Supplementary file 2:

Table S1. Results of Hydrophobic interactions of Paeoniflorin with the active site residues of TNF α.

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	57A	LEU	3.89	4325	653
2	57A	LEU	3.37	4326	655
3	59A	TYR	3.50	4325	694
4	59B	TYR	3.93	4307	2846
5	119A	TYR	3.44	4314	1471
6	119B	TYR	3.72	4312	3691

Table S2. Hydrogen bonding interactions of Paeoniflorin with the active site residues of TNF -α.

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Sidechain	Donor Atom	Acceptor Atom
1	60A	SER	1.94	2.89	171.41	✖	✖	4304 [O3]	711 [O2]
2	120A	LEU	3.21	4.00	136.19	✔	✖	1488 [Nam]	4304 [O3]
3	120B	LEU	1.83	2.73	155.17	✖	✖	4297 [O3]	3709 [O2]
4	151A	TYR	2.10	2.98	151.69	✖	✔	4303 [O3]	1970 [O3]

Table S3. Hydrophobic interactions patterns of Amoradicin with the active site residues of TNF-α.

Index	Residue	AA	Distance	Ligand Atom	Protein Atom
1	57B	LEU	3.46	4323	2811
2	59B	TYR	3.55	4302	2848
3	119A	TYR	3.00	4324	1474
4	119B	TYR	3.30	4315	3689
5	123B	VAL	3.87	4323	3745

Table S4. Hydrogen bonding interactions of Amoradicin with the active site residues of TNF alpha.

Index	Residue	AA	Distance H-A	Distance D-A	Donor Angle	Protein donor?	Sidechain	Donor Atom	Acceptor Atom
1	58A	ILE	2.60	3.25	121.70	✔	✖	668 [Nam]	4299 [O3]
2	60B	SER	2.78	3.32	116.37	✖	✖	4296 [O3]	2866 [O2]
3	60B	SER	3.63	4.04	106.63	✔	✖	2863 [Nam]	4297 [O2]
4	119A	TYR	1.98	2.92	163.55	✔	✔	1478 [O3]	4294 [O3]
5	120B	LEU	2.74	3.13	102.79	✔	✖	3706 [Nam]	4296 [O3]
6	122A	GLY	3.11	3.64	113.39	✔	✖	1514 [Nam]	4299 [O3]
7	122A	GLY	1.81	2.71	154.69	✖	✖	4299 [O3]	1517 [O2]

Table S5. π-Stacking interactions of Amoradicin with the active site residues of TNF alpha.

Index	Residue	AA	Distance	Angle	Offset	Type	Ligand Atoms
1	59B	TYR	4.85	88.18	0.57	T	4309, 4312, 4313, 4316, 4317, 4319
2	119A	TYR	5.03	75.92	1.33	T	4301, 4303, 4304, 4306, 4307, 4308