

Supplementary File 1:

Compound Name	IC50 Value (μM)	Reference
1. Luteolin	14.44	(Herath, Takano-Ishikawa, & Yamaki, 2003)
2. Genistein	65.08	(Herath et al., 2003)
3. Apigenin	3.27	(Nicholas et al., 2007)
4. Kaempferol	3.99	(Kim et al., 2007)
5. Quercetin	3.11	(Nair et al., 2006)
6. Myricetin	3.84	(Herath et al., 2003; Rathee et al., 2009)
7. Naringenin	14.41	(Herath et al., 2003; Wilcox, Borradaile, & Huff, 1999)
8. Phloretin	3.00	(Lommen, Godejohann, Venema, Hollman, & Spraul, 2000)
9. Butein	6.29	(Cheng, Kuo, Chan, Ko, & Teng, 1998)
10. Cyanidin	36.91	(Chandra, Rana, & Li, 2001)
11. Eriodictyol	50	(Wang, Li, Ho, Peng, & HO, 1998)
12. Hesperetin	50	(Swatsitang, Tucker, Robards, & Jardine, 2000)
13. Wogonin	1-50	(Lee et al., 2003)
14. Morin	1.5	(Arima & Danno, 2002)
15. Amoradecin	28.5	(Cho et al., 2000)
16. Velutin	2.5	(Xie et al., 2012)
17. Thymoquinone	25-75	(Sethi, Ahn, & Aggarwal, 2008)
18. Paeoniflorin	6.1-200	(M. Wu & Gu, 2009)
19. Paeonol	6.1-200	(M. Wu & Gu, 2009)
20. Scopoletin	10	(Moon et al., 2007)
21. Capsaicin	50	(Park et al., 2004)
22. Curcumin	2.5	(Jagetia & Aggarwal, 2007)
23. Yangonin	40	(Hashimoto et al., 2003)
24. Berberine	5	(Chen et al., 2008)
25. Ergosterol peroxide	15-60	(Kobori, Yoshida, Ohnishi-Kameyama, & Shinmoto, 2007)
26. Eudesmin	51.3	(Chae et al., 1998)
27. Magnolin	12.5	(Chae et al., 1998)
28. Magnosalin	5.9	(Ryu, Son, Lee, & Sohn, 2002)
29. Savinin	31.9	(Cho et al., 2001)
30. Arctigenin	3.88	(Zhao, Wang, & Liu, 2009)
31. Honokiol	15	(F. Wu et al., 2011)
32. Acanthoic acid	5.46	(Kang et al., 1996)
33. Silybin	140.3	(Cho et al., 2000)
34. Catechin	3.11	(Herath et al., 2003)
35. Lirioresinol-B dimethyl ether	12.5	(Chae et al., 1998)
36. Geraniin	43	(OKABE et al., 2001)
37. Corilagin	76	(OKABE et al., 2001)

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 Amoradycin 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 Amoradycin 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