

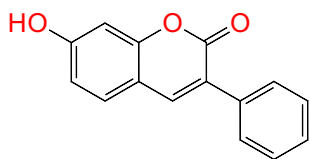
Supporting Information

Discovery of Novel Coumarin Analogs against α -
glucosidase Protein Target of Diabetes mellitus:
Pharmacophore-based QSAR, Docking, and Molecular
Dynamics Simulation Studies

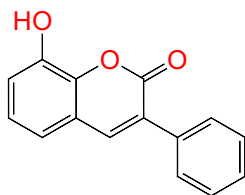
*Akhilesh Kumar Maurya, Viswajit Mulpuru, Nidhi Mishra**

Chemistry Laboratory, Department of Applied Sciences, Indian Institute of Information
Technology Allahabad, Prayagraj, U.P. India-211015

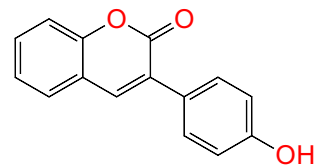
*Correspondence should be addressed to nidhimishra@iiita.ac.in



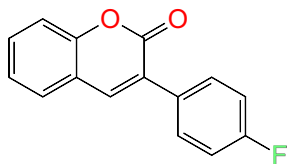
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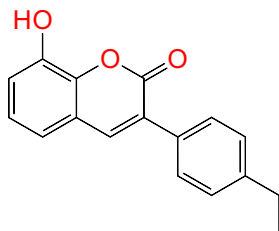
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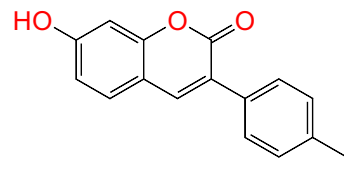
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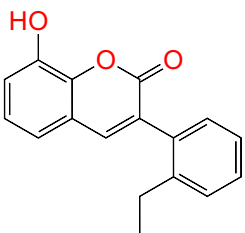
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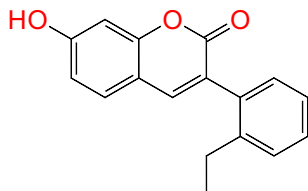
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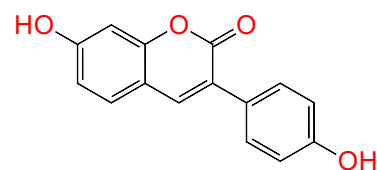
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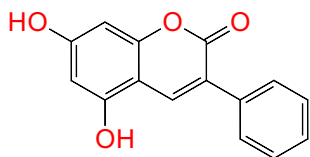
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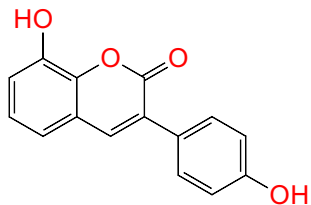
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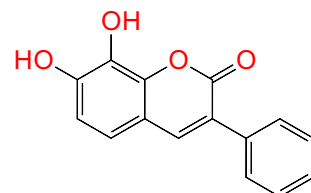
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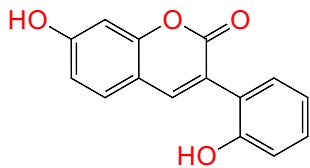
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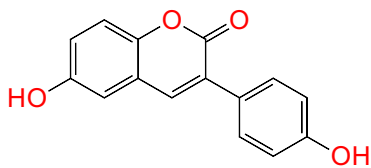
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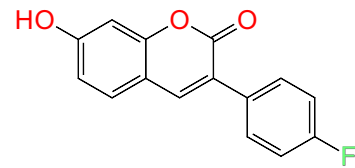
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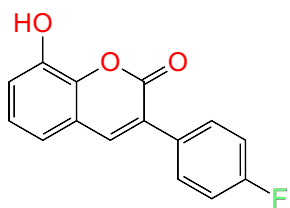
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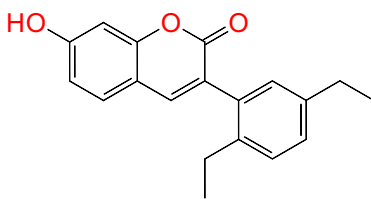
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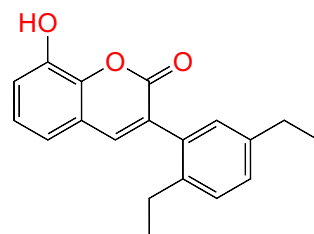
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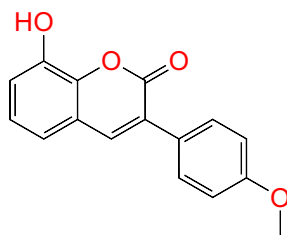
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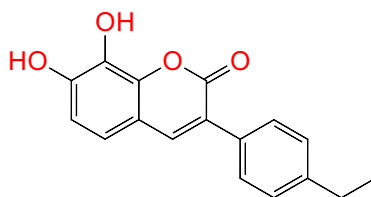
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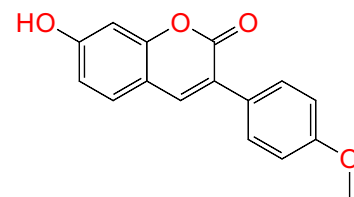
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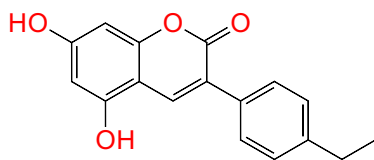
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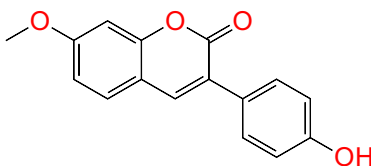
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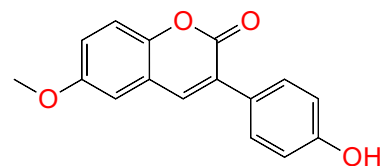
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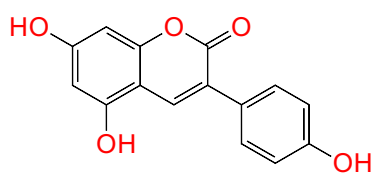
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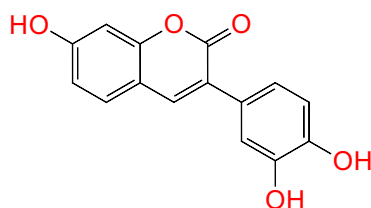
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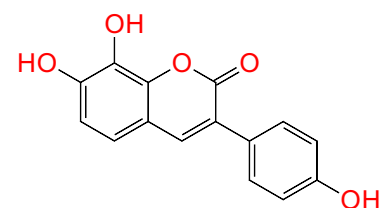
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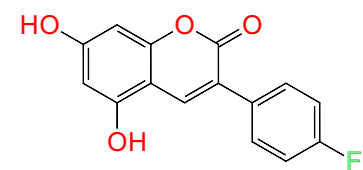
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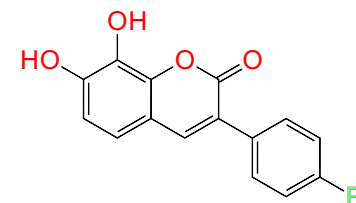
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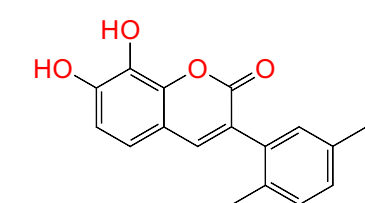
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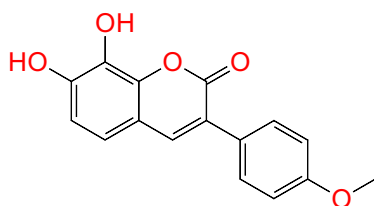
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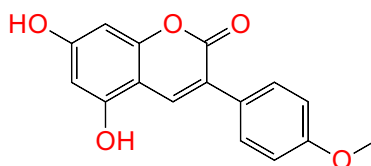
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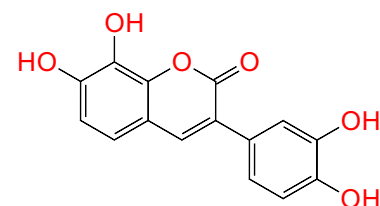
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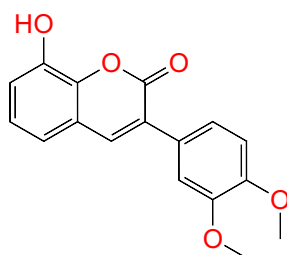
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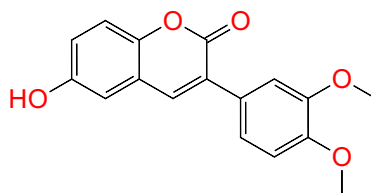
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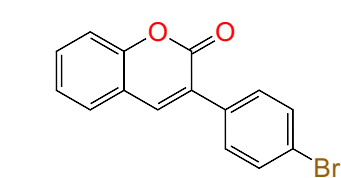
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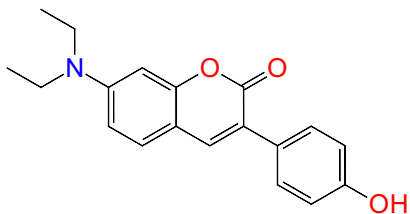
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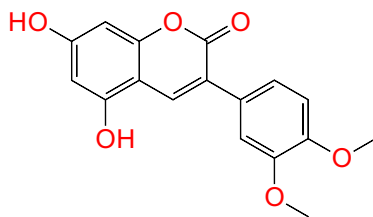
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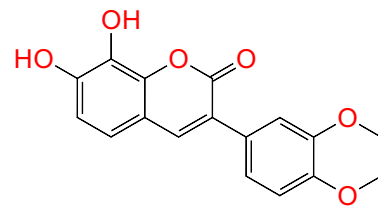
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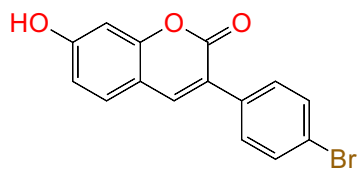
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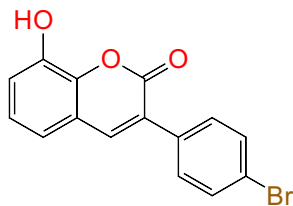
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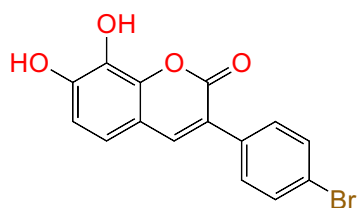
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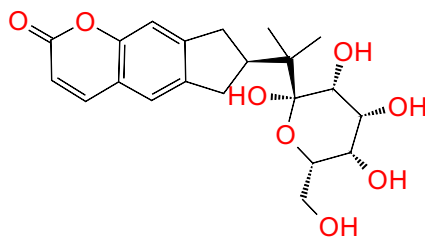
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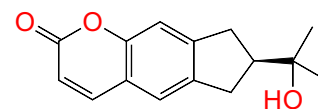


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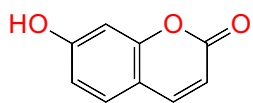


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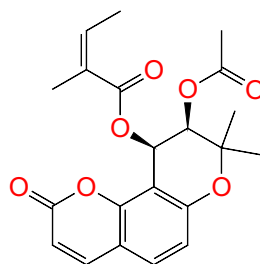
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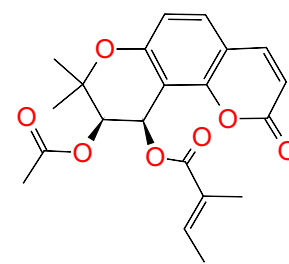
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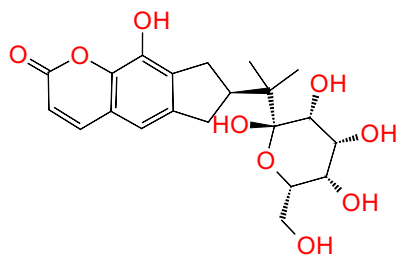
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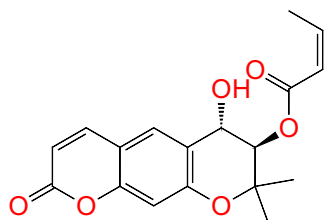
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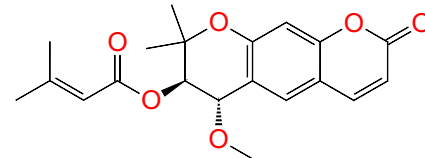
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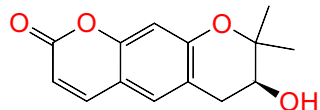
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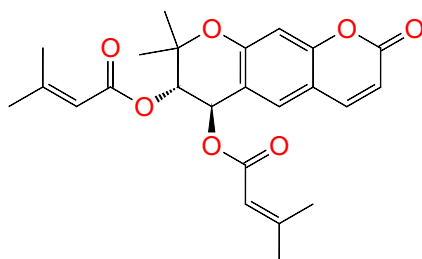
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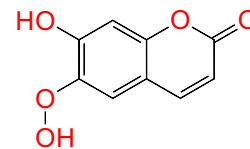
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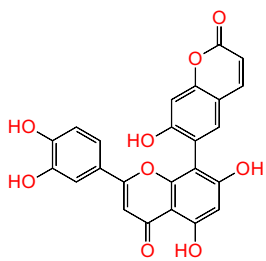
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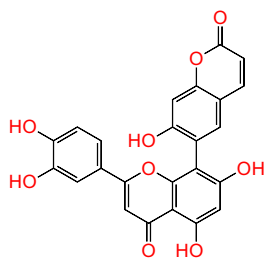
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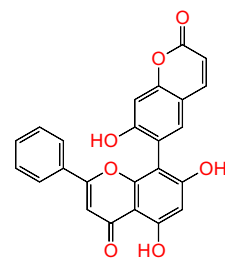
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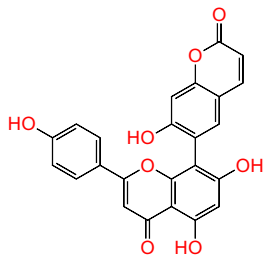
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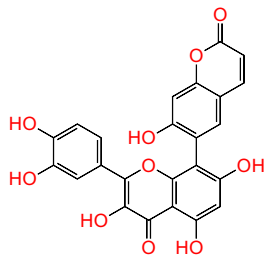
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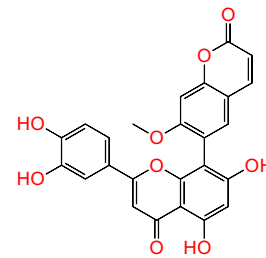
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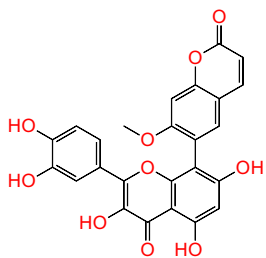
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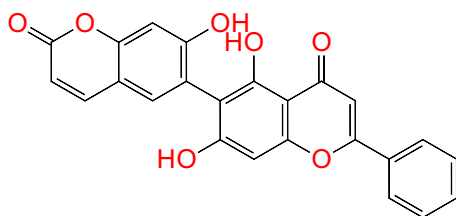
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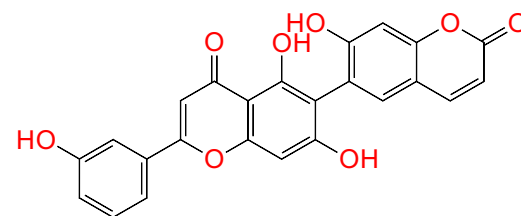
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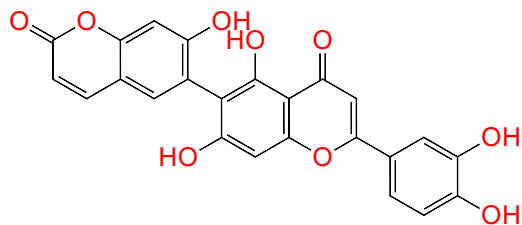
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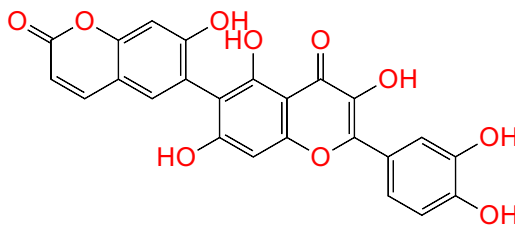
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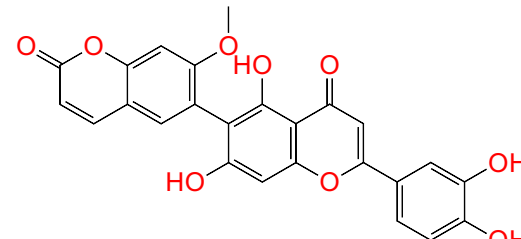
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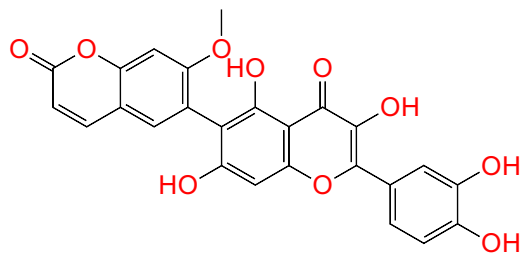
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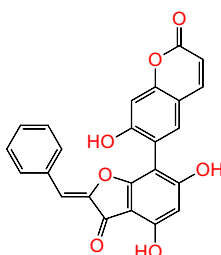
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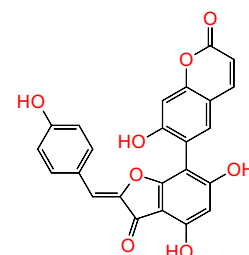
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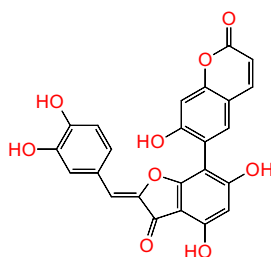
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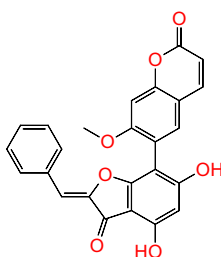
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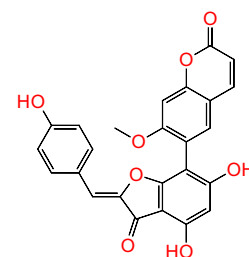
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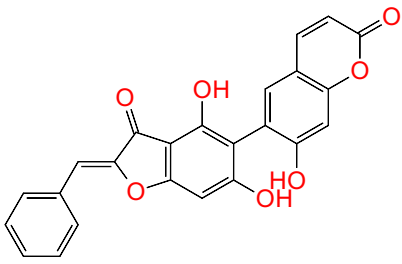
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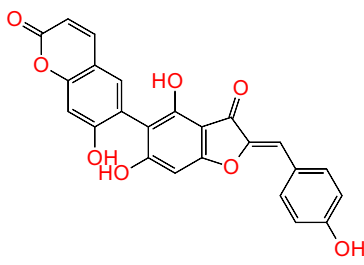
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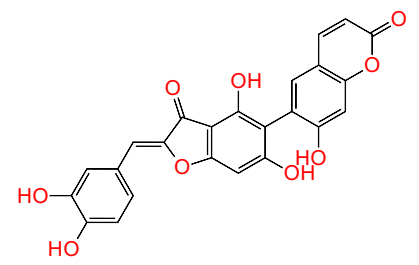
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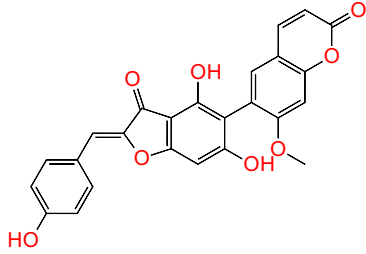
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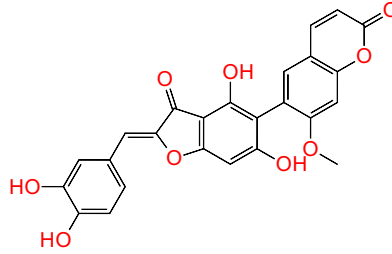
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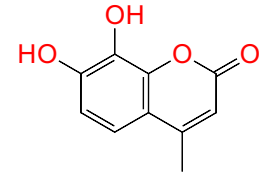
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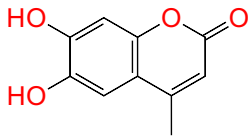
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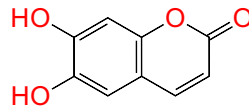
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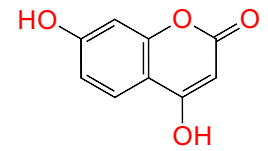
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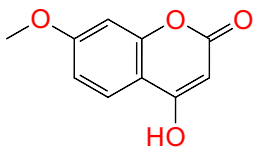
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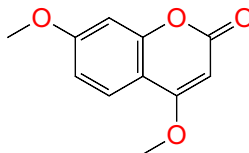
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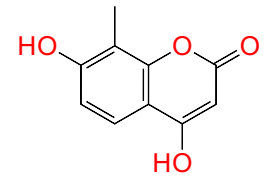
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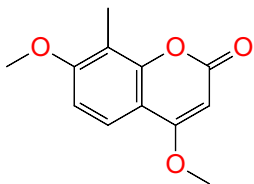
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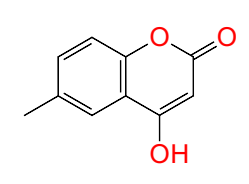
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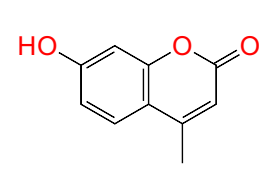
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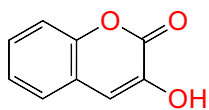
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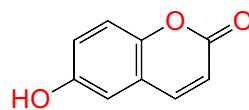
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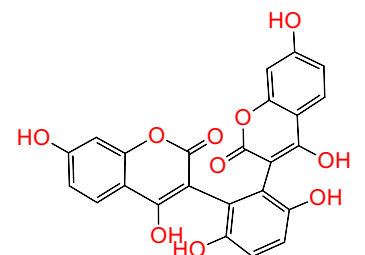
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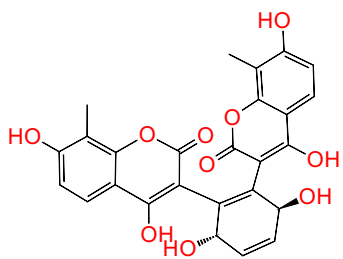
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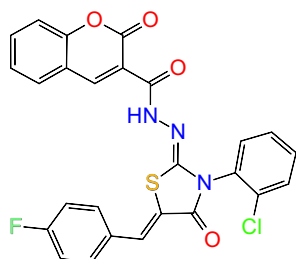
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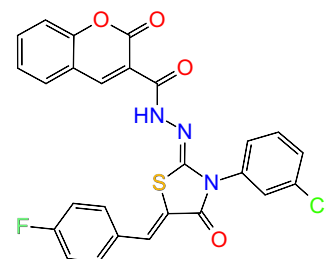
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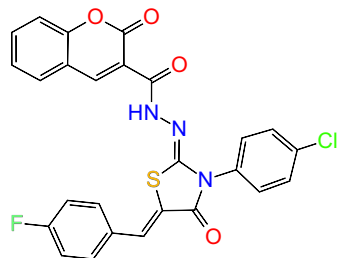
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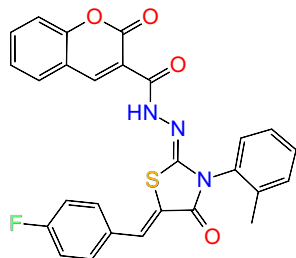
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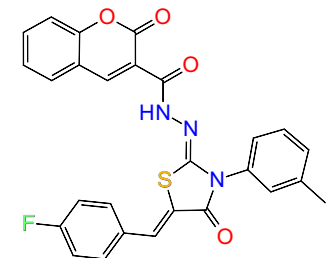
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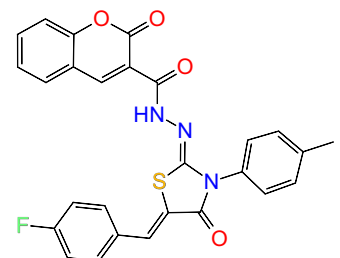
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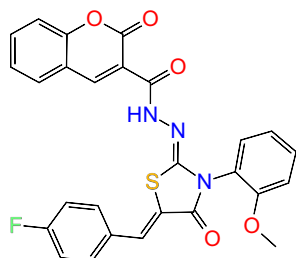
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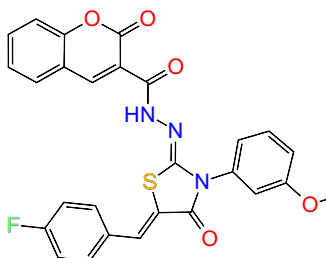
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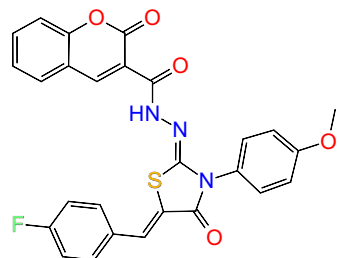
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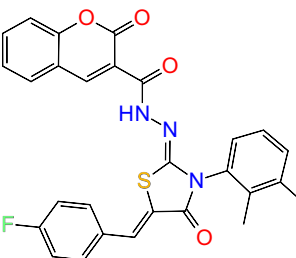
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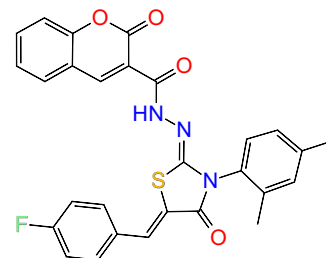
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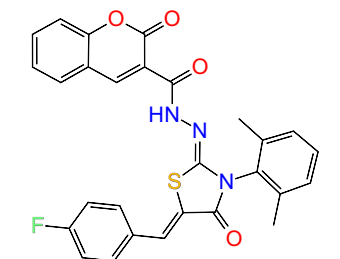
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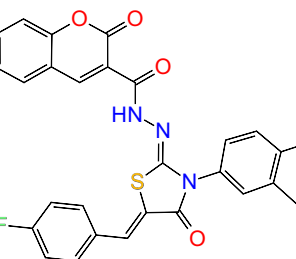
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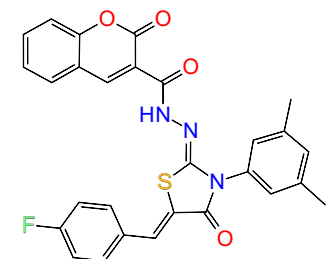
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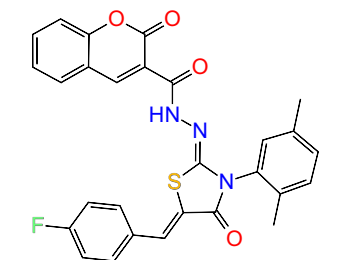
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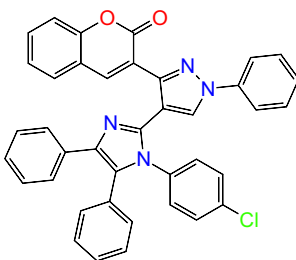
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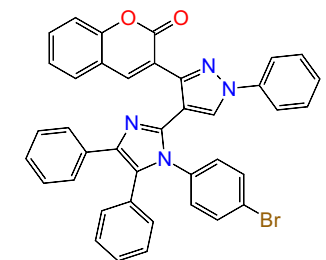
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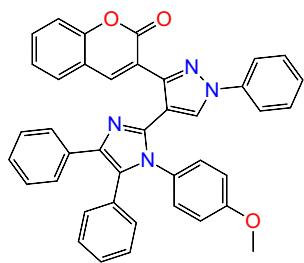
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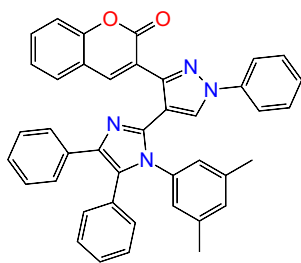
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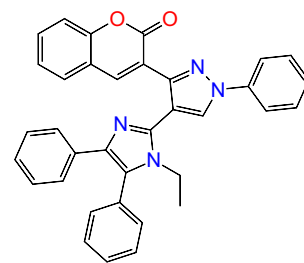
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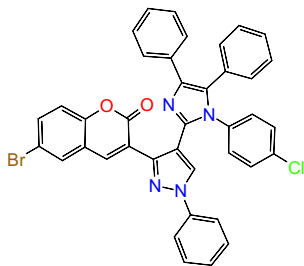
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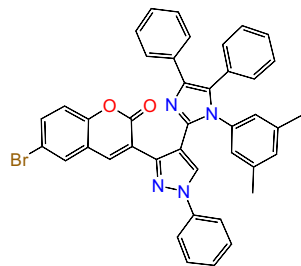
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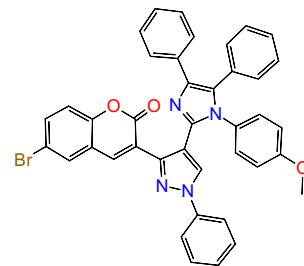
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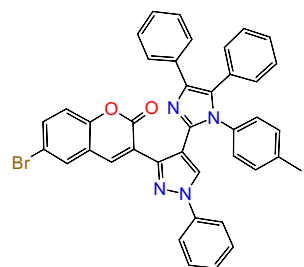
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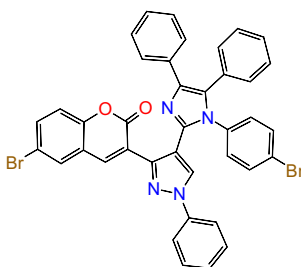
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title: 3h

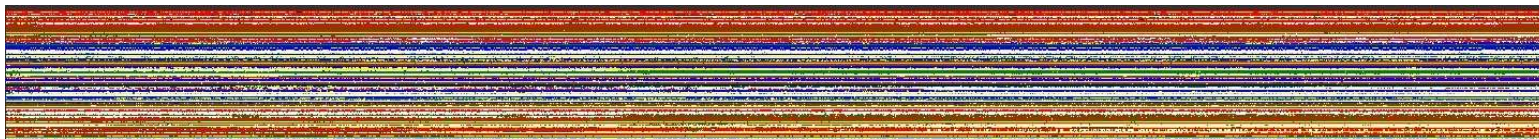


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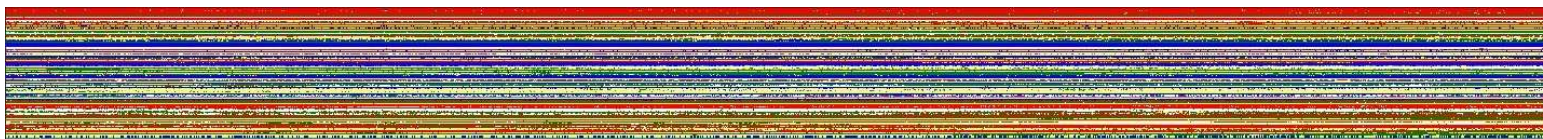


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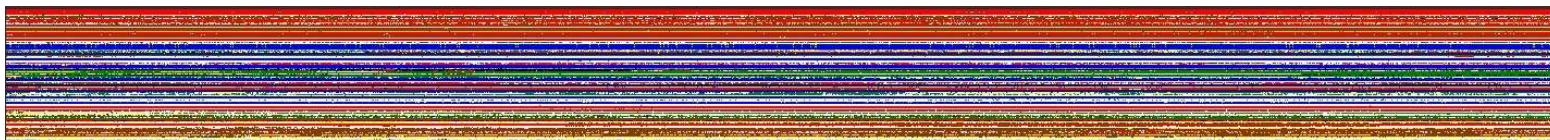
Figure S1: Structure of 116 coumarin derivatives with ligand IDs used in the study



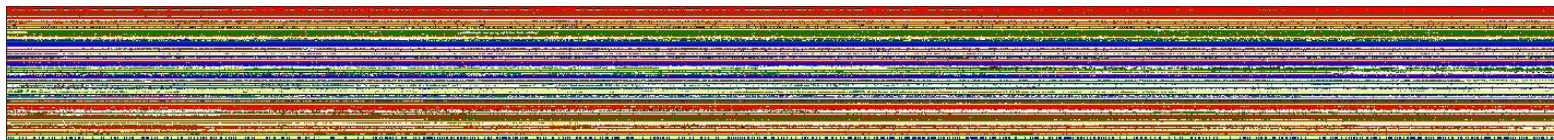
A



B



C



D

Figure S3: The secondary structure timeline evolution using DSSP. (A) unligated protein (B) Isorutarine ligated protein(C) Protein ligated with compound 10_ (D) Protein ligated with compound 36.

Table S1: Docking of coumarin derivative with Lysosomal α -glucosidase and ADME/T properties of ligands

S.N.	PSA	Ligand Title	logS	logKhsa	SASA	logB B	FISA	IC50	Caco	PISA	FOSA	dipole	%Hum anOral Absorp	HERG	logP o/w	acceptH B	logK p	MW	do no rH B	dockin g_scor e
1	161.70	Isorutarine	-2.90	-0.61	645.00	-2.64	282.35	250	20.81	137.92	224.71	3.21	36.23	-4.76	-0.23	11.55	-5.37	422.43	6	-7.64
2	59.82	10	-4.02	0.25	515.22	-0.58	106.98	1000	957.89	305.25	102.97	7.16	100	-5.25	3.02	3.25	-2.12	266.29	1	-7.12
3	126.44	36	-2.72	-0.41	509.37	-2.14	260.89	247.34	33.25	248.48	0	9.30	56.42	-5.15	0.38	5.5	-4.97	286.24	4	-6.86
4	60.96	8	-4.41	0.31	537.41	-0.68	112.55	69.6	848.29	294.60	130.21	6.83	100	-5.54	3.11	3.25	-2.26	266.29	1	-6.84
5	60.97	19	-3.83	0.08	484.07	-0.45	112.57	1000	847.87	324.49	0	8.46	95.12	-5.35	2.69	3.25	-2.25	256.23	1	-6.80
6	82.38	15	-3.20	-0.11	486.15	-1.05	159.31	29.05	305.61	326.84	0	8.5	81.84	-5.37	1.78	4	-3.01	254.24	2	-6.71
7	166.49	5a	-5.05	0.27	693.51	-2.73	295.96	1.47	15.46	308.34	89.28	5.03	60.58	-5.91	2.10	7.75	-5.31	460.39	3	-6.68
8	179.38	2'Isopropylpsoralene	-4.57	0.06	669.01	-3.21	344.40	85.82	5.36	324.60	0	4.76	47.19	-5.99	1.22	7.75	-6.14	446.36	4	-6.64
9	179.09	1	-4.86	0.14	687.89	-3.18	335.71	8.32	6.49	352.18	0	4.73	50.44	-6.22	1.53	7.75	-5.89	446.36	4	-6.64
10	69.30	22	-3.63	0.05	507.32	-0.63	112.05	1000	857.68	302.59	92.67	7.18	94.32	-5.28	2.54	4	-2.23	268.26	1	-6.52
11	185.42	5b	-4.80	0.10	705.84	-3.22	334.34	3.38	6.68	288.50	82.99	7.52	50.43	-5.92	1.48	8.5	-5.99	476.39	4	-6.50
12	60.97	45	-4.41	0.18	504.15	-0.40	112.57	1000	847.97	314.21	0	8.18	100	-5.45	3.02	3.25	-2.29	317.13	1	-6.47
13	99.14	4-hydroxyPd-C-III	-4.14	-0.03	593.51	-0.84	128.21	77.3	602.67	188.68	276.61	10.91	89.76	-5.09	2.23	6.95	-2.93	330.33	1	-6.45
14	83.51	14	-3.22	-0.11	487.40	-1.13	167.22	212.72	257.10	320.18	0	7.37	80.18	-5.35	1.72	4	-3.18	254.24	2	-6.43
15	105.67	29	-2.90	-0.26	494.13	-1.6	213.23	29.89	94.13	280.89	0	8.14	68.40	-5.13	1.04	4.75	-4.07	270.24	3	-6.43
16	90.67	34	-3.44	-0.08	521.22	-1.14	158.70	18.8	309.65	269.84	92.66	8.56	82.59	-5.24	1.89	4.75	-3.11	284.26	2	-6.43
17	60.97	5	-3.47	0.04	475.23	-0.56	112.57	280.38	847.84	362.65	0	7.11	93.75	-5.47	2.45	3.25	-2.12	238.242	1	-6.42
18	81.41	33	-4.04	0.14	535.98	-1.04	152.94	1000	351.15	227.82	155.21	8.39	86.24	-5.11	2.34	4	-3.24	282.29	2	-6.37
19	197.79	9d	-4.64	-0.08	702.96	-3.71	367.08	3.1	3.27	335.88	0	5.42	28.08	-6.42	0.83	8.5	-6.43	462.36	5	-6.264
20	98.20	43	-3.74	-0.06	560.54	-1.25	159.32	1000	305.51	215.86	185.35	8.86	83.24	-5.22	2.01	5.5	-3.21	314.29	2	-6.12
21	82.84	25	-3.99	0.12	542.70	-1.16	158.39	11.49	311.77	254.03	130.27	8.29	85.61	-5.30	2.39	4	-3.16	282.29	2	-6.09
22	139.30	Nodakenin	-3.05	-0.48	632.29	-2.09	234.45	250	59.23	168.30	229.54	8.08	61.16	-4.78	0.42	10.8	-4.48	406.43	5	-6.02
23	82.8	16	-3.08	-0.12	478.50	-0.94	151.07	10.16	365.84	327.43	0	7.20	83.45	-5.20	1.81	4	-2.86	254.24	2	-5.97
24	104.91	30	-2.96	-0.26	498.38	-1.63	213.95	19.04	92.67	284.43	0	8.71	68.30	-5.25	1.05	4.75	-4.07	270.24	3	-5.90
25	179.14	9c	-4.95	0.08	693.73	-3.3	335.35	1.71	6.54	358.37	0	6.59	49.84	-6.49	1.41	7.75	-5.86	446.36	4	-5.83
26	199.45	4c	-4.15	-0.06	670.51	-3.46	372.31	4.43	2.91	298.20	0	5.2	26.60	-5.71	0.73	8.5	-6.65	462.36	5	-5.82
27	61.60	18	-3.76	0.08	479.80	-0.43	111.64	86.91	865.37	321.16	0	8.45	95.25	-5.23	2.68	3.25	-2.25	256.23	1	-5.76
28	148.9	14b	-5.43	0.39	708.39	-2.60	266.29	11.83	29.55	339.96	102.12	5.71	69.70	-6.31	2.80	7	-4.55	444.39	2	-5.74
29	76.79	38	-3.95	0.06	549.6	-0.74	112.58	20.23	847.68	251.64	185.37	7.57	94.83	-5.35	2.64	4.75	-2.32	298.29	1	-5.67
30	82.37	23	-4.09	0.12	548.34	-1.20	159.28	25.48	305.76	258.79	130.26	8.25	85.55	-5.44	2.41	4	-3.15	282.29	2	-5.61
31	84.14	17	-3.15	-0.11	483.11	-1.10	166.30	11.54	262.32	316.81	0	5.75	80.32	-5.23	1.72	4	-3.18	254.24	2	-5.58
32	84.14	12	-3.16	-0.11	483.32	-1.10	166.29	19.39	262.38	317.03	0	7.66	80.33	-5.24	1.72	4	-3.17	254.24	2	-5.57
33	60.45	11	-3.96	0.25	512.11	-0.56	106.14	16.39	975.75	302.51	103.45	7.49	100	-5.16	3.03	3.25	-2.12	266.29	1	-5.54
34	82.37	32	-3.56	-0.07	495.06	-0.95	159.30	1000	305.64	288.75	0	9.64	83.19	-5.25	2.01	4	-3.15	272.23	2	-5.52
35	91.14	35	-3.37	-0.08	517.14	-1.12	158.46	10.81	311.30	266.00	92.67	8.62	82.58	-5.13	1.88	4.75	-3.11	284.26	2	-5.52
36	98.67	42	-3.65	-0.06	555.04	-1.22	158.42	39.08	311.58	211.27	185.34	9.00	83.30	-5.09	2.00	5.5	-3.21	314.29	2	-5.50
37	105.38	28	-2.88	-0.26	492.88	-1.59	213.06	1.37	94.50	279.82	0	8.77	68.39	-5.11	1.04	4.75	-4.07	270.24	3	-5.50

38	69.93	26	-3.64	0.06	507.70	-0.62	111.80	1000	862.22	303.21	92.68	7.75	94.47	-5.26	2.56	4	-2.22	268.26	1	-5.47
39	122.41	6h	-7.44	0.73	829.63	-1.48	159.29	0.51	305.68	499.91	105.81	12.14	75.87	-7.81	5.18	7.25	-2.11	515.51	0	-5.46
40	61.60	9	-4.33	0.30	533.16	-0.66	111.65	118.29	865.18	291.23	130.27	7.25	100	-5.44	3.11	3.25	-2.26	266.29	1	-5.42
41	63.47	41	-4.79	0.38	596.78	-0.81	110.79	13.43	881.61	270.62	215.37	5.86	100	-5.61	3.52	4.25	-2.12	309.36	1	-5.41
42	82.38	47	-3.99	0.008	513.28	-0.90	159.30	35.71	305.61	276.60	0	9.41	85.02	-5.31	2.32	4	-3.19	333.13	2	-5.36
43	82.84	46	-3.90	0.004	507.99	-0.87	158.40	1000	311.69	272.21	0	9.58	85.10	-5.17	2.31	4	-3.19	333.13	2	-5.35
44	84.55	2	-1.70	-0.48	381.3	-0.94	173.24	94.25	225.43	129.09	78.96	5.39	71.08	-3.54	0.34	4	-4.06	192.17	2	-5.34
45	60.39	20	-4.88	0.52	572.87	-0.67	105.83	1000	982.45	233.90	233.13	7.42	100	-5.23	3.68	3.25	-2.26	294.34	1	-5.30
46	82.84	31	-3.46	-0.08	489.53	-0.92	158.40	19.08	311.68	284.11	0	9.81	83.26	-5.11	1.99	4	-3.15	272.23	2	-5.27
47	59.73	21	-4.92	0.52	575.16	-0.68	105.98	1000	979.22	236.22	232.96	7.06	100	-5.3	3.68	3.25	-2.25	294.34	1	-5.19
48	69.91	27	-3.63	0.06	507.51	-0.62	111.74	70.26	863.48	303.07	92.693	6.16	94.48	-5.26	2.55	4	-2.22	268.26	1	-5.19
49	39.06	7	-3.81	0.15	467.59	0.11	57.01	1000	2852.83	363.57	0	7.19	100	-5.34	3.46	2.5	-1.19	240.23	0	-5.17
50	61.60	4	-3.36	0.04	468.89	-0.53	111.64	2567	865.34	357.25	0	7.46	93.85	-5.28	2.44	3.25	-2.12	238.24	1	-5.16
51	166.11	10a	-5.64	0.29	729.81	-2.97	295.58	4.61	15.59	342.38	91.84	8.03	61.40	-6.60	2.23	7.75	-5.18	460.39	3	-5.11
52	99.29	Umbelliferon 6-carboxylic acid	-1.19	-0.75	375.25	-1.22	199.15	172.1	128.02	176.09	0	2.80	62.13	-3.83	-0.43	5.7	-4.28	194.14	2	-5.07
53	77.43	39	-3.88	0.06	545.33	-0.72	111.69	13.09	864.39	248.27	185.36	6.02	94.95	-5.24	2.63	4.75	-2.31	298.29	1	-5.07
54	82.84	13	-3.11	-0.11	480.5	-1.02	158.41	13.46	311.63	322.08	0	8.55	81.91	-5.22	1.76	4	-3.01	254.24	2	-4.99
55	69.91	24	-3.56	0.05	503.17	-0.61	111.10	27.42	875.54	299.38	92.67	7.55	94.46	-5.16	2.53	4	-2.22	268.26	1	-4.90
56	185.28	10b	-5.32	0.11	739.31	-3.40	327.77	2.11	7.72	319.71	91.83	5.59	52.50	-6.54	1.65	8.5	-5.76	476.39	4	-4.86
57	181.79	17c	-4.81	0.01	705.49	-3.51	337.91	4.17	6.18	354.77	12.8	7.59	49.66	-6.60	1.46	7.75	-5.72	446.36	4	-4.82
58	112.92	6b	-8.02	0.88	814.17	-1.22	158.01	100	314.36	506.92	13.38	12.67	78.64	-7.80	5.62	6.5	-2.16	519.93	0	-4.76
59	168.65	18b	-5.44	0.22	737.50	-3.15	297.43	9.35	14.97	336.22	103.85	7.65	61.25	-6.65	2.26	7.75	-5.04	460.39	3	-4.60
60	112.92	6e	-7.84	0.92	821.51	-1.39	157.48	0.59	318.01	498.16	101.46	10.84	90.63	-7.78	5.44	6.5	-2.18	499.51	0	-4.58
61	147.34	18a	-5.77	0.39	728.66	-2.58	251.43	13.65	40.88	373.27	103.95	9.33	73.14	-6.80	2.96	7	-4.16	444.39	2	-4.56
62	84.64	3	-1.35	-0.59	357.59	-0.93	174.03	0	221.56	183.55	0	4.93	69.60	-3.71	0.11	4	-3.88	178.14	2	-4.52
63	39.06	40	-4.32	0.25	487.45	0.18	57.00	1000	2853.14	353.07	0	6.93	100	-5.44	3.64	2.5	-1.23	301.13	0	-4.47
64	61.60	6	-3.40	0.04	470.92	-0.54	111.67	60.88	864.76	359.24	0	6.25	93.88	-5.34	2.45	3.25	-2.12	238.24	1	-4.35
65	107.50	3'R- oAcetyl- 4'S- tigloylkh ellactone	-4.15	0.02	645.03	-0.55	100.35	93.39	1107.14	168.80	375.87	7.94	100	-4.83	3.08	7.25	-2.48	386.40	0	-4.35
66	106.50	Decursidin	-5.97	0.47	749.76	-0.75	101.71	79.09	1074.94	174.15	473.89	9.26	100	-5.69	4.17	7.25	-2.39	426.46	0	-4.34
67	61.6	44	-4.34	0.17	499.88	-0.38	111.63	1000	865.42	310.86	0	8.24	100	-5.33	3.02	3.25	-2.29	317.13	1	-4.33
68	68.48	Decursinol	-2.98	-0.18	467.64	-0.44	110.52	65.29	886.65	166.47	190.63	9.07	89.24	-4.22	1.62	4.95	-2.87	246.26	1	-4.31
69	157.66	9b	-5.25	0.25	683.07	-2.72	288.30	6.42	18.27	394.76	0	7.28	61.88	-6.61	2.11	7	-4.96	430.37	3	-4.25
70	157.26	4b	-4.91	0.23	662.33	-2.70	300.01	14.37	14.15	362.32	0	3.63	58.85	-6.14	1.93	7	-5.29	430.37	3	-4.22
71	193.36	10	-3.28	-0.36	651.57	-2.82	301.35	0.86	13.74	350.21	0	3.08	38.13	-5.77	0.64	9.5	-4.97	462.36	6	-4.19
72	65.95	3g	-12.76	2.86	993.43	-0.01	65.69	5.64	2360.2	687.09	163.26	9.84	100	-8.80	10.06	5	-0.31	689.61	0	-4.10
73	63.03	7	-1.84	-0.38	370.30	-0.49	126.36	56.2	627.46	164.98	78.95	8.10	82.69	-3.63	0.97	3.25	-3.17	176.17	1	-4.10
74	59.75	Nodakenetin	-3.64	0.16	484.64	-0.46	104.97	720.29	1000.94	168.97	210.69	8.87	95.59	-4.33	2.55	3.25	-2.66	244.29	1	-4.08

75	182.13	13c	-4.95	0.1	714.14	-3.52	341.95	17.98	5.66	359.13	13.05	7.16	50.00	-6.56	1.63	7.75	-5.78	446.36	4	-4.05
76	61.79	8	-1.43	-0.51	345.15	-0.42	119.64	35.3	726.69	225.51	0	4.59	82.68	-3.80	0.77	3.25	-2.83	162.14	1	-4.03
77	63.11	9	-1.45	-0.50	346.42	-0.48	127.09	0	617.48	219.32	0	5.83	81.12	-3.79	0.72	3.25	-2.99	162.14	1	-4.02
78	126.32	14a	-5.66	0.54	696.49	-1.95	211.99	3.55	96.73	382.51	101.99	5.57	83.15	-6.45	3.53	6.25	-3.50	428.39	1	-4.02
79	135.03	9a	-5.50	0.41	670.03	-2.06	233.71	22.73	60.20	436.32	0	8.51	75.46	-6.73	2.84	6.25	-3.90	414.37	2	-3.99
80	63.11	Umbelliferone	-1.45	-0.50	346.31	-0.48	127.07	629.87	617.78	219.23	0	7.69	81.12	-3.79	0.72	3.25	-2.99	162.14	1	-3.94
81	53.25	5'	-2.41	-0.37	454.59	-0.17	70.92	0	2105.15	114.41	269.24	7.04	96.87	-4.12	1.78	4	-2.23	220.22	0	-3.89
82	65.74	3i	-11.99	2.67	952.72	-0.006	67.008	5.83	2293.31	724.84	83.47	9.72	100	-8.76	9.65	5	-0.20	675.58	0	-3.86
83	73.98	3c	-10.83	2.33	938.58	-0.26	67.99	25.35	2244.67	780.00	90.58	9.98	100	-8.99	8.83	5.75	0.07	612.68	0	-3.84
84	60.53	6	-1.88	-0.38	372.84	-0.42	116.04	0	785.99	168.69	88.10	6.9	84.94	-3.72	1.05	3.25	-2.96	176.17	1	-3.77
85	68.84	4'	-1.63	-0.5	378.04	-0.47	116.08	96.1	785.36	169.25	92.70	7.93	83.87	-3.67	0.87	4	-2.87	192.17	1	-3.73
86	83.08	4	-1.28	-0.60	353.06	-0.88	170.73	38.85	238.14	182.33	0	7.96	70.12	-3.61	0.10	4	-3.83	178.14	2	-3.70
87	112.34	6o	-8.27	1.07	844.29	-1.33	150.54	100	370.03	463.01	166.43	10.94	80.78	-7.68	5.77	6.5	-2.18	513.54	0	-3.67
88	112.37	6d	-7.66	0.89	812.02	-1.29	150.54	1.62	370.08	519.10	78.09	11.18	91.82	-7.80	5.44	6.5	-1.98	499.51	0	-3.67
89	65.79	3j	-12.31	2.65	952.54	0.176	67.12	5.21	2287.30	731.98	0	7.83	100	-8.82	9.90	5	-0.17	740.45	0	-3.67
90	65.74	3b	-11.43	2.49	923.70	0.004	67.02	34.35	2292.29	780.58	0	8.50	100	-8.91	9.32	5	-0.00	661.55	0	-3.63
91	83.72	l	-1.77	-0.49	386.27	-0.97	173.95	52.7	221.96	133.41	78.90	9.16	70.99	-3.72	0.35	4	-4.06	192.17	2	-3.60
92	160.51	17b	-5.10	0.18	693.85	-2.93	291.23	11.62	17.14	390.18	12.43	9.32	61.62	-6.71	2.15	7	-4.84	430.37	3	-3.56
93	135.46	4a	-5.10	0.38	646.57	-2.04	242.97	11.57	49.17	403.59	0	2.96	72.73	-6.23	2.64	6.25	-4.19	414.37	2	-3.56
94	65.79	3f	-12.20	2.62	947.67	0.16	67.13	2.53	2286.97	732.75	0	7.46	100	-8.80	9.83	5	-0.17	696.00	0	-3.54
95	55.80	4"	-1.63	-0.58	413.80	-0.15	72.27	100	2044.12	155.78	185.74	7.45	94.48	-3.93	1.41	4	-2.11	206.19	0	-3.53
96	102.74	angeloylhellactone	-3.93	-0.01	633.28	-0.46	93.28	264.26	1291.96	179.66	360.32	7.47	100	-4.74	3.05	7.25	-2.31	386.40	0	-3.52
97	73.95	3h	-11.69	2.48	966.73	-0.09	68.08	9.27	2239.97	731.03	90.65	9.31	100	-8.88	9.41	5.75	-0.10	691.58	0	-3.46
98	163.08	13b	-4.80	0.20	675.61	-2.93	306.97	14.44	12.15	356.52	12.11	5.34	58.16	-6.21	2.01	7	-5.24	430.37	3	-3.45
99	65.76	3e	-9.02	1.90	822.84	-0.25	73.89	44.76	1973.11	669.51	79.43	9.58	100	-7.85	7.61	5	-0.42	534.61	0	-3.33
100	139.22	17a	-5.35	0.35	680.42	-2.27	238.11	3.87	54.68	429.61	12.68	8.80	74.93	-6.80	2.88	6.25	-3.81	414.37	2	-3.17
101	65.76	3a	-11.45	2.48	926.19	-0.02	68.10	12.71	2239.11	787.63	0	8.19	100	-9.00	9.27	5	0	617.10	0	-3.14
102	83.93	4'-methoxy Pd-C I	-4.26	-0.06	636.91	-0.50	90.74	89.19	1365.89	166.89	379.28	11.08	100	-5.12	2.75	6.95	-2.31	358.39	0	-3.11
103	110.24	6l	-7.99	1.02	829.37	-1.19	141.01	0.51	455.70	482.76	142.05	11.34	82.28	-7.64	5.75	6.5	-1.93	513.54	0	-3.04
104	112.94	6m	-8.31	1.07	846.20	-1.43	158.34	0.13	312.12	459.41	163.98	10.33	79.22	-7.68	5.73	6.5	-2.33	513.54	0	-3.03
105	80.304	5-	-1.76	-0.48	385.52	-0.85	160.77	50.53	295.99	144.97	79.77	7.47	73.96	-3.70	0.47	4	-3.78	192.17	2	-2.98
106	112.98	6f	-7.89	0.93	823.69	-1.41	158.65	0.11	309.98	498.85	101.69	10.64	90.47	-7.81	5.44	6.5	-2.20	499.51	0	-2.70
107	114.24	6n	-8.57	1.11	859.57	-1.48	160.26	0.14	299.28	445.03	189.68	10.52	79.23	-7.73	5.78	6.5	-2.42	513.54	0	-2.56
108	65.84	3d	-11.84	2.71	962.58	-0.18	65.41	46.42	2374.3	731.95	165.21	10.31	100	-8.86	9.46	5	-0.14	610.71	0	-2.56

109	183.95	11	-4.3	-0.23	716.10	-2.40	262.06	2.82	32.41	264.36	189.67	5.32	46.14	-5.73	0.87	11.4	-4.84	492.43	6	-2.54
110	121.02	6g	-7.54	0.75	835.01	-1.46	156.19	0.09	327.09	509.01	105.29	9.73	76.83	-7.90	5.25	7.25	-2.02	515.51	0	-2.43
111	140.52	13a	-5.09	0.37	664.77	-2.30	252.36	16.99	40.06	400.25	12.14	5.21	71.81	-6.36	2.76	6.25	-4.18	414.37	2	-2.31
112	113.22	6a	-7.83	0.86	808.13	-1.19	153.58	0.12	346.29	522.13	13.51	10.54	79.05	-7.82	5.56	6.5	-2.03	519.93	0	-2.23
113	121.22	6i	-7.38	0.72	826.23	-1.46	158.11	0.42	313.68	497.56	106.09	10.89	75.96	-7.77	5.16	7.25	-2.10	515.51	0	-1.69
114	112.94	6c	-8.02	0.88	814.45	-1.22	158.15	0.92	313.39	506.80	13.42	13.37	78.62	-7.80	5.62	6.5	-2.16	519.93	0	-1.52
115	112.40	6k	-8.24	1.06	842.44	-1.32	149.67	0.12	377.16	462.23	166.30	10.67	80.89	-7.66	5.76	6.5	-2.17	513.54	0	-1.44
116	112.20	6j	-8.16	1.05	838.50	-1.34	152.36	100	355.62	480.14	142.02	10.84	80.30	-7.71	5.74	6.5	-2.15	513.54	0	-1.15

Where,

MW= Molecular weight- 130.0 – 725.0

logS= Predicted aqueous solubility

log_o/w= Predicted octanol/water partition coefficient- -2.0 – 6.5

AccepH= Estimated number of hydrogen bonds that would be accepted by the solute from water molecules in an aqueous solution- 2.0 – 20.0

DonorH= Estimated number of hydrogen bonds that would be donated by the solute to water molecules in an aqueous solution- 0.0 – 6.0

QPPCaco= Predicted apparent Caco-2 cell permeability in nm/sec. Caco2 cells are a model for the gut-blood barrier- <25 poor, >500 great

QPlogBB= Predicted brain/blood partition coefficient- -3.0 – 1.2

%HumanOralAbs= Predicted human oral absorption on 0 to 100% scale-<25 poor, >80% is high

QPlog HERG= Predicted IC50 value for blockage of HERG K⁺ channels- concern below -5

SASA=Total solvent accessible surface area -300.0 – 1000.0

FOSA= Hydrophobic component of the SASA- 0.0 – 750.0

FISA=Hydrophilic component of the SASA (SASA on N, O, and H on heteroatoms) 7.0 – 330.0

PISA= π (carbon and attached hydrogen) component of the SASA- 0.0 – 450.0

Table S2: MM-GBSA of docked poses of ligand and Lysosomal α -glucosidase

Ligand Title	dG Bind	dG_Bind_Co ulomb	dG_Bind_Covalent	dG_Bind_Hbond	dG_Bind_Li po	dG_Bind_Packing	dG_Bind_So lv_GB	dG_Bind_vd W
Isorutarine	-67.7444	-9.96711	4.231813	-1.71303	-46.5353	-0.86858	20.12332	-33.0155
10	-52.2643	-13.4023	1.549819	-1.32953	-34.4134	-0.44602	15.72849	-19.9513
36	-45.3818	-11.9788	0.175291	-1.1507	-26.471	-0.42633	21.08744	-26.6177
8	-59.1848	-12.9442	0.754741	-1.2184	-32.7178	-0.48242	18.38014	-30.9568
19	-50.9809	-12.2514	1.041642	-1.22003	-26.5425	-0.42242	15.80082	-27.387
15	-53.619	-13.226	2.600868	-1.57864	-26.6499	-0.58649	9.387111	-23.566
5a	-62.151	-13.5968	1.488955	-1.24678	-32.0043	-1.70279	24.6031	-39.6925
22'- Isopropyl psoralene	-54.2447	45.00236	1.918041	-1.2347	-32.6606	-1.78536	-26.1077	-39.3768
1	-54.0868	45.02762	1.919395	-1.23554	-32.6605	-1.77218	-25.9839	-39.3818
22	-54.6778	-14.5201	0.664604	-1.16397	-30.2068	-0.03299	19.80444	-29.2231
5b	-57.214	-16.6983	3.548256	-1.44997	-29.7253	-1.47704	27.71414	-39.1258
45	-57.5478	-11.7707	0.688632	-1.21878	-31.338	-0.50067	16.24881	-29.6572
4- hydroxyPd- C-III	-63.9608	-1.41999	7.426241	-1.02575	-41.4892	-0.82467	6.996298	-33.6237
14	-49.4073	-14.8157	0.706875	-1.16409	-27.2835	-0.02702	20.55314	-27.377
29	-50.2617	-13.6034	2.242309	-0.81446	-25.8175	-0.79051	15.70535	-27.1835
34	-59.9071	-17.8571	2.614521	-1.4644	-27.6297	-0.90635	10.86982	-25.5339
5	-49.9345	-12.4994	1.243396	-1.21908	-26.435	-0.42948	16.85704	-27.452
33	-44.5103	-8.27848	1.904996	-1.32978	-33.7138	-0.53004	22.53996	-25.1032
9d	-49.8824	23.84013	0.980934	-3.26246	-26.9153	-0.00615	-9.89031	-34.6293
43	-63.1522	-13.3061	6.648104	-1.30902	-31.9031	-0.91315	10.80562	-33.1745
25	-48.8659	-15.2176	4.378871	-0.64724	-31.0833	-0.80449	21.12486	-26.617
Nodakenin	-53.2268	-2.09675	1.458297	-1.32762	-32.1728	-1.49291	16.34425	-33.9393
16	-58.385	-12.848	1.305986	-1.06063	-26.4786	-1.00672	8.414435	-26.7115
30	-56.1746	-20.2228	1.974522	-1.49599	-24.939	-0.90295	13.21329	-23.8017
9c	-49.3398	21.26295	0.987628	-3.48581	-26.4088	-0.7578	-9.11407	-31.8239
4c	-59.2077	-31.4926	5.614982	-2.34833	-29.4351	-1.16348	37.27893	-37.6621
18	-59.5895	-12.7698	0.887466	-1.06209	-26.9175	-0.9886	6.191833	-24.9308

14b	-62.9734	-16.2956	1.201922	-1.03871	-34.1519	-1.03009	24.53832	-36.1973
38	-59.0774	-9.61697	5.639837	-0.57464	-31.5138	-1.07607	12.99562	-34.9314
23	-54.2091	-12.6809	1.243776	-1.22015	-31.0747	-0.8045	19.15091	-28.8236
17	-46.6469	-10.2884	1.033163	-0.89848	-25.8679	-6.84E-06	18.79108	-29.4163
12	-57.227	-15.2557	1.108098	-1.11255	-25.6018	-0.88028	10.52304	-26.0078
11	-59.0686	-11.0202	1.172668	-1.05086	-29.7359	-0.92134	8.486529	-25.9995
32	-45.2726	-11.2019	1.678858	-1.20001	-25.5414	-0.77116	17.51959	-25.7566
35	-44.0241	-17.0792	3.592203	-0.64242	-28.9777	-0.00655	24.91974	-25.8303
42	-50.496	-16.5332	11.05031	-0.62669	-33.1481	-0.59197	24.69446	-35.3408
28	-38.9731	-17.9423	3.614301	-0.63849	-26.0789	-0.00578	25.94443	-23.8663
26	-43.1529	-8.27845	2.058553	-0.32996	-29.5591	-2.80E-07	18.90694	-25.9509
6h	-65.7036	-32.7198	18.48962	-2.7935	-37.3717	-1.3215	37.72118	-47.7079
9	-62.2711	-13.0406	2.2037	-1.10407	-30.5503	-0.88318	8.221254	-27.1179
41	-51.4623	-8.21612	4.332438	-0.33591	-36.6203	-1.52E-06	21.45822	-32.0806
47	-59.6224	-15.2646	4.409123	-1.4475	-29.6269	-0.91428	9.527505	-26.3058
46	-46.5074	-14.2039	4.459761	-0.65326	-29.9882	-0.63919	22.01994	-27.5026
2	-41.0362	-14.0232	0.987193	-1.16331	-19.0247	-0.71379	15.9733	-23.0716
20	-55.1364	-9.39554	7.167543	-1.06354	-39.0321	-0.97809	8.395224	-20.2299
31	-39.8473	-15.171	3.592753	-0.63436	-26.0765	-0.00513	21.7823	-23.3355
21	-64.4847	-12.2778	1.198346	-1.21206	-35.5881	-0.46504	18.34639	-34.4865
27	-39.8788	-7.83271	2.651738	-0.42518	-28.0704	-0.00097	16.73333	-22.9346
7	-41.8638	-1.7864	0.032126	-0.22511	-26.6854	-0.62938	13.36423	-25.9339
4	-58.115	-11.0893	0.916248	-1.06414	-26.1487	-0.85	6.748014	-26.6272
10a	-57.8203	-14.5164	1.914223	-1.23725	-32.6066	-0.56467	27.11568	-37.9253
Umbellifer on 6- carboxylic acid	-36.9464	-13.6324	0.363215	-1.55599	-16.4679	-4.12E-05	15.9701	-21.6234
39	-65.4736	-15.5285	6.343861	-1.00475	-33.0247	-0.84977	15.42157	-36.8313
13	-49.8871	-18.2786	3.302621	-1.25911	-25.2735	-1.4855	16.54275	-23.4357
24	-60.8599	-13.6175	1.947893	-1.09477	-27.9373	-0.8827	8.056534	-27.3321
10b	-60.9971	-17.4902	5.938016	-0.98503	-32.0326	-0.76427	24.51447	-40.1775
17c	-48.686	30.42226	2.394187	-1.44641	-29.9121	-0.88328	-19.1521	-30.1085
6b	-63.9293	-25.1522	19.0739	-2.29081	-41.1547	-1.00695	33.88137	-47.28
18b	-61.7045	-10.664	2.583151	-1.2274	-33.3925	-0.94095	15.63941	-33.7022
6e	-57.1023	-13.3417	21.64364	-1.50314	-41.5759	-1.64135	28.1595	-48.8434

18a	-67.2473	-17.8292	6.782858	-0.96115	-35.4741	-0.97625	15.67943	-34.4689
3	-38.7931	-11.9731	0.302792	-1.25868	-17.0609	-1.39948	11.47919	-18.883
40	-47.7854	-0.73082	-0.10912	-0.25246	-31.2546	-0.59833	13.95385	-28.7939
6	-38.5326	-4.16022	0.944024	-0.24726	-26.046	-0.55787	16.94631	-25.4116
3'R- oAcetul- 4'S- tigloylkhell actone	-55.5834	-2.78151	14.83385	-0.01807	-46.3451	-8.43E-05	19.69137	-40.9639
Decursidin	-67.9514	-3.78258	14.87031	-1.13961	-45.7718	-1.16837	13.44715	-44.4065
44	-43.8692	-3.85741	1.53433	-0.42093	-29.812	-0.69951	18.04209	-28.6557
Decursinol	-52.3766	-5.16579	0.817025	-1.08006	-29.0689	-1.32855	12.08338	-28.6338
9b	-56.3536	31.45671	1.401983	-1.24231	-30.5319	-0.00082	-18.4349	-39.0023
4b	-51.9995	31.72783	3.965605	-0.95773	-27.6469	-0.67573	-22.4262	-35.9864
10	-35.462	-17.1571	10.27557	-2.45084	-28.9311	-1.68731	38.57231	-34.0836
3g	-53.0049	-7.12633	15.42998	-1.02147	-37.7231	-0.5671	24.94159	-46.9384
7	-45.7197	-10.6331	2.229981	-1.07988	-20.406	-0.71404	5.858648	-20.9753
Nodakeneti n	-53.524	-0.74211	1.63483	-0.1997	-34.302	-4.63E-05	13.91499	-33.8299
13c	-54.7519	42.31259	-0.23174	-1.14973	-33.4895	-1.67915	-22.72	-37.7944
8	-37.3966	-5.50635	0.328576	-1.35602	-16.353	-1.51227	8.016348	-21.0139
9	-40.8394	-14.4647	0.712335	-1.00261	-16.871	-1.323	12.53706	-20.4275
14a	-64.9731	-8.86319	4.696859	-0.642	-38.1912	-0.06087	18.29533	-40.208
9a	-46.6956	30.60755	2.372651	-2.3783	-25.5085	-1.30851	-16.5508	-33.9297
Umbellifer one	-44.5095	-11.7558	0.537832	-1.04608	-16.6208	-0.92178	4.462819	-19.1658
5'	-47.4558	-3.49297	0.805648	-0.50118	-26.0639	-0.00619	13.31787	-31.515
3i	-54.2671	-7.65898	12.214	-1.05918	-38.4452	-0.59056	27.43626	-46.1634
3c	-56.0696	-7.68768	11.091	-1.0002	-34.8034	-0.69589	24.3128	-47.2862
6	-13.9321	-0.69638	0.722182	-0.8002	-19.2456	-0.86447	30.92991	-23.9775
4'	-15.3848	-8.41907	0.923188	-0.76014	-17.6251	-0.74835	33.74168	-22.497
4	-23.304	-8.73186	1.152279	-1.08295	-15.9805	-0.74462	23.10449	-21.0208
6o	-55.8555	-12.1251	10.31411	-0.75055	-44.2917	-0.98572	36.38161	-44.3981
6d	-55.6568	-6.42403	5.630088	-1.40925	-36.9818	-1.56335	27.79111	-42.6996
3j	-58.3631	-6.0109	14.21754	-0.86988	-41.605	-0.65673	27.25385	-50.692
3b	-53.7363	-5.68816	8.531591	-1.08557	-40.4457	-0.53084	31.95418	-46.4718

1	-37.256	-6.83085	-0.37954	-1.22646	-19.3466	-0.63184	12.6085	-21.4492
17b	-54.0592	29.1741	9.310025	-1.02748	-37.0781	-0.02242	-17.245	-37.1702
4a	-48.1467	34.99628	3.927855	-1.30025	-31.1907	-1.24178	-13.4668	-39.8713
3f	-56.3993	-6.94995	10.25524	-1.08626	-42.0644	-0.63093	31.03451	-46.9576
4"	-43.1194	-2.1058	1.663298	-0.79927	-25.8752	-0.54403	11.2051	-26.6635
angeloylkh ellactone	-51.0081	-6.06389	13.00795	-0.59645	-39.0317	-2.62E-10	15.44288	-33.7668
3h	-68.4125	-7.87208	6.298612	-0.01882	-43.7504	-0.84913	31.39592	-53.6166
13b	-52.3411	37.71622	1.777886	-1.05135	-34.0537	-1.62081	-19.9292	-35.1801
3e	-45.2061	-2.65949	6.74132	-0.00081	-37.0146	-0.28765	32.36566	-44.3505
17a	-37.2592	53.86887	0.772631	-0.09728	-34.006	-7.34E-07	-22.9249	-34.8726
3a	-63.4627	-7.61171	10.06993	-1.02027	-43.201	-0.62125	26.32561	-47.404
4'-methoxy Pd-C I	-60.1283	-0.62891	3.634351	-0.84289	-36.5235	-1.15883	10.80014	-35.4087
6l	-68.186	-7.93839	5.157975	-0.16094	-40.9914	-1.37937	22.64524	-45.5191
6m	-56.1854	-7.43001	6.681312	-1.4843	-36.8942	-2.04791	28.42066	-43.431
5	-16.8967	-18.1361	0.468915	-0.67594	-19.0507	-0.01123	46.99189	-26.4836
5	-16.8967	-18.1361	0.468915	-0.67594	-19.0507	-0.01123	46.99189	-26.4836
6f	-49.0039	-12.227	11.79937	-0.97344	-39.7797	-0.77044	36.19266	-43.2454
6n	-41.103	-29.5506	11.97172	-3.01524	-33.5406	-0.20124	47.52852	-34.2955
3d	-64.1257	-7.55899	8.637143	-1.05905	-39.0717	-0.62318	27.18271	-51.6326
11	-27.9311	-18.1962	4.802416	-0.64616	-36.1572	-0.79323	60.29103	-37.2318
6g	-58.4157	-5.92049	4.987861	-1.74627	-41.4604	-1.4188	31.41258	-44.2702
13a	-48.7144	36.61914	5.700669	-1.22055	-32.1202	-1.25204	-16.2307	-40.2106
6a	-60.7239	-5.6053	3.625035	-1.68974	-43.2176	-1.57192	31.73685	-44.0012
6i	-57.135	-12.9711	12.86823	-0.62746	-32.0315	-0.38663	19.83495	-43.8215
6c	-49.3718	-12.0897	13.76565	-1.23622	-41.3462	-0.76882	32.81734	-40.5139
6k	-66.8158	-1.35996	7.137454	-0.14277	-39.6212	-0.36476	18.94667	-51.4112
6j	-63.1173	-15.9823	8.121857	-0.08087	-39.4311	-0.72019	26.35665	-41.3814