

Supplementary material:

Table 1: Docking score (S) and Interaction sites of neem phytochemicals against PEPCK enzyme

No.	Compound Name	Score (S)	Interaction Sites
1	3-Deacetyl-3-cinnamoyl-azadirachtin	-37.57	A292,A297,L293,M295,G289,T343, P528,P530,G531
2	Isoazadirolide	-34.79	A292,G289
3	Meliatetraolenone	-33.20	S286,C288,G289,A292,T291,A310,A311,L290,L244,G329,A405,A287
4	Xanthophylls	-32.96	T235,A405,A403
5	7 α -Senecioid-(7-deacetyl)-23-O-methyl nimo-cinolide	-32.38	C288,G289,L290,A310,A311,A405, T291,A292,P530
6	Azadirachtanin	-31.71	C288,G289,A292,L290,V335,T291, A436
7	6-O-ACETYLNIMBANDIOL	-31.33	T291,A310,A405,L290,A311,S286, A87,T235
8	Beta-sitosterol	-30.87	P337,P402
9	Nimocinolide	-30.30	A292,G338,A436,T291,A310,A311,H264,L244,L290,A405,P333,V335
10	Rutin	-30.23	S286,C288,G289,A287,L290,A436,A292,V335,T291,A310,A311,A405