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Research article

Prediction of *annona squamosa* by using tools Swiss ADME and PubChem

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ABSTRACT

Annona squamosa L. Belongs to the Annonaceae family and is one of the basic dietary plants.It is edible fruits & called as "custard apple". In Annona squamosa consisting chemical constituent like ferulic acid,chlorogenic acid and caffeic acid etc.The main goal of our study to determination of chemical compound or phytoconstitutents which is predicted by using the ADME/T ,MOL.Soft and also Pubchem software etc.So the ferulic acid having GI absorption rate is good as compared to chlorogenic acid but the comparision between ferulic acid and caffeic acid the caffeic acid determine the high GI absortion.

By using this software we can easily determine the bioavailibity score ,BBB permeation,log k_p permeation. By the help of mol.soft and ADME/T software we can easily analyzed chemical compound. We have to stated that or assurity before any kind of clinical trials conducting. Its help to give the data. In free of cost analysis is done. It also ensure that compound would be safer or not. It also helps to researcher for investigate in vivo and in vitro studies.

Keywords: Mol.soft, Swiss ADME, PubChem, Ferulic Acid, Chromogenic acid, Caffeic acid.

INTRODUCTION

Annona Squamosa is also known as the custard apple it is belonging in an AC family in NSE family consisting 119 species. Recording to Indian council of agriculture research reported that sugar apples are found in the state in India without total planting areas of 14000 hectares. The sugar Apple has been used as a natural other food application the most important source of chemicals which is used as innovative in ingredient in the food. There are different parts of a anasthe masa which is used for the extraction many parts of A. Squamosa expect collected from barud sleeves same fruits sales and seeds which are helps to treat the this is like the area epilepsy bleeding fever and tumor etc. Ananya acetone INS are having long policket I change which has derived from the fat acid with c 35 37. Uvaricin was first reported before the introduction of more than 500 acetone having different organs of the plants belonging family Annonaceae. Custerd apple consis different types of phenolic compound like proanthocynidins & 18 various secondary metabolites mostly alkaloids & flavonoids are used for analysis according to phytochemical research. Due to its wide pharmacological properties & biologiocal activity such as antibacterial, antidiabetic ,antioxidant, antiviral ,hepatoprotective & anticancer activities which caused by presences of glycosides polysteroids sugars oils, saponines, tannins, alkaloids, phenols, flavonoids, peptides & other chemical which produce acyivities. By using this Software Mol. soft, SwissADME, PubChem which helps to analyze & evaluate phytochemicals.

MATERIAL AND METHOD

Collection of phytoconstituents

The bioactive compound of *Annona Squamosa* screening done with the help of previous research paper &

then collected from Swiss ADME software and Wikipedia. Mol.soft and PubChem [4].

Phytochemicals Obtained From A. Squamosa

⇩

By Using Wikipidia Smilies (**Simplified Molecular Input Line Entry System**) of Chemical Compound Taken

⇩

Put Into In SWISS ADME/T Software

⇩

Then it can determine their different parameter.

Methodology

Swiss ADME

It is a one of the tool which can helps to evaluate pharmacokinetics, drug likeness, Lipophilicity, solubility, physicochemical properties & also medicinal chemistry of the small molecules.

It is a free web based tool.it helps to determine ADMET properties by using Swiss ADMET software [2].

PubChem

It is free tool which can detect the following parameters like as follows: Structures, Names and identifiers, Spectral information, Chemical physical properties, Chemical vendors, Food additives and ingredients, Taxonomy, Biological test result, Toxicity [1, 3].

RESULT

Table 1: Physicochemical properties [5].

Name of Compound	Formula	Molecular weight	No. Heavy atoms	No. arom Heavy Metal atoms	Fraction Csp 3	No. Rotatable bonds	No H-Bond Acceptors	No H-Bond Donors	Molar Refractivity
Ferulic Acid	C10H10O4	194.18g/mol	14	06	0.10	03	04	02	51.63
Chromogenic acid	C16H18O9	354.31g/mol	25	06	0.38	05	09	06	83.50
Caffeic acid	C9H8O4	180.16g/mol	13	06	0.00	02	04	03	47.16

Table 2: Lipophilicity [6].

Name of Compound	Log $P_{o/w}$ (iLOGP)	Log $P_{o/w}$ (XLOGP3)	Log $P_{o/w}$ (WLOGP)	Log $P_{o/w}$ (MLOGP)	Log $P_{o/w}$ (SILICOS-IT)	Consensus Log $P_{o/w}$
Ferulic Acid	1.62	1.51	1.39	1.00	1.26	1.36
Chromogenic acid	0.87	-0.42	-0.75	-1.05	-0.61	-0.39
Caffeic acid	0.97	1.15	1.09	0.70	0.75	0.93

Table 3: Water Solubility [8].

Name of Compound	Log S(ESO)	Solubility	Class	Log S(Ali)	Solubility	Class
Ferulic Acid	-2.11	1.49 e+00mg/ml;7.68e-03mol/ I	Soluble	-2.52	5.86e-01 mg/ml ; 3.02e-03 mol/l	Soluble
Chromogenic acid	-1.62	8.50e+00 mg/ml ; 2.40e-02 mol/l	Very soluble	-2.58	9.42e-01 mg/ml ; 2.66e-03 mol/l	soluble
Caffeic acid	-1.89	2.32e+00 mg/ml ; 1.29e-02 mol/l	Very soluble	-2.38	7.55e-01 mg/ml ; 4.19e-03 mol/l	soluble

Table 4: Pharmacokinetics [9].

Name of Compound	GI absorption	BBB permeate	P-gp substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	Log K_p (skin permeation)
Ferulic Acid	Yes	X	X	X	X	X	-6.41
Chromogenic acid	low	X	X	X	X	X	-8.76cm/s
Caffeic acid	High	X	X	X	X	X	-6.58cm/s

Table 5: Drug Likeness [10].

Name of Compound	Lipinski	Ghose	Veber	Egan	Muegge	Bioavailability Score
Ferulic Acid	Yes; 0 Violation	✓	✓	✓	No;1 Violation: MW<200	0.85
Chromogenic acid	Yes;1 violation: NHorOH>5	No; 1 violation: WLOGP<-0.4	No; 1 violation: TPSA>140	No; 1 violation: TPSA>131.6	No; 2 violations: TPSA>150, H-don>5	0.11
Caffeic acid	Yes; 0 violation	✓	✓	✓	No; 1 violation: MW<200	0.56

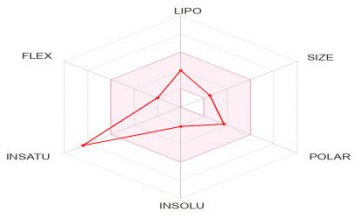
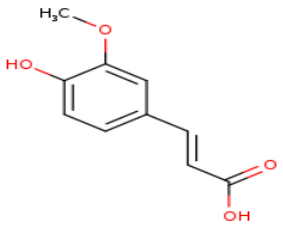
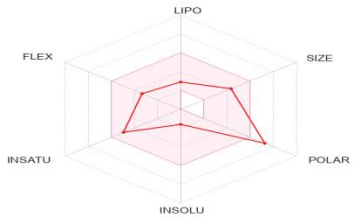
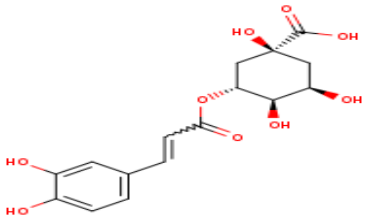
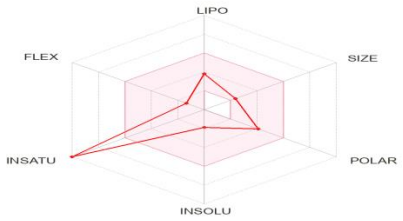
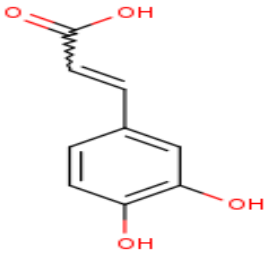
Table 6: Medicinal Chemistry [11].

Name of Compound	PAINS	Brenk	Leadlikeness	Synthetic accessibility
Ferulic Acid	0 alert	1alert:michael_acceptor _1	No;1Violation: MW<200	1.93
Chromogenic acid	1.alert: catechol	2 alerts: catechol, michael_acceptor_1	No; 1 violation: MW>350	4.16
Caffeic acid	1.alert: catechol A	2 alerts: catechol, michael_acceptor_1	No; 1 violation: MW<250	1.81

Structure Uptake From

Radar structure is obtained from SWISS ADMET & 2D chemical structure of ferulic acid ,Chromogenic acid, Caffeic acid taken from PubChem which is as follows in table :-

Table 7: Structure & Topological polar surface area of Ferulic acid, Chromogenic acid, Caffeic acid [12].

Name of Compound	Radar	Structure
Ferulic Acid		
Chlorogenic acid		
Caffeic acid		

CONCLUSION

The clinical trials required more time and more money investment after it might concluded that the molecules fails. Therefore order to reduce modify the leads structure. Which is important for the Invitro study. Swiss ADME software helps to computation of the key such as physicochemical pharmacokinetics drug like and other multiple parameters studies involve it. PubChem is the web tool which also gives the information related to molecules or lead compound. Which can determine the structure name of the chemical compound, toxicity, spectral information etc.

This is concluded that the lead compound analysis done by this two tools which is PubChem and Swiss ADME.

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