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Prediction of anti-viral activity of *Ipomoea carnea*

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Abstract

There arenumerous species of viruseswhich affects human health and causes fatalities. Some major disease causing viruses are Hepatitis B, Picornavirus, Rhinovirus, Human Immunodeficiency Virus (HIV), Herpes virus, Adenovirus, Influenza virus, Cytomegalovirus (CMV), Poxvirus, Hepatitis C etc.lpomoea carnea can be an alternative for treatment against these viral infections.
Through in-silicoprediction study, this article is aimed for prediction of anti-viral potential of active chemical constituents of Ipomoea carneausing PASS online prediction tool. From the prediction it has been concluded that Swainsonine, Squalene, 2-Ethyl-l,3-dimethylbenzene, Hexadecanoic Acid, Linoleic Acid, I-Octadecanol, Stearic Acid, 1,2-Diethylphthalate, Octacosane, Hexatriacontane and Tetracontane shows profoundanti-viral potential.

Keywords
Anti-viral, Drug design,ln-si/ico study, Ipomoea carnea, PASS online.

Introduction

In this growing world, large number of new infections and diseases comes in existence. These infections and diseases affect the health of human beings and sometimes they may be fatal. There were large number of viruses that affect human being and some of them are as follows Hepatitis B, Picornavirus, Rhinovirus, Human Immunodeficiency Virus (HIV), Herpes virus, Adenovirus, Influenza virus, Cytomegalovirus (CMV), Poxvirus, Hepatitis C etc.
Picornavirus belongs to the family Piconaviridae, order Picornavirales. Picornavirus is a

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RNA virus, infect Mammals and birds. These viruses are generally nonenveloped which show a genetic makeup of positive-sense single-stranded RNA viruses, and live in clusters forming a large family. They generally contain icosahedral capsid of 30-11m. Viruses o this family are able to cause large number of diseases paralysis, meningitis, hepatitis, poliomyelitis (Lau et al. 2011).

Rhinovirus belongs to family Picornaviridae, genus Enterovirus. Rhinovirus causes Common cold and shows its harmful effects at temperature of 33-35 ^{0}C (91—95 ^{O}F). Rhinovirus shows its effects generally over nose because nose provided the same temperature that it requires for showing its effects. Interferon-alpha is generally used Intra-nasally to provide relief from Rhinovirus infection.

Herpes simplex virus can be categorized in 2 categories, which are as follows I-ISV-I (Herpes simplex virms-l) and I-ISV-2 (Herpes simplex vilus-2). HSV-I can be noted as Human alphaherpesvinls-l and HSV-2 can be noted as Human alphaherpesvirus-2, belonging to family Herpesviridae (Chayavichitsilp et al. 2009).HSV-l & HSV-2 were generally spread by oral-to-oral contact and sexual contact respectively. According to WHO, Globally there were around 3.7 billion peoples affected by HSV-I infection that generally lies under the age 50 (67%), and 491 million peoples were affected by Hsv-2 infection. Some antiviral chugs are used to decrease the severity of HSV infection are as follows acyclovir, famciclovir and valacyclovir.

Human alpha herpesvinls 3 (HHV-3), is also known as Varicell-Zoster Virus. Varicell-Zoster Virus can be noted as Varicella Virus, and Zoster Virus, Chickenpox Virus. This virus also affects human beings and it is also capable to survive in external environments for maximum uptodays. Some antiviral dimgs are used for the treatment of HE-IV-3 and some of them are as follows, for chicken pox acyclovir is used, for Shingles famciclovir, valaciclovir is used and Varicell-Zoster Virus Immune Globulin, Vidarabine, Zoster-Immune Globulin (ZIG) can be used.

Adenovirus belongs to family Adenoviridae are generally 90-100 nm In size. They are generally nonenveloped viruses that have an icosahedral nucleocapsid which contain ds-DNA genome. They were first time named in 1953. Adenovirus affects the body in many ways by causing the illness, on young ones it show little infections of respiratory system, diseases which are fatal and are associated with more than one organ m peoples who have weak immunity. In severely affected patients cidofovir can help to relieve from complications.

Cytomegalovirus (CMV) belongs to family Herpesviridae, order Herpesvirales(Anshu et al. 2017). In the genus Cytomegalovims eight species were found and from which Human ßHerpes Virus 5 infect peoples. HI-IV-5 causes mononucleosis and pneumonia. For non severe CMV the dilig valganciclovir is used and ganciclovir is used as a drug of choice for CMV treatment(Elion et al. 1977).

Poxvirus belongs to family Poxviridae. It uses human beings, vertebrates and arthropods as a host. Poxvirus mainly causes smallpox.

There are mainly five types of hepatitis virus. Hepatitis type-B virus causes Hepatitis type-B , belongs to family hepadnavirus. Hepatitis C virus (HCV) causes Hepatitis type-C, the virus of family flaviviridae.Generally type B & C is responsible for lifelong disease which includes liver cirrhosis, cancer related deaths. According to WHO report, Globally there were around 325 million peoples are suffering from hepatitis B and/or C. Mostly observed symptoms of

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hepatitis type-A, type-B and type-C includes diarrhea, rise in body temperature, restlessness, loss of hunger, dark-coloured urine, sickness, abdominal ache and hyperbilimbinemia. Prevention and treatment of different types of Hepatitis can be possible that consists of Type A, B and C but the treatment of Type C is very costly.

Globally, 500000 to 1200000 peoples were died every year due to Hepatitis B complications. Human Immunodeficiency Virus (HIV) comes m genus Lenti-Virus (a subgroup of retrovums) and the family Retroviridae. After some time (few days to years) it causes AIDS (cause acquired immunodeficiency syndrome).Once a person reaches to this stage then his immune system progressively fails and the person will get life threatening opportunistic infections and sometimes cancer also. HIV patient can survive for 9-11 years without treatment.According to WHO, at the end of 2019 there were an estimated 38.0 million peoples infected from HIV Worldwide, 690,00 peoples were died due to HIV virus and 1.7 million new cases were found in the year 2019 Globally.

Humanparainfluenza viruses (HPIVs) causeshuman parainfluenza. HPIV belongs to family Paramyxoviridae. Ribavirin and Protein inhibitor is one of the medication that is used for provide relieve from symptoms of HPIV.

Influenza can also be noted as Flu and the organism behind causing it is influenza virus. Indications of Influenza virus are throat discomfort, muscle and joint ache, cold, Rhinorrhea, excessive rise in body temperature and fatigue. Four type f Influenza viruses are as follows Influenza viruses Type-A, Influenza viruses Type-B, and Influenza viruses Type-C &lnfluenza viruses Type-D. In 2017 around about 2,90,000 peoples were extremely infected by Influenza Virus and 6,50,000 peoples were died throughout the world.There were about 3 episodes of Influenza virus Pandemic have been already happened in 20th Century that are Spanish influenza Pandemic (1918), Asian influenza Pandemic (1957), and Hong Kong influenza Pandemic (1968).

It has long been recognized that natural products represent the richest source of high chemical diversity, providing the basis for identification of novel scaffold structures that serves as starting points for rational drug design(Dhiman, 2020). Human civilization has used natural sources for maintaining diverse health-related issues since time immortal by traditional healers (Dhiman et al., 2017). Literature revealed that the ingestion of bioactive compound from fruits and vegetables is associated with the reduced risk of many common forms of cancer and many other harmful diseases like tuberculosis(Garg V et al., 2019). The early symptoms developed can be characterized by dry cough, fever, lethargy and weight loss (Xu et al., 2021). Herbal remedies derived from plants and their products have been used since ancient times(Saini et al. 2020a;Saini et al. 2018) as therapeutic agents, attributed to various pharmacological activities v.i.z. anti-depressant, antioxidant, anti-inflammatory, analgesic, anti-fertility, antimutagenic, larvicidal, anthelmintic activity etc. (Saini et al, 2020b; Dhiman et al., 2017).Several medicinal plants are widely being used in Ayurvedic preparations (Shirwaikar et al. 2007) and contain a large number of secondary plant metabolites, which are of great therapeutic significance (Saini et al., 2016). Flavonoids are the main components of a healthy diet (Dhiman et al. 2016).

Alongwith herbal medicines, nutraceuticals and food supplements are claimed to be beneficial in several disease conditions which include cardiovascular disorder, neurodegenerative disorders, metabolic disorders and cancer prevention (Bansal & Dhiman, 2020). These may be

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explored for the production of natural medicinal formulations in pharmaceutical dimg industries for several disorders on account of potential antioxidant activity (Bhilana et al., 2018).Due to fascinating properties and biomedical applications, there is an immense necessity to explore newer prospective in the field of complementary and alternative medicine. This is one of the reasons that efforts have been directed to discover promising therapeutic agents from natural sources.

Ipomoea carnea is the herbal plant of family Convolvulaceae, is also known by its other name such as Bush Morning Glory. Ipomoea carnea is also known for its large number of biological activities such as immuno-modulatory activity (Kunal et al. 2021), antioxidant activity, anticancer activity. Immunomodulatory activity enhances immunity which ultimately helps humans to fight against bacterial and viral infections, thus it also exhibits anti-viral activity.
Antiviral activity of Ipomoea carnea were predicted from way 2 drag tool with the help of molecular structures of active chemical constituents of Ipomoea carnea(Poroikov et al.2003). The antiviral activity of active chemical constituents of Ipomoea carnea were predicted on the basis of Probable value,P= l/nEPa/(Pa+Pi). The constituent who seems to exhibit higher P value gives better biological potential.

Materials and methods

Prediction of anti-viral activity by PASS online tool

The anti-viral activity of active chemical constituents (de Balogh et al. 1999)of Ipomoea carnea was predicted by Bioinformatic tool https: www.way2drug.com on the basis of their molecular structures. This tool includes PASS online server that helps in predicting the antiviral activity of the active chemical constituents of Ipomoea carnea.

Insilicoscreening of anti- viral activity by PASS online

The antiviral activity of active chemical constituents of Ipomoea carnea was predicted by transferring the Smile structures in the search bar column and the results obtained were collected and stored in xls. format.

Data analysis

The results obtained were analyzed by observing the P_a value of the active chemical constituents of *Ipomoea carnea*. Those chemical constituents of *Ipomoea carnea* which seems to have P_a value greater than 0.5 exhibit potent antiviral activity. The predicted values of anti-viral activity of active chemical constituents present in *Ipomoea carnea*are given in Table 1,2,3,4,5.

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Table 1: Predicted values of antiviral activity against Picornavirus, Rhinovirus and Herpesvirus

Active Chemical Constituents	Antiviral (Picornavirus)		Antiviral (Rhinovirus)		Antiviral (Herpes)	
	Pa	Pi	Pa	Pi	Pa	Pi
Swainsonine	0.502	0.049	0.392	0.099	0.268	0.115
Squalene	0.597	0.019	0.571	0.009	0.423	0.026
2-Ethyl-1,3-dimethylbenzene	0.58	0.024	0.573	0.009	0.266	0.117
2-(12-Pentadecynyloxy)-tetrahydro2H-pyran	0.313	0.207	0.402	0.089	0.273	0.111
Hexadecanoic Acid	0.671	0.008	0.611	0.005	0.414	0.03
Linoleic Acid	0.597	0.02	0.623	0.005	0.421	0.027
Epiglobulol	0.442	0.08	0.335	0.185	0.31	0.085
1-Octadecanol	0.666	0.009	0.642	0.004	0.442	0.02
Stearic Acid	0.671	0.008	0.611	0.005	0.414	0.03
1, 2-diethyl phthalate	0.688	0.007	0.629	0.005	0.309	0.085
Octacosane	0.681	0.007	0.645	0.004	0.412	0.03
Hexatriacontane	0.681	0.007	0.645	0.004	0.412	0.03
Tetracontane	0.681	0.007	0.645	0.004	0.412	0.03
3-diethylamino-1-propanol	0.488	0.055	0.451	0.048	0.408	0.032
Calystegine B1	0.454	0.073	0.406	0.085	0.385	0.042
Calystegine B2	0.492	0.054	-	-	0.406	0.033
Calystegine C1	0.492	0.054	-	-	0.4	0.035

Table 2: Predicted values of antiviral activity against Herpesvirus Human, Adenovirus and CMV

Active Chemical Constituents	Antiviral (Herpesvirus 3, Human)		Antiviral (Adenovirus)		Antiviral (CMV)	
	Pa	Pi	Pa	Pi	Pa	Pi
Swainsonine	-	-	0.299	0.09	0.216	0.142
Squalene	0.013	0.006	0.48	0.008	0.366	0.008
2-Ethyl-1,3-dimethylbenzene	-	-	0.455	0.013	0.297	0.031
2-(12-Pentadecynyloxy)-tetrahydro2H-pyran	-	-	-	-	0.283	0.041
Hexadecanoic Acid	0.017	0.004	0.519	0.005	0.502	0.003
Linoleic Acid	0.017	0.004	0.461	0.011	0.533	0.002
Epiglobulol	-	-	0.332	0.065	0.26	0.064
1-Octadecanol	0.022	0.003	0.528	0.004	0.489	0.003
Stearic Acid	0.017	0.004	0.519	0.005	0.502	0.003
1, 2-diethyl phthalate	-	-	0.546	0.004	0.358	0.009
Octacosane	0.032	0.002	0.522	0.005	0.443	0.004
	0.032	0.002	0.522	0.005	0.443	0.004

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Hexatriacontane	0.032	0.002	0.522	0.005	0.443	0.004
Tetracontane	-	-	0.437	0.017	0.329	0.016
3-diethylamino-1-propanol	-	-	0.289	0.098	0.216	0.14
Calystegine B1	-	-	0.317	0.076	0.251	0.076
Calystegine B2	-	-	0.317	0.076	0.229	0.111
Calystegine C1						

Table 3: Predicted values of antiviral activity against Poxvirus and Hepatitis

Active Chemical Constituents	Antiviral (Poxvirus)		Antiviral (Hepatitis)	
	Pa	Pi	Pa	Pi
Swainsonine	0.259	0.088	0.273	0.005
Squalene	0.299	0.059	0.111	0.084
2-Ethyl-1,3-dimethylbenzene	0.194	0.168	-	-
2-(12-Pentadecynyloxy)-tetrahydro2H-pyran	-	-	-	-
Hexadecanoic Acid	0.608	0.014	0.151	0.033
Linoleic Acid	0.429	0.026	-	-
Epiglobulol	0.205	0.152	0.159	0.028
1-Octadecanol	0.431	0.025	-	-
Stearic Acid	0.608	0.014	0.151	0.033
1, 2-diethyl phthalate	0.272	0.077	-	-
Octacosane	0.486	0.021	-	-
Hexatriacontane	0.486	0.021	-	-
Tetracontane	0.486	0.021	-	-
3-diethylamino-1-propanol	0.368	0.035	-	-
Calystegine B1	0.32	0.05	-	-
Calystegine B2	0.35	0.039	-	-
Calystegine C1	0.35	0.039	-	-

Table 4: Predicted values of antiviral activity against Hepatitis B, Hepatitis C and HIV

Active Chemical Constituents	Antiviral (Hepatitis B)		Antiviral (Hepatitis C)		Antiviral (HIV)	
	Pa	Pi	Pa	Pi	Pa	Pi
Swainsonine	0.2.54	0.049	0,233	0.005	0.228	0.021
Squalene	0.232	0.061	0,100	0.061	0.142	0.075
2-Ethyl-1,3-dimethylbenzene	0.186	0.106	-	-	-	-
2-(12-Pentadecynyloxy)-tetrahydro2H-pyran	0.171	0.132	-	-	-	-
	0.321	0.028	0.132	0.026	-	-

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Hexadecanoic Acid	0.233	0.06	.	-	-	-
Linoleic Acid	0.16	0.157	0.127	0.029	-	-
Epiglobulol	0.265	0.044	-	-	-	-
1-Octadecanol	0.321	0.028	0.132	0.026	-	-
Stearic Acid	0.182	0.112	-	-	-	-
1, 2-diethyl phthalate	0.225	0.065	-	-	-	-
Octacosane	0.225	0.065	-	-	-	-
Hexatriacontane	0.225	0.065	-	-	-	-
Tetracontane	-	-	-	-	-	-
3-diethylamino-1-propanol	-	-	-	-	-	-
Calystegine B1	0.195	0.094	-	-	-	-
Calystegine B2	0.179	0.116	-	-	-	-
Calystegine C1						

Table 5: Predicted values of antiviral activity against Parainfluenza, Influenza and Influenza A

Active Chemical Constituents	Antiviral (Parainfluenza)		Antiviral (Influenza)		Antiviral (Influenza A)	
	Pa	Pi	Pa	Pi	Pa	Pi
Swainsonine	-	-	0.274	0.108	0.224	0.154
Squalene	0.114	0.004	0.434	0.036	0.356	0.016
2-Ethyl-1,3-dimethylbenzene	0.058	0.015	0.572	0.015	0.263	0.079
2-(12-Pentadecynyloxy)-tetrahydro2H-pyran	-	-	-	-	-	-
Hexadecanoic Acid	0.117	0.004	0.565	0.016	0.289	0.049
Linoleic Acid	0.069	0.01	0.599	0.013	0.247	0.104
Epiglobulol	-	-	0.226	0.161	-	-
1-Octadecanol	0.231	0.002	0.516	0.02	0.286	0.052
Stearic Acid	0.117	0.004	0.565	16	0.289	0.049
1, 2-diethyl phthalate	0.111	0.004	0.614	0.012	0.278	0.06
Octacosane	0.168	0.003	0.517	0.02	0.311	0.034
Hexatriacontane	0.168	0.003	0.517	0.02	0.311	0.034
Tetracontane	0.168	0.003	0.517	0.02	0.311	0.034
3-diethylamino-1-propanol	0.06	0.014	0.361	0.06	-	-
Calystegine B1	-	-	-	-	-	-
Calystegine B2	-	-	0.288	0.098	0.219	0.166
Calystegine C1	-	-	0.26	0.122	-	-

Results

Calculation of the data of anti-viral activity of active chemical constituents of *Ipomoea carnea* was done.

In table 1,2,3,4,5 the P_a value of Swainsonine was found to be 0.502 for Picornavirus, Squalene shows P_a value of 0.597 & 0.571 for Picornavirus and Rhinovirus respectively. 2-Ethyl-1,3-

dimethylbenzene shows P_a value of 0.580, 0.573 & 0.572 for Picornavirus, Rhinovirus & Influenza virus respectively. Hexadecanoic Acid shows P_a value of 0.671, 0.611, 0.565, 0.519, 0.502, 0.608 for Picornavirus, Rhinovirus, Influenza virus, Adenovirus, CMV &Poxvirus respectively. Linoleic Acid shows P_a value of 0.597, 0.623, 0.599, 0.533 Picornavirus, Rhinovirus, Influenza virus & CMV respectively. 1-Octadecanol shows P_a value of 0.666, 0.642, 0.516, 0.528 Picornavirus, Rhinovirus, Influenza virus & Adenovirus respectively. Stearic Acid shows P_a value of 0.671, 0.611, 0.565, 0.519, 0.502 & 0.608 for Picornavirus, Rhinovirus, Influenza virus, Adenovirus, CMV & Poxvirus respectively. 1,2-Diethylphthalate shows P_a value of 0.688, 0.629, 0.614 & 0.546 Picornavirus, Rhinovirus, Influenza virus &Adenovirus respectively. Octacosane shows P_a value of 0.681, 0.645, 0.517 & 0.522 Picornavirus, Rhinovirus, Influenza virus & Adenovirus respectively. Hexatriacontane shows P_a value of 0.681, 0.645, 0.517 & 0.522 Picornavirus, Rhinovirus, Influenza virus & Adenovirus respectively. Tetracontane shows P_a value of 0.681, 0.645, 0.517 & 0.522 Picornavirus, Rhinovirus, Influenza virus & Adenovirus respectively. Thus, Swainsonine, Squalene, 2-Ethyl-1,3-dimethylbenzene, Hexadecanoic Acid, Linoleic Acid, 1-Octadecanol, Stearic Acid, 1,2-Diethylphthalate, Octacosane, Hexatriacontane, Tetracontane exhibit potential anti-viral activity.

Conclusion

From the data it is concluded that Ipomoea carneacan be a potential herbal dilig against Picornavirus, Human Immunodeficiency Virus (HIV), Rhinovirus, Herpes virus, Influenza virus, Poxvirus, Adenovirus, Cytomegalovillls (CMV), Hepatitis B and C.

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