



Supporting Information

for

Five new sesquiterpenoids from agarwood of *Aquilaria sinensis*

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Beilstein J. Org. Chem. **2023**, *19*, 998–1007. [doi:10.3762/bjoc.19.75](https://doi.org/10.3762/bjoc.19.75)

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Figure S44: UV-vis spectra of **1–5**

Fig A: human breast cancer cell line (MCF-7) were treated with 40 μM with compounds **1–5** for 24 h, and cell viability was determined by CCK-8 assay.

Fig B: RAW 264.7 were treated with 20 μM with compounds **1–5** for 24 h, and cell viability was determined by CCK-8 assay.

Fig C: Compounds suppress LPS-induced INOS and COX-2 expression in RAW 264.7 cells.

Selected conformation of **1** and their percentage

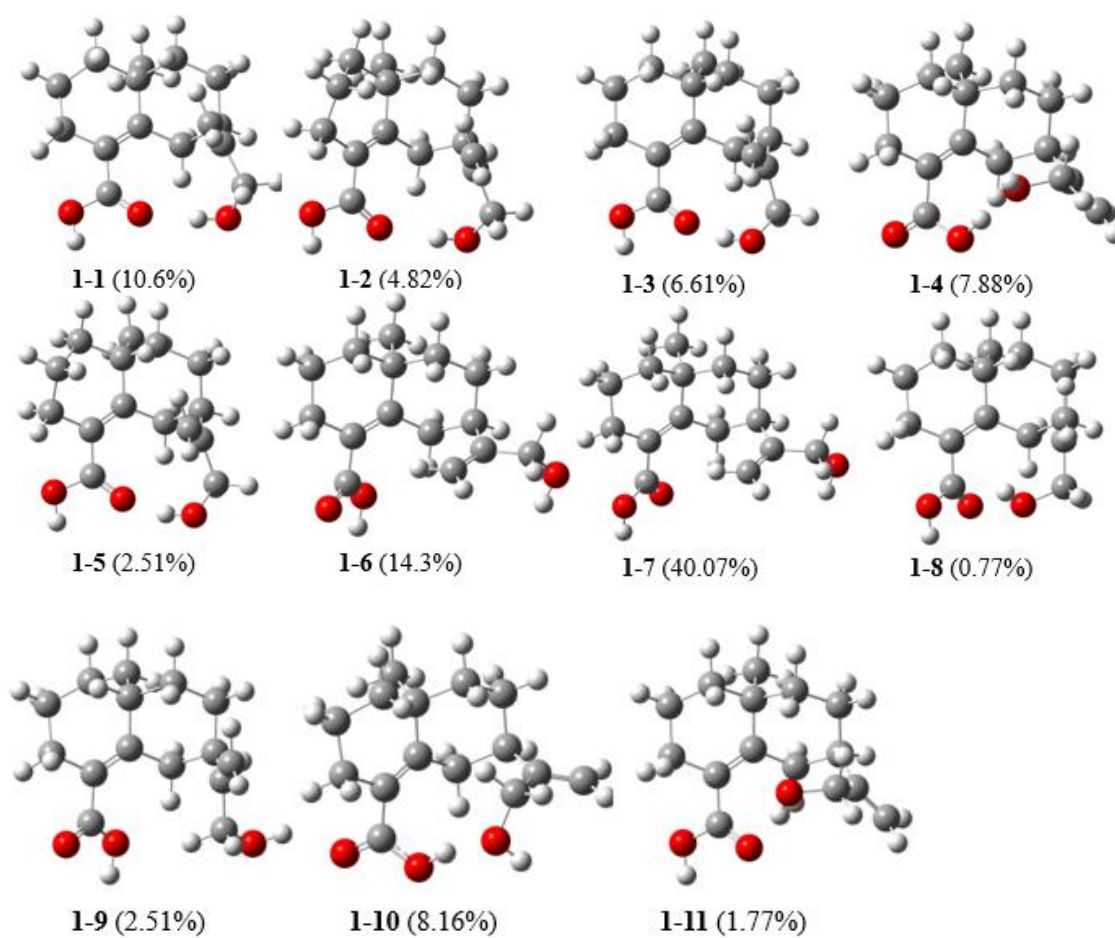


Figure S1: The lowest energy conformers of **1** (the relative populations are in parentheses).

Selected conformation of **2** and their percentage

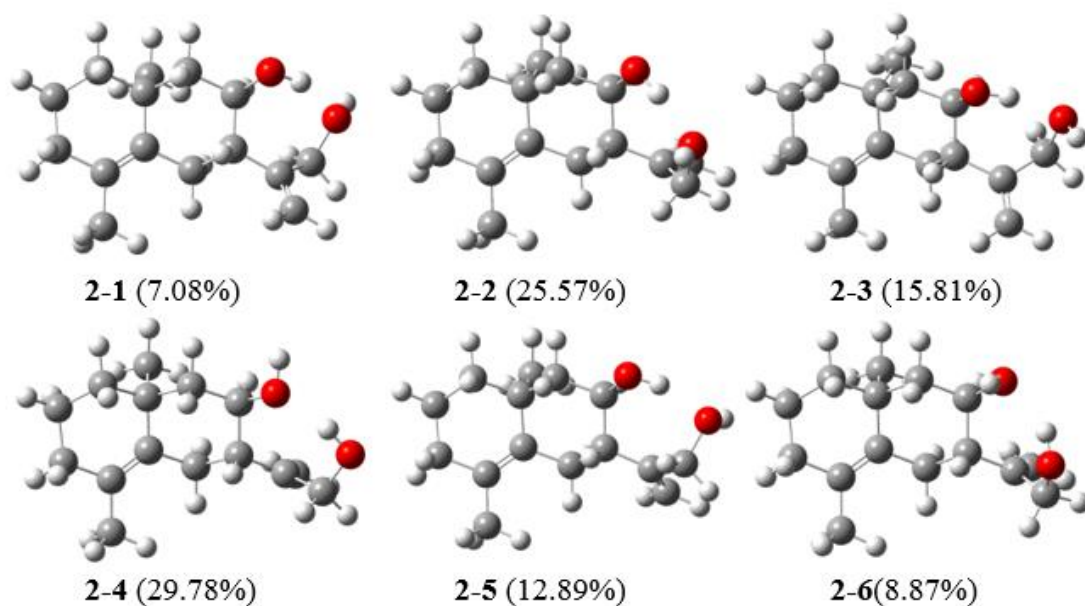


Figure S2: The lowest energy conformers of **2** (the relative populations are in parentheses).

Selected conformation of **3** and their percentage

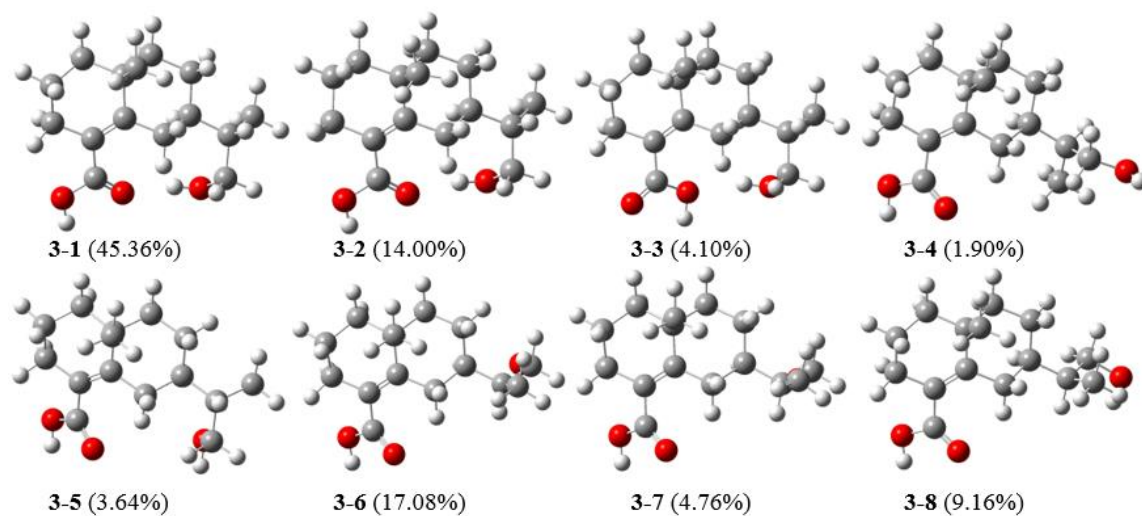


Figure S3: The lowest energy conformers of **3** (the relative populations are in parentheses).

Selected conformation of **4** and their percentage

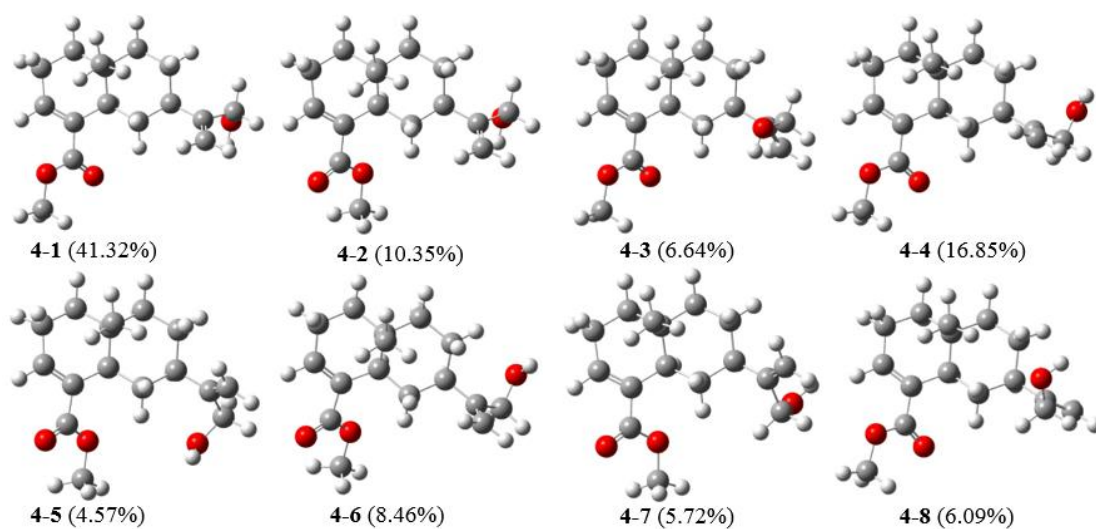


Figure S4: The lowest energy conformers of **4** (the relative populations are in parentheses).

Selected conformation of **5** and their percentage

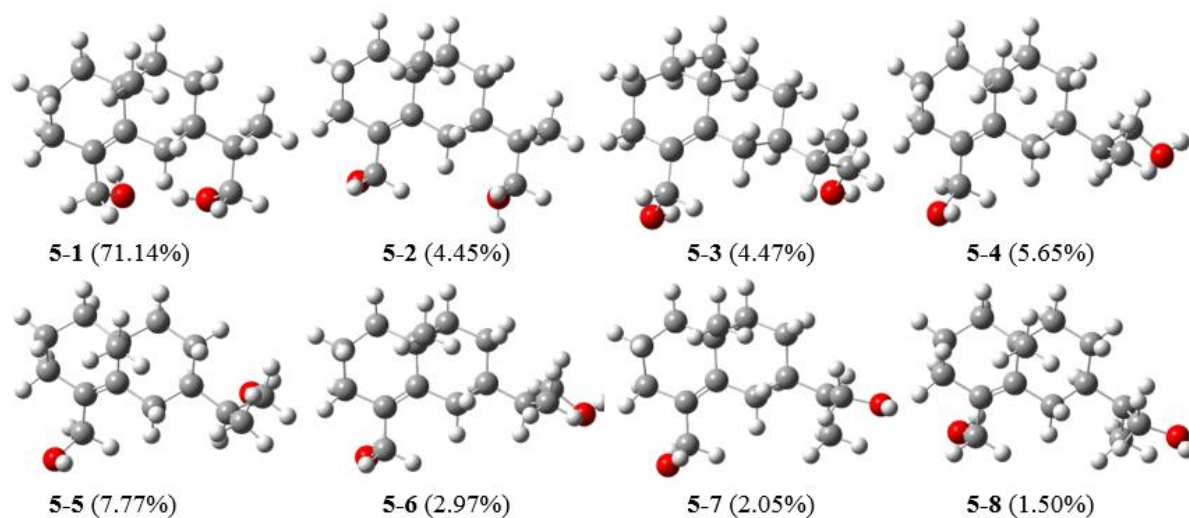


Figure S5: The lowest energy conformers of **5** (the relative populations are in parentheses).

Table S1: Extracted heats and weighting factors of the optimized conformersof **1–5** at B3LYP/6-31G(d,p) level.

		B3LYP/6-31G(d,p)	
	Conformer	Extracted heats	Boltzmann-calculated contribution (%)
1	1	-810.42627	10.6
	2	-810.425526	4.82
	3	-810.425823	6.61
	4	-810.42599	7.88
	5	-810.424909	2.51
	6	-810.426552	14.3
	7	-810.427525	40.07
	8	-810.423792	0.77
	9	-810.424911	2.51
	10	-810.426023	8.16
	11	-810.424577	1.77
2	1	-736.181953	7.08
	2	-736.183165	25.57
	3	-736.182711	15.81
	4	-736.183309	29.78
	5	-736.182518	12.89
	6	-736.182165	8.87
3	1	-811.452558	45.36
	2	-811.451448	14.00
	3	-811.450288	4.10
	4	-811.449562	1.90
	5	-811.450176	3.64
	6	-811.451636	17.08
	7	-811.45043	4.76
	8	-811.451047	9.16
4	1	-849.51583	41.32
	2	-849.514523	10.35
	3	-849.514104	6.64
	4	-849.514983	16.85
	5	-849.513751	4.57
	6	-849.514333	8.46
	7	-849.513963	5.72
	8	-849.514023	6.09
5	1	-737.384987	71.14
	2	-737.38237	4.45
	3	-737.382375	4.47
	4	-737.382596	5.65

	5	-737.382896	7.77
	6	-737.381988	2.97
	7	-737.381638	2.05
	8	-737.381342	1.5

Table S2. The Cartesian coordinates of the lowest energy conformers for **1–5**

1-1	X axis(Å)	Y axis(Å)	Z axis(Å)	1-2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-1.3963	-1.4589	-0.5995	C	-1.1888	-1.6092	-0.4689
C	-0.5173	-2.701	-0.3208	C	-0.1583	-2.6951	-0.0635
C	0.8191	-2.425	0.3812	C	1.1886	-2.1799	0.4746
C	1.6341	-1.2305	-0.1806	C	1.8169	-1.0318	-0.3549
C	0.705	-0.0307	-0.4031	C	0.7293	0.0357	-0.5441
C	-0.5323	-0.3481	-1.2251	C	-0.5008	-0.4797	-1.2678
C	2.7577	-0.9124	0.8489	C	3.0766	-0.4883	0.3789
C	3.3461	0.4785	0.6543	C	2.749	0.5582	1.4342
C	2.2608	1.538	0.8198	C	2.0205	1.7328	0.7914
C	0.9895	1.1966	0.0916	C	0.8471	1.2852	-0.0365
C	-2.2859	-0.9581	0.546	C	-2.0918	-1.0843	0.6558
C	-2.0438	-1.1379	1.8568	C	-1.7544	-1.0252	1.9567
C	-3.5769	-0.281	0.1309	C	-3.4896	-0.6732	0.2416
C	2.2979	-1.634	-1.5175	C	2.319	-1.5842	-1.7108
O	-3.3213	0.9454	-0.5273	O	-3.4539	0.4631	-0.6015
C	0.0252	2.3085	-0.0357	C	-0.2281	2.2944	-0.1656
O	-1.1235	2.3199	0.3702	O	-1.4098	2.1522	0.0906
O	0.5678	3.3554	-0.6765	O	0.2672	3.4634	-0.6052
H	-2.0994	-1.789	-1.3792	H	-1.8701	-2.1193	-1.1664
H	-1.0827	-3.4472	0.2512	H	-0.5988	-3.3884	0.6639
H	-0.295	-3.1777	-1.2852	H	0.0493	-3.3048	-0.9531
H	0.627	-2.2654	1.4465	H	1.0628	-1.8569	1.5124
H	1.4278	-3.3385	0.3396	H	1.8853	-3.0277	0.5214
H	-1.1257	0.5407	-1.445	H	-1.2006	0.3176	-1.5211
H	-0.204	-0.6831	-2.2177	H	-0.201	-0.8688	-2.2482
H	2.3638	-0.9699	1.8729	H	3.6345	-1.3128	0.8406
H	3.5563	-1.6624	0.7898	H	3.7624	-0.0278	-0.3462
H	3.8067	0.5629	-0.337	H	3.6722	0.9127	1.9066
H	4.1426	0.6532	1.3868	H	2.1337	0.1197	2.2289
H	2.6661	2.4962	0.4748	H	2.7127	2.2983	0.1552
H	2.0279	1.6563	1.8857	H	1.6904	2.4082	1.5902
H	-2.7339	-0.7711	2.6123	H	-2.4525	-0.6563	2.7036

H	-1.1652	-1.6378	2.2367	H	-0.7849	-1.3211	2.331
H	-4.1441	-0.9276	-0.5467	H	-3.9836	-1.4899	-0.2948
H	-4.2246	-0.0698	0.9887	H	-4.1186	-0.4287	1.1045
H	3.0373	-2.4288	-1.3648	H	3.1584	-2.2741	-1.5623
H	1.5745	-2.0148	-2.2455	H	1.5534	-2.1385	-2.2611
H	2.8135	-0.7872	-1.9838	H	2.6671	-0.7727	-2.3608
H	-2.6516	1.4237	0.0085	H	-2.8303	1.1008	-0.1901
H	-0.1615	4.0069	-0.7261	H	-0.5188	4.0439	-0.669
1-3	X	Y	Z	1-4	X	Y	Z
	axis(Å)	axis(Å)	axis(Å)		axis(Å)	axis(Å)	axis(Å)
C	-1.307	-1.5306	-0.7969	C	-1.8802	-0.7691	-0.9117
C	-0.4232	-2.7431	-0.4303	C	-1.5885	-2.1926	-0.4017
C	0.7957	-2.4054	0.4362	C	-0.345	-2.3143	0.4828
C	1.6531	-1.2176	-0.0725	C	0.9279	-1.6412	-0.0901
C	0.7399	-0.0351	-0.4252	C	0.6002	-0.202	-0.5014
C	-0.4157	-0.3951	-1.3458	C	-0.6068	-0.0584	-1.4116
C	2.6583	-0.8609	1.0604	C	2.0156	-1.6936	1.0218
C	3.2659	0.5227	0.8806	C	3.1573	-0.719	0.7631
C	2.1709	1.5842	0.8849	C	2.6299	0.7107	0.7019
C	0.977	1.2128	0.045	C	1.361	0.8412	-0.0943
C	-2.3004	-1.0368	0.2589	C	-2.7488	0.1006	0.0033
C	-2.3176	-1.4097	1.552	C	-3.7884	0.7807	-0.5196
C	-3.39	-0.1143	-0.2511	C	-2.4864	0.1759	1.4803
C	2.4572	-1.6461	-1.3218	C	1.4409	-2.4311	-1.3159
O	-3.5003	1.0296	0.5809	O	-1.271	0.8781	1.7043
C	0.0354	2.3212	-0.2204	C	1.0228	2.2453	-0.4303
O	-1.1633	2.3197	-0.0042	O	1.75	2.9765	-1.0804
O	0.6601	3.3839	-0.7507	O	-0.1348	2.6399	0.1357
H	-1.9356	-1.8762	-1.6316	H	-2.4887	-0.9283	-1.8166
H	-1.0209	-3.5194	0.063	H	-2.4584	-2.5939	0.1329
H	-0.0654	-3.1999	-1.3625	H	-1.4529	-2.8477	-1.2722
H	0.4533	-2.1918	1.4543	H	-0.5713	-1.888	1.4663
H	1.4217	-3.3035	0.523	H	-0.1499	-3.3796	0.6648
H	-1.0211	0.4739	-1.6147	H	-0.8391	0.9859	-1.6445
H	0.007	-0.7222	-2.305	H	-0.3333	-0.4955	-2.3817
H	2.1555	-0.8841	2.037	H	1.5738	-1.4465	1.9971
H	3.4579	-1.6104	1.1138	H	2.4151	-2.7109	1.1187
H	3.8342	0.5723	-0.0554	H	3.6696	-0.9705	-0.1727
H	3.9765	0.7268	1.6898	H	3.9053	-0.7993	1.5602
H	2.6152	2.5267	0.5447	H	3.4162	1.3511	0.2846
H	1.8292	1.7482	1.9149	H	2.4353	1.0675	1.7214
H	-3.0784	-1.02	2.2255	H	-4.4323	1.4059	0.0926
H	-1.61	-2.1001	1.9888	H	-4.0173	0.7513	-1.5813

H	-3.2104	0.2252	-1.2751	H	-3.2815	0.719	2.0035
H	-4.3513	-0.6396	-0.2508	H	-2.4313	-0.8189	1.9292
H	3.1709	-2.4409	-1.0755	H	1.7292	-3.4501	-1.0327
H	1.8171	-2.0338	-2.1204	H	0.6859	-2.5219	-2.1031
H	3.0257	-0.8094	-1.7426	H	2.3167	-1.9523	-1.7674
H	-2.6437	1.5028	0.5013	H	-1.1415	0.8692	2.6716
H	-0.0547	4.0401	-0.8827	H	-0.5778	1.9137	0.6434
1-5	X	Y	Z	1-6	X	Y	Z
	axis(Å)	axis(Å)	axis(Å)		axis(Å)	axis(Å)	axis(Å)
C	-0.9711	-1.7554	-0.6651	C	1.8218	-0.2982	0.6513
C	0.1144	-2.739	-0.1634	C	1.7048	-1.8248	0.5104
C	1.32	-2.0875	0.5347	C	0.5265	-2.2341	-0.3711
C	1.9327	-0.8921	-0.237	C	-0.8393	-1.6852	0.1148
C	0.7818	0.0755	-0.5559	C	-0.7607	-0.1738	0.3689
C	-0.3204	-0.5524	-1.3912	C	0.4738	0.2974	1.1296
C	3.0551	-0.242	0.6225	C	-1.8853	-2.0361	-0.9809
C	2.5279	0.7797	1.6183	C	-3.1912	-1.2718	-0.81
C	1.7844	1.8848	0.878	C	-2.9399	0.2306	-0.854
C	0.7455	1.3365	-0.0634	C	-1.7367	0.6625	-0.0608
C	-2.0181	-1.3068	0.3592	C	2.4584	0.3476	-0.5882
C	-1.899	-1.4174	1.6952	C	1.7965	1.0658	-1.5135
C	-3.2987	-0.7484	-0.2301	C	3.9522	0.1599	-0.7268
C	2.6247	-1.3978	-1.526	C	-1.2481	-2.386	1.4325
O	-3.6867	0.4338	0.4529	O	4.6076	0.8593	0.3203
C	-0.381	2.2603	-0.3265	C	-1.7193	2.1169	0.2031
O	-1.5705	2.0187	-0.2364	O	-1.82	2.9908	-0.6379
O	0.0694	3.475	-0.6822	O	-1.6702	2.3912	1.5166
H	-1.5396	-2.3184	-1.4208	H	2.523	-0.1069	1.4764
H	-0.3265	-3.4948	0.4983	H	2.6242	-2.257	0.0999
H	0.4865	-3.3006	-1.0304	H	1.593	-2.2698	1.5064
H	1.0232	-1.7614	1.537	H	0.7246	-1.891	-1.3952
H	2.0844	-2.86	0.6924	H	0.4887	-3.3302	-0.4223
H	-1.0771	0.1732	-1.6988	H	0.5703	1.3883	1.1278
H	0.1052	-0.897	-2.3414	H	0.3316	0.017	2.1822
H	3.624	-1.0144	1.1553	H	-1.4816	-1.8009	-1.9755
H	3.7776	0.2693	-0.0292	H	-2.0897	-3.1142	-0.9814
H	3.3605	1.2124	2.1847	H	-3.6731	-1.5436	0.136
H	1.8647	0.2974	2.3463	H	-3.8924	-1.549	-1.6057
H	2.4953	2.4974	0.3097	H	-3.8395	0.7423	-0.49
H	1.3175	2.5395	1.6242	H	-2.7968	0.5413	-1.8969
H	-2.7031	-1.085	2.3486	H	2.3092	1.5056	-2.3649
H	-1.0305	-1.8319	2.1875	H	0.7289	1.2429	-1.4726
H	-3.1976	-0.5036	-1.2914	H	4.2315	-0.8956	-0.6721

H	-4.1031	-1.4862	-0.1409	H	4.3319	0.546	-1.679
H	3.4894	-2.0263	-1.2814	H	-1.331	-3.4697	1.2907
H	1.9697	-2	-2.1617	H	-0.5252	-2.219	2.2373
H	2.985	-0.5585	-2.1328	H	-2.2147	-2.0262	1.8016
H	-2.9446	1.0643	0.3251	H	4.2495	1.7635	0.3124
H	-0.7455	3.9979	-0.8287	H	-1.705	3.3686	1.5533
1-7	X axis(Å)	Y axis(Å)	Z axis(Å)	1-8	X axis(Å)	Y axis(Å)	Z axis(Å)
C	1.8293	-0.3432	0.6339	C	1.3444	-1.528	0.7593
C	1.7029	-1.8617	0.429	C	0.4149	-2.7337	0.4954
C	0.5018	-2.2304	-0.44	C	-0.7998	-2.4008	-0.3778
C	-0.8488	-1.6948	0.0999	C	-1.6244	-1.1807	0.1031
C	-0.7564	-0.1923	0.4002	C	-0.6923	-0.0052	0.4193
C	0.4937	0.2415	1.159	C	0.5003	-0.3499	1.2984
C	-1.926	-2.0068	-0.9765	C	-2.6369	-0.8313	-1.0268
C	-3.2229	-1.2446	-0.7411	C	-3.2341	0.5618	-0.8672
C	-2.9657	0.2575	-0.7494	C	-2.133	1.6168	-0.8847
C	-1.7338	0.6644	0.0153	C	-0.9475	1.2393	-0.0451
C	2.4506	0.3496	-0.5878	C	2.3112	-1.1381	-0.3707
C	1.7737	1.0863	-1.4872	C	2.3313	-1.6843	-1.6009
C	3.9457	0.1828	-0.7403	C	3.395	-0.1443	-0.0071
C	-1.2249	-2.4384	1.4043	C	-2.4203	-1.5556	1.3754
O	4.6021	0.8514	0.326	O	2.9251	1.1842	-0.1567
C	-1.688	2.1001	0.3737	C	-0.0648	2.367	0.2974
O	-1.4899	2.5756	1.4755	O	0.009	2.9284	1.3729
O	-1.9082	2.8733	-0.7027	O	0.6949	2.7019	-0.7588
H	2.5446	-0.1913	1.4552	H	1.9998	-1.8459	1.5844
H	2.6106	-2.2774	-0.0229	H	0.9749	-3.5641	0.0484
H	1.6144	-2.3497	1.407	H	0.0577	-3.1139	1.4613
H	0.677	-1.8477	-1.4542	H	-0.4597	-2.2236	-1.4039
H	0.4568	-3.3233	-0.5333	H	-1.4455	-3.2873	-0.4321
H	0.6001	1.33	1.1999	H	1.1429	0.5127	1.4912
H	0.3671	-0.0794	2.2019	H	0.116	-0.6255	2.2896
H	-1.55	-1.7401	-1.974	H	-2.1409	-0.8753	-2.0063
H	-2.1346	-3.0837	-1.0066	H	-3.4431	-1.5748	-1.0609
H	-3.6763	-1.5423	0.2111	H	-3.8031	0.6283	0.0673
H	-3.95	-1.4956	-1.5222	H	-3.9432	0.7594	-1.6794
H	-3.8503	0.7624	-0.3422	H	-2.5563	2.5687	-0.5419
H	-2.8565	0.5927	-1.7889	H	-1.7952	1.7705	-1.9174
H	2.2759	1.5576	-2.3279	H	3.0716	-1.3836	-2.3385
H	0.7038	1.2438	-1.4346	H	1.6369	-2.4489	-1.9256
H	4.2352	-0.8713	-0.7241	H	3.7325	-0.2869	1.0244
H	4.3152	0.6059	-1.6807	H	4.276	-0.2597	-0.6481

H	-1.3187	-3.5161	1.2278	H	-3.1384	-2.3572	1.1667
H	-0.4791	-2.3037	2.194	H	-1.7741	-1.9099	2.1846
H	-2.1783	-2.0862	1.8129	H	-2.9831	-0.7013	1.7673
H	4.2086	1.7393	0.3798	H	2.2493	1.1743	-0.8607
H	-1.8525	3.7832	-0.3446	H	1.3049	3.3748	-0.386
1-9	X	Y	Z	1-10	X	Y	Z
	axis(Å)	axis(Å)	axis(Å)		axis(Å)	axis(Å)	axis(Å)
C	1.6314	-1.1012	0.6224	C	-1.9793	-0.4815	-0.9318
C	0.9696	-2.4938	0.536	C	-1.8844	-1.9812	-0.6058
C	-0.3348	-2.49	-0.2679	C	-0.775	-2.3239	0.3848
C	-1.3726	-1.4326	0.1932	C	0.6145	-1.7578	-0.0015
C	-0.7001	-0.0664	0.3949	C	0.5413	-0.2725	-0.3903
C	0.5924	-0.1087	1.1957	C	-0.6015	0.1013	-1.3212
C	-2.4861	-1.3796	-0.8926	C	1.5569	-1.9816	1.2132
C	-3.3577	-0.1363	-0.7761	C	2.8863	-1.254	1.0622
C	-2.5067	1.1208	-0.9158	C	2.67	0.2447	0.8867
C	-1.2386	1.0687	-0.11	C	1.5012	0.5986	0.0055
C	2.3411	-0.5917	-0.6466	C	-2.7782	0.29	0.1239
C	2.4906	-1.3015	-1.7811	C	-4.0928	0.5174	-0.0671
C	2.9594	0.7875	-0.5706	C	-2.1189	0.7779	1.3824
C	-2.0115	-1.88	1.5293	C	1.1647	-2.5516	-1.2132
O	3.868	0.8334	0.5195	O	-1.4594	2.0053	1.1033
C	-0.6264	2.3983	0.0843	C	1.5845	1.9836	-0.5194
O	-0.2827	3.158	-0.8022	O	2.4558	2.3474	-1.292
O	-0.5622	2.7346	1.3825	O	0.657	2.8046	-0.0017
H	2.4262	-1.1962	1.3766	H	-2.5749	-0.4212	-1.8563
H	1.6638	-3.2314	0.1164	H	-2.8416	-2.3524	-0.2179
H	0.7578	-2.8456	1.5539	H	-1.7124	-2.5329	-1.5386
H	-0.0944	-2.3253	-1.3246	H	-1.0687	-1.9723	1.3796
H	-0.7798	-3.4926	-0.2202	H	-0.7153	-3.4169	0.4755
H	1.0509	0.8758	1.311	H	-0.7006	1.1835	-1.4506
H	0.3458	-0.413	2.2216	H	-0.3422	-0.2839	-2.317
H	-2.0371	-1.3834	-1.8954	H	1.0735	-1.6251	2.1334
H	-3.1161	-2.2763	-0.8384	H	1.7427	-3.0532	1.3589
H	-3.8859	-0.1281	0.1843	H	3.4445	-1.6524	0.2074
H	-4.1277	-0.1457	-1.5562	H	3.5108	-1.4321	1.9456
H	-3.1136	1.984	-0.616	H	3.5981	0.6826	0.4997
H	-2.2436	1.2663	-1.9714	H	2.4965	0.6969	1.8719
H	3.0148	-0.8916	-2.6407	H	-4.6959	1.0518	0.6617
H	2.1116	-2.3088	-1.9059	H	-4.6092	0.171	-0.9585
H	3.5162	1.0438	-1.4787	H	-2.8463	0.9598	2.1816
H	2.2011	1.5619	-0.4348	H	-1.3882	0.0743	1.7794
H	-2.5526	-2.8256	1.4084	H	1.2981	-3.6099	-0.9611

H	-1.2677	-2.0369	2.3168	H	0.495	-2.5074	-2.0782
H	-2.7238	-1.1377	1.9063	H	2.134	-2.167	-1.5488
H	4.4936	0.1014	0.3835	H	-2.1616	2.6112	0.7918
H	-0.1597	3.6267	1.3751	H	-0.0108	2.3397	0.5608
1-11	X axis(Å)	Y axis(Å)	Z axis(Å)				
C	-1.9252	-0.6804	-0.9093				
C	-1.6901	-2.1245	-0.4318				
C	-0.4507	-2.313	0.4455				
C	0.8494	-1.682	-0.1177				
C	0.583	-0.2217	-0.5018				
C	-0.6252	-0.0122	-1.3978				
C	1.9325	-1.8065	0.9931				
C	3.1064	-0.8638	0.7681				
C	2.6251	0.5831	0.7536				
C	1.378	0.7827	-0.0628				
C	-2.7566	0.208	0.0206				
C	-3.7545	0.9567	-0.4899				
C	-2.5034	0.2274	1.5052				
C	1.3283	-2.4679	-1.3594				
O	-1.2425	0.7958	1.7981				
C	1.0178	2.1929	-0.3084				
O	-0.0237	2.7335	0.0216				
O	1.9945	2.8484	-0.9533				
H	-2.541	-0.7964	-1.8159				
H	-2.5741	-2.5026	0.0966				
H	-1.5819	-2.7656	-1.3165				
H	-0.66	-1.8959	1.437				
H	-0.299	-3.3885	0.6076				
H	-0.8176	1.0439	-1.6113				
H	-0.3741	-0.4397	-2.3783				
H	1.4976	-1.5758	1.9754				
H	2.2971	-2.8393	1.0585				
H	3.6123	-1.1014	-0.1749				
H	3.8489	-0.9947	1.5637				
H	3.4423	1.21	0.3782				
H	2.4213	0.9078	1.782				
H	-4.3712	1.5929	0.1388				
H	-3.9774	0.9672	-1.5527				
H	-3.2578	0.8212	2.0337				
H	-2.5538	-0.779	1.9291				
H	1.5678	-3.5053	-1.0985				
H	0.5721	-2.5058	-2.1498				

H	2.2272	-2.0207	-1.7977				
H	-1.1354	1.5763	1.2166				
H	1.6404	3.7549	-1.0583				
2-1	X axis(Å)	Y axis(Å)	Z axis(Å)	2-2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-3.8776	-0.7045	0.0523	C	-3.9174	-0.5331	-0.2083
C	-3.699	0.7758	-0.2565	C	-3.595	0.8762	-0.6873
C	-2.3052	1.3122	0.0044	C	-2.2171	1.3704	-0.2945
C	-1.2418	0.5013	0.2295	C	-1.2558	0.541	0.1808
C	-1.3523	-1.0342	0.1641	C	-1.4562	-0.9807	0.2827
C	-2.6914	-1.4961	-0.4724	C	-2.735	-1.453	-0.4625
C	0.1536	1.0082	0.5698	C	0.0995	1.0115	0.6822
C	1.2226	0.4443	-0.3844	C	1.2773	0.2975	-0.0145
C	1.181	-1.0995	-0.3465	C	1.1246	-1.2389	0.096
C	-0.213	-1.6114	-0.7156	C	-0.2575	-1.7023	-0.3767
C	2.5939	1.0594	-0.0844	C	2.6379	0.7833	0.5108
C	3.0542	2.0896	-0.819	C	2.9162	0.9564	1.8165
C	3.4115	0.4957	1.0424	C	3.6801	1.0743	-0.5348
O	3.9646	-0.7394	0.6084	O	4.0428	-0.1577	-1.1399
C	-2.2619	2.8206	-0.0227	C	-2.0649	2.8586	-0.4903
O	2.114	-1.6523	-1.2768	O	2.0704	-1.9327	-0.726
C	-1.2617	-1.6163	1.5946	C	-1.5721	-1.3967	1.7674
H	-3.9919	-0.852	1.1321	H	-4.1717	-0.5194	0.8577
H	-4.8033	-1.0661	-0.4103	H	-4.8028	-0.906	-0.7361
H	-4.4291	1.339	0.3381	H	-4.3591	1.5548	-0.2884
H	-3.942	0.9544	-1.3119	H	-3.6744	0.9138	-1.7814
H	-2.8533	-2.5661	-0.291	H	-2.995	-2.4776	-0.1684
H	-2.6554	-1.3742	-1.5638	H	-2.5552	-1.4847	-1.546
H	0.2119	2.0993	0.5636	H	0.2337	2.0908	0.5732
H	0.3832	0.7222	1.6043	H	0.125	0.8356	1.7641
H	0.9548	0.7443	-1.4095	H	1.2296	0.5635	-1.081
H	1.449	-1.4794	0.6455	H	1.297	-1.5669	1.1272
H	-0.395	-1.3703	-1.7731	H	-0.3	-1.5665	-1.4678
H	-0.2168	-2.7091	-0.6719	H	-0.3401	-2.7879	-0.2273
H	4.0268	2.5351	-0.6328	H	3.8932	1.2974	2.1477
H	2.4764	2.5049	-1.6399	H	2.1965	0.7385	2.5987
H	4.235	1.1629	1.3192	H	3.2857	1.7525	-1.2985
H	2.7985	0.3266	1.9329	H	4.5807	1.5264	-0.1063
H	4.5731	-1.0301	1.3099	H	4.7079	0.0539	-1.8186
H	-1.264	3.2332	-0.178	H	-1.0277	3.193	-0.5454
H	-2.8729	3.1995	-0.8501	H	-2.5271	3.1625	-1.4365
H	-2.6655	3.2242	0.9114	H	-2.5638	3.3973	0.3215
H	2.9972	-1.3905	-0.9369	H	2.9003	-1.4082	-0.7384

H	-1.3822	-2.7057	1.5823	H	-1.7764	-2.4698	1.8589
H	-0.3007	-1.4074	2.0745	H	-0.6555	-1.2005	2.3323
H	-2.0374	-1.2045	2.2493	H	-2.3814	-0.8605	2.275
2-3	X axis(Å)	Y axis(Å)	Z axis(Å)	2-4	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-3.8915	-0.693	0.0342	C	-3.9195	-0.5837	-0.2007
C	-3.7014	0.7818	-0.2938	C	-3.621	0.8253	-0.696
C	-2.3079	1.3144	-0.0241	C	-2.2503	1.3464	-0.3128
C	-1.2518	0.5013	0.2259	C	-1.2752	0.5409	0.175
C	-1.3697	-1.0339	0.181	C	-1.4523	-0.9814	0.3021
C	-2.7034	-1.4982	-0.4649	C	-2.7203	-1.486	-0.4399
C	0.1415	1.0055	0.5772	C	0.0753	1.0439	0.6623
C	1.2208	0.4263	-0.3571	C	1.2545	0.3393	-0.0409
C	1.1697	-1.1178	-0.2989	C	1.1301	-1.1912	0.1292
C	-0.223	-1.627	-0.6776	C	-0.2386	-1.6975	-0.3388
C	2.5865	1.0479	-0.0416	C	2.6273	0.8598	0.4108
C	3.0164	2.1329	-0.7127	C	2.9125	1.2392	1.6706
C	3.4279	0.4292	1.036	C	3.6796	0.9803	-0.6686
O	4.0955	-0.6937	0.4742	O	4.2499	-0.2849	-0.9527
C	-2.2556	2.822	-0.0719	C	-2.1203	2.8335	-0.5351
O	2.1073	-1.689	-1.2128	O	2.1278	-1.8525	-0.663
C	-1.2984	-1.5971	1.62	C	-1.5682	-1.3721	1.7937
H	-4.0193	-0.8242	1.1146	H	-4.1775	-0.5613	0.8642
H	-4.8136	-1.0565	-0.4341	H	-4.7966	-0.9787	-0.7262
H	-4.4354	1.3573	0.2838	H	-4.395	1.4962	-0.3033
H	-3.9309	0.9463	-1.3546	H	-3.7034	0.8486	-1.7903
H	-2.8732	-2.5646	-0.2701	H	-2.963	-2.511	-0.1326
H	-2.6539	-1.3922	-1.5575	H	-2.5368	-1.5289	-1.5224
H	0.2029	2.0963	0.5604	H	0.1881	2.1241	0.5403
H	0.3591	0.7305	1.6175	H	0.1158	0.8766	1.7453
H	0.9714	0.7151	-1.39	H	1.1678	0.569	-1.1134
H	1.4255	-1.4871	0.7004	H	1.3077	-1.4728	1.1736
H	-0.3914	-1.3984	-1.7402	H	-0.2787	-1.5905	-1.433
H	-0.2328	-2.7241	-0.6204	H	-0.3009	-2.78	-0.1609
H	3.9778	2.5933	-0.5052	H	3.9012	1.6069	1.9339
H	2.4149	2.5904	-1.4938	H	2.1963	1.1742	2.4816
H	4.1807	1.1215	1.4288	H	3.2528	1.394	-1.5881
H	2.8169	0.099	1.8813	H	4.492	1.65	-0.3668
H	4.7805	-0.3263	-0.1144	H	3.5123	-0.9319	-0.9583
H	-1.2542	3.226	-0.228	H	-1.0881	3.1801	-0.6077
H	-2.8597	3.1932	-0.9079	H	-2.5965	3.1155	-1.4812
H	-2.6618	3.2411	0.8541	H	-2.6178	3.3791	0.2729
H	2.9843	-1.5403	-0.8016	H	2.0432	-2.8079	-0.4884

H	-1.4245	-2.686	1.621	H	-1.7564	-2.4464	1.9039
H	-0.3419	-1.3868	2.1081	H	-0.6573	-1.1512	2.3587
H	-2.0794	-1.1725	2.2601	H	-2.3878	-0.8394	2.2884
2-5	X axis(Å)	Y axis(Å)	Z axis(Å)	2-6	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-3.9291	-0.6661	-0.0327	C	-3.897	-0.5156	-0.2752
C	-3.694	0.7212	-0.6159	C	-3.5606	0.9115	-0.6866
C	-2.3188	1.2924	-0.3338	C	-2.1889	1.3847	-0.2479
C	-1.2994	0.5333	0.1377	C	-1.2397	0.5356	0.217
C	-1.4284	-0.9825	0.3444	C	-1.4501	-0.9893	0.2608
C	-2.7237	-1.5529	-0.2966	C	-2.7098	-1.4279	-0.5352
C	0.0585	1.0862	0.5338	C	0.1116	0.9867	0.7533
C	1.2436	0.3958	-0.183	C	1.2803	0.2873	0.0326
C	1.1513	-1.1405	0.0214	C	1.1264	-1.2473	0.141
C	-0.2364	-1.6851	-0.3409	C	-0.2368	-1.7038	-0.3866
C	2.6139	0.9871	0.2207	C	2.6537	0.7585	0.5191
C	2.8288	1.7843	1.2855	C	2.984	0.8679	1.8189
C	3.7659	0.6847	-0.7026	C	3.6465	1.1061	-0.5613
O	4.3159	-0.5681	-0.3136	O	3.8829	-0.0341	-1.3734
C	-2.2378	2.7689	-0.6333	C	-2.0279	2.8786	-0.3891
O	2.0557	-1.8505	-0.8312	O	2.136	-1.9286	-0.6139
C	-1.4427	-1.3127	1.8546	C	-1.6122	-1.4493	1.7285
H	-4.1249	-0.5939	1.0433	H	-4.1806	-0.5452	0.783
H	-4.8252	-1.1068	-0.4847	H	-4.7685	-0.8643	-0.8413
H	-4.4631	1.3939	-0.2165	H	-4.3303	1.5757	-0.2744
H	-3.8346	0.6851	-1.7038	H	-3.6188	0.9953	-1.7794
H	-2.9226	-2.5661	0.0743	H	-2.979	-2.4626	-0.2884
H	-2.602	-1.6468	-1.3846	H	-2.5015	-1.417	-1.6139
H	0.1538	0.9627	1.62	H	0.2518	2.0682	0.6818
H	0.125	2.1641	0.3645	H	0.1346	0.7707	1.8283
H	1.1316	0.6005	-1.2583	H	1.2076	0.5607	-1.031
H	1.4002	-1.4045	1.0557	H	1.2481	-1.5705	1.1808
H	-0.347	-1.6144	-1.4337	H	-0.2477	-1.5445	-1.4749
H	-0.2613	-2.7632	-0.1285	H	-0.3241	-2.7917	-0.2611
H	3.8148	2.1899	1.4986	H	3.9696	1.2054	2.1283
H	2.0495	2.0644	1.9856	H	2.2934	0.6095	2.6153
H	3.4388	0.6237	-1.7452	H	3.2591	1.9112	-1.1937
H	4.5557	1.4424	-0.6525	H	4.6069	1.4359	-0.1517
H	4.7284	-0.4225	0.5571	H	4.009	-0.7843	-0.7589
H	-1.2201	3.1311	-0.7886	H	-0.9888	3.2107	-0.4148
H	-2.779	2.9957	-1.5591	H	-2.4724	3.2172	-1.332
H	-2.6956	3.343	0.1785	H	-2.5391	3.3907	0.4321
H	2.9677	-1.5785	-0.5956	H	2.2003	-1.4814	-1.4807

H	-1.5973	-2.3854	2.0197	H	-1.8188	-2.5245	1.7815
H	-0.5044	-1.0494	2.3525	H	-0.7146	-1.269	2.3279
H	-2.2436	-0.7779	2.3769	H	-2.4371	-0.9283	2.2266
3-1	X axis(Å)	Y axis(Å)	Z axis(Å)	3-2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	3.6311	-0.5554	-0.3088	C	3.1718	-0.4694	-1.2252
C	3.0041	0.8216	-0.5124	C	2.8989	0.8853	-0.58
C	1.5812	0.9077	-0.0232	C	1.5412	0.9426	0.0663
C	0.844	-0.1763	0.3188	C	0.8709	-0.1609	0.4756
C	1.3396	-1.6111	0.0932	C	1.4276	-1.5794	0.3003
C	2.6579	-1.647	-0.7311	C	2.887	-1.5899	-0.2351
C	-0.5552	-0.0981	0.8982	C	-0.5539	-0.1366	0.9875
C	-1.5598	-0.7406	-0.0697	C	-1.465	-0.7412	-0.0968
C	-1.1771	-2.2285	-0.2228	C	-1.0104	-2.1949	-0.3724
C	0.2676	-2.3949	-0.7165	C	0.4901	-2.2951	-0.7111
C	-3.0299	-0.53	0.3939	C	-2.9692	-0.6305	0.2842
C	-3.3956	0.9575	0.5861	C	-3.4148	0.8212	0.5602
O	-3.0859	1.7326	-0.5638	O	-3.0938	1.6888	-0.5182
C	1.5893	-2.3055	1.4503	C	1.4533	-2.3603	1.6348
C	-4.0229	-1.1555	-0.5979	C	-3.8694	-1.2231	-0.8106
C	0.9824	2.2665	-0.011	C	0.9082	2.2845	0.0815
O	-0.1517	2.5626	-0.3485	O	-0.245	2.5539	-0.2074
O	1.8515	3.1954	0.4162	O	1.7846	3.2312	0.4543
H	4.5528	-0.6278	-0.8975	H	2.5561	-0.59	-2.1245
H	3.9181	-0.686	0.7412	H	4.2177	-0.5168	-1.5496
H	3.0193	1.0725	-1.5807	H	2.9895	1.6537	-1.3574
H	3.6392	1.5544	-0.0019	H	3.663	1.0999	0.1773
H	2.444	-1.5125	-1.8002	H	3.1141	-2.5571	-0.7011
H	3.1412	-2.6279	-0.641	H	3.5919	-1.483	0.6014
H	-0.5831	-0.6145	1.8656	H	-0.6403	-0.7014	1.9222
H	-0.828	0.9266	1.1451	H	-0.8609	0.8713	1.2649
H	-1.4482	-0.2681	-1.0564	H	-1.3153	-0.1782	-1.0298
H	-1.3089	-2.7516	0.7319	H	-1.5666	-2.6143	-1.2178
H	-1.8321	-2.7237	-0.947	H	-1.2376	-2.8254	0.4954
H	0.5184	-3.4633	-0.7355	H	0.7628	-3.3551	-0.7922
H	0.2871	-2.0606	-1.7634	H	0.6326	-1.8672	-1.7124
H	-3.1725	-1.0305	1.3608	H	-3.1449	-1.2078	1.2015
H	-4.4695	1.0619	0.776	H	-4.5001	0.8619	0.7051
H	-2.8901	1.3932	1.4536	H	-2.9699	1.2175	1.4781
H	-2.1324	1.9577	-0.5324	H	-2.1492	1.9399	-0.4376
H	0.67	-2.4386	2.029	H	0.4566	-2.5578	2.0392
H	2.0175	-3.3043	1.3068	H	1.9364	-3.3361	1.504
H	2.2852	-1.733	2.0735	H	2.0146	-1.8114	2.4002

H	-5.0558	-0.9236	-0.3157	H	-4.9274	-1.0588	-0.578
H	-3.9404	-2.2462	-0.6122	H	-3.7323	-2.305	-0.8976
H	-3.8592	-0.7842	-1.6151	H	-3.6636	-0.7702	-1.7861
H	1.3443	4.032	0.3727	H	1.265	4.0608	0.4258
3-3	X	Y	Z	3-4	X	Y	Z
	axis(Å)	axis(Å)	axis(Å)		axis(Å)	axis(Å)	axis(Å)
C	3.6501	-0.5565	-0.2827	C	3.5561	-1.2164	0.2204
C	3.0367	0.827	-0.4762	C	3.342	0.2583	-0.0987
C	1.6037	0.9198	-0.0176	C	1.9129	0.7062	0.0654
C	0.8509	-0.1593	0.3045	C	0.8567	-0.1394	0.1425
C	1.3462	-1.5957	0.0843	C	1.0425	-1.664	0.0673
C	2.6713	-1.6342	-0.7284	C	2.4638	-2.0578	-0.4246
C	-0.5491	-0.0755	0.8791	C	-0.5856	0.3208	0.3104
C	-1.5561	-0.743	-0.0733	C	-1.5251	-0.3044	-0.7387
C	-1.1609	-2.2275	-0.2249	C	-1.4152	-1.8372	-0.7058
C	0.2807	-2.3814	-0.7283	C	0.0291	-2.2844	-0.9289
C	-3.0265	-0.5538	0.4028	C	-3.0043	0.1609	-0.6176
C	-3.4099	0.9247	0.6233	C	-3.6213	-0.0695	0.7698
O	-3.1298	1.7271	-0.5165	O	-5.0191	0.1964	0.7207
C	1.5861	-2.2865	1.4458	C	0.8265	-2.2647	1.4768
C	-4.0194	-1.1747	-0.5922	C	-3.1576	1.6344	-1.0262
C	1.1107	2.3165	0.0579	C	1.7503	2.1718	0.2049
O	1.7298	3.2656	0.5025	O	1.1263	2.7619	1.0665
O	-0.0911	2.4792	-0.5291	O	2.4135	2.8266	-0.7626
H	4.5771	-0.6299	-0.863	H	4.5383	-1.5323	-0.1499
H	3.926	-0.7017	0.7682	H	3.5682	-1.3688	1.3057
H	3.076	1.0928	-1.5404	H	3.6514	0.4485	-1.1345
H	3.6605	1.5539	0.0577	H	4.0028	0.85	0.5468
H	2.4674	-1.4855	-1.7978	H	2.5356	-1.9307	-1.5136
H	3.1448	-2.6204	-0.645	H	2.6554	-3.1204	-0.2291
H	-0.5758	-0.5702	1.8578	H	-0.9112	0.0587	1.3234
H	-0.8237	0.9561	1.0974	H	-0.6718	1.4062	0.2324
H	-1.4601	-0.2779	-1.065	H	-1.171	0.0153	-1.7304
H	-1.2826	-2.7494	0.7317	H	-1.783	-2.2394	0.2434
H	-1.8161	-2.7303	-0.9436	H	-2.044	-2.2708	-1.493
H	0.5386	-3.4479	-0.7538	H	0.0753	-3.3799	-0.8792
H	0.2952	-2.0404	-1.7731	H	0.3083	-2.013	-1.9564
H	-3.1563	-1.0713	1.3625	H	-3.5957	-0.4123	-1.3455
H	-4.4811	1.0129	0.8354	H	-3.4961	-1.1049	1.0968
H	-2.8919	1.3523	1.4873	H	-3.1773	0.5927	1.5199
H	-2.1606	1.7668	-0.6266	H	-5.3648	0.0716	1.6211
H	0.6635	-2.4151	2.0202	H	-0.1847	-2.0891	1.8573
H	2.0129	-3.2868	1.3081	H	0.9826	-3.3497	1.4687

H	2.279	-1.7138	2.0722	H	1.5187	-1.8365	2.2101
H	-5.0528	-0.959	-0.2991	H	-4.2147	1.9094	-1.1059
H	-3.9249	-2.2639	-0.6252	H	-2.6986	1.8185	-2.0032
H	-3.8672	-0.785	-1.6042	H	-2.6947	2.3082	-0.2984
H	-0.2338	3.4484	-0.4676	H	2.2279	3.7689	-0.5713
3-5	X	Y	Z	3-6	X	Y	Z
	axis(Å)	axis(Å)	axis(Å)		axis(Å)	axis(Å)	axis(Å)
C	3.5907	-0.9467	-0.181	C	3.375	-1.4711	-0.3348
C	3.1681	0.4942	-0.4399	C	3.2547	0.0334	-0.5463
C	1.7501	0.7875	-0.0225	C	1.9545	0.6085	-0.0462
C	0.82	-0.1675	0.2244	C	0.8584	-0.1359	0.2388
C	1.1506	-1.6598	0.0921	C	0.8571	-1.6642	0.0671
C	2.4998	-1.9029	-0.6411	C	2.0839	-2.1638	-0.7468
C	-0.6093	0.1344	0.6532	C	-0.4532	0.4438	0.7495
C	-1.6842	-0.6	-0.1794	C	-1.6651	-0.0176	-0.0866
C	-1.3695	-2.1054	-0.243	C	-1.718	-1.5513	-0.1431
C	0.0523	-2.3701	-0.7333	C	-0.4118	-2.1213	-0.6978
C	-3.1227	-0.3413	0.3779	C	-2.9899	0.6399	0.4071
C	-3.466	1.1532	0.5152	C	-4.1707	0.3872	-0.546
O	-3.2992	1.8205	-0.7275	O	-3.8622	0.802	-1.8696
C	1.2398	-2.2845	1.5043	C	0.8928	-2.3268	1.4649
C	-4.1949	-1.0166	-0.492	C	-3.3976	0.2366	1.8275
C	1.4612	2.2291	0.1639	C	1.9853	2.0733	0.1755
O	0.9254	2.7548	1.1217	O	1.6063	2.677	1.1614
O	1.8966	2.949	-0.8839	O	2.5232	2.7117	-0.8773
H	4.5229	-1.1573	-0.7179	H	4.2119	-1.8583	-0.9273
H	3.8043	-1.091	0.8842	H	3.609	-1.6864	0.714
H	3.2692	0.7096	-1.5114	H	3.3446	0.2518	-1.6182
H	3.8649	1.1572	0.0877	H	4.1024	0.5196	-0.0478
H	2.3704	-1.7745	-1.7247	H	1.9269	-1.98	-1.8187
H	2.8333	-2.9381	-0.4957	H	2.1988	-3.2496	-0.6382
H	-0.7196	-0.1267	1.713	H	-0.5686	0.1475	1.7977
H	-0.8094	1.2043	0.5777	H	-0.4495	1.5368	0.7395
H	-1.6363	-0.2089	-1.2058	H	-1.4904	0.3408	-1.1117
H	-1.5246	-2.5672	0.7388	H	-1.9132	-1.9725	0.8485
H	-2.0535	-2.6078	-0.9356	H	-2.5367	-1.8816	-0.7915
H	0.2296	-3.4534	-0.7397	H	-0.4742	-3.2171	-0.7009
H	0.1098	-2.0449	-1.7815	H	-0.3365	-1.8169	-1.7511
H	-3.1909	-0.7813	1.3819	H	-2.8143	1.725	0.411
H	-4.5052	1.2818	0.8376	H	-4.4459	-0.6714	-0.5763
H	-2.834	1.6387	1.2649	H	-5.056	0.944	-0.2193
H	-3.4779	2.7632	-0.5691	H	-3.6345	1.7468	-1.8343
H	0.2985	-2.2081	2.0577	H	0.0128	-2.0818	2.0679

H	1.4931	-3.3494	1.4465	H	0.9295	-3.4191	1.3802
H	2.0057	-1.7949	2.1157	H	1.7692	-2.0101	2.041
H	-5.201	-0.7443	-0.1542	H	-4.3004	0.7776	2.133
H	-4.1301	-2.107	-0.432	H	-2.6196	0.4781	2.5567
H	-4.1003	-0.7236	-1.5428	H	-3.6174	-0.833	1.8987
H	1.6425	3.8659	-0.6537	H	2.489	3.6547	-0.616
3-7	X axis(Å)	Y axis(Å)	Z axis(Å)	3-8	X axis(Å)	Y axis(Å)	Z axis(Å)
C	3.3776	-1.4709	-0.342	C	3.5555	-1.3215	-0.1976
C	3.2575	0.0333	-0.5564	C	3.3696	0.1683	-0.4592
C	1.9595	0.6083	-0.0529	C	2.015	0.6856	-0.0482
C	0.8638	-0.1339	0.2378	C	0.9446	-0.1083	0.1981
C	0.8605	-1.6619	0.0706	C	1.0321	-1.6384	0.0696
C	2.0842	-2.1643	-0.7465	C	2.3275	-2.0926	-0.6603
C	-0.4453	0.4514	0.7493	C	-0.4209	0.4144	0.6218
C	-1.6607	-0.0121	-0.0804	C	-1.5576	-0.1305	-0.2672
C	-1.7152	-1.5461	-0.1306	C	-1.5287	-1.6659	-0.2867
C	-0.4117	-2.1199	-0.6881	C	-0.1659	-2.1795	-0.7528
C	-2.9834	0.6486	0.4158	C	-2.9369	0.4681	0.1324
C	-4.1695	0.3916	-0.5286	C	-4.0012	0.178	-0.9398
O	-3.8542	0.8212	-1.8454	O	-5.1949	0.9069	-0.6778
C	0.9009	-2.3202	1.4702	C	1.0216	-2.2634	1.4849
C	-3.3834	0.2539	1.8409	C	-3.4383	0.0175	1.5108
C	1.9893	2.0726	0.1657	C	1.9576	2.155	0.1325
O	1.649	2.6728	1.1677	O	1.5022	2.7625	1.0828
O	2.4794	2.7123	-0.9093	O	2.5062	2.7931	-0.915
H	4.2118	-1.8601	-0.9372	H	4.4437	-1.6789	-0.7313
H	3.6161	-1.6839	0.7063	H	3.7402	-1.4965	0.8684
H	3.3436	0.2496	-1.629	H	3.5083	0.3632	-1.5304
H	4.1068	0.5208	-0.062	H	4.1612	0.7122	0.0708
H	1.923	-1.9839	-1.8183	H	2.2224	-1.9454	-1.7441
H	2.1991	-3.2499	-0.6349	H	2.4922	-3.1675	-0.5142
H	-0.5576	0.16	1.7992	H	-0.581	0.1396	1.67
H	-0.4381	1.5447	0.7346	H	-0.4716	1.5056	0.5816
H	-1.4893	0.3417	-1.1075	H	-1.3498	0.2141	-1.2915
H	-1.9071	-1.9632	0.8634	H	-1.7566	-2.0737	0.7036
H	-2.5365	-1.8783	-0.7746	H	-2.2931	-2.0533	-0.9691
H	-0.4756	-3.2157	-0.6871	H	-0.1718	-3.2769	-0.7303
H	-0.3399	-1.8193	-1.7427	H	-0.0463	-1.8964	-1.8079
H	-2.8074	1.7336	0.4109	H	-2.8232	1.5598	0.1869
H	-4.4398	-0.6684	-0.5598	H	-3.6461	0.4646	-1.9351
4-1	X axis(Å)	Y axis(Å)	Z axis(Å)	4-2	X axis(Å)	Y axis(Å)	Z axis(Å)

C	-2.8328	2.3204	-0.3816	C	3.1734	-1.9746	-0.4265
C	-2.97	0.8263	-0.3176	C	3.1453	-0.5095	-0.0984
C	-1.9228	-0.0239	-0.3179	C	2.0138	0.2202	-0.0501
C	-0.4874	0.4622	-0.4042	C	0.6457	-0.3733	-0.3128
C	-0.346	1.937	0.1035	C	0.634	-1.9205	-0.0727
C	-1.3985	2.7979	-0.6374	C	1.8139	-2.5335	-0.8679
C	0.5763	-0.4306	0.2715	C	-0.5338	0.2855	0.4337
C	2.0064	0.0687	-0.0513	C	-1.8856	-0.2777	-0.0693
C	2.1857	1.5518	0.3207	C	-1.932	-1.8143	0.0226
C	1.0734	2.4405	-0.245	C	-0.7039	-2.4834	-0.6046
C	3.1322	-0.7775	0.5482	C	-3.1207	0.3377	0.5914
C	2.9993	-1.5561	1.6378	C	-3.1334	0.8726	1.8261
C	4.4602	-0.7089	-0.1695	C	-4.3835	0.321	-0.237
O	4.322	-1.2588	-1.4704	O	-4.2159	1.1744	-1.3587
C	-0.5703	2.0826	1.6325	C	0.7858	-2.3116	1.4218
H	-0.2546	0.4553	-1.4811	H	0.4666	-0.2013	-1.3863
C	-2.1967	-1.4832	-0.3657	C	2.1802	1.668	0.2126
O	-1.5888	-2.2639	-1.0813	O	2.8502	2.1308	1.1221
O	-3.1802	-1.8064	0.513	O	1.5137	2.3706	-0.737
C	-3.4894	-3.1993	0.5442	C	1.6355	3.7854	-0.5959
H	-3.4831	2.7094	-1.1737	H	3.9067	-2.1535	-1.2214
H	-3.2018	2.7425	0.5607	H	3.529	-2.5201	0.4556
H	-3.9896	0.4464	-0.2905	H	4.1087	-0.0403	0.0967
H	-1.2042	2.7592	-1.7182	H	1.6794	-2.3229	-1.9379
H	-1.3113	3.8533	-0.3502	H	1.8229	-3.6264	-0.7715
H	0.4974	-1.4629	-0.0866	H	-0.5394	1.3689	0.2686
H	0.3963	-0.4667	1.3514	H	-0.4139	0.1433	1.5131
H	2.1009	-0.0055	-1.1444	H	-1.9313	-0.0154	-1.1364
H	3.1438	1.924	-0.0622	H	-2.0325	-2.1259	1.0692
H	2.236	1.6635	1.4104	H	-2.8246	-2.1954	-0.4887
H	1.1889	2.485	-1.3363	H	-0.7533	-2.3445	-1.6929
H	1.2132	3.4659	0.1196	H	-0.757	-3.5656	-0.4313
H	3.8309	-2.1417	2.0208	H	-4.039	1.2982	2.2504
H	2.0705	-1.6378	2.1914	H	-2.2563	0.8988	2.4634
H	4.8096	0.3234	-0.2601	H	-4.6107	-0.6876	-0.5938
H	5.2409	-1.2727	0.3524	H	-5.2538	0.6719	0.3277
H	3.8324	-2.0935	-1.3696	H	-3.8786	2.0192	-1.0147
H	-0.5371	3.1388	1.9248	H	0.8511	-3.4011	1.5268
H	-1.5367	1.6855	1.9567	H	1.6834	-1.8861	1.8801
H	0.1898	1.5659	2.2241	H	-0.0581	-1.9844	2.0346
H	-3.8444	-3.536	-0.4349	H	1.2204	4.1127	0.3625
H	-2.6169	-3.779	0.8614	H	2.682	4.092	-0.6909
H	-4.2899	-3.3524	1.2734	H	1.0627	4.2565	-1.3994

4-3	X axis(Å)	Y axis(Å)	Z axis(Å)	4-4	X axis(Å)	Y axis(Å)	Z axis(Å)
C	-2.7987	2.3179	0.1526	C	-2.7428	2.4212	-0.2863
C	-2.8931	0.8244	0.0284	C	-2.9565	0.9351	-0.2579
C	-1.8446	0.0291	-0.2667	C	-1.9558	0.0325	-0.3128
C	-0.4559	0.5839	-0.5228	C	-0.4998	0.4449	-0.4286
C	-0.2575	1.9833	0.1535	C	-0.2654	1.8971	0.1102
C	-1.4399	2.8883	-0.2716	C	-1.2937	2.8307	-0.5744
C	0.7243	-0.3469	-0.1685	C	0.5314	-0.523	0.1913
C	2.063	0.2603	-0.6396	C	1.9745	-0.078	-0.1389
C	2.281	1.6866	-0.1054	C	2.2468	1.3851	0.2492
C	1.0706	2.5919	-0.3567	C	1.1673	2.3375	-0.2727
C	3.2649	-0.6365	-0.3565	C	3.024	-1.0129	0.4534
C	4.0822	-1.0198	-1.3552	C	3.0875	-1.308	1.7646
C	3.5408	-1.0668	1.0619	C	3.9959	-1.6158	-0.5268
O	2.6614	-2.1193	1.4242	O	4.802	-0.5839	-1.0741
C	-0.2168	1.9116	1.7035	C	-0.4348	2.011	1.6488
H	-0.412	0.732	-1.6138	H	-0.2974	0.4546	-1.5116
C	-2.0911	-1.4213	-0.4711	C	-2.3072	-1.4086	-0.3922
O	-1.6097	-2.0665	-1.3897	O	-1.7676	-2.1964	-1.1532
O	-2.8896	-1.9059	0.514	O	-3.2736	-1.7074	0.5136
C	-3.1455	-3.3059	0.4113	C	-3.6523	-3.0834	0.5178
H	-3.5837	2.7814	-0.4562	H	-3.0609	2.8352	0.6778
H	-3.0078	2.5926	1.1933	H	-3.3952	2.8654	-1.0471
H	-3.8843	0.3989	0.174	H	-3.9933	0.6073	-0.2103
H	-1.4345	3.0038	-1.3643	H	-1.1343	2.8119	-1.6615
H	-1.326	3.8983	0.1418	H	-1.1429	3.8719	-0.2628
H	0.61	-1.3212	-0.6562	H	0.3987	-1.5349	-0.2079
H	0.731	-0.5438	0.9087	H	0.3708	-0.6042	1.2722
H	1.9763	0.3588	-1.7328	H	2.0618	-0.133	-1.2342
H	3.1589	2.1315	-0.5915	H	3.217	1.7003	-0.1558
H	2.5085	1.6725	0.9658	H	2.3318	1.4872	1.3374
H	0.9971	2.7808	-1.436	H	1.2542	2.3942	-1.3659
H	1.2477	3.5672	0.1138	H	1.3679	3.3484	0.1038
H	4.9477	-1.651	-1.1748	H	3.8392	-1.9846	2.1609
H	3.9091	-0.7154	-2.3836	H	2.3933	-0.8801	2.4813
H	4.5664	-1.4334	1.1794	H	4.6567	-2.3519	-0.057
H	3.4129	-0.2422	1.768	H	3.4644	-2.1189	-1.3408
H	2.6078	-2.7163	0.6578	H	5.1544	-0.0812	-0.3201
H	-0.1476	2.9189	2.1309	H	-0.3265	3.0539	1.9691
H	-1.1076	1.4388	2.1274	H	-1.4144	1.6654	1.992
H	0.6402	1.3471	2.0801	H	0.3076	1.4296	2.2016
H	-3.6687	-3.5329	-0.523	H	-4.0604	-3.3725	-0.4558

H	-2.212	-3.8732	0.4812	H	-2.7993	-3.7153	0.7846
H	-3.789	-3.5952	1.2468	H	-4.4317	-3.218	1.273
4-5	X	Y	Z	4-6	X	Y	Z
	axis(Å)	axis(Å)	axis(Å)		axis(Å)	axis(Å)	axis(Å)
C	3.3342	-1.6803	-0.3604	C	3.0164	-2.1923	-0.3565
C	3.1267	-0.2398	0.0092	C	3.1147	-0.7237	-0.0594
C	1.9207	0.3605	0.0134	C	2.0534	0.1061	-0.0491
C	0.6423	-0.3677	-0.3448	C	0.642	-0.3673	-0.3266
C	0.7881	-1.9156	-0.1563	C	0.4854	-1.9022	-0.0576
C	2.0713	-2.3664	-0.8983	C	1.6206	-2.6361	-0.8147
C	-0.6395	0.1347	0.3521	C	-0.4853	0.4136	0.3815
C	-1.8881	-0.5694	-0.2235	C	-1.8717	-0.0512	-0.1197
C	-1.7719	-2.1041	-0.1989	C	-2.0611	-1.5744	-0.0108
C	-0.4473	-2.6006	-0.7873	C	-0.8869	-2.3556	-0.6093
C	-3.1714	-0.0895	0.4453	C	-3.0173	0.6996	0.5511
C	-3.4189	-0.2572	1.7571	C	-3.1737	0.757	1.8861
C	-4.172	0.5847	-0.4553	C	-3.9765	1.4017	-0.374
O	-3.6171	1.7999	-0.9345	O	-4.6581	0.4347	-1.1573
C	0.898	-2.3425	1.3319	C	0.5714	-2.2712	1.4476
H	0.5023	-0.1764	-1.4208	H	0.4982	-0.2033	-1.4067
C	1.9115	1.8082	0.3255	C	2.3462	1.5385	0.1872
O	2.4731	2.3097	1.2864	O	3.0441	1.9581	1.0967
O	1.2275	2.4653	-0.6435	O	1.7585	2.2779	-0.786
C	1.1812	3.8794	-0.4578	C	2.0033	3.6791	-0.6694
H	4.1258	-1.7497	-1.1155	H	3.7454	-2.4543	-1.132
H	3.6983	-2.2159	0.5243	H	3.3044	-2.7478	0.5439
H	4.0204	0.3244	0.2728	H	4.1129	-0.339	0.1454
H	1.9739	-2.1321	-1.9674	H	1.5263	-2.4382	-1.8914
H	2.1957	-3.4547	-0.8352	H	1.5291	-3.723	-0.6957
H	-0.7628	1.2134	0.2006	H	-0.399	1.4871	0.1774
H	-0.5638	-0.0062	1.4365	H	-0.3925	0.3089	1.4684
H	-1.9383	-0.285	-1.285	H	-1.8993	0.1921	-1.1923
H	-2.5986	-2.5427	-0.7727	H	-2.9801	-1.8704	-0.5327
H	-1.8829	-2.4874	0.8219	H	-2.2045	-1.8718	1.0345
H	-0.4572	-2.4156	-1.8697	H	-0.9049	-2.2271	-1.6998
H	-0.3843	-3.6889	-0.6626	H	-1.0365	-3.4267	-0.4242
H	-4.3425	0.0883	2.2128	H	-3.9936	1.305	2.3417
H	-2.7065	-0.7467	2.4146	H	-2.4908	0.2544	2.5645
H	-4.4155	-0.054	-1.3103	H	-4.7238	1.9892	0.1696
H	-5.1077	0.8178	0.0635	H	-3.4404	2.0831	-1.0423
H	-3.2855	2.2778	-0.1551	H	-5.0212	-0.2178	-0.5344
H	1.0647	-3.4235	1.408	H	0.5254	-3.3589	1.5776
H	1.7234	-1.8484	1.8526	H	1.499	-1.9267	1.914

H	-0.0051	-2.119	1.9057	H	-0.2455	-1.846	2.0364
H	0.6778	4.1267	0.4821	H	1.6069	4.0605	0.2769
H	2.1903	4.3027	-0.4809	H	3.0738	3.8901	-0.7553
H	0.606	4.3107	-1.2817	H	1.4844	4.183	-1.4895
4-7	X	Y	Z	4-8	X	Y	Z
	axis(Å)	axis(Å)	axis(Å)		axis(Å)	axis(Å)	axis(Å)
C	3.2764	-1.7939	-0.4479	C	-2.6381	2.5024	0.0302
C	3.1472	-0.3479	-0.0637	C	-2.9021	1.0241	0.0493
C	1.97	0.3051	-0.0093	C	-1.9609	0.091	-0.2008
C	0.6485	-0.3644	-0.3233	C	-0.5304	0.4589	-0.5491
C	0.7323	-1.9168	-0.1407	C	-0.1516	1.8808	-0.0122
C	1.9634	-2.4231	-0.9335	C	-1.242	2.8738	-0.484
C	-0.5894	0.1965	0.4092	C	0.5538	-0.5672	-0.1508
C	-1.8871	-0.4468	-0.1289	C	1.9339	-0.1551	-0.71
C	-1.831	-1.9869	-0.0779	C	2.3249	1.2772	-0.3108
C	-0.5569	-2.5445	-0.722	C	1.214	2.2867	-0.6171
C	-3.1106	0.1692	0.5486	C	3.0072	-1.1876	-0.3769
C	-3.7058	-0.3387	1.643	C	3.5128	-1.983	-1.3381
C	-3.6355	1.436	-0.083	C	3.4648	-1.3327	1.0517
O	-4.1809	1.128	-1.3566	O	4.4069	-0.3159	1.3546
C	0.8836	-2.3495	1.3423	C	-0.0582	1.9414	1.536
H	0.4835	-0.1662	-1.3947	H	-0.5156	0.5049	-1.65
C	2.0384	1.7491	0.3118	C	-2.3771	-1.3333	-0.2637
O	2.6584	2.217	1.2535	O	-2.007	-2.1089	-1.1312
O	1.3496	2.4447	-0.6267	O	-3.1856	-1.6337	0.7848
C	1.3745	3.8578	-0.4288	C	-3.6113	-2.9955	0.8118
H	4.0315	-1.8928	-1.2363	H	-3.39	2.9955	-0.5968
H	3.6546	-2.3496	0.4183	H	-2.7751	2.8917	1.046
H	4.0745	0.1741	0.1684	H	-3.9282	0.7298	0.2619
H	1.8334	-2.1837	-1.998	H	-1.2669	2.8912	-1.5824
H	2.0421	-3.5159	-0.8747	H	-1.0004	3.8967	-0.1689
H	-0.656	1.2801	0.263	H	0.3124	-1.5565	-0.5555
H	-0.5016	0.0478	1.4922	H	0.5818	-0.6874	0.9378
H	-1.9517	-0.1956	-1.1978	H	1.8226	-0.1375	-1.8052
H	-1.8943	-2.3532	0.9515	H	3.2338	1.575	-0.8489
H	-2.7024	-2.4015	-0.6008	H	2.5711	1.3331	0.7543
H	-0.6027	-2.3592	-1.8034	H	1.1205	2.3817	-1.7071
H	-0.5386	-3.6345	-0.5974	H	1.5148	3.275	-0.2473
H	-4.572	0.1406	2.0915	H	4.2652	-2.7356	-1.1199
H	-3.3482	-1.2332	2.1411	H	3.1838	-1.9103	-2.3709
H	-4.4215	1.9045	0.5187	H	2.6308	-1.2615	1.7548
H	-2.8367	2.1725	-0.2114	H	3.9486	-2.3003	1.2242
H	-4.7801	0.3734	-1.2251	H	5.0239	-0.277	0.604

H	0.9925	-3.4382	1.4132	H	0.1523	2.9654	1.8664
H	1.7579	-1.9035	1.8253	H	-0.9831	1.6251	2.0273
H	0.0217	-2.0747	1.9556	H	0.7353	1.3068	1.939
H	0.9186	4.1188	0.5314	H	-4.1911	-3.2346	-0.0853
H	2.4002	4.2354	-0.4872	H	-2.7505	-3.6648	0.9076
H	0.7888	4.322	-1.227	H	-4.2544	-3.1323	1.6856
5-1	X axis(Å)	Y axis(Å)	Z axis(Å)	5-2	X axis(Å)	Y axis(Å)	Z axis(Å)
C	3.7578	0.1774	-0.2218	C	3.7389	-0.3445	-0.1466
C	2.949	1.4674	-0.3158	C	3.15	1.0583	-0.2113
C	1.5209	1.3324	0.1618	C	1.7041	1.1508	0.2361
C	0.9482	0.125	0.3897	C	0.9078	0.0575	0.3594
C	1.6311	-1.2063	0.055	C	1.4065	-1.3602	0.038
C	2.9438	-0.9953	-0.7494	C	2.7596	-1.3512	-0.7241
C	-0.455	-0.0224	0.9455	C	-0.5451	0.1249	0.8107
C	-1.357	-0.7259	-0.0805	C	-1.5234	-0.59	-0.1455
C	-0.775	-2.1321	-0.3368	C	-1.0545	-2.0373	-0.3772
C	0.6782	-2.0605	-0.8274	C	0.3886	-2.0885	-0.8736
C	-2.8447	-0.7502	0.3745	C	-2.9946	-0.54	0.3804
C	-3.408	0.6566	0.6688	C	-3.4826	0.8855	0.6988
O	-3.1825	1.5519	-0.4121	O	-3.2847	1.742	-0.4168
C	1.9668	-1.9669	1.357	C	1.5871	-2.1438	1.3588
C	-3.7386	-1.4269	-0.6763	C	-3.9702	-1.1811	-0.62
C	0.8006	2.6508	0.3316	C	1.2788	2.5715	0.522
O	-0.3925	2.655	-0.4509	O	0.9213	3.1961	-0.7005
H	4.6822	0.2823	-0.8013	H	3.9866	-0.6007	0.8899
H	4.0577	-0.0031	0.8171	H	4.6799	-0.3731	-0.708
H	2.9339	1.8126	-1.3573	H	3.2159	1.4344	-1.2402
H	3.4652	2.2368	0.2713	H	3.7783	1.7112	0.4068
H	2.7172	-0.8003	-1.8066	H	2.5987	-1.0996	-1.7815
H	3.555	-1.9063	-0.7342	H	3.2113	-2.3511	-0.7153
H	-0.4253	-0.5961	1.8798	H	-0.6231	-0.3103	1.8147
H	-0.8638	0.9449	1.237	H	-0.8662	1.1619	0.9069
H	-1.3063	-0.1721	-1.0292	H	-1.4868	-0.0701	-1.1137
H	-0.8341	-2.737	0.5758	H	-1.1611	-2.6229	0.5431
H	-1.3555	-2.6576	-1.102	H	-1.6785	-2.5258	-1.1332
H	1.0724	-3.0798	-0.9283	H	0.6834	-3.1382	-1.001
H	0.6525	-1.6435	-1.8441	H	0.4086	-1.6424	-1.8779
H	-2.9245	-1.3364	1.2995	H	-3.0542	-1.1186	1.3119
H	-4.4894	0.6055	0.8369	H	-4.5493	0.8828	0.9492
H	-2.978	1.0848	1.5798	H	-2.9503	1.3021	1.5595
H	-2.2829	1.9278	-0.3086	H	-3.6412	2.6145	-0.1756
H	1.0714	-2.2605	1.9136	H	0.6481	-2.2594	1.9092

H	2.5202	-2.8882	1.1413	H	1.9728	-3.1518	1.1673
H	2.5824	-1.3607	2.0308	H	2.2903	-1.6431	2.0334
H	-4.7949	-1.3581	-0.3937	H	-5.0075	-1.0539	-0.2908
H	-3.5093	-2.4924	-0.7702	H	-3.8017	-2.2581	-0.7098
H	-3.6213	-0.9611	-1.6604	H	-3.8742	-0.7332	-1.6146
H	0.5448	2.8283	1.3809	H	0.4428	2.6526	1.2196
H	1.4144	3.4921	-0.0062	H	2.0969	3.1423	0.9741
H	-0.1327	2.3401	-1.3358	H	0.2929	2.5952	-1.1393
5-3	X	Y	Z	5-4	X	Y	Z
	axis(Å)	axis(Å)	axis(Å)		axis(Å)	axis(Å)	axis(Å)
C	3.6187	-0.9022	-0.3709	C	3.6812	-0.9864	-0.27
C	3.3557	0.5919	-0.2416	C	3.4045	0.4482	-0.7002
C	1.9897	0.944	0.3179	C	2.0232	0.9586	-0.3371
C	0.9787	0.0406	0.3905	C	1.0274	0.1337	0.0747
C	1.1328	-1.4072	-0.1132	C	1.1988	-1.3952	0.1382
C	2.4106	-1.5962	-0.9749	C	2.4863	-1.8689	-0.5894
C	-0.3975	0.3542	0.963	C	-0.3431	0.6186	0.5252
C	-1.5372	-0.0098	-0.0095	C	-1.4782	-0.0608	-0.2634
C	-1.4387	-1.4907	-0.4023	C	-1.3731	-1.5875	-0.1171
C	-0.0708	-1.8008	-1.0102	C	0.0014	-2.0902	-0.5644
C	-2.9313	0.399	0.5574	C	-2.8716	0.5135	0.1197
C	-4.0524	0.2907	-0.4893	C	-3.9578	0.0412	-0.8604
O	-3.7345	1.0748	-1.6307	O	-5.1558	0.7764	-0.6403
C	1.2124	-2.3591	1.1036	C	1.2752	-1.8449	1.6162
C	-3.3433	-0.3686	1.8171	C	-3.2951	0.215	1.5642
C	1.9138	2.3818	0.7742	C	1.9059	2.4553	-0.4962
O	1.8301	3.2188	-0.3693	O	2.5094	3.0858	0.6228
H	4.4992	-1.0657	-1.0032	H	4.5715	-1.3592	-0.7895
H	3.8568	-1.3284	0.6103	H	3.9091	-1.02	0.8015
H	3.4552	1.0635	-1.2276	H	3.5221	0.5266	-1.7887
H	4.1427	1.0157	0.3941	H	4.1716	1.0905	-0.2507
H	2.2528	-1.1882	-1.9829	H	2.3347	-1.857	-1.6775
H	2.6281	-2.6632	-1.1094	H	2.7154	-2.9091	-0.3259
H	-0.5038	-0.1934	1.906	H	-0.4408	0.4094	1.5964
H	-0.5074	1.4102	1.2176	H	-0.4521	1.7017	0.4362
H	-1.3713	0.5835	-0.9204	H	-1.3188	0.1804	-1.3252
H	-1.6118	-2.1377	0.464	H	-1.5544	-1.8929	0.9188
H	-2.2067	-1.7424	-1.1414	H	-2.1355	-2.0827	-0.7284
H	-0.0235	-2.8702	-1.2536	H	0.0525	-3.1754	-0.4071
H	-0.0055	-1.267	-1.9686	H	0.0725	-1.9355	-1.6501
H	-2.8562	1.4618	0.8278	H	-2.8161	1.608	0.0346
H	-4.2123	-0.7443	-0.8067	H	-3.6453	0.2115	-1.8958
H	-4.9942	0.6676	-0.0755	H	-4.1827	-1.0219	-0.73

H	-4.4749	0.9847	-2.2549	H	-5.8112	0.4535	-1.2821
H	0.2992	-2.346	1.7067	H	0.3519	-1.6397	2.1667
H	1.3681	-3.3953	0.7815	H	1.4554	-2.9237	1.6887
H	2.038	-2.093	1.7727	H	2.0843	-1.3369	2.1523
H	-4.2942	0.0154	2.2033	H	-4.2356	0.7223	1.8056
H	-2.6064	-0.2598	2.6174	H	-2.5514	0.5678	2.2839
H	-3.4794	-1.4357	1.6161	H	-3.4504	-0.856	1.7272
H	1.0702	2.605	1.4282	H	2.4263	2.7865	-1.4016
H	2.8118	2.6563	1.3382	H	0.8796	2.8141	-0.5902
H	1.1186	2.8523	-0.923	H	2.173	2.6268	1.4114
5-5	X	Y	Z	5-6	X	Y	Z
	axis(Å)	axis(Å)	axis(Å)		axis(Å)	axis(Å)	axis(Å)
C	3.5254	-1.1044	-0.3933	C	3.7423	-0.8765	-0.1987
C	3.2871	0.349	-0.7815	C	3.4612	0.6198	-0.1856
C	1.9516	0.9088	-0.3315	C	2.061	0.9945	0.2655
C	0.9465	0.1182	0.1223	C	1.0535	0.087	0.339
C	1.0542	-1.4171	0.1474	C	1.2496	-1.3907	-0.0518
C	2.2775	-1.9295	-0.6604	C	2.5768	-1.6227	-0.8236
C	-0.3752	0.6511	0.657	C	-0.3556	0.4208	0.8112
C	-1.583	0.0371	-0.0764	C	-1.4347	-0.0271	-0.1947
C	-1.5343	-1.4954	0.0345	C	-1.2994	-1.5298	-0.4782
C	-0.2095	-2.0455	-0.4993	C	0.1035	-1.8616	-0.9861
C	-2.9286	0.6605	0.4054	C	-2.8596	0.4011	0.259
C	-4.1238	0.2421	-0.4667	C	-3.884	0.2171	-0.8726
O	-3.8817	0.5786	-1.8254	O	-5.1083	0.8498	-0.5193
C	1.193	-1.9009	1.61	C	1.2672	-2.2545	1.2316
C	-3.2567	0.3809	1.8752	C	-3.347	-0.3016	1.5334
C	1.8865	2.4115	-0.461	C	1.9522	2.4584	0.623
O	2.5663	2.9976	0.6388	O	1.9736	3.2228	-0.5734
H	4.3685	-1.5036	-0.969	H	4.6594	-1.0719	-0.7664
H	3.811	-1.1694	0.6628	H	3.9258	-1.2336	0.8211
H	3.3471	0.4444	-1.8733	H	3.6175	1.0254	-1.1933
H	4.1047	0.9496	-0.3646	H	4.2052	1.0938	0.4664
H	2.0661	-1.889	-1.7378	H	2.475	-1.2849	-1.8642
H	2.4761	-2.9835	-0.4291	H	2.8095	-2.6939	-0.8729
H	-0.4209	0.4237	1.728	H	-0.5095	-0.06	1.7835
H	-0.4417	1.7395	0.5947	H	-0.4905	1.4905	0.9832
H	-1.4694	0.2937	-1.1397	H	-1.231	0.5052	-1.1361
H	-2.3487	-1.9459	-0.5431	H	-1.5146	-2.1182	0.4198
H	-1.6712	-1.8155	1.0727	H	-2.023	-1.8418	-1.2391
H	-0.1967	-3.135	-0.3662	H	0.1754	-2.9443	-1.1519
H	-0.1925	-1.8704	-1.5841	H	0.2181	-1.3935	-1.9738
H	-2.8226	1.7488	0.2923	H	-2.8276	1.4748	0.4917

H	-4.318	-0.8328	-0.3992	H	-3.5241	0.6769	-1.7988
H	-5.0288	0.7703	-0.1468	H	-4.0901	-0.8411	-1.061
H	-4.6646	0.3036	-2.3324	H	-5.7239	0.7151	-1.26
H	0.3117	-1.6682	2.2156	H	0.3204	-2.2117	1.7791
H	1.3296	-2.9877	1.652	H	1.4512	-3.3084	0.9926
H	2.0522	-1.4394	2.109	H	2.0498	-1.9313	1.9268
H	-4.1764	0.9009	2.166	H	-4.3106	0.1066	1.8572
H	-2.4658	0.7355	2.5416	H	-2.6491	-0.1622	2.3634
H	-3.4119	-0.6863	2.0609	H	-3.4835	-1.376	1.3759
H	2.3766	2.739	-1.3845	H	1.055	2.7229	1.1833
H	0.8717	2.811	-0.5003	H	2.7988	2.7673	1.2455
H	2.2568	2.5288	1.4326	H	1.3223	2.8153	-1.1695
5-7	X	Y	Z	5-8	X	Y	Z
	axis(Å)	axis(Å)	axis(Å)		axis(Å)	axis(Å)	axis(Å)
C	3.6923	-0.8095	0.1324	C	-3.6926	-0.8724	-0.2518
C	3.3777	0.6034	-0.341	C	-3.3937	0.6185	-0.1767
C	1.9191	0.9996	-0.2135	C	-1.9307	0.9789	-0.3622
C	0.9372	0.095	0.0304	C	-0.9377	0.0561	-0.2791
C	1.217	-1.4166	0.1231	C	-1.2207	-1.4266	0.0331
C	2.6407	-1.7795	-0.3795	C	-2.6668	-1.6529	0.5507
C	-0.5235	0.4681	0.2438	C	0.5377	0.3794	-0.4811
C	-1.453	-0.2904	-0.7197	C	1.4132	-0.1144	0.6859
C	-1.2514	-1.8066	-0.5518	C	1.2076	-1.6224	0.8972
C	0.2119	-2.1953	-0.7681	C	-0.2661	-1.9397	1.1439
C	-2.9521	0.1021	-0.5917	C	2.9209	0.2381	0.5383
C	-3.5231	-0.0578	0.8252	C	3.5606	-0.2762	-0.76
O	-4.9296	0.1588	0.8012	O	4.9665	-0.0576	-0.7192
C	1.0828	-1.8759	1.5941	C	-1.0212	-2.2595	-1.2553
C	-3.1961	1.53	-1.1049	C	3.1543	1.7502	0.6828
C	1.7119	2.4839	-0.3981	C	-1.7417	2.4495	-0.6535
O	2.0593	3.1511	0.8053	O	-1.9525	3.1832	0.5435
H	4.6832	-1.1054	-0.2312	H	-4.6986	-1.0644	0.1391
H	3.7413	-0.8371	1.2269	H	-3.6969	-1.2029	-1.2967
H	3.6676	0.7027	-1.395	H	-3.7215	1.0039	0.7973
H	4.006	1.2993	0.2283	H	-4.0035	1.1201	-0.9381
H	2.6712	-1.7672	-1.4777	H	-2.7474	-1.3409	1.6012
H	2.9048	-2.8014	-0.0796	H	-2.9187	-2.7207	0.5304
H	-0.785	0.238	1.2833	H	0.8607	-0.0797	-1.4225
H	-0.6905	1.5408	0.1409	H	0.7039	1.4501	-0.5991
H	-1.1445	-0.0406	-1.7459	H	1.0579	0.3852	1.5997
H	-1.5737	-2.1392	0.44	H	1.5673	-2.1951	0.0366
H	-1.8714	-2.3455	-1.2786	H	1.7913	-1.9589	1.7626
H	0.3224	-3.275	-0.604	H	-0.3816	-3.0243	1.2673

H	0.448	-2.0216	-1.8272	H	-0.5465	-1.4913	2.1072
H	-3.5274	-0.5557	-1.2584	H	3.4555	-0.2263	1.3789
H	-3.3529	-1.0654	1.2132	H	3.3991	-1.3497	-0.8871
H	-3.0818	0.6655	1.5181	H	3.1632	0.2459	-1.636
H	-5.2525	0.0484	1.7119	H	5.3336	-0.3956	-1.5539
H	0.0685	-1.7472	1.9843	H	0.0074	-2.2176	-1.627
H	1.3309	-2.9386	1.697	H	-1.2555	-3.3159	-1.0796
H	1.7511	-1.3141	2.2559	H	-1.6658	-1.9084	-2.0686
H	-4.2685	1.7391	-1.1822	H	4.2234	1.9742	0.7624
H	-2.7655	1.6654	-2.1026	H	2.6729	2.1351	1.588
H	-2.7601	2.2813	-0.4392	H	2.7635	2.3057	-0.1754
H	2.3527	2.864	-1.2013	H	-0.7594	2.7107	-1.0482
H	0.6918	2.7598	-0.671	H	-2.4664	2.7913	-1.4003
H	1.6526	2.645	1.529	H	-1.4286	2.7403	1.2329

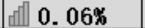
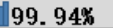

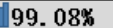
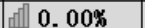
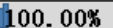
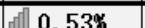

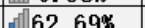
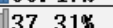
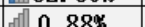
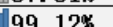
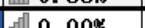
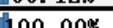
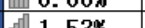
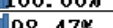
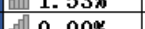
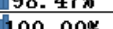
Functional mPW1PW91	Solvent? PCI		Basis Set 6-311+G(d,p)		Type of Data Unscaled Shifts	
	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	 0.06%	 99.94%	-	-	-	-
sDP4+ (C data)	 0.92%	 99.08%	-	-	-	-
sDP4+ (all data)	 0.00%	 100.00%	-	-	-	-
uDP4+ (H data)	 0.53%	 99.47%	-	-	-	-
uDP4+ (C data)	 62.69%	 37.31%	-	-	-	-
uDP4+ (all data)	 0.88%	 99.12%	-	-	-	-
DP4+ (H data)	 0.00%	 100.00%	-	-	-	-
DP4+ (C data)	 1.53%	 98.47%	-	-	-	-
DP4+ (all data)	 0.00%	 100.00%	-	-	-	-

Figure S6: DP4⁺ results of candidate(7*R*,10*R*)-1 (Isomer 1) and (7*R*,11*S*)-1 (Isomer 2).



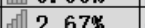
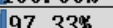
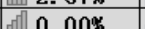
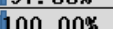
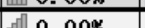
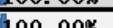
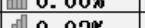
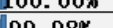
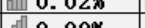
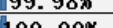


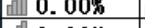
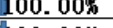
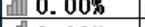
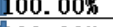
Functional mPW1PW91	Solvent? PCI		Basis Set 6-311+G(d,p)		Type of Data Unscaled Shifts	
	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	 0.00%	 100.00%	-	-	-	-
sDP4+ (C data)	 2.67%	 97.33%	-	-	-	-
sDP4+ (all data)	 0.00%	 100.00%	-	-	-	-
uDP4+ (H data)	 0.00%	 100.00%	-	-	-	-
uDP4+ (C data)	 0.02%	 99.98%	-	-	-	-
uDP4+ (all data)	 0.00%	 100.00%	-	-	-	-
DP4+ (H data)	 0.00%	 100.00%	-	-	-	-
DP4+ (C data)	 0.00%	 100.00%	-	-	-	-
DP4+ (all data)	 0.00%	 100.00%	-	-	-	-

Figure S7: DP4⁺ results of candidate(7*R*,10*R*,11*R*)-3 (Isomer 1) and (7*R*,10*R*,11*S*)-3 (Isomer 2).

Functional	Solvent?		Basis Set		Type of Data	
mPW1PW91	PCI		6-311+G(d,p)		Unscaled Shifts	
	Isomer 1	Isomer 2	Isomer 3	Isomer 4	Isomer 5	Isomer 6
sDP4+ (H data)	0.00%	100.00%	-	-	-	-
sDP4+ (C data)	62.34%	37.66%	-	-	-	-
sDP4+ (all data)	0.00%	100.00%	-	-	-	-
uDP4+ (H data)	0.00%	100.00%	-	-	-	-
uDP4+ (C data)	0.20%	99.80%	-	-	-	-
uDP4+ (all data)	0.00%	100.00%	-	-	-	-
DP4+ (H data)	0.00%	100.00%	-	-	-	-
DP4+ (C data)	0.33%	99.67%	-	-	-	-
DP4+ (all data)	0.00%	100.00%	-	-	-	-

Figure S8: DP4⁺ results of candidate(7S,10S,11S)-5 (Isomer 1) and (7R,10R,11S)-5 (Isomer 2).

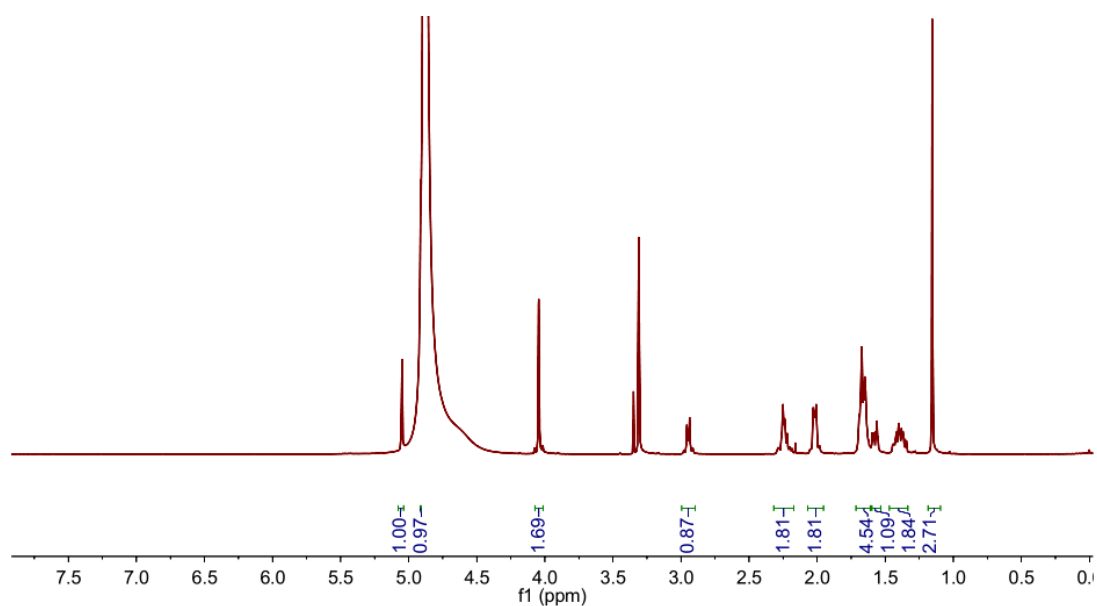


Figure S9: ¹H NMR (500 MHz) spectrum of 1 in CD₃OD.

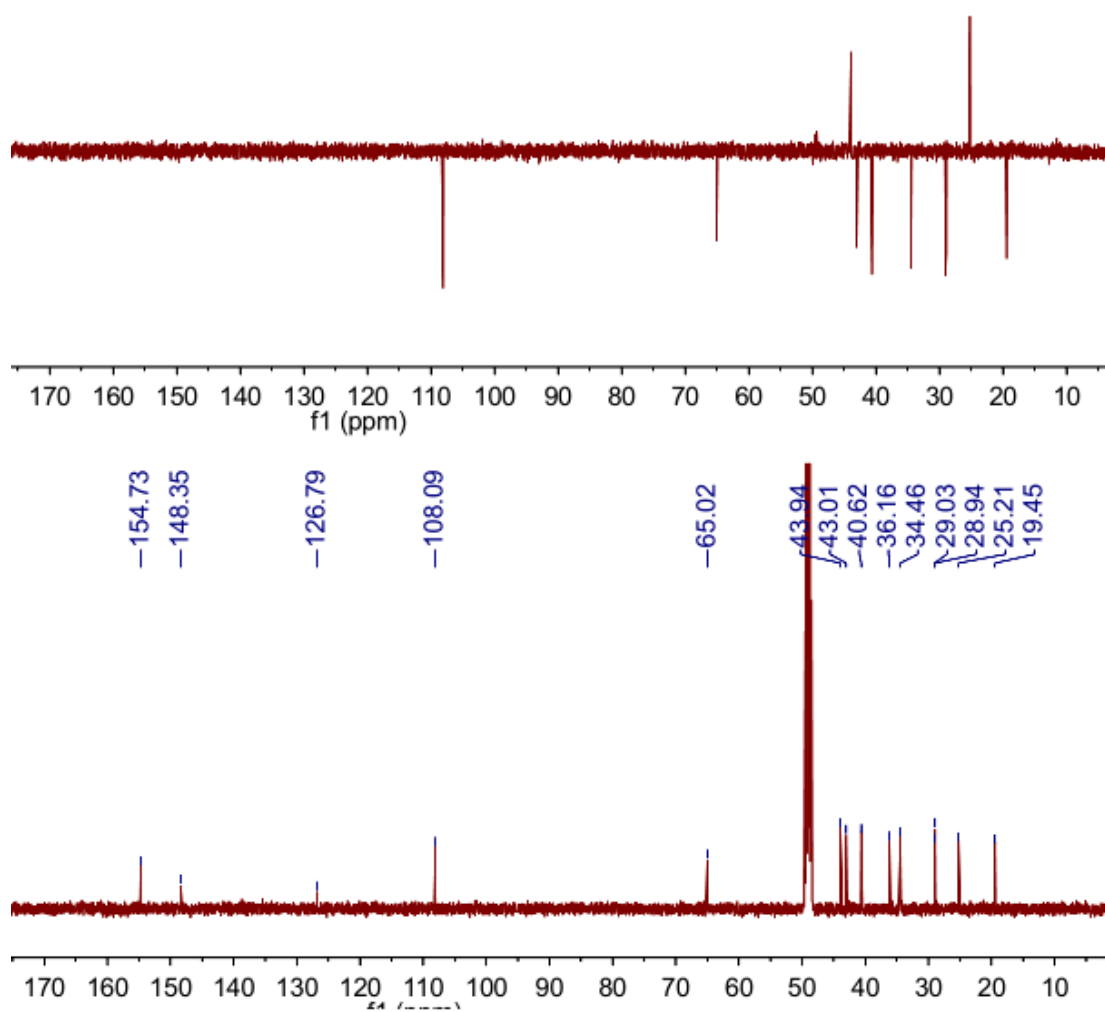


Figure S10: ^{13}C NMR and DEPT (125 MHz) spectra of **1** in CD_3OD .

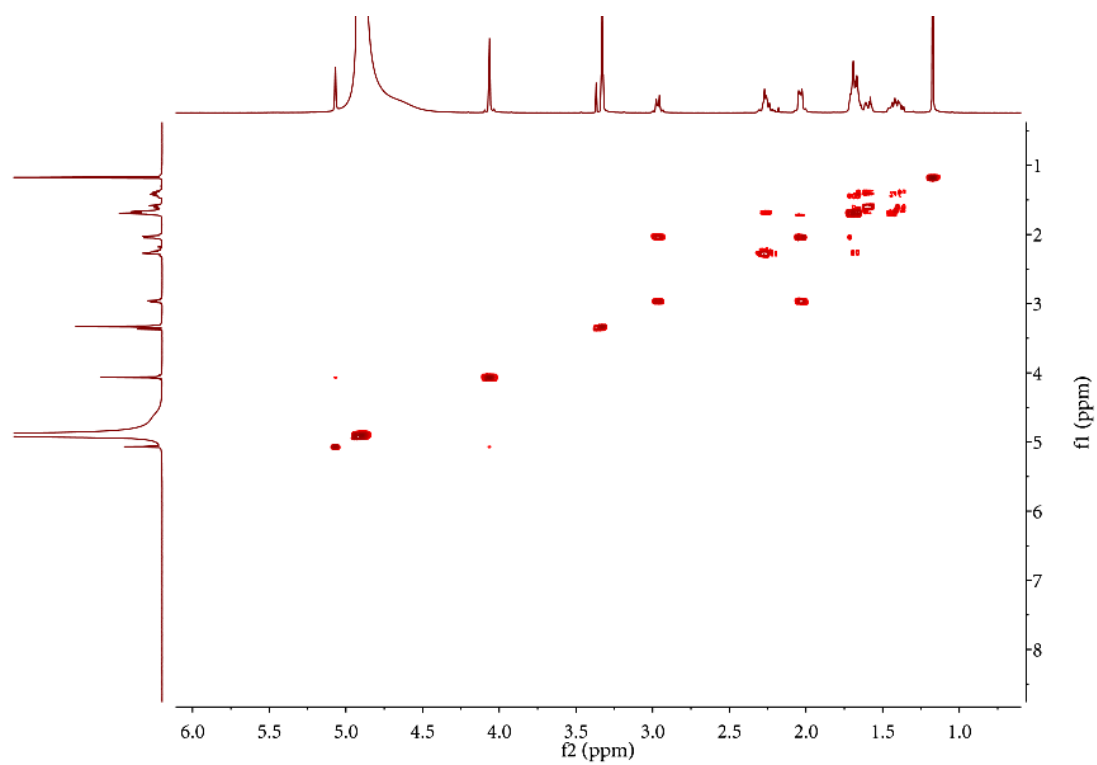


Figure S11: ^1H - ^1H COSY (500 MHz) spectrum of **1** in CD_3OD .

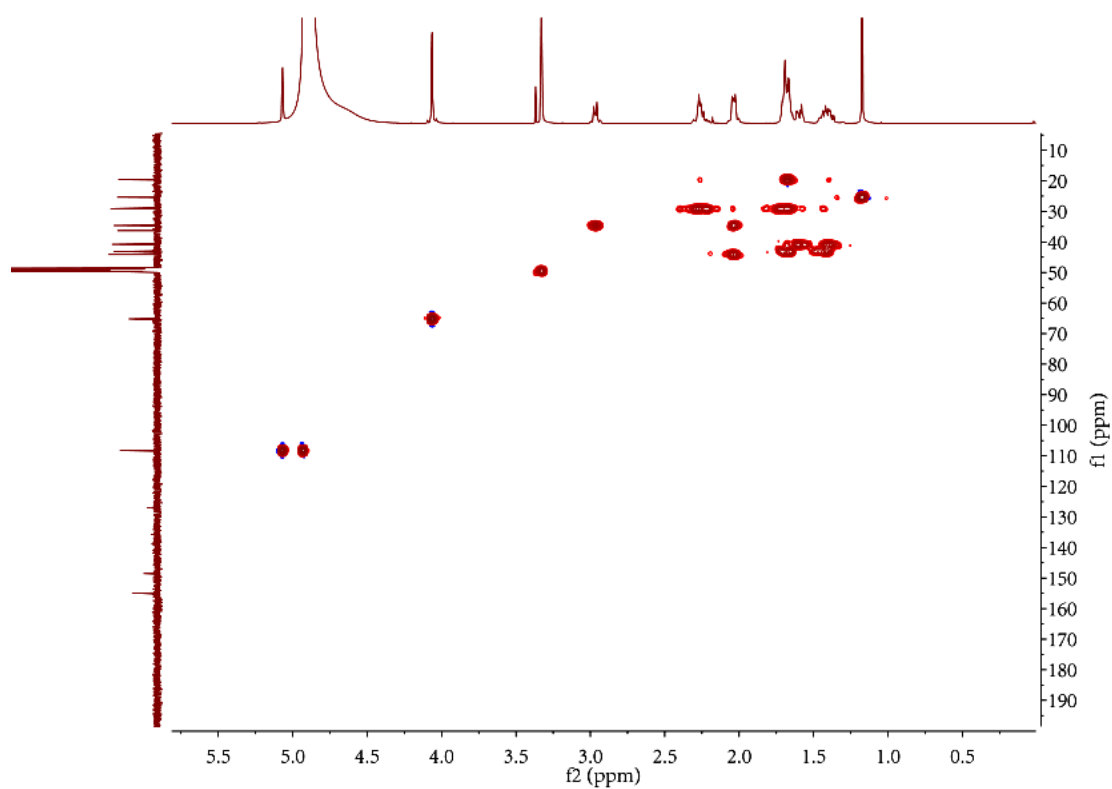


Figure S12: HSQC (500 MHz) spectrum of **1** in CD_3OD .

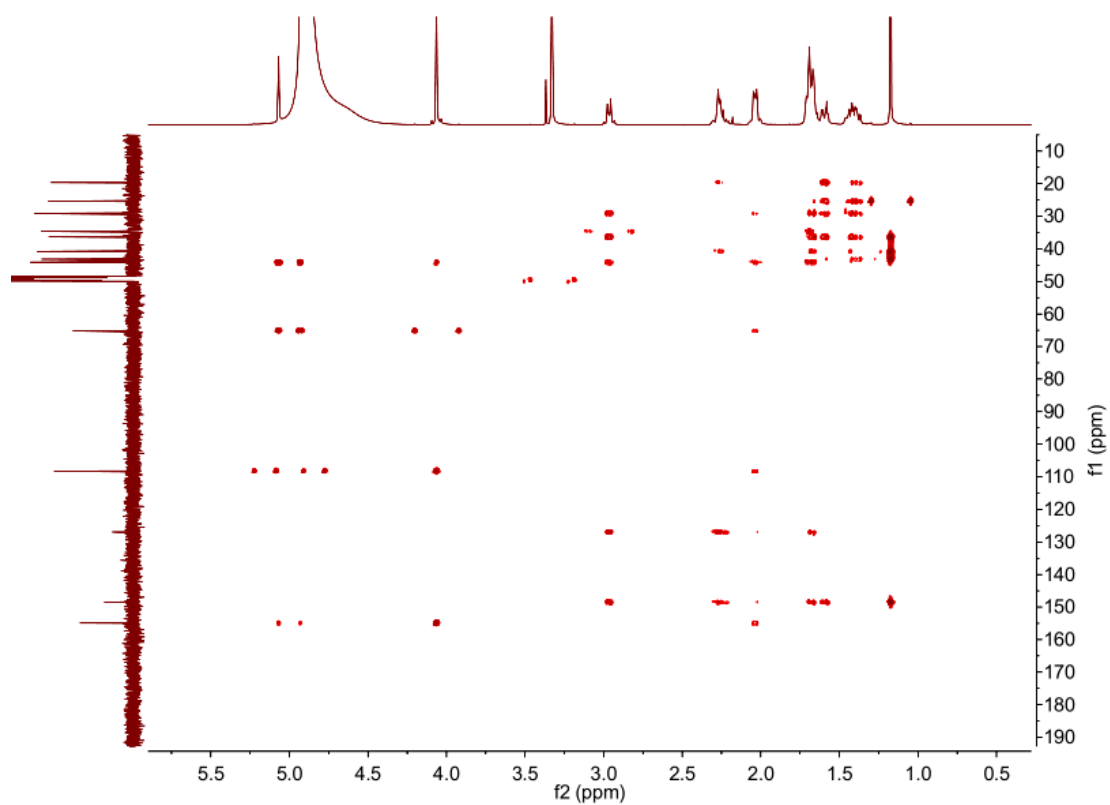


Figure S13: HSQC (500 MHz) spectrum of **1** in CD₃OD.

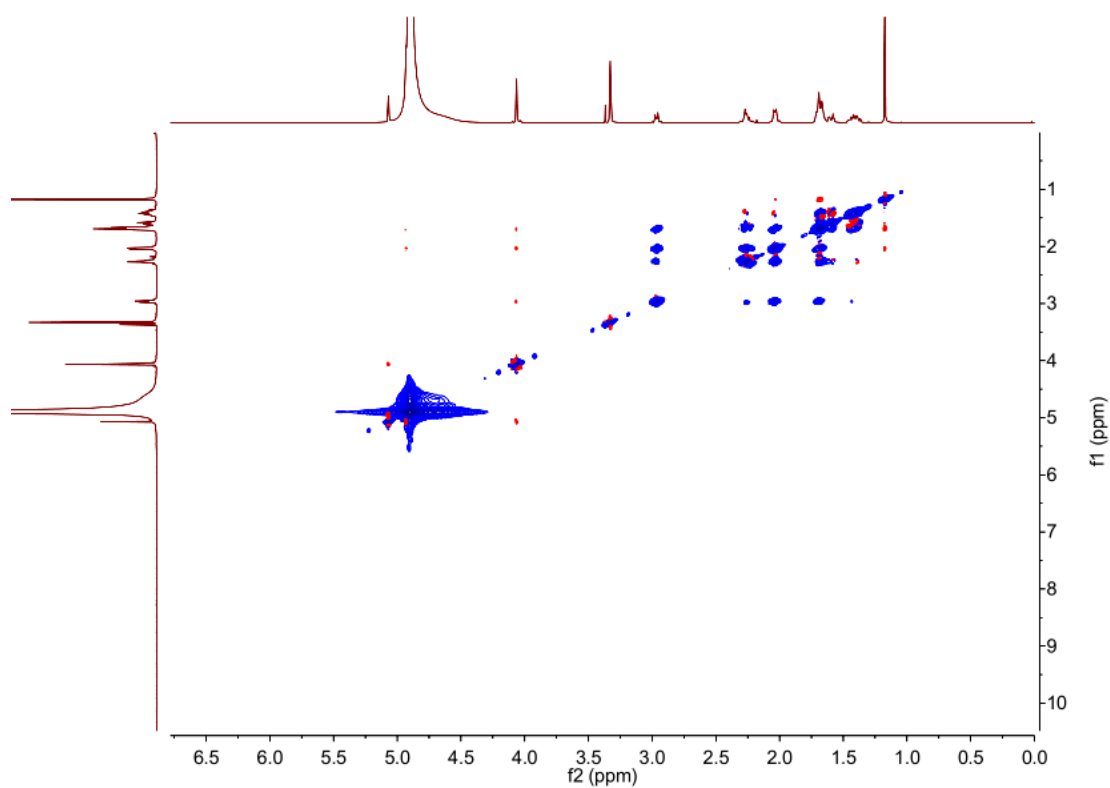


Figure S14: ROSEY (500 MHz) spectrum of **1** in CD₃OD.

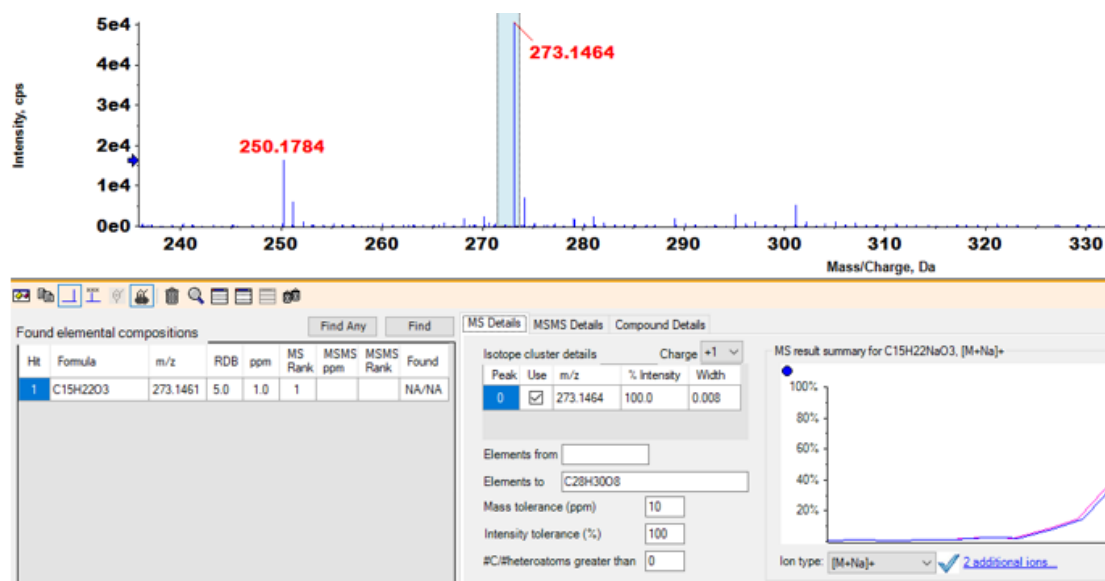


Figure S15: HRESIMS of **1**.

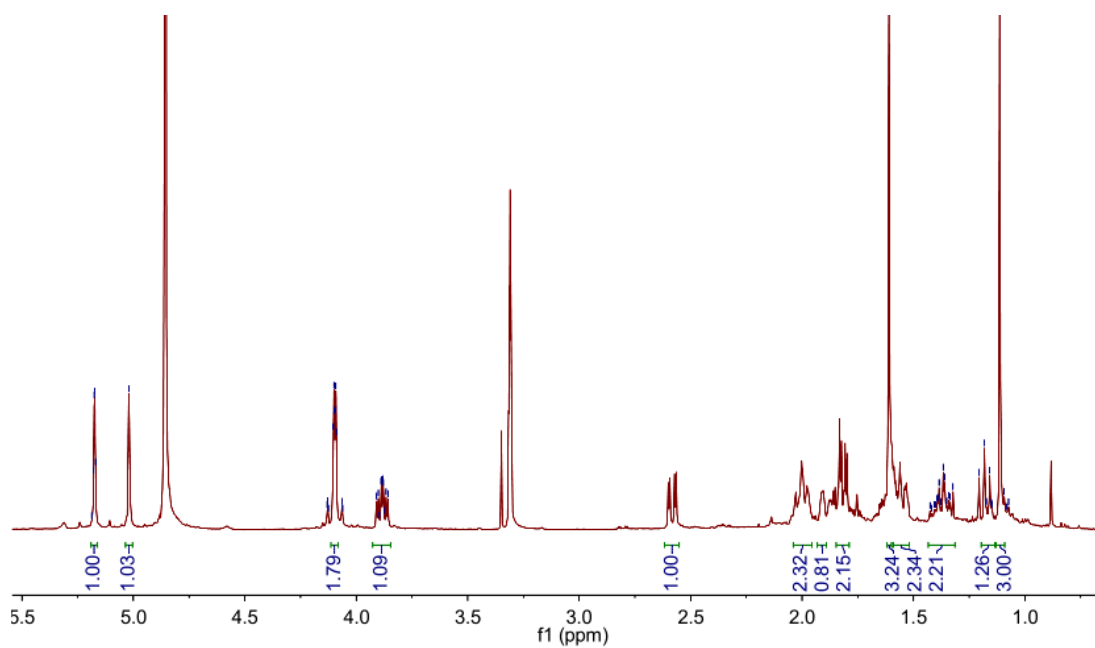


Figure S16: ¹H NMR (500 MHz) spectrum of **2** in CD₃OD.

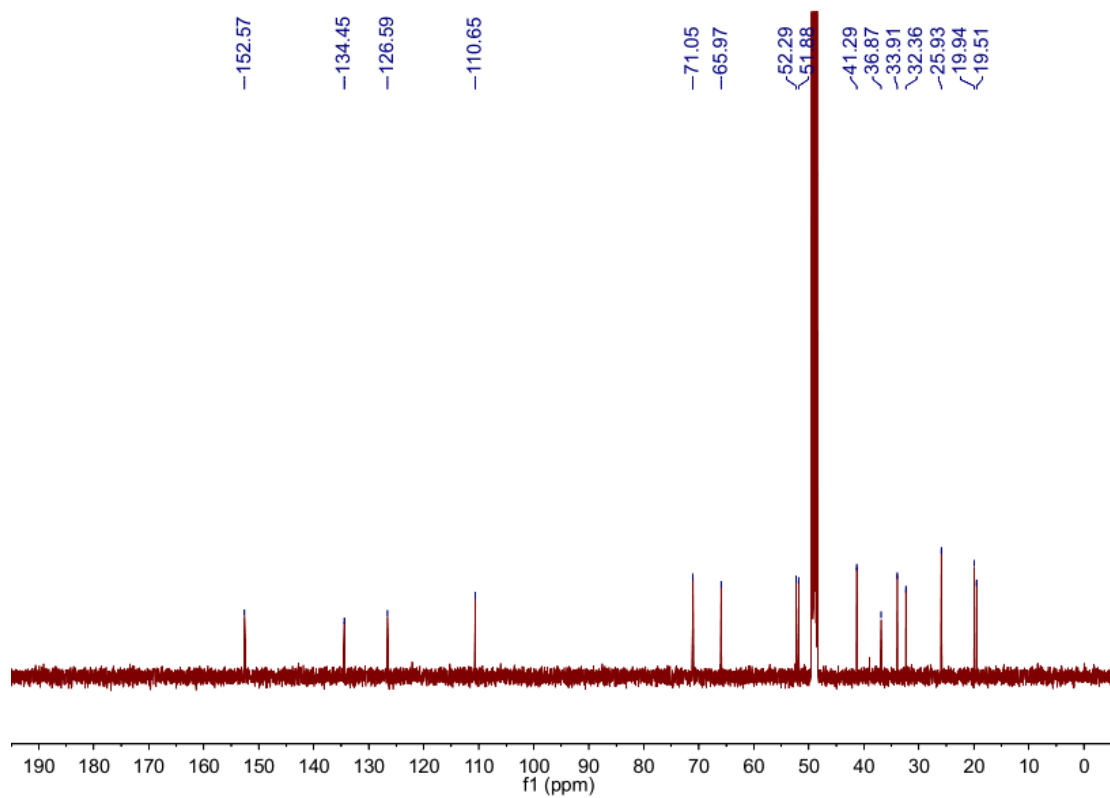


Figure S17: ^{13}C NMR (125MHz) spectrum of **2** in CD_3OD .

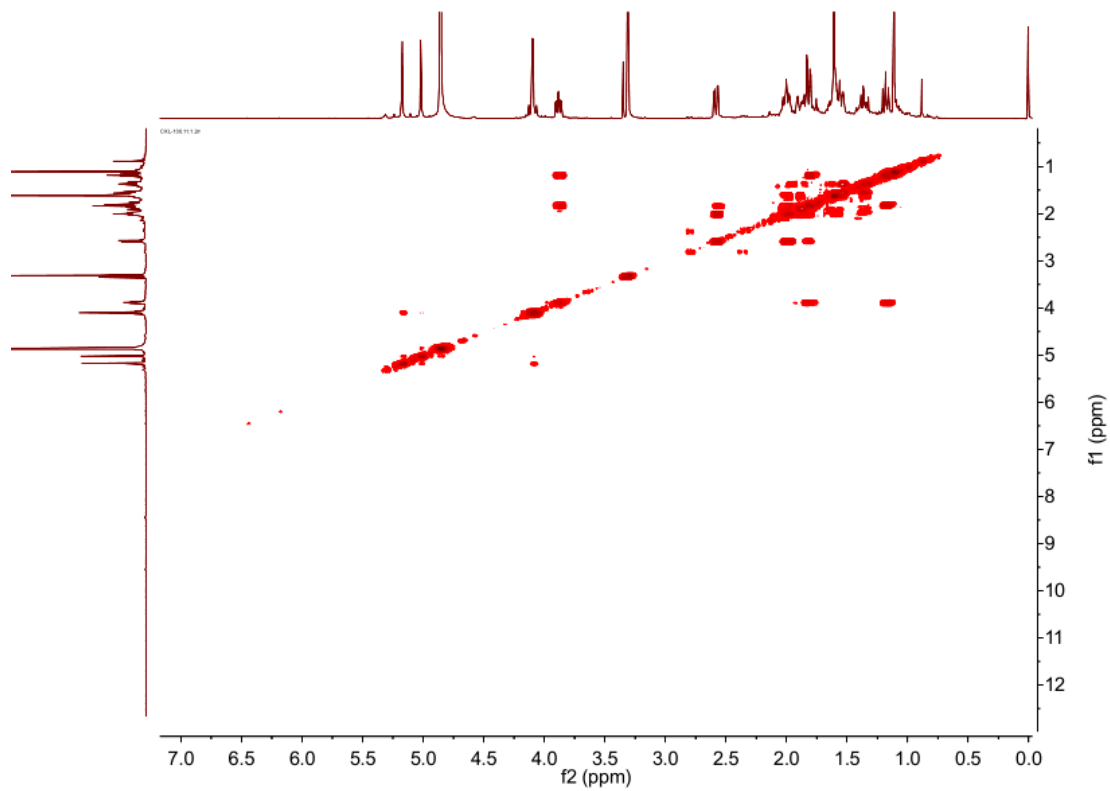


Figure S18: ^1H - ^1H COSY (500 MHz) spectrum of **2** in CD_3OD .

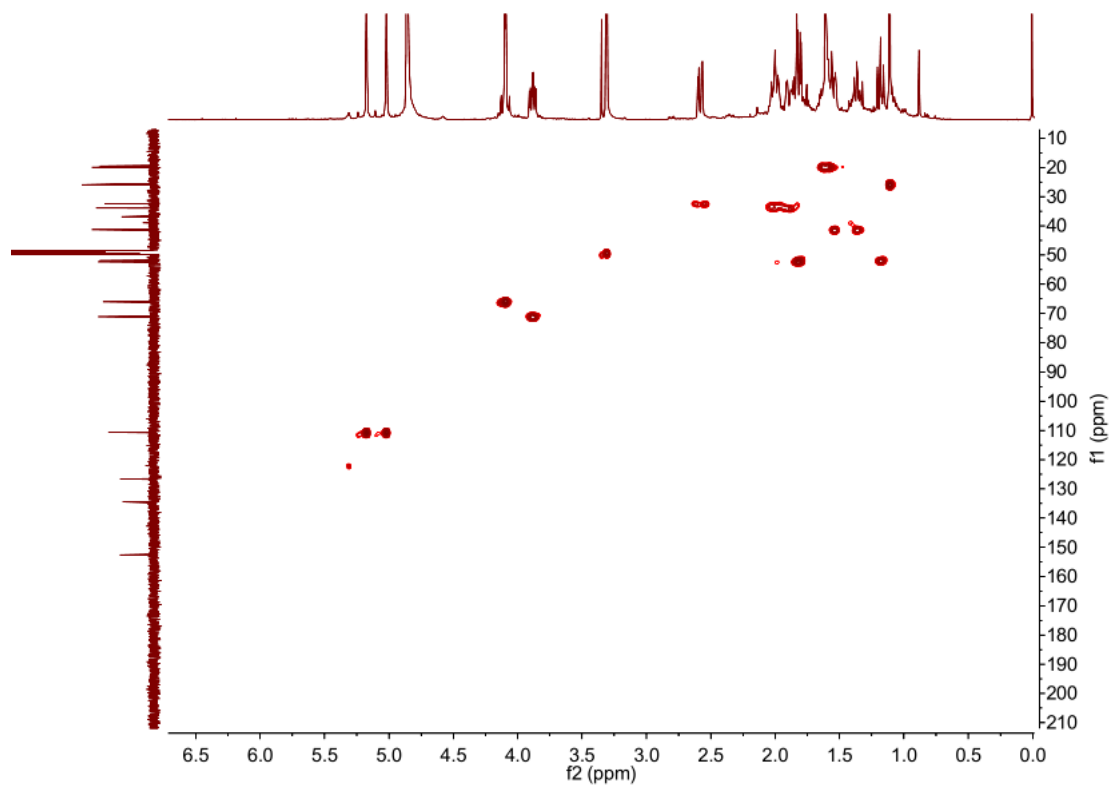


Figure S19: HSQC (500 MHz) spectrum of **2** in CD₃OD.

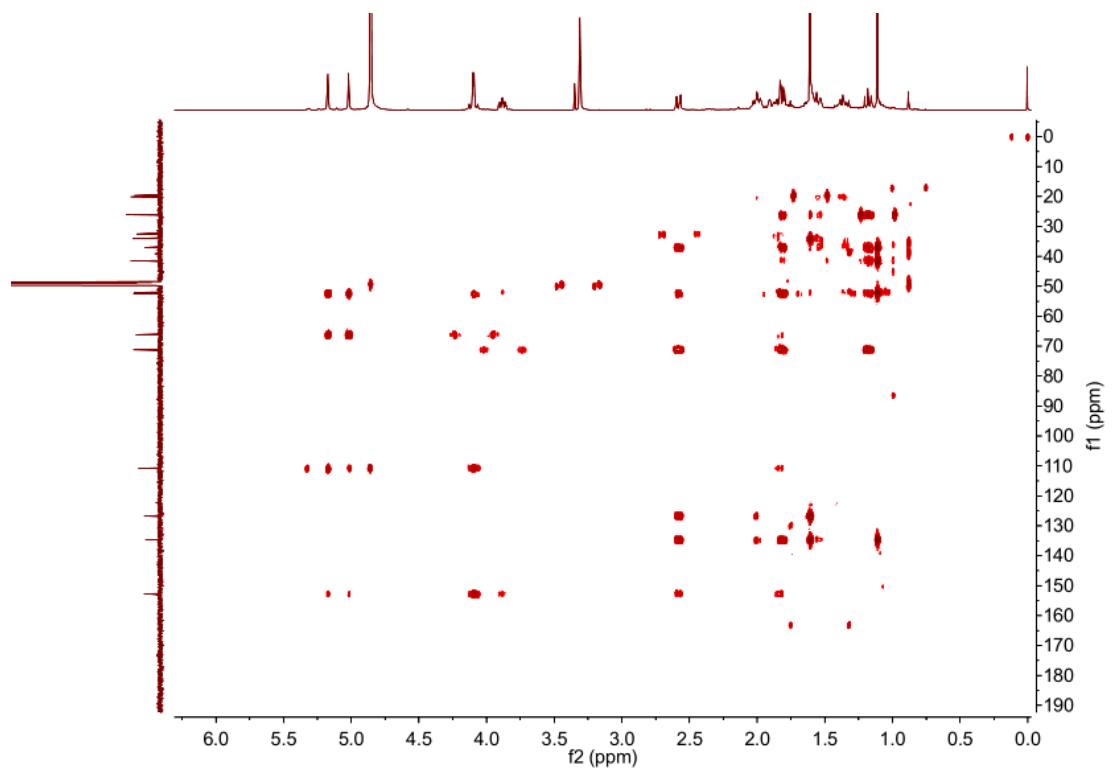


Figure S20: HSBC (500 MHz) spectrum of **2** in CD₃OD.

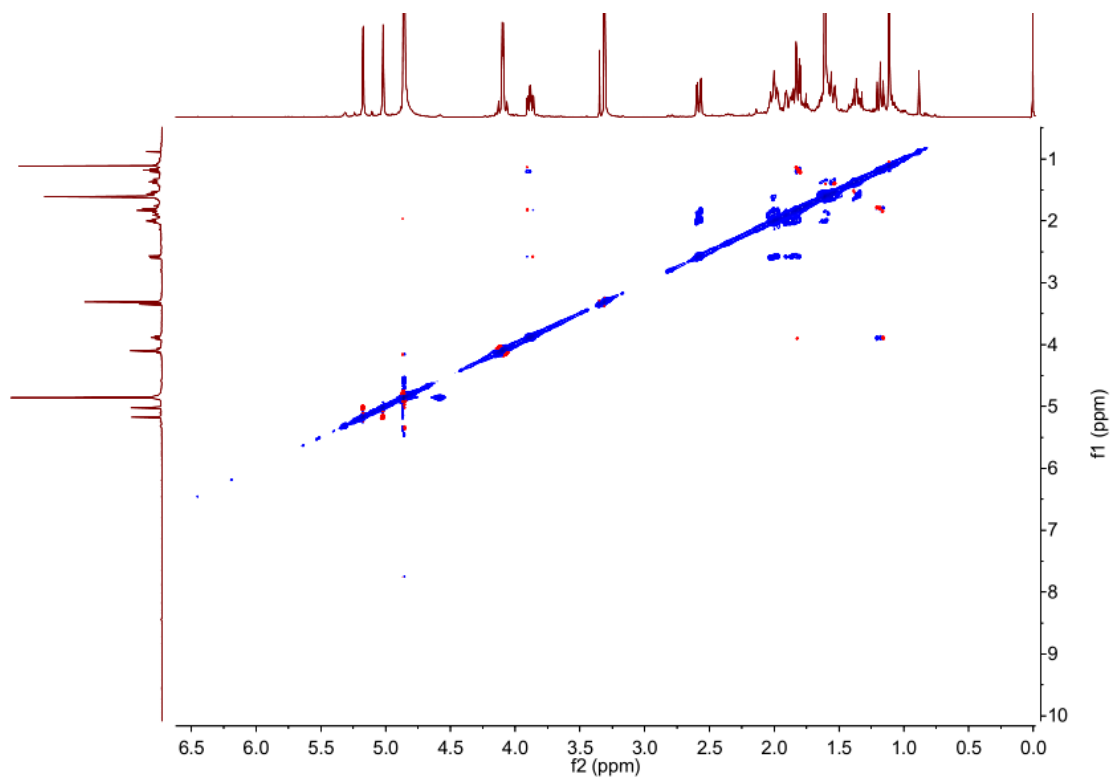


Figure S21: ROSEY (500 MHz) spectrum of **2** in CD₃OD.

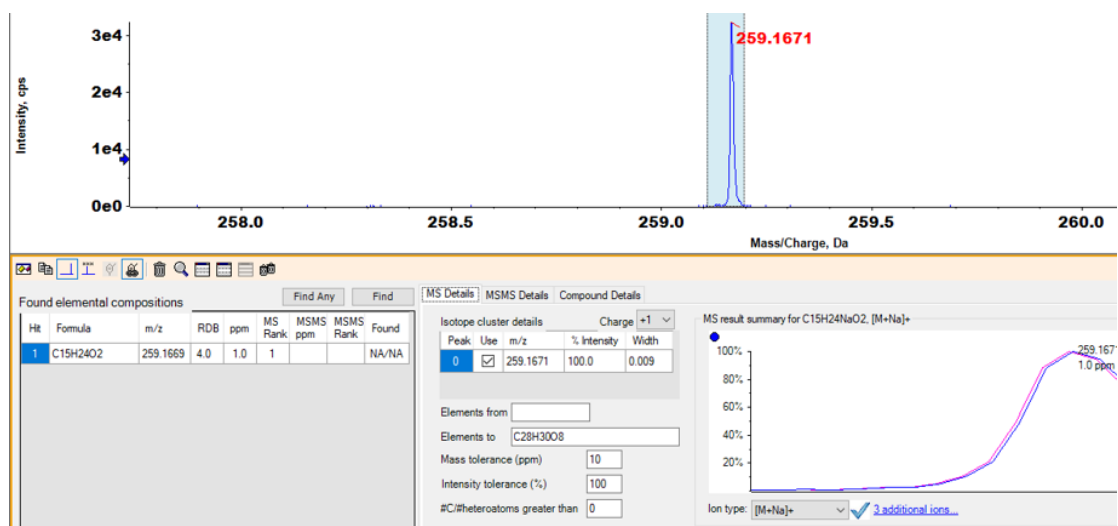


Figure S22: HRESIMS of **2**.

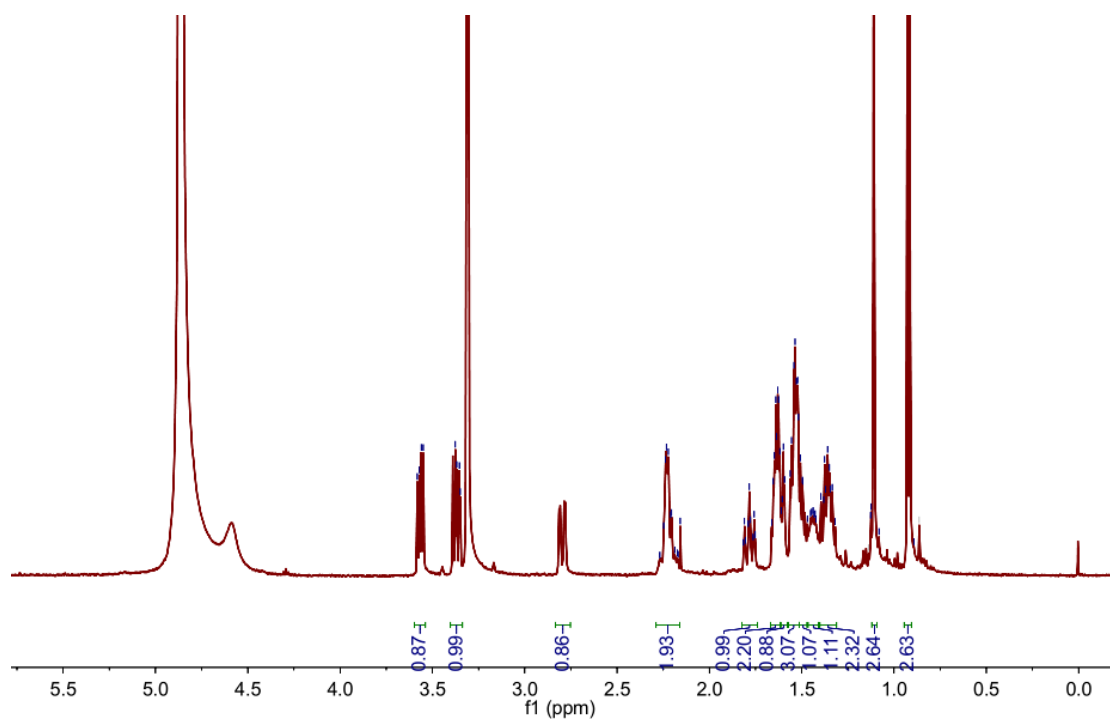


Figure S23: ^1H NMR (500 MHz) spectrum of **3** in CD_3OD .

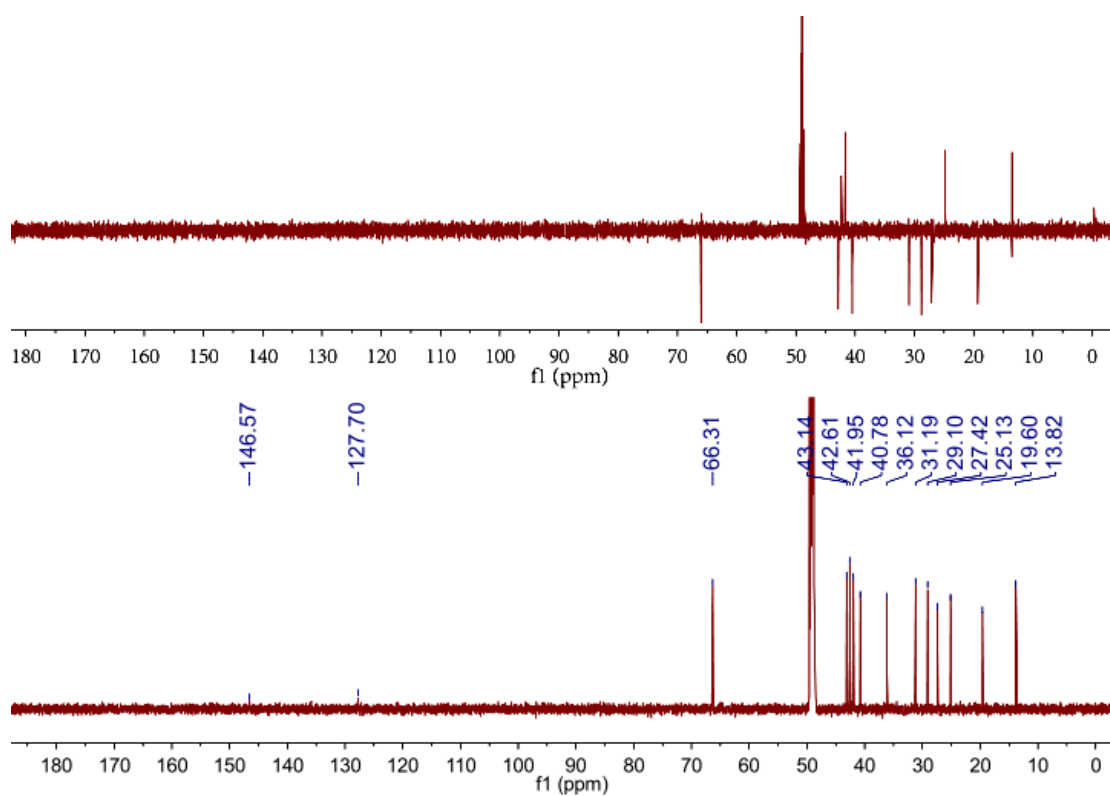


Figure S24: ^{13}C NMR and DEPT (150 MHz) spectra of **3** in CD_3OD .

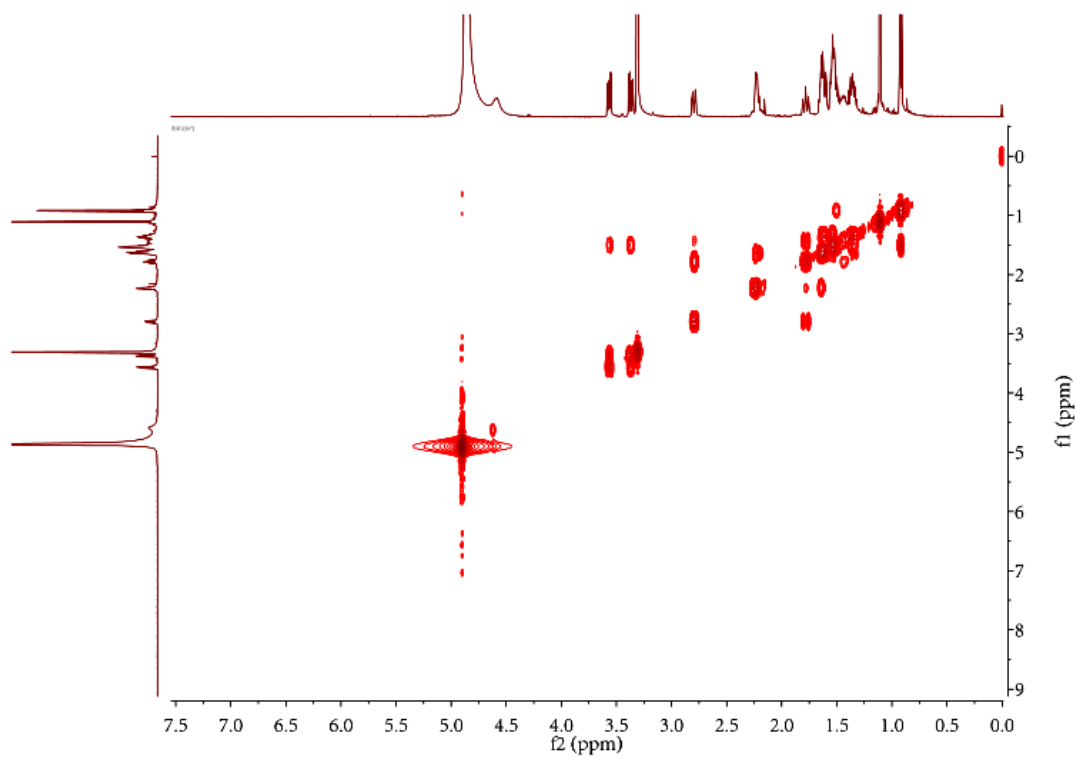


Figure S25: ^1H - ^1H COSY (600 MHz) spectrum of **3** in CD_3OD .

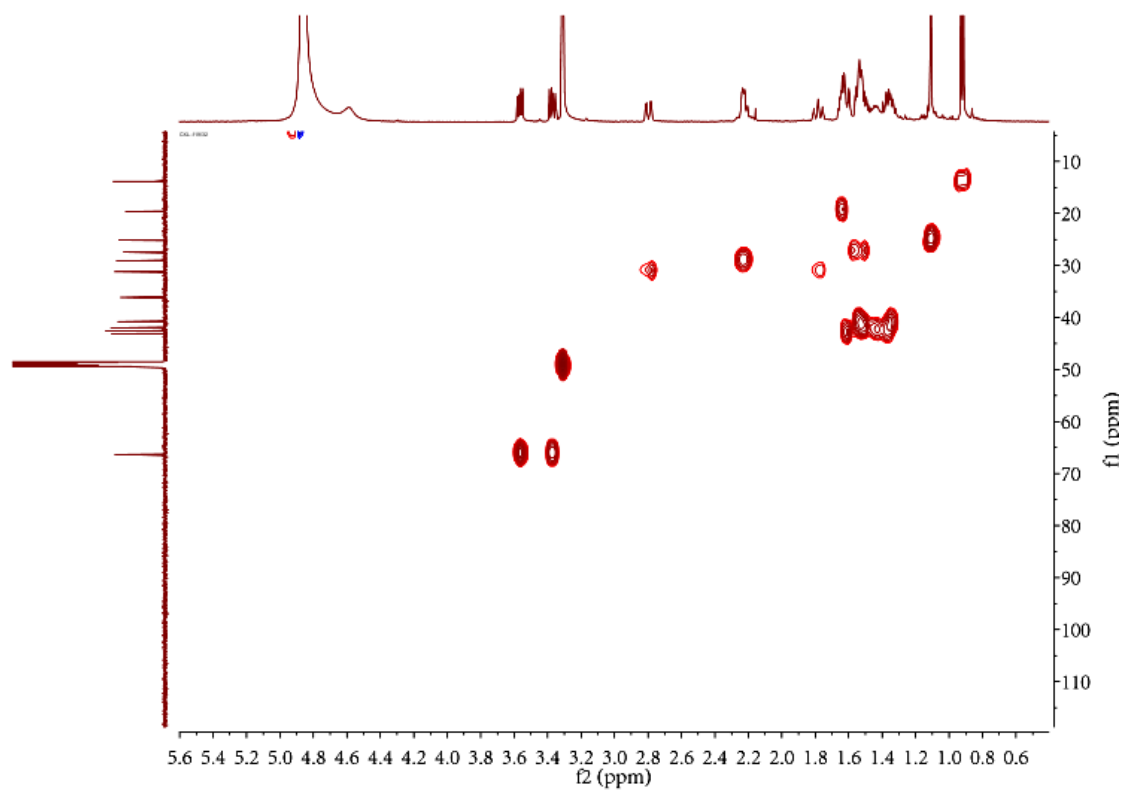


Figure S26: HSQC (600 MHz) spectrum of **3** in CD_3OD .

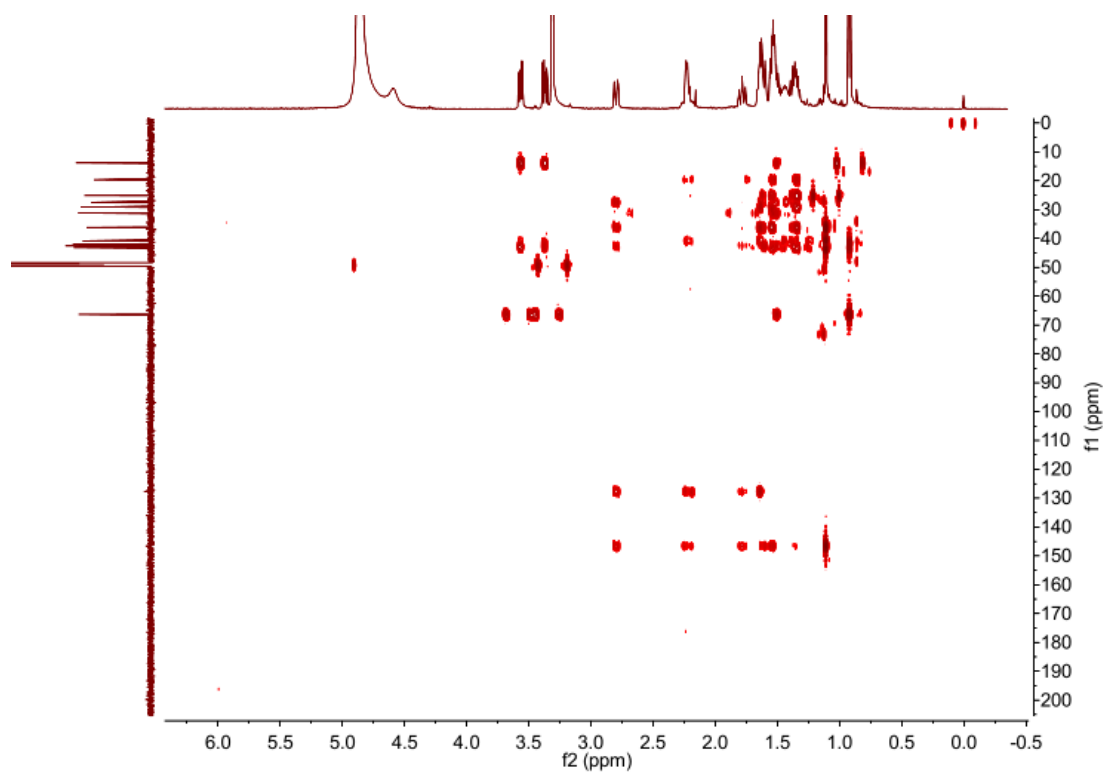


Figure S27: HSBC (600 MHz) spectrum of **3** in CD₃OD.

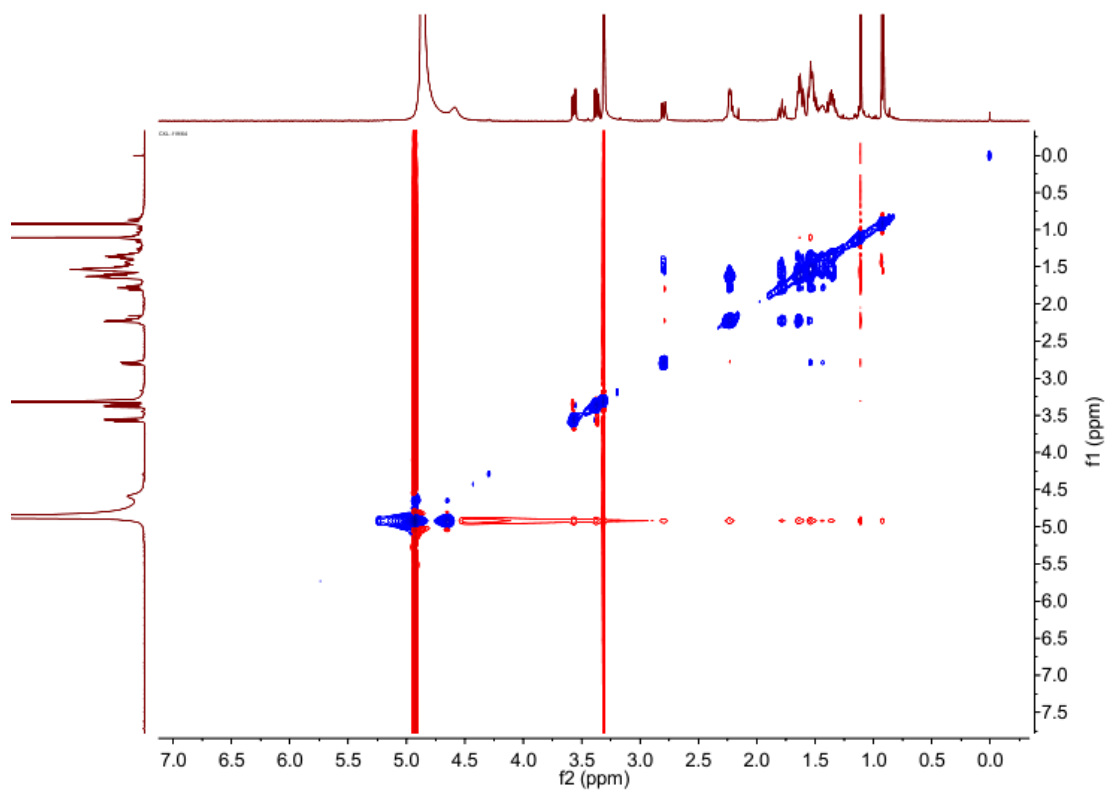


Figure S28: ROSEY (600 MHz) spectrum of **3** in CD₃OD.

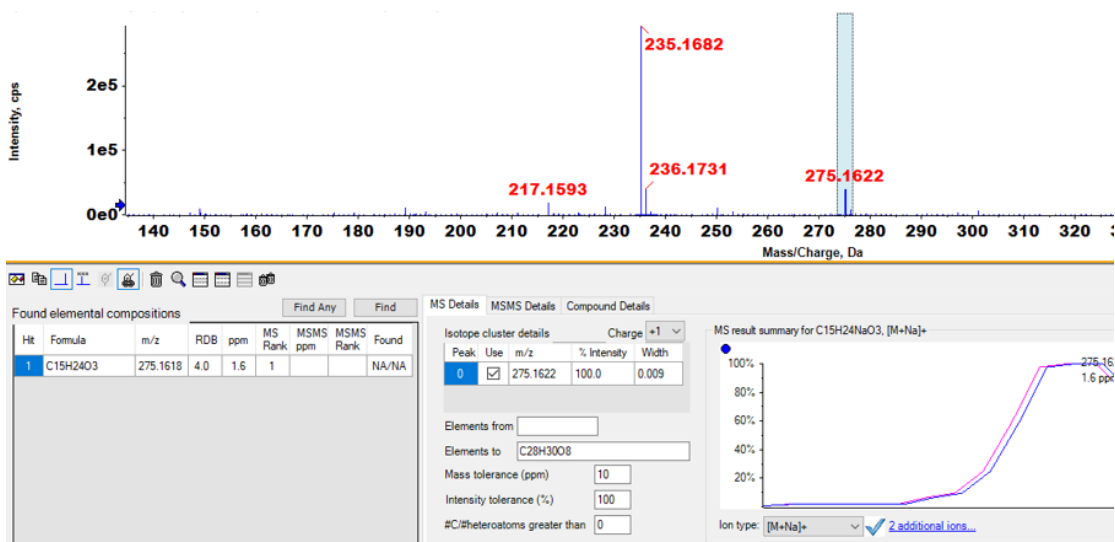


Figure S29: HRESIMS of **3**.

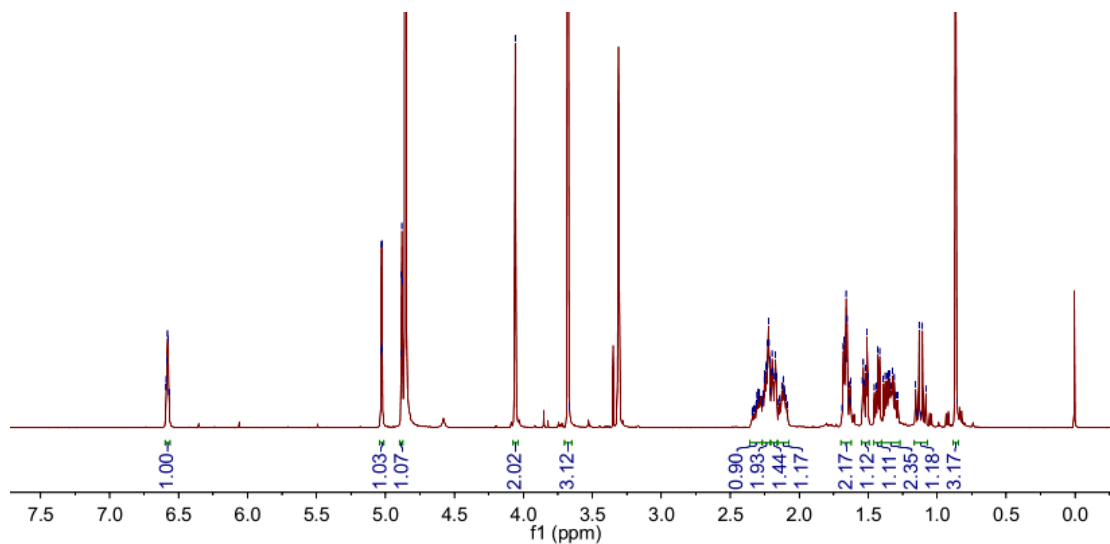


Figure S30: ¹H NMR (500 MHz) spectrum of **4** in CD₃OD.

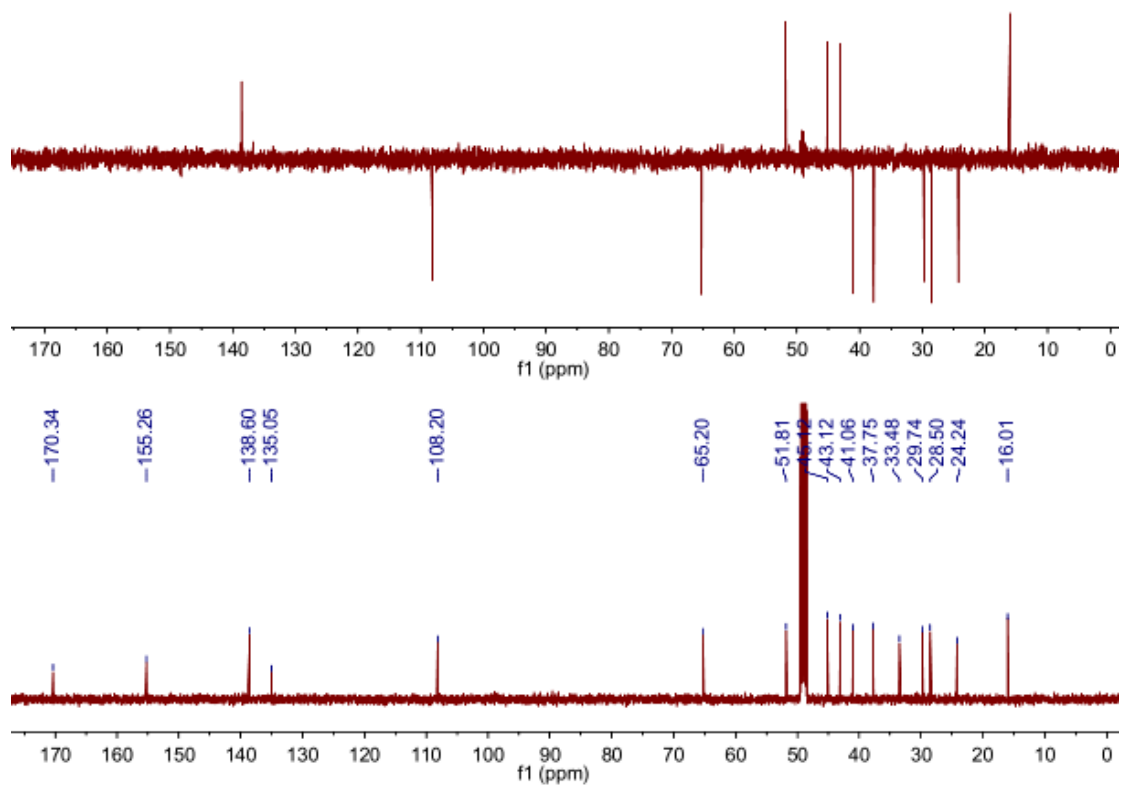


Figure S31: ^{13}C NMR and DEPT (150 MHz) spectra of **4** in CD_3OD .

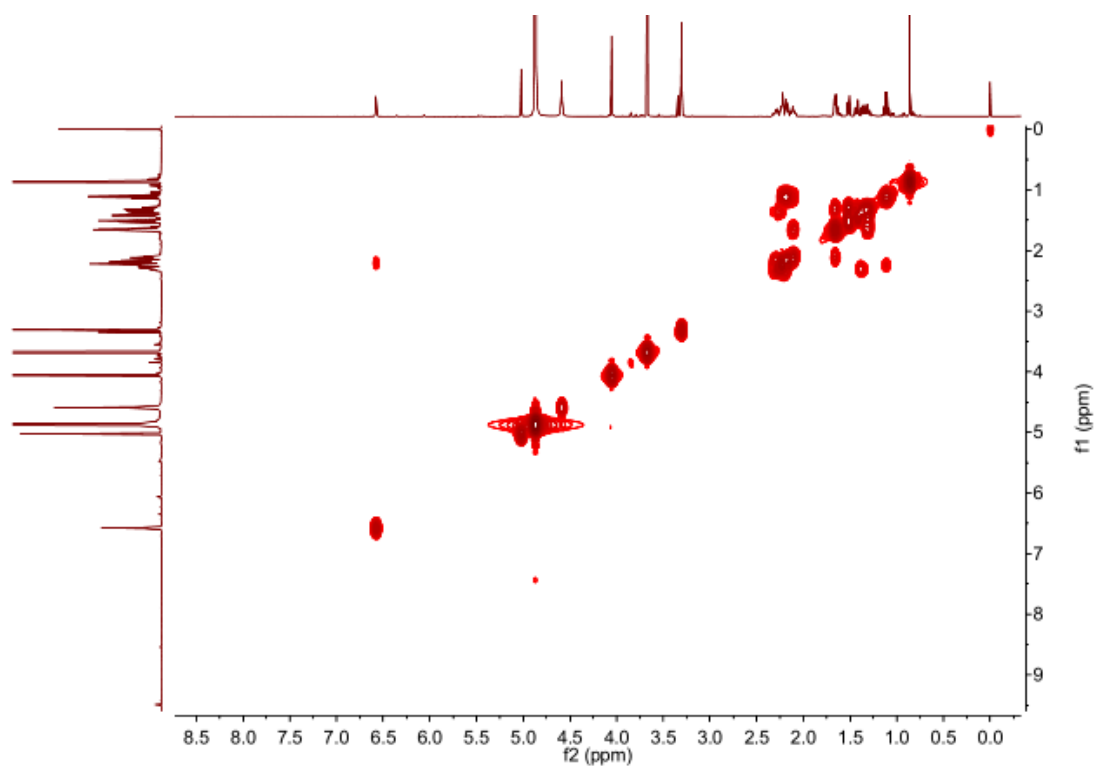


Figure S32: ^1H - ^1H COSY (600 MHz) spectrum of **4** in CD_3OD .

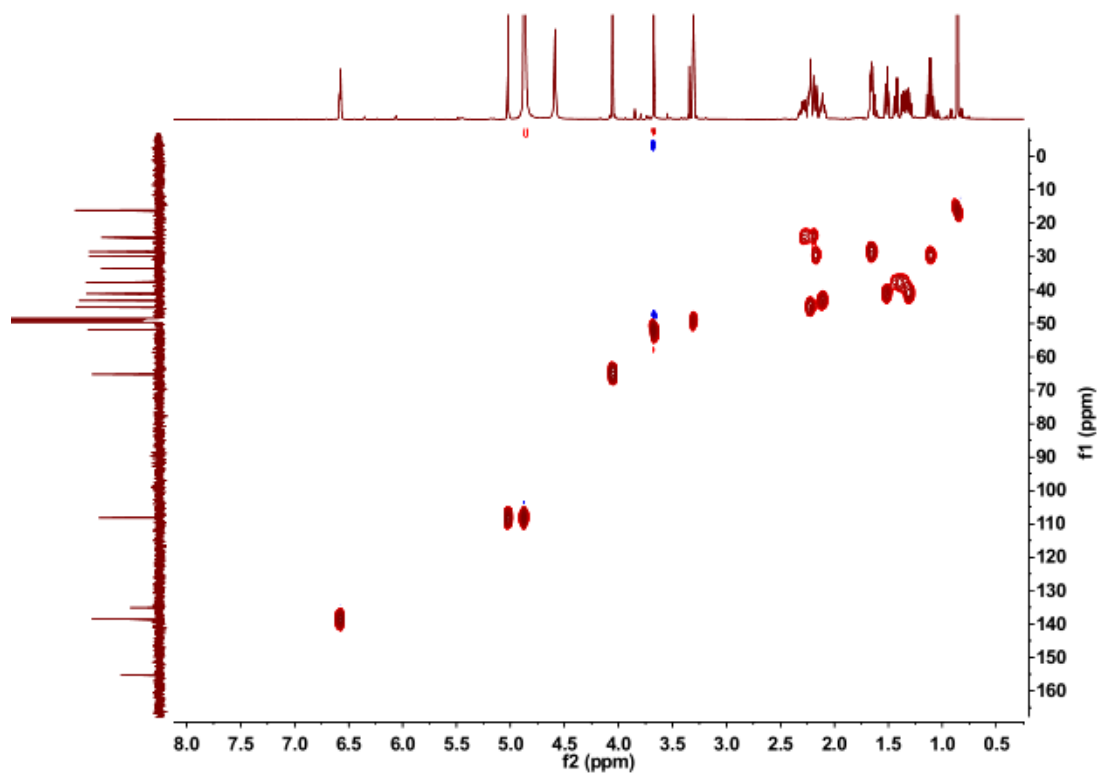


Figure S33: HSQC (600 MHz) spectrum of **4** in CD₃OD.

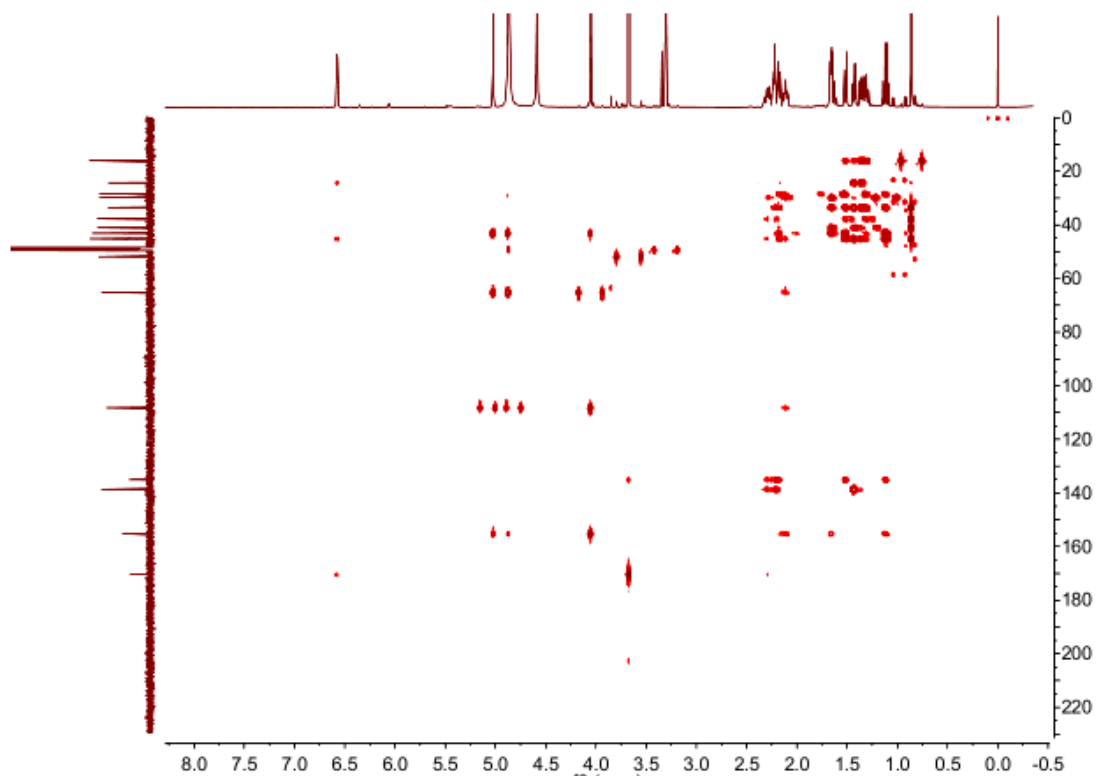


Figure S34: HSBC (600 MHz) spectrum of **4** in CD₃OD.

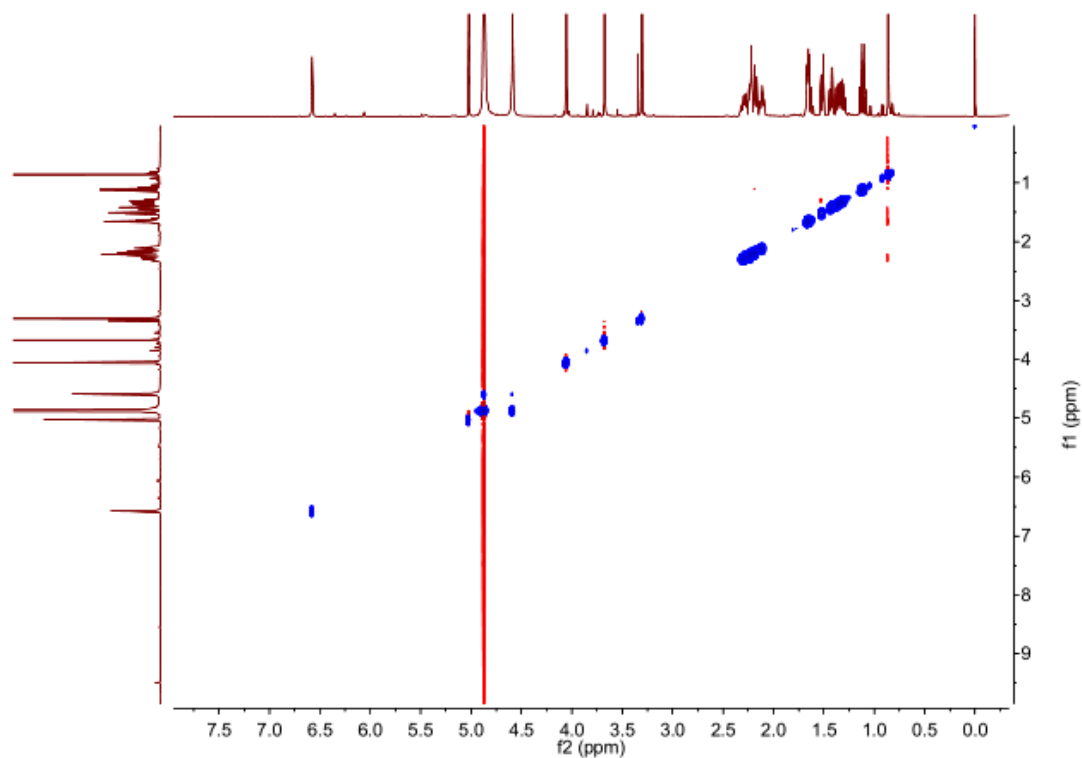


Figure S35: ROSEY (600 MHz) spectrum of **4** in CD₃OD.

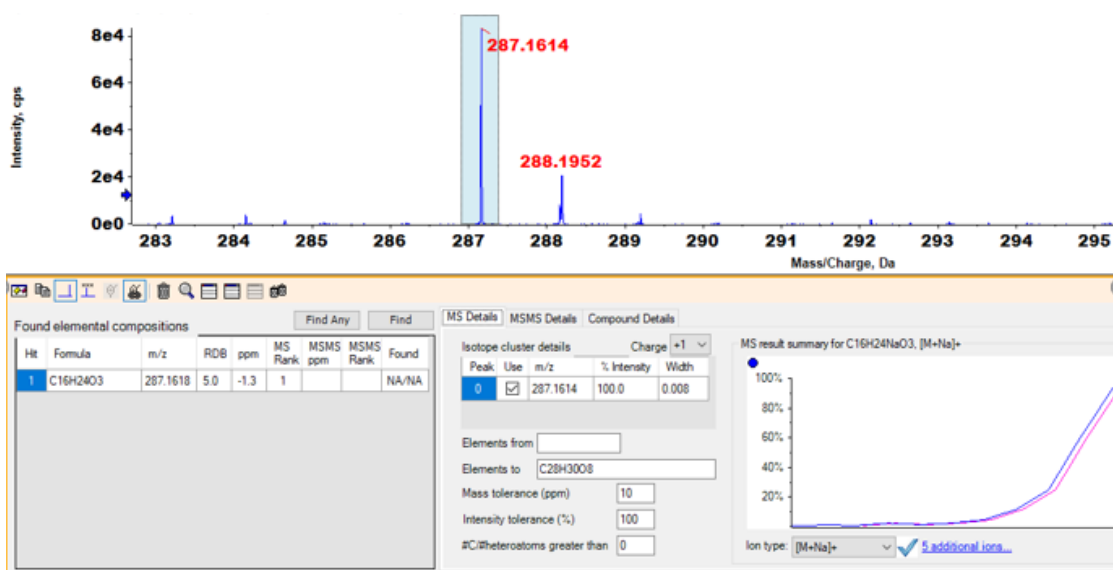


Figure S36: HRESIMS of **4**.

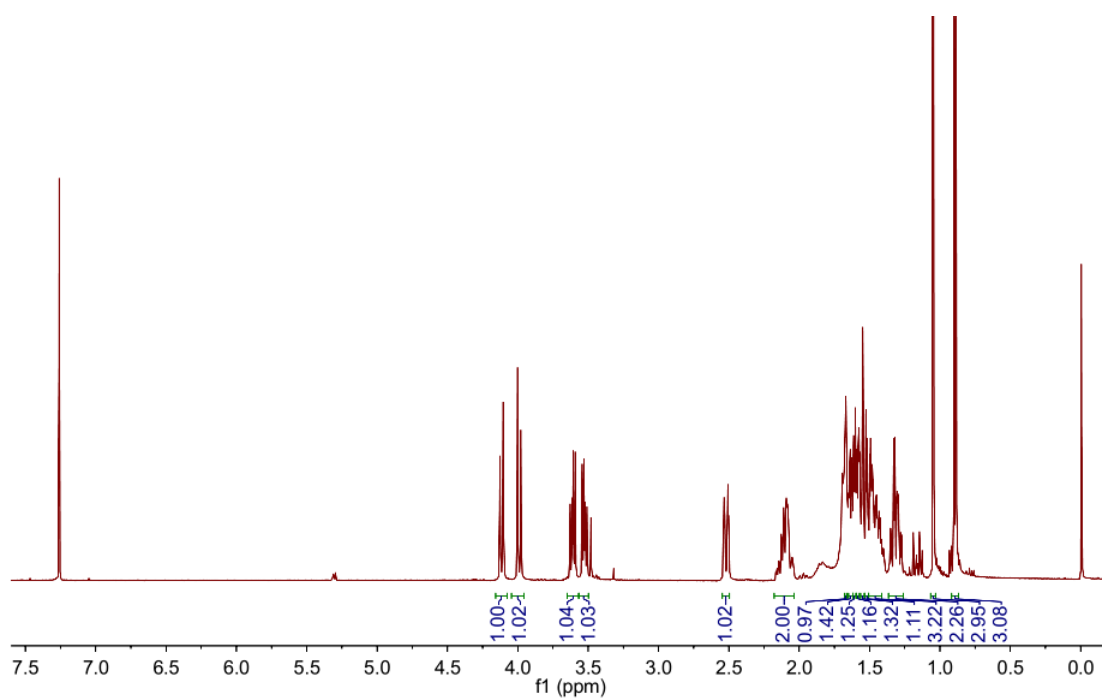


Figure S37: ^1H NMR (500 MHz) spectrum of **5** in CDCl_3 .

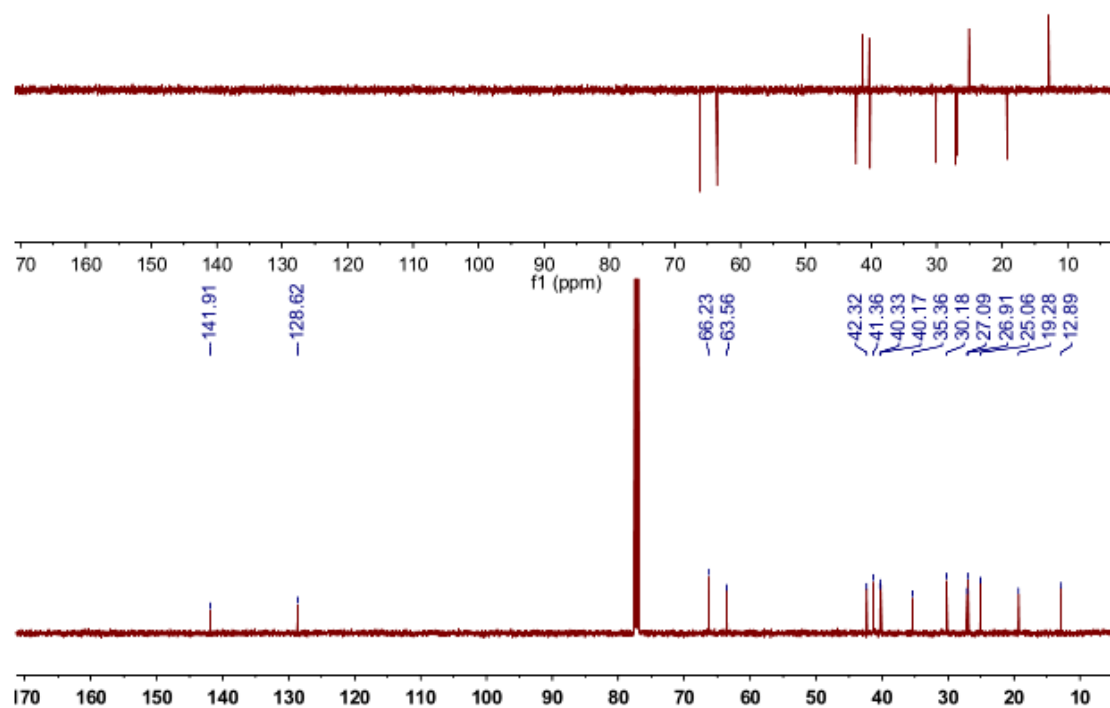


Figure S38: ^{13}C NMR and DEPT (150 MHz) spectra of **5** in CDCl_3 .

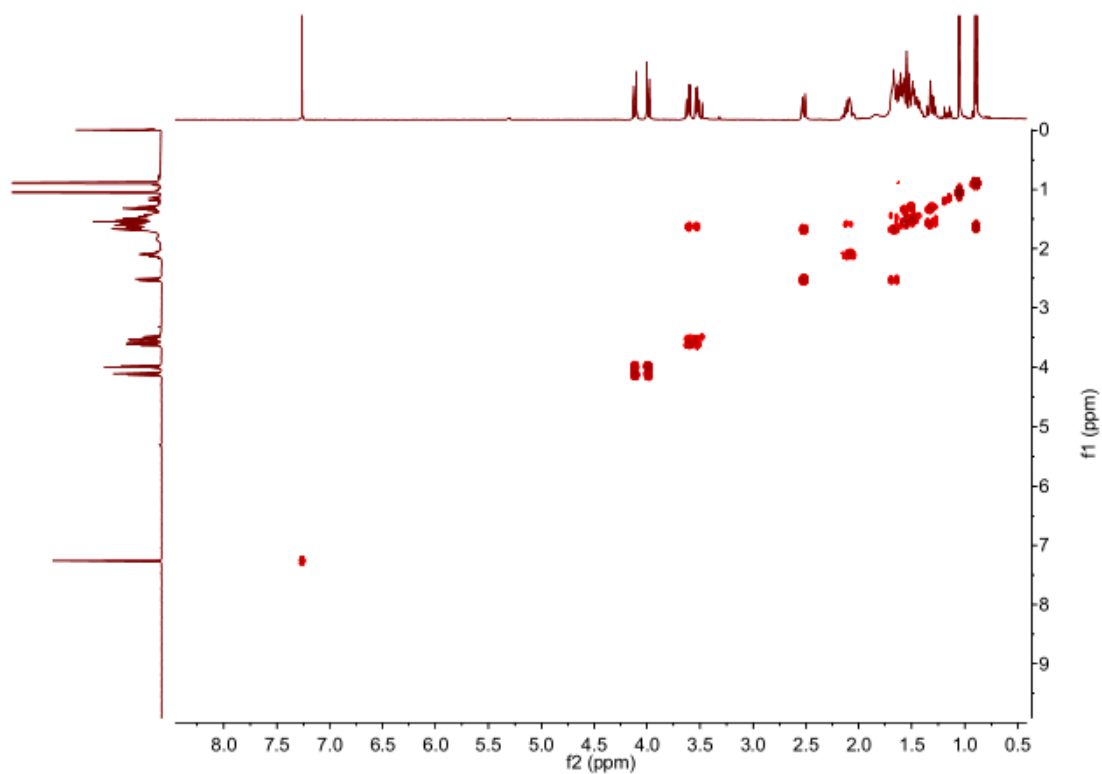


Figure S39: ^1H - ^1H COSY (600 MHz) spectrum of **5** in CDCl_3 .

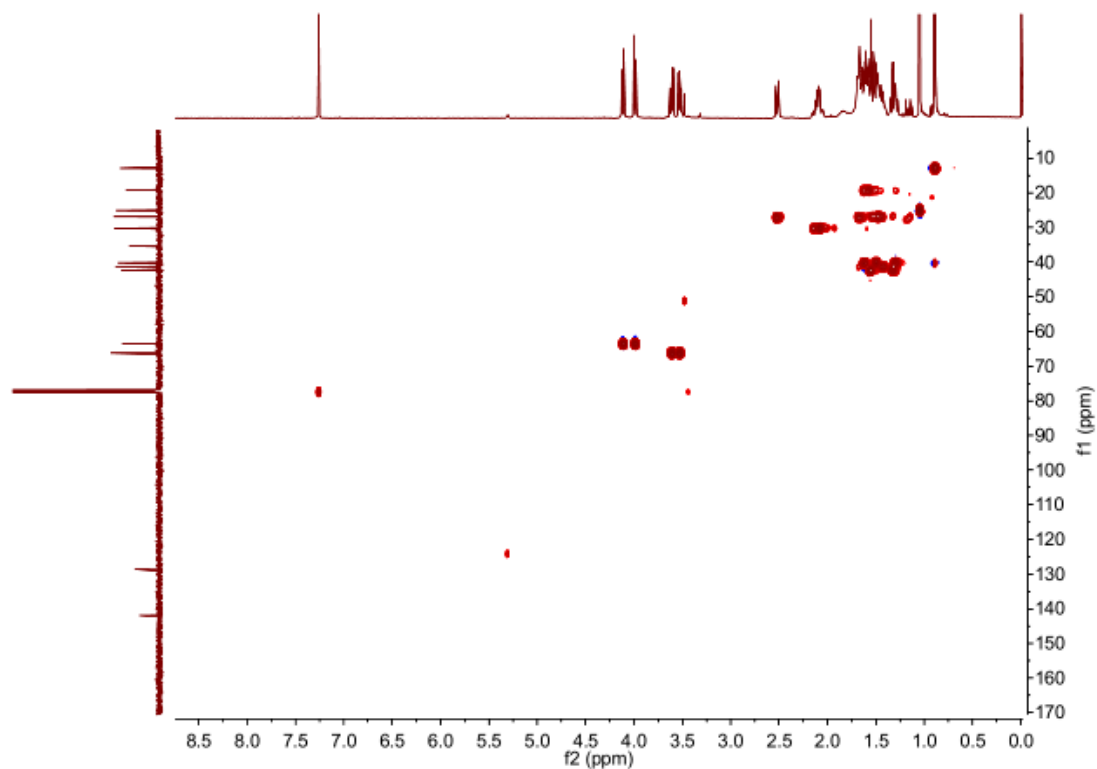


Figure S40: HSQC (600 MHz) spectrum of **5** in CDCl_3 .

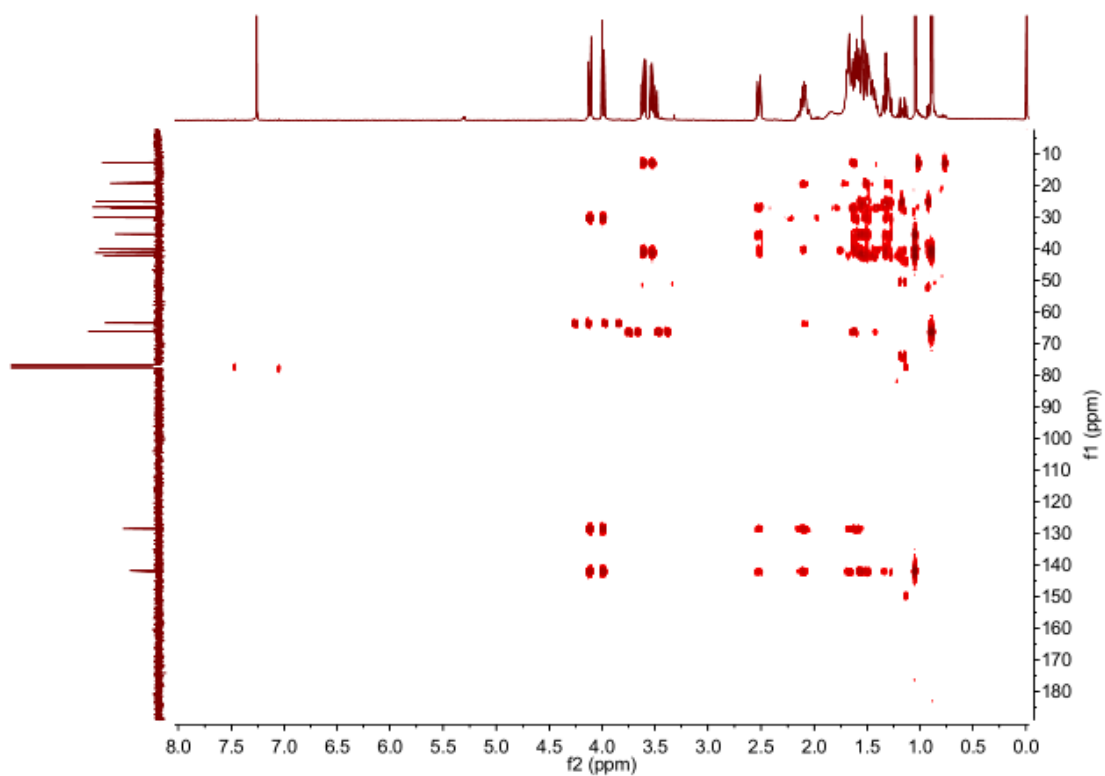


Figure S41: HSBC (600 MHz) spectrum of **5** in CDCl_3 .

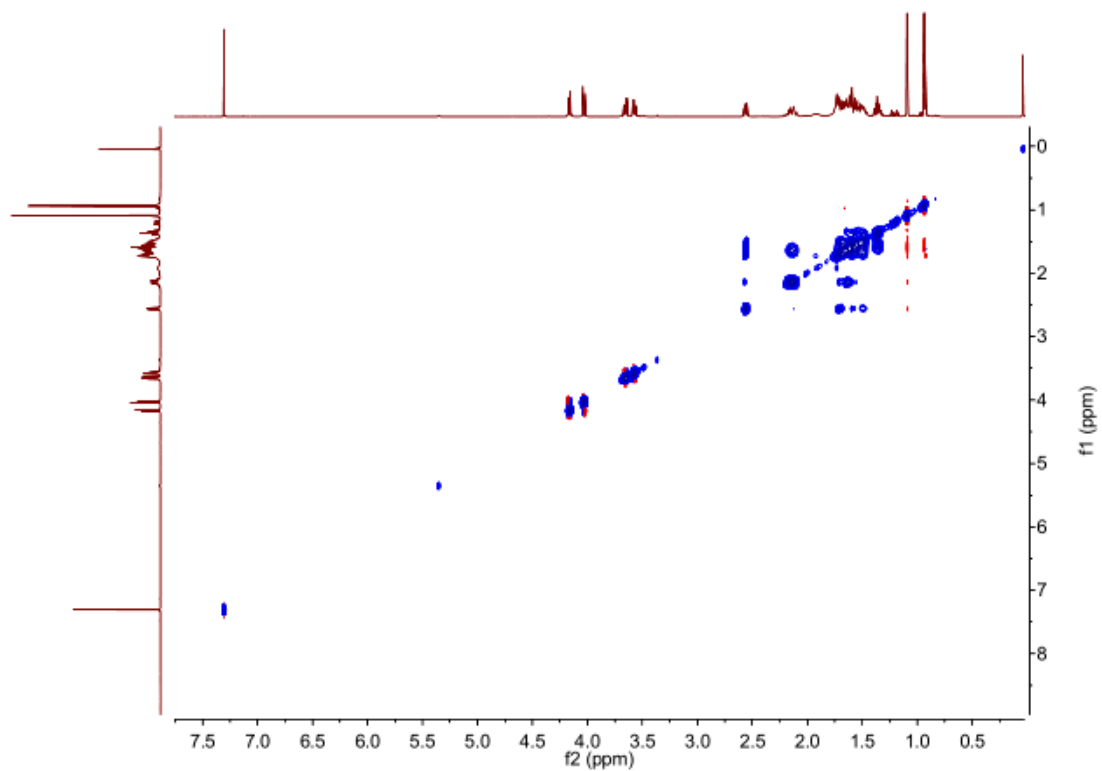


Figure S42: ROSEY (600 MHz) spectrum of **5** in CDCl_3 .

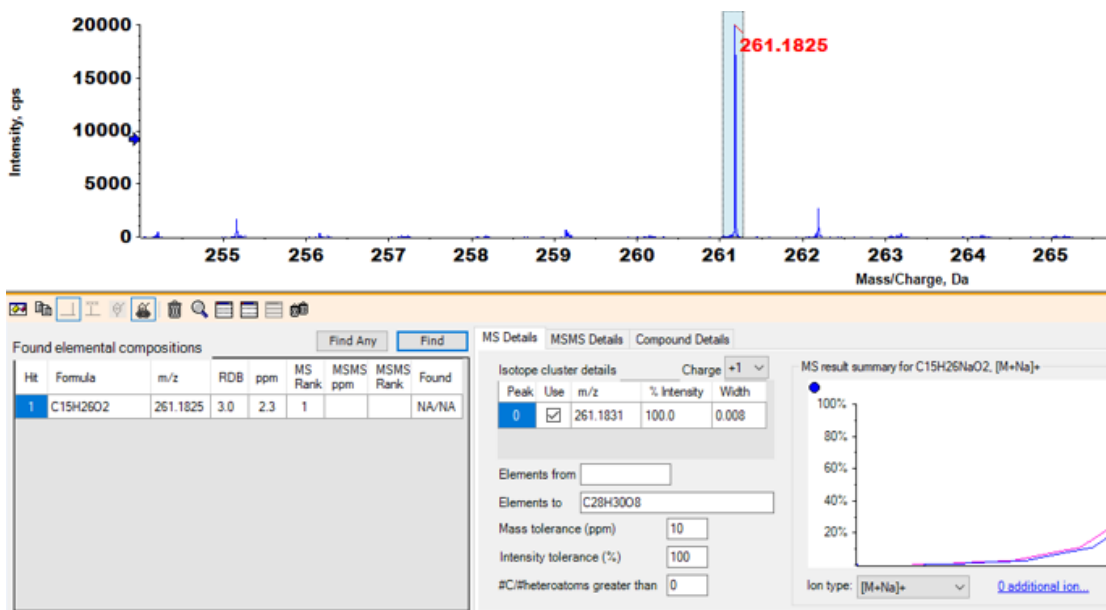
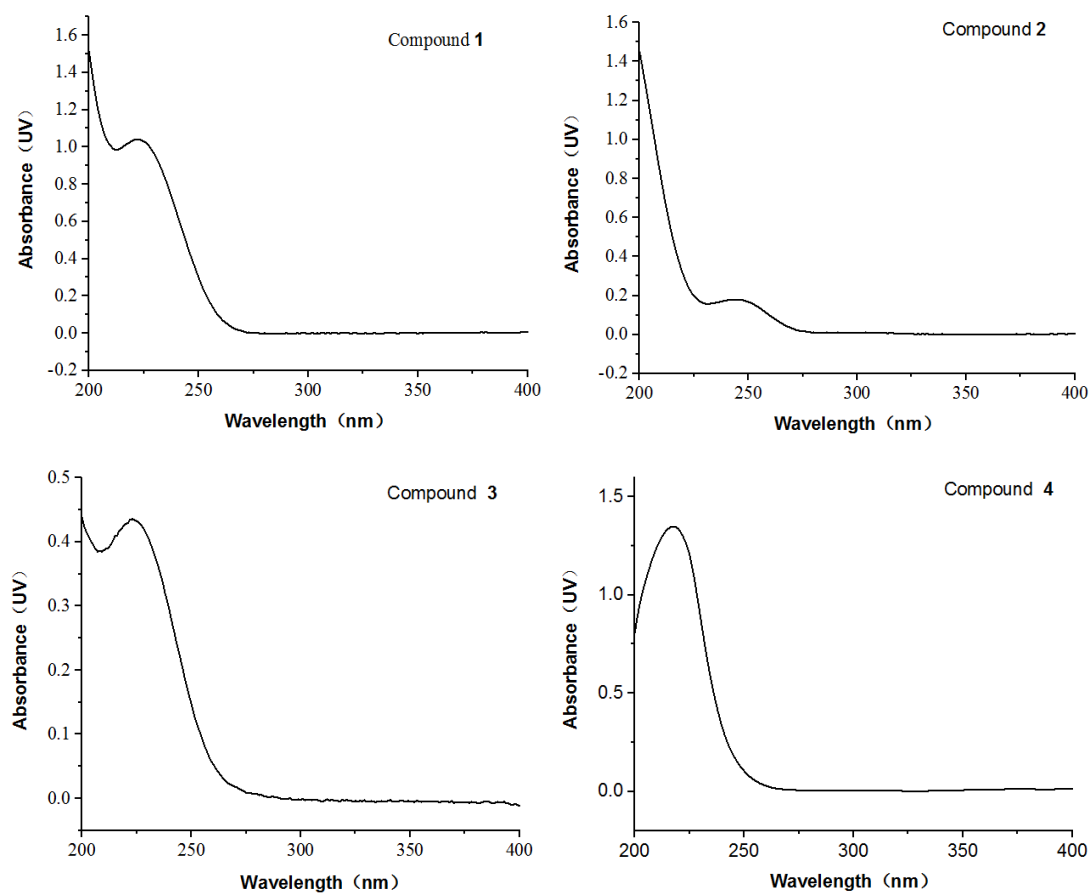


Figure S43: HRESIMS of 5.



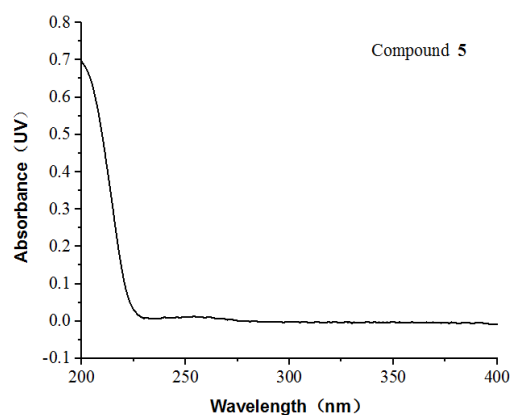


Figure S44: UV-vis spectra of 1–5

Bioactivity assay data

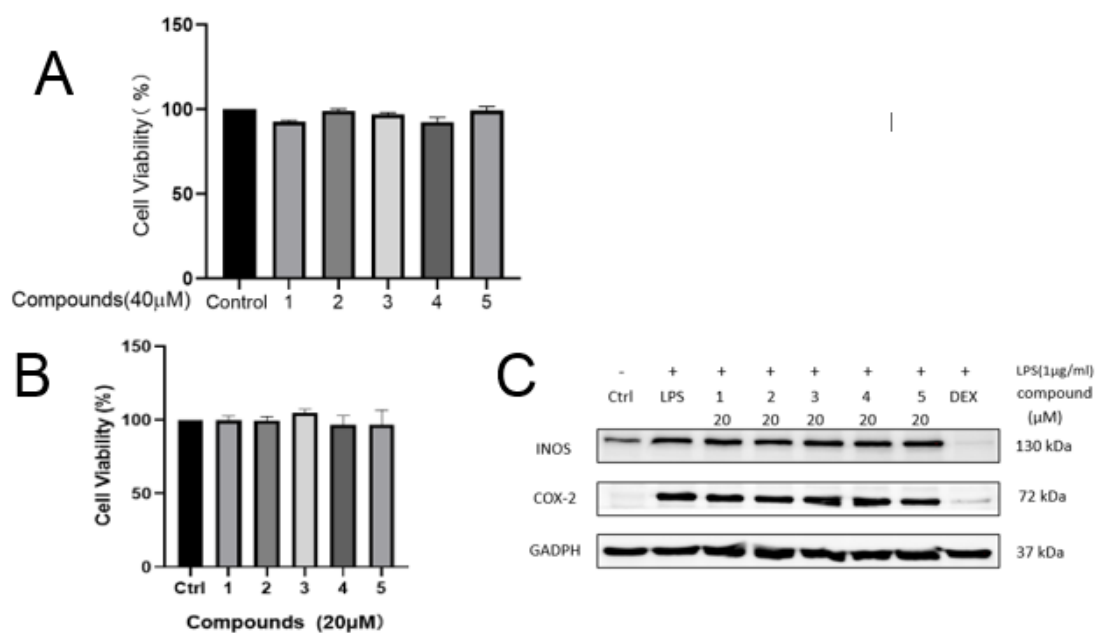


Fig A: human breast cancer cell line (MCF-7) were treated with 40 μM with compounds 1–5 for 24 h, and cell viability was determined by CCK-8 assay.

Fig B: RAW 264.7 were treated with 20 μM with compounds 1–5 for 24 h, and cell viability was determined by CCK-8 assay.

Fig C: Compounds suppress LPS-induced INOS and COX-2 expression in RAW 264.7 cells. Data represent mean ±SEM values of three experiments.