

Table S1. Tanimoto similarity and docking scores of the XP screened compounds

S.No	COCONUT ID	Docking score (kcal/mol)	Tanimoto similarity	S.No	COCONUT ID	Docking score(kcal/mol)	Tanimoto similarity
1	CNP0288601	-12.829	0.269363	100	CNP0236854	-7.084	0.234263
2	CNP0241232	-12.618	0.270499	101	CNP0259163	-7.058	0.341994
3	CNP0080250	-12.185	0.331072	102	CNP0114165	-7.045	0.299689
4	CNP0080249	-11.916	0.318373	103	CNP0240862	-7.023	0.323723
5	CNP0344609	-11.068	0.317335	104	CNP0117051	-7.016	0.288316
6	CNP0166854	-10.974	0.288668	105	CNP0222481	-6.985	0.326354
7	CNP0177079	-10.890	0.317212	106	CNP0195111	-6.974	0.301049
8	CNP0238550	-10.690	0.27046	107	CNP0232867	-6.973	0.309019
9	CNP0332060	-10.593	0.214164	108	CNP0240588	-6.961	0.326817
10	CNP0080252	-10.395	0.320113	109	CNP0295922	-6.952	0.402075
11	CNP0232558	-10.393	0.333106	110	CNP0304960	-6.920	0.312691
12	CNP0276275	-10.368	0.355526	111	CNP0186752	-6.905	0.24359
13	CNP0173564	-10.260	0.274763	112	CNP0148528	-6.904	0.294248
14	CNP0266349	-10.050	0.341146	113	CNP0172039	-6.889	0.383917
15	CNP0124430	-10.040	0.219614	114	CNP0181244	-6.863	0.303806
16	CNP0166031	-9.907	0.219064	115	CNP0377574	-6.842	0.321651
17	CNP0234527	-9.674	0.22471	116	CNP0162563	-6.779	0.297872
18	CNP0172795	-9.639	0.317824	117	CNP0276082	-6.766	0.244136
19	CNP0250275	-9.541	0.216736	118	CNP0235256	-6.765	0.260073
20	CNP0294756	-9.516	0.307692	119	CNP0257836	-6.756	0.231598
21	CNP0208621	-9.457	0.312265	120	CNP0138077	-6.724	0.259901
22	CNP0232386	-9.307	0.340489	121	CNP0292123	-6.718	0.246954
23	CNP0220888	-9.283	0.332893	122	CNP0134072	-6.718	0.311867
24	CNP0184011	-9.236	0.25852	123	CNP0243617	-6.718	0.275454
25	CNP0080230	-9.197	0.258333	124	CNP0244532	-6.717	0.305671
26	CNP0229395	-9.127	0.225514	125	CNP0309058	-6.715	0.30459
27	CNP0334271	-9.121	0.304665	126	CNP0131308	-6.700	0.346774
28	CNP0293269	-9.093	0.224558	127	CNP0373108	-6.681	0.359356
29	CNP0259095	-9.068	0.216736	128	CNP0300897	-6.654	0.271923

30	CNP0144047	-8.946	0.22755	129	CNP0243230	-6.650	0.440171
31	CNP0226348	-8.842	0.327676	130	CNP0155407	-6.650	0.357962
32	CNP0173918	-8.788	0.294286	131	CNP0199670	-6.641	0.329377
33	CNP0205945	-8.680	0.226399	132	CNP0216125	-6.640	0.356371
34	CNP0104652	-8.622	0.240329	133	CNP0146840	-6.638	0.337349
35	CNP0316445	-8.598	0.217082	134	CNP0197004	-6.624	0.273458
36	CNP0139619	-8.594	0.317539	135	CNP0377028	-6.621	0.296543
37	CNP0277873	-8.570	0.226399	136	CNP0181824	-6.612	0.224324
38	CNP0182329	-8.526	0.243056	137	CNP0312223	-6.604	0.322518
39	CNP0245710	-8.521	0.228926	138	CNP0171505	-6.603	0.341965
40	CNP0214794	-8.476	0.291076	139	CNP0170500	-6.601	0.214097
41	CNP0214412	-8.381	0.326667	140	CNP0397180	-6.600	0.44086
42	CNP0279503	-8.294	0.272806	141	CNP0166169	-6.598	0.254637
43	CNP0138643	-8.275	0.274603	142	CNP0240279	-6.579	0.281879
44	CNP0133651	-8.268	0.314176	143	CNP0268715	-6.575	0.344241
45	CNP0195932	-8.242	0.219917	144	CNP0107419	-6.567	0.32312
46	CNP0209154	-8.179	0.324503	145	CNP0174539	-6.535	0.29465
47	CNP0169391	-8.171	0.315018	146	CNP0272446	-6.534	0.3331
48	CNP0147502	-8.158	0.269929	147	CNP0291283	-6.497	0.479212
49	CNP0245121	-8.152	0.305741	148	CNP0200225	-6.491	0.22094
50	CNP0319168	-8.090	0.297778	149	CNP0177868	-6.491	0.257166
51	CNP0113508	-8.086	0.332148	150	CNP0129079	-6.490	0.225886
52	CNP0145828	-8.058	0.316056	151	CNP0174866	-6.485	0.252853
53	CNP0258154	-8.049	0.32478	152	CNP0191008	-6.470	0.390663
54	CNP0230781	-8.045	0.298361	153	CNP0277313	-6.467	0.374202
55	CNP0155859	-8.039	0.290123	154	CNP0210919	-6.455	0.281938
56	CNP0153580	-7.948	0.216918	155	CNP0131061	-6.443	0.399497
57	CNP0300194	-7.904	0.303763	156	CNP0349059	-6.432	0.371501
58	CNP0347782	-7.896	0.364109	157	CNP0085019	-6.423	0.434409
59	CNP0105429	-7.893	0.295673	158	CNP0117429	-6.420	0.320276
60	CNP0190921	-7.879	0.301304	159	CNP0085461	-6.397	0.271768
61	CNP0196231	-7.874	0.297539	160	CNP0234393	-6.394	0.34949
62	CNP0250716	-7.867	0.341176	161	CNP0164346	-6.391	0.316436

63	CNP0314566	-7.858	0.273684	162	CNP0237841	-6.387	0.357052
64	CNP0148927	-7.837	0.288889	163	CNP0224794	-6.382	0.320088
65	CNP0330352	-7.806	0.282116	164	CNP0263367	-6.378	0.253133
66	CNP0331306	-7.794	0.232358	165	CNP0117806	-6.359	0.398196
67	CNP0233323	-7.689	0.319917	166	CNP0258703	-6.352	0.287982
68	CNP0256714	-7.663	0.221761	167	CNP0244343	-6.334	0.255283
69	CNP0184645	-7.630	0.286159	168	CNP0227316	-6.317	0.405096
70	CNP0269850	-7.629	0.30593	169	CNP0249449	-6.311	0.25
71	CNP0157562	-7.615	0.3329	170	CNP0204042	-6.290	0.347769
72	CNP0204837	-7.601	0.354029	171	CNP0201102	-6.278	0.345855
73	CNP0080254	-7.595	0.288937	172	CNP0182212	-6.267	0.275444
74	CNP0156762	-7.594	0.329032	173	CNP0080245	-6.266	0.302262
75	CNP0333972	-7.566	0.272872	174	CNP0155730	-6.264	0.242735
76	CNP0329066	-7.554	0.314888	175	CNP0159795	-6.251	0.222689
77	CNP0112559	-7.547	0.259459	176	CNP0216868	-6.240	0.315673
78	CNP0189555	-7.518	0.218593	177	CNP0225025	-6.236	0.393736
79	CNP0146767	-7.452	0.264404	178	CNP0225909	-6.212	0.264186
80	CNP0249835	-7.393	0.274792	179	CNP0386711	-6.192	0.401606
81	CNP0337775	-7.389	0.382096	180	CNP0295975	-6.172	0.238565
82	CNP0153706	-7.361	0.391473	181	CNP0292269	-6.168	0.288779
83	CNP0276366	-7.341	0.291107	182	CNP0321554	-6.167	0.452381
84	CNP0290328	-7.337	0.435622	183	CNP0211522	-6.149	0.292984
85	CNP0114245	-7.308	0.321945	184	CNP0149859	-6.137	0.242123
86	CNP0175618	-7.304	0.210618	185	CNP0291183	-6.137	0.268519
87	CNP0322284	-7.301	0.316556	186	CNP0220819	-6.102	0.347625
88	CNP0130246	-7.296	0.223993	187	CNP0217259	-6.099	0.359375
89	CNP0192174	-7.271	0.295129	188	CNP0304008	-6.096	0.309826
90	CNP0370542	-7.233	0.407455	189	CNP0236109	-6.093	0.408216
91	CNP0242593	-7.228	0.258224	190	CNP0323192	-6.084	0.325181
92	CNP0330206	-7.227	0.309713	191	CNP0244923	-6.062	0.375
93	CNP0103504	-7.213	0.296296	192	CNP0256270	-6.036	0.33114
94	CNP0198200	-7.210	0.270248	193	CNP0214876	-6.028	0.316981
95	CNP0308187	-7.186	0.460938	194	CNP0329876	-6.020	0.273458

96	CNP0110235	-7.152	0.334635	195	CNP0118634	-6.000	0.285392
97	CNP0133244	-7.145	0.374179	196	CNP0295617	-5.994	0.476563
98	CNP0315919	-7.145	0.411619	197	CNP0244936	-5.980	0.311449
99	CNP0398413	-7.094	0.259473				
