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Research Article

ADMET Analysis of Biotin and Thiamine derived from *Linum usitatissimum* L. and their Antidiabetic Potential

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ABSTRACT

In the current era of eco-preservation and environmentally safe utilization, researchers worldwide are increasingly focusing on raw and sustainable materials with notable therapeutic potential, owing to their safety, versatility, biological activity, and compatibility with the environment. In the present work, we investigated *Linum usitatissimum* L. derived biotin and thiamine phytocompounds for their ADMET analysis and their antidiabetic potential against Human Acetylcholinesterase (AChE) inhibitor (PDB:4PQE). To assess the ADMET analysis and antidiabetic properties, in silico approach was used. The results have shown that the targetted drug molecules possess significant biological, ADMET profiling and remarked antidiabetic ability, attributed to the phytoconstiuent's capabilities.

1. Introduction

Nutraceuticals are referred to the hybrid form of nutrition and pharmaceutical components. In general, these are naturally occurring food components or food-derived products that provide medical or health benefits beyond basic nutritional value. Broadly, nutraceuticals include whole foods or specific parts of foods that play a functional role in regulating, restoring, and maintaining normal physiological processes essential for sustaining human health. With increasing global awareness regarding preventive healthcare and lifestyle-related diseases, the nutraceutical industry has expanded rapidly, transforming the food sector into a highly research-driven domain. Natural nutraceutical products encompass a wide range of bioactive substances such as dietary fiber, prebiotics, probiotics, polyunsaturated fatty acids, antioxidants, and various phytoconstituents from herbal and botanical sources [1-3]. These compounds are rich in polyphenols, flavonoids, alkaloids, carotenoids, vitamins, minerals, essential oils, amino acids, and other secondary metabolites that exhibit potent biological activities. Their multifunctionality includes antioxidant, anti-inflammatory, antimicrobial, antiviral, antidiabetic, anticancer, cardioprotective, neuroprotective, hepatoprotective, and immunomodulatory effects [2-6].

The therapeutic efficacy of nutraceutical-derived natural products has been well recognised in curing several health ailments/disorders, particularly obesity, cardiovascular diseases, diabetes, osteoporosis, arthritis, cancer, hypercholesterolemia, and age-related degenerative conditions. For example, curcumin from turmeric shows strong anti-inflammatory and anticancer properties; resveratrol from grapes provides cardioprotective and anti-aging benefits; catechins from green tea are powerful antioxidants; omega-3 fatty acids reduce inflammation and support heart and brain health; while probiotics enhance gut microbiota and improve immunity [7-10]. These bioactive compounds exert their effects through diverse biochemical pathways such as free radical scavenging, modulation of inflammatory mediators, regulation of metabolic enzymes, inhibition of tumour cell proliferation, and protection of cellular components from oxidative damage. A number of plants are known for their therapeutic potential as well as their parts enriched with nutritious compounds such as *Emblica officinalis* (amla), *Curcuma longa* (turmeric), *Ocimum sanctum* (tulsi), *Linum usitatissimum* (Flaxseed/Linseed), *Camellia sinensis* (green tea), *Allium sativum* (garlic), *Zingiber officinale* (ginger), *Withania somnifera* (ashwagandha), *Rubia cordifolia* (Madder), *Vitis vinifera* (grapes) etc [11-18]. The integration of plant-based nutraceuticals in daily diet offers a natural and sustainable approach towards managing lifestyle disorders and promoting long-term wellness.

Among various plant-derived nutraceutical sources, Linum usitatissimum (flaxseed) stands out for its rich and diverse phytochemical composition that significantly contributes to human health. Flaxseed is an abundant source of omega-3 fatty acids, particularly α-linolenic acid (ALA), lignans such as secoisolariciresinol diglucoside (SDG), high-quality proteins, soluble and insoluble dietary fibers, phenolic acids, flavonoids, and tocopherols. In addition to these major constituents, flaxseed also contains essential vitamins including biotin (vitamin B7) and thiamine (vitamin B1) which play vital roles in energy metabolism, enzyme function, nervous system maintenance, and cellular growth [19]. Biotin supports healthy skin, hair, and metabolic functions, while thiamine aids in carbohydrate metabolism and the proper functioning of the cardiovascular and neurological systems. Flaxseed is further enriched with minerals such as magnesium, zinc, calcium, potassium, and iron, adding to its nutritional value. These bioactive compounds collectively confer potent antioxidant, anti-inflammatory, hypolipidemic, antidiabetic, anticancer,

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cardioprotective, neuroprotective, hepatoprotective, and gastroprotective activities [11-14, 20]. The study is to investigate *Linum usitatissimum* L. derived biotin and thiamine phytocompounds for their ADMET analysis and their antidiabetic potential against Human Acetylcholinesterase (AChE) inhibitor by using CADD-based *in silico* approach as the natural products/phytoconstituents cope with the biological activity.

2. Materials and methods

2.1 Protein and Ligands preparation

The crystal structure of Human Acetylcholinesterase (AChE) inhibitor (4PQE) in PDB format was obtained from Protein Data Bank (https://www.rcsb.org/). Ligands (Table 1), Galantamine (**GalA**), Biotin and Thiamine were prepared using chemdraw software, obtained SMILES and mol2 files. The energy minimization of the modeled structures were done using Avogadro Software v1.2.0.

2.2 Biological characteristics and ADMET Properties Assay

Using Molinspiration Cheminformatics Online Server v2022.08 (https://www.molinspiration.com), the biological properties of the selected compounds **1-3** were evaluated. To evaluate ADMET properties, Swiss ADME algorithm (http://www.swissadme.ch) and pkCSM online platform (http://biosig.unimelb.edu.au/pkcsm/) were utilized [21-25].

2.3 Molecular docking studies

The Vinadock automation-assisted prediction of binding energies and interactive 3D visualization of 4PQE was obtained by CB-Dock Online platform using server2 (http://cadd.labshare.cn/cb-dock2/) [23,24,26] (Prior to docking, water molecules were removed from the uploaded protein structure).

3. Results and discussion

3.1 Biological characteristics evaluation and Prediction of ADMET properties

The biological activities of selected **Componds 1-3** were assessed and shown in Table 2. With reference to the biological activities, the selected compounds 1 and 2 demonstrated pronounced bioactive profiles. For novel drug discovery, considering pharmacokinetic and pharmacodynamic characteristics, drug validation is strongly recommended by researchers using computer aided drug design manner [27,28]. The ADMET profiles for **Compounds 1-3** have been assessed and presented in Table 3 – Table 7 computed with Swissdock ADME and pkCSM platforms integrated with biological-logarithms. A remarkable performance and notable pharmacological characteristics were observed for Biotin and Thiamine, showing activity comparable to Galantine, the standard reference drug. As shown in Table 4, the evaluated compounds demonstrated favorable absorption characteristics when compared with the reference drug, particularly in terms of Caco-2 cell permeability, human intestinal absorption, and skin permeability.

Table 1: Selected targets as ligands.

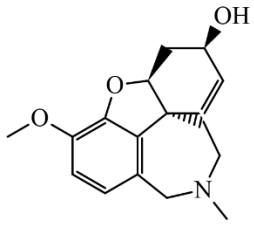
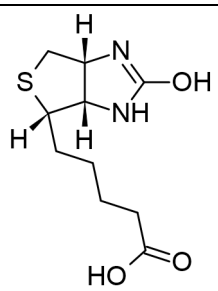
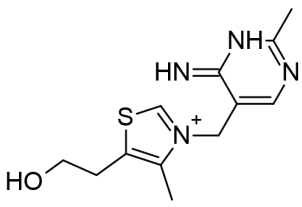
Chemical structures	Name of Compounds/Smile Codes	Molecular formula	Molecular weight	Docking Score against 4PQE (kcal/mol)
	Galantamine (**GalA**) COC1CCC2C3C1O[C@@H]1[C@@]3(CCN(C2)C)C=C[C@@H](C1)O	$C_{17}H_{21}NO_3$	287.3	-8.0
	Biotin OC=1N[C@@H]2[C@H](CCCCC(O)=O)SC[C@@H]2N=1	$C_{10}H_{16}N_2O_3S$	244.3	-7.8
	Thiamine CC=1NC(=N)C(C[n+]2csc(CCO)c2C)=CN=1	$C_{12}H_{17}N_4OS^+$	265.3	-6.7

Table 2: Molinspiration-predicted biological characteristics of selected drugs.

Ligands	GPCR ligand	Ion channel modulator	Kinase inhibitor	Nuclear receptor ligand	Protease inhibitor	Enzyme inhibitor
GalA	0.03	0.32	-0.43	-0.59	-0.36	0.24
Biotin	0.02	0.31	-0.40	-0.51	-0.33	0.26
Thiamine	0.02	0.33	-0.40	-0.54	-0.34	0.29

Table 3: Physicochemical properties, lipophilicity, druglikeness and medicinal chemistry parameters for selected drugs calculated with Swissdock ADME and pkCSM.

Drug targets	Swissdock ADME														pkCSM
	Physicochemical Properties						Lipophilicity				Druglikeness		Med. Chem.		LogP
	Fraction Csp3	NRB	HBA	HBD	M^{Ref}	TPSA (Å²)	iLOGP	XLOGP3	WLOGP	MLOGP	Lipinski violations	BioA Score	PAINS	Sy^{Ac}	
GalA	0.88	1	4	1	84.79	41.93	2.76	1.28	1.06	1.50	Yes; 0 violation	0.55	0	5.32	0.88
Biotin	0.80	5	4	3	70.62	107.22	1.53	0.46	0.24	0.74	Yes; 0 violation	0.55	0	4.02	1.14
Thiamine	0.42	4	3	3	71.94	104.88	-1.35	0.14	0.44	-0.30	Yes; 0 violation	0.55	0	3.10	3.54

NRB=No. Rotatable bonds; HBA=H-bonded acceptors; HBD=H-bonded donars; M^{Ref} =Molar refractivity; BioA=Bioavailability; Sy^{Ac} =Synthetic accessibility

Table 4: Absorption parameters for selected drugs calculated with pkCSM.

Drug target	Water solubility (log mol/L)	Caco2 permeability (log cm/s) high Caco2 permeability >0.9	Human intestinal absorption (% Absorbed) poorly absorbed <30%	Skin Permeability low skin permeability, log Kp>-2.5	P-glycoprotein substrate
GalA	Soluble	-5.020	0.986	Permeable	0.225
Biotin	Soluble	-5.71	0.952	Permeable	0.158
Thiamine	Soluble	-5.2	0.854	Permeable	0.208

Table 5: Distribution and Excretion parameters for selected drugs calculated with pkCSM.

Drug target	Distribution parameters					Excretion parameters	
	Human volume of distribution (VDss) (log L/kg) VDss low, logVDss<-0.15 VDss high, logVDss>0.45	Human fraction unbound (Fu)	BBB permeability (log BB) readily cross the BBB, logBB>0.3 poorly distributed, logBB<-1	CNS permeability (log PS) to Penetrate the CNS, logPS>-2 unable to penetrate the CNS, logPS<-3	Plasma Protein Binding Predictions	Total Clearance (log ml/min/kg)	Renal OCT2 substrate
GalA	1.570	0.270	1.000	-2.970	23.430	18.440	0.298
Biotin	0.63	0.48	0.84	-2.64	40.29	4.75	0.8
Thiamine	0.8	0.77	0.874	-3.05	61.71	7.11	0.203

Table 6: Metabolism parameters for selected drugs calculated with pkCSM.

Drug target	CYP3A4 substrate	CYP1A2 inhibitor	CYP2C19 inhibitor	CYP2C9 inhibitor	CYP2D6 inhibitor	OATP1B1 Probability
GalA	NO	NO	NO	NO	NO	0.031
Biotin	NO	NO	NO	NO	NO	0.03
Thiamine	NO	NO	NO	NO	NO	0.065

Table 7: Toxicity parameters for selected drugs calculated with pkCSM.

Drug target	AMES toxicity[a]	Maximum Human tolerated Dose[b] (log mg/kg/day) Toxic effect>0.477 log mg/kg/day	hERG I inhibitor[c]	hERG II inhibitor[d]	Oral Rat Acute Toxicity[e] (LD_{50}) (mol/kg)	Oral Rat Chronic Toxicity[f] (LOAEL) (log mg/kg bw/day)	Hepatotoxicity[g]	Skin Sensitization[h]	*T. Pyriformis* toxicity[i] (log ug/L)	Minnow toxicity[j] (log mM)	Liver Injury I (DILI) Probability
GalA	No (0.005)	-1.530	No	No	2.890	1.570	No	No	-0.960	3.470	0.191
Biotin	Yes (0.558)	-1.56	No	No	1.48	1.69	No	No	1.71	3.6	0.094
Thiamine	No (0.014)	0.39	No	No	2.71	1.56	No	No	0.58	4.02	0.465

[a]A compound with a positive values of AMES mutagenicity test is mutagenic and therefore may act as a carcinogen; A hERG [b]I/[c]II inhibitors could cause the development of the acquired long QT syndrome, which leads to fatal ventricular arrhythmia; [d]A compound with positive tests could be associated with disrupted normal function of the liver; [e]A compound with positive tests could have a high potential adverse effect for products applied to the skin, e.g. cosmetics and antifungals; mmeasured in log mg/kg/day. If value is ≤ 0.477 log mg/kg/day is considered to be low, while > 0.477 log mg/kg/day is considered to be high; [g]measured in mol/kg. [h]measured in log mg/kg_bw/day; [i]measured in log µg/L. If value is< -0.5 log µg/L is considered to be toxic; [j]measured in log mM. If log LC_{50} values < -0.3 indicate high acute toxicity.

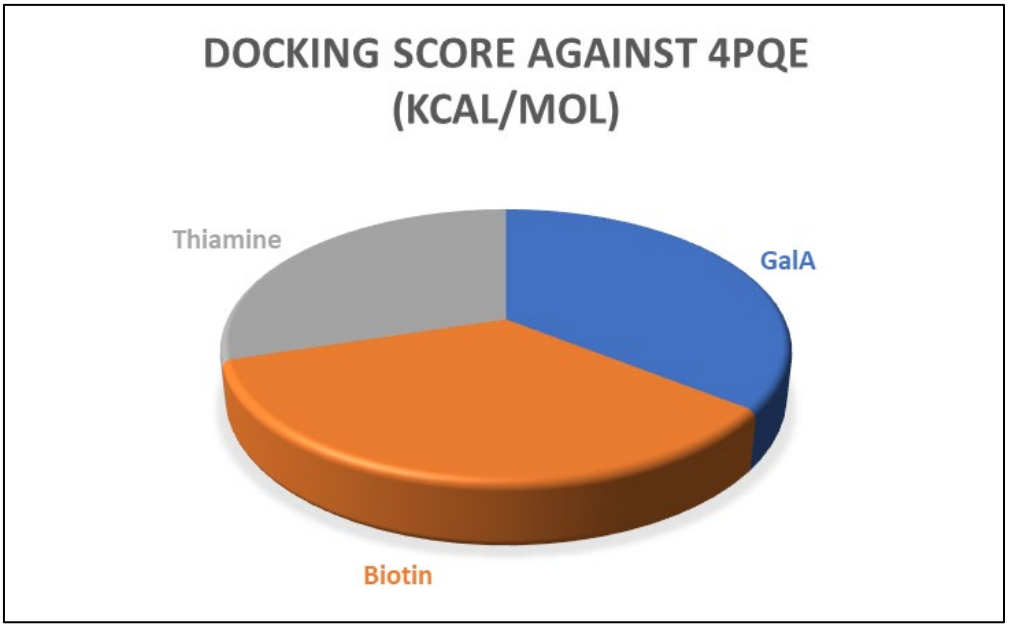


Figure 1: Comparative molecular docking score of selected compounds **1-3**.

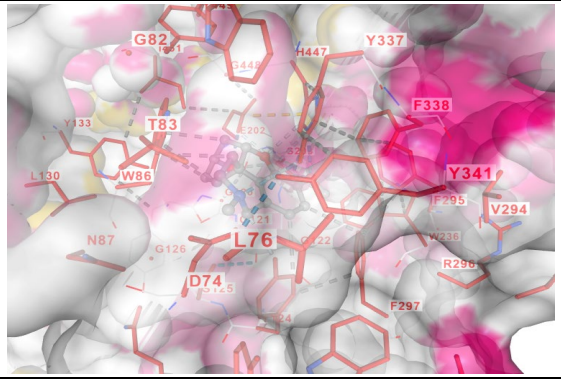
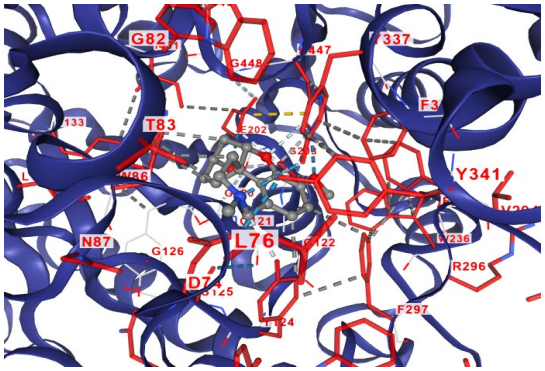
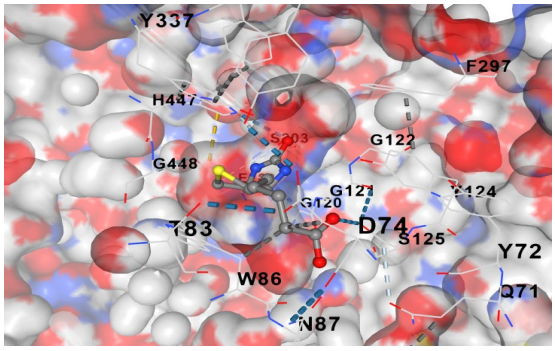
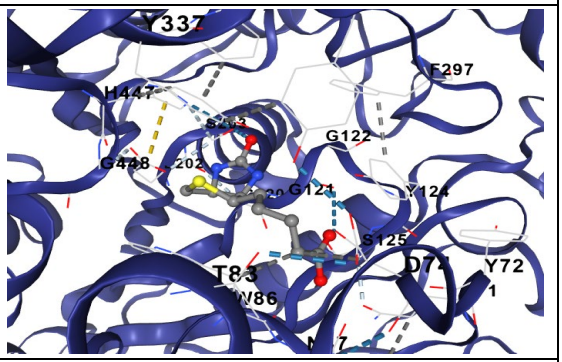
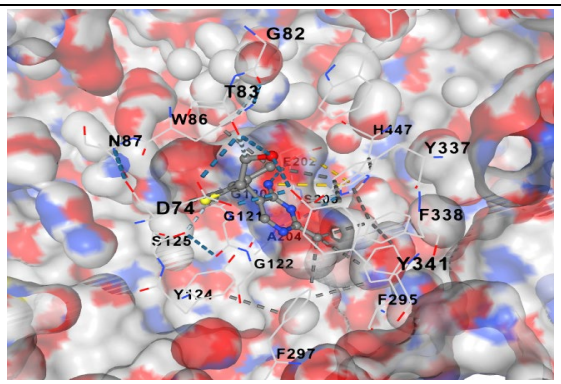
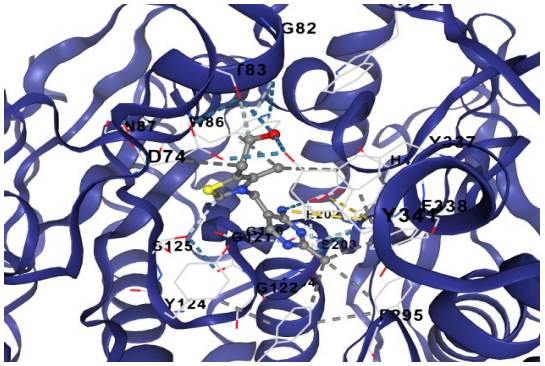
Drug target	Molecular docking pattern	
	Receptor Style: Surface	Receptor Style: Cartoon
GalA		
Biotin		
Thiamine		

Figure 2: Molecular docking pattern of selected target compounds **1-3** against 4PQE.

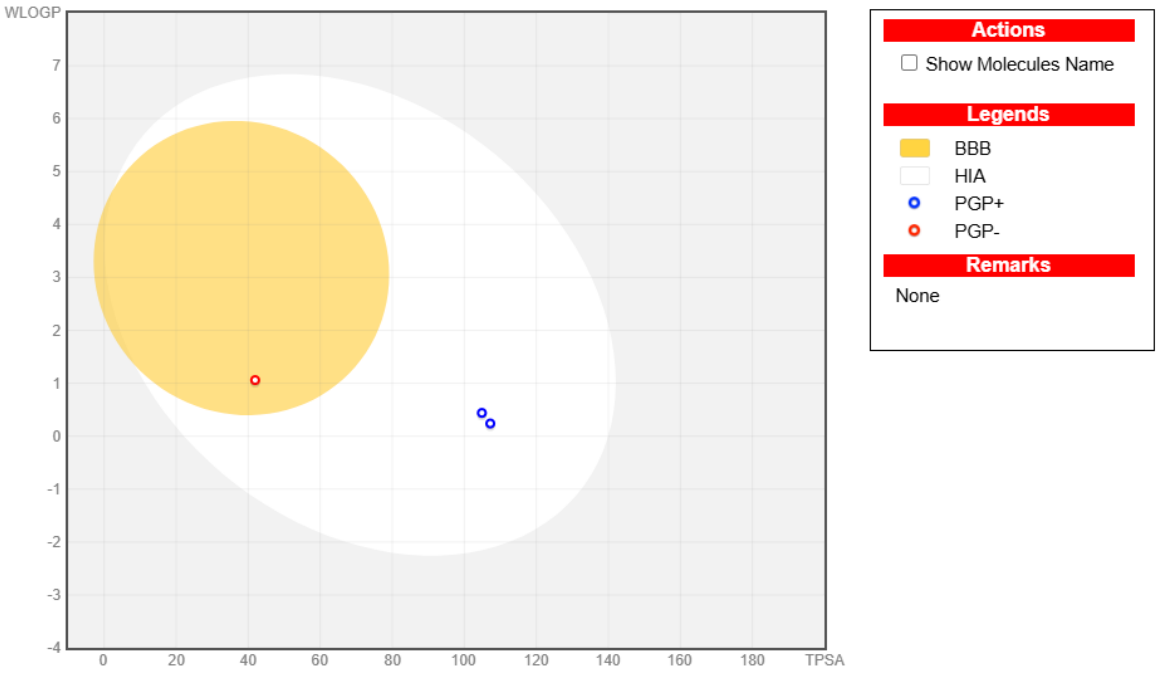


Figure 3: Boiled egg diagram for selected drug targets.

All compounds **1-3** showed considerable human volume of distribution and human fraction unbound (Fu) values, BBB, and CNS permeability and regularised excretion properties (Total Clearance and Renal OCT2 substrate) (Table 5). Moreover, the metabolism has shown considerable properties for all the selected drug targets (OATP1B1 Probability, 0.031, 0.03 & 0.065, respectively) Table 6. Table 7 depicts that the compounds **1-3** exhibited considerable results with non-hepatotoxic, and no toxicity profiling. All three compounds exhibit acceptable safety and toxicity profiles. Thiamine and Biotin demonstrate promising characteristics for drug development with no major toxicity risks besides Biotin's AMES response and Thiamine's relatively higher DILI probability. Their profiles indicate potential suitability as safe nutraceutical or therapeutic candidates when compared to the standard drug Galantamine, though further validation and dose optimisation studies are necessary.

3.2 Molecular Docking studies

Molecular docking is employed to simulate and predict the most favorable orientation and interaction of selected ligands within the target protein's active site, providing insights into binding energy and potential binding mechanisms. In the molecular docking analysis against the 4PQE receptor, it was observed that the three compounds exhibited stable binding interactions, as reflected by their negative docking scores (Fig. 1 and Fig. 2). The reference drug, galantamine, exhibited the highest binding affinity docking score of -8.0 kcal/mol, predicting a strong interaction within the active site. Biotin had a very close docking score of -7.8 kcal/mol with a similar binding tendency and thus might be predicted for an efficient competitive interaction with the standard. Thiamine, with a -6.7 kcal/mol docking score, demonstrated a moderate binding tendency; however, it was lesser than galantamine and biotin and thus would correspondingly interact weaklier within the binding pocket. Fig. 3 explains the boiled egg diagram that showed good ability to be digestion. The docking interactions of compounds 1–3 have shown satisfactory binding within the active site, primarily due to hydrogen bonding and other stabilizing interactions given by their functional groups and active moieties. All such interactions are evidence of good ligand–receptor affinity and support their potential as bioactive candidates (Fig. 2). Plant-derived natural products, including these compounds, have attracted great pharmaceutical interest due to their inherent biological activities such as antioxidant, antimicrobial, antidiabetic, and other therapeutic properties, linked with the advantage of eco-sustainability and environmental compatibility [2-6,13,15,29-32]. Our study demonstrates that the selected compounds biotin as well as thiamine bears remarked bioactivities to have mobile superior docking scores/ negative binding energies with respect to the reference drugs attributed to the strong hydrogen-bonding interactions both inter and intra assemblies towards antidiabetic capabilities.

4. Conclusion

Linum usitatissimum L. is a nutritionally valuable plant enriched with multiple phytoconstituents, exhibiting promising biological and therapeutic activities such as antimicrobial, anticancer, and antidiabetic effects, alongside its potential to alleviate various other health-associated ailments. In the present study, Biotin and Thiamine of the chief phytoconstituents present in *Linum usitatissimum* for human anticholinesterase (AChE) inhibitor (4PQE as an emerging scaffold. Our study reveals that the selected compounds observed considerable biological, ADMET profiling and docking scores/ negative binding energies against 4PQE with respect to the reference drug galantamine attributed to the strong hydrogen-bonding interactions both inter as well as intra assemblies towards antidiabetic capabilities. After following clinical evaluations, these compounds hold promise for development as oral therapeutic agents. Moreover, structural derivatives could find the way for extensive biomedical applications, ultimately advancing nature-based drug candidates with potential efficacy against diabetes, subject to further research validation.

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Contribution

Sandeep K. Chaurasiya: Concept, literature review, data interpretation, drafting the manuscript and approval for final submission.

Mohd Yusuf: Concept, data analysis, editing, technical support, drafting the manuscript and approval for final submission and correspondence.

Shafat Ahmad Khan: Data analysis, editing, technical support, drafting the manuscript and approval for final submission.

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Conflicts of Interest

The authors declare no conflict of interest.

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