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Nutritional and phytochemical characterisation of yellow passion fruit pomace: GC-MS/MS, LC-MS/MS, molecular docking, and ADMET Insights

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Abstract
Yellow passion fruit (Passiflora edulis f. flavicarpa) pomace is an underutilised processing by-product with potential as a source of nutrients and bioactive compounds. The present study evaluated its nutritional, mineral, phytochemical, and in silico bioactivity profiles. Fresh pomace contained 58.00% moisture, 6.01% protein, 19.06% dietary fibre, 7.41% fat, 7.76% carbohydrates, and 2.04% pectin. Total phenolic and flavonoid contents were 11.84 mg GAE/g and 8.23 mg QE/g, respectively. Potassium (185.00 mg/100 g) was the predominant mineral, followed by phosphorus (105.33 mg/100 g). GC-MS/MS and LC-MS/MS profiling identified diverse phytoconstituents. Molecular docking demonstrated favourable interactions with key anti-diabetic and hypocholesterolemic targets, while ADMET analysis indicated variable pharmacokinetic profiles and generally favourable predicted safety characteristics. Overall, YPF pomace represents a promising source of nutritionally relevant minerals and bioactive compounds with potential for functional and nutraceutical applications.

Keywords: Yellow passion fruit pomace, Passiflora edulis, nutritional profiling, mineral composition, GC-MS/MS, LC-MS/MS, molecular docking, ADMET analysis

Introduction

Yellow passion fruit (Passiflora edulis f. flavicarpa) is an economically important tropical fruit widely processed into juices, concentrates, and other food products. Processing generates substantial by-products, including peel, seeds, residual pulp, and fibrous materials, collectively referred to as pomace. Although often discarded or underutilised, passion fruit pomace contains valuable macronutrients, minerals, and diverse bioactive compounds, including fatty acids, organic acids, phenolic acids, flavonoids, stilbenes, and other phytochemicals. These constituents highlight its potential as a source of functional ingredients and nutraceutical compounds, supporting its valorisation within a circular bioeconomy framework (Matsui *et al*., 2010 [11]; He *et al*., 2020; Weyya *et al*., 2024) [16].

Nutritional and mineral profiling provides fundamental information on the chemical composition and potential applications of passion fruit pomace. Nutritional analysis of moisture, protein, lipid, dietary fibre, carbohydrate, acidity, and pectin contents, together with the quantification of essential minerals, enables evaluation of its nutritional characteristics and potential utilisation as a value-added ingredient. However, comprehensive characterisation of its metabolite composition requires complementary analytical platforms due to the chemical diversity and structural heterogeneity of the matrix (Kawakami *et al*., 2021) [10]

GC-MS/MS is particularly suitable for profiling volatile and semi-volatile metabolites, including fatty acids, organic acids, sugars, amino acids, and related primary metabolites. In contrast, LC-MS/MS enables the detection and characterisation of non-volatile and thermolabile phytochemicals, including phenolic acids, flavonoids, stilbenes, and glycosides. The combined application of GC-MS/MS and LC-MS/MS therefore provides complementary coverage of the metabolome and facilitates the identification of chemically diverse metabolites present in passion fruit pomace (Dos Santos *et al*., 2021) [7]

The biological relevance of identified metabolites can be further investigated through ADMET (absorption, distribution, metabolism, excretion, and toxicity) analysis. Prediction of gastrointestinal absorption, bioavailability-related properties, cytochrome P450 interactions, drug-likeness, and toxicity provides preliminary information regarding the pharmacokinetic and safety profiles of candidate compounds (Venkatraman, 2021; Dulsat *et al*., 2023) [8, 15]. Thus, the integration of nutritional and mineral analysis, GC-MS/MS and LC-MS/MS metabolite profiling, and ADMET prediction provides a comprehensive approach for characterising passion fruit pomace and prioritising potentially bioactive compounds for further experimental investigation.

Materials and Methods

1. Sample preparation

Fresh yellow passion fruits (YPF) were collected from the Department of Fruit Science, College of Agriculture, Kerala Agricultural University, Vellanikkara, Thrissur, Kerala. The fruits were carefully selected to ensure uniform maturity and the absence of physical damage or microbial spoilage. They were washed thoroughly with potable water to remove adhering dirt and impurities. The fruits were manually cut open, and the pulp containing seeds was separated from the rind. The pulp was subjected to juice extraction, and the residual material consisting of seeds and adhering pulp (pomace) was collected immediately after juice extraction. The fresh pomace was used directly for subsequent analysis.

2. Analytical methods

2.1 Nutritional and mineral analysis

The moisture, crude protein, crude fat, and titratable acidity of yellow passion fruit (YPF; Passiflora edulis f. flavicarpa) pomace were determined according to AOAC International (2023). Total carbohydrates were estimated using the anthrone method. Dietary fibre was determined by the enzymatic-gravimetric procedure (AOAC 991.43), and pectin was determined by acid extraction followed by alcohol precipitation and gravimetric recovery. Mineral elements were analysed after nitric-perchloric acid digestion. Calcium, magnesium, and sodium were quantified by atomic absorption spectrophotometry, phosphorus by the molybdenum-blue method, and potassium by flame photometry. Results were expressed as percentages for nutritional constituents and mg/100 g for minerals on a fresh-weight basis.

2.2 Preparation of extracts for GC-MS/MS and LC-MS/MS

Fresh yellow passion fruit (YPF) pomace (100 g), collected immediately after juice extraction, was extracted separately with n-hexane and methanol (200 mL each) at a 1:2 (w/v) ratio by cold maceration for 24 h. Each extraction was performed in triplicate, and the respective extracts were concentrated under reduced pressure using a rotary evaporator. The extraction yields, calculated based on the initial fresh weight of the pomace, were 5% (w/w) for the n-hexane extract and 7% (w/w) for the methanolic extract. Before instrumental analysis, both extracts were filtered through a 0.22 µm PVDF syringe filter. The n-hexane extract was used for GC–MS/MS analysis, whereas the methanolic extract was used for LC–MS/MS analysis.

2.3 GC-MS/MS analysis

The hexane extract of yellow passion fruit (Passiflora edulis f. flavicarpa) pomace was analysed at the Kerala Forest Research Institute (KFRI), Peechi, Kerala, India, using a Shimadzu GC–MS/MS system (Shimadzu Corporation, Kyoto, Japan). Data acquisition and processing were performed using Shimadzu GCMS solution software. Chromatographic separation was carried out on a Restek XTI-5 fused-silica capillary column (60 m × 0.25 mm i.d., 0.25 µm film thickness). Helium (99.999% purity) was used as the carrier gas at a constant flow rate of 1.0 mL min^{-1}. A 1.0 µL aliquot of the sample was injected in split mode with a split ratio of 20:1. The injector temperature was maintained at 280°C. The oven temperature programme was as follows: the initial oven temperature was maintained at 70°C, increased at 8°C min^{-1} to 260°C and held for 2 min, followed by an increase at 4°C min^{-1} to 280°C and held for 5 min. The interface temperature was maintained at 280°C, while the ion source temperature was maintained at 220°C. Mass spectrometric detection was performed using electron ionisation (EI) at 70 eV. Data were acquired in scan mode over an m/z range of 50–500, and the solvent cut time was set at 3.10 min. The acquired chromatograms and mass spectra were processed using Shimadzu GCMSsolution software. Compound identification was performed by comparing the obtained mass spectra with the NIST mass spectral library and relevant published literature. Compound assignments were based on spectral matching. Since authentic reference standards were not analysed, all compounds identified in this study were considered putatively (tentatively) identified.

2.4 HRLC-MS/MS analysis

The methanolic extract of yellow passion fruit (Passiflora edulis f. flavicarpa) pomace was analysed at the Sophisticated Analytical Instrument Facility (SAIF), IIT Bombay, using a high-resolution Agilent 6550 Quadrupole Time-of-Flight (Q-TOF) LC–MS/MS system (Agilent Technologies, USA) equipped with a Dual Agilent Jet Stream electrospray ionisation (Dual AJS ESI) source. Data acquisition and processing were performed using Agilent MassHunter Acquisition software and Agilent MassHunter Qualitative Analysis B.06 software, respectively. Before analysis, the extract was filtered through a 0.22 µm PVDF syringe filter, and 5 µL of the sample was injected into the LC–MS/MS system. Chromatographic separation was performed on a ZORBAX Eclipse Plus C18 column (150 × 2.1 mm, 5 µm; Agilent Technologies, USA). The mobile phase consisted of 0.1% formic acid in Milli-Q water (solvent A) and acetonitrile (solvent B). The mobile phase was delivered at a constant flow rate of 0.30 mL min^{-1}. The gradient programme was maintained at 95% A and 5% B from 0 to 1 min, gradually changed to 100% B at 25 min, maintained until 30 min, and then returned to the initial composition (95% A and 5% B) from 31 to 35 min for column re-equilibration. The column compartment temperature was maintained at 40°C. Mass spectra were acquired in positive electrospray ionisation (ESI+) mode over an m/z range of 120–1200 using Auto MS/MS acquisition mode. The ion source parameters were as follows: capillary voltage, 3500 V; nozzle voltage, 1000 V; fragmentor voltage, 175 V; skimmer voltage, 65 V; nebulizer pressure, 35 psi; drying gas temperature, 250°C; drying gas flow, 13 L min^{-1}; sheath gas temperature, 300°C; and sheath gas flow, 11 L min^{-1}. MS/MS spectra were acquired at a scan rate of one spectrum per second using a medium (~4 amu) precursor isolation width. Metabolite annotation was performed using Agilent MassHunter Qualitative Analysis B.06 by comparing accurate mass measurements, molecular formula predictions, isotope patterns, retention times and MS/MS fragmentation spectra with the available compound database. Compound assignments were supported by calculated mass errors (ppm). Since authentic reference standards were not analysed, all metabolites reported in this study were considered putatively (tentatively) identified, and further confirmation using authentic standards is required.

2.5 Molecular docking

The selected ligand molecules were downloaded from PubChem maintained by National Centre for Biotechnology Information (https://pubchem.ncbi.nlm.nih.gov). A literature survey was conducted on the antidiabetic and hypocholestrolemic activity of passion fruit pomace. The proteins involved in the pathways were identified and selected for the docking study. The 3D crystal structure of receptor molecules was analysed and downloaded from protein databank (http://www.rcsb.org). The receptor molecules with high resolution were selected for molecular docking against the selected ligands. Molecular docking studies were performed using CB-Dock to predict the binding sites of the protein and calculate cavity centres and sizes with novel curvature-based cavity detection approach, and perform docking with a popular docking program, AutoDock Vina. Docking results were visualied and analysed using PyMol open-source software.

2.6 ADMET analysis

Selected ligands were subjected to in silico ADMET analysis using SwissADME and ADMETlab 2.0. Physicochemical properties, predicted gastrointestinal absorption, blood-brain barrier permeability, P-glycoprotein substrate status, CYP2D6 inhibition, clearance, half-life, and toxicity-related endpoints were evaluated.

2.7 Statistical analysis

All analyses were carried out in triplicate (n = 3), and the experimental results are presented as mean ± standard deviation (SD). The mean and standard deviation were calculated using Microsoft Excel to describe the central tendency and variability of the experimental data.

Results and Discussion

1. Nutritional, phytochemical and mineral composition of YPF pomace

The nutritional and phytochemical composition of YPF pomace is presented in Table 1. The moisture content of yellow passion fruit (YPF) pomace in the present study was 58.00%, closely aligning with the 57.09% reported for yellow passion fruit seeds by dos Reis *et al*. (2018) [6]. This moisture level may be associated with the seed fraction present in the pomace and indicates that fresh YPF pomace contains considerable water, which may influence its storage stability and necessitate appropriate drying or preservation before further utilisation. Crude protein, dietary fibre, crude fat, and carbohydrate contents were 6.01%, 19.06%, 7.41%, and 7.76%, respectively. The relatively high fibre content indicates the retention of structural components within the pomace following fruit processing, while the presence of protein and lipid fractions demonstrates its potential nutritional value. The heterogeneous composition of passion fruit processing residues, which may contain residual pulp, seeds, peel-derived material, and fibrous tissues, contributes to variations in their nutritional composition (He *et al*., 2020; Campos-Rodriguez *et al*., 2023) [3].

The total phenolic content (TPC) and total flavonoid content (TFC) of fresh yellow passion fruit pomace were 11.84 mg GAE/g and 8.23 mg QE/g, respectively. These values demonstrate the retention of bioactive phytochemicals in the pomace after processing. Similar phenolic-rich profiles have been reported in passion fruit by-products and other fruit pomaces, supporting their potential as sources of natural bioactive compounds (He *et al*., 2020; Weyya *et al*., 2024) [16].

The yellow passion fruit (YPF) pomace contained potassium (185.00 mg/100 g) as the predominant mineral, followed by phosphorus (105.33 mg/100 g), magnesium (42.00 mg/100 g), sodium (29.00 mg/100 g), and calcium (25.00 mg/100 g) (Table 1). Kawakami *et al*. (2021) [10] reported potassium (112–760 mg/100 g), phosphorus (63–310 mg/100 g), calcium (6–173.1 mg/100 g), sodium (3.46–241.7 mg/100 g), and magnesium (138.3–290 mg/100 g) in passion fruit seed-derived samples. Nagarajaiah *et al*. (2016) reported calcium contents of 303 mg/100 g in orange pomace and 581 mg/100 g in sweet lemon pomace. The differences in mineral concentrations may be related to fruit species, tissue composition, cultivar, processing conditions, and moisture basis. Overall, the mineral profile of YPF pomace, particularly its potassium and phosphorus contents, indicates its potential as a nutritionally valuable fruit-processing by-product.

Table 1: Nutritional, phytochemical and mineral composition of YPF pomace

Parameters	Value (Mean ± SD)
Moisture (%)	58.00 ± 0.00
Crude Protein (%)	6.01 ± 0.07
Dietary Fibre (%)	19.06 ± 0.20
Crude Fat (%)	7.41 ± 0.11
Carbohydrates (%)	7.76 ± 0.12
Titratable Acidity (%)	3.65 ± 0.07
Pectin (%)	2.04 ± 0.10
Total phenolic content (mg GAE/g)	11.84 ± 0.18
Total flavonoid content (mg QE/g)	8.23 ± 0.11
Mineral composition (mg/100 g)	
Calcium	25.00 ± 1.22
Phosphorus	105.33 ± 2.50
Sodium	29.00 ± 1.22
Potassium	185.00 ± 4.18
Magnesium	42.00 ± 2.12

2. GC-MS/MS and LC-MS/MS analyses

GC–MS/MS and LC–MS/MS analyses revealed a diverse range of volatile and non-volatile phytochemicals in yellow passion fruit (YPF) pomace (Table 2). The volatile fraction consisted of terpenes (β-myrcene), esters (ethyl hexanoate and ethyl oleate), aldehydes [(E,E)-2,4-decadienal], unsaturated fatty acids (oleic, linoleic and linolenic acids), long-chain hydrocarbons (pentacosane, hexacosane, heptacosane, octacosane, nonacosane, triacontane, hentriacontane, dotriacontane and tetratriacontane), fatty alcohols and squalene. The non-volatile fraction comprised several biologically important compounds, including kaempferol, genistein, neoastilbin, kaempferitrin, forsythiaside A, silibinin, butin, naringenin 7-O-glucoside, xanthyletine, isobarbaloin and 4-O-caffeoyl-3-O-feruloylquinic acid. The presence of these phytochemicals indicates that YPF pomace is a valuable source of bioactive compounds with potential applications in functional foods and nutraceuticals.

Previous studies have also demonstrated that passion fruit by-products are rich sources of flavonoids, phenolic acids, carotenoids and other phytochemicals with antioxidant and therapeutic properties (Corrêa *et al*., 2016). Likewise, Zhang *et al*. (2023) [4, 18] reported that Passiflora residues contain flavonoids such as kaempferol derivatives together with unsaturated fatty acids that contribute to their biological activity. He *et al*. (2020) further described Passiflora edulis

as an excellent source of flavonoids, terpenoids and phenolic compounds associated with antioxidant, anti-inflammatory and antidiabetic activities. The identification of squalene, oleic acid, linoleic acid and linolenic acid in the present study further supports their reported occurrence in fruit by-products possessing cardioprotective and hypolipidaemic properties (Corrêa *et al*., 2016) [4].

Table 2: Volatile and non-volatile compounds identified in YPF pomace by GC-MS/MS and LC-MS/MS

S. No.	Volatile Compounds	Non-volatile Compounds
1	β-Myrcene	D-Erythroascorbic acid 1′-α-D-glucoside
2	Ethyl hexanoate	Sagecoumarin
3	(E,E)-2,4-Decadienal	S-Methyl-1-thio-D-glycerate
4	Linolenic acid	L-Malic acid
5	Linoleic acid	Icodulinum
6	12-Octadecadienoate	Methylisocitric acid
7	Oleic acid	Eremopetasitenin C3
8	Heneicosane	Digalacturonate
9	Ethyl oleate	4-O-Caffeoyl-3-O-feruloylquinic acid
10	9-Tricosene (Z)	Isobarbaloin
11	Tetracosanol	Neoastilbin
12	Pentacosane	Butin
13	Hexacosane	Naringenin 7-O-glucoside
14	Heptacosane	Kaempferitrin
15	1-Heptacosanol	Forsythiaside A
16	Octacosane	6-Demethoxycapillarisin
17	Nonacosane	4-Caffeoyl-1,5-quinolactone
18	Triacontane	Genistein
19	Hentriacontane	Kaempferol
20	Dotriacontane	Flazine
21	Tritriacontane	Arbutin
22	Squalene	Xanthyletine
23	Tetratriacontane	Silibinin

3. Therapeutic potential of YPF pomace

Molecular docking was performed to evaluate the anti-diabetic and hypocholesterolemic potential of phytoconstituents identified from yellow passion fruit (YPF) pomace, with the results summarised in Table 3. The identified compounds showed favourable binding affinities and stable interactions with key active-site residues. Neoastilbin exhibited the strongest binding to α-glucosidase (−8.4 kcal/mol) with seven hydrogen bonds, while sagecoumarin showed the highest affinity toward DPP-4 (−10.6 kcal/mol), followed by forsythiaside A (−9.5 kcal/mol) with 11 hydrogen bonds. Kaempferol interacted with PTP1B at −7.0 kcal/mol with three hydrogen bonds. Similar favourable interactions of fruit-derived phenolics with digestive enzymes have been reported through molecular docking studies (Zhang *et al*., 2018; Bie *et al*., 2024; Shi *et al*., 2022) [2, 14, 19]. The observed binding affinities and hydrogen-bond interactions suggest that YPF pomace-derived phytochemicals may possess multi-target anti-diabetic potential.

Molecular docking analysis also indicated favourable hypocholesterolemic interactions of YPF pomace-derived phytoconstituents with key lipid-metabolism targets (Table 3). Among the ligands, 4-O-caffeoyl-3-O-feruloylquinic acid showed strong binding to HMG-CoA reductase (−9.4 kcal/mol) with eight hydrogen bonds, while kaempferol exhibited an affinity of −8.7 kcal/mol. Against pancreatic lipase, isobarbaloin showed the strongest binding (−8.0 kcal/mol), followed by kaempferitrin (−7.6 kcal/mol) and neoastilbin (−7.4 kcal/mol). Genistein showed favourable binding to PPAR-α (−8.4 kcal/mol) with three hydrogen bonds, whereas forsythiaside A showed a strong affinity (−10.0 kcal/mol) with six hydrogen bonds. Similar studies have reported that phenolic compounds from fruit-derived materials can interact with HMG-CoA reductase, pancreatic lipase, and other lipid-metabolism targets, supporting their potential hypolipidemic activity (Nagarajaiah *et al*., 2016; He *et al*., 2020). Overall, the favourable binding affinities and multiple hydrogen-bond interactions observed in the present study suggest that YPF pomace phytoconstituents may exert potential multi-target effects against cholesterol biosynthesis and lipid metabolism.

Table 3: Molecular docking interactions of selected YPF pomace phytochemicals with anti-diabetic and hypocholesterolaemic targets

Potential	Target protein	Ligand	Binding affinity (kcal/mol)	H-bonds	Interaction residues
Anti-diabetic	α-Glucosidase	Kaempferol	-7.7	1	THR 384; GLN 630
Anti-diabetic	α-Glucosidase	Genistein	-8.0	2	ILE 276; TYR 275
Anti-diabetic	α-Glucosidase	Neoastilbin	-8.4	7	TYR 294; GLN 574; LYS 498; ASN 575
Anti-diabetic	α-Glucosidase	Isobarbaloin	-7.4	2	GLN 386; ALA 655
Anti-diabetic	Dipeptidyl peptidase-4	Forsythiaside A	-9.5	11	LYS 271; GLN 269; TYR 629
Anti-diabetic	Dipeptidyl peptidase-4	6-Demethoxycapillarisin	-8.5	2	HIS 752; ARG 590
Anti-diabetic	Dipeptidyl peptidase-4	Sagecoumarin	-10.6	7	ASP 620; ARG 59; LYS 735; SER 852; ASN 755
Anti-diabetic	Protein tyrosine phosphatase 1B	Silibinin	-7.4	5	ARG 254; MET 74; GLU 76; ARG 238
Anti-diabetic	Protein tyrosine phosphatase 1B	Kaempferol	-7.0	3	ASP 6; ARG 221; TYR 46; GLU 2
Hypocholesterolaemic	HMG-CoA reductase	4-O-Caffeoyl-3-O-feruloylquinic acid	-9.4	8	ALA 757; MET 657; SER 852; VAL 863
Hypocholesterolaemic	HMG-CoA reductase	Genistein	-7.0	3	ALA 217; PHE 3; ASP 6
Hypocholesterolaemic	HMG-CoA reductase	Kaempferol	-8.7	5	LYS 691; SER 865; LYS 591
Hypocholesterolaemic	Pancreatic lipase	Neoastilbin	-7.4	2	SER 129; ILE 97; PHE 96; GLY 100
Hypocholesterolaemic	Pancreatic lipase	Isobarbaloin	-8.0	3	THR 54; ASP 24
Hypocholesterolaemic	Pancreatic lipase	Kaempferitrin	-7.6	4	ILE 97; GLU 102; ALA 131
Hypocholesterolaemic	PPAR-α	Genistein	-8.4	3	GLU 286; TYR 324; THR 283
Hypocholesterolaemic	PPAR-α	Forsythiaside A	-10.0	6	THR 279; ASN 219; LEU 331; ALA 333; SER 280

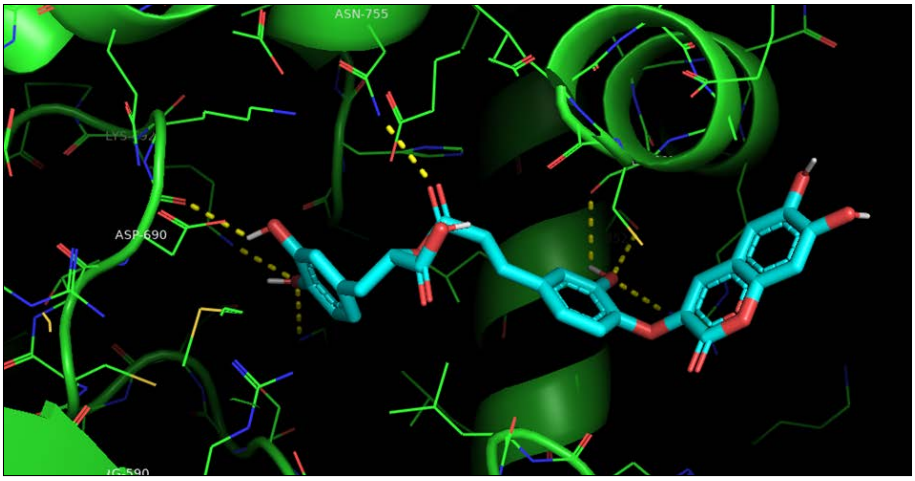

Fig 1: Highest-affinity antidiabetic docking interaction of sagecoumarin with dipeptidyl peptidase-4 (DPP-4) (binding affinity −10.6 kcal/mol; 7 hydrogen bonds).

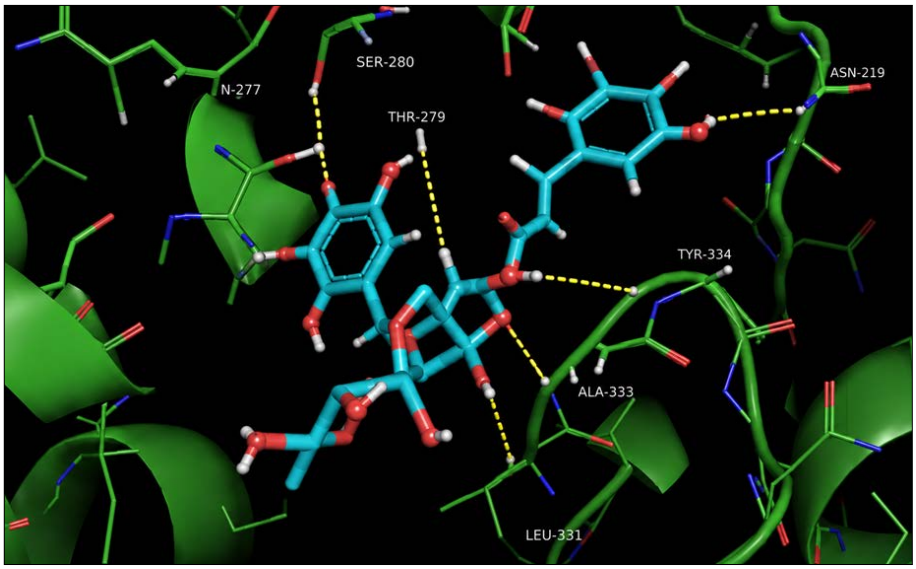

Fig 2: Highest-affinity hypocholesterolemic docking interaction of forsythiaside A with peroxisome proliferator-activated receptor alpha (PPAR-α) (binding affinity −10.0 kcal/mol; 6 hydrogen bonds).

The highest-affinity docking interactions for the two biological activity groups are shown in Figures 1 and 2. Sagecoumarin showed the strongest antidiabetic interaction with DPP-4 (−10.6 kcal/mol), whereas forsythiaside A showed the strongest hypocholesterolemic interaction with PPAR-α (−10.0 kcal/mol). The complete docking results are retained in Table 3.

4. ADMET properties of selected phytochemicals identified in YPF pomace

The predicted ADMET properties of selected YPF pomace phytochemicals are presented in Table 4. Kaempferol, genistein, 6-demethoxycapillarisin, sagecoumarin, and several lipid-derived compounds showed high predicted gastrointestinal absorption, whereas neoastilbin, isobarbaloin, forsythiaside A, silibinin, 4-O-caffeoyl-3-O-feruloylquinic acid, kaempferitrin, and pentacosane showed low absorption. None of the selected compounds were predicted to be P-glycoprotein substrates or CYP2D6 inhibitors. Sagecoumarin and several lipid-derived compounds, including oleic, linoleic and linolenic acids, ethyl oleate and 12-octadecadienoate, were predicted to permeate the blood-brain barrier, whereas the remaining compounds were not. These predictions indicate variable absorption and distribution characteristics among YPF pomace phytochemicals and support further experimental pharmacokinetic evaluation (Pires *et al*., 2015; Daina *et al*., 2017) [5, 13].

Table 4: Predicted ADMET properties of selected phytochemicals identified in YPF pomace

S. No.	Ligand	GI Absorption	BBB Permeant	P-gp Substrate	CYP2D6 Inhibitor
1	Kaempferol	High	No	No	No
2	Genistein	High	No	No	No
3	Neoastilbin	Low	No	No	No
4	Isobarbaloin	Low	No	No	No
5	Forsythiaside A	Low	No	No	No

6	6-Demethoxycapillarisin	High	No	No	No
7	Sagecoumarin	High	Yes	No	No
8	Silibinin	Low	No	No	No
9	4-O-Caffeoyl-3-O-feruloylquinic acid	Low	No	No	No
10	Kaempferitrin	Low	No	No	No
11	Oleic acid	High	Yes	No	No
12	Linoleic acid	High	Yes	No	No
13	Linolenic acid	High	Yes	No	No
14	Ethyl oleate	High	Yes	No	No
15	12-Octadecadienoate	High	Yes	No	No
16	Squalene	High	No	No	No
17	Pentacosane	Low	No	No	No

5. Excretion and toxicity profile of selected phytochemicals identified in YPF pomace

The predicted excretion and toxicity profiles of selected YPF pomace phytochemicals are presented in Table 5. The predicted total clearance ranged from 0.11 to 0.79 log mL/min/kg, while the estimated half-life varied from 2.8 to 9.4 h, indicating differences in compound persistence and elimination. None of the compounds showed predicted hepatotoxicity or carcinogenicity, whereas isobarbaloin and sagecoumarin showed possible skin-sensitization potential. Kaempferitrin, 4-O-caffeoyl-3-O-feruloylquinic acid, and forsythiaside A exhibited relatively lower clearance and longer half-lives, suggesting greater systemic persistence. Similar studies have highlighted the importance of clearance, half-life, and toxicity prediction in the early assessment of plant-derived bioactive compounds (Pires *et al*., 2015; Daina *et al*., 2017; Dulsat *et al*., 2023) [5, 8, 13]. Overall, the absence of predicted hepatotoxicity and carcinogenicity indicates a favourable preliminary safety profile, although experimental validation is required.

Table 5: Predicted excretion and toxicity profile of selected phytochemicals identified in YPF pomace

S. No.	Ligands	Total Clearance (log mL/min/kg)	Half-life (h)	Hepatotoxicity	Carcinogenicity	Skin Sensitization
1	Kaempferol	0.46	2.8	No	No	No
2	Genistein	0.61	3.2	No	No	No
3	Neoastilbin	0.18	6.4	No	No	No
4	Isobarbaloin	0.39	5.1	No	No	Possible
5	Forsythiaside A	0.11	7.3	No	No	No
6	6-Demethoxycapillarisin	0.54	3.5	No	No	No
7	Sagecoumarin	0.58	3.1	No	No	Possible
8	Silibinin	0.24	6.2	No	No	No
9	4-O-Caffeoyl-3-O-feruloylquinic acid	0.16	7.8	No	No	No
10	Kaempferitrin	0.13	8.4	No	No	No
11	Oleic acid	0.73	4.2	No	No	No
12	Linoleic acid	0.77	4.0	No	No	No
13	Linolenic acid	0.79	3.9	No	No	No
14	Ethyl oleate	0.69	3.8	No	No	No
15	12-Octadecadienoate	0.71	3.9	No	No	No
16	Squalene	0.31	8.7	No	No	No
17	Pentacosane	0.28	9.4	No	No	No

Conclusion

The present study demonstrated that yellow passion fruit (Passiflora edulis f. flavicarpa) pomace is a valuable source of nutrients, minerals, phenolics, flavonoids, and diverse bioactive phytoconstituents. The presence of substantial dietary fibre, pectin, potassium, phosphorus, and bioactive compounds highlights its potential for value-added utilisation. GC-MS/MS and LC-MS/MS profiling, together with molecular docking, revealed favourable interactions of selected phytochemicals with key anti-diabetic and hypocholesterolemic targets. ADMET analysis further indicated generally favourable predicted pharmacokinetic and safety profiles for several identified compounds. Overall, YPF pomace represents a promising underutilized fruit-processing by-product for potential application in functional foods, nutraceuticals, and other bioactive product development. However, further in vitro and *in vivo* studies are required to validate the predicted biological activities and establish its safety and efficacy.

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