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Alpha-glucosidase activity of phytochemicals from *Phyllanthus amarus* leaves via *in-silico* approaches

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ABSTRACT

Diabetes mellitus is a metabolic disease that poses a serious global health challenge. The provision of alternative and complementary medicine to combat the disease has attracted the attention of numerous scientists. In this study, anti- α-glucosidase activities of selected seven compounds obtained from *Phyllanthus amarus* leaves were explored using computational chemistry approach. The absorption, distribution, metabolism and excretion (ADME) properties of the compound with the best binding affinity and metformin were examined. The descriptors obtained from the optimized compounds accurately describe anti- α-glucosidase activities of the studied compounds. The results showed that Compound **1**[(1*S*,19*R*,21*S*,22*R*,23*R*)-6,7,8,11,12,13,22,23-octahydroxy-3,16-dioxo-2,17,20-trioxatetracyclo[17.3.1.0^{4,9}.0^{10,15}] tricosa-4,6,8,10,12,14-hexaen-21-yl] 3,4,5-trihydroxybenzoate possesses greater capacity to inhibit α-glucosidase than other studied compounds selected from *Phyllanthus amarus* leaves as well as Metformin.

1. Introduction

Increase in blood sugar level in human body has been one of the major challenges facing people globally [1]. Improper supply of insulin in patients with diabetes leads to increased level of blood sugar [2]. Diabetes has been rated to be the third leading disease with high mortality rate and this has drawn the attention of many researchers to finding lasting solution to this menace [3]. Alpha-glucosidase as a vital enzyme which is located in human small intestine and plays a major role in breaking down of carbohydrates to glucose [4]. It is a carbohydrate-hydrolase which discharges α-glucosidase and inhibition of α-glucosidase can help to decrease the discharge of glucose into human bloodstream [5]. Series of drug-like molecules such as acarbose and voglibose have been reported as anti-α-Glucosidase thereby down-regulating diabetes mellitus; nevertheless, several side effects such as diarrhea, hepatic disorders, and gastrointestinal diseases have been reported to accompany their therapeutic effects in human beings [6–8].

Phyllanthus amarus has been reported to exert effects against several diseases such as microbial infection, diabetes, plasmodial, inflammation and cancer [9–12]. *Phyllanthus amarus* can be found in several parts of the world such as Africa, Asia, America and China. The leafy medicinal plant belongs to Euphorbiaceae family and it is observed to be one of the plants with low toxicity [13,14]. Series of organic molecules with vital therapeutic activities such as flavonoids, polyphenols, triterpenes, sterols and alkaloids are present in *Phyllanthus amarus* [15].

Moreover, the use of computational approach via density functional theory in probing the anti-diabetic activities of drug-like molecular compounds obtained from herbal plants still remain at its highest peak [16]. Its usefulness can be linked to its immeasurably significant role played in elucidating the electronic structure as well as reactivity of drug-like molecules [17]. Moreso, density functional theory method among other computational chemistry methods has proven to be efficient in clarifying and understanding chemical progressions and this has drawn the attention of many researchers to its use [18].

Therefore, this work was aimed at identifying the molecular descriptors responsible for anti-diabetic activity of *Phyllanthus amarus* leaves as well as investigating the non-bonding interactions between the studied compounds obtained from *Phyllanthus amarus* and α-glucosidase [19].

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2. Materials and methods

2.1. Computational details

2.1.1. Theoretical calculations via density functional theory

Seven molecular compounds [20] were subjected to optimization process using density functional theory method via Spartan 14 software [21,22]. In density functional theory method, three-parameter density functional which includes Becke's gradient exchange correction [23] and the Lee, Yang, Parr correlation functional was used. According to Semire et al., 2017, accuracy of quantum chemical calculation via density functional theory method could be attributed to the chosen basis set; thus, 6–31G* was used for optimization of the studied molecular compounds [24]. The IUPAC name of the studied compounds obtained from *Phyllanthus amarus* leaves are listed in Table 1.

2.2. Preparation of studied protein and compounds obtained from phyllanthus amarus Leaves

The 3D structure of the studied receptor (α-glucosidase with PDB ID 3wy1[19]) was downloaded from protein data bank and subjected to molecular docking software in order to obtain non-bonding interactions as well as binding affinity. The studied receptor (α-glucosidase) was also treated to obtain a clean receptor using pymol software. The active site in the treated receptor was located using autodock tool software and further saved in pdbqt format so as to be accepted by autodock vina software for docking calculations. The details for the active site in the studied receptor were as follows: center (X = -9.31, Y = -12.598, Z = 11.653) and size (X = 56, Y = 5654, Z = 84) and spacing was set to be 1.00 Å.

3. Result and discussion

3.1. Calculated descriptors obtained from the studied compounds

Series of descriptors obtained from the optimized compounds from *Phyllanthus amarus* were highest occupied molecular orbital energy, lowest unoccupied molecular orbital energy, dipole moment, area, volume, polar surface area, ovality, polarizability, hydrogen bond donor and hydrogen bond acceptor (Table 2). According to Oyebamiji et al., [25], optimized compound with highest calculated E_{HOMO} value is expected to possess greatest ability to release electron to the nearby compounds; therefore, compound **5** with -5.45 kcal/mol was expected to interact well with the studied receptor. Also, the molecular compound(s) with lowest E_{LUMO} value reveals its ability to accept electron from neighboring compound thereby leads to better interaction [26]; thus, compound **4** with -1.96 kcal/mol was expected to accept electron from the nearby compounds than other studied compounds.

The role played by dipole moment as one of the imperative non-bonded interactions between compound-receptor complexes cannot be overemphasized [27]. The acceptable dipole moment value for any drug-like molecules was expected to fall within the range of 3 kJ/mol to 5 kJ/mol; thus, compound 3, 5, 6 and 7 were within the acceptable range and expected to form robust non-bonded interaction with the studied receptor. More so, the calculated log P for drug-like compounds exposed their dissolving capacity [28] and problems in oral use may occur if the calculated log P is greater than 5 [29]. Hence, all the studied compounds are expected to possess the affinity to be administered via oral cavity. Other calculated descriptors were reported in Table 2.

3.2. Molecular docking calculations

Seven optimized molecular compounds were docked against α-glucosidase with PDB ID 3wy1 for investigating the non-bonding interactions and binding affinity between the studied complexes. As shown

Table 1
Schematic Structure of the studied compounds.

1	[(1*S*,19*R*,21*S*,22*R*,23*R*)-6,7,8,11,12,13,22,23-octahydroxy-3,16-dioxo-2,17,20-trioxatetracyclo[17.3.1.$0^{4,9}$.$0^{10,15}$]tricosa-4,6,8,10,12,14-hexaen-21-yl] 3,4,5-trihydroxybenzoate
2	(2*R*,3*R*)-2-(3,4-dihydroxyphenyl)-3,4-dihydro-2*H*-chromene-3,5,7-triol
3	(7*R*,8*R*,9*S*)-9-(3,4-dimethoxyphenyl)-4-methoxy-7,8-bis(methoxymethyl)-6,7,8,9-tetrahydrobenzo[g][1,3]benzodioxole
4	methyl 7,8,9-trihydroxy-3,5-dioxo-1,2-dihydrocyclopenta[c]isochromene-1-carboxylate
5	6-[(2*S*,3*S*)-3-[(3,4-dimethoxyphenyl)methyl]-4-methoxy-2-(methoxymethyl)butyl]-4-methoxy-1,3-benzodioxole
6	(5*R*,6*S*,7*S*)-5-(3,4-dimethoxyphenyl)-4-methoxy-6,7-bis(methoxymethyl)-5,6,7,8-tetrahydrobenzo[f][1,3]benzodioxole
7	4-[(2*S*,3*S*)-3-[(3,4-dimethoxyphenyl)methyl]-4-methoxy-2-(methoxymethyl)butyl]-1,2-dimethoxybenzene

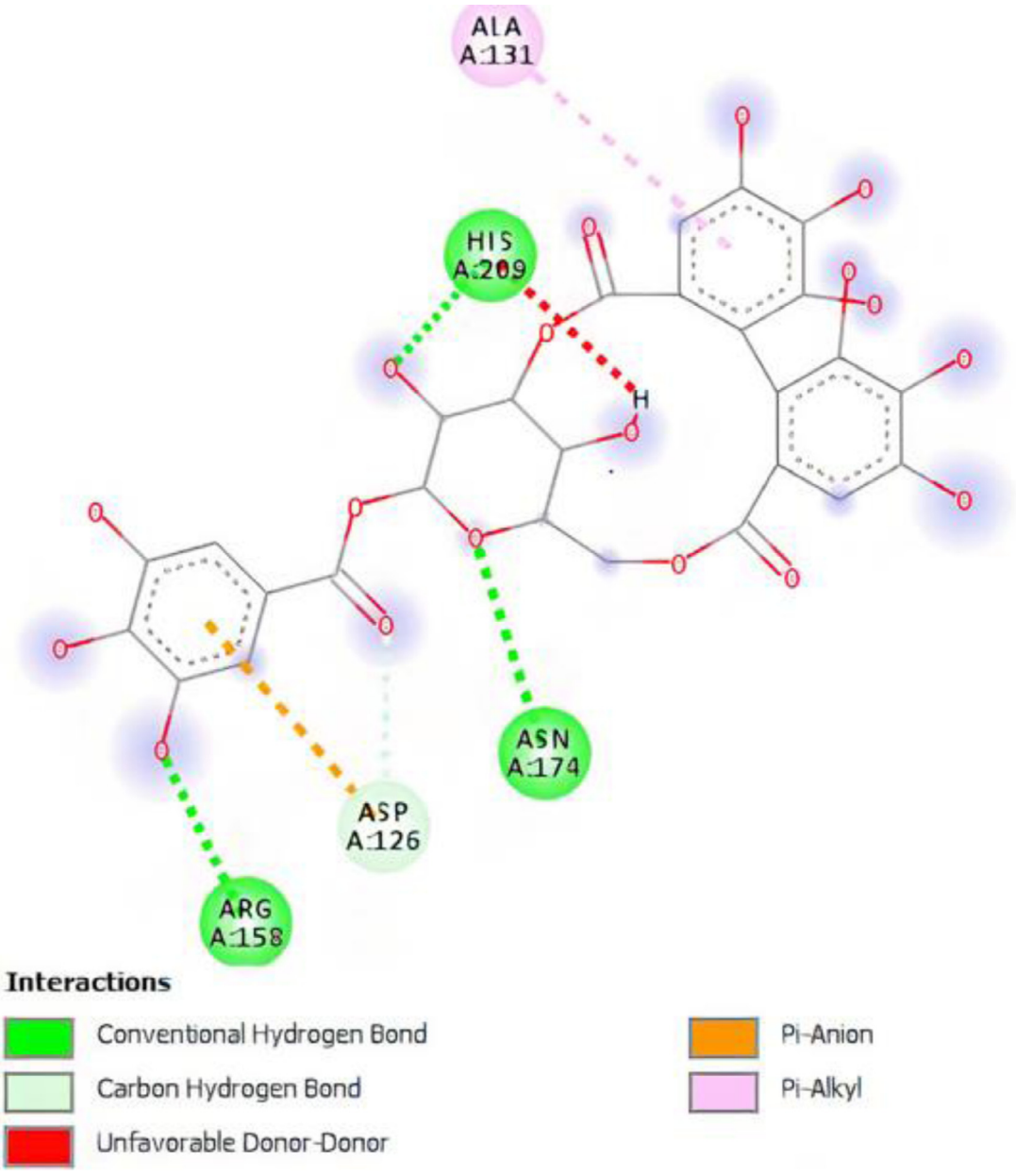

Fig. 1. 2D structures of interaction between compound 1 and α-glucosidase (PDB ID 3wy1).

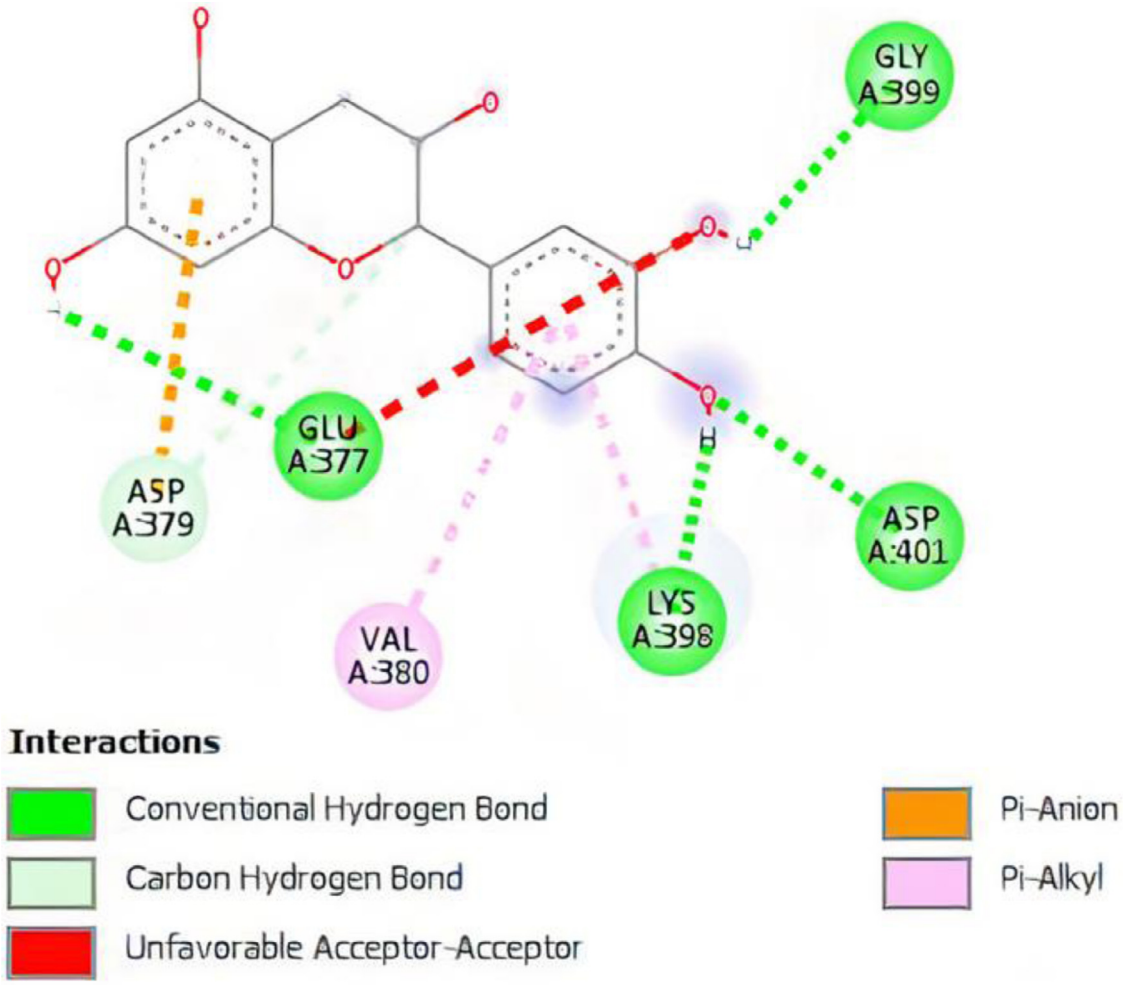

Fig. 2. 2D structures of interaction between compound 2 and α-glucosidase (PDB ID 3wy1).

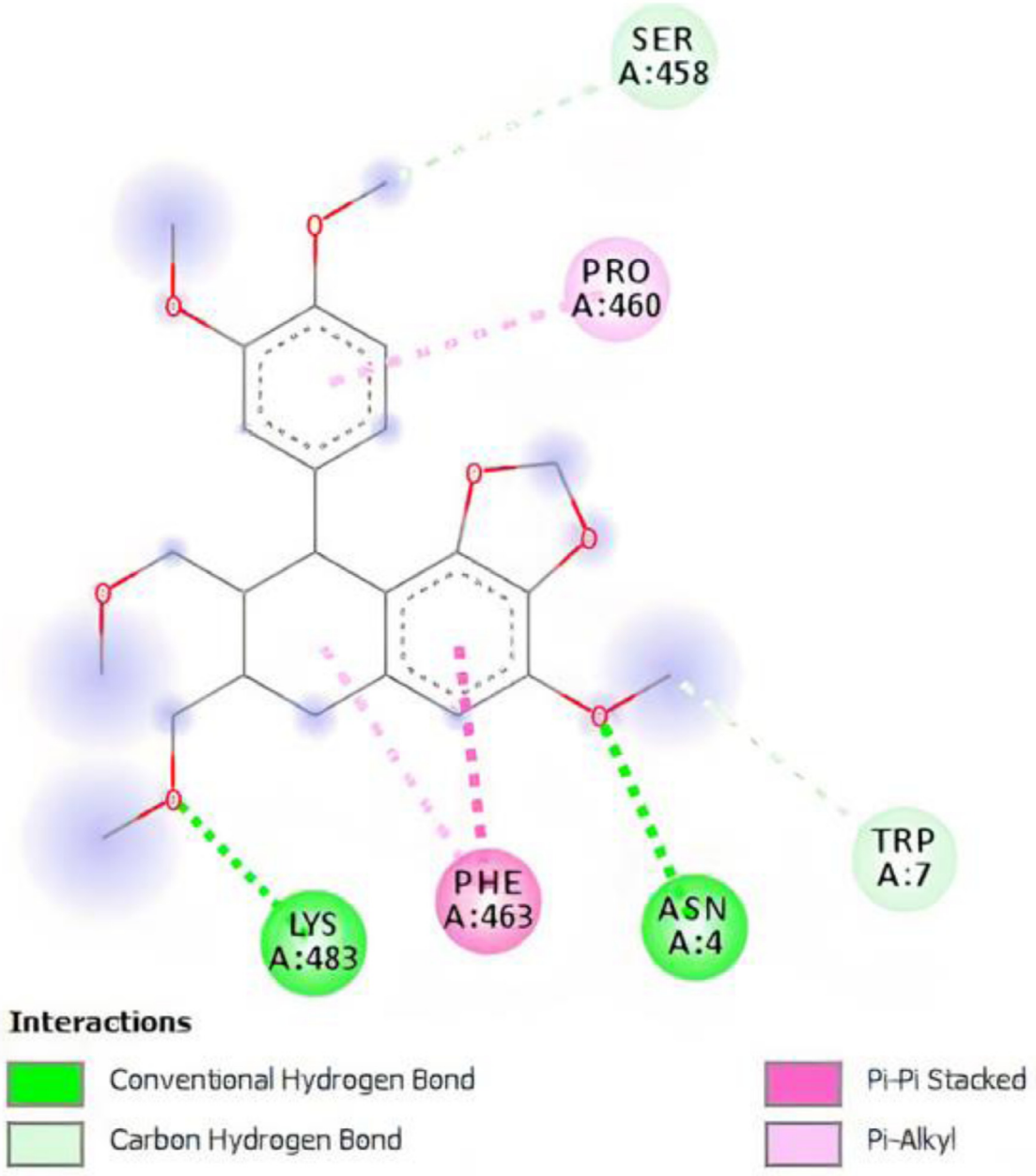

Fig. 3. 2D structures of interaction between compound 3 and α-glucosidase (PDB ID 3wy1).

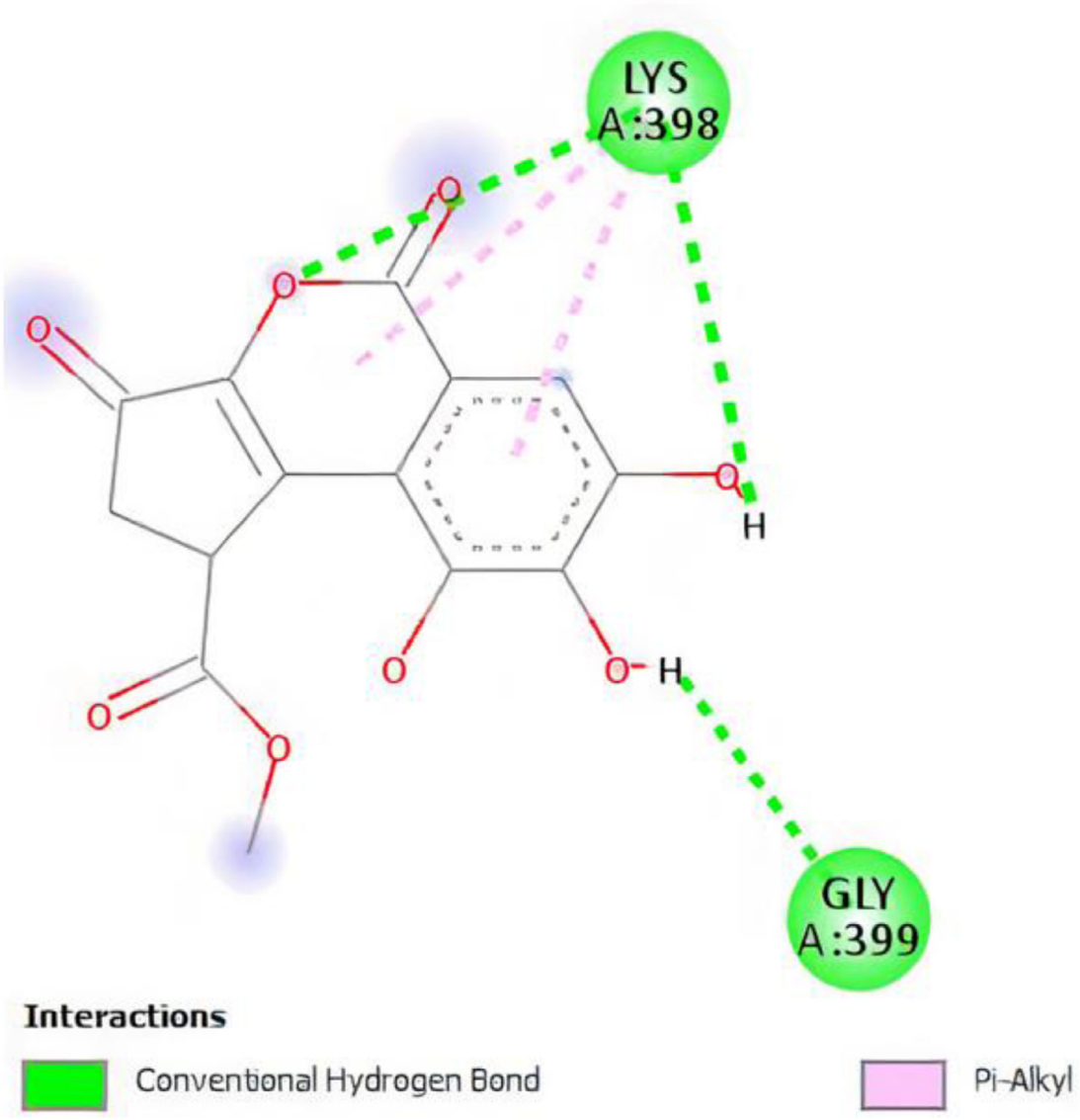

Fig. 4. 2D structures of interaction between compound 4 and α-glucosidase (PDB ID 3wy1).

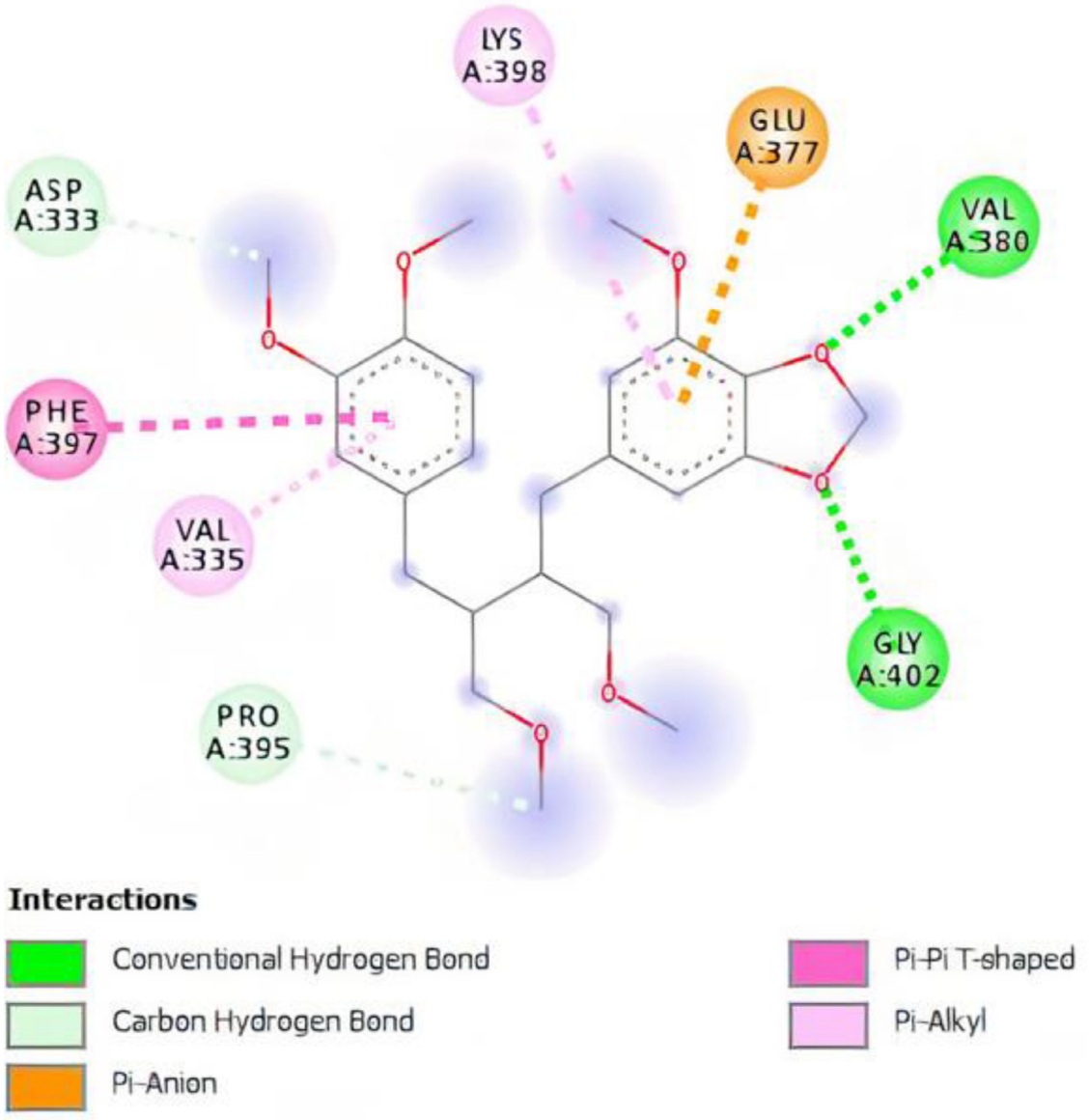

Fig. 5. 2D structures of interaction between compound 5 and α-glucosidase (PDB ID 3wy1).

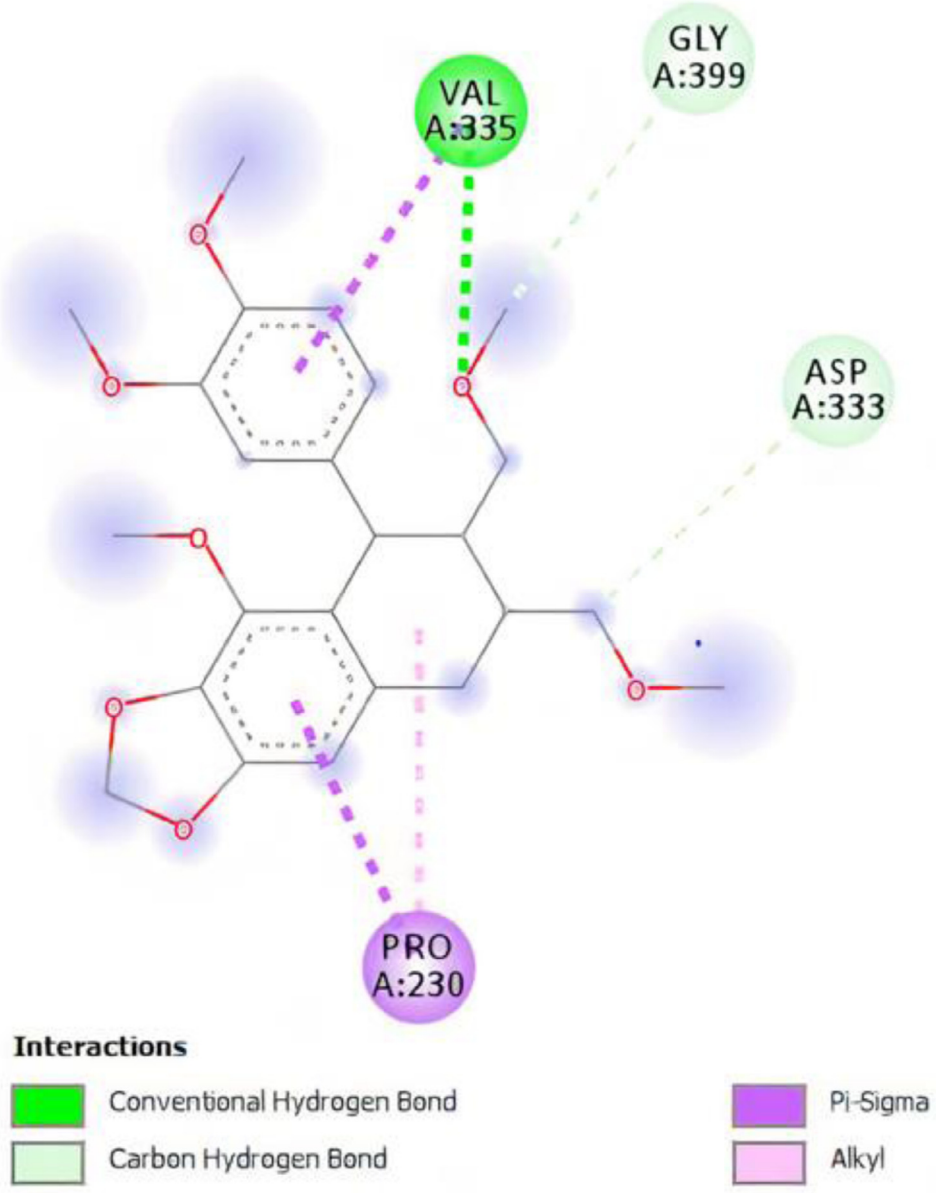

Fig. 6. 2D structures of interaction between compound 6 and α-glucosidase (PDB ID 3wy1).

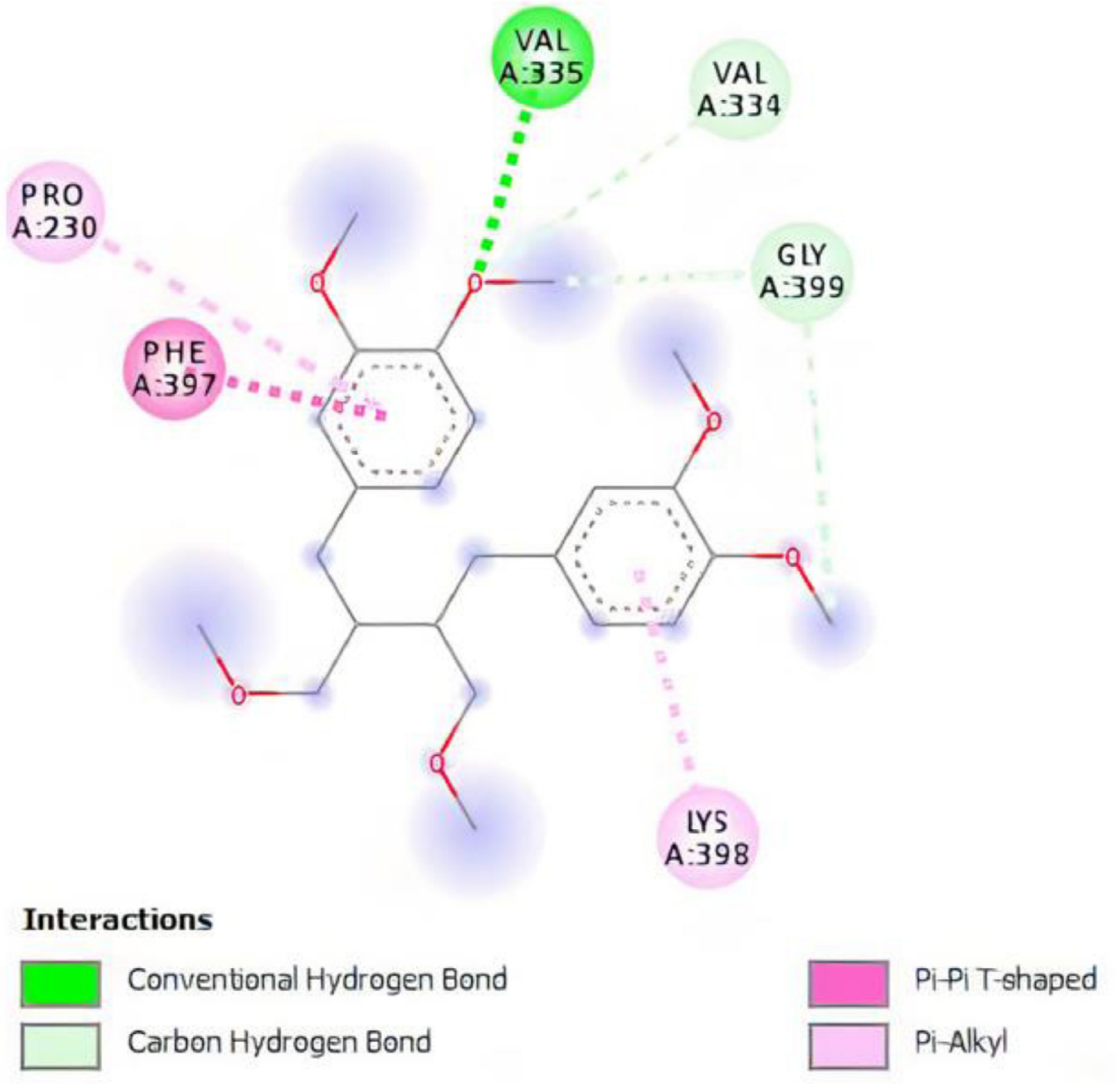

Fig. 7. 2D structures of interaction between compound 7 and α-glucosidase (PDB ID 3wy1).

Table 2
Calculated descriptors obtained from compounds from Phyllanthus amarus Leaves.

	E_{HOMO}(kcal/mol)	E_{LUMO}(kcal/mol)	DM(Debye)	MW(amu)	AREA(Å^2)	VOL (Å^3)	PSA (Å^2)	OVA-LITY	POL	HBD	HBA	Log P
1	-6.00	-1.30	9.16	634.45	505.94	521.26	251.78	1.62	82.55	11	15	-9.12
2	-5.70	-0.02	7.37	290.27	286.78	269.58	101.37	1.42	61.90	5	6	-3.72
3	-5.47	-0.13	3.25	430.49	459.93	440.08	49.06	1.64	75.81	0	7	-2.77
4	-6.17	-1.96	11.46	306.22	277.67	262.28	109.78	1.40	61.65	3	6	-3.65
5	-5.45	0.07	1.11	432.51	485.08	453.81	51.58	1.70	76.88	0	7	-1.94
6	-5.46	-0.18	1.71	430.49	456.31	439.24	48.912	1.63	75.76	0	7	-2.77
7	-5.53	0.09	1.91	418.53	484.64	453.79	42.71	1.70	76.86	0	6	-1.00

Table 3
Calculated binding affinity, types of interaction and amino acid residues involved in the interaction.

	Binding Affinity (kcal/mol)	Residues involved in the interactions	Types of Non-bonding interaction involved
1	-7.6	Ala131, His209, Asn174, Asp126, Arg158	Conventional Hydrogen Bond, Carbon Hydrogen bond, Unfavourbale Donor-Donor, Pi-Anion, Pi-Alkyl
2	-7.4	Asp379, Glu377, Val380, Lys398, Asp401, Gly399	Conventional Hydrogen Bond, Carbon Hydrogen bond, Unfavourbale Acceptor-Acceptor, Pi-Anion, Pi-Alkyl
3	-6.7	Ser458, Pro460, Lys483, Phe463, Asn4, Trp7	Conventional Hydrogen Bond, Carbon Hydrogen bond, Pi-Pi Stacked, Pi-Alkyl
4	-7.2	Lys398, Gly399	Conventional Hydrogen Bond, Pi-Alkyl
5	-5.9	Asp333, Phe397, Val335, Pro395, Gly402, Val380, Glu377, Lys398	Conventional Hydrogen Bond, Carbon Hydrogen bond, Pi-Anion, Pi-Pi T-Shaped, Pi-Alkyl
6	-6.5	Val335, Gly399, Asp333, Pro230	Conventional Hydrogen Bond, Carbon Hydrogen bond, Pi-Sigma, Alkyl
7	-5.1	Pro230, Phe397, Val335, Val334, Gly399, Lys398	Conventional Hydrogen Bond, Carbon Hydrogen bond, Pi-Pi T-Shaped, Pi-Alkyl
Metformin	-6.0	-	-

in Table 3, the calculated binding affinity for compound **1** to **7** were -7.6 kcal/mol, -7.4 kcal/mol, -6.7 kcal/mol, -7.2 kcal/mol, -5.9 kcal/mol, -6.5 kcal/mol, and -5.1 kcal/mol. The calculated binding affinity for compound **5** and **7** showed that they were not as efficient as other studied compounds as well as the referenced drug in inhibiting α-glucosidase.

According to Oyewole et al., [30], higher the binding affinity (in term of negativity) is expected to bring about utmost inhibitory activity of such drug-like compounds; thus, compound **1** with -7.6 kcal/mol proved to be more potent than other studied compound including the referenced drug (Metformin). The residues involve in the interaction for each ligand was Ala131, His209, Asn174, Asp126, Arg158 for compound **1**; Asp379, Glu377, Val380, Lys398, Asp401, Gly399 for compound **2**; Ser458, Pro460, Lys483, Phe463, Asn4, Trp7 for compound **3**; Lys398, Gly399 for compound **4**; Asp333, Phe397, Val335, Pro395, Gly402, Val380, Glu377, Lys398 for compound **5**; Val335, Gly399, Asp333, Pro230 for compound **6** and Pro230, Phe397, Val335, Val334, Gly399, Lys398 for compound **7**. Also, series of interactions observed in the docking calculation are shown in Table 3 and Figs. 1–7.

3.3. Predicted ADME properties

Absorption, distribution, metabolism and excretion (ADME) properties of the studied compounds were examined using swissadme online software [31]. Compound with highest calculated binding affinity and referenced drug were considered and the predicted reports were displayed in Table 4. As shown in Table 4, different categories of factors describing the ADME properties of the studied compounds were physicochemical, lipophilicity, water solubility, pharmacokinetics, druglikeness and medicinal chemistry. The calculated lipophilicity for any drug-like compound was expected to obey the standard rule (-0.7 < XLOGP3 < 0.5) and it was observed that the calculated lipophilicity for compound **1** were within the accepted range; thus, compound 1 has the ability to dissolve in lipophilic solutions which is one of the essential criteria for drug-like molecules to infuse through many biological membranes.

The flexibility of drug-like compound could be determined based on the rotatable bond which was expected to fall within 0 - 9; therefore, compound **1** fairly correlated to the referenced drug in term of flexibility. As shown in Table 4, compound **1** and **Metformin** are non-inhibitors of CYP1A2, CYP2C19, CYP2C9, CYP2D6 and CYP3A4. Other predicted ADME properties are shown in Table 3.

4. Conclusion

In this work, seven molecular compounds were selected among the compounds present in *Phyllanthus amarus* leaves and subjected to *in-silico* study. The calculated descriptors from the optimized compounds from *Phyllanthus amarus* leaves perfectly showed potential anti-diabetic activities of the studied compounds. [(1*S*,19*R*,21*S*,22*R*,23*R*)-6,7,8,11,12,13,22,23-octahydroxy-3,16-dioxo-2,17,20-trioxatetracyclo[17.3.1.$0^{4,9}$.$0^{10,15}$]tricosa-4,6,8,10,12,14-hexaen-21-yl] 3,4,5-trihydroxybenzoate (**Compound 1**) with -7.6 kcal/mol proved to have ability to inhibit α-glucosidase (PDB ID 3wy1) than other studied compounds as well as Metformin (Referenced Drug). Also, fair correlation was observed between the ADME properties of compound **1** and Metformin.

Availability of data and materials

All data generated or analysed during this study are included in this published article.

Ethics approval, guidelines and consent to participate

Not Applicable

Consent for publication

Not Applicable

Table 4
ADME properties of the studied compounds.

	Compound 1	Metformin
Physicochemical Properties		
Num. heavy atoms	45	9
Num. arom. heavy atoms	18	0
Fraction Csp3	0.22	0.50
Num. rotatable bonds	3	2
Num. H-bond acceptors	18	2
Num. H-bond donors	11	3
Molar Refractivity	141.85	36.93
TPSA	310.66 Å^2	91.49 Å^2
Lipophilicity		
Log $P_{o/w}$ (iLOGP)	0.92	0.34
Log $P_{o/w}$ (XLOGP3)	0.07	-1.27
Log $P_{o/w}$ (WLOGP)	-0.30	-1.24
Log $P_{o/w}$ (MLOGP)	-2.42	-0.96
Log $P_{o/w}$ (SILICOS-IT)	-2.15	-1.74
Consensus Log $P_{o/w}$	-0.78	-0.98
Water Solubility		
Log S (ESOL)	-3.92	0.29
Solubility	7.70e-02 mg/ml; 1.21e-04 mol/l	2.53e+02 mg/ml; 1.96e+00 mol/l
Class	Soluble	Highly soluble
Log S (Ali)	-6.15	-0.15
Solubility	4.52e-04 mg/ml; 7.12e-07 mol/l	9.05e+01 mg/ml; 7.00e-01 mol/l
Class	Poorly soluble	Very soluble
Log S (SILICOS-IT)	-0.51	0.58
Solubility	1.95e+02 mg/ml; 3.07e-01 mol/l	4.90e+02 mg/ml; 3.79e+00 mol/l
Class	Soluble	Soluble
Pharmacokinetics		
GI absorption	Low	High
BBB permeant	No	No
P-gp substrate	Yes	No
CYP1A2 inhibitor	No	No
CYP2C19 inhibitor	No	No
CYP2C9 inhibitor	No	No
CYP2D6 inhibitor	No	No
CYP3A4 inhibitor	No	No
Log K_p (skin permeation)	-10.12 cm/s	-7.99 cm/s
Druglikeness		
Lipinski	No; 3 violations: MW>500, NorO>10, NHorOH>5	Yes; 0 violation
Ghose	No; 2 violations: MW>480, MR>130	No; 3 violations: MW<160, WLOGP<-0.4, MR<40
Veber	No; 1 violation: TPSA>140	Yes
Egan	No; 1 violation: TPSA>131.6	Yes
Muegge	No; 4 violations: MW>600, TPSA>150, H-acc>10, H-don>5	No; 2 violations: MW<200, #C<5
Bioavailability Score	0.17	0.55
Medicinal Chemistry		
PAINS	1 alert: catechol_A	0 alert
Brenk	2 alerts: catechol, more_than_2_esters	2 alerts: imine_1, imine_2
Leadlikeness	No; 1 violation: MW>350	No; 1 violation: MW<250
Synthetic accessibility	6.66	3.02

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Declaration of Competing Interest

The authors declare no conflict of interest.

CRediT authorship contribution statement

Abel K. Oyebamiji: Conceptualization, Methodology, Writing – review & editing, Writing – original draft, Data curation, Investigation. **Emmanuel A. Soetan:** Methodology, Writing – review & editing, Writing – original draft. **Sunday A. Akintelu:** Methodology, Writing – original draft, Investigation, Data curation, Writing – review & editing. **Ademola O. Ayeleso:** Supervision, Writing – review & editing, Writing – original draft. **Emmanuel Mukwevho:** Supervision, Writing – review & editing, Writing – original draft.

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