Supplementary material

S1 Glide molecular docking result

For the receptor 3NRZ (antioxidant target protein) Figure S1 is the visual display of β-Maaliene interaction with this antioxidant target. It shows a glide docking score of −6.999 kcal/mol and hydrogen bonding is not obserbved. LEU257, VA258, VAL259, ILE264, PRO281, LEU287, ALA301, ALA302, ILE353, LEU398, ILE403, and LEU404 are hydrophobically involved amino acids whereas SER347 and THR354 are polar amino acids.

Figure S2 is the pictorial display of γ-eudesmol interaction with the antioxidant target receptor 3NRZ. It shows a glide score of −6.879 kcal/mol and hydrogen bonding is evident with VAL259 (1.90 Å), and ASN261 (2.11 Å). LEU257,

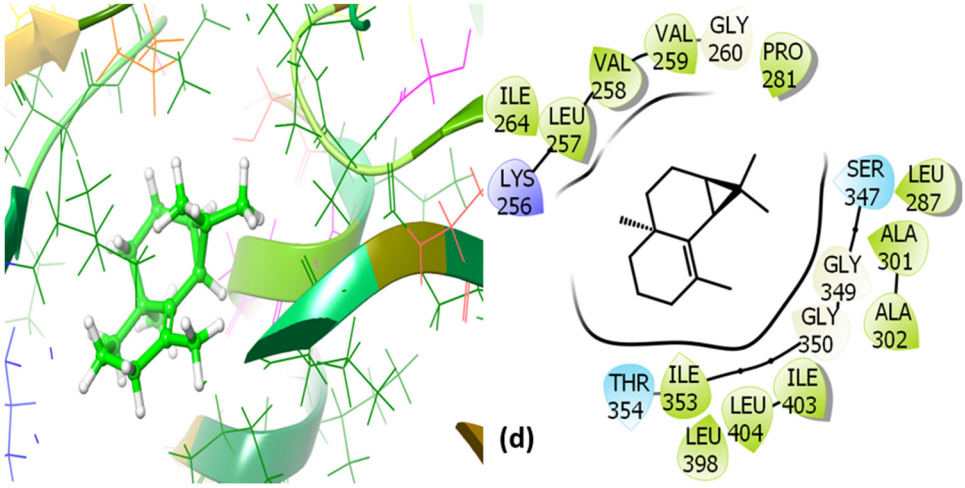

Figure S1: 3D and 2D interactive view of β-Maaliene (d) with antioxidant target protein (3NRZ).

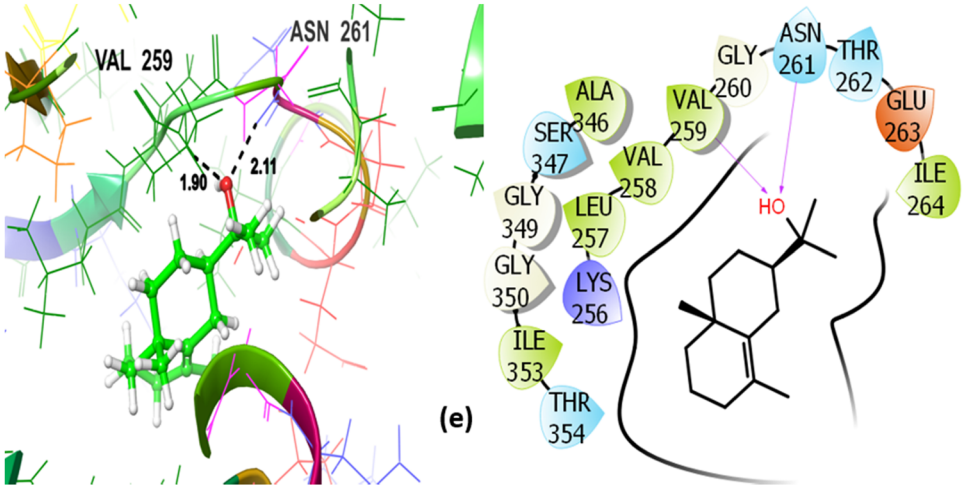

Figure S2: 3D and 2D interactive view of γ-eudesmol (e) with antioxidant target protein (3NRZ).

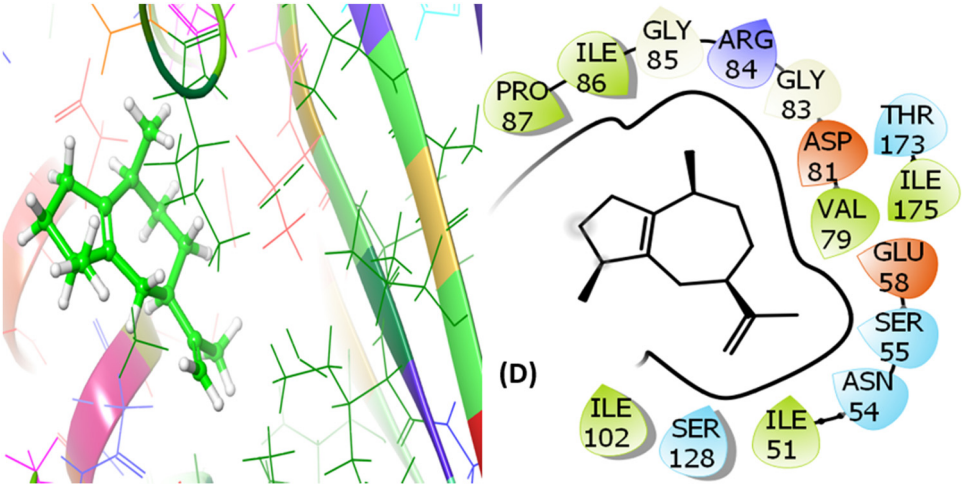

Figure S3: 3D and 2D interactive view of *α*-Guaiene (D) with antibacterial target protein (4URO).

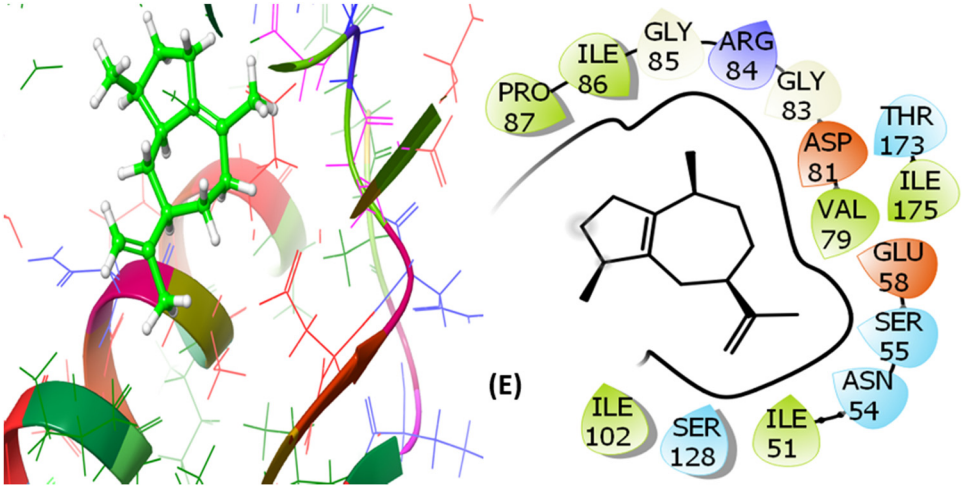

Figure S4: 3D and 2D interactive view of *δ*-Guaiene (E) with antibacterial target protein (4URO).

VA258, VAL259, ILE264, ALA346, and ILE353 are hydrophobically engaged amino acids. The polar amino acid residues are ASN261, THR262, SER347, and THR354.

For the receptor 4URO (antibacterial target protein), *α*-Guaiene and *δ*-Guaiene as shown in Figures S3 and S4 respectively, exhibits a prominent glide score of −5.345 kcal/mol and a-5.336 −5.345 kcal/mol. They both show no hydrogen bonding and hydrophobic interactions are seen with ILE51, VAL79, ILE86, PRO87, ILE102, and ILE175. The polar amino acid residues are ASN54, SER55, SER128, and THR173.

Table S1: Glide molecular docking data of bioactive constituents investigated for antioxidant and antibacterial activity

Ligands	Docking score (kcal/mol)	Glide score (kcal/mol)	Glide emodel (kcal/mol)	H-bonding and distance in Å	Polar amino acid residues	Hydrophobic interactions
	3NRZ (Antioxidant)					
(d)*β*-Maaliene (101596917)	−6.999	−6.999	−27.469	Not found	SER347, THR354	LEU257, VA258, VAL259, ILE264, PRO281, LEU287, ALA301, ALA302, ILE353, LEU398, ILE403, LEU404
(e)*γ*-eudesmol (6432005)	−6.879	−6.879	−43.715	VAL259 (1.90), ASN261 (2.11)	ASN261, THR262, SER347, THR354	LEU257, VA258, VAL259, ILE264, ALA346, ILE353
	4URO (Antibacterial)					
(D)*α*-Guaiene (5317844)	−5.345	−5.345	−32.643	Not found	ASN54, SER55, SER128, THR173	ILE51, VAL79, ILE86, PRO87, ILE102, ILE175
(E)*δ*-Guaiene (94275)	−5.336	−5.336	−35.144	Not found	ASN54, SER55, SER128, THR173	ILE51, VAL79, ILE86, PRO87, ILE102, ILE175

Table S2: Glide molecular docking score data of bioactive constituents investigated for antioxidant activity

S#	Ligand (pubchem id)	Docking score	Glide gscore	Glide emodel
1	Co-crystallized ligand-3NRZ (Antioxidant)	−8.288	−10.375	−90.026
2	bulnesol (90785)	−8.013	−8.013	−47.856
3	champacol (227829)	−7.645	−7.645	−47.716
4	*β*-Maaliene (101596917)	−6.999	−6.999	−27.469
5	*γ*-eudesmol (6432005)	−6.879	−6.879	−43.715
6	*α*-humulene (5281520)	−6.651	−6.651	−42.580
7	*α*-Terpineol (17100)	−6.599	−6.599	−39.130
8	*β*-Caryophyllene (5281515)	−6.548	−6.548	−26.828
9	humulene oxide II (91749531)	−6.347	−6.347	−31.949
10	*δ*-Guaiene (94275)	−6.324	−6.324	−43.166
11	aromadendrene (91354)	−6.311	−6.311	−38.338
12	*β*-eudesmol (91457)	−6.215	−6.215	−41.626
13	*γ*-caryophyllene (5281522)	−6.164	−6.164	−28.974
14	Eucalyptol (2758)	−6.158	−6.158	−26.647
15	selina-3,7(11)-diene (6432648)	−6.110	−6.110	−36.184
16	*α*-Guaiene (5317844)	−6.107	−6.107	−35.969
17	9-epi-*β*-caryophyllene (6429301)	−6.030	−6.030	−18.316
18	*α*-trans-Bergamotene (6429302)	−5.951	−5.951	−28.183
19	*γ*-Gurjunene (90805)	−5.934	−5.934	−38.915
20	(-) -*β*-Selinene (28237)	−5.886	−5.886	−29.449
21	caryophyllene oxide (1742210)	−5.877	−5.877	−20.250
22	*α*-Bisabolol (1549992)	−5.865	−5.865	−37.015
23	*α*-pinene (6654)	−5.842	−5.842	−22.534
24	*β*-pinene (14896)	−5.792	−5.792	−21.205
25	*β*-bisabolene (10104370)	−5.733	−5.733	−34.430
26	(E)-*α*-bisabolene (5315468)	−5.689	−5.689	−32.590
27	D-Limonene (440917)	−5.567	−5.567	−27.691
28	*β*-OCIMENE (5320250)	−3.249	−3.249	−22.820
29	*β*-Myrcene (31253)	−2.865	−2.865	−21.966
30	*α*-farnesene (5281516)	−2.289	−2.289	−31.192
31	*E*-nerolidol (5284507)	−2.057	−2.057	−31.768
32	(E)-*β*-farnesene (5281517)	−1.165	−1.165	−26.598

Table S3: Glide molecular docking score data of bioactive constituents investigated for antibacterial activity

S#	Ligand	Docking score	Glide gscore	Glide emodel
1	Co-crystallized ligand-4URO-(Antibacterial)	−5.809	−5.904	−62.448
2	bulnesol (90785)	−5.771	−5.771	−40.741
3	champacol (227829)	−5.492	−5.492	−39.316
4	*α*-Guaiene (5317844)	−5.345	−5.345	−32.643
5	*δ*-Guaiene (94275)	−5.336	−5.336	−35.144
6	caryophyllene oxide (1742210)	−5.317	−5.317	−22.026
7	aromadendrene (91354)	−5.229	−5.229	−32.264
8	*β*-Maaliene (101596917)	−5.220	−5.220	−31.347
9	D-Limonene (440917)	−4.892	−4.892	−25.122
10	*γ*-Gurjunene (90805)	−4.880	−4.880	−31.233
11	*β*-eudesmol (91457)	−4.777	−4.777	−32.539
12	selina-3,7(11)-diene (6432648)	−4.693	−4.693	−29.674
13	*α*-humulene (5281520)	−4.568	−4.568	−26.733
14	*γ*-caryophyllene (5281522)	−4.454	−4.454	−22.064
15	(E)-*α*-bisabolene (5315468)	−4.374	−4.374	−26.066
16	*α*-Terpineol (17100)	−4.297	−4.297	−25.327
17	humulene oxide II (91749531)	−4.292	−4.292	−26.507
18	*γ*-eudesmol (6432005)	−4.276	−4.276	−30.449
19	Eucalyptol (2758)	−4.253	−4.253	−22.595
20	*α*-pinene (6654)	−4.142	−4.142	−13.335
21	9-epi-*β*-caryophyllene (6429301)	−4.009	−4.009	−20.697
22	*β*-pinene (14896)	−4.007	−4.007	−16.943
23	*β*-Caryophyllene (5281515)	−3.995	−3.995	−20.801
24	*β*-bisabolene (10104370)	−3.962	−3.962	−25.170
25	(-) -*β*-Selinene (28237)	−3.897	−3.897	−27.275
26	*α*-Bisabolol (1549992)	−3.861	−3.861	−25.854
27	*α*-trans-Bergamotene (6429302)	−3.450	−3.450	−20.769
28	*β*-OCIMENE (5320250)	−2.795	−2.795	−20.398
29	*β*-Myrcene (31253)	−2.467	−2.467	−22.748
30	*E*-nerolidol (5284507)	−1.132	−1.132	−26.731
31	*α*-farnesene (5281516)	−0.709	−0.709	−22.932
32	(E)-*β*-farnesene (5281517)	−0.067	−0.067	−23.939