Supplementary Data

Table S1. List of some synthetic and semi-synthetic compounds screened against NQO1.

1	2244	Aspirin
2	89105	Tretazicar
3	216210	Dabigatran
4	54678486	Warfarin
5	1183	Vanillin
6	98527	Dimethoxy-4-Bromophenetholamine
7	154482	Hexabromo-1,1 Biphenyl
8	332529	9-(3,4-Dimethoxyphenyl)-5-hydroxy-6H-[2]benzofuro[5,6-f][1,3]Benzodioxol-8-One
9	442664	Vicenin
10	442882	Justicidin
11	3633866	Naphthalen-2-Ylsulfonyl
12	4470790	ES-936
13	10397115	2-(Aziridin-1-yl)-5-methyl-1,4-benzoquinone
14	101916320	4-0-Demethyl Suchilactone

Table S2. Binding affinity and hydrogen bonding interaction of molecular docking analysis of phytobioactives against NQO1 (2F1O) Protein.

Sl No	**Compound CID**	**Ligand**	**Binding Affinity Kcal/mol**	**Hydrogen bonding forming Amino Acid residues**
1	87310	Alliin	-4.2	Lue 103, Tyr 155(2), Gly 150, Tpr 105
2	54670067	Ascorbic acid	-5.1	Phe 106, Lys A 113.
3	1183	Vanillin	-4.8	Ala 223.
4	5576	Trimethadi	-6	Trp 105 (2), Gly149,

		one		Gly 150.
5	11958	Benzoquinone	-4.8	Tyr 155, Trp 105.
6	370	Gallic acid	-4.8	Val 108.
7	2153	Theophylline	-4.9	Lue 103, Tyr 102.
8	89105	Tretazicar	-6.8	Lue 103, Gly 150.
9	16871	Napthoquinone	-5.4	Trp 105, His161, Tyr 155.
10	5746	MYTOMYCIN	-8.1	Trp 105, Gly 149.
11	10280735	Edoxaban	-7.8	His 11, His 194.
12	5884	NADPH	-7.3	Gln 187 (2), Pro 186, Lue 188 (2), Tyr 190, Gly 206, Arg 210, Lys 270.
13	10429233	Dihydrocurcumin	-5.2	Trp 105, Tyr 155.
14	5280445	Luteolin	-6.6	Pro 68, Gly 122.
15	4470790	ES-936	-7.4	Tyr 67.
16	295934	Deoxynyboquinone	-6.5	Gly 149, Tyr 105, Tyr 155, His 169.
17	9875401	Rivaroxaban	-7.2	Lys 270, Tyr 190
18	11250888	β-NADH	-7.5	Gly 149, Tyr 155.
19	117587706	Dihydronapthalene	-6.3	Tyr 126.
20	101916320	Demethyl Suchilaceone	-7	Ile 50, Lys 270.

21	5281675	ORIENTIN	-6.6	Tyr190, Gly150.
22	11617	DIALLYL SULFIDE	-2.9	Phe 106.
23	5386591	Ajoene	-3.3	Ile 164
24	896	Melatonin	-5.6	Leu 157, Asp 266.
25	54676038	Dicumarol	-6.9	Val 108, Phe 106.
26	4055	Menadione	-5.2	Lys 113.
27	5281672	Myricetin	-6.6	Phe 178, Pro 68.