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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". It has consisting different phytochemicals such as ferullic acid, chlorogenic acid, caffeic acid. The aim of our study was to carry out to PASS predication investigate potential prediction of activity of phytochemicals. For this purpose computer mechanics developed. In this approaches different software used such as Pubchem, Mol.soft, Swiss ADME/T. The results of these study helps to researcher for investigate *in vivo* & *in vitro* studies. These ensuring that compounds safe for human.

Keywords: Mol.soft, SwissADME, Pubchem, ferrulic acid, chlorogenic 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 rane of 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.

Materials & Methods
Collection of compounds
The bioactive compound of *Annona Squamosa* screening done with the help of previous research paper & then collected from Swiss ADME software and wikipidia.

Methodology
a) 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.

b) 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.'

Result

1. Physicochemical properties

Sr. No.	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
1.	Ferullic Acid	C10H10O4	194.18g/mol	14	06	0.10	03	04	02	51.63
2.	Chlorogenic acid	C16H18O9	354.31g/mol	25	06	0.38	05	09	06	83.50
3.	Caffeic acid	C9H8O4	180.16g/mol	13	06	0.00	02	04	03	47.16

2. Lipophilicity

Sr. No.	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 $P_{o/w}$
1.	Ferullic Acid	1.62	1.51	1.39	1.00	1.26	1.36
2.	Chlorogenic acid	0.87	-0.42	-0.75	-1.05	-0.61	-0.39
3.	Caffeic acid	0.97	1.15	1.09	0.70	0.75	0.93

3. Water Solubility

Sr. No.	Name of Compound	Log S(ESOL)	Solubility	Class	Log S(Ali)	Solubility	Class	Log S (SILICOS-IT)	Solubility	Class
1.	Ferullic 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	-1.42	7.43e+00 mg/ml; 3.83e-02 mol/l	Soluble
2.	Chlorogenic 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	0.40	8.94e+02 mg/ml; 2.52e+00 mol/l	soluble
3.	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	-0.71	3.51e+01 mg/ml; 1.95e-01 mol/l	soluble

4. Pharmacokinetics

Sr. No.	Name of Compound	GI absorption	BBB permeate	P- gp substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor	Log K_p (skin permeation)
1.	Ferullic Acid	Yes	No	No	No	No	No	No	No	-6.41
2.	Chlorogenic acid	Low	No	No	No	No	No	No	No	-8.76cm/s
3.	Caffeic acid	High	No	No	No	No	No	No	No	-6.58cm/s

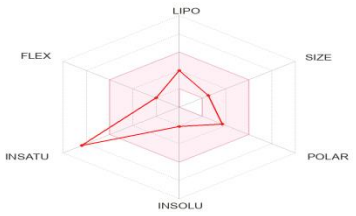
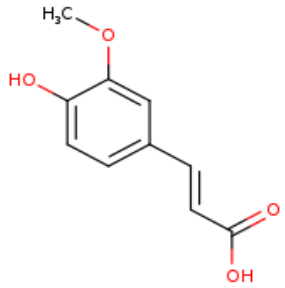
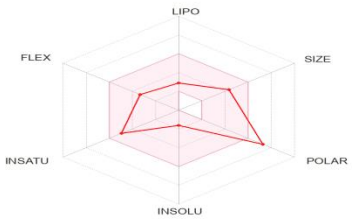
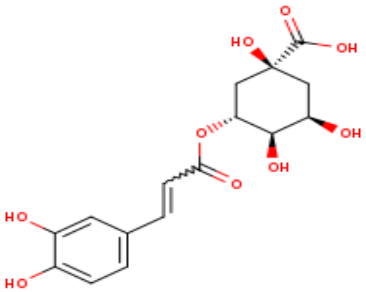
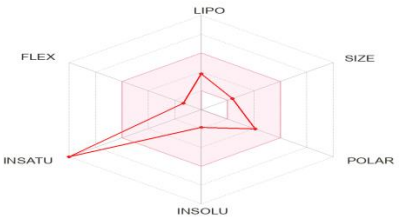
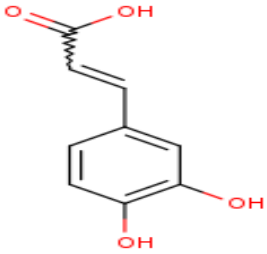
5. Drug Likeness

Sr. No.	Name of Compound	Lipinski	Ghose	Veber	Egan	Muegge	Bioavailability Score
1.	Ferrulic Acid	Yes; 0 Violation	Yes	Yes	Yes	No;1 Violation: MW<200	0.85
2.	Chlorogenic 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
3.	Caffeic acid	Yes; 0 violation	Yes	Yes	Yes	No; 1 violation: MW<200	0.56

6. Medicinal Chemistry

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

Structure & Topological polar surface area of Ferullic acid, Chlorogenic acid, Caffeic acid

Sr. No.	Name of Compound	Radar	Structure
1	Ferullic Acid		
2	Chlorogenic acid		
3	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 *in vitro* 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 another 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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