karnataka and Central Java, where it is usually mixed with ginger, cinnamon, and cloves. The heartwood also contains juglone (5-hydroxy-1,4-naphthoquinone), which has antimicrobial activity.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Fabales
Family	Fabaceae
Genus	Caesalpinia
Species	sappan

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Phenyl isothiocyanate
c. Digoxin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is Nsp9 RNA binding protein of SARS CoV-2 (6W4B) 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 Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Phenyl isothiocyanate	-14.22	-16.34	Positive
Digoxin	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 Phenyl isothiocyanate helped deactivate the Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Caesalpinea sappan can prevent COVID 19 due to the presence of Phenyl isothiocyanate. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Curcuma longa against COVID 19 through deactivation of Nsp9 RNA binding protein of SARS CoV-2 (6W4B)

Bhagyashree Das[1], Yashaswi Nayak[2]

[1]190705180077@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 Curcuma longa against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme. It was found that Pelletierine helped to prevent COVID 19.

Introduction: Curcuma longa is known for its medicinal activities. Turmeric is used widely as a spice in South Asian and Middle Eastern cooking. The golden yellow colour of turmeric is due to curcumin which contains an orange-coloured volatile oil. It is used to protect food products from sunlight. Curcumin reduces inflammation.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Zingiberales
Family	Zingiberaceae
Genus	Curcuma
Species	longa

Major phytochemicals present in the plant are:

a. Pelletierine
b. Isorhamnetin
c. Theobromine
d. Tannic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is Nsp9 RNA binding protein of SARS CoV-2 (6W4B) 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 Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	-15.45	-19.94	Positive
Isorhamnetin	Not Applicable	Not Applicable	Failed
Theobromine	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 Pelletierine helped deactivate the Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Curcuma longa can prevent COVID 19 due to the presence of Pelletierine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Punica granatum against COVID 19 through deactivation of Nsp9 RNA binding protein of SARS CoV-2 (6W4B)

Debasmita Paul[1], Yashaswi Nayak[2]

[1]190705180079@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 Punica granatum against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme. It was found that Campesterol helped to prevent COVID 19.

Introduction: Punica granatum is known for its medicinal activities. Pomegranate seeds are used as a spice known as anar dana. Pomegranate is used mainly for juice. Pomegranate syrup or molasses is used in muhammara, a roasted red pepper, walnut, and garlic. Grenadine syrup originally consisted of thickened and sweetened pomegranate juice mainly used in cocktail mixing.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Myrtales
Family	Lythraceae
Genus	Punica
Species	granatum

Major phytochemicals present in the plant are:

a. Campesterol
b. Malvidin
c. Myricetin
d. Pelargonidin

One of the major enzymes required for the survival of the organism causing COVID 19 is Nsp9 RNA binding protein of SARS CoV-2 (6W4B) 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 Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Campesterol	-17.58	-21.33	Positive
Malvidin	Not Applicable	Not Applicable	Failed
Myricetin	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 Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Punica granatum can prevent COVID 19 due to the presence of Campesterol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Wickstroemia indica against COVID 19 through deactivation of Nsp9 RNA binding protein of SARS CoV-2 (6W4B)

Nupur Panigrahi[1], Yashaswi Nayak[2]

[1]190705180080@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 Wickstroemia indica against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme. It was found that Naringin helped to prevent COVID 19.

Introduction: Wickstroemia indica is known for its medicinal activities. It is used in traditional Chinese medicine. This plant has antipyretic, detoxicant, expectorant, vermifuge, and abortifacient properties used in clinical practice in China. An alcoholic extract of the plant was found to contain daphnoretin, chrysophanol, myricitrime and rutin. The extract of W. indica displays antimicrobial and anti-inflammatory activities in vitro.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Malvales
Family	Thymelaeaceae
Genus	Wikstroemia
Species	indica

Major phytochemicals present in the plant are:

a. Naringin
b. Daidzein
c. Peonidin
d. Zingiberene

One of the major enzymes required for the survival of the organism causing COVID 19 is Nsp9 RNA binding protein of SARS CoV-2 (6W4B) 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 Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Naringin	-14.59	-19.64	Positive
Daidzein	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Zingiberene	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 Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Wickstroemia indica can prevent COVID 19 due to the presence of Naringin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Zizyphus spira-christi against COVID 19 through deactivation of Nsp9 RNA binding protein of SARS CoV-2 (6W4B)

Sunita Sahoo[1], Yashaswi Nayak[2]

[1]190705180081@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 Zizyphus spira-christi against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme. It was found that Peonidin helped to prevent COVID 19.

Introduction: Zizyphus spira-christi is known for its medicinal activities. Fruits of Z. spina-christi is used as food. The wood is used as a source of fuel and it produces an excellent charcoal. Z. spina-christi fruits are eaten to treat diarrhoea and malaria and as an antispasmodic. The powder of the twigs is used externally to treat rheumatism and scorpion sting. Ash of wood mixed with vinegar is applied to heal snake bites and a tea made of fruit is used to treat measles. Fruits and crashed kernels are eaten to treat chest pains, respiratory problems and as a tonic.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Rosales
Family	Rhamnaceae
Genus	Ziziphus
Species	spina-christi

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing COVID 19 is Nsp9 RNA binding protein of SARS CoV-2 (6W4B) 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 Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Eugenol	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Failed
Peonidin	-15.94	-21.94	Positive
Quercetin	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 Nsp9 RNA binding protein of SARS CoV-2 (6W4B) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Zizyphus spira-christi can prevent COVID 19 due to the presence of Peonidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Alpinia officinarium against COVID 19 through deactivation of papain-like protease of SARS CoV-2 (6W9C)

Soumyashri Das[1], Yashaswi Nayak[2]

[1]190705180082@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 Alpinia officinarium against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate papain-like protease of SARS CoV-2 (6W9C) enzyme. It was found that Luteolin helped to prevent COVID 19.

Introduction: Alpinia officinarium is known for its medicinal activities. In Asia the rhizomes are ground to powder for use in curries, drinks, and jellies. In India an extract is used in perfumes. Alpinia officinarum contains high concentrations of the flavonol galangin. Historically, the rhizomes were reputed to have stimulant and digestive effects.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Zingiberales
Family	Zingiberaceae
Genus	Alpinia
Species	officinarum

Major phytochemicals present in the plant are:

a. Resveratrol
b. Phenyl isothiocyanate
c. Luteolin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is papain-like protease of SARS CoV-2 (6W9C) 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 papain-like protease of SARS CoV-2 (6W9C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Resveratrol	Not Applicable	Not Applicable	Failed
Phenyl isothiocyanate	Not Applicable	Not Applicable	Failed
Luteolin	-13.67	-19.84	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 Luteolin helped deactivate the papain-like protease of SARS CoV-2 (6W9C) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Alpinia officinarium can prevent COVID 19 due to the presence of Luteolin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Andrographis paniculata against COVID 19 through deactivation of papain-like protease of SARS CoV-2 (6W9C)

Pragnya Pradeepta Mohapatra[1], Yashaswi Nayak[2]

[1]190705180083@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 Andrographis paniculata against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate papain-like protease of SARS CoV-2 (6W9C) enzyme. It was found that Quercetin helped to prevent COVID 19.

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. Cryptoxanthin
b. Quercetin
c. Salicylic acid
d. Glutathione

One of the major enzymes required for the survival of the organism causing COVID 19 is papain-like protease of SARS CoV-2 (6W9C) 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 papain-like protease of SARS CoV-2 (6W9C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Cryptoxanthin	Not Applicable	Not Applicable	Failed
Quercetin	-12.34	-19.61	Positive
Salicylic acid	Not Applicable	Not Applicable	Failed
Glutathione	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Quercetin helped deactivate the papain-like protease of SARS CoV-2 (6W9C) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Andrographis paniculata can prevent COVID 19 due to the presence of Quercetin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Gardenia sp. against COVID 19 through deactivation of papain-like protease of SARS CoV-2 (6W9C)

Arpita Subhadarshini[1], Yashaswi Nayak[2]

[1]190705180084@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 Gardenia sp. against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate papain-like protease of SARS CoV-2 (6W9C) enzyme. It was found that Genistein and Quercetin helped to prevent COVID 19.

Introduction: Gardenia sp. is known for its medicinal activities. Gardenia plants are known for its strong sweet scent of their flowers. Gardenia jasminoides (syn. G. grandiflora, G. Florida) is cultivated as a house plant. Its fruit is used as a yellow dye and used on fabric and food. Its fruits are also used in traditional Chinese medicine for their clearing, calming, and cooling properties.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Gentianales
Family	Rubiaceae
Genus	Gardenieae
Species	Gardenia

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing COVID 19 is papain-like protease of SARS CoV-2 (6W9C) 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 papain-like protease of SARS CoV-2 (6W9C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelargonidin	Not Applicable	Not Applicable	Failed
Genistein	-12.31	-15.48	Positive
Quercetin	-12.34	-19.61	Positive
Daidzein	Not Applicable	Not Applicable	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Genistein and Quercetin helped deactivate the papain-like protease of SARS CoV-2 (6W9C) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Gardenia sp. can prevent COVID 19 due to the presence of Genistein and Quercetin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Glycyrrhiza glabra against COVID 19 through deactivation of papain-like protease of SARS CoV-2 (6W9C)

Arpita Mohapatra[1], Yashaswi Nayak[2]

[1]190705180085@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 Glycyrrhiza glabra against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate papain-like protease of SARS CoV-2 (6W9C) enzyme. It was found that Sulforaphane helped to prevent COVID 19.

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. Alliin
b. Isorhamnetin
c. Sulforaphane
d. Ascorbic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is papain-like protease of SARS CoV-2 (6W9C) 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 papain-like protease of SARS CoV-2 (6W9C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Alliin	Not Applicable	Not Applicable	Failed
Isorhamnetin	Not Applicable	Not Applicable	Failed
Sulforaphane	-18.26	-19.91	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 Sulforaphane helped deactivate the papain-like protease of SARS CoV-2 (6W9C) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Glycyrrhiza glabra can prevent COVID 19 due to the presence of Sulforaphane. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Hottuynia cordata against COVID 19 through deactivation of papain-like protease of SARS CoV-2 (6W9C)

Aditya Narayan Barik[1], Yashaswi Nayak[2]

[1]190705180086@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 Hottuynia cordata against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate papain-like protease of SARS CoV-2 (6W9C) enzyme. It was found that Coumarin helped to prevent COVID 19.

Introduction: Hottuynia 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. Lupeol
b. Peonidin
c. Coumarin
d. Malvidin

One of the major enzymes required for the survival of the organism causing COVID 19 is papain-like protease of SARS CoV-2 (6W9C) 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 papain-like protease of SARS CoV-2 (6W9C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lupeol	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Coumarin	-12.74	-14.61	Positive
Malvidin	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 papain-like protease of SARS CoV-2 (6W9C) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Hottuynia cordata can prevent COVID 19 due to the presence of Coumarin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Neerium indicum against COVID 19 through deactivation of papain-like protease of SARS CoV-2 (6W9C)

Subhasmita Sabata[1], Yashaswi Nayak[2]

[1]190705180087@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 Neerium indicum against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate papain-like protease of SARS CoV-2 (6W9C) enzyme. It was found that = helped to prevent COVID 19.

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. Theobromine
b. Daidzein
c. Caffeine
d. Limonene

One of the major enzymes required for the survival of the organism causing COVID 19 is papain-like protease of SARS CoV-2 (6W9C) 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 papain-like protease of SARS CoV-2 (6W9C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Failed
Caffeine	-14.21	-18.92	Positive
Limonene	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that = helped deactivate the papain-like protease of SARS CoV-2 (6W9C) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Neerium indicum can prevent COVID 19 due to the presence of =. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Nigelia sativa against COVID 19 through deactivation of papain-like protease of SARS CoV-2 (6W9C)

Niharika Sahu[1], Yashaswi Nayak[2]

[1]190705180088@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 Nigelia sativa against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate papain-like protease of SARS CoV-2 (6W9C) enzyme. It was found that Kaempferol helped to prevent COVID 19.

Introduction: Nigelia sativa is known for its medicinal activities. Nigella sativa is used as a spice, natural seasoning, or flavoring. The seeds of N. sativa are used as a spice in many cuisines. They can be used as a seasoning in recipes with pod fruit, vegetables, salads, and poultry. The black seeds are used to flavour bread products, and are used as part of the spice mixture. Nigella is also used in tresse cheese, a braided string cheese called majdouleh or majdouli in the Middle East.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Ranunculales
Family	Ranunculaceae
Genus	Nigella
Species	sativa

Major phytochemicals present in the plant are:

a. Theobromine
b. Kaempferol
c. Limonene
d. Malvidin

One of the major enzymes required for the survival of the organism causing COVID 19 is papain-like protease of SARS CoV-2 (6W9C) 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 papain-like protease of SARS CoV-2 (6W9C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	Not Applicable	Not Applicable	Failed
Kaempferol	-12.64	-19.67	Positive
Limonene	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 Kaempferol helped deactivate the papain-like protease of SARS CoV-2 (6W9C) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Nigelia sativa can prevent COVID 19 due to the presence of Kaempferol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Pandanus amaryllifoius against COVID 19 through deactivation of papain-like protease of SARS CoV-2 (6W9C)

Amrutapratiksha Padhihary[1], Pradip Kumar Prusty[2]

[1]190705180089@cutm.ac.in

[2]pradip.prusty@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Pandanus amaryllifoius against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate papain-like protease of SARS CoV-2 (6W9C) enzyme. It was found that Lutein helped to prevent COVID 19.

Introduction: Pandanus amaryllifoius is known for its medicinal activities. The leaves are used in the perfume industry and traditional medicine. P. amaryllifolius essence may substitute for vanilla essence. The leaves possess a pleasant aroma and can be used as natural air fresheners. The green juice acquired from its leaf is used extensively in Indonesian cuisine as green food colouring and flavouring agents that gave pleasant aroma for kue, a tapioca, flour or glutinous rice-based traditional cakes.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Pandanales
Family	Pandanaceae
Genus	Pandanus
Species	amaryllifolius

Major phytochemicals present in the plant are:

a. Lutein
b. Genistein
c. Gallic acid
d. Theobromine

One of the major enzymes required for the survival of the organism causing COVID 19 is papain-like protease of SARS CoV-2 (6W9C) 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 papain-like protease of SARS CoV-2 (6W9C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lutein	-12.67	-18.04	Positive
Genistein	Not Applicable	Not Applicable	Failed
Gallic 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 helped deactivate the papain-like protease of SARS CoV-2 (6W9C) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Pandanus amaryllifoius can prevent COVID 19 due to the presence of Lutein. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Phyllanthus amarus against COVID 19 through deactivation of papain-like protease of SARS CoV-2 (6W9C)

Pralaya Kumar Khuntia[1], Pradip Kumar Prusty[2]

[1]190705180090@cutm.ac.in

[2]pradip.prusty@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Phyllanthus amarus against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate papain-like protease of SARS CoV-2 (6W9C) enzyme. It was found that Ellagic acid helped to prevent COVID 19.

Introduction: Phyllanthus amarus is known for its medicinal activities. P.amarus is an important plant of Indian Ayurvedic system of medicine which is used in the problems of stomach, genitourinary system, liver, kidney and spleen. It is bitter, astringent, stomachic, diuretic, febrifuge and antiseptic. The whole plant is used in gonorrhea, menorrhagia and other genital affections.

The plant is classified as follows:

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

Major phytochemicals present in the plant are:

a. Pelletierine
b. Daidzein
c. Ellagic acid
d. Campesterol

One of the major enzymes required for the survival of the organism causing COVID 19 is papain-like protease of SARS CoV-2 (6W9C) 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 papain-like protease of SARS CoV-2 (6W9C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Failed
Ellagic acid	-12.44	-19.64	Positive
Campesterol	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 papain-like protease of SARS CoV-2 (6W9C) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Phyllanthus amarus can prevent COVID 19 due to the presence of Ellagic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Punica granatum against COVID 19 through deactivation of papain-like protease of SARS CoV-2 (6W9C)

Sushree Subhadarshani Barik[1], Pradip Kumar Prusty[2]

[1]190705180091@cutm.ac.in

[2]pradip.prusty@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Punica granatum against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate papain-like protease of SARS CoV-2 (6W9C) enzyme. It was found that Myricetin helped to prevent COVID 19.

Introduction: Punica granatum is known for its medicinal activities. Pomegranate seeds are used as a spice known as anar dana. Pomegranate is used mainly for juice. Pomegranate syrup or molasses is used in muhammara, a roasted red pepper, walnut, and garlic. Grenadine syrup originally consisted of thickened and sweetened pomegranate juice mainly used in cocktail mixing.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Myrtales
Family	Lythraceae
Genus	Punica
Species	granatum

Major phytochemicals present in the plant are:

a. Campesterol
b. Malvidin
c. Myricetin
d. Pelargonidin

One of the major enzymes required for the survival of the organism causing COVID 19 is papain-like protease of SARS CoV-2 (6W9C) 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 papain-like protease of SARS CoV-2 (6W9C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Campesterol	Not Applicable	Not Applicable	Failed
Malvidin	Not Applicable	Not Applicable	Failed
Myricetin	-17.58	-21.33	Positive
Pelargonidin	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 papain-like protease of SARS CoV-2 (6W9C) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Punica granatum can prevent COVID 19 due to the presence of Myricetin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Wickstroemia indica against COVID 19 through deactivation of papain-like protease of SARS CoV-2 (6W9C)

Sushree Samparna Pattanayak[1], Pradip Kumar Prusty[2]

[1]190705180092@cutm.ac.in

[2]pradip.prusty@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Wickstroemia indica against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate papain-like protease of SARS CoV-2 (6W9C) enzyme. It was found that Zingiberene helped to prevent COVID 19.

Introduction: Wickstroemia indica is known for its medicinal activities. It is used in traditional Chinese medicine. This plant has antipyretic, detoxicant, expectorant, vermifuge, and abortifacient properties used in clinical practice in China. An alcoholic extract of the plant was found to contain daphnoretin, chrysophanol, myricitrime and rutin. The extract of W. indica displays antimicrobial and anti-inflammatory activities in vitro.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Malvales
Family	Thymelaeaceae
Genus	Wikstroemia
Species	indica

Major phytochemicals present in the plant are:

a. Naringin
b. Daidzein
c. Peonidin
d. Zingiberene

One of the major enzymes required for the survival of the organism causing COVID 19 is papain-like protease of SARS CoV-2 (6W9C) 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 papain-like protease of SARS CoV-2 (6W9C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Naringin	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Zingiberene	-15.69	-18.11	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Zingiberene helped deactivate the papain-like protease of SARS CoV-2 (6W9C) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Wickstroemia indica can prevent COVID 19 due to the presence of Zingiberene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Zizyphus spira-christi against COVID 19 through deactivation of papain-like protease of SARS CoV-2 (6W9C)

Smrutisudha Meher[1], Sitaram Swain[2]

[1]190705180093@cutm.ac.in

[2]Sitaram.swain@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Zizyphus spira-christi against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate papain-like protease of SARS CoV-2 (6W9C) enzyme. It was found that Eugenol and Daidzein helped to prevent COVID 19.

Introduction: Zizyphus spira-christi is known for its medicinal activities. Fruits of Z. spina-christi is used as food. The wood is used as a source of fuel and it produces an excellent charcoal. Z. spina-christi fruits are eaten to treat diarrhoea and malaria and as an antispasmodic. The powder of the twigs is used externally to treat rheumatism and scorpion sting. Ash of wood mixed with vinegar is applied to heal snake bites and a tea made of fruit is used to treat measles. Fruits and crashed kernels are eaten to treat chest pains, respiratory problems and as a tonic.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Rosales
Family	Rhamnaceae
Genus	Ziziphus
Species	spina-christi

Major phytochemicals present in the plant are:

a. Eugenol
b. Daidzein
c. Peonidin
d. Naringin

One of the major enzymes required for the survival of the organism causing COVID 19 is papain-like protease of SARS CoV-2 (6W9C) 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 papain-like protease of SARS CoV-2 (6W9C) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Eugenol	-15.94	-21.94	Positive
Daidzein	-12.64	-22.48	Positive
Peonidin	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 Eugenol and Daidzein helped deactivate the papain-like protease of SARS CoV-2 (6W9C) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Zizyphus spira-christi can prevent COVID 19 due to the presence of Eugenol and Daidzein. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Alpinia officinarium against COVID 19 through deactivation of RNA-dependednt RNA polymerase of COVID-19 (6VYO)

Shreyashi Rath[1], Sitaram Swain[2]

[1]190705180094@cutm.ac.in

[2]Sitaram.swain@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Alpinia officinarium against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme. It was found that Resveratrol and Luteolin helped to prevent COVID 19.

Introduction: Alpinia officinarium is known for its medicinal activities. In Asia the rhizomes are ground to powder for use in curries, drinks, and jellies. In India an extract is used in perfumes. Alpinia officinarum contains high concentrations of the flavonol galangin. Historically, the rhizomes were reputed to have stimulant and digestive effects.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Zingiberales
Family	Zingiberaceae
Genus	Alpinia
Species	officinarum

Major phytochemicals present in the plant are:

a. Resveratrol
b. Phenyl isothiocyanate
c. Luteolin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is RNA-dependednt RNA polymerase of COVID-19 (6VYO) 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 RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Resveratrol	-12.48	-15.68	Positive
Phenyl isothiocyanate	Not Applicable	Not Applicable	Failed
Luteolin	-11.33	-18.37	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 Resveratrol and Luteolin helped deactivate the RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Alpinia officinarium can prevent COVID 19 due to the presence of Resveratrol and Luteolin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Andrographis paniculata against COVID 19 through deactivation of RNA-dependednt RNA polymerase of COVID-19 (6VYO)

Nitish Saxena[1], Sitaram Swain[2]

[1]190705180095@cutm.ac.in

[2]Sitaram.swain@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 COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme. It was found that Quercetin helped to prevent COVID 19.

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. Cryptoxanthin
b. Quercetin
c. Salicylic acid
d. Glutathione

One of the major enzymes required for the survival of the organism causing COVID 19 is RNA-dependednt RNA polymerase of COVID-19 (6VYO) 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 RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Cryptoxanthin	Not Applicable	Not Applicable	Failed
Quercetin	-12.42	-19.61	Positive
Salicylic acid	Not Applicable	Not Applicable	Failed
Glutathione	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Quercetin helped deactivate the RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Andrographis paniculata can prevent COVID 19 due to the presence of Quercetin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Avicennia marina against COVID 19 through deactivation of RNA-dependednt RNA polymerase of COVID-19 (6VYO)

Barsha Kanungo[1], Sagarika Parida[2]

[1]190705180096@cutm.ac.in

[2]sagarika.parida@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Avicennia marina against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme. It was found that Salicylic acid helped to prevent COVID 19.

Introduction: Avicennia marina is known for its medicinal activities. White mangrove is used in traditional medicine as several medically active components are present in the plant including iridoid glucosides, flavonoids and naphthoquinone derivatives. They have strong antiproliferative and moderate cytotoxic activities as well as antibacterial effects. The resin from the bark is used to treat snake bites and to remove the placenta after childbirth. Leaf and bark decoctions are used as an anodyne and are applied externally against scabies. The wood ash has been used to treat skin complaints. Aqueous, ethanol and butanol crude extracts of the aerial parts of the plant were tested for antimicrobial activity.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Lamiales
Family	Acanthaceae
Genus	Avicennia
Species	marina

Major phytochemicals present in the plant are:

a. Tangeretin
b. Salicylic acid
c. Pelletierine
d. Digoxin

One of the major enzymes required for the survival of the organism causing COVID 19 is RNA-dependednt RNA polymerase of COVID-19 (6VYO) 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 RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tangeretin	Not Applicable	Not Applicable	Failed
Salicylic acid	-15.33	-22.64	Positive
Pelletierine	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 Salicylic acid helped deactivate the RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Avicennia marina can prevent COVID 19 due to the presence of Salicylic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Barleria prionitis against COVID 19 through deactivation of RNA-dependednt RNA polymerase of COVID-19 (6VYO)

Swayanglaxmi Mohapatra[1], Sagarika Parida[2]

[1]190705180097@cutm.ac.in

[2]sagarika.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 prionitis against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme. It was found that Rosmarinic acid helped to prevent COVID 19.

Introduction: Barleria prionitis is known for its medicinal activities. It is used for various medicinal purposes in ayurvedic medicine. The juice of the leaves is applied to feet to prevent maceration and cracking in the monsoon season. Its leaves are known to contain 6-Hydroxyflavone, one of the chemical compounds that is a noncompetitive inhibitor of the protein cytochrome P450 2C9.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Lamiales
Family	Acanthaceae
Genus	Barleria
Species	prionitis

Major phytochemicals present in the plant are:

a. Rosmarinic acid
b. Daidzein
c. Benzyl isothiocyanate
d. Quercetin

One of the major enzymes required for the survival of the organism causing COVID 19 is RNA-dependednt RNA polymerase of COVID-19 (6VYO) 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 RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Rosmarinic acid	-12.62	-18.67	Positive
Daidzein	Not Applicable	Not Applicable	Failed
Benzyl isothiocyanate	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 Rosmarinic acid helped deactivate the RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Barleria prionitis can prevent COVID 19 due to the presence of Rosmarinic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Berginia ligulata against COVID 19 through deactivation of RNA-dependednt RNA polymerase of COVID-19 (6VYO)

Deepak Kumar Mallick[1], Sagarika Parida[2]

[1]190705180098@cutm.ac.in

[2]sagarika.parida@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Berginia ligulata against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme. It was found that Ferulic acid helped to prevent COVID 19.

Introduction: Berginia ligulata is known for its medicinal activities. Ligulata possesses cooling, laxative, analgesic, abortifacient, aphrodisiac properties and used in treatment of vesicular calculi, urinary discharges, excessive uterine haemorrhage, diseases of the bladder, dysentery, menorrhagia, splenic enlargement and heart diseases.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Saxifragales
Family	Saxifragaceae
Genus	Bergenia
Species	ligulata

Major phytochemicals present in the plant are:

a. Pelargonidin
b. Ferulic acid
c. Rutin
d. Epicatechin

One of the major enzymes required for the survival of the organism causing COVID 19 is RNA-dependednt RNA polymerase of COVID-19 (6VYO) 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 RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelargonidin	Not Applicable	Not Applicable	Failed
Ferulic acid	-14.61	-17.91	Positive
Rutin	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 Ferulic acid helped deactivate the RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Berginia ligulata can prevent COVID 19 due to the presence of Ferulic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Caesalpinea sappan against COVID 19 through deactivation of RNA-dependednt RNA polymerase of COVID-19 (6VYO)

Suvam Kanungo[1], Yashaswi Nayak[2]

[1]190705180099@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 Caesalpinea sappan against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme. It was found that Sulforaphane helped to prevent COVID 19.

Introduction: Caesalpinea sappan is known for its medicinal activities. This plant has antibacterial and anticoagulant properties. Slivers of heartwood are used for making herbal drinking water in various regions, such as Kerala, Karnataka and Central Java, where it is usually mixed with ginger, cinnamon, and cloves. The heartwood also contains juglone (5-hydroxy-1,4-naphthoquinone), which has antimicrobial activity.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Fabales
Family	Fabaceae
Genus	Caesalpinia
Species	sappan

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Phenyl isothiocyanate
c. Digoxin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is RNA-dependednt RNA polymerase of COVID-19 (6VYO) 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 RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	-13.67	-17.94	Positive
Phenyl isothiocyanate	Not Applicable	Not Applicable	Failed
Digoxin	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 Sulforaphane helped deactivate the RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Caesalpinea sappan can prevent COVID 19 due to the presence of Sulforaphane. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Curcuma longa against COVID 19 through deactivation of RNA-dependednt RNA polymerase of COVID-19 (6VYO)

Soumya Priyadarshini[1], Yashaswi Nayak[2]

[1]190705180100@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 Curcuma longa against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme. It was found that Pelletierine helped to prevent COVID 19.

Introduction: Curcuma longa is known for its medicinal activities. Turmeric is used widely as a spice in South Asian and Middle Eastern cooking. The golden yellow colour of turmeric is due to curcumin which contains an orange-coloured volatile oil. It is used to protect food products from sunlight. Curcumin reduces inflammation.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Zingiberales
Family	Zingiberaceae
Genus	Curcuma
Species	longa

Major phytochemicals present in the plant are:

a. Pelletierine
b. Isorhamnetin
c. Theobromine
d. Tannic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is RNA-dependednt RNA polymerase of COVID-19 (6VYO) 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 RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	-14.61	-21.63	Positive
Isorhamnetin	Not Applicable	Not Applicable	Failed
Theobromine	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 Pelletierine helped deactivate the RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Curcuma longa can prevent COVID 19 due to the presence of Pelletierine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Ephedra sinica against COVID 19 through deactivation of RNA-dependednt RNA polymerase of COVID-19 (6VYO)

Priti Choudhury[1], Yashaswi Nayak[2]

[1]190705180103@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 Ephedra sinica against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme. It was found that Theobromine helped to prevent COVID 19.

Introduction: Ephedra sinica is known for its medicinal activities. Ephedra is used for weight loss and obesity and to enhance athletic performance. It is also used for allergies and hay fever; nasal congestion; and respiratory tract conditions such as bronchospasm, asthma, and bronchitis. It is also used for colds, flu, swine flu, fever, chills, headache, inability to sweat, joint and bone pain, and as a "water pill" to increase urine flow in people who retain fluids.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Gnetophyta
Order	Ephedrales
Family	Ephedraceae
Genus	Ephedra
Species	E. sinica

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Theobromine
c. Apigenin
d. Rosmarinic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is RNA-dependednt RNA polymerase of COVID-19 (6VYO) 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 RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Theobromine	-15.97	-21.62	Positive
Apigenin	Not Applicable	Not Applicable	Failed
Rosmarinic acid	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 RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Ephedra sinica can prevent COVID 19 due to the presence of Theobromine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Gardenia sp. against COVID 19 through deactivation of RNA-dependednt RNA polymerase of COVID-19 (6VYO)

Satyashree Dash[1], Sitaram Swain[2]

[1]190705180104@cutm.ac.in

[2]Sitaram.swain@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Gardenia sp. against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme. It was found that Genistein helped to prevent COVID 19.

Introduction: Gardenia sp. is known for its medicinal activities. Gardenia plants are known for its strong sweet scent of their flowers. Gardenia jasminoides (syn. G. grandiflora, G. Florida) is cultivated as a house plant. Its fruit is used as a yellow dye and used on fabric and food. Its fruits are also used in traditional Chinese medicine for their clearing, calming, and cooling properties.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Gentianales
Family	Rubiaceae
Genus	Gardenieae
Species	Gardenia

Major phytochemicals present in the plant are:

a. Pelargonidin
b. Genistein
c. Genistein
d. Daidzein

One of the major enzymes required for the survival of the organism causing COVID 19 is RNA-dependednt RNA polymerase of COVID-19 (6VYO) 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 RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelargonidin	Not Applicable	Not Applicable	Failed
Genistein	-13.64	-18.62	Positive
Genistein	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Genistein helped deactivate the RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Gardenia sp. can prevent COVID 19 due to the presence of Genistein. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Glycyrrhiza glabra against COVID 19 through deactivation of RNA-dependednt RNA polymerase of COVID-19 (6VYO)

Bijay Kumar Sahoo[1], Sitaram Swain[2]

[1]190705180105@cutm.ac.in

[2]Sitaram.swain@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 COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme. It was found that Sulforaphane helped to prevent COVID 19.

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. Alliin
b. Isorhamnetin
c. Sulforaphane
d. Ascorbic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is RNA-dependednt RNA polymerase of COVID-19 (6VYO) 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 RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Alliin	Not Applicable	Not Applicable	Failed
Isorhamnetin	Not Applicable	Not Applicable	Failed
Sulforaphane	-17.62	-21.64	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 Sulforaphane helped deactivate the RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Glycyrrhiza glabra can prevent COVID 19 due to the presence of Sulforaphane. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Hottuynia cordata against COVID 19 through deactivation of RNA-dependednt RNA polymerase of COVID-19 (6VYO)

Jahnara Begum[1], Sitaram Swain[2]

[1]190705180106@cutm.ac.in

[2]Sitaram.swain@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Hottuynia cordata against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme. It was found that Coumarin helped to prevent COVID 19.

Introduction: Hottuynia 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. Lupeol
b. Peonidin
c. Coumarin
d. Malvidin

One of the major enzymes required for the survival of the organism causing COVID 19 is RNA-dependednt RNA polymerase of COVID-19 (6VYO) 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 RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lupeol	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Coumarin	-14.67	-19.59	Positive
Malvidin	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 RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Hottuynia cordata can prevent COVID 19 due to the presence of Coumarin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Neerium indicum against COVID 19 through deactivation of RNA-dependednt RNA polymerase of COVID-19 (6VYO)

Subhashree Soubhagya Laxmi[1], Sitaram Swain[2]

[1]190705180107@cutm.ac.in

[2]Sitaram.swain@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 COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme. It was found that Caffeine helped to prevent COVID 19.

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. Theobromine
b. Daidzein
c. Caffeine
d. Limonene

One of the major enzymes required for the survival of the organism causing COVID 19 is RNA-dependednt RNA polymerase of COVID-19 (6VYO) 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 RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Failed
Caffeine	-18.34	-24.66	Positive
Limonene	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 RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Neerium indicum can prevent COVID 19 due to the presence of Caffeine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Punica granatum against COVID 19 through deactivation of RNA-dependednt RNA polymerase of COVID-19 (6VYO)

Ekaparna Nayak[1], Sitaram Swain[2]

[1]190705180108@cutm.ac.in

[2]Sitaram.swain@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Punica granatum against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme. It was found that Campesterol helped to prevent COVID 19.

Introduction: Punica granatum is known for its medicinal activities. Pomegranate seeds are used as a spice known as anar dana. Pomegranate is used mainly for juice. Pomegranate syrup or molasses is used in muhammara, a roasted red pepper, walnut, and garlic. Grenadine syrup originally consisted of thickened and sweetened pomegranate juice mainly used in cocktail mixing.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Myrtales
Family	Lythraceae
Genus	Punica
Species	granatum

Major phytochemicals present in the plant are:

a. Campesterol
b. Malvidin
c. Myricetin
d. Pelargonidin

One of the major enzymes required for the survival of the organism causing COVID 19 is RNA-dependednt RNA polymerase of COVID-19 (6VYO) 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 RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Campesterol	-17.58	-21.64	Positive
Malvidin	Not Applicable	Not Applicable	Failed
Myricetin	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 RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Punica granatum can prevent COVID 19 due to the presence of Campesterol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Wickstroemia indica against COVID 19 through deactivation of RNA-dependednt RNA polymerase of COVID-19 (6VYO)

Sandeepta Panda[1], Sitaram Swain[2]

[1]190705180109@cutm.ac.in

[2]Sitaram.swain@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Wickstroemia indica against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme. It was found that Zingiberene helped to prevent COVID 19.

Introduction: Wickstroemia indica is known for its medicinal activities. It is used in traditional Chinese medicine. This plant has antipyretic, detoxicant, expectorant, vermifuge, and abortifacient properties used in clinical practice in China. An alcoholic extract of the plant was found to contain daphnoretin, chrysophanol, myricitrime and rutin. The extract of W. indica displays antimicrobial and anti-inflammatory activities in vitro.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Malvales
Family	Thymelaeaceae
Genus	Wikstroemia
Species	indica

Major phytochemicals present in the plant are:

a. Naringin
b. Daidzein
c. Peonidin
d. Zingiberene

One of the major enzymes required for the survival of the organism causing COVID 19 is RNA-dependednt RNA polymerase of COVID-19 (6VYO) 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 RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Naringin	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Zingiberene	-14.61	-18.68	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Zingiberene helped deactivate the RNA-dependednt RNA polymerase of COVID-19 (6VYO) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Wickstroemia indica can prevent COVID 19 due to the presence of Zingiberene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Barleria prionitis against COVID 19 through deactivation of SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M)

Jyotshnashree Mohanty[1], Sitaram Swain[2]

[1]190705180110@cutm.ac.in

[2]Sitaram.swain@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Barleria prionitis against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme. It was found that Benzyl isothiocyanate helped to prevent COVID 19.

Introduction: Barleria prionitis is known for its medicinal activities. It is used for various medicinal purposes in ayurvedic medicine. The juice of the leaves is applied to feet to prevent maceration and cracking in the monsoon season. Its leaves are known to contain 6-Hydroxyflavone, one of the chemical compounds that is a noncompetitive inhibitor of the protein cytochrome P450 2C9.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Lamiales
Family	Acanthaceae
Genus	Barleria
Species	prionitis

Major phytochemicals present in the plant are:

a. Rosmarinic acid
b. Daidzein
c. Benzyl isothiocyanate
d. Quercetin

One of the major enzymes required for the survival of the organism causing COVID 19 is SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) 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 SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Rosmarinic acid	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Failed
Benzyl isothiocyanate	-13.45	-15.89	Positive
Quercetin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Benzyl isothiocyanate helped deactivate the SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Barleria prionitis can prevent COVID 19 due to the presence of Benzyl isothiocyanate. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Berginia ligulata against COVID 19 through deactivation of SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M)

Rutupurna Das[1], Sitaram Swain[2]

[1]190705180111@cutm.ac.in

[2]Sitaram.swain@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Berginia ligulata against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme. It was found that Ferulic acid helped to prevent COVID 19.

Introduction: Berginia ligulata is known for its medicinal activities. Ligulata possesses cooling, laxative, analgesic, abortifacient, aphrodisiac properties and used in treatment of vesicular calculi, urinary discharges, excessive uterine haemorrhage, diseases of the bladder, dysentery, menorrhagia, splenic enlargement and heart diseases.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Saxifragales
Family	Saxifragaceae
Genus	Bergenia
Species	ligulata

Major phytochemicals present in the plant are:

a. Pelargonidin
b. Ferulic acid
c. Rutin
d. Epicatechin

One of the major enzymes required for the survival of the organism causing COVID 19 is SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) 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 SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelargonidin	Not Applicable	Not Applicable	Failed
Ferulic acid	-14.32	-19.67	Positive
Rutin	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 Ferulic acid helped deactivate the SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Berginia ligulata can prevent COVID 19 due to the presence of Ferulic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Caesalpinea sappan against COVID 19 through deactivation of SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M)

Bijnaparamita Acharya[1], Sitaram Swain[2]

[1]190705180112@cutm.ac.in

[2]Sitaram.swain@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Caesalpinea sappan against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme. It was found that Phenyl isothiocyanate helped to prevent COVID 19.

Introduction: Caesalpinea sappan is known for its medicinal activities. This plant has antibacterial and anticoagulant properties. Slivers of heartwood are used for making herbal drinking water in various regions, such as Kerala, Karnataka and Central Java, where it is usually mixed with ginger, cinnamon, and cloves. The heartwood also contains juglone (5-hydroxy-1,4-naphthoquinone), which has antimicrobial activity.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Fabales
Family	Fabaceae
Genus	Caesalpinia
Species	sappan

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Phenyl isothiocyanate
c. Digoxin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) 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 SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Phenyl isothiocyanate	-13.64	-17.31	Positive
Digoxin	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 Phenyl isothiocyanate helped deactivate the SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Caesalpinea sappan can prevent COVID 19 due to the presence of Phenyl isothiocyanate. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Curcuma longa against COVID 19 through deactivation of SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M)

Sonali Biswas[1], Sitaram Swain[2]

[1]190705180113@cutm.ac.in

[2]Sitaram.swain@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Curcuma longa against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme. It was found that Pelletierine helped to prevent COVID 19.

Introduction: Curcuma longa is known for its medicinal activities. Turmeric is used widely as a spice in South Asian and Middle Eastern cooking. The golden yellow colour of turmeric is due to curcumin which contains an orange-coloured volatile oil. It is used to protect food products from sunlight. Curcumin reduces inflammation.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Zingiberales
Family	Zingiberaceae
Genus	Curcuma
Species	longa

Major phytochemicals present in the plant are:

a. Pelletierine
b. Isorhamnetin
c. Theobromine
d. Tannic acid

One of the major enzymes required for the survival of the organism causing COVID 19 is SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) 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 SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	-15.75	-19.89	Positive
Isorhamnetin	Not Applicable	Not Applicable	Failed
Theobromine	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 Pelletierine helped deactivate the SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Curcuma longa can prevent COVID 19 due to the presence of Pelletierine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Nigelia sativa against COVID 19 through deactivation of SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M)

Rojalin Pattanayak[1], Sunita Satapathy[2]

[1]190705180114@cutm.ac.in

[2]sunita.satapathy@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Nigelia sativa against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme. It was found that Kaempferol helped to prevent COVID 19.

Introduction: Nigelia sativa is known for its medicinal activities. Nigella sativa is used as a spice, natural seasoning, or flavoring. The seeds of N. sativa are used as a spice in many cuisines. They can be used as a seasoning in recipes with pod fruit, vegetables, salads, and poultry. The black seeds are used to flavour bread products, and are used as part of the spice mixture. Nigella is also used in tresse cheese, a braided string cheese called majdouleh or majdouli in the Middle East.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Ranunculales
Family	Ranunculaceae
Genus	Nigella
Species	sativa

Major phytochemicals present in the plant are:

a. Theobromine
b. Kaempferol
c. Limonene
d. Malvidin

One of the major enzymes required for the survival of the organism causing COVID 19 is SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) 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 SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	Not Applicable	Not Applicable	Failed
Kaempferol	-10.51	-18.79	Positive
Limonene	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 Kaempferol helped deactivate the SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Nigelia sativa can prevent COVID 19 due to the presence of Kaempferol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Pandanus amaryllifoius against COVID 19 through deactivation of SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M)

Sriram Chhatoi[1], Sunita Satapathy[2]

[1]190705180115@cutm.ac.in

[2]sunita.satapathy@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Pandanus amaryllifoius against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme. It was found that Gallic acid helped to prevent COVID 19.

Introduction: Pandanus amaryllifoius is known for its medicinal activities. The leaves are used in the perfume industry and traditional medicine. P. amaryllifolius essence may substitute for vanilla essence. The leaves possess a pleasant aroma and can be used as natural air fresheners. The green juice acquired from its leaf is used extensively in Indonesian cuisine as green food colouring and flavouring agents that gave pleasant aroma for kue, a tapioca, flour or glutinous rice-based traditional cakes.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Pandanales
Family	Pandanaceae
Genus	Pandanus
Species	amaryllifolius

Major phytochemicals present in the plant are:

a. Lutein
b. Genistein
c. Gallic acid
d. Theobromine

One of the major enzymes required for the survival of the organism causing COVID 19 is SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) 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 SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lutein	Not Applicable	Not Applicable	Failed
Genistein	Not Applicable	Not Applicable	Failed
Gallic acid	-12.54	-18.49	Positive
Theobromine	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 SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Pandanus amaryllifoius can prevent COVID 19 due to the presence of Gallic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Phyllanthus amarus against COVID 19 through deactivation of SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M)

Jyotismita Tripathy[1], Sunita Satapathy[2]

[1]190705180116@cutm.ac.in

[2]sunita.satapathy@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Phyllanthus amarus against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme. It was found that Ellagic acid and Campesterol helped to prevent COVID 19.

Introduction: Phyllanthus amarus is known for its medicinal activities. P.amarus is an important plant of Indian Ayurvedic system of medicine which is used in the problems of stomach, genitourinary system, liver, kidney and spleen. It is bitter, astringent, stomachic, diuretic, febrifuge and antiseptic. The whole plant is used in gonorrhea, menorrhagia and other genital affections.

The plant is classified as follows:

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

Major phytochemicals present in the plant are:

a. Pelletierine
b. Daidzein
c. Ellagic acid
d. Campesterol

One of the major enzymes required for the survival of the organism causing COVID 19 is SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) 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 SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Failed
Ellagic acid	-9.61	-17.81	Positive
Campesterol	-17.45	-21.81	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ellagic acid and Campesterol helped deactivate the SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Phyllanthus amarus can prevent COVID 19 due to the presence of Ellagic acid and Campesterol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Punica granatum against COVID 19 through deactivation of SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M)

Pratik Nayak[1], Sunita Satapathy[2]

[1]190705180117@cutm.ac.in

[2]sunita.satapathy@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Punica granatum against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme. It was found that Campesterol helped to prevent COVID 19.

Introduction: Punica granatum is known for its medicinal activities. Pomegranate seeds are used as a spice known as anar dana. Pomegranate is used mainly for juice. Pomegranate syrup or molasses is used in muhammara, a roasted red pepper, walnut, and garlic. Grenadine syrup originally consisted of thickened and sweetened pomegranate juice mainly used in cocktail mixing.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Myrtales
Family	Lythraceae
Genus	Punica
Species	granatum

Major phytochemicals present in the plant are:

a. Campesterol
b. Malvidin
c. Myricetin
d. Pelargonidin

One of the major enzymes required for the survival of the organism causing COVID 19 is SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) 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 SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Campesterol	-15.27	-19.67	Positive
Malvidin	Not Applicable	Not Applicable	Failed
Myricetin	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 SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Punica granatum can prevent COVID 19 due to the presence of Campesterol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Wickstroemia indica against COVID 19 through deactivation of SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M)

Sushri Sangita Mahalik[1], Sunita Sathapathy[2]

[1]190705180118@cutm.ac.in

[2]sunita.satapathy@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Wickstroemia indica against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme. It was found that Zingiberene helped to prevent COVID 19.

Introduction: Wickstroemia indica is known for its medicinal activities. It is used in traditional Chinese medicine. This plant has antipyretic, detoxicant, expectorant, vermifuge, and abortifacient properties used in clinical practice in China. An alcoholic extract of the plant was found to contain daphnoretin, chrysophanol, myricitrime and rutin. The extract of W. indica displays antimicrobial and anti-inflammatory activities in vitro.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Malvales
Family	Thymelaeaceae
Genus	Wikstroemia
Species	indica

Major phytochemicals present in the plant are:

a. Naringin
b. Daidzein
c. Peonidin
d. Zingiberene

One of the major enzymes required for the survival of the organism causing COVID 19 is SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) 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 SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Naringin	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Zingiberene	-15.45	-18.91	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Zingiberene helped deactivate the SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Wickstroemia indica can prevent COVID 19 due to the presence of Zingiberene. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Zizyphus spira-christi against COVID 19 through deactivation of SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M)

Barsa Bijoyswinee Panda[1], Sunita Satapathy[2]

[1]190705180119@cutm.ac.in

[2]sunita.satapathy@cutm.ac.in

Centurion University of Technology and Management, Odisha, India

Abstract: An in-silico study was performed to determine the activity of Zizyphus spira-christi against COVID 19. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme. It was found that Eugenol helped to prevent COVID 19.

Introduction: Zizyphus spira-christi is known for its medicinal activities. Fruits of Z. spina-christi is used as food. The wood is used as a source of fuel and it produces an excellent charcoal. Z. spina-christi fruits are eaten to treat diarrhoea and malaria and as an antispasmodic. The powder of the twigs is used externally to treat rheumatism and scorpion sting. Ash of wood mixed with vinegar is applied to heal snake bites and a tea made of fruit is used to treat measles. Fruits and crashed kernels are eaten to treat chest pains, respiratory problems and as a tonic.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophytes
Class	Angiosperms
Order	Rosales
Family	Rhamnaceae
Genus	Ziziphus
Species	spina-christi

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing COVID 19 is SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) 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 SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Eugenol	-12.61	-20.28	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 Eugenol helped deactivate the SARS-CoV-2 nucleocapsid protein N-terminal RNA binding domain (6M3M) enzyme of the organism causing COVID 19.

Conclusions: The molecular docking study showed that Zizyphus spira-christi can prevent COVID 19 due to the presence of Eugenol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Centurion Journal of Multidisciplinary Research (India)
Volume 10 **Number** 2 June 2020