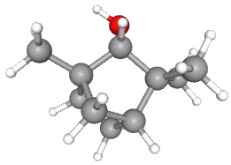
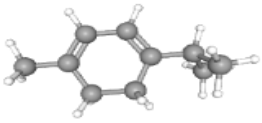
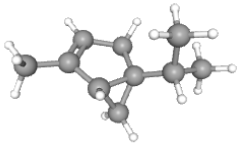
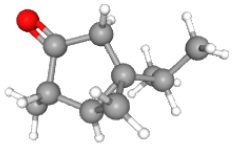
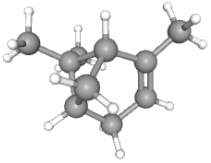
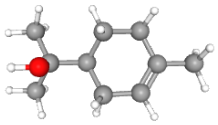
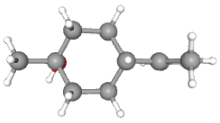
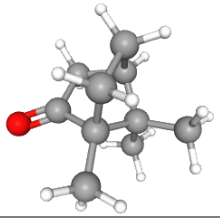
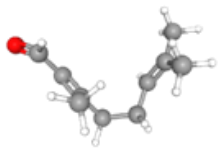
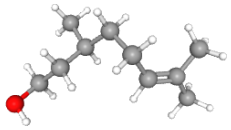
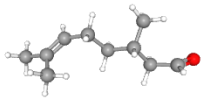
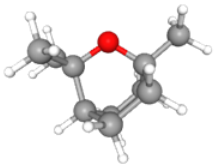
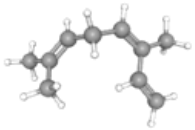
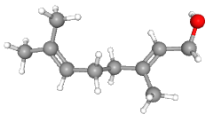
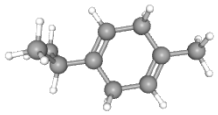
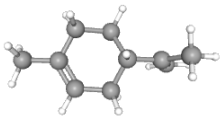
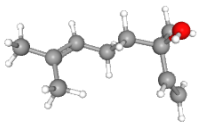
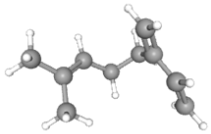
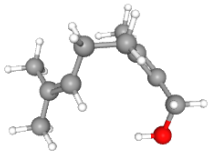
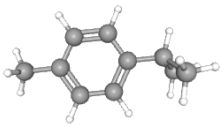
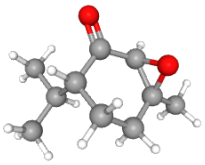
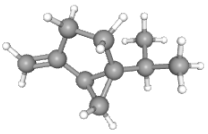
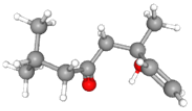
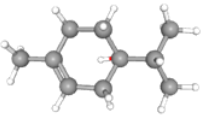
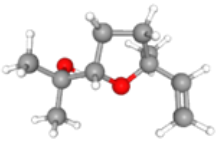
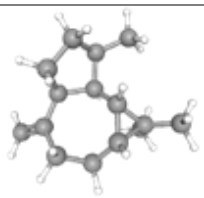
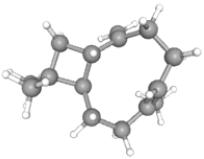
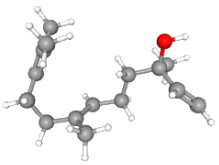
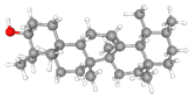
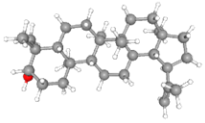
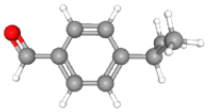
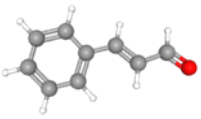
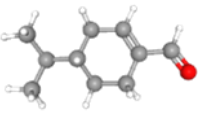
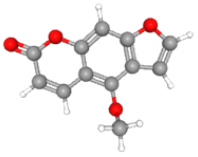
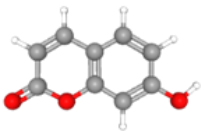
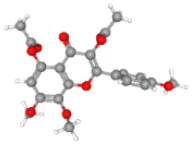
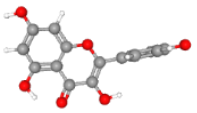
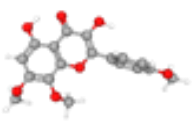
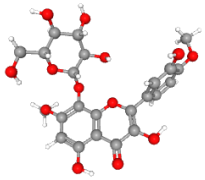
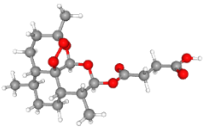
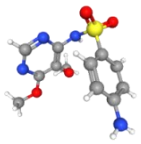
Supplementary Table 1. The molecular weight, molecular formula, and structure of the specific phytochemicals from *Z. armatum.*

Sr. No.	Ligand name	PubChem CID	Molecular formula	Molecular weight	Structure
1.	α -Fenchol	CID 439711	$C_{10}H_{18}O$	154.25g/mol	
2.	α -Terpinene	CID 7462	$C_{10}H_{16}$	136.23 g/mol	
3.	α -Thujene	CID 6453408	$C_{10}H_{16}$	136.23 g/mol	
4.	α -Thujone	CID 261491	$C_{10}H_{16}O$	152.23 g/mol	
5.	α-Pinene	CID 6654	$C_{10}H_{16}$	136.23 g/mol	
6.	α-Terpineol	CID 17100	$C_{10}H_{18}O$	154.25 g/mol	
7.	β-Terpineol	CID 8748	$C_{10}H_{18}O$	154.25 g/mol	
8.	Camphor	CID 2537	$C_{10}H_{16}O$	152.23 g/mol	

9.	Citral	CID 638011	$C_{10}H_{16}O$	152.23 g/mol	
10.	Citronellol	CID 8842	$C_{10}H_{20}O$	156.26 g/mol	
11.	Citronellal	CID 7794	$C_{10}H_{18}O$	154.25 g/mol	
12.	1,8-cineole	CID2758	$C_{10}H_{18}O$	154.25 g/mol	
13.	Cis -ocimene	CID 5320250	$C_{10}H_{16}$	136.23 g/mol	
14.	Geraniol	CID637566	$C_{10}H_{18}O$	154.25 g/mol	
15.	ɣ-terpinene	CID7461	$C_{10}H_{16}$	136.23 g/mol	
16.	Limonene	CID22311	$C_{10}H_{16}$	136.23 g/mol	
17.	Linalool	CID6549	$C_{10}H_{18}O$	154.25 g/mol	
18.	Myrcene	CID31253	$C_{10}H_{16}$	136.23 g/mol	

19.	Nerol	CID643820	$C_{10}H_{18}O$	154.25 g/mol	
20.	P-cymene	CID7463	$C_{10}H_{14}$	134.22 g/mol	
21.	Piperitone	CID 6987	$C_{10}H_{16}O$	152.23 g/mol	
22.	Sabinene	CID 18818	$C_{10}H_{16}$	136.23 g/mol	
23.	Tagetonol	CID 522417	$C_{10}H_{18}O2$	170.25 g/mol	
24.	Terpinen-4-ol	CID11230	$C_{10}H_{18}O$	154.25 g/mol	
25.	(*Z*)-Linalool oxide	CID6431477	$C_{10}H_{18}O2$	170.25g/mol	
26.	*allo*-Aromadenderene	CID10899740	$C_{15}H_{24}$	204.35 g/mol	
27.	β-caryophllene	CID 5281515	$C_{15}H_{24}$	204.35 g/mol	
28.	(*E*)-nerolidol	CID 5284507	$C_{15}H_{26}O$	222.37g/mol	

29.	α-Amyrins	CID 73170	$C_{30}H_{50}O$	426.7g/mol	
30.	lupeol	CID259846	$C_{30}H_{50}O$	426.7g/mol	
31.	Cuminal	CID325	$C_{10}H_{14}O$	150.22 g/mol	
32.	Cinnamic aldehyde	CID637511	C_9H_8O	132.16g/mol	
33.	Phellandral	CID 89488	$C_{10}H_{16}O$	152.23g/mol	
34.	2-Tridecanone	CID 11622	$C_{13}H_{26}O$	198.34g/mol	
35.	Bergapten	CID 2355	$C_{12}H_8O_4$	216.19g/mol	
36.	Umbelliferon	CID5281426	$C_9H_6O_3$	162.14 g/mol	
37.	3,5-Diacetyltambulin	CID5316626	$C_{22}H_{20}O_9$	428.4 g/mol	
38.	Kaempferol	CID5280863	$C_{51}H_{10}O_6$	286.24 g/mol	
39.	Tambulin	CID5281700	$C_{18}H_{16}O_7$	344.3 g/mol	

40.	Tambuletin	CID 9936050	$C_{23}H_{24}O_{13}$	508.4g/mol	
Artesunate		6917864	384.4 g/mol	$C_{19}H_{28}O_8$	
Sulfadoxine		CID 17134	$C_{12}H_{14}N_4O_4S$	310.33g/mol	

Supplementary Table 2. Lipinski rule of 5 properties of phytochemicals of *Z. armatum*.

Ligands	M log p <4.15	MW g/mol<500g/mol	NOHNH <5	NON < 10	TPSA(A^2)<140ºA	Number of rotatable bonds (<10)	Lipinski's Violation
α-Fenchol	2.50	154.25	1	1	20.23	0	Yes'0 violation
α-Terpinene	3.30	136.23	0	0	0.00	1	Yes'0 violation
α-Thujene	3.15	136.23	0	0	0.00	1	Yes'0 violation
α-Thujone	2.35	15.23	1	0	17.07	1	Yes'0 violation
α-Pinene	3.44	136.23	0	0	0.00	0	Yes'0 violation
α-Terpineol	2.58	154.25	1	0	20.23	1	Yes'0 violation
β-Terpineol	2.44	154.25	1	1	20.23	1	Yes'0 violation
Citral	2.71	152.23	1	0	17.07	4	Yes'0 violation
Camphor	2.37	152.23	1	0	17.07	0	Yes'0 violation
Citronellol	2.92	156.27	1	1	20.23	5	Yes'0 violation
Citronellal	2.94	154.25	1	0	17.07	5	Yes'0 violation
1,8cineole	2.67	154.25	1	0	9.23	0	Yes'0 violation
Cis-ocimene	3.40	136.23	0	0	0.00	3	Yes'0 violation
Geraniol	2 78	154.25	1	1	20.23	4	Yes'0 violation
γ-terpinene	3.35	136.23	0	0	0.00	1	Yes '0 violation
Limonene	3.37	136.23	0	0	0.00	1	Yes'0 violation
Linalool	2.05	170.25	2	1	29.46	2	Yes'0 violation
Myrcene	3 43	136.23	0	0	0.00	4	Yes'0 violation
Nerol	2.78	154.25	1	1	20.23	4	Yes'0 violation
P-cymene	3.50	134.25	0	0	0.00	1	Yes'0 violation
Piperitone	2.52	152.23	1	0	17.07	1	Yes'0 violation
Sabinene	3.25	136.23	0	0	0.00	1	Yes'0violation
Tagetonol	1.92	170.25	2	1	37.30	5	Yes '0 violation

Terpinen-4-ol	2.60	154.25	1	1	20.23	1	Yes'0 violation
(*Z*)-Linalool oxide	2.05	170.25	2	1	29.46	2	Yes '0 violation
***allo*-Aromadendrene**	4.19	204.35	0	1	0.00	0	Yes"1violationMLOGP>4.15
β-caryophyllene	4.24	204.35	0	0	0.00	0	Yes'1violationMLOGP>4.15
(*E*)-Nerolidol	4.19	222.37	1	1	20.23	7	Yes'1violationMLOGP>4.15
α-Amyrins	7.05	426.72	1	1	20.23	0	Yes'1violationMLOGP>4.15
lupeol	7.26	426.72	1	1	20.23	1	Yes'1violation MLOGP>4.15
Cuminal	2.48	148.20	1	0	17.07	2	Yes'0 violation
Cinamic aldehyde	2.48	148.20	1	0	17.07	2	Yes'0 violation
Phellandral	2.48	148.20	1	0	17.07	2	Yes'0 violation
2-Tridecanone	4.25	198.34	1	0	17.07	10	Yes'0 violation
Umbelliferon	1.51	162.14	3	1	50.44	0	Yes'0 violation
Bergapten	2.16	216.19	4	0	52.58	1	Yes'0 violation
3,5-Diacetyltambulin	3.01	428.39	9	0	110.50	8	Yes'0 violation
Kaempferol	1.58	286.24	6	4	111.13	1	Yes'0 violation
Tambuletin	0.09	508.43	13	7	208.74	6	No 3 violation MW<500,N or0<10,NH orOH<5
Tambulin	2.49	344.32	7	2	98.36	4	Yes'0 violation
Artesunate	2.92	384.5	1	8	100	5	0
Sulfadoxine	0.36	310.33	3	8	116.44	5	0

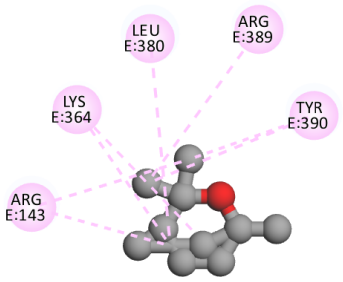
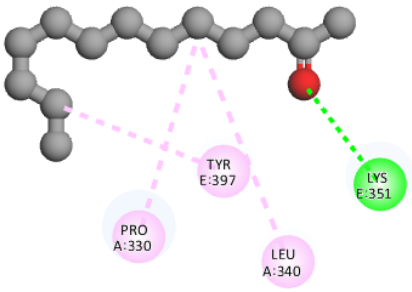
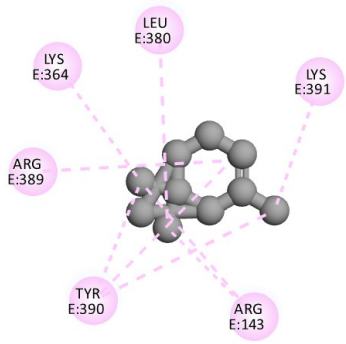
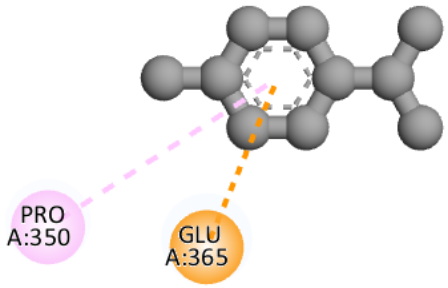
Supplementary Table 3. Drug likeness properties of phytochemicals of *Z. armatum*

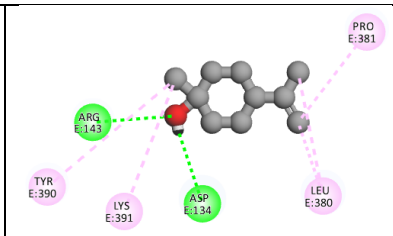
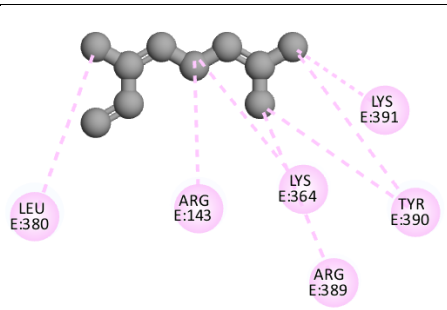
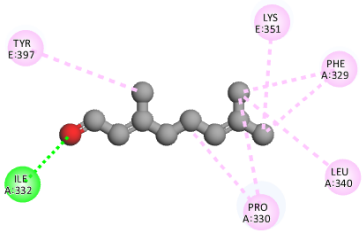
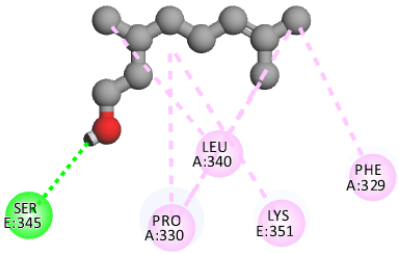
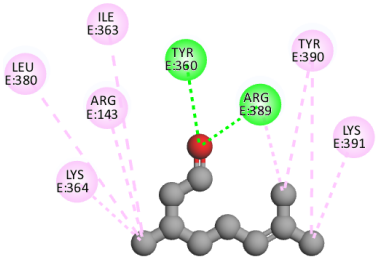
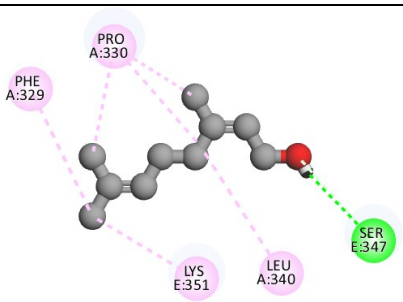
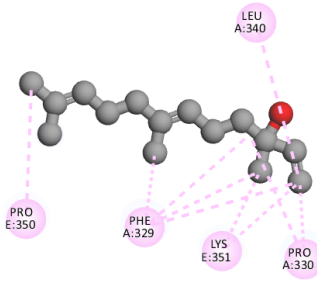
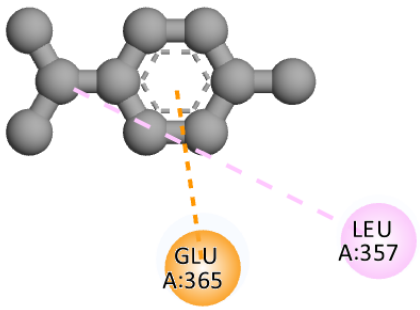
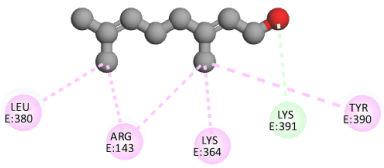
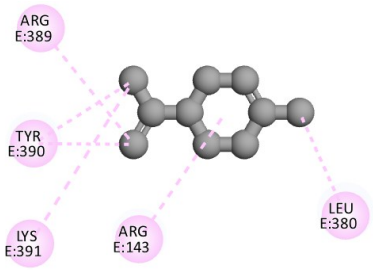
ligand	Ghoshe	Veber	Egen	Muegge	Bioavailability score
α-Fenchol	No; 1 violation: #atoms<20	yes	Yes	No ;1violation: MW<200	0.55
α-Terpinene	No; 1 violation: #atoms<20	yes	Yes	No ;1violation:MW<200	0.55
α-Thujene	No; 1 violation: MW<160	yes	Yes	No ;1violation: MW<200	0.55
α-Thujone	No;1 violation: MW<160	no	No	No; 2 violations: MW<200, Heteroatoms<2	0.55
α-Pinene	No; 1 violation: MW<16	yes	Yes	No; 2 violations: MW<200, Heteroatoms<2	0.55
α-Terpineol	No; 1 violation: MW<160	yes	Yes	No; 2 violations: MW<200, Heteroatoms<2	0.55
β-Terpineol	No,1 violationMW<160	Yes	Yes	No;2 violation: MW<200, Hetero atoms<2	0.55
Citral	No,1 violation MW<160	Yes	Yes	No;2 violation MW<200, Hetero atoms<2	0.55
Camphor	No,1 violation MW<160	Yes	Yes	No;2 violation MW<200. Hetero atoms <2	0.55
Citronellol	No,1 violation MW<160	Yes	Yes	No;2 violation MW<200. Hetero atoms <2	0.55
Citronellal	No,1 violation MW<160	Yes	Yes	No;2 violation MW<200. Hetero atoms <2	0.55
1,8cineole	No,1 violation MW<160	Yes	Yes	No;2 violation MW<200. Hetero atoms <2	0.55
Cis-ocimene	No,1 violation MW<160	Yes	Yes	No;2 violation MW<200. Hetero atoms <2	0.55
Geraniol	No,1 violation MW<160	Yes	Yes	No;2 violation MW<200. Hetero atoms <2	0.55
γ-terpinene	No,1 violation MW<160	Yes	Yes	No;2 violation MW<200. Hetero atoms <2	0.55
Limonene	No,1 violation	Yes	Yes	No;2 violation	0.55

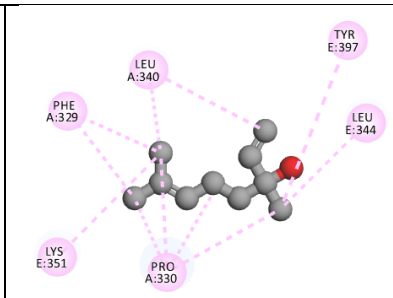
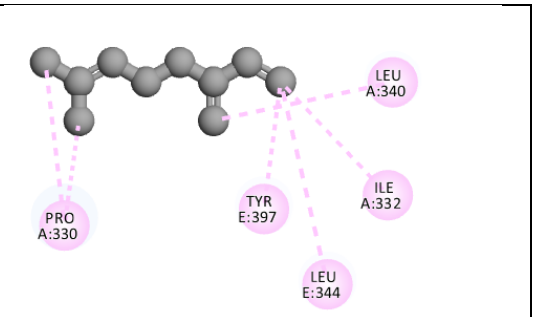
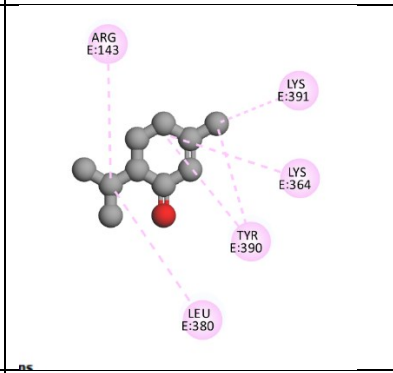
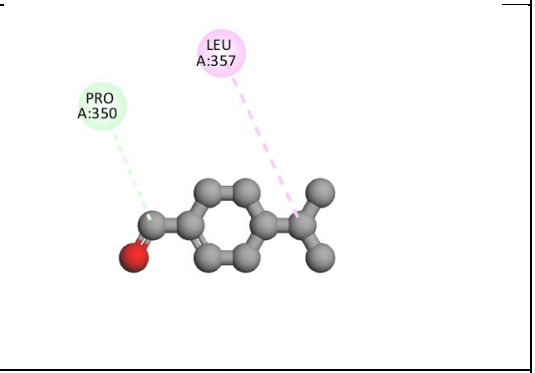
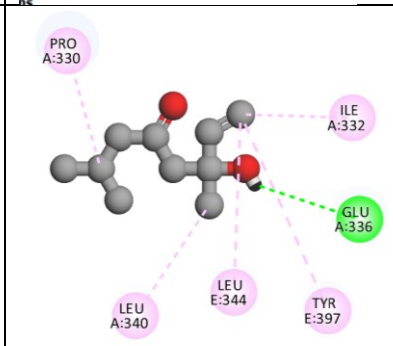
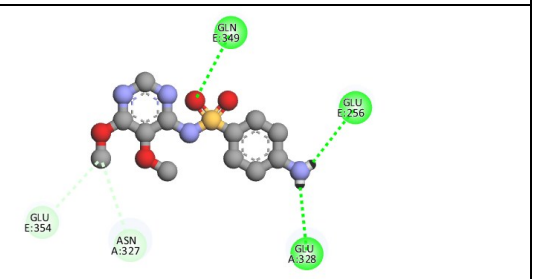
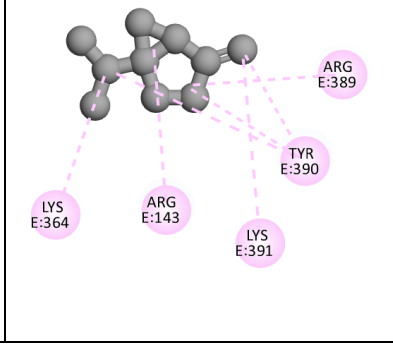
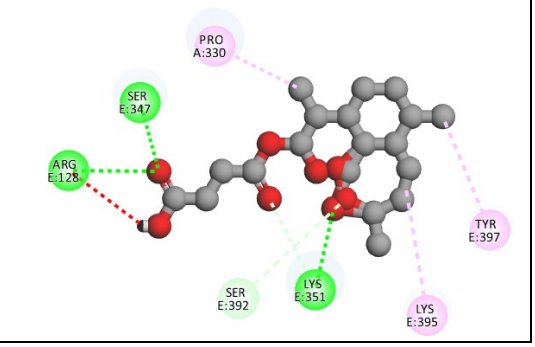
	MW< 160			MW<200. Hetero atoms <2	
Linalool	Yes	Yes	Yes	No,1 violation MW<200	0.55
Myrecene	No,1 violation MW< 160	Yes	Yes	No;2 violation MW<200. Hetero atoms <2	0.55
Nerol	No,1 violation MW< 160	Yes	Yes	No;2 violation MW<200. Hetero atoms <2	0.55
P-cymene	No,1 violation MW< 160	Yes	Yes	No;2 violation MW<200. Hetero atoms <2	0.55
Piperitone	No,1 violation MW< 160	Yes	Yes	No;2 violation MW<200. Hetero atoms <2	0.55
Sabinene	No,1 violation MW< 160	Yes	Yes	No;2 violation MW<200. Hetero atoms <2	0.55
Tagetonol	No,1 violation MW< 160	Yes	Yes	No;2 violation MW<200. Hetero atoms <2	0.55
Terpinene-4-ol	No,1 violation MW< 160	Yes	Yes	No;2 violation MW<200. Hetero atoms <2	0.55
(*Z*)-Linalool oxide	Yes	Yes	Yes	No,1 violation MW<200	0.55
***allo*-Aromadendrene**	Yes	Yes	Yes	No,1 violation MW<200	0.55
β-caryophellene	Yes	Yes	Yes	No; 1 violation: Heteroatoms<2	0.55
(*E*)-Nerolidol	Yes	Yes	Yes	No,1 violation MW<200	0.55
α-Amyrins	No; 3 violations: WLOGP>5.6, MR>130, #atoms>70	Yes	No; 1 violation: WLOGP>5.88	No; 2 violations: XLOGP3>5, Heteroatoms<2	0.55
lupeol	No; 3 violations: WLOGP>5.6, MR>130, #atoms>70	Yes	No; 1 violation: WLOGP>5.88	No; 2 violations: XLOGP3>5, Heteroatoms<2	0.55
Bergapten	yes	yes	Yes	yes	0.55
Umbelliferone	No; 1 violation: #atoms<20	yes	Yes	No ;1violation: MW<200	0.55
cuminal	No;1 violation: MW<160	yes	Yes	No ;2 violation: MW<200,heteroatoms <2	0.55

Cinnamic aldehyde	No;1 violation: MW<160	yes	Yes	No ;2 violation: MW<200,heteroatoms <2	0.55
Phellandral	No;1 violation: MW<160	yes	Yes	No ;2 violation: MW<200,heteroatoms <2	0.55
2-Tridecanone	No;1 violation: MW<160	yes	Yes	No ;2 violation: MW<200,heteroatoms <2	0.55
Tambuletin	No; 1 violation: MW>480	No; 1 violation: TPSA>140	No; 1 violation: TPSA>131.6	No; 3 violations: TPSA>150, H-acc>10, H-don>5	0.17
tambulin	yes	yes	Yes	yes	0.55
3,5 Diacetyl-tambulin	yes	yes	Yes	yes	0.55
kaempferol	yes	yes	Yes	yes	0.55
Artesunate	Yes; 0 violation	Yes	Yes	Yes	0.56

Supplementary table 4. Docking interaction poses of *Pf*AMA-1 with different phytoconstituents of *Z.armatum*

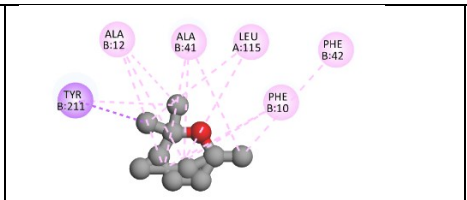
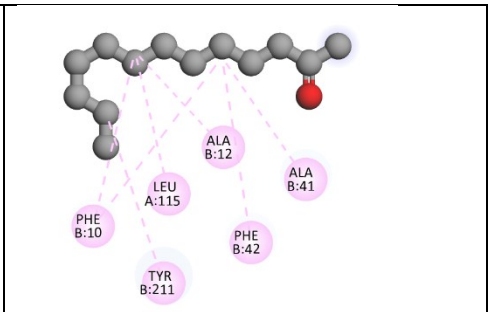
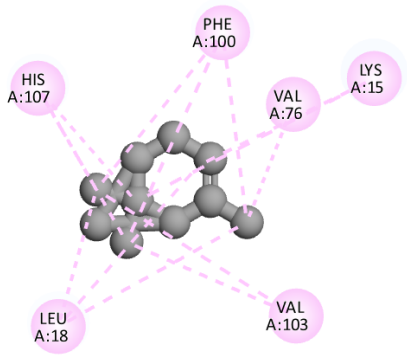
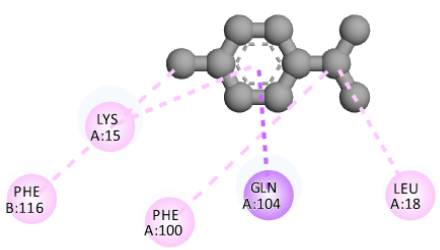
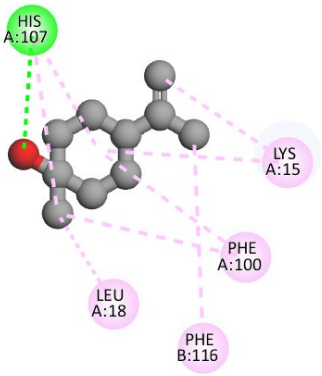
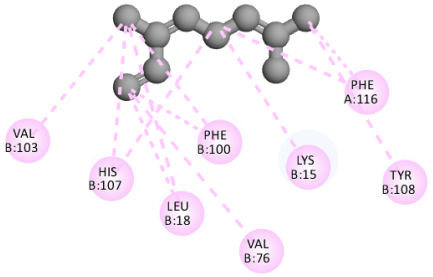
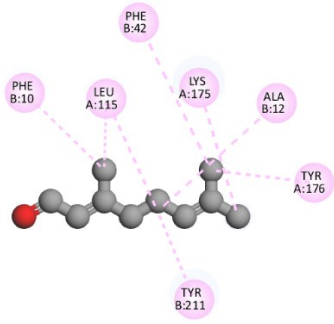
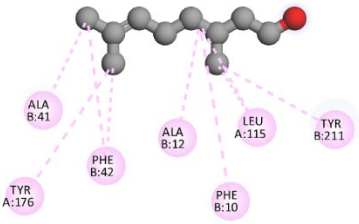
ligands	2D interactions	Ligands	2D interactions
1,8-cineole		**2-tridecanone**	
α-Pinene		**α-Terpinene**	

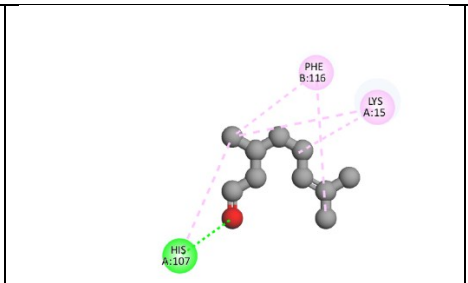
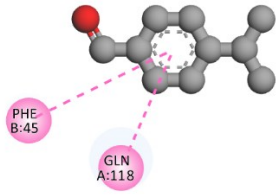
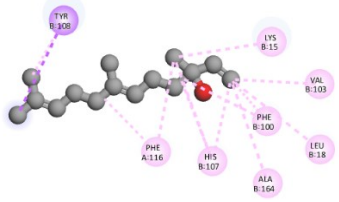
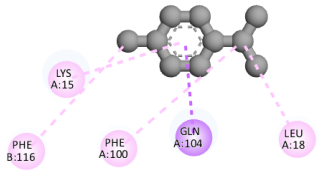
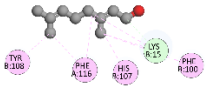
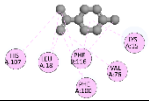
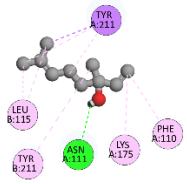
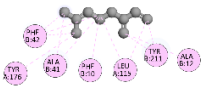
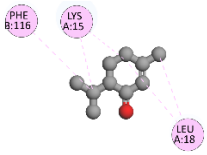
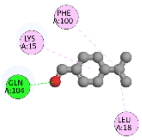
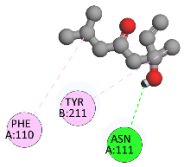
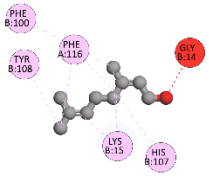
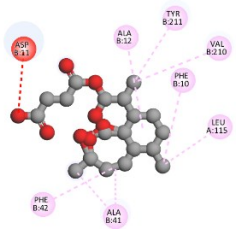
β-terpineol		**Cis-ocimene**	
citral		**Citronellol**	
Citronellal		**Nerol**	
(E)-Nerolidol		**γ-Terpinene**	
Geraniol		**Limonene**	

Linalool		**Myrcene**	
Piperitone		**Phellandral**	
Tagetonol		**Sulfadoxine**	
Sabinene		**Artesunate**	

Supplementary Table 5: Docking interaction poses of *Pf*GST with different phytoconstituents of *Z.armatum*

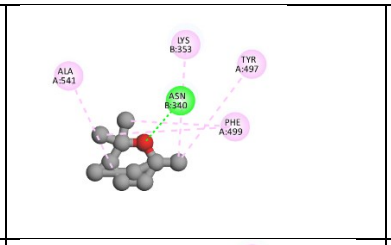
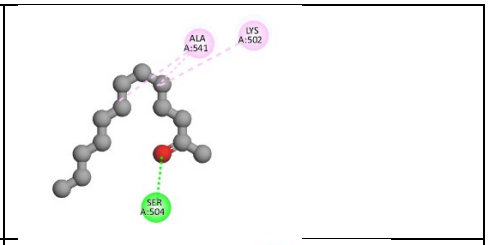
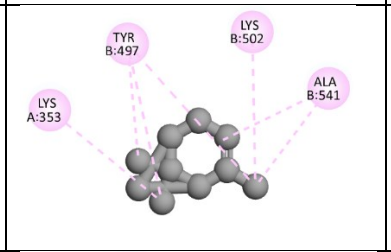
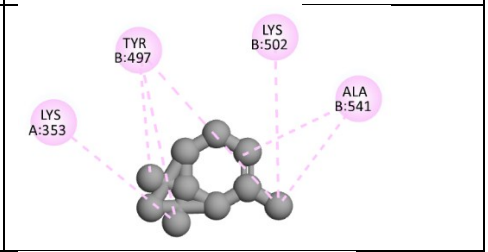
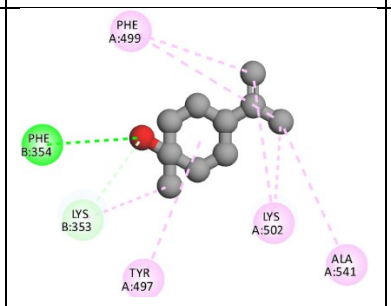
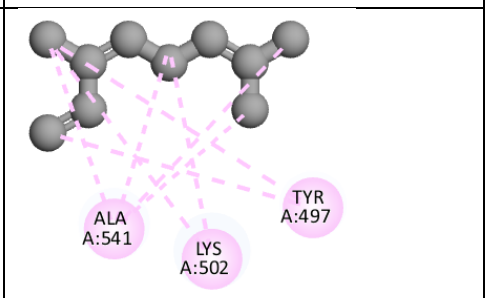
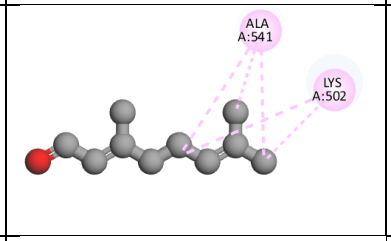
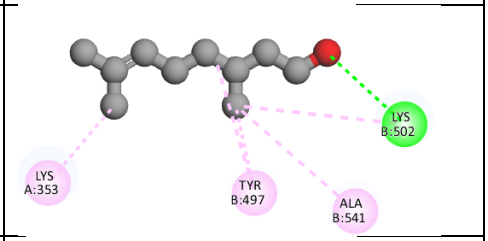
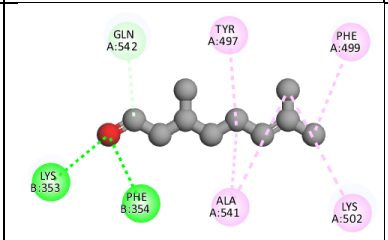
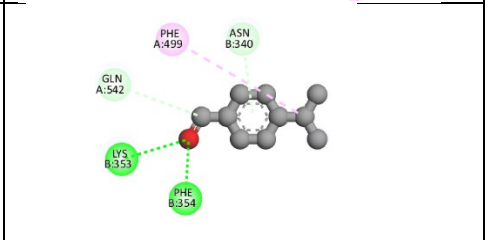
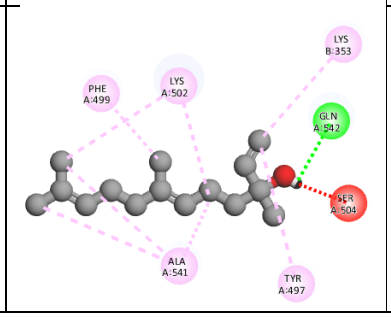
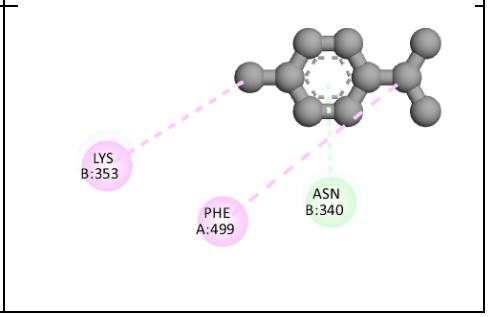
ligand		**ligand**	

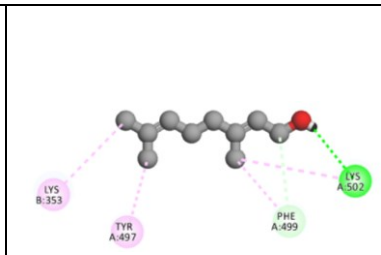
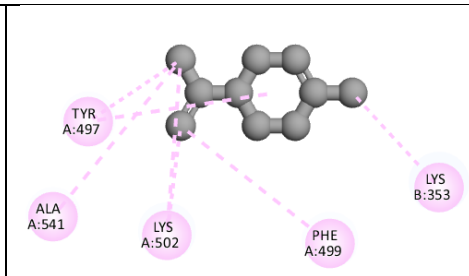
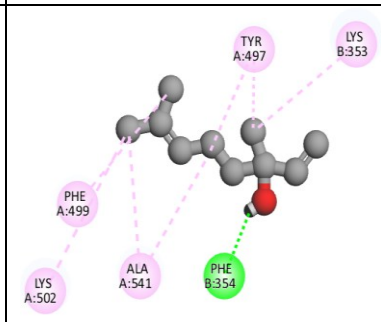
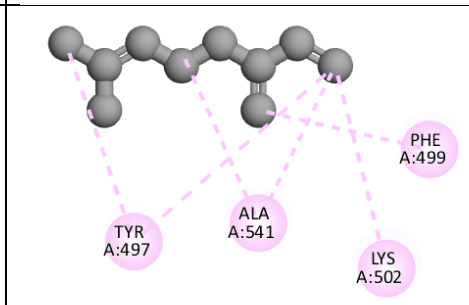
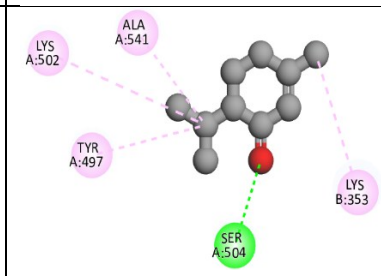
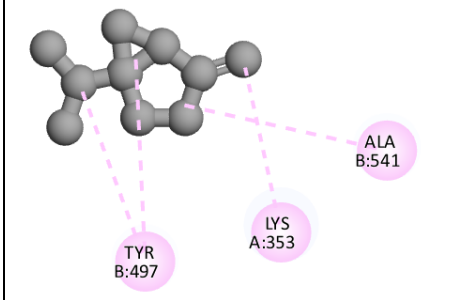
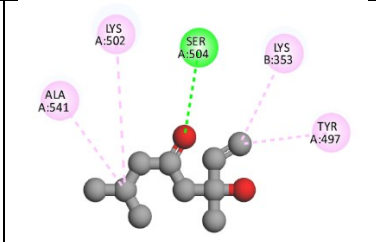
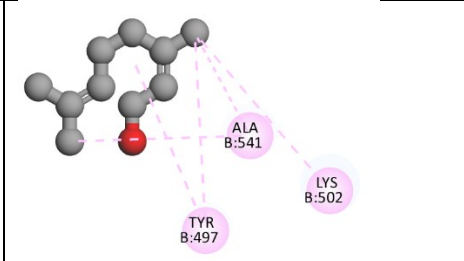
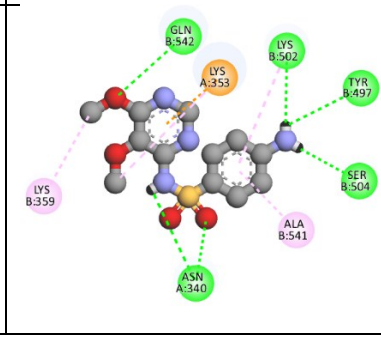
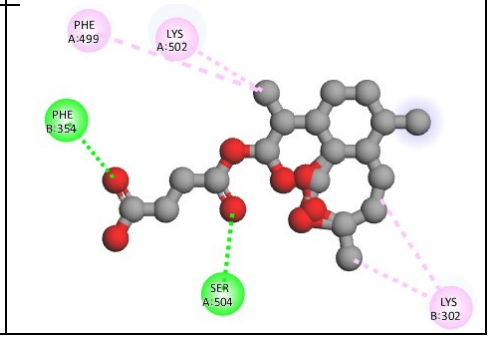
1,8-Cineole		**2-Tridecanone**	
α-Pinene		**α-Terpinene**	
β-terpineol		**Cis-ocimene**	
Citral		**Citronellol**	

Citronellal		**Cuminal**	
(E)-Nerolidol		**γ-Terpinene**	
Geraniol		**Limonene**	
Linalool		**Myrcene**	
Piperitone		**Phellandral**	
Tagetonol		**Nerol**	
Sulfadoxine	**No interactions**	**Artesunate**	

Supplementary table 6: Docking interaction poses of *Pf*DHFR with different phytoconstituents of *Z.armatum*

ligand	2D image	**ligand**	2D image

1,8-Cineole		**2-Tridecanone**	
α-Pinene		**α- Terpinene**	
β-terpineol		**Cis-ocimene**	
Citral		**Citronellol**	
Citronellal		**Cuminal**	
(E)-Nerolidol		**γ-Terpinene**	

Geraniol		**Limonene**	
Linalool		**Myrcene**	
Piperitone		**Sabinene**	
Tagetonol		**Nerol**	
Sulfadoxine		**Artesunate**	

Supplementary Table 7. 23 Common Targets from Genecard, Disgenet and Drug targets of 3 Selected Phytochemicals.

Sr. No.	Common Target Genes
1.	NOS2
2.	TYMS
3.	GSR
4.	IDO1
5.	G6PD
6.	ACP1
7.	ALB
8.	MPO
9.	ACHE
10.	IL6
11.	TTR
12.	CYP2C19
13.	CEL
14.	NR1I3
15.	TNF
16.	PTPRC
17.	HMOX1
18.	ADAM17
19.	CXCL8
20.	CTSL
21.	CD81
22.	ANPEP
23.	CCR5