

Table S1 List of natural compounds considered for molecular docking from NPACT database.

Alliin	Quercetin	Podophyllotoxin bromide	Fangchinoline
Allyl isothiocyanate	Resveratrol	Protopine	Galangin
Andrographidoid D	Silymarin	Psoralen	Gallic acid (1)
Anneoplaston A10	Theflavin	Quassin	Genistein (1)
Apigenin	Zeaxanthin	Rubiadin	Germacronolide
Apiole	10-Gingerol	Spartine	Germacrone
Capsaicin	Aloe-emodin	Tetrandrine	Ginkgetin
Catechin	Bergenin	Thymoquinone	Ginkgolides A
Chlorogenic acid	Bruceantin	Ursolic acid	Ginkgolides B
Chlorogenic acid	Cardiac glucosides (Ouabain)	Withferin A	Hyperoside
Coumarin	Cicutoxin	(E)-gamma-Bisabolene	Licoagrochalcone A
Curcumin	Damnacanthol	Andrographolide	Mangiferin
Cyanidin	Diterpenes (aconitine)	Bavachinin	Oridonin
Diallyl sulphide	Elliptinium	Berberine(2)	Podophyllotoxin
Ellagic acid	Embelin	Berberine	Ponicidine
Epigallocatechin gallate (EGCG)	Epipodophyllotoxin	Chelidonine	Psoralidin
Gallic acid	Flavonol 3-O-glycoside	Combretastatins	Psorospermin
Genistein	Ginsenosides C-K	Costunolide	Quassinoid
Gingerol	Homoharringtonine	Curcumol	Quercetin (1)
Gossypol	Lupeol	Curdione	Quercetin-3-gluconide
Hesperidin	Mallatophenone	Cynaropicrin	Rhamnetin
Indole-3-carbinol	Naringenin	Daidzein	Rubescensine
Kaempferol	Neohesperidin	Dehydrocostuslactone	Spirosolane
Methyl allyl trisulfide	Nitidine chloride	Dithymoquinone	Trichothecenes
Piperine	Pinocembrin	Emodin tetra acetate	Withnolide D
			Xanthone