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Research Article

Computational Study of Alkaloids Targeting O-GlcNAc Transferase as Antidiabetic Agents

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Abstract:
O-GlcNAc Transferase (OGT) plays a pivotal role in glucose metabolism and insulin signaling, making it an attractive therapeutic target for the management of diabetes mellitus. In the present study, a comprehensive in silico approach was employed to investigate the inhibitory potential of selected alkaloids against human OGT, with an emphasis on their binding affinity and pharmacokinetic suitability. Molecular docking analysis was performed using AutoDock Vina to elucidate the interaction patterns between the selected compounds and the active site of OGT. The docking results revealed that berberine exhibited the strongest binding affinity (−7.8 kcal/mol), slightly surpassing that of the native ligand (−7.7 kcal/mol), and formed stable hydrogen bonding and hydrophobic interactions with key catalytic residues such as LYS898, ASN838, and PRO559. In contrast, castanospermine and swainsonine showed comparatively weaker binding affinities, attributed to limited interaction networks within the binding pocket. To further assess the drug development potential of the studied compounds, in silico ADMET analysis was carried out using SwissADME and ADMETlab 3.0. Berberine demonstrated favorable physicochemical properties, superior drug-likeness (highest QED score), and acceptable absorption and toxicity profiles compared to the native ligand and other alkaloids. Although potential cytochrome P450 interactions and moderate bioaccumulation were predicted for berberine, its overall pharmacokinetic profile was well balanced. Collectively, the integrated docking and ADMET results highlight berberine as a promising lead alkaloid targeting OGT, warranting further in vitro and in vivo validation for its potential development as an antidiabetic agent.

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Graphical Abstract

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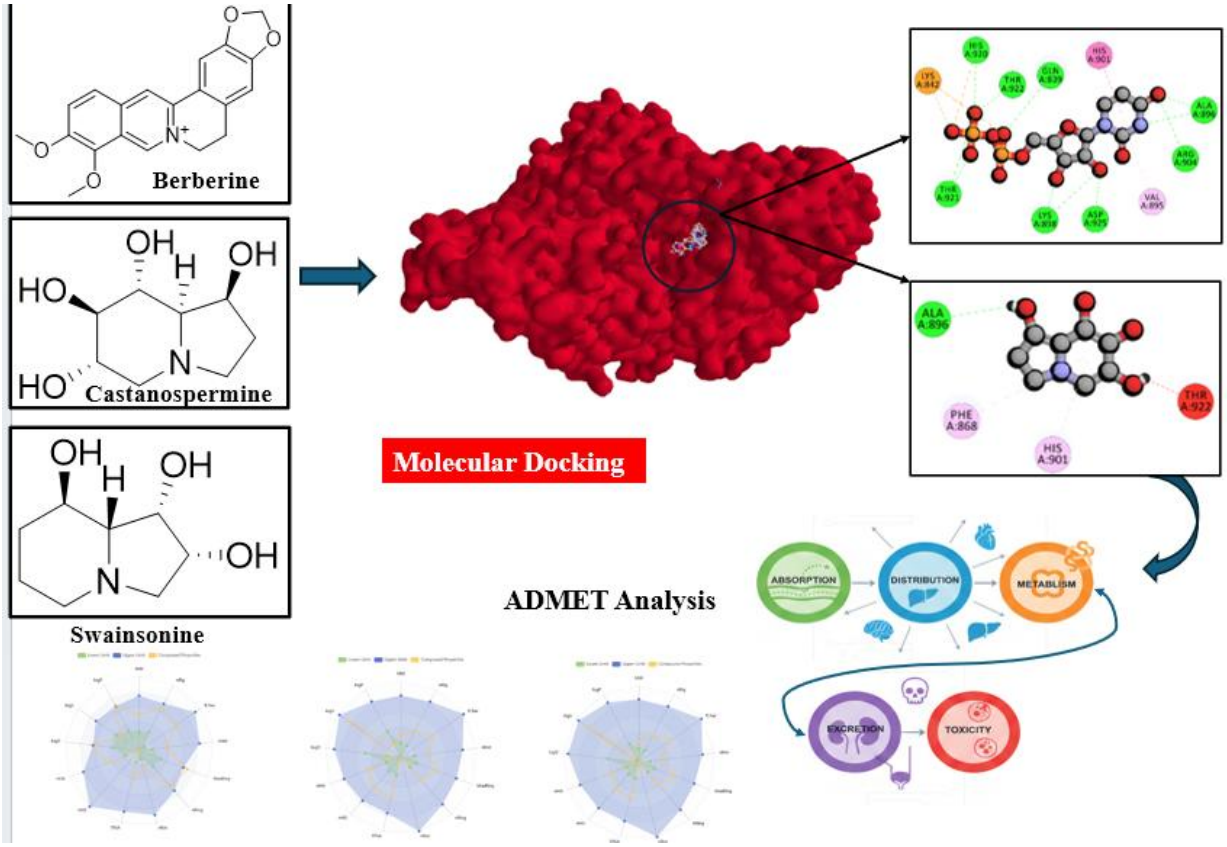

1. Introduction

Diabetes mellitus is a multifactorial metabolic disorder characterized by chronic hyperglycemia arising from defects in insulin secretion, insulin action, or both (1). The global prevalence of diabetes continues to rise at an alarming rate, posing a significant burden on healthcare systems worldwide (2). Although several classes of antidiabetic drugs are currently available, their long-term use is often limited by adverse effects, reduced efficacy over time, and the inability to adequately prevent disease-associated complications (3). Therefore, the identification of novel molecular targets and safer, more effective therapeutic agents remains a critical objective in diabetes research. O-GlcNAc Transferase (OGT) has recently emerged as a crucial regulator of glucose homeostasis and insulin signaling (4). OGT catalyzes the transfer of N-acetylglucosamine to serine and threonine residues of nuclear and cytoplasmic proteins, a reversible post-translational modification known as O-GlcNAcylation (5,6). This modification functions as a cellular nutrient sensor and plays a key role in regulating transcription, signal transduction, and metabolic pathways (7). Under hyperglycemic conditions, excessive O-GlcNAcylation driven by elevated OGT activity disrupts insulin signaling cascades, promotes insulin resistance, and contributes to β-cell dysfunction. Increasing evidence links abnormal OGT activity to the onset and progression of diabetes and its associated complications, highlighting OGT as a promising therapeutic target for antidiabetic drug development (8,9).

Natural products have historically served as a rich source of bioactive compounds for the treatment of metabolic disorders (10). Among them, alkaloids are of particular interest due to their diverse chemical scaffolds and broad spectrum of pharmacological activities. Alkaloids such as berberine, castanospermine, and swainsonine have demonstrated antihyperglycemic, insulin-sensitizing, and enzyme-inhibitory properties in previous studies (11). The selection of these specific alkaloids was guided by their reported antidiabetic activities, structural diversity, and complementary mechanisms of action. Berberine is well known for its ability to modulate glucose metabolism and improve insulin sensitivity, which is consistent with its strong binding affinity and favorable pharmacokinetic profile observed in this study. In contrast, castanospermine and

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swainsonine are iminosugar alkaloids recognized for their glycosidase inhibitory activity and influence on carbohydrate metabolism, offering a distinct mechanistic approach toward enzyme inhibition (12). The inclusion of these structurally diverse compounds enables a comparative evaluation of their interaction with the OGT active site and provides insight into how differences in polarity, molecular size, and functional groups affect binding efficiency and drug-likeness. However, despite their reported antidiabetic potential, the molecular basis of their interaction with OGT and their comparative inhibitory efficiency against this enzyme remain inadequately explored. Recent advances in computational drug discovery have enabled efficient screening and evaluation of potential drug candidates prior to experimental studies (13). Molecular docking provides detailed insights into ligand–protein binding modes, interaction patterns, and binding affinity, while in silico ADMET analysis allows early prediction of pharmacokinetic behavior, drug-likeness, toxicity, and environmental safety. The integration of these approaches significantly reduces time and cost in the early stages of drug development and enhances the success rate of lead identification (14).

Therefore, this study aimed to identify and evaluate alkaloids targeting O-GlcNAc transferase using computational approaches for their potential antidiabetic activity. Molecular docking was employed to elucidate the binding interactions and stability of the alkaloids within the active site of OGT, in comparison with the native ligand. Furthermore, ADMET profiling was conducted to assess the pharmacokinetic suitability and safety profiles of the compounds. The combined analysis aimed to identify a potent and drug-like alkaloid candidate capable of modulating OGT activity, thereby providing a strong foundation for future in vitro and in vivo validation and the development of novel antidiabetic agents. Thus, the present computational approach, which integrates molecular docking and ADMET analysis, directly addresses this research gap by systematically evaluating the binding interactions and pharmacokinetic potential of selected alkaloids against OGT, enabling the identification of promising lead candidates.

2. Experimental

2.1 Molecular Docking

Molecular docking was performed to predict the binding affinity and interaction pattern of the selected phytochemicals with the target protein (figure 1). The chemical structures of the ligands were retrieved from the PubChem database and sketched/refined using ChemDraw. All ligands were geometry-optimized and saved in the appropriate file format prior to docking studies. The three-dimensional crystal structure of the target protein was obtained from the Protein Data Bank (PDB) (PDB ID: 4GZ3). Protein preparation involved the removal of water molecules, heteroatoms, and co-crystallized ligands, followed by the addition of polar hydrogen atoms and the assignment of Kollman charges using Discovery Studio (15,16). Docking simulations were performed using PyRx and the AutoDock Vina algorithm. The grid box was defined using the coordinates X = −17.460480, Y = 28.190000, and Z = 12.357080 to encompass the active binding sites. The docking results were ranked based on the binding energy scores, and the best ligand–protein complexes were visualized and analyzed for key molecular interactions using Discovery Studio.

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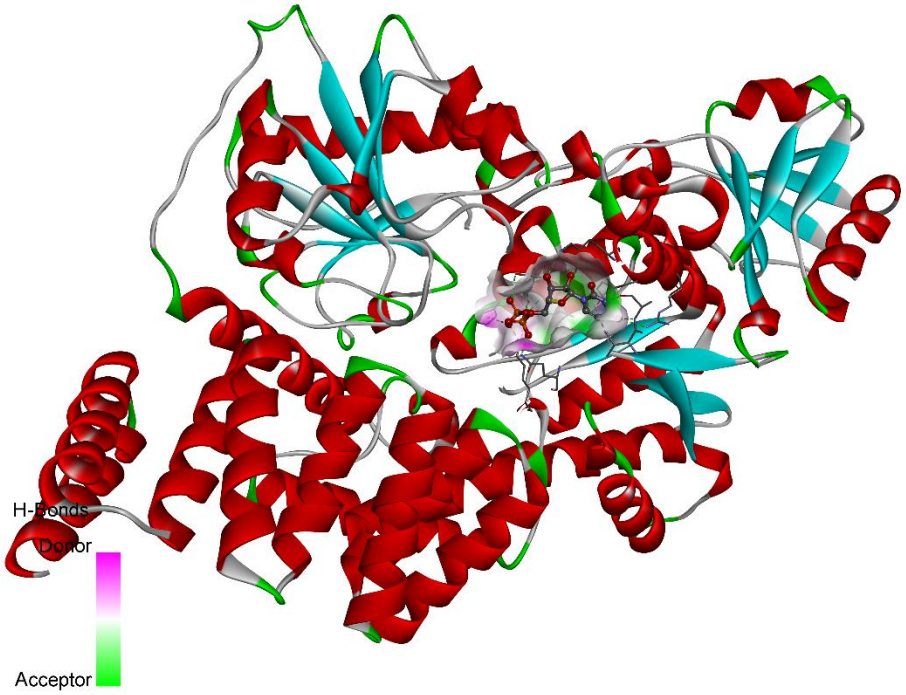

Figure 1. 3D line ribbon representation of Human O-GlcNAc Transferase (OGT) With Native Ligand

2.2 ADMET Analysis

In silico ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) analysis was conducted to evaluate the drug-likeness and pharmacokinetic suitability of the selected phytochemicals (17,18). The canonical SMILES of each compound were generated and analyzed using SwissADME and ADMETlab 3.0. The analysis revealed that most compounds possessed favorable physicochemical properties, good absorption potential, and acceptable metabolic stability, with minimal toxicity risks. Overall, the results indicate that these phytochemicals exhibit promising pharmacokinetic profiles and are suitable candidates for further studies.

3. Results and Discussion

3.1 Molecular Docking

Molecular docking analysis was performed to compare the binding affinity and interaction profiles of selected phytochemicals with the native ligand at the active site of human O-GlcNAc Transferase (OGT) (Table 1 and Table 2). The native ligand exhibited a docking score of −7.7 kcal/mol with a relatively high ligand energy of 1261.05 kcal/mol, indicating stable binding supported by multiple interactions within the catalytic pocket. Notably, the native ligand formed several conventional hydrogen bonds with key active-site residues, including THR922, ASP925, ALA896, GLN839, LYS842, and LYS898, along with carbon hydrogen bonds and hydrophobic π-alkyl interactions, reflecting optimal accommodation within the binding cavity. Among the screened phytochemicals, berberine showed the most favorable binding performance, with a docking score of −7.8 kcal/mol, slightly surpassing that of the native ligand, and a markedly lower ligand energy of 403.87 kcal/mol. Berberine established a conventional hydrogen bond with LYS898, along with carbon hydrogen bonding and hydrophobic alkyl/π-alkyl interactions involving ASN838 and PRO559. These interactions suggest enhanced binding stability and efficient molecular recognition at the active site, supporting berberine's potential as a strong OGT inhibitor.

In contrast, castanospermine and swainsonine displayed comparatively weaker binding affinities, with docking scores of −5.7 and −5.4 kcal/mol, respectively. Although both compounds formed conventional

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hydrogen bonds with ALA896, their interaction profiles were limited, involving fewer hydrophobic contacts, which likely contributed to the reduced binding stability. Overall, the docking results highlight berberine as the most promising lead compound among the tested phytochemicals for further validation.

Table 1. Binding interaction of selected compounds With Human O-GlcNAc Transferase (OGT)

Amino Acid	Bond Length	Bond Type	Bond Category	Ligand Energy (Kcal/mol)	Docking Score
Native Ligand					
THR922	3.11456	Hydrogen Bond	Conventional Hydrogen Bond	1261.05	-7.7
ASP925	2.6029				
ALA896	2.23786				
GLN839	1.78872				
GLN839	1.89487				
LYS842	2.08068				
LYS898	2.52354				
HIS920	2.85482				
THR921	2.7179				
THR922	2.27543				
THR921	3.11118		Carbon Hydrogen Bond		
LYS898	4.33458	Hydrophobic	Pi-Alkyl		
berberine					
LYS898	2.75469	Hydrogen Bond	Conventional Hydrogen Bond	403.87	-7.8
ASN838	3.25231		Carbon Hydrogen Bond		
PRO559	5.17747	Hydrophobic	Alkyl		
LYS898	4.85911		Pi-Alkyl		
PRO559	5.01635				
Castanospermine					
ALA896	2.65359	Hydrogen Bond	Conventional Hydrogen Bond	1049.45	-5.7
PHE868	5.49065	Hydrophobic	Pi-Alkyl		
HIS901	3.90911				
Swainsonine					
ALA896	1.99907	Hydrogen Bond	Conventional Hydrogen Bond	1058.59	-5.4
LYS898	4.84308	Hydrophobic	Alkyl		

Table 2. The 2D and 3D binding interaction poses of the most potent Compounds with Human O-GlcNAc Transferase (OGT) enzyme

3D Interaction	2D Interaction
Native Ligand	

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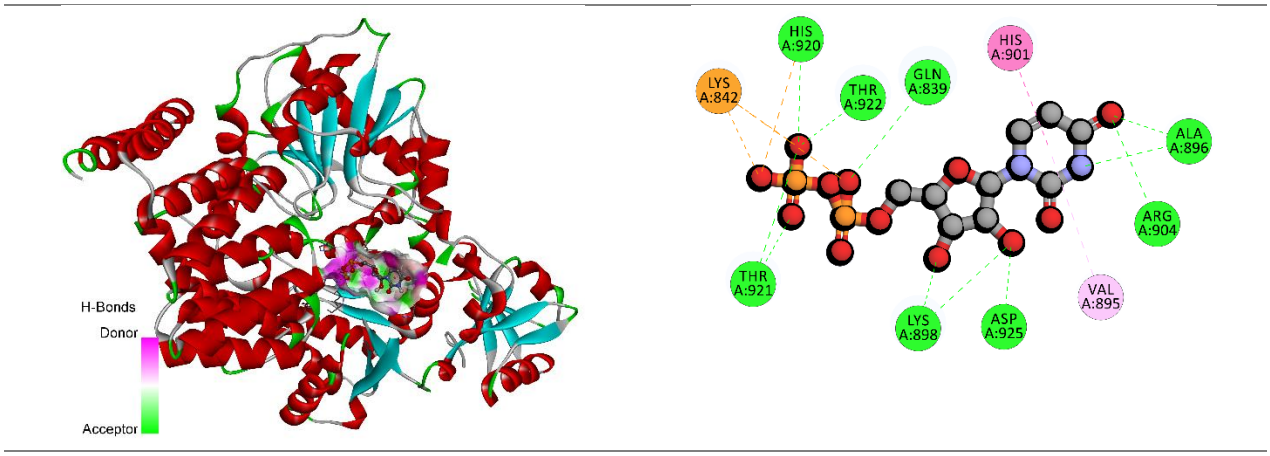

Berberine

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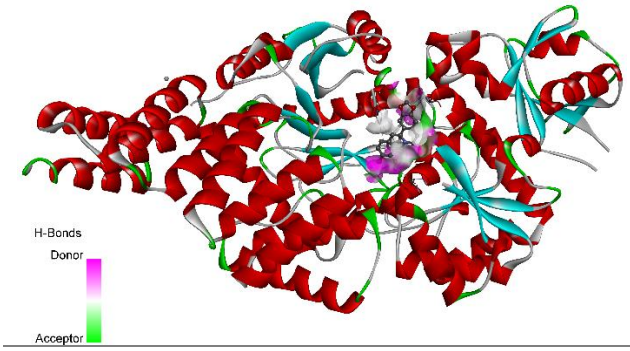
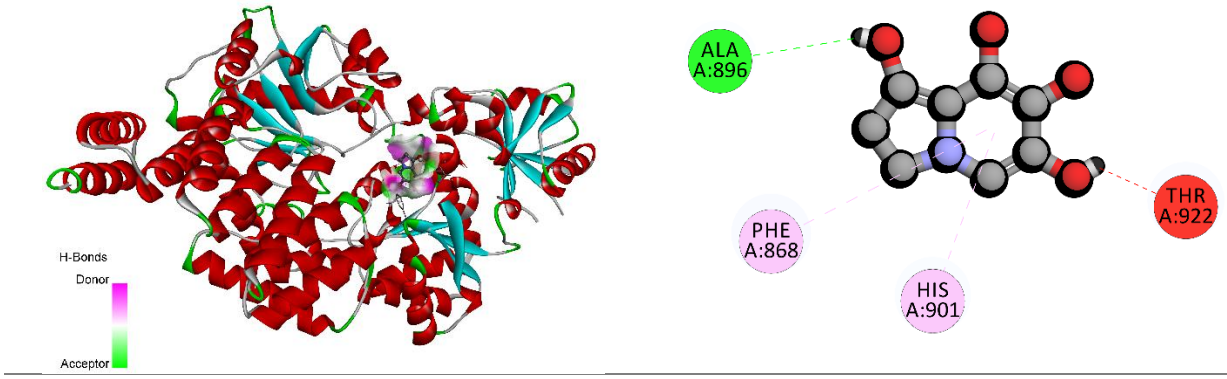
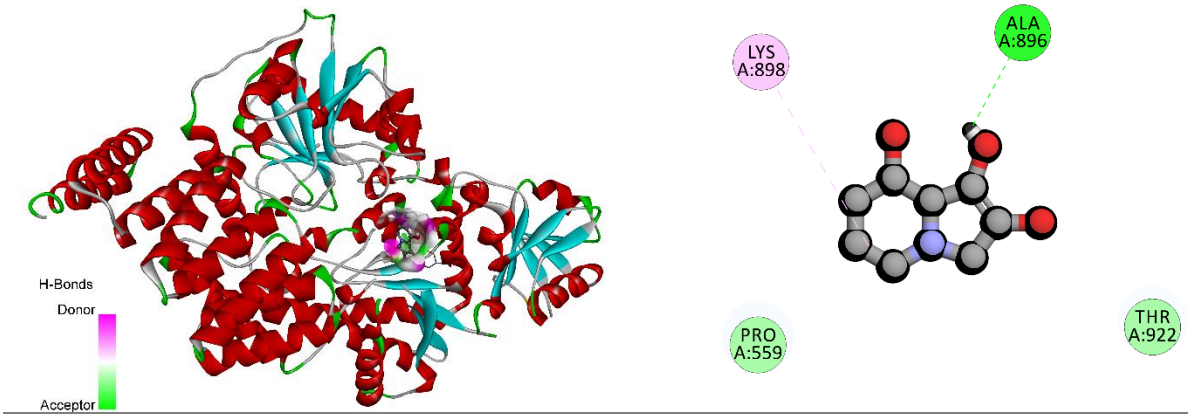


Castanospermine



Swainsonine



3.2 ADMET Analysis

The ADMET properties of the native ligands berberine, castanospermine, and swainsonine were systematically evaluated to understand their physicochemical behavior, drug-likeness, pharmacokinetics, toxicity, and environmental safety. The complete numerical results are presented in Tables 3–8, and all compounds are discussed comparatively. The ADMET radar representation summarizing the overall pharmacokinetic and drug-likeness characteristics of the native ligand and selected alkaloids is shown in Table 9.

Physicochemical analysis showed that the native ligand possessed the highest molecular weight (404 Da) and Topological Polar Surface Area (TPSA) (217.84 Å²), which may negatively influence membrane permeability despite good aqueous solubility (logS −1.12). Berberine exhibited a moderate molecular weight (336.12 Da), optimal lipophilicity (logP 3.11), and low TPSA (40.8 Å²), indicating favorable permeability but reduced solubility. Castanospermine and swainsonine are low-molecular-weight polar compounds with negative logP values, suggesting good solubility but limited lipophilic membrane diffusion.

Drug-likeness assessment revealed that berberine achieved the highest Quantitative Estimation of Drug-likeness (QED) score (0.674), indicating superior overall drug-likeness. The native ligand exhibited the lowest QED (0.269), indicating poor oral drug suitability. Castanospermine (0.339) and swainsonine (0.419) displayed moderate drug-likeness, with partial compliance with the Golden Triangle criteria, suggesting a potential but suboptimal pharmacokinetic balance.

Absorption parameters indicated that berberine had relatively better Caco-2 and MDCK permeability and high fractional absorption (F20% and F50%), although it was predicted to be a P-gp substrate, which may affect its bioavailability. The native ligand showed moderate human intestinal absorption but poor permeability. Castanospermine exhibited moderate absorption, whereas swainsonine exhibited lower HIA values, consistent with its higher polarity.

Distribution and metabolism profiles demonstrated that berberine had high plasma protein binding and moderate BBB permeability, whereas the native ligand and swainsonine showed negligible BBB permeabilities. Castanospermine exhibited the highest free fraction in the plasma. CYP interaction analysis suggested that berberine may interact with multiple CYP450 isoforms, indicating possible metabolic concerns, whereas castanospermine and swainsonine exhibited lower CYP inhibition and substrate probabilities.

Excretion and toxicity predictions showed acceptable plasma clearance and half-life values for all the compounds. The native ligand exhibited a higher probability of drug-induced liver injury (DILI). Berberine showed a comparatively lower hepatotoxicity risk and acceptable acute toxicity. Castanospermine and swainsonine exhibited moderate toxicity profiles with lower respiratory and carcinogenic risks.

Environmental toxicity evaluation revealed that berberine had the highest bioaccumulation factor, whereas castanospermine and swainsonine exhibited lower aquatic toxicity, indicating better environmental safety. Overall, while all compounds demonstrated acceptable ADMET characteristics to varying extents, berberine emerged as the most balanced candidate, combining favorable physicochemical properties, superior drug-likeness, reasonable absorption, and manageable toxicity compared to the native ligand, castanospermine, and swainsonine.

Table 3. Predicted physicochemical properties of the native ligand and selected alkaloids relevant to drug-likeness and membrane permeability.

Compounds	MW	Volume	Dense	nHA	nHD	nRot	nRing	TPSA	logS	logP

Native Ligand	404	306.3288	1.318844	14	6	6	2	217.84	-1.12019	-3.00449
Berberine	336.12	338.0781	0.994208	5	0	2	5	40.8	-5.05883	3.119507
Castanospermine	189.1	175.9691	1.074621	5	4	0	2	84.16	-0.11082	-1.44162
Swainsonine	173.11	167.1789	1.035478	4	3	0	2	63.93	-0.23966	-0.72997

Table 4. In silico drug-likeness assessment of the native ligand and selected alkaloids based on QED, NP score, and multiple medicinal chemistry rule filters.

Compounds	QED	NP Score	Lipinski rule	Pfizer Rule	GSK Rule	GoldenTriangle	Chelator Rule
Native Ligand	0.269	1.516	1	0	1	0	0
Berberine	0.674	1.302	0	1	0	0	0
Castanospermine	0.339	1.843	0	0	0	1	0
Swainsonine	0.419	1.566	0	0	0	1	0

Table 5. Predicted absorption parameters of the native ligand and selected alkaloids, including permeability, P-glycoprotein interaction, and intestinal absorption indices.

Compounds	Caco-2 Permeability	MDCK Permeability	Pgp-inhibitor	Pgp-substrate	HIA	F20%	F30%	F50%
Native Ligand	-5.99235	-5.08587	2.53E-06	1.03E-06	0.800362	0.006233	0.905809	0.515016
Berberine	-5.00954	-4.7	0.007298	0.999569	0.032294	0.939769	0.287881	0.998183
Castanospermine	-5.92489	-4.95837	0.002412	0.970653	0.372886	0.364888	0.732719	0.792294
Swainsonine	-4.75319	-5.03948	0.006607	0.895686	0.031992	0.245102	0.123522	0.679225

Table 6. Predicted distribution and metabolism profiles of the native ligand and selected alkaloids, including plasma protein binding, BBB permeability, and CYP450 interactions.

Compounds	Distribution				Metabolism									
					CYP1A2		CYP2C19		CYP2C9		CYP2D6		CYP3A4	
	PPB %	VD	BBB	Fu	Inhibitor	Substrate	Inhibitor	Substrate	Inhibitor	Substrate	Inhibitor	Substrate	Inhibitor	Substrate
Native Ligand	28.13776	-0.51719	0.00247	63.02791	2.06E-18	1.92E-18	6.61E-15	1.84E-11	8.24E-09	0.820943	1.75E-10	3.77E-13	2.97E-14	1.92E-07

Berberine	68.37754	0.072918	0.116582	37.94892	0.87697	0.994421	0.055071	0.389114	0.001165	0.840826	0.994708	0.995421	0.953667	0.026405
Castanospermine	22.04954	-0.36591	0.281576	77.64304	0.148536	0.004771	0.004158	0.076254	0.022958	0.008444	0.032682	0.003056	0.012237	0.047378
Swainsonine	30.17758	-0.3193	0.004901	70.61276	0.003047	0.03759	0.000447	0.163163	0.003389	0.01383	0.007759	0.002233	0.00239	0.113551

Table 7. Predicted excretion and toxicity profiles of the native ligand and selected alkaloids based on clearance, half-life, and safety-related endpoints.

Compounds	Excretion			Toxicity								
	CL-plasma	T1/2	H-HT	DILI	Ames Toxicity	Rat Oral Acute Toxicity	FDAMDD	Skin Sensitization	Carcinogenicity	Eye Corrosion	Eye Irritation	Respiratory Toxicity
Native Ligand	1.793813	2.539129	0.060686	0.963272	0.026782	0.01134	0.922616	0.969896	0.259088	0.023858	0.722965	0.942033
Berberine	5.281618	1.287795	0.138465	0.1773	0.421178	0.867958	0.913553	0.959617	0.807932	0.0257	0.975493	0.919293
Castanospermine	2.999568	2.975583	0.381752	0.081394	0.480415	0.109135	0.08831	0.705731	0.275691	0.072372	0.862467	0.168689
Swainsonine	4.079789	3.255498	0.371986	0.063684	0.387199	0.105902	0.091936	0.603741	0.256965	0.064388	0.859147	0.130667

Table 8. Environmental toxicity assessment of the native ligand and selected alkaloids based on bioaccumulation and aquatic toxicity parameters.

Compounds	BCF	IGC50	LC50FM	LC50DM
Native Ligand	0.024629	2.377931	3.400926	3.833741
Berberine	2.074011	4.275215	5.140494	6.015509
Castanospermine	0.158303	1.635194	2.085806	2.930232
Swainsonine	0.127632	1.617952	1.873178	2.778767

Table 9. ADMET radar representation summarizing the overall pharmacokinetic and drug-likeness characteristics of the native ligand and selected alkaloids.

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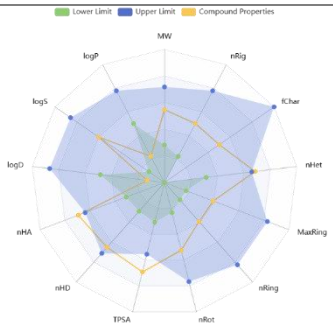
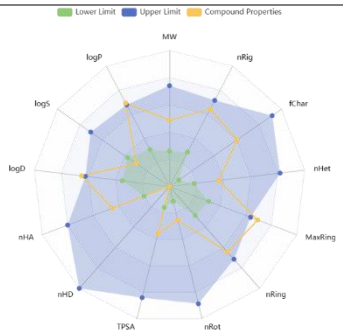
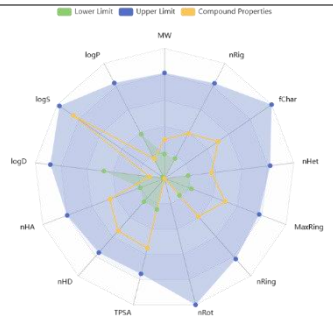


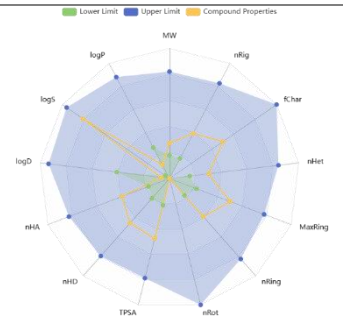
Native Ligand



Berberine



Castanospermine



Swainsonine

4. Conclusion

The present study employed an integrated in silico strategy combining molecular docking and ADMET profiling to identify potential inhibitors of Human O-GlcNAc Transferase (OGT). Molecular docking results demonstrated that berberine exhibited the most favorable binding affinity (−7.8 kcal/mol), comparable to and slightly better than the native ligand, with stable hydrogen bonding and hydrophobic interactions involving key active-site residues of OGT. In contrast, castanospermine and swainsonine showed weaker binding energies and limited interaction networks, suggesting lower inhibitory potential. ADMET analysis further supported these findings by revealing that berberine possesses a balanced pharmacokinetic profile, including optimal lipophilicity, superior drug-likeness (highest QED value), acceptable absorption parameters, and manageable toxicity risks. Although berberine showed potential CYP interactions and higher bioaccumulation compared to other compounds, its overall ADMET performance was superior to the native ligand and the remaining phytochemicals. Castanospermine and swainsonine, while exhibiting good solubility and lower environmental toxicity, were limited by weaker binding affinity and suboptimal absorption characteristics. Overall, the combined docking and ADMET results identify berberine as the most promising lead compound for OGT inhibition. These findings provide a strong rationale for further in vitro and in vivo experimental validation to confirm its therapeutic potential.

Acknowledgments
None

Conflict of Interest
The authors declare no conflict of interest.

Authors' Contribution

Authors contribution includes "Conceptualization, and methodology, software, validation, and formal analysis investigation, resources, data curation, writing—original draft preparation, writing—review and editing, visualization, supervision, project administration, Pardaev Jamshid and Umida Sadikova acquisition. All authors have read and agreed to the published version of the manuscript.

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