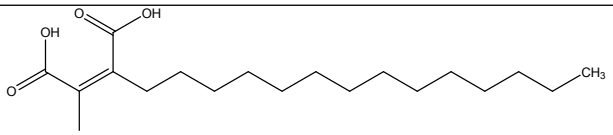
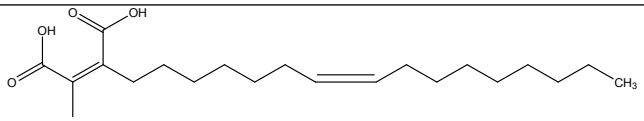
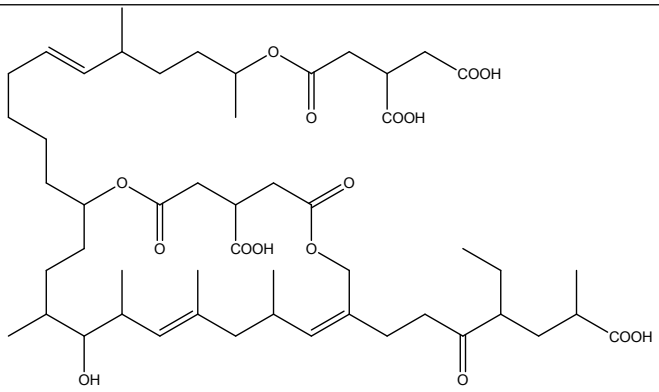
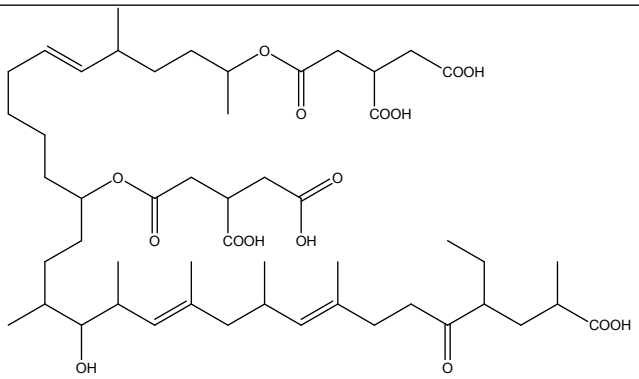
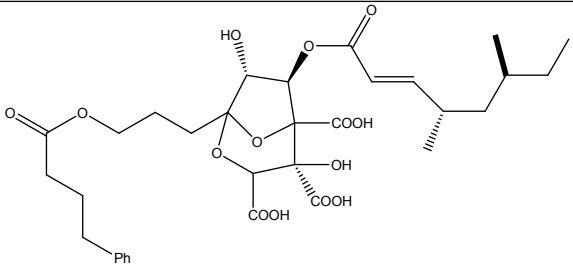
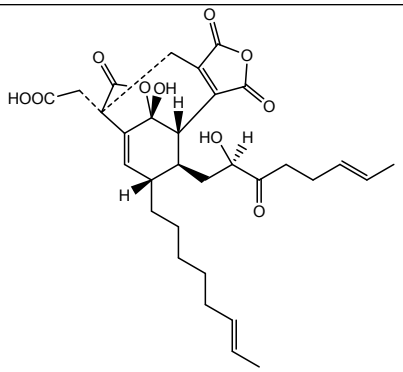
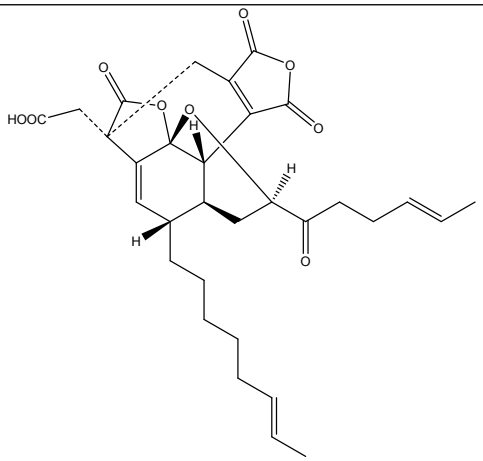
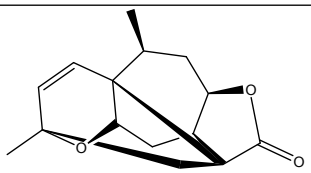
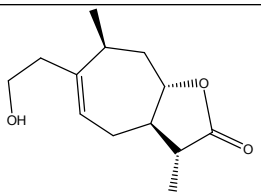
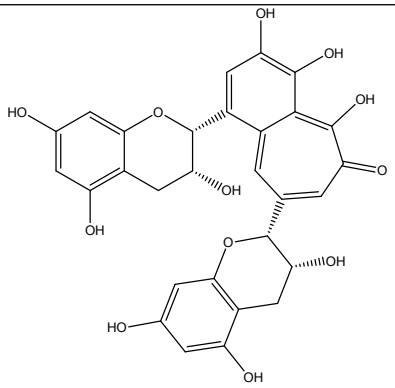
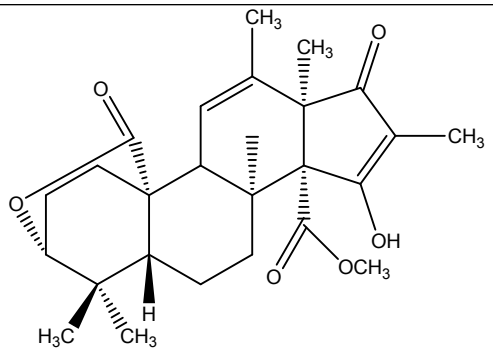
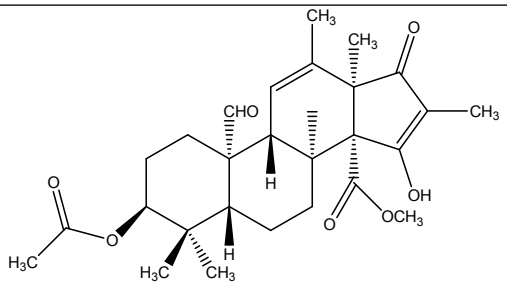
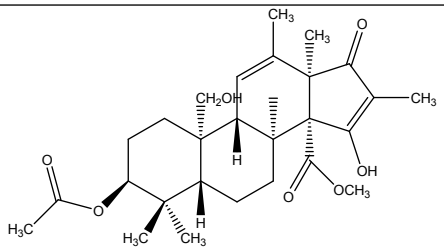
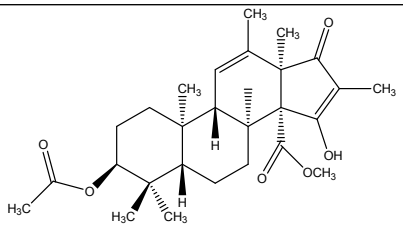
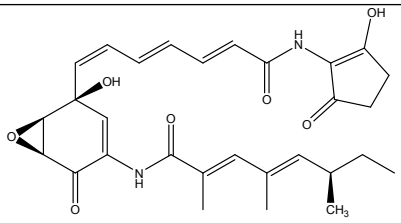
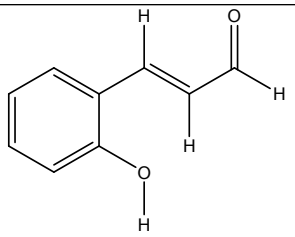
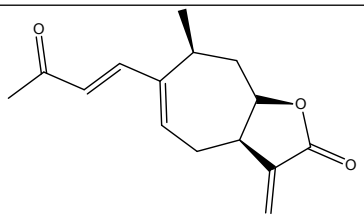
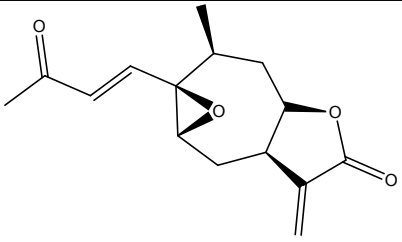
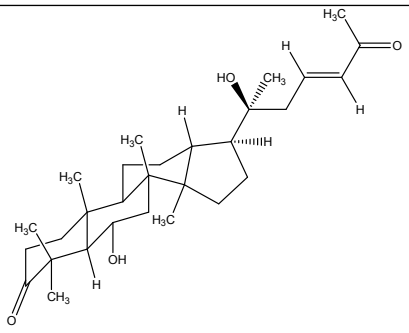
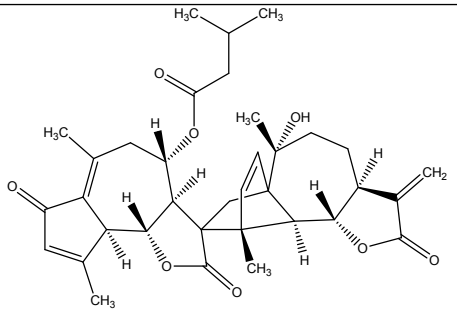
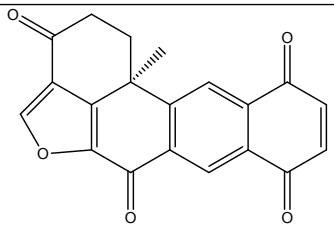
Supplementary data

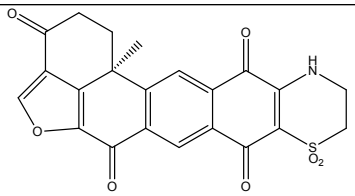
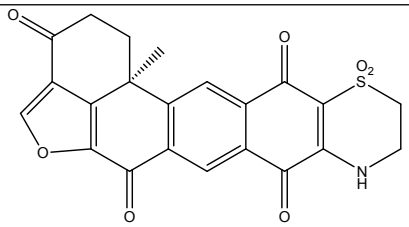
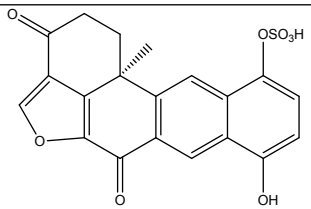
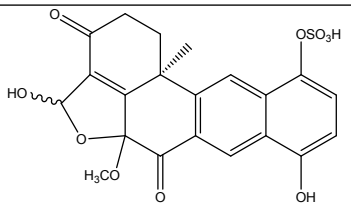
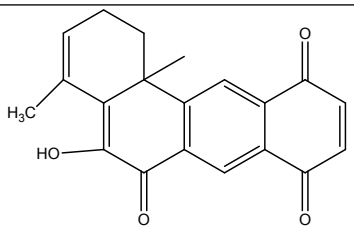
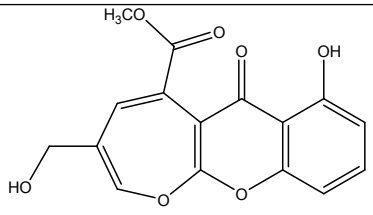
Table S1: Structure of the natural compounds considered for the studies

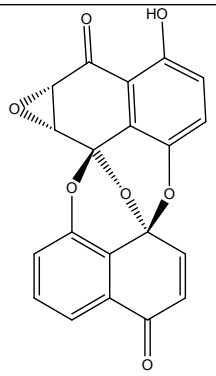
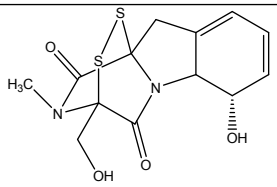
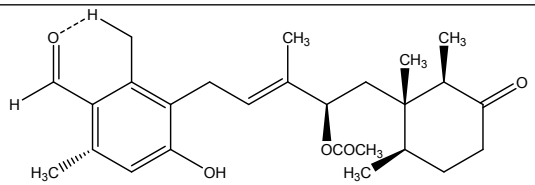
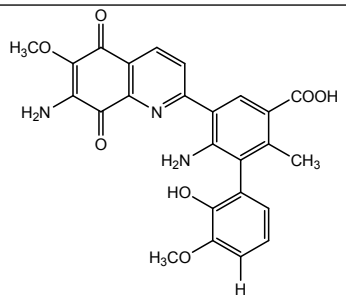
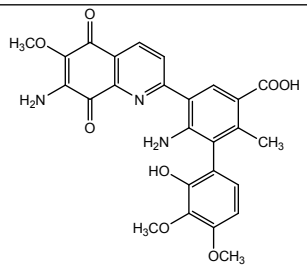
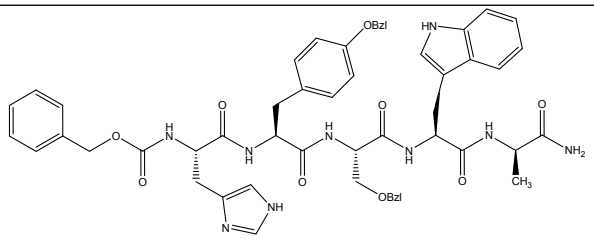
Comp Code	Structure	Reference
Nat-1		1, 2
Nat-2		1, 2
Nat-3		1, 2
Nat-4		1, 2
Nat-5		1, 2

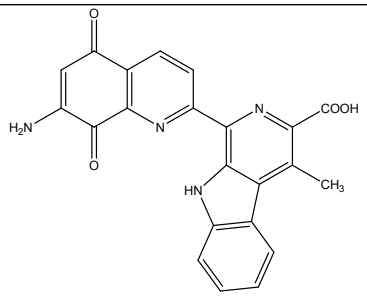
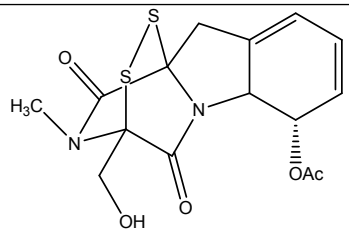
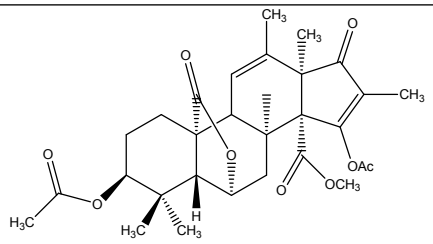
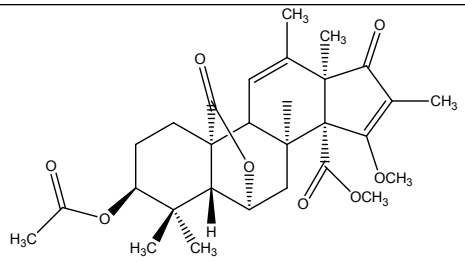
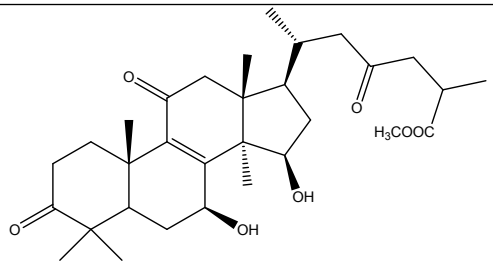
Nat-6		1
Nat-7		1
Nat-8		3
Nat-9		3
Nat-10		4

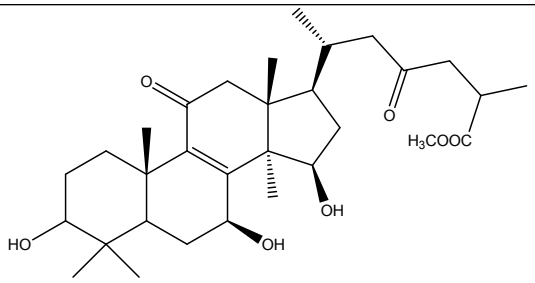
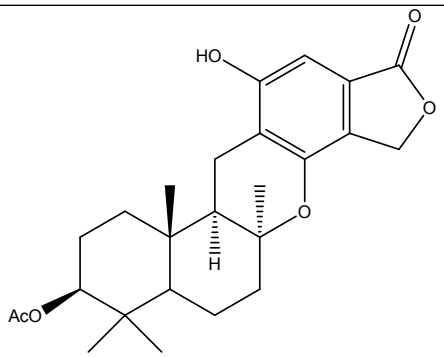
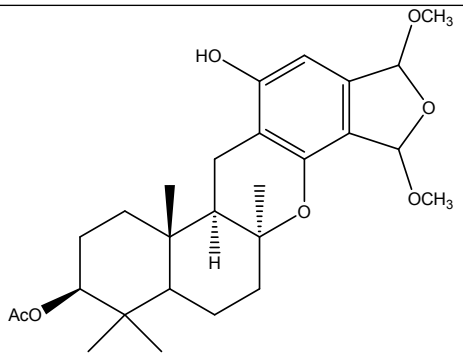
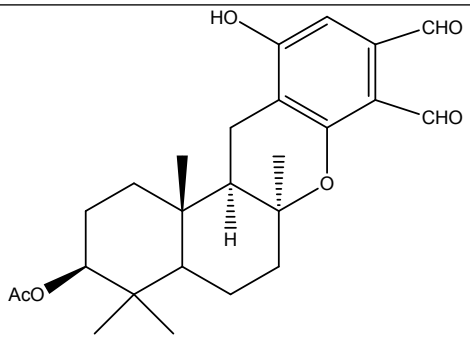
Nat-11		5
Nat-12		5,6
Nat-13		5,6
Nat-14		5,6
Nat-15		7,8

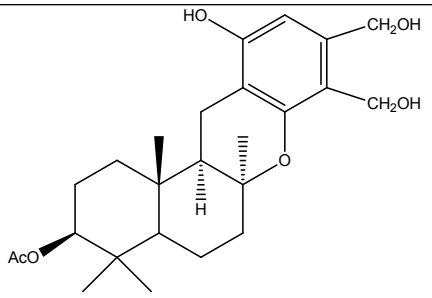
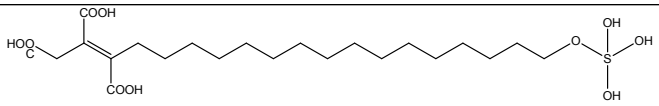
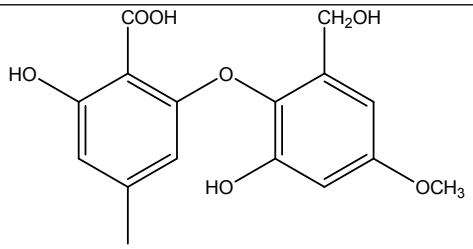
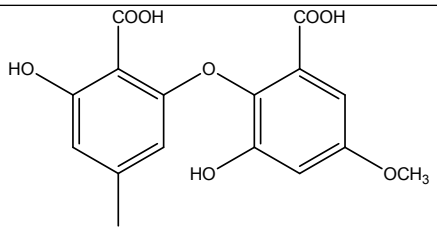
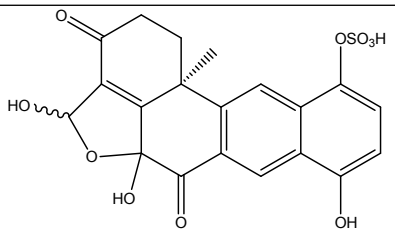
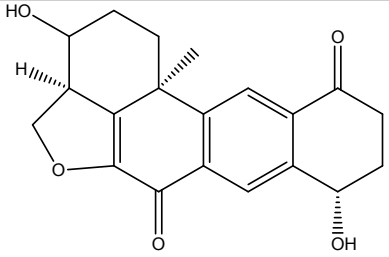
Nat-16		9
Nat-17		10
Nat-18		10
Nat-19		9
Nat-20		1,9
Nat-21		11

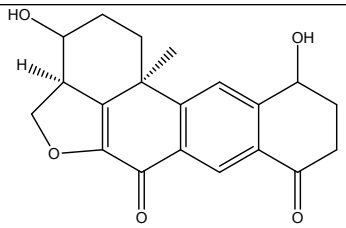
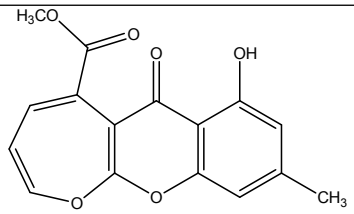
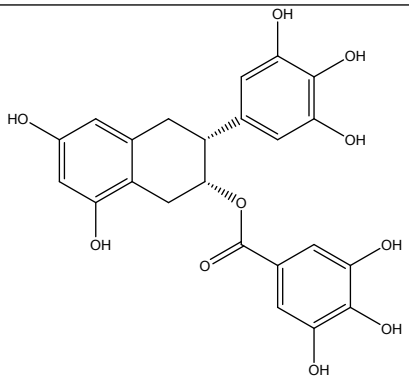
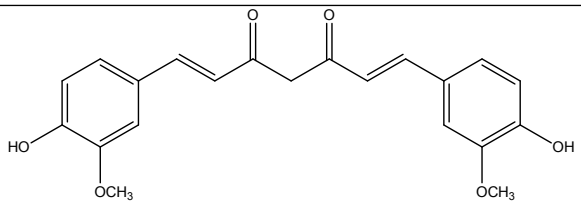
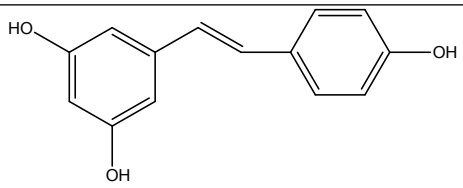
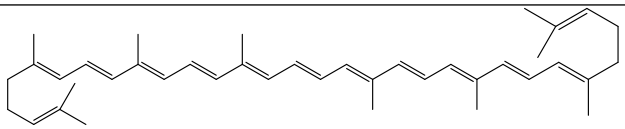
Nat-22		11
Nat-23		11
Nat-24		11
Nat-25		11
Nat-26		11
Nat-27		1,8

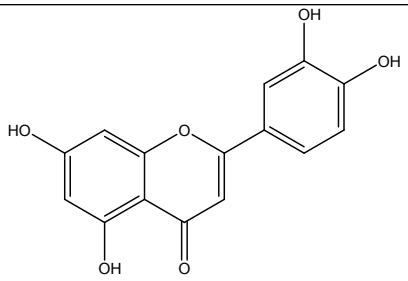
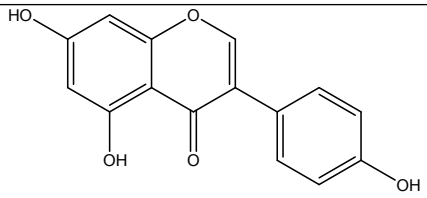
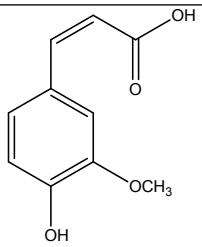
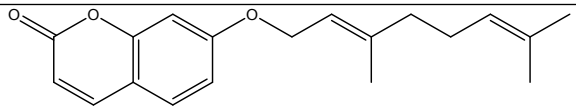
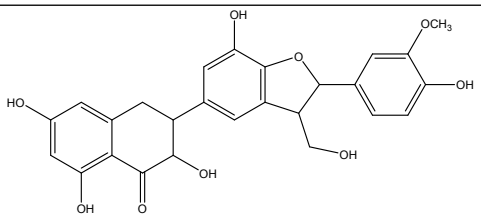
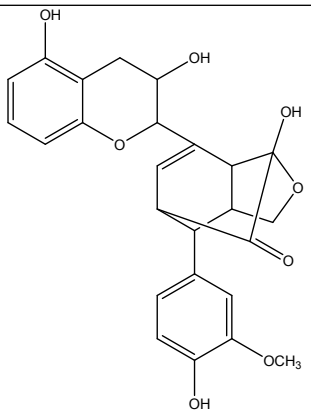
Nat-28		1,2,8
Nat-29		1
Nat-30		1
Nat-31		12
Nat-32		12
Nat-33		2

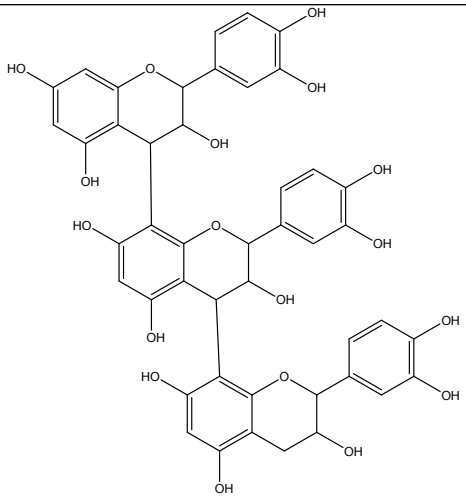
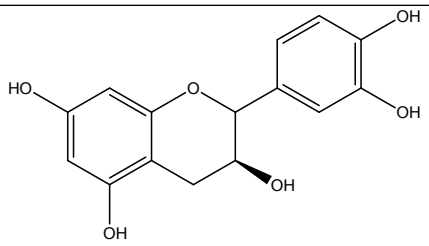
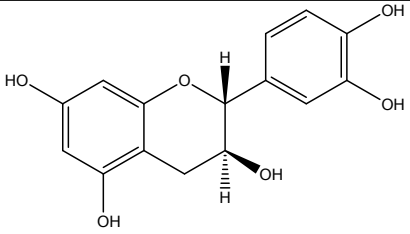
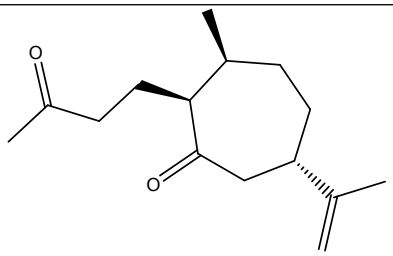
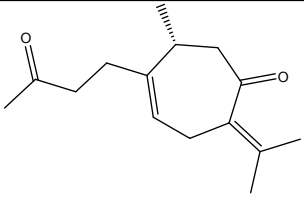
Nat-34		12
Nat-35		2
Nat-36		2
Nat-37		2
Nat-38		2

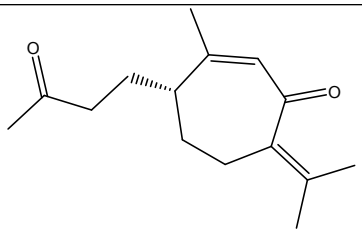
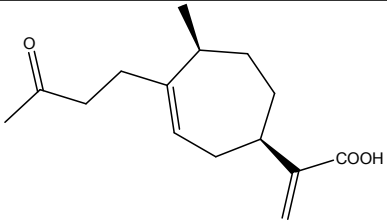
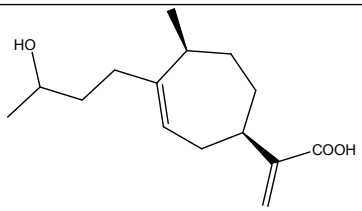
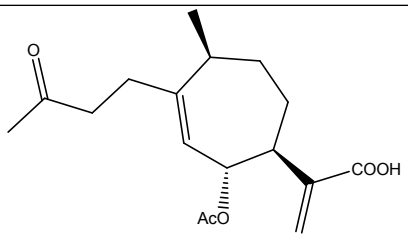
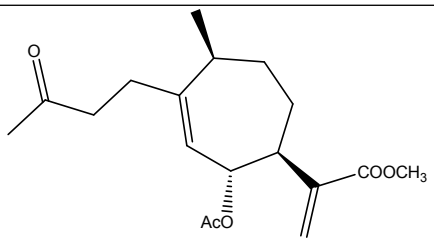
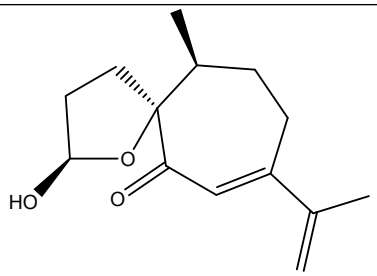
Nat-39		2
Nat-40		2
Nat-41		2
Nat-42		2

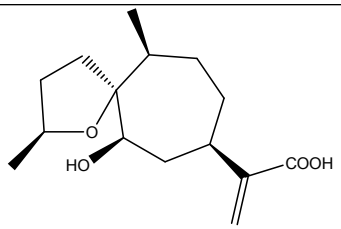
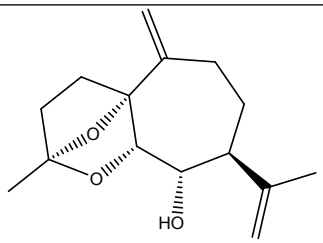
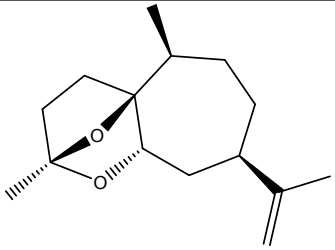
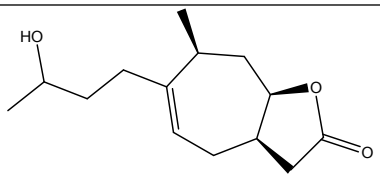
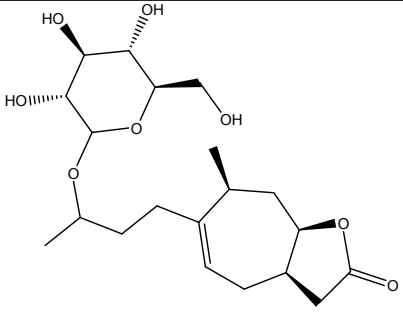
Nat-43		2
Nat-44		2
Nat-45		2
Nat-46		2
Nat-47		2
Nat-48		11

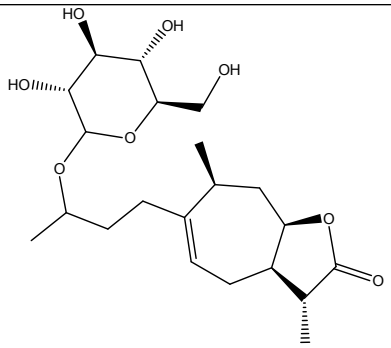
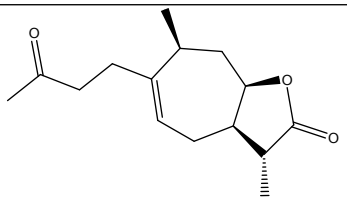
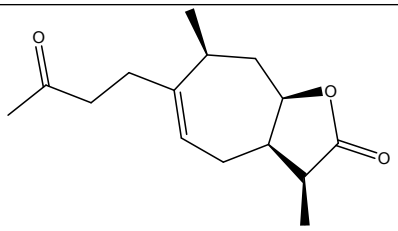
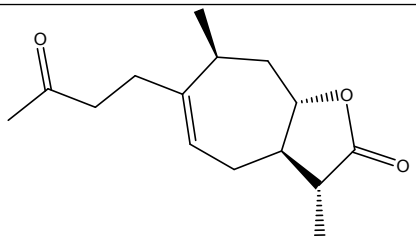
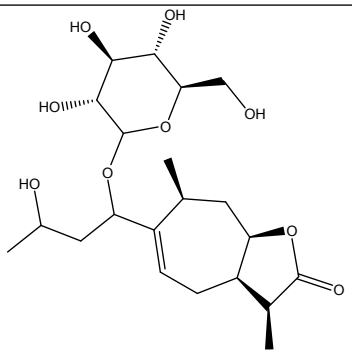
Nat-49		11
Nat-50		2
Nat-51		13
Nat-52		14
Nat-53		14
Nat-54		14

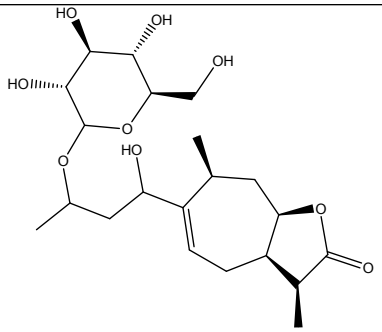
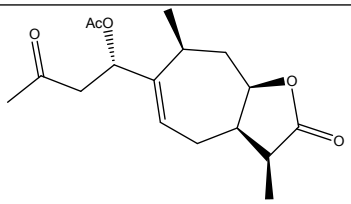
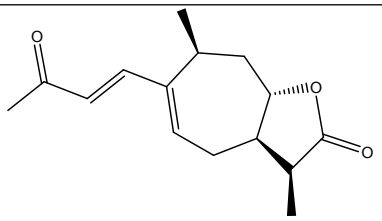
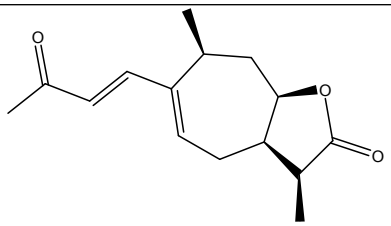
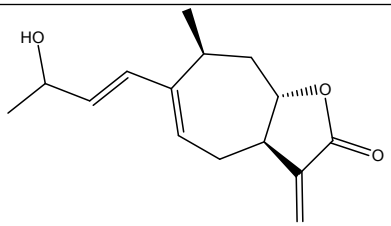
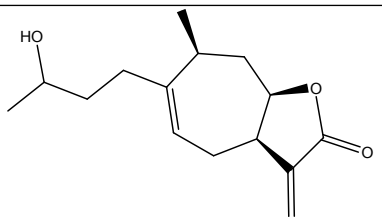
Nat-55		14
Nat-56		14
Nat-57		13
Nat-58		13
Nat-59		13
Nat-60		13

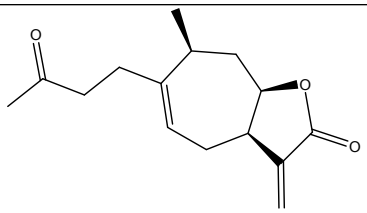
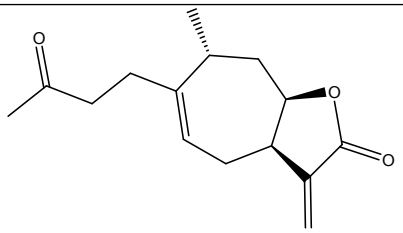
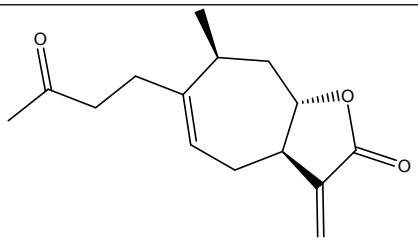
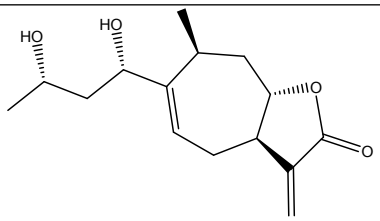
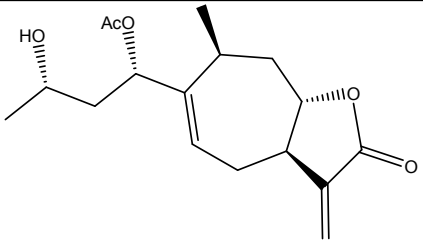
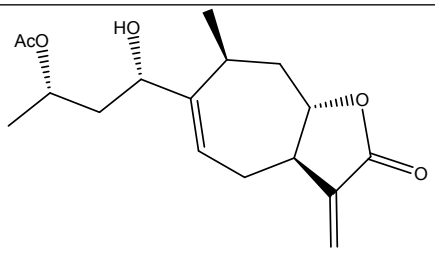
Nat-61		13
Nat-62		13
Nat-63		13
Nat-64		3
Nat-65		3

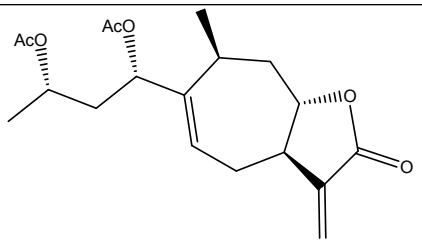
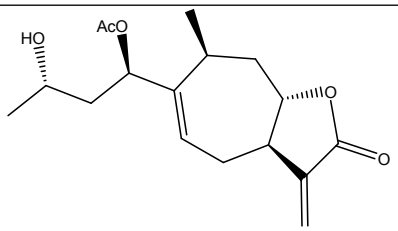
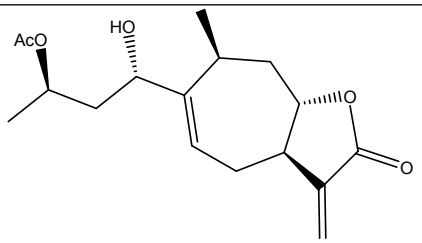
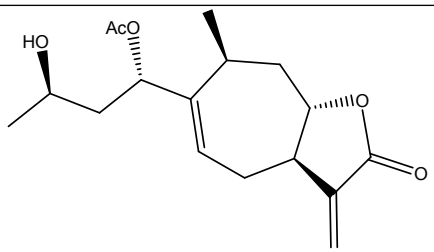
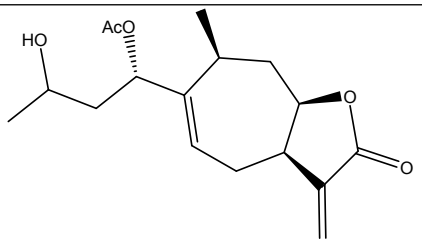
Nat-66		3
Nat-67		3
Nat-68		3
Nat-69		3
Nat-70		3
Nat-71		3

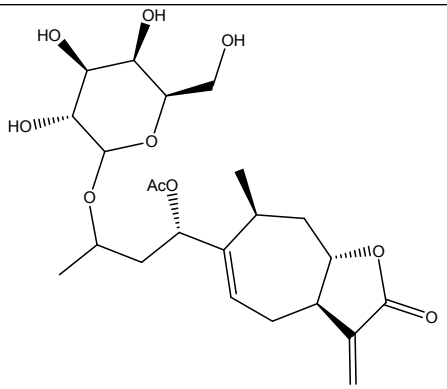
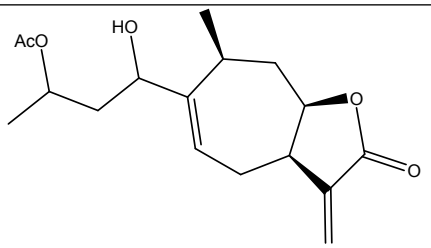
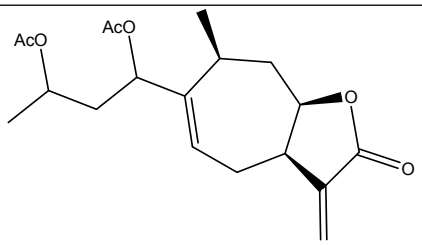
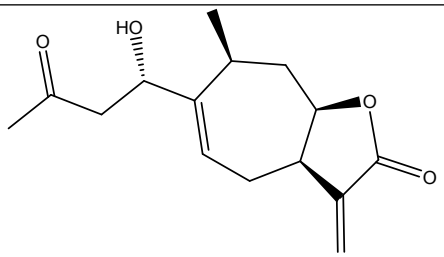
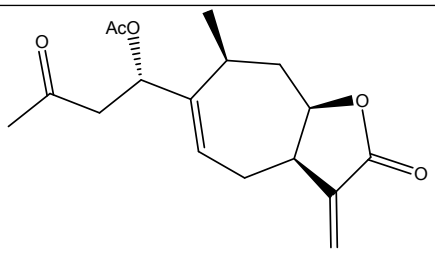
Nat-72		3
Nat-73		3
Nat-74		3
Nat-75		3
Nat-76		3

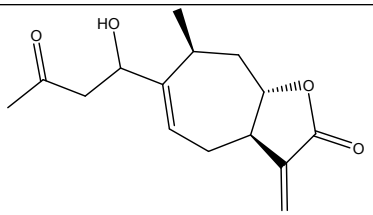
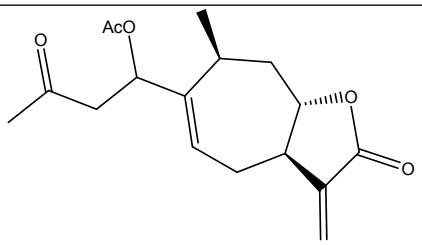
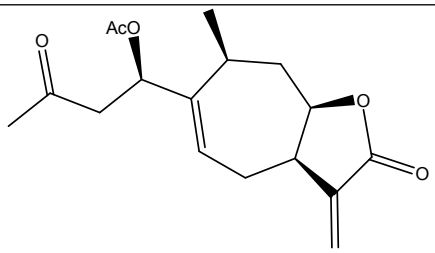
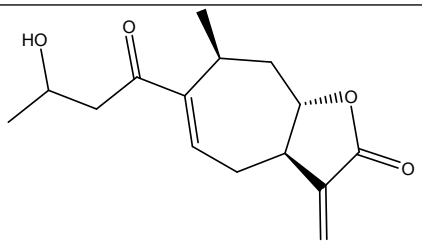
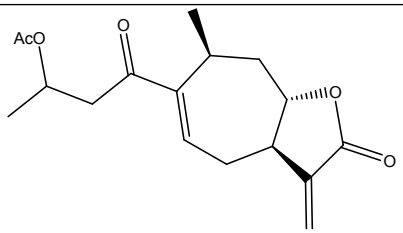
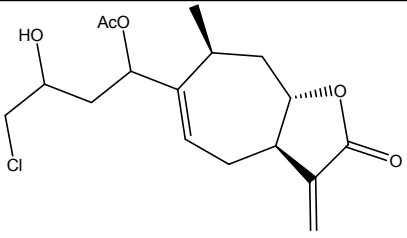
Nat-77		3
Nat-78		3
Nat-79		3
Nat-80		3
Nat-81		3

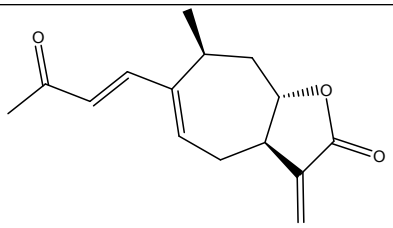
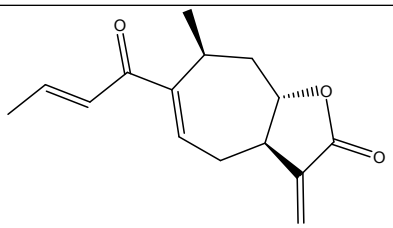
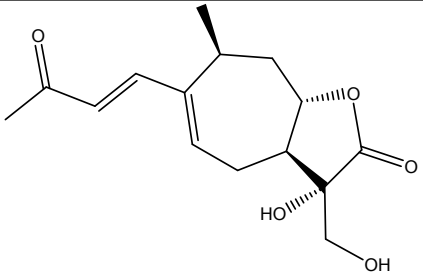
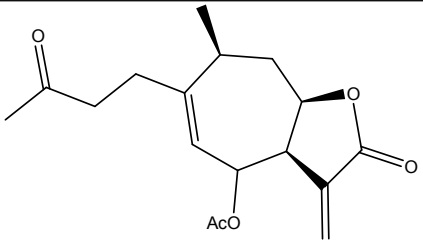
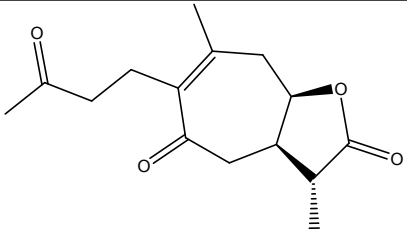
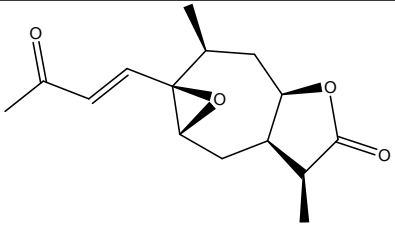
Nat-82		3
Nat-83		3
Nat-84		3
Nat-85		3
Nat-86		3
Nat-87		3

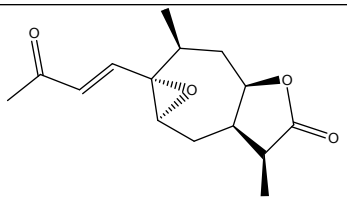
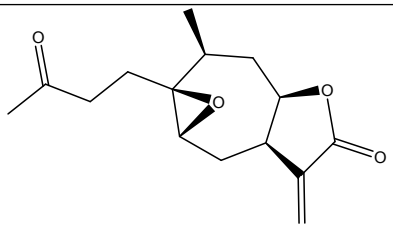
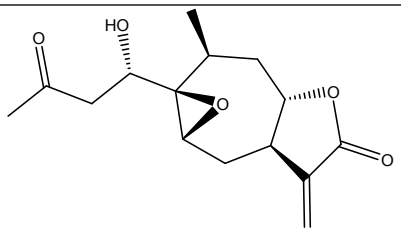
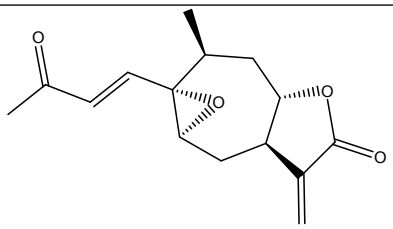
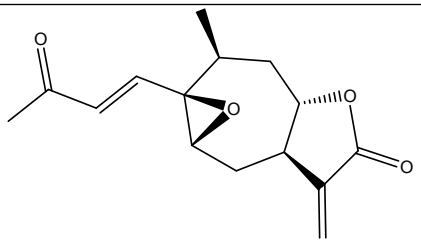
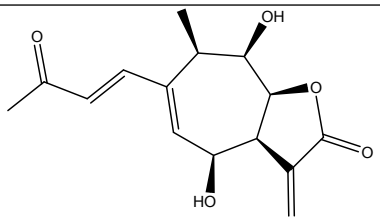
Nat-88		3
Nat-89		3
Nat-90		3
Nat-91		3
Nat-92		3
Nat-93		3

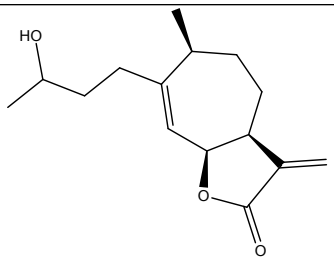
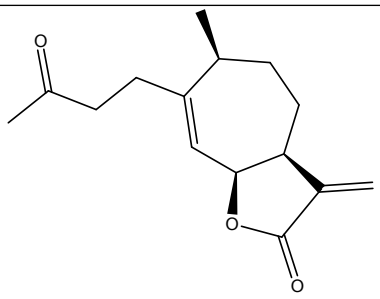
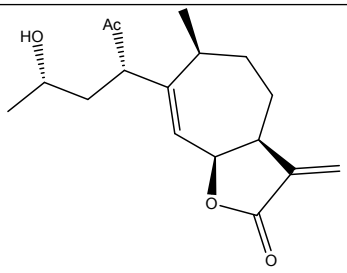
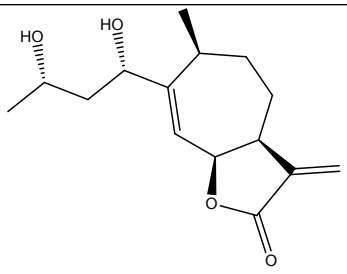
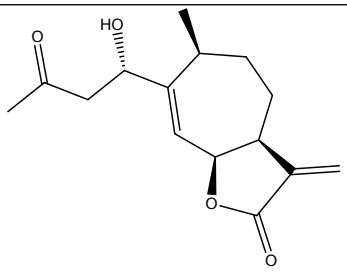
Nat-94		3
Nat-95		3
Nat-96		3
Nat-97		3
Nat-98		3

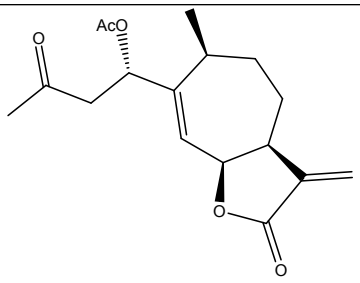
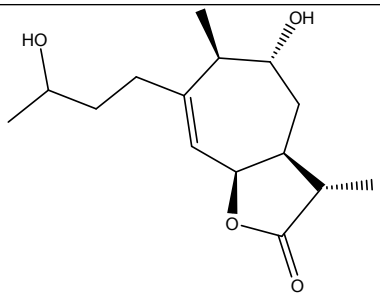
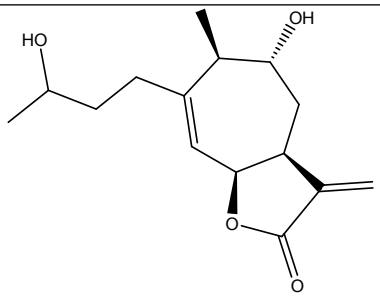
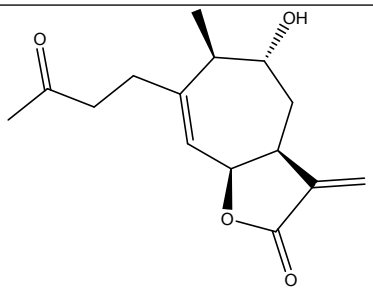
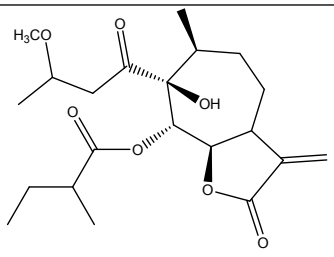
Nat-99		3
Nat-100		3
Nat-101		3
Nat-102		3
Nat-103		3

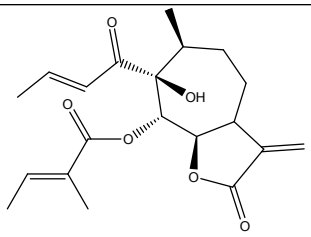
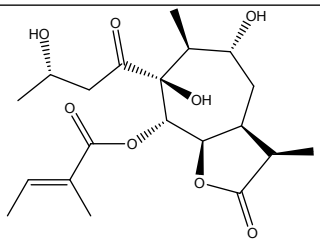
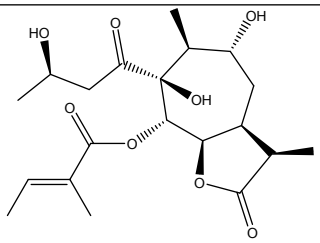
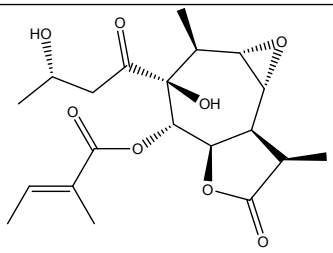
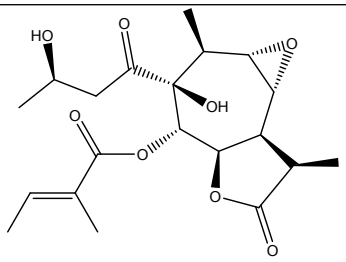
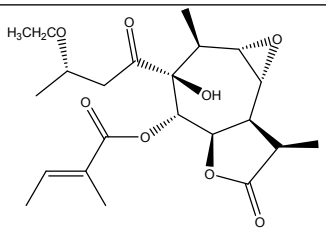
Nat-104		3
Nat-105		3
Nat-106		3
Nat-107		3
Nat-108		3
Nat-109		3

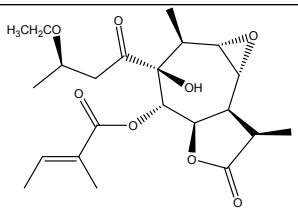
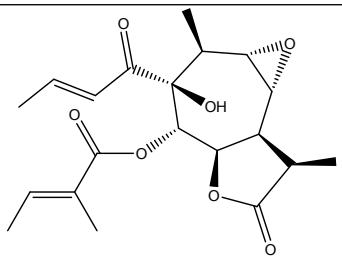
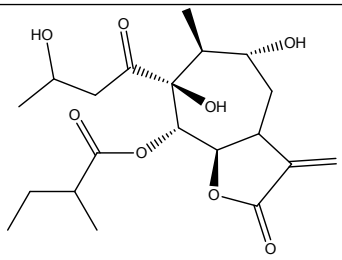
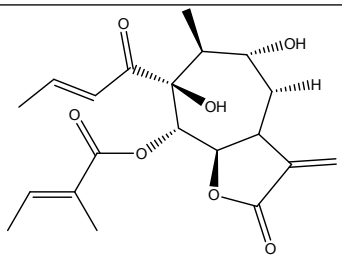
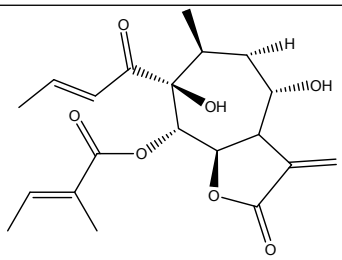
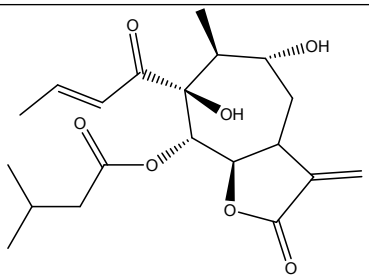
Nat-110		3
Nat-111		3
Nat-112		3
Nat-113		3
Nat-114		3
Nat-115		3

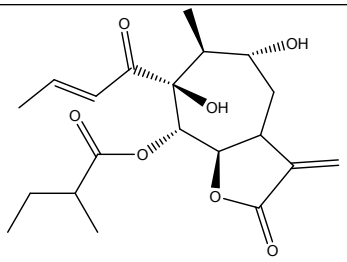
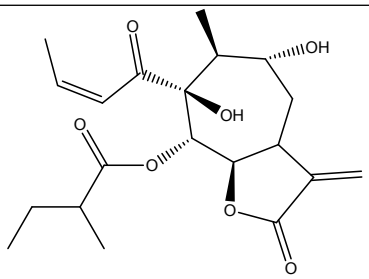
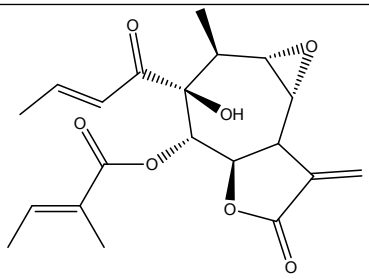
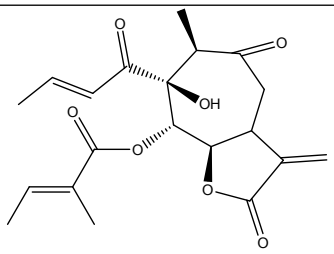
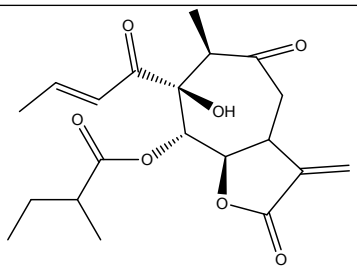
Nat-116		3
Nat-117		3
Nat-118		3
Nat-119		3
Nat-120		3
Nat-121		3

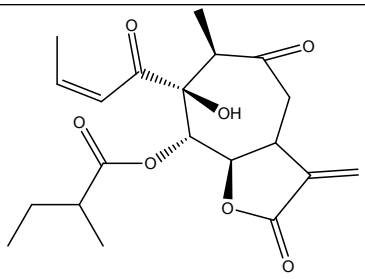
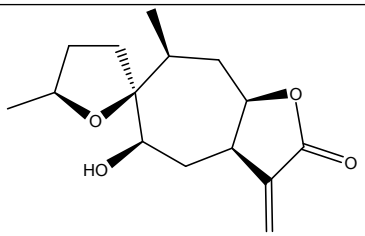
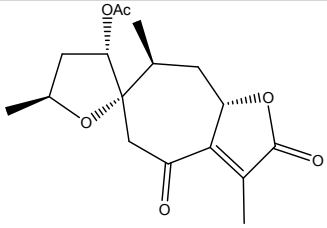
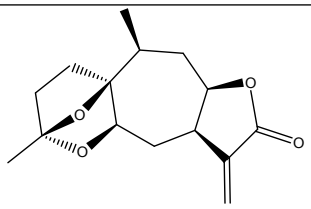
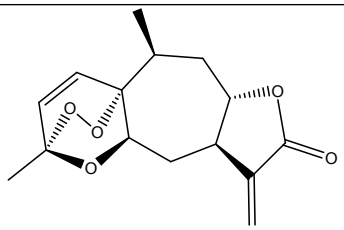
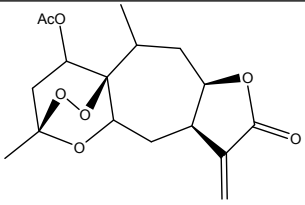
Nat122		3
Nat-123		3
Nat-124		3
Nat-125		3
Nat-126		3

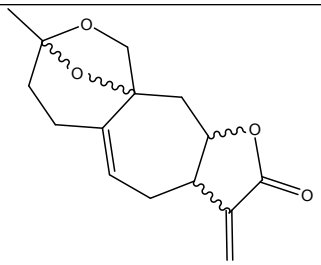
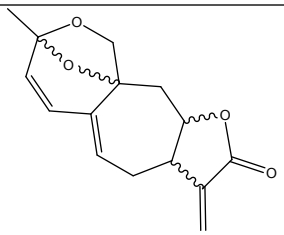
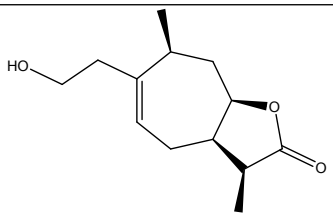
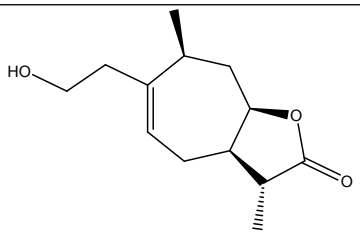
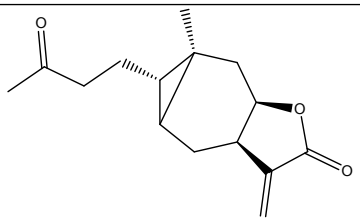
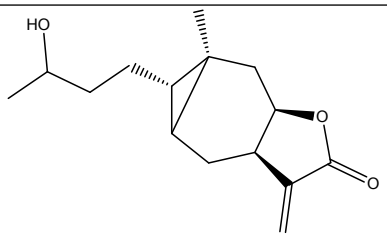
Nat-127		3
Nat-128		3
Nat-129		3
Nat-130		3
Nat-131		3

Nat-132		3
Nat-133		3
Nat-134		3
Nat-135		3
Nat-136		3
Nat-137		3

Nat-138		3
Nat-139		3
Nat-140		3
Nat-141		3
Nat-142		3
Nat-143		3

Nat-144		3
Nat-145		3
Nat-146		3
Nat-147		3
Nat-148		3

Nat-149		3
Nat-150		3
Nat-151		3
Nat-152		3
Nat-153		3
Nat-154		3

Nat-155		3
Nat-156		3
Nat-157		3
Nat-158		3
Nat-159		3
Nat-160		3

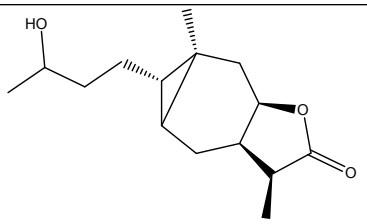
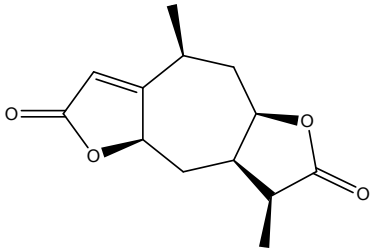
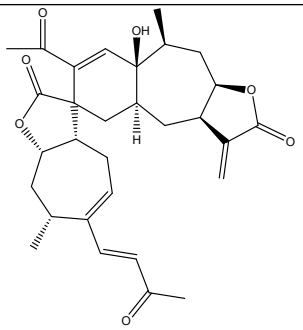
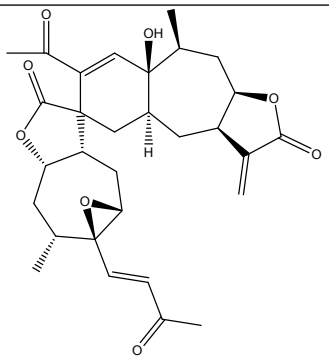
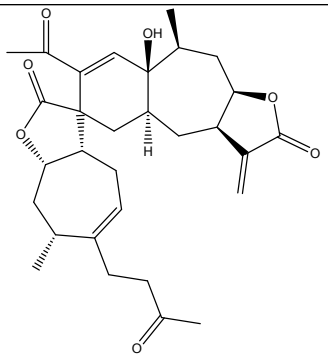
Nat-161		3
Nat-162		3
Nat-163		3
Nat-164		3
Nat-165		3

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Table S2: Validation results of REN inhibitors

BindingDB ID	Ki (μM)	ΔG_{bind} (kcal/ mol)	Predicted ΔG_{bind} (kcal/mol)							
			Model 1		Model 2			Model 3		
			Predicted	LOO	Predicted	LOO	Test	Predicted	LOO	Test
912	13	-6.67	-9.3041	-4.0002	-8.9500	-4.3399	--	-9.0764	-4.2164	--
17941	0.0007	-12.49	-9.3590	-15.6642	-9.0144	-16.0440	--	-9.1381	-15.9095	--
21642	0.0017	-11.96	-9.3590	-14.5969	--	--	-11.0143	--	--	-9.1381
32392	5.7	-7.15	-9.3350	-4.9351	-8.9862	-5.2730	--	-9.1110	-5.1499	--
32394	16	-6.54	-9.2914	-3.7515	--	--	-8.9352	-9.0621	-3.9686	--
50012322	0.000051	-14.04	-9.3590	-18.7856	--	--	-9.0144	--	--	-12.1381
50017487	1	-8.18	-9.3548	-6.9890	-9.0094	-7.3319	--	-9.1333	-7.2075	--
50021129	0.0012	-12.17	-9.3590	-15.0198	-9.0144	-15.3968	--	-9.1381	-15.2630	--
50022507	0.008	-11.05	-9.3590	-12.7643	--	--	-9.0143	--	--	-9.1380
50022512	0.099	-9.55	-9.3586	-9.7440	-9.0139	-10.0982	--	-9.1376	-9.9707	--
50022515	1.1	-8.13	-9.3544	-6.8887	-9.0089	-7.2313	--	-9.1329	-7.1070	--
50022517	1.7	-7.87	-9.3519	-6.3677	-9.0059	-6.7085	--	-9.1300	-6.5847	--
50022519	0.016	-10.63	-9.3590	-11.9186	-9.0143	-12.2821	--	--	--	-9.1380
50022520	0.009	-10.98	-9.3590	-12.6234	--	--	-9.0143	--	--	-9.1380
50022905	2	-7.77	-9.3506	-6.1676	--	--	-9.0045	--	--	-9.1286

50023050	0.052	-9.94	-9.3588	-10.5292	-9.0141	-10.8868	--	-9.1378	-10.7583	--
50023051	0.154	-9.29	-9.3583	-9.2207	-9.0136	-9.5726	--	-9.1373	-9.4457	--
50023052	1.2	-8.08	-9.3540	-6.7885	-9.0084	-7.1307	--	-9.1324	-7.0065	--
50023053	0.12	-9.44	-9.3585	-9.5226	--	--	-9.0138	--	--	-9.1375
50023054	0.007	-11.12	-9.3590	-12.9050	--	--	-9.0143	--	--	-9.1380
50023055	16	-6.54	-9.2915	-3.7515	--	--	-8.9352	-9.0621	-3.9686	--
50023056	12	-6.71	-9.3084	-4.0764	-8.9550	-4.4157	--	-9.0811	-4.2922	--
50025931	0.0048	-11.35	-9.3590	-13.3685	--	--	-9.0143	-9.1380	-13.6065	--
50025932	0.0036	-11.52	-9.3590	-13.7108	--	--	-9.0143	-9.1381	-13.9499	--
50025933	0.043	-10.05	-9.3589	-10.7507	-9.0142	-11.1092	--	-9.1379	-10.9805	--
50025934	0.000064	-13.91	-9.3590	-16.5238	--	--	-9.0144	--	--	-9.1381
50025935	0.000026	-14.44	-9.3590	-16.5911	--	--	-12.0144	-9.1381	-16.8487	--
50025937	0.00052	-12.66	-9.3590	-16.0065	--	--	-9.0144	-9.1381	-16.2529	--
50025939	0.049	-9.97	-9.3588	-10.5896	-9.0141	-10.9474	--	-9.1378	-10.8189	--
50025940	0.21	-9.11	-9.3587	-8.8584	-9.0133	-9.2089	--	-9.1371	-9.0824	--
50025941	0.0011	-12.22	-9.3590	-15.1205	-9.0144	-15.4979	--	-9.1381	-15.3640	--
50025942	0.19	-9.17	-9.3582	-8.9792	-9.0134	-9.3301	--	-9.1372	-9.2035	--
50025943	4.1	-7.35	-9.3417	-5.3310	-8.9941	-5.6692	--	-9.1186	-5.5461	--
50025944	0.58	-8.51	-9.3566	-7.6517	-9.0115	-7.9972	--	-9.1353	-7.8721	--
50025945	0.00088	-12.35	-9.3590	-15.3823	-9.0144	-15.7608	--	-9.1381	-15.6266	--
50025946	0.0077	-11.07	-9.3590	-12.8046	--	--	-9.0143	-9.1380	-13.0409	--
50025948	0.014	-10.71	-9.3590	-12.0797	--	--	-9.0143	--	--	-9.1380
50025949	0.93	-8.23	-9.3551	-7.0894	--	--	-9.0098	-9.1337	-7.3082	--
50027353	0.8	-8.32	-9.3557	-7.2700	-9.0104	-7.6141	--	--	--	-9.1343
50027354	2.5	-7.64	-9.3485	-5.9080	--	--	-9.0020	-9.1262	-6.1240	--

50027355	2.2	-7.72	-9.3497	-6.0678	--	--	-9.0035	-9.1276	-6.2841	--
50027356	42	-5.97	-9.1816	-2.7167	-8.8065	-3.0745	--	-8.9387	-2.9459	--
50027357	0.8	-8.32	-9.3557	-7.2701	-9.0104	-7.6141	--	--	--	-9.1343
50027358	0.6	-8.49	-9.3565	-7.6115	--	--	-9.0114	-9.1352	-7.8318	--
50027359	0.1	-9.55	-9.3586	-9.7440	-9.0139	-10.0982	--	-9.1376	-9.9707	--
50027360	0.1	-9.55	-9.3586	-9.7440	-9.0139	-10.0982	--	-9.1376	-9.9707	--
50027361	1	-8.18	-9.3548	-6.9890	-9.0094	-7.3319	--	-9.1333	-7.2075	--
50027362	0.001	-12.28	-9.3590	-15.2413	-9.0144	-15.6193	--	--	--	-9.1381
50027364	4	-7.36	-9.3426	-5.3507	--	--	-8.9946	--	--	-9.1191
50027365	0.3	-8.9	-9.3578	-8.4359	-9.0129	-8.7846	--	--	--	-9.1366
50027895	1000	-4.09	-5.1342	-2.9893	-4.0154	-4.1741	--	-4.3906	-3.7656	--
50028489	670	-4.33	-6.5284	-2.0735	-5.6982	-2.8874	--	-5.9573	-2.6429	--
50028490	600	-4.39	-6.8241	-1.9012	-6.0447	-2.6612	--	-6.2896	-2.4316	--
50028491	1780	-3.75	-1.8388	-6.0343	-0.2043	-5.3290	--	-0.6876	-7.7881	--
50028492	1140	-4.01	-4.5427	-3.4396	-3.3720	-4.7553	--	-3.7260	-4.3240	--
50028493	230	-4.96	-8.3873	-1.4919	-7.8760	-1.9886	--	-8.0462	-1.8239	--
50028494	530	-4.47	-7.1199	-1.7694	-6.3911	-2.4782	--	-6.6219	-2.2619	--
50028495	980	-4.1	-5.2187	-2.9232	-4.1639	-4.0286	--	-4.4856	-3.6852	--
50028496	300	-4.81	-8.0916	-1.4871	-7.5295	-2.0337	--	--	--	-7.7138
50028527	2440	-3.56	0.9496	-6.1397	--	--	-3.0624	--	--	-2.4457
50028528	1010	-4.09	-5.0919	-3.0328	--	--	-4.0154	-4.3431	-3.8164	--
50077669	0.0007	-12.49	-9.3590	-15.6642	-9.0144	-16.0440	--	-9.1381	-15.9095	--
50084688	0.014	-10.71	-9.3590	-12.0797	--	--	-9.0143	-9.1380	-12.3137	--
50139109	1.9	-7.8	-9.3510	-6.2276	-9.0050	-6.5680	--	--	--	-9.1290
50139110	24.4	-6.29	-9.2560	-3.2846	-8.8936	-3.6305	--	-9.0222	-3.5052	--

50139111	73.6	-5.64	-9.0481	-2.1893	-8.6501	-2.5703	--	-8.7886	-2.4353	--
50139112	10.9	-6.77	-9.3130	-4.1925	--	--	-8.9604	-9.0863	-4.4080	--
50281636	0.212	-9.1	-9.3586	-8.8383	-9.0133	-9.1886	--	--	--	-9.1371
50281638	0.002	-11.87	-9.3590	-14.4156	-9.0144	-14.7900	--	-9.1381	-14.6570	--
50281642	1.2	-8.08	-9.3540	-6.7885	--	--	-9.0084	--	--	-9.1324
50333943	0.021	-10.47	-9.3590	-11.5964	-9.0143	-11.9586	--	--	--	-9.1380
50333944	0.094	-9.59	-9.3586	-9.8246	-9.0139	-10.1791	--	--	--	-9.1376
50333947	0.34	-8.82	-9.3576	-8.2750	-9.0127	-8.6230	--	-9.1364	-8.4972	--
50333948	0.13	-9.39	-9.3585	-9.4219	-9.0137	-9.7748	--	-9.1374	-9.6476	--
50333949	0.45	-8.66	-9.3571	-7.9532	-9.0121	-8.2999	--	-9.1359	-8.1745	--
50333951	0.94	-8.22	-9.3551	-7.0693	-9.0097	-7.4125	--	-9.1336	-7.2880	--
50366324	0.002	-11.87	-9.3590	-14.4156	-9.0144	-14.7900	--	-9.1381	-14.6570	--
50367081	230	-4.96	-8.3873	-3.4919	--	--	-7.8760	-8.0461	-1.8239	--
50367082	1520	-3.84	-2.9373	-4.8635	--	--	-1.4916	-1.9219	-6.1599	--
50367083	1140	-4.01	-4.5427	-3.4396	--	--	-3.3720	-3.7260	-4.3240	--
50367084	440	-4.58	-7.5001	-1.6137	-6.8366	-2.2586	--	-7.0492	-2.0582	--
50367085	960	-4.12	-5.3032	-2.8778	-4.2629	-3.9610	--	-4.5805	-3.6261	--
50367086	520	-4.48	-7.1621	-1.7477	-6.4406	-2.4492	--	-6.6694	-2.2348	--
50368274	0.000043	-14.14	-9.3590	-16.9870	--	--	-9.0144	--	--	-12.1381
50368278	0.00004	-14.18	-9.3590	-17.0675	--	--	-12.0144	-9.1381	-16.3235	--
50405192	0.018	-10.56	-9.3590	-11.7776	-9.0143	-12.1406	--	-9.1380	-12.0107	--

Table S3: Validation results of ACE inhibitors

BindingDB MonomerID	Ki (μM)	ΔG_{bind} (kcal/mol)	Predicted ΔG_{bind} (kcal/mol)							
			Model A		Model B			Model C		
			Predicted	LOO	Predicted	LOO	Test	Predicted	LOO	Test
21642	0.0017	-11.96	-10.2945	-13.6556	--	--	-10.5040	-10.2593	-13.7071	--
50011270	0.0012	-12.17	-10.2946	-14.0794	-10.5041	-13.8792	--	-10.2593	-14.1328	--
50018848	0.015	-10.67	-10.2940	-11.0528	-10.5030	-10.8414	--	--	--	-10.2588
50018850	0.0004	-12.82	-10.2946	-14.3912	-10.5041	-15.1960	--	--	--	-11.2593
50020843	0.0014	-12.08	-10.2946	-13.8978	--	--	-10.5041	-10.2593	-13.9503	--
50021114	0.0014	-12.08	-10.2946	-13.8978	-10.5041	-13.6969	--	-10.2593	-13.9503	--
50021116	0.008	-11.05	-10.2943	-11.8194	-10.5035	-11.6107	--	-10.2590	-11.8625	--
50021117	55	-5.81	-8.1757	-4.3598	-6.1618	-5.4025	--	-8.3296	-3.1864	--
50021118	0.0012	-12.17	-10.2946	-14.0794	-10.5041	-13.8792	--	-10.2593	-14.1328	--
50021119	0.0005	-12.69	-10.2946	-15.1288	-10.5041	-14.9326	--	--	--	-10.2593
50021120	42	-5.97	-8.6765	-5.1950	-7.1882	-4.6435	--	-8.7857	-3.0661	--
50021121	0.0014	-12.08	-10.2946	-13.8978	-10.5041	-13.6969	--	-10.2593	-13.9503	--
50021122	0.8	-8.32	-10.2638	-6.3414	--	--	-10.4410	-10.2313	-6.3573	--
50021123	0.0012	-12.17	-10.2946	-14.0794	-10.5041	-13.8792	--	--	--	-10.2593
50021124	0.0026	-11.71	-10.2945	-13.1512	-10.5040	-12.9473	--	-10.2592	-13.2003	--
50024096	0.13	-9.39	-10.2896	-8.4741	-10.4939	-8.2576	--	-10.2548	-8.5017	--
50027141	0.1	-9.55	-10.2908	-8.7958	-10.4963	-8.5792	--	-10.2558	-8.8250	--
50027353	0.1	-9.55	-10.2908	-8.7958	--	--	-10.4963	--	--	-10.2558
50036060	94	-5.49	-6.6732	-4.1959	-3.0827	-6.5582	--	-6.9612	-3.8725	--
50044868	0.000004	-15.55	-10.2946	-16.9006	--	--	-10.5042	--	--	-12.2593
50044869	0.002	-11.87	-10.2945	-13.474	-10.5040	-13.2715	--	--	--	-10.2592
50047222	70	-5.67	-7.5978	-3.6400	-4.9775	-6.5603	--	-7.8033	-3.4123	--
50073120	0.006	-11.22	-10.2944	-12.1624	--	--	-10.5037	-10.2591	-12.2071	--

50084628	0.0098	-10.92	-10.2942	-11.5571	-10.5034	-11.3474	--	-10.2590	-11.5990	--
50121928	50	-5.87	-8.3683	-3.2937	-6.5566	-5.0956	--	--	--	-8.5050
50155447	250.2	-4.91	-0.6554	-6.0716	--	--	-6.2496	-1.4807	-5.4157	--
50189452	7	-7.03	-10.0249	-5.9854	-9.9515	-4.0433	--	--	--	-10.0137
50189454	26.3	-6.25	-9.2814	-5.1641	-8.4277	-3.9841	--	--	--	-9.3365
50279944	0.01	-10.91	-10.2942	-11.5369	--	--	-10.5034	-10.2590	-11.5788	--
50281462	50	-5.87	-8.3683	-3.2937	--	--	-6.5566	-8.5050	-3.1377	--
50281463	0.35	-8.81	-10.2811	-7.3124	-10.4765	-7.1007	--	--	--	-10.2470
50281632	0.0017	-11.96	-10.2945	-13.6556	-10.5040	-13.4538	--	-10.2593	-13.7071	--
50286715	0.03	-10.26	-10.2934	-10.2259	-10.5018	-10.0119	--	-10.2583	-10.2618	--
50286724	0.52	-8.57	-10.2746	-6.8348	-10.4631	-6.6286	--	-10.2411	-6.8538	--
50292544	14.2	-6.61	-9.7475	-3.4218	-9.3831	-3.7699	--	--	--	-8.7611
50292546	126	-5.32	-5.4403	-5.1781	--	--	-3.5562	-5.8384	-4.7043	--
50292547	34.2	-6.09	-8.9770	-5.1425	--	--	-7.8040	-9.0594	-3.0394	--
50303319	0.00041	-12.81	-10.2946	-14.3710	--	--	-10.5041	-10.2593	-15.4302	--
50303321	0.0004	-12.82	-10.2946	-14.3912	-10.5041	-15.1960	--	-10.2593	-15.4504	--
50303324	0.013	-10.76	-10.2941	-11.2343	--	--	-10.5031	--	--	-10.2589
50303325	0.005	-11.32	-10.2944	-12.3642	-10.5038	-12.1574	--	-10.2591	-12.4098	--
50303329	0.025	-10.37	-10.2936	-10.4477	-10.5022	-10.2344	--	-10.2584	-10.4846	--
50303330	0.012	-10.8	-10.2941	-11.3150	-10.5032	-11.1045	--	--	--	-10.2589
50303331	0.02	-10.5	-10.2938	-10.7099	-10.5026	-10.4973	--	-10.2586	-10.7480	--
50367249	0.0005	-12.69	-10.2946	-15.1288	-10.5041	-14.9326	--	-10.2593	-15.1869	--
50367254	0.0014	-12.08	-10.2946	-13.8978	--	--	-10.5041	-10.2593	-13.9503	--
50369460	0.00016	-13.36	-10.2946	-14.4810	-10.5042	-16.2900	--	--	--	-11.2593
50411605	0.49	-8.61	-10.2757	-6.9143	--	--	-10.4655	-10.2421	-6.9337	--

50411722	0.016	-10.63	-10.2940	-10.9721	-10.5029	-10.7604	--	-10.2588	-11.0114	--
50411723	0.21	-9.11	-10.2865	-7.9122	-10.4876	-7.6969	--	-10.2520	-7.9371	--
50411724	0.84	-8.29	-10.2622	-6.2825	-10.4379	-6.0880	--	-10.2299	-6.2980	--
50411725	2.7	-7.6	-10.1906	-4.9643	--	--	-10.2910	-10.1646	-4.9681	--
50411727	13	-6.67	-9.7938	-5.4958	-9.4778	-3.7963	--	--	--	-9.8032
50411728	0.62	-8.47	-10.2707	-6.6370	-10.4552	-6.4343	--	-10.2376	-6.6547	--
50411729	0.2	-9.14	-10.2869	-7.9724	-10.4884	-7.7569	--	-10.2523	-7.9975	--
50411730	0.0093	-10.96	-10.2942	-11.6378	-10.5034	-11.4284	--	--	--	-10.2590
50411731	0.0086	-11	-10.2943	-11.7185	-10.5035	-11.5094	--	--	--	-10.2590
50411732	3.4	-7.46	-10.1636	-5.7098	-10.2357	-4.6190	--	--	--	-10.1400
50411733	0.2	-9.14	-10.2869	-7.9724	--	--	-10.4884	-10.2523	-7.9975	--
50411734	0.021	-10.47	-10.2938	-10.6494	-10.5025	-10.4367	--	-10.2586	-10.6872	--
50411735	0.093	-9.59	-10.2910	-8.8763	-10.4968	-8.6597	--	--	--	-10.2561
50411736	0.0032	-11.59	-10.2945	-12.9090	-10.5039	-12.7043	--	-10.2592	-12.9570	--
50411737	0.7	-8.4	-10.2676	-6.4989	-10.4489	-6.2992	--	-10.2348	-6.5158	--

Table S4: ΔG_{bind} values of natural compounds calculated from docking and correlation studies

REN							**ACE**						
		ΔG_{bind} (kcal/mol)							**ΔG_{bind} (kcal/mol)**				
			Correlation Analysis							**Correlation Analysis**			
Inhibitor	**Ki (µM)**	**Docking**	**Model 1**	**Model 2**	**Model 3**	**Average**	**Inhibitor**	**Ki (µM)**	**Docking**	**Model A**	**Model B**	**Model C**	**Average**
Nat-20	1.46E-02	-10.69	-9.3590	-9.0143	-9.1380	-9.1704	**Nat-34**	7.10E-04	-12.48	-10.2946	-10.5041	-10.2593	-10.3527
Nat-38	1.94E-02	-10.52	-9.3590	-9.0143	-9.1380	-9.1704	**Nat-7**	7.72E-04	-12.43	-10.2946	-10.5041	-10.2593	-10.3527

Nat-39	4.15E-02	-10.07	-9.3590	-9.0141	-9.1379	-9.1703	**Nat-6**	1.20E-03	-12.17	-10.2946	-10.5041	-10.2593	-10.3527
Nat-59	3.06E-02	-10.25	-9.3589	-9.0142	-9.1379	-9.1703	**Nat-31**	6.82E-03	-11.14	-10.2943	-10.5036	-10.2591	-10.3523
NLC-1	6.33E-02	-9.82	-9.3588	-9.0140	-9.1378	-9.1702	**Nat-59**	7.54E-03	-11.08	-10.2943	-10.5036	-10.2591	-10.3523
Nat-165	6.43E-02	-9.81	-9.3588	-9.0140	-9.1378	-9.1702	**NLC-1**	1.38E-02	-10.72	-10.2941	-10.5031	-10.2588	-10.352
Nat-7	7.36E-02	-9.73	-9.3587	-9.0140	-9.1377	-9.1702	**Nat-61**	2.11E-02	-10.47	-10.2938	-10.5025	-10.2586	-10.3516
Nat-19	8.43E-02	-9.65	-9.3587	-9.0139	-9.1377	-9.1701	**Nat-69**	2.26E-02	-10.43	-10.2937	-10.5024	-10.2585	-10.3515
Nat-132	8.72E-02	-9.63	-9.3587	-9.0139	-9.1377	-9.1701	**Nat-72**	2.34E-02	-10.41	-10.2937	-10.5023	-10.2585	-10.3515
Nat-14	1.63E-01	-9.26	-9.3584	-9.0135	-9.1373	-9.1697	**Nat-10**	2.46E-02	-10.38	-10.2937	-10.5022	-10.2585	-10.3515
Nat-12	1.77E-01	-9.21	-9.3583	-9.0135	-9.1372	-9.1697	**Nat-47**	2.81E-02	-10.3	-10.2935	-10.5019	-10.2583	-10.3512
Nat-77	2.21E-01	-9.08	-9.3581	-9.0133	-9.1370	-9.1695	**Nat-165**	2.86E-02	-10.29	-10.2935	-10.5019	-10.2583	-10.3512
Nat-15	2.28E-01	-9.06	-9.3581	-9.0132	-9.1370	-9.1694	**Nat-38**	2.96E-02	-10.27	-10.2935	-10.5018	-10.2583	-10.3512
Nat-99	2.28E-01	-9.06	-9.3581	-9.0132	-9.1370	-9.1694	**Nat-39**	3.45E-02	-10.18	-10.2933	-10.5014	-10.2581	-10.3509
Nat-141	2.32E-01	-9.05	-9.3581	-9.0132	-9.1370	-9.1694	**Nat-40**	3.50E-02	-10.17	-10.2933	-10.5014	-10.2581	-10.3509
Nat-23	2.53E-01	-9	-9.3580	-9.0131	-9.1370	-9.1693	**Nat-67**	3.69E-02	-10.14	-10.2932	-10.5013	-10.2580	-10.3508
Nat-24	2.66E-01	-8.97	-9.3579	-9.0130	-9.1368	-9.1693	**Nat-19**	4.08E-02	-10.08	-10.2930	-10.5009	-10.2579	-10.3506
Nat-81	2.89E-01	-8.92	-9.3578	-9.0129	-9.1367	-9.1692	**Nat-24**	4.08E-02	-10.08	-10.2930	-10.5009	-10.2579	-10.3506
Nat-22	2.89E-01	-8.92	-9.3578	-9.0129	-9.1367	-9.1692	**Nat-68**	5.25E-02	-9.93	-10.2926	-10.5000	-10.2575	-10.35
Nat-163	2.99E-01	-8.9	-9.3578	-9.0129	-9.1367	-9.1691	**Nat-99**	5.25E-02	-9.93	-10.2926	-10.5000	-10.2575	-10.35
Nat-82	3.25E-01	-8.85	-9.3577	-9.0128	-9.1365	-9.1690	**Nat-15**	5.43E-02	-9.91	-10.2925	-10.4999	-10.2574	-10.3499