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Research paper

GCMS and ADME Profiling of Extract from Seeds of *Passiflora edulis*

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ABSTRACT

Passiflora edulis is a tropical fruit from the family *passifloraceae*. It is used as a traditional medicine in the treatment of several ailments. However, preliminary studies and several literature have mentioned these seeds to possess huge medicinal properties. This study is based on Gas Chromatography-Mass Spectrometry (GCMS) and in-silico techniques (ADME) applied to identify the bioactive phytocompounds present in extracts of the seeds in the fruit. The parameters considered for analysis were molecular weight, lipophilicity, GI absorption, water solubility, drug-likeness, Lipinski rule of 5, blood-brain barrier permeability, synthetic accessibility, bioavailability, and lead likeness. Among the eleven phytocomponents subjected to ADME analysis, ten of them were found to possess medicinal properties and four were identified as novel to these extracts. The compounds found in the GCMS analysis were propanedioic acid, oxirane derivative, anthranilanilide, a cytotoxic agent, an anticancer agent, and an antiproliferative agent. The chemical compounds present in the seeds impart them with medicinal properties, which would allow one to understand the relationship between the different bioactive compounds in seeds and the human body. Further studies need to be performed to identify its potential in ameliorating the neurological properties.

1. Introduction

Passiflora edulis is a tropical fruit from the family *passifloraceae* and is a native fruit of South America. The fruit is characterised by its peculiar flavour and health value. The round to oval shaped fruit is filled with juicy pulp and hundreds of small seeds (Zibadi et al., 2004). These seeds are by-products of the fruit juice processing industry and generally considered as a waste. However, preliminary studies and several literature have mentioned these seeds to possess huge medicinal properties and being used as a traditional medicine in treatment of several ailments. The bioactive compounds present in seeds impart them with medicinal properties. In-depth study of these phytocompounds (plant based bioactive compounds) helps in understanding their mode of action and therapeutic properties. To reduce cost and save time, in-silico methods can also be utilised to study the drug likeness of the phytocompound. The studies regarding ADME mechanisms would allow one to understand the relationship between the different bioactive phytocompounds in *Passiflora edulis* seeds and the human body. Absorption defines how the phytocompound moves from the site of administration into the blood. Distribution is about the phytocompound entering systemic circulation, and getting distributed to all parts of the body (tissues and organs). Metabolism determines the phase of body's enzymes, (primarily located in the liver), breaking down the phytocompound molecules.

Excretion explains the final phase of removing the phytocompound and its metabolites from the body (Testa, et al., 2008).

This can be carried out by using the available online software tools that predict the crucial properties of a bioactive phytocompound in being a drug molecule. This study is based on GCMS and in-silico techniques (ADME) applied to identify the phytocompounds present in extracts of *passiflora edulis* seeds.

2. Materials and methods

2.1 Preparation of sample

Healthy and fresh passion fruits were procured naturally, and the seeds were separated from the pulp. The seeds were washed thoroughly and dried in partial sunlight for 3 days. Then, the seeds were crushed using a pestle and mortar. 0.1 g of this crushed seed powder was mixed with methanol, distilled water, and chloroform in three separate tubes. These tubes were placed in a shaker incubator for 72 hours at 35 degrees centigrade. All the chemicals used in the extraction procedure were of analytical grade (SD Fine Chem. Ltd.).

2.2 Gas chromatography-mass spectroscopy (GCMS)

Preliminary tests were performed on all the three extracts and based on those results, methanolic extract was subjected to GCMS analysis. GCMS analysis was carried out at Meuriex Life Sciences - Rajajinagar, Bengaluru. One microliter volume of samples were injected into the instrument (Agilent). The Rtx-5ms with a length of 30 m and internal diameter of 0.25 mm, with a film thickness of 0.25 µm was used. The injector temperature was 250°C and helium was used as the carrier gas at a flow rate of 1 mm per minute. The interface temperature (between the GC and MS) was maintained at 280°C. The MS scanned a mass range from 40 to 600 m/z. The NIST 23 mass spectral library was used for compound identification.

2.3 ADME analysis

The phytocompounds identified from the GCMS analysis were further analyzed for their ADME properties using the software SwissADME (Daina et al., 2017). The SMILES format of the phytocompounds was retrieved from the PubChem database and used in the SwissADME software. The results obtained were analyzed based on the acceptable ranges for 10 selected parameters. The parameters considered for analysis were molecular weight, lipophilicity, GI absorption, water solubility, drug-likeness, Lipinski rule of 5, blood-brain barrier permeability, synthetic accessibility, bioavailability and lead likeness.

The acceptable ranges of parameters were as follows: molecular weight of the phytocompound must be within 150.0 to 500 g/mol, lipophilicity or the log P (o/w) value is acceptable if the compound contains high lipophilicity value. The water solubility or the log S value considered here is of ESOL model and the scale is value ≤ 10 (insoluble), value ≤ 6 (poorly soluble), value ≤ 4 (moderately soluble), value ≤ 2 (soluble) and value < 0 (highly soluble). The gastrointestinal absorption was high to low and the ability for crossing the blood brain barrier was yes or no. The drug likeness parameter considers Lipinski's rule of five and the acceptable bioavailability score was a value of 0.56. The synthetic accessibility scores ranges from 1 being very easy to 10 being very difficult (Doogue et al., 2013).

3. Results and Discussions

3.1 Gas Chromatography - Mass Spectrometry:

11 phytocompounds were observed in the GCMS analysis and they were identified from the NIST database. The identified phytocompounds and their spectral graph is as shown in (Fig 1) and (Table 1).

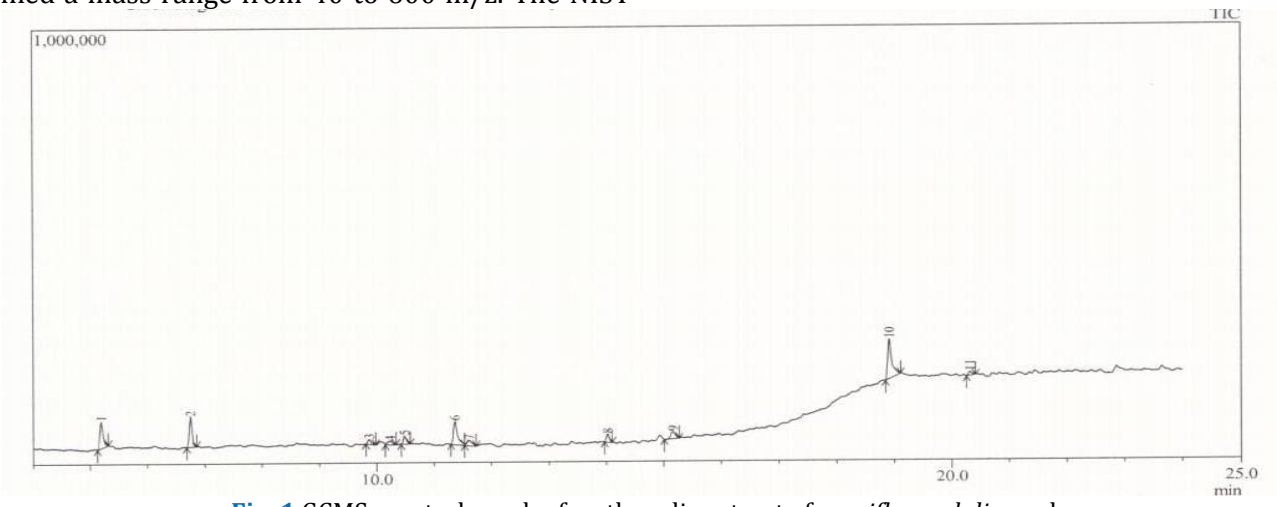

Fig. 1 GCMS spectral graph of methanolic extract of *passiflora edulis* seeds

Table 1 Compounds and their RT time observed in GCMS analysis of the methanolic extract of *Passiflora edulis* seeds

Compound	Area %	RT time
Phenol	15.24	5.194
Undecane	14.61	6.748
13-Methylheptacosane	2.71	9.863
Normorphine,2TMS derivative	2.99	10.230
Propanedioic acid, (ethoxy methylene),diethyl ester	4.52	10.485
Diethyl phthalate	16.08	11.368
2,4-Dihydroxybenzoic acid,3TMS derivative	4.21	11.610
n-Hexadecanoic acid	3.92	14.021
Distearyl thiodipropionate	5.53	15.157
Oxirane,2,2-dimethyl-3-(3,7,12,16,20-pentamethyl-3,7,11,15,19-heneicosapentaenyl)-,(all-E)-	27.74	18.910
Anthranilanilide,2TMS	2.43	20.318

3.2 ADME

The compounds subjected to ADME analysis, and the results obtained are mentioned in table 2. The spider web representation of each phytocompound reveals the actual values and the acceptable ranges of their significant properties (Fig 2).

Table 2 ADME properties of phytocompounds in methanolic extract of passion fruit seeds

Compound	Molecular Weight	Canonical SMILE Formula	Molecular Formula	Log P	Lipinski	Gi Absorption	BBB	Water Solubility	Bioavailability Score	Leadlikeness	Synthetic Accessibility
Phenol	94.11 g/mol	C1=CC=C(C=C1)O	C6H6O	1.41	Yes, 0 Violation	High	Yes	(Soluble) -1.98	0.55	No (1), MW<250	1
Undecane	156.31 g/mol	CCCCCCCCCCC	C11H24	4.56	Yes, 1 Violation	Low	No	(Soluble) -3.78	0.55	No (3), MW<250	1.72
13 -Methylheptacosane	394.8 g/mol	CCCCCCCCCCCCCCCC(C)CCCCCCCCCCC	C28H58	10.79	Yes, 1 Violation	Low	No	(Insoluble)-10.21	0.55	No (3), MW>350	4.14
Normorphine,2TMS Derivative	415.7 g/mol	C[Si](C)(C)OC1C=CC2C3CC4=C5C2(C1OC5=C(C=C4)O[Si](C)(C)C)CCN3	C22H33NO3Si2	3.38	Yes, 0 Violation	High	Yes	(Moderately Soluble)-5.33	0.55	No (2), MW>350	6.04
Propanedioic acid, (ethoxymethylene)-, diethyl ester	160.17 g/mol	CCOC(=O)CC(=O)OCC	C7H12O4	1	Yes, 0 Violation	High	No	(Very Soluble) -1.04	0.55	No (1), MW<250	1.63
Diethyl Phthalate	222.24 g/mol	CCOC(=O)C1=CC=CC=C1C(=O)OCC	C12H14O4	2.3	Yes, 0 Violation	High	Yes	(Soluble) -2.62	0.55	No (1), MW<250	1.93
2,4-Dihyroxybenzoic acid, 3TMS derivative	154.12 g/mol	C1=CC(=C(C=C1O)O)C(=O)O	C7H6O4	0.77	Yes, 0 Violation	High	No	(Soluble) -2.16	0.56	No (1), MW<250	1.1
n-Hexadecanoic acid	256.42 g/mol	CCCCCCCCCCCCCCCC(=O)O	C16H32O2	5.2	Yes, 1 Violation	High	Yes	(Moderately Soluble) -5.02	0.85	No (2)	2.31
Distearyl thiodipropionate	683.2 g/mol	CCCCCCCCCCCCCCCCCCCCOC(=O)CCSCCC(=O)OCCCCCCCCCCCCCCCCCC	C42H82O4S	13.35	No, 2 Violation	Low	No	(Insoluble) -12.76	0.17	No (3), MW>350	6.44
Oxirane, 2,2-dimethyl-3-(3,7,12,16,20-pentamethyl -3,7,11,15,19-heneicosapentaenyl)-,(all-E)	426.7 g/mol	CC(=CCCC(=CCCC(=CCCC=C(C)CCC=C(C)CCC1C(O1)(C)C)C)C)C	C30H50O	8.55	Yes, 1 Violation	Low	No	(Poorly Soluble) -7.97	0.55	No (3), MW>350	5.08
Anthranilanilide, 2TMS	212.25 g/mol	C1=CC=C(C=C1)NC(=O)C2=CC=CC=C2N	C13H12N2O	2.25	Yes, 0 Violation	High	Yes	(Moderately Soluble) -3.37	0.55	No (1), MW<250	1.3

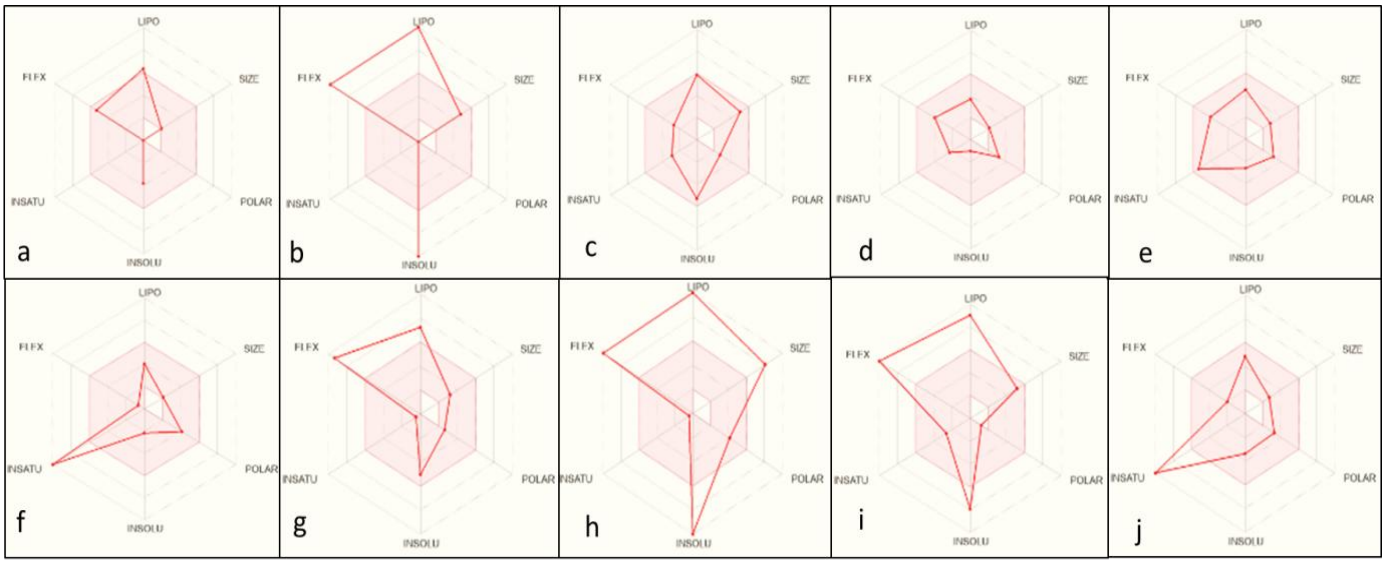

Fig. 2 Spider web view of phytocompounds in passion fruit seed extract
a.Undecane, b.13 - Methylheptacosane, c.Normorphine, d.Propanedioic acid, e.Diethyl Phthalate, f. 2,4- Dihyroxybenzoic acid, g. n- Hexadecanoic acid, h. Distearyl thiodipropionate, i. Oxirane, j. Anthranilanilide

Among the eleven phytocompounds subjected to ADME analysis, ten of them were found to possess medicinal properties and four phytocompounds were identified as novel to these extracts. The four compounds are undecane, normorphine, propanedioic acid and diethyl phthalate.

Diethyl phthalate is a colorless, and odorless liquid. Diethylphthalate is used as an alcohol denaturant, solvent and carrier in fragrance and cosmetics. Hence, the compound has found wide application in the field of aromatherapy, cosmetic products and fragrances industries (ApI A. M., 2001).

2,4- Dihyroxybenzoic acid possesses a strong antibacterial activity against a series of microorganisms, and several studies have revealed its ability to suppress both gram-positive and gram-negative bacteria. Therefore, the compound holds a promise as a therapeutic agent against bacterial infections. The compound has also been researched for its antiproliferative activity against cancer cell lines. The cytotoxic activity of this compound has been proved in human breast cancer cell lines. (Łukasz Popiołek et al., 2023).

n- Hexadecanoic acid is found to regulate inflammation by inhibiting phospholipase and act as an anti-inflammatory agent. It has been linked to neurotrophic effects making it a promising prophylactic and therapeutic agent for neuropathy. It possesses antibacterial properties specifically against *Salmonella typhi*. It has applications in the production of soaps, cosmetics, whereas in the food industry it is used as flavour enhancer, flavouring agent or adjuvant (Aparna et al., 2012).

Distearyl thiodipropionate is known for its antioxidant properties. Generally this compound is incorporated in the production of cosmetics and is also acknowledged by FDA as a GRAS for use in the food packaging and cosmetics industry (Diamante et al., 2010).

Oxirane and its derivative compounds are known to have robust antibacterial activity. Several oxirane derivatives have demonstrated active antibacterial activity aganist gram-positive and gram-negative bacteria. Oxirane derivatives may interfere with inflammatory mechanisms, which could make them useful in therapies and conditions involving chronic inflammation. The other biological properties of these compounds include antioxidant and neuroprotective activities (Jayalekshmi C et al., 2024).

Anthranilanilide is a chemical compound with antimycobacterial properties. It acts as an allosteric inhibitor of the ribosome inactivating protein (RIP). Thereby inhibiting the production of preinflammatory cytokine TNF-α. Several scientific studies have proven the anticancer property of this compound by in-vivo inhibition of the tumor growth in the in-vitro assays. It is also reported as the compound binds to the sulfonic acid groups present on the surface of bacterial cell walls and inhibits the synthesis of vital proteins involved in cell division (Stolfa et al., 2012).

4. Conclusion

All the phytocompounds were screened on the basis of ten parameters and their acceptable range selected. Among them, undecane had few parameters in the acceptable range, such as its molecular weight of 156.31 g/mol and easing the permeability through cell membrane. The phytocompound is unable to pass the blood brain barrier, soluble in water with acceptable bio availability value. The synthetic accessibility value is 1.72 making the compound more easy to produce artificially. The phytocompound normorphine has an acceptable molecular weight of 415.7 g/mol and follows all the lipinski rules without

violations. It has high absorption in the gastrointestinal tract and a good bioavailability score.

The phytocompound propanedioic acid has an acceptable molecular weight of 160.17 g/mol with 0 violations in Lipinski rule. It has high absorbity in the gastrointestinal tract and also is not able to cross the blood brain barrier. The phytocompound is very soluble in water hence attaining an acceptable bioavailability score (0.55) and it is also easy to synthesize artificially (1.60). The phytocompound diethyl phthalate has an acceptable molecular weight of 222.24 g/mol with 0 violations in Lipinski rule and is highly absorbable in the gastrointestinal tract. As the phytocompound has the potential to cross the blood brain barrier, further studies need to be performed to identify its potential in ameliorating the neurological properties. The phytocompound is soluble in water with a good bioavailability score (0.55) and is also easily accessible to artificially synthesize (1.93).

However, additional scientific studies are required to validate the therapeutic claims of these phytocompounds. Subsequent scientific investigate-ons can be helpful in modifying their three dimensional structures to enhance their therapeutic properties.

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Declaration of Conflict

“The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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