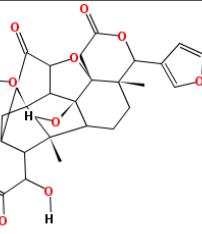
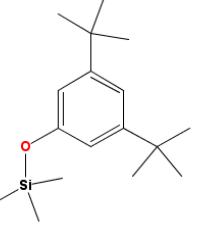
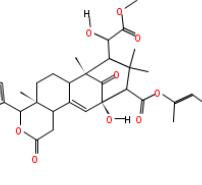
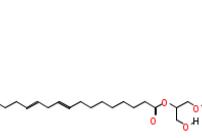
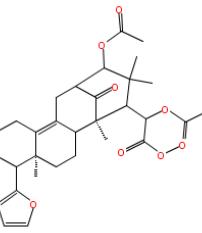
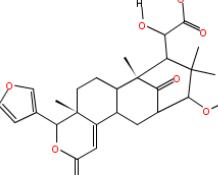
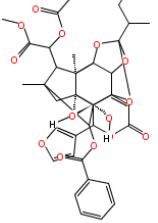
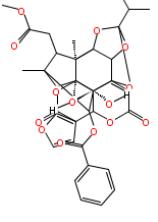
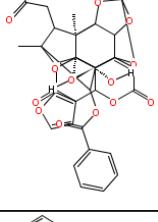
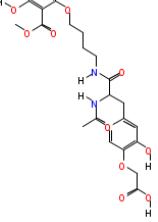


Swietenia macrophylla Phytochemicals

No	ID	Structure	MW (g/mol)	XLogP	H-Don	H-Acc	rot. bonds	ring count	top. PSA	PAIN	PubChem CID
1	74138		308.3	12.5	0	0	19	0	0.0		74138
2	12395		224.3	9.1	0	0	13	0	0.0		12395
3	101076684		560.2	0.6	3	11	6	7	158.1		101076684
4	101076684		560.2	0.6	3	11	6	7	158.1		101076684

5	91895449		516.2	-0.5	3	10	4	7	148.8		91895449
6	528937		278.2	7.2	0	1	4	1	9.2		528937
7	76326957		584.3	2.6	2	10	7	5	145.7		76326957
8	5365676		354.3	6.8	2	4	18	0	66.8		5365676
9	44575317		570.2	1.7	0	10	8	5	131.5		44575317

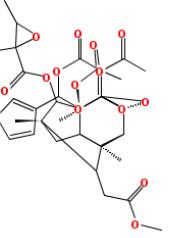
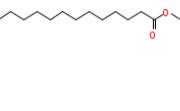
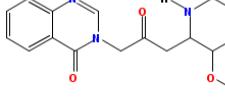
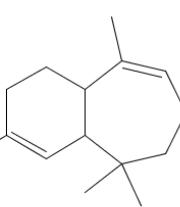
10	21672225		486.2	0.9	2	8	4	5	119.4		21672225
11	102279627		762.3	3.8	2	14	11	9	182.6		102279627
12	102279629		762.3	3.5	2	14	11	9	182.6		102279629
13	102279631		748.3	2.9	2	14	10	9	182.6		102279631
14	448214		518.2	1.9	5	12	17	2	180.7		448214

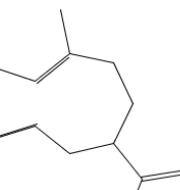
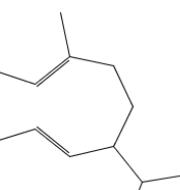
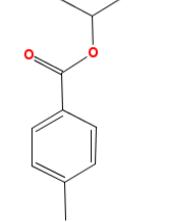
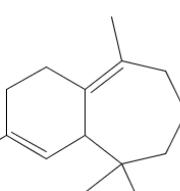
15	23258996		610.3	3.3	0	10	9	5	131.5		23258996
16	101396725		584.3	1.2	2	10	7	5	145.7		101396725
17	5362709		196.2	7.8	0	0	10	0	0.0		5362709
18	348289626		428.4	9.5	1	2	6	4	37.3		
19	5364600		280.3	11.2	0	0	16	0	0.0		5364600

20	101498001		726.3	2.5	2	14	10	8	182.6		101498001
21	102279626		740.3	3.0	2	14	11	8	182.6		102279626
22	71300386		438.2	2.2	0	6	1	6	82.2		71300386
23	3931		280.2	7.9	1	2	14	0	37.3		3931
24	965		282.3	8.2	1	2	15	0	37.3		965

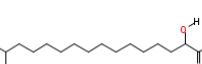
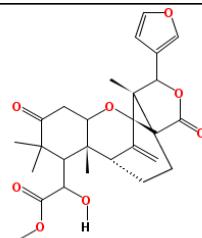
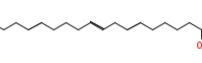
25	102279628		740.3	2.8	2	14	11	8	182.6		102279628
26	102279630		726.3	2.2	2	14	10	8	182.6		102279630
27	266444		468.2	2.3	0	7	5	5	91.4		266444
28	60123241		412.4	11.6	0	1	6	4	17.1		60123241
29	6427091		204.2	6.1	0	0	1	2	0.0		6427091

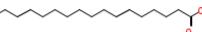
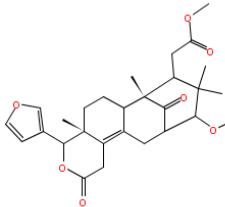
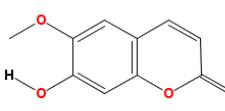
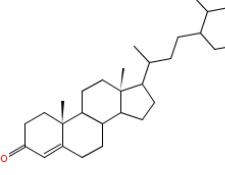
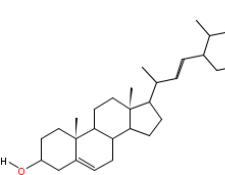
30	21672224		728.3	1.4	2	14	12	5	198.3		21672224
31	9064		290.1	1.5	5	6	1	3	110.4	catechol_A(92)	9064
32	520449		336.4	13.7	0	0	0	1	0.0		520449
33	70697958		568.3	1.9	1	9	7	5	125.4		70697958
34	unnamed_1		290.1	1.5	5	6	1	3	110.4	catechol_A(92)	

35	101321330		740.3	1.8	0	15	11	9	181.0		101321330
36	12366		284.3	8.3	0	2	16	0	26.3		12366
37	unnamed_1		284.3	8.3	0	2	16	0	26.3		
38	unnamed_1		301.1	0.7	2	6	4	3	82.0		
39	577062		204.2	6.0	0	0	0	2	0.0		577062

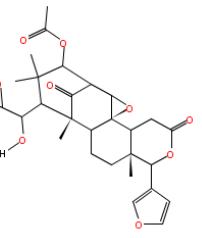
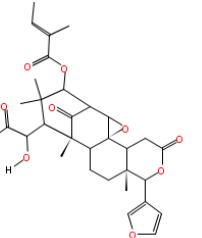
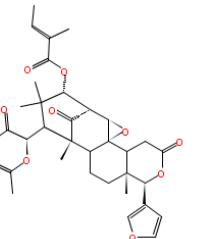
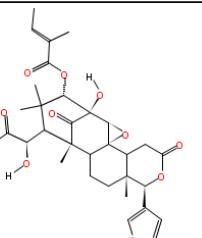
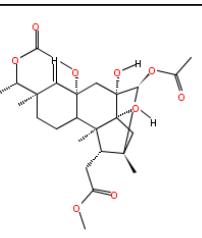
40	5835162		204.2	5.6	0	0	1	1	0.0		5835162
41	5373727		204.2	6.3	0	0	1	1	0.0		5373727
42	985		256.2	7.6	1	2	14	0	37.3		985
43	230182		178.1	3.3	0	2	3	1	26.3		230182
44	11586487		204.2	5.6	0	0	0	2	0.0		11586487

45	100953349		684.3	2.7	0	13	11	6	170.3		100953349
46	101936275		502.2	1.6	2	9	4	6	128.6		101936275
47	76330468		516.2	0.1	3	10	4	7	152.1		76330468
48	76319611		518.2	-0.1	4	10	4	7	152.0		76319611
49	unnamed_1		552.3	2.7	0	8	7	5	105.2		

50	530317		300.3	7.4	1	3	15	0	46.5		530317
51	unnamed_1		486.2	1.1	1	8	4	5	108.4		
52	5280590		296.3	8.5	0	2	16	0	26.3		5280590
53	5284421		294.3	8.2	0	2	15	0	26.3		5284421
54	8181		270.3	7.9	0	2	15	0	26.3		8181

55	unnamed_1		298.3	9.0	0	2	17	0	26.3		
56	23258999		470.2	0.9	1	7	4	5	99.1		23258999
57	5280460		192.0	1.0	1	4	1	2	55.8		5280460
58	5484202		412.4	11.6	0	1	6	4	17.1		5484202
59	5280794		412.4	11.1	1	1	5	4	20.2		5280794

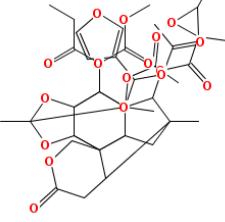
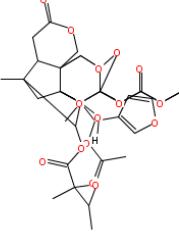
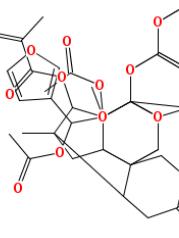
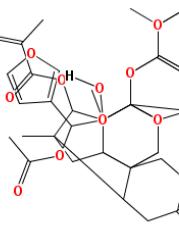
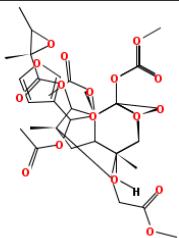
60	101889628		586.3	2.3	1	10	8	6	138.0		101889628
61	101471349		756.3	1.8	4	15	12	6	221.6		101471349
62	102033438		482.1	2.3	6	10	4	5	166.1	catechol_A(92)	102033438
63	14262267		558.2	1.4	1	10	7	6	138.0		14262267
64	102056053		600.3	2.2	0	11	9	6	144.0		102056053

65	14587344		544.2	1.2	1	10	6	6	138.0		14587344
66	21636354		584.3	2.2	1	10	7	6	138.0		21636354
67	unnamed_1		626.3	2.9	0	11	9	6	144.0		
68	unnamed_1		600.3	1.7	2	11	7	6	158.2		
69	unnamed_1		544.2	0.9	3	10	6	6	148.8		

70	14262276		568.3	2.6	1	9	7	5	125.4		14262276
71	101486442		800.3	2.3	0	17	14	9	207.2		101486442
72	101889628		586.3	2.3	1	10	8	6	138.0		101889628
73	101471349		756.3	1.8	4	15	12	6	221.6		101471349
74	102033438		482.1	2.3	6	10	4	5	166.1	catechol_A(92)	102033438

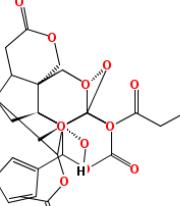
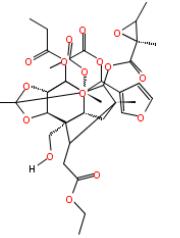
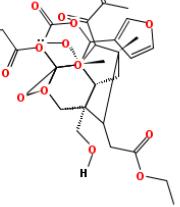
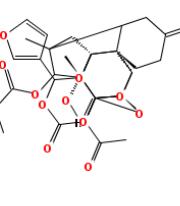
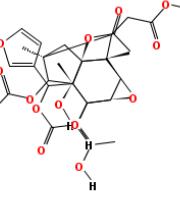
75	14262267		558.2	1.4	1	10	7	6	138.0		14262267
76	102056053		600.3	2.2	0	11	9	6	144.0		102056053
77	14587344		544.2	1.2	1	10	6	6	138.0		14587344
78	21636354		584.3	2.2	1	10	7	6	138.0		21636354
79	unnamed_1		626.3	2.9	0	11	9	6	144.0		

80	unnamed_1		600.3	1.7	2	11	7	6	158.2		
81	unnamed_1		544.2	0.9	3	10	6	6	148.8		
82	14262276		568.3	2.6	1	9	7	5	125.4		14262276
83	101486442		800.3	2.3	0	17	14	9	207.2		101486442
84	101486443		800.3	2.3	0	17	14	9	207.2		101486443

85	101486444		814.3	2.6	0	17	15	9	207.2		101486444
86	101486445		772.3	1.9	1	16	13	9	201.2		101486445
87	101486446		798.3	3.6	0	16	15	8	194.7		101486446
88	101486447		770.3	3.2	1	15	13	8	188.7		101486447
89	101486448		832.3	1.9	1	18	17	8	227.5		101486448

90	101486449		872.3	4.0	0	18	20	7	221.0		101486449
91	101486450		822.3	1.1	2	18	17	8	222.8		101486450
92	101486452		848.3	2.9	1	18	19	7	216.3		101486452
93	101486453		862.3	1.3	2	19	18	8	247.7		101486453
94	101486454		904.3	2.0	1	20	20	8	253.8		101486454

95	101486451		864.3	1.9	1	19	19	8	228.9		101486451
96	101786375		756.3	3.0	0	15	12	9	181.0		101786375
97	101786376		742.3	2.7	0	15	11	9	181.0		101786376
98	101786377		740.3	4.0	0	14	12	8	168.4		101786377
99	101786378		682.3	2.1	1	13	9	8	162.4		101786378

100	101786379		642.2	1.7	1	13	6	9	162.4		101786379
101	101786380		786.3	2.3	1	16	14	9	201.2		101786380
102	101786381		712.3	2.8	2	13	11	8	173.4		101786381
103	101786383		664.3	1.6	1	12	6	9	153.1		101786383
104	101786384		684.3	3.1	3	13	9	7	187.6		101786384

105	101786385		698.3	3.3	3	13	10	7	187.6		101786385
106	23258997		570.2	1.6	0	10	8	5	131.5		23258997
107	21636326		486.2	0.2	2	8	4	5	119.4		21636326
108	44575315		486.2	0.2	2	8	4	5	119.4		44575315
109	98042580		568.3	1.9	1	9	7	5	125.4		98042580

110	101471346		684.3	3.2	1	12	10	8	145.3		101471346
111	101471347		670.3	2.8	1	12	9	8	145.3		101471347
112	101471348		700.3	2.1	2	13	10	8	165.5		101471348
113	222284		414.4	11.6	1	1	6	4	20.2		222284