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Special issue :
Proceedings of
National Conference on Molecular Docking (Series II):
Phytochemicals against Hepatitis C
20-22 Dec 2019

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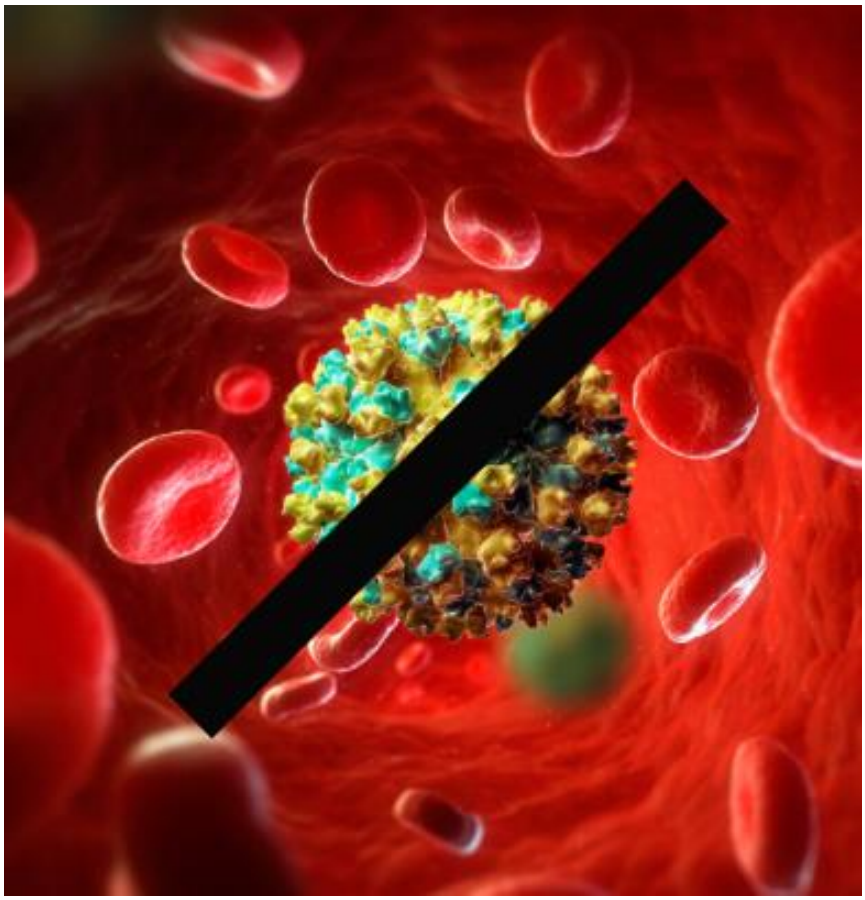

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Special Issue: Dec 2019

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THE VISION

Objective

Viruses cause a wide range of human diseases, ranging from acute self-resolving conditions to acute fatal diseases. Effects that arise long after the primary infection can also increase the propensity for chronic conditions or lead to the development of cancer. Recent advances in the fields of virology and pathology have been fundamental in improving our understanding of viral pathogenesis, in providing improved vaccination strategies and in developing newer, more effective treatments for patients worldwide.

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

Introduction

More than twenty years of study has provided a better understanding of hepatitis C virus (HCV) life cycle, including the general properties of viral RNA and proteins (Albert et al., 1999). This effort facilitates the development of sensitive diagnostic tools and effective antiviral treatments (Hoofnagle 2002). At present, serologic screening test is recommended to perform on individuals in the high risk groups and nucleic acid tests are recommended to confirm the active HCV infections. Quantization and genotyping of HCV RNAs are important to determine the optimal duration of anti-viral therapy and predict the likelihood of response (Chen and Morgan 2006). In the early 2000s, pegylated interferon plus ribavirin became the standard anti-HCV treatment. However, this therapy is not ideal. Some of the viral diseases can be cured by approved antiviral drugs, but for others still do not have any vaccines or drugs available. Most of the approved antiviral drugs are somehow directly or indirectly associated with side effects, which eventually raise the need for the development of antivirals based on natural phytochemicals (Lakeman et al., 1995; Perry et al., 1996). Globally, the development of antivirals is shifting towards the plant-derived products as they are less toxic and has less chance to develop resistance (Balfour 1998). Phytochemicals have been exploited traditionally for the cure of many diseases, and also have been reported to inhibit viral replication/transcription (Anand et al., 2003; Aati 2020). Most of them inhibit the

viruses either during the viral entry inside the host cell or during their replication. Moreover, 50% of the drugs derived from plants are being used in the Western nations (DeLano 2002). Plants have a variety of phytochemicals like flavonoids, terpenoids, lignins, alkaloids, and coumarins that are having antioxidant activity, and help to inhibit viral genome (Dallakyan et al., 2015; Alamri 2020).

Viral Protein Structure and Phytochemical dataset collection

The 3D structure of the viral protein was accessed from Protein Data Bank with accessions 5PZL, 3M5O and 3T4B (Fig. 1). Phytochemical list in different plants (Fig. 2) was obtained and consequently both the protein and the ligands were used for *in silico* analysis.

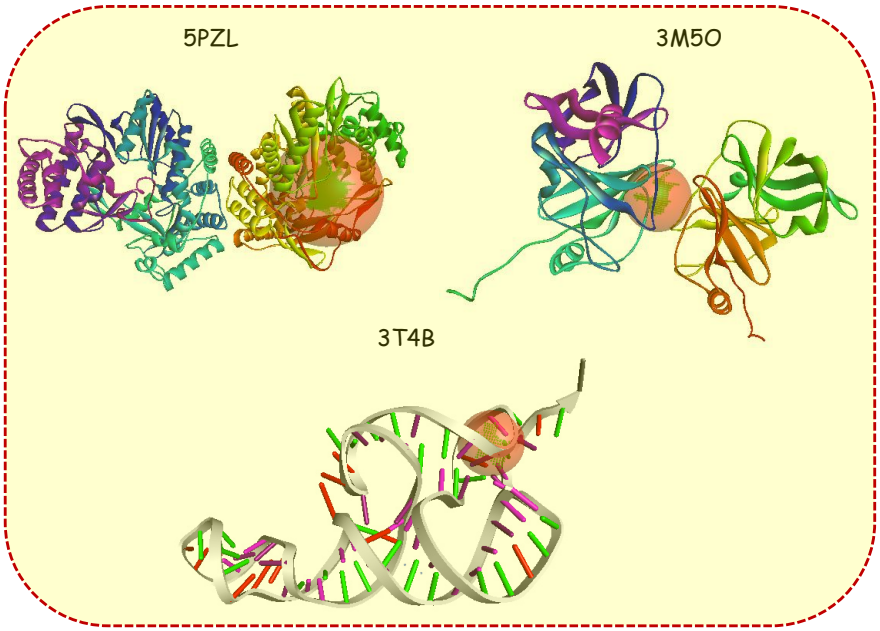

Figure 1. Different enzymes available in hepatitis virus

Molecular docking

For the *in silico* molecular docking, BIOVIA's Discovery Studio docking suite was used for molecular docking. The catalytic pocket of the viral proteins were specified and targeted for binding of the ligand(s). -CDOCKER Energy and -CDOCKER Interaction Energy signify the affinity of the ligands with the protein receptors. Basically, high positive values of the CDOCKER Energy, CDOCKER Interaction Energy and a diminutive difference between the -CDOCKER Energy and -CDOCKER Interaction Energy are considered to be the most

favourable. Discovery Studio is a software suite for performing computational analysis of data relevant to Life Sciences research.

Conclusion

Nowadays, research and development programs are continuously adopting approaches based on plant-based products for the development of drugs. Pure compounds and plant extracts have been investigated for the synthesis of new pharmaceuticals and therapeutics. Traditional plants have been continuously used in the field of medicine for the treatment of various infections. Therapies based on natural products (phytochemicals) for human health are associated with less toxicity and minimal side effects. Thus, the researchers are focusing to elucidate the new plant-based compounds for the treatment of many diseases. Different plant secondary metabolites have been studied and used for various human-based treatments because of antioxidant, anticancerous, antibacterial, and antiviral properties. Several in silico and in vitro studies have revealed the promising use of photochemicals for the treatment of viral infections. Among all the phytochemicals, flavonoids have been widely exploited and studied for the treatment of several viral diseases. Phytochemicals having antiviral activity can be nanoencapsulated for better delivery, prolonged action, and enhanced bioavailability. Moreover, excessive research on different biodiversity-rich regions could be explored to get more potent phytochemicals and metabolites as antiviral agents.

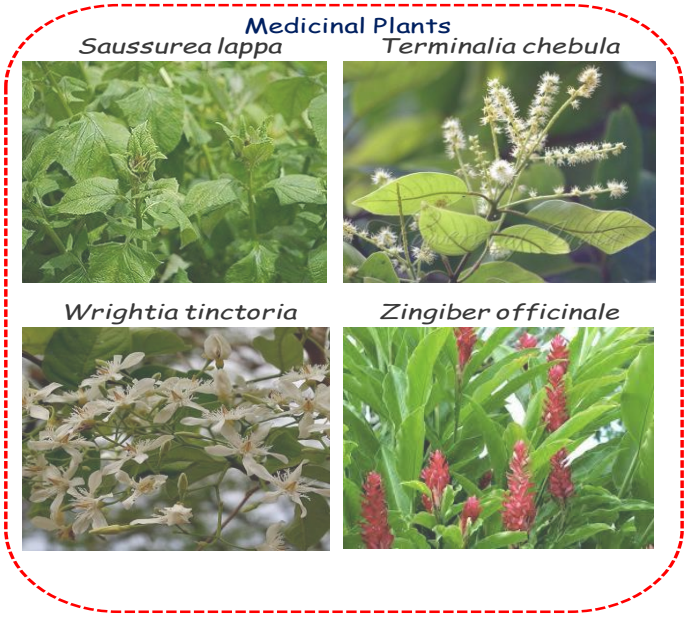

Figure 2. Plants that can fight against hepatitis C

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Index

Articles	Page no.
Activity of Agrimonia eupatoria against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)	1 to 2
Activity of Alpinea galanga against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)	3 to 4
Activity of Bupleurum sp. against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)	5 to 6
Activity of Glycyrrhiza glabra against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)	7 to 8
Activity of Hypericum perforatum against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)	9 to 10
Activity of Pericampylus glaucus against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)	11 to 12
Activity of Phyllanthus amarus against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)	13 to 14
Activity of Phyllanthus urinaria against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)	15 to 16
Activity of Picrorhiza kurroa against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)	17 to 18
Activity of Potentila anserine against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)	19 to 20
Activity of Ranunculus scleratus against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)	21 to 22
Activity of Rubia cardifolia against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)	23 to 24

Activity of Saussurea lappa against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)	25 to 26
Activity of Terminalia chebula against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)	27 to 28
Activity of Wrightia tinctoria against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)	29 to 30
Activity of Zingiber officinale against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)	31 to 32
Activity of Agrimonia eupatoria against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain (3T4B)	33 to 34
Activity of Alpinea galanga against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain (3T4B)	35 to 36
Activity of Bupleurum sp. against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain (3T4B)	37 to 38
Activity of Glycyrrhiza glabra against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain (3T4B)	39 to 40
Activity of Hypericum perforatum against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain (3T4B)	41 to 42
Activity of Oenanthe javanica against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain (3T4B)	43 to 44
Activity of Pericampylus glaucus against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain (3T4B)	45 to 46
Activity of Phyllanthus amarus against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain (3T4B)	47 to 48
Activity of Phyllanthus urinaria against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain (3T4B)	49 to 50
Activity of Picrorhiza kurroa against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain (3T4B)	51 to 52

Activity of Potentila anserine against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain (3T4B)	53 to 54
Activity of Ranunculus scleratus against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain (3T4B)	55 to 56
Activity of Rubia cardifolia against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain (3T4B)	57 to 58
Activity of Saussurea lappa against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain (3T4B)	59 to 60
Activity of Terminalia chebula against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain (3T4B)	61 to 62
Activity of Wrightia tinctoria against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain (3T4B)	63 to 64
Activity of Zingiber officinale against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain (3T4B)	65 to 66
Activity of Zingiber officinale against Hepatitis C through deactivation of Hepatitis C Virus protease (3M5O)	67 to 68
Activity of Agrimonia eupatoria against Hepatitis C through deactivation of Hepatitis C Virus protease (3M5O)	69 to 70
Activity of Alpinea galanga against Hepatitis C through deactivation of Hepatitis C Virus protease (3M5O)	71 to 72
Activity of Bupleurum sp. against Hepatitis C through deactivation of Hepatitis C Virus protease (3M5O)	73 to 74
Activity of Glycyrrhiza glabra against Hepatitis C through deactivation of Hepatitis C Virus protease (3M5O)	75 to 76
Activity of Hypericum perforatum against Hepatitis C through deactivation of Hepatitis C Virus protease (3M5O)	77 to 78
Activity of Oenanthe javanica against Hepatitis C through deactivation of Hepatitis C Virus protease (3M5O)	79 to 80

Activity of Pericampylus glaucus against Hepatitis C through deactivation of Hepatitis C Virus protease (3M5O)	81 to 82
Activity of Phyllanthus amarus against Hepatitis C through deactivation of Hepatitis C Virus protease (3M5O)	83 to 84
Activity of Phyllanthus urinaria against Hepatitis C through deactivation of Hepatitis C Virus protease (3M5O)	85 to 86
Activity of Picrorhiza kurroa against Hepatitis C through deactivation of Hepatitis C Virus protease (3M5O)	87 to 88
Activity of Potentila anserine against Hepatitis C through deactivation of Hepatitis C Virus protease (3M5O)	89 to 90
Activity of Ranunculus scleratus against Hepatitis C through deactivation of Hepatitis C Virus protease (3M5O)	91 to 92
Activity of Rubia cardifolia against Hepatitis C through deactivation of Hepatitis C Virus protease (3M5O)	93 to 94
Activity of Saussurea lappa against Hepatitis C through deactivation of Hepatitis C Virus protease (3M5O)	95 to 96
Activity of Terminalia chebula against Hepatitis C through deactivation of Hepatitis C Virus protease (3M5O)	97 to 98
Activity of Wrightia tinctoria against Hepatitis C through deactivation of Hepatitis C Virus protease (3M5O)	99 to 100
Activity of Oenanthe javanica against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)	101 to 102

Activity of Agrimonia eupatoria against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)

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Abstract: An in-silico study was performed to determine the activity of Agrimonia eupatoria against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. It was found that Ferulic acid helped to prevent Hepatitis C.

Introduction: Agrimonia eupatoria is known for its medicinal activities. It is used as a folk remedy for asthma, bronchitis, dermatitis, entorrhagia, enuresis, gastrorrhagia, hematuria, hepatosis, metrorrhagia and neuralgia.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Rosales
Family	Rosaceae
Genus	Agrimonia
Species	eupatoria

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Resveratrol	Not Applicable	Not Applicable	Failed
Phenyl isothiocyanate	Not Applicable	Not Applicable	Failed
Rutin	Not Applicable	Not Applicable	Failed
Ferulic acid	-12.54	-15.66	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ferulic acid helped deactivate the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme of the organism causing Hepatitis C.

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

Activity of Alpinea galanga against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)

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Abstract: An in-silico study was performed to determine the activity of Alpinea galanga against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. It was found that Tangeretin helped to prevent Hepatitis C.

Introduction: Alpinea galanga is known for its medicinal activities. Alpinia is a plant related to ginger. The horizontal underground stem (rhizome) is used to make medicine. Alpinia is used to treat fever, muscle spasms, intestinal gas, and swelling (inflammation); to kill bacteria; and as a stimulant.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Zingiberales
Family	Zingiberaceae
Genus	Alpinea
Species	galanga

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Cryptoxanthin	Not Applicable	Not Applicable	Failed
Tangeretin	-12.57	-18.69	Positive
Salicylic acid	Not Applicable	Not Applicable	Failed
Limonene	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Tangeretin helped deactivate the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme of the organism causing Hepatitis C.

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

Activity of Bupleurum sp. against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)

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Abstract: An in-silico study was performed to determine the activity of Bupleurum sp. against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. It was found that Pelletierine helped to prevent Hepatitis C.

Introduction: Bupleurum sp. is known for its medicinal activities. Bupleurum is used for respiratory infections, including the flu (influenza), swine flu, the common cold, bronchitis, and pneumonia; and symptoms of these infections, including fever and cough.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Apiales
Family	Apiaceae
Genus	Bupleurum
Species	scorzonerifolium

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tangeretin	Not Applicable	Not Applicable	Failed
Tannic acid	Not Applicable	Not Applicable	Failed
Pelletierine	-15.37	-19.77	Positive
Digoxin	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 Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme of the organism causing Hepatitis C.

Conclusions: The molecular docking study showed that Bupleurum sp. can prevent Hepatitis C due to the presence of Pelletierine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Glycyrrhiza glabra against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)

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Abstract: An in-silico study was performed to determine the activity of Glycyrrhiza glabra against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. It was found that Genistein and Daidzein helped to prevent Hepatitis C.

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. Genistein
b. Daidzein
c. Theobromine
d. Quercetin

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Genistein	-12.66	-15.38	Positive
Daidzein	-11.78	-15.93	Positive
Theobromine	Not Applicable	Not Applicable	Failed
Quercetin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Genistein and Daidzein helped deactivate the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme of the organism causing Hepatitis C.

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

Activity of Hypericum perforatum against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)

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Abstract: An in-silico study was performed to determine the activity of Hypericum perforatum against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. It was found that Pelargonidin helped to prevent Hepatitis C.

Introduction: Hypericum perforatum is known for its medicinal activities. It is used tropically for the treatment of wounds, abrasions, burns, sunburns and inflammatory skin disorders. Its use in wound healing could be justified with its anti-inflammatory, antimicrobial and astringent effects.

The plant is classified as follows:

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

Major phytochemicals present in the plant are:

a. Pelargonidin
b. Limonene
c. Rutin
d. Azadirichtin

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelargonidin	-15.64	-18.78	Positive
Limonene	Not Applicable	Not Applicable	Failed
Rutin	Not Applicable	Not Applicable	Failed
Azadirichtin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Pelargonidin helped deactivate the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme of the organism causing Hepatitis C.

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

Activity of Pericampylus glaucus against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)

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Abstract: An in-silico study was performed to determine the activity of Pericampylus glaucus against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. It was found that Tannic acid helped to prevent Hepatitis C.

Introduction: Pericampylus glaucus is known for its medicinal activities. The mucilage resulting from soaking the pounded leaves overnight is taken orally to cure a swollen spleen and accompanying fever.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Ranunculales
Family	Menispermaceae
Genus	Pericampylus
Species	glaucus

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	-13.55	-14.27	Positive
Alliin	Not Applicable	Not Applicable	Failed
Theobromine	Not Applicable	Not Applicable	Failed
Tannic acid	-12.08	-15.27	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Tannic acid helped deactivate the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme of the organism causing Hepatitis C.

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

Activity of Phyllanthus amarus against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)

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Abstract: An in-silico study was performed to determine the activity of Phyllanthus amarus against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. It was found that Rosmarinic acid helped to prevent Hepatitis C.

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. Sulforaphane
b. Digoxin
c. Isorhamnetin
d. Rosmarinic acid

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Digoxin	Not Applicable	Not Applicable	Failed
Isorhamnetin	Not Applicable	Not Applicable	Failed
Rosmarinic acid	-11.25	-18.66	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Rosmarinic acid helped deactivate the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme of the organism causing Hepatitis C.

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

Activity of Phyllanthus urinaria against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)

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Abstract: An in-silico study was performed to determine the activity of Phyllanthus urinaria against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. It was found that Limoene and Daidzein helped to prevent Hepatitis C.

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

The plant is classified as follows:

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

Major phytochemicals present in the plant are:

a. Limonene
b. Naringin
c. Genistein
d. Daidzein

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme.

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

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Limoene and Daidzein helped deactivate the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme of the organism causing Hepatitis C.

Conclusions: The molecular docking study showed that Phyllanthus urinaria can prevent Hepatitis C due to the presence of Limoene and Daidzein. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Picrorhiza kurroa against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)

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Abstract: An in-silico study was performed to determine the activity of Picrorhiza kurroa against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. It was found that Curcumin helped to prevent Hepatitis C.

Introduction: Picrorhiza kurroa is known for its medicinal activities. Picrorhiza kurroa is a well-known herb in the Ayurvedic system of medicine and has traditionally been used to treat disorders of the liver and upper respiratory tract, reduce fevers, and to treat dyspepsia, chronic diarrhea, and scorpion sting.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Eudicots
Order	Lamiales
Family	Phyllanthaceae
Genus	Picrorhiza
Species	kurroa

Major phytochemicals present in the plant are:

a. Luteolin
b. Isorhamnetin
c. Curcumin
d. Ascorbic acid

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Luteolin	Not Applicable	Not Applicable	Failed
Isorhamnetin	Not Applicable	Not Applicable	Failed
Curcumin	-18.22	-20.38	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 Curcumin helped deactivate the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme of the organism causing Hepatitis C.

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

Activity of Potentila anserine against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)

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Abstract: An in-silico study was performed to determine the activity of Potentila anserine against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. It was found that Limonene helped to prevent Hepatitis C.

Introduction: Potentila anserine is known for its medicinal activities. The whole plant is antispasmodic, mildly astringent, diuretic, foot care, haemostatic, odontalgic and tonic.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Rosales
Family	Rosaceae
Genus	Potentilla
Species	anserine

Major phytochemicals present in the plant are:

a. Lupeol
b. Peonidin
c. Limonene
d. Malvidin

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lupeol	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Limonene	-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 Limonene helped deactivate the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme of the organism causing Hepatitis C.

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

Activity of Ranunculus scleratus against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)

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Abstract: An in-silico study was performed to determine the activity of Ranunculus scleratus against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. It was found that Limonene helped to prevent Hepatitis C.

Introduction: Ranunculus scleratus is known for its medicinal activities. The whole plant has anti-inflammatory, analgesic, sedative and expectorant properties and it is recommended against skin diseases such as eczema, herpes, pruritus, burns and swellings.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Ranunculales
Family	Ranunculaceae
Genus	Ranunculus
Species	sceleratus

Major phytochemicals present in the plant are:

a. Theobromine
b. Daidzein
c. Peonidin
d. Limonene

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Limonene	-12.47	-17.29	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Limonene helped deactivate the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme of the organism causing Hepatitis C.

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

Activity of Rubia cardifolia against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)

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Abstract: An in-silico study was performed to determine the activity of Rubia cardifolia against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. It was found that Theobromine helped to prevent Hepatitis C.

Introduction: Rubia cardifolia is known for its medicinal activities. Rubia cordifolia role in supporting heart health is evidenced by traditional and reported activities which show that it act as potent blood purifier, antioxidant, diuretic, calcium channel blocker, antiplatelet, antidiabetic, antiinflammatory, antistress, immunomodulator etc.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Gentianales
Family	Rubiaceae
Genus	Rubia
Species	cordifolia

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	-10.84	-18.27	Positive
Peonidin	Not Applicable	Not Applicable	Failed
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 Theobromine helped deactivate the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme of the organism causing Hepatitis C.

Conclusions: The molecular docking study showed that Rubia cardifolia can prevent Hepatitis C due to the presence of Theobromine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Saussurea lappa against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)

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Abstract: An in-silico study was performed to determine the activity of Saussurea lappa against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. It was found that Lutein helped to prevent Hepatitis C.

Introduction: Saussurea lappa is known for its medicinal activities. In Unani system of medicine it is used for carminative, aphrodisiac, anthelmintic, tonic, stimulates the brain, used in diseases of liver, kidney and blood. It also used for treating deaf, headache, paralysis, asthma, cough, old fever, inflammation, and ophthalmic conditions.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Asterales
Family	Asteraceae
Genus	Saussurea
Species	lappa

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lutein	-11.36	-17.59	Positive
Genistein	Not Applicable	Not Applicable	Failed
Daidzein	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 Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme of the organism causing Hepatitis C.

Conclusions: The molecular docking study showed that Saussurea lappa can prevent Hepatitis C due to the presence of Lutein. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Terminalia chebula against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)

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Abstract: An in-silico study was performed to determine the activity of Terminalia chebula against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. It was found that Campesterol helped to prevent Hepatitis C.

Introduction: Terminalia chebula is known for its medicinal activities. Its powder is a good astringent dentifrice in loose gums, bleeding and ulceration in gums. It is good to increase appetite, digestive aid, liver stimulant, stomachic, gastrointestinal prokinetic agent, and mild laxative. The powder of T. chebula fruits has been used in chronic diarrhea.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Myrtales
Family	Combretaceae
Genus	Terminalia
Species	chebula

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Failed
Alliin	Not Applicable	Not Applicable	Failed
Campesterol	-12.47	-16.91	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Campesterol helped deactivate the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme of the organism causing Hepatitis C.

Conclusions: The molecular docking study showed that Terminalia chebula can prevent Hepatitis C due to the presence of Campesterol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Wrightia tinctoria against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)

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Abstract: An in-silico study was performed to determine the activity of Wrightia tinctoria against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. It was found that Campesterol helped to prevent Hepatitis C.

Introduction: Wrightia tinctoria is known for its medicinal activities. It is the most commonly prescribed Siddha herbal medication for skin diseases, in specific psoriasis. The "777 oil" made from the fresh leaves of the plant exhibits various analgesic, anti-inflammatory, and antipyretic activities and it is a highly cited medication for the treatment of psoriasis.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Gentianales
Family	Apocynaceae
Genus	Wrightia
Species	tinctoria

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 Hepatitis C is Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) 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 Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme of the organism causing Hepatitis C.

Conclusions: The molecular docking study showed that Wrightia tinctoria can prevent Hepatitis C due to the presence of Campesterol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Zingiber officinale against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)

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Abstract: An in-silico study was performed to determine the activity of Zingiber officinale against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. It was found that Naringin and Zingiberene helped to prevent Hepatitis C.

Introduction: Zingiber officinale is known for its medicinal activities. It is a spice consumed worldwide for culinary and medicinal purposes. The plant has a number of chemicals responsible for its medicinal properties, such as antiarthritis, antiinflammatory, antidiabetic, antibacterial, antifungal, anticancer, etc.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Zingiberales
Family	Zingiberaceae
Genus	Zingiber
Species	officinale

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 Hepatitis C is Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) 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 Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme of the organism causing Hepatitis C.

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

Activity of Agrimonia eupatoria against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain

(3T4B)

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Abstract: An in-silico study was performed to determine the activity of Agrimonia eupatoria against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. It was found that Phenyl isothiocyanate helped to prevent Hepatitis C.

Introduction: Agrimonia eupatoria is known for its medicinal activities. It is used as a folk remedy for asthma, bronchitis, dermatitis, entorrhagia, enuresis, gastrorrhagia, hematuria, hepatosis, metrorrhagia and neuralgia.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Rosales
Family	Rosaceae
Genus	Agrimonia
Species	eupatoria

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Resveratrol	Not Applicable	Not Applicable	Failed
Phenyl isothiocyanate	-10.61	-19.37	Positive
Rutin	Not Applicable	Not Applicable	Failed
Ferulic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Phenyl isothiocyanate helped deactivate the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme of the organism causing Hepatitis C.

Conclusions: The molecular docking study showed that Agrimonia eupatoria can prevent Hepatitis C due to the presence of Phenyl isothiocyanate. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Alpinea galanga against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain

(3T4B)

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Abstract: An in-silico study was performed to determine the activity of Alpinea galanga against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. It was found that Limonene helped to prevent Hepatitis C.

Introduction: Alpinea galanga is known for its medicinal activities. Alpinia is a plant related to ginger. The horizontal underground stem (rhizome) is used to make medicine. Alpinia is used to treat fever, muscle spasms, intestinal gas, and swelling (inflammation); to kill bacteria; and as a stimulant.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Zingiberales
Family	Zingiberaceae
Genus	Alpinea
Species	galanga

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Cryptoxanthin	Not Applicable	Not Applicable	Failed
Tangeretin	Not Applicable	Not Applicable	Failed
Salicylic acid	Not Applicable	Not Applicable	Failed
Limonene	-11.95	-19.48	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Limonene helped deactivate the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme of the organism causing Hepatitis C.

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

Activity of Bupleurum sp. against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain

(3T4B)

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Abstract: An in-silico study was performed to determine the activity of Bupleurum sp. against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. It was found that Tangeretin helped to prevent Hepatitis C.

Introduction: Bupleurum sp. is known for its medicinal activities. Bupleurum is used for respiratory infections, including the flu (influenza), swine flu, the common cold, bronchitis, and pneumonia; and symptoms of these infections, including fever and cough.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Apiales
Family	Apiaceae
Genus	Bupleurum
Species	scorzonerifolium

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tangeretin	-9.47	-18.31	Positive
Tannic acid	Not Applicable	Not Applicable	Failed
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 Tangeretin helped deactivate the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme of the organism causing Hepatitis C.

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

Activity of Glycyrrhiza glabra against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain

(3T4B)

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Abstract: An in-silico study was performed to determine the activity of Glycyrrhiza glabra against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. It was found that Genistein and Quercetin helped to prevent Hepatitis C.

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. Genistein
b. Daidzein
c. Theobromine
d. Quercetin

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Genistein	-9.33	-21.54	Positive
Daidzein	Not Applicable	Not Applicable	Failed
Theobromine	Not Applicable	Not Applicable	Failed
Quercetin	-12.37	-19.67	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Genistein and Quercetin helped deactivate the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme of the organism causing Hepatitis C.

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

Activity of Hypericum perforatum against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain

(3T4B)

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Abstract: An in-silico study was performed to determine the activity of Hypericum perforatum against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. It was found that Rutin helped to prevent Hepatitis C.

Introduction: Hypericum perforatum is known for its medicinal activities. It is used tropically for the treatment of wounds, abrasions, burns, sunburns and inflammatory skin disorders. Its use in wound healing could be justified with its anti-inflammatory, antimicrobial and astringent effects.

The plant is classified as follows:

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

Major phytochemicals present in the plant are:

a. Pelargonidin
b. Limonene
c. Rutin
d. Azadirichtin

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelargonidin	Not Applicable	Not Applicable	Failed
Limonene	Not Applicable	Not Applicable	Failed
Rutin	-12.66	-19.12	Positive
Azadirichtin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Rutin helped deactivate the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme of the organism causing Hepatitis C.

Conclusions: The molecular docking study showed that Hypericum perforatum can prevent Hepatitis C due to the presence of Rutin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Oenanthe javanica against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain

(3T4B)

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Abstract: An in-silico study was performed to determine the activity of Oenanthe javanica against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. It was found that Digoxin helped to prevent Hepatitis C.

Introduction: Oenanthe javanica is known for its medicinal activities. Oenanthe javanica, popularly known as water dropwort, has long been used in various ethnomedical systems in Asia, especially in China, Korean, and Japan, for treating various chronic and acute hepatitis, jaundice, alcohol hangovers, abdominal pain, and inflammatory conditions.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Apiales
Family	Apiaceae
Genus	Oenanthe
Species	javanica

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Astaxanthin
c. Digoxin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Astaxanthin	Not Applicable	Not Applicable	Failed
Digoxin	-11.68	-23.64	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 Digoxin helped deactivate the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme of the organism causing Hepatitis C.

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

Activity of Pericampylus glaucus against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain

(3T4B)

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Abstract: An in-silico study was performed to determine the activity of Pericampylus glaucus against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. It was found that Pelletierine and Alliin helped to prevent Hepatitis C.

Introduction: Pericampylus glaucus is known for its medicinal activities. The mucilage resulting from soaking the pounded leaves overnight is taken orally to cure a swollen spleen and accompanying fever.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Ranunculales
Family	Menispermaceae
Genus	Pericampylus
Species	glaucus

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	-14.69	-22.31	Positive
Alliin	-12.15	-18.64	Positive
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 and Alliin helped deactivate the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme of the organism causing Hepatitis C.

Conclusions: The molecular docking study showed that Pericampylus glaucus can prevent Hepatitis C due to the presence of Pelletierine and Alliin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Phyllanthus amarus against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain

(3T4B)

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Abstract: An in-silico study was performed to determine the activity of Phyllanthus amarus against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. It was found that Digoxin helped to prevent Hepatitis C.

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. Sulforaphane
b. Digoxin
c. Isorhamnetin
d. Rosmarinic acid

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Digoxin	-10.67	-17.95	Positive
Isorhamnetin	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 Digoxin helped deactivate the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme of the organism causing Hepatitis C.

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

Activity of Phyllanthus urinaria against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain

(3T4B)

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Abstract: An in-silico study was performed to determine the activity of Phyllanthus urinaria against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. It was found that Naringin and Daidzein helped to prevent Hepatitis C.

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

The plant is classified as follows:

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

Major phytochemicals present in the plant are:

a. Limonene
b. Naringin
c. Genistein
d. Daidzein

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Limonene	Not Applicable	Not Applicable	Failed
Naringin	-6.67	-13.91	Positive
Genistein	-14.38	-22.37	Positive
Daidzein	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Naringin and Daidzein helped deactivate the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme of the organism causing Hepatitis C.

Conclusions: The molecular docking study showed that Phyllanthus urinaria can prevent Hepatitis C due to the presence of Naringin and Daidzein. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Picrorhiza kurroa against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain

(3T4B)

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Abstract: An in-silico study was performed to determine the activity of Picrorhiza kurroa against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. It was found that Isorhamnetin helped to prevent Hepatitis C.

Introduction: Picrorhiza kurroa is known for its medicinal activities. Picrorhiza kurroa is a well-known herb in the Ayurvedic system of medicine and has traditionally been used to treat disorders of the liver and upper respiratory tract, reduce fevers, and to treat dyspepsia, chronic diarrhea, and scorpion sting.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Eudicots
Order	Lamiales
Family	Phyllanthaceae
Genus	Picrorhiza
Species	kurroa

Major phytochemicals present in the plant are:

a. Luteolin
b. Isorhamnetin
c. Curcumin
d. Ascorbic acid

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Luteolin	Not Applicable	Not Applicable	Failed
Isorhamnetin	-19.64	-21.84	Positive
Curcumin	Not Applicable	Not Applicable	Failed
Ascorbic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Isorhamnetin helped deactivate the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme of the organism causing Hepatitis C.

Conclusions: The molecular docking study showed that Picrorhiza kurroa can prevent Hepatitis C due to the presence of Isorhamnetin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Potentila anserine against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain

(3T4B)

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Abstract: An in-silico study was performed to determine the activity of Potentila anserine against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. It was found that Lupeol helped to prevent Hepatitis C.

Introduction: Potentila anserine is known for its medicinal activities. The whole plant is antispasmodic, mildly astringent, diuretic, foot care, haemostatic, odontalgic and tonic.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Rosales
Family	Rosaceae
Genus	Potentilla
Species	anserine

Major phytochemicals present in the plant are:

a. Lupeol
b. Peonidin
c. Limonene
d. Malvidin

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lupeol	-12.37	-18.67	Positive
Peonidin	Not Applicable	Not Applicable	Failed
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 Lupeol helped deactivate the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme of the organism causing Hepatitis C.

Conclusions: The molecular docking study showed that Potentila anserine can prevent Hepatitis C due to the presence of Lupeol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Ranunculus scleratus against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain

(3T4B)

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Abstract: An in-silico study was performed to determine the activity of Ranunculus scleratus against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. It was found that Daidzein helped to prevent Hepatitis C.

Introduction: Ranunculus scleratus is known for its medicinal activities. The whole plant has anti-inflammatory, analgesic, sedative and expectorant properties and it is recommended against skin diseases such as eczema, herpes, pruritus, burns and swellings.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Ranunculales
Family	Ranunculaceae
Genus	Ranunculus
Species	sceleratus

Major phytochemicals present in the plant are:

a. Theobromine
b. Daidzein
c. Peonidin
d. Limonene

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	Not Applicable	Not Applicable	Failed
Daidzein	-9.64	-17.84	Positive
Peonidin	Not Applicable	Not Applicable	Failed
Limonene	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Daidzein helped deactivate the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme of the organism causing Hepatitis C.

Conclusions: The molecular docking study showed that Ranunculus scleratus can prevent Hepatitis C due to the presence of Daidzein. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Rubia cardifolia against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain

(3T4B)

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Abstract: An in-silico study was performed to determine the activity of Rubia cardifolia against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. It was found that Limonene helped to prevent Hepatitis C.

Introduction: Rubia cardifolia is known for its medicinal activities. Rubia cordifolia role in supporting heart health is evidenced by traditional and reported activities which show that it act as potent blood purifier, antioxidant, diuretic, calcium channel blocker, antiplatelet, antidiabetic, antiinflammatory, antistress, immunomodulator etc.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Gentianales
Family	Rubiaceae
Genus	Rubia
Species	cordifolia

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Limonene	-10.08	-18.54	Positive
Malvidin	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Limonene helped deactivate the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme of the organism causing Hepatitis C.

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

Activity of Saussurea lappa against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain

(3T4B)

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Abstract: An in-silico study was performed to determine the activity of Saussurea lappa against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. It was found that Daidzein helped to prevent Hepatitis C.

Introduction: Saussurea lappa is known for its medicinal activities. In Unani system of medicine it is used for carminative, aphrodisiac, anthelmintic, tonic, stimulates the brain, used in diseases of liver, kidney and blood. It also used for treating deaf, headache, paralysis, asthma, cough, old fever, inflammation, and ophthalmic conditions.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Asterales
Family	Asteraceae
Genus	Saussurea
Species	lappa

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lutein	Not Applicable	Not Applicable	Failed
Genistein	Not Applicable	Not Applicable	Failed
Daidzein	-12.68	-22.64	Positive
Theobromine	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Daidzein helped deactivate the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme of the organism causing Hepatitis C.

Conclusions: The molecular docking study showed that Saussurea lappa can prevent Hepatitis C due to the presence of Daidzein. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Terminalia chebula against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain

(3T4B)

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Abstract: An in-silico study was performed to determine the activity of Terminalia chebula against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. It was found that Daidzein helped to prevent Hepatitis C.

Introduction: Terminalia chebula is known for its medicinal activities. Its powder is a good astringent dentifrice in loose gums, bleeding and ulceration in gums. It is good to increase appetite, digestive aid, liver stimulant, stomachic, gastrointestinal prokinetic agent, and mild laxative. The powder of T. chebula fruits has been used in chronic diarrhea.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Myrtales
Family	Combretaceae
Genus	Terminalia
Species	chebula

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	Not Applicable	Not Applicable	Failed
Daidzein	-15.68	-21.52	Positive
Alliin	Not Applicable	Not Applicable	Failed
Campesterol	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Daidzein helped deactivate the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme of the organism causing Hepatitis C.

Conclusions: The molecular docking study showed that Terminalia chebula can prevent Hepatitis C due to the presence of Daidzein. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Wrightia tinctoria against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain

(3T4B)

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Abstract: An in-silico study was performed to determine the activity of Wrightia tinctoria against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. It was found that Malvidin helped to prevent Hepatitis C.

Introduction: Wrightia tinctoria is known for its medicinal activities. It is the most commonly prescribed Siddha herbal medication for skin diseases, in specific psoriasis. The "777 oil" made from the fresh leaves of the plant exhibits various analgesic, anti-inflammatory, and antipyretic activities and it is a highly cited medication for the treatment of psoriasis.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Gentianales
Family	Apocynaceae
Genus	Wrightia
Species	tinctoria

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 Hepatitis C is Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Campesterol	Not Applicable	Not Applicable	Failed
Malvidin	-16.78	-21.37	Positive
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 Malvidin helped deactivate the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme of the organism causing Hepatitis C.

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

Activity of Zingiber officinale against Hepatitis C through deactivation of Hepatitis C Virus IRES Pseudoknot domain

(3T4B)

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Abstract: An in-silico study was performed to determine the activity of Zingiber officinale against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. It was found that Peonidin helped to prevent Hepatitis C.

Introduction: Zingiber officinale is known for its medicinal activities. It is a spice consumed worldwide for culinary and medicinal purposes. The plant has a number of chemicals responsible for its medicinal properties, such as antiarthritis, antiinflammatory, antidiabetic, antibacterial, antifungal, anticancer, etc.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Zingiberales
Family	Zingiberaceae
Genus	Zingiber
Species	officinale

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 Hepatitis C is Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Naringin	Not Applicable	Not Applicable	Failed
Daidzein	Not Applicable	Not Applicable	Failed
Peonidin	-11.29	-16.27	Positive
Zingiberene	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 Hepatitis C Virus IRES Pseudoknot domain

(3T4B) enzyme of the organism causing Hepatitis C.

Conclusions: The molecular docking study showed that Zingiber officinale can prevent Hepatitis C due to the presence of Peonidin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Zingiber officinale against Hepatitis C through deactivation of Hepatitis C Virus protease (3M5O)

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Abstract: An in-silico study was performed to determine the activity of Zingiber officinale against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus protease (3M5O) enzyme. It was found that Naringin and Zingiberene helped to prevent Hepatitis C.

Introduction: Zingiber officinale is known for its medicinal activities. It is a spice consumed worldwide for culinary and medicinal purposes. The plant has a number of chemicals responsible for its medicinal properties, such as antiarthritis, antiinflammatory, antidiabetic, antibacterial, antifungal, anticancer, etc.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Zingiberales
Family	Zingiberaceae
Genus	Zingiber
Species	officinale

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 Hepatitis C is Hepatitis C Virus protease (3M5O) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus protease (3M5O) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Naringin	-13.28	-18.61	Positive
Daidzein	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Zingiberene	-7.59	-12.54	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Naringin and Zingiberene helped deactivate the Hepatitis C Virus protease (3M5O) enzyme of the organism causing Hepatitis C.

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

Activity of Agrimonia eupatoria against Hepatitis C through deactivation of Hepatitis C Virus protease

(3M5O)

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Abstract: An in-silico study was performed to determine the activity of Agrimonia eupatoria against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus protease

(3M5O) enzyme. It was found that Phenyl isothiocyanate helped to prevent Hepatitis C.

Introduction: Agrimonia eupatoria is known for its medicinal activities. It is used as a folk remedy for asthma, bronchitis, dermatitis, entorrhagia, enuresis, gastrorrhagia, hematuria, hepatosis, metrorrhagia and neuralgia.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Rosales
Family	Rosaceae
Genus	Agrimonia
Species	eupatoria

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus protease

(3M5O) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus protease

(3M5O) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Resveratrol	Not Applicable	Not Applicable	Failed
Phenyl isothiocyanate	-13.63	-17.25	Positive
Rutin	Not Applicable	Not Applicable	Failed
Ferulic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Phenyl isothiocyanate helped deactivate the Hepatitis C Virus protease

(3M5O) enzyme of the organism causing Hepatitis C.

Conclusions: The molecular docking study showed that Agrimonia eupatoria can prevent Hepatitis C due to the presence of Phenyl isothiocyanate. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Alpinea galanga against Hepatitis C through deactivation of Hepatitis C Virus protease

(3M5O)

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Abstract: An in-silico study was performed to determine the activity of Alpinea galanga against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus protease

(3M5O) enzyme. It was found that Tangeretin helped to prevent Hepatitis C.

Introduction: Alpinea galanga is known for its medicinal activities. Alpinia is a plant related to ginger. The horizontal underground stem (rhizome) is used to make medicine. Alpinia is used to treat fever, muscle spasms, intestinal gas, and swelling (inflammation); to kill bacteria; and as a stimulant.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Zingiberales
Family	Zingiberaceae
Genus	Alpinea
Species	galanga

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus protease

(3M5O) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus protease

(3M5O) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Cryptoxanthin	Not Applicable	Not Applicable	Failed
Tangeretin	-12.15	-15.37	Positive
Salicylic acid	Not Applicable	Not Applicable	Failed
Limonene	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Tangeretin helped deactivate the Hepatitis C Virus protease

(3M5O) enzyme of the organism causing Hepatitis C.

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

Activity of Bupleurum sp. against Hepatitis C through deactivation of Hepatitis C Virus protease

(3M5O)

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Abstract: An in-silico study was performed to determine the activity of Bupleurum sp. against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus protease

(3M5O) enzyme. It was found that Tannic acid helped to prevent Hepatitis C.

Introduction: Bupleurum sp. is known for its medicinal activities. Bupleurum is used for respiratory infections, including the flu (influenza), swine flu, the common cold, bronchitis, and pneumonia; and symptoms of these infections, including fever and cough.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Apiales
Family	Apiaceae
Genus	Bupleurum
Species	scorzonerifolium

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus protease

(3M5O) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus protease

(3M5O) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Tangeretin	Not Applicable	Not Applicable	Failed
Tannic acid	-13.61	-18.34	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 Tannic acid helped deactivate the Hepatitis C Virus protease

(3M5O) enzyme of the organism causing Hepatitis C.

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

Activity of Glycyrrhiza glabra against Hepatitis C through deactivation of Hepatitis C Virus protease

(3M5O)

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Abstract: An in-silico study was performed to determine the activity of Glycyrrhiza glabra against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus protease

(3M5O) enzyme. It was found that Daidzein and Quercetin helped to prevent Hepatitis C.

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. Genistein
b. Daidzein
c. Theobromine
d. Quercetin

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus protease

(3M5O) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus protease

(3M5O) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Genistein	Not Applicable	Not Applicable	Failed
Daidzein	-10.57	-14.57	Positive
Theobromine	Not Applicable	Not Applicable	Failed
Quercetin	-12.08	-15.27	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Daidzein and Quercetin helped deactivate the Hepatitis C Virus protease

(3M5O) enzyme of the organism causing Hepatitis C.

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

Activity of Hypericum perforatum against Hepatitis C through deactivation of Hepatitis C Virus protease

(3M5O)

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Abstract: An in-silico study was performed to determine the activity of Hypericum perforatum against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus protease

(3M5O) enzyme. It was found that Azadirichtin helped to prevent Hepatitis C.

Introduction: Hypericum perforatum is known for its medicinal activities. It is used tropically for the treatment of wounds, abrasions, burns, sunburns and inflammatory skin disorders. Its use in wound healing could be justified with its anti-inflammatory, antimicrobial and astringent effects.

The plant is classified as follows:

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

Major phytochemicals present in the plant are:

a. Pelargonidin
b. Limonene
c. Rutin
d. Azadirichtin

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus protease

(3M5O) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus protease

(3M5O) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelargonidin	Not Applicable	Not Applicable	Failed
Limonene	Not Applicable	Not Applicable	Failed
Rutin	Not Applicable	Not Applicable	Failed
Azadirichtin	-15.49	-19.62	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Azadirichtin helped deactivate the Hepatitis C Virus protease

(3M5O) enzyme of the organism causing Hepatitis C.

Conclusions: The molecular docking study showed that Hypericum perforatum can prevent Hepatitis C due to the presence of Azadirichtin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Oenanthe javanica against Hepatitis C through deactivation of Hepatitis C Virus protease

(3M5O)

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Abstract: An in-silico study was performed to determine the activity of Oenanthe javanica against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus protease

(3M5O) enzyme. It was found that Ferulic acid helped to prevent Hepatitis C.

Introduction: Oenanthe javanica is known for its medicinal activities. Oenanthe javanica, popularly known as water dropwort, has long been used in various ethnomedical systems in Asia, especially in China, Korean, and Japan, for treating various chronic and acute hepatitis, jaundice, alcohol hangovers, abdominal pain, and inflammatory conditions.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Apiales
Family	Apiaceae
Genus	Oenanthe
Species	javanica

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Astaxanthin
c. Digoxin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus protease

(3M5O) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus protease

(3M5O) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Astaxanthin	Not Applicable	Not Applicable	Failed
Digoxin	Not Applicable	Not Applicable	Failed
Ferulic acid	-12.31	-20.54	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Ferulic acid helped deactivate the Hepatitis C Virus protease

(3M5O) enzyme of the organism causing Hepatitis C.

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

Activity of Pericampylus glaucus against Hepatitis C through deactivation of Hepatitis C Virus protease

(3M5O)

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Abstract: An in-silico study was performed to determine the activity of Pericampylus glaucus against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus protease

(3M5O) enzyme. It was found that Theobromine and Tannic acid helped to prevent Hepatitis C.

Introduction: Pericampylus glaucus is known for its medicinal activities. The mucilage resulting from soaking the pounded leaves overnight is taken orally to cure a swollen spleen and accompanying fever.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Ranunculales
Family	Menispermaceae
Genus	Pericampylus
Species	glaucus

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus protease

(3M5O) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus protease

(3M5O) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	Not Applicable	Not Applicable	Failed
Alliin	Not Applicable	Not Applicable	Failed
Theobromine	-14.29	-15.37	Positive
Tannic acid	-11.38	-17.24	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Theobromine and Tannic acid helped deactivate the Hepatitis C Virus protease

(3M5O) enzyme of the organism causing Hepatitis C.

Conclusions: The molecular docking study showed that Pericampylus glaucus can prevent Hepatitis C due to the presence of Theobromine and Tannic acid. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Phyllanthus amarus against Hepatitis C through deactivation of Hepatitis C Virus protease

(3M5O)

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Abstract: An in-silico study was performed to determine the activity of Phyllanthus amarus against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus protease

(3M5O) enzyme. It was found that Sulforaphane and Rosmarinic acid helped to prevent Hepatitis C.

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. Sulforaphane
b. Digoxin
c. Isorhamnetin
d. Rosmarinic acid

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus protease

(3M5O) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus protease

(3M5O) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	-12.57	-16.54	Positive
Digoxin	Not Applicable	Not Applicable	Failed
Isorhamnetin	Not Applicable	Not Applicable	Failed
Rosmarinic acid	-9.64	-12.32	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Sulforaphane and Rosmarinic acid helped deactivate the Hepatitis C Virus protease

(3M5O) enzyme of the organism causing Hepatitis C.

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

Activity of Phyllanthus urinaria against Hepatitis C through deactivation of Hepatitis C Virus protease

(3M5O)

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Abstract: An in-silico study was performed to determine the activity of Phyllanthus urinaria against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus protease

(3M5O) enzyme. It was found that Daidzein helped to prevent Hepatitis C.

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

The plant is classified as follows:

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

Major phytochemicals present in the plant are:

a. Limonene
b. Naringin
c. Genistein
d. Daidzein

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus protease

(3M5O) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus protease

(3M5O) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Limonene	Not Applicable	Not Applicable	Failed
Naringin	Not Applicable	Not Applicable	Failed
Genistein	Not Applicable	Not Applicable	Failed
Daidzein	-13.64	-19.61	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Daidzein helped deactivate the Hepatitis C Virus protease

(3M5O) enzyme of the organism causing Hepatitis C.

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

Activity of Picrorhiza kurroa against Hepatitis C through deactivation of Hepatitis C Virus protease

(3M5O)

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Abstract: An in-silico study was performed to determine the activity of Picrorhiza kurroa against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus protease

(3M5O) enzyme. It was found that Luteolin helped to prevent Hepatitis C.

Introduction: Picrorhiza kurroa is known for its medicinal activities. Picrorhiza kurroa is a well-known herb in the Ayurvedic system of medicine and has traditionally been used to treat disorders of the liver and upper respiratory tract, reduce fevers, and to treat dyspepsia, chronic diarrhea, and scorpion sting.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Eudicots
Order	Lamiales
Family	Phyllanthaceae
Genus	Picrorhiza
Species	kurroa

Major phytochemicals present in the plant are:

a. Luteolin
b. Isorhamnetin
c. Curcumin
d. Ascorbic acid

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus protease

(3M5O) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus protease

(3M5O) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Luteolin	-17.54	-19.66	Positive
Isorhamnetin	Not Applicable	Not Applicable	Failed
Curcumin	Not Applicable	Not Applicable	Failed
Ascorbic acid	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Luteolin helped deactivate the Hepatitis C Virus protease

(3M5O) enzyme of the organism causing Hepatitis C.

Conclusions: The molecular docking study showed that Picrorhiza kurroa can prevent Hepatitis C due to the presence of Luteolin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Potentila anserine against Hepatitis C through deactivation of Hepatitis C Virus protease

(3M5O)

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Abstract: An in-silico study was performed to determine the activity of Potentila anserine against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus protease

(3M5O) enzyme. It was found that Lupeol helped to prevent Hepatitis C.

Introduction: Potentila anserine is known for its medicinal activities. The whole plant is antispasmodic, mildly astringent, diuretic, foot care, haemostatic, odontalgic and tonic.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Rosales
Family	Rosaceae
Genus	Potentilla
Species	anserine

Major phytochemicals present in the plant are:

a. Lupeol
b. Peonidin
c. Limonene
d. Malvidin

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus protease

(3M5O) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus protease

(3M5O) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lupeol	-14.23	-18.94	Positive
Peonidin	Not Applicable	Not Applicable	Failed
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 Lupeol helped deactivate the Hepatitis C Virus protease

(3M5O) enzyme of the organism causing Hepatitis C.

Conclusions: The molecular docking study showed that Potentila anserine can prevent Hepatitis C due to the presence of Lupeol. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Ranunculus scleratus against Hepatitis C through deactivation of Hepatitis C Virus protease

(3M5O)

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Abstract: An in-silico study was performed to determine the activity of Ranunculus scleratus against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus protease

(3M5O) enzyme. It was found that Theobromine helped to prevent Hepatitis C.

Introduction: Ranunculus scleratus is known for its medicinal activities. The whole plant has anti-inflammatory, analgesic, sedative and expectorant properties and it is recommended against skin diseases such as eczema, herpes, pruritus, burns and swellings.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Ranunculales
Family	Ranunculaceae
Genus	Ranunculus
Species	sceleratus

Major phytochemicals present in the plant are:

a. Theobromine
b. Daidzein
c. Peonidin
d. Limonene

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus protease

(3M5O) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus protease

(3M5O) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	-13.22	-16.54	Positive
Daidzein	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Limonene	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Theobromine helped deactivate the Hepatitis C Virus protease

(3M5O) enzyme of the organism causing Hepatitis C.

Conclusions: The molecular docking study showed that Ranunculus scleratus can prevent Hepatitis C due to the presence of Theobromine. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Rubia cardifolia against Hepatitis C through deactivation of Hepatitis C Virus protease

(3M5O)

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Abstract: An in-silico study was performed to determine the activity of Rubia cardifolia against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus protease

(3M5O) enzyme. It was found that Malvidin helped to prevent Hepatitis C.

Introduction: Rubia cardifolia is known for its medicinal activities. Rubia cordifolia role in supporting heart health is evidenced by traditional and reported activities which show that it act as potent blood purifier, antioxidant, diuretic, calcium channel blocker, antiplatelet, antidiabetic, antiinflammatory, antistress, immunomodulator etc.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Gentianales
Family	Rubiaceae
Genus	Rubia
Species	cordifolia

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus protease

(3M5O) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus protease

(3M5O) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Theobromine	Not Applicable	Not Applicable	Failed
Peonidin	Not Applicable	Not Applicable	Failed
Limonene	Not Applicable	Not Applicable	Failed
Malvidin	-11.31	-18.38	Positive

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Malvidin helped deactivate the Hepatitis C Virus protease

(3M5O) enzyme of the organism causing Hepatitis C.

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

Activity of Saussurea lappa against Hepatitis C through deactivation of Hepatitis C Virus protease

(3M5O)

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Abstract: An in-silico study was performed to determine the activity of Saussurea lappa against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus protease

(3M5O) enzyme. It was found that Daidzein helped to prevent Hepatitis C.

Introduction: Saussurea lappa is known for its medicinal activities. In Unani system of medicine it is used for carminative, aphrodisiac, anthelmintic, tonic, stimulates the brain, used in diseases of liver, kidney and blood. It also used for treating deaf, headache, paralysis, asthma, cough, old fever, inflammation, and ophthalmic conditions.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Asterales
Family	Asteraceae
Genus	Saussurea
Species	lappa

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus protease

(3M5O) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus protease

(3M5O) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Lutein	Not Applicable	Not Applicable	Failed
Genistein	Not Applicable	Not Applicable	Failed
Daidzein	-10.55	-14.94	Positive
Theobromine	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Daidzein helped deactivate the Hepatitis C Virus protease

(3M5O) enzyme of the organism causing Hepatitis C.

Conclusions: The molecular docking study showed that Saussurea lappa can prevent Hepatitis C due to the presence of Daidzein. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Terminalia chebula against Hepatitis C through deactivation of Hepatitis C Virus protease

(3M5O)

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Abstract: An in-silico study was performed to determine the activity of Terminalia chebula against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus protease

(3M5O) enzyme. It was found that Daidzein helped to prevent Hepatitis C.

Introduction: Terminalia chebula is known for its medicinal activities. Its powder is a good astringent dentifrice in loose gums, bleeding and ulceration in gums. It is good to increase appetite, digestive aid, liver stimulant, stomachic, gastrointestinal prokinetic agent, and mild laxative. The powder of T. chebula fruits has been used in chronic diarrhea.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Myrtales
Family	Combretaceae
Genus	Terminalia
Species	chebula

Major phytochemicals present in the plant are:

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

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus protease

(3M5O) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus protease

(3M5O) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Pelletierine	Not Applicable	Not Applicable	Failed
Daidzein	-11.66	-17.45	Positive
Alliin	Not Applicable	Not Applicable	Failed
Campesterol	Not Applicable	Not Applicable	Failed

Based on the values of C-Docker energy and C-Docker interaction energy it was found that Daidzein helped deactivate the Hepatitis C Virus protease

(3M5O) enzyme of the organism causing Hepatitis C.

Conclusions: The molecular docking study showed that Terminalia chebula can prevent Hepatitis C due to the presence of Daidzein. Experimental studies are required to validate the results obtained by *in-silico* analysis.

Activity of Wrightia tinctoria against Hepatitis C through deactivation of Hepatitis C Virus protease

(3M5O)

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Abstract: An in-silico study was performed to determine the activity of Wrightia tinctoria against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus protease

(3M5O) enzyme. It was found that Myricetin helped to prevent Hepatitis C.

Introduction: Wrightia tinctoria is known for its medicinal activities. It is the most commonly prescribed Siddha herbal medication for skin diseases, in specific psoriasis. The "777 oil" made from the fresh leaves of the plant exhibits various analgesic, anti-inflammatory, and antipyretic activities and it is a highly cited medication for the treatment of psoriasis.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Gentianales
Family	Apocynaceae
Genus	Wrightia
Species	tinctoria

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 Hepatitis C is Hepatitis C Virus protease

(3M5O) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus protease

(3M5O) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Campesterol	Not Applicable	Not Applicable	Failed
Malvidin	Not Applicable	Not Applicable	Failed
Myricetin	-16.59	-21.64	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 Hepatitis C Virus protease

(3M5O) enzyme of the organism causing Hepatitis C.

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

Activity of Oenanthe javanica against Hepatitis C through deactivation of Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL)

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Abstract: An in-silico study was performed to determine the activity of Oenanthe javanica against Hepatitis C. Molecular docking using Biovia Discovery Studio was performed to identify the phytochemical responsible to deactivate Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. It was found that Astaxanthin helped to prevent Hepatitis C.

Introduction: Oenanthe javanica is known for its medicinal activities. Oenanthe javanica, popularly known as water dropwort, has long been used in various ethnomedical systems in Asia, especially in China, Korean, and Japan, for treating various chronic and acute hepatitis, jaundice, alcohol hangovers, abdominal pain, and inflammatory conditions.

The plant is classified as follows:

Kingdom	Plantae
Division	Tracheophyta
Class	Magnoliopsida
Order	Apiales
Family	Apiaceae
Genus	Oenanthe
Species	javanica

Major phytochemicals present in the plant are:

a. Sulforaphane
b. Astaxanthin
c. Digoxin
d. Ferulic acid

One of the major enzymes required for the survival of the organism causing Hepatitis C is Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme. The objective of this work is to find the phytochemical that can deactivate the enzyme, thereby preventing the physiological activity of the organism.

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

Results and discussion: The result of molecular docking is presented in Table 1. "Positive" in the remarks column indicated that the phytochemical is capable of deactivating the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme.

Phytochemical	CDocker energy	CDocker interaction energy	Remarks
Sulforaphane	Not Applicable	Not Applicable	Failed
Astaxanthin	-13.82	-22.54	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 Astaxanthin helped deactivate the Hepatitis C Virus RNA-Dependent RNA polymerase (5PZL) enzyme of the organism causing Hepatitis C.

Conclusions: The molecular docking study showed that Oenanthe javanica can prevent Hepatitis C due to the presence of Astaxanthin. Experimental studies are required to validate the results obtained by *in-silico* analysis.

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