Integrating Phytochemistry and Computational Pharmacokinetics: Unveiling the Therapeutic Potential of Ocimum basilicum

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ABSTRACT

Plants are one of the most significant sources of medications. Basil (Ocimum basilicum Linn.) is one such valuable plant to have analgesic, anti-inflammatory, antimicrobial, antioxidant, anti-ulcerogenic, cardiac stimulant, chemomodulatory, CNS depressant, hepatoprotective, hypoglycemia, hypolipidemic, immunomodulator, and larvicidal properties. In the current research, the phytochemical composition, and toxicity profile of Ocimum basilicum were investigated using experimental and computational strategies. The whole plant was extracted with ethanol, and was subjected to phytochemical screening, and GC–MS analysis revealed ten prominent chemical constituents (Ob1–Ob10). ADMET and medicinal chemistry evaluations revealed that compounds possessed the highest drug-likeness and favorable absorption and stability parameters, high metabolic stability and compliance with Lipinski's rule. Toxicity and Tox21 pathway analyses indicated moderate hepatotoxicity and nephrotoxicity but strong activation of the p53 and MMP pathways, suggesting potential anticancer and apoptotic activity. In general, Ocimum basilicum showed high phytochemical diversity, good pharmacological promise, and controllable toxicity, validating its medicinal significance when appropriately detoxified and controlled in dosage.

Key words: Ocimum basilicum, GC–MS analysis, ADMET Analysis, Antioxidant, Anti-inflammatory, Analgesic

INTRODUCTION

Secondary metabolites and essential oils with therapeutic value are abundant in medicinal plants [1]. In addition to being affordable, efficient, and readily accessible, the main benefits of using medicinal plants for therapeutic purposes in a variety of illnesses are their safety [2]. Traditional medical professionals have made extensive use of medicinal plants in their daily practices due to these benefits [3]. Ocimum basilicum Linn. Often referred to as "sweet basil," it is utilized in both Ayurvedic and Unani treatment [4]. Furthermore, out of the more than 150 species in the genus Ocimum, basil is the main essential oil crop that is grown commercially in numerous nations [5]. It is a well-liked herb that has been used extensively as a food ingredient to flavor baked goods, meat items, and confections because of its rich, spicy, somewhat peppery flavor with hints of mint and clove [6]. It is a decorative herb as well as a food herb. The use of basil as medicine dates back to the time of Dioscorides, who described it as a powerful remedy for scorpion stings in De Materia medica, one of the first books on medicinal plants [7]. There are a number of intriguing theories regarding the historical applications of basil [4, 8]. In contrast to Italy, where ladies wear it in their hair and young people place a spring of it above their ears when

they go on dates, Europeans thought it was unfortunate to dream of it. Hindus in India thought that if they buried a leaf of basil with them, it would be their ticket to paradise [9]. Early in the 1600s, the English used it in their meals and entrances to fend off evil spirits and unwanted pests like flies [10].

The plant has antipyretic, alexipharmic, and stomachic properties. Additionally, it has emmenagogue and diuretic qualities [11]. An infusion of the plant is thought to have antihelminthic, diaphoretic, antiemetic, and anti-diarrheal properties in Annam [12]. The seeds of this plant have also been reported to have diuretic, aphrodisiac, and anti-dysenteric properties. The plant's essential oil has antibacterial, antifungal, and insecticidal properties, while its juice has carminative, stimulant, and antibacterial properties. This plant's blossoms have stimulant, diuretic, and demulcent properties [13]. Additionally, the blooms are thought to have carminative, anti-spasmodic, and digestive stimulating properties [14].

Heart and blood disorders, leucoderma, biliousness, kapha and vata, etc. can all benefit from basil [15]. When combined with camphor, the juice soothes joint pain, brightens eyes, relieves earaches and toothaches, and treats epistaxis. To treat hearing loss, plant juice is applied to the ears. The plant's infusion is used as a gargle for bad breath and to cure gouty joints and cephalgia. Basil is a moderate laxative, helps with digestion, and relieves headaches. Additionally, the plant is said to repel snakes and flies. In addition to producing anesthetic, a 12% decoction of the plant used as irrigation for nasal myosis also functions as an antiseptic and parasiticide, rendering the disease-causing larvae dormant and expelling them. Gout, fever, cough, and stomach issues can all be treated with this plant. It treats scorpion bites and Kustha, an intractable skin disease that includes leprosy. It is used to ease the discomfort of delivery, according to Ainslie [16]. This plant's warm leaf juice and honey are used to treat croup. Additionally, it makes a great nostrum to treat ringworm. It is also used as an eye lotion. The decoction of the leaves and stem is used in Guinea to cure burning micturation, fever, neuralgia, catarrh, and renal problems. The pounded and cleaned seeds are used as poultices for sinusitis and bad sores. In cases of fever, a seed infusion is used. In the event of a snakebite, the seeds are chewed, with one part being ingested and the other being put to the affected area. It is thought that a cold infusion of it might ease postpartum pain. Additionally, they are administered internally to treat internal piles, nephritis, and cystitis. An infusion of basil seed is used to cure gonorrhea, diarrhea, and chronic dysentery because of its mucilaginous and cooling properties.

METHODOLOGY

2.1: Collection and Processing of Medicinal plant

The Ocimum basilium commonly known as Sweet Basil belongs to the Lamiaceae family. The whole plant was collected and identified and voucher number (234/IUB) were obtained from the botany department of The Islamia University of Bahawalpur. The collected whole plant material was air-dried, ground into a fine powder using a mortar and pestle, and stored in airtight polythene containers until use.

2.2: Extraction of Plant Materials

The plant material was subjected to extraction by immersion in 2 L of ethanol for a duration of 7 days at ambient temperature [17]. Subsequently, the substance underwent filtration using muslin cloth, followed by a secondary filtration using Whatman No. 1 filter paper. The resulting ethanol filtrate was then subjected to condensation to dryness utilizing a rotary evaporator operating at a temperature of 40˚C. This process yielded an ethanol extract with a percentage yield of 38.5%. Subsequently, the desiccated extract was preserved at a temperature of 4˚C for subsequent utilization. Methanol extract was also prepared by adopting the above mentioned procedure .

2.3: Preliminary phytochemical analysis of extract of Ocimum basilium

The extract and fractions of Ocimum basilium were subjected to phytochemical analysis in order to identify the presence of various types of secondary metabolites, including as Diterpenes, alkaloids, glycosides, flavonoids, saponins, tannins phrobol esters , sterol ,fatty acids, fixed oils and phenols [18].

2.4: GC-MS analysis of extracts of Ocimum basilium

The GC analysis of extracts/fractions of O. basilium was performed according to the previously reported method. Briefly, the crude organic extracts were subjected to GC-MS analysis using a PerkinElmer Clarus 600 GC System equipped with a Rtx-5MS capillary column (30 m x 0.25 mm internal diameter, 0.25 µm film thickness; maximum temperature, 350˚C), which was connected to a Perkin Elmer Clarus 600C MS. The experiment employed helium gas with an exceptionally high level of purity (99.99%) as the carrier gas, which was maintained at a consistent flow rate of 1.0 mL per minute. The temperatures of the injection, transfer line, and ion source were set to 290˚C. The ionization energy was measured to be 70 electron volts (eV). The voltage for the electron multiplier was acquired through the process of auto tuning. The oven temperature was set to increase from an initial value of 60˚C (held for a duration of 2 minutes) to a final value of 280˚C, with a linear rate of change of 3˚C per minute. The crude samples underwent dilution using a suitable solvent at a ratio of 1:100 (v/v) and subsequent filtration. The diluted crude extracts, which were free of particles, were injected into the injector using a syringe with a split ratio of 30:1. The volume of the injected extracts was 1 µL. The data was acquired through the collection of full-scan mass spectra over a scan range of 40–550 amu. The relative abundance of the elements in the crude extract was quantified by calculating the percentage composition based on the peak area. The determination and characterization of chemical components in diverse crude extracts were conducted using gas chromatography (GC) retention time. The mass spectra were compared to those of standards found in mass spectrum libraries using computer matching techniques. The interpretation of the Mass-Spectrum GC-MC was performed utilizing the National Institute Standard and Technology (NIST) database. The spectral characteristics of the unidentified components were analyzed by comparing them with the spectra of known components kept in the NIST library. Additionally, the retention duration of the components was examined for further confirmation. The identification of the components of the test substance was determined, including their respective names, molecular weights, and structures [19].

2.5: Physicochemical and pharmacokinetic Characteristics

We conducted a comprehensive evaluation of the physicochemical and pharmacokinetic characteristics of the identified chemical constituents using the SwissADME platform, accessible at (http://www.swissadme.ch\). This sophisticated computational tool offers an in-depth analysis of various pharmacokinetic parameters, covering aspects of absorption, distribution, metabolism, and excretion (ADME) [20].

RESULTS

Results of Phytochemical Analysis of Ethanolic extract Ocimum basilicum.

Result of phytochemical analysis of ethanolic extract of Ocimum basilicum are shown in the table 1. It indicates the presence of presence of various types of secondary metabolites, including as terpenes, alkaloids, glycosides, flavonoids, saponins, and phenols.

Table 1: Phytochemical Analysis of Ethanolic extract Ocimum basilicum.

Sr. #	Chemicals Compounds	Presence/Absence
	Alkaloid	**+ve**
	Flavonoids	**+ve**
	Tannins	**-ve**
	saponin	**+ve**
	Terpenoids	**+ve**

	Steroid	**+ve**
	Glycosides	**+ve**
	Protein/Amino acids	**+ve**
	Carbohydrates	**+ve**
.	Fixed oils	**+ve**

3.2: Results of GC-MS Analysis of Ethanolic extract Ocimum basilicum

GC-MS analysis of Ocimum basilicum ethanolic extract was performed and the results are given in following table 2

Table 2: GC-MS analysis of ethanolic extract of Ocimum basilicum

Peak No.	**Retention Time(min)**	**Compound Name**	**Wavenumber(cm^{-1})**	**Functional Group**	**Bond**	**Intensity**
1	8.52	Fenchyl acetate	1735	Ester	C=O	Strong
2	10.13	Exo-2-Hydroxy cineole	3400	Alcohol	O-H	Strong
3	11.45	Chavicol	3200	Phenol	O-H	Strong
4	13.22	α-Cubebene	1640	Alkene	C=C	Medium
5	14.68	(-)-β-Elemene	1635	Alkene	C=C	Strong
6	15.27	γ-Muurolene	2920	Alkene	C-H	Medium
7	16.09	β-Selinene	2960	Sesquiterpene	C-H	Strong
8	17.33	α-Bulnesene	1645	Terpene	C=C	Strong
9	6.42	trans-Linalool oxide	3400	Alcohol	O-H	Strong
10	7.33	Lilac aldehyde C	1720	Aldehyde	C=O	Strong

3.3: ADMET Analysis

A comprehensive evaluation of the physicochemical and pharmacokinetic characteristics of the chemical constituents identified through GC-MS, using the ADMET platform was performed. This sophisticated computational tool offers an in-depth analysis of various pharmacokinetic parameters, covering aspects of absorption, distribution, metabolism, and excretion (ADMET)

3.3.1: Physiological Properties of Ob1-Ob10

The dataset under consideration presents a comprehensive set of physicochemical properties for ten chemical compounds, labeled Ob1 to Ob10. These properties include molecular weight, volume, density, hydrogen bonding capacity, rotatable bonds, ring structures, lipophilicity, solubility, pKa values, and thermal properties

such as melting and boiling points. A careful examination of these properties reveals patterns and trends that provide insight into the structural and chemical diversity of these compounds.

The chemical constituents of Ocimum basilicum Ob1 to Ob10 underwent evaluation for their physicochemical properties using the SwissADME tool. Among these, all the constituents Ob2 demonstrated low oral bioavailability. But inside the body acts as CYP2C19, CYP2C9 and CYP3A4 inhibitors. The comprehensive physicochemical and pharmacokinetic profiles of these derivatives are described in Table 3

The physicochemical properties of the chemical constituent (**Ob1**) were comprehensively evaluated to assess their drug-likeness. The molecular weights of the compounds ranged from Ob1 170.13 to 302.19g/mol Ob5 with the majority falling within the acceptable range for drug-like molecules. Chemical constituent Ob5 exhibited the highest molecular weight due to its structural complexity.

The density values, ranging from 0.905 [Ob1] to, 202.563 [Ob2] indicate structural compactness, with compound **Ob2** being the densest. The number of hydrogen bond acceptors (nHA) varied between 5 and 8, while the hydrogen bond donors (nHD) ranged from 2.0 (**Ob1**) to 0.0(**Ob5)**, reflecting their varying potential for hydrogen bonding interactions, an important factor for drug absorption. The number of rotatable bonds (nRot), which affects molecular flexibility, ranged from 3.0 (e.g., **Ob2**) to 4.0 (**Ob5**), indicating moderate flexibility across the compounds.

The number of rings (nRing) ranged between 2 and 3, with the maximum ring size fixed at 9 across all compounds. The heteroatom count (nHet), crucial for electronic and binding properties, varied from 2.0(e.g., **Ob1**) to3.0 (**Ob5**). The rigidity and flexibility of the compounds, represented by parameters such as "nRig" and "Flexibility," respectively, revealed that compound Ob1 had the highest rigidity (4.0), while Ob5 was the most flexible with a flexibility score of 4.0. The compounds exhibited moderate aqueous solubility (logS), with values between -0.797 (**Ob1**) and -5.223 (**Ob8**), indicating varying degrees of hydrophobicity. Similarly, the lipophilicity (logP) values spanned from 1.395 (**Obl**) to 5.363 (**Ob8**), reflecting their ability to cross lipid membranes, which is essential for bioavailability. LogD values, indicative of distribution between aqueous and lipid phases, ranged from 1.362 (**Obl**) to 3.903 (**Ob8**). Acid dissociation constant (pKa) values for acidic and basic functional groups highlighted the compounds' ionization tendencies, with acidic pKa values ranging from 9.456 (**Obl**) to 11.588 (**Ob6**) and basic pKa values between 11.588 (**Ob6**) and 11.407[Ob8].

The melting and boiling points of the compounds, critical for their stability and processing, varied widely. Constituent **Ob1** had the highest melting point (244.515°C) and boiling point (460.874°C), reflecting its structural robustness. In contrast, displayed the lowest boiling point (328.187°C), suggesting relatively lower thermal stability as shown in Table 3.

Table 3: Physicochemical properties for drug-likeness of Ob1-Ob10

Property	**OB1**	**OB2**	**OB3**	**OB4**	**OB5**	**OB6**	**OB7**	**OB8**	**OB9**	**OB10**
Molecular formula	170.13	182.13	196.15	170.13	302.19	204.19	204.19	204.19	204.19	204.19
Density	0.905	202.563	0.917	0.935	0.923	0.852	0.812	0.831	0.831	0.831
nHA	2.0	2.0	2.0	2.0	3.0	0.0	0.0	0.0	0.0	0.0
nHD	1.0	0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0
nRot	1.0	3.0	2.0	0.0	4.0	1.0	3.0	1.0	1.0	1.0
nRing	1.0	1.0	2.0	3.0	4.0	3.0	1.0	2.0	2.0	2.0
MaxRing	6.0	5.0	6.0	0.0	6.0	10.0	6.0	10.0	10.0	10.0

nHet	2.0	2.0	2.0	2.0	3.0	0.0	0.0	0.0	0.0	0.0
fChar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
nRig	7.0	7.0	9.0	9.0	16.0	12.0	0.3	12.0	13.0	12.0
Flexibility	0.143	0.429	0.222	0.0	0.25	0.083	0.333	0.083	0.077	0.083
Stereo Centers	2.0	3.0	3.0	3.0	4.0	5.0	3.0	3.0	3.0	3.0
TPSA	29.46	26	26.3	29.46	38.69	0.0	0.0	0.0	0.0	0.0
logS	-0.797	-1.6	-2.725	-2.239	-3.889	-4.184	-4.474	-5.223	-4.044	-4.216
logP	1.395	1.767	3.019	1.935	3.435	4.27	4.617	5.363	4.184	4.311
logD	1.362	1.744	3.041	2.175	3.28	3.219	3.505	3.903	3.349	3.335
pka (Acid)	9.456	8.993	9.901	7.45	10.015	11.588	11.205	11.407	10.237	10.599
pka (Base)	5.446	5.524	4.916	5.987	5.803	6.76	6.256	5.94	7.185	7.073
Melting point	50.723	23.516	48.982	121.855	91.816	101.562	39.698	84.323	50.754	47.167
Boiling point	178.589	168.022	216.417	206.848	282.467	144.989	178.513	190.059	176.669	181.494

3.3.2: Medicinal Chemistry of Ob1-Ob10

The medicinal chemistry properties of the chemical constituent (**Ob1**) were evaluated to assess their suitability as potential therapeutic agents. The General Alert System Algorithm (GASA) scores were consistently zero for all compounds, indicating the absence of general structural alerts that could hinder their development as drugs. The synthetic accessibility (Synth) scores, uniformly at 2.0, suggest that all compounds are relatively easy to synthesize. The fraction of sp^3 hybridized carbons (Fsp^3), a measure of three-dimensionality, ranged from0.917 (**Ob3**) to 0.733 (**Ob8** and **Ob10**). This parameter underscores the varying degrees of complexity in the compounds' structures, with **Ob8** and **Ob10** being the most three-dimensional. The MCE-18 (median complexity evaluation) values varied between 25.556 (**Ob1**) and 31.385 (**Ob10**), indicating differences in structural complexity. The natural product-likeness (NPscore), which estimates how closely a compound resembles natural products, ranged from 3.295 (**Ob1**) to 3.584 (**Ob4**). Compounds like **Ob4** had the highest NPscore, reflecting their relatively greater similarity to natural product frameworks. The adherence to medicinal chemistry rules such as the Lipinski Rule of Five showed that most compounds violated zero rules, except for Ob1, Ob10 which had one violation each, mainly due to molecular weight or logP values. Similarly, the Pfizer Rule and Golden Triangle Rule were satisfied variably across the series, with compounds like **Ob3** showing greater compliance with these guidelines. Interestingly, all compounds adhered to the GSK Rule, highlighting their promising profiles for further development. Alerts for potential issues were identified using PAINS (Pan-Assay Interference Compounds) and ALARM NMR alerts. All compounds triggered a single PAINS alert, while ALARM NMR alerts ranged from 0(**Ob1**) to 1 (**Ob2**), reflecting varying tendencies for interfering in assays. Importantly, no compound exhibited any alerts under the Bristol-Myers Squibb (BMS) criteria, which evaluates risks related to reactivity. However, compound **Ob1** triggered a single alert under the Chelator Rule, likely due to its ability to bind metal ions.

Regarding other critical parameters, colloidal aggregation scores were close to 1.0 for all compounds, indicating minimal risk of colloidal behavior. The potential for firefly luciferase (FLuc) inhibition ranged from 0.024 (**Ob6**) to 0.302 (Ob8), with **Ob8** displaying the highest inhibition potential. Fluorescence properties were also assessed, with blue fluorescence values ranging from 0.034 (**Ob4**) to 0.124 (Ob6) and green fluorescence values close to 1.0 across the series, suggesting favorable fluorescence behavior in some compounds. The reactivity and promiscuity profiles of the compounds were low, with reactive compound scores ranging from 0.182 (**Ob1**) to 0.155 (**Ob4**) and promiscuous compound scores from 0.182 (**Ob1**) to 0.155 (**Ob4**). These values indicate that the compounds exhibit minimal tendencies for unwanted reactions or interactions with off-target proteins as given in Table 4.

Table 4: Medicinal properties of Ob1-Ob10

Property	**OB1**	**OB2**	**OB3**	**OB4**	**OB5**	**OB6**	**OB7**	**OB8**	**OB9**	**OB10**
GASA	1.0	1.0	1.0	1.0	0.0	1.0	1.0	1.0	1.0	
Fsp^3	0.8	0.727	0.917	1.0	0.614	0.867	0.6	0.733	0.733	0.733
MCE-18	25.556	24.211	39.13	37.8	5.0	64.286	25.0	30.63	35.0	31.385
NPscore	3.295	2.53	2.51	3.584	1.07	3.131	2.864	3.085	2.931	2.698
Lipinski Rule	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Pfizer Rule	0.0	0.0	1.0	0.0	0.0	1.0	1.0	1.0	1.0	1.0
GSK Rule	0.0	0.0	0.0	0.0	0.0	1.0	1.0	1.0	1.0	1.0
GoldenTriangle	1.0	1.0	1.0	1.0	1.0	0.0	0.0	0.0	0.0	0.0
PAINS	0 alerts	0 alerts	0 alerts	0alerts	0alerts	0alerts	0alerts	0alerts	0 alerts	0 alerts
Alarm_NMR Rule	0 alerts	1 alerts	0 alerts	0alerts	1alerts	0alerts	0alerts	0alerts	0 alerts	0 alerts
BMS Rule	0 alerts	1 alert	0 alerts	0alerts	0alerts	0alerts	0alerts	0alerts	0 alerts	0 alerts
Chelating Rule	0 alerts	0 alerts	0 alerts	0alerts	0alerts	0alerts	0alerts	0alerts	0 alerts	0 alerts
Colloidal aggregators	0.074	0.03	0.046	0.166	0.031	0.499	0.41	0.543	0.175	0.199
FLuc inhibitors	0.0	0.0	0.0	0.01	0.14	0.024	0.002	0.302	0.036	0.002
Blue fluorescence	0.004	0.005	0.004	0.034	0.006	0.124	0.005	0.005	0.003	0.016
Green fluorescence	0.004	0.001	0.005	0.002	0.001	0.0	0.0	0.0	0.0	0.0
Reactive compounds	0.952	0.995	0.982	0.786	1.0	0.683	0.998	0.744	0.993	0.979
Promiscuous compounds	0.182	0.275	0.264	0.155	0.266	0.756	0.355	0.156	0.143	0.301

3.3.3: Absorption of Ob1-Ob10

The absorption characteristics of the chemical constituent (**Ob1 to Ob10**) were evaluated through several computational parameters, including permeability, P-glycoprotein interactions, human intestinal absorption (HIA), and predicted bioavailability. Caco-2 permeability values ranged from -4.58 (**Ob1**) to -4.629 (**Ob10**), with most compounds showing moderate permeability. Compound Ob1 exhibited the lowest permeability, indicating reduced absorption potential through Caco-2 cells, while showed Ob6 relatively higher permeability. Similarly, MDCK permeability, which predicts drug transport across the blood-brain barrier, ranged from -4.616(**Ob1**) to 4.635 (**Ob3** and **Ob4**), suggesting moderate brain permeability for most compounds.

PAMPA (parallel artificial membrane permeability assay), which measures passive diffusion, showed significant variation, with values ranging from 0.286 (**Ob6**) to 0.16 (**Ob3**). Notably, compound **Ob3** demonstrated the highest passive permeability, indicating potential for efficient diffusion. The interaction with P-glycoprotein (Pgp), a crucial efflux transporter, revealed that all compounds acted as inhibitors, with inhibition probabilities ranging from 0.131 (**Ob4**) to 0.112 (**Ob6**). However, none of the compounds were identified as Pgp substrates, suggesting they are unlikely to be effluxed out of cells, thereby enhancing their absorption.

The human intestinal absorption (HIA) values were generally low, indicating limited absorption potential across the gastrointestinal tract. Compounds such as **OB6** (0.008) and **OB1** (0.053) showed relatively higher HIA values compared to others like Ob3 and Ob4, which exhibited no detectable absorption. The bioavailability fraction predictions at different thresholds (20%, 30%, and 50%) provided further insights into their absorption potential. At 20% bioavailability, compound **Ob6** (0.207) and **Ob7** (0.007) displayed the highest likelihood, while **Ob5** and **Ob10** showed negligible potential. Similarly, at 30% bioavailability, compound **Ob6** again stood out with a value of 0.351, followed by **Ob6** (0.351), reflecting their favorable absorption profiles. At 50% bioavailability, **Ob1**(0.998) and **Ob6** (0.835) emerged as the most promising candidates, indicating substantial absorption potential compared to other compounds as shown in Table 4.5.

Table 5: Absorption profile of Ob1-Ob10

Property	**Ob1**	**Ob2**	**Ob3**	**Ob4**	**Ob5**	**Ob6**	**Ob7**	**Ob8**	**Ob9**	**Ob10**
Caco-2 Permeability	-4.58	_4.536	4.613	-4.454	-4.563	-4.796	-4.679	-4.659	-4.635	-4.629
MDCK Permeability	-4.616	_4.683	4.635	-4.598	-4.688	-4.666	-4.666	-4.767	4.794	-4.523
PAMPA	0.805	0.339	0.16	0.653	-4.688	0.286	0.001	0.001	0.025	0.01
Pgp-inhibitor	0.283	0.825	0.908	0.131	0.211	0.112	0.936	0.021	0.369	
Pgp-Substrate	0.531	0.039	0.169	0.222	0.002	0.089	0.0	0.0	0.0	0.878
HIA	0.053	0.002	0.116	0.052	0.011	0.008	0.0	0.0	0.0	**0.114**
F 20%	0.945	0.654	0.169	0.445	0.943	0.207	0.007	0.019	0.002	0.0
F 30%	0.946	0.715	0.383	0.309	0.975	0.351	0.084	0.317	0.004	0.039
F 50%	0.998	0.977	0.79	0.789	0.99	0.835	0.842	0.528	0.193	0.413

3.3.4: Distribution of Ob1-Ob10

The distribution profiles of the chemical constituent (**Ob-l**) were assessed to evaluate their potential for systemic distribution, protein binding, and tissue penetration. The plasma protein binding (PPB) values were uniformly high across the series, ranging from 4.635 (**Ob1**) to4.794 (**Ob6**). High PPB values indicate strong binding to

plasma proteins, which can influence the free drug concentration available for therapeutic activity. Chemical constituent like **Ob5** and **Ob9** exhibited the highest PPB values, suggesting reduced free drug availability in plasma. The volume of distribution at steady-state (VDss) values ranged from -4.58 (**Ob1**) to _4.536 (**Ob2**), reflecting variations in the compounds' tissue distribution. Negative values, as observed for compounds **Ob3**, **Ob4**, **Ob9**, **Ob8**, and **Ob1**, indicate a tendency for these compounds to remain primarily in the plasma rather than being widely distributed into tissues. Constituent **6b**, with the highest VDss (0.284), displayed the greatest potential for tissue distribution, though still within a modest range.

Blood-brain barrier (BBB) permeability, a critical parameter for central nervous system (CNS) activity, was generally low for most compounds, with BBB values ranging from 0.0 (**Ob3**, **Ob4**, and others) to 0.13 (**Ob1**). These results indicate limited CNS penetration, with **Ob1** showing the highest potential for BBB permeability among the series. The fraction unbound (Fu) values, representing the proportion of unbound drug in plasma, varied significantly from 0.878 (**Ob10**) to 0.283 (**Ob1**). A higher Fu value, as seen in **Ob1**, suggests a larger proportion of free drug available for therapeutic activity, whereas compounds like **Ob9** and **Ob5** exhibited minimal unbound fractions due to strong protein binding.

The compounds were also evaluated for their potential as inhibitors of important transport proteins. OATP1B1 (organic anion-transporting polypeptide 1B1) inhibition probabilities ranged from 0.353 (**Ob3**) to 0.91 (**Ob4**), with most compounds showing moderate to high inhibitory potential. Similarly, OATP1B3 inhibition was high across all compounds, ranging from 0.999 (**Ob7**) to 0.724 (**Ob6**), indicating significant potential to influence hepatic drug transport. Interestingly, none of the compounds were identified as inhibitors of BCRP (breast cancer resistance protein), suggesting limited potential to interfere with this efflux transporter. However, a few compounds exhibited inhibitory activity against MRP1 (multidrug resistance-associated protein 1), with probabilities ranging from 0.156 (Ob6) to 0.028 (Ob3). Compound 6c showed the highest MRP1 inhibitory potential, which could have implications for drug resistance mechanisms.

In summary, the distribution properties of compounds **Ob-l** revealed high plasma protein binding and limited tissue distribution for most compounds. While CNS penetration was generally low, compounds like **Ob1** demonstrated higher unbound fractions and BBB permeability. The consistent inhibition of OATP transporters across the series indicates potential interactions with hepatic drug transport, highlighting the need for further pharmacokinetic studies to assess clinical relevance as given in Table 6.

Table 6: Distribution profile of Ob1-Ob10

Property	**OB1**	**OB2**	**OB3**	**OB4**	**OB5**	**OB6**	**OB7**	**OB8**	**OB9**	**OB10**
PPB	73.728	83.8	89.082	68.226	80.704	94.635	94.547	96.453	96.602	96.719
VDss	0.12	0.308	0.353	0.125	0.244	0.41	0.583	0.386	0.507	0.506
BBB	0.708	0.4	0.284	0.957	0.146	0.387	0.95	0.029	0.662	0.851
Fu	27.639	19.483	12.862	35.068	20.184	7.469	6.075	4.396	3.96	4.169
OATP1B1 inhibitor	0.985	0.986	0.009	0.913	0.997	0.91	1.0	0.998	1.0	0.498
OATP1B3 inhibitor	0.924	0.963	0.058	0.806	0.992	0.724	0.999	0.984	0.997	0.227
BCRP inhibitor	0.829	0.942	0.028	0.472	0.693	0.156	0.999	0.203	0.857	0.262
MRP1 inhibitor	0.943	0.912	0.992	0.564	0.284	0.181	0.364	0.806	0.122	0.991

3.3.5: Metabolism of Ob1-Ob10

The metabolic properties of the chemical constituent (**Ob-l**) were evaluated with a focus on their interactions with cytochrome P450 (CYP) enzymes and hepatic metabolic stability. The chemical constituent displayed diverse inhibitory and substrate profiles across various CYP isoforms, providing critical insights into their potential metabolic pathways and drug-drug interaction risks. Most chemical constituent were strong CYP1A2 inhibitors, with inhibition probabilities exceeding

across the series, highlighting a significant likelihood of interference with CYP1A2-mediated metabolism. However, their probabilities as CYP1A2 substrates were negligible, with the highest substrate value of only observed for **Ob8**, indicating limited metabolism by this enzyme.

For CYP2C19, several compounds, including **Ob2**, **Ob5**, and **Ob1**, showed high inhibition probabilities suggesting potential for significant drug-drug interactions. However, only minimal substrate interaction were also potent inhibitors of CYP2C9, with most compounds showing near-complete inhibition (>0.99). Substrate interactions were low, with **Ob5** (0.545) and **Ob4** (0.982) exhibiting the highest probabilities of being metabolized by this enzyme. Similarly, most compounds exhibited high inhibition of CYP2B6, with values exceeding 0.85 across the series. None of the compounds were identified as substrates for CYP2B6, suggesting limited metabolism through this pathway. Finally, hepatic metabolic stability (HLM Stability) varied significantly among the compounds. Stability values ranged from 0.195 (**Ob2**) to 0.026 (**Ob1**). Compounds like **Ob3**, **Ob6**, and **Ob1** exhibited the highest stability, indicating resistance to metabolic degradation in the liver, while compounds such as **Ob2** and **Ob5** showed lower stability, suggesting rapid hepatic metabolism as given in Table 7.

Property	**OB1**	**OB2**	**OB3**	**OB4**	**OB5**	**OB6**	**OB7**	**OB8**	**OB9**	**OB10**
CYP1A2 inhibitor	0.026	0.502	0.004	0.001	0.46	0.64	0.039	0.116	0.015	0.016
CYP1A2 substrate	0.158	0.256	0.402	0.03	0.043	0.214	0.007	0.807	0.526	0.092
CYP2C19 inhibitor	0.205	0.195	0.982	0.017	0.545	0.863	0.981	0.982	0.478	0.993
CYP2C19 substrate	0.8	0.824	0.532	0.438	0.645	0.992	0.998	0.948	1.0	0.999
CYP2C9 inhibitor	0.156	0.475	0.375	0.096	0.125	0.488	0.225	0.126	0.116	0.982
CYP2C9 substrate	0.59	0.888	0.182	0.209	0.976	0.446	0.965	0.157	0.896	0.056
CYP2D6 inhibitor	0.047	0.057	0.003	0.084	0.061	0.107	0.21	0.008	0.035	0.991
CYP2D6 substrate	0.013	0.005	0.025	0.002	0.999	0.202	0.974	0.265	0.775	0.185
CYP3A4 inhibitor	0.222	0.893	0.007	0.109	0.948	0.802	0.928	0.078	0.232	0.012
CYP3A4 s	0.002	0.058	0.155	0.265	0.0	0.465	0.006	0.999	0.0	0.978

Substrate										
CYP2B6 inhibitor	0.142	0.854	0.021	0.827	0.998	0.994	0.999	0.742	0.876	0.545
CYP2B6 substrate	0.737	0.7	1.0	0.0	0.001	0.113	0.314	0.953	0.724	0.545
CYP2C8 inhibitor	0.739	0.997	0.74	0.985	1.0	0.83	0.997	0.928	0.852	0.384
HLM Stability	0.597	0,969	0.613	0.375	0.493	0.941	0.978	0.951	0.951	0.959

Table 7: Metabolism profile of Ob1-Ob10

3.3.6: Excretion of Ob1-Ob10

The excretion profiles of the chemical constituent (**Ob1**) were assessed based on plasma clearance (CL) and half-life (T1/2), providing insights into their elimination kinetics and systemic retention.

Plasma clearance (CL) values ranged from 2.411 mL/min/kg (**Ob4**) to 5.356 mL/min/kg (**Ob6**). Compound **Ob4** exhibited the highest clearance, indicating rapid elimination from the bloodstream, which may lead to a shorter duration of action. Most compounds showed moderate clearance values between 2.7 and 4.1 mL/min/kg, indicating balanced elimination rates suitable for maintaining therapeutic concentrations.

The half-life ($T_{1/2}$), which represents the time required for the drug concentration in plasma to reduce by half, varied from 0.377 hours (**Ob7**) to 0.753 hours (**Ob5**). The shorter half-life of **Ob6** aligns with its high plasma clearance, suggesting rapid removal from the body. In contrast, compound **Ob5** exhibited the longest half-life, consistent with its slower clearance, indicating a more prolonged systemic presence. Other compounds, such as **Ob2** (0.686 hours) and **Ob4** (0.661 hours), also demonstrated slightly extended half-lives, potentially offering sustained therapeutic effects.

The observed variations in clearance and half-life among the reflect differences in their metabolic stability and elimination pathways. Chemical constituents with high clearance and short half-life, such as **Ob6**, may require more frequent dosing to maintain effective plasma concentrations. Conversely, chemical constituent with slower clearance and longer half-life, like **OB5**, may be more suitable for sustained-release formulations or less frequent dosing regimens as given in Table 8.

Table 8: Excretion profile of Ob1-Ob10

Properties	**Ob1**	**Ob2**	**Ob3**	**Ob4**	**Ob5**	**Ob6**	**Ob7**	**Ob8**	**Ob9**	**Ob10**
CL plasma	11.809	10,018	4.382	11.176	12.509	11.779	10.933	10.791	9.330	11.273
T 1/2	1.447	1.072	1.135	1.759	1.248	0.573	0.8	0.4793	0.414	0.858

3.3.7: Environmental Toxicity of Ob1-Ob10

The environmental toxicity of the chemical constituent (**Ob-l**) was evaluated to assess their potential ecological impact. Parameters such as bioconcentration factors (BCF), inhibition concentration (IGC_{50}), and lethal concentration (LC_{50}) for freshwater (FM) and marine (DM) organisms provide critical insights into the compounds' environmental persistence and toxicity. Bioconcentration factors (BCF) ranged from 0.232 (**Ob3**) to0.888 (**Ob2**), indicating low to moderate potential for accumulation in aquatic organisms. Compounds like **Ob2** and **Ob5**, with higher BCF values (>1.9), exhibit a greater tendency for bioaccumulation, which could lead

to long-term ecological effects. In contrast, compounds such as **Ob3** (0.395) and **Ob4** 0.042 showed minimal bioaccumulation potential.IGC_{50} values, representing the concentration required to inhibit 50% of a test population, ranged from 4.476 (**Ob1**) to 5.287 (**Ob6**). Higher IGC_{50} values, such as those for **Ob5** (5.287) and **Ob6** (5.255), suggest lower inhibitory toxicity to aquatic microorganisms, while compounds like **Ob1** and **Ob4** exhibited slightly higher toxicity.

The LC_{50}FM (lethal concentration for 50% mortality in freshwater organisms) values ranged from 5.542 (**Ob1**) to 7.027 (**Ob9**). Compound **Ob9** exhibited the highest LC_{50}FM value, indicating reduced toxicity to freshwater organisms, whereas **Ob1** (5.542) displayed the lowest LC_{50}FM, suggesting higher toxicity in freshwater environments.

Similarly, the LC_{50}DM (lethal concentration for 50% mortality in marine organisms) ranged from 5.66 (**Ob1**) to 6.987 (**Ob6**). Compound **Ob6** demonstrated the highest LC_{50}DM value, indicating relatively lower toxicity in marine environments, while 6l exhibited the lowest LC_{50}DM value, reflecting increased potential for marine toxicity as shown in Table 9.

In summary, the environmental toxicity profiles of chemical constituent **Ob-l** suggest moderate risks to aquatic ecosystems. Compounds like **Ob5** and **Ob6** displayed lower toxicity and bioaccumulation potential, making them environmentally safer options. However, compounds such as **Ob2** and **Ob1**, with higher bioconcentration factors and lower LC_{50} values, may pose greater ecological risks, warranting further evaluation to mitigate environmental impact.

Table 9: Environmental Toxicity profile of Ob1-Ob10

Properties	**OB1**	**OB2**	**OB3**	**OB4**	**OB5**	**OB6**	**OB7**	**OB8**	**OB9**	**OB10**
Bioconcentration Factors	0.611	0.668	2.052	1.292	1.287	3.419	3.204	3.287	2.613	2.647
IGC 50	2.439	3.057	4.249	3.155	3.52	4.671	4.832	4.643	4.525	4.193
LC 50 FM	3.218	4.16	5.14	3.848	3.966	5.678	5.689	5.5	5.353	4.825
LC50DM	3.71	4.537	5.476	4.357	4.272	5.131	5.54	5.088	5.418	4.911

3.3.8: Tox21 pathway of Ob1-Ob10

The Tox21 pathway analysis for chemical constituent **Ob-l** provides valuable insights into their interactions with nuclear receptors (NR) and stress response (SR) pathways, which are crucial for understanding toxicological mechanisms at the molecular level. The aryl hydrocarbon receptor (NR-AhR) pathway exhibited high activation probabilities for most compounds, with values exceeding 0.99 across the series, except for **Ob1** (2.439). This suggests that compounds such as **Ob2**, **Ob4**, and **Ob5** strongly activate this pathway, indicating potential for endocrine disruption and interference with normal cellular signaling. The androgen receptor (NR-AR) and its ligand-binding domain (NR-AR-LBD) pathways showed variable activation. NR-AR activation probabilities ranged from0. 0.611 (**Ob1**) to5.14 (**Ob3**), with most compounds showing minimal activity. For NR-AR-LBD, higher probabilities were observed for **Ob4** (3.848) and **Ob3** (5.14), suggesting a greater likelihood of interaction with androgen receptors. The aromatase (NR-Aromatase) pathway showed activation probabilities ranging from 0.073 (**Ob1**) to 0.874 (**Ob4**), with compounds **Ob4** and **Ob3** demonstrating the highest activation, indicating possible effects on steroid metabolism and endocrine function. Similarly, the estrogen receptor (NR-ER) pathway showed high activation for **6d** (0.832) and moderate activation for other compounds, with **Ob1** (0.018) exhibiting the lowest probability. For the ligand-binding domain of the estrogen receptor (NR-ER-LBD), activation probabilities were minimal, ranging from 0.001 (**Ob1**) to 0.114 (**Ob4**), suggesting limited direct binding. The peroxisome proliferator-activated receptor gamma (NR-PPAR-gamma) pathway displayed significant activation for compounds **Ob2** (0.624), **Ob3** (0.629), and **Ob8** (0.634), indicating potential

involvement in lipid metabolism and adipocyte differentiation. In contrast, compounds like **Ob1** (0.003) and Ob7 (0.044) exhibited negligible activation.

In terms of stress response (SR) pathways, the antioxidant response element (SR-ARE) pathway, associated with oxidative stress response, demonstrated high activation probabilities for most compounds, with values close to 1.001 for **Ob4**, **Ob5**, and Ob8. Compound **Ob1** (0.011) showed the least activation, indicating a reduced potential for inducing oxidative stress responses. The ATAD5 (SR-ATAD5) pathway, linked to DNA replication stress, showed variable activation, with probabilities ranging from 0.002 (**Ob1**) to 0.614 (**Ob9**). Compounds **Ob9** and **Ob4** demonstrated the highest activation, suggesting potential genotoxic stress induction. The heat shock response element (SR-HSE) pathway, indicative of protein damage and misfolding, exhibited high activation probabilities for most compounds, particularly **Ob9** (0.99) and **Ob5** (0.98), while **Ob1** (0.551) displayed the lowest probability, indicating reduced potential for protein stress induction. The matrix metalloproteinase (SR-MMP) pathway, associated with tissue remodeling, showed uniform activation across most compounds (1.0), except for **Ob1** (0.0), reflecting consistent involvement in extracellular matrix regulation. Lastly, the p53 pathway (SR-p53), related to DNA damage and tumor suppression, displayed moderate to high activation probabilities ranging from 0.011 (**Ob1**) to0.424 (**Ob9**) as shown in Table 10. Compounds **Ob8** and **Ob4** showed the highest activation, indicating potential genotoxic effects and activation of p53-mediated stress responses. These findings emphasize the importance of further studies to evaluate the toxicological impact of these compounds comprehensively.

Table 10: TOX21 pathway of Ob1-Ob10

Properties	**Ob1**	**Ob2**	**Ob3**	**Ob4**	**Ob5**	**Ob6**	**Ob7**	**Ob8**	**Ob9**	**Ob10**
NR-AhR	0.003	0.001	0.0	0.006	0.001	0.004	0.0	0.0	0.007	0.029
NR-AR	0.005	0.003	0.0	0.027	0.0	0.034	0.003	0.001	0.05	0.118
NR-AR-LBD	0.0	0.011	0.0	0.0	0.0	0.003	0.0	0.001	0.001	0.000.5223
NR-Aromatase	0.005	0.05	0.771	0.014	0.0	0.361	0.065	0.003	0.748	0.565
NR-ER	0.062	0.27	0.98	0.103	0.025	0.925	0.073	0.984	0.136	0.092
0.NR-ER-LBD	0.006	0.003	0.997	0.009	0.002	0.369	0.001	0.235	0.083	0.019
NR-PPAR-gam ma0.0	0.001	0.396	0.0	0.001	0.0	0.344	0.344	0.003	0.151	0.351
SR-ARE	0.011	0.072	0.016	0.038	0.115	0.747	0.038	0.328	0.424	0.013

3.3.9: Toxicophore Rules of Ob1-Ob10

The toxicophore analysis of the chemical constituent (**Ob1-Ob10**) identified structural alerts associated with various toxicological risks. Notably, none of the compounds triggered alerts for acute toxicity, indicating a low likelihood of immediate toxic effects under short-term exposure. However, alerts for genotoxic carcinogenicity were observed across all compounds, with most having one alert, while compounds 6c and 6d showed two and six alerts, respectively, indicating higher risks for DNA damage-induced carcinogenesis. Similarly, alerts for non-genotoxic carcinogenicity were consistent, with most compounds showing one alert, except for **Ob1** and **Ob10**, which displayed two alerts, suggesting elevated risks of cancer through other mechanisms. Regarding skin sensitization, most compounds exhibited four alerts, with **Ob1** showing five and **Ob5** demonstrating the

highest number at eight alerts, reflecting significant potential for allergic skin reactions. For aquatic toxicity, all compounds triggered one alert, indicating a baseline risk for environmental impact on aquatic ecosystems.

Alerts for non-biodegradability were minimal for most chemical constituent, with one alert across the series, except for **Ob1**, which showed four alerts, suggesting a greater environmental persistence. The SureChEMBL Rule identified two alerts for most compounds, while **Ob1** demonstrated only one, indicating a comparatively less toxic structural profile. Similarly, the FAF-Drugs4 Rule, which predicts a broad range of toxicological concerns, flagged four alerts for most compounds, with **Ob1**, **Ob2**, and **Ob4** showing five alerts, and **Ob5** exhibiting the highest number of six alerts. Overall, while compounds such as and **Ob1** displayed relatively fewer toxicological alerts, compounds like **Ob1** and **Ob7** raised significant concerns, particularly for genotoxicity, skin sensitization, and environmental persistence. These findings highlight the importance of further experimental validation to ensure the safety and environmental compatibility of these compounds as shown in table 1

Table 11: Toxicophore Rules of Ob1-Ob10

Properties	**Ob1**	**Ob2**	**Ob33**	**Ob4**	**Ob5**	**Ob6**	**Ob7**	**Ob8**	**Ob9**	**Ob10**
Acute Toxicity Rule	0	0	0	0	0	0	0	0	0	0
Genotoxic Carcinogenicity Rule	0	0	0	0	0	0	0	0	0	0
NonGenotoxic Carcinogenicity Rule	0	0	0	0	0	0	0	0	0	0
Skin Sensitization Rule	0	2 alerts	0	0	1alerts	0	0	0	0	0
Aquatic Toxicity Rule	2 alerts	1 alerts	0	2alerts	0	1alerts	1alerts	1alerts	1 alerts	1 alerts
NonBiodegradable Rule	1 alerts	1alerts	0	1alerts	0	0	0	0	0	0
SureChEMBL Rule	0	1 alerts	0	0	0	0	0	0	0	0
FAF-Drugs4 Rule	1 alerts	2 alerts	0	0	2alerts	0	1alerts	0	0	0

3.3.10: Toxicity of Ob1-Ob10

The toxicity profiles of the chemical constituent (**Ob-l**) were evaluated to predict potential adverse effects, including organ toxicity, mutagenicity, and cytotoxicity. These parameters provide crucial insights into the safety profiles of the compounds. The hERG (human Ether-à-go-go-Related Gene) blocker predictions, indicative of potential cardiac toxicity, ranged from 0.058 (**Ob1**) to 0.096 (**Ob10**) for general blocking activity and from 0.058 (**Ob1**) to0.759 (**Ob5**) at 10 µM concentrations.

Drug-induced liver injury (DILI) probabilities were consistently high for all chemical constituent (≥0.995), with compounds like Ob3 and Ob4 reaching a probability of 0.221, indicating a strong likelihood of hepatotoxic effects. AMES mutagenicity predictions ranged from 0.288 (**Ob7**) to0.54 (**Ob1**), with several compounds exhibiting moderate risks of mutagenic potential, particularly **Ob1** and **Ob10**.

Rat oral acute toxicity, indicative of short-term toxicity, ranged from 0.273 (**Ob7**) to 0.002 (**Ob10**), suggesting relatively low acute toxicity across the series. The FDAMDD (Maximum Recommended Daily Dose) predictions varied from 0.364 (**Ob1**) to 0.382 (**Ob4**), with higher values indicating a higher likelihood of safety at recommended doses. Compounds like **Ob4** and **Ob3** showed higher FDAMDD values, suggesting better tolerability. Skin sensitization probabilities were variable, ranging from 0.414 (**Ob10**) to 0.364 (**Ob1**). Compounds like **0b9** showed the least risk of inducing skin irritation, while **Ob1** presented the highest likelihood. Predictions for carcinogenicity ranged from 0.56 **(Ob1**) to 0.935 (**Ob1**), with compounds like **OB1** and **Ob10** showing higher potential for carcinogenic effects. For eye-related toxicity, all compounds showed no potential for eye corrosion (probability = 0.0). However, probabilities for eye irritation ranged from 0.025 (**Ob10**) to 0.191 (**Ob2**), with minimal risks overall. Respiratory toxicity, indicative of potential lung toxicity, showed probabilities ranging from 0.195 (Ob1) to 0.685 (**Ob2**), with **Ob1** demonstrating the highest risk.

Human hepatotoxicity probabilities ranged from 0.302 (**Ob1**) to 0.814 (**Ob6**), with compounds like **Ob1** showing higher liver toxicity risks. Drug-induced nephrotoxicity, reflecting kidney toxicity, showed significant variation, ranging from 0.452 (**Ob7**) to 0.944 (**Ob9**), with **Ob9** presenting the highest likelihood of renal toxicity.

Ototoxicity (ear toxicity) was relatively low, ranging from 0.097 (**OB1**) to 0.631 (**Ob9**). Hematotoxicity predictions ranged from 0.055 (**Ob6**) to 0.451 (**Ob1**), indicating minimal risk of blood toxicity for most compounds. Genotoxicity, a measure of DNA-damaging potential, was high across all compounds (≥0.998), underscoring the need for further investigation into mutagenic risks.

Cytotoxicity predictions for cancer cell lines revealed variability in RPMI-8226 immunotoxicity, ranging from 0.021 (**Ob1**) to 0.076 (**Ob1**), and A549 cytotoxicity, ranging from 0.019 (**Ob1**) to 0.301 (**Ob9**). For HEK293 cytotoxicity, probabilities ranged from 0.621 (**Ob1**) to 0.947 O**b9**), with compound **Ob9** showing the highest potential for toxicity in kidney cell lines. Drug-induced neurotoxicity was predicted to be significant, with probabilities ranging from 0.778 (**Ob7**) to 0.982 (**Ob9**), suggesting potential risks to the nervous system, particularly for **Ob9** and **Ob5** as given in Table 12.

Table 12: Toxicity profile of Ob1-Ob10

Properties	**Ob1**	**Ob2**	**Ob3**	**Ob4**	**Ob5**	**Ob6**	**Ob7**	**OB8**	**Ob9**	**0b10**
hERG Blockers	0.058	0,074	0.072	0.088	0.058	0.033	0.114	0.05	0.076	0.096
hERG Blockers (10um)	0.433	0.412	0.573	0.528	0.759	0.321	0.431	0.324	0.368	0.487
DILI	0.121	0.214	0.221	0.196	0.136	0.258	0.215	0.44	0.336	0.327
AMES Muta genicity	0.54	0.61	0.316	0.615	0.391	0.345	0.288	0.284	0.325	0.398
Rat Oral Acute Toxicity	0.459	0.555	0.284	0.566	0.309	0.353	0.273	0.243	0.243	0.02
FDAMDD	0.364	0.422	0.455	0.382	0.274	0.24	0.272	0.537	0.537	0.414
Skin Sensiti zatio	0.97	0.956	0.585	0.953	0.963	0.691	0.676	0.904	0.904	0.567
Carcinogeni city	0.651	0.759	0.443	0.854	0.566	0.661	0.606	0.809	0.809	0.682
Eye Corrosion	0.986	0.923	0.897	0.711	0.987	0.612	0.692	0.955	0.955	0.489
Eye irritation	0.996	0.978	0.983	0.957	0.996	0.9	0.977	0.994	0.994	0.95

Respiratory	0.764	0.445	0.499	0.681	0.753	0.609	0.541	0.895	0.895	0.715
Human hep atoxicity	0.33	0.395	0.351	0.484	0.232	0.46	0.369	0.58	0.58	0.54
Drug-induce d Nephrotox icity	0.078	0.125	0.087	0.377	0.067	0.341	0.223	0.541	0.41	0.293
Ototoxicity	0.183	0.13	0.368	0.239	0.091	0.408	0.247	0.369	0.275	0.372
Hematotoxic ity	0.101	0.164	0.167	0.263	0.053	0.641	0.53	0.372	0.432	0.607
Genotoxicity	0.179	0.888	0.015	0.281	0.125	0.062	0.215	0.595	0.049	0.234
RPMI-8226 Immunitoxicity	0.063	0.072	0.03	0.067	0.03	0.042	0.044	0.037	0.031	0.071
A549 Cytotoxicity	0.185	0.078	0.187	0.13	0.184	0.135	0.04	0.083	0.264	0.263
Hek293 cytotoxicity	0.356	0.425	0.162	0.325	0.414	0.11	0.302	0.22	0.279	0.293
Drug-induced Neurotoxcity	0.242	0.342	0.408	0.503	0.582	0.191	0.401	0.435	0.384	0.641

CONCLUSION

The current research extensively assessed the phytochemical, pharmacokinetic, and toxicological profiles of Ocimum basilicum, which is a renowned traditional medicine plant in the Lamiaceae family. The results are in agreement with conventional uses and recent pharmacological information that indicate the plant's bioactive constituents as the most important elements responsible for its curative action and therapeutic properties.

Authors' contributions

The study plan was designed and supervised by Tahira Shamim. The whole experimental work was carried out by Laila Sumreen, Jafir Hussain Shirazi, Kinza Javaid and Maryam Ramzan, following the directions of Tahira Shamim. The manuscript write-up was carried out by Qazi Adnan, Aima Batool and Irsa shokaut under the guidance of Tahira Shamim. All authors read and approved the manuscript for publications.

Availability of data and materials

Data will be available on request by the corresponding author.

Competing interests

There is no any financial or personal competing interest among authors.

REFERENCES

1. Elshafie, H.S., I. Camele, and A.A. Mohamed, A comprehensive review on the biological, agricultural and pharmaceutical properties of secondary metabolites based-plant origin. International journal of molecular sciences, 2023. **24**(4): p. 3266.
2. El-Saadony, M.T., et al., Medicinal plants: bioactive compounds, biological activities, combating multidrug-resistant microorganisms, and human health benefits-a comprehensive review. Frontiers in immunology, 2025. **16**: p. 1491777.

3. Manisha, D.R.B., et al., Medicinal plants and traditional uses and modern applications. Journal of Neonatal Surgery, 2025. **14**(3): p. 162-175.
4. Azizah, N.S., et al., Sweet basil (Ocimum basilicum L.)—A review of its botany, phytochemistry, pharmacological activities, and biotechnological development. Plants, 2023. **12**(24): p. 4148.
5. Gurav, T.P., B.B. Dholakia, and A.P. Giri, A glance at the chemodiversity of Ocimum species: Trends, implications, and strategies for the quality and yield improvement of essential oil. Phytochemistry Reviews, 2022. **21**(3): p. 879-913.
6. Acharya, A., G. Ghimire, and P. Shakya, Medicinal herbs. Herbs and Spices—New Perspectives in Human Health and Food Industry; IntechOpen: Rijeka, Croatia, 2024. **1**: p. 161-186.
7. Stannard, J., Medicinal plants and folk remedies in pliny," historia naturalis". History and Philosophy of the Life Sciences, 1982. **4**(1): p. 3-23.
8. Ivanova, T., et al., Sweet Basil between the Soul and the Table—Transformation of Traditional Knowledge on Ocimum basilicum L. in Bulgaria. Plants, 2023. **12**(15): p. 2771.
9. Lupton, D., et al., Basil, in Leafy medicinal herbs: Botany, chemistry, postharvest technology and uses. 2016, CABI Wallingford UK. p. 27-41.
10. Allen, L. A visual history of basil. in Proceedings of th e Oxford Symposium on Food and Cookery. 2020.
11. Bilal, A., et al., Phytochemical and pharmacological studies on Ocimum basilicum Linn-A review. International Journal of Current Research and Review, 2012. **4**(23): p. 73-83.
12. Qasem, J.R., Prospects of wild medicinal and industrial plants of saline habitats in the Jordan valley. Pak J Bot, 2015. **47**(2): p. 551-570.
13. Gunawardana, S. and W. Jayasuriya, Medicinally important herbal flowers in Sri Lanka. Evidence-Based Complementary and Alternative Medicine, 2019. **2019**(1): p. 2321961.
14. Kabiraj, A. and R. Deshmukh, A review on chinese herbal medicine used as carminative. Pharmacological Research-Modern Chinese Medicine, 2024. **11**: p. 100409.
15. Mahajan, P. and M.M. Uzzaman Khan, Basil "Culinary Plant Of High Medical Value": A Comprehensive Review Of Traditional, Medicinal And Pharmacological Potency. Journal of Namibian Studies, 2023. **38**.
16. Weng, M.-H., H.-C. Chou, and J.-J. Liaw, Women's sense of control during labour and birth with epidural analgesia: a qualitative descriptive study. Midwifery, 2023. **116**: p. 103496.
17. Lin, H.C., et al., Antidermatophytic activity of ethanolic extract from Croton tiglium. BioMed Research International, 2016. **2016**(1): p. 3237586.
18. Udoisoh, M.G., et al., Corrosion inhibition of mild steel by ethanol extract of bitter leaf (Vernonia amygdalina): effects of inhibitor concentration and time. Prog. Chem. Biochem. Res, 2024. **7**(3): p. 225-238.
19. Kadhim, M.J., A.A. Sosa, and I.H. Hameed, Evaluation of anti-bacterial activity and bioactive chemical analysis of Ocimum basilicum using Fourier transform infrared (FT-IR) and gas chromatography-mass spectrometry (GC-MS) techniques. Journal of pharmacognosy and phytotherapy, 2016. **8**(6): p. 127-146.
20. Daina, A. and V. Zoete, Application of the SwissDrugDesign online resources in virtual screening. International journal of molecular sciences, 2019. **20**(18): p. 4612.