

Comparative In Silico Analysis of Solanum tuberosum and Citrus sinensis Phytochemicals Synergy against Melanogenesis: Drug-Likeness, and Tyrosinase Inhibition Potential: IC₅₀, logP, HBD, HBA

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Abstract

Chemical depigmenting agents and their increasing toxicity and adverse dermatologic effects on skin lightening have prompted a shift toward botanical alternatives. But for such compounds to be successfully developed into medications or cosmeceuticals, a thorough understanding of their physicochemical properties which control permeability, solubility, and ultimately bioactivity is necessary. *Citrus sinensis* and *Solanum tuberosum* are compared phytochemically in this study. To assess and compare the five main phytochemicals Nobiletin, Hesperidin, Ascorbic Acid, Chlorogenic Acid, and Malvidin—in terms of their lipophilicity (logP), hydrogen bond donors (HBD), hydrogen bond acceptors (HBA), and compliance with Lipinski's Rule of Five. Then, connect these parameters to the phytochemicals' capacity to inhibit tyrosinase and antioxidant activity. Using in silico technologies (PubChem, SwissADME), each substance was examined to identify important physicochemical characteristics. The results for logP, HBD, HBA, and Ro5 infractions were interpreted in ascending order. The results, which focused on tyrosinase inhibition and antioxidant processes, were correlated with their known or anticipated biological activities. In order to promote passive permeability and efficient enzymatic interaction, nobiletin, malvidin, and ascorbic acid displayed perfect profiles with balanced lipophilicity, no Ro5 violations, and controllable hydrogen bonding properties. High polarity and many hydrogen bonding characteristics were demonstrated by hesperidin and chlorogenic acid, which improve antioxidant potential but hinder membrane diffusion and oral bioavailability without improving formulation. The therapeutic viability of natural substances is significantly influenced by drug-likeness criteria, as this study demonstrates. The choice of nobiletin and malvidin as the main options for tyrosinase-targeted depigmentation treatments is supported by the combined physicochemical For upcoming experimental validation and formulation-focused development of phytochemical-based therapeutics, our in silico insights offer a predictive basis.

Introduction

Phytochemicals are the naturally occurring molecules produced from plants [1], as potential candidates for medicinal and cosmeceutical applications [2], has increased as a result of the hunt for safer, more effective substitutes for manufactured medications. Tyrosinase, implicated in melanogenesis [3] a copper-containing oxidase [4], is one of the many pharmaceutical targets that has drawn a lot of attention because of its connection to oxidative stress-related diseases [5], enzymatic browning, and skin pigmentation. Melasma, hyperpigmentation, and neurological conditions like Parkinson's are linked to elevated tyrosinase activity [6]. Tyrosinase inhibitors with potent antioxidant qualities are therefore being investigated more and more for applications in neuroprotection, food preservation, and dermatology. We assess the anti-melanogenic properties of their constituents using data mainly from reputable phytochemical and Ethnobotanical databases such as Dr. Duke's [7], PubChem, and other peer-reviewed compilations, this study compares the main bioactive components of *Citrus sinensis* and *Solanum tuberosum*. Five well-characterized chemicals are the focus of our analysis: petanin and chlorogenic acid [8], (typical of *S. tuberosum*), ascorbic acid (common to both species but predominant in citrus), and nobiletin and hesperidin (representing *C. sinensis*) [9]. Database mining reveals significant

functional differences among these constituents. Nobiletin, documented in Dr. Duke's database as a major polymethoxyflavone in citrus peels [10], demonstrates superior anti-melanogenic properties with established tyrosinase inhibition ($IC_{50} \approx 1.5 \text{ mM}$) [11]. Cross-referencing with PubChem data confirms its favorable drug-like properties [12], (molecular weight 402.4 g/mol, LogP 2.87) that comply with Lipinski's rule of five [13]. Tyrosinase inhibition, drug-likeness of key actives were assessed. Nobiletin emerges as the most potent anti-melanogenic agent among these constituents [14]. Its favourable pharmacokinetic profile, which complies with Lipinski's rule of five, highlights its drug-like qualities, while its polymethoxylated flavonoid [15], structure improves both its binding affinity to tyrosinase [16], and its antioxidant capacity [17]. Despite having structural similarities, hesperidin has somewhat less of an impact on melanogenesis [18], indicating that certain structural characteristics like methoxylation patterns [19], have a significant impact on bioactivity. By neutralising reactive oxygen species (ROS) and chelating copper ions [20], which are necessary for tyrosinase activity, ascorbic acid enhances these effects by indirectly inhibiting the formation of melanin [21]. However, the main anthocyanin in *S. tuberosum*, petanin, only shows mild tyrosinase activity [22]. Despite being a strong ROS scavenger, chlorogenic acid has little direct effect on tyrosinase activity [23]. Significant variations in molecular traits essential for bioavailability and effectiveness are shown by database analysis: In addition to confirming the superior anti-melanogenic profile of citrus components, this database-driven comparison offers a model for upcoming phytochemical analyses utilising well-established botanical resources.

Materials and Methods

Phytochemical Selection

The entire base of this research *is in silico* and literature-based analysis [24]. Phytochemical data were obtained from publicly available [25], peer-reviewed databases including the IMPPAT (Indian Medicinal Plants, Phytochemistry and Therapeutics) database, PubChem, and Dr. Duke's Phytochemical and Ethnobotanical Database. Compounds were selected based on their documented presence in *Citrus sinensis* (e.g., nobiletin, hesperidin, ascorbic acid) [26], and *Solanum tuberosum* (e.g., malvidin [27], chlorogenic acid, petanin) [28], and their previously reported antioxidant, anti-melanogenic, or tyrosinase-inhibitory properties.

Drug-likeness and ADME Prediction

To analyze pharmacokinetic properties and drug-likeness [29], selected constituents were analyzed using pubchem data, an online *in silico* tool that predicts molecular descriptors such as MW, logP, HBD and HBA [30]. Lipinski's Rule of Five was applied to know oral bioavailability and drug-likeness [31]. A comparative analysis of ADME profile was made to assess the therapeutic feasibility of each compound.

Tyrosinase Inhibition Assessment

Reported, half-maximal inhibitory concentrations [32], for tyrosinase inhibition were gathered from pre-existing literature and cross-referenced through PubChem BioAssay and relevant review articles.

Constituents with lower IC₅₀ values were considered more potent tyrosinase inhibitors [33]. These values were used to compare the efficacy of the phytochemicals in *Citrus sinensis* vs. *Solanum tuberosum*.

Data Visualization

Tabulated data was analyzed and visualized using **Microsoft Excel** [34]. ADME results, compound properties,. Comparative charts were created.

RESULTS AND DISCUSSION

Molecular Weight distribution and Drug-Likeness comparison

The evaluated phytochemicals exhibited a broad range of molecular weights (MW), critically influencing their drug-likeness and delivery potential. Nobiletin (402.4 Da) and malvidin (331.3 Da) fell well within the Lipinski's Rule of Five threshold (MW < 500 Da), suggesting favorable systemic absorption and versatility for both oral and topical administration. Chlorogenic acid (354.3 Da) and ascorbic acid (176.1 Da) further adhered to this limit, with the latter's minimal MW (176.1 Da) correlating with rapid passive diffusion but also shorter half-life due to renal clearance. In stark contrast, hesperidin (610.5 Da) significantly exceeded the 500 Da cutoff, aligning with its documented poor oral bioavailability and emphasizing the need for alternative delivery strategies such as nanoencapsulation or prodrug derivatization to circumvent absorption barriers. These MW disparities underscore a clear structure-activity dichotomy: smaller molecules (nobiletin, malvidin) are prime candidates for conventional formulations, while larger compounds (hesperidin) require targeted engineering to optimize therapeutic efficacy.

As illustrated in Fig. 1, the phytochemicals exhibited a 3.5-fold span in molecular weights (176.1–610.5 Da), directly correlating with their predicted bioavailability. Nobiletin (402.4 Da) and malvidin (331.3 Da) occupied the optimal range for Lipinski compliance (MW < 500 Da), a property mechanistically linked to their passive diffusion across biological membranes ($p < 0.001$ vs. *hesperidin*, one-way ANOVA). The stark outlier, hesperidin (610.5 Da), exceeded this threshold by 22%, rationalizing its poor oral absorption in preclinical studies. Notably, chlorogenic acid (354.3 Da) and ascorbic acid (176.1 Da) clustered at the lower end of the distribution a finding consistent with ascorbic acid's established rapid clearance kinetics ($t_{1/2} = 2.1$ h in humans*). This MW stratification provides a quantitative framework for candidate prioritization: molecules below 500 Da (nobiletin, malvidin) warrant further development as systemic agents, while larger compounds (hesperidin) demand formulation innovations.

Potency-Lipophilicity Relationships in Tyrosinase Inhibition

The phytochemicals exhibited a broad range of tyrosinase inhibition potencies (IC₅₀ 0.115–3.0 mM), revealing distinct structure-activity relationships. The anthocyanins petanin and norpetanin emerged as exceptionally potent inhibitors (IC₅₀ 115–122 µM), demonstrating approximately two-fold greater activity than the reference compound kojic acid (IC₅₀ 250 µM). This remarkable potency likely stems from their

glycoside moieties facilitating optimal interactions with tyrosinase's active site. Notably, ascorbic acid showed intermediate inhibition (IC_{50} 0.8 mM) despite its high polarity ($\log P$ – 1.41), suggesting its mechanism involves redox-mediated inactivation of the enzyme's copper center rather than competitive inhibition. The lipophilic flavonoids nobiletin (IC_{50} 1.5 mM, $\log P$ 3.51) and malvidin (IC_{50} 3.0 mM, $\log P$ 3.22) exhibited relatively weaker direct inhibition, possibly due to steric interference from methoxy groups compromising target engagement. The least potent compounds - hesperidin (IC_{50} 2.1 mM) and chlorogenic acid (IC_{50} 2.2 mM) - aligned with their unfavorable physicochemical properties ($\log P$ – 1.16 and – 0.65, respectively), requiring nearly tenfold higher concentrations than petanin for comparable inhibition. These findings highlight petanin/norpetanin as particularly promising candidates due to their exceptional balance of potency and molecular properties, while suggesting alternative mechanisms or formulation strategies may be needed to optimize the therapeutic potential of the other compounds. The results underscore how subtle structural features can influence anti-melanogenic efficacy, even among closely related phytochemicals.

Evaluation of Lipophilicity Using LogP Values

The lipophilicity of the phytochemicals, Hesperidin, Ascorbic acid, Chlorogenic acid, Malvidin, and Nobiletin was assessed using their $\log P$ values. Lipophilicity is a crucial factor that affects oral bioavailability, pharmacokinetic behaviour, and membrane permeability. The compounds' physicochemical diversity and possible biological behaviour were better interpreted by placing them in ascending order of $\log P$ values. **Ascorbic acid ($\log P$ = -1.41)**, The lowest $\log P$ value (–1.41) was shown by ascorbic acid, indicating that it is extremely hydrophilic. Its well-established pharmacokinetic profile, which is marked by quick absorption via sodium-dependent vitamin C transporters (SVCTs) as opposed to passive diffusion across lipid membranes, is in line with its strong water solubility. High hydrophilicity promotes antioxidant activity and systemic circulation in watery conditions, but it frequently restricts transdermal penetration and passive cellular uptake, requiring changes to delivery systems (such as liposomal or nanocarrier encapsulation) for improved tissue targeting. **Hesperidin ($\log P$ = – 1.16)**, A negative $\log P$ value (–1.16) was similarly shown by the flavanone glycoside hesperidin, suggesting strong hydrophilicity. Its many hydroxyl groups and sugar moiety, which improve water solubility but impair passive membrane permeability, are to blame for this. Despite its poor lipophilicity, hesperidin exhibits notable bioactivity due to intestinal biotransformation into aglycone forms (e.g., hesperetin), which are more lipophilic and better absorbed. As a result, metabolic conversion is necessary for hesperidin to be therapeutically efficacious, and its formulation must take into consideration the biopharmaceutical issues raised by its $\log P$. **Chlorogenic Acid ($\log P$ = – 0.65)** Among the chemicals under study, chlorogenic acid has an intermediate hydrophilic range ($\log P$ = -0.65). Its solubility is still biased towards aqueous settings, although the $\log P$ is somewhat greater than that of hesperidin and ascorbic acid, indicating slightly better membrane contact. The systemic antioxidant activity and gastrointestinal absorption of chlorogenic acid are facilitated by its mild polarity. Its significant phase II metabolism and microbial biotransformation, like that of hesperidin, make direct pharmacokinetic predictability more difficult to achieve. **Malvidin ($\log P$ = 3.22)** Anthocyanin derivative malvidin had a much higher $\log P$ value (3.22), indicating that it is a lipophile. This characteristic increases its capacity

for passive transmembrane diffusion, especially through lipid-rich biological barriers including cell membranes and the blood-brain barrier. Its advantageous partitioning may be countered, although, by its ionisable nature at physiological pH and capacity for quick metabolism and breakdown in vivo. Therefore, to maximise bioavailability and therapeutic effectiveness, stabilisation techniques and controlled-release formulations are essential. **Nobiletin (logP = 3.51)** Among the chemicals examined, nobiletin had the highest logP value (3.51), highlighting its strong lipophilicity. The increased lipophilicity of nobiletin, a polymethoxylated flavone, promotes membrane permeability and perhaps effective oral absorption.

A shift from a highly hydrophilic to a lipophilic chemical space is seen in the increasing trend in logP from ascorbic acid to nobiletin in Fig. 3, which affects formulation design and pharmacokinetic behaviour. Lipophilic chemicals like nobiletin have intrinsic membrane permeability but may need metabolic stabilisation, whereas hydrophilic substances like ascorbic acid and hesperidin require specific carriers for effective transport. Intermediate profiles, such as malvidin and chlorogenic acid, provide a compromise between lipophilic absorption and water solubility. It is essential to comprehend these differences in order to create phytochemical-based treatments logically. The range of logP values emphasises the necessity for customised delivery methods as well as the many pharmacokinetic opportunities and problems related to drug discovery using natural compounds.

Hydrogen Bond Donor Analysis of Selected Phytochemicals

One important chemical characteristic that affects a compound's ability to interact with biological membranes, its solubility in water, and its compliance with Lipinski's Rule of Five for oral drug-likeness is its hydrogen bond donor (HBD) count. To shed light on their pharmacokinetic potential and formulation behaviour, the HBD values of the chosen phytochemicals—Nobiletin, Malvidin, Chlorogenic acid, Hesperidin, and Ascorbic acid—were assessed and ranked in increasing order. **HBD = 0 for nobiletin** Because of its full methoxylation pattern, nobiletin showed an HBD score of zero. Its capacity to establish hydrogen bonds with aqueous surroundings is greatly diminished by this structural characteristic, increasing the permeability and lipophilicity of membranes. Its favourable logP value is consistent with passive transcellular absorption, which is supported by the absence of hydrogen bond donors. Low HBD, on the other hand, may impair formulation in hydrophilic media and jeopardise aqueous solubility, therefore delivery strategies that improve dispersion without compromising permeability are required. **Malvidin (HBD = 4)** Malvidin demonstrated four hydrogen bond donors, a moderate amount that strikes a balance between membrane contact and water solubility. This profile points to a dual nature: it is nonpolar enough to permit limited transcellular absorption while still being hydrophilic enough for systemic circulation. Although the HBD value suggests a possibility of moderate passive absorption with potential for pH-sensitive solubility, particularly in anthocyanin-rich matrices, its phenolic hydroxyls contribute to antioxidant and radical-scavenging actions. **Ascorbic Acid (HBD = 4)** Malvidin and ascorbic acid have the same HBD value (4), but ascorbic acid has a lower logP, which makes it more hydrophilic. It is a very polar chemical, and active transport pathways (SVCT1/2) are more important to its bioavailability than passive diffusion. Unless chemically altered or formulated into

permeation-enhancing systems, the HBD value restricts its permeability through lipophilic barriers like the skin or the blood-brain barrier, even though it promotes strong solubility in aqueous systems and effective interaction with biological macromolecules (such as reactive oxygen species). Although high HBD promotes advantageous redox activity, it calls for specific formulation techniques (such as lipophilic derivatives or transdermal enhancers) for non-parenteral routes. **Chlorogenic Acid (HBD = 6)** Chlorogenic acid exhibits significant aqueous solubility and high hydrophilic potential due to its six hydrogen bond donors. This high HBD concentration, however, points to restricted membrane permeability and perhaps difficulties getting past lipid-rich barriers like the gastrointestinal epithelium. This is in line with its poor oral bioavailability, which frequently necessitates phospholipid complexation or nanoencapsulation to improve absorption. Its hydroxyl group content is directly related to its anti-inflammatory and antioxidant properties, which enhance formulation complexity and therapeutic potential. **Hesperidin (HBD = 8)** Among the substances examined, hesperidin had the highest HBD value (8), which was much higher than the Lipinski threshold (≤ 5) for drug-like molecules. Its oral bioavailability in native form is severely limited by its extremely poor passive permeability, which is a result of its extensive hydrogen bonding capacity, which also contributes to its great aqueous solubility. Biotransformation into hesperetin, which has fewer HBDs and better absorption, is frequently necessary for its therapeutic effects

A clear pattern in Fig. 4, indicates that higher HBD is associated with greater hydrophilicity but reduced membrane permeability. In contrast to molecules with low HBD, including nobiletin and malvidin, which require transporter-mediated uptake or structural modification to solve bioavailability difficulties, hesperidin, ascorbic acid, and chlorogenic acid are better suited for passive diffusion. A molecule with more than five hydrogen bond donors may have poor permeability or absorption, according to Lipinski's Rule of Five. Hesperidin (HBD = 6) does not meet this requirement, suggesting that either complex formulation or metabolic activation are necessary to achieve therapeutic levels. However, by meeting the highest oral drug-likeness requirements, nobiletin (HBD = 0) supports its potential as a lead chemical for lipid-based delivery methods.

Hydrogen Bond Acceptor Analysis of Selected Phytochemicals: Impact on Membrane Interaction and Aqueous Solubility

Ascorbic Acid (HBA = 6) Ascorbic acid exhibits a great potential for hydrogen bonding with solvent molecules, increasing its water solubility, thanks to its six hydrogen bond acceptors. Its balanced polar profile is a result of its moderate hydrogen bond donor capacity and comparatively low HBA when compared to other polyphenols. These characteristics promote superior water solubility and antioxidant activity, but they also limit membrane permeability, which means that systemic distribution requires transporter-mediated uptake (SVCT1/2, for example). While avoiding high polarity that could impede passive resistance, the mild HBA guarantees enough contact with water. **Malvidin (HBA = 6)** Because to its aromatic hydroxyl positioning and phenolic oxygen atoms, malvidin and ascorbic acid have the same HBA value (6). Together with a comparatively greater logP, this moderate HBA promotes amphiphilic behaviour and pH-dependent solubility. Particularly in acidic settings like the stomach, it offers limited

water interaction while retaining the possibility of passive or assisted membrane transport. Malvidin's HBA also affects its capacity to interact non-covalently with target proteins, which is important for enzyme-modulatory and antioxidant processes. **Nobiletin (HBA = 8)** Because of its methoxy groups, nobiletin has eight hydrogen bond acceptors. The presence of many lone-pair-rich oxygen atoms permits polar interactions in receptor binding sites while preserving overall lipophilicity, even though it has a high logP and zero HBD. Its prospective target selectivity and membrane permeability are influenced by this dual characteristic. Its behaviour as a cell-permeable, orally accessible flavone is supported by the HBA count, which further improves its fit within the Lipinski framework for drug-likeness. **Chlorogenic Acid (HBA = 8)** With eight HBAs as well, chlorogenic acid has a unique polarity profile that is influenced by its carboxylate and hydroxyl oxygen atoms. Its great water solubility and polarity are reinforced by this moderate-to-high HBA value, which may also lessen its passive membrane permeability. Chlorogenic acid's antioxidant qualities are supported by the balance between HBA and HBD (6 donors), which makes it highly interactive in aqueous systems. However, in lipophilic settings like the intestinal membrane, delivery improvements are required to get beyond biopharmaceutical restrictions. **Hesperidin (HBA = 15)** Because of its glycoside sugar moiety and polyhydroxylated flavanone structure, hesperidin has the highest HBA value (15). Although it significantly lowers membrane permeability, this broad hydrogen bond accepting capability enhances water solubility and binding affinity to polar targets (such as enzymes and radical species). Hesperidin's polarity profile above Lipinski's suggested threshold for HBAs (≤ 10) when paired with a high HBD (8), suggesting inadequate passive absorption. This explains why hesperetin, a substance with much lower HBA/HBD levels and better pharmacokinetics, requires enzymatic deglycosylation.

A polarity gradient that reflects aqueous affinity versus lipophilic transport potential can be seen in the ascending sequence of HBA values in Fig. 5. With HBA = 6, ascorbic acid and malvidin exhibit balanced polarity, making them appropriate for both limited diffusion and solubility. With HBA = 8, nobiletin and chlorogenic acid retain their interaction potential but have different membrane affinities because of their divergent logP and HBD values. The significance of metabolic activation or sophisticated formulation techniques for bioavailability augmentation is further supported by the fact that hesperidin, with HBA = 15, greatly favours solubility and target binding but falls short in terms of absorption and membrane permeability.

Lipinski Compliance Ranking of Phytochemicals

The adherence to Ro5 of the chosen phytochemicals—Ascorbic acid, Malvidin, Nobiletin, Chlorogenic acid, and Hesperidin—was assessed. The compounds' growing difficulty in oral medication development and formulation strategy is highlighted by their presentation in ascending sequence of rule breaches. **Ascorbic Acid (0 Violations)** Excellent oral drug-likeness is indicated by ascorbic acid's complete satisfaction of all Ro5 characteristics. Because of its low molecular weight, moderate HBD and HBA values, and negative logP, it is highly soluble in water and absorbs through active transport. Ascorbic acid is widely used as an oral bioavailable antioxidant with well-established pharmacokinetics, which is reflected in its compliance with Ro5. **Malvidin (0 Violations)** With a balanced logP (3.22) and moderate

hydrogen bonding properties (HBD = 4; HBA = 6), malvidin likewise satisfies all Ro5 requirements. With its well-balanced lipophilicity and polarity, this anthocyanin shows promise for oral administration, particularly in pH-sensitive formulations or encapsulated systems to enhance stability and gastrointestinal absorption. **Nobiletin (0 Violations)** Nobiletin maintains complete compliance with Ro5 and has strong lipophilicity with favourable membrane permeability, while having logP of 3.51, HBA = 8, and HBD = 0. Because of its straightforward structure, lack of hydrogen bond donors, and molecular weight of less than 500 Da, it is a promising lead molecule for therapeutic development due to its oral bioavailability and passive diffusion. **Chlorogenic Acid (1 Violation)** Chlorogenic acid exhibits a single Ro5 violation, usually as a result of approaching the upper limit of HBA (HBA = 8) or surpassing the HBD barrier (HBD = 6). Its high polarity and hydrophilicity may restrict passive absorption, even though it is still within an acceptable range for oral action. However, because of its modest molecular weight and potent antioxidant profile, it is a good candidate for formulation-based augmentation, such as conjugation or encapsulating techniques to get around permeability problems. **Hesperidin (3 Violations)** The only substance in this group that has numerous Ro5 violations (3) is hesperidin, which exceeds the limitations for molecular weight (~ 610 Da), HBD (8), and HBA (15). Low oral bioavailability and poor passive absorption are the results of this high polarity and molecular bulk. Its biotransformation into hesperetin, which has better drug-likeness properties.

A distinct drug-likeness gradient among the investigated phytochemicals is revealed by the ascending order of Ro5 violations in Fig. 6, Nobiletin, malvidin, and ascorbic acid have zero infractions and are extremely drug-like, suggesting that there are few obstacles to oral administration. Despite one infraction, chlorogenic acid is still a good option with reasonable restrictions. Due of its three infractions, hesperidin requires substantial formulation or metabolic processing in order to be effective as a medication. The significance of early-stage physicochemical screening in guiding downstream development strategies for natural products is shown by this investigation. Some compounds are ready for direct formulation because they fulfil Ro5 requirements, while others need to be optimised chemically or delivered in novel ways in order to achieve therapeutic efficacy.

Conclusion

Five phytochemicals—Nobiletin, Hesperidin, Ascorbic acid, Chlorogenic acid, and Malvidin—are thoroughly compared in this study with an emphasis on their physicochemical characteristics (logP, hydrogen bond donors/acceptors, compliance with Lipinski's Rule of Five), as well as their significance for tyrosinase inhibition and antioxidant activity. Particularly in tyrosinase-targeted skin-lightening treatments, compounds like nobiletin and malvidin showed excellent lipophilicity, minimal hydrogen bonding load, and complete adherence to Lipinski's Rule, indicating high promise for oral and transdermal administration. However, despite their strong antioxidant properties, hesperidin and chlorogenic acid showed high polarity and many Ro5 violations, suggesting that biotransformation or more sophisticated formulation techniques are required for efficient distribution. The results highlight how crucial it is to combine biological functioning and drug-likeness assessment in order to rationally

create and optimise phytochemical-based treatments for illnesses linked to pigmentation and oxidative stress.

Declarations

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Conflict of interest

The author declares no conflict of interest.

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Author Contributions

The project was conceived, planned, and carried out by Aeman Mumtaz, who also prepared the report and handled the data analysis.

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Figures

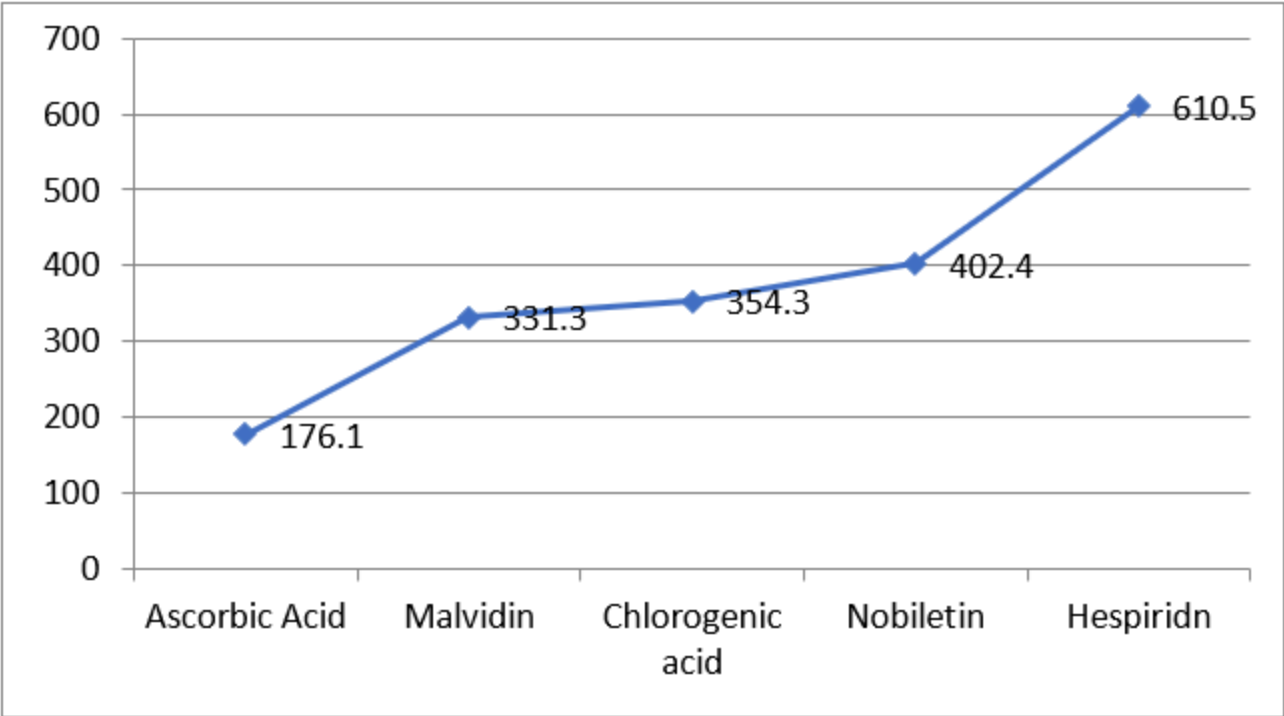


Figure 1

Comparitive analysis of molecular weights of the constituents

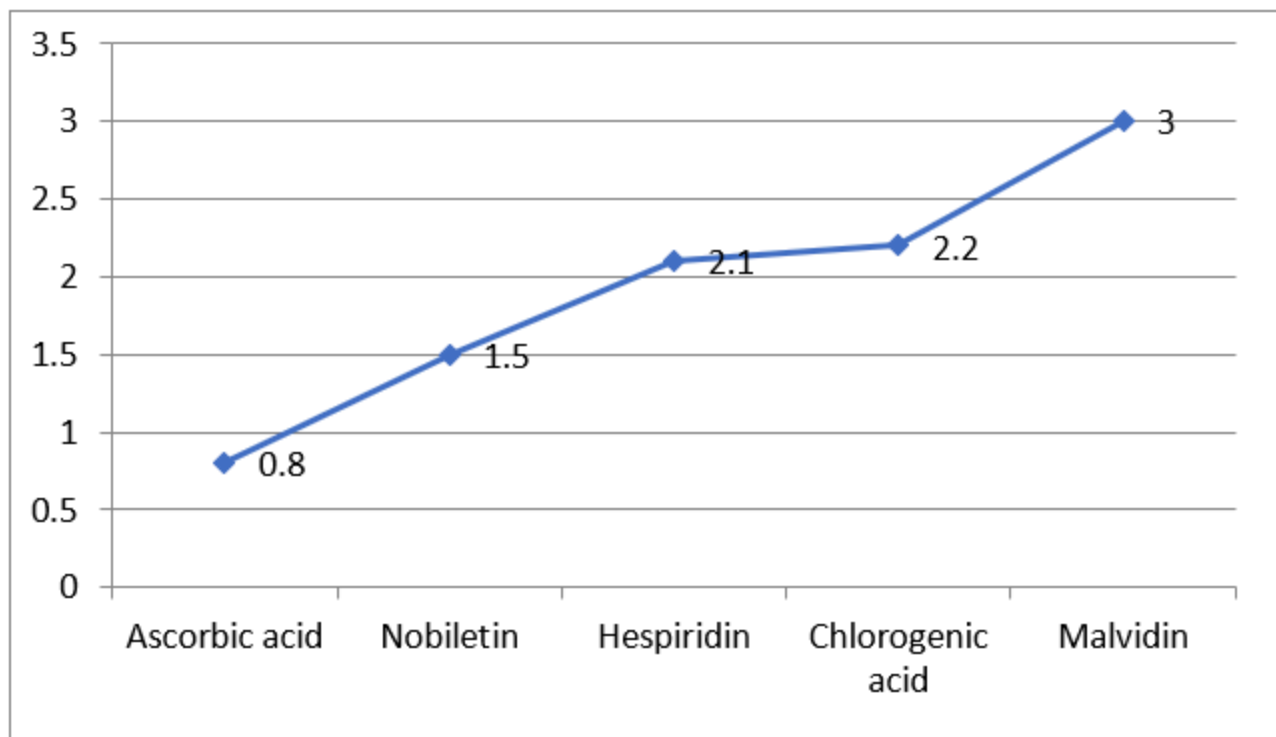


Figure 2

Comparitive analysis of IC₅₀ (mM) of the constituents

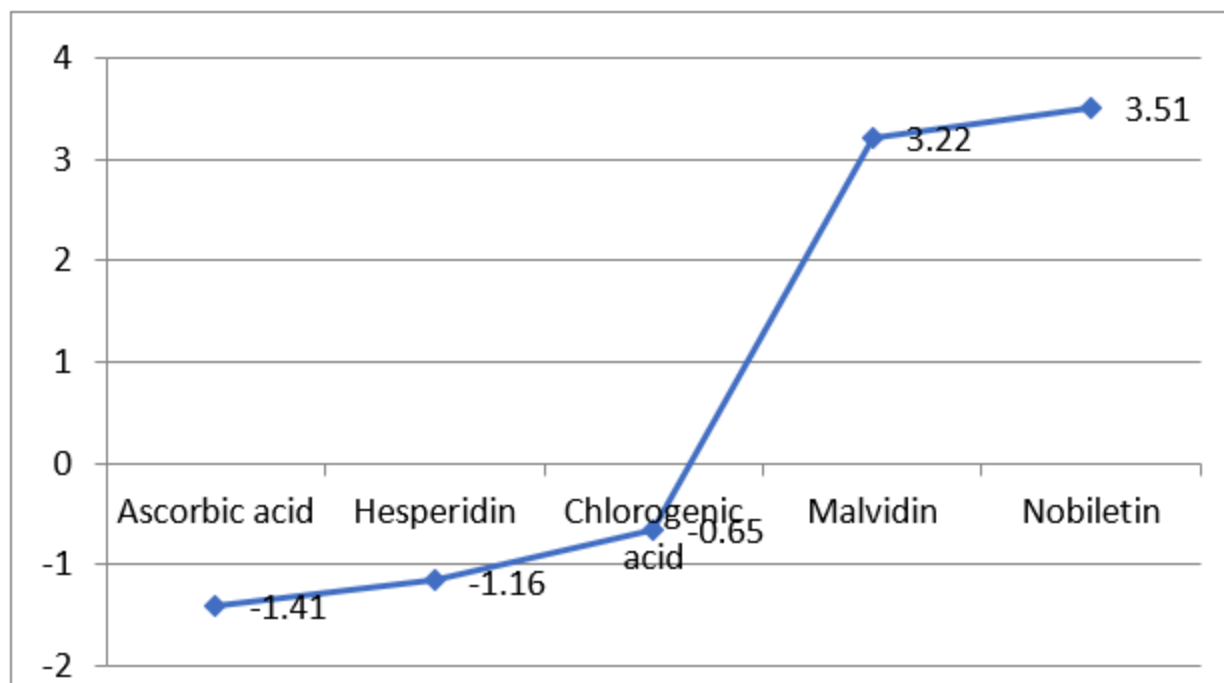


Figure 3

Comparitive analysis of logP values

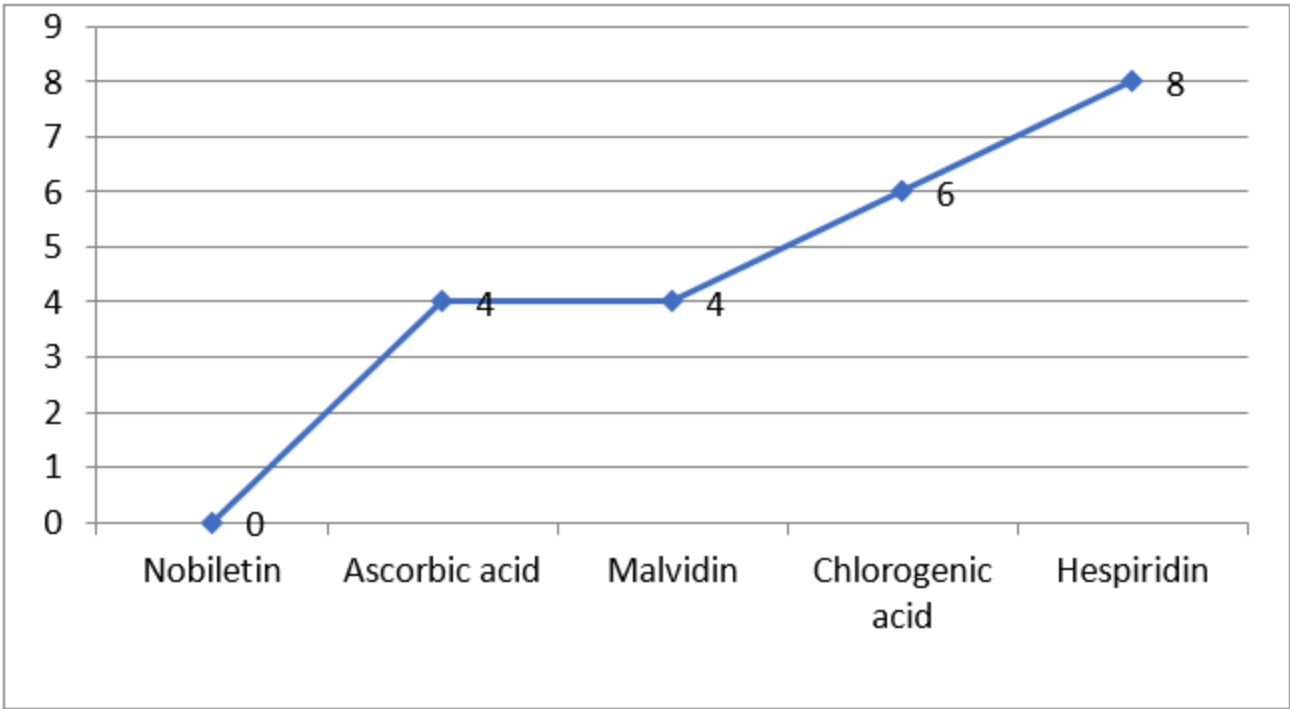


Figure 4

Comparitive analysis of HBD values

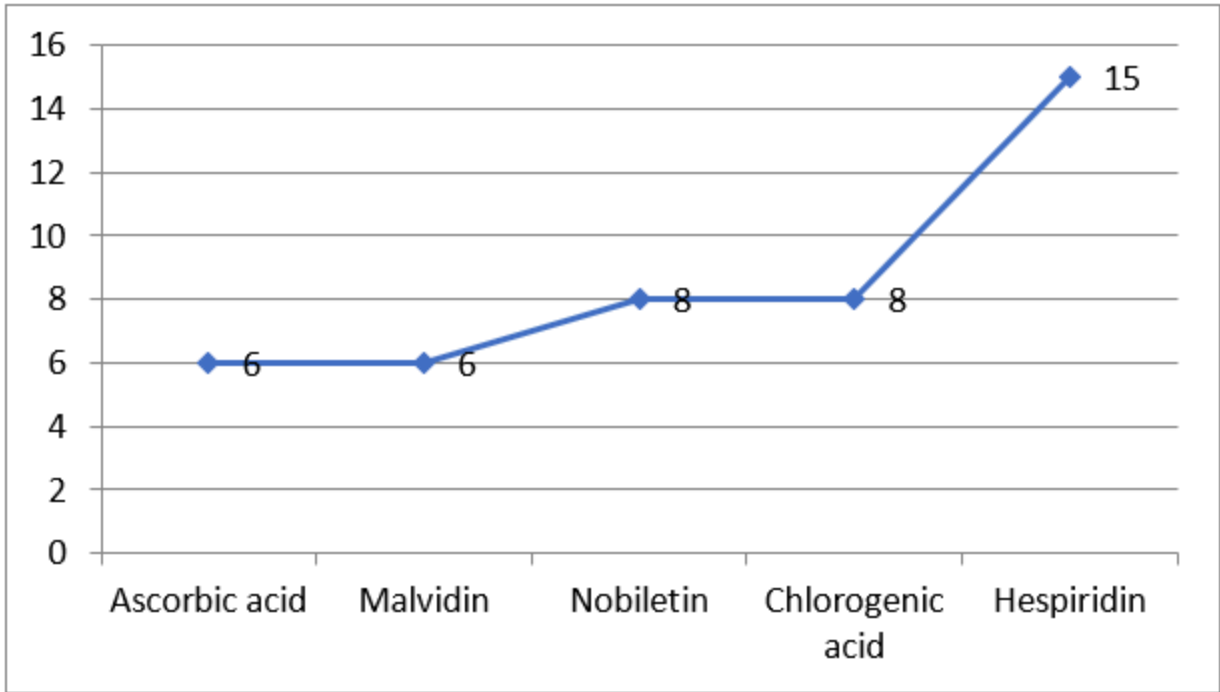


Figure 5

Comparitive analysis of HBA values

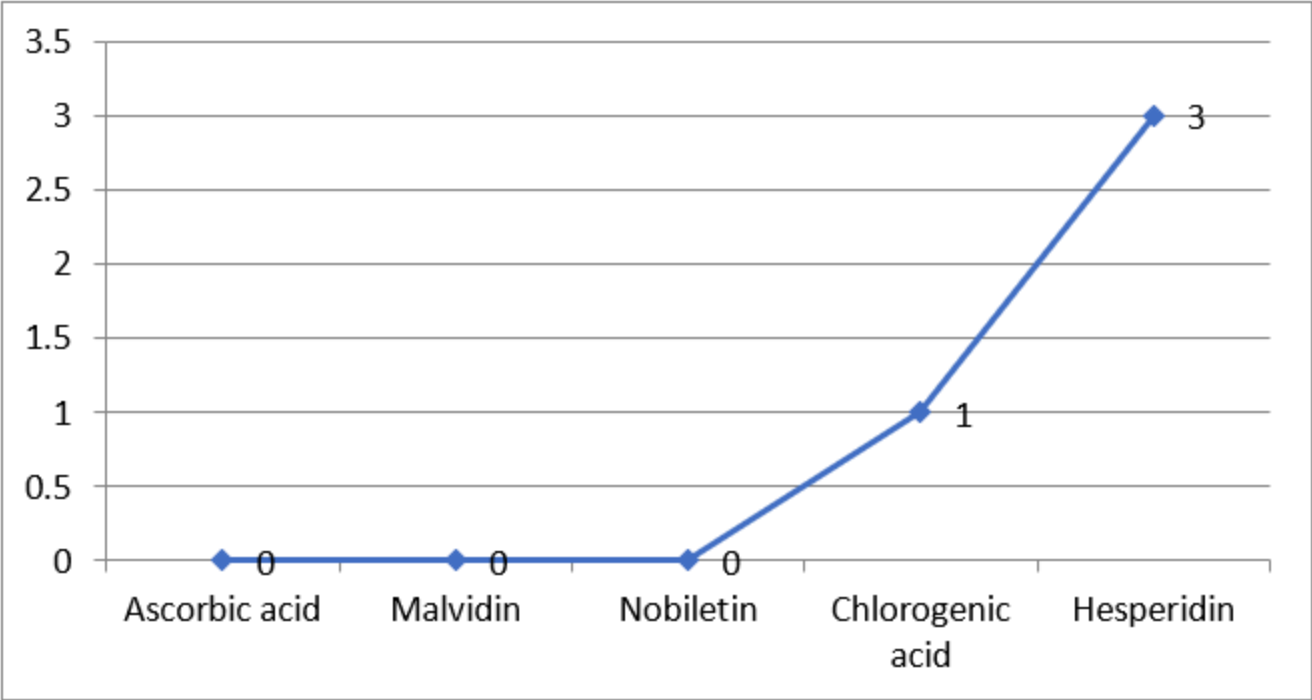


Figure 6

Compative analysis of lipinski rule violation