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Development of PARP-1 inhibitors for Breast cancer therapy: *In-silico* scrutinising of potent phytochemicals

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SUPPLEMENTARY MATERIAL

Table S1: Phytochemicals that failed to dock in the binding pocket of PARP-1 protein.

Entry No.	Code	Title	Smiles	Docking score (Kcal/mol)
1	**P29**	Matairesinol	c1cc(O)c(OC)cc1C[C@@H](C(=O)OC2)[C@H]2Cc3cc(OC)c(O)cc3	-8.296
2	**P30**	Luteolin	Oc1cc(O)cc(c12)oc(cc2=O)-c3cc(O)c(O)cc3	-8.29
3	**P31**	Silibinin	c1cc(O)c(OC)cc1[C@@H](O2)[C@@H](CO)Oc(c23)ccc(c3)[C@H]([C@@H](O)C4=O)Oc(c45)cc(O)cc5O	-8.246
4	**P32**	Apigenin-7-O-glucoside	O[C@H]1[C@H](O)[C@@H](CO)O[C@H]([C@@H]1O)O[C@H](C2)C[C@@H](O)[C@H]([C@H]23)[C@H](O)C[C@H](O3)[C@@H]4CC[C@H](O)CC4	-8.222
5	**P33**	3'-Hydroxy-O-desmethylangolensin	c1cc(O)c(O)c(O)c1C(=O)[C@@H](C)c2ccc(O)cc2	-8.184

6	**P34**	Morin	Oc1cc(O)cc(c12)oc(c(O)c2=O)-c3c(O)cc(O)cc3	-8.177
7	**P35**	Isovitexin	O[C@@H]1[C@@H](O)[C@H](O)[C@@H](CO)O[C@H]1c(c2O)c([O-])cc(c23)oc(cc3=O)-c4ccc(O)cc4	-8.14
8	**P36**	Gallic acid	O[C@H](C1)[C@@H](O)[C@@H](O)C[C@H]1C(O)O	-8.126
9	**P37**	Epigallocatechin Gallate	Oc1cc(O)cc(c12)O[C@H](c3cc(O)c(O)c(O)c3)[C@@H](C2)OC(=O)c4cc(O)c(O)c([O-])c4	-7.975
10	**P38**	Enterodiol	c1ccc(O)cc1C[C@@H](CO)[C@H](CO)Cc2cc(O)ccc2	-7.954
11	**P39**	Pinoresinol	c1cc(O)c(OC)cc1[C@H]2OC[C@@H]([C@@H]23)[C@H](OC3)c4cc(OC)c(O)cc4	-7.95
12	**P40**	Fisetin	c1cc(O)cc(c12)oc(c(O)c2=O)-c3cc(O)c(O)cc3	-7.939
13	**P41**	Quinizarin	O[C@@H]1CC[C@H](O)[C@H]([C@@H]12)[C@H](O)[C@@H]3[C@H]([C@H]2O)CCCC3	-7.928
14	**P42**	5'-Hydroxy-O-desmethylangolensin	Oc(c1)c(O)cc(O)c1C(=O)[C@H](C)c2ccc(O)cc2	-7.871
15	**P43**	Caffeic acid phenethyl ester	c1ccccc1CCOC(=O)\C=C\c2cc(O)c(O)cc2	-7.839
16	**P44**	Meso-dihydroguaiaretic acid	c1cc(O)c(OC)cc1C[C@H](C)[C@H](C)Cc2cc(OC)c(O)cc2	-7.83
17	**P45**	Baicalein	Oc1c(O)c(O)cc(c12)oc(cc2=O)-c3ccccc3	-7.824
18	**P46**	Epicatechin	Oc1cc(O)cc(c12)O[C@@H]([C@H](O)C2)c3cc(O)c(O)cc3	-7.824
19	**P47**	Butein	c1cc(O)cc(O)c1C(=O)\C=C\c2cc(O)c(O)cc2	-7.813
20	**P48**	9-epoxylignan	C1C[C@H](O)[C@@H](OC)C[C@H]1C[C@H](CO[C@@H]2OC)[C@@H]2C[C@@H]3C[C@H](OC)[C@H](O)CC3	-7.776
21	**P49**	Kaempferol	Oc1cc(O)cc(c12)oc(c(O)c2=O)-c3ccc(O)cc3	-7.736
22	**P50**	Emodin	C1[C@H](C)C[C@H](O)[C@H]([C@@H]12)[C@H](O)[C@@H]3[C@@H]([C@H]2O)C[C@@H](O)C[C@H]3O	-7.709
23	**P51**	Rosmarinic acid	c1cc(O)c(O)cc1C[C@H](C([O-])=O)OC(=O)/C=C/c2cc(O)c(O)cc2	-7.673

24	**P52**	Juglone	O[C@@H]1CCC[C@@H]([C@H]12)[C@@H](O)CC[C@H]2O	-7.617
25	**P53**	Sesamin	O1COc(c12)ccc(c2)[C@H]3OC[C@@H]([C@@H]34)[C@H](OC4)c(c5)ccc(c56)OCO6	-7.593
26	**P54**	Isoamaranthin	O[C@@H]1[C@@H](O)[C@H](O)[C@@H](C([O-])=O)O[C@H]1O[C@@H]2[C@@H](O)[C@H](O)[C@@H](CO)O[C@H]2Oc(c3)c(O)cc(c34)N([C@H](C4)C([O-])=O)/C=C/C5=CC(C([O-])=O)=[NH+][C@@H](C5)C([O-])=O	-7.55
27	**P55**	Thalirugine	COc(c1)c(OC)c(O)c(c12)CC[N@@H+](C)[C@H]2Cc3ccc(cc3)Oc(c(OC)cc4)cc4C[C@@H]5[N@H+](C)CCc(c56)cc(OC)c(O)c6	-7.478
28	**P56**	Catechin	O[C@H]1C[C@@H](O)C[C@H]([C@@H]12)O[C@@H]([C@@H](O)C2)[C@@H]3C[C@H](O)[C@H](O)CC3	-7.455
29	**P57**	Hesperetin	Oc1cc(O)cc(c12)O[C@@H](CC2=O)c3cc(O)c(OC)cc3	-7.418
30	**P58**	Noroxyhydrastinine	O1COc(c2)c1cc(c23)C(=O)NCC3	-7.399
31	**P59**	Alizarin	O[C@@H]1[C@@H](O)CC[C@@H]([C@H]12)[C@@H](O)[C@H]3[C@H]([C@@H]2O)CCCC3	-7.379
32	**P60**	Aloe-emodin	OC[C@H](C1)C[C@@H](O)[C@@H]([C@H]12)[C@@H](O)[C@H]3[C@H]([C@@H]2O)CCC[C@@H]3O	-7.365
33	**P61**	Vitexin	O[C@@H]1[C@@H](O)[C@H](O)[C@@H](CO)O[C@H]1c2c([O-])cc(O)c(c23)c(=O)cc(o3)-c4ccc(O)cc4	-7.357
34	**P62**	Galangin	Oc1cc(O)cc(c12)oc(c(O)c2=O)-c3ccccc3	-7.304
35	**P63**	Alpha-D-Glucose	OC[C@H]1O[C@H](O)[C@H](O)[C@@H](O)[C@@H]1O	-7.279
36	**P64**	Theaflavin-3,3-digallate	c1c(O)c([O-])c(O)cc1C(=O)O[C@H](Cc(c23)c(O)cc(c3)O)[C@H](O2)c(c4)cc(O)c(=[OH+])c(c45)c(O)c(O)cc5[C@H](Oc(c67)cc(O)cc7O)[C@H](C6)OC(=O)c8cc(O)c(O)c(c8)O	-7.261

37	**P65**	Beta-Sitosterol-beta-D-Glucoside	O[C@H]1[C@H](O)[C@@H](CO)O[C@H]([C@@H]1O)O[C@@H](CC2)CC(=CC3)[C@@]2(C)[C@@H](CC4)[C@@H]3[C@@H]([C@]45C)CC[C@@H]5[C@H](C)CC[C@H](C(C)C)CC	-7.255
38	**P66**	Apigenin	Oc1cc(O)cc(c12)oc(cc2=O)-c3ccc(O)cc3	-7.25
39	**P67**	Physicon	C1[C@@H](C)C[C@H](O)[C@H]([C@@H]12)[C@H](O)[C@@H]3[C@@H]([C@H]2O)C[C@@H](OC)C[C@H]3O	-7.237
40	**P68**	3,3'-Diindolylmethane	c1cccc(c12)[nH]cc2Cc3c[nH]c(c34)cccc4	-7.167
41	**P69**	Rutin	O[C@@H]1[C@@H](O)[C@H](C)O[C@H]([C@@H]1O)OC[C@H]2O[C@H]([C@H](O)[C@@H](O)[C@@H]2O)Oc(c3=O)c(-c4cc(O)c(O)cc4)oc(c35)cc([O-])cc5O	-7.036
42	**P70**	Capsaicin	CC(C)/C=C/CCCCC(=O)NCc1cc(OC)c(O)cc1	-7.019
43	**P71**	Resveratrol	Oc(c1)cc(O)cc1/C=C/c2ccc(O)cc2	-7.014
44	**P72**	7,8-benzoflavone	c1ccccc1-c(o2)cc(=O)c3ccc(c4c23)cccc4	-7.004
45	**P73**	Genistein	Oc1cc(O)cc(c12)occ(c2=O)-c3ccc(O)cc3	-6.981
46	**P74**	4-hydroxychalcone	c1cc(O)ccc1/C=C/C(=O)c2ccccc2	-6.978
47	**P75**	Naringenin	Oc1cc(O)cc(c12)O[C@@H](CC2=O)c3ccc(O)cc3	-6.952
48	**P76**	Isoliquiritigenin	c1cc(O)cc(O)c1C(=O)\C=C\c2ccc(O)cc2	-6.884
49	**P77**	3'-O-Methylequol	c1cc(O)cc(c12)OC[C@@H](C2)c3cc(OC)c(O)cc3	-6.822
50	**P78**	Flavone	c1cccc(c12)oc(cc2=O)-c3ccccc3	-6.788
51	**P79**	Niazinin	CO[C@@H]([S-])[NH2+]C[C@H](CC1)CC[C@H]1O[C@@H]([C@@H]2O)O[C@@H](C)[C@H](O)[C@H]2O	-6.783
52	**P80**	Isoxanthohumol	c1cc(O)ccc1[C@@H](O2)CC(=O)c(c23)c(OC)cc(O)c3CC=C(C)C	-6.776
53	**P81**	7,4'-Dihydroxyflavone	Oc1ccc(cc1)-c(cc2=O)oc(c23)cc(O)cc3	-6.769

54	**P82**	Ellagic Acid	O=c1oc2c(O)c([O-])cc3c(=O)oc4c(O)c(O)cc1c4c23	-6.765
55	**P83**	Oxymatrine	[O-][N@@+]12[C@@H]3[C@H](CCC1)[C@@H]4N(C(=O)CCC4)C[C@@H]3CCC2	-6.711
56	**P84**	Enterolactone	c1ccc(O)cc1C[C@@H](C(=O)OC2)[C@H]2Cc3cc(O)ccc3	-6.699
57	**P85**	Acacetin	Oc1cc(O)cc(c12)oc(cc2=O)-c3ccc(OC)cc3	-6.673
58	**P86**	Chrysin	Oc1cc(O)cc(c12)oc(cc2=O)-c3ccccc3	-6.66
59	**P87**	Carnosol	Oc1c(O)c(C(C)C)cc(c1[C@]234)[C@@H](OC4=O)C[C@H]2C(C)(C)CCC3	-6.612
60	**P88**	Taxifolin	Oc1cc([O-])cc(c12)O[C@@H]([C@@H](O)C2=O)c3cc(O)c(O)cc3	-6.552
61	**P89**	Quercetin	Oc1cc([O-])cc(c12)oc(c(O)c2=O)-c3cc(O)c(O)cc3	-6.548
62	**P90**	Biochanin A	Oc1cc(O)cc(c12)occ(c2=O)-c3ccc(OC)cc3	-6.537
63	**P91**	Hispidulin	Oc1c(OC)c(O)cc(c12)oc(cc2=O)-c3ccc(O)cc3	-6.526
64	**P92**	Isocorydine	C[N@H+]1CCc(c2[C@@H]13)cc(OC)c(OC)c2c4c(C3)ccc(OC)c4O	-6.517
65	**P93**	Chryophanol	C1[C@@H](C)C[C@@H](O)[C@@H]([C@H]12)[C@H](O)[C@H]3[C@H]([C@@H]2O)CCC[C@@H]3O	-6.489
66	**P94**	Gingerol	CCCCC[C@H](O)CC(=O)CCc1cc(OC)c(O)cc1	-6.481
67	**P95**	3-(4-bromophenyl)-7-hydroxy-4-phenylcoumarin	c1ccccc1-c(c(c23)ccc(c3)O)c(c(=O)o2)-c4ccc(Br)cc4	-6.462
68	**P96**	Thalirugidine	COc(c1)c(OC)c(O)c(c12)CC[N@@H+](C)[C@H]2Cc3cc(c(OC)cc3)Oc(cc4)ccc4C[C@@H]5[N@@H+](C)CCc(c56)c(O)c(OC)c(c6)OC	-6.437
69	**P97**	Equol	c1cc(O)cc(c12)OC[C@@H](C2)c3ccc(O)cc3	-6.435
70	**P98**	Piperolein B	C1CCCCN1C(=O)CCCCCC/C=C/c(c2)ccc(c23)OCO3	-6.428

71	**P99**	2'-Hydroxychalcone	c1cccc(O)c1C(=O)\C=C\c2ccccc2	-6.425
72	**P100**	8-Prenylnaringenin	C1C[C@@H](O)CC[C@H]1[C@@H](O2)C[C@H](O)[C@@H]([C@H]23)[C@@H](O)C[C@@H](O)[C@H]3CCC(C)C	-6.406
73	**P101**	Tambulin	Oc1cc(OC)c(OC)c(c12)oc(c(O)c2=O)-c3ccc(OC)cc3	-6.401
74	**P102**	O-Desmethylangolensin	c1cc(O)cc(O)c1C(=O)[C@@H](C)c2ccc(O)cc2	-6.399
75	**P103**	6-O-Methylequol	COc(c1)c(O)cc(c12)OC[C@@H](C2)c3ccc(O)cc3	-6.395
76	**P104**	4-Benzyl-3(4'-chlorophenyl)-7-hydroxycoumarin	c1ccccc1Cc(c(c23)ccc(c3)O)c(c(=O)o2)-c4ccc(Cl)cc4	-6.365
77	**P105**	Coumestrol	Oc(c1)ccc2c1oc(c23)c4c(oc3=O)cc(O)cc4	-6.341
78	**P106**	Armatamide	O1CO[C@@H]([C@H]12)CC[C@@H](C2)CC[C@H](O)[NH2+]CC[C@@H]3CC[C@H](OC)CC3	-6.244
79	**P107**	Plumbagin	c1ccc(O)c(c12)C(=O)C=C(C2=O)C	-6.18
80	**P108**	Caffeic Acid	c1cc(O)c(O)cc1/C=C/C([O-])=O	-6.155
81	**P109**	Flavanone	c1cccc(c12)O[C@@H](CC2=O)c3ccccc3	-6.153
82	**P110**	Xanthyletin	O1C(C)(C)C=Cc(c12)cc3c(c2)oc(=O)cc3	-6.147
83	**P111**	Eriodictyol	Oc1cc([O-])cc(c12)O[C@@H](CC2=O)c3cc(O)c(O)cc3	-6.129
84	**P112**	6'-Hydroxy-O-desmethylangolensin	c1cc(O)ccc1[C@H](C)C(=O)c2c([O-])cc(O)cc2O	-6.071
85	**P113**	Daidzein	c1cc(O)cc(c12)occ(c2=O)-c3ccc(O)cc3	-6.012
86	**P114**	Betanidin	O=C(C1)C(=O)C=C(C=12)N([C@@H](C2)C([O-])=O)/C=C/C(C3)=CC(=C(O)O)[N-][C@@H]3C([O-])=O	-5.986
87	**P115**	Theaflavin 3-gallate	[O-]c(c1)c(O)c(O)cc1C(=O)O[C@@H](C2)[C@@H](Oc(c23)cc(O)cc3O)c4cc(O)c(O)c(c45)c(=[OH+])c(O)cc(c5)[C@H]([C@H](O)C6)Oc(c67)cc(O)cc7O	-5.929
88	**P116**	Xanthohumol	CC(C)=CCc1c(O)c(c(OC)cc1O)C(=O)/C=C/c2ccc(O)cc2	-5.921

89	**P117**	Curcumin	c1cc(O)c(OC)cc1/C=C/C(/O)=C\C(=O)\C=C\c2cc(OC)c(O)cc2	-5.866
90	**P118**	Rohitukine	C[N@@H+]1C[C@@H](O)[C@H](CC1)c2c([O-])cc(O)c(c23)c(=O)cc(o3)C	-5.851
91	**P119**	Germacranolide	C[C@@H]1C(=O)O[C@@H]([C@H]12)/C=C(C)\CC[C@H](O)/C(C)=C\[C@@H]2O	-5.848
92	**P120**	Protocatechuic acid	c1cc(O)c(O)cc1C([O-])=O	-5.793
93	**P121**	Rubiadin	O[C@@H]1[C@H](C)[C@H](O)C[C@@H]([C@@H]12)[C@H](O)[C@@H]3[C@@H]([C@H]2O)CCCC3	-5.791
94	**P122**	Dantron	C1CC[C@@H](O)[C@H]([C@H]2O)[C@@H]1[C@H](O)[C@H]([C@H]23)CCC[C@@H]3O	-5.774
95	**P123**	Methoxyeugenol	COc(c1)c(O)c(OC)cc1CC=C	-5.749
96	**P124**	Indole-3-carbinol	OCc1c[nH]c(c12)cccc2	-5.718
97	**P125**	Piperlongumine	COc(c1)c(OC)c(OC)cc1\C=C\C(=O)N2CCC=CC2=O	-5.687
98	**P126**	Anthrarufin	O[C@@H]1CCC[C@@H]([C@@H]2O)[C@H]1[C@@H](O)[C@@H]([C@@H]23)CCC[C@H]3O	-5.684
99	**P127**	Alpha-Mangostin	CC(C)=CCc(c([O-])c1)c(O)c(c2=O)c1oc(c23)cc(O)c(OC)c3CC=C(C)C	-5.672
100	**P128**	Eugenol	C=CCc1cc(OC)c(O)cc1	-5.65
101	**P129**	5,6-benzoflavone	c1ccccc1-c(cc2=O)oc3ccc(c4c23)cccc4	-5.643
102	**P130**	Piperolein A	C1CCCCN1C(=O)CCCC/C=C/c(c2)ccc(c23)OCO3	-5.615
103	**P131**	Thymoquinone	O=C1C=C(C)C(=O)C=C1C(C)C	-5.527
104	**P132**	Vinylguaiacol	C1CC[C@@H](OC)[C@@H](O)[C@@H]1CC	-5.527
105	**P133**	Epigallocatechin	Oc1cc(O)cc(c12)O[C@@H]([C@H](O)C2)c3cc(O)c(O)c([O-])c3	-5.503
106	**P134**	6-hydroxy-3-(4-methoxyphenyl)-4-methylcoumarin	c1cc(O)cc(c12)c(C)c(c(=O)o2)-c3ccc(cc3)OC	-5.5

107	**P135**	N-(4-hydroxyundecanoyl) anabasine	c1ncccc1[C@H](CCCC2)N2C(=O)CC[C@@H](O)CCCCCCC	-5.444
108	**P136**	Thalicarpine	C[N@@H+]1CCc(c2[C@@H]13)cc(OC)c(OC)c2c4c(C3)cc(c(c4)OC)Oc(cc(OC)c(c5)OC)c5C[C@@H]6[N@H+](C)CCc(c67)cc(OC)c(c7)OC	-5.386
109	**P137**	Thymol	CC(C)c1c(O)cc(C)cc1	-5.369
110	**P138**	Ginkoglide b	O[C@H]1C(=O)O[C@H]([C@@]12[C@]345)O[C@]3([C@]6(O)[C@H]([C@@H]5O)OC(=O)[C@H]6C)C(=O)O[C@@H]4C[C@H]2C(C)(C)C	-5.354
111	**P139**	4-O-Methyl equol	c1cc(O)cc(c12)OC[C@@H](C2)c3ccc(OC)cc3	-5.302
112	**P140**	Shogaol	c1cc(O)c(OC)cc1CCC(=O)\C=C\CCCCC	-5.302
113	**P141**	Syringol	CO[C@H]1[C@H](O)[C@H](OC)CCC1	-5.241
114	**P142**	Hexadecanoic acid	OC(O)CCCCCCCCCCCCCCC	-5.24
115	**P143**	Perillyl alcohol	OCC(=CC1)CC[C@@H]1C(C)=C	-5.23
116	**P144**	Nimbiol	c1c(C)c(O)cc2c1C(=O)C[C@H]([C@@]23C)C(C)(C)CCC3	-5.192
117	**P145**	Acetic acid	OC(O)C	-5.103
118	**P146**	Anthrone	C1CCC[C@H]([C@@H]12)[C@H](O)[C@@H]3[C@@H](C2)CCCC3	-5.101
119	**P147**	Sterol	C1C[C@@H](O)C[C@@H](CC2)[C@H]1[C@@H]([C@H]23)CC[C@H]4[C@H]3CCC4	-5.078
120	**P148**	Octadecenoic acid	OC(O)CCCCCCCCCCCCCCCCC	-5.026
121	**P149**	Anthraquinone	C1CCC[C@@H]([C@@H]2O)[C@@H]1[C@H](O)[C@H]([C@@H]23)CCCC3	-5.012
122	**P150**	Nobiletin	COc1c(OC)c(OC)c(OC)c(c12)oc(cc2=O)-c3cc(OC)c(OC)cc3	-4.998
123	**P151**	Pterostilbene	COc(c1)cc(OC)cc1/C=C/c2ccc(O)cc2	-4.997

124	**P152**	Ferulic acid	c1cc(O)c(OC)cc1/C=C/C([O-])=O	-4.971
125	**P153**	8-Oxyberberine	O1CO[C@H](C2)[C@H]1C[C@H](CC3)[C@@H]2[C@H]([N@H+]34)C[C@@H]5[C@H]([C@H]4O)[C@@H](OC)[C@H](OC)CC5	-4.96
126	**P154**	Linoleic acid	OC(O)CCCCCCCCCCCCCCCCC	-4.942
127	**P155**	Guaiol	OC(C)(C)[C@@H](C1)CC[C@H](C)C(=C12)CC[C@@H]2C	-4.915
128	**P156**	Heptadecanoic acid	OC(O)CCCCCCCCCCCCCCCCC	-4.913
129	**P157**	Safrole	O1COc(c12)ccc(c2)CC=C	-4.885
130	**P158**	Cucubitacin B	CC(=O)OC(C)(C)/C=C/C(=O)[C@](C)(O)[C@@H]([C@@H](C1)O)[C@](C)([C@@]12C)CC(=O)[C@]3(C)[C@H]2CC=C4[C@H]3C[C@H](O)C(=O)C4(C)C	-4.867
131	**P159**	Mesitol	C[C@H]1[C@@H](O)[C@H](C)C[C@@H](C1)C	-4.818
132	**P160**	Columbamine	C1C[C@H](OC)[C@@H](OC)[C@H](C2)[C@@H]1C[C@@H]([N@@H+]23)[C@H]4[C@@H](CC3)C[C@@H](OC)[C@@H](O)C4	-4.809
133	**P161**	4-Hydroxycinnamic acid	c1cc(O)ccc1/C=C/C([O-])=O	-4.798
134	**P162**	Sulfrophane	C[S@@](=O)CCCCN=C=S	-4.771
135	**P163**	Isoelemicin	COc(c1)c(OC)c(OC)cc1/C=C/C	-4.762
136	**P164**	Benzeneethanamine	[NH3+]CCC1CCCCC1	-4.758
137	**P165**	Delta cadinene	CC(=C1)CCC([C@@H]12)=C(C)CC[C@H]2C(C)C	-4.729
138	**P166**	Jatrorrhizine	c1cc(OC)c(OC)c(c2)c1cc([n+]23)c4c(CC3)cc(O)c(c4)OC	-4.708
139	**P167**	Nerol	OC/C=C(C)\CCC=C(C)C	-4.68
140	**P168**	Glabridin	C1=CC(C)(C)Oc(cc2)c1c(c23)OC[C@H](C3)c4c(O)cc(O)cc4	-4.679
141	**P169**	Carveol	C1C=C(C)[C@H](O)C[C@@H]1C(C)=C	-4.676
142	**P170**	Bornyl acetate	O[C@@H](C)O[C@@H]1C[C@H](CC2)C(C)(C)[C@@]12C	-4.66

143	**P171**	Anisaldehyde	CO[C@H]1CC[C@@H](CC1)CO	-4.655
144	**P172**	Parthenolide	C[C@@]12[C@H](O1)[C@@H]3[C@H](C(C(O3)=O)=C)CC/C(C)=C\CC2	-4.622
145	**P173**	Pterygospermin	C1CCCCC1CN2[C@@H](S)O[C@@]2(CC3)CC[C@]34O[C@H](S)N4CC5CCCCC5	-4.597
146	**P174**	Myristicin	O1COc(c12)cc(CC=C)cc2OC	-4.546
147	**P175**	Geranyl acetate	O=C(C)OC\C=C(C)\CCC=C(C)C	-4.532
148	**P176**	Piperine	C1CCCCN1C(=O)/C=C/C=C/c(c2)ccc(c23)OCO3	-4.497
149	**P177**	Carnosic acid	Oc1c(O)c(C(C)C)cc(c1[C@]23C(=O)[O-])CC[C@H]2C(C)(C)CCC3	-4.497
150	**P178**	Glyceollin	Oc(c1)ccc2c1O[C@H]([C@]23O)c4c(OC3)c5c(cc4)OC(C)(C)C=C5	-4.48
151	**P179**	Geraniol	OC\C=C(C)\CCC=C(C)C	-4.471
152	**P180**	Sanguinarine	O1COc(cc2)c1c(c[n+]3C)c2c(c34)ccc5c4cc6c(c5)OCO6	-4.417
153	**P181**	Linalool	C=C[C@@](O)(C)CCC=C(C)C	-4.382
154	**P182**	Centratherin	O=C1C=C(O[C@@]12C)/C(C[O-])=C\[C@@H]3[C@H](C(C(O3)=O)=C)[C@H](C2)OC(=O)/C(C)=C\C	-4.381
155	**P183**	Spathulenol	C1C[C@@](O)(C)[C@@H]2[C@@H]1C(=C)CC[C@H]([C@H]23)C3(C)C	-4.345
156	**P184**	Terpinolene	CC(C)=C1CCC(C)=CC1	-4.298
157	**P185**	Campesterol	C1C[C@H](O)CC(=CC2)[C@@]1(C)[C@@H](CC3)[C@@H]2[C@@H]([C@]34C)CC[C@@H]4[C@H](C)CC[C@@H](C)C(C)C	-4.288
158	**P186**	Oxyberberine	O1COc(c2)c1cc(CC3)c2c(n34)cc5c(c4=O)c(OC)c(OC)cc5	-4.248
159	**P187**	4-benzyl-7-methoxy-3-phenylcoumarin	c1cc(OC)cc(c12)oc(=O)c(-c3ccccc3)c2Cc4ccccc4	-4.222
160	**P188**	Elemicin	CO[C@H](C1)[C@H](OC)[C@@H](OC)C[C@@H]1CCC	-4.204
161	**P189**	Rotenone	O=C1c2ccc(O[C@H](C3)C(C)=C)c3c2O[C@@H]([C@@H]14)COc5c4cc(OC)c(c5)OC	-4.199

162	**P190**	Vernosterol	C1C[C@H](O)C[C@@H]2CCC([C@H]3[C@@]12C)=C4[C@](C)(CC3)[C@H](C=C4)[C@H](C)CC/C(C(C)C)=C/C	-4.197
163	**P191**	Citral alpha	OCC[C@H](C)CCCC(C)C	-4.184
164	**P192**	4-terpinol	CC(C)[C@]1(O)CC[C@@H](C)CC1	-4.146
165	**P193**	Benzyl isothiocyanate	S=C=[NH+]Cc1ccccc1	-4.116
166	**P194**	Stigmasterol	C1C[C@H](O)CC(=CC2)[C@@]1(C)[C@@H](CC3)[C@@H]2[C@@H]([C@]34C)CC[C@@H]4[C@H](C)/C=C/[C@H](C(C)C)CC	-4.1
167	**P195**	Citronellal	OCC[C@@H](C)CCCC(C)C	-4.05
168	**P196**	Carvacrol	O[C@H]1[C@H](C)CC[C@@H](C1)C(C)C	-4.048
169	**P197**	Hypericin	c12c3c4c5c6c1c(c(=O)cc6C)c(O)c7c2c(c(O)cc7O)c8c3c(c(O)cc8O)c(O)c4c(=O)cc5C	-4.047
170	**P198**	Camphor	C[C@@]12[C@@H](O)C[C@@H](CC1)C2(C)C	-4.024
171	**P199**	p-Tolualdehyde	OC[C@H](CC1)CC[C@H]1C	-3.967
172	**P200**	Berberine	O1CO[C@H](C2)[C@H]1C[C@H](CC3)[C@@H]2[C@H]([N@H+]34)C[C@@H]5[C@H](C4)[C@@H](OC)[C@H](OC)CC5	-3.919
173	**P201**	Pelargic acid	OC(O)CCCCCCCCC	-3.876
174	**P202**	1,2-dithiocane	S1SCCCCCC1	-3.869
175	**P203**	1'-Acetoxychavicol acetate	O=C(C)O[C@@H](C=C)c1ccc(cc1)OC(=O)C	-3.861
176	**P204**	Cinnamic acid	[O-]C(=O)\C=C\c1ccccc1	-3.848
177	**P205**	Estragole	C1C[C@H](OC)CC[C@H]1CCC	-3.822
178	**P206**	Lambertine	O1COc(c2)c1cc(CC3)c2C(N34)=Cc5c(C4)c(OC)c(OC)cc5	-3.802
179	**P207**	(E)-Ajoene	CCC[S+](O)CCCSSCCC	-3.789
180	**P208**	Brassicasterol	C1C[C@H](O)CC(=CC2)[C@@]1(C)[C@@H](CC3)[C@@H]2[C@@H]([C@]34C)CC[C@@H]4[C@H](C)/C=C/[C@H](C)C(C)C	-3.742
181	**P209**	Trans-Nerolidol	C=C[C@@](O)(C)CC/C=C(C)/CCC=C(C)C	-3.702

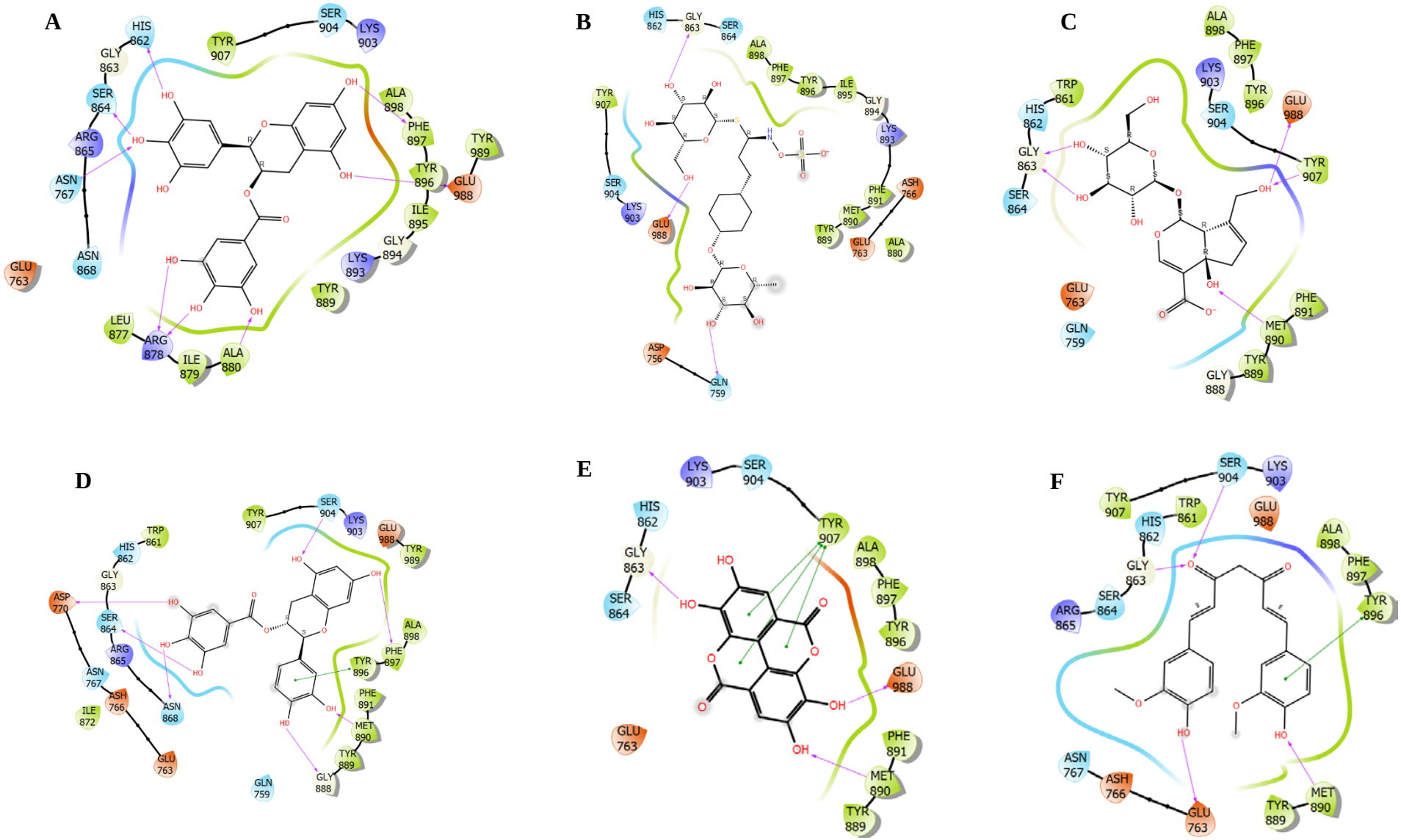
182	**P210**	D-limonene	CC(C)[C@@H]1CC[C@@H](C)CC1	-3.692
183	**P211**	Stearic acid	[O-]C(=O)CCCCCCCCCCCCCCCCCC	-3.686
184	**P212**	Beta_Bisabolene	CC1=CC[C@H](CC1)C(=C)CCC=C(C)C	-3.683
185	**P213**	Lemonene	CC(=C)[C@H]1CCC(C)=CC1	-3.68
186	**P214**	s allylmercaptocysteine	C=CCSSC[C@@H](C(=O)[O-])[NH3+]	-3.674
187	**P215**	Phytic acid	[O-]P(=O)(O)O[C@H]1[C@H](OP([O-])(=O)O)[C@H](OP([O-])(=O)O)[C@H](OP([O-])(=O)O)[C@@H](OP([O-])(=O)O)[C@H]1OP([O-])(=O)O	-3.404
188	**P216**	Allicin	CCC[S+](O)SCCC	-3.27
189	**P217**	Hirsutine	COC(=O)C(=C\OC)\[C@H]([C@H](C1)CC)C[C@@H](N12)c3c(CC2)c4c([nH]3)cccc4	-3.27
190	**P218**	1-cyanocychexylpyrrolidin	C1CCC[NH+]1C2CCCCC2	-3.241
191	**P219**	Piperazine	[NH2+]1CCNCC1	-3.225
192	**P220**	Sabinene	CC(C)[C@@]12[C@@H](C1)C(=C)CC2	-3.158
193	**P221**	Beta pinene	CC([C@@H]12)(C)[C@@H](C2)C(=C)CC1	-3.15
194	**P222**	1,2-Didehydropinidinol	O[C@H](C)C[C@@H]1N=C(C)CCC1	-3.131
195	**P223**	Caryophyllene oxide	C[C@@]12[C@H](O1)CC[C@@H](C)[C@@H]3[C@H](C(C3)(C)C)CC2	-3.086
196	**P224**	Alpha pinene	CC1(C)[C@H](C2)C(C)=CC[C@@H]12	-2.975
197	**P225**	Thalisopine	C[N@@H+]1CCc(c2[C@@H]13)c([O-])c(OC)c(OC)c2Oc4cc5c(cc4OC)CC[N@@H+](C)[C@H]5Cc6cc(c(OC)cc6)Oc7ccc(C3)cc7	-2.797

198	**P226**	Oxycanthine	C[N@H+]1CCc(c2[C@H]13)cc(OC)c(OC)c2Oc4cc5c(cc4OC)CC[N@@H+](C)[C@@H]5Cc6cc(c(O)cc6)Oc7ccc(C3)cc7	-2.774
199	**P227**	Palmitic acid	[O-]C(=O)CCCCCCCCCCCCCCC	-2.709
200	**P228**	Beta-Sitosterol	C1C[C@H](O)CC(=CC2)[C@@]1(C)[C@@H](CC3)[C@@H]2[C@@H]([C@]34C)CC[C@@H]4[C@H](C)CC[C@H](C(C)C)CC	-2.696
201	**P229**	Myrcene	CC(C)=CCCC(=C)C=C	-2.516
202	**P230**	Ursolic acid	C1C[C@@H](C)[C@H](C)[C@H]([C@]12C(=O)[O-])C=3[C@@](C)(CC2)[C@@]4(C)[C@H](CC3)[C@]5(C)[C@@H](CC4)C(C)(C)[C@@H](O)CC5	-2.488
203	**P231**	Palmatine	COc(c1)c(OC)cc(CC2)c1c([n+]23)cc4c(c3)c(OC)c(OC)cc4	-2.486
204	**P232**	Diallyldisulfide	C=CCSSCC=C	-2.469
205	**P233**	Beta-Caryophyllene oxide	C[C@]12[C@H](O2)CCC(=C)[C@@H]3[C@@H](CC1)C(C3)(C)C	-2.454
206	**P234**	N-valeramide	O[C@H]([NH3+])CCCC	-2.44
207	**P235**	Lauric acid	[O-]C(=O)CCCCCCCCCCC	-2.278
208	**P236**	Azelaic acid	[O-]C(=O)CCCCCCCC([O-])=O	-2.221
209	**P237**	Anthocyanin	c1cccc(c12)[o+]c(cc2)-c3ccccc3	-2.185
210	**P238**	Octadecane	CCCCCCCCCCCCCCCCCC	-2.085
211	**P239**	Myristic acid	[O-]C(=O)CCCCCCCCCCCCC	-2.059
212	**P240**	Camphene	[C@@H]12C(C)(C)[C@H](C)[C@@H](C1)CC2	-2.038
213	**P241**	Daucosterol	O[C@@H]1[C@@H](O)[C@H](O)[C@@H](CO)O[C@H]1O[C@@H](CC2)CC(=CC3)[C@@]2(C)[C@@H](CC4)[C@@H]3[C@@H]([C@]45C)CC[C@@H]5[C@H](C)CC[C@H](C(C)C)CC	-1.957

214	**P242**	Lupeol	C1C[C@H](O)C(C)(C)[C@H](CC2)[C@@]1(C)[C@H]3CC[C@@H]([C@]4(C)[C@]23C)[C@@H]5[C@@](C)(CC4)CC[C@H]5C(C)=C	-1.708
215	**P243**	Colchicine	O=C(C)N[C@H]1CCc(cc(OC)c(OC)c2OC)c2c(c13)ccc(OC)c(=O)c3	-1.674
216	**P244**	Olenolic acid	C1C[C@H](O)C(C)(C)[C@@H]([C@]12C)CC[C@]3(C)[C@@H]2CC=C4[C@@]3(C)CC[C@]5(C(=O)[O-])[C@H]4CC(C)(C)CC5	-1.556
217	**P245**	Vinyllithium	[CH-]=C	-1.492
218	**P246**	Thalrugosidine	C[N@@H+]1CCc(c2[C@@H]13)cc(OC)c([O-])c2Oc4c5c(cc(OC)c4OC)[C@@H]([N@H+](C)CC5)Cc6ccc(cc6)Oc7cc(C3)ccc7OC	-1.2
219	**P247**	Thalidasine	C[N@H+]1CCc(c2[C@@H]13)cc(OC)c(OC)c2Oc4c5c(cc(OC)c4OC)[C@@H](N(C)CC5)Cc6ccc(cc6)Oc7cc(C3)ccc7OC	0.075

Table S2: ADME profile of compounds P1 and Ct

Entry no.	Compounds	Mol. Wt. (g/mol)	Num. H-bond acceptors	Num. H-bond donors	TPSA (A^2)	Water solubility	GI absorption	BBB penetration	Cytochrome inhibition
1	**P1**	458.37	11	8	197.37	Soluble	Low	No	No
2	**Ct**	244.29	3	3	83.80	Very soluble	High	No	No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ARG 865
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GLU 763
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TYR 889
LEU 877
ARG 878
ILE 879
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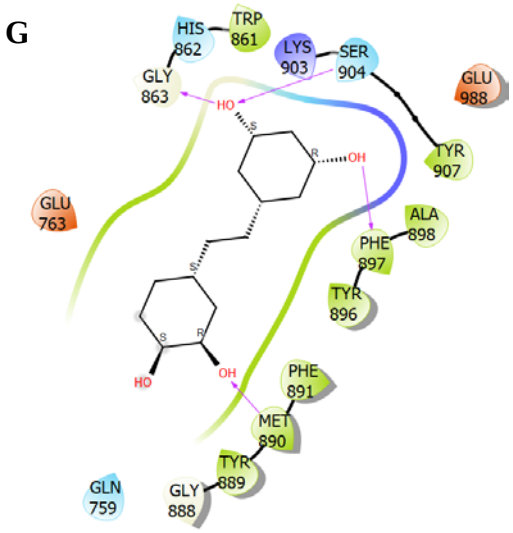

Figure S1: Protein-ligand interactions A) Epigallocatechin gallate-PARP-1 complex and B) Glucomoringin-PARP-1 complex C) Theveside-PARP-1 complex D) Catechin gallate-PARP-1 complex E) Ellagic acid-PARP-1 complex F) Curcumin-PARP-1 complex G) Piceatannol-PARP-1 complex