Supporting Information

Highly oxygenated Steroids with Immunosuppressive activity from *Solanum undatum*

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Table S1. ^{13}C NMR Data of 4, 1-dehydronuatigenone, 5 and cilistol a in $CDCl_3$

no.	4	1-dehydronuatigenone	5	cilistol a
	δ_C		δ_C	
1	156.1	156.2	204.5	204.5
2	127.9	127.9	127.8	127.9
3	186.7	186.8	145.3	145.3
4	124.3	124.3	33.4	33.5
5	169.4	169.5	135.6	135.7
6	33.1	33.2	124.8	124.8
7	34.0	34.1	30.7	30.8
8	35.5	35.5	33.4	33.5
9	52.7	52.8	42.5	42.8
10	42.3	44.0	50.3	50.5
11	23.0	23.1	36.6	36.8
12	39.7	39.8	32.2	32.3
13	41.2	41.3	47.8	47.9
14	55.4	55.5	50.3	50.7
15	32.2	32.3	23.7	24.0
16	81.2	81.3	23.3	23.6
17	62.1	62.2	85.4	85.5
18	16.5	16.6	14.8	15.1
19	19.1	19.1	18.8	19.2
20	38.2	38.3	42.8	43.0
21	15.0	15.1	9.4	9.4
22	120.6	120.6	65.5	65.6
23	34.3	34.4	32.6	32.6
24	30.7	30.8	65.4	65.5
25	86.4	86.4	63.5	63.6
26	69.0	69.1	91.6	91.9
27	24.2	24.3	16.4	15.5
28			18.8	19.0

Table S2. ^{13}C NMR Data of 6, cilistol d, 7 and cilistepoxide

no.	6[a]	cilistol d[b]	7[a]	cilistepoxide[a]
	δ_C		δ_C	
1	204.4	203.9	203.4	203.0
2	127.9	127.9	129.3	129.7
3	145.2	145.8	144.2	142.4
4	33.5	33.9	32.9	34.3
5	135.7	136.3	63.5	64.9
6	124.8	124.9	61.9	58.9
7	30.7	31.2	30.0	29.1
8	33.4	33.7	31.1	31.3
9	42.5	43.3	42.7	38.0
10	50.4	51.0	48.3	48.5
11	36.8	37.8	36.7	36.9
12	32.2	32.8	32.1	32.3
13	47.8	48.2	47.8	48.0
14	50.1	50.7	49.9	50.8
15	23.7	24.1	23.5	23.9
16	23.4	24.0	23.2	22.7
17	85.5	84.9	85.3	85.4
18	14.8	15.1	14.7	15.1
19	18.5	18.6	18.8	19.1
20	42.7	44.1	44.2	43.1
21	10.0	10.2	9.5	9.7
22	67.3	67.7	65.5	65.8
23	33.3	33.6	32.7	32.9
24	60.9	61.3	65.3	65.6
25	61.5	61.3	63.2	63.7
26	99.3	99.8	91.6	91.9
27	17.0	17.3	14.8	15.7
28	18.9	19.0	16.4	16.7
26-OMe	55.8	55.4		

[a]Measured in $CDCl_3$. [b]Measured in Pyridine-d_5.

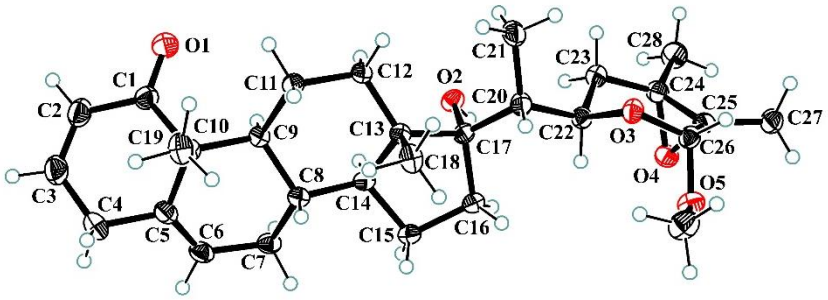


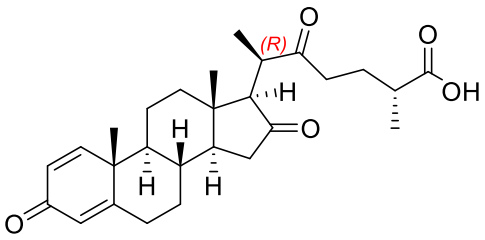
Figure S1. X-ray ORTEP drawing of **6**.

Figure S2. Comparison of the experimental and calculated NMR data for **1**

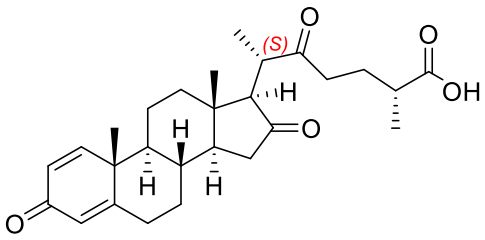
Functional		Solvent?		Basis Set		Type of Data	
mPW1PW91		PCM		6-31+G(d,p)		Unscaled Shifts	
		DP4+	0.00%	100.00%	-	-	-
Nuclei	sp2?	Experimental	Isomer-1-1	Isomer-1-2			
C	x	155.00	158.1895165	158.1009367			
C	x	127.80	126.8036182	126.8100775			
C	x	186.20	182.699865	182.8891986			
C	x	124.20	123.0690721	122.9894084			
C	x	168.00	172.7667428	172.8707636			
C		32.40	36.63686595	36.85940072			
C		33.40	37.68987803	37.46539303			
C		34.40	36.90013131	36.86460902			
C		51.60	55.13905767	55.2798087			
C		43.30	49.09504597	48.97804661			
C		22.20	25.8502012	25.89591864			
C		38.20	40.70980964	40.47072898			
C		41.90	46.69130277	46.29277843			
C		50.10	50.76783376	52.25007934			
C		37.10	42.58657367	40.98330859			
C	x	217.30	221.3363249	222.0173491			
C		66.10	67.57661005	70.9773715			
C		13.10	15.60151646	14.43498969			
C		18.70	20.27537449	20.3248236			
C		43.20	47.6420415	47.46928289			
C		15.30	17.97943636	18.03523247			
C	x	212.70	216.4766113	217.0588864			
C		39.80	42.5586939	42.84633014			
C		27.00	30.07206723	29.26813448			
C		38.30	40.40358528	40.05890808			
C	x	180.00	177.2445156	177.4014608			
C		17.30	19.8878328	20.9008816			
H	x	7.04	7.641577598	7.636112953			
H	x	6.27	6.513949669	6.503849281			
H	x	6.10	6.340213047	6.370246947			
H		2.40	2.281192378	2.266790191			
H		2.48	2.648750584	2.653651259			
H		1.16	1.14987074	1.168529022			
H		1.89	1.856603834	1.826107252			
H		1.80	1.946584597	2.012202827			
H		1.28	1.188874027	1.20956043			
H		1.78	1.625379813	1.651305081			
H		1.83	1.824481227	1.931750402			
H		1.55	1.191813822	1.516743292			
H		2.06	1.457866282	1.997079759			
H		1.61	1.415707966	1.526535821			
H		1.77	2.029873306	1.930767478			
H		2.22	2.265981589	2.12776418			
H		2.61	2.292986634	2.714270325			
H		0.85	0.865593063	0.910829288			
H		1.26	1.266997045	1.398481974			
H		2.61	2.859369588	2.643834566			
H		1.04	1.361790771	0.938088432			
H		2.68	2.669275972	2.792442627			
H		2.77	2.761275817	3.056887792			
H		1.88	1.648225461	1.657486736			
H		1.90	1.741283906	1.74186541			
H		2.54	2.698644372	2.833050163			
H		1.23	1.183535159	1.227955324			

Figure S3. DP4+ probabilities for each candidate isomer of **1**

Functional	Solvent?		Basis Set		Type of Data	
mPW1PW91	PCM		6-31+G(d,p)		Unscaled Shifts	
	Isomer-1-1	Isomer-1-2				
sDP4+ (H data)	0.01%	99.99%	-	-	-	-
sDP4+ (C data)	44.77%	55.23%	-	-	-	-
sDP4+ (all data)	0.01%	99.99%	-	-	-	-
uDP4+ (H data)	0.13%	99.87%	-	-	-	-
uDP4+ (C data)	46.09%	53.91%	-	-	-	-
uDP4+ (all data)	0.11%	99.89%	-	-	-	-
DP4+ (H data)	0.00%	100.00%	-	-	-	-
DP4+ (C data)	40.94%	59.06%	-	-	-	-
DP4+ (all data)	0.00%	100.00%	-	-	-	-



Isomer-1-1



Isomer-1-2

Table S3. B3LYP/6-31G (d) optimized conformers of **Isomer-1-1**

Conf.	*G* (kcal/mol)	Δ*G* (kcal/mol)	Boltzmann factor	Equilibrium mole fraction	Imaginary frequency
Conf-1	-895035.9083	0.0000	1.0000	0.3167	0
Conf-2	-895035.8957	0.0126	0.9790	0.3101	0
Conf-3	-895035.0888	0.8195	0.2504	0.0793	0
Conf-4	-895035.0486	0.8597	0.2340	0.0741	0
Conf-5	-895034.8359	1.0724	0.1633	0.0517	0
Conf-6	-895034.7612	1.1471	0.0829	0.0456	0
Conf-7	-895034.7474	1.1609	0.1440	0.0445	0
Conf-8	-895034.4644	1.4439	0.1406	0.0276	0
Conf-9	-895034.1770	1.7313	0.0872	0.0170	0
Conf-10	-895033.9542	1.9541	0.0536	0.0117	0
Conf-11	-895033.7666	2.1417	0.0368	0.0085	0
Conf-12	-895033.3512	2.5571	0.0268	0.0042	0
Conf-13	-895033.3418	2.5665	0.0133	0.0041	0
Conf-14	-895033.2213	2.6870	0.0107	0.0034	0
Conf-15	-895032.3798	3.5285	0.0026	0.0008	0
Conf-16	-895032.2424	3.6659	0.0020	0.0006	0

Table S4. B3LYP/6-31G (d) optimized conformers of **Isomer-1-2**

Conf.	*G* (kcal/mol)	Δ*G* (kcal/mol)	Boltzmann factor	Equilibrium mole fraction	Imaginary frequency
Conf-1	-895037.6208	0.0000	1.0000	0.5543	0
Conf-2	-895037.0591	0.5616	0.3871	0.2146	0
Conf-3	-895036.7755	0.8452	0.2397	0.1329	0
Conf-4	-895036.2798	1.3410	0.1037	0.0575	0
Conf-5	-895035.6554	1.9654	0.0361	0.0200	0
Conf-6	-895035.0066	2.6142	0.0121	0.0067	0
Conf-7	-895034.8798	2.7410	0.0097	0.0054	0
Conf-8	-895034.6533	2.9675	0.0066	0.0037	0
Conf-9	-895034.5918	3.0290	0.0060	0.0033	0
Conf-10	-895033.6373	3.9834	0.0012	0.0007	0
Conf-11	-895033.2006	4.4202	0.0006	0.0003	0
Conf-12	-895033.0851	4.5356	0.0005	0.0003	0
Conf-13	-895032.5699	5.0508	0.0002	0.0001	0
Conf-14	-895032.5097	5.1111	0.0002	0.0001	0
Conf-15	-895032.5078	5.1129	0.0002	0.0001	0
Conf-16	-895031.9826	5.6832	0.0001	0.0000	0

Table S5. Cartesian coordinates of all conformers for **Isomer-1-1**

Conf-1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	5.237946	-2.814983	-0.440691	35	1	1.301333	1.371019	-1.341003
2	6	6.299112	-1.94639	-0.977566	36	1	-1.025528	1.375401	-1.565779
3	6	6.192141	-0.521298	-0.643249	37	1	5.312491	-3.874531	-0.671992
4	6	5.199462	-0.011772	0.111036	38	1	6.966762	0.123208	-1.053398
5	6	4.087446	-0.872963	0.682854	39	1	3.494339	-3.002073	0.712325
6	6	4.240737	-2.322625	0.307396	40	1	5.929606	1.989695	-0.104056
7	6	5.085468	1.466667	0.356429	41	1	5.124885	1.678355	1.433648
8	6	3.751924	1.98783	-0.2057	42	1	3.646971	3.054399	0.023221
9	6	2.561065	1.2045	0.356501	43	1	3.762786	1.892898	-1.300459
10	6	2.722818	-0.317612	0.108867	44	1	0.143906	-0.735294	-1.083731
11	6	1.244978	1.65393	-0.277876	45	1	-0.662873	-1.156026	0.416366
12	6	-0.009839	0.927426	0.283118	46	1	1.432212	-1.092369	1.677279
13	6	0.163831	-0.570604	0.000741	47	1	1.580547	-2.156673	0.293866
14	6	1.485665	-1.105517	0.582788	48	1	1.099704	3.603772	0.733288
15	6	0.870408	3.136713	-0.233425	49	1	1.344026	3.752088	-1.004641
16	6	-0.649782	3.129442	-0.420144	50	1	5.120082	-1.110101	2.59144
17	6	-1.131701	1.669421	-0.508743	51	1	3.922787	0.195604	2.609793
18	8	7.220614	-2.392198	-1.667817	52	1	3.394173	-1.491172	2.670753
19	6	4.130166	-0.809601	2.235222	53	1	-0.379342	2.223699	2.030274
20	6	-0.207036	1.167978	1.794206	54	1	-1.075691	0.609376	2.158328
21	6	-2.598103	1.4422	-0.113076	55	1	0.653399	0.840177	2.381415
22	6	-2.986903	-0.027138	-0.251866	56	1	-2.754748	1.761311	0.923513
23	6	-3.591197	2.211286	-1.01666	57	1	-4.623569	1.947585	-0.763695
24	6	-3.762455	-0.645182	0.89817	58	1	-3.451005	3.285349	-0.90223
25	8	-2.718507	-0.654862	-1.264165	59	1	-3.422788	1.938582	-2.063793
26	8	-1.33895	4.12978	-0.449397	60	1	-3.042001	-0.780003	1.719725
27	6	-4.426854	-1.978406	0.557782	61	1	-4.48332	0.093297	1.270914
28	6	-5.583118	-1.869053	-0.463146	62	1	-3.674284	-2.652715	0.136251
29	6	-6.130547	-3.255443	-0.818882	63	1	-4.810098	-2.441424	1.474367
30	6	-6.683122	-1.009808	0.12852	64	1	-5.205307	-1.37374	-1.361385
31	8	-7.498805	-1.381249	0.948404	65	1	-6.9258	-3.189204	-1.568693
32	8	-6.644871	0.264472	-0.328958	66	1	-5.329868	-3.881784	-1.224774
33	1	2.515353	1.393084	1.437615	67	1	-6.542403	-3.743981	0.069346
34	1	2.793508	-0.447678	-0.981827	68	1	-7.361167	0.758344	0.127538

Conf-2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	4.46474	-2.615995	-1.117537	35	1	1.050529	2.107751	-1.031186
2	6	5.660777	-1.761747	-1.208269	36	1	-1.183981	2.481022	-1.501709
3	6	5.618137	-0.514306	-0.436496	37	1	4.488962	-3.548621	-1.675534
4	6	4.565684	-0.149313	0.320656	38	1	6.494935	0.12489	-0.516356
5	6	3.314423	-1.000587	0.439487	39	1	2.555521	-2.937411	-0.306267

6	6	3.407249	-2.264555	-0.372482	40	1	5.477492	1.710088	0.865101
7	6	4.53397	1.178428	1.024339	41	1	4.425497	1.033027	2.107804
8	6	3.346995	2.0124	0.512567	42	1	3.294355	2.957003	1.065855
9	6	2.026754	1.245979	0.642737	43	1	3.515729	2.266441	-0.543183
10	6	2.101547	-0.126341	-0.075962	44	1	-0.297736	0.183241	-1.631766
11	6	0.858489	2.034274	0.050914	45	1	-1.337141	-0.605095	-0.446741
12	6	-0.516743	1.322665	0.18766	46	1	0.525199	-1.202612	0.974113
13	6	-0.424819	-0.013896	-0.559482	47	1	0.803365	-1.76905	-0.657521
14	6	0.749434	-0.864976	-0.043584	48	1	0.724655	3.552594	1.640507
15	6	0.594205	3.45571	0.554924	49	1	1.213434	4.229035	0.089483
16	6	-0.883523	3.688361	0.221534	50	1	4.017592	-1.961014	2.269707
17	6	-1.445448	2.413411	-0.432471	51	1	2.946459	-0.583912	2.577847
18	8	6.63835	-2.076965	-1.893741	52	1	2.273501	-2.119041	2.013638
19	6	3.12321	-1.437306	1.918901	53	1	-1.060748	2.02558	2.208014
20	6	-0.909242	1.088001	1.662034	54	1	-1.840493	0.518251	1.724734
21	6	-2.97356	2.23841	-0.354864	55	1	-0.152751	0.515435	2.202633
22	6	-3.367059	0.938087	-1.060852	56	1	-3.281683	2.190263	0.695716
23	6	-3.737242	3.384542	-1.048883	57	1	-3.516554	4.335911	-0.566686
24	6	-4.099508	-0.104907	-0.242795	58	1	-3.4468	3.439005	-2.10278
25	8	-3.108632	0.773092	-2.242202	59	1	-4.817821	3.204993	-1.005941
26	8	-1.490916	4.707748	0.48303	60	1	-3.550124	-0.231859	0.696703
27	6	-4.269079	-1.442931	-0.95909	61	1	-5.071509	0.3239	0.047441
28	6	-4.701492	-2.578539	-0.027593	62	1	-5.0052	-1.34078	-1.763501
29	6	-5.007178	-3.870688	-0.812104	63	1	-3.323463	-1.714903	-1.438632
30	6	-3.628614	-2.876038	1.007322	64	1	-5.606601	-2.292281	0.524373
31	8	-2.462714	-2.532376	0.947388	65	1	-5.32392	-4.675751	-0.143539
32	8	-4.1113	-3.617153	2.0269	66	1	-5.806952	-3.684877	-1.535794
33	1	1.837797	1.084611	1.712444	67	1	-4.12117	-4.204855	-1.363622
34	1	2.329077	0.090073	-1.131039	68	1	-3.360376	-3.804706	2.631004

Conf-3

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	4.930646	-2.830059	-0.881214	35	1	1.43437	1.812903	-1.121096
2	6	6.106582	-1.96115	-1.057788	36	1	-0.826267	2.098444	-1.603574
3	6	6.050124	-0.659931	-0.381368	37	1	4.966483	-3.802386	-1.365966
4	6	5.001687	-0.258724	0.362772	38	1	6.912467	-0.011986	-0.523368
5	6	3.76952	-1.122222	0.565543	39	1	3.04201	-3.127032	-0.015383
6	6	3.877439	-2.443508	-0.147849	40	1	5.883229	1.653474	0.752208
7	6	4.952421	1.117875	0.964003	41	1	4.859491	1.053988	2.0567
8	6	3.743831	1.887939	0.404887	42	1	3.678507	2.870882	0.885046
9	6	2.439564	1.110106	0.608762	43	1	3.896342	2.063486	-0.669119
10	6	2.533861	-0.3134	0.000461	44	1	0.119126	-0.176976	-1.54715
11	6	1.252577	1.826836	-0.034774	45	1	-0.907933	-0.872564	-0.304938
12	6	-0.109855	1.10777	0.172381	46	1	0.995602	-1.31961	1.161314
13	6	0.003036	-0.284776	-0.461521	47	1	1.261585	-2.023486	-0.420697
14	6	1.196134	-1.070527	0.113143	48	1	1.094643	3.468659	1.423362
15	6	0.968119	3.280877	0.349169	49	1	1.577973	4.021328	-0.177656
16	6	-0.511414	3.464407	-0.004742	50	1	4.517338	-1.919732	2.454897

17	6	-1.063641	2.125331	-0.527235	51	1	3.417053	-0.548085	2.669956
18	8	7.078471	-2.307557	-1.735837	52	1	2.775253	-2.138348	2.236855
19	6	3.606437	-1.445917	2.076893	53	1	-1.430837	0.434595	1.77249
20	6	-0.492949	0.988352	1.662255	54	1	-0.637624	1.965182	2.136149
21	6	-2.583071	1.932211	-0.392582	55	1	0.263031	0.455022	2.242492
22	6	-2.994151	0.58147	-0.981302	56	1	-2.86671	1.969315	0.665132
23	6	-3.393746	3.001624	-1.15688	57	1	-3.126739	2.98218	-2.218409
24	6	-3.851429	-0.315712	-0.112882	58	1	-4.468044	2.799401	-1.0744
25	8	-2.672863	0.273878	-2.117901	59	1	-3.187498	3.992698	-0.755075
26	8	-1.126689	4.500905	0.147637	60	1	-3.291713	-0.505606	0.813234
27	6	-4.25647	-1.619284	-0.796441	61	1	-4.727778	0.265471	0.209614
28	6	-5.15449	-2.538455	0.0684	62	1	-4.768597	-1.390541	-1.736313
29	6	-4.483063	-2.985284	1.369234	63	1	-3.354196	-2.179498	-1.066805
30	6	-6.464197	-1.825494	0.349062	64	1	-5.390276	-3.416547	-0.543892
31	8	-6.736089	-1.217682	1.366229	65	1	-5.090472	-3.735835	1.884775
32	8	-7.306371	-1.893475	-0.705044	66	1	-3.503427	-3.42613	1.155952
33	1	2.261597	1.031068	1.689684	67	1	-4.348575	-2.145184	2.05538
34	1	2.74227	-0.178534	-1.071859	68	1	-8.104362	-1.370691	-0.472529

Conf-4

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	-4.3912	2.703359	0.427333	35	1	-0.472068	-1.129967	-1.484782
2	6	-5.360388	2.226283	-0.573336	36	1	1.843094	-1.271618	-1.339047
3	6	-5.354258	0.782242	-0.834885	37	1	-4.394649	3.769656	0.638785
4	6	-4.527544	-0.078311	-0.210198	38	1	-6.059641	0.431502	-1.585293
5	6	-3.513534	0.373435	0.825214	39	1	-2.879185	2.247511	1.80998
6	6	-3.558697	1.860397	1.054314	40	1	-5.261371	-1.75021	-1.32902
7	6	-4.498914	-1.53639	-0.57326	41	1	-4.734568	-2.152737	0.30493
8	6	-3.100835	-1.917642	-1.089172	42	1	-3.066689	-2.992218	-1.301837
9	6	-2.00831	-1.54034	-0.083347	43	1	-2.91475	-1.3954	-2.038061
10	6	-2.082994	-0.037111	0.29051	44	1	0.683946	0.578718	-0.199385
11	6	-0.612793	-1.822186	-0.639173	45	1	1.202998	0.25719	1.449117
12	6	0.537264	-1.509319	0.358615	46	1	-1.079126	-0.076595	2.217538
13	6	0.459536	-0.014909	0.694751	47	1	-0.942228	1.456961	1.38031
14	6	-0.931732	0.373198	1.229323	48	1	-0.698565	-4.018788	-0.518548
15	6	-0.290139	-3.225327	-1.157655	49	1	-0.633825	-3.42817	-2.176817
16	6	1.237973	-3.289218	-1.090292	50	1	-4.863886	-0.069226	2.482422
17	6	1.763272	-1.96956	-0.488133	51	1	-3.722313	-1.382676	2.149565
18	8	-6.129106	2.996616	-1.156856	52	1	-3.170503	0.081949	2.972661
19	6	-3.834201	-0.296642	2.190432	53	1	0.526567	-3.430882	1.440347
20	6	0.462247	-2.356436	1.645691	54	1	1.292477	-2.098662	2.309021
21	6	3.153813	-2.096206	0.172667	55	1	-0.466885	-2.187223	2.194716
22	6	3.503197	-0.838597	0.967733	56	1	3.123275	-2.913343	0.900726
23	6	4.250971	-2.395462	-0.868438	57	1	4.06637	-3.366235	-1.327867
24	6	3.860485	0.411046	0.180905	58	1	4.264391	-1.639017	-1.660845
25	8	3.514182	-0.848799	2.189611	59	1	5.239764	-2.411382	-0.396394
26	8	1.902955	-4.249351	-1.423392	60	1	4.863979	0.243312	-0.234383
27	6	3.831729	1.685739	1.023514	61	1	3.193354	0.500755	-0.682118

28	6	4.154035	2.970523	0.246759	62	1	2.844622	1.788325	1.484438
29	6	5.52479	2.939237	-0.456578	63	1	4.548277	1.58794	1.845448
30	6	3.050725	3.332717	-0.734568	64	1	4.178612	3.79962	0.968609
31	8	2.042099	2.689317	-0.956255	65	1	5.773383	3.918544	-0.871728
32	8	3.305031	4.502923	-1.358752	66	1	6.302117	2.658408	0.261752
33	1	-2.157749	-2.14655	0.820192	67	1	5.541351	2.211883	-1.274859
34	1	-1.953401	0.52221	-0.648584	68	1	2.554536	4.673637	-1.968184

Conf-5

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	4.326617	-2.89521	-0.609661	35	1	1.002702	1.830102	-1.309894
2	6	5.514124	-2.133938	-1.033047	36	1	-1.290436	2.155035	-1.616368
3	6	5.574339	-0.737561	-0.585153	37	1	4.276429	-3.934342	-0.924878
4	6	4.619595	-0.162063	0.170557	38	1	6.443713	-0.170404	-0.910983
5	6	3.380221	-0.911579	0.626141	39	1	2.519794	-2.940703	0.457223
6	6	3.365431	-2.335708	0.138362	40	1	5.608778	1.73704	0.149731
7	6	4.683073	1.295444	0.532061	41	1	4.695323	1.417384	1.623712
8	6	3.456396	2.028017	-0.037645	42	1	3.477222	3.078804	0.272863
9	6	2.149533	1.367268	0.413072	43	1	3.508741	2.015226	-1.135224
10	6	2.127577	-0.139812	0.047506	44	1	-0.423934	-0.120678	-1.272439
11	6	0.93324	2.033783	-0.229615	45	1	-1.344373	-0.545442	0.158337
12	6	-0.427927	1.435346	0.223363	46	1	0.673202	-0.861103	1.494738
13	6	-0.432657	-0.044552	-0.177924	47	1	0.751336	-1.821949	0.032296
14	6	0.778671	-0.793836	0.406026	48	1	0.99087	3.900948	0.935468
15	6	0.747574	3.544607	-0.073989	49	1	1.328964	4.15194	-0.774628
16	6	-0.751538	3.749558	-0.312543	50	1	4.277905	-1.430918	2.546802
17	6	-1.409599	2.375448	-0.542826	51	1	3.261604	0.017777	2.627524
18	8	6.402568	-2.641056	-1.724243	52	1	2.515349	-1.582896	2.527763
19	6	3.354235	-0.974176	2.178936	53	1	0.123508	1.098313	2.329078
20	6	-0.661104	1.57957	1.741533	54	1	-0.710279	2.626651	2.059287
21	6	-2.913136	2.30915	-0.225693	55	1	-1.608746	1.111466	2.027671
22	6	-3.461788	0.905693	-0.487389	56	1	-3.078479	2.57375	0.824727
23	6	-3.746712	3.264119	-1.109803	57	1	-4.815011	3.16081	-0.886953
24	6	-4.312109	0.285751	0.605973	58	1	-3.447125	4.296863	-0.936822
25	8	-3.272982	0.354779	-1.560608	59	1	-3.596453	3.017917	-2.16586
26	8	-1.306851	4.829638	-0.278856	60	1	-3.73113	0.295088	1.537966
27	6	-4.86466	-1.102133	0.284196	61	1	-5.138577	0.987608	0.794814
28	6	-3.798282	-2.205066	0.207034	62	1	-5.60805	-1.378907	1.039796
29	6	-3.079816	-2.458263	1.547431	63	1	-5.39371	-1.057831	-0.672695
30	6	-4.425484	-3.502491	-0.269293	64	1	-3.049063	-1.929831	-0.543015
31	8	-5.615336	-3.740107	-0.327516	65	1	-2.557463	-1.559202	1.887796
32	8	-3.486157	-4.410586	-0.618902	66	1	-3.797633	-2.744964	2.324648
33	1	2.077562	1.476757	1.50358	67	1	-2.340289	-3.25711	1.447874
34	1	2.234265	-0.193964	-1.046646	68	1	-3.961324	-5.224789	-0.891942

Conf-6

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z

1	6	-4.467615	2.359889	0.239053	35	1	-0.255382	-1.266189	-1.460982
2	6	-5.407889	1.708879	-0.689388	36	1	2.071389	-1.168105	-1.373039
3	6	-5.275184	0.253337	-0.821796	37	1	-4.568456	3.435684	0.358739
4	6	-4.359719	-0.469254	-0.148034	38	1	-5.960863	-0.225825	-1.517387
5	6	-3.368322	0.164545	0.811088	39	1	-2.895223	2.167609	1.616721
6	6	-3.548118	1.655534	0.913476	40	1	-4.958416	-2.295885	-1.091705
7	6	-4.202845	-1.945751	-0.381328	41	1	-4.36081	-2.498357	0.554719
8	6	-2.787193	-2.244773	-0.904377	42	1	-2.657354	-3.326987	-1.017907
9	6	-1.710462	-1.676064	0.025936	43	1	-2.673236	-1.80025	-1.902913
10	6	-1.921186	-0.157343	0.262297	44	1	0.735564	0.64202	-0.410087
11	6	-0.308291	-1.880615	-0.547863	45	1	1.351826	0.572374	1.242211
12	6	0.829337	-1.363299	0.376769	46	1	-0.859579	0.092956	2.144764
13	6	0.613067	0.143283	0.559887	47	1	-0.899639	1.539681	1.160368
14	6	-0.789437	0.451673	1.1122	48	1	-0.172552	-4.052644	-0.212216
15	6	0.137891	-3.291268	-0.939442	49	1	-0.210972	-3.626348	-1.92113
16	6	1.666333	-3.200223	-0.9213	50	1	-4.623633	-0.246586	2.548557
17	6	2.075054	-1.786134	-0.458859	51	1	-3.379199	-1.479793	2.287166
18	8	-6.25415	2.351919	-1.317435	52	1	-2.937324	0.094341	2.961302
19	6	-3.586703	-0.408315	2.239123	53	1	1.679646	-1.682122	2.353098
20	6	0.863836	-2.078677	1.742759	54	1	1.026365	-3.157255	1.639505
21	6	3.486722	-1.727296	0.16738	55	1	-0.065245	-1.944312	2.301254
22	6	3.728373	-0.399423	0.883619	56	1	3.560982	-2.500514	0.938926
23	6	4.580417	-1.972241	-0.891486	57	1	4.49568	-1.26288	-1.722147
24	6	3.885751	0.844011	0.024531	58	1	5.578318	-1.86496	-0.451797
25	8	3.801397	-0.344171	2.101726	59	1	4.481616	-2.980856	-1.292935
26	8	2.416564	-4.11611	-1.190558	60	1	4.861747	0.775021	-0.474083
27	6	3.777431	2.149768	0.818063	61	1	3.151759	0.808464	-0.788404
28	6	3.454484	3.385438	-0.059343	62	1	3.008821	2.050184	1.590391
29	6	4.489886	3.625649	-1.160599	63	1	4.716335	2.340195	1.348492
30	6	2.065161	3.216554	-0.645508	64	1	3.417746	4.252258	0.610213
31	8	1.809754	2.770232	-1.748117	65	1	4.285511	4.558308	-1.695851
32	8	1.098179	3.571833	0.230508	66	1	5.492098	3.693634	-0.724694
33	1	-1.779383	-2.205156	0.985715	67	1	4.482076	2.814918	-1.893754
34	1	-1.875294	0.318491	-0.72939	68	1	0.236454	3.411943	-0.211859

Conf-7

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	6.095526	0.780365	-0.916942	35	1	0.998259	0.75767	1.868186
2	6	6.636373	-0.19084	0.048977	36	1	-0.758778	2.271422	1.908632
3	6	5.702689	-1.224663	0.510337	37	1	6.781936	1.54217	-1.277801
4	6	4.425113	-1.306834	0.091784	38	1	6.097978	-1.933888	1.234519
5	6	3.828032	-0.322318	-0.897722	39	1	4.472653	1.431261	-2.078206
6	6	4.824951	0.715542	-1.339073	40	1	4.013105	-2.980075	1.362762
7	6	3.482995	-2.332212	0.65742	41	1	3.096155	-2.977042	-0.143328
8	6	2.300349	-1.631161	1.347389	42	1	1.586301	-2.380845	1.706508
9	6	1.602976	-0.646233	0.403459	43	1	2.669705	-1.089154	2.229205
10	6	2.610394	0.38293	-0.175683	44	1	1.102404	2.732853	0.507389
11	6	0.49506	0.127396	1.116513	45	1	0.254054	2.833971	-1.034159

12	6	-0.28195	1.106519	0.187036	46	1	1.568597	1.00801	-1.981201
13	6	0.728666	2.13549	-0.335862	47	1	2.636467	2.228659	-1.320073
14	6	1.915431	1.453649	-1.042561	48	1	-1.035623	-1.447901	1.256765
15	6	-0.602855	-0.639483	1.861296	49	1	-0.303134	-1.068964	2.821351
16	6	-1.679093	0.421791	2.057144	50	1	4.229011	-1.628084	-2.600262
17	6	-1.332713	1.649461	1.198387	51	1	2.580896	-1.796002	-1.972848
18	8	7.804308	-0.135929	0.445933	52	1	3.020665	-0.380369	-2.937304
19	6	3.380657	-1.080712	-2.178476	53	1	-1.699531	-0.354797	-0.664095
20	6	-0.954044	0.375384	-0.989659	54	1	-1.445029	1.093762	-1.64952
21	6	-2.54114	2.54002	0.802518	55	1	-0.224695	-0.166789	-1.595581
22	6	-3.434578	1.985322	-0.312046	56	1	-3.169874	2.541313	1.706045
23	6	-2.116212	3.976853	0.485345	57	1	-2.992718	4.619545	0.35955
24	6	-4.29322	0.775463	0.010313	58	1	-1.503362	4.383287	1.296527
25	8	-3.503202	2.531065	-1.402185	59	1	-1.542293	4.025456	-0.442729
26	8	-2.635124	0.33744	2.80482	60	1	-3.804735	0.166126	0.76954
27	6	-4.662363	-0.060489	-1.216528	61	1	-5.202384	1.16495	0.495423
28	6	-5.322502	-1.391678	-0.844577	62	1	-5.337314	0.506248	-1.865175
29	6	-5.782617	-2.168644	-2.094821	63	1	-3.762072	-0.264263	-1.805111
30	6	-4.373282	-2.273801	-0.050619	64	1	-6.199417	-1.212073	-0.209571
31	8	-3.157461	-2.201222	-0.059332	65	1	-6.264499	-3.111794	-1.821704
32	8	-5.033756	-3.208638	0.660552	66	1	-6.497635	-1.565981	-2.663522
33	1	1.160546	-1.225566	-0.416825	67	1	-4.929504	-2.389673	-2.746
34	1	3.049978	0.902538	0.689528	68	1	-4.3601	-3.760403	1.114684

Conf-8

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	5.504592	0.990918	-1.857058	35	1	0.214999	0.552514	0.510427
2	6	5.942018	1.845755	-0.740477	36	1	-1.829089	-0.00587	-0.384383
3	6	5.417233	1.490309	0.583408	37	1	5.899177	1.234384	-2.840269
4	6	4.586331	0.451607	0.794454	38	1	5.729946	2.129349	1.406498
5	6	4.106897	-0.448959	-0.330265	39	1	4.401269	-0.670619	-2.509898
6	6	4.674088	-0.0433	-1.664506	40	1	4.412472	0.887797	2.883752
7	6	4.007758	0.178794	2.154621	41	1	4.289243	-0.827325	2.49392
8	6	2.473668	0.274782	2.097913	42	1	2.051435	0.019604	3.076623
9	6	1.892987	-0.641307	1.015999	43	1	2.18708	1.313963	1.88413
10	6	2.529329	-0.346308	-0.369736	44	1	0.062023	-0.047753	-1.797757
11	6	0.38049	-0.47025	0.885175	45	1	-0.046048	-1.728343	-2.315806
12	6	-0.258589	-1.416015	-0.165986	46	1	2.17547	-2.231917	-1.39995
13	6	0.349566	-1.073566	-1.529278	47	1	2.26988	-0.84709	-2.4677
14	6	1.885699	-1.180058	-1.4989	48	1	-0.25156	-1.504768	2.720794
15	6	-0.515818	-0.625877	2.117315	49	1	-0.528635	0.234246	2.793048
16	6	-1.905382	-0.848601	1.512998	50	1	5.673764	-1.921843	0.043701
17	6	-1.755168	-1.037891	-0.003104	51	1	4.141902	-2.325673	0.836157
18	8	6.702947	2.802997	-0.91034	52	1	4.323639	-2.554726	-0.908212
19	6	4.58559	-1.904348	-0.068986	53	1	-0.460738	-3.182199	1.135689
20	6	-0.043843	-2.905552	0.161964	54	1	-0.527855	-3.53188	-0.594271
21	6	-2.801588	-1.906126	-0.758547	55	1	1.014115	-3.176052	0.174502
22	6	-3.831961	-0.961855	-1.376965	56	1	-2.280401	-2.344117	-1.61731

23	6	-3.450534	-3.035847	0.05685	57	1	-2.691659	-3.723699	0.439103
24	6	-4.917768	-0.388829	-0.47777	58	1	-4.010914	-2.65207	0.91039
25	8	-3.754696	-0.652359	-2.555951	59	1	-4.131161	-3.612796	-0.578769
26	8	-2.944995	-0.833956	2.143805	60	1	-5.770828	-1.080978	-0.539876
27	6	-5.358912	1.016066	-0.897479	61	1	-4.58995	-0.412812	0.565645
28	6	-4.256443	2.072824	-0.715215	62	1	-5.652838	1.004873	-1.951326
29	6	-4.711073	3.451021	-1.228391	63	1	-6.231049	1.313987	-0.30632
30	6	-3.889659	2.203178	0.751378	64	1	-3.36304	1.768748	-1.269987
31	8	-4.684611	2.331315	1.659444	65	1	-3.919909	4.199918	-1.116714
32	8	-2.549321	2.197071	0.956984	66	1	-4.972658	3.384973	-2.289161
33	1	2.109229	-1.679039	1.302272	67	1	-5.590845	3.793357	-0.673712
34	1	2.314177	0.711136	-0.586718	68	1	-2.412265	2.308773	1.923472

Conf-9

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	4.522564	-2.339283	-1.081573	35	1	0.76821	2.124353	-1.08691
2	6	5.652614	-1.401928	-1.197692	36	1	-1.492334	2.310503	-1.558321
3	6	5.520408	-0.142495	-0.455759	37	1	4.613414	-3.28037	-1.618007
4	6	4.446413	0.162274	0.29763	38	1	6.347366	0.557416	-0.555142
5	6	3.262004	-0.776724	0.443957	39	1	2.64568	-2.781746	-0.254235
6	6	3.444865	-2.049057	-0.339609	40	1	5.219414	2.096718	0.792718
7	6	4.318385	1.500823	0.969225	41	1	4.224013	1.374587	2.056391
8	6	3.071659	2.231928	0.442634	42	1	2.950889	3.183512	0.972606
9	6	1.812126	1.373818	0.599945	43	1	3.217524	2.470981	-0.619951
10	6	1.986119	-0.007415	-0.084271	44	1	-0.41656	0.09351	-1.638105
11	6	0.585839	2.059858	-0.002577	45	1	-1.409569	-0.738395	-0.454201
12	6	-0.732604	1.251199	0.156834	46	1	0.497226	-1.152713	1.010348
13	6	-0.537606	-0.088519	-0.562747	47	1	0.807894	-1.759543	-0.607091
14	6	0.690951	-0.841286	-0.023507	48	1	0.333415	3.592914	1.556599
15	6	0.21613	3.467327	0.472379	49	1	0.779273	4.27512	-0.005289
16	6	-1.273127	3.584318	0.129305	50	1	4.043515	-1.637913	2.291345
17	6	-1.742288	2.252672	-0.485795	51	1	2.873103	-0.33853	2.574804
18	8	6.648126	-1.661647	-1.880003	52	1	2.31591	-1.933127	2.051118
19	6	3.110843	-1.191099	1.934289	53	1	-1.368201	1.952163	2.149762
20	6	-1.099156	1.021267	1.639188	54	1	-1.949935	0.340703	1.731495
21	6	-3.254407	1.969902	-0.392712	55	1	-0.278483	0.570774	2.201459
22	6	-3.547556	0.61565	-1.043316	56	1	-3.554381	1.940781	0.660866
23	6	-4.099595	3.030015	-1.126822	57	1	-5.164561	2.777361	-1.067837
24	6	-4.174768	-0.454002	-0.172307	58	1	-3.943824	4.013339	-0.685008
25	8	-3.290962	0.426228	-2.221265	59	1	-3.818917	3.061521	-2.184278
26	8	-1.951855	4.566356	0.353901	60	1	-3.666489	-0.44108	0.798166
27	6	-4.159418	-1.854491	-0.792606	61	1	-5.201209	-0.127781	0.055264
28	6	-4.155423	-2.986102	0.260369	62	1	-5.029838	-1.990133	-1.443327
29	6	-4.27381	-4.363398	-0.405285	63	1	-3.279837	-1.960153	-1.436194
30	6	-2.906792	-2.864593	1.114538	64	1	-4.993193	-2.83438	0.949918
31	8	-2.865245	-2.387992	2.232708	65	1	-4.248869	-5.169989	0.334819
32	8	-1.794617	-3.299094	0.477684	66	1	-5.22146	-4.430623	-0.949519
33	1	1.642261	1.225772	1.674598	67	1	-3.457091	-4.525395	-1.11467

34	1	2.189477	0.196192	-1.146622	68	1	-1.04363	-3.171101	1.09593

Conf-10

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	6.13092	-1.744132	-0.937061	35	1	1.50632	1.783792	-0.966863
2	6	6.982829	-0.624909	-0.500705	36	1	-0.453944	1.726288	-2.007665
3	6	6.374308	0.311053	0.451995	37	1	6.576015	-2.453443	-1.630213
4	6	5.1169	0.17973	0.916309	38	1	6.999061	1.145058	0.76468
5	6	4.204391	-0.95495	0.485602	39	1	4.290603	-2.744833	-0.808833
6	6	4.875918	-1.886154	-0.488302	40	1	5.247098	1.983087	2.063693
7	6	4.508297	1.212003	1.823487	41	1	4.202212	0.752548	2.7731
8	6	3.27347	1.834443	1.149968	42	1	2.799026	2.546274	1.835044
9	6	2.267579	0.760701	0.721786	43	1	3.595314	2.403093	0.266417
10	6	2.934749	-0.300769	-0.193741	44	1	1.018173	-0.174349	-2.318023
11	6	1.088145	1.368973	-0.035887	45	1	-0.009251	-1.469357	-1.701357
12	6	0.016469	0.327821	-0.474726	46	1	1.5768	-1.977334	0.096572
13	6	0.695511	-0.6857	-1.400647	47	1	2.401055	-1.992058	-1.449103
14	6	1.916848	-1.333295	-0.721985	48	1	0.057662	2.293058	1.67686
15	6	0.270975	2.490994	0.61817	49	1	0.726361	3.484424	0.564121
16	6	-1.046838	2.463465	-0.160614	50	1	4.7258	-2.172895	2.220363
17	6	-1.000829	1.293201	-1.15112	51	1	3.237246	-1.241056	2.452054
18	8	8.137759	-0.483916	-0.913615	52	1	3.229109	-2.681067	1.425196
19	6	3.820068	-1.811012	1.724571	53	1	-1.267235	-1.194987	0.415674
20	6	-0.605115	-0.391575	0.741141	54	1	-1.188089	0.285638	1.374181
21	6	-2.367624	0.865209	-1.741873	55	1	0.158612	-0.841244	1.378816
22	6	-3.180134	-0.076824	-0.85109	56	1	-2.939258	1.801271	-1.809061
23	6	-2.213414	0.267459	-3.145628	57	1	-1.660877	-0.674068	-3.117661
24	6	-3.975347	0.553559	0.275813	58	1	-3.193128	0.061703	-3.58813
25	8	-3.206591	-1.278928	-1.071578	59	1	-1.681804	0.966095	-3.800149
26	8	-1.968189	3.244653	-0.026533	60	1	-3.338264	1.285456	0.783706
27	6	-4.574501	-0.43752	1.274935	61	1	-4.764546	1.164586	-0.185199
28	6	-5.729428	-1.286796	0.729375	62	1	-3.788259	-1.117636	1.622232
29	6	-6.178292	-2.347599	1.754497	63	1	-4.931547	0.119413	2.147941
30	6	-6.924323	-0.427465	0.36389	64	1	-5.40348	-1.802778	-0.178066
31	8	-7.141692	0.70128	0.761485	65	1	-6.995764	-2.958283	1.361019
32	8	-7.776867	-1.080687	-0.457141	66	1	-5.33888	-3.007627	1.99556
33	1	1.894922	0.272143	1.631327	67	1	-6.516106	-1.872642	2.682875
34	1	3.323819	0.245892	-1.066403	68	1	-8.539333	-0.482836	-0.614595

Conf-11

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	-6.269662	1.085726	0.973546	35	1	-1.290123	0.379689	-1.947574
2	6	-6.934237	0.123475	0.078477	36	1	0.539584	1.635821	-2.185368
3	6	-6.123029	-1.023533	-0.346406	37	1	-6.865275	1.931485	1.307665
4	6	-4.847738	-1.211612	0.043679	38	1	-6.609336	-1.727495	-1.018398
5	6	-4.1252	-0.240485	0.960483	39	1	-4.556079	1.630819	2.055552
6	6	-4.999709	0.915581	1.36689	40	1	-4.643431	-2.984783	-1.139425

7	6	-4.030223	-2.356221	-0.485989	41	1	-3.68439	-2.992298	0.340111
8	6	-2.80663	-1.81591	-1.245474	42	1	-2.18271	-2.651755	-1.58194
9	6	-1.985091	-0.857379	-0.376992	43	1	-3.148644	-1.286413	-2.145621
10	6	-2.86537	0.298079	0.170526	44	1	-1.176965	2.448977	-0.686807
11	6	-0.828652	-0.241759	-1.163643	45	1	-0.254456	2.550463	0.813375
12	6	0.062245	0.721045	-0.324413	46	1	-1.694921	0.897606	1.905016
13	6	-0.824731	1.865844	0.175123	47	1	-2.669889	2.185726	1.228312
14	6	-2.03806	1.333646	0.960389	48	1	0.481455	-2.009923	-1.240822
15	6	0.176759	-1.161683	-1.868147	49	1	-0.165556	-1.575809	-2.821188
16	6	1.389401	-0.253515	-2.083855	50	1	-4.602669	-1.405817	2.743331
17	6	1.112728	1.096966	-1.409851	51	1	-2.998774	-1.771925	2.086778
18	8	-8.102318	0.275213	-0.291325	52	1	-3.267475	-0.269172	2.979937
19	6	-3.71732	-0.969837	2.270921	53	1	1.418005	-0.783735	0.550469
20	6	0.717188	-0.005017	0.868661	54	1	1.264959	0.701757	1.494177
21	6	2.356372	1.98764	-1.161109	55	1	-0.025759	-0.48889	1.50588
22	6	3.153614	1.638548	0.096754	56	1	3.017888	1.76867	-2.011877
23	6	1.997919	3.477822	-1.172535	57	1	2.899988	4.092823	-1.098955
24	6	4.046023	0.412512	0.034871	58	1	1.479899	3.737298	-2.101715
25	8	3.110679	2.346081	1.090991	59	1	1.353869	3.738807	-0.329975
26	8	2.395621	-0.546478	-2.699385	60	1	3.542654	-0.374793	-0.530804
27	6	4.50768	-0.069375	1.408965	61	1	4.906636	0.689982	-0.593831
28	6	5.396019	-1.336538	1.361901	62	1	5.043725	0.737087	1.916349
29	6	4.673311	-2.555886	0.784896	63	1	3.630843	-0.296238	2.026714
30	6	6.663092	-1.036121	0.582853	64	1	5.700674	-1.546466	2.394665
31	8	6.913681	-1.419812	-0.542288	65	1	5.288664	-3.456027	0.87849
32	8	7.498391	-0.232929	1.279807	66	1	3.734671	-2.725559	1.323603
33	1	-1.578131	-1.43409	0.463728	67	1	4.449342	-2.422516	-0.276599
34	1	-3.276214	0.815604	-0.709869	68	1	8.269312	-0.047599	0.701082

Conf-12

Center Number	Atomic Number	Coordinates (Angstroms)			Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z			X	Y	Z
1	6	6.358099	-1.619256	-0.518978	35	1	1.260802	1.005048	-1.428084
2	6	7.055748	-0.333324	-0.687961	36	1	-0.794213	0.225646	-2.095738
3	6	6.375112	0.843528	-0.13504	37	1	6.860069	-2.500637	-0.909987
4	6	5.18564	0.781617	0.493642	38	1	6.884189	1.795359	-0.271115
5	6	4.43085	-0.522379	0.681019	39	1	4.704058	-2.669663	0.233407
6	6	5.171475	-1.696885	0.099461	40	1	5.113219	2.902875	0.776769
7	6	4.486938	2.025409	0.966481	41	1	4.318145	1.979174	2.050907
8	6	3.129696	2.164102	0.255888	42	1	2.59813	3.040152	0.644479
9	6	2.273716	0.904826	0.428573	43	1	3.302207	2.340729	-0.814954
10	6	3.036046	-0.360776	-0.046629	44	1	0.972586	-1.354197	-1.777117
11	6	0.971103	0.997775	-0.364842	45	1	0.215542	-2.378379	-0.560063
12	6	0.03637	-0.235398	-0.187194	46	1	1.979487	-1.904726	1.064241
13	6	0.801211	-1.463245	-0.697339	47	1	2.68214	-2.467815	-0.437824
14	6	2.154891	-1.625137	0.019549	48	1	-0.098423	2.440523	0.90282
15	6	0.049181	2.204326	-0.159932	49	1	0.373315	3.125859	-0.651804
16	6	-1.28001	1.723213	-0.741989	50	1	5.24235	-0.823794	2.684731
17	6	-1.169483	0.224107	-1.056503	51	1	3.645398	-0.057294	2.69347

18	8	8.146062	-0.252492	-1.261491	52	1	3.795074	-1.7873	2.357471
19	6	4.262135	-0.811317	2.198744	53	1	-0.958575	0.403282	1.671321
20	6	-0.383187	-0.442349	1.280213	54	1	-1.002099	-1.336561	1.376296
21	6	-2.516862	-0.534956	-1.136101	55	1	0.479658	-0.569502	1.937356
22	6	-3.258929	-0.730198	0.189553	56	1	-3.166542	0.124938	-1.725224
23	6	-2.39048	-1.873485	-1.869509	57	1	-3.386064	-2.271059	-2.087182
24	6	-3.936004	0.477517	0.826309	58	1	-1.853739	-1.744704	-2.815192
25	8	-3.354408	-1.833203	0.705976	59	1	-1.863061	-2.614428	-1.265342
26	8	-2.250722	2.422463	-0.958283	60	1	-3.22051	0.922876	1.531553
27	6	-5.222151	0.117236	1.580162	61	1	-4.113262	1.243786	0.068691
28	6	-6.281459	-0.609172	0.715106	62	1	-4.985662	-0.536452	2.425482
29	6	-7.616614	-0.729473	1.458284	63	1	-5.658128	1.03764	1.98532
30	6	-6.404026	0.092317	-0.621174	64	1	-5.897543	-1.605187	0.480946
31	8	-5.843878	-0.263429	-1.64211	65	1	-8.357156	-1.275566	0.864448
32	8	-7.156025	1.211495	-0.563118	66	1	-7.469188	-1.272802	2.397745
33	1	2.034546	0.80624	1.495475	67	1	-8.027146	0.257193	1.692054
34	1	3.281737	-0.191864	-1.106244	68	1	-7.133612	1.620204	-1.455664

Conf-13

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	6.108517	0.814074	-0.992076	35	1	1.054671	0.720055	1.886086
2	6	6.6925	-0.11353	-0.008557	36	1	-0.703219	2.1451	1.956173
3	6	5.795465	-1.158084	0.499715	37	1	6.767075	1.583866	-1.386304
4	6	4.514178	-1.287815	0.105676	38	1	6.222345	-1.834195	1.237473
5	6	3.873958	-0.350874	-0.903075	39	1	4.449502	1.386023	-2.143312
6	6	4.833588	0.701897	-1.390234	40	1	4.169598	-2.932952	1.432417
7	6	3.610508	-2.32173	0.716904	41	1	3.229783	-3.001046	-0.057888
8	6	2.419766	-1.633388	1.405445	42	1	1.733759	-2.39133	1.800522
9	6	1.67933	-0.69826	0.443556	43	1	2.787743	-1.053652	2.263411
10	6	2.646472	0.340483	-0.184876	44	1	1.097802	2.668533	0.452154
11	6	0.560011	0.063207	1.15245	45	1	0.209745	2.700429	-1.071005
12	6	-0.254185	1.003128	0.21485	46	1	1.544551	0.867145	-1.986246
13	6	0.718769	2.036769	-0.363025	47	1	2.596638	2.139743	-1.401492
14	6	1.903759	1.3583	-1.075225	48	1	-0.892971	-1.574798	1.348919
15	6	-0.512343	-0.717374	1.920478	49	1	-0.203359	-1.093216	2.900054
16	6	-1.642508	0.301169	2.066406	50	1	4.289618	-1.69546	-2.571442
17	6	-1.293011	1.546753	1.238608	51	1	2.655608	-1.891358	-1.916359
18	8	7.865086	-0.015912	0.365177	52	1	3.041619	-0.493185	-2.928394
19	6	3.43156	-1.159915	-2.154261	53	1	-1.694945	-0.48148	-0.555801
20	6	-0.940102	0.220887	-0.922198	54	1	-1.429896	0.907572	-1.614716
21	6	-2.489655	2.463252	0.870227	55	1	-0.221443	-0.361226	-1.502935
22	6	-3.346291	1.972043	-0.299193	56	1	-3.139742	2.418762	1.756657
23	6	-2.049267	3.912891	0.642046	57	1	-1.438664	4.005946	-0.258518
24	6	-4.288099	0.810914	-0.034701	58	1	-2.919414	4.564318	0.515753
25	8	-3.315223	2.5249	-1.387288	59	1	-1.469184	4.275551	1.496957
26	8	-2.638061	0.160869	2.749969	60	1	-3.870713	0.170166	0.744418
27	6	-4.64556	0.015074	-1.289906	61	1	-5.195053	1.248399	0.412692
28	6	-5.51832	-1.211893	-0.990385	62	1	-5.172735	0.660316	-1.999667

29	6	-5.815613	-2.013167	-2.272364	63	1	-3.727405	-0.310516	-1.789648
30	6	-4.89663	-2.141599	0.036725	64	1	-6.467583	-0.890798	-0.54684
31	8	-5.4962	-2.684672	0.941007	65	1	-6.458583	-2.87384	-2.062005
32	8	-3.573682	-2.354232	-0.180587	66	1	-6.32548	-1.373741	-3.000196
33	1	1.242314	-1.315349	-0.352069	67	1	-4.887117	-2.37603	-2.725479
34	1	3.082693	0.902444	0.655158	68	1	-3.273686	-2.987081	0.507194

Conf-14

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	-6.100081	-0.243067	-1.489891	35	1	-1.229066	-1.520271	1.418687
2	6	-6.768655	0.105891	-0.224964	36	1	0.562842	-2.800485	0.942175
3	6	-5.937089	0.788786	0.773185	37	1	-6.709856	-0.735345	-2.243238
4	6	-4.640323	1.091785	0.572023	38	1	-6.42702	1.034566	1.712982
5	6	-3.913273	0.743917	-0.714663	39	1	-4.360713	-0.197935	-2.663706
6	6	-4.808997	0.046799	-1.70358	40	1	-4.425437	1.914733	2.537241
7	6	-3.806759	1.714136	1.656837	41	1	-3.402641	2.678821	1.321148
8	6	-2.637243	0.781851	2.016933	42	1	-1.999612	1.263718	2.766812
9	6	-1.813684	0.411774	0.778793	43	1	-3.036574	-0.134259	2.473997
10	6	-2.70947	-0.205532	-0.327173	44	1	-1.130793	-2.557009	-0.758216
11	6	-0.714006	-0.594126	1.116842	45	1	-0.157706	-1.869998	-2.057237
12	6	0.185792	-0.979729	-0.095724	46	1	-1.483703	0.184238	-2.081555
13	6	-0.722302	-1.616862	-1.153993	47	1	-2.528596	-1.21246	-2.243445
14	6	-1.88251	-0.679954	-1.539033	48	1	0.650116	0.769409	2.172959
15	6	0.282995	-0.264083	2.232124	49	1	-0.091397	-0.413053	3.249185
16	6	1.447313	-1.211317	1.947699	50	1	-4.271248	2.7184	-1.573355
17	6	1.180224	-1.940773	0.623959	51	1	-2.684719	2.57922	-0.79792
18	8	-7.955985	-0.162284	-0.018511	52	1	-2.968923	1.826977	-2.373155
19	6	-3.423205	2.048306	-1.403311	53	1	1.467317	-0.040483	-1.579585
20	6	0.916106	0.243137	-0.682267	54	1	1.637226	0.67111	0.022461
21	6	2.420596	-2.597829	-0.037187	55	1	0.222078	1.041923	-0.952014
22	6	3.480005	-1.632087	-0.586812	56	1	2.901029	-3.141309	0.786968
23	6	2.024121	-3.600025	-1.12976	57	1	1.664423	-3.083233	-2.021224
24	6	4.629188	-1.269106	0.336225	58	1	2.887612	-4.205501	-1.424679
25	8	3.442149	-1.237358	-1.742026	59	1	1.23995	-4.275155	-0.772281
26	8	2.414714	-1.371064	2.668518	60	1	4.249178	-1.158192	1.355051
27	6	5.459516	-0.073417	-0.129017	61	1	5.265229	-2.168477	0.372975
28	6	4.68761	1.253661	-0.114751	62	1	6.345923	0.021675	0.507596
29	6	4.231047	1.680981	1.29512	63	1	5.819605	-0.2599	-1.144971
30	6	5.532072	2.359802	-0.718912	64	1	3.801088	1.161139	-0.751842
31	8	6.727401	2.311382	-0.930061	65	1	3.681593	2.62554	1.257018
32	8	4.792122	3.459407	-0.992184	66	1	3.581751	0.923939	1.743265
33	1	-1.350281	1.331508	0.398951	67	1	5.094882	1.811277	1.957326
34	1	-3.176778	-1.098035	0.116508	68	1	5.406073	4.134725	-1.352982

Conf-15

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	6.119344	1.219871	-0.390247	35	1	0.884885	0.140631	1.875651

2	6	6.671741	0.047124	0.308456	36	1	-0.981293	1.453856	2.202707
3	6	5.792274	-1.124815	0.3894	37	1	6.767799	2.088641	-0.470767
4	6	4.551702	-1.155306	-0.134503	38	1	6.195334	-1.986826	0.916822
5	6	3.942801	0.034858	-0.853907	39	1	4.524622	2.081992	-1.448825
6	6	4.884669	1.207407	-0.91197	40	1	4.189774	-3.139861	0.583572
7	6	3.655852	-2.348123	0.048421	41	1	3.364852	-2.759302	-0.927692
8	6	2.386394	-1.936073	0.813599	42	1	1.709459	-2.794171	0.892762
9	6	1.675756	-0.762329	0.131624	43	1	2.662861	-1.647622	1.837452
10	6	2.637739	0.439887	-0.057674	44	1	0.921461	2.407284	1.140386
11	6	0.474191	-0.28251	0.944082	45	1	0.167281	2.904769	-0.37205
12	6	-0.322262	0.871844	0.263474	46	1	1.657643	1.493929	-1.688862
13	6	0.642544	2.059591	0.135639	47	1	2.592052	2.533284	-0.632759
14	6	1.916189	1.67248	-0.63958	48	1	-0.920246	-1.936959	0.534606
15	6	-0.598524	-1.291746	1.360851	49	1	-0.327608	-1.939102	2.200167
16	6	-1.778776	-0.404841	1.72858	50	1	4.53328	-0.716196	-2.816636
17	6	-1.472186	1.039517	1.302946	51	1	2.866604	-1.136544	-2.387419
18	8	7.805669	0.052989	0.797303	52	1	3.263015	0.513574	-2.884251
19	6	3.625595	-0.353349	-2.324989	53	1	-1.579025	-0.35417	-1.066653
20	6	-0.868753	0.474979	-1.119214	54	1	-1.389012	1.321205	-1.571747
21	6	-2.710982	1.955208	1.103973	55	1	-0.067156	0.173666	-1.79783
22	6	-3.72077	1.5296	0.022865	56	1	-3.248011	1.879816	2.058155
23	6	-2.314728	3.42047	0.878103	57	1	-3.189239	4.072492	0.977233
24	6	-4.927585	0.75516	0.514699	58	1	-1.565884	3.739922	1.609753
25	8	-3.615483	1.896014	-1.136344	59	1	-1.909512	3.563215	-0.125457
26	8	-2.785183	-0.775107	2.308122	60	1	-4.610492	0.058794	1.294151
27	6	-5.805791	0.072218	-0.539013	61	1	-5.536111	1.506188	1.045843
28	6	-5.198555	-1.161633	-1.278084	62	1	-6.719436	-0.247691	-0.028734
29	6	-4.529334	-0.819127	-2.611554	63	1	-6.100961	0.8031	-1.298748
30	6	-4.247826	-1.921357	-0.374995	64	1	-6.033906	-1.847778	-1.474034
31	8	-3.066577	-2.113852	-0.599151	65	1	-4.139061	-1.720435	-3.093747
32	8	-4.847154	-2.358017	0.750599	66	1	-5.263243	-0.358799	-3.280982
33	1	1.324485	-1.107328	-0.849029	67	1	-3.708777	-0.114443	-2.474252
34	1	2.988064	0.714714	0.949119	68	1	-4.13899	-2.694088	1.341967

Conf-16

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-6.11832	1.217071	0.392452	35	1	-0.88377	0.147318	-1.87758
2	6	-6.66985	0.044191	-0.306711	36	1	0.984517	1.462213	-2.202022
3	6	-5.789071	-1.126644	-0.389142	37	1	-6.767743	2.085009	0.474118
4	6	-4.548015	-1.155993	0.133676	38	1	-6.191504	-1.988806	-0.9168
5	6	-3.939953	0.034382	0.85348	39	1	-4.523725	2.080387	1.450276
6	6	-4.883186	1.205738	0.913126	40	1	-4.184444	-3.139619	-0.586132
7	6	-3.650937	-2.347603	-0.050984	41	1	-3.358359	-2.759107	0.924524
8	6	-2.3828	-1.933361	-0.817165	42	1	-1.70491	-2.790564	-0.897773
9	6	-1.672953	-0.759493	-0.134637	43	1	-2.660634	-1.644299	-1.840475
10	6	-2.635953	0.441567	0.056486	44	1	-0.92034	2.41173	-1.140091
11	6	-0.472342	-0.277572	-0.94713	45	1	-0.166925	2.907964	0.373118
12	6	0.323823	0.875825	-0.264518	46	1	-1.656982	1.495859	1.688185

13	6	-0.641589	2.063075	-0.135635	47	1	-2.591893	2.534789	0.632152
14	6	-1.915311	1.674541	0.638883	48	1	0.922208	-1.932874	-0.541955
15	6	0.600246	-1.285753	-1.366557	49	1	0.329043	-1.931055	-2.207359
16	6	1.780477	-0.398211	-1.732279	50	1	-4.527957	-0.719042	2.816042
17	6	1.474372	1.045183	-1.302955	51	1	-2.861041	-1.13679	2.385251
18	8	-7.80425	0.048977	-0.794471	52	1	-3.259323	0.512383	2.883723
19	6	-3.621134	-0.354564	2.323997	53	1	1.578299	-0.353041	1.064949
20	6	0.869659	0.477463	1.11795	54	1	1.391352	1.322671	1.570807
21	6	2.713867	1.959327	-1.100581	55	1	0.067618	0.17734	1.796577
22	6	3.722603	1.529767	-0.02002	56	1	3.251641	1.885795	-2.054517
23	6	2.318391	3.424242	-0.871478	57	1	3.193416	4.075977	-0.967817
24	6	4.925878	0.749679	-0.511976	58	1	1.911979	3.564742	0.131916
25	8	3.619579	1.89703	1.139135	59	1	1.570639	3.745965	-1.603252
26	8	2.786682	-0.767126	-2.312957	60	1	5.53768	1.498148	-1.042992
27	6	5.801156	0.0631	0.541772	61	1	4.605919	0.054819	-1.29158
28	6	5.18901	-1.168691	1.279997	62	1	6.713696	-0.260153	0.031612
29	6	4.51748	-0.823815	2.611766	63	1	6.098942	0.792455	1.301948
30	6	4.2385	-1.926531	0.375124	64	1	6.022188	-1.8568	1.478343
31	8	3.055842	-2.11418	0.596037	65	1	5.250917	-0.364575	3.282448
32	8	4.839474	-2.36804	-0.747674	66	1	3.698747	-0.117457	2.472398
33	1	-1.320647	-1.105175	0.845401	67	1	4.124267	-1.723965	3.093729
34	1	-2.987406	0.716842	-0.949783	68	1	4.131609	-2.703896	-1.339608

Table S6. Cartesian coordinates of all conformers for **Isomer-1-2**

Conf-1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	6.461208	0.834455	1.148655	35	1	0.804197	-0.491714	0.943401
2	6	6.796898	-0.577667	1.398172	36	1	-1.181815	0.8148	1.191342
3	6	5.981063	-1.566862	0.684022	37	1	7.066595	1.576904	1.662439
4	6	4.984395	-1.23324	-0.158127	38	1	6.218252	-2.610332	0.88036
5	6	4.606494	0.209767	-0.441052	39	1	5.273918	2.236899	0.134551
6	6	5.468944	1.182782	0.317641	40	1	4.475785	-3.280578	-0.525378
7	6	4.121965	-2.282353	-0.801952	41	1	4.186734	-2.209886	-1.896156
8	6	2.656845	-2.088579	-0.375577	42	1	2.023548	-2.819902	-0.890448
9	6	2.170389	-0.665395	-0.669133	43	1	2.567457	-2.286842	0.701604
10	6	3.096048	0.390113	-0.009181	44	1	1.012438	1.852856	1.307087
11	6	0.748955	-0.438674	-0.155673	45	1	0.783916	3.021942	0.011683
12	6	0.181976	0.976515	-0.4789	46	1	2.671125	2.120287	-1.256513
13	6	1.094182	1.993199	0.220567	47	1	3.169324	2.527271	0.372787
14	6	2.56415	1.823718	-0.207043	48	1	-0.318647	-1.65776	-1.647811
15	6	-0.361275	-1.405261	-0.579804	49	1	-0.384117	-2.349952	-0.028274
16	6	-1.631593	-0.599004	-0.321666	50	1	5.8493	0.287558	-2.233849
17	6	-1.255135	0.829177	0.091519	51	1	4.151566	-0.077602	-2.584284
18	8	7.708632	-0.906587	2.162913	52	1	4.633625	1.570869	-2.161922
19	6	4.816913	0.513697	-1.950747	53	1	-0.545578	0.546488	-2.512385
20	6	0.108342	1.255461	-1.992725	54	1	-0.291013	2.258363	-2.175093
21	6	-2.369501	1.821144	-0.275039	55	1	1.087894	1.204901	-2.473176
22	6	-3.638169	1.434501	0.496741	56	1	-2.580225	1.752981	-1.34794
23	6	-2.037709	3.280997	0.080493	57	1	-2.90296	3.929183	-0.09954
24	6	-4.924158	1.340688	-0.29575	58	1	-1.211045	3.660225	-0.52486
25	8	-3.596222	1.288147	1.709097	59	1	-1.765252	3.364864	1.136942
26	8	-2.769734	-1.007694	-0.456958	60	1	-5.149645	2.356234	-0.657931
27	6	-6.107418	0.781942	0.493179	61	1	-4.733781	0.742319	-1.191488
28	6	-5.941781	-0.683954	0.913952	62	1	-6.250227	1.378993	1.400184
29	6	-7.099565	-1.138839	1.824323	63	1	-7.015803	0.878602	-0.111412
30	6	-5.863072	-1.607043	-0.286578	64	1	-5.004966	-0.799507	1.467196
31	8	-6.188875	-1.331146	-1.425765	65	1	-6.97219	-2.178387	2.138713
32	8	-5.416455	-2.834552	0.057405	66	1	-7.137199	-0.508745	2.718767
33	1	2.179011	-0.525533	-1.758402	67	1	-8.061344	-1.049812	1.305642
34	1	3.077957	0.183024	1.071703	68	1	-5.401961	-3.372067	-0.762967

Conf-2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	6.667851	-1.464058	-0.979441	35	1	1.34023	0.866773	-1.026545
2	6	7.262449	-0.140931	-1.233834	36	1	-0.834502	-0.052882	-1.339138
3	6	6.613428	0.993286	-0.565751	37	1	7.148152	-2.313846	-1.457853
4	6	5.540993	0.86215	0.238346	38	1	7.043283	1.972603	-0.765263
5	6	4.896714	-0.482852	0.523221	39	1	5.208221	-2.608449	0.002815

6	6	5.597641	-1.610706	-0.185907	40	1	5.398303	2.97468	0.557816
7	6	4.858808	2.062599	0.832039	41	1	4.866625	2.001695	1.928848
8	6	3.400482	2.127988	0.346988	42	1	2.890668	2.972073	0.825096
9	6	2.653091	0.822466	0.638309	43	1	3.390619	2.316919	-0.735506
10	6	3.396623	-0.395798	0.030669	44	1	1.13373	-1.483336	-1.35218
11	6	1.23477	0.846261	0.069891	45	1	0.647922	-2.566438	-0.052967
12	6	0.408908	-0.436642	0.387078	46	1	2.618274	-1.997131	1.279698
13	6	1.147414	-1.615041	-0.261593	47	1	3.095909	-2.517693	-0.32313
14	6	2.606573	-1.705748	0.223445	48	1	0.357836	2.273703	1.500922
15	6	0.303469	2.005929	0.437262	49	1	0.469004	2.925259	-0.132606
16	6	-1.08364	1.434446	0.150141	50	1	6.0341	-0.748408	2.367231
17	6	-0.95453	-0.042103	-0.24357	51	1	4.418715	-0.075089	2.641746
18	8	8.246124	0.002747	-1.965988	52	1	4.609329	-1.791742	2.260941
19	6	4.989587	-0.789606	2.044065	53	1	1.182058	-0.789174	2.41925
20	6	0.228785	-0.666864	1.900292	54	1	-0.300469	0.161531	2.383997
21	6	-2.242884	-0.809702	0.078427	55	1	-0.356702	-1.57432	2.079686
22	6	-3.38619	-0.250615	-0.778246	56	1	-2.500475	-0.668154	1.134279
23	6	-2.160444	-2.31865	-0.21673	57	1	-3.138563	-2.793923	-0.079802
24	6	-4.70487	-0.013714	-0.075948	58	1	-1.455521	-2.817469	0.452596
25	8	-3.236867	-0.077629	-1.977043	59	1	-1.842423	-2.489723	-1.2498
26	8	-2.134883	2.037151	0.2578	60	1	-4.960297	-0.921096	0.487943
27	6	-5.839101	0.383326	-1.015732	61	1	-4.518117	0.767037	0.674369
28	6	-7.144554	0.718358	-0.288506	62	1	-5.52943	1.255813	-1.600781
29	6	-8.215488	1.251285	-1.26243	63	1	-6.021252	-0.425637	-1.731148
30	6	-7.708346	-0.493539	0.43151	64	1	-6.960483	1.488925	0.471342
31	8	-7.456411	-1.654896	0.174628	65	1	-8.446137	0.502436	-2.028419
32	8	-8.583308	-0.139215	1.398709	66	1	-9.140006	1.5052	-0.736058
33	1	2.594549	0.705243	1.728751	67	1	-7.844646	2.149611	-1.76596
34	1	3.458431	-0.210175	-1.052485	68	1	-8.939391	-0.969207	1.783507

Conf-3

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	6.678585	-1.296476	-0.664248	35	1	1.169598	0.493548	-1.188597
2	6	7.159088	0.006717	-1.154045	36	1	-0.906414	-0.663721	-1.350437
3	6	6.396296	1.179706	-0.711019	37	1	7.244455	-2.171557	-0.973646
4	6	5.320293	1.099906	0.095089	38	1	6.742557	2.141279	-1.083999
5	6	4.79022	-0.223862	0.616371	39	1	5.302564	-2.370927	0.500978
6	6	5.606328	-1.393198	0.134115	40	1	4.982985	3.213174	0.020056
7	6	4.519859	2.320728	0.452725	41	1	4.506139	2.461629	1.542065
8	6	3.073825	2.163255	-0.047813	42	1	2.479611	3.029333	0.264862
9	6	2.437888	0.868499	0.469221	43	1	3.073906	2.15241	-1.146668
10	6	3.302293	-0.365358	0.100062	44	1	1.181859	-1.885403	-1.087015
11	6	1.038285	0.6596	-0.107429	45	1	0.759916	-2.759408	0.381044
12	6	0.321398	-0.616296	0.428167	46	1	2.63591	-1.782759	1.609281
13	6	1.178277	-1.818562	0.009546	47	1	3.200146	-2.534679	0.131253
14	6	2.626515	-1.686759	0.517748	48	1	0.00129	2.23167	1.035759
15	6	-0.000846	1.776004	0.036531	49	1	0.098022	2.591076	-0.686776
16	6	-1.323722	1.038437	-0.158055	50	1	5.896226	-0.046587	2.489766

17	6	-1.055022	-0.467028	-0.27613	51	1	4.222536	0.518941	2.618874
18	8	8.142966	0.103563	-1.89356	52	1	4.569295	-1.214475	2.561709
19	6	4.868092	-0.238729	2.168568	53	1	1.069847	-0.527454	2.497663
20	6	0.123232	-0.588412	1.956259	54	1	-0.490274	0.260329	2.277958
21	6	-2.278721	-1.279062	0.168702	55	1	-0.383325	-1.499592	2.290467
22	6	-3.447581	-0.976373	-0.777995	56	1	-2.567829	-0.980127	1.182606
23	6	-2.057537	-2.80223	0.14067	57	1	-2.991685	-3.333453	0.356783
24	6	-4.787221	-0.699015	-0.131592	58	1	-1.323242	-3.111663	0.888116
25	8	-3.295964	-1.027225	-1.987829	59	1	-1.70746	-3.12012	-0.846215
26	8	-2.426408	1.552006	-0.175081	60	1	-5.00352	-1.524922	0.560974
27	6	-5.917503	-0.493923	-1.137268	61	1	-4.649317	0.184935	0.503854
28	6	-7.266096	-0.081689	-0.496664	62	1	-5.613946	0.26827	-1.861112
29	6	-7.826515	-1.133074	0.463103	63	1	-6.075388	-1.417105	-1.706205
30	6	-7.094287	1.255417	0.200133	64	1	-7.972378	0.076437	-1.320736
31	8	-6.982475	1.423016	1.398958	65	1	-8.82934	-0.857292	0.804207
32	8	-7.029423	2.274263	-0.685024	66	1	-7.890017	-2.10475	-0.038041
33	1	2.361469	0.944645	1.56213	67	1	-7.196044	-1.236791	1.349971
34	1	3.376996	-0.371933	-0.998067	68	1	-6.857249	3.092726	-0.171086

Conf-4

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	6.29205	-2.222874	-0.453162	35	1	1.188156	0.465593	-1.162716
2	6	6.926109	-1.291814	-1.401953	36	1	-1.060338	-0.190975	-0.762716
3	6	6.462104	0.099288	-1.34277	37	1	6.637445	-3.253313	-0.47777
4	6	5.518759	0.527679	-0.482235	38	1	6.919668	0.784204	-2.053516
5	6	4.838196	-0.400759	0.507774	39	1	4.927829	-2.524773	1.112937
6	6	5.348063	-1.813446	0.405733	40	1	5.565402	2.51927	-1.267527
7	6	5.015093	1.943339	-0.516805	41	1	5.185389	2.432184	0.452069
8	6	3.507539	1.954352	-0.822583	42	1	3.132747	2.983654	-0.791016
9	6	2.728116	1.075302	0.161182	43	1	3.346175	1.584075	-1.844565
10	6	3.290148	-0.370343	0.186631	44	1	0.781029	-1.689614	-0.231165
11	6	1.245482	1.002659	-0.202537	45	1	0.422644	-1.914688	1.477159
12	6	0.392968	0.164418	0.797111	46	1	2.602446	-1.025705	2.14311
13	6	0.947476	-1.265851	0.768648	47	1	2.801274	-2.3287	0.989343
14	6	2.453188	-1.296338	1.091755	48	1	0.688336	3.053386	0.382173
15	6	0.457322	2.303822	-0.386394	49	1	0.59468	2.789024	-1.357512
16	6	-0.991466	1.854176	-0.207072	50	1	6.219941	0.130408	2.111824
17	6	-1.018723	0.371444	0.184036	51	1	4.713804	1.061689	2.159978
18	8	7.793793	-1.66189	-2.198488	52	1	4.728162	-0.626508	2.687649
19	6	5.138267	0.07571	1.956455	53	1	1.431357	0.761746	2.645065
20	6	0.422434	0.737218	2.227517	54	1	0.027777	1.758262	2.271864
21	6	-2.294128	0.040113	0.966613	55	1	-0.190252	0.123468	2.895682
22	6	-3.511069	0.229076	0.05436	56	1	-2.391254	0.722918	1.818388
23	6	-2.355919	-1.410243	1.481554	57	1	-3.333737	-1.62215	1.930144
24	6	-4.71885	0.910324	0.665781	58	1	-1.598276	-1.593938	2.246882
25	8	-3.507967	-0.206127	-1.086409	59	1	-2.201123	-2.115769	0.659452
26	8	-1.973426	2.564913	-0.308055	60	1	-4.83805	0.561261	1.699659
27	6	-6.00649	0.770753	-0.144267	61	1	-4.437607	1.969085	0.7506

28	6	-6.531012	-0.669332	-0.244552	62	1	-6.783644	1.40341	0.298218
29	6	-6.894502	-1.285468	1.121466	63	1	-5.829881	1.151472	-1.154906
30	6	-7.748776	-0.719345	-1.148594	64	1	-5.766977	-1.29955	-0.712893
31	8	-8.41296	0.233379	-1.505563	65	1	-7.301529	-2.292662	0.999042
32	8	-8.046644	-1.987341	-1.514926	66	1	-6.01063	-1.356735	1.762366
33	1	2.82594	1.520487	1.160402	67	1	-7.640025	-0.670738	1.639322
34	1	3.200892	-0.753798	-0.841234	68	1	-8.85443	-1.94261	-2.070402

Conf-5

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	6.50754	-1.640956	0.203113	35	1	1.325481	0.312487	-1.57603
2	6	7.176036	-0.518755	-0.477089	36	1	-0.813493	-0.728002	-1.807444
3	6	6.473836	0.769222	-0.431948	37	1	7.024916	-2.596894	0.188351
4	6	5.291578	0.944668	0.188984	38	1	6.960305	1.594921	-0.946924
5	6	4.568324	-0.186931	0.897075	39	1	4.882732	-2.329463	1.339666
6	6	5.328346	-1.484028	0.820641	40	1	5.17259	2.999433	-0.401973
7	6	4.569463	2.261806	0.136826	41	1	4.415538	2.652075	1.152062
8	6	3.200174	2.08152	-0.540751	42	1	2.653526	3.031163	-0.524644
9	6	2.376296	0.983238	0.139736	43	1	3.35442	1.816567	-1.596033
10	6	3.161859	-0.352873	0.193748	44	1	1.095775	-1.973094	-0.953895
11	6	1.058679	0.732278	-0.592922	45	1	0.389083	-2.456485	0.583307
12	6	0.152685	-0.337804	0.087765	46	1	2.153299	-1.335036	1.8512
13	6	0.942513	-1.653958	0.086132	47	1	2.847312	-2.444554	0.686821
14	6	2.309199	-1.496111	0.7786	48	1	0.020141	2.581358	-0.000507
15	6	0.122357	1.912895	-0.865922	49	1	0.40432	2.535804	-1.720078
16	6	-1.221408	1.231954	-1.11467	50	1	5.409944	0.351696	2.83772
17	6	-1.090541	-0.271813	-0.84276	51	1	3.797118	1.033732	2.569994
18	8	8.260668	-0.656309	-1.050689	52	1	3.979734	-0.683544	2.951707
19	6	4.423949	0.153994	2.406568	53	1	0.60477	0.187352	2.178463
20	6	-0.257002	0.055819	1.520303	54	1	-0.830381	0.988933	1.544339
21	6	-2.436575	-0.884532	-0.423734	55	1	-0.887509	-0.722047	1.962732
22	6	-3.431985	-0.731471	-1.584543	56	1	-2.829091	-0.346024	0.445782
23	6	-2.337355	-2.384991	-0.092597	57	1	-3.328211	-2.813717	0.0895
24	6	-4.788713	-0.140316	-1.265844	58	1	-1.736249	-2.554877	0.803548
25	8	-3.13801	-1.127086	-2.701466	59	1	-1.883752	-2.928451	-0.92703
26	8	-2.24816	1.793757	-1.44586	60	1	-4.608166	0.846631	-0.826993
27	6	-5.603205	-0.997333	-0.280537	61	1	-5.336618	-0.011231	-2.204745
28	6	-6.88534	-0.301217	0.186881	62	1	-5.869132	-1.949645	-0.754265
29	6	-7.784492	-1.25067	1.004001	63	1	-5.003929	-1.230079	0.605561
30	6	-6.55331	0.908049	1.04455	64	1	-7.456434	0.056041	-0.678978
31	8	-5.517591	1.075391	1.659323	65	1	-8.696579	-0.745122	1.333935
32	8	-7.577073	1.785847	1.090813	66	1	-8.068623	-2.113035	0.392768
33	1	2.153253	1.315029	1.162532	67	1	-7.252802	-1.618995	1.88857
34	1	3.390144	-0.618858	-0.849638	68	1	-7.309565	2.513053	1.694006

Conf-6

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z

1	6	5.774874	-1.6086	-1.313625	35	1	1.292095	2.013199	-0.662714
2	6	6.661673	-0.650615	-0.632046	36	1	-0.814906	2.085501	-1.847091
3	6	6.070061	0.082821	0.492789	37	1	6.206837	-2.17036	-2.13801
4	6	4.797641	-0.089222	0.900025	38	1	6.72103	0.799889	0.988502
5	6	3.849411	-1.059595	0.218785	39	1	3.891826	-2.528606	-1.431572
6	6	4.5048	-1.787375	-0.924135	40	1	4.974534	1.41396	2.414621
7	6	4.210864	0.746519	2.002764	41	1	3.867357	0.104538	2.825266
8	6	3.015075	1.553208	1.467865	42	1	2.553813	2.115715	2.287404
9	6	1.976894	0.645899	0.800242	43	1	3.377434	2.288998	0.736378
10	6	2.625904	-0.213555	-0.319967	44	1	0.726744	0.462799	-2.375163
11	6	0.840312	1.450416	0.171559	45	1	-0.338211	-0.911044	-2.071775
12	6	-0.264657	0.560653	-0.46074	46	1	1.233182	-1.881199	-0.471691
13	6	0.3871	-0.236753	-1.598402	47	1	2.0736	-1.519357	-1.964127
14	6	1.591196	-1.056921	-1.097389	48	1	-0.30722	2.051197	1.942682
15	6	0.064682	2.479207	1.002458	49	1	0.611027	3.394567	1.243924
16	6	-1.130858	2.78418	0.098262	50	1	4.276602	-2.649408	1.652157
17	6	-1.262492	1.652221	-0.937478	51	1	2.825319	-1.719845	2.061881
18	8	7.831332	-0.476795	-0.987929	52	1	2.777813	-2.900351	0.746031
19	6	3.399269	-2.145366	1.235571	53	1	-0.17033	-1.128854	0.930231
20	6	-0.900222	-0.409192	0.552718	54	1	-1.33161	0.110792	1.408682
21	6	-2.701284	1.264171	-1.30978	55	1	-1.698203	-0.984626	0.072777
22	6	-3.632407	1.117061	-0.111731	56	1	-2.685183	0.274649	-1.788981
23	6	-3.307852	2.266194	-2.318878	57	1	-4.324196	1.987607	-2.61246
24	6	-5.042328	0.610842	-0.399213	58	1	-2.694478	2.29386	-3.225238
25	8	-3.297174	1.387933	1.02993	59	1	-3.325195	3.268862	-1.884265
26	8	-1.79039	3.804868	0.11532	60	1	-5.68175	1.496023	-0.523458
27	6	-5.603362	-0.257327	0.73244	61	1	-5.062678	0.082227	-1.357665
28	6	-4.780898	-1.536907	1.018081	62	1	-5.626495	0.330087	1.655471
29	6	-5.431447	-2.376249	2.123719	63	1	-6.635001	-0.538332	0.492087
30	6	-4.585177	-2.304418	-0.272713	64	1	-3.779846	-1.231148	1.33327
31	8	-3.603455	-2.221219	-0.990231	65	1	-4.845182	-3.275441	2.339862
32	8	-5.650528	-3.063479	-0.59966	66	1	-5.498354	-1.785567	3.043263
33	1	1.560116	-0.013441	1.572247	67	1	-6.440683	-2.688166	1.839921
34	1	3.062712	0.499572	-1.035763	68	1	-5.451431	-3.486549	-1.463224

Conf-7

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-6.693052	1.223588	-0.114742	35	1	-1.218096	-0.225163	-1.435888
2	6	-7.186229	-0.003025	-0.763787	36	1	0.802551	1.015747	-1.600555
3	6	-6.352672	-1.198855	-0.592959	37	1	-7.309014	2.112804	-0.222449
4	6	-5.204438	-1.204897	0.110915	38	1	-6.708904	-2.101481	-1.084898
5	6	-4.660443	0.038493	0.791464	39	1	-5.23676	2.15311	1.077192
6	6	-5.55005	1.235195	0.585205	40	1	-4.821256	-3.262264	-0.342498
7	6	-4.340952	-2.432798	0.186122	41	1	-4.215549	-2.747003	1.231225
8	6	-2.956217	-2.135861	-0.414566	42	1	-2.311474	-3.015378	-0.306542
9	6	-2.306217	-0.916668	0.248081	43	1	-3.065451	-1.94691	-1.491584
10	6	-3.234485	0.323391	0.170478	44	1	-1.282368	2.102361	-0.941177
11	6	-0.97614	-0.558847	-0.41424	45	1	-0.740909	2.743939	0.605376

12	6	-0.242211	0.641779	0.255398	46	1	-2.457233	1.501357	1.82531
13	6	-1.16803	1.858749	0.12397	47	1	-3.184757	2.461103	0.553286
14	6	-2.554426	1.585669	0.737087	48	1	0.203006	-2.256145	0.348942
15	6	0.100079	-1.639512	-0.553894	49	1	-0.045443	-2.325115	-1.394201
16	6	1.381629	-0.827932	-0.735695	50	1	-5.573545	-0.483953	2.703921
17	6	1.062306	0.665516	-0.588592	51	1	-3.881472	-0.993837	2.583543
18	8	-8.236448	-0.021105	-1.412681	52	1	-4.27609	0.710456	2.844809
19	6	-4.586847	-0.20042	2.325518	53	1	-0.778927	0.183889	2.342443
20	6	0.107066	0.373229	1.732451	54	1	0.771803	-0.489832	1.848925
21	6	2.293313	1.457778	-0.136896	55	1	0.619767	1.237949	2.165979
22	6	3.372498	1.415077	-1.225293	56	1	2.706013	1.015132	0.776852
23	6	2.00462	2.949614	0.128402	57	1	2.931762	3.499875	0.323666
24	6	4.818196	1.416249	-0.760189	58	1	1.35844	3.078568	0.999551
25	8	3.079017	1.468781	-2.407846	59	1	1.515871	3.405879	-0.738191
26	8	2.489492	-1.292428	-0.922187	60	1	5.441018	1.752555	-1.595586
27	6	5.277647	0.024717	-0.289812	61	1	4.922211	2.137095	0.060034
28	6	6.764952	0.001179	0.138516	62	1	4.6588	-0.312343	0.549651
29	6	7.063102	0.891925	1.345625	63	1	5.120818	-0.692909	-1.098841
30	6	7.139695	-1.439497	0.436852	64	1	7.367826	0.319107	-0.722044
31	8	7.269246	-1.922728	1.543858	65	1	8.10897	0.797301	1.652604
32	8	7.284855	-2.162654	-0.695742	66	1	6.874812	1.943421	1.111517
33	1	-2.120433	-1.165942	1.30136	67	1	6.439419	0.60608	2.198566
34	1	-3.4166	0.505557	-0.899652	68	1	7.475745	-3.086963	-0.426393

Conf-8

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-4.446865	2.553302	0.808561	35	1	-0.359561	-0.849316	-1.509833
2	6	-5.353895	2.235061	-0.306929	36	1	1.920041	-0.916555	-1.246624
3	6	-5.302893	0.854169	-0.801344	37	1	-4.486486	3.569166	1.193513
4	6	-4.488035	-0.085786	-0.284806	38	1	-5.963031	0.6221	-1.634441
5	6	-3.534067	0.203853	0.859845	39	1	-2.995054	1.896182	2.17476
6	6	-3.626403	1.630585	1.330105	40	1	-5.128898	-1.560942	-1.698619
7	6	-4.408928	-1.463671	-0.879821	41	1	-4.673472	-2.219185	-0.127616
8	6	-2.979517	-1.736398	-1.379008	42	1	-2.911647	-2.762243	-1.758572
9	6	-1.943913	-1.510608	-0.272281	43	1	-2.760379	-1.065933	-2.2217
10	6	-2.071664	-0.087337	0.332836	44	1	0.696074	0.646111	0.063332
11	6	-0.517754	-1.673956	-0.796006	45	1	1.161666	0.087269	1.666302
12	6	0.578234	-1.50283	0.296545	46	1	-1.148028	-0.399544	2.277027
13	6	0.450187	-0.077271	0.850996	47	1	-1.019816	1.245178	1.687127
14	6	-0.971609	0.197379	1.375237	48	1	-0.463409	-3.861294	-0.998586
15	6	-0.125226	-2.960525	-1.529011	49	1	-0.484384	-3.038103	-2.559198
16	6	1.403146	-2.920645	-1.49316	50	1	-4.944162	-0.527716	2.357055
17	6	1.844135	-1.779962	-0.563912	51	1	-3.76314	-1.751936	1.862385
18	8	-6.109444	3.080854	-0.795398	52	1	-3.276527	-0.438472	2.941778
19	6	-3.898557	-0.689547	2.078153	53	1	0.606318	-3.55592	1.100779
20	6	0.444229	-2.527645	1.438665	54	1	1.18258	-2.31092	2.214927
21	6	3.260823	-1.991878	0.034996	55	1	-0.542383	-2.490509	1.906205
22	6	3.6189	-0.779762	0.890893	56	1	3.923558	-1.977419	-0.841627

23	6	3.503977	-3.307203	0.78254	57	1	3.006114	-3.326971	1.751149
24	6	3.99408	0.489367	0.146163	58	1	4.577085	-3.427432	0.965317
25	8	3.60487	-0.827344	2.111074	59	1	3.168344	-4.157589	0.185226
26	8	2.149128	-3.651148	-2.113828	60	1	5.042969	0.359962	-0.161094
27	6	3.820043	1.757191	0.983775	61	1	3.418002	0.555886	-0.781251
28	6	4.064646	3.063357	0.215427	62	1	2.806387	1.773189	1.39526
29	6	5.460675	3.146064	-0.431129	63	1	4.502111	1.720733	1.839258
30	6	2.97298	3.325011	-0.810642	64	1	3.987917	3.893789	0.932246
31	8	2.02484	2.602176	-1.055321	65	1	6.228787	2.942394	0.322274
32	8	3.158286	4.50134	-1.446491	66	1	5.574592	2.413698	-1.237083
33	1	-2.123049	-2.257034	0.512647	67	1	5.639948	4.138909	-0.849802
34	1	-1.919058	0.616092	-0.499867	68	1	2.418178	4.605462	-2.083087

Conf-9

Center Number	Atomic Number	Coordinates (Angstroms)			Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z			X	Y	Z
1	6	6.499922	-1.462662	-0.640161	35	1	1.258499	0.976935	-1.045889
2	6	7.138547	-0.138218	-0.72321	36	1	-0.861527	0.143368	-1.227563
3	6	6.420386	0.962433	-0.07007	37	1	7.029004	-2.288552	-1.890546
4	6	5.249958	0.800445	0.576374	38	1	6.88422	1.943754	-1.108876
5	6	4.558156	-0.546858	0.682077	39	1	4.910222	-2.6392	-0.144393
6	6	5.332959	-1.639454	-0.004903	40	1	5.091591	2.889509	0.062637
7	6	4.509801	1.972648	1.156808	41	1	4.37242	1.838813	1.018678
8	6	3.129018	2.100429	0.49094	42	1	2.570559	2.92102	2.238453
9	6	2.334071	0.794298	0.59054	43	1	3.26429	2.361735	0.955342
10	6	3.13728	-0.396231	0.0049	44	1	1.068555	-1.342074	-0.567852
11	6	1.005597	0.886222	-0.159135	45	1	0.399428	-2.497034	-1.736531
12	6	0.126215	-0.39509	-0.044589	46	1	2.175581	-2.054417	-0.58998
13	6	0.932397	-1.544328	-0.665254	47	1	2.858547	-2.484967	1.031366
14	6	2.311142	-1.697768	0.004121	48	1	-0.034273	2.235882	-0.523344
15	6	0.049316	2.038733	0.159572	49	1	0.300487	2.989243	1.236619
16	6	-1.296562	1.518871	-0.344582	50	1	5.438891	-0.956325	-0.320854
17	6	-1.134288	0.071137	-0.825062	51	1	3.808928	-0.270271	2.636884
18	8	8.212211	0.033196	-1.308315	52	1	4.028962	-1.96156	2.74211
19	6	4.445871	-0.955163	2.177444	53	1	0.608791	-0.896076	2.273929
20	6	-0.262506	-0.718498	1.411648	54	1	-0.841769	0.088906	2.046151
21	6	-2.454952	-0.701332	-0.748633	55	1	-0.880976	-1.620832	1.872795
22	6	-3.465506	-0.119847	-1.745318	56	1	-2.884477	-0.627511	1.449495
23	6	-2.315706	-2.195798	-1.106641	57	1	-3.298349	-2.676495	0.256236
24	6	-4.924894	-0.200972	-1.341668	58	1	-1.735582	-2.731033	-1.163732
25	8	-3.114086	0.302217	-2.834948	59	1	-1.821334	-2.316535	-0.351616
26	8	-2.340115	2.142541	-0.329023	60	1	-5.53497	-0.154547	-2.075944
27	6	-5.308378	0.929775	-0.363076	61	1	-5.094813	-1.166179	-2.24796
28	6	-6.608706	0.662693	0.406272	62	1	-4.500077	1.088235	-0.851778
29	6	-7.818132	0.376305	-0.501241	63	1	-5.41037	1.864715	0.35273
30	6	-6.408405	-0.437019	1.438154	64	1	-6.842531	1.563834	-0.924136
31	8	-5.360027	-1.0052	1.681023	65	1	-7.691536	-0.561001	0.992857
32	8	-7.548199	-0.720443	2.104371	66	1	-8.738926	0.303755	-1.052772
33	1	2.128258	0.606003	1.652809	67	1	-7.930809	1.18462	0.081877

34	1	3.343768	-0.141704	-1.045889	68	1	-7.332545	-1.42102	-1.231231

Conf-10

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	-6.45404	-1.428766	0.859767	35	1	-1.357221	1.355291	1.159347
2	6	-7.146451	-0.150918	0.621789	36	1	0.673252	0.773278	2.091438
3	6	-6.433814	0.817922	-0.21934	37	1	-6.978839	-2.161083	1.468042
4	6	-5.221345	0.580348	-0.75539	38	1	-6.939358	1.766993	-0.384688
5	6	-4.471751	-0.720509	-0.528357	39	1	-4.781642	-2.647509	0.509278
6	6	-5.244927	-1.678624	0.33808	40	1	-5.119319	2.530059	-1.634854
7	6	-4.494572	1.636279	-1.540184	41	1	-4.287322	1.279519	-2.558233
8	6	-3.162461	1.975839	-0.850081	42	1	-2.608628	2.703272	-1.454463
9	6	-2.312849	0.721551	-0.62169	43	1	-3.371216	2.453344	0.117422
10	6	-3.103092	-0.353084	0.17402	44	1	-1.11009	-0.791396	2.189025
11	6	-1.035335	1.038483	0.154113	45	1	-0.317249	-2.131205	1.359488
12	6	-0.119859	-0.196809	0.369605	46	1	-2.033741	-2.164564	-0.389843
13	6	-0.904785	-1.218948	1.197626	47	1	-2.791379	-2.249375	1.186608
14	6	-2.237184	-1.584786	0.517052	48	1	0.10113	2.043956	-1.437019
15	6	-0.080875	2.123123	-0.356473	49	1	-0.397134	3.151377	-0.159269
16	6	1.227583	1.815877	0.380034	50	1	-5.210649	-1.590823	-2.388727
17	6	1.072649	0.470417	1.106344	51	1	-3.608509	-0.854531	-2.558293
18	8	-8.258128	0.088754	1.102384	52	1	-3.784207	-2.414055	-1.742661
19	6	-4.249058	-1.435328	-1.890457	53	1	0.971296	-1.700436	-0.766018
20	6	0.341117	-0.828607	-0.958089	54	1	-0.501148	-1.165753	-1.565728
21	6	2.327538	-0.366834	1.43277	55	1	0.917413	-0.130662	-1.574205
22	6	3.201756	-0.841655	0.266839	56	1	1.966385	-1.300146	1.880257
23	6	3.215615	0.34522	2.477263	57	1	4.110684	-0.244003	2.696114
24	6	3.871049	0.171393	-0.648263	58	1	2.651196	0.474074	3.407423
25	8	3.389895	-2.040015	0.114782	59	1	3.523601	1.331703	2.126503
26	8	2.19906	2.546626	0.40541	60	1	3.092279	0.576306	-1.30773
27	6	4.997786	-0.41796	-1.498998	61	1	4.203327	1.033256	-0.062642
28	6	6.225824	-0.89933	-0.695084	62	1	4.61519	-1.272102	-2.06659
29	6	7.306885	-1.455744	-1.629437	63	1	5.328794	0.338483	-2.219903
30	6	6.777716	0.264455	0.103409	64	1	5.902161	-1.673408	0.004524
31	8	7.38474	1.208336	-0.362554	65	1	8.160694	-1.845147	-1.064801
32	8	6.488984	0.166465	1.42173	66	1	6.897223	-2.271742	-2.23343
33	1	-2.039775	0.318219	-1.605527	67	1	7.671617	-0.672242	-2.300781
34	1	-3.385792	0.118311	1.12771	68	1	6.84184	0.973389	1.857021

Conf-11

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	4.432677	-2.724883	-0.895935	35	1	1.045769	2.008093	-1.17456
2	6	5.631017	-1.888833	-1.078882	36	1	-1.172188	2.282577	-1.663499
3	6	5.605899	-0.578376	-0.418592	37	1	4.444827	-3.703469	-1.369169
4	6	4.566331	-0.141945	0.318297	38	1	6.484533	0.045945	-0.566636
5	6	3.312162	-0.971263	0.527645	39	1	2.534273	-2.96252	-0.032135
6	6	3.387696	-2.302868	-0.170227	40	1	5.494902	1.752582	0.684586

7	6	4.55138	1.242557	0.903394	41	1	4.458778	1.192909	1.99691
8	6	3.360976	2.036777	0.338633	42	1	3.320942	3.025287	0.810198
9	6	2.039044	1.292163	0.553218	43	1	3.515543	2.198904	-0.73718
10	6	2.098647	-0.13723	-0.049074	44	1	-0.302613	0.065766	-1.605217
11	6	0.865336	2.031624	-0.087989	45	1	-1.346894	-0.626488	-0.362272
12	6	-0.512006	1.335439	0.126631	46	1	0.526439	-1.12417	1.093458
13	6	-0.429816	-0.052693	-0.520884	47	1	0.792293	-1.815786	-0.491552
14	6	0.744051	-0.86697	0.051107	48	1	0.667994	3.672997	1.361776
15	6	0.608015	3.497252	0.278968	49	1	1.273236	4.220314	-0.201995
16	6	-0.838649	3.714686	-0.170995	50	1	4.029685	-1.776721	2.425643
17	6	-1.42892	2.365063	-0.593787	51	1	2.977735	-0.365714	2.626202
18	8	6.596273	-2.268585	-1.748856	52	1	2.280751	-1.935931	2.206094
19	6	3.136295	-1.27501	2.041728	53	1	-0.066285	0.725915	2.189443
20	6	-0.866741	1.205153	1.621825	54	1	-1.065294	2.173405	2.091533
21	6	-2.976712	2.325882	-0.558019	55	1	-1.756126	0.582309	1.750269
22	6	-3.425003	1.023683	-1.229444	56	1	-3.273467	3.11996	-1.255571
23	6	-3.644913	2.643314	0.785891	57	1	-4.728151	2.73759	0.652668
24	6	-4.096286	-0.042961	-0.386773	58	1	-3.276817	3.600357	1.163487
25	8	-3.205277	0.851266	-2.418463	59	1	-3.469226	1.885889	1.550747
26	8	-1.420797	4.781025	-0.200672	60	1	-3.544754	-0.133001	0.554673
27	6	-4.190557	-1.39716	-1.086017	61	1	-5.093741	0.326044	-0.103934
28	6	-4.682135	-2.518085	-0.165745	62	1	-4.863815	-1.321297	-1.946054
29	6	-4.891729	-3.83563	-0.939861	63	1	-3.207727	-1.666382	-1.486294
30	6	-3.704486	-2.77094	0.969781	64	1	-5.638796	-2.236308	0.293627
31	8	-2.537513	-2.426305	0.998965	65	1	-5.256304	-4.629178	-0.281863
32	8	-4.273679	-3.474731	1.970778	66	1	-5.623433	-3.683483	-1.739437
33	1	1.868362	1.223611	1.635427	67	1	-3.952648	-4.166924	-1.397189
34	1	2.318852	-0.009842	-1.120071	68	1	-3.578139	-3.637094	2.644513

Conf-12

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	6.133377	1.028369	-0.693682	35	1	0.905539	0.593925	1.812878
2	6	6.669666	0.025561	0.242024	36	1	-0.900194	1.978738	1.872302
3	6	5.765623	-1.077597	0.587253	37	1	6.799686	1.841371	-0.970784
4	6	4.516996	-1.191826	0.095308	38	1	6.15717	-1.812112	1.287877
5	6	3.92404	-0.175159	-0.863979	39	1	4.543922	1.674662	-1.902582
6	6	4.89131	0.931776	-1.188333	40	1	4.123246	-2.95943	1.237967
7	6	3.598255	-2.292237	0.547001	41	1	3.281989	-2.901258	-0.310668
8	6	2.351558	-1.688566	1.21606	42	1	1.656803	-2.489624	1.49308
9	6	1.6553	-0.680138	0.296713	43	1	2.651639	-1.185588	2.145987
10	6	2.638926	0.42858	-0.16712	44	1	0.999956	2.655178	0.584538
11	6	0.47549	-0.003905	0.992806	45	1	0.21331	2.830346	-0.985548
12	6	-0.287626	0.998398	0.085313	46	1	1.654255	1.117729	-1.983535
13	6	0.691593	2.105023	-0.315814	47	1	2.636971	2.339231	-1.201651
14	6	1.938524	1.520173	-1.005274	48	1	-0.967845	-1.67081	0.949166
15	6	-0.636339	-0.859142	1.608863	49	1	-0.396456	-1.303947	2.57937
16	6	-1.801929	0.117909	1.747647	50	1	4.471775	-1.354469	-2.617267
17	6	-1.417597	1.437791	1.058059	51	1	2.802926	-1.6311	-2.091391

18	8	7.81014	0.110667	0.70757	52	1	3.226574	-0.140773	-2.944003
19	6	3.578639	-0.871041	-2.210086	53	1	-0.103921	-0.184348	-1.75523
20	6	-0.874886	0.317941	-1.166851	54	1	-1.626008	-0.438083	-0.918491
21	6	-2.502717	2.434581	0.578756	55	1	-1.343067	1.060597	-1.815936
22	6	-3.436125	1.967074	-0.541573	56	1	-1.957091	3.277343	0.138413
23	6	-3.334193	2.965319	1.765322	57	1	-4.052983	3.720484	1.429481
24	6	-4.484471	0.91186	-0.236627	58	1	-2.671702	3.436364	2.499834
25	8	-3.368056	2.473962	-1.650927	59	1	-3.873704	2.160359	2.267785
26	8	-2.835809	-0.122882	2.346798	60	1	-4.229871	0.399158	0.690447
27	6	-4.686922	-0.073017	-1.403977	61	1	-5.423554	1.444726	-0.028305
28	6	-5.235324	-1.442124	-0.948963	62	1	-5.362585	0.354365	-2.150901
29	6	-5.383908	-2.400814	-2.137172	63	1	-3.732355	-0.244326	-1.911492
30	6	-4.258814	-2.004489	0.068637	64	1	-6.201942	-1.305112	-0.452616
31	8	-3.108023	-2.315908	-0.185724	65	1	-6.046537	-1.966121	-2.892393
32	8	-4.774451	-2.065124	1.308166	66	1	-4.40819	-2.587594	-2.596488
33	1	1.284457	-1.227712	-0.578909	67	1	-5.805991	-3.362003	-1.825283
34	1	3.00891	0.913449	0.749325	68	1	-4.036209	-2.261141	1.926081

Conf-13

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	6.501085	-1.079078	0.600147	35	1	1.285948	-0.280922	-1.839578
2	6	7.063731	-0.009502	-0.241423	36	1	-0.558344	-1.624493	-2.016386
3	6	6.188894	1.143903	-0.483041	37	1	7.145735	-1.931128	0.800473
4	6	4.94403	1.245756	0.020739	38	1	6.599706	1.928529	-1.1149
5	6	4.324607	0.161925	0.885164	39	1	4.895613	-1.79087	1.749315
6	6	5.262077	-0.995466	1.104578	40	1	4.596317	3.119571	-0.955593
7	6	4.054829	2.407078	-0.325315	41	1	3.757685	2.944468	0.585482
8	6	2.790559	1.901276	-1.040791	42	1	2.117897	2.743154	-1.240766
9	6	2.068519	0.831047	-0.215977	43	1	3.074718	1.477841	-2.014229
10	6	3.023251	-0.341179	0.139978	44	1	1.323058	-2.446237	-0.806215
11	6	0.871507	0.252006	-0.968657	45	1	0.535072	-2.74333	0.7439
12	6	0.081435	-0.809296	-0.156571	46	1	2.027407	-1.170987	1.88988
13	6	1.031752	-1.972544	0.141752	47	1	2.97247	-2.339305	0.990634
14	6	2.295908	-1.487133	0.875943	48	1	-0.509977	1.952307	-0.777064
15	6	-0.215004	1.187878	-1.508773	49	1	0.041404	1.712344	-2.433781
16	6	-1.407306	0.251827	-1.739113	50	1	4.906488	1.158385	2.73783
17	6	-1.057231	-1.129444	-1.163028	51	1	3.247083	1.531987	2.24372
18	8	8.201824	-0.081347	-0.714569	52	1	3.625498	-0.042508	2.955069
19	6	3.999435	0.741168	2.290256	53	1	0.29269	0.155515	1.806541
20	6	-0.490942	-0.238101	1.155951	54	1	-1.199989	0.577987	0.982345
21	6	-2.184902	-2.101523	-0.755881	55	1	-1.013434	-1.017893	1.715013
22	6	-3.114755	-1.682088	0.390112	56	1	-1.689166	-3.000275	-0.370761
23	6	-3.033454	-2.516902	-1.977468	57	1	-3.811352	-3.229719	-1.683806
24	6	-3.974258	-0.443866	0.239596	58	1	-2.394534	-3.004069	-2.722418
25	8	-3.193531	-2.391216	1.382673	59	1	-3.502378	-1.650867	-2.447238
26	8	-2.433701	0.564837	-2.311125	60	1	-3.318195	0.406798	0.035925
27	6	-4.863861	-0.177635	1.451457	61	1	-4.578908	-0.553586	-0.667551
28	6	-5.738698	1.077955	1.31803	62	1	-5.501131	-1.048597	1.62796

29	6	-4.9325	2.364538	1.056226	63	1	-4.236039	-0.066645	2.342932
30	6	-6.829992	0.890651	0.276259	64	1	-6.273508	1.216114	2.269384
31	8	-7.04059	-0.121242	-0.363837	65	1	-5.571939	3.247559	1.12302
32	8	-7.590575	1.999358	0.1388	66	1	-4.133504	2.457453	1.799837
33	1	1.712441	1.303868	0.708653	67	1	-4.472135	2.357017	0.062789
34	1	3.379327	-0.748211	-0.818768	68	1	-8.271736	1.796132	-0.538091

Conf-14

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	6.474697	-1.192568	0.517887	35	1	1.272879	-0.125012	-1.858906
2	6	7.056006	-0.070122	-0.237768	36	1	-0.592908	-1.418933	-2.137837
3	6	6.199405	1.111618	-0.391988	37	1	7.105827	-2.067242	0.653187
4	6	4.954714	1.193477	0.115919	38	1	6.623859	1.936004	-0.961072
5	6	4.316546	0.056017	0.893691	39	1	4.855009	-1.966057	1.605704
6	6	5.235612	-1.129074	1.024943	40	1	4.637935	3.141532	-0.714837
7	6	4.08421	2.391525	-0.14127	41	1	3.793735	2.862366	0.807724
8	6	2.813551	1.961793	-0.89417	42	1	2.154171	2.826721	-1.02941
9	6	2.073699	0.842965	-0.153918	43	1	3.09266	1.609614	-1.89701
10	6	3.009799	-0.368021	0.110111	44	1	1.278284	-2.363798	-1.0003
11	6	0.867397	0.344141	-0.947991	45	1	0.485119	-2.772692	0.521484
12	6	0.061412	-0.765604	-0.220219	46	1	1.999379	-1.319471	1.788876
13	6	0.993718	-1.963504	-0.017132	47	1	2.927704	-2.426577	0.799184
14	6	2.264288	-1.557755	0.752963	48	1	-0.48483	2.048746	-0.62243
15	6	-0.204702	1.336867	-1.410709	49	1	0.05845	1.925616	-2.294234
16	6	-1.413679	0.441588	-1.706866	50	1	4.90765	0.899866	2.817974
17	6	-1.082999	-0.986629	-1.246246	51	1	3.254788	1.332992	2.351405
18	8	8.194455	-0.122872	-0.71248	52	1	3.609913	-0.296225	2.94115
19	6	3.996084	0.530613	2.338572	53	1	0.289963	0.038053	1.812631
20	6	-0.500474	-0.290407	1.134647	54	1	-1.195632	0.548801	1.027585
21	6	-2.225168	-1.970513	-0.916698	55	1	-1.034894	-1.103252	1.632126
22	6	-3.145251	-1.632631	0.262221	56	1	-1.743314	-2.905252	-0.607129
23	6	-3.081963	-2.272605	-2.165668	57	1	-3.868375	-2.997532	-1.92949
24	6	-3.987823	-0.371736	0.223613	58	1	-2.450779	-2.705738	-2.94944
25	8	-3.233965	-2.419237	1.193376	59	1	-3.539107	-1.364749	-2.562643
26	8	-2.439547	0.814368	-2.242266	60	1	-3.324004	0.48716	0.09322
27	6	-4.864631	-0.203924	1.462804	61	1	-4.586471	-0.385943	-0.696513
28	6	-5.752729	1.063664	1.427002	62	1	-5.496604	-1.087689	1.587535
29	6	-4.94831	2.362853	1.34641	63	1	-4.227587	-0.151399	2.352821
30	6	-6.734902	0.962068	0.274151	64	1	-6.347522	1.057315	2.349025
31	8	-6.689772	1.601745	-0.75768	65	1	-5.601345	3.234597	1.452227
32	8	-7.681424	0.02386	0.505831	66	1	-4.202262	2.39385	2.147792
33	1	1.724589	1.249049	0.804412	67	1	-4.435792	2.454144	0.385114
34	1	3.36174	-0.703905	-0.877326	68	1	-8.251234	-0.01246	-0.292598

Conf-15

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	-6.154184	-0.051519	-1.509346	35	1	-1.227602	-1.721281	1.104627

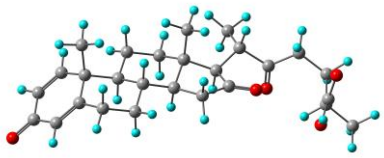
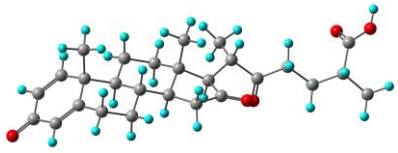
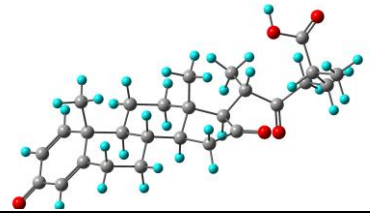
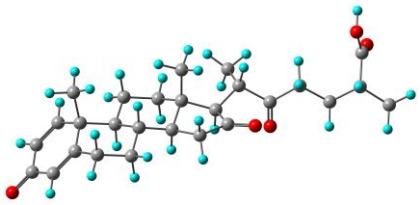
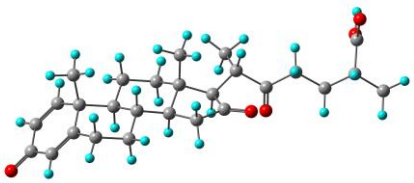
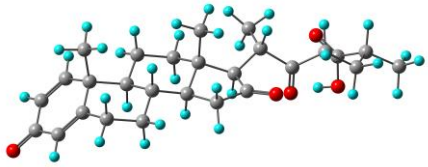
2	6	-6.812911	0.070961	-0.197919	36	1	0.572667	-2.868353	0.38299
3	6	-5.978736	0.588659	0.893132	37	1	-6.766233	-0.4185	-2.329354
4	6	-4.688201	0.939631	0.7342	38	1	-6.461377	0.666894	1.865024
5	6	-3.970921	0.822075	-0.599079	39	1	-4.429303	0.215473	-2.674668
6	6	-4.869336	0.288403	-1.682856	40	1	-4.462632	1.424211	2.807803
7	6	-3.851132	1.384174	1.900853	41	1	-3.464621	2.397847	1.728505
8	6	-2.664698	0.423269	2.088174	42	1	-2.024597	0.78167	2.902466
9	6	-1.850296	0.279476	0.798483	43	1	-3.045804	-0.562854	2.388085
10	6	-2.750892	-0.161579	-0.387227	44	1	-1.151174	-2.38687	-1.204812
11	6	-0.731276	-0.749386	0.95214	45	1	-0.196701	-1.494536	-2.391297
12	6	0.146086	-0.909923	-0.319595	46	1	-1.559529	0.522087	-2.077822
13	6	-0.760044	-1.390804	-1.455866	47	1	-2.590743	-0.846369	-2.44297
14	6	-1.938041	-0.423102	-1.673621	48	1	0.6417	0.437708	2.19511
15	6	0.290498	-0.59698	2.083981	49	1	-0.054318	-0.925041	3.069028
16	6	1.467434	-1.459316	1.618514	50	1	-4.362995	2.906548	-1.113847
17	6	1.171371	-1.957822	0.197444	51	1	-2.767794	2.663171	-0.383428
18	8	-7.994552	-0.244306	-0.028878	52	1	-3.056418	2.179862	-2.059935
19	6	-3.504652	2.229897	-1.063716	53	1	0.140238	1.222651	-0.848403
20	6	0.849526	0.403776	-0.711604	54	1	1.57056	0.728709	0.046441
21	6	2.332032	-2.445229	-0.707061	55	1	1.396588	0.27494	-1.646852
22	6	3.44287	-1.428726	-1.006289	56	1	1.879635	-2.637567	-1.687245
23	6	2.911788	-3.768183	-0.16998	57	1	3.704055	-4.146367	-0.824807
24	6	4.590526	-1.270659	-0.022495	58	1	2.123246	-4.527473	-0.128833
25	8	3.431054	-0.809604	-2.06021	59	1	3.316503	-3.64644	0.836976
26	8	2.449523	-1.709415	2.293029	60	1	4.211211	-1.354986	0.998146
27	6	5.425154	-0.00816	-0.245075	61	1	5.230479	-2.155409	-0.160142
28	6	4.660831	1.295001	0.029667	62	1	6.31118	-0.04399	0.397993
29	6	4.228322	1.451911	1.50206	63	1	5.785011	0.006002	-1.277809
30	6	5.506723	2.49225	-0.359778	64	1	3.765769	1.328792	-0.600659
31	8	6.708632	2.488978	-0.536577	65	1	3.680797	2.38713	1.649359
32	8	4.761148	3.616437	-0.468715	66	1	3.585253	0.624475	1.813017
33	1	-1.405739	1.257313	0.572858	67	1	5.10396	1.458059	2.161537
34	1	-3.201959	-1.120776	-0.090146	68	1	5.377201	4.347982	-0.688977

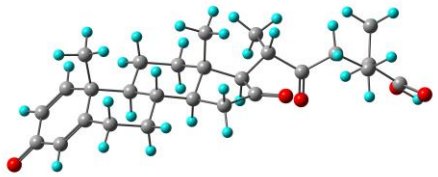
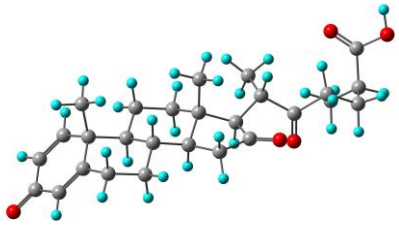
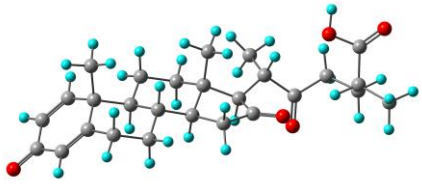
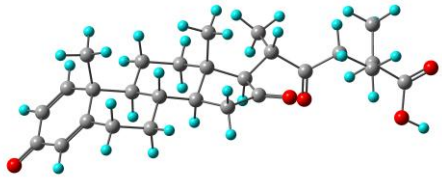
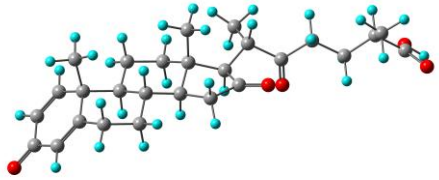
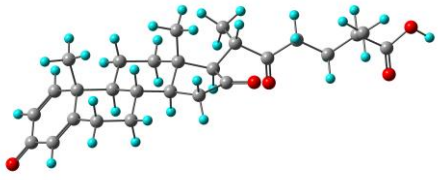
Conf-16

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	6.137669	1.211574	-0.539768	35	1	0.884307	0.423	1.800815
2	6	6.691265	0.161926	0.332243	36	1	-0.982805	1.755135	1.891676
3	6	5.821631	-0.994887	0.574941	37	1	6.779327	2.065584	-0.741493
4	6	4.58831	-1.116349	0.047216	38	1	6.225717	-1.765101	1.228531
5	6	3.977744	-0.05256	-0.847631	39	1	4.5504	1.8892	-1.734274
6	6	4.910172	1.108348	-1.068326	40	1	4.236615	-2.976937	1.047017
7	6	3.701641	-2.278934	0.395224	41	1	3.425642	-2.832977	-0.512184
8	6	2.419876	-1.771182	1.077855	42	1	1.749769	-2.614865	1.27847
9	6	1.705728	-0.72164	0.220539	43	1	2.682131	-1.329362	2.049393
10	6	2.658009	0.452239	-0.136447	44	1	0.913178	2.555632	0.736307
11	6	0.489807	-0.137477	0.937242	45	1	0.161853	2.818487	-0.838916
12	6	-0.294264	0.891934	0.078754	46	1	1.696426	1.247969	-1.920764

13	6	0.650133	2.063012	-0.210643	47	1	2.609125	2.438001	-1.015193
14	6	1.937618	1.580943	-0.905674	48	1	-0.900744	-1.837485	0.760785
15	6	-0.596214	-1.07025	1.482483	49	1	-0.346688	-1.578009	2.418881
16	6	-1.789591	-0.140691	1.682279	50	1	4.601866	-1.077486	-2.671039
17	6	-1.460719	1.220307	1.050418	51	1	2.934816	-1.451847	-2.202694
18	8	7.818345	0.252576	0.828555	52	1	3.318538	0.111878	-2.933828
19	6	3.68387	-0.657996	-2.248488	53	1	-0.013598	-0.095539	-1.859502
20	6	-0.823162	0.291287	-1.23623	54	1	-1.525116	-0.529706	-1.067843
21	6	-2.607343	2.163049	0.596179	55	1	-1.346753	1.058363	-1.811133
22	6	-3.670138	1.569	-0.345423	56	1	-2.127518	2.943245	-0.006612
23	6	-3.25975	2.830258	1.822939	57	1	-3.677089	2.085646	2.505122
24	6	-4.85983	0.855205	0.268991	58	1	-4.056672	3.520685	1.526568
25	8	-3.599188	1.765358	-1.548891	59	1	-2.507082	3.406909	2.371383
26	8	-2.804514	-0.430725	2.29217	60	1	-4.533699	0.278862	1.136465
27	6	-5.72627	0.015042	-0.677455	61	1	-5.489622	1.655838	0.686719
28	6	-5.113206	-1.313746	-1.218009	62	1	-6.641014	-0.229892	-0.129148
29	6	-4.399636	-1.173371	-2.564937	63	1	-6.020226	0.621648	-1.53979
30	6	-4.203851	-1.952088	-0.187217	64	1	-5.953393	-2.010913	-1.343155
31	8	-3.024987	-2.209457	-0.351601	65	1	-5.103455	-0.7964	-3.313887
32	8	-4.83816	-2.195609	0.976648	66	1	-3.566086	-0.473473	-2.504445
33	1	1.370638	-1.213488	-0.701417	67	1	-4.017866	-2.140921	-2.904361
34	1	2.992254	0.877567	0.822315	68	1	-4.152127	-2.454093	1.629841

Table S7. Re-optimized conformers, energies and proportions for **1**

Conf.	Conformer	Energy (hartree)	Proportion (%)
Conf-1		-1426.340600	33.27
Conf-2		-1426.339655	12.22
Conf-3		-1426.338117	2.39
Conf-4		-1426.339168	7.29
Conf-5		-1426.338778	4.82
Conf-6		-1426.338234	2.71

Conf-7		-1426.339259	8.03
Conf-8		-1426.337710	1.55
Conf-9		-1426.337837	1.78
Conf-10		-1426.339108	6.84
Conf-11		-1426.338684	4.36
Conf-12		-1426.338391	3.20

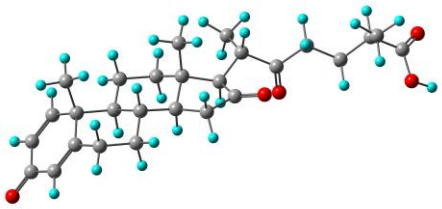
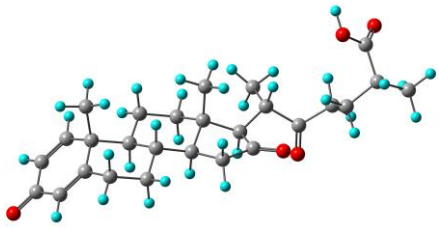
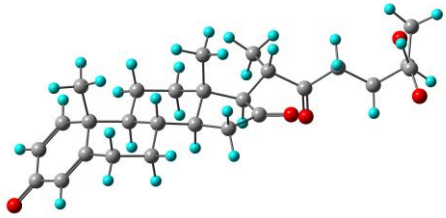
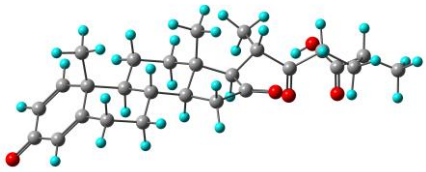
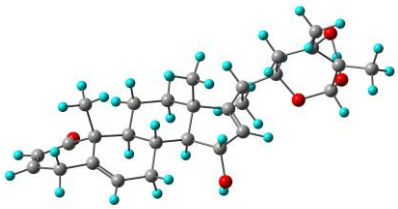
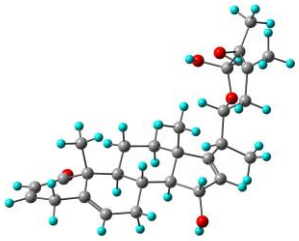
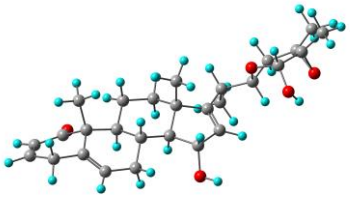
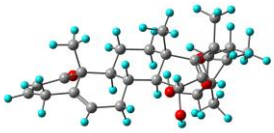
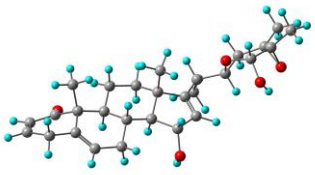
Conf-13		-1426.337708	1.55
Conf-14		-1426.337895	1.89
Conf-15		-1426.337731	1.59
Conf-16		-1426.339062	6.51

Table S8. Re-optimized conformers, energies and proportions for **2**

Conf.	Conformer	Energy (hartree)	Proportion (%)
Conf-1		-1465.520681	39.06
Conf-2		-1465.518887	5.83
Conf-3		-1465.518155	2.68
Conf-4		-1465.519742	14.44
Conf-5		-1465.520188	23.16

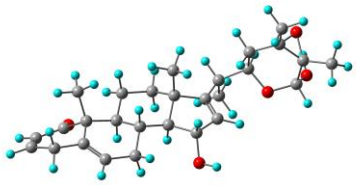
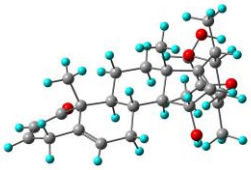
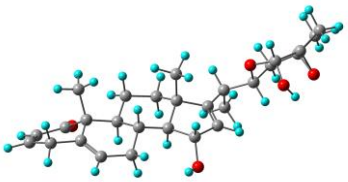
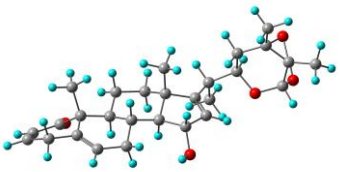
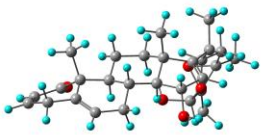
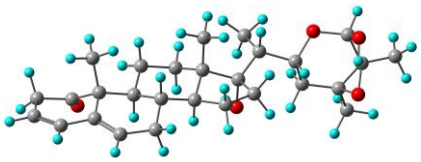
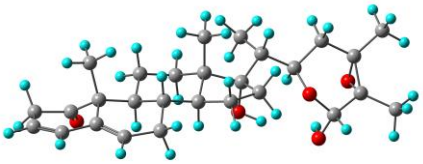
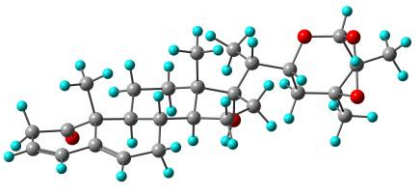
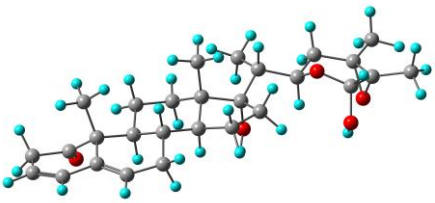
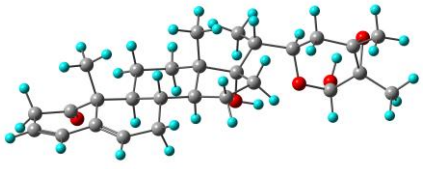
Conf-6		-1465.518849	5.60
Conf-7		-1465.517779	1.80
Conf-8		-1465.517822	1.89
Conf-9		-1465.518446	3.65
Conf-10		-1465.517819	1.88

Table S9. Re-optimized conformers, energies and proportions for **3**

Conf.	Conformer	Energy (hartree)	Proportion (%)
Conf-1		-1466.726535	41.07
Conf-2		-1466.724386	4.21
Conf-3		-1466.725747	17.81
Conf-4		-1466.723848	2.38
Conf-5		-1466.724380	4.18

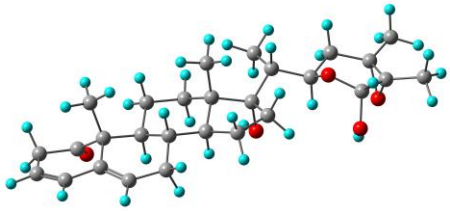
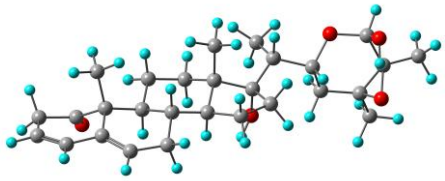
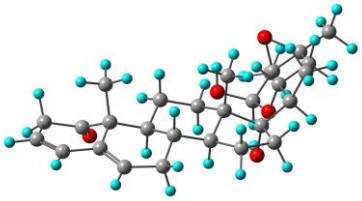
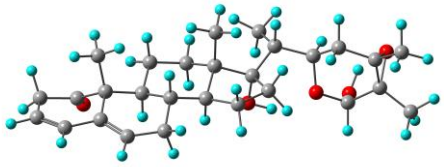
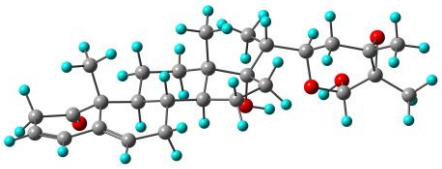
Conf-6		-1466.723817	2.30
Conf-7		-1466.725749	17.85
Conf-8		-1466.724160	3.31
Conf-9		-1466.724509	4.79
Conf-10		-1466.723724	2.09

Table S10. Cartesian coordinates of all optimized conformers of **1**

Conf-1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	6.472014	0.842535	1.122623	35	1	0.812681	-0.480848	0.962832
2	6	6.80723	-0.56634	1.382441	36	1	-1.170699	0.829326	1.206622
3	6	5.988077	-1.561911	0.684441	37	1	7.080147	1.590828	1.625176
4	6	4.985728	-1.235748	-0.155143	38	1	6.224756	-2.604276	0.8886
5	6	4.607603	0.204211	-0.449381	39	1	5.2789	2.236589	0.103137
6	6	5.474383	1.183821	0.294217	40	1	4.474933	-3.286386	-0.49899
7	6	4.119666	-2.290778	-0.783171	41	1	4.177376	-2.228125	-1.878292
8	6	2.657055	-2.091755	-0.349695	42	1	2.02141	-2.828023	-0.854324
9	6	2.170215	-0.671477	-0.655736	43	1	2.573441	-2.278951	0.729932
10	6	3.099195	0.390038	-0.01041	44	1	1.023837	1.866519	1.301925
11	6	0.75201	-0.438489	-0.136423	45	1	0.790058	3.023503	-0.004366
12	6	0.184423	0.973547	-0.471683	46	1	2.669453	2.108451	-1.272711
13	6	1.100193	1.996622	0.21374	47	1	3.176249	2.531294	0.349739
14	6	2.567878	1.82221	-0.219936	48	1	-0.324163	-1.669049	-1.612531
15	6	-0.360707	-1.408538	-0.546055	49	1	-0.379802	-2.349079	0.012927
16	6	-1.628114	-0.600331	-0.287101	50	1	5.839718	0.263324	-2.251094
17	6	-1.250552	0.832331	0.10693	51	1	4.138919	-0.102572	-2.586465
18	8	7.725532	-0.888982	2.145945	52	1	4.626169	1.549204	-2.182488
19	6	4.809473	0.493765	-1.963413	53	1	1.081459	1.180455	-2.471793
20	6	0.104175	1.237922	-1.987764	54	1	-0.553205	0.525121	-2.497828
21	6	-2.365058	1.821286	-0.268018	55	1	-0.293569	2.240057	-2.177953
22	6	-3.639297	1.438495	0.494298	56	1	-2.568855	1.750207	-1.342091
23	6	-2.035484	3.282746	0.084074	57	1	-2.90046	3.929838	-0.101007
24	6	-4.916745	1.338606	-0.311087	58	1	-1.207335	3.659358	-0.520629
25	8	-3.611947	1.303122	1.709295	59	1	-1.764963	3.37048	1.140775
26	8	-2.768356	-1.011684	-0.406346	60	1	-5.137	2.352041	-0.682279
27	6	-6.110216	0.78612	0.466521	61	1	-4.715025	0.73566	-1.201224
28	6	-5.955072	-0.678051	0.897293	62	1	-6.262737	1.388533	1.368439
29	6	-7.124469	-1.122415	1.798337	63	1	-7.01183	0.882961	-0.148151
30	6	-5.868014	-1.610736	-0.295723	64	1	-5.024441	-0.794133	1.460914
31	8	-6.186574	-1.340517	-1.439353	65	1	-8.080227	-1.032723	1.268835
32	8	-5.42594	-2.834448	0.060036	66	1	-7.005228	-2.160413	2.120989
33	1	2.173143	-0.5435	-1.74641	67	1	-7.169545	-0.486203	2.688095
34	1	3.086456	0.193347	1.07256	68	1	-5.415274	-3.38885	-0.752552

Conf-2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	6.671306	-1.452212	-0.977363	35	1	1.345291	0.86071	-1.029158
2	6	7.2611	-0.127127	-1.224385	36	1	-0.824633	-0.06668	-1.355022
3	6	6.610558	1.002014	-0.552764	37	1	7.153083	-2.299735	-1.458956
4	6	5.53697	0.86462	0.250041	38	1	7.037109	1.984207	-0.746633
5	6	4.896608	-0.482876	0.528053	39	1	5.213819	-2.605495	-0.001735

6	6	5.60051	-1.605497	-0.184911	40	1	5.390294	2.975194	0.57918
7	6	4.851617	2.060822	0.847411	41	1	4.855297	1.993814	1.943773
8	6	3.394589	2.125029	0.357503	42	1	2.882517	2.966316	0.837903
9	6	2.649343	0.817124	0.642801	43	1	3.387482	2.317804	-0.724353
10	6	3.396362	-0.398272	0.033762	44	1	1.142917	-1.490338	-1.357226
11	6	1.234022	0.838939	0.066737	45	1	0.653978	-2.574783	-0.059298
12	6	0.408354	-0.445135	0.379053	46	1	2.616764	-2.000044	1.28159
13	6	1.151891	-1.622239	-0.266599	47	1	3.101852	-2.522051	-0.318447
14	6	2.609089	-1.71007	0.224997	48	1	0.341508	2.257861	1.495783
15	6	0.298869	1.996826	0.429702	49	1	0.470785	2.919523	-0.132953
16	6	-1.08323	1.426315	0.124412	50	1	6.031924	-0.750984	2.373815
17	6	-0.951966	-0.052063	-0.260102	51	1	4.412261	-0.086628	2.646667
18	8	8.24671	0.022741	-1.956808	52	1	4.612267	-1.800841	2.258761
19	6	4.988335	-0.795963	2.047944	53	1	1.170463	-0.796092	2.414959
20	6	0.219691	-0.676987	1.890876	54	1	-0.315017	0.149237	2.372326
21	6	-2.240665	-0.820439	0.060434	55	1	-0.363242	-1.586907	2.06625
22	6	-3.388386	-0.255594	-0.784278	56	1	-2.493261	-0.68817	1.118686
23	6	-2.158088	-2.327249	-0.246776	57	1	-3.135187	-2.80471	-0.110024
24	6	-4.701031	-0.019482	-0.070857	58	1	-1.450905	-2.829396	0.417342
25	8	-3.250681	-0.079933	-1.985281	59	1	-1.84172	-2.490685	-1.28165
26	8	-2.135977	2.032708	0.207393	60	1	-4.963761	-0.939823	0.469012
27	6	-5.835762	0.417259	-0.992426	61	1	-4.503976	0.735778	0.702223
28	6	-7.135988	0.733387	-0.247486	62	1	-5.523942	1.309099	-1.546789
29	6	-8.206839	1.310246	-1.196103	63	1	-6.02599	-0.364162	-1.735871
30	6	-7.707433	-0.502428	0.424961	64	1	-6.94283	1.472309	0.540765
31	8	-7.49222	-1.653121	0.092337	65	1	-7.833183	2.226111	-1.664821
32	8	-8.540523	-0.181322	1.435788	66	1	-8.444898	0.593445	-1.990031
33	1	2.586604	0.697452	1.732667	67	1	-9.128232	1.548361	-0.656766
34	1	3.458604	-0.210874	-1.049136	68	1	-8.911458	-1.021075	1.791908

Conf-3

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	6.339236	-1.46345	0.103244	35	1	1.028425	0.180614	-1.599694
2	6	6.931594	-0.313633	-0.598061	36	1	-1.054037	-0.952366	-1.791319
3	6	6.161897	0.933314	-0.553922	37	1	6.906829	-2.390789	0.088709
4	6	4.98205	1.050344	0.086635	38	1	6.591709	1.779883	-1.085729
5	6	4.336018	-0.111114	0.81913	39	1	4.774789	-2.229103	1.274968
6	6	5.163747	-1.365078	0.740856	40	1	4.740866	3.088483	-0.5232
7	6	4.188313	2.325004	0.033596	41	1	4.02962	2.716817	1.047411
8	6	2.819654	2.06175	-0.618149	42	1	2.223146	2.980801	-0.602279
9	6	2.069544	0.928859	0.090288	43	1	2.969819	1.792508	-1.672945
10	6	2.927466	-0.361628	0.144593	44	1	0.938688	-2.104284	-0.949001
11	6	0.755976	0.596408	-0.616543	45	1	0.285122	-2.609637	0.605232
12	6	-0.079219	-0.512633	0.090602	46	1	1.998622	-1.370991	1.83219
13	6	0.782861	-1.782845	0.089939	47	1	2.735735	-2.459857	0.674623
14	6	2.148431	-1.540469	0.760027	48	1	-0.361538	2.397655	-0.024547
15	6	-0.247171	1.720835	-0.882045	49	1	-0.020356	2.343453	-1.75299
16	6	-1.561869	0.972099	-1.081812	50	1	5.182029	0.496606	2.738163

17	6	-1.342529	-0.524368	-0.817432	51	1	3.527924	1.082163	2.493276
18	8	8.014459	-0.397165	-1.190301	52	1	3.815733	-0.617681	2.889335
19	6	4.201162	0.23788	2.327968	53	1	0.372705	0.08643	2.162376
20	6	-0.48915	-0.12605	1.526046	54	1	-1.138367	0.756083	1.548996
21	6	-2.62495	-1.22738	-0.362644	55	1	-1.045012	-0.943814	1.995995
22	6	-3.686069	-1.207081	-1.465067	56	1	-3.034165	-0.721734	0.517771
23	6	-2.414037	-2.714759	-0.001666	57	1	-3.370614	-3.214282	0.184773
24	6	-5.141776	-1.31769	-1.033895	58	1	-1.811582	-2.816999	0.903167
25	8	-3.383671	-1.194555	-2.647941	59	1	-1.908532	-3.242027	-0.81711
26	8	-2.624338	1.493037	-1.36758	60	1	-5.651974	-1.933413	-1.781682
27	6	-5.868673	0.04143	-0.948505	61	1	-5.219069	-1.828028	-0.067496
28	6	-5.397366	0.977712	0.174552	62	1	-5.757911	0.567766	-1.903232
29	6	-6.246834	2.262366	0.206157	63	1	-6.936394	-0.161637	-0.808939
30	6	-5.498857	0.300129	1.526077	64	1	-4.356731	1.255978	0.005956
31	8	-6.442466	-0.364653	1.910121	65	1	-5.899293	2.948756	0.985276
32	8	-4.411224	0.533128	2.293113	66	1	-6.176403	2.776827	-0.75762
33	1	1.846726	1.261597	1.112812	67	1	-7.299289	2.026398	0.397035
34	1	3.150058	-0.628608	-0.899864	68	1	-4.556046	0.088377	3.16048

Conf-4

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	6.65039	-1.440019	-1.005264	35	1	1.324883	0.874702	-1.025614
2	6	7.240966	-0.111365	-1.23027	36	1	-0.844854	-0.047026	-1.368382
3	6	6.589836	1.007194	-0.541733	37	1	7.132464	-2.279856	-1.499841
4	6	5.515268	0.857397	0.257523	38	1	7.016922	1.992186	-0.719542
5	6	4.874316	-0.494188	0.513343	39	1	5.191287	-2.608188	-0.049884
6	6	5.578628	-1.605566	-0.21661	40	1	5.368594	2.962535	0.619822
7	6	4.829553	2.04413	0.873092	41	1	4.832252	1.959823	1.968261
8	6	3.37296	2.116376	0.383029	42	1	2.860638	2.94996	0.876407
9	6	2.627246	0.804194	0.646721	43	1	3.36681	2.326411	-0.695603
10	6	3.374613	-0.401392	0.018896	44	1	1.122198	-1.470637	-1.391582
11	6	1.212503	0.83548	0.069664	45	1	0.631965	-2.575701	-0.111649
12	6	0.386326	-0.453302	0.360632	46	1	2.593707	-2.022928	1.240034
13	6	1.130187	-1.620009	-0.303214	47	1	3.080057	-2.519139	-0.367807
14	6	2.586952	-1.715954	0.188244	48	1	0.318977	2.231856	1.520262
15	6	0.277376	1.987755	0.45014	49	1	0.450158	2.919199	-0.097652
16	6	-1.104406	1.422682	0.134385	50	1	6.007703	-0.792834	2.355636
17	6	-0.973275	-0.049468	-0.273504	51	1	4.388531	-0.131082	2.637576
18	8	8.227245	0.049902	-1.959352	52	1	4.586975	-1.839155	2.222644
19	6	4.964356	-0.831472	2.028187	53	1	1.146813	-0.837038	2.391095
20	6	0.1964	-0.709543	1.868355	54	1	-0.338736	0.108713	2.362761
21	6	-2.262766	-0.821823	0.034379	55	1	-0.386477	-1.622295	2.028529
22	6	-3.409442	-0.241571	-0.800478	56	1	-2.515088	-0.7067	1.094714
23	6	-2.181792	-2.323396	-0.297894	57	1	-3.159116	-2.802536	-0.168625
24	6	-4.720852	-0.009167	-0.081582	58	1	-1.474736	-2.836808	0.357633
25	8	-3.274247	-0.048142	-1.99875	59	1	-1.865933	-2.469816	-1.335439
26	8	-2.157305	2.027613	0.226006	60	1	-4.976567	-0.930962	0.461579
27	6	-5.854334	0.437361	-1.000893	61	1	-4.523139	0.741151	0.695529

28	6	-7.157875	0.779681	-0.251891	62	1	-5.533858	1.322256	-1.56117
29	6	-8.234147	1.287796	-1.220379	63	1	-6.062804	-0.343602	-1.741266
30	6	-7.65585	-0.460173	0.467813	64	1	-6.943737	1.545902	0.501457
31	8	-8.125148	-1.438111	-0.083427	65	1	-9.148817	1.57095	-0.688727
32	8	-7.495118	-0.383005	1.804334	66	1	-7.868076	2.165756	-1.762086
33	1	2.563467	0.667053	1.734462	67	1	-8.488607	0.510429	-1.947303
34	1	3.437994	-0.196548	-1.060762	68	1	-7.814092	-1.231911	2.189872

Conf-5

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	6.647291	-1.476048	-0.972748	35	1	1.329593	0.85824	-1.042206
2	6	7.242904	-0.155374	-1.22929	36	1	-0.844098	-0.063236	-1.360107
3	6	6.596534	0.981588	-0.566884	37	1	7.125765	-2.32918	-1.44768
4	6	5.521994	0.854787	0.236385	38	1	7.027222	1.960486	-0.768116
5	6	4.876092	-0.487937	0.52454	39	1	5.18457	-2.615809	0.010887
6	6	5.575507	-1.618858	-0.179686	40	1	5.383657	2.96843	0.548987
7	6	4.841356	2.058331	0.824337	41	1	4.844839	1.999873	1.921192
8	6	3.384559	2.124598	0.334052	42	1	2.875955	2.971623	0.808002
9	6	2.634165	0.821924	0.629567	43	1	3.378039	2.309005	-0.749259
10	6	3.376258	-0.400983	0.029553	44	1	1.118022	-1.494194	-1.35292
11	6	1.218723	0.845014	0.053849	45	1	0.625338	-2.567309	-0.046996
12	6	0.388354	-0.433603	0.376075	46	1	2.590726	-1.990775	1.289009
13	6	1.126897	-1.618244	-0.261373	47	1	3.073262	-2.525997	-0.307421
14	6	2.583887	-1.708248	0.230396	48	1	0.332602	2.2785	1.472585
15	6	0.288197	2.009237	0.408651	49	1	0.463194	2.926836	-0.161372
16	6	-1.096181	1.441697	0.108748	50	1	6.010216	-0.746616	2.37239
17	6	-0.970725	-0.039898	-0.265278	51	1	4.393281	-0.073585	2.640086
18	8	8.22963	-0.015235	-1.962136	52	1	4.586303	-1.791519	2.265301
19	6	4.966459	-0.789818	2.046829	53	1	1.150218	-0.772094	2.414092
20	6	0.19959	-0.653576	1.88966	54	1	-0.331969	0.178035	2.365279
21	6	-2.262118	-0.800574	0.062689	55	1	-0.386323	-1.5602	2.072128
22	6	-3.408739	-0.23615	-0.782905	56	1	-2.51198	-0.660199	1.120559
23	6	-2.186757	-2.309775	-0.234792	57	1	-3.165413	-2.782519	-0.092637
24	6	-4.719187	0.012731	-0.067484	58	1	-1.480239	-2.810193	0.43127
25	8	-3.275403	-0.068812	-1.985266	59	1	-1.873287	-2.481425	-1.269201
26	8	-2.146952	2.051962	0.188553	60	1	-4.975614	-0.8999	0.491385
27	6	-5.855645	0.43784	-0.992755	61	1	-4.519517	0.778187	0.694427
28	6	-7.152742	0.786112	-0.241875	62	1	-5.542072	1.31644	-1.567165
29	6	-8.262832	1.216687	-1.216107	63	1	-6.055794	-0.355504	-1.720838
30	6	-7.626408	-0.373309	0.614974	64	1	-6.953247	1.603098	0.46064
31	8	-7.819152	-0.327203	1.814858	65	1	-8.493287	0.412405	-1.921548
32	8	-7.823439	-1.49537	-0.109893	66	1	-9.181938	1.480995	-0.682424
33	1	2.571263	0.710894	1.720315	67	1	-7.936611	2.092584	-1.786426
34	1	3.439238	-0.221823	-1.054696	68	1	-8.13399	-2.195193	0.50878

Conf-6

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z

1	6	6.135977	-2.20281	-0.330776	35	1	1.061061	0.492579	-1.186221
2	6	6.793176	-1.287534	-1.276894	36	1	-1.196773	-0.152044	-0.82511
3	6	6.334875	0.104738	-1.249016	37	1	6.476305	-3.235531	-0.332673
4	6	5.37444	0.549296	-0.414725	38	1	6.809545	0.778951	-1.959202
5	6	4.670227	-0.36204	0.573479	39	1	4.736574	-2.478023	1.209496
6	6	5.175084	-1.777657	0.502243	40	1	5.447246	2.528869	-1.22739
7	6	4.878225	1.965986	-0.480669	41	1	5.028837	2.467279	0.485001
8	6	3.377383	1.978021	-0.819006	42	1	3.00751	3.009468	-0.810355
9	6	2.574106	1.117631	0.161834	43	1	3.235831	1.592859	-1.838444
10	6	3.128459	-0.3299	0.220732	44	1	0.625792	-1.646651	-0.228992
11	6	1.099519	1.043878	-0.233127	45	1	0.229156	-1.842188	1.474989
12	6	0.221639	0.225165	0.760349	46	1	2.396452	-0.947428	2.173398
13	6	0.771404	-1.207297	0.767379	47	1	2.615699	-2.272183	1.048652
14	6	2.269484	-1.236848	1.124251	48	1	0.533671	3.101783	0.313246
15	6	0.320784	2.344723	-0.453481	49	1	0.485717	2.818929	-1.425889
16	6	-1.132464	1.900649	-0.307821	50	1	6.021853	0.187278	2.197939
17	6	-1.176099	0.427151	0.112542	51	1	4.517517	1.123212	2.20206
18	8	7.678925	-1.672874	-2.049807	52	1	4.51585	-0.557704	2.753078
19	6	4.943304	0.133452	2.021459	53	1	1.22079	0.85155	2.620185
20	6	0.220935	0.82066	2.181763	54	1	-0.173502	1.842604	2.201626
21	6	-2.467242	0.106415	0.876106	55	1	-0.40637	0.217611	2.845931
22	6	-3.668915	0.301649	-0.052815	56	1	-2.573507	0.795881	1.72167
23	6	-2.536398	-1.339435	1.403512	57	1	-3.530961	-1.559169	1.801976
24	6	-4.862355	1.03134	0.533204	58	1	-1.803941	-1.503321	2.197441
25	8	-3.661292	-0.138865	-1.191881	59	1	-2.341678	-2.049751	0.594071
26	8	-2.109379	2.611559	-0.459901	60	1	-5.035568	0.665183	1.554095
27	6	-6.138121	0.972996	-0.308702	61	1	-4.523433	2.0701	0.645114
28	6	-7.016053	-0.277413	-0.066339	62	1	-6.759004	1.846402	-0.080182
29	6	-8.327982	-0.187576	-0.855779	63	1	-5.873671	1.0303	-1.369976
30	6	-6.237829	-1.542974	-0.36989	64	1	-7.236446	-0.329102	1.006378
31	8	-5.632634	-2.1945	0.462869	65	1	-8.957593	-1.067707	-0.6886
32	8	-6.263634	-1.878241	-1.672945	66	1	-8.890193	0.697907	-0.540912
33	1	2.652649	1.578336	1.155609	67	1	-8.134109	-0.108547	-1.929381
34	1	3.057531	-0.729113	-0.802648	68	1	-5.688105	-2.668849	-1.781539

Conf-7

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	6.301635	-2.206135	-0.484157	35	1	1.194409	0.478164	-1.158937
2	6	6.932738	-1.257673	-1.415283	36	1	-1.052109	-0.194497	-0.775682
3	6	6.466973	0.130043	-1.334132	37	1	6.648788	-3.235789	-0.524601
4	6	5.520903	0.541859	-0.4673	38	1	6.922872	0.829251	-2.032343
5	6	4.841998	-0.404784	0.505344	39	1	4.936266	-2.538505	1.075213
6	6	5.355282	-1.813652	0.38091	40	1	5.56487	2.546274	-1.218882
7	6	5.014328	1.956381	-0.479198	41	1	5.180506	2.428512	0.498528
8	6	3.507129	1.968164	-0.788095	42	1	3.130601	2.99607	-0.739316
9	6	2.728569	1.071075	0.179781	43	1	3.348443	1.614698	-1.816447
10	6	3.293797	-0.373475	0.181869	44	1	0.791571	-1.693507	-0.26342
11	6	1.247312	0.999157	-0.189634	45	1	0.42953	-1.947173	1.44085

12	6	0.394633	0.142464	0.793739	46	1	2.603836	-1.061174	2.126673
13	6	0.953568	-1.285572	0.743702	47	1	2.809949	-2.34586	0.953958
14	6	2.458446	-1.316199	1.070958	48	1	0.678167	3.035022	0.432101
15	6	0.45553	2.300699	-0.353718	49	1	0.598439	2.806085	-1.313818
16	6	-0.991392	1.84177	-0.194	50	1	4.728348	-0.667889	2.680344
17	6	-1.016116	0.354824	0.179213	51	1	6.219457	0.10359	2.121347
18	8	7.803662	-1.612942	-2.218812	52	1	4.709944	1.029092	2.181151
19	6	5.138227	0.048093	1.962676	53	1	1.425385	0.714828	2.653048
20	6	0.417393	0.691471	2.23342	54	1	0.016969	1.709446	2.294276
21	6	-2.290668	0.008484	0.956904	55	1	-0.192746	0.062728	2.889914
22	6	-3.512226	0.223375	0.0593	56	1	-2.382268	0.668928	1.826835
23	6	-2.353751	-1.454515	1.436208	57	1	-3.331059	-1.67638	1.880913
24	6	-4.715568	0.884205	0.701528	58	1	-1.595378	-1.655934	2.19612
25	8	-3.519885	-0.176779	-1.095289	59	1	-2.199078	-2.140242	0.597398
26	8	-1.977171	2.548413	-0.30126	60	1	-4.828651	0.499357	1.723192
27	6	-6.007774	0.774465	-0.105755	61	1	-4.432633	1.938981	0.823515
28	6	-6.547338	-0.658234	-0.228851	62	1	-6.776214	1.407423	0.35152
29	6	-6.954156	-1.275068	1.124731	63	1	-5.830062	1.171691	-1.109976
30	6	-7.741456	-0.691232	-1.165108	64	1	-5.778714	-1.296292	-0.679374
31	8	-8.386	0.273146	-1.531105	65	1	-7.361675	-2.280305	0.988581
32	8	-8.040048	-1.951301	-1.548024	66	1	-6.090464	-1.350545	1.792005
33	1	2.822701	1.500505	1.186136	67	1	-7.712302	-0.657701	1.620518
34	1	3.20694	-0.740137	-0.852395	68	1	-8.837189	-1.902941	-2.123332

Conf-8

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	6.178718	-2.133373	-0.660852	35	1	1.228993	0.874782	-1.157586
2	6	6.932647	-1.003442	-1.226193	36	1	-1.055639	0.238712	-1.219274
3	6	6.482054	0.333881	-0.828809	37	1	6.512202	-3.130904	-0.936638
4	6	5.444235	0.546035	0.004257	38	1	7.029983	1.170462	-1.257918
5	6	4.637996	-0.590863	0.604636	39	1	4.629402	-2.801336	0.588058
6	6	5.140689	-1.939322	0.165472	40	1	5.609646	2.673479	-0.17253
7	6	4.964653	1.935666	0.315151	41	1	5.018837	2.123985	1.395942
8	6	3.506148	2.099745	-0.146302	42	1	3.142467	3.094852	0.133436
9	6	2.602698	1.01674	0.452383	43	1	3.46726	2.038325	-1.24282
10	6	3.14082	-0.401995	0.12982	44	1	0.688964	-1.434657	-0.930369
11	6	1.175164	1.116115	-0.084013	45	1	0.120559	-2.115001	0.590788
12	6	0.198196	0.070438	0.532342	46	1	2.211299	-1.548341	1.727718
13	6	0.735642	-1.317968	0.161051	47	1	2.536381	-2.483251	0.282651
14	6	2.189701	-1.506252	0.633048	48	1	0.575859	2.941401	0.995787
15	6	0.429929	2.450692	0.024152	49	1	0.689356	3.183394	-0.746331
16	6	-1.034486	2.035302	-0.095494	50	1	5.818266	-0.594066	2.441573
17	6	-1.126162	0.505506	-0.152337	51	1	4.327427	0.353305	2.577726
18	8	7.888898	-1.174483	-1.992163	52	1	4.258545	-1.41412	2.602424
19	6	4.763358	-0.554192	2.153662	53	1	1.01175	0.079289	2.578946
20	6	0.060229	0.216031	2.060541	54	1	-0.327505	1.199378	2.348739
21	6	-2.488148	0.024452	0.354448	55	1	-0.633598	-0.534202	2.453192
22	6	-3.591705	0.512818	-0.586826	56	1	-2.680044	0.445912	1.348092

23	6	-2.633973	-1.508391	0.438136	57	1	-3.662356	-1.786377	0.694506
24	6	-4.886065	0.94632	0.074638	58	1	-1.97622	-1.925277	1.204458
25	8	-3.440701	0.513347	-1.798306	59	1	-2.382468	-1.970275	-0.522224
26	8	-1.988729	2.791529	-0.09547	60	1	-5.025668	0.378133	1.001269
27	6	-6.131064	0.901491	-0.815295	61	1	-4.692348	1.981051	0.392696
28	6	-6.773985	-0.501554	-0.997313	62	1	-6.889312	1.567934	-0.391468
29	6	-5.93006	-1.486408	-1.810065	63	1	-5.874107	1.287073	-1.80717
30	6	-7.099863	-1.071136	0.370092	64	1	-7.728119	-0.337646	-1.512151
31	8	-6.415633	-1.869611	0.985092	65	1	-6.492956	-2.406462	-1.999784
32	8	-8.233729	-0.547122	0.877738	66	1	-5.652377	-1.042148	-2.769466
33	1	2.582216	1.160073	1.540918	67	1	-5.013888	-1.761294	-1.285407
34	1	3.173758	-0.476855	-0.967899	68	1	-8.351601	-0.916632	1.783004

Conf-9

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	-6.474746	1.386904	-0.339809	35	1	-1.044513	-0.393952	-1.377473
2	6	-7.005793	0.13602	-0.903726	36	1	1.018519	0.709793	-1.58886
3	6	-6.234348	-1.077352	-0.61766	37	1	-7.044389	2.292265	-0.535185
4	6	-5.106154	-1.078363	0.119381	38	1	-6.617427	-2.000426	-1.04827
5	6	-4.525119	0.189244	0.718146	39	1	-5.008247	2.344082	0.817687
6	6	-5.350826	1.403888	0.391337	40	1	-4.80777	-3.17991	-0.161153
7	6	-4.303294	-2.333253	0.315197	41	1	-4.219033	-2.56815	1.384896
8	6	-2.891206	-2.145216	-0.265921	42	1	-2.292136	-3.042015	-0.072009
9	6	-2.203103	-0.9091	0.322366	43	1	-2.96341	-2.034899	-1.356914
10	6	-3.069334	0.361724	0.124113	44	1	-1.011223	1.965919	-1.054192
11	6	-0.84254	-0.660665	-0.327948	45	1	-0.480251	2.693616	0.457962
12	6	-0.06752	0.551261	0.270649	46	1	-2.2782	1.615101	1.714897
13	6	-0.933518	1.795384	0.028356	47	1	-2.928814	2.516935	0.36162
14	6	-2.345484	1.628223	0.621278	48	1	0.228566	-2.352754	0.589452
15	6	0.183889	-1.795804	-0.355849	49	1	0.031136	-2.530631	-1.152488
16	6	1.509252	-1.061488	-0.548181	50	1	-5.515282	-0.145821	2.635301
17	6	1.255046	0.452149	-0.5437	51	1	-3.84195	-0.727882	2.608008
18	8	-8.041411	0.112536	-1.579973	52	1	-4.174523	1.005589	2.724083
19	6	-4.50725	0.06916	2.267974	53	1	-0.667956	0.271429	2.37134
20	6	0.238819	0.374029	1.771179	54	1	0.857633	-0.509163	1.964296
21	6	2.50167	1.245432	-0.142663	55	1	0.784841	1.241356	2.155321
22	6	3.576579	1.152657	-1.224948	56	1	2.934393	0.828648	0.774199
23	6	2.243293	2.751904	0.082534	57	1	3.181631	3.290341	0.250919
24	6	5.002637	1.521597	-0.825342	58	1	1.612342	2.916478	0.958124
25	8	3.316945	0.871695	-2.384156	59	1	1.74832	3.195342	-0.787664
26	8	2.59551	-1.601416	-0.640118	60	1	5.276187	2.410751	-1.407268
27	6	5.999732	0.397355	-1.149581	61	1	5.051989	1.797055	0.232613
28	6	5.84607	-0.862171	-0.268111	62	1	5.862266	0.103846	-2.195965
29	6	6.811973	-1.963583	-0.720785	63	1	7.022083	0.779065	-1.046284
30	6	6.123746	-0.487348	1.174674	64	1	4.814375	-1.214959	-0.337561
31	8	7.227	-0.280195	1.64321	65	1	6.687745	-2.872662	-0.122769
32	8	4.992673	-0.366989	1.904777	66	1	6.625974	-2.21771	-1.769222
33	1	-2.055815	-1.085619	1.396306	67	1	7.849782	-1.630567	-0.621116

34	1	-3.211147	0.472369	-0.961881	68	1	5.253755	-0.083451	2.811581

Conf-10

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	6.32049	-2.074215	-0.802966	35	1	1.18168	0.626291	-1.072284
2	6	6.944345	-0.988674	-1.575738	36	1	-1.059208	-0.117563	-0.791687
3	6	6.462218	0.36554	-1.287879	37	1	6.678657	-3.082168	-0.998079
4	6	5.509223	0.631003	-0.372833	38	1	6.912095	1.167324	-1.870097
5	6	4.839419	-0.459148	0.443197	39	1	4.954012	-2.653832	0.681279
6	6	5.367405	-1.827487	0.107439	40	1	5.532388	2.726174	-0.812961
7	6	4.987394	2.025612	-0.172337	41	1	5.147579	2.346337	0.865942
8	6	3.480474	2.068148	-0.479681	42	1	3.092974	3.073095	-0.277978
9	6	2.711178	1.027863	0.341053	43	1	3.326348	1.871445	-1.549811
10	6	3.290945	-0.394824	0.126378	44	1	0.800056	-1.657652	-0.512546
11	6	1.230605	0.9973	-0.036101	45	1	0.443511	-2.167778	1.13445
12	6	0.388041	-0.004989	0.808637	46	1	2.609945	-1.374705	1.944956
13	6	0.960085	-1.404068	0.544339	47	1	2.826932	-2.465866	0.592067
14	6	2.465776	-1.469045	0.862903	48	1	0.643091	2.912036	0.882512
15	6	0.426082	2.300965	-0.003965	49	1	0.562264	2.945385	-0.877939
16	6	-1.016004	1.809566	0.086197	50	1	6.21135	-0.185254	2.119707
17	6	-1.026038	0.283644	0.234403	51	1	4.69044	0.701922	2.316481
18	8	7.822786	-1.208389	-2.418564	52	1	4.730051	-1.050693	2.553154
19	6	5.130847	-0.229327	1.95284	53	1	1.418803	0.291068	2.731768
20	6	0.410043	0.322367	2.314431	54	1	0.001493	1.316343	2.527695
21	6	-2.295589	-0.187381	0.952816	55	1	-0.193173	-0.402734	2.870257
22	6	-3.520523	0.150436	0.098621	56	1	-2.390646	0.333569	1.912466
23	6	-2.34422	-1.706514	1.205523	57	1	-3.318158	-2.002309	1.612961
24	6	-4.724531	0.705707	0.832436	58	1	-1.581831	-2.013366	1.925014
25	8	-3.529773	-0.07616	-1.102045	59	1	-2.185675	-2.255865	0.27237
26	8	-2.008729	2.514694	0.084616	60	1	-4.839296	0.173123	1.784912
27	6	-6.016608	0.716276	0.017332	61	1	-4.445506	1.732002	1.108861
28	6	-6.555108	-0.694599	-0.330646	62	1	-6.785858	1.2612	0.578753
29	6	-6.893963	-1.534805	0.901461	63	1	-5.841666	1.263531	-0.913257
30	6	-7.774165	-0.538356	-1.220249	64	1	-5.788658	-1.197738	-0.930571
31	8	-8.924031	-0.766776	-0.896204	65	1	-7.62192	-1.020143	1.537005
32	8	-7.443239	-0.080339	-2.446836	66	1	-7.326406	-2.49679	0.611165
33	1	2.801153	1.302419	1.400538	67	1	-5.997838	-1.736008	1.495724
34	1	3.206975	-0.602402	-0.951373	68	1	-8.27899	0.029377	-2.954858

Conf-11

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	6.714803	-1.486878	-0.891096	35	1	1.274171	0.5494	-1.098369
2	6	7.221847	-0.224539	-1.451643	36	1	-0.857526	-0.509999	-1.077739
3	6	6.54767	0.996629	-1.000598	37	1	7.2148	-2.398848	-1.208308
4	6	5.525541	0.994309	-0.122397	38	1	6.91167	1.929331	-1.426963
5	6	4.972293	-0.285041	0.477862	39	1	5.371348	-2.45765	0.396996
6	6	5.695587	-1.506857	-0.019995	40	1	5.284698	3.118177	-0.246815

7	6	4.810721	2.263462	0.246132	41	1	4.87782	2.437351	1.328631
8	6	3.327726	2.161315	-0.150512	42	1	2.798875	3.065654	0.170796
9	6	2.66953	0.917596	0.455793	43	1	3.251009	2.114297	-1.245736
10	6	3.445679	-0.369555	0.072305	44	1	1.180074	-1.823199	-0.908433
11	6	1.225307	0.758379	-0.017763	45	1	0.821342	-2.623762	0.617958
12	6	0.488157	-0.461385	0.612452	46	1	2.821414	-1.698229	1.67732
13	6	1.256042	-1.718443	0.182517	47	1	3.245045	-2.529479	0.194988
14	6	2.740501	-1.640708	0.586124	48	1	0.341124	2.415448	1.13389
15	6	0.25117	1.928515	0.15347	49	1	0.339984	2.71402	-0.603287
16	6	-1.11349	1.250506	0.071531	50	1	6.216063	-0.101772	2.263057
17	6	-0.92472	-0.268964	-0.004093	51	1	4.581568	0.5438	2.48792
18	8	8.161079	-0.197925	-2.256291	52	1	4.84757	-1.204885	2.465979
19	6	5.160283	-0.25638	2.020759	53	1	1.380366	-0.338719	2.621597
20	6	0.396732	-0.371549	2.148246	54	1	-0.152368	0.517066	2.478675
21	6	-2.150299	-1.003811	0.554396	55	1	-0.127161	-1.245018	2.5497
22	6	-3.371828	-0.676418	-0.311646	56	1	-2.349485	-0.660549	1.575997
23	6	-2.004545	-2.53695	0.564129	57	1	-2.945176	-3.014098	0.862347
24	6	-4.650967	-0.338942	0.424412	58	1	-1.235248	-2.85749	1.270338
25	8	-3.31449	-0.754755	-1.529001	59	1	-1.738555	-2.903203	-0.432283
26	8	-2.191237	1.81677	0.101063	60	1	-4.834502	-1.126252	1.171553
27	6	-5.856437	-0.163436	-0.494063	61	1	-4.438841	0.570471	0.999287
28	6	-7.171456	0.10191	0.276255	62	1	-5.667694	0.666763	-1.185672
29	6	-7.149203	1.407952	1.072595	63	1	-5.971742	-1.061243	-1.108986
30	6	-8.320205	0.101826	-0.716586	64	1	-7.339475	-0.745938	0.95432
31	8	-8.929701	1.083132	-1.096054	65	1	-8.11233	1.586369	1.560044
32	8	-8.58665	-1.141309	-1.171703	66	1	-6.378225	1.377747	1.847464
33	1	2.673515	1.034046	1.547795	67	1	-6.946059	2.258039	0.413483
34	1	3.440326	-0.416577	-1.027445	68	1	-9.309032	-1.063629	-1.835734

Conf-12

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	6.735891	-1.433562	-0.935696	35	1	1.291517	0.595106	-1.071659
2	6	7.240319	-0.145508	-1.43695	36	1	-0.834228	-0.470128	-1.113775
3	6	6.560839	1.051832	-0.932939	37	1	7.239927	-2.328573	-1.292364
4	6	5.536251	1.006348	-0.05875	38	1	6.923014	2.004093	-1.315347
5	6	4.985148	-0.300709	0.480683	39	1	5.391948	-2.466097	0.302896
6	6	5.71421	-1.496327	-0.069553	40	1	5.28894	3.132959	-0.086741
7	6	4.816218	2.25513	0.365079	41	1	4.879521	2.379596	1.454597
8	6	3.334747	2.16684	-0.04066	42	1	2.801973	3.05359	0.320687
9	6	2.678322	0.894198	0.504539	43	1	3.261654	2.170754	-1.137131
10	6	3.460395	-0.371334	0.065278	44	1	1.205711	-1.784729	-0.993585
11	6	1.236782	0.752647	0.017356	45	1	0.841288	-2.656955	0.49163
12	6	0.50038	-0.497804	0.585345	46	1	2.832138	-1.773768	1.60465
13	6	1.275142	-1.730823	0.101492	47	1	3.266863	-2.535292	0.088349
14	6	2.757061	-1.66694	0.51675	48	1	0.340519	2.349535	1.242143
15	6	0.257903	1.910277	0.238821	49	1	0.3485	2.731621	-0.478643
16	6	-1.10392	1.232654	0.115984	50	1	6.221231	-0.195791	2.277537
17	6	-0.909442	-0.280879	-0.030322	51	1	4.58377	0.433882	2.52506

18	8	8.181771	-0.079647	-2.236749	52	1	4.855265	-1.311082	2.42372
19	6	5.166921	-0.342182	2.023998	53	1	1.380285	-0.465523	2.603556
20	6	0.39961	-0.480739	2.123093	54	1	-0.155806	0.388812	2.491476
21	6	-2.136593	-1.045437	0.482919	55	1	-0.122422	-1.374495	2.479904
22	6	-3.35169	-0.684325	-0.379305	56	1	-2.346834	-0.750062	1.517196
23	6	-1.983599	-2.57675	0.423917	57	1	-2.924715	-3.071148	0.690853
24	6	-4.640445	-0.388447	0.357446	58	1	-1.219389	-2.926079	1.121947
25	8	-3.280052	-0.705282	-1.598286	59	1	-1.706453	-2.895742	-0.585626
26	8	-2.183588	1.793856	0.164961	60	1	-4.823213	-1.209956	1.067324
27	6	-5.838369	-0.17639	-0.562928	61	1	-4.437053	0.494082	0.976491
28	6	-7.15058	0.046394	0.198698	62	1	-5.648947	0.677627	-1.222216
29	6	-7.155993	1.345353	1.030878	63	1	-5.943671	-1.045002	-1.221402
30	6	-8.324488	0.073637	-0.764307	64	1	-7.32625	-0.794694	0.8836
31	8	-8.251955	0.21936	-1.969417	65	1	-6.972697	2.214229	0.388208
32	8	-9.502239	-0.061463	-0.118058	66	1	-8.116444	1.483538	1.534485
33	1	2.67706	0.959735	1.600792	67	1	-6.373489	1.316785	1.794311
34	1	3.459723	-0.367486	-1.035478	68	1	-10.21685	-0.000853	-0.792246

Conf-13

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	6.715842	-1.34757	-1.063553	35	1	1.264052	0.644179	-1.018437
2	6	7.205984	-0.02623	-1.486227	36	1	-0.854218	-0.430954	-1.113298
3	6	6.525642	1.130977	-0.896876	37	1	7.221013	-2.214063	-1.483452
4	6	5.511526	1.021692	-0.016172	38	1	6.877511	2.108617	-1.220346
5	6	4.974537	-0.321336	0.442986	39	1	5.392944	-2.467739	0.120348
6	6	5.704917	-1.473571	-0.191665	40	1	5.251845	3.14393	0.097897
7	6	4.788302	2.235333	0.495085	41	1	4.86004	2.288434	1.589852
8	6	3.304118	2.163841	0.096204	42	1	2.768991	3.021928	0.518178
9	6	2.660152	0.854557	0.563717	43	1	3.22201	2.237956	-0.997131
10	6	3.44589	-0.375844	0.039545	44	1	1.192065	-1.737836	-1.085237
11	6	1.215952	0.734287	0.078536	45	1	0.844291	-2.700297	0.347378
12	6	0.490577	-0.553036	0.573453	46	1	2.83836	-1.871306	1.497107
13	6	1.269445	-1.749478	0.010581	47	1	3.265926	-2.538892	-0.064861
14	6	2.754211	-1.700783	0.418015	48	1	0.317487	2.246284	1.404987
15	6	0.232079	1.870175	0.376551	49	1	0.314514	2.735254	-0.288565
16	6	-1.126249	1.193471	0.217845	50	1	6.229117	-0.324184	2.230073
17	6	-0.924112	-0.307435	-0.02005	51	1	4.590409	0.276685	2.534588
18	8	8.136142	0.098098	-2.292288	52	1	4.87186	-1.456172	2.317658
19	6	5.173109	-0.461278	1.978382	53	1	1.382354	-0.637652	2.584894
20	6	0.398905	-0.630646	2.109908	54	1	-0.160371	0.210606	2.533994
21	6	-2.144312	-1.108594	0.45312	55	1	-0.114693	-1.548342	2.414277
22	6	-3.365987	-0.699451	-0.377406	56	1	-2.348613	-0.87888	1.505092
23	6	-1.984627	-2.632361	0.29786	57	1	-1.213361	-3.020149	0.967201
24	6	-4.649568	-0.445662	0.384319	58	1	-1.713667	-2.88649	-0.73155
25	8	-3.304779	-0.651806	-1.596137	59	1	-2.921254	-3.147333	0.540527
26	8	-2.208948	1.744455	0.303149	60	1	-4.839327	-1.314585	1.033024
27	6	-5.846909	-0.158768	-0.516758	61	1	-4.440557	0.389984	1.062988
28	6	-7.162427	0.024558	0.269671	62	1	-5.649951	0.738264	-1.11326

29	6	-7.145157	1.264747	1.179163	63	1	-5.959754	-0.984751	-1.228864
30	6	-8.327452	0.08674	-0.699605	64	1	-7.339966	-0.869404	0.878298
31	8	-9.212143	-0.743399	-0.787892	65	1	-6.928107	2.167449	0.599855
32	8	-8.277804	1.181989	-1.486779	66	1	-8.110713	1.401531	1.677674
33	1	2.666743	0.850154	1.661907	67	1	-6.382611	1.161152	1.956565
34	1	3.433812	-0.304334	-1.058816	68	1	-9.05425	1.14627	-2.090737

Conf-14

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	6.520331	-1.491989	-0.566478	35	1	1.254577	0.848602	-1.291365
2	6	7.145598	-0.175775	-0.769588	36	1	-0.866492	-0.057504	-1.852401
3	6	6.428983	0.971242	-0.203893	37	1	7.048846	-2.352229	-0.97021
4	6	5.267604	0.856853	0.470032	38	1	6.882781	1.946768	-0.367115
5	6	4.588863	-0.480999	0.699239	39	1	4.949559	-2.616257	0.255004
6	6	5.3628	-1.622507	0.097666	40	1	5.098888	2.974873	0.73476
7	6	4.525895	2.069196	0.957524	41	1	4.40122	2.02623	2.04799
8	6	3.13632	2.12981	0.299774	42	1	2.577935	2.983537	0.699858
9	6	2.353408	0.831866	0.522519	43	1	3.25665	2.299769	-0.779233
10	6	3.157831	-0.399259	0.030137	44	1	1.075964	-1.507261	-1.595271
11	6	1.01544	0.849045	-0.215939	45	1	0.430669	-2.56331	-0.343389
12	6	0.148135	-0.423487	0.020943	46	1	2.223218	-1.969312	1.20948
13	6	0.954872	-1.617018	-0.508872	47	1	2.889895	-2.528357	-0.310732
14	6	2.343053	-1.702024	0.153617	48	1	-0.020578	2.304296	1.072304
15	6	0.054294	2.018688	0.014405	49	1	0.294971	2.927307	-0.546025
16	6	-1.290586	1.450042	-0.430851	50	1	5.497696	-0.718564	2.670304
17	6	-1.125344	-0.033965	-0.78125	51	1	3.864581	-0.035081	2.738184
18	8	8.212246	-0.047315	-1.382846	52	1	4.089938	-1.75887	2.411239
19	6	4.498897	-0.761909	2.22554	53	1	0.660423	-0.736711	2.139767
20	6	-0.220391	-0.623215	1.504112	54	1	-0.801963	0.215717	1.902005
21	6	-2.44074	-0.800914	-0.61305	55	1	-0.827378	-1.525926	1.627461
22	6	-3.482647	-0.296897	-1.616989	56	1	-2.83622	-0.648694	0.398143
23	6	-2.30592	-2.318154	-0.860203	57	1	-3.287348	-2.805095	-0.854563
24	6	-4.93041	-0.328879	-1.164517	58	1	-1.701523	-2.791811	-0.083629
25	8	-3.169182	0.029873	-2.750827	59	1	-1.837115	-2.50916	-1.830752
26	8	-2.339569	2.06604	-0.465489	60	1	-5.564283	-0.361408	-2.054805
27	6	-5.283087	0.892841	-0.292545	61	1	-5.101779	-1.248835	-0.589875
28	6	-6.675304	0.789865	0.375515	62	1	-4.526289	1.027508	0.483279
29	6	-7.826478	0.695456	-0.626033	63	1	-5.25625	1.794792	-0.912589
30	6	-6.684469	-0.386564	1.335423	64	1	-6.794824	1.694162	0.986664
31	8	-7.320179	-1.413635	1.194369	65	1	-8.793421	0.725582	-0.114703
32	8	-5.854236	-0.183364	2.380744	66	1	-7.782193	1.534222	-1.328493
33	1	2.162361	0.735308	1.599679	67	1	-7.784506	-0.23738	-1.194573
34	1	3.348321	-0.234723	-1.041456	68	1	-5.880669	-0.993057	2.940008

Conf-15

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	6.685752	-1.337347	-0.585457	35	1	1.195136	0.464055	-1.227208

2	6	7.178468	-0.05424	-1.110509	36	1	-0.885005	-0.687374	-1.373345
3	6	6.419413	1.136476	-0.716478	37	1	7.248407	-2.226538	-0.859496
4	6	5.333599	1.089525	0.080281	38	1	6.774395	2.084182	-1.116573
5	6	4.790988	-0.212867	0.639123	39	1	5.290288	-2.36592	0.598359
6	6	5.603967	-1.401897	0.204202	40	1	5.011211	3.200957	-0.068482
7	6	4.537741	2.326154	0.388417	41	1	4.512683	2.502201	1.472335
8	6	3.095997	2.160259	-0.122503	42	1	2.504903	3.040113	0.155402
9	6	2.447034	0.887683	0.431813	43	1	3.107076	2.112374	-1.220317
10	6	3.306793	-0.363266	0.112912	44	1	1.192249	-1.910351	-1.04484
11	6	1.052896	0.666935	-0.153717	45	1	0.748556	-2.731729	0.44789
12	6	0.322366	-0.585752	0.416666	46	1	2.615059	-1.7228	1.663722
13	6	1.176276	-1.80656	0.048727	47	1	3.191744	-2.530015	0.220217
14	6	2.619129	-1.665434	0.56953	48	1	0.010768	2.279597	0.926076
15	6	0.018771	1.7933	-0.058761	49	1	0.132439	2.584982	-0.805691
16	6	-1.304565	1.057571	-0.247788	50	1	5.879563	0.020871	2.517302
17	6	-1.045372	-0.452392	-0.308262	51	1	4.20748	0.598927	2.609371
18	8	8.173807	0.012957	-1.842011	52	1	4.545411	-1.137454	2.613449
19	6	4.853673	-0.176715	2.191995	53	1	-0.406448	-1.403914	2.299299
20	6	0.106457	-0.505709	1.940458	54	1	1.047011	-0.428963	2.490195
21	6	-2.277283	-1.241257	0.155055	55	1	-0.507643	0.35536	2.226508
22	6	-3.445531	-0.955745	-0.795454	56	1	-2.563853	-0.914701	1.161185
23	6	-2.068134	-2.76678	0.167642	57	1	-1.339604	-3.060812	0.926644
24	6	-4.782656	-0.661936	-0.150575	58	1	-1.714885	-3.11335	-0.808475
25	8	-3.299976	-1.034567	-2.005592	59	1	-3.007145	-3.285076	0.39363
26	8	-2.404533	1.577131	-0.303314	60	1	-4.994189	-1.470833	0.563039
27	6	-5.918096	-0.483337	-1.155419	61	1	-4.641195	0.236793	0.462782
28	6	-7.277665	-0.092925	-0.525051	62	1	-5.632721	0.283582	-1.882701
29	6	-7.827528	-1.15565	0.43172	63	1	-6.056729	-1.412008	-1.720508
30	6	-7.145332	1.289381	0.091425	64	1	-7.97995	0.037078	-1.357023
31	8	-7.139656	2.323135	-0.55047	65	1	-7.181457	-1.293945	1.302189
32	8	-6.979817	1.267606	1.429831	66	1	-8.821759	-0.879938	0.797299
33	1	2.359438	1.001926	1.520461	67	1	-7.911258	-2.11462	-0.091154
34	1	3.391632	-0.407724	-0.983679	68	1	-6.863157	2.200124	1.724635

Conf-16

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	6.153155	-2.18507	-0.332271	35	1	1.053365	0.47185	-1.181212
2	6	6.799608	-1.273434	-1.289256	36	1	-1.198669	-0.182128	-0.800085
3	6	6.331737	0.11584	-1.271237	37	1	6.50054	-3.215429	-0.326985
4	6	5.372377	0.561013	-0.436055	38	1	6.798274	0.787106	-1.989555
5	6	4.679447	-0.346551	0.563538	39	1	4.76317	-2.456551	1.217157
6	6	5.193416	-1.759337	0.501759	40	1	5.427136	2.533838	-1.26633
7	6	4.866295	1.97377	-0.511352	41	1	5.019505	2.484382	0.449025
8	6	3.363383	1.973365	-0.840643	42	1	2.986984	3.002475	-0.838269
9	6	2.571646	1.115991	0.15218	43	1	3.218115	1.578827	-1.855958
10	6	3.135735	-0.327444	0.2188	44	1	0.638221	-1.662427	-0.206618
11	6	1.094957	1.03027	-0.232433	45	1	0.254444	-1.849587	1.501304
12	6	0.228932	0.213413	0.77311	46	1	2.419539	-0.93684	2.179981

13	6	0.787563	-1.215659	0.78588	47	1	2.640009	-2.267293	1.062282
14	6	2.287954	-1.23363	1.133483	48	1	0.521927	3.089558	0.301983
15	6	0.307083	2.325017	-0.456723	49	1	0.461496	2.792073	-1.434308
16	6	-1.142354	1.874431	-0.295583	50	1	6.035971	0.225445	2.176005
17	6	-1.1745	0.403108	0.133689	51	1	4.525577	1.151532	2.180161
18	8	7.68455	-1.659265	-2.062824	52	1	4.53791	-0.524565	2.745582
19	6	4.956882	0.163071	2.005786	53	1	1.237579	0.858792	2.621257
20	6	0.234846	0.81896	2.190274	54	1	-0.16537	1.838734	2.205703
21	6	-2.458945	0.08223	0.908613	55	1	-0.384007	0.217213	2.863553
22	6	-3.667987	0.270387	-0.013543	56	1	-2.56105	0.775602	1.751409
23	6	-2.516725	-1.359814	1.446502	57	1	-3.499613	-1.572659	1.87746
24	6	-4.860168	0.993353	0.579823	58	1	-1.76572	-1.520499	2.223223
25	8	-3.66497	-0.172696	-1.151646	59	1	-2.340049	-2.076555	0.637984
26	8	-2.124644	2.579101	-0.441504	60	1	-5.050724	0.594148	1.585328
27	6	-6.125699	0.982927	-0.278885	61	1	-4.51387	2.024387	0.732622
28	6	-7.028313	-0.264906	-0.122029	62	1	-6.739505	1.850057	-0.011225
29	6	-8.345122	-0.081577	-0.882679	63	1	-5.849145	1.095692	-1.333032
30	6	-6.319258	-1.516124	-0.605508	64	1	-7.232232	-0.399217	0.947371
31	8	-6.368045	-1.963834	-1.733745	65	1	-9.005801	-0.944215	-0.748816
32	8	-5.607789	-2.106606	0.381456	66	1	-8.867715	0.810451	-0.522871
33	1	2.653649	1.585203	1.141669	67	1	-8.155611	0.033131	-1.954108
34	1	3.061931	-0.734654	-0.801216	68	1	-5.134767	-2.873087	-0.015806

Table S11. Cartesian coordinates of all optimized conformers of **2**

Conf-1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	7.017024	-1.064123	-0.02577	37	1	1.144712	0.198156	-1.631626
2	6	7.527429	0.140136	0.272406	38	1	7.652915	-1.919794	-0.240045
3	6	6.67088	1.34508	0.514982	39	1	8.606487	0.272723	0.341229
4	6	5.223642	1.133801	0.127947	40	1	6.757796	1.612731	1.582039
5	6	4.621578	-0.22901	0.47029	41	1	7.083539	2.204879	-0.027815
6	6	5.56526	-1.302903	-0.125515	42	1	5.061522	3.027574	-0.739176
7	6	4.542877	2.099135	-0.497309	43	1	2.99252	1.802126	-1.946683
8	6	3.094929	2.007163	-0.869607	44	1	2.605073	2.976071	-0.718902
9	6	2.371596	0.920991	-0.068433	45	1	0.489354	-2.581967	0.54449
10	6	3.183201	-0.402271	-0.113013	46	1	0.986713	-2.047609	-1.062905
11	6	0.983665	0.634142	-0.630437	47	1	2.984697	-2.508879	0.306679
12	6	0.20353	-0.444753	0.154622	48	1	2.384853	-1.48968	1.596363
13	6	0.973936	-1.762365	-0.002621	49	1	-0.118368	2.444144	-0.040243
14	6	2.418554	-1.597384	0.508903	50	1	-2.235744	1.310529	-1.436023
15	6	-0.058741	1.738455	-0.881121	51	1	5.64601	-0.184754	2.417777
16	6	-1.325621	0.910621	-1.002981	52	1	3.931352	0.250259	2.485741
17	6	-1.181946	-0.319667	-0.486781	53	1	4.421159	-1.446367	2.296535
18	6	4.658436	-0.418049	2.012925	54	1	-0.637622	-0.830236	2.12915
19	6	0.027174	-0.098831	1.654227	55	1	0.969602	-0.107378	2.206825
20	6	-2.190691	-1.440497	-0.409649	56	1	-0.424966	0.889717	1.780064
21	6	-3.625798	-1.009512	-0.071446	57	1	-1.889762	-2.100234	0.417056
22	6	-2.169898	-2.279236	-1.701797	58	1	-2.49714	-1.671133	-2.548947
23	8	5.147871	-2.34009	-0.632616	59	1	-1.162494	-2.651287	-1.90973
24	1	-4.224454	-1.926716	0.018858	60	1	-2.843222	-3.140262	-1.614195
25	8	-4.144405	-0.227895	-1.155614	61	1	-5.718666	0.763217	-1.855793
26	6	-5.537803	-0.005303	-1.099691	62	1	-3.041446	0.62966	1.195643
27	6	-6.029255	0.479881	0.273258	63	1	-3.463462	-0.842494	2.078196
28	6	-5.137743	0.336573	1.441569	64	1	-4.954311	0.616689	3.561233
29	6	-3.741893	-0.211692	1.223902	65	1	-4.674109	2.082437	2.607793
30	6	-5.292579	1.181132	2.684739	66	1	-6.328312	1.481084	2.851987
31	6	-7.169274	1.465858	0.190744	67	1	-6.822385	2.418006	-0.226552
32	8	-6.210764	-0.622379	1.202135	68	1	-7.615416	1.653015	1.168561
33	8	-6.285999	-1.132127	-1.488199	69	1	-7.946759	1.068388	-0.471431
34	8	0.205143	2.568193	-2.013886	70	1	-6.422035	-1.668956	-0.681342
35	1	3.31285	-0.634158	-1.180356	71	1	0.265352	1.974622	-2.787238
36	1	2.294577	1.26603	0.97216					

Conf-2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	6.130899	-2.163235	-0.692559	37	1	1.36071	1.806851	-1.198615
2	6	6.900832	-1.603371	0.252659	38	1	6.515714	-2.919634	-1.372422
3	6	6.407697	-0.519261	1.161592	39	1	7.932155	-1.930392	0.379572

4	6	5.07475	0.05455	0.734194	40	1	6.347976	-0.934505	2.182292
5	6	4.040731	-0.944924	0.216093	41	1	7.158352	0.278786	1.223242
6	6	4.727385	-1.763699	-0.90513	42	1	5.659853	2.018353	1.142103
7	6	4.852594	1.370928	0.797714	43	1	3.615275	2.496567	-0.541277
8	6	3.550402	2.026099	0.452476	44	1	3.348524	2.851926	1.14391
9	6	2.390756	1.025401	0.473417	45	1	-0.51439	-1.27941	-1.099505
10	6	2.766575	-0.238754	-0.345659	46	1	0.446918	-0.173057	-2.081527
11	6	1.125403	1.619216	-0.136895	47	1	1.878543	-1.996538	-1.225546
12	6	-0.08736	0.652242	-0.159307	48	1	1.339088	-1.698518	0.413447
13	6	0.290439	-0.533661	-1.055699	49	1	0.457767	3.001701	1.439014
14	6	1.573735	-1.207449	-0.535134	50	1	-1.460681	3.754136	-0.45892
15	6	0.514893	2.949259	0.342967	51	1	4.61042	-2.354842	1.80722
16	6	-0.860182	2.863873	-0.297206	52	1	3.12767	-1.445194	2.135455
17	6	-1.181977	1.611719	-0.655416	53	1	3.117101	-2.794111	0.980333
18	6	3.703092	-1.950197	1.352666	54	1	-0.724921	1.004721	1.912014
19	6	-0.450178	0.163883	1.268135	55	1	-1.297808	-0.527476	1.246537
20	6	-2.394013	1.165724	-1.436236	56	1	0.378751	-0.361383	1.747588
21	6	-3.254318	0.174514	-0.634372	57	1	-2.021331	0.574062	-2.286541
22	6	-3.21207	2.329337	-2.007138	58	1	-2.600044	2.925965	-2.690686
23	8	4.137874	-2.111453	-1.924264	59	1	-3.576065	2.997513	-1.219887
24	1	-2.607362	-0.644184	-0.306737	60	1	-4.076672	1.947189	-2.556089
25	8	-4.242613	-0.366133	-1.522848	61	1	-5.720697	-1.688789	-1.687194
26	6	-4.870257	-1.526926	-1.019625	62	1	-4.573631	1.620807	0.275123
27	6	-5.358187	-1.384875	0.43168	63	1	-3.227833	1.133357	1.307551
28	6	-4.868565	-0.252403	1.243035	64	1	-4.90044	0.66305	3.182336
29	6	-3.960284	0.765494	0.580512	65	1	-6.290918	1.070279	2.163949
30	6	-5.612695	0.259735	2.453461	66	1	-6.193584	-0.523947	2.942432
31	6	-6.631204	-2.144623	0.715515	67	1	-6.85241	-2.179572	1.78324
32	8	-4.280174	-1.579484	1.388116	68	1	-7.477319	-1.681878	0.194973
33	8	-4.056992	-2.672272	-1.123216	69	1	-6.529894	-3.173186	0.351445
34	8	1.245459	4.118564	-0.026512	70	1	-3.518618	-2.710109	-0.307016
35	1	3.036239	0.12578	-1.347718	71	1	1.337454	4.097697	-0.998821
36	1	2.214307	0.742621	1.52007					

Conf-3

Center Number	Atomic Number	Coordinates (Angstroms)			Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z			X	Y	Z
1	6	6.985845	-1.317303	0.003125	37	1	1.256205	0.452962	-1.670036
2	6	7.547771	-0.184117	0.450099	38	1	7.58296	-2.18072	-0.28049
3	6	6.748308	1.035837	0.792118	39	1	8.628547	-0.123232	0.572294
4	6	5.30938	0.952109	0.332304	40	1	6.804857	1.181998	1.884495
5	6	4.620313	-0.402032	0.500961	41	1	7.229461	1.923285	0.361836
6	6	5.528687	-1.458661	-0.175023	42	1	5.286591	2.934143	-0.327134
7	6	4.708636	2.016879	-0.207709	43	1	3.206861	1.968254	-1.737213
8	6	3.275574	2.049315	-0.641782	44	1	2.832133	3.023267	-0.403709
9	6	2.459716	0.928332	0.007987	45	1	0.366863	-2.503001	0.179991
10	6	3.199936	-0.427865	-0.14849	46	1	0.959176	-1.833322	-1.342754
11	6	1.082778	0.782096	-0.633217	47	1	2.871447	-2.551992	0.036003
12	6	0.215755	-0.323978	0.012607	48	1	2.276313	-1.640676	1.406262

13	6	0.918058	-1.660745	-0.259076	49	1	0.069925	2.579367	0.116457
14	6	2.347625	-1.635464	0.315417	50	1	-2.070699	1.748978	-1.41128
15	6	0.118825	1.962326	-0.797412	51	1	5.563751	-0.625915	2.477054
16	6	-1.192338	1.233453	-1.031597	52	1	3.873015	-0.103685	2.530701
17	6	-1.136644	-0.047822	-0.645452	53	1	4.280043	-1.795246	2.174671
18	6	4.583004	-0.757683	2.013977	54	1	-0.733325	-0.850203	1.902384
19	6	0.000575	-0.124446	1.533948	55	1	0.916672	-0.253783	2.115197
20	6	-2.226632	-1.090561	-0.704518	56	1	-0.397138	0.872637	1.74365
21	6	-3.612098	-0.48778	-0.452173	57	1	-2.046151	-1.821014	0.097207
22	6	-2.170166	-1.837254	-2.051989	58	1	-1.156582	-2.198535	-2.245717
23	8	5.07799	-2.408998	-0.808257	59	1	-2.446469	-1.165738	-2.873063
24	1	-3.804415	0.286298	-1.206647	60	1	-2.84209	-2.701243	-2.067731
25	8	-3.574639	0.112141	0.849444	61	1	-4.57909	1.173218	2.195603
26	6	-4.665527	0.959429	1.126832	62	1	-4.499626	-2.353473	0.16656
27	6	-6.027537	0.314412	0.827335	63	1	-4.898286	-1.894799	-1.494313
28	6	-6.063289	-0.905476	-0.003334	64	1	-7.018676	-2.666623	0.777308
29	6	-4.75231	-1.503367	-0.481006	65	1	-8.158198	-1.391008	0.296839
30	6	-7.216967	-1.880016	0.040611	66	1	-7.3362	-2.359488	-0.937742
31	6	-7.115332	0.718086	1.792593	67	1	-8.099974	0.391913	1.454394
32	8	-6.369374	0.397959	-0.582489	68	1	-6.924446	0.29295	2.784485
33	8	-4.582223	2.200213	0.464457	69	1	-7.128979	1.809701	1.888432
34	8	0.529882	2.78407	-1.896477	70	1	-5.001176	2.078124	-0.411271
35	1	3.360833	-0.554051	-1.229157	71	1	-0.064426	3.557107	-1.916069
36	1	2.355524	1.164223	1.076273					

Conf-4

Center Number	Atomic Number	Coordinates (Angstroms)			Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z			X	Y	Z
1	6	5.267263	-2.828839	0.228003	37	1	0.437476	0.837827	-1.212541
2	6	6.33026	-2.103138	-0.150236	38	1	5.3343	-3.901606	0.392779
3	6	6.247637	-0.63497	-0.436999	39	1	7.302756	-2.580352	-0.265225
4	6	4.8258	-0.125738	-0.524086	40	1	6.808279	-0.104068	0.351445
5	6	3.837928	-0.691667	0.495715	41	1	6.784954	-0.411067	-1.367251
6	6	3.929175	-2.235088	0.406557	42	1	5.238212	1.077956	-2.181115
7	6	4.479255	0.755309	-1.467349	43	1	2.566875	0.877029	-2.425074
8	6	3.114926	1.358939	-1.60028	44	1	3.195522	2.412034	-1.892347
9	6	2.308817	1.23062	-0.303854	45	1	-0.600138	-0.15536	2.098697
10	6	2.372444	-0.22883	0.218592	46	1	-0.487282	-0.604996	0.393718
11	6	0.84284	1.59349	-0.518257	47	1	1.423582	-1.538472	1.644653
12	6	-0.040794	1.477719	0.752982	48	1	1.811653	0.036371	2.304769
13	6	-0.022284	0.002409	1.178419	49	1	0.970811	3.780769	-0.714031
14	6	1.424095	-0.470459	1.416578	50	1	-1.763521	3.599802	-1.273515
15	6	0.416434	2.934354	-1.143373	51	1	5.37444	-0.540665	2.064655
16	6	-1.049907	2.957614	-0.762106	52	1	4.184939	0.770465	2.079964
17	6	-1.345699	2.099086	0.223927	53	1	3.754496	-0.839814	2.692609
18	6	4.316929	-0.305103	1.923259	54	1	0.479238	3.429794	1.616244
19	6	0.480276	2.374917	1.906211	55	1	-0.159058	2.272587	2.78803
20	6	-2.740924	1.871527	0.755055	56	1	1.496905	2.114132	2.209539
21	6	-3.240611	0.443408	0.460692	57	1	-3.400441	2.552354	0.198795

22	6	-2.877626	2.197482	2.253691	58	1	-2.343355	1.469019	2.873334
23	8	2.945861	-2.961827	0.516114	59	1	-3.926613	2.197139	2.564991
24	1	-2.666159	-0.271548	1.059343	60	1	-2.466521	3.18846	2.466371
25	8	-3.008047	0.192317	-0.932066	61	1	-3.201604	-1.097843	-2.429419
26	6	-3.197881	-1.143309	-1.337115	62	1	-5.298157	1.062172	0.270966
27	6	-4.507305	-1.764137	-0.831447	63	1	-4.922208	0.312982	1.827898
28	6	-5.252525	-1.07317	0.238555	64	1	-7.313601	-0.557264	-0.092853
29	6	-4.728562	0.255212	0.750612	65	1	-6.962758	-1.169334	1.53171
30	6	-6.729209	-1.295068	0.468288	66	1	-7.046157	-2.294456	0.166056
31	6	-5.121378	-2.749266	-1.796224	67	1	-4.356685	-3.463158	-2.122237
32	8	-4.394694	-2.211597	0.546026	68	1	-5.938995	-3.308343	-1.338925
33	8	-2.123192	-1.986367	-0.983536	69	1	-5.501834	-2.230314	-2.683314
34	8	0.644303	3.04406	-2.549861	70	1	-2.297458	-2.297816	-0.072198
35	1	2.003733	-0.856986	-0.605594	71	1	0.172719	2.297643	-2.967735
36	1	2.761554	1.902422	0.438532					

Conf-5

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	6.973288	-1.336738	0.012299	37	1	1.266002	0.456357	-1.665942
2	6	7.540749	-0.206508	0.459829	38	1	7.566113	-2.203026	-0.271531
3	6	6.747386	1.017408	0.802064	39	1	8.621782	-0.151029	0.582243
4	6	5.308555	0.941291	0.340784	40	1	6.803434	1.162452	1.894588
5	6	4.6124	-0.409198	0.509538	41	1	7.233543	1.902652	0.372914
6	6	5.515543	-1.470674	-0.166023	42	1	5.297405	2.923013	-0.320271
7	6	4.714493	2.008959	-0.200909	43	1	3.216326	1.966714	-1.732517
8	6	3.281878	2.04922	-0.636372	44	1	2.843891	3.02591	-0.400264
9	6	2.459741	0.932601	0.013418	45	1	0.347879	-2.488155	0.176584
10	6	3.192797	-0.427552	-0.141114	46	1	0.9523	-1.824821	-1.344025
11	6	1.084651	0.794378	-0.630866	47	1	2.852304	-2.549341	0.049328
12	6	0.207361	-0.308766	0.003614	48	1	2.254086	-1.629473	1.412821
13	6	0.905413	-1.649359	-0.260925	49	1	0.069571	2.603195	0.104317
14	6	2.331767	-1.629031	0.322339	50	1	-2.057402	1.77806	-1.439649
15	6	0.122115	1.983597	-0.802257	51	1	5.553081	-0.640462	2.486014
16	6	-1.186868	1.256945	-1.051113	52	1	3.866218	-0.105741	2.538966
17	6	-1.13664	-0.026545	-0.669124	53	1	4.260844	-1.800115	2.182327
18	6	4.571637	-0.764758	2.022366	54	1	-0.765147	-0.828175	1.883241
19	6	-0.02294	-0.10727	1.522402	55	1	0.88705	-0.24189	2.111993
20	6	-2.226228	-1.067991	-0.746697	56	1	-0.41701	0.892025	1.728279
21	6	-3.610279	-0.471865	-0.471502	57	1	-2.040874	-1.817054	0.036294
22	6	-2.175664	-1.781831	-2.11201	58	1	-2.848899	-2.644228	-2.146043
23	8	5.059688	-2.418562	-0.799226	59	1	-1.163079	-2.139764	-2.317746
24	1	-3.810534	0.315999	-1.209487	60	1	-2.453939	-1.090302	-2.915585
25	8	-3.56074	0.103375	0.840491	61	1	-4.553122	1.135984	2.21732
26	6	-4.651634	0.941456	1.145942	62	1	-4.484473	-2.352945	0.117889
27	6	-6.014273	0.295748	0.850961	63	1	-4.904146	-1.860919	-1.528187
28	6	-6.05511	-0.907926	-0.002882	64	1	-6.992318	-2.688561	0.755373
29	6	-4.747754	-1.490331	-0.508571	65	1	-8.143749	-1.409438	0.314258
30	6	-7.203613	-1.888788	0.036691	66	1	-7.333106	-2.349765	-0.949226

31	6	-7.091601	0.67488	1.837643	67	1	-8.079023	0.351344	1.505065
32	8	-6.374221	0.404891	-0.55254	68	1	-6.886538	0.230339	2.818139
33	8	-4.580874	2.194044	0.505384	69	1	-7.108625	1.764225	1.956051
34	8	0.484326	2.90489	-1.833123	70	1	-5.00888	2.086197	-0.367809
35	1	3.354342	-0.555561	-1.221537	71	1	0.541908	2.389068	-2.660473
36	1	2.354334	1.170009	1.081245					

Conf-6

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	7.018878	-1.058039	-0.02416	37	1	1.141774	0.200758	-1.642364
2	6	7.526623	0.146131	0.278764	38	1	7.656661	-1.912066	-0.2394
3	6	6.667459	1.348879	0.522818	39	1	8.605305	0.280256	0.350613
4	6	5.221233	1.136365	0.132508	40	1	6.752151	1.613961	1.590709
5	6	4.620647	-0.228685	0.468528	41	1	7.079716	2.210759	-0.01703
6	6	5.567707	-1.299023	-0.128223	42	1	5.057159	3.033117	-0.727359
7	6	4.539592	2.10284	-0.489981	43	1	2.991055	1.810461	-1.943783
8	6	3.092938	2.009317	-0.86617	44	1	2.600582	2.976511	-0.711017
9	6	2.369067	0.918482	-0.072168	45	1	0.49321	-2.588079	0.534045
10	6	3.183759	-0.402929	-0.118857	46	1	0.987805	-2.049388	-1.072865
11	6	0.982886	0.628339	-0.639763	47	1	2.988786	-2.511729	0.291784
12	6	0.205014	-0.450424	0.149332	48	1	2.388483	-1.499085	1.586238
13	6	0.976428	-1.766832	-0.011911	49	1	-0.117135	2.4316	-0.043539
14	6	2.42132	-1.601992	0.498311	50	1	-2.236572	1.295369	-1.444409
15	6	-0.05558	1.726822	-0.890932	51	1	5.64037	-0.186943	2.418582
16	6	-1.324333	0.900411	-1.009759	52	1	3.924124	0.242231	2.483686
17	6	-1.18182	-0.327055	-0.488305	53	1	4.420035	-1.452222	2.290996
18	6	4.654524	-0.422356	2.010726	54	1	-0.633554	-0.837851	2.124512
19	6	0.032428	-0.107177	1.649982	55	1	0.975222	-0.118895	2.201941
20	6	-2.19203	-1.446418	-0.404293	56	1	-0.417198	0.882288	1.77774
21	6	-3.626161	-1.011853	-0.066606	57	1	-1.891257	-2.101833	0.426005
22	6	-2.174231	-2.293009	-1.691237	58	1	-1.167418	-2.667005	-1.898462
23	8	5.153788	-2.335654	-0.639328	59	1	-2.502018	-1.689743	-2.541641
24	1	-4.226439	-1.927493	0.02843	60	1	-2.848171	-3.153001	-1.597622
25	8	-4.144961	-0.234064	-1.153803	61	1	-5.718567	0.756102	-1.856725
26	6	-5.537956	-0.009431	-1.097507	62	1	-3.038305	0.632511	1.19138
27	6	-6.027504	0.482212	0.273822	63	1	-3.460997	-0.834506	2.082042
28	6	-5.134912	0.343027	1.44179	64	1	-4.668711	2.093811	2.599589
29	6	-3.739902	-0.207676	1.224988	65	1	-6.32301	1.494699	2.848528
30	6	-5.28769	1.193263	2.681356	66	1	-4.948694	0.632628	3.560001
31	6	-7.166691	1.468915	0.188201	67	1	-7.61131	1.661292	1.165694
32	8	-6.20927	-0.615877	1.207548	68	1	-6.819595	2.418711	-0.23428
33	8	-6.288274	-1.136668	-1.480466	69	1	-7.945458	1.068949	-0.470964
34	8	0.273964	2.451604	-2.081159	70	1	-6.423985	-1.670116	-0.671314
35	1	3.316244	-0.631262	-1.18653	71	1	-0.380555	3.168896	-2.172731
36	1	2.288125	1.258946	0.969657					

Conf-7

Center	Atomic	Coordinates (Angstroms)	Center	Atomic	Coordinates (Angstroms)

Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	-5.239879	-2.78488	0.021669	37	1	-0.330569	0.887697	1.129888
2	6	-6.284444	-2.023759	0.381194	38	1	-5.324724	-3.864138	-0.080768
3	6	-6.176057	-0.543197	0.583752	39	1	-7.260467	-2.479579	0.543419
4	6	-4.746232	-0.049465	0.607976	40	1	-6.749252	-0.048983	-0.219366
5	6	-3.790628	-0.687043	-0.400118	41	1	-6.687457	-0.260679	1.512665
6	6	-3.898099	-2.220835	-0.216193	42	1	-5.102439	1.253646	2.201687
7	6	-4.365395	0.879548	1.490068	43	1	-2.428475	1.029764	2.393474
8	6	-2.990472	1.470804	1.555263	44	1	-3.051034	2.539968	1.78781
9	6	-2.218709	1.256458	0.249289	45	1	0.621949	-0.303823	-2.130611
10	6	-2.313697	-0.228806	-0.186212	46	1	0.545768	-0.645619	-0.415883
11	6	-0.743093	1.611092	0.405249	47	1	-1.412799	-1.629223	-1.555575
12	6	0.104844	1.416006	-0.881828	48	1	-1.803131	-0.092416	-2.296832
13	6	0.0593	-0.080839	-1.218292	49	1	-0.855195	3.804014	0.493591
14	6	-1.39731	-0.549669	-1.38996	50	1	1.882846	3.663118	0.952569
15	6	-0.291821	2.977138	0.94868	51	1	-5.363154	-0.606458	-1.938685
16	6	1.158313	2.979244	0.51537	52	1	-4.157355	0.684217	-2.059133
17	6	1.427991	2.070352	-0.43553	53	1	-3.76284	-0.965027	-2.585792
18	6	-4.299579	-0.378315	-1.836248	54	1	-0.436259	3.319359	-1.83838
19	6	-0.443884	2.249964	-2.069725	55	1	0.175547	2.097424	-2.958131
20	6	2.817744	1.868134	-1.002628	56	1	-1.467221	1.974225	-2.334356
21	6	3.560449	0.624871	-0.466397	57	1	3.415164	2.711227	-0.627357
22	6	2.88416	1.903894	-2.537232	58	1	2.327382	1.074821	-2.97917
23	8	-2.925286	-2.965288	-0.296586	59	1	3.925104	1.81919	-2.869836
24	1	4.610329	0.735144	-0.772414	60	1	2.477905	2.844148	-2.921995
25	8	3.02607	-0.550274	-1.081087	61	1	3.145419	-2.527402	-1.22559
26	6	3.800185	-1.71512	-0.899076	62	1	2.452201	0.489145	1.375341
27	6	4.237938	-1.943885	0.555707	63	1	4.001666	1.312703	1.536616
28	6	4.120184	-0.831081	1.518604	64	1	4.4865	-0.205537	3.538736
29	6	3.497614	0.468015	1.049058	65	1	4.579038	-1.960561	3.315995
30	6	4.046016	-1.058789	3.010361	66	1	3.000393	-1.145135	3.326745
31	6	4.296131	-3.401218	0.944575	67	1	4.779113	-3.54414	1.912298
32	8	5.403745	-1.148426	0.902114	68	1	3.286862	-3.826176	0.988053
33	8	4.932267	-1.755299	-1.735629	69	1	4.865659	-3.956213	0.190588
34	8	-0.473815	3.160894	2.354097	70	1	5.649759	-1.292987	-1.257108
35	1	-1.932223	-0.81355	0.663838	71	1	0.003931	2.432078	2.795306
36	1	-2.681207	1.8912	-0.519169					

Conf-8

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	6.972255	-1.337125	-0.007738	37	1	1.265622	0.454618	-1.659983
2	6	7.544176	-0.205985	0.431439	38	1	7.562054	-2.20442	-0.294704
3	6	6.754455	1.018864	0.778035	39	1	8.62627	-0.150283	0.543705
4	6	5.310638	0.942357	0.332503	40	1	6.820904	1.166998	1.86952
5	6	4.615493	-0.407182	0.507724	41	1	7.236312	1.902939	0.341747
6	6	5.513052	-1.470927	-0.172647	42	1	5.292291	2.926255	-0.323261
7	6	4.711179	2.011959	-0.198678	43	1	3.188902	2.001151	-1.708972
8	6	3.272415	2.056561	-0.61245	44	1	2.848522	3.031766	-0.334657

9	6	2.45353	0.930565	0.02638	45	1	0.353848	-2.49334	0.198586
10	6	3.191757	-0.426178	-0.133306	46	1	0.956058	-1.836538	-1.325988
11	6	1.081485	0.787288	-0.626491	47	1	2.857683	-2.547887	0.071809
12	6	0.205936	-0.315405	0.012387	48	1	2.258046	-1.619184	1.429194
13	6	0.908588	-1.655202	-0.243966	49	1	0.036571	2.588952	0.09347
14	6	2.334766	-1.627181	0.338522	50	1	-2.051177	1.746463	-1.478004
15	6	0.11268	1.970022	-0.816467	51	1	5.571122	-0.636733	2.477187
16	6	-1.184255	1.233596	-1.071858	52	1	3.885602	-0.098754	2.542323
17	6	-1.134727	-0.042978	-0.669416	53	1	4.2742	-1.79444	2.185407
18	6	4.585788	-0.759982	2.021463	54	1	-0.772772	-0.8306	1.890172
19	6	-0.031868	-0.108441	1.529136	55	1	0.875879	-0.237043	2.123705
20	6	-2.225738	-1.083869	-0.73527	56	1	-0.430572	0.890335	1.729052
21	6	-3.608963	-0.481892	-0.468446	57	1	-2.042629	-1.82334	0.057314
22	6	-2.175445	-1.81528	-2.091163	58	1	-2.452618	-1.134076	-2.903867
23	8	5.051464	-2.420737	-0.79852	59	1	-1.163002	-2.176502	-2.29175
24	1	-3.80581	0.299537	-1.214082	60	1	-2.849383	-2.67754	-2.114332
25	8	-3.56046	0.105514	0.838384	61	1	-4.553428	1.151759	2.204443
26	6	-4.649398	0.949354	1.134269	62	1	-4.49087	-2.354071	0.13791
27	6	-6.013508	0.30634	0.840435	63	1	-4.904115	-1.877622	-1.514377
28	6	-6.056289	-0.90498	-0.002401	64	1	-7.33687	-2.350379	-0.939764
29	6	-4.749472	-1.497089	-0.498171	65	1	-7.003209	-2.674747	0.769044
30	6	-7.208867	-1.880818	0.042284	66	1	-8.148017	-1.395197	0.312212
31	6	-7.092724	0.699062	1.81975	67	1	-6.892919	0.263032	2.805142
32	8	-6.368262	0.404062	-0.565212	68	1	-8.080277	0.376378	1.48674
33	8	-4.572693	2.197002	0.48469	69	1	-7.105729	1.789544	1.927755
34	8	0.429507	2.814582	-1.930462	70	1	-4.996757	2.083619	-0.389736
35	1	3.345965	-0.554473	-1.214631	71	1	1.021687	3.517134	-1.609888
36	1	2.344551	1.160592	1.095374					

Conf-9

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	7.013579	-1.073084	-0.055885	37	1	1.144347	0.206772	-1.618492
2	6	7.53073	0.129882	0.235361	38	1	7.644478	-1.930594	-0.277347
3	6	6.680381	1.3369	0.488134	39	1	8.610832	0.259931	0.290923
4	6	5.227478	1.129966	0.120321	40	1	6.780669	1.604491	1.554008
5	6	4.625348	-0.231166	0.466806	41	1	7.0883	2.195715	-0.05973
6	6	5.560237	-1.308149	-0.138241	42	1	5.059172	3.028649	-0.735728
7	6	4.541498	2.100919	-0.48982	43	1	2.959729	1.845581	-1.915778
8	6	3.086552	2.019355	-0.836047	44	1	2.615608	2.99239	-0.638052
9	6	2.367823	0.921068	-0.046929	45	1	0.492737	-2.581855	0.563344
10	6	3.181754	-0.400061	-0.103922	46	1	0.988176	-2.049877	-1.045653
11	6	0.9822	0.633254	-0.616269	47	1	2.986802	-2.505586	0.324486
12	6	0.201895	-0.446045	0.168096	48	1	2.38784	-1.480656	1.61063
13	6	0.975259	-1.76245	0.013938	49	1	-0.145674	2.432801	-0.031568
14	6	2.419934	-1.593939	0.523501	50	1	-2.225151	1.29199	-1.459956
15	6	-0.063205	1.732602	-0.879904	51	1	5.668692	-0.1927	2.404252
16	6	-1.319699	0.898146	-1.012852	52	1	3.956759	0.250519	2.488937
17	6	-1.179148	-0.325824	-0.482222	53	1	4.436356	-1.448358	2.29399

18	6	4.676061	-0.421042	2.008913	54	1	-0.648579	-0.833326	2.138514
19	6	0.017521	-0.101013	1.666782	55	1	0.957179	-0.10863	2.224338
20	6	-2.18943	-1.445015	-0.400275	56	1	-0.436201	0.887152	1.790876
21	6	-3.625301	-1.011263	-0.069134	57	1	-1.891672	-2.099047	0.432104
22	6	-2.165786	-2.293454	-1.685988	58	1	-2.490731	-1.691761	-2.538557
23	8	5.134587	-2.345195	-0.638401	59	1	-1.157914	-2.66706	-1.888666
24	1	-4.224474	-1.92765	0.025907	60	1	-2.83945	-3.153761	-1.593511
25	8	-4.140891	-0.236833	-1.159916	61	1	-5.712885	0.75066	-1.870326
26	6	-5.534359	-0.013932	-1.1097	62	1	-3.046016	0.637856	1.186849
27	6	-6.030682	0.478016	0.259043	63	1	-3.467296	-0.828402	2.079625
28	6	-5.142553	0.342732	1.430822	64	1	-4.966325	0.634882	3.549505
29	6	-3.745179	-0.204408	1.220176	65	1	-4.685287	2.095712	2.588808
30	6	-5.302659	1.193905	2.668803	66	1	-6.33935	1.49327	2.831112
31	6	-7.172269	1.461375	0.167572	67	1	-6.82592	2.411871	-0.253919
32	8	-6.21322	-0.619473	1.193403	68	1	-7.621826	1.653027	1.142954
33	8	-6.281495	-1.14261	-1.494833	69	1	-7.946888	1.05873	-0.494825
34	8	0.163821	2.479541	-2.081663	70	1	-6.418483	-1.676283	-0.686052
35	1	3.301228	-0.629234	-1.172917	71	1	0.710725	3.250864	-1.852505
36	1	2.290189	1.254839	0.997223					

Conf-10

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	5.27589	-2.833268	0.203656	37	1	0.449174	0.85277	-1.225681
2	6	6.341542	-2.100525	-0.152824	38	1	5.34273	-3.908433	0.352147
3	6	6.259641	-0.628139	-0.417161	39	1	7.315742	-2.574756	-0.265841
4	6	4.838014	-0.119116	-0.509424	40	1	6.81258	-0.109171	0.384577
5	6	3.841026	-0.702357	0.491545	41	1	6.805176	-0.389132	-1.338864
6	6	3.935273	-2.244027	0.378853	42	1	5.264622	1.111817	-2.142435
7	6	4.499138	0.776889	-1.441293	43	1	2.595081	0.914868	-2.416318
8	6	3.135353	1.380382	-1.578053	44	1	3.217564	2.438792	-1.850565
9	6	2.315758	1.230332	-0.292674	45	1	-0.606108	-0.189243	2.072189
10	6	2.37718	-0.236864	0.208287	46	1	-0.487736	-0.614125	0.361433
11	6	0.849466	1.59224	-0.514824	47	1	1.416955	-1.57045	1.604373
12	6	-0.03811	1.461878	0.753154	48	1	1.801905	-0.007978	2.294622
13	6	-0.024091	-0.019469	1.156589	49	1	0.97992	3.777035	-0.671338
14	6	1.419938	-0.498576	1.394992	50	1	-1.755774	3.601885	-1.255682
15	6	0.428332	2.934901	-1.123371	51	1	5.363579	-0.57329	2.076007
16	6	-1.04067	2.956639	-0.748981	52	1	4.170378	0.734312	2.102503
17	6	-1.340588	2.091491	0.229068	53	1	3.739276	-0.886839	2.685203
18	6	4.306658	-0.338208	1.929415	54	1	-0.163686	2.226857	2.799263
19	6	0.4801	2.34021	1.92204	55	1	1.494483	2.072569	2.226948
20	6	-2.737583	1.866313	0.757732	56	1	0.483332	3.399137	1.64713
21	6	-3.244758	0.441656	0.459925	57	1	-3.393777	2.551456	0.202698
22	6	-2.87537	2.189054	2.257103	58	1	-3.92498	2.196263	2.566309
23	8	2.952273	-2.974009	0.467837	59	1	-2.456572	3.175977	2.47356
24	1	-2.67218	-0.278093	1.054707	60	1	-2.348327	1.454531	2.875846
25	8	-3.017798	0.193499	-0.934121	61	1	-3.220901	-1.091221	-2.43476
26	6	-3.216074	-1.13976	-1.342614	62	1	-5.299428	1.072845	0.279643

27	6	-4.528612	-1.754035	-0.836726	63	1	-4.923013	0.314351	1.831863
28	6	-5.266899	-1.062371	0.237532	64	1	-7.3253	-0.532462	-0.088618
29	6	-4.733015	0.260347	0.753744	65	1	-7.068397	-2.27199	0.165257
30	6	-6.744552	-1.27542	0.469512	66	1	-6.975394	-1.151002	1.533688
31	6	-5.151185	-2.731355	-1.803947	67	1	-5.971798	-3.286574	-1.347286
32	8	-4.416021	-2.207752	0.538787	68	1	-5.529622	-2.206569	-2.688468
33	8	-2.146665	-1.990919	-0.992821	69	1	-4.391907	-3.449174	-2.13399
34	8	0.653383	2.92979	-2.537767	70	1	-2.321312	-2.302469	-0.081636
35	1	2.01645	-0.852856	-0.628398	71	1	0.435397	3.821342	-2.867754
36	1	2.759678	1.891114	0.464811					

Table S12. Cartesian coordinates of all optimized conformers of **3**

Conf-1

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	7.108416	-1.420268	-0.136728	38	1	7.287676	-1.767725	0.893796
2	6	7.721251	-0.061166	-0.353899	39	1	7.553662	-2.172739	-0.797209
3	6	6.975575	1.044903	-0.502235	40	1	8.805361	-0.010382	-0.425269
4	6	5.51456	1.047642	-0.414877	41	1	7.457306	1.99837	-0.712764
5	6	4.853457	-0.195634	0.199332	42	1	5.333211	2.952289	-1.264104
6	6	5.608192	-1.399675	-0.38754	43	1	2.934764	2.06298	-1.875597
7	6	4.797084	2.098435	-0.848758	44	1	2.980134	3.173969	-0.525924
8	6	3.301973	2.172561	-0.841157	45	1	0.654654	-2.260569	0.880378
9	6	2.649427	1.105432	0.046511	46	1	0.986717	-1.723184	-0.765821
10	6	3.342603	-0.26354	-0.142997	47	1	3.070165	-2.343194	0.375914
11	6	1.163505	0.964909	-0.27938	48	1	2.725576	-1.242722	1.69634
12	6	0.412934	-0.104187	0.553999	49	1	0.412395	2.886898	-1.030125
13	6	1.103508	-1.453769	0.292072	50	1	0.504103	2.78077	0.724128
14	6	2.605759	-1.383371	0.617181	51	1	-1.715186	2.03976	0.732814
15	6	0.273265	2.209083	-0.182835	52	1	-1.74229	1.875253	-1.01928
16	6	-1.165971	1.63445	-0.122186	53	1	4.477692	0.592705	2.196778
17	6	-1.046359	0.085954	-0.009545	54	1	4.888349	-1.132395	2.199257
18	6	5.110781	-0.168389	1.731964	55	1	6.150138	0.087575	1.949115
19	6	0.431865	0.216383	2.062282	56	1	1.450585	0.339667	2.436646
20	6	-2.194923	-0.528091	0.831916	57	1	-0.10987	1.137052	2.297242
21	6	-3.590174	-0.105301	0.329276	58	1	-0.026946	-0.593829	2.638283
22	6	-2.109297	-2.050411	1.018725	59	1	-2.129078	-0.073742	1.826583
23	8	5.068213	-2.274691	-1.043044	60	1	-1.293306	-2.325014	1.690853
24	8	-1.10801	-0.383232	-1.371647	61	1	-1.953281	-2.582976	0.073116
25	1	-3.594164	0.978065	0.173278	62	1	-3.040797	-2.42061	1.455891
26	8	-4.503309	-0.410773	1.401869	63	1	-0.9785	-1.347857	-1.37586
27	6	-5.77331	0.186654	1.270544	64	1	-6.3872	-0.30891	2.027741
28	6	-6.402173	0.004696	-0.119173	65	1	-4.017315	-1.872956	-0.839447
29	6	-5.543318	-0.446036	-1.231014	66	1	-3.467029	-0.492043	-1.788777
30	6	-4.093519	-0.783971	-0.941439	67	1	-7.118922	-0.77197	-2.690453
31	6	-6.105258	-1.108774	-2.46704	68	1	-5.470371	-0.880631	-3.330754
32	6	-7.90399	-0.143586	-0.087801	69	1	-6.117685	-2.197072	-2.339031
33	8	-5.880334	0.966337	-1.075783	70	1	-8.337983	-0.088106	-1.087255
34	8	-5.767443	1.557336	1.597451	71	1	-8.185088	-1.100906	0.365676
35	1	3.278084	-0.504012	-1.213887	72	1	-8.336275	0.659449	0.519854
36	1	2.766124	1.425983	1.090987	73	1	-5.550019	2.03902	0.773987
37	1	1.106485	0.614334	-1.319051					

Conf-2

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	7.004829	-1.096722	-1.073109	38	1	7.235133	-1.945478	-0.408712
2	6	7.633594	0.1704	-0.554562	39	1	7.395369	-1.364528	-2.061291

3	6	6.904497	1.17043	-0.035129	40	1	8.712783	0.265644	-0.651016
4	6	5.451135	1.106657	0.125822	41	1	7.393843	2.09171	0.276897
5	6	4.798832	-0.279122	0.00609	42	1	5.263874	3.164799	0.45813
6	6	5.493221	-0.962682	-1.18289	43	1	2.816482	2.722572	-0.39481
7	6	4.733301	2.215751	0.374484	44	1	2.961434	2.920322	1.336331
8	6	3.243058	2.255507	0.508982	45	1	0.603575	-2.435521	-0.283231
9	6	2.61729	0.869455	0.70965	46	1	0.835103	-1.096398	-1.399003
10	6	3.269716	-0.170842	-0.22774	47	1	2.983665	-2.211701	-0.877671
11	6	1.113185	0.9137	0.444262	48	1	2.726789	-1.979876	0.841464
12	6	0.375891	-0.442068	0.601209	49	1	0.390804	2.927216	0.939727
13	6	1.031699	-1.433543	-0.375812	50	1	0.541992	1.848656	2.321596
14	6	2.549304	-1.529594	-0.141288	51	1	-1.727617	1.279742	1.983593
15	6	0.262737	1.888999	1.261581	52	1	-1.761146	2.082639	0.433359
16	6	-1.18469	1.384644	1.039356	53	1	4.555161	-0.703022	2.130293
17	6	-1.097976	0.007254	0.290956	54	1	4.925988	-2.149237	1.173784
18	6	5.143842	-1.083442	1.290689	55	1	6.199399	-0.973823	1.549155
19	6	0.46437	-0.961687	2.052453	56	1	1.499448	-1.011078	2.398253
20	6	-2.236601	-0.976553	0.704569	57	1	-0.078388	-0.322553	2.754366
21	6	-3.601001	-0.574786	0.098562	58	1	0.050128	-1.969579	2.14038
22	6	-1.98751	-2.426589	0.254798	59	1	-2.321036	-0.950355	1.798007
23	8	4.898861	-1.349018	-2.175048	60	1	-2.884385	-3.040295	0.38843
24	8	-1.167839	0.214813	-1.131123	61	1	-1.186773	-2.905376	0.819138
25	1	-3.636308	-0.973928	-0.922356	62	1	-1.721442	-2.44747	-0.806419
26	8	-3.727449	0.854983	0.022345	63	1	-1.983603	0.725131	-1.284981
27	6	-4.770898	1.294105	-0.822272	64	1	-4.849756	2.365388	-0.621205
28	6	-6.112258	0.601549	-0.544107	65	1	-4.738542	-0.742261	1.916919
29	6	-6.116263	-0.618452	0.288425	66	1	-4.807179	-2.193683	0.910626
30	6	-4.802548	-1.098156	0.880723	67	1	-7.352783	-0.683679	2.045684
31	6	-7.347294	-1.087856	1.02719	68	1	-8.268115	-0.784879	0.526326
32	6	-7.308566	1.499394	-0.746807	69	1	-7.341641	-2.181344	1.10034
33	8	-6.188313	-0.707976	-1.165732	70	1	-7.337989	2.278037	0.023739
34	8	-4.437435	1.16439	-2.184897	71	1	-7.234063	1.991043	-1.723378
35	1	3.138572	0.201003	-1.254003	72	1	-8.244342	0.939517	-0.716453
36	1	2.797256	0.573573	1.752422	73	1	-4.716388	0.267757	-2.462806
37	1	0.99272	1.189265	-0.612496					

Conf-3

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	7.115087	-1.411878	-0.119417	38	1	7.286374	-1.76676	0.909918
2	6	7.726564	-0.049773	-0.320843	39	1	7.567892	-2.15813	-0.781818
3	6	6.979611	1.055532	-0.468217	40	1	8.811173	0.004215	-0.381474
4	6	5.517692	1.053551	-0.39515	41	1	7.46075	2.011791	-0.667044
5	6	4.854568	-0.194926	0.206404	42	1	5.33955	2.962389	-1.236053
6	6	5.617012	-1.392895	-0.383018	43	1	2.950548	2.066846	-1.87718
7	6	4.801933	2.104637	-0.830948	44	1	2.978198	3.173392	-0.523151
8	6	3.306631	2.1742	-0.838536	45	1	0.652823	-2.259466	0.880421
9	6	2.650197	1.102163	0.039859	46	1	0.960016	-1.739157	-0.768675
10	6	3.346249	-0.2658	-0.14704	47	1	3.072748	-2.34693	0.361853

11	6	1.166985	0.955853	-0.297433	48	1	2.72551	-1.251916	1.685518
12	6	0.4123	-0.112419	0.534912	49	1	0.420676	2.871236	-1.072889
13	6	1.102968	-1.461668	0.281583	50	1	0.485241	2.772136	0.682365
14	6	2.605328	-1.388953	0.605673	51	1	-1.731459	2.039337	0.655503
15	6	0.26941	2.196456	-0.225212	52	1	-1.735052	1.843694	-1.089922
16	6	-1.168727	1.615339	-0.1819	53	1	4.460899	0.579176	2.206079
17	6	-1.047189	0.061387	-0.037143	54	1	4.879653	-1.143812	2.200671
18	6	5.100954	-0.175977	1.74102	55	1	6.137498	0.083546	1.967058
19	6	0.426377	0.224688	2.03948	56	1	1.443649	0.347207	2.418109
20	6	-2.191286	-0.534196	0.814804	57	1	-0.11404	1.148852	2.264664
21	6	-3.589172	-0.107382	0.321003	58	1	-0.037779	-0.579867	2.61865
22	6	-2.104322	-2.055831	0.99625	59	1	-2.116979	-0.069513	1.803667
23	8	5.084864	-2.263394	-1.050679	60	1	-1.295293	-2.32827	1.678438
24	8	-1.158141	-0.571394	-1.324173	61	1	-1.924404	-2.559916	0.043307
25	1	-3.590139	0.974826	0.156625	62	1	-3.038054	-2.432721	1.423966
26	8	-4.491807	-0.397697	1.408001	63	1	-0.547501	-0.134143	-1.944245
27	6	-5.759405	0.20509	1.286729	64	1	-6.367425	-0.280018	2.055457
28	6	-6.406335	0.01614	-0.093638	65	1	-4.038282	-1.88087	-0.827409
29	6	-5.563167	-0.447946	-1.211868	66	1	-3.493405	-0.514158	-1.793784
30	6	-4.112516	-0.792968	-0.937172	67	1	-7.158752	-0.774218	-2.650067
31	6	-6.143902	-1.114378	-2.437206	68	1	-5.518605	-0.893577	-3.309813
32	6	-7.908521	-0.123279	-0.043183	69	1	-6.159389	-2.201956	-2.303649
33	8	-5.890774	0.968287	-1.062948	70	1	-8.354123	-0.071683	-1.037739
34	8	-5.742878	1.579162	1.601576	71	1	-8.189542	-1.076119	0.419712
35	1	3.29047	-0.503294	-1.21914	72	1	-8.329071	0.686044	0.564385
36	1	2.754417	1.420442	1.085932	73	1	-5.52981	2.051014	0.771398
37	1	1.14896	0.602032	-1.342616					

Conf-4

Center Number	Atomic Number	Coordinates (Angstroms)			Center Number	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z			X	Y	Z
1	6	7.138552	-1.212991	-0.509831	38	1	7.335778	-1.832389	0.380267
2	6	7.69854	0.173715	-0.327313	39	1	7.60898	-1.728977	-1.354324
3	6	6.910927	1.247555	-0.160022	40	1	8.779655	0.283368	-0.373812
4	6	5.451161	1.170418	-0.085966	41	1	7.355347	2.238863	-0.08718
5	6	4.839967	-0.219977	0.145259	42	1	5.194746	3.229875	-0.359548
6	6	5.637313	-1.17853	-0.754021	43	1	2.830784	2.462611	-1.21802
7	6	4.692864	2.273687	-0.208419	44	1	2.836991	3.144572	0.392088
8	6	3.19601	2.286898	-0.191934	45	1	0.730183	-2.545148	0.21589
9	6	2.588145	0.98747	0.350384	46	1	0.984168	-1.564633	-1.218107
10	6	3.331459	-0.244334	-0.212814	47	1	3.130751	-2.392795	-0.303227
11	6	1.108054	0.885987	-0.015576	48	1	2.761604	-1.719652	1.272429
12	6	0.391202	-0.394032	0.490163	49	1	0.292254	2.907886	-0.261238
13	6	1.132468	-1.58987	-0.13286	50	1	0.40017	2.366596	1.40855
14	6	2.635353	-1.555883	0.196832	51	1	-1.780097	1.549521	1.247333
15	6	0.177114	2.034059	0.387509	52	1	-1.872774	1.879971	-0.455723
16	6	-1.242979	1.417175	0.308315	53	1	4.443343	-0.045273	2.281684
17	6	-1.079756	-0.105367	-0.007768	54	1	4.918902	-1.683394	1.797414
18	6	5.102896	-0.618875	1.624315	55	1	6.132783	-0.396138	1.911863

19	6	0.401102	-0.489515	2.028673	56	1	1.415961	-0.462493	2.43273
20	6	-2.221845	-0.96698	0.603127	57	1	-0.154685	0.327775	2.497575
21	6	-3.594005	-0.489312	0.075291	58	1	-0.052356	-1.429474	2.359731
22	6	-2.011169	-2.46884	0.361245	59	1	-2.235154	-0.79288	1.685274
23	8	5.1282	-1.850981	-1.634597	60	1	-1.09924	-2.815017	0.848303
24	8	-1.17398	-0.342051	-1.427656	61	1	-1.926846	-2.690431	-0.706889
25	1	-3.470933	-0.198298	-0.971787	62	1	-2.833531	-3.058195	0.774368
26	8	-3.976897	0.663213	0.850746	63	1	-0.701867	0.368852	-1.895041
27	6	-5.011663	1.427566	0.279368	64	1	-5.293431	2.136597	1.062491
28	6	-6.227967	0.585755	-0.132287	65	1	-4.816734	-1.877293	1.199658
29	6	-6.071475	-0.879462	-0.210137	66	1	-4.556566	-2.356325	-0.483006
30	6	-4.737779	-1.497358	0.172669	67	1	-8.170668	-1.368362	-0.476425
31	6	-7.24772	-1.822766	-0.1125	68	1	-7.052572	-2.723084	-0.706311
32	6	-7.548266	1.293748	0.051107	69	1	-7.396716	-2.133539	0.927742
33	8	-6.029057	-0.060624	-1.417689	70	1	-8.370228	0.746668	-0.413032
34	8	-4.590221	2.20093	-0.821761	71	1	-7.768678	1.424047	1.116719
35	1	3.272559	-0.174126	-1.308497	72	1	-7.494167	2.287399	-0.407939
36	1	2.691226	1.002545	1.444021	73	1	-4.655086	1.6229	-1.608623
37	1	1.090768	0.824332	-1.116597					

Conf-5

Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z	Center Number	Atomic Number	Coordinates (Angstroms) X	Y	Z
1	6	7.128497	-1.144088	-0.291382	38	1	7.364861	-1.514917	0.719309
2	6	7.641691	0.260257	-0.475947	39	1	7.600957	-1.840674	-0.99302
3	6	6.819062	1.317394	-0.560534	40	1	8.717103	0.387353	-0.57774
4	6	5.3647	1.21708	-0.429993	41	1	7.228651	2.308382	-0.749591
5	6	4.808123	-0.0888	0.157596	42	1	5.029804	3.133257	-1.203
6	6	5.622429	-1.217681	-0.494764	43	1	2.67863	2.101165	-1.77746
7	6	4.565121	2.231004	-0.804029	44	1	2.690666	3.168879	-0.392694
8	6	3.0694	2.202394	-0.75079	45	1	0.787144	-2.43898	0.932113
9	6	2.518463	1.064516	0.117673	46	1	0.975172	-1.84939	-0.713458
10	6	3.294344	-0.24657	-0.140679	47	1	3.168572	-2.354536	0.313176
11	6	1.036928	0.831261	-0.171761	48	1	2.810545	-1.320043	1.681549
12	6	0.377823	-0.300699	0.661419	49	1	0.128197	2.688227	-0.904229
13	6	1.146772	-1.59417	0.336935	50	1	0.325619	2.622974	0.842642
14	6	2.654427	-1.433946	0.603451	51	1	-1.779075	1.699362	1.052183
15	6	0.077806	2.019748	-0.039519	52	1	-2.00381	1.621227	-0.690214
16	6	-1.317217	1.36397	0.120108	53	1	4.445706	0.601751	2.193093
17	6	-1.103239	-0.183748	0.142488	54	1	4.972845	-1.089568	2.119511
18	6	5.113896	-0.096881	1.681623	55	1	6.140046	0.222742	1.876205
19	6	0.422995	-0.019374	2.175607	56	1	1.445523	0.131696	2.528981
20	6	-2.202781	-0.923201	0.967028	57	1	-0.147239	0.872232	2.452758
21	6	-3.662924	-0.622474	0.525009	58	1	0.010575	-0.864765	2.737145
22	6	-1.99726	-2.445571	0.972642	59	1	-2.133778	-0.565206	2.001025
23	8	5.121945	-2.105847	-1.163741	60	1	-1.964653	-2.829689	-0.051044
24	8	-1.082933	-0.69201	-1.198149	61	1	-2.816997	-2.941717	1.503539
25	1	-4.257352	-1.508906	0.774458	62	1	-1.067798	-2.727176	1.469097
26	8	-3.723724	-0.442814	-0.905083	63	1	-2.007043	-0.637589	-1.507093

27	6	-5.023112	-0.551752	-1.462633	64	1	-4.908589	-0.172275	-2.480858
28	6	-6.074428	0.269846	-0.70305	65	1	-3.776788	1.488849	1.028085
29	6	-5.745606	0.793515	0.638413	66	1	-4.407771	0.405128	2.269976
30	6	-4.347417	0.570946	1.186525	67	1	-5.949088	2.90295	1.001164
31	6	-6.472678	1.971434	1.243786	68	1	-7.501648	2.046196	0.888676
32	6	-7.147241	0.840405	-1.599058	69	1	-6.493921	1.873049	2.335075
33	8	-6.541248	-0.419364	0.486765	70	1	-7.974976	1.257672	-1.024052
34	8	-5.451741	-1.882257	-1.572552	71	1	-6.732148	1.625787	-2.240766
35	1	3.210629	-0.454956	-1.216917	72	1	-7.542173	0.047743	-2.244373
36	1	2.645725	1.357525	1.169196	73	1	-5.87969	-2.115259	-0.723552
37	1	0.977734	0.490955	-1.213815					

Conf-6

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	7.139093	-1.209485	-0.520036	38	1	7.340008	-1.829399	0.368915
2	6	7.698161	0.177679	-0.338401	39	1	7.607312	-1.724493	-1.36637
3	6	6.909913	1.250753	-0.16923	40	1	8.779071	0.288281	-0.387244
4	6	5.450447	1.172366	-0.091881	41	1	7.353614	2.242456	-0.097327
5	6	4.841152	-0.218458	0.14105	42	1	5.191343	3.23124	-0.365936
6	6	5.636986	-1.177546	-0.758944	43	1	2.825618	2.461219	-1.218433
7	6	4.690547	2.274696	-0.213209	44	1	2.835365	3.143893	0.391221
8	6	3.193748	2.28634	-0.193345	45	1	0.735041	-2.549194	0.194258
9	6	2.587387	0.986779	0.350652	46	1	1.022502	-1.55361	-1.22986
10	6	3.332051	-0.243313	-0.21401	47	1	3.134279	-2.392973	-0.302229
11	6	1.106335	0.887484	-0.011695	48	1	2.761122	-1.719481	1.272787
12	6	0.392911	-0.394791	0.491851	49	1	0.286281	2.907758	-0.236696
13	6	1.137677	-1.587951	-0.138208	50	1	0.413882	2.361165	1.43066
14	6	2.639367	-1.55563	0.197084	51	1	-1.76809	1.535692	1.288512
15	6	0.180173	2.031654	0.410421	52	1	-1.871494	1.880453	-0.416197
16	6	-1.239428	1.416355	0.343053	53	1	4.449087	-0.043214	2.278279
17	6	-1.080089	-0.094975	0.008353	54	1	4.923101	-1.681789	1.793295
18	6	5.106963	-0.617256	1.619636	55	1	6.137579	-0.395024	1.904951
19	6	0.407385	-0.507862	2.02924	56	1	1.423222	-0.47874	2.430119
20	6	-2.226943	-0.964494	0.614592	57	1	-0.150516	0.303047	2.505927
21	6	-3.596927	-0.489919	0.080992	58	1	-0.040486	-1.452582	2.354758
22	6	-2.020175	-2.468352	0.379064	59	1	-2.2446	-0.796729	1.69793
23	8	5.125475	-1.853705	-1.635382	60	1	-1.09819	-2.814689	0.846291
24	8	-1.145491	-0.167445	-1.431441	61	1	-1.970018	-2.717059	-0.688489
25	1	-3.468677	-0.206437	-0.968326	62	1	-2.834839	-3.053785	0.811526
26	8	-3.980302	0.667163	0.846987	63	1	-0.929512	-1.075588	-1.70686
27	6	-5.013127	1.430012	0.268966	64	1	-5.298197	2.140399	1.049609
28	6	-6.227469	0.586982	-0.14548	65	1	-4.826687	-1.868041	1.210189
29	6	-6.072882	-0.878881	-0.213854	66	1	-4.560464	-2.360856	-0.467903
30	6	-4.742301	-1.496419	0.180601	67	1	-8.171008	-1.365982	-0.489656
31	6	-7.251022	-1.819928	-0.117787	68	1	-7.053955	-2.723817	-0.705514
32	6	-7.547887	1.29789	0.025426	69	1	-7.406642	-2.124632	0.923273
33	8	-6.021133	-0.067415	-1.425641	70	1	-8.367625	0.749713	-0.441335
34	8	-4.587163	2.201212	-0.831204	71	1	-7.775161	1.434029	1.088864

35	1	3.270474	-0.174185	-1.309557	72	1	-7.489003	2.289028	-0.438371
36	1	2.695715	1.001993	1.444088	73	1	-4.642313	1.620897	-1.617136
37	1	1.059482	0.830182	-1.107962					

Conf-7

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	7.115051	-1.411783	-0.119781	38	1	7.286321	-1.766834	0.909498
2	6	7.726495	-0.049592	-0.320941	39	1	7.567889	-2.15788	-0.782318
3	6	6.979534	1.055753	-0.46798	40	1	8.811103	0.004412	-0.38164
4	6	5.517635	1.053797	-0.394783	41	1	7.460698	2.01204	-0.666619
5	6	4.854542	-0.194913	0.206333	42	1	5.339419	2.96297	-1.234922
6	6	5.616986	-1.392703	-0.38347	43	1	2.950428	2.067828	-1.876297
7	6	4.801838	2.105056	-0.830108	44	1	2.978084	3.173632	-0.521667
8	6	3.306529	2.174619	-0.837604	45	1	0.652935	-2.259877	0.879677
9	6	2.650119	1.102122	0.04027	46	1	0.960086	-1.739039	-0.769262
10	6	3.346232	-0.265731	-0.147152	47	1	3.072857	-2.347052	0.361056
11	6	1.166924	0.955873	-0.297129	48	1	2.725605	-1.252453	1.685069
12	6	0.412278	-0.112729	0.534828	49	1	0.420492	2.871527	-1.071864
13	6	1.103027	-1.461859	0.281082	50	1	0.485088	2.771752	0.683355
14	6	2.605381	-1.38918	0.605187	51	1	-1.731614	2.038883	0.656154
15	6	0.269291	2.196415	-0.224449	52	1	-1.73512	1.843878	-1.089347
16	6	-1.168826	1.615217	-0.181371	53	1	4.460886	0.578576	2.206257
17	6	-1.047196	0.061207	-0.037191	54	1	4.879565	-1.144436	2.200304
18	6	5.100895	-0.176466	1.740946	55	1	6.137439	0.082949	1.967121
19	6	0.426317	0.22383	2.039525	56	1	1.443582	0.346182	2.418225
20	6	-2.19126	-0.534792	0.814516	57	1	-0.114105	1.147905	2.265066
21	6	-3.589134	-0.107627	0.321075	58	1	-0.03786	-0.580941	2.618374
22	6	-2.104327	-2.056532	0.995036	59	1	-2.116876	-0.070696	1.803649
23	8	5.084818	-2.262979	-1.051408	60	1	-1.295201	-2.329412	1.676935
24	8	-1.158098	-0.571134	-1.324435	61	1	-1.924568	-2.560065	0.041771
25	1	-3.590163	0.974729	0.157723	62	1	-3.038035	-2.433626	1.422634
26	8	-4.491827	-0.399023	1.407715	63	1	-0.547819	-0.133344	-1.944484
27	6	-5.759191	0.204348	1.286924	64	1	-6.367324	-0.281008	2.055412
28	6	-6.40631	0.01627	-0.093545	65	1	-4.038041	-1.880039	-0.829069
29	6	-5.563134	-0.446935	-1.212104	66	1	-3.493418	-0.512354	-1.794166
30	6	-4.112439	-0.792033	-0.937775	67	1	-7.158513	-0.771493	-2.650807
31	6	-6.144024	-1.112642	-2.437767	68	1	-5.518319	-0.8922	-3.310174
32	6	-7.90845	-0.123393	-0.042912	69	1	-6.160509	-2.200234	-2.30445
33	8	-5.890978	0.969212	-1.062215	70	1	-8.354327	-0.07202	-1.037357
34	8	-5.741965	1.578229	1.602407	71	1	-8.189286	-1.076213	0.420153
35	1	3.290489	-0.50285	-1.219339	72	1	-8.328996	0.685898	0.564718
36	1	2.754257	1.419936	1.086495	73	1	-5.530336	2.050519	0.772108
37	1	1.14892	0.602423	-1.342439					

Conf-8

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	5.542719	-2.823468	0.289018	38	1	5.439662	-3.185988	1.324773

2	6	6.692197	-1.856102	0.176022	39	1	5.7012	-3.711129	-0.333615
3	6	6.504733	-0.543264	-0.030801	40	1	7.696947	-2.269009	0.23089
4	6	5.181594	0.077237	-0.112279	41	1	7.364178	0.112264	-0.16198
5	6	3.992135	-0.75373	0.392675	42	1	5.919777	1.855858	-0.932634
6	6	4.230601	-2.178819	-0.132574	43	1	3.457211	2.043524	-1.838074
7	6	5.029475	1.319876	-0.602077	44	1	3.812796	3.069935	-0.467872
8	6	3.715258	2.01752	-0.765842	45	1	-0.732811	-0.827853	0.551678
9	6	2.576199	1.351425	0.016186	46	1	-0.041818	-0.538437	-1.033503
10	6	2.642723	-0.187462	-0.12035	47	1	1.460194	-1.940719	0.324184
11	6	1.217973	1.838395	-0.485715	48	1	1.469269	-0.755914	1.616376
12	6	-0.006119	1.211544	0.230002	49	1	1.466191	3.881438	-1.258097
13	6	0.076469	-0.308737	0.030292	50	1	1.226043	3.786507	0.483178
14	6	1.420419	-0.867018	0.527902	51	1	-1.060095	4.112092	0.04768
15	6	0.925666	3.34248	-0.47394	52	1	-0.880706	3.767191	-1.664129
16	6	-0.611106	3.417984	-0.664078	53	1	3.760148	0.172951	2.351847
17	6	-1.166836	1.96562	-0.524457	54	1	3.402043	-1.563555	2.360627
18	6	4.061945	-0.796274	1.944848	55	1	5.080297	-0.996395	2.28531
19	6	-0.016282	1.539448	1.735093	56	1	0.926552	1.261386	2.21207
20	6	-2.629067	1.93466	0.041567	57	1	-0.174101	2.602279	1.933281
21	6	-3.239158	0.522306	0.183181	58	1	-0.80765	0.983126	2.246751
22	6	-2.888527	2.703168	1.354901	59	1	-3.208329	2.437157	-0.746277
23	8	3.452463	-2.762116	-0.868176	60	1	-2.290396	3.612183	1.426345
24	8	-1.22723	1.491342	-1.883664	61	1	-2.672145	2.098381	2.23974
25	1	-2.660572	-0.054247	0.914303	62	1	-3.937432	3.007192	1.412401
26	8	-3.171294	-0.139034	-1.098325	63	1	-1.758462	0.67213	-1.861536
27	6	-3.513881	-1.516349	-1.123612	64	1	-3.644935	-1.733434	-2.186493
28	6	-4.79911	-1.83562	-0.355155	65	1	-5.25997	1.246801	-0.027641
29	6	-5.371317	-0.809862	0.535755	66	1	-4.79473	0.91278	1.644195
30	6	-4.706122	0.54986	0.615131	67	1	-7.245065	-1.822248	0.957004
31	6	-6.827333	-0.814518	0.939276	68	1	-6.936914	-0.381162	1.93987
32	6	-5.583278	-2.980303	-0.950425	69	1	-7.413505	-0.204174	0.243168
33	8	-4.567884	-1.900047	1.07713	70	1	-6.380622	-3.312702	-0.284387
34	8	-2.480067	-2.350343	-0.674523	71	1	-6.024395	-2.684926	-1.909088
35	1	2.602491	-0.409727	-1.19633	72	1	-4.911047	-3.826297	-1.131258
36	1	2.698345	1.623574	1.073615	73	1	-2.546392	-2.388497	0.30144
37	1	1.139011	1.509278	-1.530608					

Conf-9

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	7.132032	-1.123427	-0.296146	38	1	7.368061	-1.504764	0.710694
2	6	7.639569	0.285121	-0.463723	39	1	7.608652	-1.809943	-1.004847
3	6	6.812624	1.33979	-0.53644	40	1	8.714517	0.417868	-0.563147
4	6	5.358609	1.2321	-0.408202	41	1	7.218307	2.33461	-0.71341
5	6	4.806593	-0.083427	0.161885	42	1	5.016594	3.156811	-1.156508
6	6	5.626684	-1.200568	-0.503384	43	1	2.669777	2.124424	-1.745502
7	6	4.555248	2.247691	-0.769429	44	1	2.677073	3.172708	-0.34599
8	6	3.059607	2.212714	-0.717274	45	1	0.793928	-2.462857	0.891143
9	6	2.512159	1.060654	0.134647	46	1	0.986045	-1.847053	-0.744377

10	6	3.293995	-0.243452	-0.14099	47	1	3.177587	-2.357928	0.284282
11	6	1.031859	0.826099	-0.160163	48	1	2.809722	-1.343634	1.665208
12	6	0.376087	-0.322722	0.652244	49	1	0.118241	2.694175	-0.858108
13	6	1.152178	-1.607355	0.310564	50	1	0.308617	2.593263	0.887878
14	6	2.657915	-1.443883	0.585123	51	1	-1.798311	1.659545	1.064039
15	6	0.066981	2.007567	-0.00771	52	1	-2.007715	1.6087	-0.679764
16	6	-1.325808	1.342112	0.13078	53	1	4.438454	0.58037	2.205225
17	6	-1.103214	-0.205096	0.129762	54	1	4.97143	-1.108112	2.111391
18	6	5.109854	-0.109551	1.686206	55	1	6.134567	0.211163	1.886518
19	6	0.414473	-0.064936	2.170909	56	1	1.434717	0.089262	2.529586
20	6	-2.20182	-0.961925	0.938768	57	1	-0.164095	0.817361	2.460225
21	6	-3.66147	-0.657625	0.491514	58	1	0.007557	-0.922409	2.71795
22	6	-1.989302	-2.482966	0.92665	59	1	-2.137389	-0.617472	1.977508
23	8	5.131167	-2.081972	-1.184881	60	1	-1.062924	-2.766872	1.427827
24	8	-1.076749	-0.694496	-1.217765	61	1	-1.945755	-2.853615	-0.101733
25	1	-4.245149	-1.570484	0.655859	62	1	-2.811332	-2.989572	1.444051
26	8	-3.70571	-0.359551	-0.919578	63	1	-1.996562	-0.615798	-1.534474
27	6	-4.996482	-0.428864	-1.503107	64	1	-4.870429	0.03942	-2.482272
28	6	-6.066164	0.314799	-0.691278	65	1	-3.800256	1.40009	1.16992
29	6	-5.760557	0.726065	0.69386	66	1	-4.442092	0.210541	2.305028
30	6	-4.36828	0.468721	1.240679	67	1	-7.533096	1.935764	1.024987
31	6	-6.507888	1.841605	1.386304	68	1	-6.541596	1.651811	2.465121
32	6	-7.13285	0.949015	-1.551145	69	1	-5.99151	2.795314	1.229543
33	8	-6.541081	-0.477777	0.429146	70	1	-7.973064	1.307418	-0.954926
34	8	-5.412005	-1.747331	-1.736183	71	1	-6.717696	1.790384	-2.117401
35	1	3.212863	-0.43706	-1.220188	72	1	-7.50979	0.2103	-2.267301
36	1	2.636876	1.339305	1.190363	73	1	-5.850542	-2.057301	-0.917706
37	1	0.974977	0.503743	-1.208046					

Conf-10

Center	Atomic	Coordinates (Angstroms)			Center	Atomic	Coordinates (Angstroms)		
Number	Number	X	Y	Z	Number	Number	X	Y	Z
1	6	7.109417	-1.226002	-0.252445	38	1	7.343303	-1.553081	0.773802
2	6	7.647378	0.158439	-0.50489	39	1	7.565943	-1.963462	-0.922128
3	6	6.843889	1.225561	-0.635777	40	1	8.724424	0.260639	-0.616884
4	6	5.388593	1.158514	-0.494549	41	1	7.270693	2.198794	-0.87287
5	6	4.811261	-0.107958	0.155823	42	1	5.084493	3.042537	-1.354477
6	6	5.601437	-1.280674	-0.446928	43	1	2.712093	2.029381	-1.870121
7	6	4.605618	2.168499	-0.911869	44	1	2.75084	3.158749	-0.535735
8	6	3.109889	2.170027	-0.850806	45	1	0.752083	-2.348027	1.049234
9	6	2.542425	1.08345	0.071175	46	1	0.946039	-1.835838	-0.621087
10	6	3.293656	-0.25186	-0.12879	47	1	3.13298	-2.333744	0.423789
11	6	1.055645	0.863824	-0.202048	48	1	2.797781	-1.230177	1.743125
12	6	0.379867	-0.216926	0.683627	49	1	0.180385	2.70576	-1.009676
13	6	1.125063	-1.537177	0.416561	50	1	0.377177	2.707266	0.738437
14	6	2.636044	-1.391622	0.671923	51	1	-1.75191	1.840217	0.976086
15	6	0.118535	2.073539	-0.118852	52	1	-1.961275	1.67738	-0.76402
16	6	-1.287894	1.449816	0.066807	53	1	4.470976	0.683677	2.157975
17	6	-1.101759	-0.098609	0.165305	54	1	4.967279	-1.018529	2.1619

18	6	5.124056	-0.050205	1.677321	55	1	6.15669	0.259471	1.85276
19	6	0.435087	0.133605	2.183045	56	1	1.461174	0.284401	2.526097
20	6	-2.207986	-0.779534	1.030251	57	1	-0.11998	1.046188	2.419869
21	6	-3.666302	-0.503126	0.579903	58	1	0.011013	-0.677761	2.784549
22	6	-2.011689	-2.301119	1.123592	59	1	-2.138206	-0.362182	2.041995
23	8	5.081385	-2.188523	-1.073255	60	1	-1.956216	-2.741326	0.123963
24	8	-1.096247	-0.66854	-1.151175	61	1	-2.846905	-2.764163	1.659838
25	1	-4.281655	-1.314624	0.981455	62	1	-1.096223	-2.558895	1.657701
26	8	-3.754769	-0.56801	-0.8608	63	1	-2.025402	-0.648773	-1.448033
27	6	-5.064961	-0.760015	-1.360644	64	1	-4.986534	-0.459799	-2.413225
28	6	-6.127935	0.102228	-0.674439	65	1	-3.770572	1.67067	0.65211
29	6	-5.749378	0.895843	0.515789	66	1	-4.324647	0.860997	2.120764
30	6	-4.319178	0.803484	1.024226	67	1	-6.455518	2.2788	1.997258
31	6	-6.47286	2.163327	0.907338	68	1	-5.972942	3.035335	0.470594
32	6	-7.276106	0.455099	-1.592919	69	1	-7.514673	2.160058	0.582736
33	8	-6.502888	-0.335301	0.650956	70	1	-8.092397	0.93132	-1.048104
34	8	-5.48249	-2.096301	-1.246274	71	1	-6.943257	1.129771	-2.389793
35	1	3.201189	-0.508543	-1.193825	72	1	-7.662227	-0.45816	-2.058929
36	1	2.679115	1.422408	1.107613	73	1	-4.881754	-2.63443	-1.798946
37	1	0.985809	0.478531	-1.22778					

Figure S4. ^{1}H NMR spectrum of solaundaic acid A (**1**) in $CDCl_3$

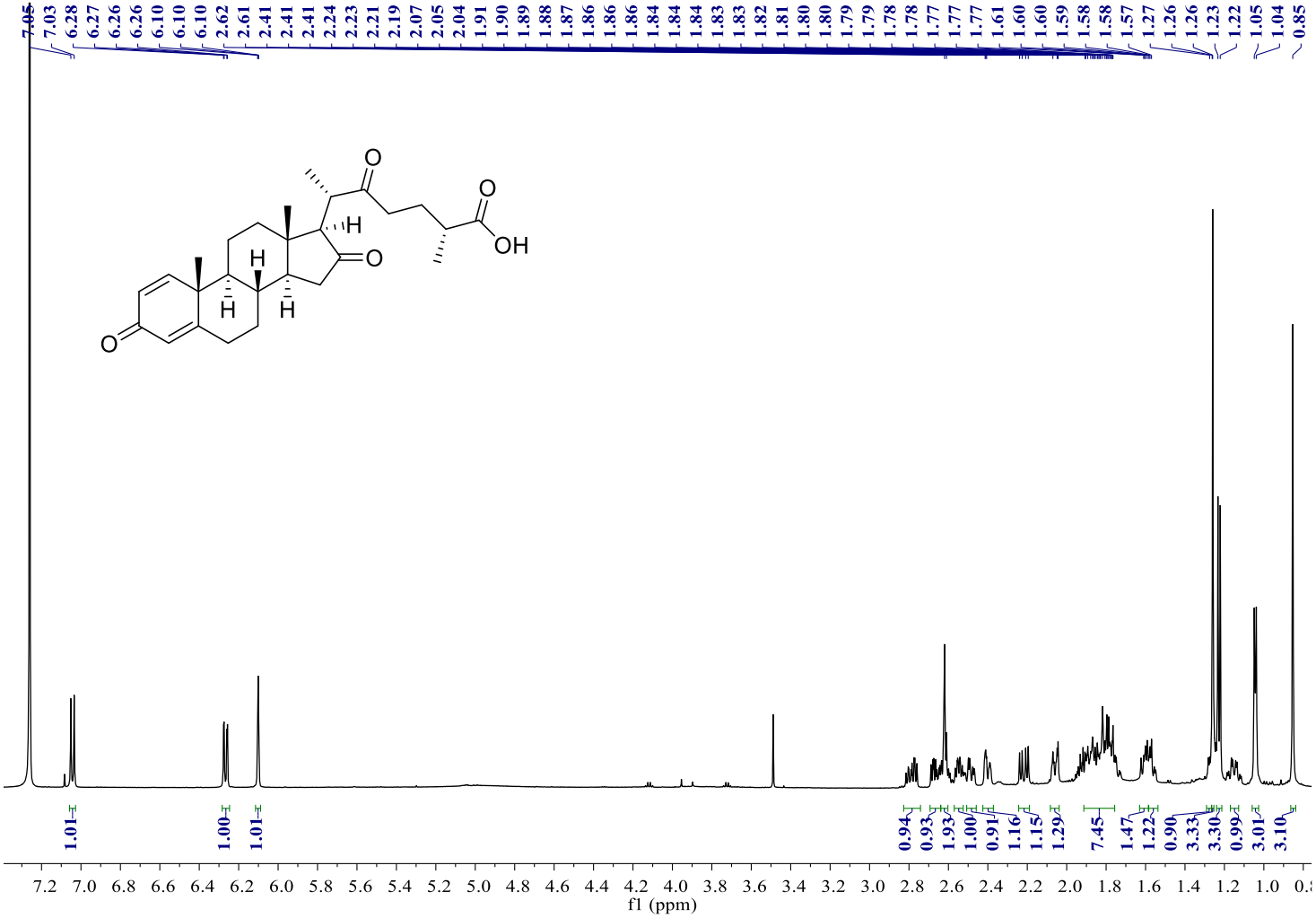


Figure S5. ^{13}C NMR spectrum of solaundaic acid A (**1**) in $CDCl_3$

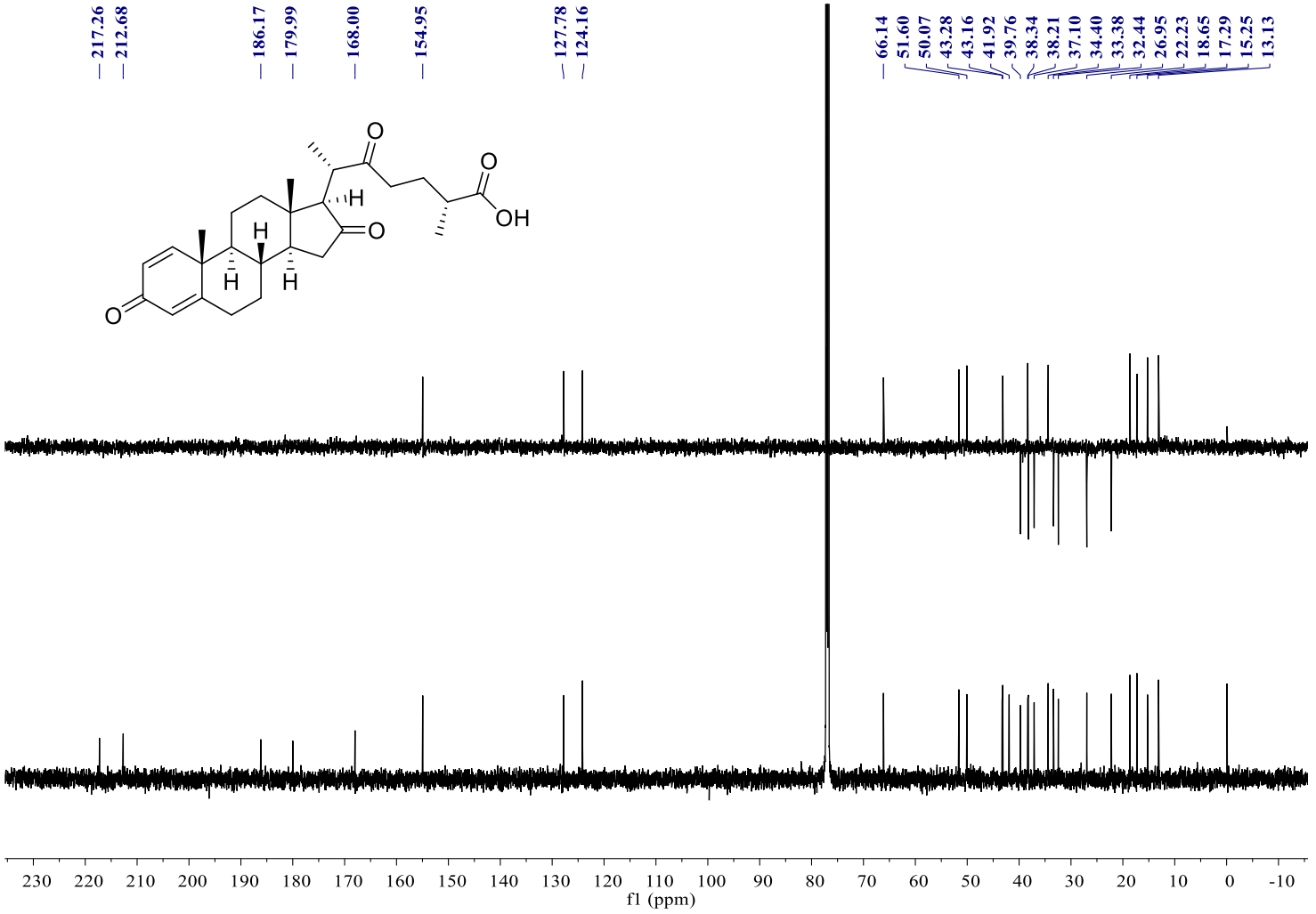


Figure S6. HSQC spectrum of solaundaic acid A (**1**) in $CDCl_3$

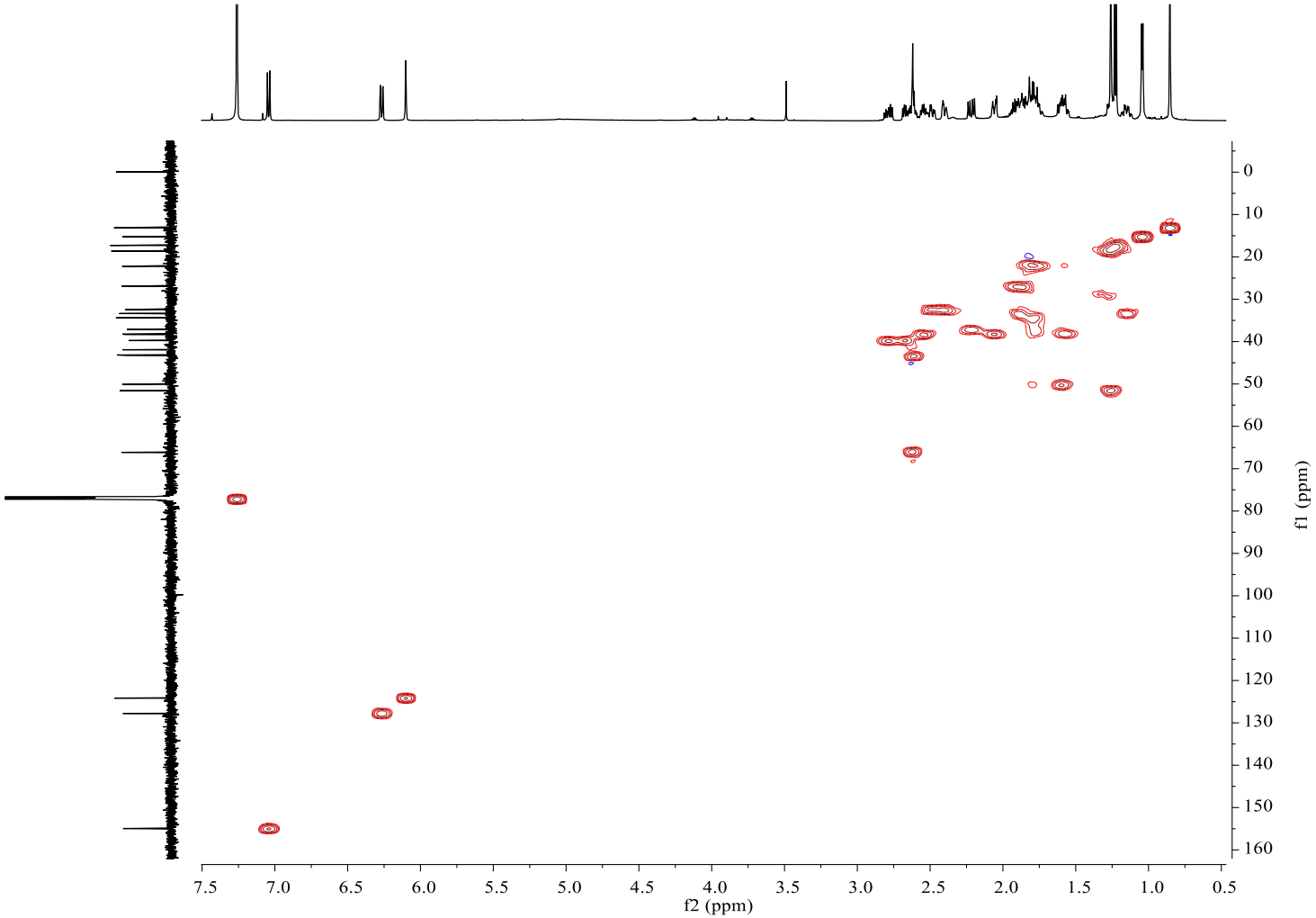


Figure S7. HMBC spectrum of solaundaic acid A (**1**) in $CDCl_3$

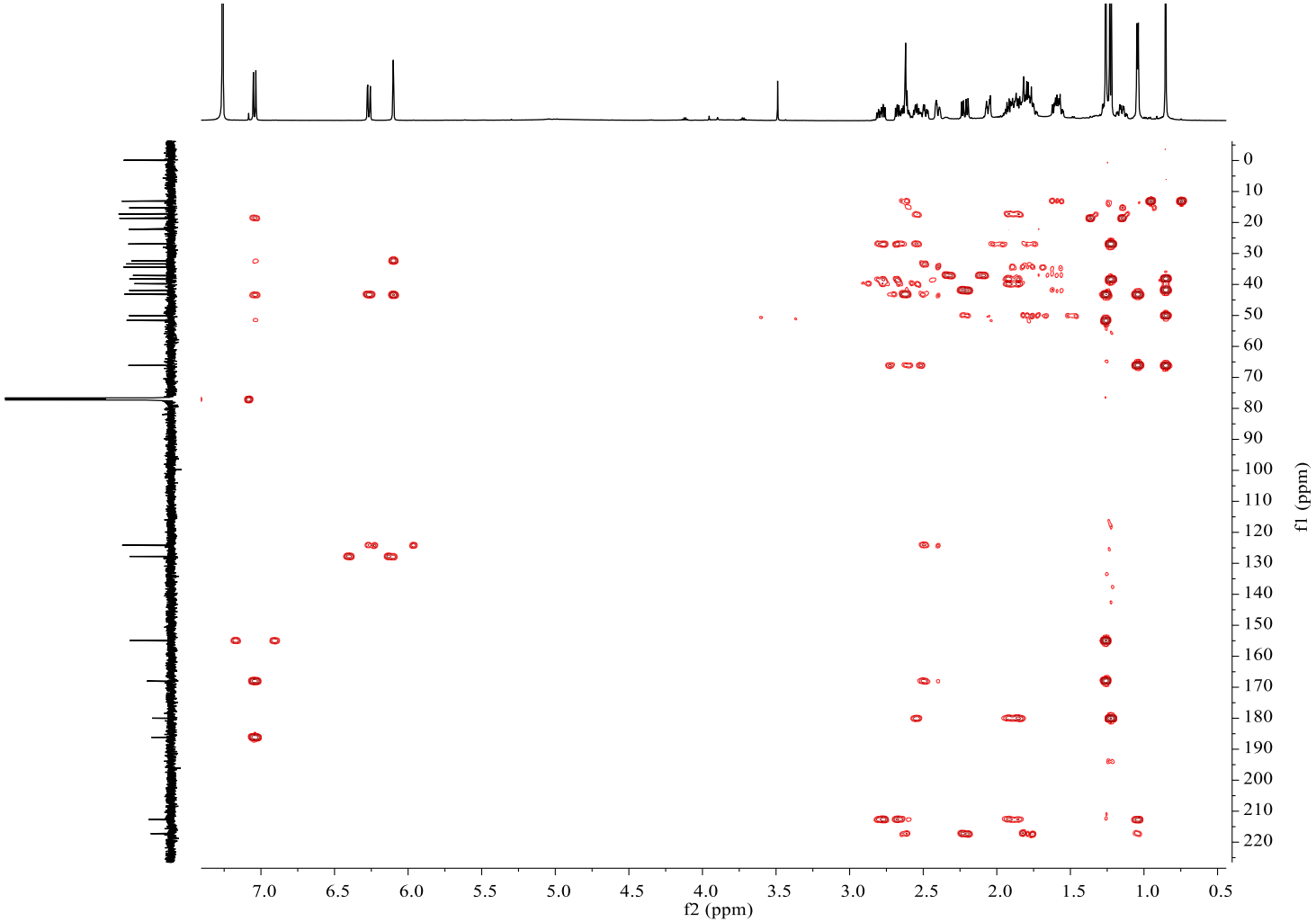


Figure S8. ^{1}H-^{1}H COSY spectrum of solaundaic acid A (**1**) in $CDCl_3$

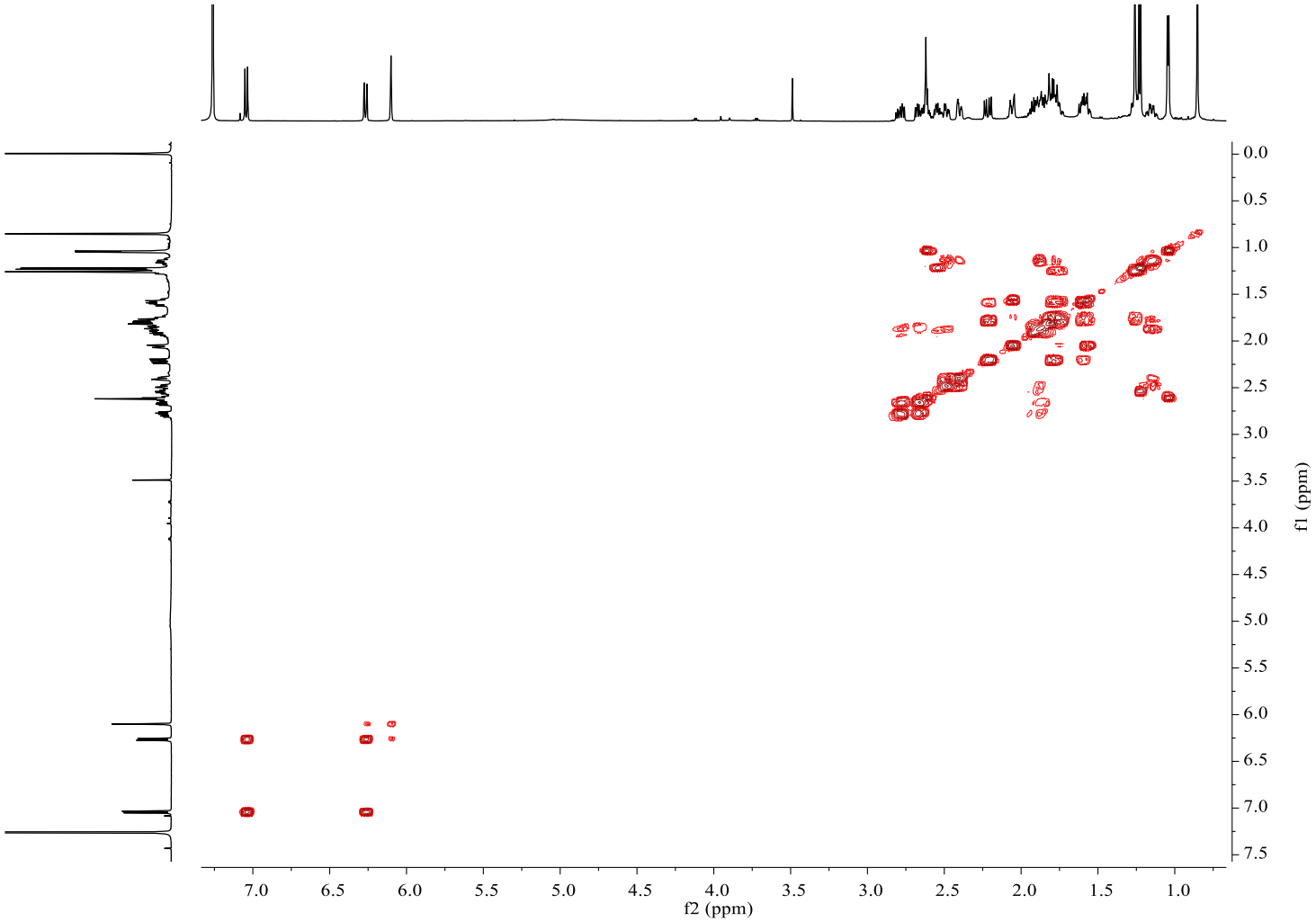


Figure S9. NOESY spectrum of solaundaic acid A (**1**) in $CDCl_3$

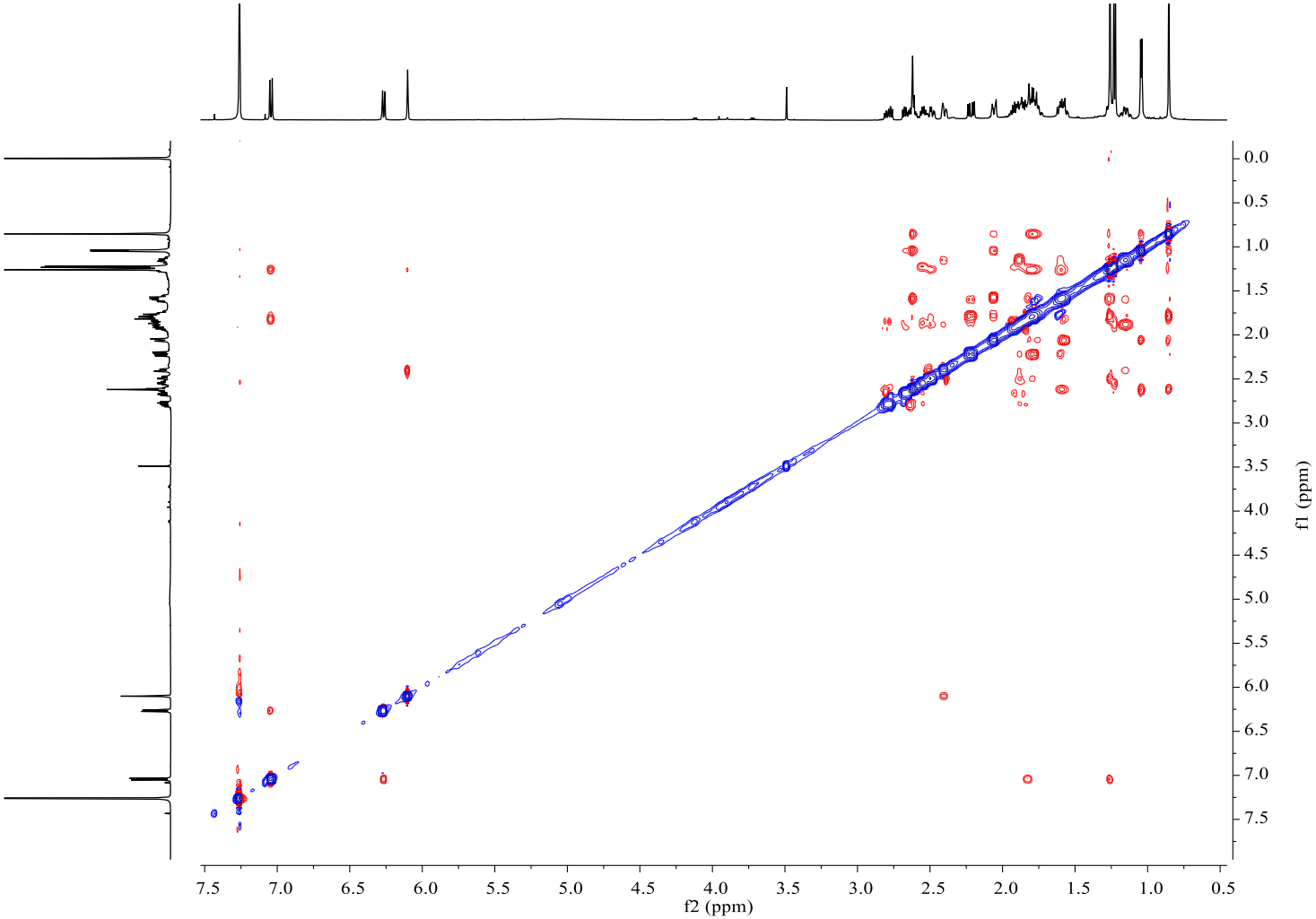


Figure S10. (–)-ESIMS spectrum of solaundaic acid A (**1**)

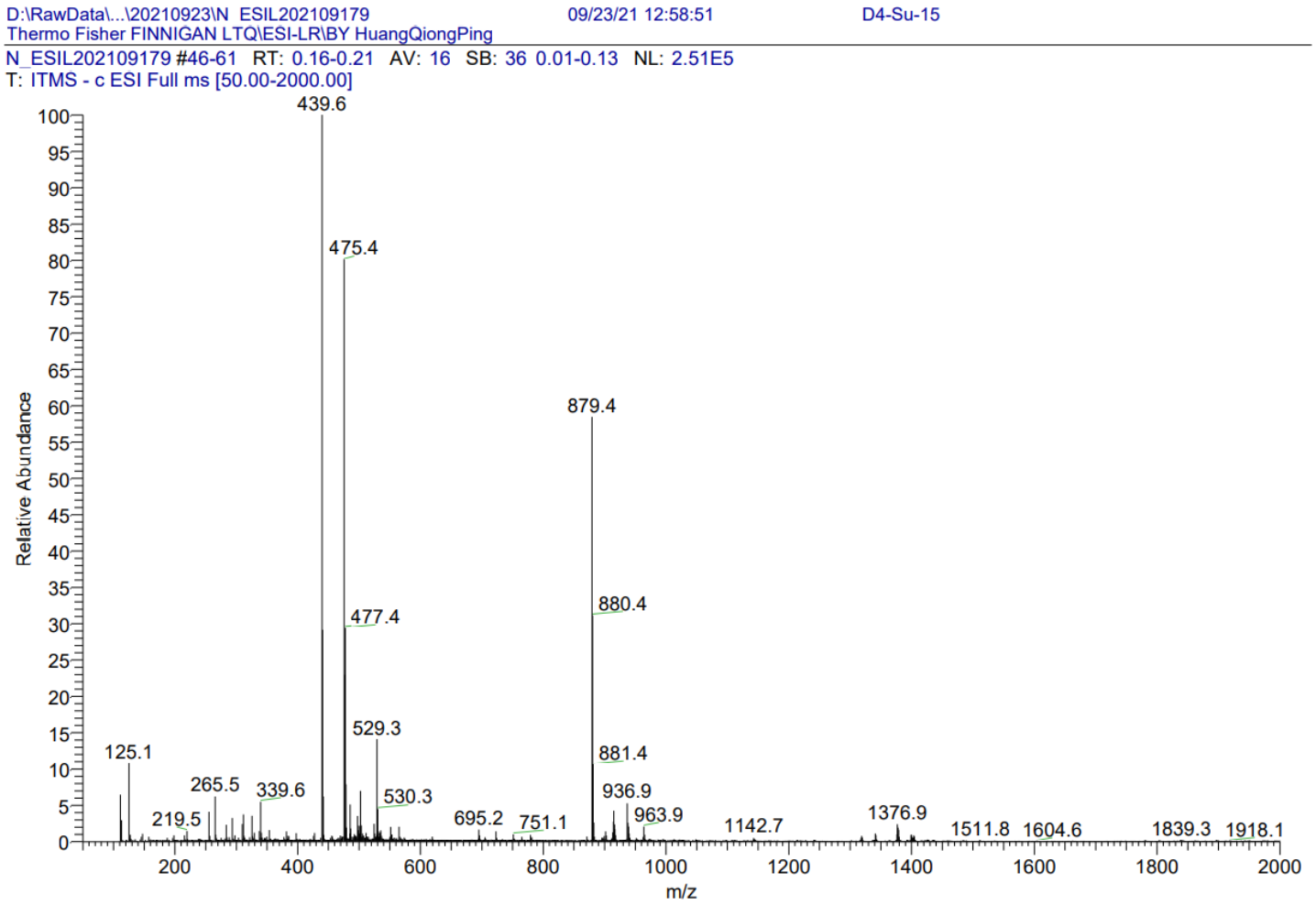


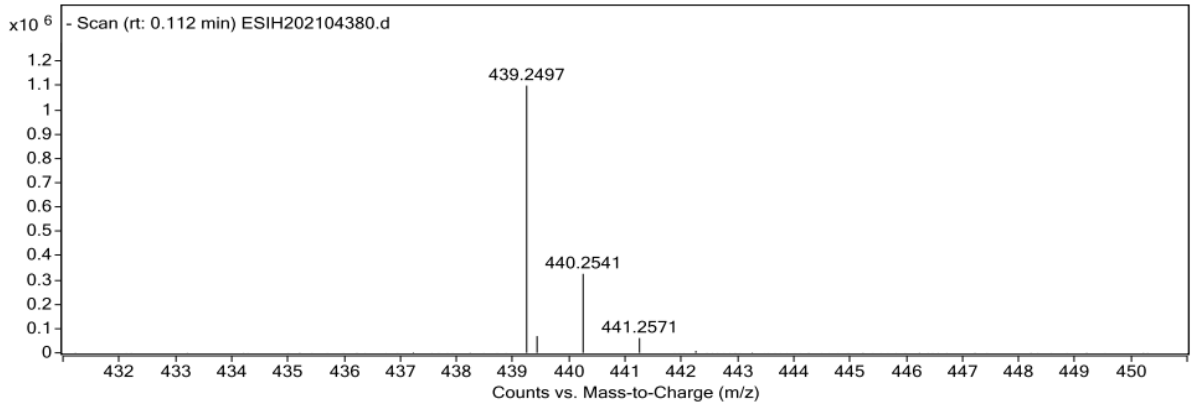
Figure S11. (–)-HRESIMS spectrum of solaundaic acid A (**1**)

Qualitative Analysis Report

Data Filename	ESIH202104380.d	**Sample Name**	D4-SU-15
Sample ID		**Position**	P1-B1
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160324_MS_ESIH_NEG_1min.m
Acquired Time	9/24/2021 17:48:37	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by fangsu

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
439.2497	439.249	-0.66	-1.5	C27 H35 O5	(M-H)-

--- End Of Report ---

Figure S12. IR spectrum of solaundaic acid A (**1**)

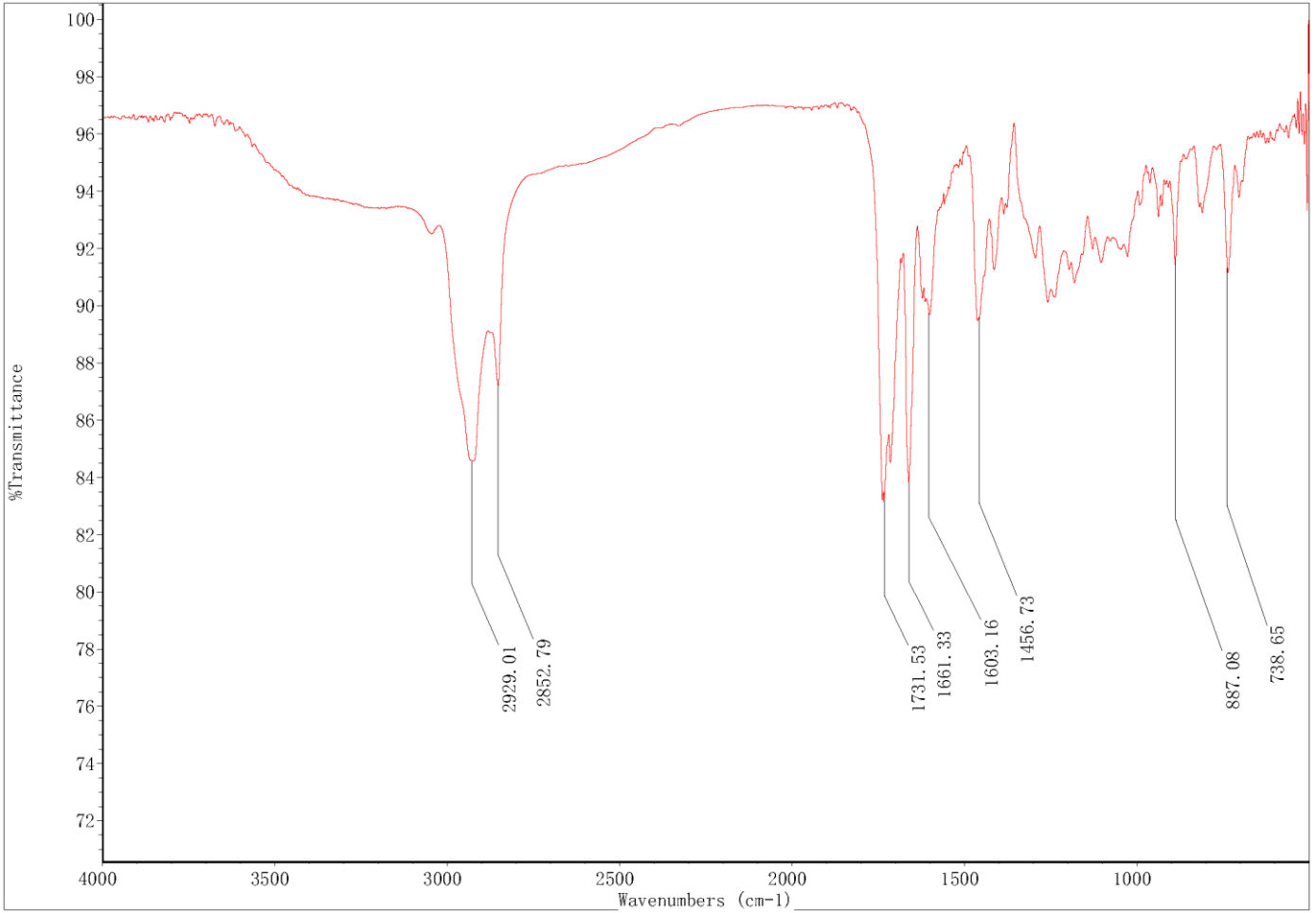


Figure S13. ^{1}H NMR spectrum of solaundalide A (**2**) in $CDCl_3$

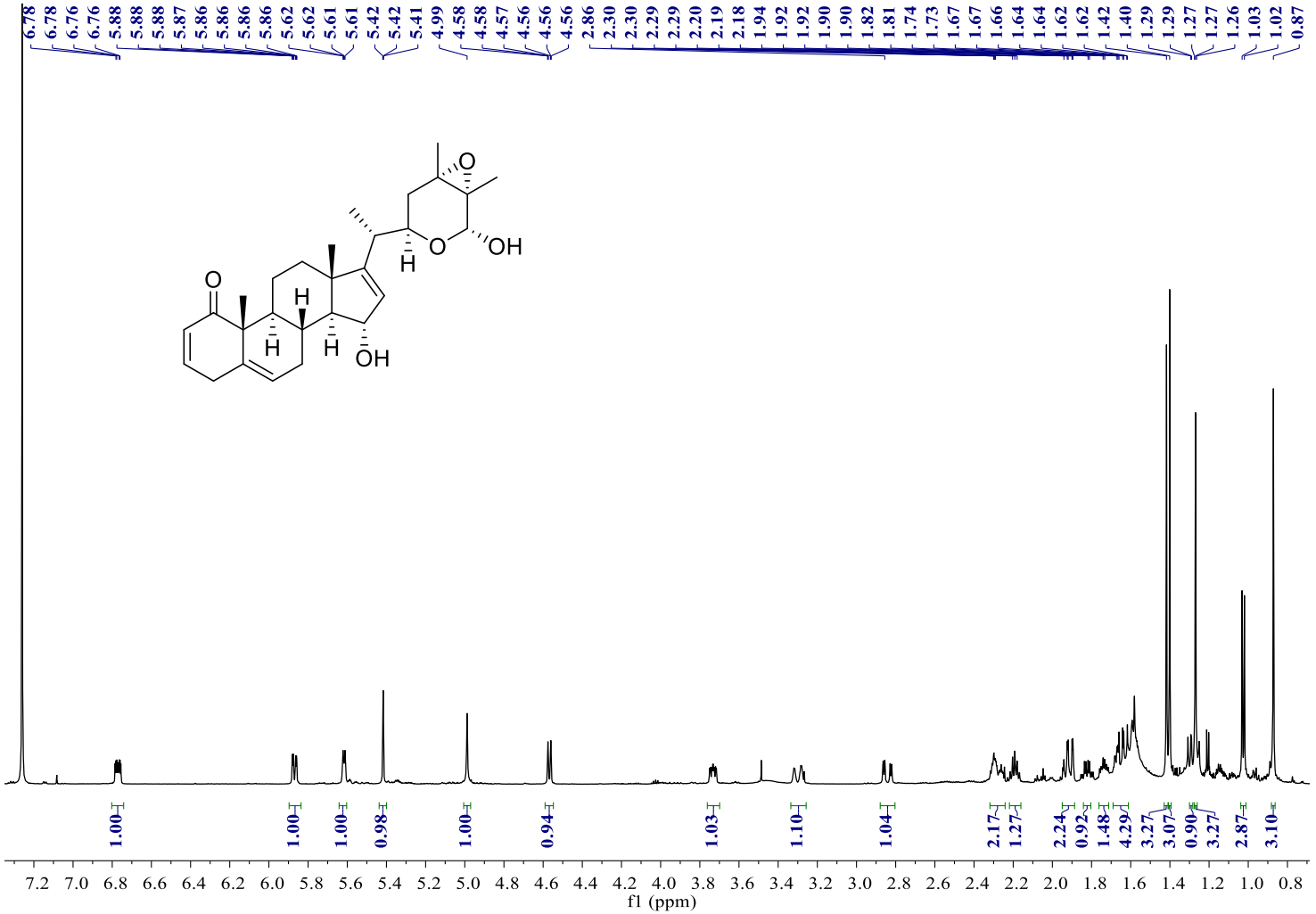


Figure S14. ^{13}C-NMR spectrum of solaundalide A (**2**) in $CDCl_3$

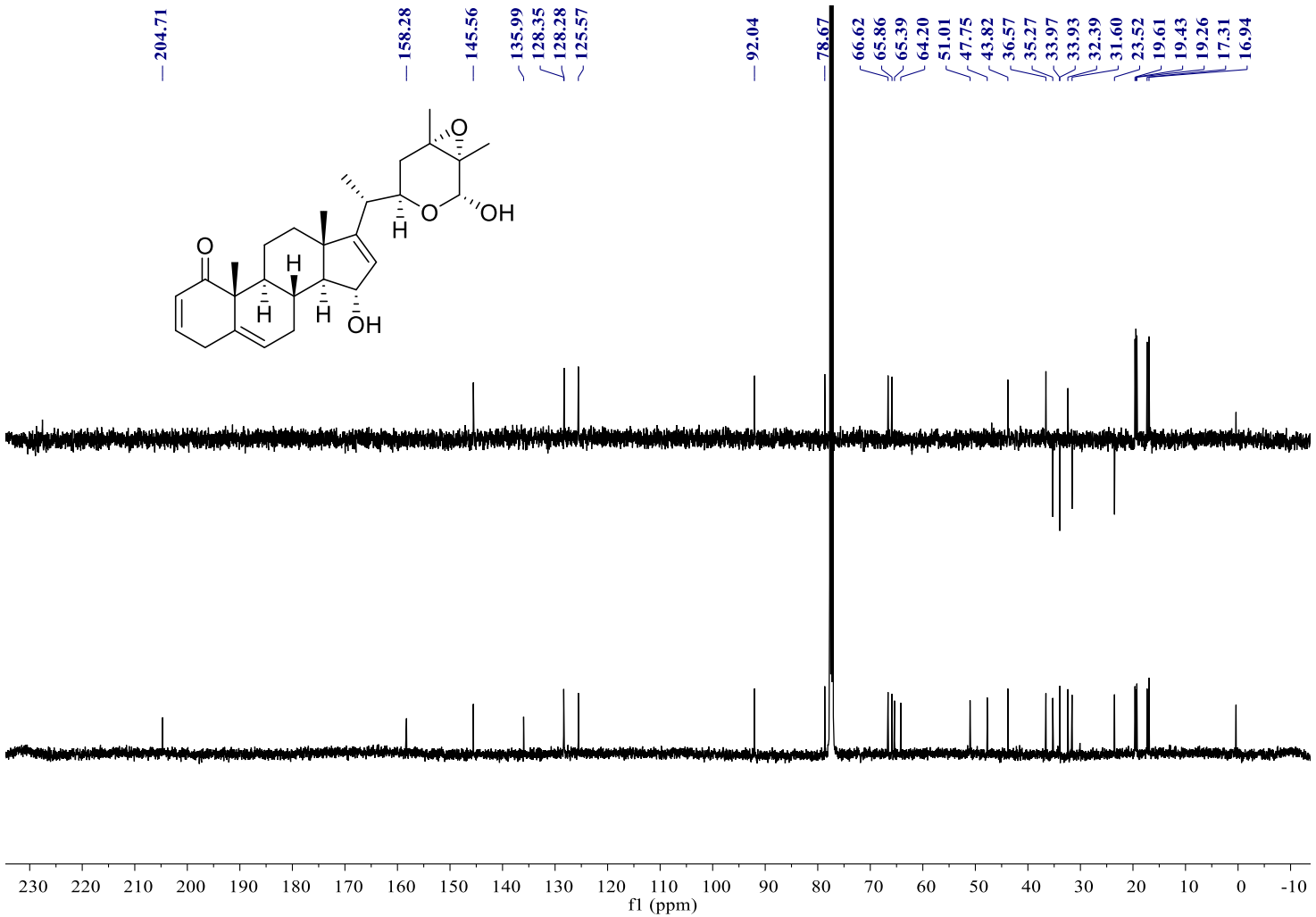


Figure S15. HSQC spectrum of solaundalide A (**2**) in $CDCl_3$

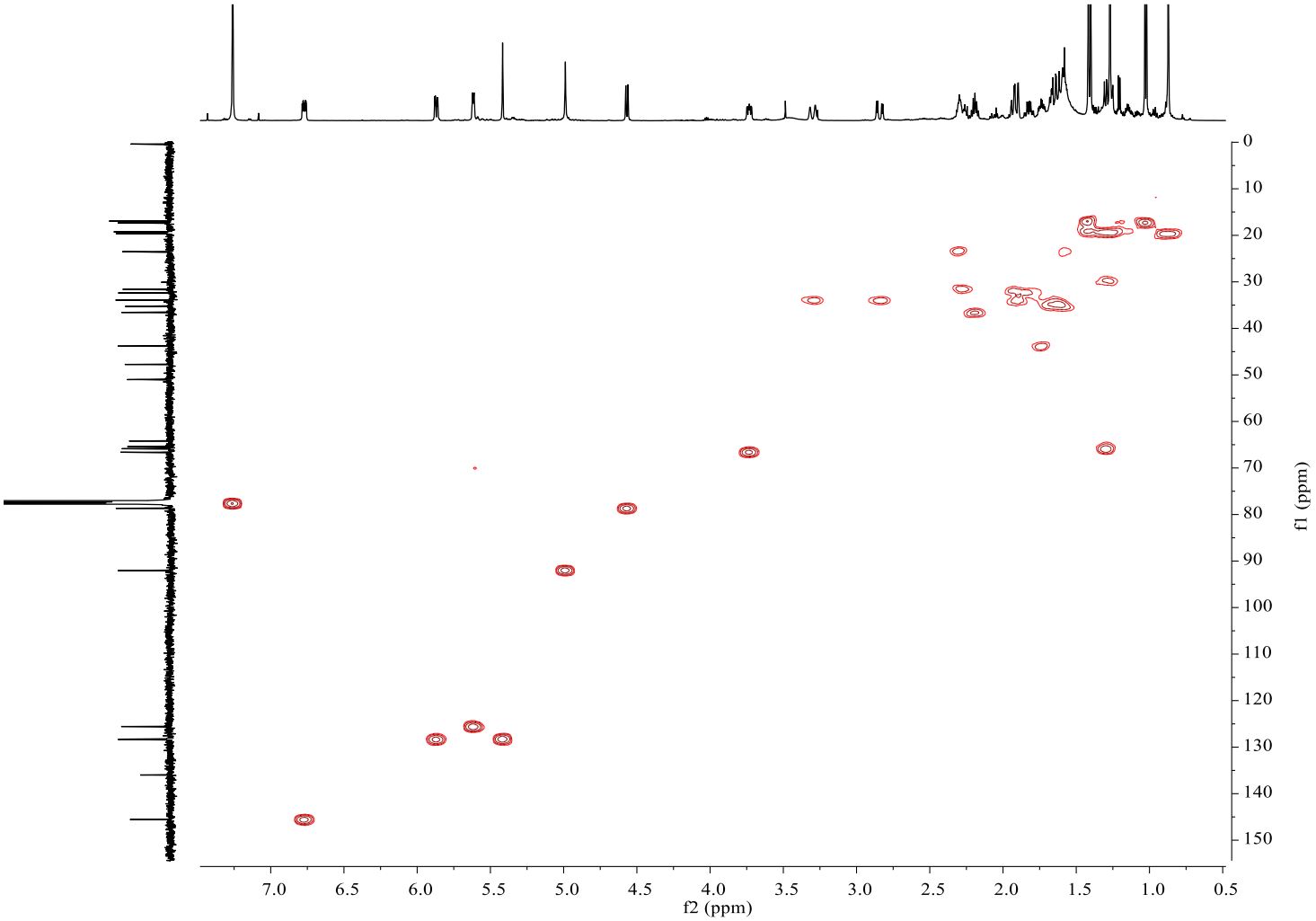


Figure S16. HMBC spectrum of solaundalide A (**2**) in $CDCl_3$

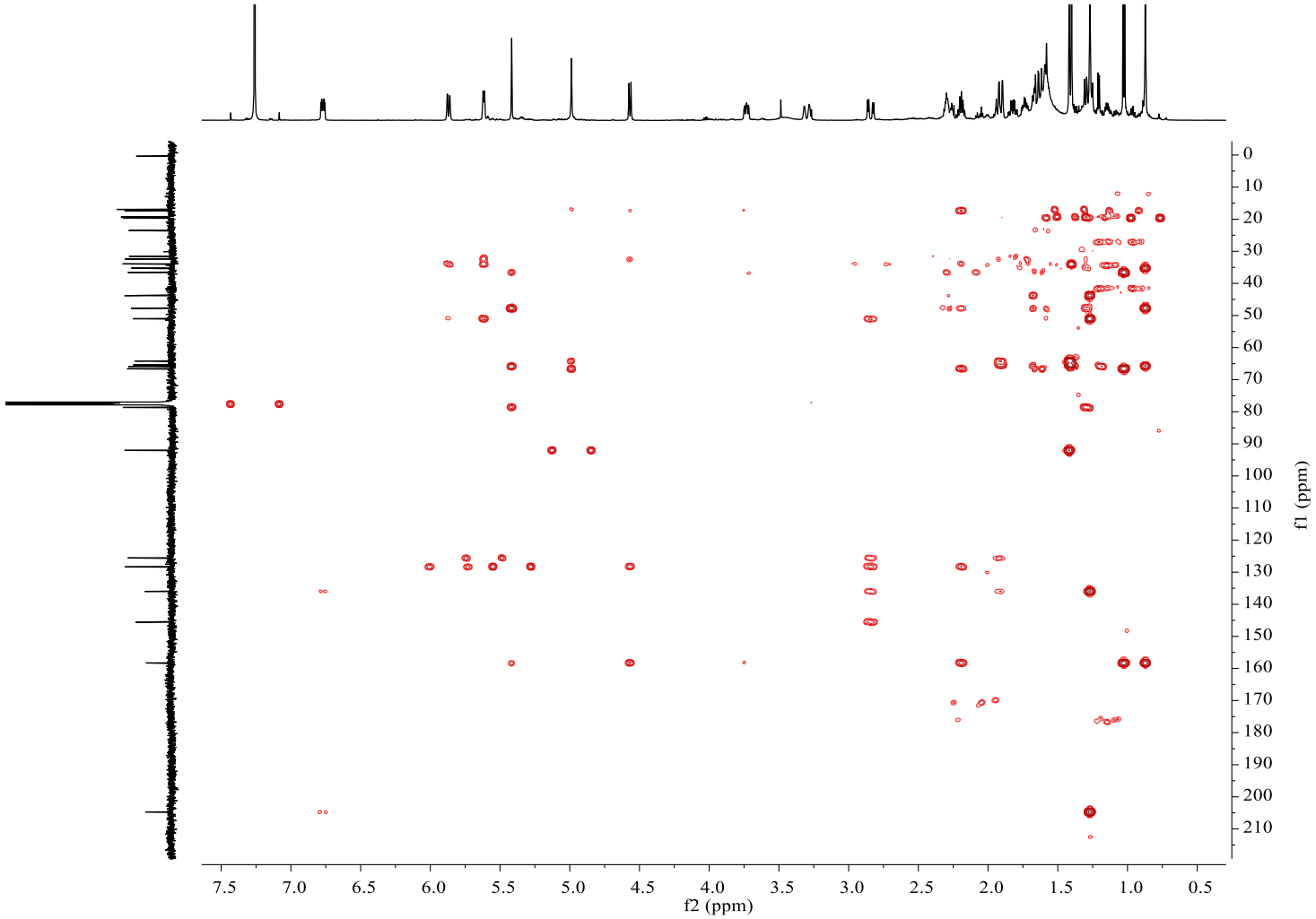


Figure S17. ^{1}H-^{1}H COSY spectrum of solaundalide A (**2**) in $CDCl_3$

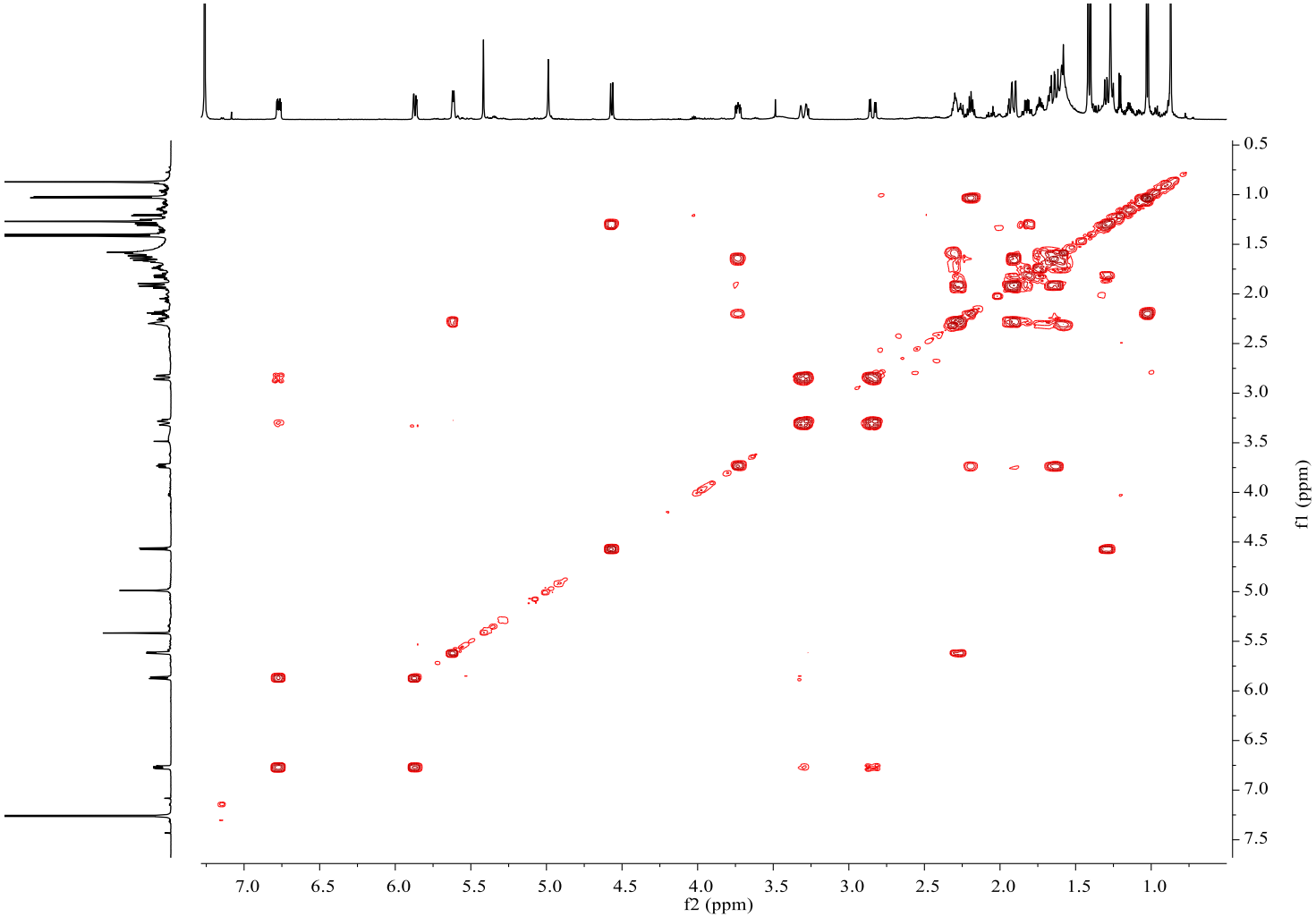


Figure S18. NOESY spectrum of solaundalide A (**2**) in $CDCl_3$

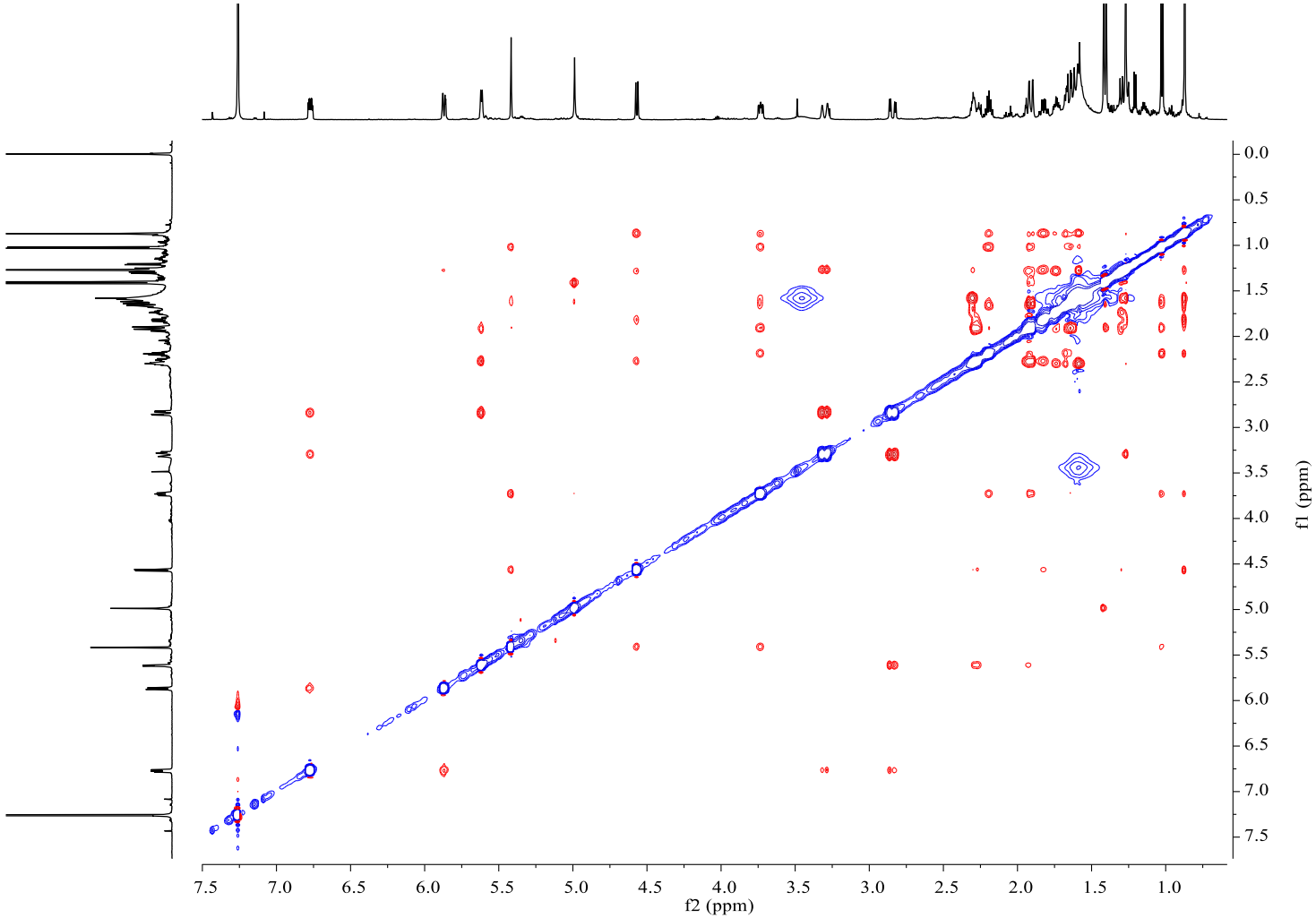


Figure S19. (+)-ESIMS spectrum of solaundalide A (**2**)

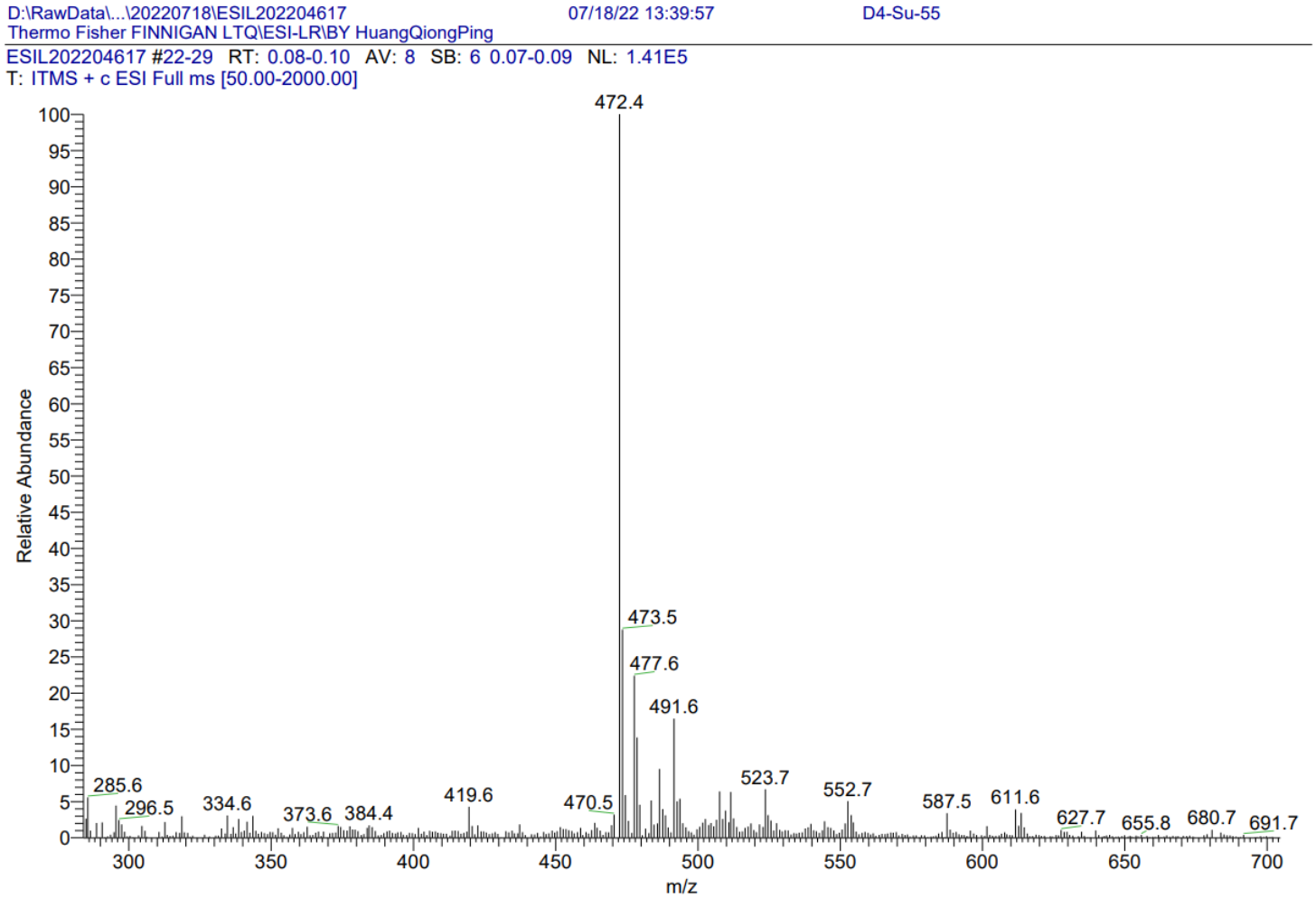


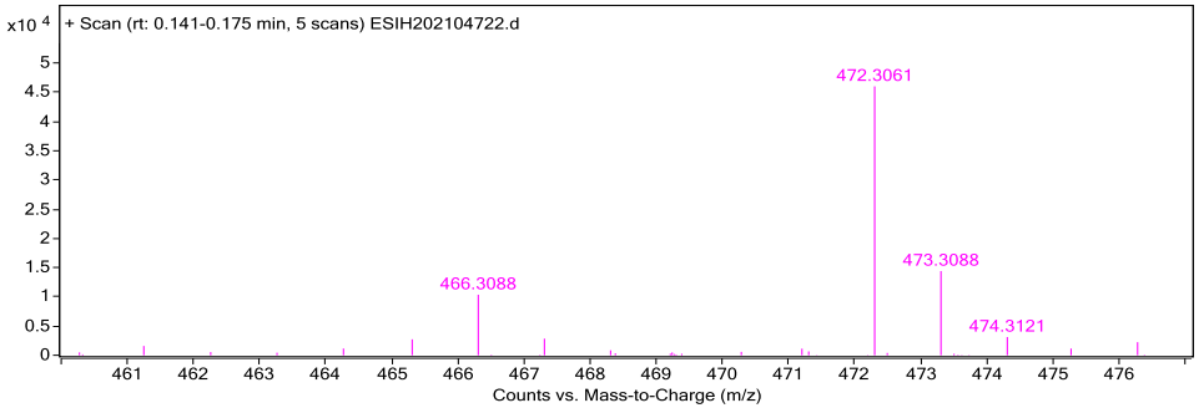
Figure S20. (+)-HRESIMS spectrum of solaundalide A (**2**)

Qualitative Analysis Report

Data Filename	ESIH202104722.d	**Sample Name**	D4-Su-55
Sample ID		**Position**	P1-C4
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	10/22/2021 19:21:26	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by zhuzhenyun

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
472.3061	472.3057	-0.31	-0.65	C28 H42 N O5	(M+NH4)+

--- End Of Report ---

Figure S21. IR spectrum of solaundalide A (**2**)

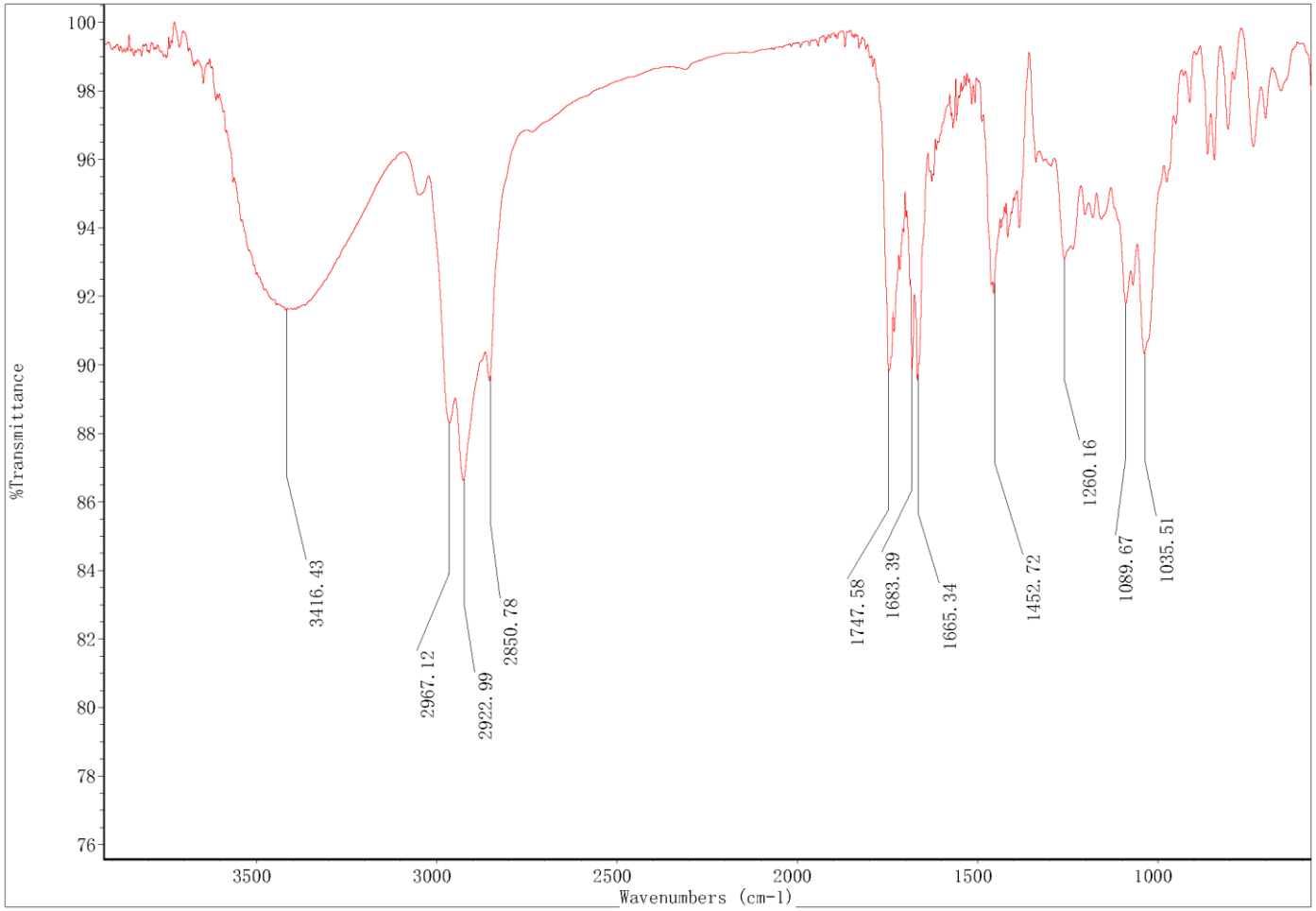


Figure S22. ^{1}H NMR spectrum of solaundaolide B (**3**) in CD_3OD

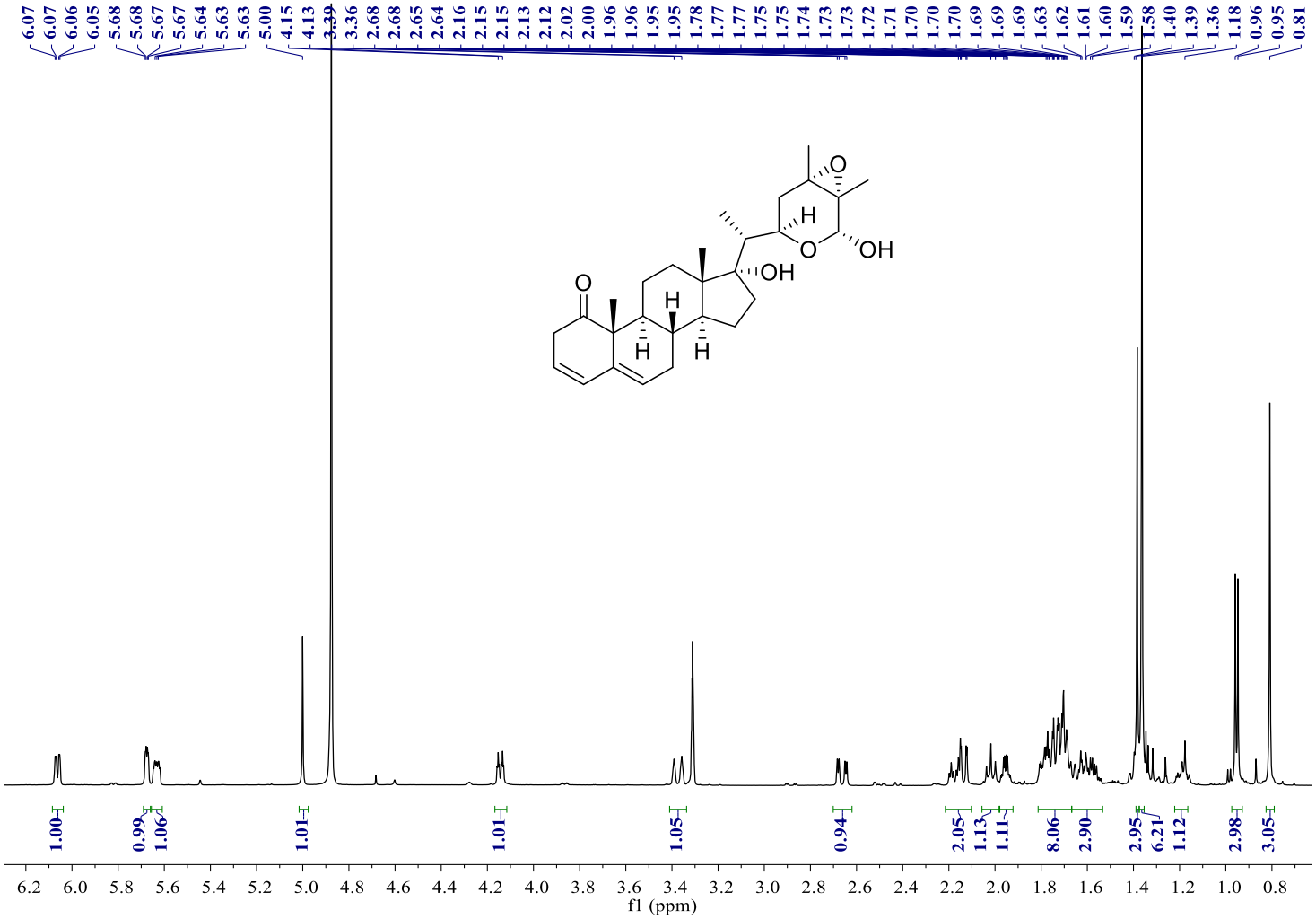


Figure S23. ^{13}C NMR spectrum of solaundaolide B (**3**) in CD_3OD

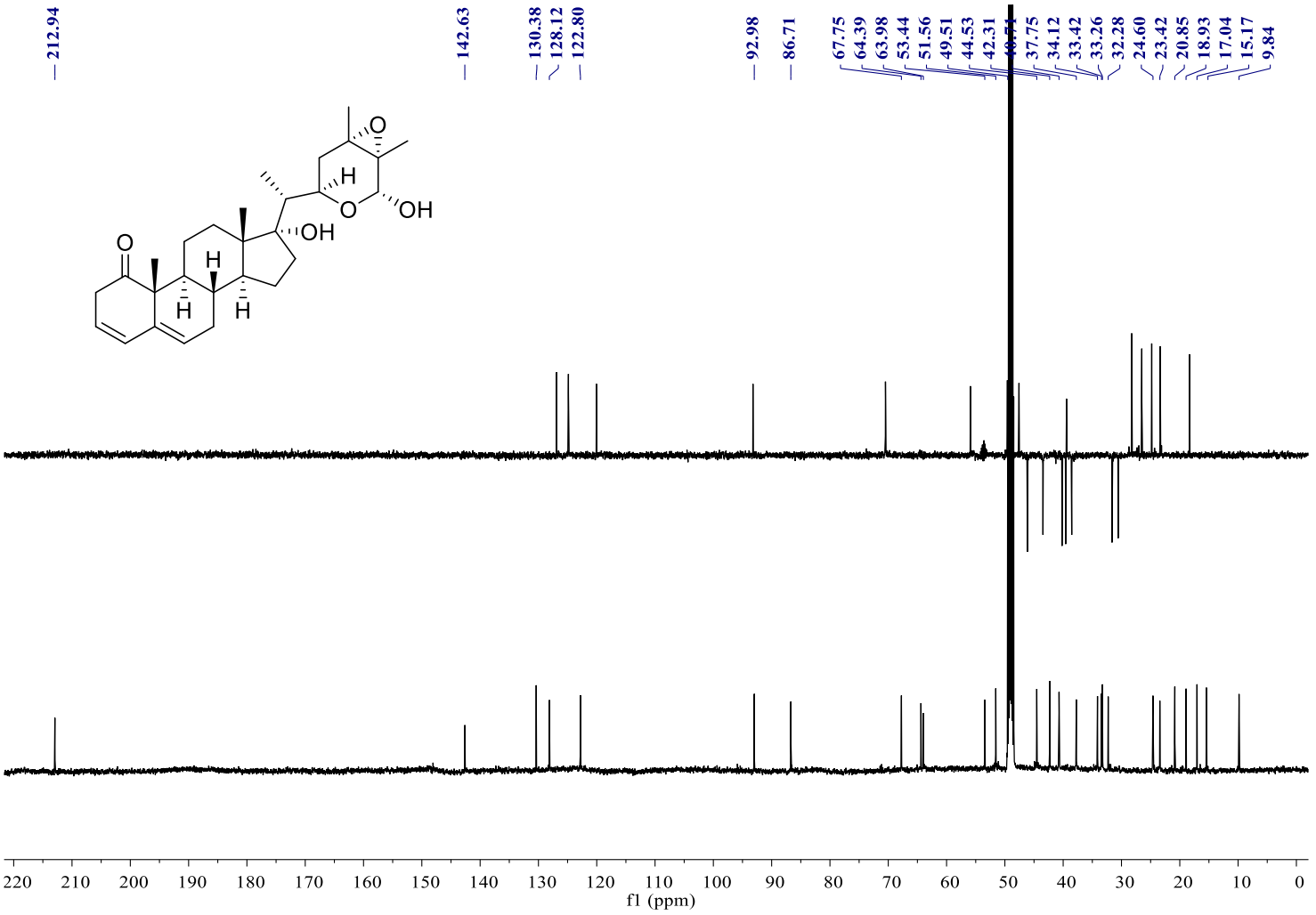


Figure S24. HSQC spectrum of solaundaolide B (**3**) in CD_3OD

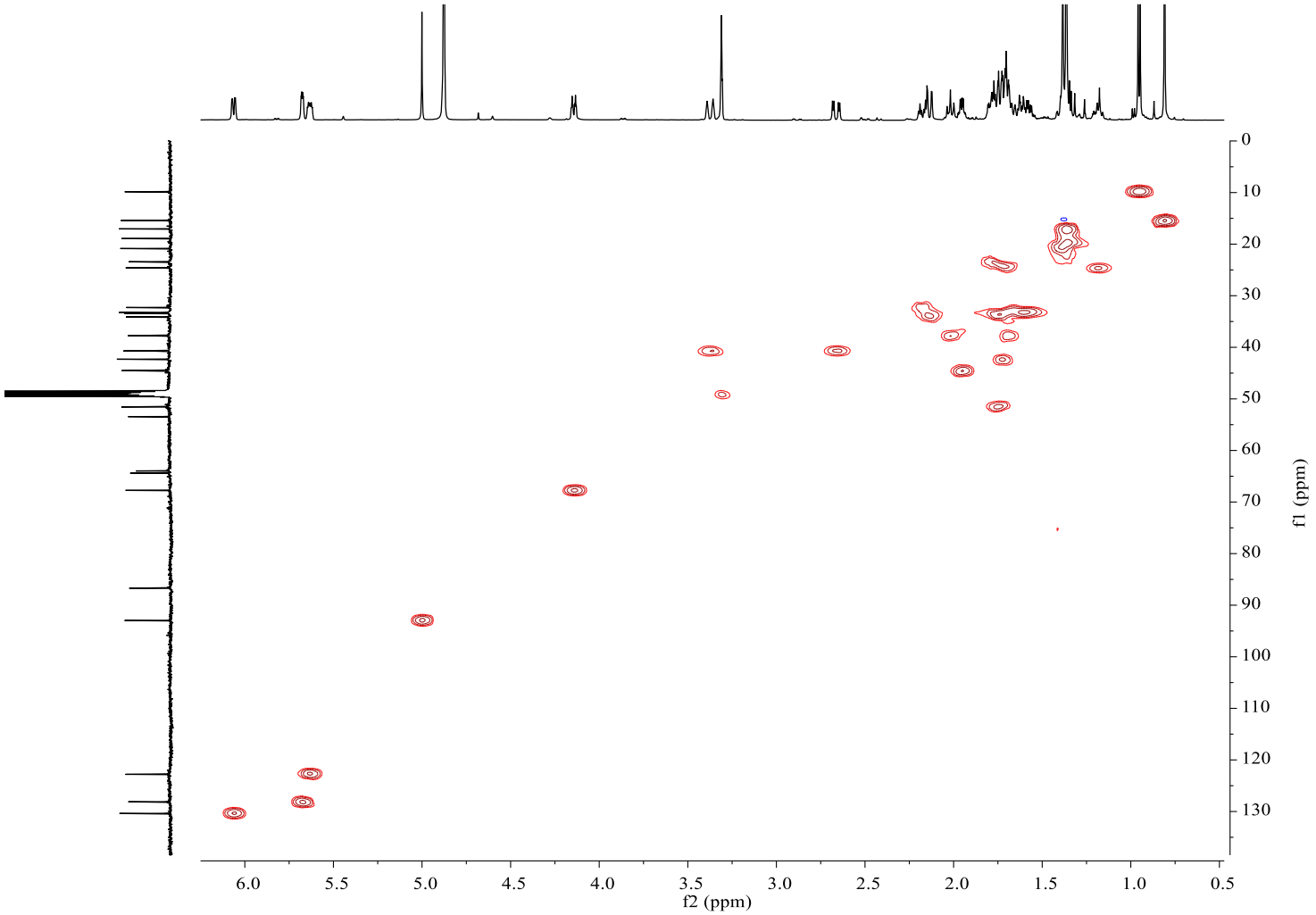


Figure S25. HMBC spectrum of solaundaolide B (**3**) in CD_3OD

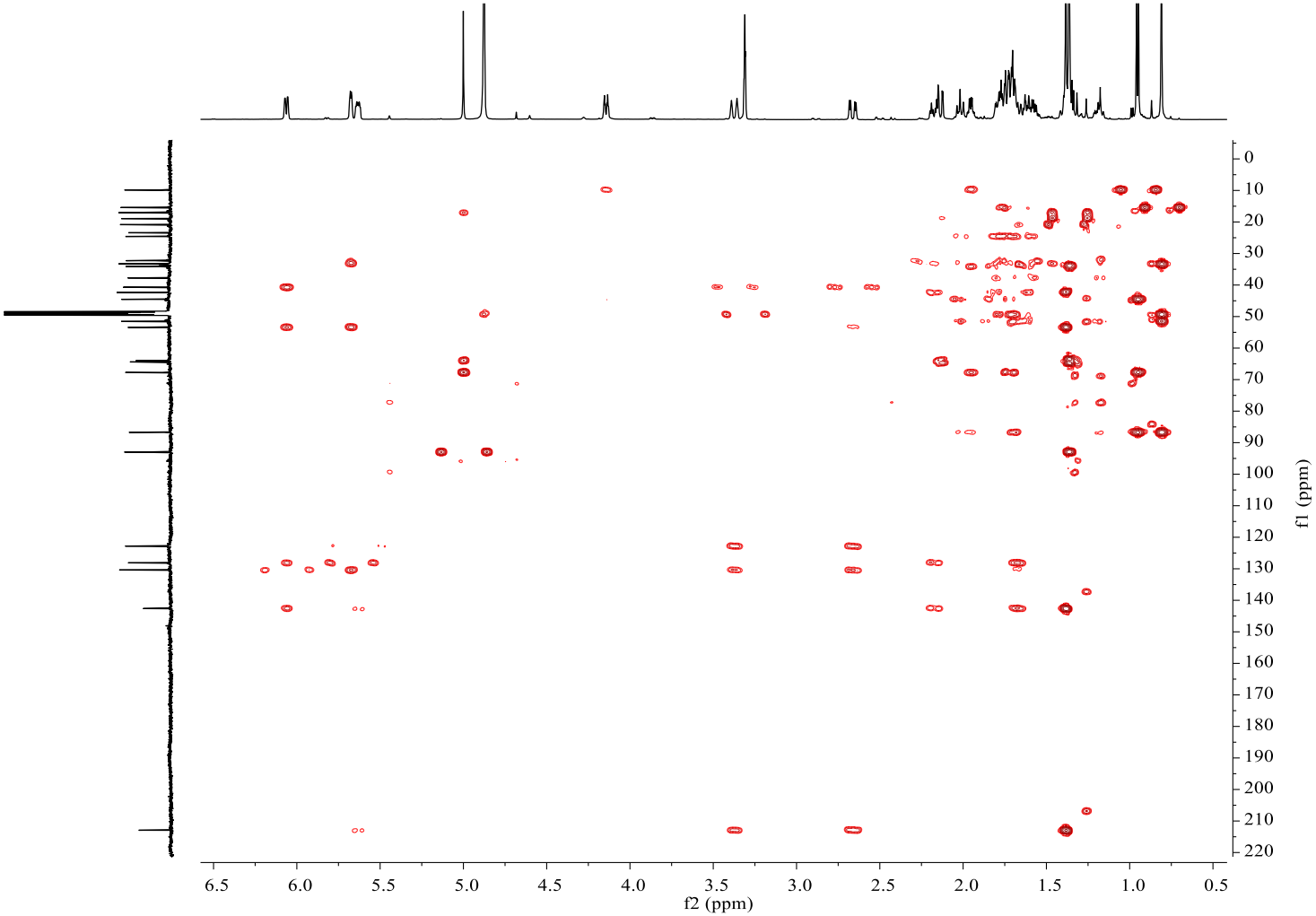


Figure S26. ^{1}H-^{1}H COSY spectrum of solaundaolide B (**3**) in CD_3OD

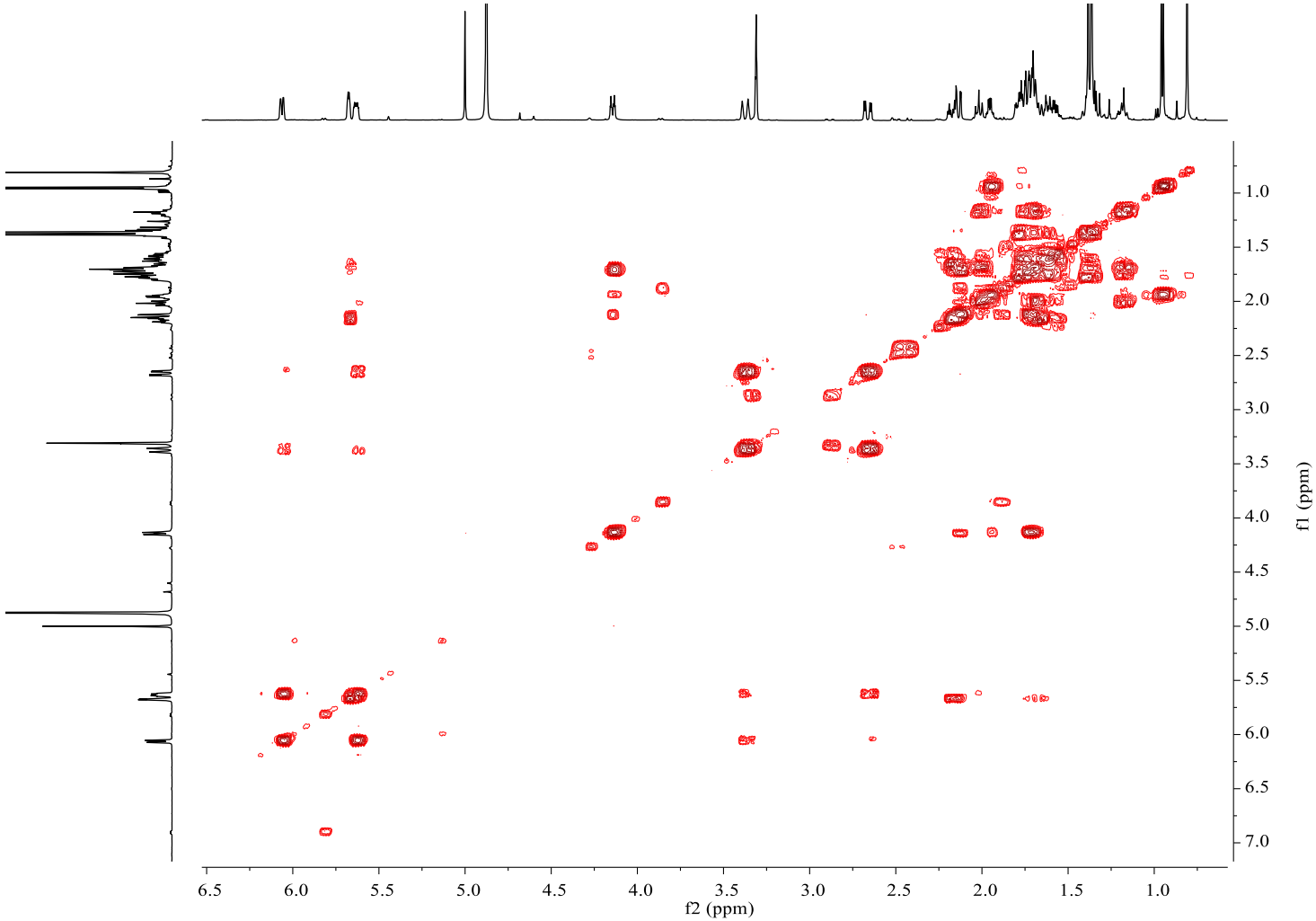


Figure S27. NOESY spectrum of solaundaolide B (**3**) in CD_3OD

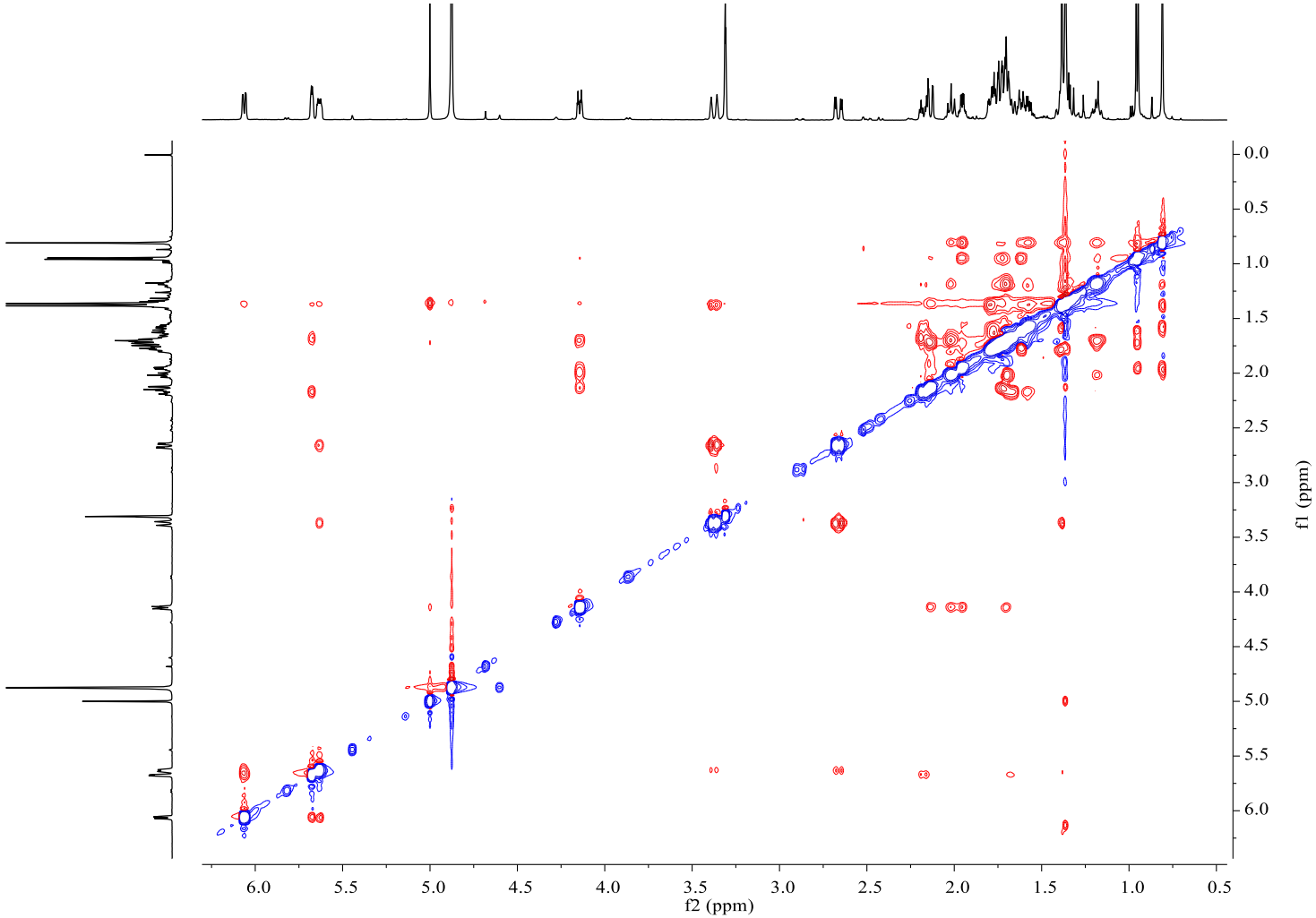


Figure S28. (+)-ESIMS spectrum of solaundaolide B (**3**)

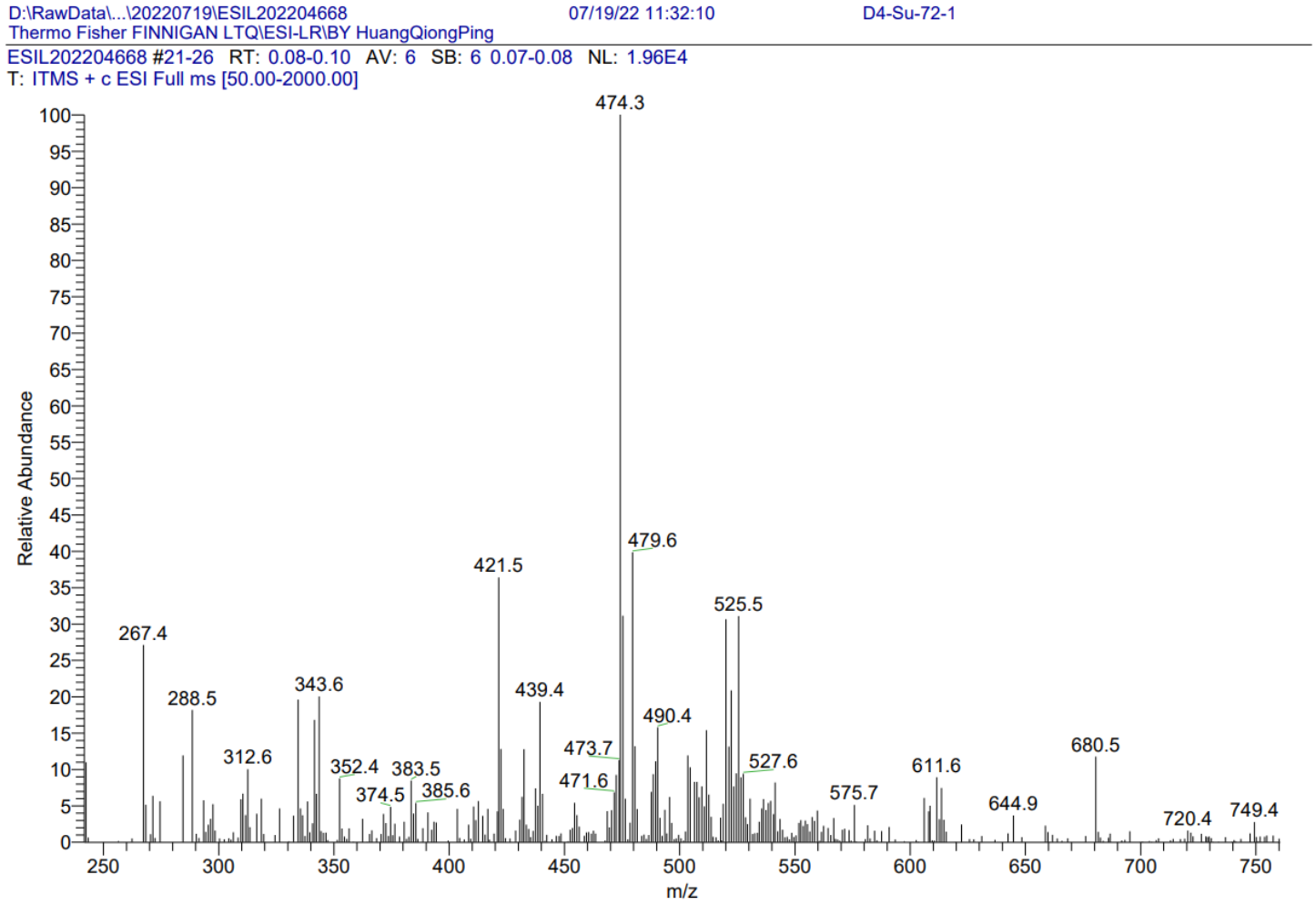


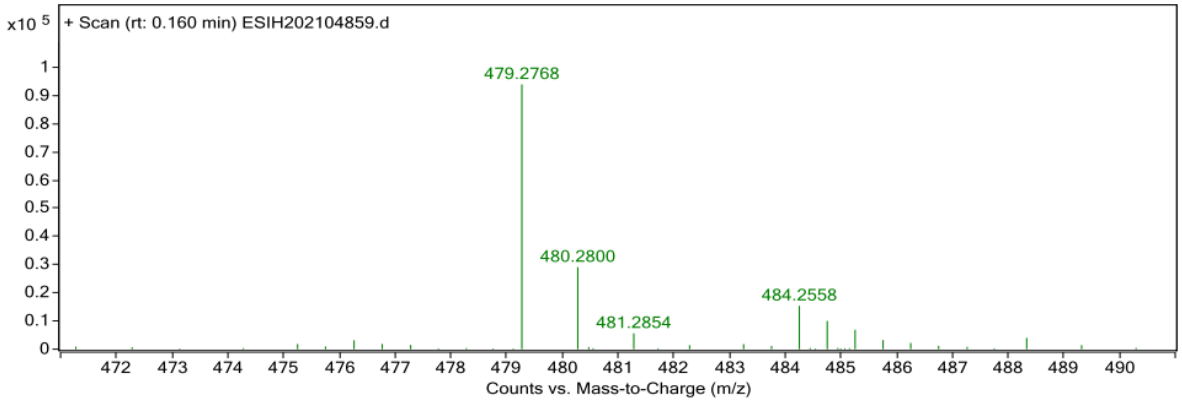
Figure S29. (+)-HRESIMS spectrum of solaundaolide B (**3**)

Qualitative Analysis Report

Data Filename	ESIH202104859.d	**Sample Name**	D4-Su-72
Sample ID		**Position**	P1-A2
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	11/4/2021 11:27:14	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by fangsu

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
479.2768	479.2768	-0.01	-0.02	C28 H40 Na O5	(M+Na)+

--- End Of Report ---

Figure S30. IR spectrum of solaundaolide B (**3**)

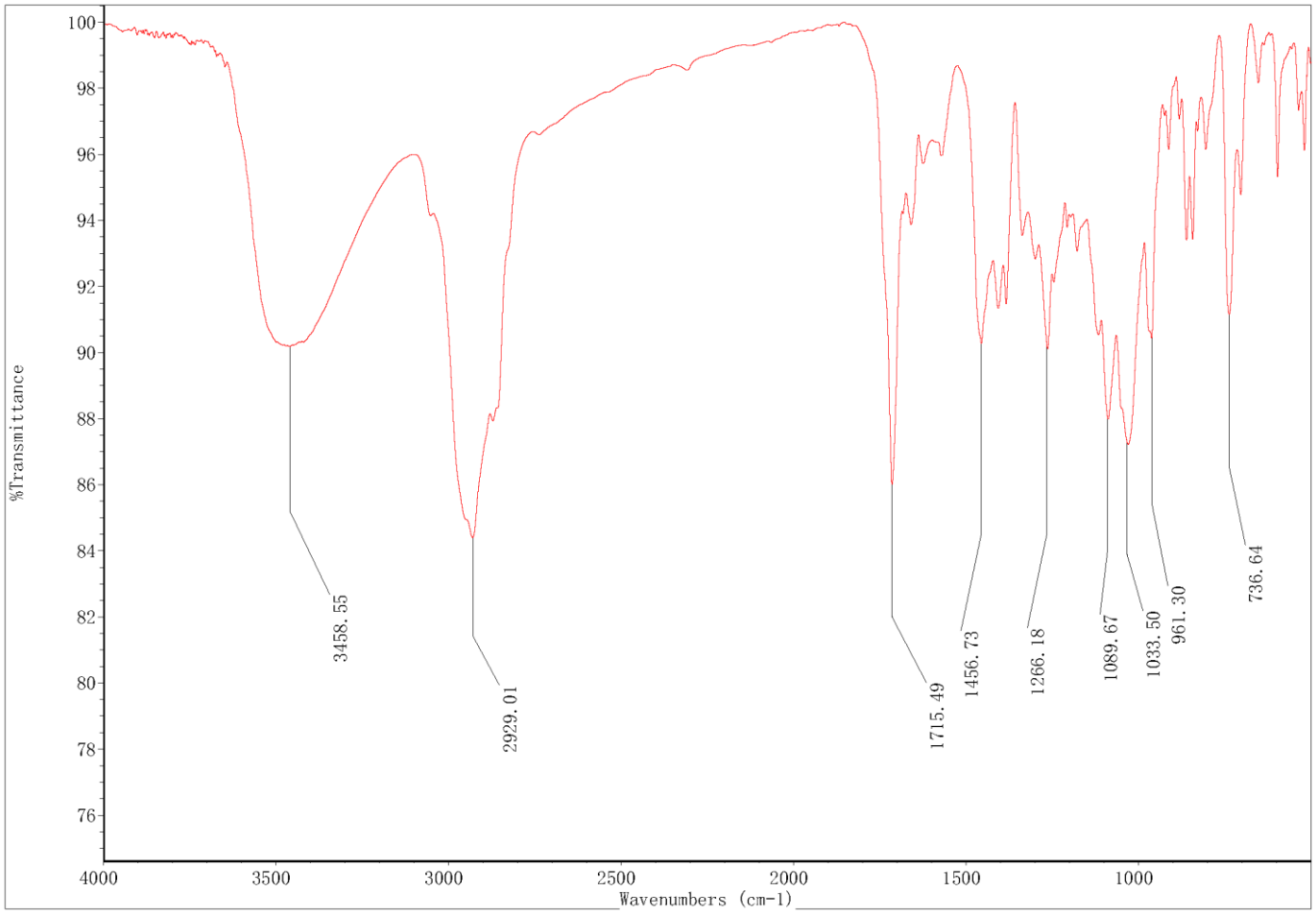


Figure S31. ^{1}H NMR spectrum of the (*S*)-PGME amide (**1a**) of solaundaic acid A (**1**) in $CDCl_3$

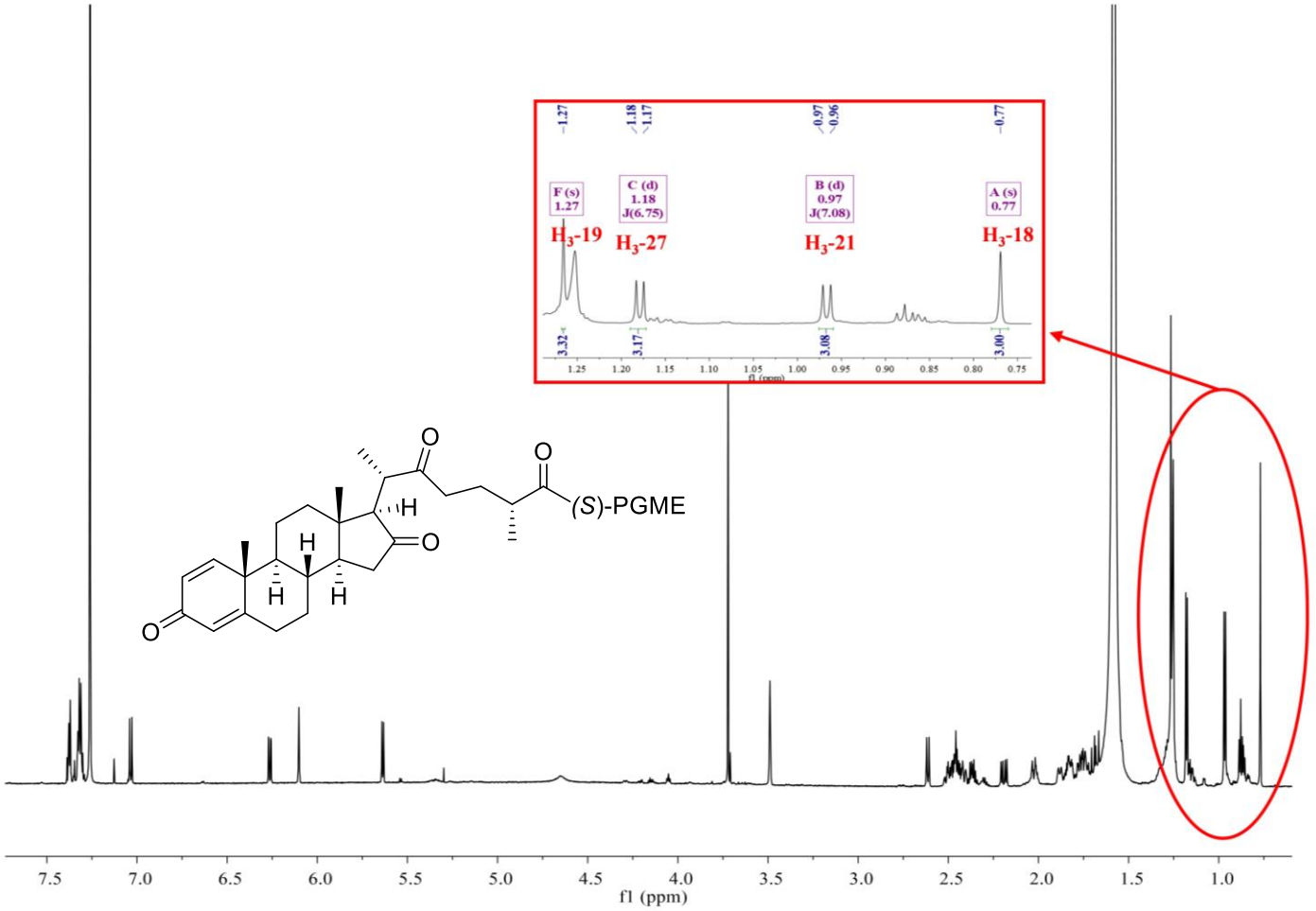


Figure S32. (+)-ESIMS spectrum of the (*S*)-PGME amide (**1a**) of solaundaic acid A (**1**)

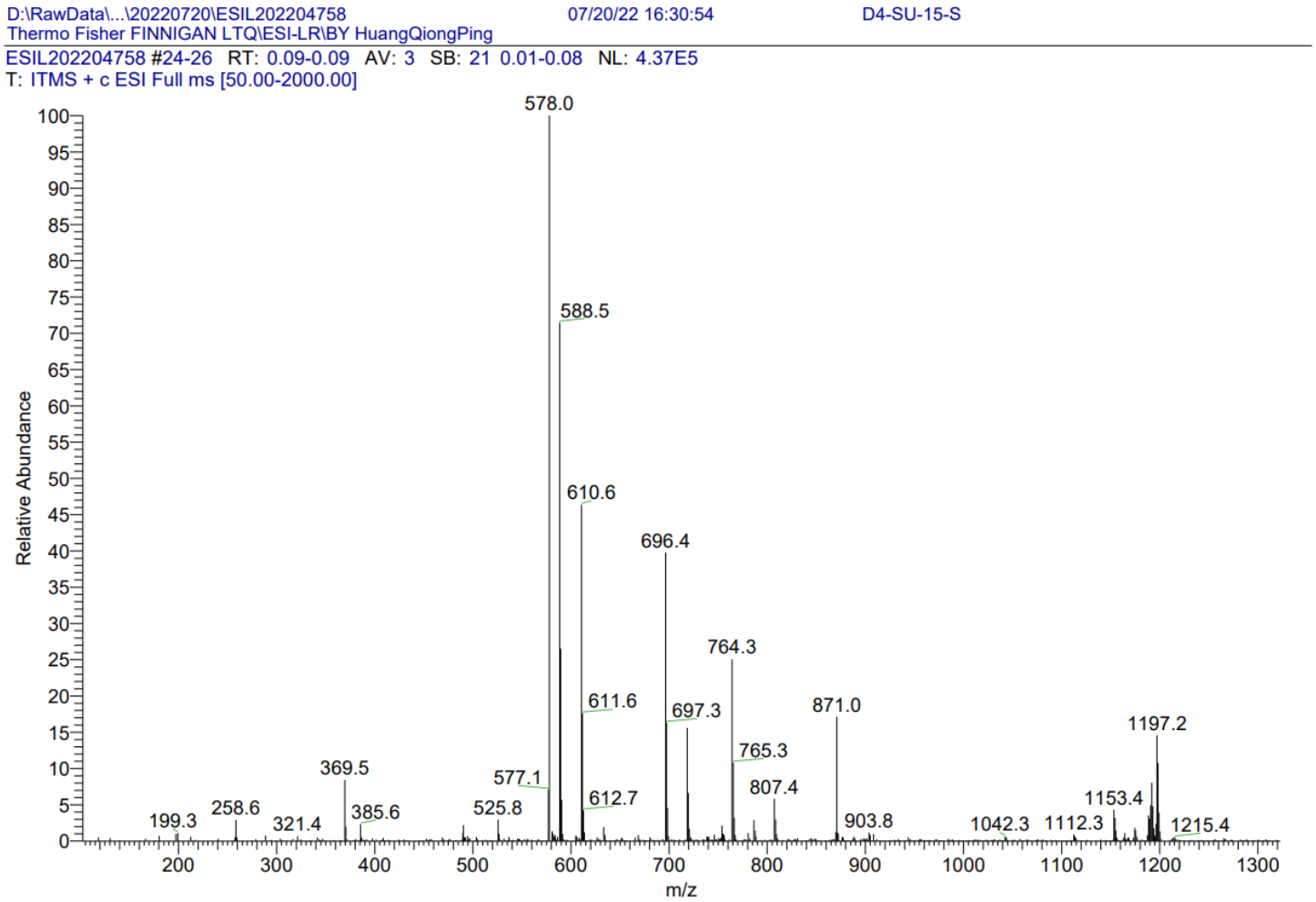


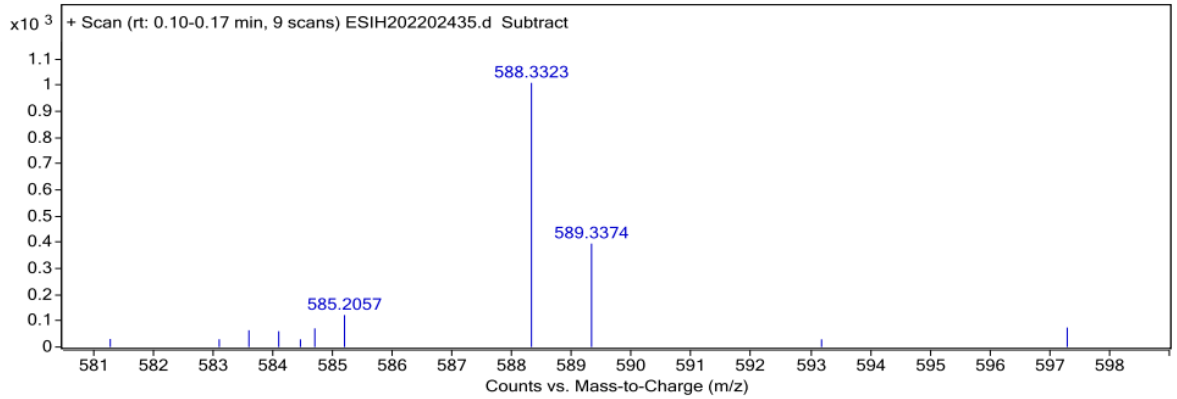
Figure S33. (+)-HRESIMS spectrum of the (*S*)-PGME amide (**1a**) of solaundaic acid A (**1**)

Qualitative Analysis Report

Data Filename	ESIH202202435.d	**Sample Name**	D4-SU-15-S
Sample ID		**Position**	P1-A9
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	7/21/2022 10:00:33	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by fangsu

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
588.3323	588.332	-0.32	-0.55	C36 H46 N O6	(M+H)+

--- End Of Report ---

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Figure S34. ^{1}H NMR spectrum of the (*R*)-PGME amide (**1b**) of solaundaic acid A (**1**) in $CDCl_3$

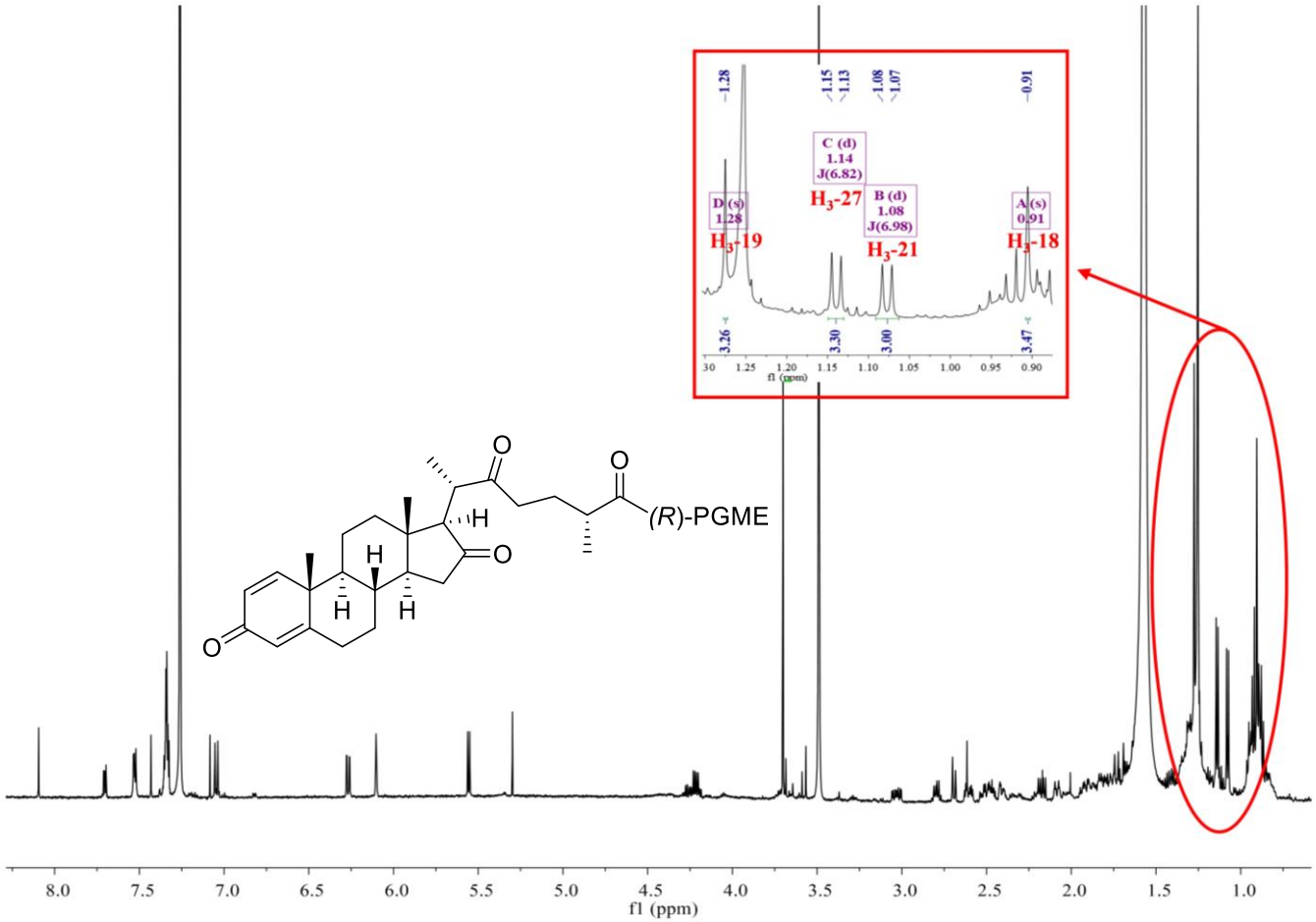


Figure S35. (+)-ESIMS spectrum of the (*R*)-PGME amide (**1b**) of Solaundaic acid A (**1**)

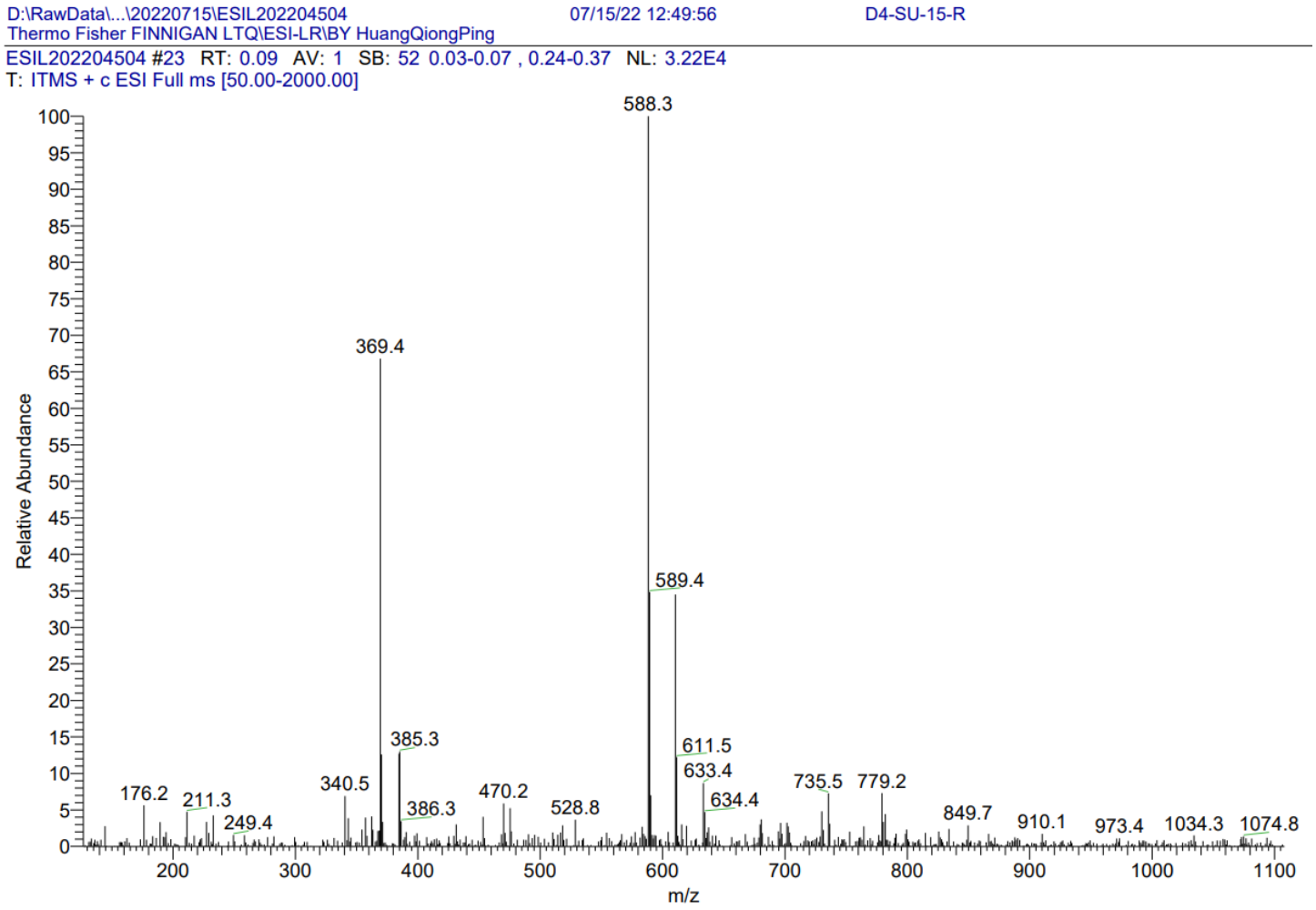


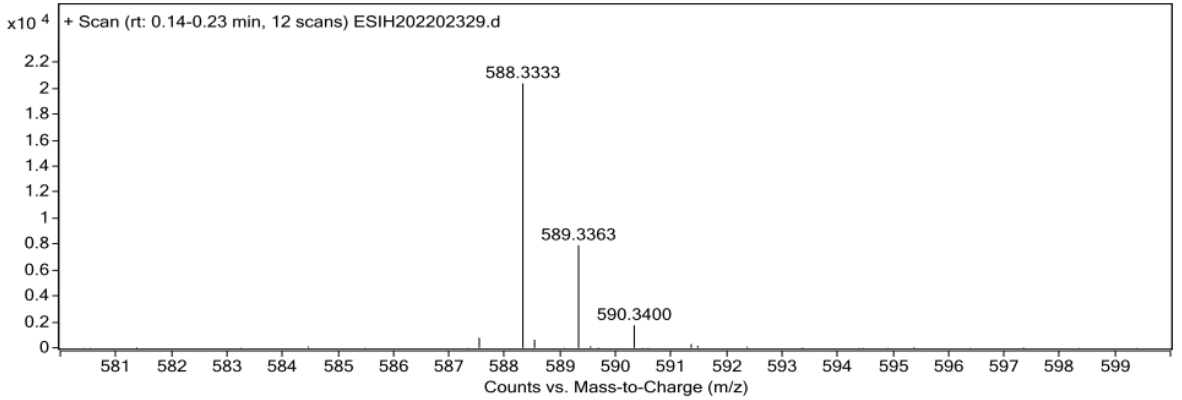
Figure S36. (+)-HRESIMS spectrum of the (*R*)-PGME amide (**1b**) of Solaundaic acid A (**1**)

Qualitative Analysis Report

Data Filename	ESIH202202329.d	**Sample Name**	D4-SU-15-R
Sample ID		**Position**	P1-B3
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	7/15/2022 17:23:22	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by fangsu

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
588.3333	588.332	-1.32	-2.24	C36 H46 N O6	(M+H)+

--- End Of Report ---

Figure S37. ^{1}H NMR spectrum of 1-dehydronuatigenone (**4**) in $CDCl_3$

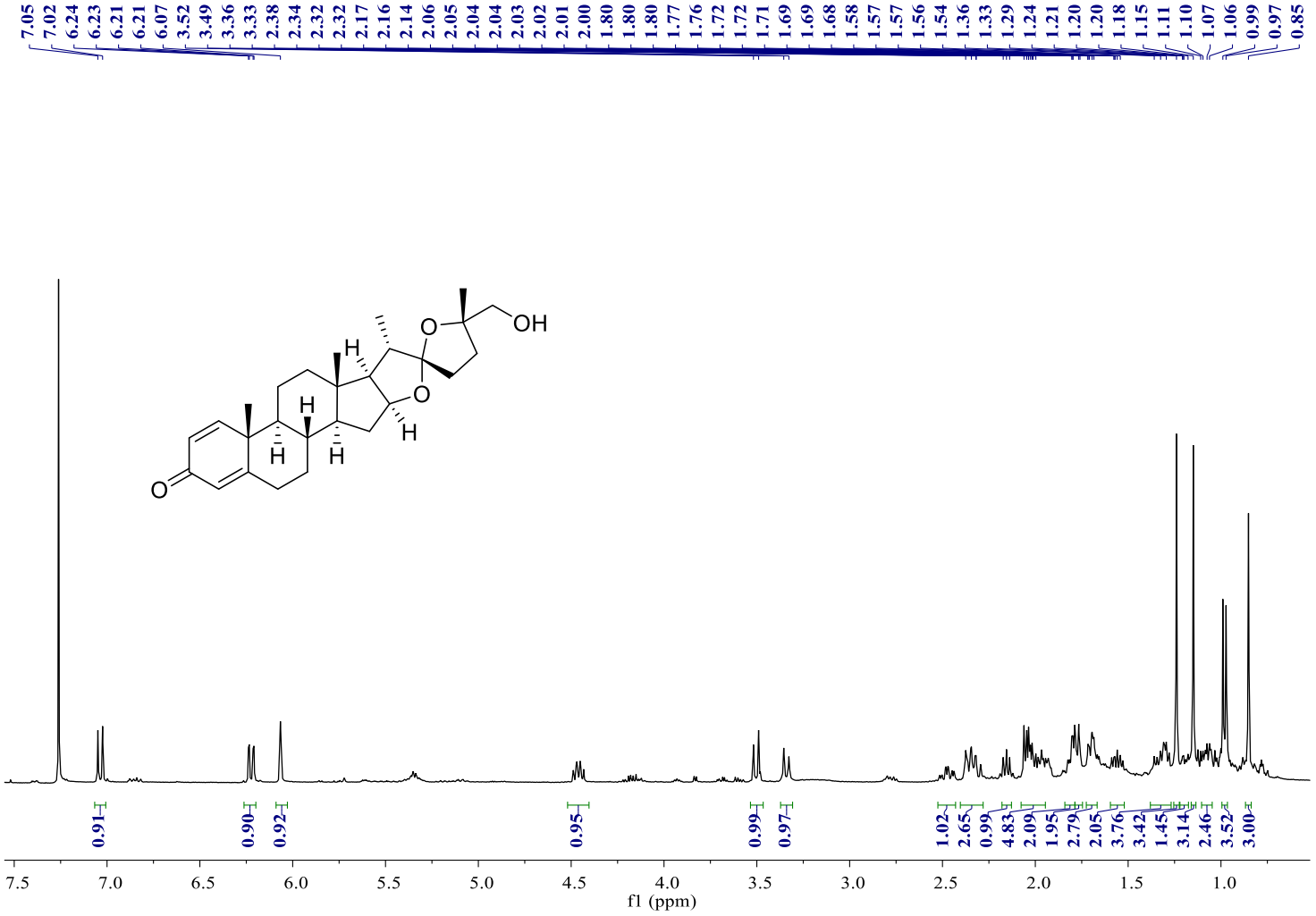


Figure S38. ^{13}C NMR spectrum of 1-dehydronuatigenone (**4**) in $CDCl_3$

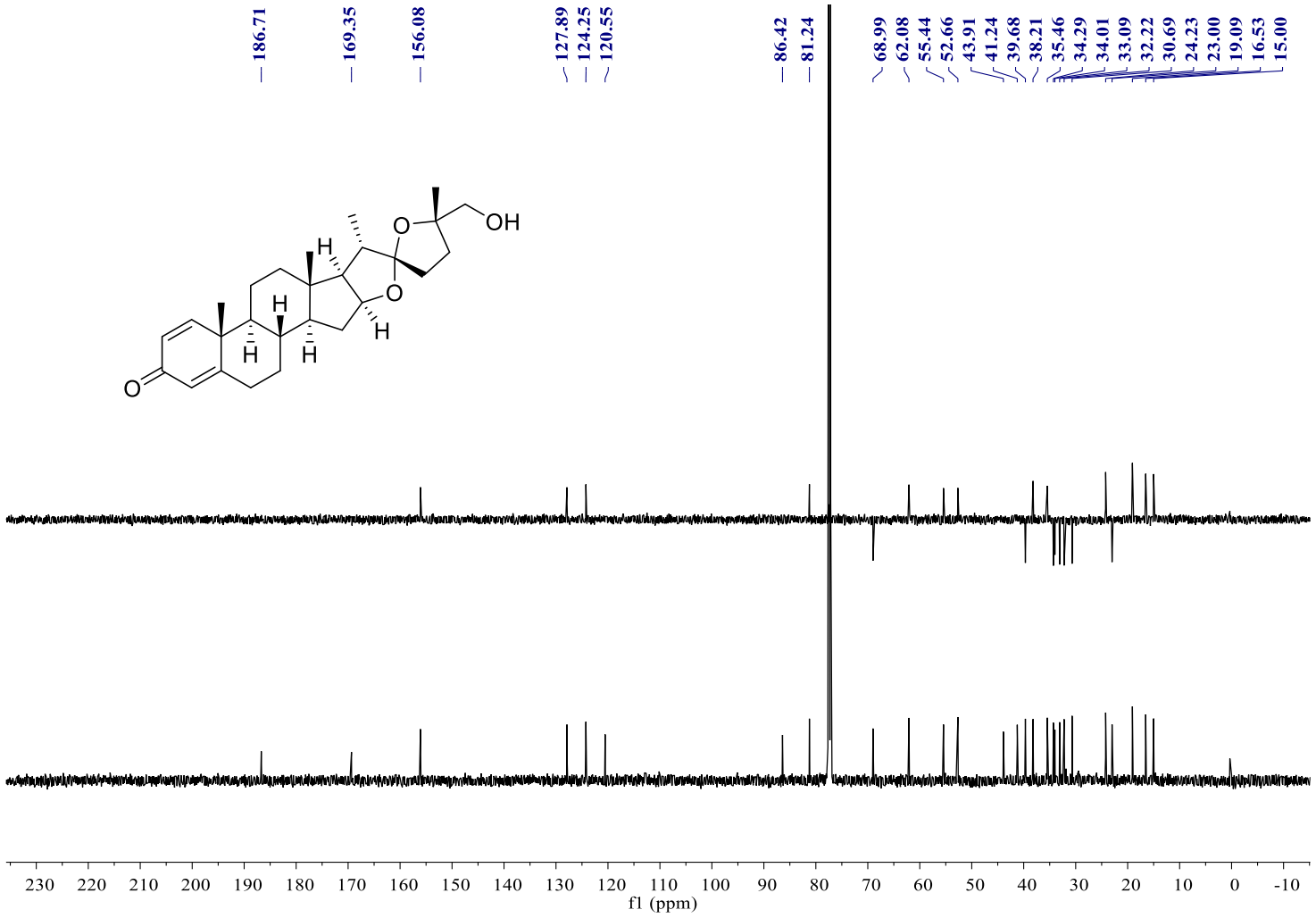


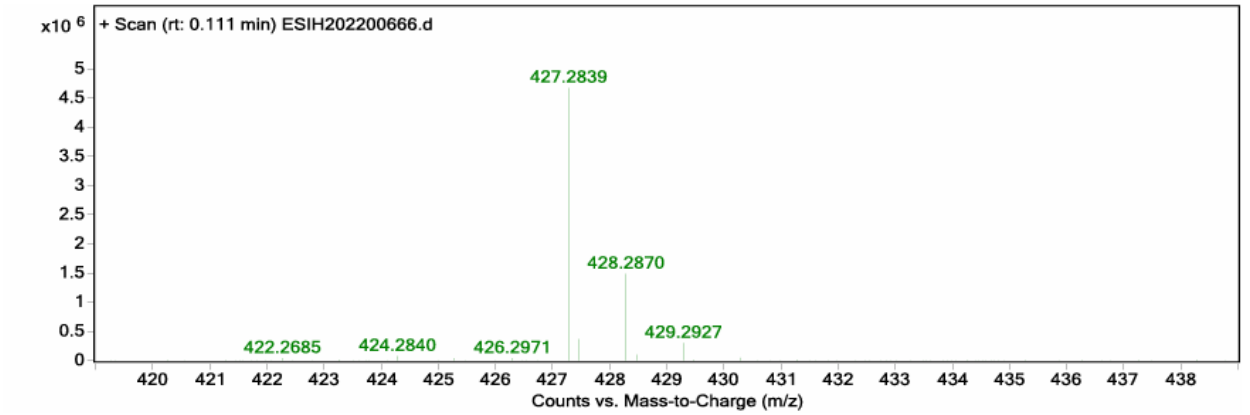
Figure S39. (+)-HRESIMS spectrum of 1-dehydronuatigenone (**4**)

Qualitative Analysis Report

Data Filename	ESIH202200666.d	**Sample Name**	D4-Su-92
Sample ID		**Position**	P1-A1
Instrument Name	Agilent G6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	2/16/2022 11:31:58	**IRM Calibration Status**	Success
DA Method	small molecular data analysis method.m	**Comment**	ESIH by fangsu

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
175	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
427.2839	427.2843	0.38	0.9	C27 H39 O4	(M+H)+

--- End Of Report ---

Figure S40. ^{1}H NMR spectrum of cilistol a (**5**) in $CDCl_3$

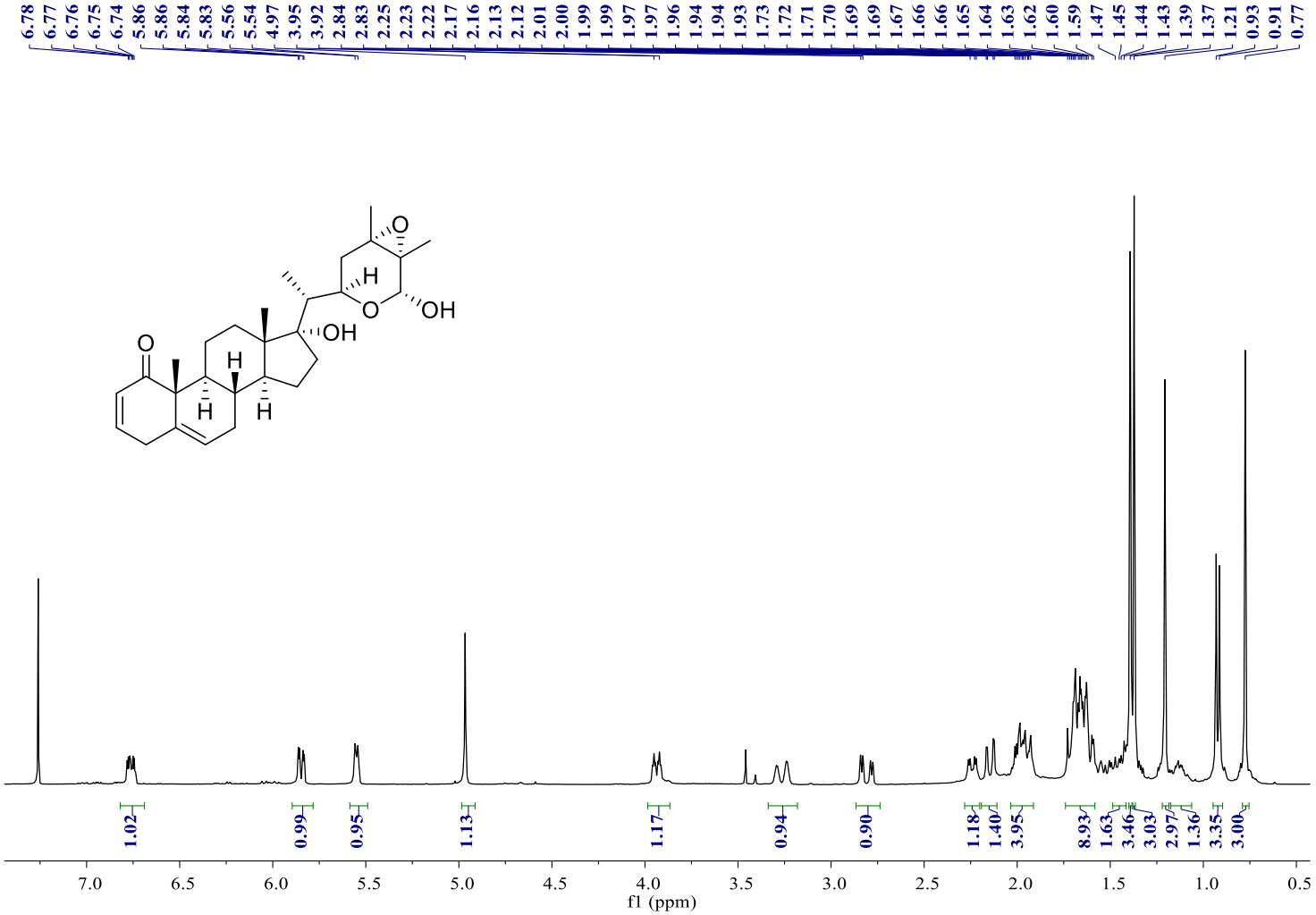


Figure S41. ^{13}C NMR spectrum of cilistol a (**5**) in $CDCl_3$

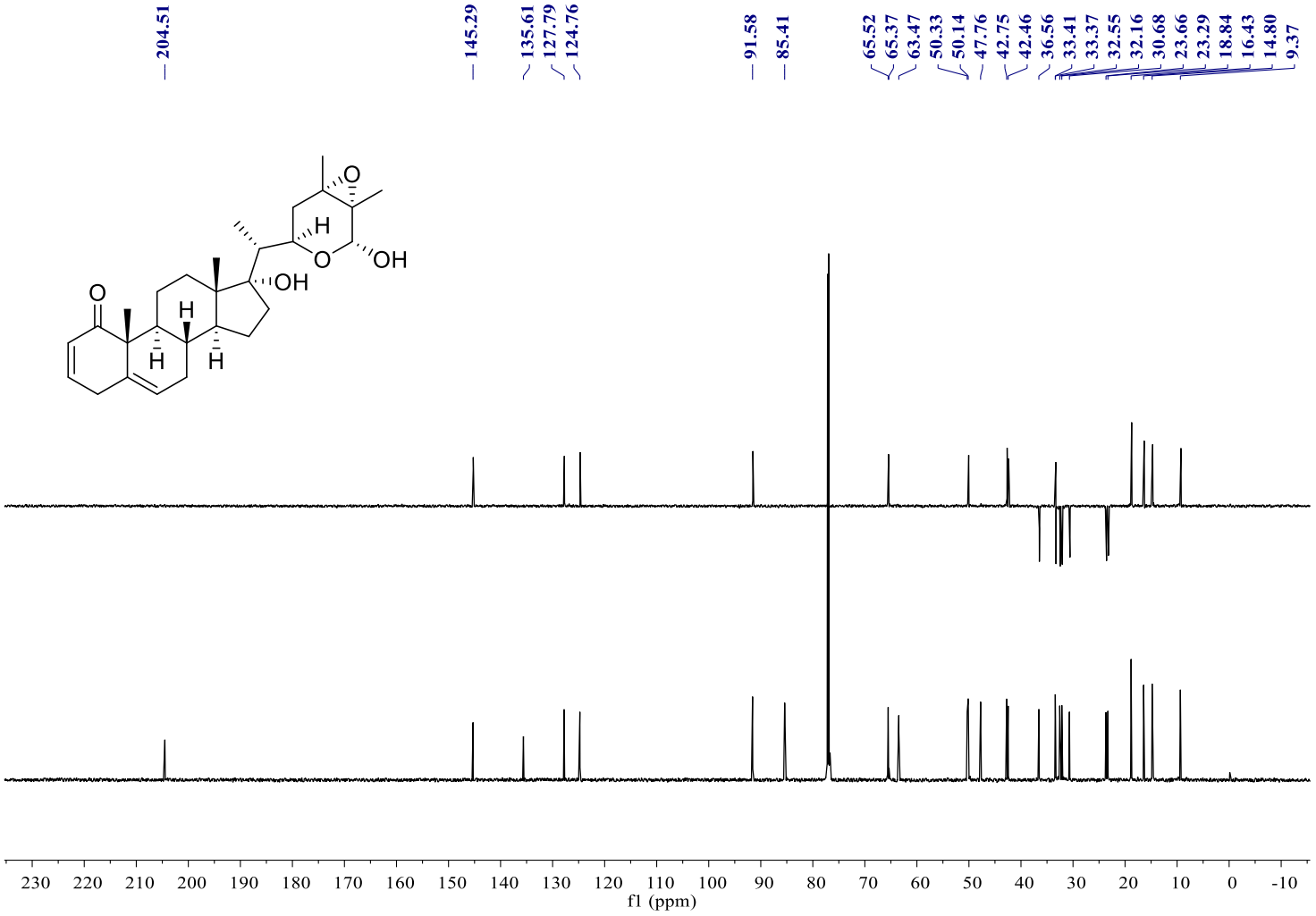


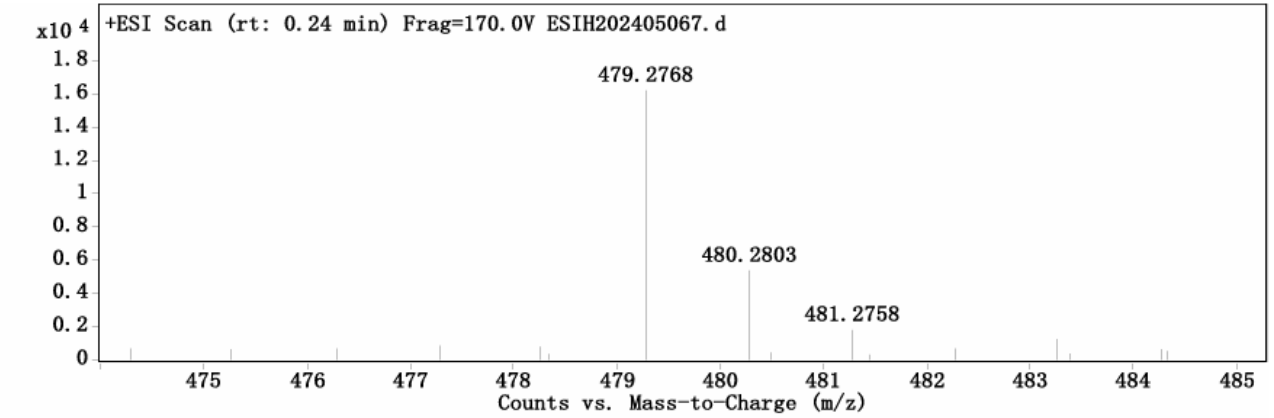
Figure S42. (+)-HRESIMS spectrum of cilistol a (**5**)

Qualitative Analysis Report

Data Filename	ESIH202405067.d	**Sample Name**	D4-SU-39
Sample ID		**Position**	P1-A9
Instrument Name	Agilent 6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	10/25/2024 4:30:41 PM	**DA Method**	ESI-HR-20231114.m
Comment	ESIH by fangsu		

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
170	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
479.2768	479.2768	-0.02	-0.03	C28 H40 Na O5	(M+Na)+

--- End Of Report ---

Figure S43. ^{1}H NMR spectrum of cilistol d (**6**) in $CDCl_3$

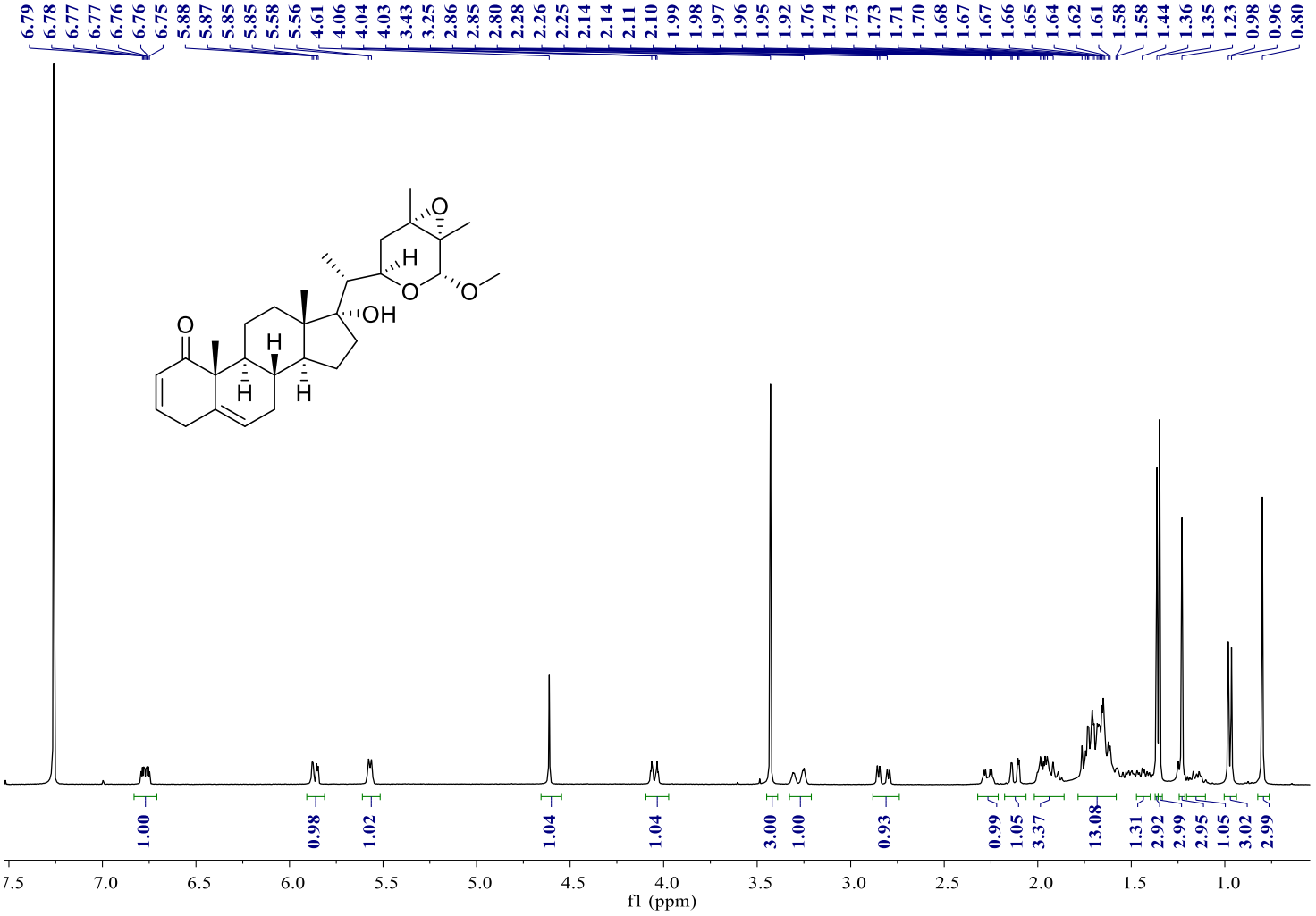


Figure S44. ^{13}C NMR spectrum of cilistol d (**6**) in $CDCl_3$

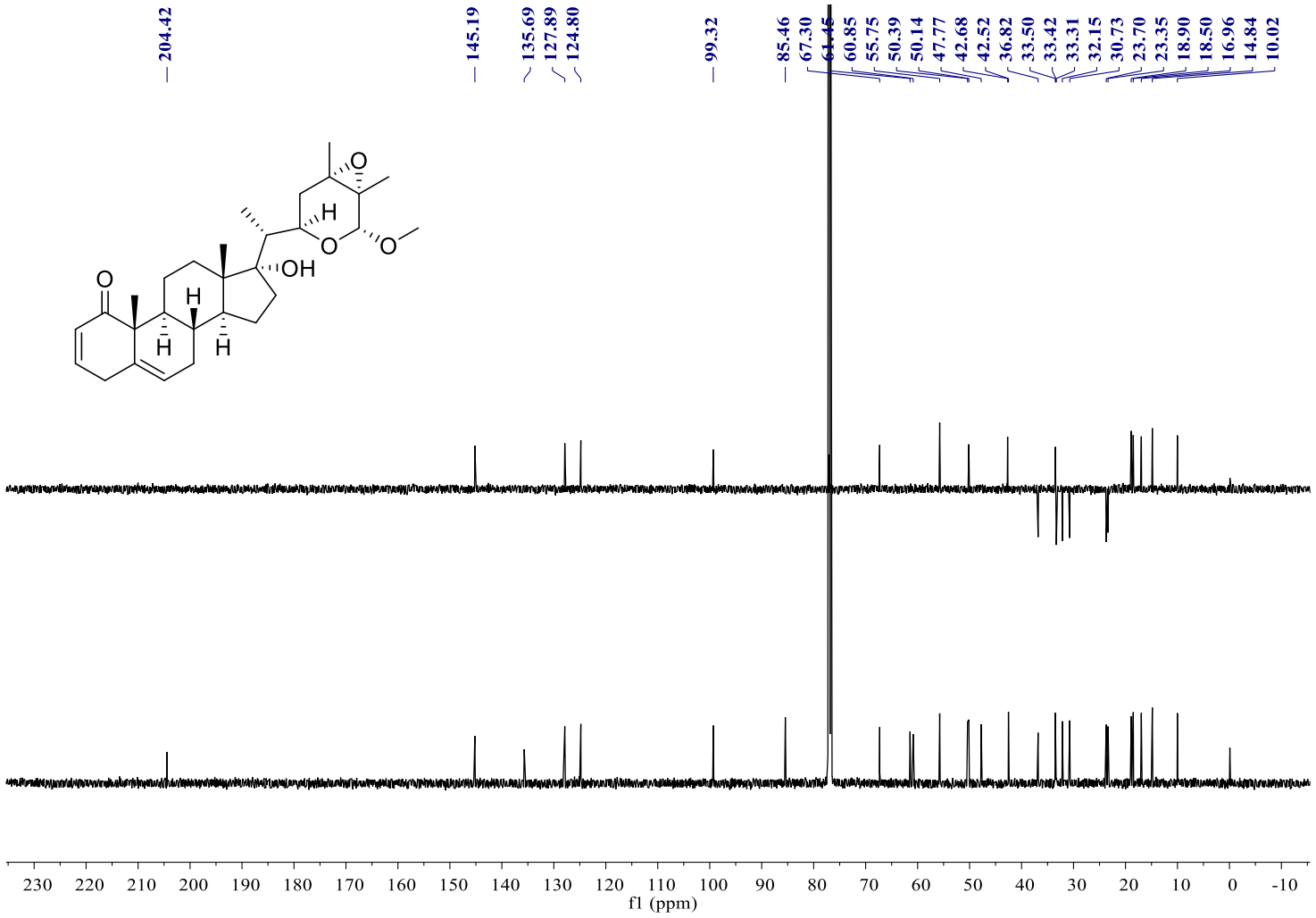


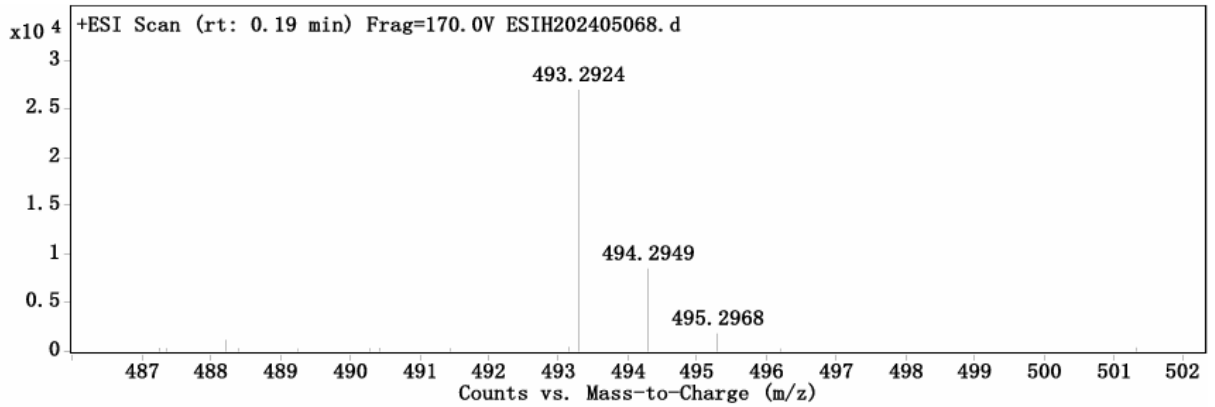
Figure S45. (+)-HRESIMS spectrum of cilistol d (**6**)

Qualitative Analysis Report

Data Filename	ESIH202405068.d	**Sample Name**	D4-SU-41
Sample ID		**Position**	P1-B1
Instrument Name	Agilent 6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	10/25/2024 4:25:28 PM	**DA Method**	ESI-HR-20231114.m
Comment	ESIH by fangsu		

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
170	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
493.2924	493.2924	0.08	0.16	C29 H42 Na O5	(M+Na)+

--- End Of Report ---

Figure S46. ^{1}H NMR spectrum of cilistepoxide (**7**) in $CDCl_3$

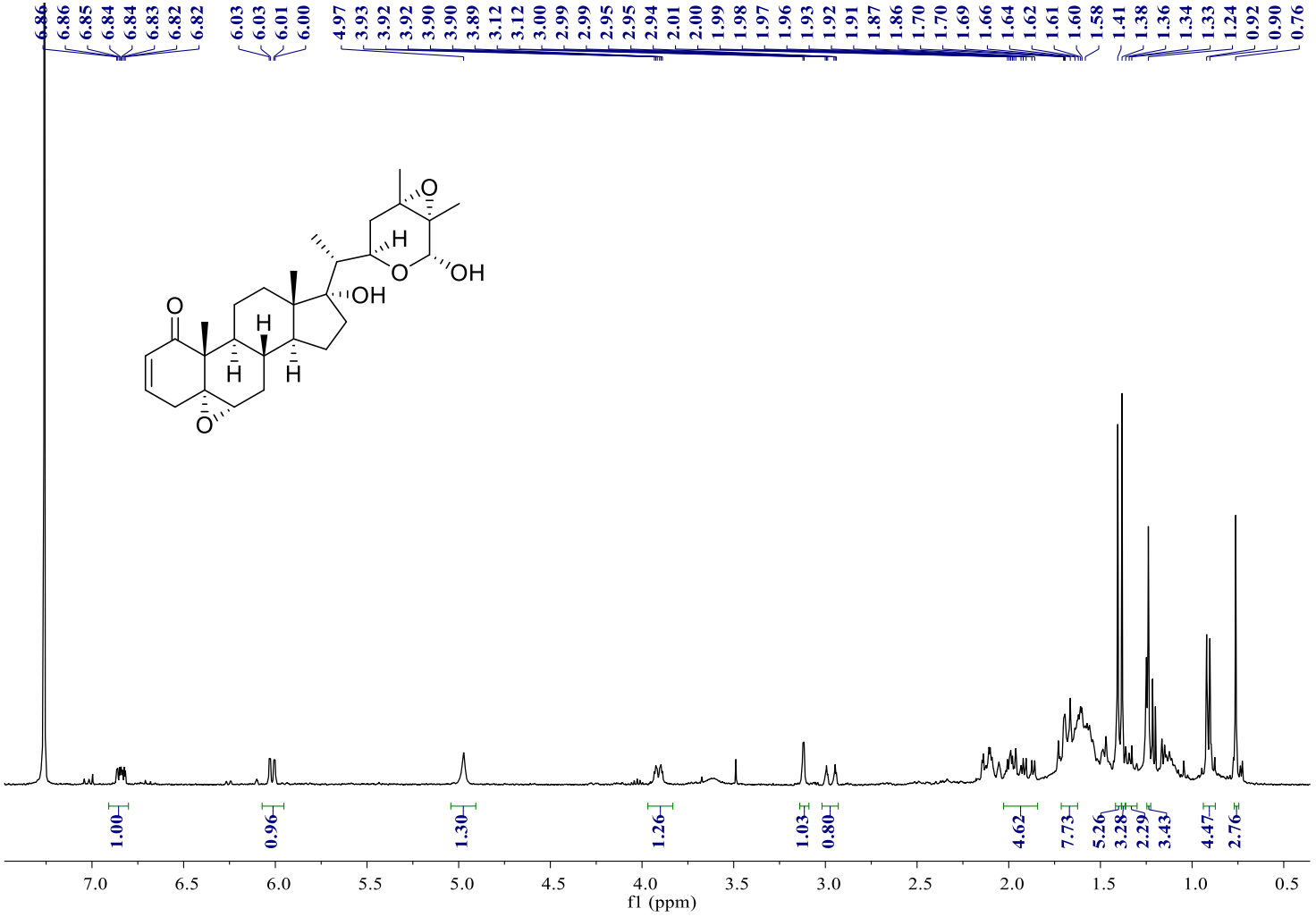


Figure S47. ^{13}C NMR spectrum of cilistepoxide (**7**) in $CDCl_3$

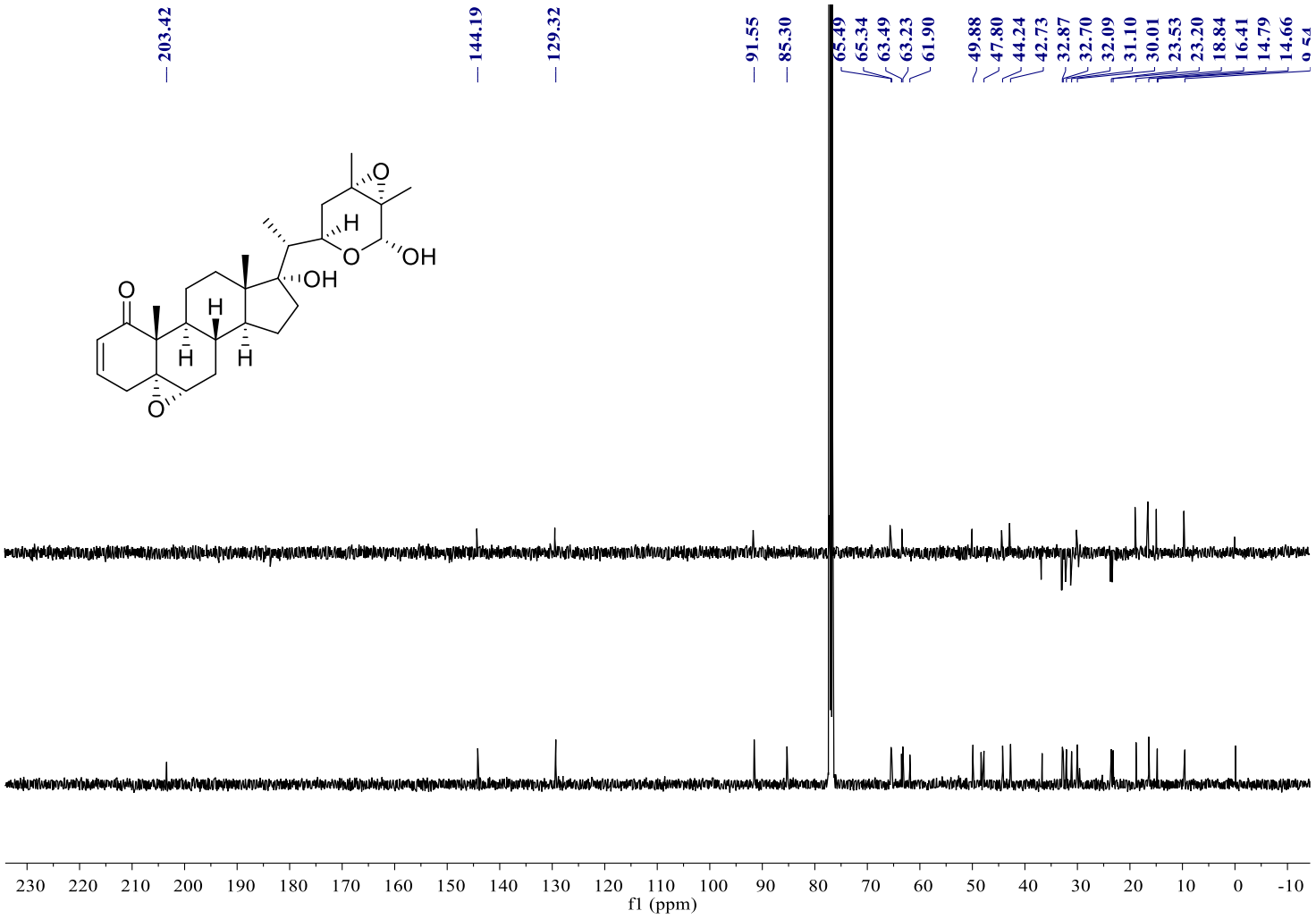


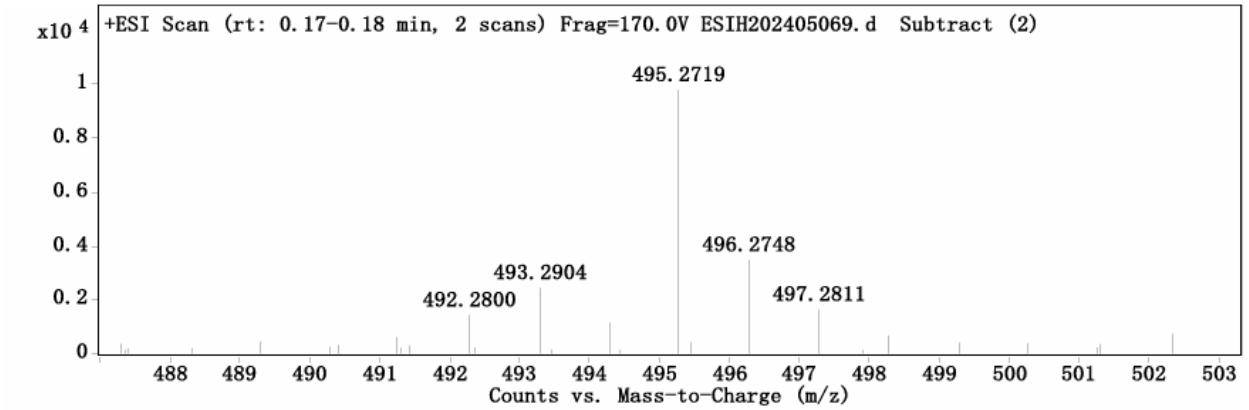
Figure S48. (+)-HRESIMS spectrum of cilistepoxide (**7**)

Qualitative Analysis Report

Data Filename	ESIH202405069.d	**Sample Name**	D4-SU-54
Sample ID		**Position**	P1-B2
Instrument Name	Agilent 6520 Q-TOF	**Acq Method**	20160322_MS_ESIH_POS_1min.m
Acquired Time	10/25/2024 4:26:46 PM	**DA Method**	ESI-HR-20231114.m
Comment	ESIH by fangsu		

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
170	0	ESI



Formula Calculator Results

m/z	Calc m/z	Diff (mDa)	Diff (ppm)	Ion Formula	Ion
495.2719	495.2717	-0.18	-0.37	C28 H40 Na O6	(M+Na)+

--- End Of Report ---

Figure S49. Cytotoxicity of compounds **1**−**7** on the murine splenocyte

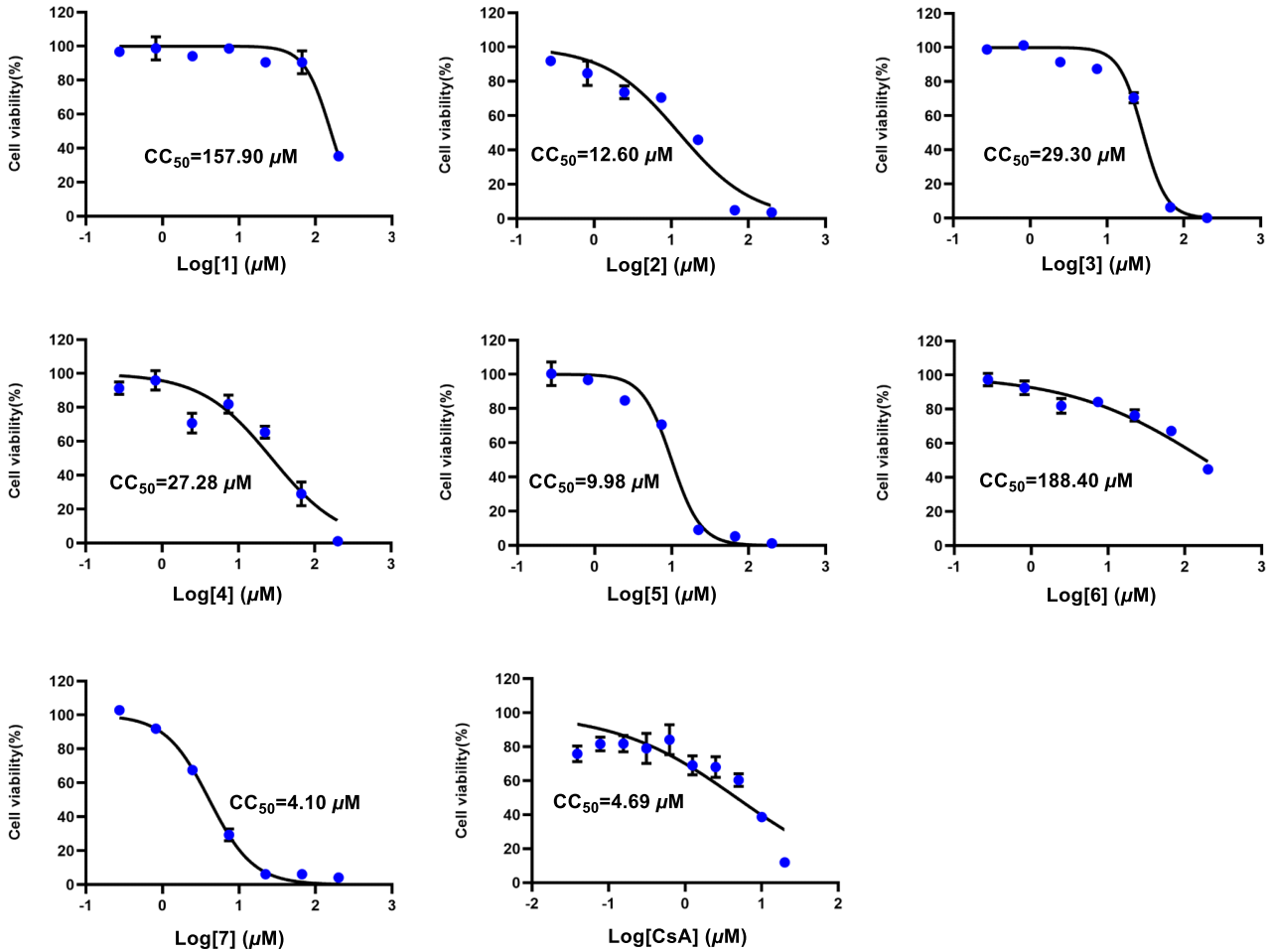


Figure S50. Inhibitory effects of compounds **1**−**7** on ConA-induced proliferation of lymphocytes

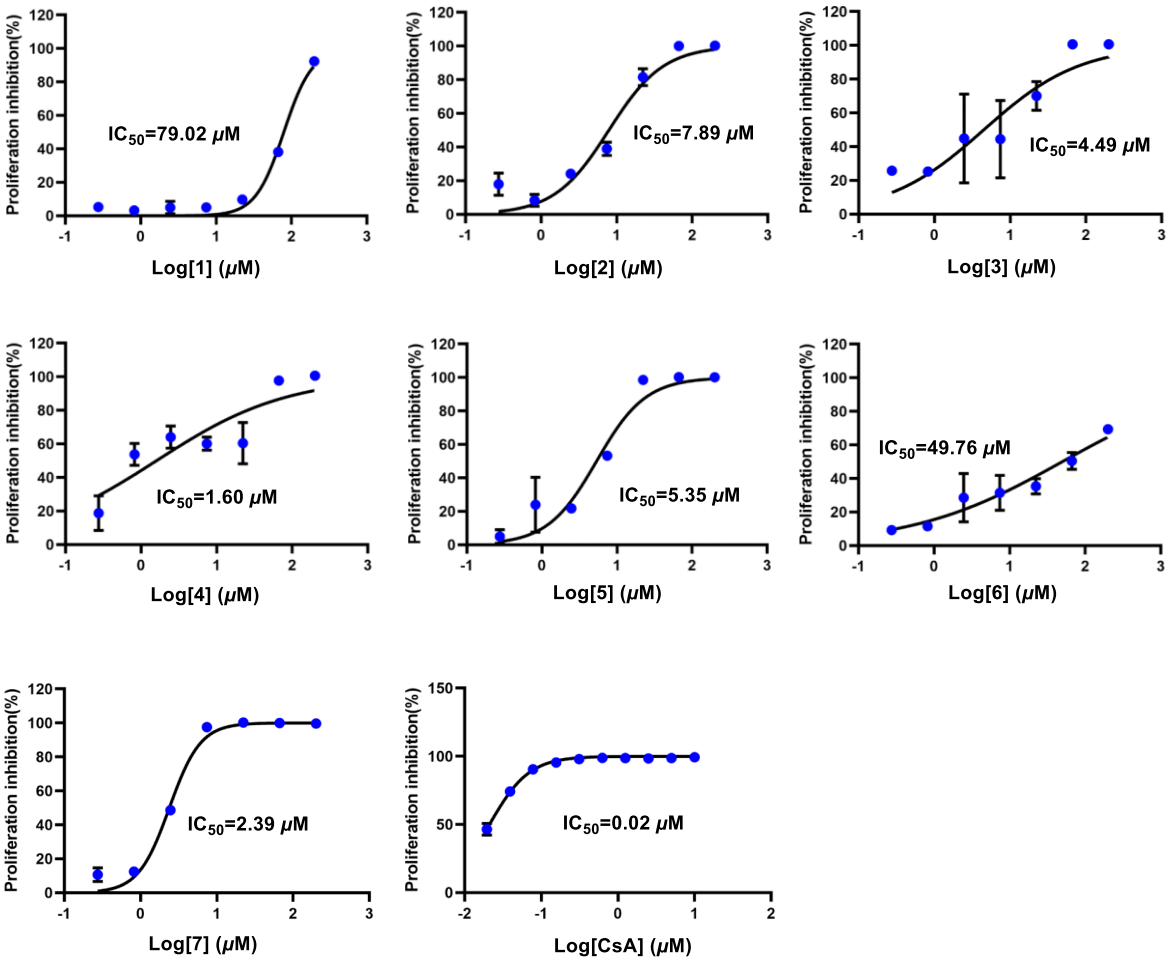


Figure S51. Inhibitory effects of compounds **1**−**7** on LPS-induced proliferation of lymphocytes