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1 Supplementary Tables

Table S1

Virtual Screening Results

Ranking	Chem ID	Code	Predicted Binding Energy
1	443917	Pg5	-13.6
2	12137511	M6	-12.6
3	44256862	Pn38	-10.5
4	131751177	C222	-10.3
5	90658134	C174	-10.2
6	44256911	D69	-10.2
7	44256966	Pt16	-10.2
8	5282068	C15	-10.1
9	44256762	C84	-10.1
10	102515358	C208	-10.1
11	441702	D5	-10.1
12	44256878	D45	-10.1
13	44256932	D90	-10.1
14	44256849	Pn26	-10.1
15	23724730	C34	-10.0
16	44256771	C92	-10.0
17	23724706	D27	-10.0
18	90657578	Pg95	-10.0
19	102515095	Pg112	-10.0
20	102515504	Pg116	-10.0
21	44256855	Pn31	-10.0
22	131752297	Pn54	-10.0
23	44256763	C85	-9.9
24	44256765	C87	-9.9
25	44256823	C141	-9.9
26	70698351	C155	-9.9
27	132526878	C248	-9.9
28	6444318	D11	-9.9
29	23724707	D28	-9.9
30	44256943	D94	-9.9
31	44256946	D97	-9.9
32	101699074	D127	-9.9
33	46878535	Pg88	-9.9
34	102174360	Pg111	-9.9
35	44256850	Pn27	-9.9
36	44256860	Pn36	-9.9
37	101945205	Pn49	-9.9
38	11239215	M5	-9.9

39	5282067	C14	-9.8
40	21576546	C31	-9.8
41	44256711	C47	-9.8
42	44256744	C69	-9.8
43	44256769	C90	-9.8
44	44256819	C137	-9.8
45	131750824	C219	-9.8
46	5320022	D9	-9.8
47	23724731	D29	-9.8
48	44256665	Pg54	-9.8
49	44256681	Pg69	-9.8
50	44256687	Pg75	-9.8
51	44256692	Pg80	-9.8
52	45266708	Pg87	-9.8
53	44256851	Pn28	-9.8
54	72193654	Pn44	-9.8
55	44256967	Pt17	-9.8
56	72193655	Pt28	-9.8
57	72193651	M47	-9.8
58	101332736	M52	-9.8
59	23724699	C33	-9.7
60	44256728	C57	-9.7
61	44256759	C82	-9.7
62	44256800	C119	-9.7
63	101268575	C182	-9.7
64	102163929	C199	-9.7
65	131752266	C230	-9.7
66	44256949	D100	-9.7
67	71308288	D105	-9.7
68	72193639	D106	-9.7
69	44256628	Pg26	-9.7
70	90658862	Pg97	-9.7
71	44256745	C70	-9.6
72	44256752	C75	-9.6
73	44256820	C138	-9.6
74	131752260	C226	-9.6
75	44256872	D39	-9.6
76	44256874	D41	-9.6
77	44256905	D66	-9.6
78	44256910	D68	-9.6
79	44256920	D78	-9.6
80	44256928	D86	-9.6
81	44256930	D88	-9.6
82	131750957	D133	-9.6
83	44256680	Pg68	-9.6
84	21594268	Pn10	-9.6
85	44256846	Pn23	-9.6
86	72193653	Pn43	-9.6
87	6540681	Pt3	-9.6

88	44256965	Pt15	-9.6
89	118797967	M55	-9.6
90	44256705	C41	-9.5
91	44256707	C43	-9.5
92	44256712	C48	-9.5
93	44256746	C71	-9.5
94	44256766	C88	-9.5
95	131753191	C244	-9.5
96	132526875	C246	-9.5
97	23250609	D23	-9.5
98	44256893	D56	-9.5
99	44256917	D75	-9.5
100	44256927	D85	-9.5
101	44256931	D89	-9.5
102	90658852	D122	-9.5
103	23724733	Pg12	-9.5
104	23724700	Pn11	-9.5
105	44256975	Pt25	-9.5
106	101204175	Pt33	-9.5
107	131752300	Pt37	-9.5
108	23724702	M7	-9.5
109	44256991	M20	-9.5
110	443921	C12	-9.4
111	44256764	C86	-9.4
112	44256794	C113	-9.4
113	44256818	C136	-9.4
114	44256821	C139	-9.4
115	44256824	C142	-9.4
116	50909830	C152	-9.4
117	71587512	C160	-9.4
118	102385315	C202	-9.4
119	25244498	D34	-9.4
120	44256879	D46	-9.4
121	44256881	D48	-9.4
122	44256904	D65	-9.4
123	72734296	D107	-9.4
124	443919	Pg6	-9.4
125	44256636	Pg33	-9.4
126	44256638	Pg35	-9.4
127	44256653	Pg47	-9.4
128	44256688	Pg76	-9.4
129	102515242	Pg113	-9.4
130	131753202	Pn55	-9.4
131	44256963	Pt13	-9.4
132	44256976	Pt26	-9.4
133	100926551	Pt31	-9.4
134	101513454	Pt34	-9.4
135	44257004	M30	-9.4
136	44257013	M39	-9.4

137	74977114	M48	-9.4
138	100926552	D125	-9.4
139	44256702	C38	-9.3
140	44256747	C72	-9.3
141	44256753	C76	-9.3
142	44256774	C95	-9.3
143	74976921	C164	-9.3
144	101545480	C185	-9.3
145	101545483	C188	-9.3
146	101575201	C190	-9.3
147	102515449	C210	-9.3
148	131752265	C229	-9.3
149	131753047	C237	-9.3
150	10100905	D12	-9.3
151	11972331	D17	-9.3
152	44256916	D74	-9.3
153	90657963	D116	-9.3
154	44256616	Pg17	-9.3
155	44256627	Pg25	-9.3
156	44256640	Pg36	-9.3
157	44256667	Pg56	-9.3
158	44256676	Pg64	-9.3
159	44256678	Pg66	-9.3
160	44256856	Pn32	-9.3
161	44256958	Pt9	-9.3
162	44256964	Pt14	-9.3
163	44256970	Pt20	-9.3
164	72193656	Pt29	-9.3
165	44256989	M19	-9.3
166	44257000	M26	-9.3
167	44257007	M33	-9.3
168	44257014	M40	-9.3
169	131752271	M56	-9.3
170	44256756	C79	-9.3
171	90659011	C176	-9.2
172	29232	C1	-9.2
173	5316221	C16	-9.2
174	14655733	C25	-9.2
175	44256729	C58	-9.2
176	44256734	C61	-9.2
177	44256802	C121	-9.2
178	44256804	C123	-9.2
179	44256806	C125	-9.2
180	44256826	C144	-9.2
181	44256830	C148	-9.2
182	73981555	C162	-9.2
183	74976932	C165	-9.2
184	132470936	C245	-9.2
185	132526876	C247	-9.2

186	15922818	D22	-9.2
187	25244733	D35	-9.2
188	44256882	D49	-9.2
189	44256890	D53	-9.2
190	44256898	D60	-9.2
191	44256902	D64	-9.2
192	44256919	D77	-9.2
193	44256921	D79	-9.2
194	102028681	D128	-9.2
195	131752146	D134	-9.2
196	44256632	Pg29	-9.2
197	44256637	Pg34	-9.2
198	44256652	Pg46	-9.2
199	44256682	Pg70	-9.2
200	101731795	Pg108	-9.2
201	44256836	Pn14	-9.2
202	44256960	Pt10	-9.2
203	134732297	Pt40	-9.2
204	44256981	M11	-9.2
205	44257006	M32	-9.2
206	44257010	M36	-9.2
207	72193647	M46	-9.2
208	132531494	M57	-9.2
209	9897848	Pt4	-9.2
210	4481457	C13	-9.1
211	6602295	C18	-9.1
212	44256717	C50	-9.1
213	44256730	C59	-9.1
214	44256775	C96	-9.1
215	44256784	C104	-9.1
216	44256787	C107	-9.1
217	44256831	C149	-9.1
218	56776253	C154	-9.1
219	101545484	C189	-9.1
220	131752762	C232	-9.1
221	5316496	D7	-9.1
222	25201660	D33	-9.1
223	44256889	D52	-9.1
224	44256892	D55	-9.1
225	44256895	D57	-9.1
226	44256922	D80	-9.1
227	167643	Pg2	-9.1
228	23724704	Pg11	-9.1
229	44256615	Pg16	-9.1
230	44256618	Pg19	-9.1
231	44256629	Pg27	-9.1
232	44256663	Pg52	-9.1
233	44256664	Pg53	-9.1
234	44256675	Pg63	-9.1

235	44256679	Pg67	-9.1
236	44256689	Pg77	-9.1
237	44256691	Pg79	-9.1
238	101545485	Pg101	-9.1
239	101682297	Pg107	-9.1
240	131751360	Pg118	-9.1
241	5488811	Pn3	-9.1
242	44256843	Pn20	-9.1
243	44256995	M23	-9.1
244	25203612	C36	-9.0
245	441681	C7	-9.0
246	44256701	C37	-9.0
247	44256737	C63	-9.0
248	44256772	C93	-9.0
249	44256814	C132	-9.0
250	101268577	C184	-9.0
251	131752264	C228	-9.0
252	131753044	C234	-9.0
253	131753049	C239	-9.0
254	131753050	C240	-9.0
255	131753090	C243	-9.0
256	5493095	D10	-9.0
257	11972332	D18	-9.0
258	14311158	D20	-9.0
259	23724705	D26	-9.0
260	44256899	D61	-9.0
261	44256908	D67	-9.0
262	44256912	D70	-9.0
263	44256929	D87	-9.0
264	44256933	D91	-9.0
265	44256947	D98	-9.0
266	90657987	D117	-9.0
267	90658465	D121	-9.0
268	44256624	Pg23	-9.0
269	44256642	Pg38	-9.0
270	44256644	Pg40	-9.0
271	44256649	Pg43	-9.0
272	90659020	Pg98	-9.0
273	14757905	Pn8	-9.0
274	44256842	Pn19	-9.0
275	44256844	Pn21	-9.0
276	44256859	Pn35	-9.0
277	44256865	Pn41	-9.0
278	75184857	Pt30	-9.0
279	44256985	M15	-9.0
280	44256988	M18	-9.0
281	71308234	M44	-9.0
282	181258	C3	-8.9
283	441688	C8	-8.9

284	10312147	C21	-8.9
285	15714477	C29	-8.9
286	44256709	C45	-8.9
287	44256726	C55	-8.9
288	44256742	C67	-8.9
289	44256757	C80	-8.9
290	44256758	C81	-8.9
291	44256782	C102	-8.9
292	44256786	C106	-8.9
293	44256810	C129	-8.9
294	56671053	C153	-8.9
295	74976920	C163	-8.9
296	74976937	C167	-8.9
297	101114060	C181	-8.9
298	101697180	C194	-8.9
299	101921444	C197	-8.9
300	131751173	C221	-8.9
301	3083066	D6	-8.9
302	90657596	D115	-8.9
303	25195385	Pg13	-8.9
304	44256614	Pg15	-8.9
305	44256641	Pg37	-8.9
306	44256651	Pg45	-8.9
307	44256660	Pg49	-8.9
308	44256683	Pg71	-8.9
309	44256686	Pg74	-8.9
310	44256690	Pg78	-8.9
311	101545491	Pg104	-8.9
312	101860769	Pg109	-8.9
313	101931855	Pg110	-8.9
314	131751760	Pg120	-8.9
315	131751762	Pg122	-8.9
316	44256847	Pn24	-8.9
317	44256861	Pn37	-8.9
318	131752296	Pn53	-8.9
319	102174359	Pt36	-8.9
320	44256980	M10	-8.9
321	44256983	M13	-8.9
322	44257002	M28	-8.9
323	101701148	M54	-8.9
324	11169452	C22	-8.9
325	6602304	C19	-8.8
326	44256706	C42	-8.8
327	44256714	C49	-8.8
328	44256721	C51	-8.8
329	44256768	C89	-8.8
330	44256770	C91	-8.8
331	44256781	C101	-8.8
332	102385316	C203	-8.8

333	102515296	C207	-8.8
334	122396785	C213	-8.8
335	131750819	C215	-8.8
336	131752267	C231	-8.8
337	192918	D3	-8.8
338	23724698	D24	-8.8
339	44256880	D47	-8.8
340	44256883	D50	-8.8
341	44256897	D59	-8.8
342	44256918	D76	-8.8
343	44256926	D84	-8.8
344	44256950	D101	-8.8
345	44256951	D102	-8.8
346	74977047	D112	-8.8
347	101243495	D126	-8.8
348	102515146	D129	-8.8
349	21603999	Pg9	-8.8
350	44256650	Pg44	-8.8
351	44256685	Pg73	-8.8
352	44256698	Pg85	-8.8
353	44256699	Pg86	-8.8
354	102515511	Pg117	-8.8
355	185595	Pn1	-8.8
356	44256841	Pn18	-8.8
357	44256853	Pn29	-8.8
358	44256864	Pn40	-8.8
359	44256955	Pt6	-8.8
360	44256961	Pt11	-8.8
361	131752301	Pt38	-8.8
362	44256979	M9	-8.8
363	44256982	M12	-8.8
364	44256994	M22	-8.8
365	44257005	M31	-8.8
366	44257012	M38	-8.8
367	44256891	D54	-8.8
368	15126294	C27	-8.7
369	23724697	C32	-8.7
370	23724737	C35	-8.7
371	44256708	C44	-8.7
372	44256722	C52	-8.7
373	44256773	C94	-8.7
374	44256783	C103	-8.7
375	44256795	C114	-8.7
376	44256797	C116	-8.7
377	44256817	C135	-8.7
378	44256832	C150	-8.7
379	44256833	C151	-8.7
380	101545481	C186	-8.7
381	131750823	C218	-8.7

382	131750956	C220	-8.7
383	131753043	C233	-8.7
384	131753089	C242	-8.7
385	11972329	D16	-8.7
386	15385440	D21	-8.7
387	25200736	D31	-8.7
388	44256884	D51	-8.7
389	44256896	D58	-8.7
390	44256925	D83	-8.7
391	44256948	D99	-8.7
392	44256622	Pg21	-8.7
393	44256625	Pg24	-8.7
394	44256630	Pg28	-8.7
395	44256634	Pg31	-8.7
396	44256670	Pg59	-8.7
397	44256673	Pg61	-8.7
398	44256674	Pg62	-8.7
399	44256677	Pg65	-8.7
400	44256684	Pg72	-8.7
401	44256693	Pg81	-8.7
402	44256697	Pg84	-8.7
403	101545489	Pg103	-8.7
404	101545495	Pg106	-8.7
405	131751479	Pg119	-8.7
406	44256839	Pn16	-8.7
407	44256857	Pn33	-8.7
408	74977015	Pn46	-8.7
409	100958662	Pn47	-8.7
410	44256956	Pt7	-8.7
411	44256973	Pt23	-8.7
412	71587075	Pt27	-8.7
413	100987512	Pt32	-8.7
414	44256710	C46	-8.6
415	44256731	C60	-8.6
416	44256739	C64	-8.6
417	44256816	C134	-8.6
418	44256825	C143	-8.6
419	74976933	C166	-8.6
420	76322875	C169	-8.6
421	102438708	C204	-8.6
422	102588654	C212	-8.6
423	131753045	C235	-8.6
424	131753051	C241	-8.6
425	441689	D4	-8.6
426	25200961	D32	-8.6
427	44256868	D37	-8.6
428	44256873	D40	-8.6
429	44256924	D82	-8.6
430	44256941	D92	-8.6

431	73774601	D109	-8.6
432	44256617	Pg18	-8.6
433	44256633	Pg30	-8.6
434	44256659	Pg48	-8.6
435	44256668	Pg57	-8.6
436	74315894	Pn45	-8.6
437	101268578	Pn48	-8.6
438	131752295	Pn52	-8.6
439	44256971	Pt21	-8.6
440	101922116	Pt35	-8.6
441	443652	M2	-8.6
442	44256986	M16	-8.6
443	44256997	M24	-8.6
444	44257003	M29	-8.6
445	12137508	D19	-8.6
446	182463	C4	-8.5
447	441671	C6	-8.5
448	10143380	C20	-8.5
449	44256724	C54	-8.5
450	44256736	C62	-8.5
451	44256761	C83	-8.5
452	44256811	C130	-8.5
453	44256815	C133	-8.5
454	71296189	C156	-8.5
455	71296190	C157	-8.5
456	101666798	C191	-8.5
457	101692563	C193	-8.5
458	101710212	C195	-8.5
459	102227471	C200	-8.5
460	44256900	D62	-8.5
461	86289400	D113	-8.5
462	90658013	D119	-8.5
463	90659258	D124	-8.5
464	44256623	Pg22	-8.5
465	44256648	Pg42	-8.5
466	44256669	Pg58	-8.5
467	44256696	Pg83	-8.5
468	72734294	Pg91	-8.5
469	90657500	Pg94	-8.5
470	44256835	Pn13	-8.5
471	44256858	Pn34	-8.5
472	44256863	Pn39	-8.5
473	72193652	Pn42	-8.5
474	122706400	Pn50	-8.5
475	443651	Pt1	-8.5
476	132569542	Pt39	-8.5
477	441765	M1	-8.5
478	44256984	M14	-8.5
479	44257016	M42	-8.5

480	5319251	M4	-8.5
481	185664	C5	-8.5
482	5491619	C17	-8.4
483	14779570	C26	-8.4
484	15719498	C30	-8.4
485	44256777	C98	-8.4
486	44256785	C105	-8.4
487	44256799	C118	-8.4
488	71315020	C158	-8.4
489	87984599	C170	-8.4
490	101805622	C196	-8.4
491	102445481	C205	-8.4
492	23724703	D25	-8.4
493	44256923	D81	-8.4
494	74977043	D111	-8.4
495	90658074	D120	-8.4
496	102515301	D131	-8.4
497	44256661	Pg50	-8.4
498	54602214	Pg89	-8.4
499	71627264	Pg90	-8.4
500	101257894	Pg100	-8.4
501	44256834	Pn12	-8.4
502	44256840	Pn17	-8.4
503	44256845	Pn22	-8.4
504	44256854	Pn30	-8.4
505	131753204	Pn57	-8.4
506	44256987	M17	-8.4
507	44256999	M25	-8.4
508	44257011	M37	-8.4
509	44257017	M43	-8.4
510	100926553	M51	-8.4
511	12137509	C24	-8.4
512	44256703	C39	-8.3
513	44256741	C66	-8.3
514	44256743	C68	-8.3
515	44256755	C78	-8.3
516	44256776	C97	-8.3
517	44256796	C115	-8.3
518	44256829	C147	-8.3
519	72812405	C161	-8.3
520	126455742	C214	-8.3
521	131750821	C216	-8.3
522	131751484	C223	-8.3
523	44256866	D36	-8.3
524	44256875	D42	-8.3
525	44256914	D72	-8.3
526	44256944	D95	-8.3
527	44256945	D96	-8.3
528	44256635	Pg32	-8.3

529	44256643	Pg39	-8.3
530	44256645	Pg41	-8.3
531	74976917	Pg93	-8.3
532	90659377	Pg99	-8.3
533	102515381	Pg115	-8.3
534	443654	Pn2	-8.3
535	14861214	Pn9	-8.3
536	44256838	Pn15	-8.3
537	6325802	Pt2	-8.3
538	44256968	Pt18	-8.3
539	44256974	Pt24	-8.3
540	44257008	M34	-8.3
541	44256727	C56	-8.2
542	44256740	C65	-8.2
543	44256754	C77	-8.2
544	44256813	C131	-8.2
545	100917934	C180	-8.2
546	102025500	C198	-8.2
547	131750822	C217	-8.2
548	131751767	C225	-8.2
549	165558	D1	-8.2
550	176440	D2	-8.2
551	44256870	D38	-8.2
552	73157738	D108	-8.2
553	90659256	D123	-8.2
554	443648	Pg3	-8.2
555	5320457	Pg8	-8.2
556	44256662	Pg51	-8.2
557	44256666	Pg55	-8.2
558	44256694	Pg82	-8.2
559	90658189	Pg96	-8.2
560	101545493	Pg105	-8.2
561	102515300	Pg114	-8.2
562	131751761	Pg121	-8.2
563	13832989	Pn6	-8.2
564	131752294	Pn51	-8.2
565	131753203	Pn56	-8.2
566	44256972	Pt22	-8.2
567	44256977	M8	-8.2
568	44256992	M21	-8.2
569	44257009	M35	-8.2
570	74977116	M49	-8.2
571	44256723	C53	-8.1
572	44256779	C100	-8.1
573	44256792	C112	-8.1
574	44256798	C117	-8.1
575	44256803	C122	-8.1
576	71315022	C159	-8.1
577	101268576	C183	-8.1

578	102318121	C201	-8.1
579	102514964	C206	-8.1
580	131753046	C236	-8.1
581	131753048	C238	-8.1
582	44256901	D63	-8.1
583	44256913	D71	-8.1
584	44256942	D93	-8.1
585	74818467	D110	-8.1
586	11454027	Pn4	-8.1
587	44256848	Pn25	-8.1
588	131753205	Pn58	-8.1
589	44256962	Pt12	-8.1
590	176458	C2	-8.0
591	441699	C9	-8.0
592	44256704	C40	-8.0
593	44256748	C73	-8.0
594	44256788	C108	-8.0
595	44256789	C109	-8.0
596	44256807	C126	-8.0
597	74976939	C168	-8.0
598	131752261	C227	-8.0
599	102515282	D130	-8.0
600	44256613	Pg14	-8.0
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602	14311169	Pn7	-8.0
603	3568969	M3	-8.0
604	101697438	M53	-8.0
605	443915	C11	-7.9
606	44256778	C99	-7.9
607	44256828	C146	-7.9
608	90659301	C179	-7.9
609	44256915	D73	-7.9
610	44256619	Pg20	-7.9
611	74976872	Pg92	-7.9
612	14311149	Pt5	-7.9
613	44256969	Pt19	-7.9
614	44257001	M27	-7.9
615	72193646	M45	-7.9
616	74977121	M50	-7.9
617	44256827	C145	-7.8
618	131751485	C224	-7.8
619	44256877	D44	-7.8
620	132575728	M58	-7.8
621	44256790	C110	-7.7
622	44256801	C120	-7.7
623	44256809	C128	-7.7
624	101545482	C187	-7.7
625	10843319	D15	-7.7
626	44256952	D103	-7.7

627	23724696	Pg10	-7.7
628	44256671	Pg60	-7.7
629	443623	C10	-7.6
630	90657364	D114	-7.6
631	131852234	D135	-7.6
632	443913	Pg4	-7.6
633	44257015	M41	-7.6
634	11953846	C23	-7.6
635	44256805	C124	-7.5
636	44256876	D43	-7.5
637	167642	Pg1	-7.5
638	5282162	Pg7	-7.5
639	101545487	Pg102	-7.5
640	131751763	Pg123	-7.5
641	101682300	C192	-7.4
642	44256791	C111	-7.3
643	54605857	D104	-7.3
644	5316498	D8	-7.2
645	15433396	C28	-7.1
646	134775899	D136	-7.1
647	90658006	D118	-7.0
648	44256808	C127	-6.9
649	44256957	Pt8	-6.8
650	10100906	D13	-6.6
651	10196837	D14	-6.6
652	102515359	D132	-6.6
653	90657732	C172	-6.6
654	90659093	C177	-6.5
655	134742266	C249	-6.5
656	44256749	C74	-6.4
657	24187921	D30	-6.2
658	134755516	C250	-6.1
659	44256822	C140	-5.8
660	90658034	C173	-5.6
661	102515400	C209	-5.4
662	90658522	C175	-5.4
663	90659261	C178	-5.3
664	90657144	C171	-5.0
665	102515473	C211	-4.7

Table 2 Summary of 3D-QSAR model statistics

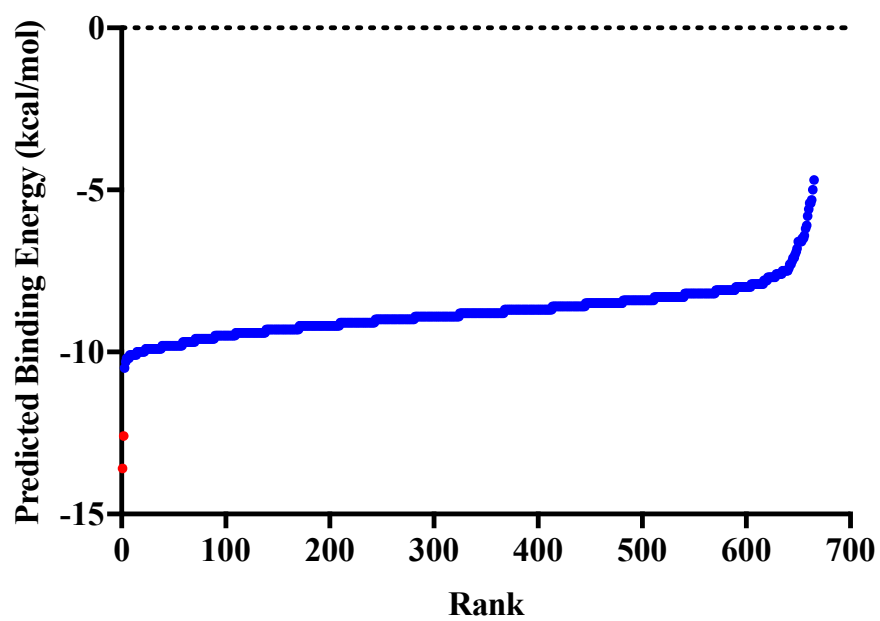
	naïve alignment	docking alignment
no. of components	7	5
r²	0.999	0.989
std error of estimate	0.032	0.074
F value	669.9	138.8

Table S3**Calculated Secondary Structure Fractions**

M3A (μM)	0	50	100	M3G (μM)	0	100	200	Pt3A (μM)	0	250	500	Pn3A (μM)	0	50	100
α-helix	0.24	0.17	0.14		0.24	0.34	0.34		0.34	0.23	0.24		0.20	0.21	0.24
β-sheet	0.17	0.26	0.29		0.09	0.00	0.00		0.00	0.12	0.11		0.16	0.16	0.11
Turn	0.20	0.24	0.22		0.22	0.09	0.10		0.10	0.21	0.21		0.22	0.25	0.22
Random	0.36	0.29	0.34		0.44	0.58	0.58		0.52	0.40	0.42		0.37	0.36	0.40
Total	0.97	0.96	0.99		0.99	1.01	1.02		0.96	0.96	0.98		0.95	0.98	0.97

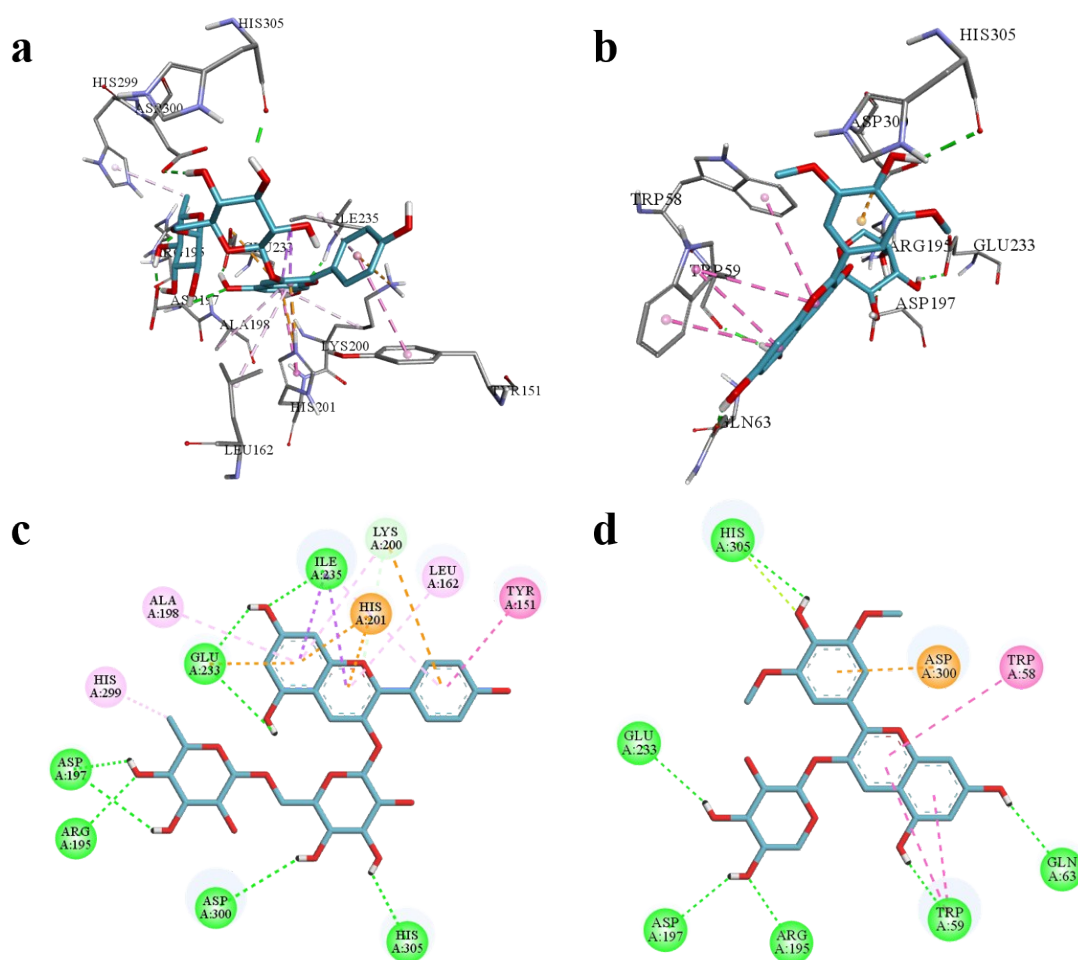
2 Supplementary Figures

Figure S1



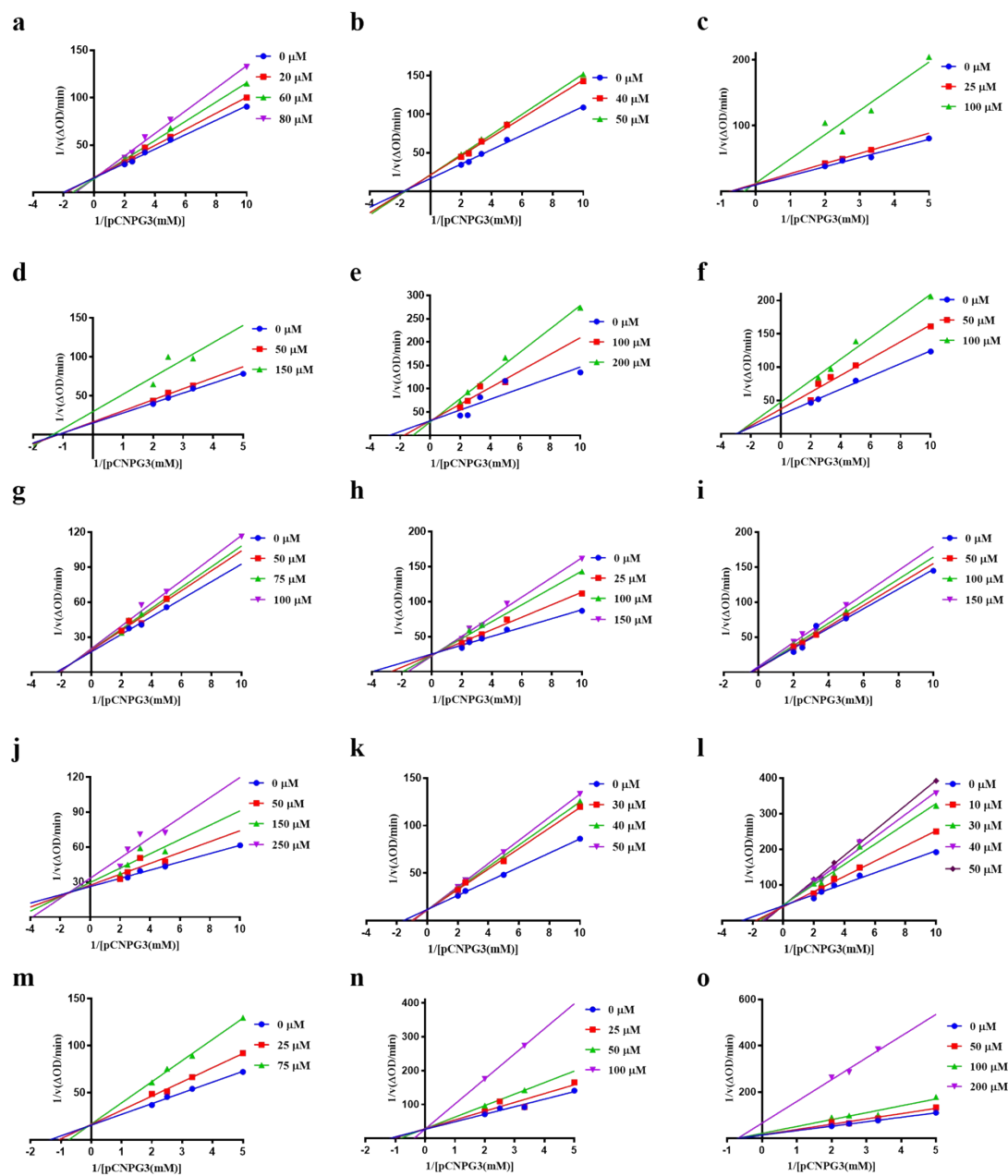
Ranking of virtual screening results. Red points indicate the top 2 ranked anthocyanins.

Figure S2



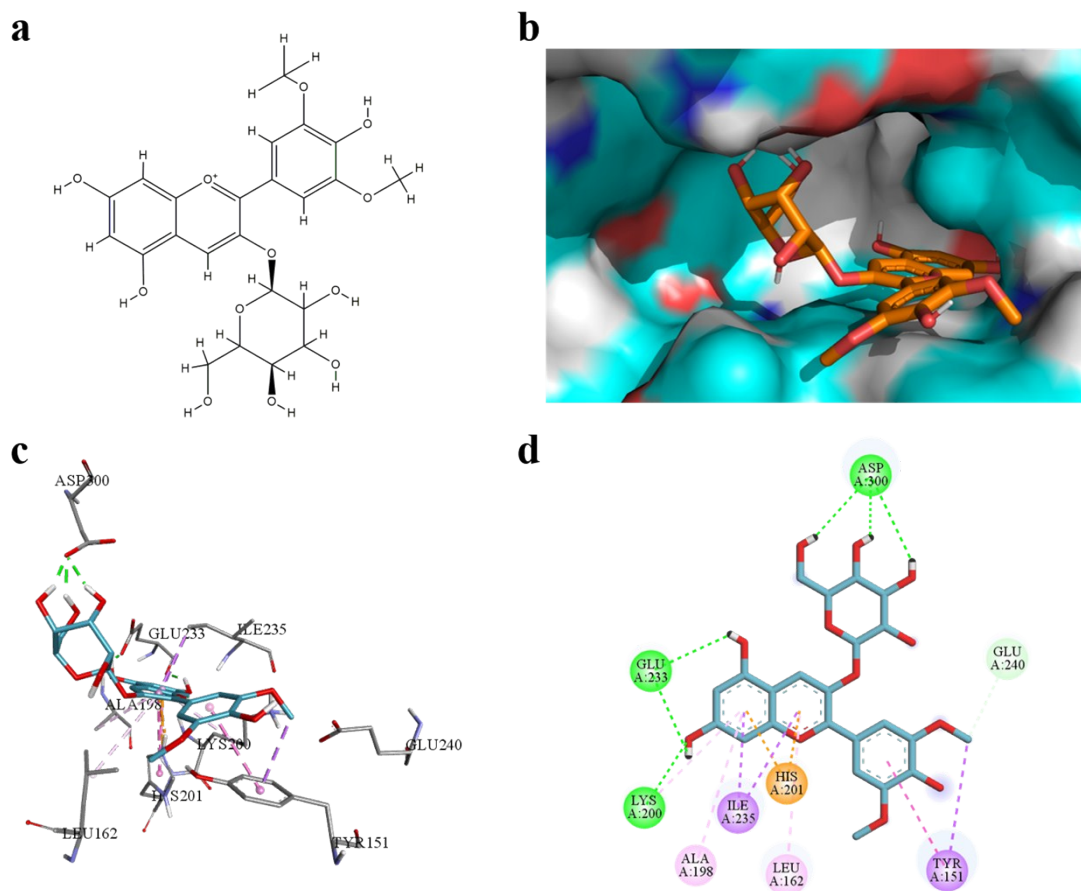
Predicted interactions of Pg3R and M3A with HPA in molecular docking. Pg3R and M3A are colored in cyan, and their oxygen atoms are colored in red. Hydrogen bonding interactions are colored in green, hydrophobic interactions are colored in orange, light pink and pink. a. Predicted interactions of Pg3R with HPA. b. Predicted interactions of M3A with HPA. c. Predicted interactions of Pg3R with HPA in 2D dimension. d. Predicted interactions of M3A with HPA in 2D dimension.

Figure S3



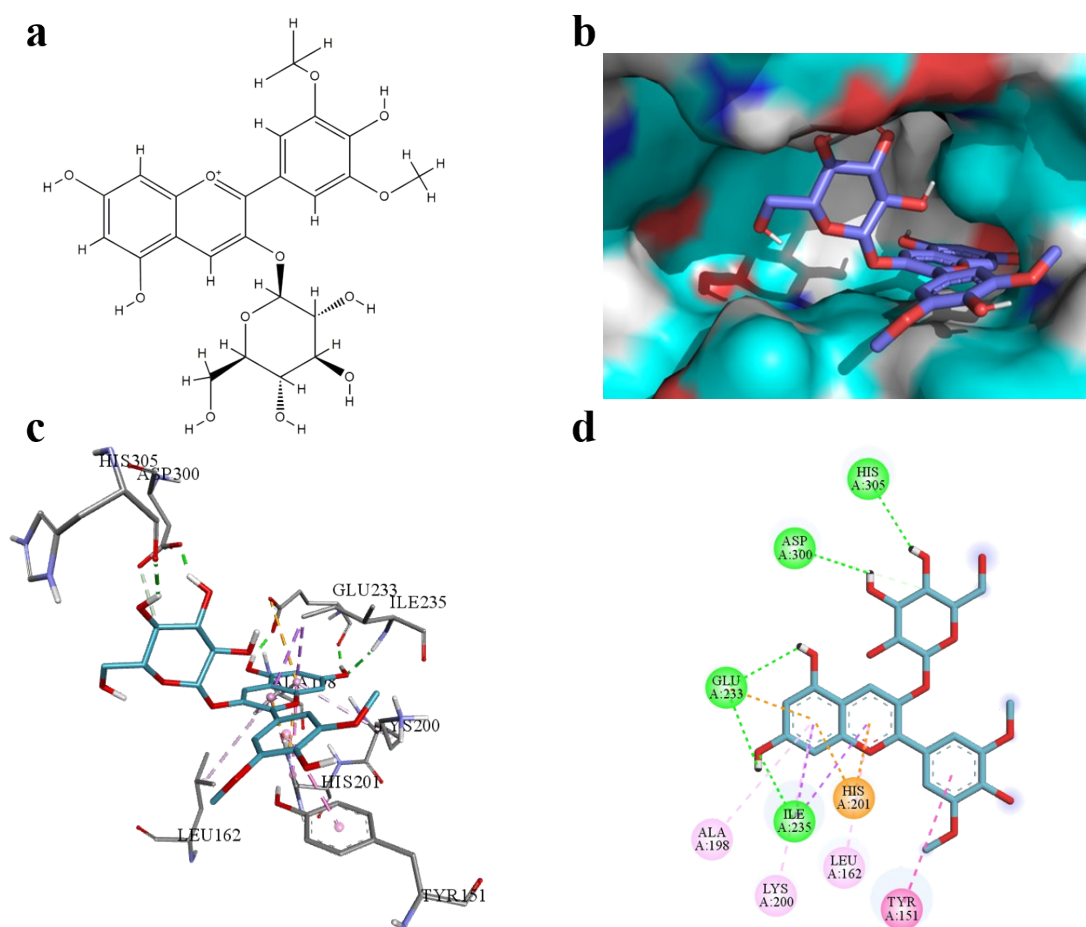
Enzyme kinetic results of 15 anthocyanins in Lineweaver-Burk plots. a. C3A. b. C3Ga. c. C3G. d. C3R. e. C3S. f. D3A. g. D3Ga. h. D3G. i. D3R. j. D3S. k. Pn3A. l. Pn3Ga. m. Pet3A. n. Pet3Ga. o. Pet3G.

Figure S4



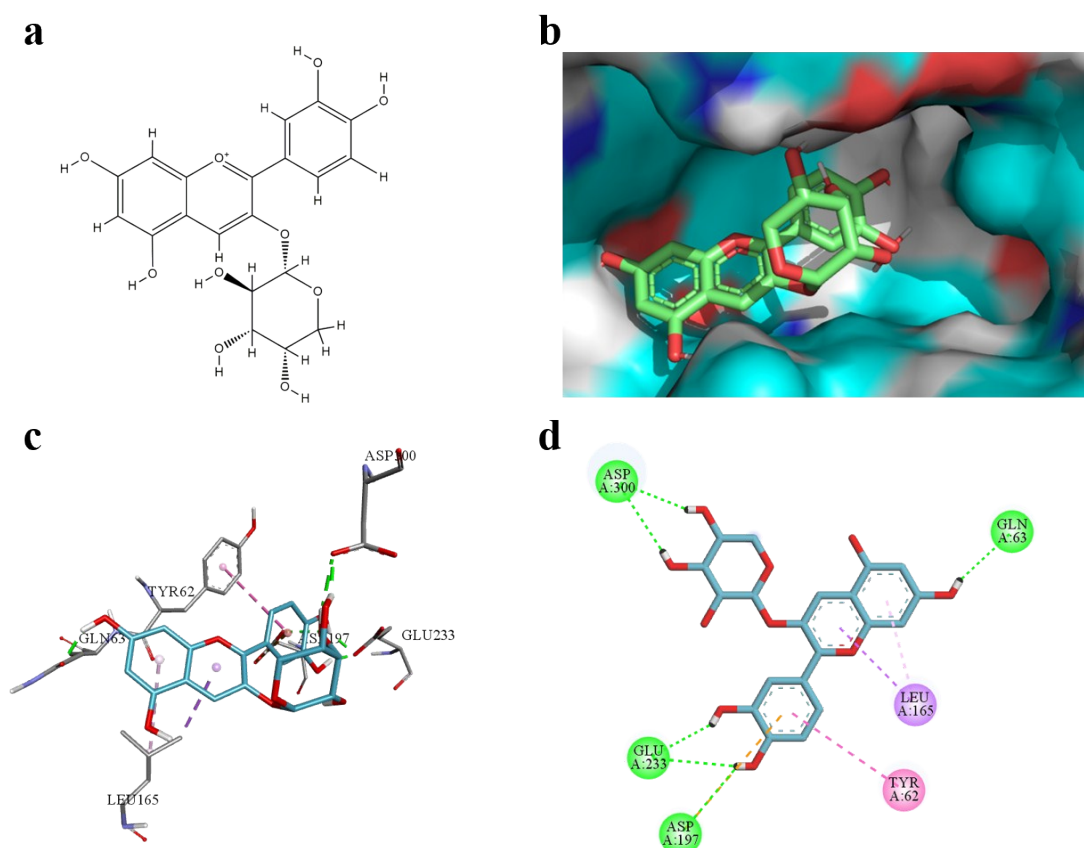
Molecular docking results of M3Ga with HPA. a. Chemical structure of M3Ga. b. Predicted binding conformation of M3Ga in the active pocket of HPA, M3Ga is colored in orange, and its oxygen atoms are colored in red. c. Predicted interactions of M3Ga with HPA d. Predicted interactions of M3Ga with HPA in 2D dimension. M3Ga is colored in cyan, and its oxygen atoms are colored in red. Hydrogen bonding interactions are colored in light green and green, hydrophobic interactions are colored in orange, light pink and purple.

Figure S5



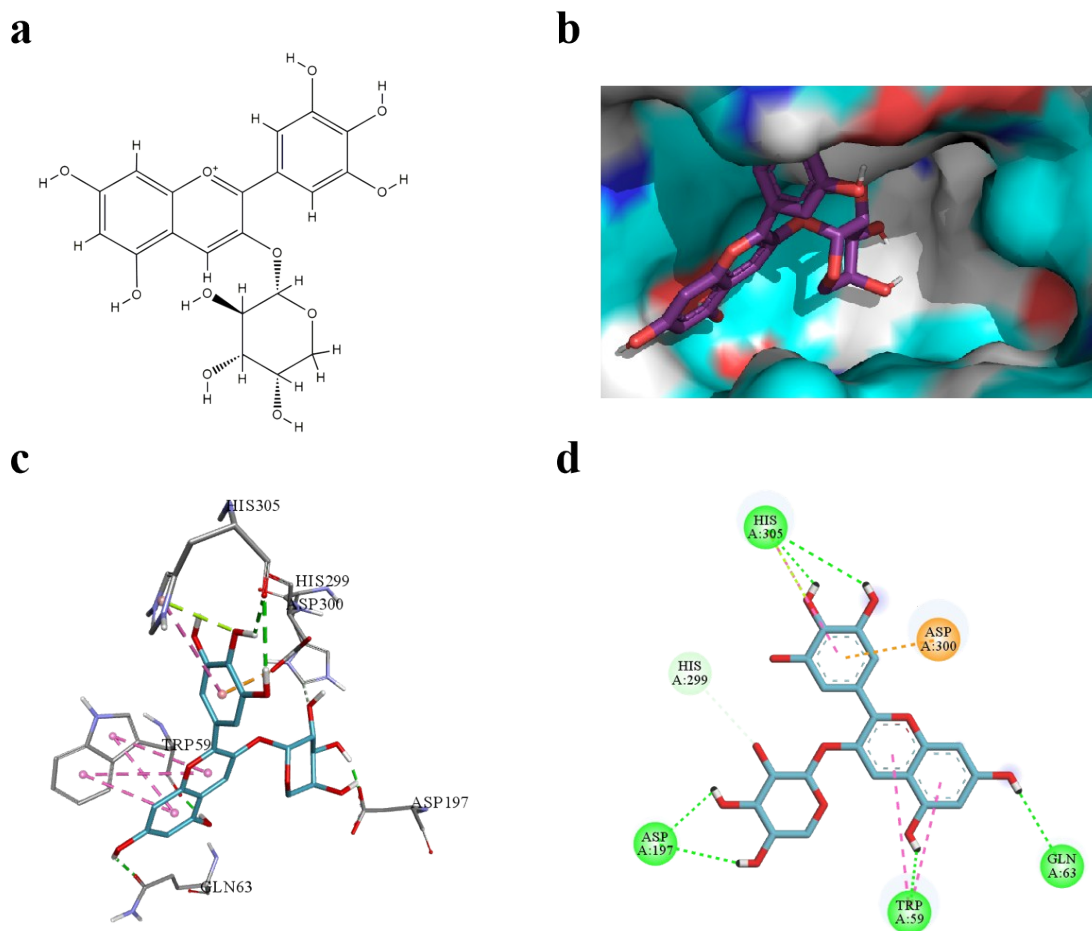
Molecular docking results of M3G with HPA. a. Chemical structure of M3G. b. Predicted binding conformation of M3G in the active pocket of HPA, M3G is colored in purple, and its oxygen atoms are colored in red. c. Predicted interactions of M3G with HPA d. Predicted interactions of M3G with HPA in 2D dimension. M3G is colored in cyan, and its oxygen atoms are colored in red. Hydrogen bonding interactions are colored in green, hydrophobic interactions are colored in orange, light pink and pink.

Figure S6



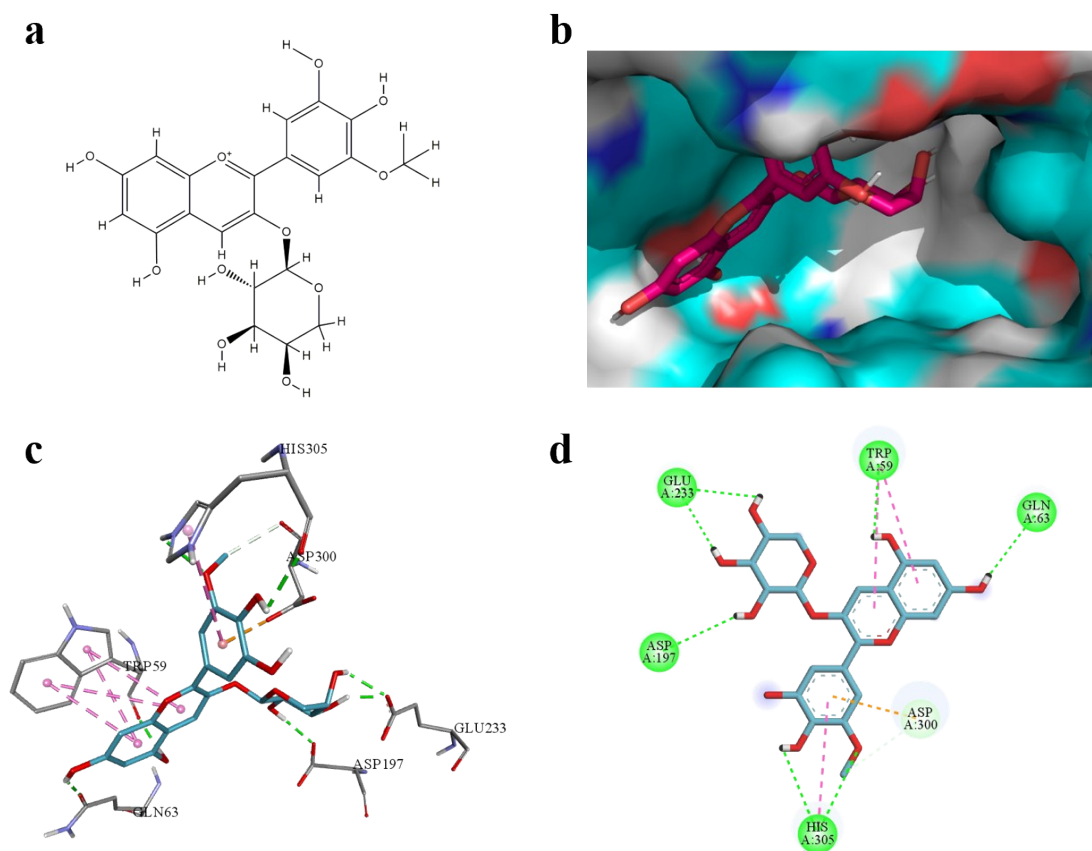
Molecular docking results of C3A with HPA. a. Chemical structure of C3A. b. Predicted binding conformation of C3A in the active pocket of HPA, C3A is colored in green, and its oxygen atoms are colored in red. c. Predicted interactions of C3A with HPA d. Predicted interactions of C3A with HPA in 2D dimension. C3A is colored in cyan, and its oxygen atoms are colored in red. Hydrogen bonding interactions are colored in green, hydrophobic interactions are colored in pink and purple.

Figure S7



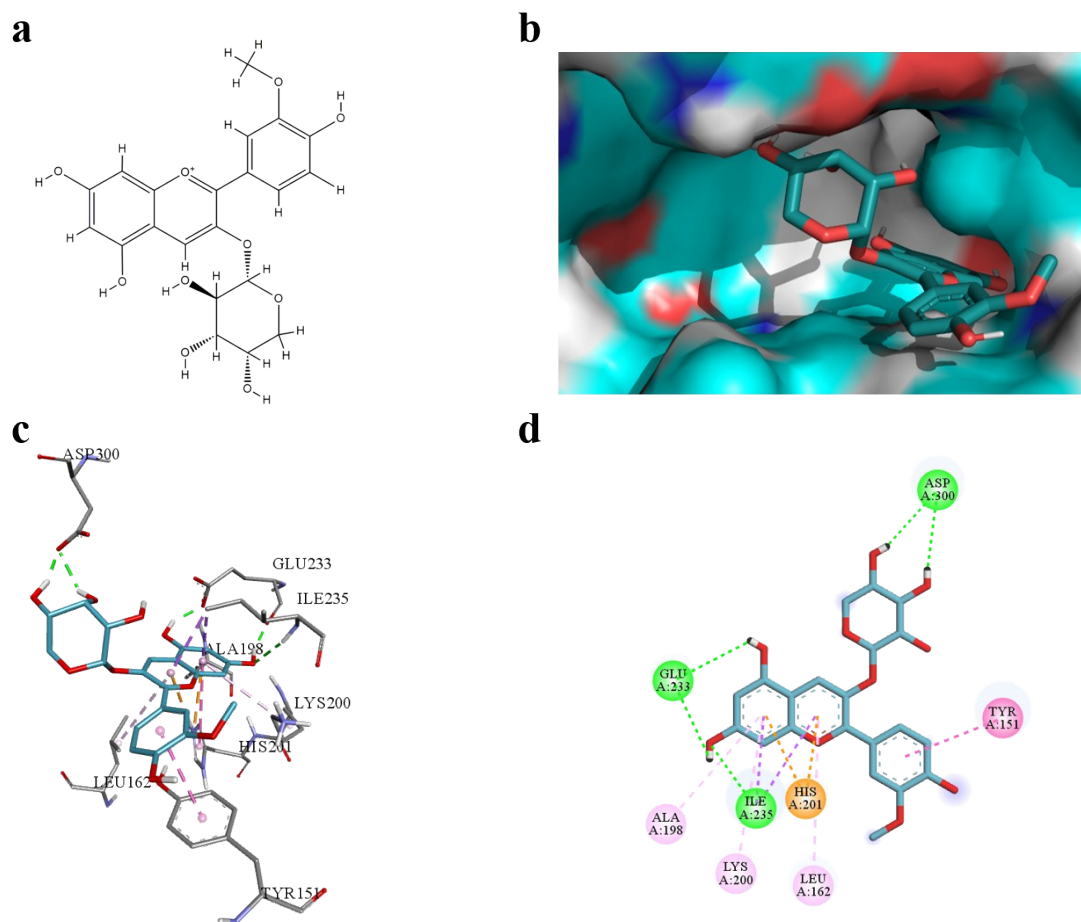
Molecular docking results of D3A with HPA. a. Chemical structure of D3A. b. Predicted binding conformation of D3A in the active pocket of HPA, D3A is colored in purple, and its oxygen atoms are colored in red. c. Predicted interactions of D3A with HPA d. Predicted interactions of D3A with HPA in 2D dimension. Pt3A is colored in cyan, and its oxygen atoms are colored in red. Hydrogen bonding interactions are colored in green, hydrophobic interactions are colored in pink and orange.

Figure S8



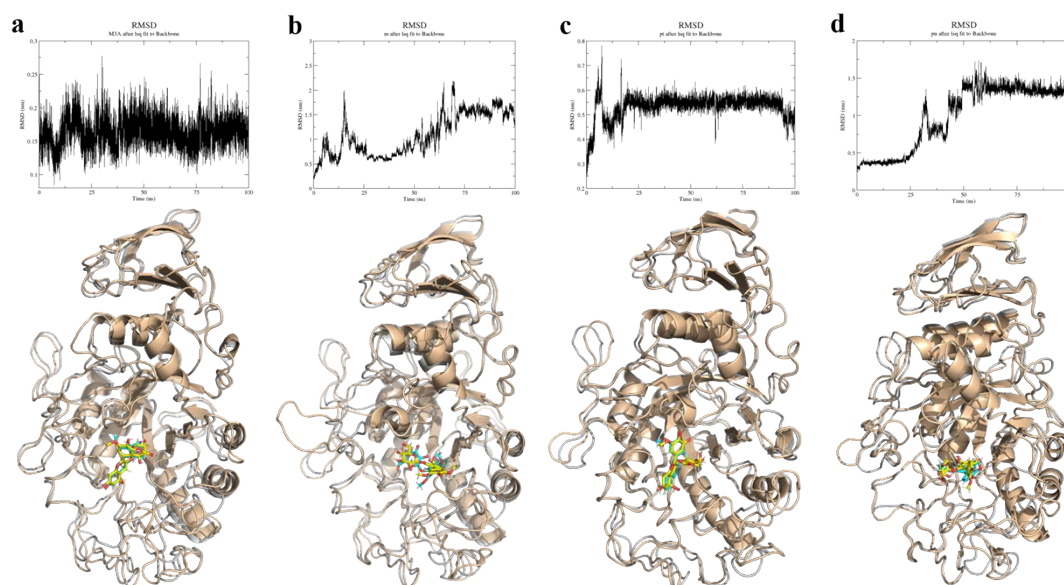
Molecular docking results of Pt3A with HPA. a. Chemical structure of Pt3A. b. Predicted binding conformation of Pt3A in the active pocket of HPA, Pt3A is colored in pink, and its oxygen atoms are colored in red. c. Predicted interactions of Pt3A with HPA d. Predicted interactions of Pt3A with HPA in 2D dimension. Pt3A is colored in cyan, and its oxygen atoms are colored in red. Hydrogen bonding interactions are colored in green, hydrophobic interactions are colored in pink and orange.

Figure S9



Molecular docking results of Pn3A with HPA. a. Chemical structure of Pn3A. b. Predicted binding conformation of Pn3A in the active pocket of HPA, Pn3A is colored in indigo, and its oxygen atoms are colored in red. c. Predicted interactions of Pn3A with HPA d. Predicted interactions of Pn3A with HPA in 2D dimension. Pn3A is colored in cyan, and its oxygen atoms are colored in red. Hydrogen bonding interactions are colored in green, hydrophobic interactions are colored in light pink and

Figure S10



RMSD and conformation analysis of molecular dynamic results. Conformation of HPA before molecular dynamic simulation is colored in gray, conformation of HPA after molecular dynamic simulation is colored in wheat, conformation of anthocyanin before molecular dynamic simulation is colored in blue, and conformation of anthocyanin after molecular dynamic simulation is colored in yellow. a. M3A. b. M3G. c. Pt3A. d. Pn3A.