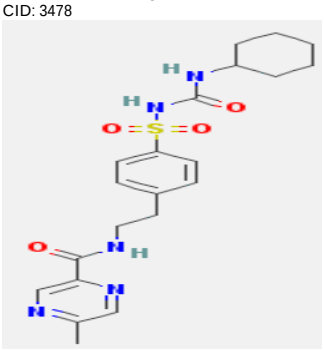
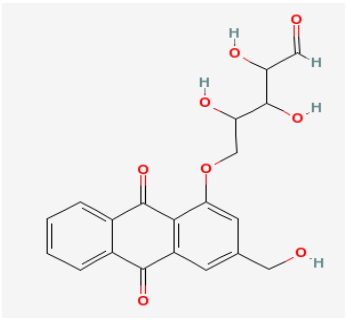
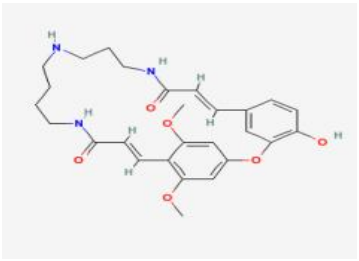
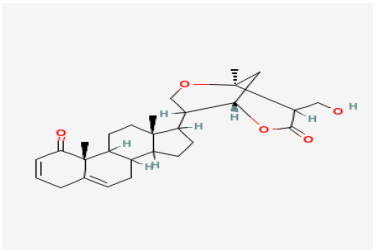
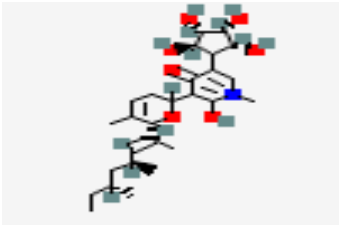
BIOINFORMATION open access

Supplementary material:

Table 1: Comparative study representation of drug likeness and biochemical properties, docking score (using Hex and Quantum) and binding pocket analysis for AhG compounds vs. bench mark drug satisfying Protein-Ligand Interaction study (Stage I and II).

Sl. No.	Name of the plant (the compound)	Chemical properties of the compound	Docking score	Binding Analysis	Pocket
Std Drug	Flax plant (Glipizide) **Structure of the compound** CID: 3478  **Canonical smile:** CC1=NC=C(N=C1)C(=O)NCCC2=CC=C(C=C2)S(=O)(=O)NC(=O)NC3CCCCC3	**Lipinski Rule:** Molecular Weight : 445.53518 [g/mol] Molecular Formula : $C_{21}H_{27}N_5O_4S$ XLogP3-AA : 1.9 H-Bond Donor : 3 H-Bond Acceptor : 6 **Chemical/Bio-activity** miLogP: 2.313 GPCR ligand: 0.31 Ion channel Modulator: -0.01 Kinase inhibitor: -0.17 Nuclear receptor Ligand: -0.40	**Hex Score:** **Energy minimized (Kcal/mol)** / **Docking results (E-Total)** 151.85 / -257.66 **Quantum Score:** **Gibbs free energy (kcal/mol)** / **Root Mean Square Deviation (A°)** -19.38 / 47.39	**Amino acid base** LEU 32 **Rank:**	**H-Bond distance (A°)** 1.63
1.	Aloe barbadensis (Aloins) **Structure of the compound** CID: 221037  **Canonical smile:** C1=CC=C2C(=C1)C(=O)C3=CC(=CC(=C3C2=O)OCC(C(C(C=O)O)O)O)CO	**Lipinski Rule:** Molecular Weight : 386.35212 [g/mol] Molecular Formula : $C_{20}H_{18}O_8$ XLogP3-AA :- 0.4 H-Bond Donor : 4 H-Bond Acceptor : 8 **Chemical/Bio-activity** miLogP: 1.071 GPCR ligand: -0.02 Ion channel Modulator: -0.03 Kinase inhibitor: -0.02 Nuclear receptor Ligand: 0.15	**Hex Score:** **Energy minimized (Kcal/mol)** / **Docking results (E-Total)** 50.12 / -260.48 **Quantum Score:** **Gibbs free energy (kcal/mol)** / **Root Mean Square Deviation (A°)** -20.07 / 25.92	**Amino acid base** GLU 30 **Rank: FOURTH**	**H-Bond distance (A°)** 2.50
2.	Capparis decidua (Capparisin-ine) **Structure of the compound** CID: 16058118  **Canonical smile:** COC1=CC2=CC(=C1C=CC(=O)NCCCCNCCCNC(=O)C=CC3=CC(=C(C=C3)O)O2)OC	**Lipinski Rule:** Molecular Weight : 495.56742 [g/mol] Molecular Formula : $C_{27}H_{33}N_3O_6$ XlogP3-AA : 3 H-Bond Donor : 4 H-Bond Acceptor : 7 **Chemical/Bio-activity** miLogP: 2.734 GPCR ligand: 0.12 Ion channel Modulator: -0.07 Kinase inhibitor: -0.01 Nuclear receptor Ligand: 0.07	**Hex Score:** **Energy minimized (Kcal/mol)** / **Docking results (E-Total)** 150.29 / -283.00 **Quantum Score:** **Gibbs free energy (kcal/mol)** / **Root Mean Square Deviation (A°)** -20.40 / 32.96	**Amino acid base** GLY 59 **Rank: THIRD**	**H-Bond distance (A°)** 1.73
3.	Desmodium Gangeticum (Daturilinol) **Structure of the compound** CID: 5316315  **Canonical smile:** CC12CCC3C(C1CCC2C4COC5(CC4OC(=O)C5CO)C)CC=C6C3(C(=O)C=CC6)C	**Lipinski Rule:** Molecular Weight: 454.59832 [g/mol] Molecular Formula: $C_{28}H_{38}O_5$ XLogP3-AA: 4.8 H-Bond Donor: 1 H-Bond Acceptor: 5 **Chemical/Bio-activity** miLogP: 4.607 GPCR ligand: 0.14 Ion channel Modulator: 0.17 Kinase inhibitor: -0.56 Nuclear receptor Ligand: 0.63	**Hex Score:** **Energy minimized (Kcal/mol)** / **Docking results (E-Total)** 371.14 / -267.19 **Quantum Score:** **Gibbs free energy (kcal/mol)** / **Root Mean Square Deviation (A°)** -11.16 / 26.69	**Amino acid base** LEU 32, GLY 59 **Rank: SIXTH**	**H-Bond distance (A°)** 1.60, 1.70

4. Senna occidentalis (L.)
(Funiculosin)
Structure of the compound
CID: 6444332



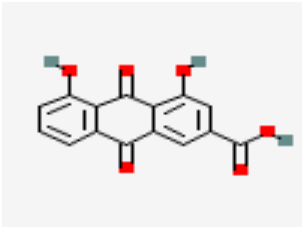
Canonical smile:
CCC(C)CC(C)C=C(C)C1C(=CCC(O1)C2=C(N(C=C(C2=O)C3C(C(C(C3O)O)O)O)C)O)C

Lipinski Rule:
Molecular Weight : 491.61694 [g/mol]
Molecular Formula : $C_{27}H_{41}NO_7$
XLogP3-AA: 2.1
H-Bond Donor: 5
H-Bond Acceptor: 8

Chemical/Bio-activity
miLogP: 2.323
GPCR ligand: 0.20
Ion channel Modulator: -0.03
Kinase inhibitor: -0.06
Nuclear receptor Ligand: 0.28

Hex Score:	Amino acid base	H-Bond (Aº)	distance
Energy minimized (Kcal/mol)	Docking results (E-Total)		
91.58	-269.31	GLU 13	1.21
Quantum Score:	Rank: FIRST		
Gibbs free energy (kcal/mol)	Root Mean Square Deviation (Aº)		
-37.52	38.95		

5. Senna occidentalis (L.)
(Rhein)
Structure of the compound
CID: 10168



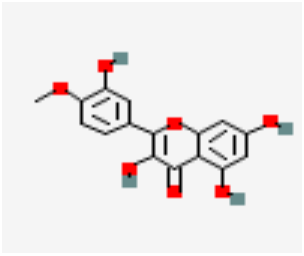
Canonical smile:
C1=CC2=C(C(=C1)O)C(=O)C3=C(C=C(C=C3C2=O)C(=O)O)O

Lipinski Rule:
Molecular Weight: 284.22042 [g/mol]
Molecular Formula: $C_{15}H_8O_6$
XLogP3-AA: 2.2
H-Bond Donor: 3
H-Bond Acceptor: 6

Chemical/Bio-activity
miLogP: 2.997
GPCR ligand: -0.08
Ion channel Modulator: -0.10
Kinase inhibitor: 0.01
Nuclear receptor Ligand: 0.29

Hex Score:	Amino acid base	H-Bond (Aº)	distance
Energy minimized (Kcal/mol)	Docking results (E-Total)		
37.06	-258.48	LEU 32, GLY 59	1.56, 2.17
Quantum Score:	Rank: SECOND		
Gibbs free energy (kcal/mol)	Root Mean Square Deviation (Aº)		
-27.32	39.09		

6. Costus spicatus
(Tamarixetin)
Structure of the compound
CID: 5281699



Canonical smile:
COC1=C(C=C(C=C1)C2=C(C(=O)C3=C(C=C(C=C3O2)O)O)O)O

Lipinski Rule:
Molecular Weight : 316.26228 [g/mol] Molecular Formula : $C_{16}H_{12}O_7$ XLogP3-AA : 1.9 H-Bond Donor : 4 H-Bond Acceptor : 7

Chemical/Bio-activity
miLogP: 1.99
GPCR ligand: -0.10
Ion channel Modulator: -0.26
Kinase inhibitor: 0.25
Nuclear receptor Ligand: 0.28

Hex Score:	Amino acid base	H-Bond (Aº)	distance
Energy minimized (Kcal/mol)	Docking results (E-Total)		
-17.56	-258.00	ILE 25	1.54
Quantum Score:	Rank: FIFTH		
Gibbs free energy (kcal/mol)	Root Mean Square Deviation (Aº)		
-15.65	19.70		

Table 2: Pharmacokinetic and pharmodynamic studies for AhG compounds on various body organelles.

Sl. No.	Compound	ADME Properties					Toxicity Properties					
		Oral Availability	Solubility	Drug binding to plasma protein	Volume of Distrib-ution	AMES	Health effect					
							B^a	C^a	G^a	K^a	Li^a	Lu^a
Drug	Glipizide	%F(Oral) > 30%: 0.886 %F(Oral) > 70%: 0.732	-3.15	%PPB: 99.13% LogKa HSA : 4.86	0.19 L / kg	0.000	0.46	0.92	0.97	0.31	0.28	0.23
1	Aloins	%F(Oral) > 30%: 0.086 %F(Oral) > 70%: 0.040	-3.53	%PPB: 15.83% LogKa HSA: 2.94	1.29 L / kg	0.739	0.20	0.85	0.35	0.30	0.18	0.20
2	Capparisi-nine	%F(Oral) > 30%: 0.729 %F(Oral) > 70%: 0.521	-2.13	%PPB: 61.93% LogKa HSA: 3.92	3.42 L / kg	0.207	0.00	0.02	0.92	0.18	0.14	0.00
3	Funiculosin	%F(Oral) > 30%: 0.773 %F(Oral) > 70%: 0.148	-3.66	%PPB: 98.55% LogKa HSA: 4.04	0.36 L / kg	0.018	0.98	0.99	0.99	0.97	0.94	0.99
4	Rhein	%F(Oral) > 30%: 0.296 %F(Oral) > 70%: 0.080	-2.99	%PPB: 97.49% LogKa HSA: 5.16	0.23 L / kg	0.977	0.15	0.34	0.23	0.09	0.06	0.41

B^a= Blood; C^a= Cardiovascular system; G^a= Gastrointestinal system; K^a= Kidney; Li^a= Liver; Lu^a= Lungs