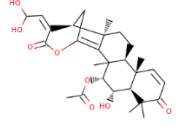
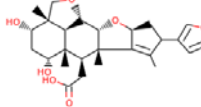
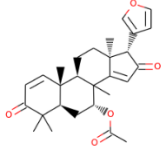
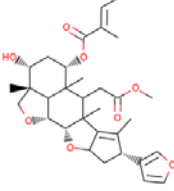
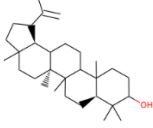
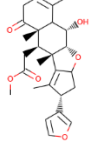
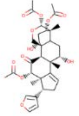
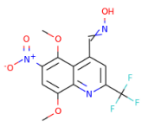
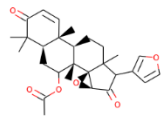
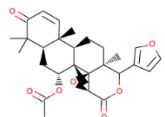
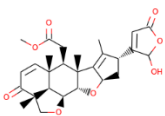
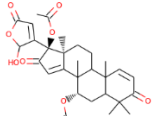
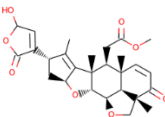
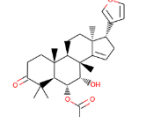
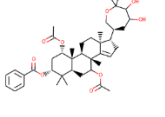
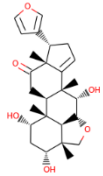
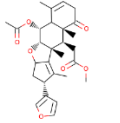
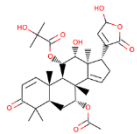
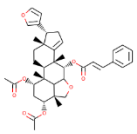
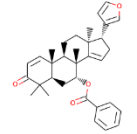
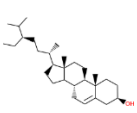
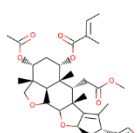
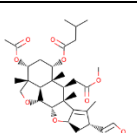
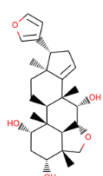
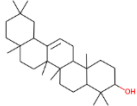

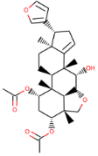
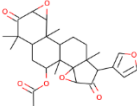
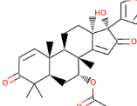
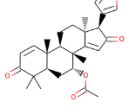
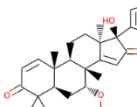
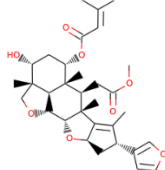
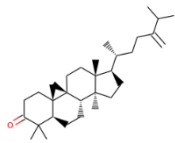
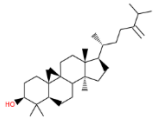
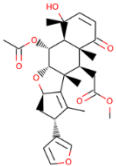
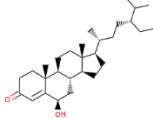
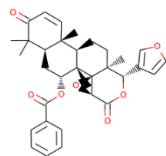
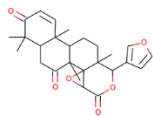
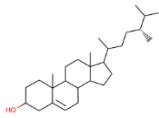
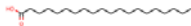


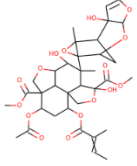
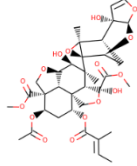
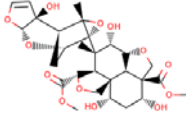
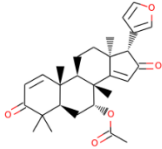
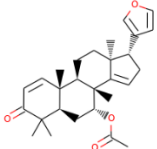


Compound name	Phytochemical name	Docking score	Structure
CID:6442906	Nimocinolide	-8.3	
CASID:29803858	((2aR)-8t-[3]furyl-3t,5t-dihydroxy-2a,5a,6a,7-tetramethyl-(2ar,5ac,6ac,9at,10ac,10bc,10ct)-Δ6b-dodecahydro-cyclopenta[d']naphtho[1,8-bc:2,3-b']difuran-6c-yl)-acetic acid	-8.7	
CHEMSPIDER:156225	(5α,7α,8β,13α,17α)-17-(3-Furyl)-4,4,8-trimethyl-3,16-dioxoandrosta-1,14-dien-7-yl acetate	-8.1	
CID:6450192	3-Deacetylsalannin	-8.9	
CID:16219576	3β-Hydroxy-20(29)-lupene	-7.1	
CID:102285347	6-Deacetylnimbinene	-8.1	
CID:102146586	Azadirachtanin	-8.2	

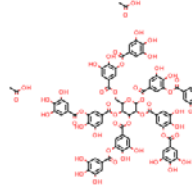
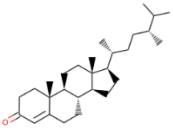

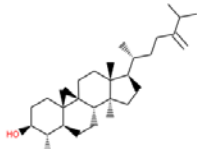
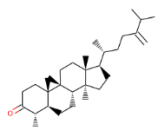
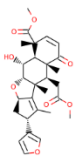
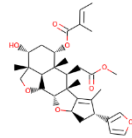

CID:102285346	Desacetylnimbinolide	-7.0	
CID:122801	Epoxyzadiradione	-8.3	
CID:114923	Gedunin	-8.5	
CASID:105377740	Isomargosinolide	-8.0	
CASID:106807345	Isonimolicinolide	-7.3	
CASID:105404759	Margosinolide	-8.1	
CID:101289833	Meldenin	-6.9	
CID:101650342	Melianin B	-7.9	

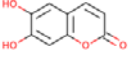
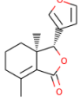
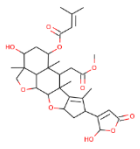
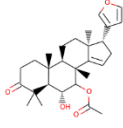
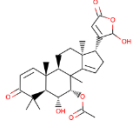
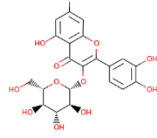
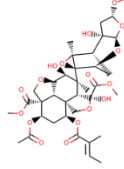
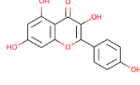
CID:101306757	Nimbidinin	-8.5	
CID:44715635	Nimbinene	-8.3	
CID:13875774	Nimbocinolide	-8.2	
CID:101650373	Nimbolin A	-7.6	
CASID:104522761	Nimocin	-6.9	
CID:12303662	Phytosterols	-5.9	
CID:118701505	Salannin	-8.8	
CID:14194026	Salannol acetate	-8.3	
CID:102090424	Vilasinin	-7.1	

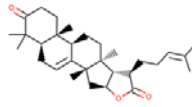
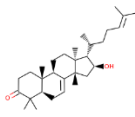
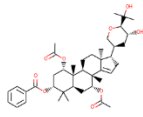
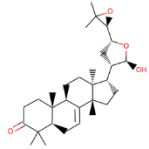
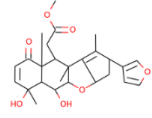
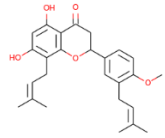
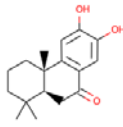
CID:225689	Beta-Amyrin	-4.9	
CID:8067	1-Pentanethiol	-5.1	
CID:52952013	1,3-Diacetylvilasinin	-7.0	
CHEMSPIDER:298060	17-(3-Furyl)-4,4,8-trimethyl-3,16-dioxo-1,2:14,15-diepoxyandrostan-7-yl acetate	-6.9	
CID:52951894	17-epi-17-Hydroxyazadiradione	-8.9	
CID:12308716	17-Epiazadiradione	-8.0	
CID:52951892	17-Hydroxyazadiradione	-8.1	
CID:91886694	2',3'-Dehydrosalannol	-7.7	

CID:14635659	24-Methylenecycloartan-3-one	-6.6	
CID:9547213	24-Methylenecycloartanol	-7.1	
CID:52952216	6-Acetylnimbandiol	-8.8	
CID:9823926	6beta-Hydroxystigmast-4-en-3-one	-6.1	
CID:52952112	7-Deacetyl-7-benzoylgedunin	-7.9	
CID:1886	7-Deacetyl-7-oxogedunin	-7.2	
CID:10134	AC1L1UKB	-9.5	
CID:10467	Arachidic acid	-3.9	

CID:2263	Azadirachtin	-7.9	
CID:16126804	Azadirachtin B	-8.5	
CID:23256847	Azadirachtol	-8.4	
CID:12308714	Azadiradione	-7.9	
CID:10906239	Azadirone	-6.9	
CID:244	Benzyl alcohol	-5.2	
CID:5280489	Beta-carotene	-4.8	

CID:76419085	Bis (acetic acid); tannins	-8.8	
CID:11988279	Campest-4-en-3-one	-6.9	
CID:444539	Cinnamic acid	-5.9	
CID:101690	Cycloeucalenol	-6.2	
CID:21594790	Cycloeucalenone	-7.3	
CID:10505484	Deacetylnimbin	-8.9	
CID:14458886	Deacetylsalannin	-8.0	
CID:8215	Docosanoic acid	-3.9	

CID:5281416	Esculetin	-6.8	
CID:124039	Fraxinellone	-8.3	
CID:101425842	Isozadirolide	-8.7	
CID:76316558	Isomeldenin	-7.9	
CID:184310	Isonimocinolide	-8.9	
CID:10813969	Isoquercetin	-8.8	
CID:24796982	Isovepaol	-8.9	
CID:5280863	Kaempferol	-9.1	

CID:15560423	Kulactone	-8.5	
CID:44567124	Kulinone	-8.0	
CID:101277363	Melianin A	-8.9	
CID:44575793	Melianone	-8.1	
CASID:78916537	Methyl 2-(2-(furan-3-yl)-5,6-dihydroxy-1,6,9a,10a-tetramethyl-9-oxo-3,3a,4a,5,5a,6,9,9a,10,10a-decahydro-2H-cyclopenta[b]naphtho[2,3-d]furan-10-yl)acetate	-8.3	
CID:14492795	Nimbaflavone	-9.7	
CID:11119228	Nimbidiol	-9.0	

Supplementary Fig. 5. List of compounds and docking score.