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ORIGINAL ARTICLE

Phytochemical Profiling and *In Silico* Evaluation of Antioxidant and Neuropharmacologically Active Constituents of the Methanolic Stem Bark Extract of *Magnolia officinalis* Using HPLC-UV

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ABSTRACT

Neuropsychiatric disorders, including anxiety, bipolar disorder, and schizophrenia, are associated with neurotransmitter dysregulation, oxidative stress, and neuroinflammation, necessitating novel multi-target therapeutics from natural sources. This study investigated the phytochemical composition, antioxidant activity, and neuropharmacological potential of the methanolic bark extract of *Magnolia officinalis* using integrated in-vitro and computational approaches to identify potential central nervous system (CNS)-active compounds. Qualitative and quantitative phytochemical analyses and antioxidant assays [2,2-diphenyl-1-picrylhydrazyl (DPPH), ferric reducing antioxidant power (FRAP), nitric oxide (NO), and cupric ion reducing antioxidant capacity (CUPRAC)] were performed. High-performance liquid chromatography coupled with ultraviolet detection (HPLC-UV), molecular docking against $GABA_A$, serotonin ($5\text{-}HT_{1A}$ and $5\text{-}HT_{2A}$), dopamine D_2, histamine H_1, and α_2C-adrenergic receptors, and ADMET analysis were conducted. The extract contained 45.00 ± 0.25 mg gallic acid equivalents (GAE)/g total phenolics and 744.44 ± 19.25 mg quercetin equivalents (QE)/g total flavonoids. Antioxidant activity yielded DPPH, FRAP, and NO IC_{50}/EC_{50} values of 805.36 ± 3.29, 398.68 ± 0.13, and 1333.26 ± 33.80 µg/mL, respectively, compared with 13.23 ± 0.67, 64.78 ± 0.07, and 582.39 ± 35.90 µg/mL for ascorbic acid, while the CUPRAC value was 8210.00 ± 493.66 µg AAE/g extract. HPLC-UV identified 22 phytochemicals including quercetin, magnolol and honokiol. Molecular docking showed that honokiol, magnolol, and obovatol consistently exhibited the strongest binding affinities across multiple CNS targets. ADMET predicted favourable drug-likeness, pharmacokinetics, blood-brain barrier permeability, and safety profiles for these compounds. These findings highlight *M. officinalis* as a promising source of antioxidant, multi-target CNS-active compounds, warranting further in vitro and in vivo validation.

Keywords: *Magnolia* officinalis; Phytochemical screening; Antioxidant potential; Molecular docking; Neuropsychological disorders; ADMET

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1.0 INTRODUCTION

Magnolia officinalis, a well-established traditional medicinal plant, has been widely used throughout East Asia, particularly in Chinese, Korean, and Japanese medicine (Olas, 2025), to treat gastrointestinal disorders, anxiety, depression, respiratory ailments, and cardiovascular conditions. Studies have shown that the primary medicinal part, the dried bark (referred to as "Houpo" in Traditional Chinese Medicine), contains a rich array of bioactive compounds, including phenolics, alkaloids, steroids, and volatile oils (Olas, 2025). Among these constituents, the phenolic compounds such as magnolol and honokiol are considered the most pharmacologically significant, known for their antioxidant, anti-inflammatory, anticancer, and neuroprotective effects (Liou et al., 2003; Fried & Arbiser, 2009; Sulakhiya et al., 2015; Li et al., 2016; Lee et al., 2017; Niu et al., 2021; Olas, 2025). These compounds, among others, found predominantly in the bark but also present in other plant parts, have been the major focus of increasing pharmacological interest because of their potential therapeutic applications. Neuropsychiatric disorders, including anxiety, depression, bipolar disorder, and schizophrenia, are multifactorial conditions characterized by dysregulation of γ-aminobutyric acid (GABA), serotonin, dopamine, histamine, and adrenergic neurotransmission, together with oxidative stress and neuroinflammation, which contribute to neuronal dysfunction and disease progression (Barnes & Sharp, 1999; Beaulieu & Gainetdinov, 2011; Salim, 2017). Oxidative stress results from an imbalance between reactive oxygen and nitrogen species and endogenous antioxidant defenses, leading to lipid peroxidation, protein oxidation, DNA damage, mitochondrial dysfunction, and neuronal injury (Sies, 2017). Consequently, antioxidant assays such as 2,2-diphenyl-1-picrylhydrazyl (DPPH), ferric reducing antioxidant power (FRAP), nitric oxide (NO) scavenging, and cupric ion reducing antioxidant capacity (CUPRAC) are widely employed to evaluate the capacity of natural products to neutralize free radicals and reduce oxidative damage associated with neurodegenerative and neuropsychiatric disorders. Given the historical importance and pharmacological potential of *M. officinalis*, there is a critical need for comprehensive scientific validation of its medicinal properties, especially in the treatment of depression and anxiety. Such validation requires a multidisciplinary approach combining phytochemical screening, advanced chromatographic analysis, and computational modeling. High-performance liquid chromatography coupled with ultraviolet detection (HPLC-UV) plays a pivotal role in the identification and quantification of key constituents, enabling the standardization and quality assurance of plant-based preparations. The neuropharmacological activity of phytochemicals can be explored through their interactions with molecular targets involved in neurotransmission. The γ-aminobutyric acid type A ($GABA_A$) receptor mediates inhibitory neurotransmission and is a principal target for anxiolytic and sedative

drugs (Olsen & Sieghart, 2008). Serotonin receptors, particularly 5-HT_{1A} and 5-HT_{2A}, regulate mood, cognition, and emotional behaviour and are major therapeutic targets in anxiety, depression, and schizophrenia (Barnes & Sharp, 1999). Dopamine D_2 receptors play central roles in psychosis, schizophrenia, and reward signaling (Beaulieu & Gainetdinov, 2011), whereas histamine H_1 receptors influence cognition, arousal, and sedation (Panula et al., 2015). The α_{2C}-adrenergic receptor regulates noradrenergic neurotransmission and has emerged as a promising target for the treatment of cognitive impairment, anxiety, and depression (Uys et al., 2017). Therefore, simultaneous modulation of these receptors may provide a multi-target strategy for the management of complex neuropsychiatric disorders.

In recent years, *in silico* techniques such as molecular docking and pharmacokinetic modeling have emerged as valuable tools in natural product research (Adekilekun et al., 2026). These approaches help predict molecular targets, binding affinities, and drug-like properties, thereby accelerating the discovery and safety assessment of plant-derived therapeutic agents (Abdulameed et al., 2026). Although the neuroprotective activities of isolated constituents such as honokiol and magnolol have been extensively investigated, few studies have comprehensively characterized the phytochemical composition of the methanolic bark extract of *M. officinalis* using HPLC-UV while simultaneously evaluating its antioxidant activity and predicting the multi-target neuropharmacological potential of its constituents through molecular docking and ADMET analysis. Moreover, the possible contributions of less-studied phytochemicals within the extract to CNS activity remain poorly understood. This represents an important knowledge gap that may limit the discovery of additional bioactive compounds with therapeutic potential. Therefore, this study aimed to validate the traditional medicinal claims of *Magnolia officinalis* through an integrative experimental and computational approach by characterizing the phytochemical composition of its methanolic bark extract, evaluating its antioxidant potential using DPPH, FRAP, nitric oxide (NO), and cupric ion reducing antioxidant capacity (CUPRAC) assays, identifying its major phytochemical constituents by HPLC-UV, and investigating their interactions with $GABA_A$, serotonin (5-HT_{1A} and 5-HT_{2A}), dopamine D_2, histamine H_1, and α_2C-adrenergic receptors through molecular docking and ADMET analyses. By combining qualitative and quantitative phytochemical screening with experimental and computational methodologies, the study sought to identify promising CNS-active phytochemicals, enhance understanding of the pharmacological potential of *M. officinalis*, and contribute to the development of standardized, evidence-based herbal therapeutics.

2. MATERIALS AND METHODS

2.1 Collection of plant material and preparation of methanolic extract

The *Magnolia officinalis* tree does not grow in Nigeria. The pulverized bark powder was purchased from Biotech and Pharmaceutical Valley, Nanjing, China. The powder is marketed as a plant supplement. The extraction was carried out by dissolving 120 g of the powder in 360 mL of 96% methanol, and the mixture was constantly shaken for 48 hours on an orbital shaker. The extract was filtered using Whatman No 1 Filter Paper, and a Büchi Rotavapor R-200 rotary evaporator was used to concentrate the filtrate to dryness. The final crude extracts (30 g) were weighed, representing a 25% extraction yield, and stored in airtight, opaque containers for subsequent phytochemical analysis.

2.2 Qualitative and quantitative phytochemical screening

The herbal extract was distributed into separate test tubes for qualitative analysis to investigate the presence of various phytochemicals, including flavonoids, saponins, steroids, carbohydrates, phenols, tannins, glycosides, terpenoids, and alkaloids. The screening followed standard protocols established by Sofowora (1993), Trease & Evans (1989), and Harborne (1973), with slight modifications as described by Yadav & Agarwala (2011). The total phenolic content was determined using the method described by Yadav & Agarwala (2011), while the total flavonoid content was determined by aluminum chloride colorimetric assay adapted from Muthukumaran et al. (2016) with slight modification.

2.3 Antioxidant assay

The 2,2-diphenyl-1-picrylhydrazyl (DPPH) free radical scavenging assay, ferric reducing antioxidant power (FRAP) assay, nitric oxide (NO) radical scavenging assay, and cupric reducing antioxidant capacity (CUPRAC) assay were performed according to the methods of Erhirhie et al. (2020), Habibur et al. (2013), Atere et al. (2018), and Alaribe et al. (2020), respectively.

2.4 HPLC-UV analysis

High-performance liquid chromatography coupled with ultraviolet detection (HPLC-UV) was performed using a Shimadzu Nexera MX system equipped with a diode array detector (DAD) operated at 254 nm. Chromatographic separation was achieved on a uBondapak C18 column (100 × 4.6 mm, 7 µm) using an acetonitrile/water mobile phase at a flow rate of 1.0 mL/min with an injection volume of 10 µL. The dried methanolic bark extract of *Magnolia officinalis* (10g) was reconstituted in acetonitrile, filtered through a 0.45 µm syringe filter, and analyzed under the chromatographic conditions described above. Authentic reference standards were analyzed prior to sample analysis to establish the retention times and UV spectral profiles of target phytochemicals. Compounds in the extract were identified by comparing their retention times and UV spectra with those of the corresponding reference standards. Compound identification was achieved by comparing the retention times of chromatographic peaks with those of authentic reference standards analyzed under identical chromatographic conditions. The relative abundance (%) of each phytochemical is calculated as;

$$\text{Relative abundance (\%)} = \frac{\text{Peak area of compound}}{\text{Sum of peak areas of identified compounds}} \text{x100} \quad (1)$$

2.5 *In silico* analysis for *Magnolia officinalis* phytochemicals

Three-dimensional X-ray diffraction structures of target proteins relevant to anxiety and depression, which include α-$_2$C Adrenergic Receptor (6KUW), Gamma-Aminobutyric Acid ($GABA_A$) Receptor (8DD2), Histamine H_1 Receptor (3RZE), Serotonin 5-hydroxytryptamine 1A (5-HT_1A) receptor (7E2Y), Serotonin 5-hydroxytryptamine 2A (5-HT_2A) receptor (6A93), and Dopamine D2 Receptor (6CM4) were retrieved from the Protein Data Bank (PDB) using their respective PDB IDs. Protein preparation was conducted using PyMOL and PyRx. The phytochemicals identified from HPLC analysis and reference drug, Diazepam, were located and obtained from the PubChem database and saved in SDF format. Ligand structures were concatenated using Open Babel software. Energy minimization and subsequent conversion to PDBQT format was performed using PyRx software. Molecular docking was performed with PyRx software and binding affinities were recorded in kcal/mol. Docked complexes were visualized and analyzed using PyMOL software and Discovery Studio Visualizer. Predicted absorption, distribution, metabolism, excretion and toxicity (ADMET) properties of the ligands were predicted using the SwissADME online tool and Protox 3 online server.

Statistical analysis

Data analysis was performed using Microsoft Excel (2016), with results expressed as mean ± standard deviation (SD). IC_{50} values were calculated through regression analysis within the Excel platform.

3. RESULTS

3.1 Quantitative phytochemical analysis

The methanol extraction of *M. officinalis* bark yielded 25.00 ± 0.22% extract. Quantitative phytochemical analysis of the methanol extract of *M. officinalis* bark revealed substantial levels of bioactive compounds. The total phenolic content (TPC) was 45.00 ± 0.25 mg gallic acid equivalents (GAE)/g extract, while the total flavonoid content (TFC) was 744.44 ± 19.25 mg quercetin equivalents (QE)/g extract, indicating a high abundance of flavonoids.

3.2 *In vitro* antioxidant profile analysis

The antioxidant activity of *M. officinalis* methanol extract was evaluated using multiple in vitro assays. In the DPPH assay, the extract showed an IC_{50} of 805.36 ± 3.29 µg/mL, compared to 13.23 ± 0.67 µg/mL for ascorbic acid. The FRAP assay yielded an EC_{50} of 398.68 ± 0.13 µg/mL, whereas ascorbic acid exhibited 64.78 ± 0.07 µg/mL. The nitric oxide scavenging assay, the extract demonstrated an IC_{50} of 1333.26 ± 33.80 µg/mL, relative to 582.39 ± 35.90 µg/mL for the standard. Additionally, the CUPRAC value was 8210.00 ± 493.66 µg AAE/g extract. Overall, the extract exhibited measurable but comparatively much lower antioxidant activity than ascorbic acid across all assays.

3.3 HPLC-UV analysis

The HPLC-UV chromatogram of the *Magnolia officinalis* methanolic bark extract in Figure 1 revealed a complex phytochemical profile comprising 22 identified compounds with distinct retention times (RT) and peak areas (Table 1). Compound identification was achieved by comparing the retention times and UV spectral profiles of sample peaks with those of authentic reference standards. The identified phytochemicals eluted over a retention time range of 1.266–26.533 min. Early-eluting compounds included 4-hydroxybenzoic acid (RT = 1.266 min), β-caryophyllene (2.516 min), magnolol (4.450 min), honokiol (5.466 min), gallic acid (6.483 min), and caffeic acid (7.333 min). Compounds detected at intermediate retention times included catechin (7.950 min), epicatechin (8.783 min), sitosterol (9.350 min), humulene (9.883 min), and quercetin (11.050 min). Later-eluting compounds comprised elemicin (12.166 min), isorhamnetin (13.700 min), apigenin (16.850 min), luteolin (17.616 min), myricetin (18.900 min), maglifloenone (19.416 min), bisabolene (21.133 min), naringenin (22.766 min), germacrene D (24.133 min), α-pinene (24.550 min), and obovatol (26.533 min). Relative abundance, estimated by peak area normalization, indicated that quercetin was the predominant phytochemical, accounting for 41.91% of the total chromatographic peak area. Elemicin (16.82%), isorhamnetin (13.57%), β-caryophyllene (10.88%), and 4-hydroxybenzoic acid (4.84%) were also present in relatively high abundance, whereas magnolol contributed 3.05% of the total peak area. The remaining identified phytochemicals each accounted for less than 2% of the total chromatographic peak area.

.Table **1**. HPLC-UV identified compounds in *M.officinalis* and their relative abundance

Phytochemical	Retention	Area	Height	Relative abundance (%)
4-Hydroxybenzoic Acid	1.266	1181.3855	33.553	4.84
Beta-Caryophyllene	2.516	2658.315	24.849	10.88
Magnolol	4.45	744.0795	12.809	3.05
Honokiol	5.466	312.409	7.886	1.28
Gallic Acid	6.483	199.6535	6.04	0.82
Caffiec Acid	7.333	61.059	4.121	0.30
Catechin	7.95	72.216	3.412	0.30
Epicatechin	8.783	95.626	7.584	0.39
Sitosterol	9.35	101.463	4.646	0.42
Humulene	9.883	55.754	6.456	0.23
Quercetin	11.05	10237.005	169.394	41.91
Elemicin	12.166	4108.1185	72.814	16.82
Isorhamnetin	13.7	3315.377	46.496	13.57
Apigenin	16.85	84.0755	7.752	0.34
Luteolin	17.616	477.434	6.998	1.95
Myricetin	18.9	60.3305	7.656	0.25
Magliflonenone	19.416	94.247	6.004	0.39
Bisabolene	21.133	72.2665	3.8	0.30
Naringenin	22.766	73.096	7.189	0.30
Germacrene D	24.133	145.655	9.298	0.60
Alpha-Pinene	24.55	67.416	7.977	0.28
Obovatol	26.533	83.082	6.542	0.34

3.4 *In silico* analysis of *M. officinalis* phytochemicals

The molecular docking analysis of phytochemicals from *Magnolia officinalis* against six neuropharmacological protein targets (α-$_2$C Adrenergic receptor (6KUW), Gamma-Aminobutyric Acid ($GABA_A$) receptor (8DD2), Histamine H_1 receptor (3RZE), Serotonin 5-hydroxytryptamine 1A (5-HT_1A) receptor (7E2Y), Serotonin 5-hydroxytryptamine 2A (5-HT_2A) receptor (6A93), and Dopamine D2 receptor (6CM4)) revealed varying binding affinities as summarized in Table 2. Several compounds demonstrated binding energies comparable to or exceeding those of the reference drug, diazepam. Among the screened compounds, sitosterol exhibited the highest binding affinity against 6KUW (-9.5 kcal/mol), surpassing diazepam (-7.7 kcal/mol). Other notable compounds with strong binding affinities across multiple targets included maglifloenone (-8.3 kcal/mol), luteolin (-7.9 kcal/mol), isorhamnetin (-7.9 kcal/mol), naringenin (-7.9 kcal/mol), and myricetin (-7.9 kcal/mol). Importantly, luteolin demonstrated consistently high binding affinities across all protein targets, suggesting a multi-target binding profile. Similarly, other flavonoids such as quercetin, isorhamnetin, myricetin, naringenin, apigenidin sitosterol, maglifloenone, catechin, epicatechin, magnolol, honokiol and obovatol also demonstrated notable multi-target activities Conversely, compounds such as 4-hydroxybenzoic acid, gallic acid, caffeic acid, elemicin, alpha-pinene, and germacrene D showed comparatively weaker binding affinities, indicating lower interaction potential with the selected targets. Binding interaction analysis summarized in Table 3 revealed that the active compounds engaged in key stabilizing interactions, including conventional hydrogen bonds, carbon-hydrogen bonds, pi–pi stacking, and pi-alkyl interactions. Residues such as arginine (ARG), tyrosine (TYR), alanine (ALA) and lysine (LYS) were frequently involved in ligand binding. Flavonoids such as luteolin, quercetin, and isorhamnetin exhibited multiple hydrogen bonding interactions alongside pi-interactions, contributing to stable ligand-protein complexes. Lignans such as honokiol and magnolol primarily formed hydrophobic and pi-alkyl interactions.

.Table **2**. Molecular docking profiles of phytochemicals from the methanol extract of *Magnolia officinalis* against protein targets

PHYTOCHEMICAL	PUB CHEM ID	α-$_2$C Adrenergic receptor (6KUW) Binding Affinity (Kcal/mol)	Gamma-Aminobutyric Acid (8DD2) Binding Affinity (Kcal/mol)	Histamine H_1 receptor (3RZE) Binding Affinity (Kcal/mol)	Serotonin 5-hydroxytryptamine 1A (5-HT_1A) receptor 7E2Y Binding Affinity (Kcal/mol)	Serotonin 5-hydroxytryptamine 2A (5-HT_2A) receptor (6A93) Binding Affinity (Kcal/mol)	Dopamine D2 receptor (6CM4) Binding Affinity (Kcal/mol)
4-Hydroxybenzoic acid	135	-5.3	-4.4	-4.6	-4.6	-5.0	-5.5
Alpha pinene	5317570	-6.9	-4.9	-5.7	-5.7	-6.5	-6.3
Apigenidin	5280443	-7.8	-6.1	-7.0	-7.0	-7.5	-7.7
Beta-caryophyllene	5281515	-7.2	-4.9	-5.6	-5.6	-7.1	-6.2
Bisabolene	3033866	-6.6	-5.5	-6.0	-6.0	-6.4	-7.4
Caffeic acid	689043	-6.3	-5.6	-5.4	-5.4	-5.6	-6.4
Catechin	9064	-7.6	-5.9	-6.8	-6.8	-7.2	-6.4
Elemicin	10248	-5.3	-4.8	-4.7	-4.7	-5.4	-5.5

Epicatechin	72276	-7.6	-5.9	-6.8	-6.8	-7.2	-6.4
Gallic acid	370	-5.7	-5.0	-5.0	-5.0	-5.3	-5.2
Germacrene D	5317570	-6.7	-5.0	-5.7	-5.7	-6.7	-5.9
Honokiol	72303	-7.2	-6.2	-6.5	-6.5	-6.9	-7.5
Humulene	5281520	-6.9	-4.8	-5.4	-5.4	-6.5	-6.1
Isorhamnetin	5281654	-7.9	-6.3	-6.9	-6.9	-7.4	-6.5
Luteolin	5280445	-7.9	-6.2	-7.1	-7.1	-7.6	-6.8
Maglifloenone	21723002	-8.3	-5.5	-6.4	-6.4	-7.2	-7.0
Magnolol	72300	-7.5	-6.5	-6.1	-6.1	-6.8	-7.2
Myricetin	5281672	-7.9	-6.0	-7.2	-7.2	-7.2	-6.5
Naringenin	439246	-7.9	-5.8	-6.8	-6.8	-7.5	-6.9
Obovatol	100771	-7.3	-6.6	-6.4	-6.4	-6.9	-7.6
Quercetin	5280343	-7.7	-6.2	-6.9	-6.9	-7.3	-6.7
Sitosterol	222284	-9.5	-5.4	-6.5	-6.5	-7.4	-7.9
Diazepam (Control)	3016	-7.7	-6.2	-6.7	-6.4	-7.0	-6.8

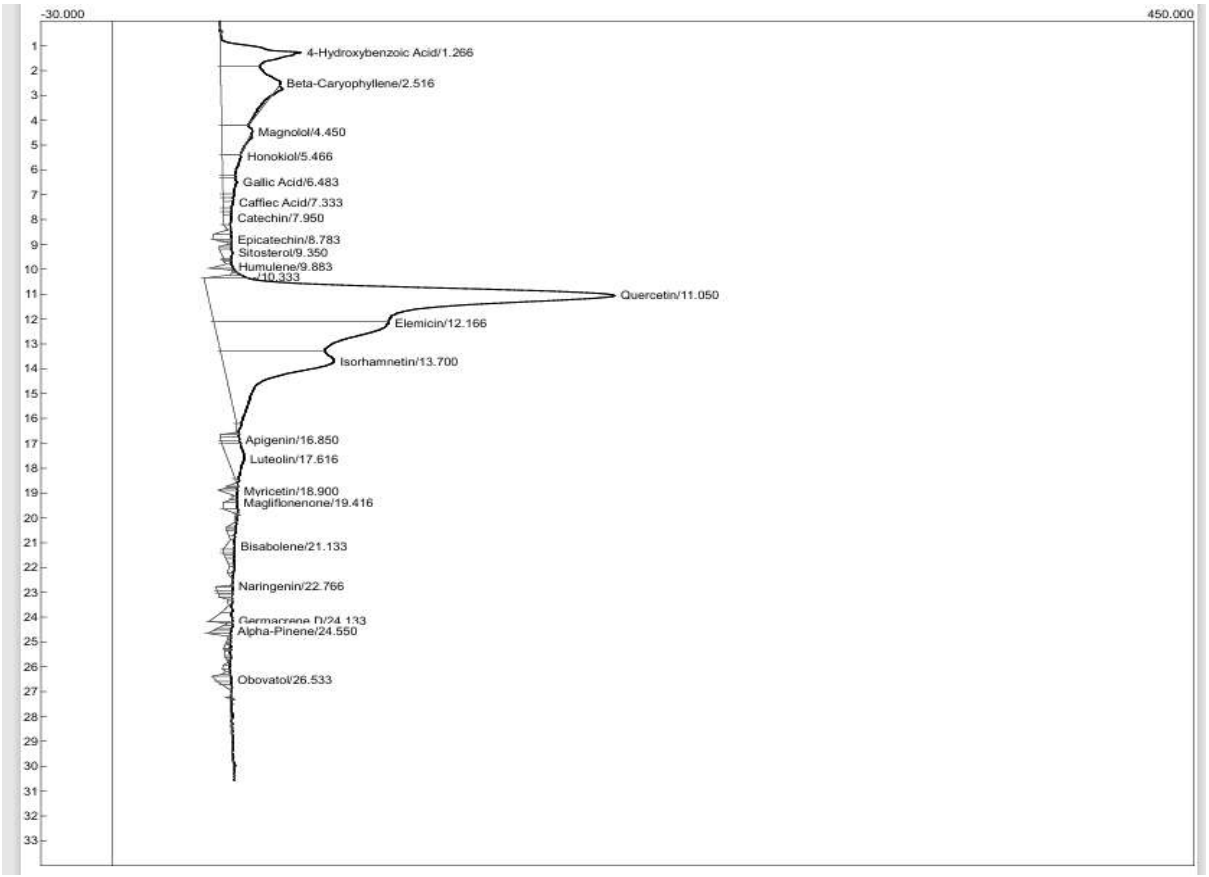


Figure **1**. HPLC-UV chromatogram for *M. officinalis* bark methanol extract

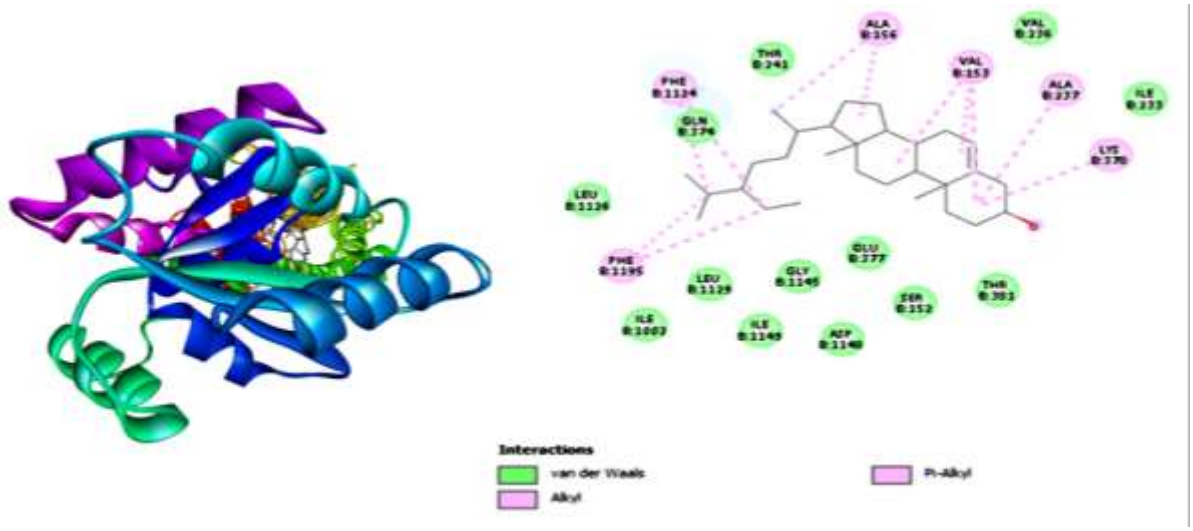


Figure **2**. 3D and 2D Sitosterol-6KUW binding site interaction analysis

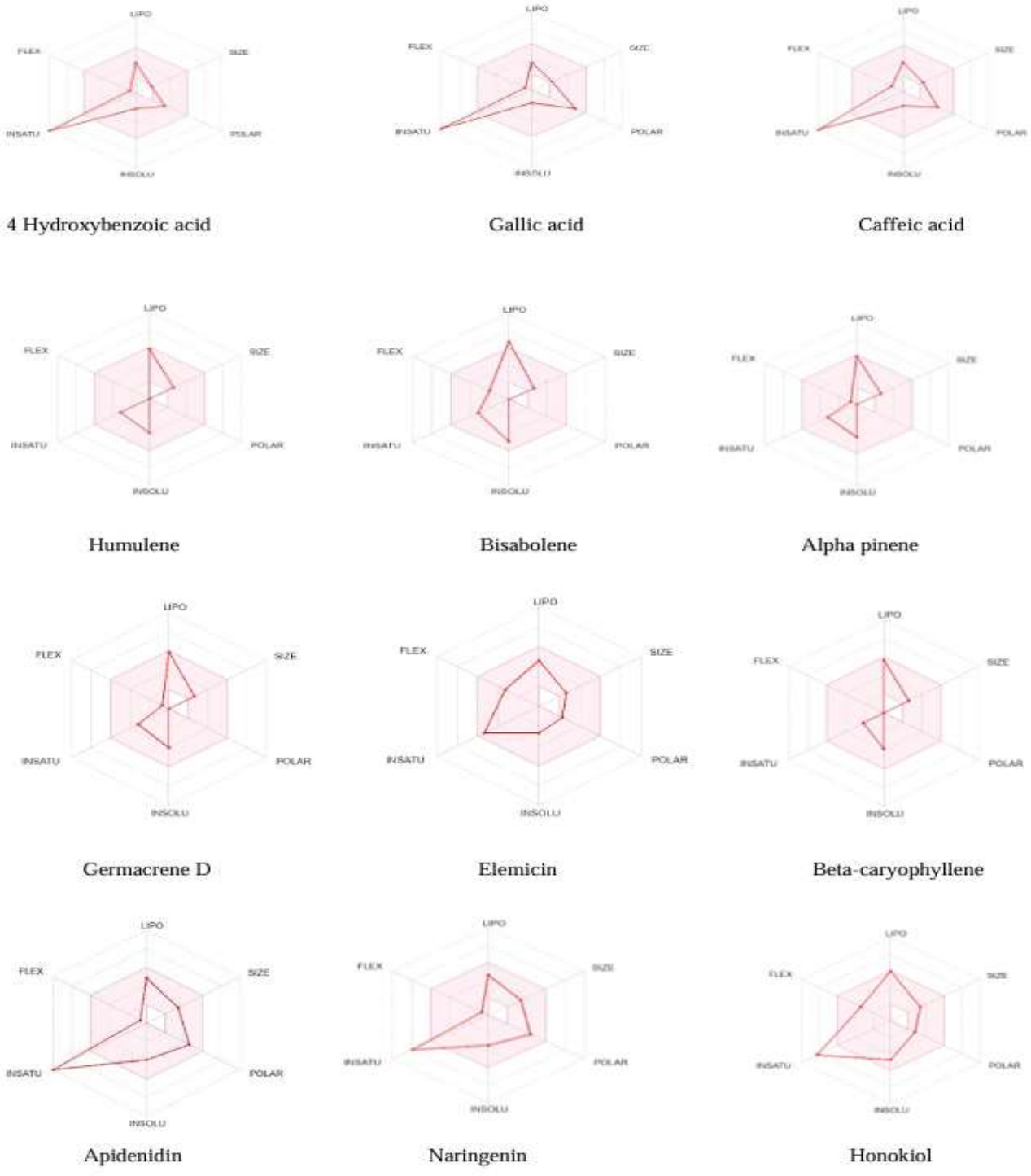


Figure **3**. Bioavailability Radar Plot Prediction for *M. officinalis* Phytochemicals

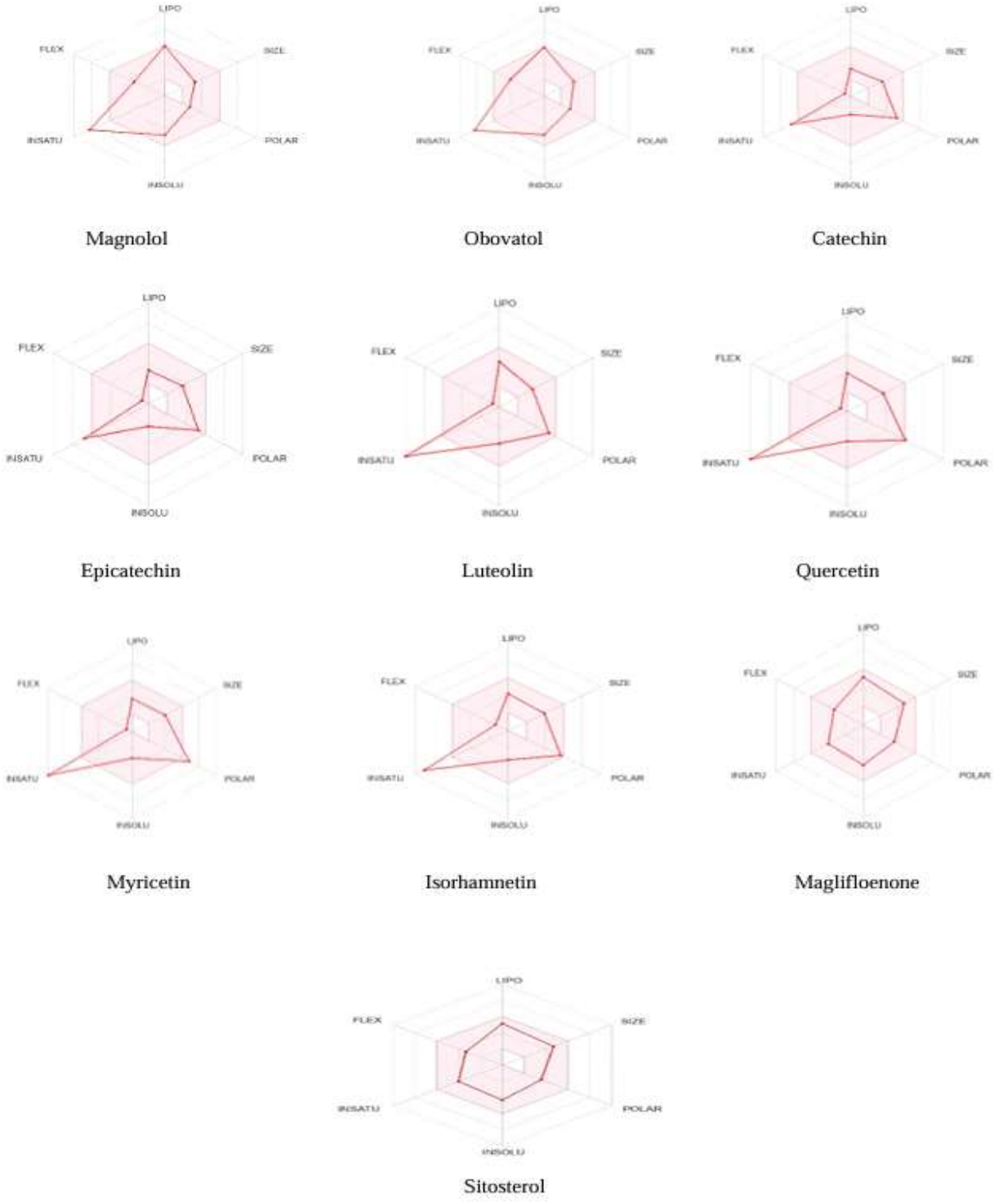


Figure **4**. Bioavailability radar plot prediction for *M. officinalis* phytochemicals (Continued)

3.5 Drug likeness and bioavailability radar plot of *M. officinalis* phytochemicals

The drug-likeness and bioavailability screening results of *M. officinalis* phytochemicals presented in Table 4 and Figures 3 and 4, respectively, were performed using SwissADME. The compounds spanned a broad molecular weight range (138.12 - 386.44 g/mol) and largely complied with Lipinski, Veber, Ghose, and Amgen rules, indicating overall favourable drug-like properties. TPSA varied widely, from nonpolar terpenoids (0 Å²) to highly polar flavonoids such as quercetin (131.36 Å²) and myricetin (151.59 Å²), with higher values suggesting reduced membrane permeability. In contrast, honokiol, magnolol, and obovatol exhibited low TPSA (<50Å²) and moderate lipophilicity (XLOGP3 ≈ 4.8-4.9), supporting good permeability. Lipophilicity ranged from 0.7 to 6.33; compounds within the optimal range (1-5) showed balanced solubility and permeability, while highly lipophilic molecules may have reduced bioavailability. Solubility screening results aligned with this trend, with polar compounds moderately soluble and lipophilic ones poorly soluble. All compounds met flexibility criteria (≤ 9 rotatable bonds), and Fsp^3 values ranged from 0 to 0.6, with some CNS-active compounds below the preferred threshold yet retaining acceptable profiles. Bioavailability radar analysis identified seven compounds, including two hit compounds, maglifloenone, and sitosterol, as having optimal physicochemical balance, highlighting their potential for oral and CNS-targeted applications.

3.6 Pharmacokinetic screening of *M. officinalis* phytochemicals

In silico pharmacokinetics profiling of *Magnolia officinalis* phytochemicals using SwissADME in Table 5 identified several

compounds with favourable pharmacokinetic properties for CNS targeting. Key selection criteria included high gastrointestinal absorption, blood-brain barrier (BBB) permeability, absence of p-glycoprotein (p-gp) efflux, and minimal cytochrome P450 (CYP) inhibition. 4-Hydroxybenzoic acid exhibited the most optimal overall pharmacokinetic profile, followed by elemicin, which showed similar properties but with CYP1A2 inhibition. Sitosterol, maglifloenone, honokiol, magnolol, and obovatol demonstrated high gastrointestinal absorption and BBB permeability; however, all showed potential inhibition of CYP450 isoforms. Sitosterol and maglifloenone consistently displayed favorable performance across ADMET parameters and molecular docking, indicating strong CNS drug candidacy. In contrast, elemicin and 4-hydroxybenzoic acid, despite excellent pharmacokinetic profiles, showed comparatively weaker docking affinities.

3.6.1 Toxicity screening

ProTox-3 toxicity screening results in Table 6 indicated that *M. officinalis* phytochemicals exhibit a broad range of acute oral toxicity (LD_{50}: 159 - 10,000 mg/kg), with most compounds classified as toxicity classes 4 - 6 (low toxicity), while quercetin, myricetin, and isorhamnetin (LD_{50} = 159 mg/kg) fell into class 3. Hepatotoxicity was not predicted for any compound. Nephrotoxicity was observed in several phenolics and flavonoids, whereas neurotoxicity was limited to caffeic acid, alpha-pinene, naringenin, and sitosterol. Respiratory toxicity was predicted for multiple flavonoids and maglifloenone, while cardiotoxicity was absent. *In silico* toxicity assessment identified germacrene D, β-caryophyllene, maglifloenone, and sitosterol as having carcinogenic potential. Immunotoxicity and mutagenicity were mainly associated with flavonoids, while cytotoxicity was predicted only for naringenin. $GABA_A$ receptor interaction was identified for apigenidin, honokiol, and magnolol. The compounds demonstrated predominantly low toxicity with selective organ- and endpoint-specific liabilities.

Table **4**. *In silico* drug likeness prediction for *M. officinale* phytochemicals

Phytocompounds	MW g/mol	TPSA Å²	XLOGP3	Log *S* (ESOL)	F.Csp3	NRB	LV	GV	VB	EV	MV	BS
4-Hydroxybenzoic acid	138.12	57.53	1.58	-2.07	0	1	0	3	0	0	1	0.85
Gallic acid	170.12	97.99	0.7	-1.64	0	1	0	2	0	0	1	0.56
Caffeic acid	180.16	77.76	1.15	-1.89	0	2	0	0	0	0	1	0.56
Humulene	204.35	0	4.55	-3.97	0.6	0	1	0	0	0	1	0.55
Bisabolene	204.35	0	6.33	-4.9	0.6	3	1	0	0	0	2	0.55
Alpha pinene	204.35	0	4.74	-4.03	0.6	1	1	0	0	0	1	0.55
Germacrene D	204.35	0	4.74	-4.03	0.6	1	1	0	0	0	1	0.55
Elemicin	208.25	27.69	2.53	-2.69	0.33	5	0	0	0	0	0	0.55
Beta caryophelene	204.35	0	4.38	-3.87	0.73	0	1	0	0	0	1	0.55
Apigenidin	270.24	90.9	3.02	-3.94	0	1	0	0	0	0	0	0.55
Naringenin	272.25	86.99	2.52	-3.49	0.13	1	0	0	0	0	0	0.55
Honokiol	266.33	40.46	4.98	-4.74	0.11	5	0	0	0	0	0	0.55
Magnolol	266.33	40.46	4.98	-4.74	0.11	5	0	0	0	0	0	0.55
Obovatol	282.33	49.69	4.88	-4.69	0.11	6	0	0	0	0	0	0.55
Catechin	290.27	110.38	0.36	-2.22	0.2	1	0	0	0	0	0	0.55
Epicatechin	290.27	110.38	0.36	-2.22	0.2	1	0	0	0	0	0	0.55
Luteolin	286.24	111.13	2.53	-3.71	0	1	0	0	0	0	0	0.55
Quercetin	302.24	131.36	1.54	-3.16	0	1	0	0	0	0	0	0.55
Myricetin	318.24	151.59	1.18	-3.01	0	1	1	0	1	1	2	0.55
Isorhamnetin	316.26	120.36	1.87	-3.36	0.06	2	0	0	0	0	0	0.55
Maglifloenone	386.44	63.22	3.56	-4.31	0.5	5	0	0	0	0	0	0.85
Sitosterol	386.44	63.22	3.56	-4.31	0.5	5	0	0	0	0	0	0.85

MW-Molecular weight, TP-Topological Polar Surface Area, NRB-Number of Rotable Bonds, LV-Lipinski Violations, GV-Ghose Violations, Veber Violations, Egan Violations, Muegge Violations, BS- Bioavailability score, F.Csp3- fraction of sp^3-hybridized carbons, XLOGp3- logarithm of the octanol–water partition coefficient, Log S - predicted aqueous solubility.

Table **5**. *In silico* pharmacokinetics prediction for *M. officinalis* phytochemicals

Phytochemicals	ESOL (LogS)	GIA	BBB Permeant	P-gp substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	CYP3A4 inhibitor
4-Hydroxybenzoic acid	-2.07	High	Yes	No	No	No	No	No	No
Gallic acid	-1.64	High	No	No	No	No	No	No	Yes
Caffeic acid	-1.89	High	No	No	No	No	No	No	No
Humulene	-3.97	Low	No	No	No	No	Yes	No	No
Bisabolene	-4.9	Low	No	No	Yes	No	Yes	No	No
Alpha pinene	-4.03	Low	No	No	No	No	Yes	No	No
Germacrene D	-4.03	Low	No	No	No	No	Yes	No	No
Elemicin	-2.69	High	Yes	No	Yes	No	No	No	No
Beta caryophelene	-3.87	Low	No	No	No	Yes	Yes	No	No
Apigenidin	-3.94	High	No	No	Yes	No	No	Yes	Yes
Naringenin	-3.49	High	No	Yes	Yes	No	No	No	Yes
Honokiol	-4.74	High	Yes	No	Yes	Yes	Yes	Yes	Yes
Magnolol	-4.74	High	Yes	No	Yes	Yes	Yes	Yes	Yes
Obovatol	-4.69	High	Yes	No	Yes	Yes	Yes	Yes	Yes
Catechin	-2.22	High	No	Yes	No	No	No	No	No
Epicatechin	-2.22	High	No	Yes	No	No	No	No	No
Luteolin	-3.71	High	No	No	Yes	No	No	Yes	Yes
Quercetin	-3.16	High	No	No	Yes	No	No	Yes	Yes
Myricetin	-3.01	Low	No	No	Yes	No	No	No	Yes
Isorhamnetin	-3.36	High	No	No	Yes	No	No	Yes	Yes
Maglifloenone	-4.31	High	Yes	No	No	No	Yes	Yes	Yes
Sitosterol	-4.31	High	Yes	No	No	No	Yes	Yes	Yes

4.0 DISCUSSION

Neuropsychiatric disorders such as anxiety, bipolar disorder, and schizophrenia are multifactorial conditions characterized by dysregulation of neurotransmitter systems, oxidative stress, and neuroinflammatory processes. In this study, a structured workflow integrating phytochemical screening, antioxidant evaluation, chromatographic profiling, molecular docking, and ADMET prediction was employed to identify CNS-active compounds from *Magnolia officinalis* bark extract. Quantitative analysis revealed appreciable levels of the constituents of *Magnolia officinalis* bark methanolic extract. Although total phenolic content was lower than that reported by Cristea et al. (2024), the relatively high flavonoid content suggests meaningful neuropharmacological relevance. Oxidative stress is a well-established contributor to anxiety, bipolar disorder, and schizophrenia, with clinical studies reporting elevated oxidative damage and reduced antioxidant defenses in affected individuals (Palta et al., 2014; Liu et al., 2015, Ait Tayeb et al., 2023). Research studies further indicates that increased antioxidant intake correlates with reduced symptom severity (Abshirini et al., 2019; Luo et al., 2024). In this context, the antioxidant activity observed in *M. officinalis* extract supports its therapeutic relevance. Although much less potent than ascorbic acid, the extract exhibited improved activity compared to previously reported study with ethanol extracts (IC_{50} = 2130 ± 50 µg/mL) (Wang et al., 2021). This suggests that extraction conditions may significantly influence bioactivity (Dai & Mumper, 2010; Iloki-Assanga et al., 2015; Yeo & Shahidi, 2019; Bako et al., 2024; Yamauchi, 2024). Even little antioxidant effects may contribute to restoring redox balance and reducing neuroinflammation, which are key mechanisms in neuropsychiatric disorders (Vollbracht & Werner, 2024). HPLC-UV was selected because it provides a robust, reproducible, and cost-effective approach for the separation and detection of UV-absorbing phytochemicals. The technique offers excellent chromatographic resolution and reliable quantitative performance for compounds containing UV-active chromophores, making it well suited for phytochemical profiling and the identification of major bioactive constituents. Although HPLC-UV does not detect compounds lacking significant UV absorbance and provides less structural information than HPLC-MS-based techniques, it remains a widely accepted method for routine phytochemical analysis and quality assessment of plant extracts. HPLC-UV analysis identified twenty-two (22) phytochemicals spanning phenolics, flavonoids, terpenoids, and sterols (Sakaue et al 2016; Wang, et al., 2019; Huang et al., 2020; Usach, et al., 2021). The major constituents based on relative abundance in Table 1 are quercetin, isorhamnetin, elemicin, and beta-caryophyllene, while honokiol was present in lower abundance. The relative abundance values were estimated from normalized HPLC-UV peak areas and should be interpreted as relative detector responses rather than absolute concentrations, as differences in molar absorptivity among compounds may influence detector response. However, biological activity is not solely dependent on concentration but also on receptor affinity and pharmacokinetic behaviour, underscoring the importance of *in silico* prioritization (Lipinski et al., 2001; Hughes et al., 2011; Daina et al., 2017). The analysis confirmed the presence of phenolics, flavonoids, tannins, glycosides, and steroids. These phytochemical classes are strongly associated with neuroprotective and anti-inflammatory effects relevant to neuropsychiatric disorders. Phenolic and flavonoid compounds, in particular, modulate oxidative stress and inflammatory pathways implicated in neuronal dysfunction (Barakat et al., 1993; Okwu, 2004; Okwu, & Omodamino, 2005).

Molecular docking against key CNS targets including Gamma-Aminobutyric Acid ($GABA_A$) (8DD2), serotonin 5-HT_1A (7E2Y), serotonin 5-HT_2A (6A93), dopamine D_2 (6CM4), histamine H_1 (3RZE), and α_2C-adrenergic (6KUW) receptors (Shimamura et al., 2011; Wang et al., 2018; Kimura et al., 2019; Xu et al., 2021; Zhu et al., 2022) revealed several strong multi-target interactions. Notably, luteolin demonstrated consistent binding across all receptors, reflecting a broad-spectrum interaction profile. Such behaviour is characteristic of multi-target compounds, which can interact with multiple proteins due to structural features such as planar aromaticity and hydrogen-bonding capacity. While this property may be advantageous for complex disorders like schizophrenia and bipolar disorder, it may also increase off-target effects and reduce selectivity. Previous studies support this concept of polypharmacology, highlighting that some flavonoids exhibit multi-target activity across CNS receptors (Medina-Franco, et al., 2013). However, despite its strong docking performance, luteolin and other flavonoids, including quercetin, myricetin and catechin, were limited by poor BBB permeability probably due to their high polarity, which constrains their CNS permeability. Similarly, naringenin and isorhamnetin showed favourable binding and drug-likeness but insufficient CNS bioavailability, highlighting the critical importance of pharmacokinetic constraints in neurotherapeutic discovery. *M. officinalis* compounds were prioritized based on their ability to satisfy key pharmacodynamic and pharmacokinetic criteria, with particular emphasis on blood–brain barrier (BBB) permeability, a critical determinant in the development of central nervous system (CNS)-active agents. Within this framework, beta-sitosterol, maglifloenone, honokiol, magnolol, and obovatol emerged as the most promising candidates. These compounds were predicted to have BBB penetration, strong binding affinities, and favourable drug-likeness profiles, supporting their progression through the selection pipeline. In particular, the observed pharmacological profiles of honokiol, magnolol, and obovatol are consistent with the reported neuroprotective activity of Magnolia-derived neolignans. (Yang et al., 2013). In contrast, although elemicin and 4-hydroxybenzoic acid exhibited favorable pharmacokinetic properties, their weak receptor binding affinities limited their neuropharmacological relevance. Among the prioritized compounds, honokiol and magnolol demonstrated notable predicted mechanistic relevance through in silico modulation of GABAergic signaling. This computational finding aligns with previous experimental evidence indicating that both compounds act as positive allosteric modulators of $GABA_A$ receptors, consistent with their reported anxiolytic and neuroprotective effects in vivo (Li, et al., 2011). Beta-sitosterol, maglifloenone, honokiol, magnolol, and obovatol exhibited strong molecular docking performance and favourable predicted gastrointestinal absorption profiles, reinforcing their classification as potential CNS-active candidates. ADMET profiling further refined compound prioritization by integrating pharmacokinetic and safety parameters. These *in silico* findings are consistent with experimental evidence confirming the neuroactivity and safety of honokiol and magnolol (Choi et al., 2012; Sarrica et al., 2018; Anand et al., 2021). Although toxicity of the compounds was predicted computationally, empirical studies indicate that honokiol and magnolol are non-genotoxic and well tolerated, with a no observed adverse effect level exceeding 240 mg/kg/day and no adverse effects reported in long-term human studies (Sarrica et al., 2018). Despite these promising attributes, certain limitations were identified. Predicted interactions with cytochrome P450 (CYP450) isoforms, particularly for honokiol, magnolol and obovatol, alongside the provisional safety profiles of beta-sitosterol and maglifloenone, highlight the need for further medicinal chemistry optimization. Addressing these potential metabolic liabilities will be essential to enhance their safety profiles and ensure translational viability. This study demonstrates that a multi-layered analytical pipeline integrating phytochemical profiling, antioxidant assessment, molecular docking, and ADMET prediction is effective for identifying CNS-active compounds. Multi-target compounds such as luteolin highlight the potential of poly-pharmacology in complex neuropsychiatric disorders. Compounds such as honokiol, magnolol, obovatol, sitosterol and maglifloenone demonstrate a more optimal balance between target specificity and pharmacokinetic suitability. These findings support *Magnolia officinalis* as a promising source of lead compounds for the development of therapeutics targeting anxiety, bipolar disorder, and schizophrenia, warranting further experimental validation.

Conclusion

Magnolia officinalis bark methanol extract contains a diverse range of bioactive phytochemicals, including phenolics, flavonoids, terpenoids, and sterols, which support its pharmacological relevance. The extract demonstrated antioxidant activity, indicating potential to mitigate oxidative stress implicated in neuropsychiatric disorders such as anxiety, bipolar disorder, and schizophrenia. HPLC profiling confirmed substantial chemical diversity, while molecular docking identified multiple compounds with strong affinity toward key CNS targets involved in neurotransmission and mood regulation. Among these, honokiol, magnolol, and obovatol consistently showed the most favourable binding profiles and safety profiles. ADMET analysis further prioritized these compounds as the most promising CNS-active candidates, with additional potential observed for beta-sitosterol and maglifloenone. Overall, the integrated experimental and computational approach effectively identified lead neuroactive phytochemicals from *M. officinalis*, supporting its potential for further development in neuropsychiatric drug discovery.

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Conflict of interest
There is no actual or potential conflict of interest in this article.

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Table **3**. Binding site interaction analysis with hit compounds and protein targets

Phytochemical	6KUW binding site interactions	8DD2 binding site interactions	3RZE binding site interactions	7E2Y Binding site interactions	6A93 Binding site interactions	6CM4 Binding site interactions
Apigenidin	**CH-Bond**: SER152, VAL153; **Carbon-H-Bond**: LYS378; **Pi-sigma**: VAL153, ALA237; **Pi-alkyl:** ALA237, LYS378		**CH-Bond**: ASN 408; Pi-**Pi-T-shaped**: HIS220; **Amide-Pi-stacked**: ALA414, LYS415; **Pi-Alkyl:** ARG411, ALA414, LYS415, LYS412	**CH-Bond**: ARG242, GLY202; **Pi-sigma**: ALA41; **Pi-alkyl:** ALA205, ALA245, LEU249	**CH-Bond**: ALA108, LYS195, GLU318, SER188; **Pi-cation:** ASP 173; **Pi-anion:** ASP172; **Pi-alkyl:** ALA108, ALA176, ARG173	**CH-Bond**: ALA122; **Carbon-H-Bond**: LEU206; **Pi-sigma**: THR 205; **Pi-Alkyl:** LEU206**,** ALA379**,** ILE383, LEU125, ALA379
Beta-caryophyllene					**Alkyl:** ALA321, LEU325, LYS320, LEU105, LEU115, VAL324; **Pi-alkyl:** TYR387	
Bisabolene						**Alkyl:** ALA376, ALA379, LEU206, ILE 383, LEU 125; **Pi-alkyl:** PHE202, TYR209, PHE382
Caffeic acid			**CH-Bond:** THR60, ASN63; Amide **Pi-stacked:** ARG409, GLU410; **Pi-Alkyl:** ALA413	**CH-Bond**: GLY42; **Pi-sigma**: LEU249;		
Catechin			**CH-Bond**: ASN408, **Amide-Pi-stacked:** ALA414; **Alkyl:** LYS415; **Pi-Alkyl:** ALA414, LYS415, ARG411, LYS412	**CH-Bond**: SER246, SER206 **Carbon-HB:** ARG205 **Pi-sigma:** ALA41 **Alkyl:** LEU249 **Pi-alkyl:** ALA245, LEU249	**CH-Bond**: ALA108, GLU318, SER188; **Alkyl:** ALA108; **Pi-alkyl:** ARG173, ALA176	
Epicatechin			**Amide-Pi-stacked:** ALA414; **Alkyl:** LYS415; **Pi-alkyl:** ALA414, LYS415, ARG411, LYS412	**CH-Bond**: ARG242, SER246, SER206; **Pi-sigma:** ALA41 **Alkyl:** LEU249 **Pi-alkyl:** ALA245, LEU249		
Honokiol		**Pi-Pi-stacked**: TYR220; **Alkyl**: LEU268; **Pi-alkyl**: HIS267		**Alkyl:** ALA41, LEU39, ARG208, LEU249, ILE253 **Pi-alkyl:** TRY211, ALA41		
Isorhamnetin	**CH-Bond**: VAL153, ALA237; **Carbon-HB:** LYS378, SER 152; **Pi-sigma:** VAL153, ALA237; **Pi-alkyl:** ALA237, LYS378	**CH-Bond**: TYR143, TYR271; **Carbon-HB**: MET49,SER5 1;**Pi-anion**: GLU52;Alkyl: VAL50,LEU18 3,PRO184; **Pi-alkyl**:PHE186, PRO184	**CH-Bond**: TYR458,THR112; **Alkyl**: TYR108,TRP428, PHE432, PHE435	**CH-Bond**: ARG242, SER246; **Carbon-HB:** ARG205, SER246; **Pi-sigma:** ALA41, LEU246; **Pi-alkyl:** ALA245, LEU249, PHE223	**CH-Bond**: ALA108, glu108; **Pi-cation:** ARG173**,** LYS195; **Pi-anion:** ASP172; **Pi-alkyl:** ALA108, ALA176, ARG173	
Luteolin	**CH-Bond**: VAL153; **Carbon-HB:** LYS378; **Pi-sigma**: VAL153; **Pi-alkyl:** ALA237, LYS378	**CH-Bond**: PRO184; **Pi-Pi stacked:** TYR220	**CH-Bond**: ASN474, ARG139, ASN472; **Pi-Alkyl:** ARG409, LYS412, ALA413	**CH-Bond**: ARG242, GLN204, SER206; **Pi-sigma:** ALA41; **Pi-alkyl:** ARG205, ALA245, LEU249	**CH-Bond**: ALA108, SER188, GLU318; **Pi-cation:** ARG173 **Pi-anion:** ASP172 **Pi-alkyl:** ALA108, ALA176, ARG173	**CH-Bond**: TYR209, PHE202; **Carbon-HB:** GLY380; **PI-Pi-T-shaped:** TYR209; **Pi-Alkyl:** LEU206, ALA376
Maglifloenone	**CH-Bond**: THR241; **Pi-sigma:**			**CH-Bond**: ARG208; **Carbon-HB:** ASP200;	**CH-Bond**: ASN107, ARG173, ASN179; **Carbon-HB:** ARG173;	**CH-Bond**: ARG220,GLN373;

	ALA156; **Alkyl**: VAL 153; **Pi-Alkyl**: PHE 1124			**Pi-Lone-pair:** GLY202 **Alkyl:** LYS46	**Alkyl:** ALA108, ALA176, ARG173, ILE177; **Pi-Alkyl:** ALA376, TYR209, TYR213	**Carbon-HB:** ALA376; **PI-Pi-stacked:** TYR209; **Pi-Alkyl:** ALA376, TYR209, TYR213
Magnolol		**Pi-Pi-stacked**: TYR220; **Alkyl:** LEU268; **PI-Alkyl:** TYR220, PHE221				**Pi-sigma:**: TYR209; **Alkyl:** ILE212**,** LEU216, ALA379,ILE383; **Pi-Alkyl:** LEU206,ALA376,PHE202, TYR213
Myricetin	**CH-Bond**: VAL153, SER152, LYS378; **Pi-sigma:** VAL153, ALA237; **Pi-alkyl:** ALA 237, LYS378		**CH-Bond**: ARG125, ASN472; **Pi-sigma:** ALA413; **Pi-alkyl:** ARG409, LYS412	**CH-Bond**: ARG242, SER246; **Pi-sigma:** ALA41; **Pi-alkyl:** ALA245, LEU249	**CH-Bond**: ASN107, GLU318; **Pi-cation:** ARG173; **Pi-alkyl:** ALA108, ALA176	
Naringenin	**CH-Bond**: TYR234; **Carbon-HB:** LYS378; **Pi-sigma:** VAL153**; Pi-alkyl:** ALA237, LYS378		**Pi-cation**: LYS412; **Pi-sigma:** LYS412; **Pi alkyl:** ALA413, ARG409	**CH-Bond**: ARG208, ARG242, GLY202, SER206; **Pi-sigma:** ALA41; **Pi-alkyl:** ARG205, ALA245, LEU249	**CH-Bond**: ALA108; **Pi-cation:** ARG173; **Pi-anion:** ASP172 **Pi-alkyl:** ALA108, ARG173, ALA176	**CH-Bond:** ALA122; **Carbon-HB:** LEU206; **Pi-sigma:** THR205 **Pi-Alkyl**: LEU125, ALA379, ILE383
Obovatol		**CH-Bond:** GLU52; **Pi-Pi-stacked:** TYR220; **Alkyl:** LEU268; **Pi-Alkyl**: TYR220, PHE221		**CH-Bond**: GLY202, VAL201; **Alkyl**: ALA245, LEU249, LEU39, ARG208, ILE212, ILE253 **Pi-alkyl:** ARG41, ALA249, TRP211		**PI-PI-stacked:** TYR209; **Alkyl:** LEU125, ALA379, ILE383, ILE212, LEU216; **Pi-alkyl:** ALA376, LEU206, ALA379, TYR213
Quercetin	**CH-Bond:** VAL153 **Pi-sigma:** VAL153 **Pi-Alkyl**: ALA237,LYS378	**CH-Bond**: PRO184; **Pi-Pi-stacked:** TYR220	**CH-Bond**: ASN474, ARG125, ASN472; **Pi-alkyl:** ARG409, LYS412, ALA413	**Alkyl:** ARG205, LEU39, LEU249, VAL201, LEU234, ALA245, LEU249; **Pi-alky:** TRP211	**CH-Bond**: ALA108, SER188; GLU318 **Pi-cation:** LYS195; **Pi-alkyl:** ALA108, ALA176, ARG173	
Sitosterol	**Alkyl:** VAL153, ALA156, ALA237, LYS378 **Pi-Alkyl:** PHE1124, PHE1195			**Alkyl:** ARG205, LEU39, LEU249, VAL201, LEU234, ALA245; **Pi-alkyl:** TRP211	**Alkyl:** ALA321, VAL324; **Pi-Alkyl:** TYR380, TYR387	**Alkyl:** ILE212, LEU216, ILE383, ALA379, ALA376; **Pi-alkyl**: PHE202, TYR213

CH-Bond: Conventional hydrogen bond; Carbon-HB: Carbon hydrogen bonds

Table **6**. Toxicity prediction results for *M. officinalis* phytochemicals

Phytochemical	**Oral**	**Toxicity prediction**	**Organ**	**toxicity**	**prediction**			**Toxicity**	**end points**	**prediction**		**Molecular initiating events**
	LD50 (Mg/kg)	Predicted toxicity class	Hepato toxicity	Neuro toxicity	Nephro toxicity	Respiratory toxicity	Cardio toxicity	Carcino Genicity	Immuno toxicity	Muta genicity	Cyto toxicity	GABA receptor (GABAR)
4-Hydroxybenzoic acid	2200	5	Inactive	Inactive	Active	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
Gallic acid	2000	4	Inactive	Inactive	Active	Active	Inactive	Active	Inactive	Inactive	Inactive	Inactive
Caffeic acid	2980	5	Inactive	Active	Inactive	Inactive	Inactive	Active	Inactive	Inactive	Inactive	Inactive
Humulene	3650	5	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
Bisabolene	4390	5	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
Alpha pinene	3700	5	Inactive	Active	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
Germacrene D	5300	5	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Active	Inactive	Inactive	Inactive
Elemicin	1930	4	Inactive	Inactive	Inactive	Inactive	Inactive	Active	Inactive	Active	Inactive	Inactive
Beta-caryophyllene	5300	5	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Active	Inactive	Inactive	Inactive
Apigenidin	1070	4	Inactive	Inactive	Inactive	Active	Inactive	Inactive	Inactive	Inactive	Inactive	Active
Naringenin	2000	4	Inactive	Active	Active	Inactive	Inactive	Inactive	Inactive	Inactive	Active	Inactive
Honokiol	1649	4	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Active
Magnolol	2200	5	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Active
Obovatol	1930	4	Inactive	Inactive	Active	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
Catechin	10000	6	Inactive	Inactive	Active	Active	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
Epicatechin	10000	6	Inactive	Inactive	Active	Active	Inactive	Inactive	Inactive	Inactive	Inactive	Inactive
Luteolin	3919	5	Inactive	Inactive	Active	Active	Inactive	Active	Inactive	Active	Inactive	Inactive
Quercetin	159	3	Inactive	Inactive	Active	Active	Inactive	Active	Inactive	Active	Inactive	Inactive
Myricetin	159	3	Inactive	Inactive	Active	Active	Inactive	Active	Inactive	Active	Inactive	Inactive
Isorhamnetin	159	3	Inactive	Inactive	Active	Active	Inactive	Active	Inactive	Active	Inactive	Inactive
Maglifloenone	687	4	Inactive	Inactive	Inactive	Active	Inactive	Active	Active	Inactive	Inactive	Inactive
Sitosterol	890	4	Inactive	Active	Inactive	Active	Inactive	Inactive	Active	Inactive	Inactive	Inactive