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Assessing the Druglikeness of *Isoberlinia tomentosa* Phytochemicals: A Computational Study



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Abstract

The hunt for novel therapeutic agents from plants has gained significant attention because of the increasing need for more effective and safer options to synthetic drugs. This study focused on *Isoberlinia tomentosa*, a Fabaceae family species traditionally used to treat fever, arthritis, wounds, and gastrointestinal disorders, to evaluate its phytochemical composition, pharmacokinetic behavior, drug-likeness, and toxicity profile using *in-silico* computational approaches. GC-FID (Gas Chromatography–Flame Ionization Detection) identified twenty-three bioactive phytochemicals in the ethanolic fruit extract. Canonical SMILES data retrieved from PubChem and ChemSpider were subjected to pharmacokinetic (ADMET) and medicinal chemistry analyses through established computational servers. Results revealed that most of the phytochemicals complied with Lipinski's rule of five, Pfizer, GSK, and Golden Triangle drug-likeness criteria, indicating favorable oral bioavailability, solubility, and absorption profiles. About 82% of the compounds exhibited optimal molecular weight, logP, and TPSA values consistent with good intestinal permeability and metabolic stability. ADMET predictions showed desirable absorption and distribution features, with most compounds demonstrating non-inhibitory effects on key cytochrome P450 isoenzymes (CYP1A2, CYP2C9, CYP3A4, and CYP2D6), implying minimal drug–drug interaction potential. Toxicological evaluations using ProTox-II, StopTox, and ADMETlab servers indicated low mutagenic, hepatotoxic, and carcinogenic risks for most compounds, suggesting a broad safety margin. PASS analysis predicted diverse pharmacological activities, including anti-carcinogenic, antioxidant, kinase inhibitory, anti-inflammatory, antimicrobial potentials, while only a few compounds showed low probabilities for adverse effects such as myocardial infarction, nephrotoxicity, or hepatotoxicity. Overall, *Isoberlinia tomentosa* demonstrated promising therapeutic potential with promising pharmacokinetic and safety features, supporting its consideration as a source of lead compounds for future pharmacological validation and drug development.

Keywords: *Isoberlinia tomentosa*, phytochemicals, ADMET, *in-silico* analysis, drug-likeness, toxicity prediction

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INTRODUCTION

Searching for new drugs from natural plants using computational methods has gaining momentum therefore the need for plants phytochemical profiling, curative advantage and toxicity potentials. Bioactive substances mostly from plant have the features of novel structures, high activities, and likely few side effects, therefore they are presently being adopted as substitute treatment options in many therapy (Heise et al., 2023; Das et al., 2022). Over the years, some medicines have been removed from the market because of toxicity and serious adverse effect on major organs which lead to death or require organ transplantation (Jothimani et al., 2020; Isabel et al., 2020). Current medicines offer some assistance in the management of various diseases, but many other ailments are currently in need of better treatment option where the options could be from plant-based preparations (Dickson et al., 2020). Globally, people are sifting to the use of traditional medicine from conventional drugs because the herbal medicines are been scientifically and clinically proved to be effective, moreover, the synthetic drugs are considered to be associated with many adverse drug reactions (Jahan et al., 2020; Borwin et al., 2023). *Isobertonia tomentosa* is a deciduous tree found in tropical Africa and belongs to the family of Fabaceae (ceasalpinoideae). It exists as shrub or tree with the fruits having two-valved pod which twist during dehiscence; obliquely oblong, compressed, and becoming woody (Hadiza et al., 2020; Yilangai et al., 2023; Adekilekun et al., 2025). There is report about a species called *Isobertonia doka* which has been scientifically reported in severally publications including phytochemicals presence, antioxidant activities, and enhance sexuality in male Wistar rats (Hadiza et al., 2020), but reports about *I. tomentosa* is scanty. It is therefore necessary to determine the phytochemical constituents of *I. tomentosa* fruit, and predict their biological activity and toxicity so that further *in-vitro* and *in-vivo* studies would be more direct and focused. *I. tomentosa* is traditionally reported to be used as therapy in conditions such as fever, arthritis, wounds, and gastrointestinal disturbances. The limited scientific evidence on the pharmacological properties of this plant necessitated this study by evaluating the phytochemical composition then examine the drug-likeness and toxicity potentials of active compounds using computational study. Computational pharmacology involves the use of databases and software to generate and analyze biological activities and molecular information of phytochemicals from plants, this remain a major method in drug discovery and development stages in other to screen and identify a lead compound. This method has helped in solving the challenges encountered in developmental stage of new drugs because of less information about the pharmacokinetics, toxicity profile and pharmacogenomics. Computer-aided methods have exposed informations on toxicity, pharmacokinetic and pharmacogenomics profile through predictions, this has helped in reducing risks taken by pharmaceutical manufacturers (Bitew et al., 2021; Oyewusi et al., 2022; Adekilekun et al., 2024). The present

study revealed the reported phytochemicals and detailed of an *in-silico* drug-likeness, pharmacokinetic (ADME) properties, toxicity, and pharmacogenomics profiles of phytochemicals from *I. tomentosa* using various online software and databases to screen for new or novel classes of drugs or drug-like species which may support future drug discovery.

Material and Methods

Collection, Identification and Preparation of Plant's Part

Fresh fruit of *I. tomentosa* plant was identified using their morphological features reported by Hadiza et al. (2020) and was collected from Igangan village (9.4140°N latitude and 4.1058°E longitude) of Oyo State, Nigeria, after which the authentication and deposit were done (voucher specimen: 1142093) at Forestry Research Institute of Nigeria (FRIN), Ibadan, Oyo State. The fruits were washed in running clean water in order to remove all foreign matters, sliced into pieces before air-dried under the shade to obtain a constant weight, then pulverized into coarse powder with mortar and pestle before storage at room temperature until further experiment.

Analysis of Phytochemicals

Gas Chromatography–Flame Ionization Detection (GC-FID)

Gas Chromatography (BUCK (M910) Scientific, USA) was used for the quantification of phytochemicals in the extracts. The specific gas chromatography was with a flame ionization detector, a RESTEK 15 m MKT-1 column (15 m× 20 m×0.15 µm). The injection temperature was set at 280 °C while the injection velocity 30cm/s was used with 2 µL splitless injection of the samples. Helium (5.0pa) was used as carrier gas at 40 mL/min as flow rate. Then, the initial oven temperature was at 200 °C, the oven was also heated to attain a temperature of 330 °C at the rate of 3 °C/min while the detector was also operated at 320 °C. Phytochemicals were therefore determined by the ratio between area and mass of internal standard therefore the concentrations of individual phytochemicals were expressed in µg/mL (Forghe, & Nna, 2020).

Determination of Availability of Molecular Formulae, Molecular Weights and Canonical SMILE Formats of Identified Phytochemicals

The information about the identified phytochemicals were extracted from ChemSpider (<http://www.chemspider.com/>) and PubChem database (<https://pubchem.ncbi.nlm.nih.gov/>) to retrieve their canonical SMILE formats, molecular weights, and molecular numbers which were used for subsequent analysis (Adekilekun et al., 2024).

Evaluation of Drug Profile of Identified Phytochemicals

Evaluation of Drug Likeness

Pharmacokinetic (PK) analysis of biologically active compounds is normally conducted to select drug candidates using the canonical smile numbers of the

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identified phytochemicals that are downloaded from the PubChem and ChemSpider databases and uploaded in the open source SwissADME and ADMETlab2 web servers (<http://admet.scbdd.com>). The drug-like features of the phytocompounds were evaluated using multiple parameters such as Lipinski rule of 5 lipophilicity (iLogP), water solubility (ESol), topological polar surface area (TPSA). Furthermore, lipophilicity (WLOGP), TPSA and bioavailability of these bioactive compounds were determined using PGP (p-glycoprotein) responses.

Absorption, Distribution, Metabolism, Excretion and Toxicity (ADMET) Analyses

The drug profile assessment for the identified phytochemicals were done via ADME/T analysis. ADMETlab2 servers were utilized for analysing different pharmacokinetic properties connected to ADMET analysis for their critical roles in deciding the pharmacological action and performance of drugs (Liu et al., 2022). For best prediction, Canonical SMILES format files were produced for the identified phytochemicals with the aid of Open Babel v.2.3.1 in the Linux command line that were afterward introduced to the SwissADME and ADMETlab2 servers for the prediction of ADME properties. Moreso, two different servers were used for toxicity analysis, such as ProToxII (<https://tox-new.charite.de>) and StopTox (<https://stoptox.mml.unc.edu>). ProTox-II server is known to predict different toxicity endpoints, like acute toxicity, hepatotoxicity, carcinogenicity, cytotoxicity, mutagenicity, immunotoxicity, adverse outcomes (Tox21) pathways, and toxicity targets with the operations that depend on fragment propensities, molecular similarity, most frequent features, and machine learning methods (Banerjee et al., 2018). StopTox server utilizes a collection of QSAR (quantitative structure-activity relationship) principles that measure the toxicity of compounds for different toxicity end points like acute inhalation toxicity, skin sensitization, acute oral toxicity, eye irritation and corrosion, etc. after compilation, curating, and integration using the largest widely available datasets (Borba et al., 2022).

Biological Activity and Adverse Drug Reaction Predictions

The biological properties and adverse reaction on major organs by the identified compounds were also predicted using PASS (prediction of activity spectra for substances; www.way2drug.com/passonline) webserver. The PASS webserver assesses the biological activities of compounds based on their structure-activity relationship. It compares the structure of the demanded compounds with the stored and documented set of known compounds with their different biological properties and ADVERPred *in-silico* prediction of adverse effects such as Nephrotoxicity, Arrhythmia, Cardiac failure, Hepatotoxicity, and Myocardial infarction. These servers give brief list of potential biological activities as predicted on the ratio of Pa (probability of being active) and Pi (probability of being inactive), where higher Pa value suggests a higher possibility of such biological property for a compound being considered.

Results

Isoberlinia tomentosa Phytochemicals

The GC-FID analysis of *I. tomentosa* ethanolic fruit extract identified and quantified twenty-three (23) bioactive compounds present in this plant species (Table 1; Figure 1).

Molecular Formulae, Molecular Weights and Canonical SMILE Formats Analysis of Identified Phytochemicals

The study revealed that all the identified phytochemicals were deposited at PubChem and ChemSpider databases therefore their molecular weight, molecular formulae and Canonical SMILE numbers are listed in Table 2. Also, these recognized canonical SMILES numbers were used for further pharmacokinetics analysis

Table 1: GC-FID Analysis of Different Parts of *Isoberlinia tomentosa* Ethanolic Extract

S/N	Compound	Retention Time	Peak Area
1	Beta-Carotene	3.033	436.7920
2	Fisetin	3.616	361.0450
3	Betain	4.400	959.0340
4	Betalain	5.016	291.1100
5	Catechin	8.166	688.8100
6	Epicatechin	9.366	695.2900
7	Gallocatechin	9.750	1041.4755
8	Orientin	10.933	1119.8920
9	Taxifolin	11.216	2141.6660
10	Aromadendrene	12.116	854.2250
11	Quercetin	12.600	2100.3680
12	Genistein	12.950	171.0630
13	Delphinidin	13.416	1192.1920
14	Kaempferol	13.900	1493.1860
15	Rutin	14.550	1018.0185
16	Apigenin	15.150	2000.4480
17	Isorhamnetin	15.783	745.7050
18	Apigenin	16.300	2266.9115

19	Luteolin	17.383	880.0725
20	Myricetin	18.083	181.3510
21	Vitexin	18.433	961.6460
22	Cyanidin	19.433	574.2540
23	Betacyanin	20.383	448.8850

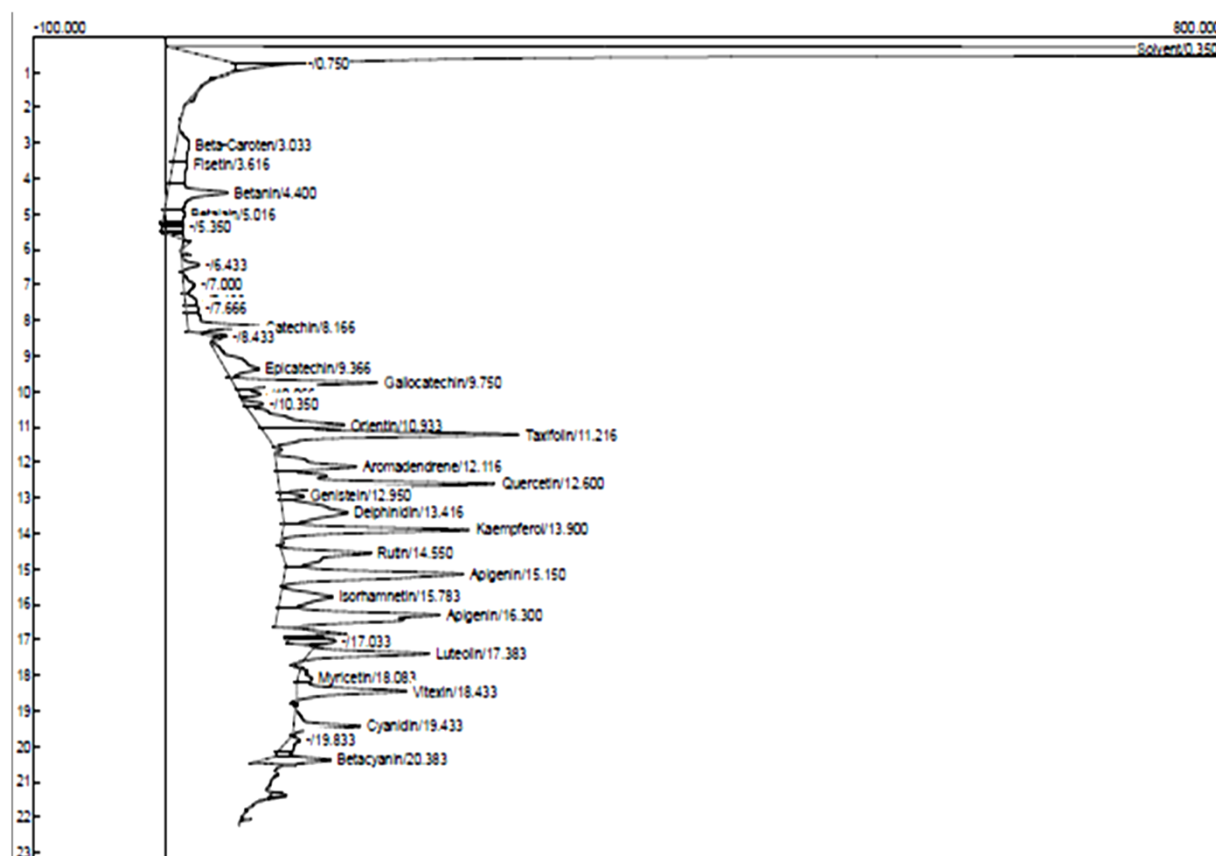


Figure 1: GC-FID chromatogram of ethanolic extract of *I. tomentosa* Fruit

Pharmacokinetics Properties

Analysis of Physicochemical Properties for Drug-likeness

Lipinski's rule of five (RO5) proposes that bioactive molecules tend to display good smooth membrane permeability, oral bioavailability, and high gastrointestinal absorption properties in human gut when their MW \leq 500 Da; log P \leq 5; HBDs \leq 5; and HBAs \leq 10 (Naidoo et al., 2020). It was revealed in this study that molecular weights of all identified phytochemicals falls within the acceptable values of less than 500 except for Betacyanin with 726.18 and few compounds including Beta-Carotene, Betanin, Betalain, and Rutin are with values a little above 500 Da (Table A1; Table A2). Also, the number of hydrogen-bond-acceptors (NHBAs) and hydrogen-bond-donor of all the phytochemicals were less than 10 and 5 respectively, except Betanin, Orientin, Rutin, Betacyanin with higher values. Out of the twenty-two phytochemicals analyzed, twenty of the compounds are within the normal range of LogP accepted value (logP \leq 3) except Aromadendrene and Beta-Carotene. Furthermore, compounds with TPSA values \geq 140 \AA^2 will be poorly absorbed (i.e., less than 10% fractional absorption), while those with lesser TPSA \AA^2

(\leq 140 \AA^2) values would be well absorbed. As can be seen, many of the phytochemicals identified have TPSA values less than 140 \AA^2 indicating the good absorption characteristics, except for Betalain, Orientin, Myricetin, Vitexin, and Betacyanin with higher values. The solubility properties of the compounds depend on the LogS with the acceptable range of -4 to 5. The study predicted that majority of the phytochemicals showed that LogS results are within the acceptable value except for Beta-Carotene and Aromadendrene. The computed results of the distribution coefficient (logD) showed that almost all the identified phytochemicals have LogD values within the acceptable range of 1 to 3 except Beta-Carotene and Aromadendrene. Lastly, logP explained the hydrophilicity and lipophilicity of compounds. The present study showed that out of the 22 identified phytochemicals with smiles identity, only Beta-Carotene and Aromadendrene exhibited higher values of LogP denoting high metabolic turnover, poor oral absorption, and low solubility. Betalain, Betanin and Rutin have negative values, suggesting that they have higher affinity for the aqueous medium or more hydrophilic in nature, while other 18 compounds possess positive value for logP denoting a higher lipophilic.

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Medicinal Chemistry Properties

This analysis predicts the determination of corresponding drug-likeness rules such as Lipinski's rule-of-five, GSK, Pfizer, and Golden Triangle rules which were born out of the long-term practice in drug discovery by the world-giant pharmaceutical companies. Moreso, some other quantitative measures, like Quantitative Estimate of Drug-likeness (QED), MCE-18, Fsp³, natural product score (NPscore), and synthetic accessibility score (SAscore), and the quantitative parameters evaluated medicinal chemistry evolution, molecular drug-likeness, natural product likeness, synthetic feasibility, respectively (Naidoo et al., 2020). The study observed that majority of these compounds were accepted by the Lipinski's rule-of-five except six (Beta-Carotene, Betanin, Betalain, Orientin, Rutin, and Betacyanin) that violated the rule and thereby rejected (Table A3; Table A4). As stated earlier, the study investigated other rules that are more rigid or flexible and imposes more limitations on the molecules (Table 4). For example, compounds with molecular weights higher than 200 violate the Golden Triangle rule but will normally pass Lipinski's rule-of-five, this was used to further refine molecules based on medicinal chemistry principles.

QED is an alternative metric for drug-like compounds which is measured ranging from 0 (synthesis too complex) to 1 (synthesis attractive) that captures the abstract notion of aesthetics in medicinal chemistry, penalizing molecular patterns commonly found in common drugs and penalizing patterns that lead to toxicity or difficulty in synthesizability (Natesh et al., 2021). This study computed QED scores for the identified phytochemicals from *Isoberberlinia tomentosa*, as can be observed in Table A3 and A4 predicting complexity in their synthesis. Fsp³ is also considered in this prediction which is a simple measure and interpretable metric for molecular saturation, and it is defined as the fraction of sp³ carbon atoms (the number of sp³ hybridized carbons/total carbon count). It is closely linked to solubility and melting points. Table A3 and A4 depicted the Fsp³ of identified phytochemicals where 18.2% have appropriate value (≥ 0.42 : suitable value). Because this result could not completely reflect true 3D-complexity of molecules and their synthetic feasibility, other parameters like medicinal chemistry evolution-18 (MCE-18) can be readily applied for the assessment of novelty of pharmacologically relevant molecules and may help researchers in designing new chemical entities which have great potential in modern drug design. So also Table A3 and A4 shows that 50% of the compounds possess acceptable MCE-18 values (suitable value: $18 \geq 45$).

Synthesizing natural compounds is a better way of minimizing the resources required to extract compounds from their natural origin. Therefore, a molecule with an SA score less than 5.00 indicate not difficult to synthesize, then it requires likely consideration for further optimization studies. As depicted in Table A3 and A4, all the identified phytochemicals have a synthetic accessibility (SA) score of less than 5.00 also indicate their easy synthetic accessibility. On the other hand, The NPscore is a useful means of guiding new molecules design through interesting areas of chemical space which have been

considered by natural evolution as "bioactive regions". Moreover, the calculated NPscore is classically in the range from -5 (high NPscore) to 5 (low NPscore). The higher the NPscore, the higher the probability that the molecules are natural products. In this present study, all the compounds has NPscore below 5, though values above -5 predict the probability of being natural products (Table A3 and A4).

Absorption, Distribution, Metabolism, Excretion and Toxicity (ADMET) Analyses

ADME/T estimation predicted the pharmacokinetics parameters of compounds such as absorption, distribution, metabolism, excretion, and even toxicity. For absorption to take place, human intestinal absorption (HIA) is considered for bioavailability, thus Caco-2 permeability presumed to mimic the HIA *in-vitro* system (Natesh et al., 2021).

Absorption

To assess the absorption phase, the study predicted Caco-2-Permeability, Human intestinal absorption (HIA), P-glycoprotein inhibitor or substrate, 30% bioavailability (F30) and 20% bioavailability (F20) as listed in (Table A5 and A6). HIA depicts human intestinal permeability and any value closer to 1 denotes better absorption via the intestine (Elekofehinti et al., 2018). Out of the 22 phytochemicals, about 63% were showing undesirable Caco-2-Permeability (cm/s) values indicating a very low permeability, while other 36% with values ranges from -4.4 to -5.2 suggesting a low to moderate permeability (Table A5). As can be seen, only 6 (Rutin, Vitexin, Betacyanin, Betanin, Betalain, and Orientin) showed high HIA with a value $\geq 30\%$ while the other 16 phytochemicals depicted HIA below 30% indicating their HIA is low (Table A5 and A6). Majority of the phytochemicals identified from *Isoberberlinia tomentosa* were considered desirable by having predicted Bioavailability scores of greater than either 30 or 20% (Table A5 and A6). The present study predicted that majority of the phytochemicals revealed are potential substrate of P-glycoprotein (P-gp), except Apigenin, Rutin, Vitexin, Betacyanin, Betanin, Betalain, and Orientin that were non-substrate of P-glycoprotein (P-gp) (Table A6). However, compounds or drugs that are predicted as substrates for P-glycoprotein normally have increased metabolism and clearance causing therapeutic failure because the drug concentration will be lower than expected (Nguyen et al., 2021).

Distribution

Plasma Protein Binding (PPB), Blood Brain Barrier (BBB) permeability, and Volume of distribution (VD) are factors considered to account for distribution of identified phytochemicals (Table A5 and A6). The drugs' plasma proteins binding result into the pharmacokinetic functions that affect drug clearance, volume of distribution, and its efficacy because only the free fraction of the compounds that cross the membranes including anatomical barriers like BBB, thus, responsible for stimulating a pharmacological response (Charlier et al., 2021). The present analysis showed that majority of phytochemicals (about 60.6%) have PPB values greater than acceptable value (PPB < 90%) (Table A5 and A6), showing that their distribution beyond these barriers will be very low as

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compared to the other 40% have PPB values less than 90% which suggests their high availability for absorption and distribution. Moreover, [Table A5 and A6](#) also showed BBB results obtained from ADMETlab with all the phytochemicals predicted to have desirable BBB penetration. The volumes of distribution (VD) value in L/Kg are considered satisfactory if the values are between 0.04 – 20 L/kg. The high VD implies the poor ability of bioactive compounds to diffuse or transverse across a cell membrane ([Charlier et al., 2021](#)). The study revealed that all the phytochemicals are ideal candidates for uniform distribution in blood plasma ([Table A5 and A6](#)).

Metabolism and excretion

Five principal isoforms of Cytochrome P450 inhibition profile (1A2, 2C9, 2C19, 2D6, and 3A4) were assessed in order to support the cleanest profile and predict the compound(s) with lower probability of causing drug-drug interactions due to CYP inhibition ([Elekofehinti et al., 2018](#)). The study revealed that some phytochemicals are CYP enzyme substrates making them to be quickly metabolized by the enzymes, while some possessed CYP enzyme inhibitory actions, which might hinder their metabolism ([Table A6](#)). CYP enzyme inhibitors especially CYP3A4 and CYP2D6 inhibitors are vital determinants in the therapeutic efficacy and even toxicity of various compounds. Ten (10) phytochemicals are predicted to act as CYP1A2 and CYP2C9 inhibitors, while three (3) phytochemicals (Beta-Carotene, Genistein and Apigenin) are inhibitors of CYP2C19 ([Table A6](#)). Additionally, the study revealed that eight (8) are CYP2D6 inhibitors and nine (9) exhibited CYP3A4 inhibitors. The interactions with CYP3A are frequently considered as the manifestation of drug-drug interactions. Moreover, majority of the phytochemicals showed good or moderate clearance values of greater than 5ml/min/kg except Rutin, Vitexin, Betacyanin, Beta-Carotene, Betanin, and Betalain ([Table A5 and A6](#)).

Toxicity Profile/Toxicological Endpoints

Toxicity properties were therefore analyzed with the aid of two different online servers for dependability of prediction whereas the servers provided coherent and satisfactory results ([Tables A6 & Table A7](#)). ProToxII and StopTox servers disclosed significant results in the different parameters. The ADMETlab descriptors such as human hepatotoxicity (H-HT), hERG Blockers (hERG), Skin sensitization (SkinSen), Ames Mutagenicity (AMES) were applied to predict the toxicity of the phytochemicals from *Isoblerlinia tomentosa*. The numbers 1 and 0 in the group section shown in [Table A6](#) denote positive and negative respectively for toxicity prediction values. All the phytochemicals from *Isoblerlinia tomentosa* are predicted not to block the hERG (human ether-a-go-go related gene). Nevertheless, only Catechin was predicted to show carcinogenicity, with only few have toxic to respiratory, eye and skin ([Table A7 and Table A8](#)). Besides the ADMETlab analysis, ProTox II prediction descriptors such as the organ toxicity (hepatotoxicity) and the toxicological endpoints (cytotoxicity, mutagenicity, carcinogenicity, and immunotoxicity) of the bioactive compounds were predicted and presented in [Table A7 and Table A8](#). As can

be seen, the predicted cytotoxicity and drug induced liver injury (DILI) results demonstrate that majority of the identified phytochemicals are non-cytotoxic, this correlates with the results from ADMETlab prediction in [Table 5](#). Most of the phytochemicals were foreseen with inactivity to induce liver injury except Fisetin, Betanin, Betalain, Orientin, Taxifolin and Quercetin. The results also signal the disposition of these phytochemicals to cause liver cancer ([Table A7 and Table A8](#)). Fisetin, Betalain, Betanin, Orientin, Taxifolin, Quercetin, Luteolin, Myricetin, Vitexin, Cyanidin, and Betacyanin are the ones showed two or three toxicological endpoints each ([Table A7 and Table A8](#)). StopTox server used to evaluate toxicity from five toxicity endpoints, like eye irritation and corrosion, acute inhalation toxicity, skin irritation and corrosion, acute oral toxicity and skin sensitization criteria where most of the phytochemicals were found to be harmless and thus satisfactory ([Table A7 and Table A8](#)). Most of the phytochemicals showed none active condition for all the parameters while some indicated active status under the Tox21-Stress response pathway and Tox21-Nuclear receptor signalling pathway ([Table A7 and Table A8](#)). Among all the compounds only Catechin, Epicatechin, and Gallocatechin are predicted to have LD₅₀ greater than 5000mg/kg body weight, this shows that majority of the compounds are potentially safe.

Biological Activity and Adverse Reaction Prediction

The biological activity and adverse reactions of identified phytochemicals from *I. tomentosa* were determined using Prediction of Activity Spectra for Substances (PASS) approach. PASSonline usually predicts pharmacological effects, particular toxicity, and mechanisms of action of the studied compounds by comparing with similar structure regions of known biologically active substances available in the data bank, with 95% accuracy ([Genovese et al., 2021](#)). PASSonline provides concurrent predictions of many forms of biological activity based on the structure of drug-like compounds. Our findings revealed that these phytochemicals identified from *I. tomentosa* except have a potential Tp53 expression enhancement, kinase inhibitor, Anticarcinogenic, antioxidant, Antineoplastic, Antiinflammatory, Antifungal, Antibacterial, Chemoprotective and Antioxidant effects ([Table A9](#)). This indicated that *I. tomentosa* phytochemicals can be use in the treatment or management of numerous diseases such as cancer. This server could not give any predictable uses for Delphinidin and Cyanidin. Moreover the adverse reaction as predicted showed that Gallocatechin, Aromadendrene, Delphinidin and Cyanidin were not predicted for any reaction yet. Beta-Carotene, Betanin, Betalain, and Betacyanin were predicted to present Myocardial infarction with Betanin, Betalain, and Betacyanin having Nephrotoxicity as second adverse reaction. Other phytochemicals presented to have both Hepatotoxicity and Nephrotoxicity ([Table 3](#)). The crude extract of *I. tomentosa* has shown to have antioxidant and antiinflammatory effects ([Adekilekun et al., 2025](#)). Apiginin, Catechin and Cyanidin have shown some anticancer effects ([Shikha et al., 2024; Adekilekun et al., 2024; Rauf et al., 2025](#)), Betalain, Catechin and Beta-Carotene have also shown antioxidant

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activities (Sadowska-Bartosz, & Bartosz, 2021; Shikha et al., 2024; Dağlıoğlu, 2025).

Table 2: Phytochemical components of *Isoberlinia tomentosa*

S/N	Compound	Molecular Formula	Molecular Weight	Canonical SMILE Number
1	Beta-Carotene (CID: 5280489)	C ₄₀ H ₅₆	536.9	CC1=C(C(CCC1)(C)C)/C=C/C(=C/C=C/C(=C/C=C/C=C(/C=C/C=C(/C=C/C2=C(CCCC2(C)C)C)\C)/C)/C
2	Fisetin (CID: 5281614)	C ₁₅ H ₁₀ O ₆	286.24	C1=CC(=C(C=C1C2=C(C(=O)C3=C(O2)C=C(C=C3)O)O)O)O
3	Betanin (CID: 6540685)	C ₂₄ H ₂₆ N ₂ O ₁₃	550.5	C1[C@@H](N=C(C=C1/C=C/N2[C@@H](CC3=CC(=C(C=C32)O)O)[C@H]4[C@@H]([C@H]([C@@H]([C@H](O4)CO)O)O)O)C(=O)O)C(=O)O)C(=O)O
4	Betalain (CID: 56841626)	C ₂₄ H ₂₆ N ₂ O ₁₃	550.5	C1[C@@H]([N+](=C/C=C/2\CC(NC(=C2)C(=O)O)C(=O)O)C3=CC(=C(C=C31)O)[C@@H]4[C@@H]([C@H]([C@@H]([C@H](O4)CO)O)O)O)O)C(=O)[O-]
5	Catechin (CID: 9064)	C ₁₅ H ₁₄ O ₆	290.27	C1[C@@H]([C@H](OC2=CC(=CC(=C21)O)O)C3=CC(=C(C=C3)O)O)O
6	Epicatechin (CID: 72276)	C ₁₅ H ₁₄ O ₆	290.27	C1[C@H]([C@H](OC2=CC(=CC(=C21)O)O)C3=CC(=C(C=C3)O)O)O
7	Gallocatechin (CID: 65084)	C ₁₅ H ₁₄ O ₇	306.27	C1[C@@H]([C@H](OC2=CC(=CC(=C21)O)O)C3=CC(=C(C=C3)O)O)O
8	Orientin (CID: 5281675)	C ₂₁ H ₂₀ O ₁₁	448.4	C1=CC(=C(C=C1C2=CC(=O)C3=C(O2)C(=C(C=C3)O)[C@H]4[C@@H]([C@H]([C@@H]([C@H](O4)CO)O)O)O)O)O
9	Taxifolin (CID: 439533)	C ₁₅ H ₁₂ O ₇	304.25	C1=CC(=C(C=C1[C@@H]2[C@H](C(=O)C3=C(C=C(C=C3O2)O)O)O)O)O
10	Aromadendrene (CID: 11095734)	C ₁₅ H ₂₄	204.35	C[C@@H]1CC[C@@H]2[C@@H]1[C@H]3[C@H](C3(C)C)CCC2=C
11	Quercetin (CID: 5280343)	C ₁₅ H ₁₀ O ₇	302.23	C1=CC(=C(C=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O)O
12	Genistein (CID: 5280961)	C ₁₅ H ₁₀ O ₅	270.24	C1=CC(=CC=C1C2=COC3=CC(=CC(=C3C2=O)O)O)O
13	Delphinidin (CID: 68245)	C ₁₅ H ₁₁ ClO ₇	338.69	C1=C(C=C(C(=C1O)O)O)C2=[O+]C3=CC(=CC(=C3C=C2O)O)O.[Cl-]
14	Kaempferol (CID: 5280863)	C ₁₅ H ₁₀ O ₆	286.24	C1=CC(=CC=C1C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O
15	Rutin (CID: 5280805)	C ₂₇ H ₃₀ O ₁₆	610.5	C[C@H]1[C@@H]([C@H]([C@H]([C@@H](O1)OC[C@@H]2[C@H]([C@@H]([C@H]([C@@H](O2)OC3=C(OC4=CC(=CC(=C4C3=O)O)O)C5=CC(=C(C=C5)O)O)O)O)O)O)O
16	Apigenin (CID: 5280443)	C ₁₅ H ₁₀ O ₅	270.24	C1=CC(=CC=C1C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O
17	Isorhamnetin (CID: 5281654)	C ₁₆ H ₁₂ O ₇	316.26	COC1=C(C=CC(=C1)C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O
19	Luteolin (CID: 5280445)	C ₁₅ H ₁₀ O ₆	286.24	C1=CC(=C(C=C1C2=CC(=O)C3=C(C=C(C=C3O2)O)O)O)O
20	Myricetin (CID: 5281672)	C ₁₅ H ₁₀ O ₈	318.23	C1=C(C=C(C(=C1O)O)O)C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O
21	Vitexin (CID: 5280441)	C ₂₁ H ₂₀ O ₁₀	432.4	C1=CC(=CC=C1C2=CC(=O)C3=C(O2)C(=C(C=C3)O)[C@H]4[C@@H]([C@H]([C@@H]([C@H](O4)CO)O)O)O)O
22	Cyanidin (CID: 128861)	C ₁₅ H ₁₁ O ₆ ⁺	287.24	C1=CC(=C(C=C1C2=[O+]C3=CC(=CC(=C3C=C2O)O)O)O)O
23	Betacyanin (CID: 6325284)	C ₃₀ H ₃₄ N ₂ O ₁₉	726.6	C\1[C@H](NC(=C/C1=C/C=[N+]2[C@@H](CC3=CC(=C(C=C32)O)O)[C@H]4[C@@H]([C@H]([C@@H]([C@H](O4)CO)O)O)O)[C@H]5[C@@H]([C@H]([C@@H]([C@H](O5)C(=O)O)O)O)O)C(=O)[O-])C(=O)O)C(=O)O

Table 3. Prediction of Activity Spectra for Substances (PASS) Analysis for Potential Adverse Reactions of *Isoberlinia tomentosa* Identified Phytochemicals.

Adverse Reactions Compound	Myocardial infarction		Hepatotoxicity		Nephrotoxicity	
	Pa	Pi	Pa	Pi	Pa	Pi
Beta-Carotene	0.915	0.004				
Fisetin			0.773	0.070		
Betanin	0.298	0.204			0.527	0.041
Betalain	0.306	0.187			0.511	0.046
Catechin					0.242	0.236
Epicatechin					0.242	0.236
Gallocatechin	-----		-----		-----	
Orientin					0.499	0.050
Taxifolin					0.245	0.230
Aromadendrene	-----		-----		-----	
Quercetin			0.559	0.165		
Genistein			0.342	0.308		
Delphinidin	----		-----		-----	
Kaempferol			0.525	0.182		
Rutin			0.384	0.271	0.247	0.228
Apigenin			0.525	0.182		
Isorhamnetin			0.365	0.286		
Luteolin			0.559	0.165		
Myricetin			0.637	0.126		
Vitexin					0.510	0.047
Cyanidin	-----		-----		-----	
Betacyanin	0.285	0.236			0.518	0.044

Discussion

Computer aided techniques are used to process information pertaining to chemical molecules depending on their structures to search and predict for biologically active molecules through data mining tools in the pharmaceutical researches thereby supporting the discovery of novel drugs (Gautam et al., 2023). PubChem and ChemSpider servers were used to reveal the documented or confirmed information about the identified phytochemicals of *I. tomentosa*. In this study, twenty-three phytochemicals identified through GC-FID which are also available in the PubChem and ChemSpider database servers (Table 1). Most importantly, the study also retrieves the canonical SMILES numbers of all the twenty-two phytochemicals that were used for further analysis (Table 2). Drug designing procedure involves prediction of pharmacokinetic properties in human, which will support advancement of drug candidates if it will be successful in the clinic (Sadybekov, & Katritch, 2023). A molecule or phytochemical with poor pharmacokinetics especially absorption and elimination might not be seriously considered to have good fits to the receptor, this might predict a failure in the development. Predicting physicochemical characteristics of a drug candidate is considered to be related to its therapeutic accuracy, safety and efficiency obtainable in the laboratory (Naidoo et al., 2020). Other features like number of hydrogen bond acceptors or donors, number of rotatable bonds, topological polar surface area (TPSA [Å]), molecular weight, logarithm of distribution coefficient (log D), and logarithm of partial coefficient (log P) [at pH = 7.4] were also appraised carefully for the phytochemicals identified from *I. tomentosa* (Table A1 & A2). Physicochemical and

medicinal chemistry properties of the phytochemicals were assessed based the conventional guidelines of drug-likeness that are applicable in emerging stages of drug discovery, including Lipinski's rule-of-five, GSK, Pfizer, and Golden Triangle rules. These rules suggest that a drug or bioactive molecule tends to exhibit smooth membrane permeability, decent oral bioavailability, and high gastrointestinal absorption in human gut when all the criteria are met as stated in (Table A3 & Table A4). Going by the Lipinski's rule-of-five, only six (Beta-Carotene, Betanin, Betalain, Orientin, Rutin, Betacyanin) violated the rule while others obeyed (Table A1 & A2), which strongly imply others could be more preferable. It was also revealed that majority of the identified compounds showed good medicinal chemistry property. Solubility and intestinal absorption of a compound are vital pharmacokinetic indices linked with drug's action and efficacy (Vinarov et al., 2021). Likewise, bioavailability is determined using the absorbance in the small intestine methods especially through oral route of administration, therefore, reduced solubility and poor intestinal absorption are main obstacles that affect its accuracy and execution (Tsume et al., 2023; Awais et al., 2023). It is worth mentioning that majority of identified phytochemicals of *I. tomentosa* showed good intestinal absorbance especially Genistein, Delphinidin, Kaempferol, Apigenin, Isorhamnetin, Luteolin, Fisetin, Aromadendrene describing their better bioavailability after oral administration. Moreover, this study also demonstrated that all the bioactive compounds are P-glycoprotein I/II inhibitors which are very important feature in pharmacokinetics studies (Table 5). A molecule with capacity of inhibit these transporters could also

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obstruct the pharmacokinetics of another compound (Nguyen et al., 2021). Subsequently, it can be predicted that majority of these phytochemicals can be adjuvant agents with any other bioactive thus considered as safe and effective. Interestingly, majority of phytochemicals assessed were predicted to show high gastrointestinal absorption, good solubility and excretion in the human system, these features might establish them as favourable therapeutic candidates (Table A5 & A6). Other factors that can influence pharmacokinetic interactions include drug-metabolizing enzymes and total clearance, which measures the rate of drug removal from plasma or blood. Cytochrome P450, a key detoxification enzyme primarily found in the human liver, plays a major role in this process. Any adjustment in the activity of these enzymes could lead to disruptions in the pharmacokinetics of drugs metabolized by them. Cytochrome P2D6 and cytochrome P3A4 are the two most essential isoforms of cytochrome P450 (Morales et al., 2023). Table A5 & A6 shows that those compounds don't affect or inhibit these enzymes. Therefore, it can be understood that all these compounds are safe as supportive agents with other drugs. The Clearance or drug elimination results from both liver and kidney. Total clearance (CL_{tot}) represents the combined effect of renal and hepatic clearance. It is closely associated with bioavailability and plays a crucial role in determining dosing rates required to achieve steady-state plasma concentrations. A steady-state level is obtained when the drug administered is at appropriate dose and concentration to ensure sufficient bioavailability. The rate of compound excretion is directly dependent on the clearance value (Morales et al., 2023; Tuloup et al., 2023; Domínguez-Villa et al., 2021). Table 5 shows the total clearance predicted values of the compounds exposing their rate of excretion. Rutin, Vitexin, Beta-Carotene, Betanin, and Betalain showed the undesirable clearance proportion as compared to the others (Table A5 & A6).

In-silico toxicity valuation, in connection with AMES mutagenicity dataset, was done using ProTox-II and StopTox webservers and the results were further corroborated with admetLab. Toxicity prediction of the compound can be done by AMES toxicity which also predicts if any compound has carcinogenic or mutagenic or cytotoxic potential or not (Morales et al., 2023). The study revealed toxicity prediction pertaining to carcinogenicity, mutagenicity, and cytotoxicity of the phytochemicals (Table A7 & A8). It was revealed that some of the phytochemicals have no mutagenic effects. Also an important aspect to be considered is determining the likelihood of any drug to induce liver injury. As can be seen from Table A7 & A8 all of the phytochemicals are not hepatotoxic. Carcinogens or mutagens are referred to as the chemicals/ compounds that stimulate formation, growth, and proliferation of tumours, thus, inducing cancer. The carcinogenicity predictions revealed that most of the phytochemicals were potential non-carcinogens or non-mutagens (Table A7 & A8). Furthermore, most of the phytochemicals were predicted not to display any irritation effects (Table A7 & A8). Generally, majority of these phytochemicals showed no presence of toxicity which is a

main factor considered in choosing a therapeutic candidate. Several possible biological activities and adverse reactions of the identified phytochemicals were predicted by means of the prediction of activity spectra for substances (PASS) webserver. Two factors are used to evaluate the active compounds; Pa indicates the probability "to be active", and Pi suggests the probability "to be inactive", with the values ranging from 0 to 1. At this point, the study noticed that most of the phytochemical's function as potent anticarcinogenic, anti-inflammatory, antimicrobial, and antioxidants (Table A9). Besides, they also have antineoplastic, kinase inhibitor, and TP53 enhancement, especially against the cancerous growth. Therefore, it can be predicted that phytochemicals from *I. tomentosa* might be used in many disease therapy. PASS analysis also predicted some major side effects of these active compounds. Three predicted adverse reaction include Myocardial infarction, Nephrotoxicity and Hepatotoxicity, and it was shown in Table 3, that majority of these compounds have less probability of causing these damages.

Conclusion

This comprehensive *in-silico* study of *Isoberlinia tomentosa* phytochemicals reveals promising potential for drug discovery and development. The analysis of 23 identified compounds using various computational tools provides valuable perceptions into their pharmacokinetic properties, drug-likeness, and potential biological activities. Most compounds revealed favorable drug-like properties, observing to Lipinski's rule of five and other medicinal chemistry criteria. The majority of phytochemicals also showed good absorption and distribution profiles, with acceptable bioavailability and plasma protein binding. Several compounds exhibited potential as P-glycoprotein inhibitors, suggesting possible roles as adjuvant agents in combination therapies. Toxicity predictions were largely favorable, with most compounds showing low potential for mutagenicity, carcinogenicity, and organ toxicity. Biological activity predictions highlighted potential anticarcinogenic, anti-inflammatory, antimicrobial, and antioxidant properties for many compounds. These results underscore the therapeutic potential of *I. tomentosa* phytochemicals, particularly in areas such as cancer treatment, inflammation, and oxidative stress-related disorders. While further *in-vitro* and *in-vivo* studies are necessary to validate these outcomes, this computational analysis provides a solid foundation for targeted experimental investigations and rational drug design efforts. The study demonstrates the power of *in-silico* approaches in streamlining the drug discovery practice, offering a cost-effective and efficient method for initial screening of natural products. As research continues, *I. tomentosa* and its bioactive compounds may emerge as valuable resources in the discovery of novel, effective, safe therapeutic candidates.

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Supplementary Tables

Table A1: Physicochemical properties of *Isoberlinia tomentosa* phytochemicals

Properties	Rules	Beta-Carotene	Fisetin	Betanin	Betalain	Catechin	Epicatechin	Gallocatechin	Orientin	Taxifolin	Aromadendrene	Quercetin
Mw	≤600	536.44	286.05	550.14	550.14	290.08	290.08	306.07	448.1	304.06	204.19	302.04
(g/mol)												
nHA	≤12	0	6	15	15	6	6	7	11	7	0	7
nHD	≤7	0	4	8	8	5	5	6	8	5	0	5
TPSA	≤140 Å ²	0.0	111.13	247.11	249.38	110.38	110.38	130.61	201.28	127.45	0.0	131.36
LogS	-4 – 0.5	-5.026	-3.704	-1.576	-0.627	-2.739	-2.72	-2.596	-3.697	-3.521	-6.086	-3.671
LogP	≤3	7.687	2.428	-0.201	-1.425	1.343	1.213	0.9	0.757	1.056	5.193	2.155
LogD	1 – 3	5.523	2.043	-0.07	-1.013	1.62	1.243	0.715	-0.024	1.009	5.432	1.767

Table A2: Physicochemical properties of *Isoberlinia tomentosa* phytochemicals

Properties	Rules	Genistein	Delphinidin	Kaempferol	Rutin	Apigenin	Isorhamnetin	Luteolin	Myricetin	Vitexin	Cyanidin	Betacyanin
Mw (g/mol)	≤600	270.05	338.02	286.05	610.15	270.05	316.06	286.05	318.04	432.11	287.06	726.18
nHA	≤12	5	7	6	16	5	7	6	8	10	6	21
nHD	≤7	3	6	4	10	3	4	4	6	7	5	11
TPSA	≤140 Å ²	90.9	132.68	111.13	269.43	90.9	120.36	111.13	151.59	181.05	112.45	345.6
LogS	-4 – 0.5	-3.44	-3.428	-3.624	-3.742	-3.606	-3.748	-3.629	-3.665	-3.78	-3.432	-0.237
LogP	≤3	2.506	2.533	2.656	-0.038	3.307	2.541	2.902	1.747	1.232	2.895	-2.169
LogD	1 – 3	2.577	1.86	2.233	-0.21	2.704	2.262	2.361	0.9	0.145	2.83	-1.344

Table A3: Medicinal chemistry properties of *Isoberlinia tomentosa* phytochemicals

Properties	Beta-Carotene	Fisetin	Betanin	Betalain	Catechin	Epicatechin	Gallocatechin	Orientin	Taxifolin	Aromadendrene	Quercetin
QED (>0.67: attractive; 0.49 - 0.67: unattractive; <0.34: too complex)	0.244	0.511	0.178	0.152	0.51	0.51	0.437	0.247	0.501	0.517	0.434
SA score (≥ 6: difficult to synthesise; <6: easy to synthesise)	3.693	2.359	5.06	5.36	3.344	3.344	3.521	4.072	3.361	4.223	2.545
Fsp³ (≥0.42: suitable value)	0.45	0.0	0.417	0.417	0.2	0.2	0.2	0.286	0.133	0.867	0.0
MCE-18 (18≥45: suitable value)	25.517	18.0	102.353	102.353	60.0	60.0	63.333	91.0	61.471	48.857	19.0
NP score (-5: high; 5: low)	1.127	1.335	1.365	-	2.304	2.304	2.272	2.014	2.298	3.363	1.701
Lipinski Rule (MW ≤ 500; logP ≤ 5; nHA ≤ 10; nHD ≤ 5)	Rejected	Accepted	Rejected	Rejected	Accepted	Accepted	Accepted	Rejected	Accepted	Accepted	Accepted
Pfizer Rule (logP > 3; TPSA < 75)	Rejected	Accepted	Accepted	Accepted	Accepted	Accepted	Accepted	Accepted	Accepted	Rejected	Accepted
GSK Rule (MW ≤ 400; logP ≤ 4)	Rejected	Accepted	Rejected	Rejected	Accepted	Accepted	Accepted	Rejected	Accepted	Rejected	Accepted
Golden Triangle 200 ≤ MW ≤ 50; -2 ≤ logD ≤ 5	Rejected	Accepted	Rejected	Rejected	Accepted	Accepted	Accepted	Accepted	Accepted	Rejected	Accepted

Table A4: Medicinal Chemistry Properties of *Isoberlinia tomentosa* Phytochemicals

Properties	Genistein	Delphinidin	Kaempferol	Rutin	Apigenin	Isorhamnetin	Luteolin	Myricetin	Vitexin	Cyanidin	Betacyanin
QED (>0.67: attractive; 0.49 - 0.67: unattractive; <0.34: too complex)	0.632	0.263	0.546	0.14	0.632	0.572	0.511	0.371	0.3	0.347	0.1
SA score (≥ 6: difficult to synthesise; <6: easy to synthesise)	2.297	3.331	2.375	4.783	2.253	2.453	2.42	2.733	3.954	3.038	5.897
Fsp³ (≥0.42: suitable value)	0.0	0.0	0.0	0.444	0.0	0.062	0.0	0.0	0.286	0.0	0.5
MCE-18 (18≥45: suitable value)	17.0	17.0	18.0	122.949	17.0	19.0	18.0	20.0	87.63	18.0	137.644
NP score (-5: high; 5: low)	1.355	1.64	1.546	2.015	1.358	1.566	1.499	1.698	1.978	1.745	2.298
Lipinski Rule (MW ≤ 500; logP ≤ 5; nHA ≤ 10; nHD ≤ 5)	Accepted	Accepted	Accepted	Rejected	Accepted	Accepted	Accepted	Accepted	Accepted	Accepted	Rejected
Pfizer Rule (logP > 3; TPSA < 75)	Accepted	Accepted	Accepted	Accepted	Accepted	Accepted	Accepted	Accepted	Accepted	Accepted	Accepted
GSK Rule (MW ≤ 400; logP ≤ 4)	Accepted	Accepted	Accepted	Rejected	Accepted	Accepted	Accepted	Accepted	Rejected	Accepted	Rejected
Golden Triangle 200 ≤ MW ≤ 50; -2 ≤ logD ≤ 5	Accepted	Accepted	Accepted	Rejected	Accepted	Accepted	Accepted	Accepted	Accepted	Accepted	Rejected

Table A5: ADMET Properties of *Isoberlinia tomentosa* Phytochemicals

Class	Properties	Genistein	Delphinidin	Kaempferol	Rutin	Apigenin	Isorhamnetin	Luteolin	Myricetin	Vitexin	Cyanidin	Betacyanin
Absorption	Caco-2 permeability (>-5.15 cm/s)	-4.764	-4.978	-4.974	-6.47	-4.847	-5.056	-5.028	-5.653	-6.222	-5.344	-7.405
	Pgp-inhibitor (category 1: inhibitor; 0: non-inhibitor)	0.007	0.005	0.004	0.005	0.004	0.008	0.004	0.004	0.005	0.012	0.0
	Pgp-substrate (category 1: substrate; 0: non-substrate)	0.693	0.008	0.011	0.997	0.82	0.042	0.274	0.006	0.991	0.022	0.998
	HIA (≥30%: high, <30%: low)	0.01	0.009	0.008	0.876	0.015	0.024	0.047	0.035	0.841	0.28	0.933
	Bioavailability scores (≥20%: high, <20%: low)	0.863	0.923	0.856	0.038	0.995	0.03	0.998	0.977	0.934	0.997	0.923
	Bioavailability scores (≥30%: high, <30%: low)	0.992	0.994	0.993	0.999	0.999	0.978	1.0	0.999	1.0	0.998	1.0
	PPB (<90%)	97.55%	97.04%	97.86%	87.11%	97.25%	96.23%	95.43%	92.76%	89.60%	95.43%	35.98%

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Distribution	VD (0.04 – 20 L/kg)	0.471	0.477	0.522	0.701	0.51	0.647	0.533	0.633	0.903	0.609	0.478
	BBB Penetration (category 1: BBB+; 0: BBB-)	0.02	0.009	0.009	0.041	0.012	0.005	0.009	0.006	0.017	0.011	0.242
Metabolism	CYP1A2 inhibitor	0.981	0.95	0.972	0.121	0.988	0.96	0.981	0.846	0.211	0.735	0.01
	CYP1A2 substrate	0.132	0.114	0.11	0.041	0.145	0.736	0.154	0.108	0.039	0.186	0.001
(Category 1: inhibitor; 0: non-inhibitor)	CYP2C19 inhibitor	0.59	0.097	0.181	0.035	0.588	0.111	0.124	0.027	0.023	0.035	0.028
	CYP2C19 substrate	0.048	0.046	0.046	0.048	0.051	0.049	0.046	0.037	0.053	0.046	0.019
inhibitor)	CYP2C9 inhibitor	0.615	0.535	0.653	0.018	0.602	0.657	0.576	0.574	0.067	0.168	0.032
	CYP2C9 substrate	0.935	0.689	0.867	0.139	0.939	0.827	0.842	0.32	0.526	0.616	0.045
Excretion	CYP2D6 inhibitor	0.863	0.532	0.722	0.056	0.792	0.585	0.568	0.098	0.094	0.146	0.006
	CYP2D6 substrate	0.716	0.329	0.283	0.129	0.778	0.304	0.559	0.169	0.167	0.265	0.047
Toxicity	CYP3A4 inhibitor	0.813	0.62	0.697	0.039	0.833	0.52	0.549	0.187	0.065	0.174	0.019
	CYP3A4 substrate	0.109	0.098	0.08	0.003	0.126	0.086	0.092	0.025	0.02	0.065	0.0
hERG I/II (category 1: active; 0: inactive)	Clearance rate (>15 ml/min/kg: high; 5ml/ min/kg<Cl < >15 ml/min/kg: moderate; <5ml/ min/kg: low)	7.844	8.273	6.868	1.502	7.022	6.991	8.146	7.716	4.091	15.311	1.459
	H-HT (Human Hepatotoxicity)	0.048	0.043	0.07	0.227	0.057	0.061	0.064	0.145	0.11	0.085	0.019
DILI (category 1: high risk; 0: no risk)	DILI (category 1: high risk; 0: no risk)	0.092	0.127	0.098	0.083	0.072	0.064	0.084	0.099	0.175	0.165	0.228
	Skin sensitization (category 1: sensitizer; 0: non-sensitizer)	0.51	0.978	0.979	0.982	0.854	0.978	0.905	0.982	0.978	0.969	0.98
Carcinogenicity (category 1: carcinogens; 0: non-carcinogens)	Skin sensitization (category 1: sensitizer; 0: non-sensitizer)	0.926	0.919	0.856	0.929	0.928	0.774	0.946	0.943	0.67	0.941	0.792
	Carcinogenicity (category 1: carcinogens; 0: non-carcinogens)	0.316	0.147	0.097	0.055	0.277	0.047	0.095	0.028	0.072	0.069	0.399
Eye corrosion (category 1: corrosives; 0: non-corrosives)	Eye corrosion (category 1: corrosives; 0: non-corrosives)	0.05	0.004	0.009	0.003	0.011	0.007	0.009	0.008	0.003	0.008	0.003
	Eye Irritation (category 1: irritants; 0: non-irritants)	0.962	0.93	0.929	0.609	0.945	0.919	0.944	0.93	0.134	0.949	0.019
Respiratory Toxicity (category 1: toxicants; 0: non-toxicants)	Respiratory Toxicity (category 1: toxicants; 0: non-toxicants)	0.087	0.074	0.09	0.025	0.266	0.121	0.22	0.065	0.085	0.126	0.656

The prediction property values indicate desirable Fairly desirable Undesirable

Table A6: ADMET Properties of *Isoberlinia tomentosa* Phytochemicals

Class	Properties	Beta-Carotene	Fisetin	Betanin	Betalain	Catechin	Epicatechin	Gallocatechin	Orientin	Taxifolin	Aromadendrene	Quercetin
Absorption	Caco-2 permeability (>-5.15 cm/s)	-5.459	-4.978	-6.784	-6.769	-6.052	-6.213	-6.362	-6.293	-6.311	-4.598	-5.204
	Pgp-inhibitor (category 1: inhibitor; 0: non-inhibitor)	0.0	0.005	0.0	0.0	0.00	0.007	0.007	0.007	0.006	0.002	0.004
	Pgp-substrate (category 1: substrate; 0: non-substrate)	0.0	0.008	0.994	0.993	0.01	0.004	0.02	0.99	0.001	0.0	0.005
	HIA (≥30%: high, <30%: low)	0.009	0.009	0.917	0.829	0.03	0.037	0.096	0.912	0.046	0.002	0.014
	Bioavailability scores (≥20%: high, <20%: low)	0.002	0.923	0.306	0.946	0.99	0.998	1.0	0.954	0.976	0.056	0.93
	Bioavailability scores (≥30%: high, <30%: low)	0.014	0.994	0.998	0.999	1.0	0.999	1.0	1.0	0.998	0.142	0.997
Distribution	PPB (<90%)	105.8%	97.04%	49.41%	49.45%	89.2	92.35%	88.61%	88.77%	93.58%	93.22%	95.49%
	VD (0.04 – 20 L/kg)	1.175	0.477	0.447	0.359	0.65	0.652	0.649	0.842	0.603	0.996	0.579
	BBB Penetration (category 1: BBB+; 0: BBB-)	0.0	0.009	0.173	0.198	0.02	0.025	0.022	0.013	0.021	0.174	0.008
Metabolism	CYP1A2 inhibitor	0.475	0.95	0.038	0.025	0.36	0.393	0.142	0.199	0.557	0.856	0.943
	CYP1A2 substrate	0.95	0.114	0.006	0.004	0.23	0.224	0.121	0.039	0.101	0.516	0.115
(Category 1: inhibitor; 0: non-inhibitor)	CYP2C19 inhibitor	0.542	0.097	0.024	0.028	0.03	0.031	0.02	0.02	0.048	0.326	0.053
	CYP2C19 substrate	0.957	0.046	0.028	0.032	0.05	0.054	0.05	0.048	0.051	0.912	0.041
	CYP2C9 inhibitor	0.545	0.535	0.006	0.048	0.29	0.323	0.221	0.071	0.426	0.385	0.598
	CYP2C9 substrate	1.0	0.689	0.103	0.063	0.81	0.827	0.466	0.241	0.676	0.291	0.643
	CYP2D6 inhibitor	0.926	0.532	0.01	0.016	0.18	0.139	0.039	0.028	0.28	0.018	0.411
	CYP2D6 substrate	0.991	0.329	0.084	0.085	0.38	0.31	0.22	0.158	0.225	0.64	0.205
	CYP3A4 inhibitor	0.845	0.62	0.021	0.02	0.43	0.371	0.179	0.058	0.771	0.202	0.348

	CYP3A4 substrate	0.275	0.098	0.0	0.0	0.17	0.18	0.125	0.011	0.132	0.407	0.046
Excretion	Clearance rate (>15 ml/min/kg: high; 5ml/min/kg<Cl<>15 ml/min/kg: moderate; <5ml/ min/kg: low)	0.576	8.273	1.391	1.623	17.301	16.512	16.047	5.439	10.511	8.981	8.284
Toxicity	hERG I/II (category 1: active; 0; inactive)	0.097	0.043	0.031	0.013	0.033	0.03	0.103	0.126	0.051	0.029	0.099
	H-HT (Human Hepatotoxicity)	0.076	0.127	0.497	0.384	0.103	0.099	0.135	0.169	0.112	0.233	0.1
	DILI (category 1: high risk; 0; no risk)	0.064	0.978	0.989	0.975	0.073	0.101	0.123	0.98	0.931	0.373	0.98
	Skin sensitization (category 1: sensitizer; 0; non-sensitizer)	0.537	0.919	0.648	0.605	0.136	0.947	0.964	0.903	0.93	0.087	0.919
	Carcinogenicity (category 1: carcinogens; 0; non-carcinogens)	0.065	0.147	0.024	0.673	0.953	0.159	0.053	0.039	0.053	0.024	0.05
	Eye corrosion (category 1: corrosives; 0; non-corrosives)	0.003	0.004	0.003	0.003	0.185	0.003	0.004	0.003	0.003	0.947	0.007
	Eye Irritation (category 1: irritants; 0; non-irritants)	0.886	0.93	0.015	0.011	0.004	0.914	0.909	0.508	0.929	0.899	0.936
	Respiratory Toxicity (category 1: toxicants; 0: non-toxicants)	0.381	0.074	0.642	0.412	0.915	0.117	0.086	0.071	0.089	0.368	0.072

The prediction property values indicate desirable (green), Fairly desirable (yellow), and Undesirable (red).

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Table A7: Prediction and Probability Toxicity and Toxicity End Predictions of *Isoberlinia tomentosa* Phytochemicals Based on ProToxII and StopTox Servers.

Classification	Target	Probability										
		Beta-Carotene	Fisetin	Betanin	Betalain	Catechin	Epicatechin	Gallocatechin	Orientin	Taxifolin	Aromadendrene	Quercetin
LD50 Prediction (mg/kg)		1510	159	305	305	10000	10000	10000	1213	2000	5000	159
Organ Toxicity	Hepatotoxicity	Inactive (0.85)	Inactive (0.7)	Inactive (0.64)	Inactive (0.64)	Inactive (0.72)	Inactive (0.72)	Inactive (0.72)	Inactive (0.81)	Inactive (0.69)	Inactive (0.81)	Inactive (0.69)
Toxicity end points	Carcinogenicity	Inactive (0.86)	Active (0.71)	Inactive (0.62)	Inactive (0.51)	Active (0.51)	Inactive (0.51)	Inactive (0.51)	Inactive (0.72)	Active (0.68)	Inactive (0.65)	Active (0.68)
	Immunotoxicity	Inactive (0.88)	Active (0.51)	Active (0.63)	Active (0.96)	Inactive (0.96)	Inactive (0.96)	Inactive (0.92)	Active (0.52)	Inactive (0.76)	Inactive (0.86)	Inactive (0.87)
	Mutagenicity	Active (0.71)	Active (0.53)	Active (0.78)	Active (0.55)	Inactive (0.55)	Inactive (0.55)	Inactive (0.55)	Active (0.52)	Active (0.51)	Inactive (0.76)	Active (0.51)
	Cytotoxicity	Inactive (0.81)	Inactive (0.98)	Inactive (0.67)	Inactive (0.67)	Inactive (0.84)	Inactive (0.84)	Inactive (0.84)	Inactive (0.87)	Inactive (0.99)	Inactive (0.69)	Inactive (0.99)
Acute inhalation toxicity		No	No	No	No	No	No	No	No	No	No	No
Acute oral toxicity		No	No	No	No	No	No	No	No	No	No	No
Acute Dermal toxicity		No	Yes	No	No	Yes	Yes	Yes	No	Yes	No	Yes
Eye irritation and corrosion		No	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	No	Yes
Skin irritation and corrosion		Yes	No	No	No	No	No	Yes	No	No	Yes	No

Table A8: Prediction and Probability Toxicity and Toxicity End Predictions of *Isoberlinia tomentosa* Phytochemicals Based on ProToxII and StopTox Servers

Classification	Target	Probability										
		Genistein	Delphinidin	Kaempferol	Rutin	Apigenin	Isorhamnetin	Luteolin	Myricetin	Vitexin	Cyanidin	Betacyanin
LD50 Prediction (mg/kg)		2500	5000	3919	5000	2500	5000	3919	159	832	5000	305
Organ Toxicity	Hepatotoxicity	Inactive (0.69)	Inactive (0.71)	Inactive (0.68)	Inactive (0.80)	Inactive (0.68)	Inactive (0.72)	Inactive (0.69)	Inactive (0.69)	Inactive (0.81)	Inactive (0.72)	Inactive (0.64)
Toxicity end points	Carcinogenicity	Inactive (0.69)	Inactive (0.71)	Inactive (0.72)	Inactive (0.91)	Inactive (0.62)	Inactive (0.68)	Active (0.68)	Active (0.68)	Active (0.72)	Active (0.61)	Active (0.62)
	Immunotoxicity	Inactive (0.97)	Inactive (0.86)	Inactive (0.96)	Active (0.98)	Inactive (0.99)	Active (0.58)	Inactive (0.97)	Inactive (0.86)	Inactive (0.82)	Active (0.93)	Active (0.99)
	Mutagenicity	Active (0.74)	Inactive (0.76)	Inactive (0.52)	Inactive (0.88)	Inactive (0.57)	Inactive (0.94)	Active (0.51)	Active (0.51)	Active (0.52)	Inactive (0.58)	Inactive (0.57)
	Cytotoxicity	Inactive (0.91)	Inactive (0.85)	Inactive (0.98)	Inactive (0.64)	Inactive (0.87)	Inactive (0.95)	Inactive (0.99)	Inactive (0.99)	Inactive (0.87)	Inactive (0.94)	Active (0.57)
Acute inhalation toxicity		No	No	No	No	No	No	No	No	No	No	No
Acute oral toxicity												
Acute Dermal toxicity		No	No	No	No	No	No	No	No	No	No	No
Eye irritation and corrosion		Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes	No
Skin irritation and corrosion		No	Yes	No	No	Yes	Yes	Yes	Yes	No	Yes	Yes
		No	No	No	No	No	No	No	No	No	No	No

Table A9: Prediction of Activity Spectra for Substances (PASS) Analysis for Potential Biological Activities of *Isoberlinia tomentosa* Identified Phytochemicals

Compound	Pa	Pi	Biological activity	Compound	Pa	Pi	Biological activity
Betalain	0.329	0.136	Antineoplastic	Catechin	0.548	0.044	Antiinflammatory
	0.175	0.117	Chemoprotective		0.687	0.009	Anticarcinogenic
	0.265	0.074	Anticarcinogenic		0.959	0.003	TP53expression enhance
	0.486	0.018	Antibacterial		0.552	0.023	Antifungal
	0.326	0.019	Antioxidant		0.675	0.030	Antineoplastic
	0.762	0.002	Chemoprotective		0.788	0.004	Chemoprotective
Beta-Carotene	0.931	0.005	Antineoplastic	Fisetin	0.950	0.002	Kinase inhibitor
	0.775	0.004	Antioxidant		0.943	0.001	Antimutagenic
	0.765	0.002	Chemoprotective		0.912	0.005	TP53expression enhance
	0.690	0.009	Anticarcinogenic		0.787	0.004	Antioxidant
	0.690	0.017	Antiinflammatory		0.727	0.022	Antineoplastic
	0.686	0.019	Immunosuppressant		0.680	0.009	Anticarcinogenic
	0.383	0.054	Antifungi		0.640	0.004	Chemoprotective
	0.316	0.051	Antiparasitic		0.643	0.024	Antiinflammatory
	0.431	0.010	Antioxidant		0.810	0.003	Antioxidant
	0.297	0.059	Anticarcinogenic		0.795	0.005	Anticarcinogenic
Betanin	0.182	0.107	Chemoprotective	Epicatechin	0.788	0.004	Chemopreventive
	0.424	0.095	Antineoplastic		0.743	0.009	Kinase inhibitor
					0.675	0.030	Antineoplastc
					0.552	0.023	Antifungal
					0.548	0.044	Antiinflammatory
Gallocatechin	0.963	0.003	TP53 expression enhancer	Orientin	0.959	0.003	TP53expression enhance
	0.870	0.003	Antioxidant		0.974	0.003	TP53 expression enhancer
	0.815	0.005	Anticarcinogenic		0.881	0.003	Chemoprotective
	0.808	0.004	Chemopreventive		0.872	0.003	Anticarcinogenic
	0.742	0.019	Antineoplastic		0.852	0.004	Kinase inhibitor
	0.721	0.011	Kinase inhibitor		0.828	0.003	Antioxidant
			0.714	0.009	Antifungal		

	0.611	0.029	Antiinflammatory		0.626	0.027	Antiinflammatory	
	0.597	0.019	Antifungal		0.541	0.013	Antibacterial	
	0.459	0.009	Antiviral		0.368	0.019	Antiviral	
	0.970	0.003	TP53 expression enhancer		0.341	0.178	TP53 expression enhancer	
Taxifolin	0.938	0.002	Antioxidant	Aromadendrene	0.826	0.009	Antineoplastic	
	0.850	0.004	Kinase inhibitor		0.515	0.028	Antifungi	
	0.821	0.005	Anticarcinogenic		0.380	0.035	Antibacterial	
	0.744	0.005	Chemopreventive		0.335	0.034	Antiprotozoa	
	0.729	0.021	Antineoplastic		0.297	0.057	Antiparasitic	
	0.628	0.026	Antiinflammatory					
	0.511	0.029	Antifungal					
Quercetin	0.872	0.003	Antioxidant	Genistein	0.844	0.004	Kinase inhibitor	
	0.844	0.008	TP53 expression enhancer		0.824	0.009	TP53 expression enhancer	
	0.809	0.005	Kinase inhibitor		0.765	0.004	Antioxidant	
	0.797	0.012	Antineoplastic		0.750	0.018	Antineoplastic	
	0.757	0.007	Anticarcinogenic		0.715	0.008	Anticarcinogenic	
	0.717	0.006	Chemopreventive		0.609	0.010	Chemopreventive	
	0.689	0.017	Antiinflammatory		0.626	0.027	Antiinflammatory	
	0.490	0.032	Antifungal		0.502	0.030	Antifungal	
Kaempferol	0.959	0.001	Kinase inhibitor	Rutin	0.983	0.001	Anticarcinogenic	
	0.931	0.004	TP53 expression enhancer		0.968	0.001	Chemopreventive	
	0.858	0.003	Antioxidant		0.923	0.003	Antioxidant	
	0.791	0.013	Antineoplastic		0.893	0.005	TP53 expression enhancer	
	0.715	0.008	Anticarcinogenic		0.849	0.007	Antineoplastic	
	0.669	0.008	Chemopreventive		0.819	0.005	Kinase Inhibitor	
	0.676	0.019	Antiinflammatory		0.784	0.006	Antifungi	
	0.495	0.031	Antifungi		0.728	0.013	Antiinflammatory	
	0.461	0.013	Antiprotozoal		0.677	0.005	Antibacterial	
			Antibacteria		0.484	0.011	Antiprotozoal	
		0.941	0.002		Kinase inhibitor	0.945	0.002	Kinase inhibitor

Apigenin	0.873	0.006	TP53 expression enhancer		0.944	0.002	TP53 expression enhancer	
	0.774	0.015	Antineoplastic	Isorhamnetin	0.803	0.011	Antioxidant	
	0.732	0.004	Antioxidant		0.779	0.006	Anticarcinogenic	
	0.641	0.011	Anticarcinogenic		0.772	0.004	Chemopreventive	
	0.644	0.024	Antiinflammatory		0.663	0.021	Antiinflammatory	
	0.593	0.010	Chemopreventive		0.468	0.036	Antifungal	
	0.524	0.027	Antifungal		0.403	0.019	Antiprotozoal	
	0.441	0.023	Antiparasitic		0.375	0.037	Antibacterial	
	0.940	0.002	Kinase inhibitor			0.958	0.001	Kinase inhibitor
Luteolin		0.916	0.004	TP53 expression enhancer		0.944	0.004	TP53 expression enhancer
	0.775	0.004	Antioxidant	Myricetin	0.924	0.003	Antioxidant	
	0.783	0.014	Antineoplastic		0.841	0.008	Antineoplastic	
	0.690	0.009	Anticarcinogenic		0.784	0.006	Anticarcinogenic	
	0.648	0.008	Chemopreventive		0.734	0.005	Chemopreventive	
	0.661	0.021	Antiinflammatory		0.720	0.013	Antiinflammatory	
	0.520	0.027	Antifungal		0.508	0.029	Antifungal	
	0.401	0.031	Antiparasitic		0.482	0.012	Antiprotozoal	
			0.427		0.025	Antibacterial		
Vitexin	0.973	0.003	TP53 expression enhancer				TP53 expression enhancer	
	0.877	0.003	Anticarcinogenic	Betacyanin	0.355	0.040	Anticarcinogenic	
	0.606	0.030	Antiinflammatory					Antiinflammatory
	0.864	0.003	Chemopreventive		0.260	0.045	Chemopreventive	
	0.722	0.009	Antifungal		0.322	0.073	Antifungal	
	0.541	0.013	Antibacterial		0.530	0.014	Antibacterial	
	0.847	0.004	Kinase inhibitor		0.189	0.116	Antiprotozoal	
	0.836	0.008	Antineoplastic		0.426	0.095	Antineoplastic	
0.780	0.004	Antioxidant	0.393		0.013	Antioxidant		