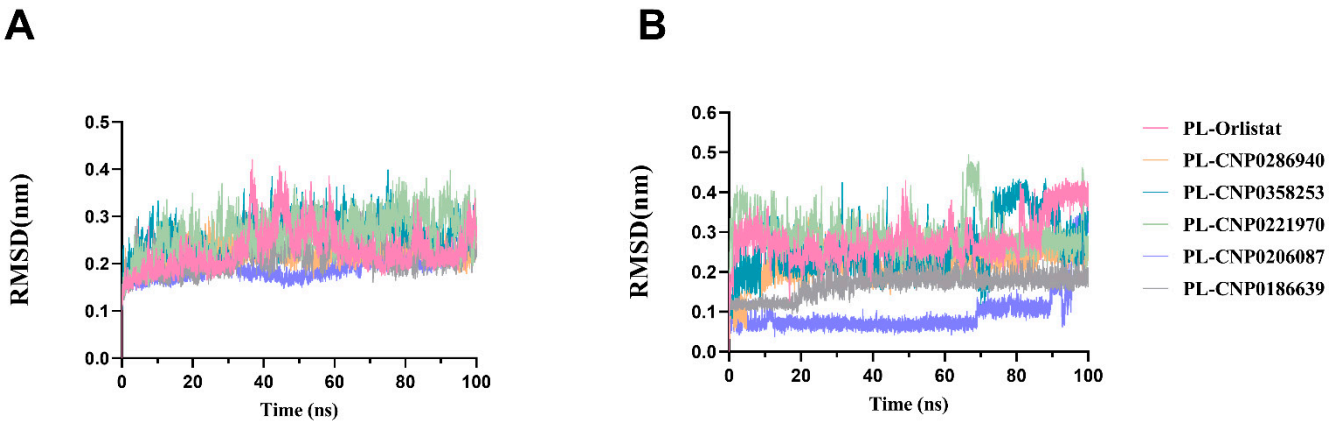
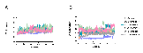


Figure S1. RMSD analysis of complex (A) and ligand (B) of PL-Orlistat, PL-CNP0286940, PL-CNP0358253, PL-CNP0221970, PL-CNP0206087 and PL-CNP0186639.

Table S1. Reference sources for each compound in the dataset.

Number	Name of compound	References
1	Daidzein	
2	genistein	
3	formononetin	
4	3',4',7-Trihydroxyisoflavone	
5	CHEMBL4870006	
6	7,8-Dihydroxy-4'-methoxyisoflavone	[1]
7	Maduraktermol H	
8	CHEMBL4878391	
9	CHEMBL4859886	
10	7,3',4'-Trimethoxyisoflavone	
11	wogonin	[2]

12	oroxylin A	
13	(−)-epiafzelechin 3-O-gallate	
14	(−)-epicatechin 3-O-gallate	
15	(−)-epicatechin 3-O-(3′-O-methyl)gallate	
16	(−)-epigallocatechin 3,5-di-O-gallate	
17	(−)-epigallocatechin 3-O-p-coumaroate	
18	(−)-epigallocatechin 3-O-gallate	[3]
19	(−)-catechin 3-O-gallate	
20	(−)-catechin 3-O-gallate	
21	8-C-ascorbyl (−)-epigallocatechin	
22	 8-C-ascorbyl (−)-epigallocatechin 3-O-gallate	
23	tangeretin	
24	nobiletin	[4]
25	5-demethyltangeretin	
26	5-demethylnobiletin	
27	Isoginkgetin	
28	Bilobetin	[5]
29	Ginkgetin	
30	Sciadopitysin	
31	5,7,3′,5′-tetrahydroxyflavanone	
32	8-prenylnaringenin	[6]
33	cudraflavanone D	

34	cudraflavanone A	
35	2′,5,7-trihydroxy-4,5′-(2,2-dimethylchromeno)-8-(3-hydroxy-3-methylbuthyl)flavanone	
36	cudracuspiflavanone A	
37	Luteolin	
38	Kaempferol-3-Orutinoside	[7]
39	Rutin	
40	Quercetin	

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Table S2. Molecular descriptors of potential PL inhibitors screened.

Name	MATS1p	ATSC6e	GATS2p	SpMin8_Bhi	VR2_DzZ
CNP0186639	0.244810577	0.796184389	1.176948987	0.947291746	13.86796247
CNP0221970	0.244810577	1.661881994	1.176948987	0.968044715	12.85192419
CNP0358253	0.244810577	2.010529781	1.176948987	0.96789442	12.44882367
CNP0286940	0.233223414	1.584163789	1.177845666	0.950973695	13.17518648
CNP0206087	0.199429013	1.535463529	1.182106191	0.953684305	13.15952316