Electronic Supplementary Information (ESI)

Synthesis and environment-dependent fluorescence behavior of a biaryl-conjugated (diphenylmethylene)imidazolinone

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1. Experimental section

1.1. Theoretical calculations

The theoretical calculations were performed using Spartan'18 ver. 12.0 for Windows (Wavefunction, Inc., Irvine) under the default settings in the gas phase. The structures of DAINs **1a**–**h** and **2-*H*** were constructed and optimized through the following two steps: 1) systematic conformational search at the molecular mechanics (MMFF), 2) geometry optimization of the lowest energy conformer obtained in step 1 at the DFT/CAM-B3LYP/6-31G* level. Frequencies were confirmed at this stage. Molecular orbitals were calculated at the DFT/CAM-B3LYP/6-31+G* level for the optimized structure obtained in step 2.

1.2. Evaluation of optical properties

Absorption spectra were measured at a concentration of 1.0×10^{-5} M. Fluorescence spectra in tricaprylin were measured at a concentration of 1.0×10^{-4} M under the irradiation of λ_{max} (Table S1) for the excitation. The spectra in tricaprylin were corrected by subtracting the background emission from tricaprylin. Fluorescence spectra of AIE (suspension and powder) were measured under the irradiation of λ_{ex} that was obtained from their excitation spectra. The suspension for AIE was prepared by mixing the DAIN solution in DMSO (1.0×10^{-2} M) and water (volume ratio: 1/999, final concentration: 1.0×10^{-5} M).

Table S1: Excitation wavelengths (nm) of DAINs **1** and **2-*H***.

	1a	**1b**	**1c**	**1d**	**1e**	**1f**	**1g**	**1h**	**2-*H***
λ_{max}	399	401	401	404	404	406	400	401	391
$\lambda_{ex(sus)}$	403	403	404	405	406	406	—	—	—
$\lambda_{ex(pow)}$	369	370	369	370	368	369	369	369	—

Dimyristoylphosphatidylcholine (DMPC) vesicle was prepared by a common method, which involved thin film hydration and sonication.[1] The fluorescence spectra of the mixture of **1e** and the DMPC vesicle were measured after addition of a DMPC vesicle solution in water (2.0×10^{-3} M) to a suspension of **1e** in water containing 0.125% DMSO (1.25×10^{-5} M), (volume ratio: 1/4, final concentration of DMPC: 4.0×10^{-4} M, **1e**: 1.0×10^{-5} M).

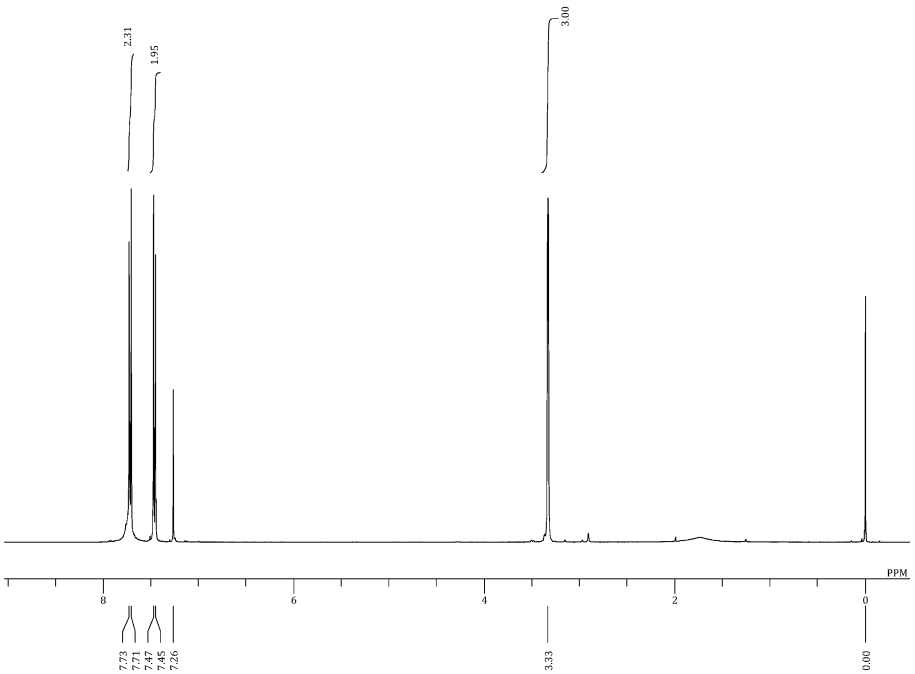
Reference:

1) A. Akbarzadeh, R. Rezaei-Sadabady, S. Davaran, S. W. Joo, N. Zarghami, Y. Hanifehpour, M. Samiei, M. Kouhi and K. Nejati-Koshki, *Nanoscale Res. Lett.*, 2013, **8**, 102.

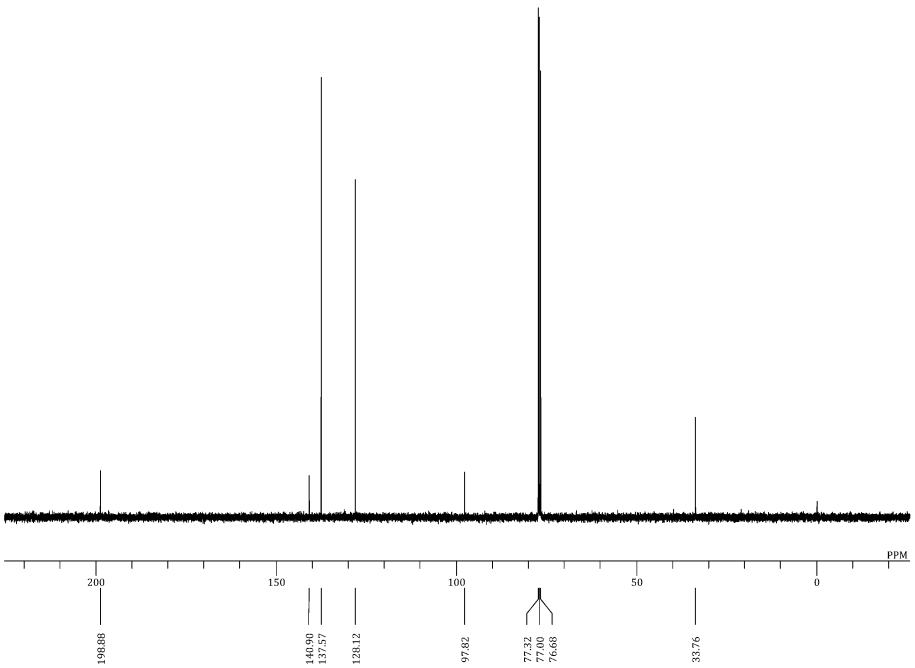
2. ^{1}H and ^{13}C NMR spectra of new compounds

Compound **5**

^{1}H-NMR



^{13}C-NMR



Compound **6**

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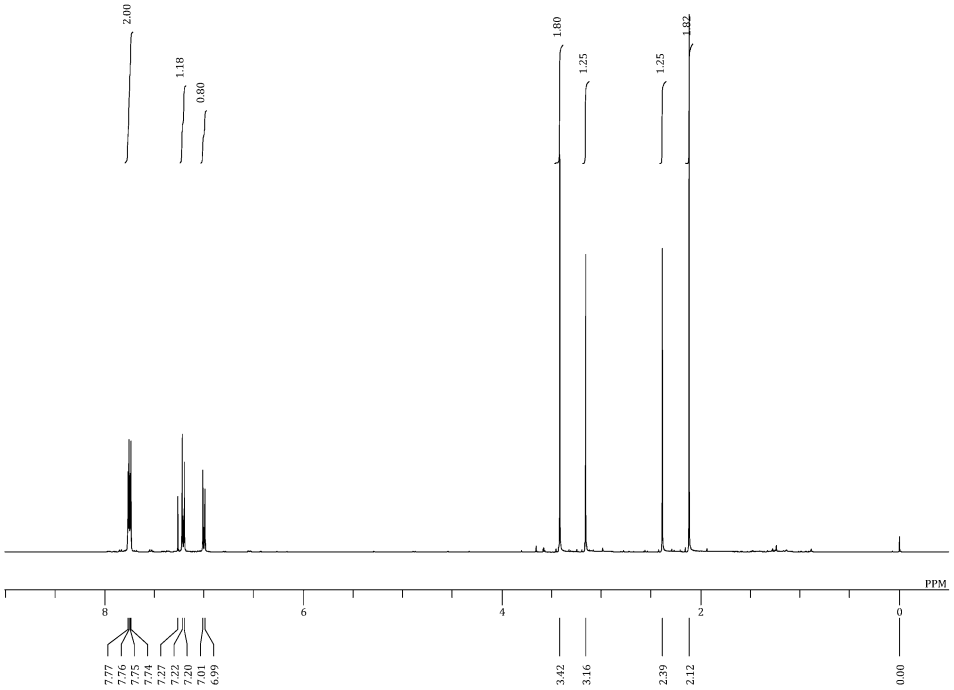

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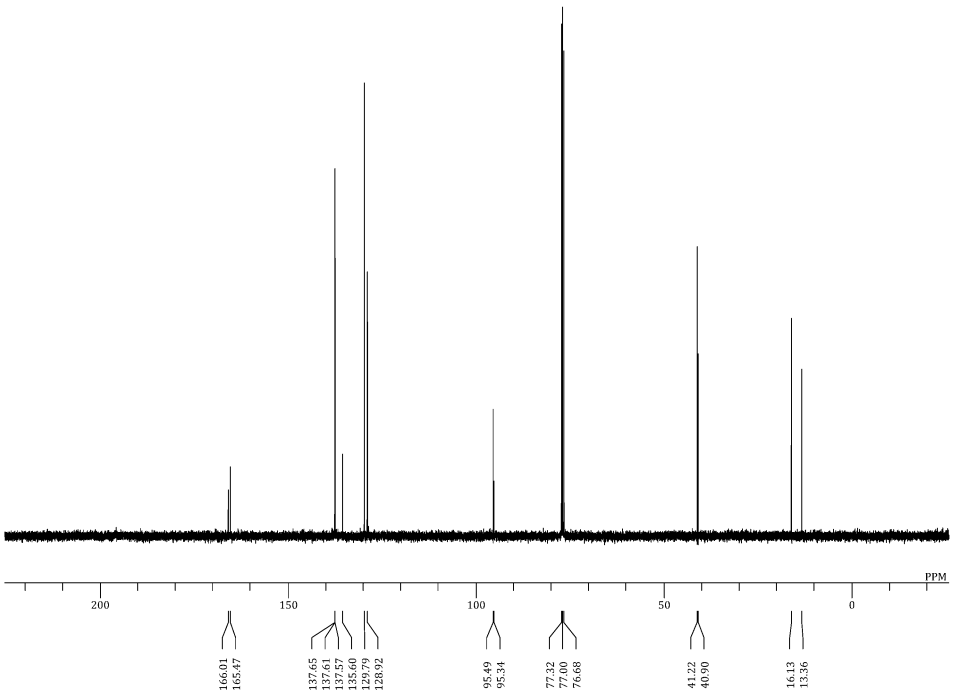

Compound **2-*I***

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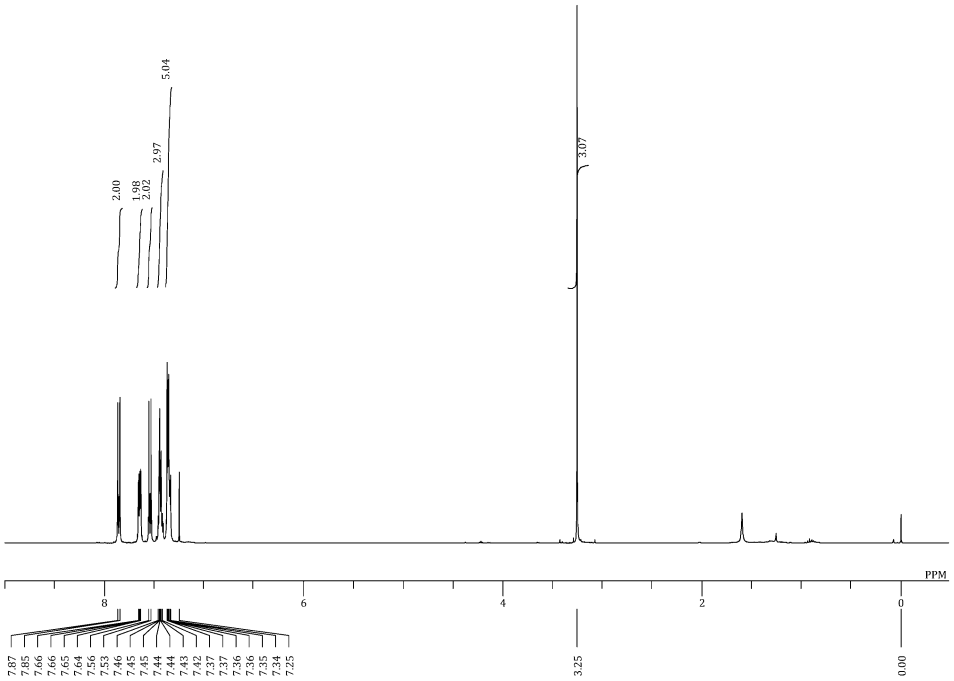

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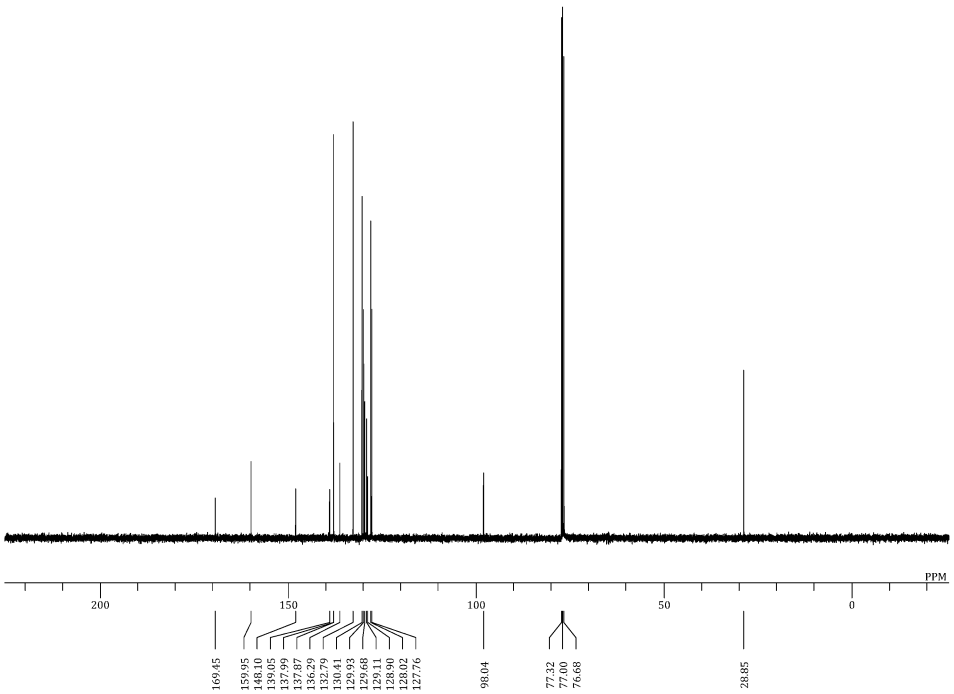
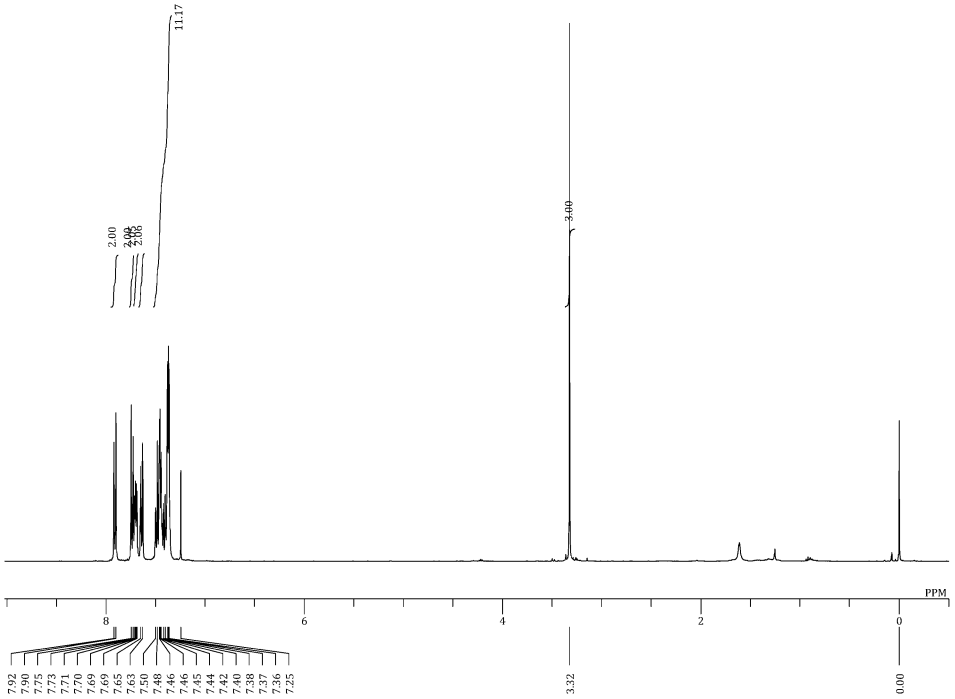


Compound **1a**

^{1}H-NMR



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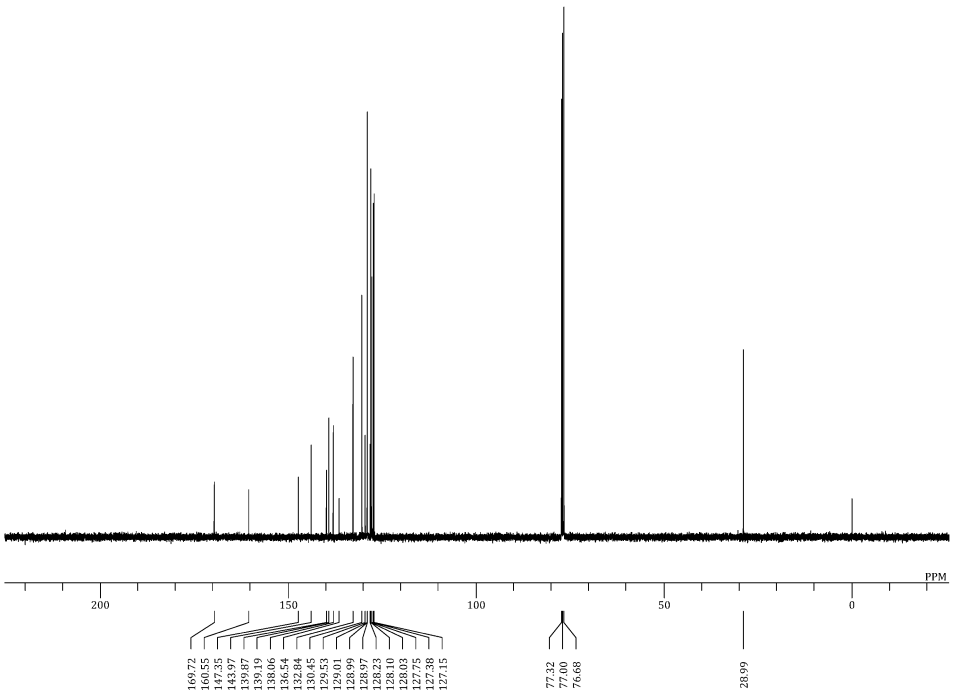

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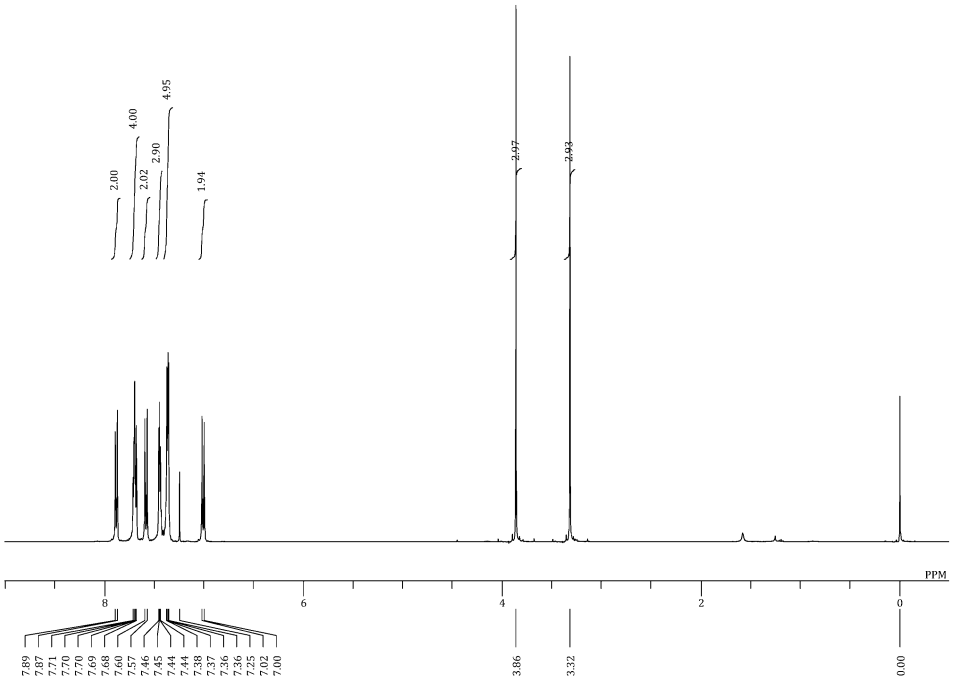

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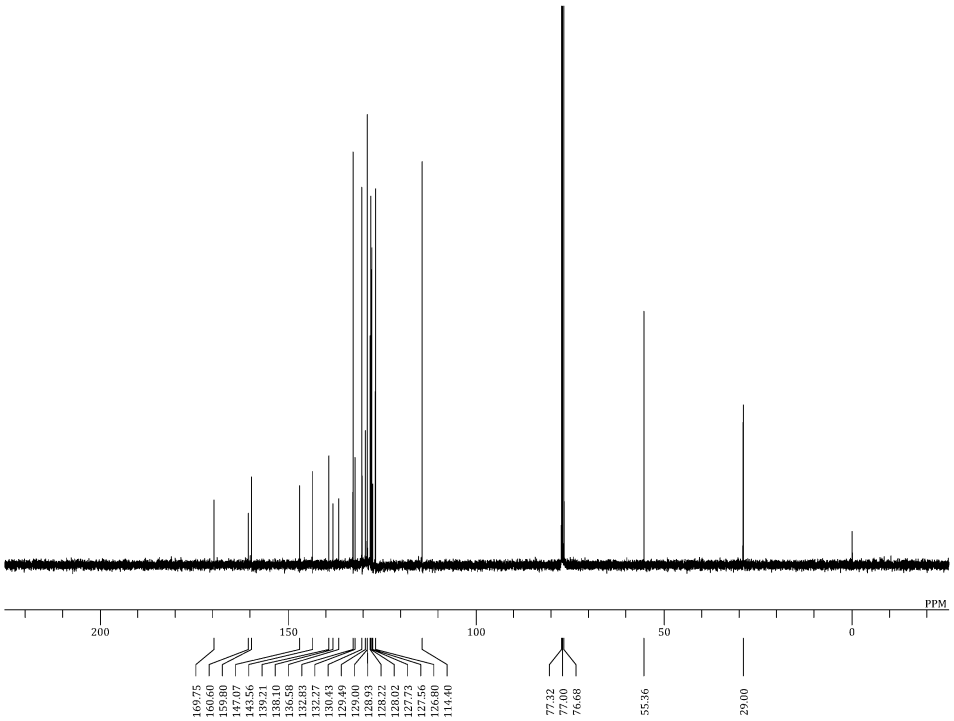

Compound **1c**

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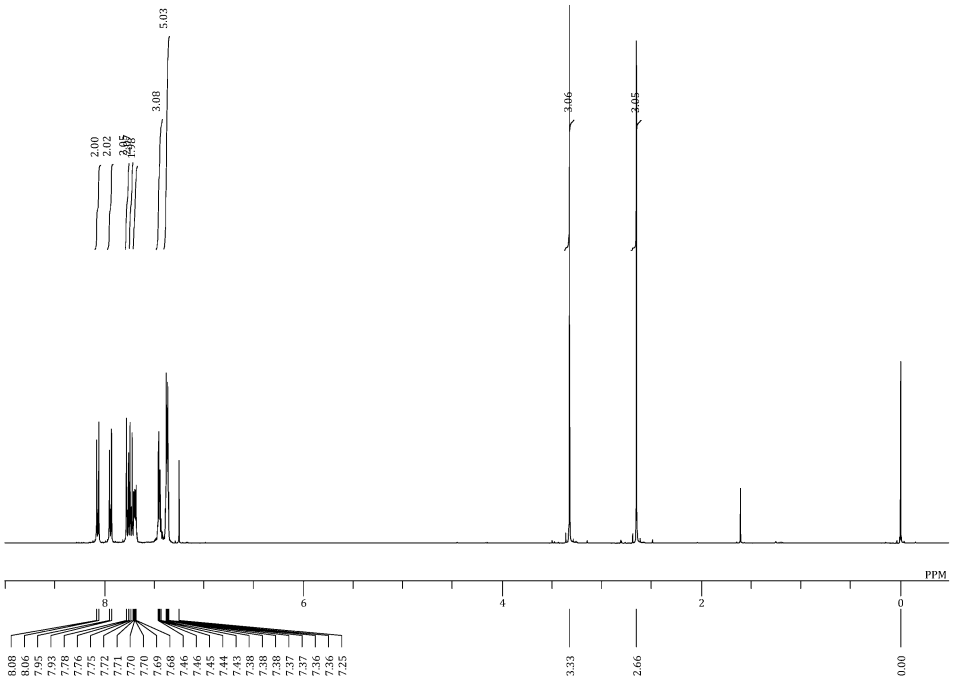

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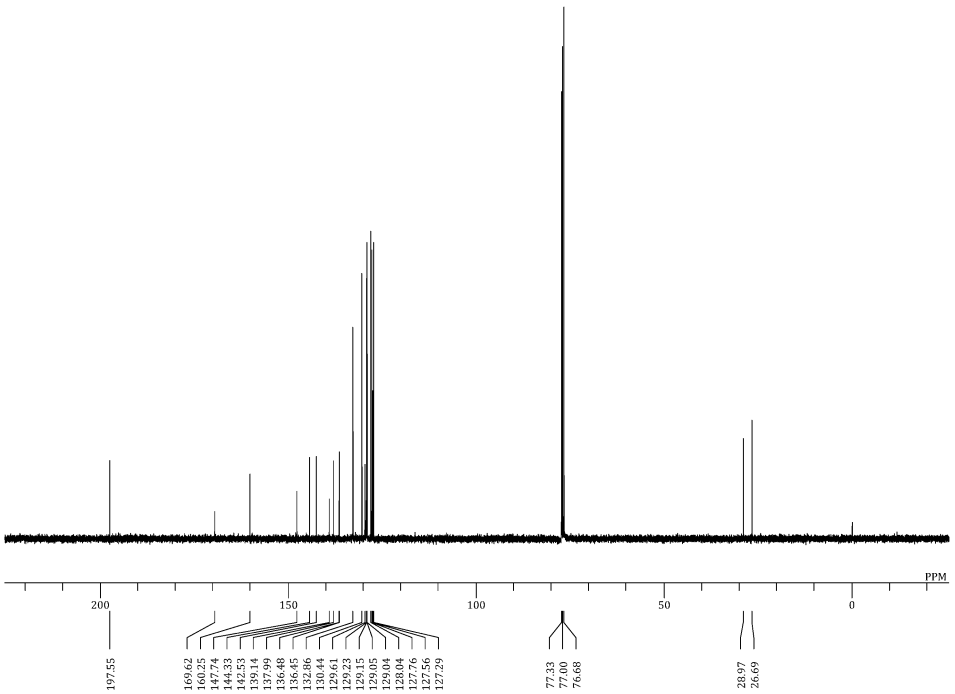

Compound **1d**

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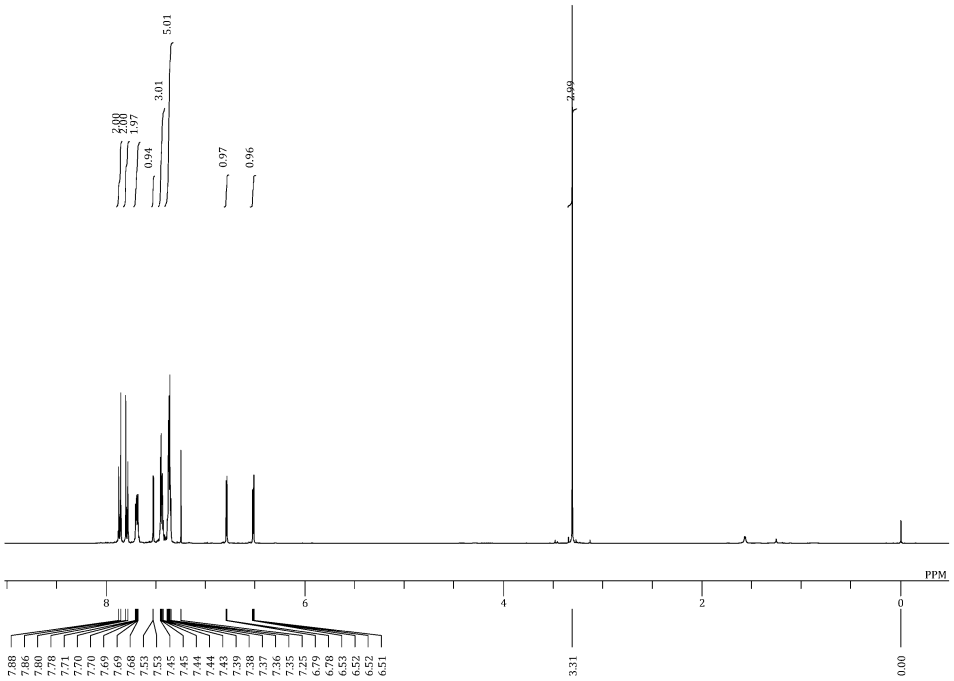

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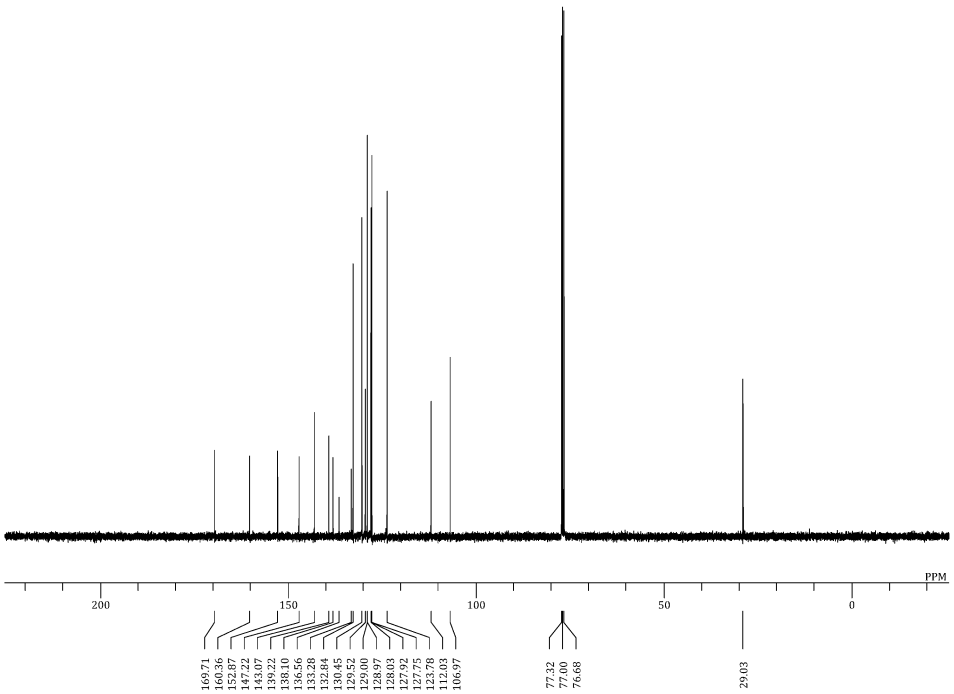

Compound **1e**

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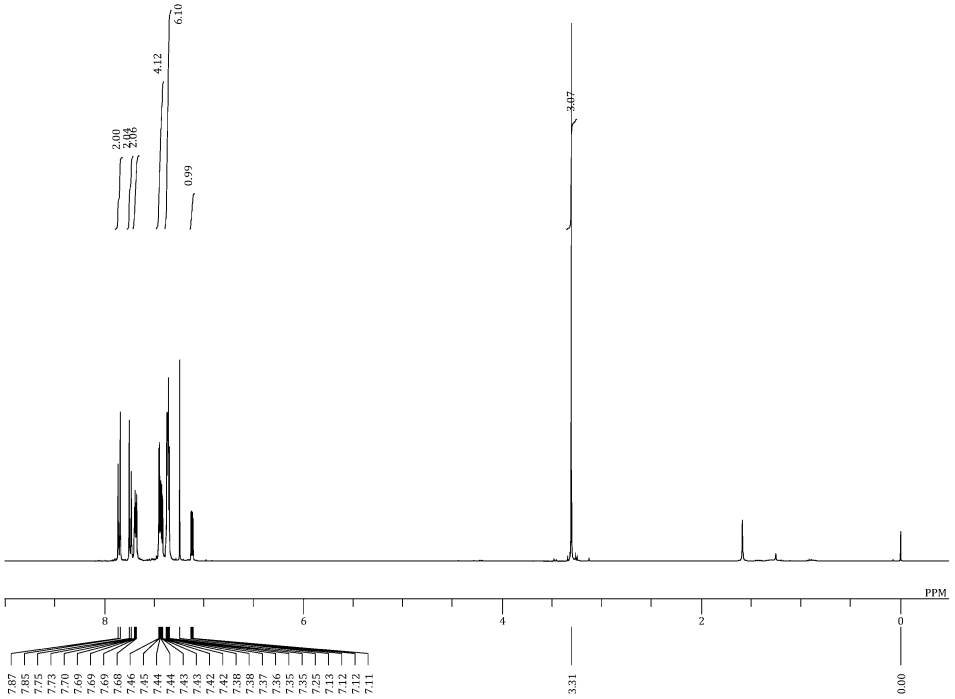

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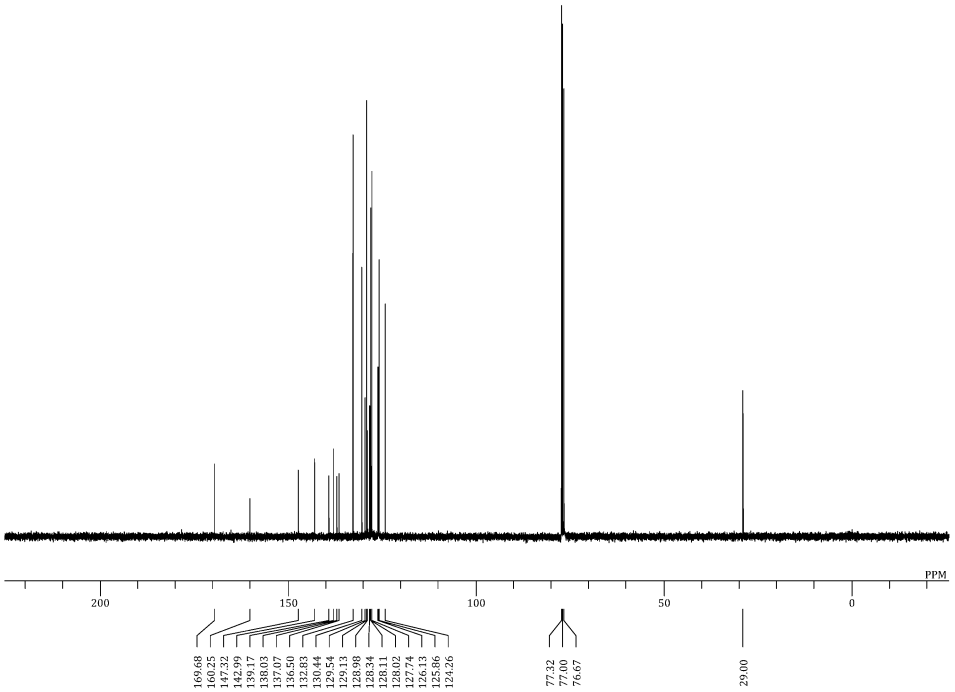
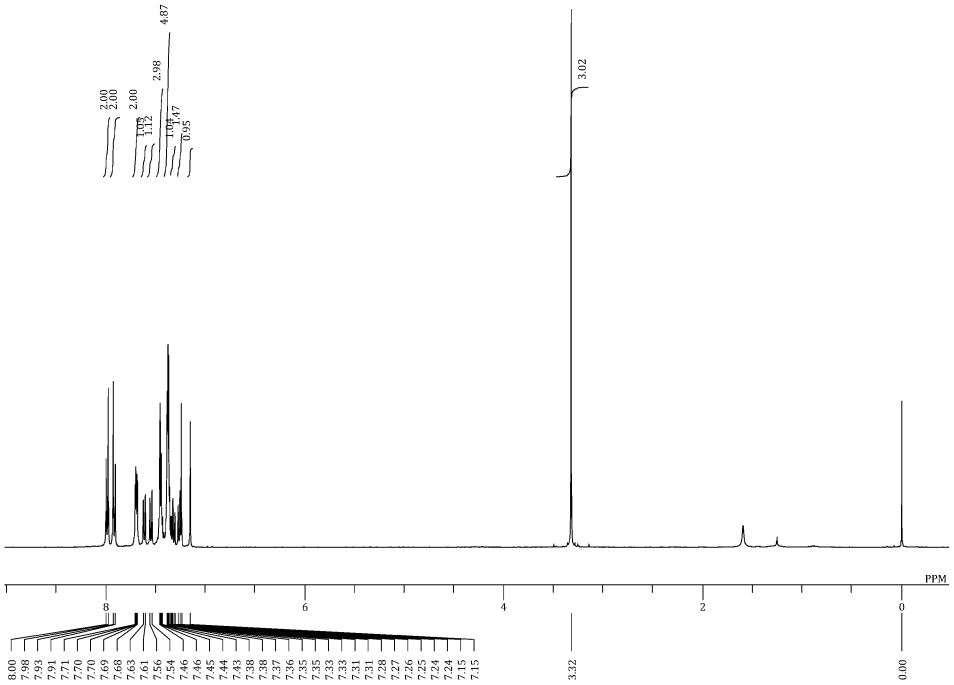


Compound **1f**

^{1}H-NMR



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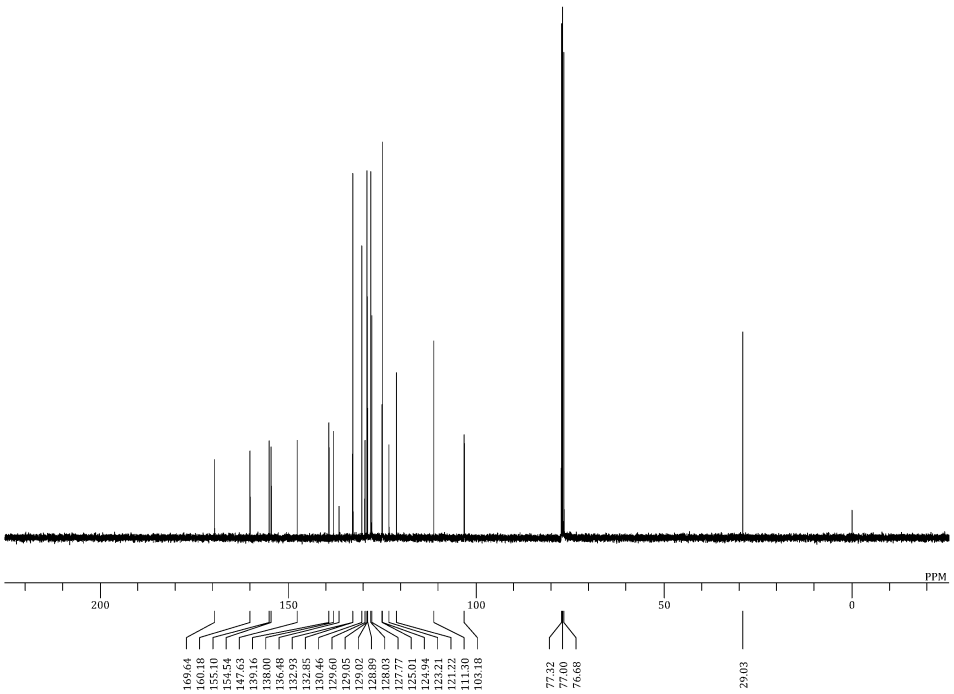
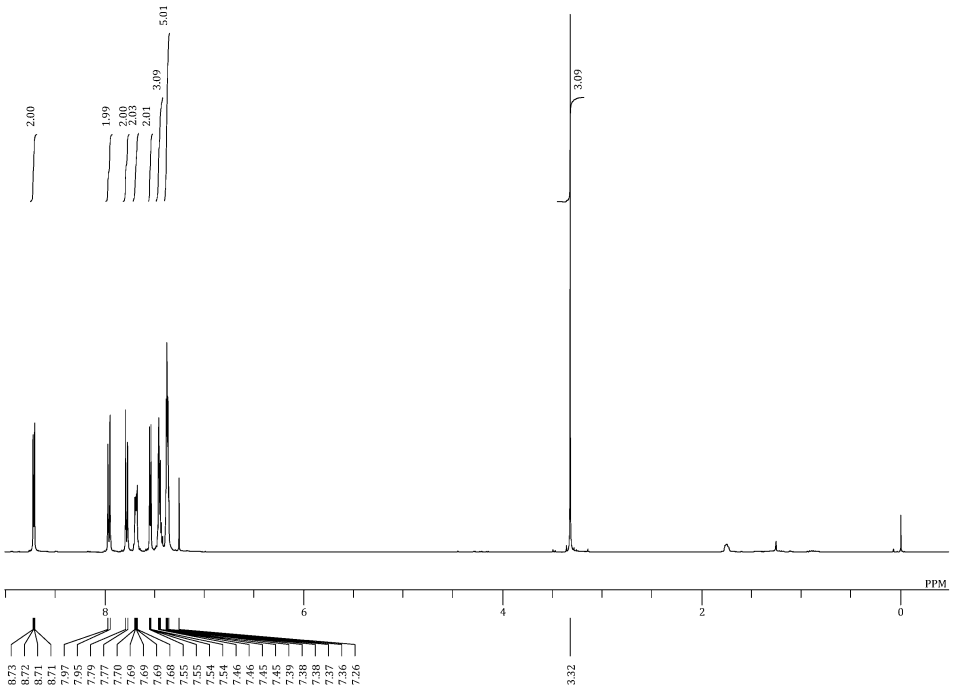


Compound **1g**

^{1}H-NMR



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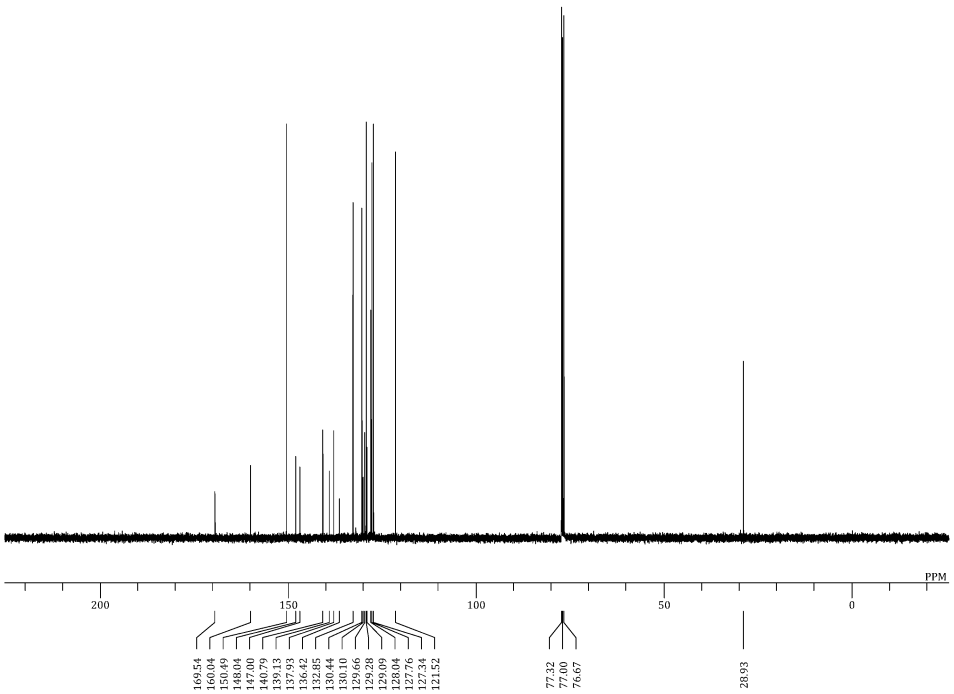

Compound **1h**

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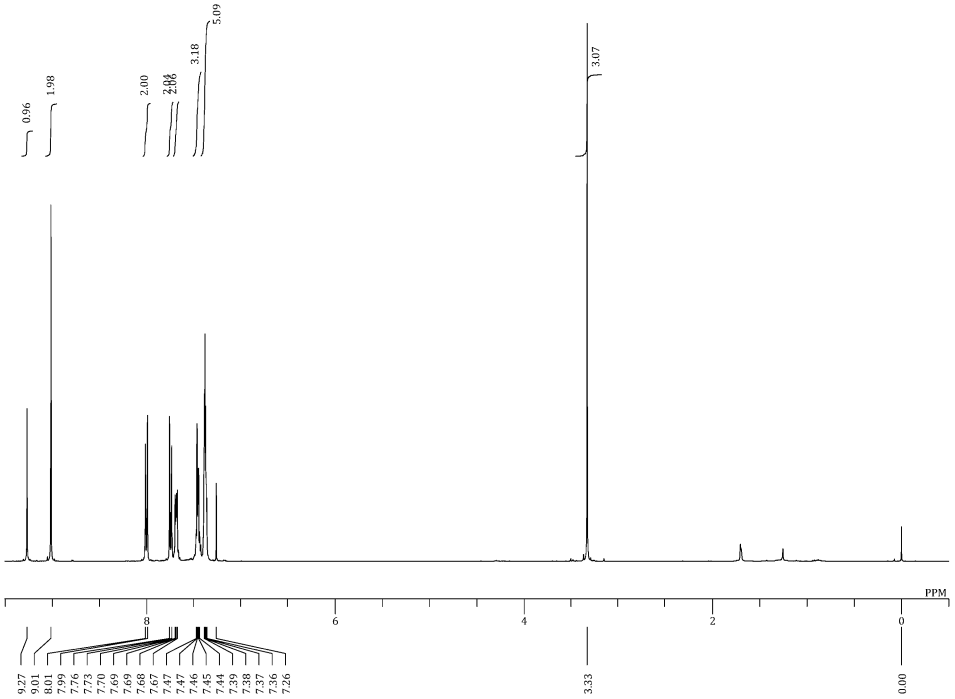

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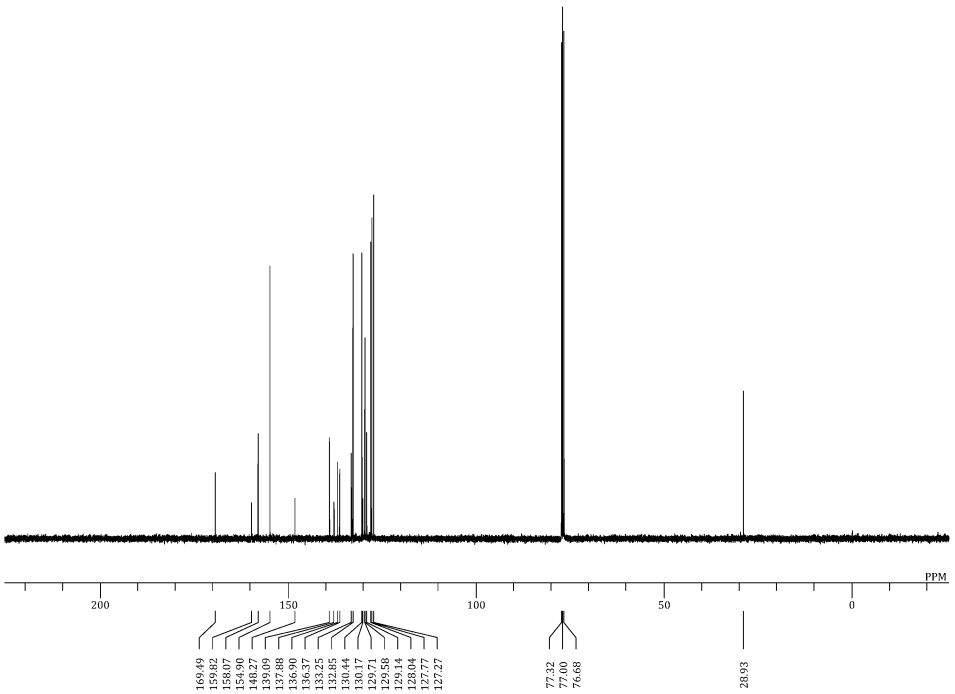

3. Mol2 files, energies and number of imaginary frequencies for computed structures

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38	C38	2.138708928	1.602276311	0.833329650	C.ar	1	noname
39	H39	1.589150089	-3.762323943	-0.980287870	H	1	noname
40	H40	2.503839098	-1.727372872	-1.072433589	H	1	noname
41	H41	0.080549332	1.043900372	1.115918065	H	1	noname
42	H42	4.426207104	-0.239849992	-0.845677850	H	1	noname
43	H43	2.035548665	2.531057718	1.385219582	H	1	noname
44	C44	4.556732253	2.148789184	0.439006601	C.ar	1	noname
45	C45	6.784982298	3.847240159	0.706176403	C.ar	1	noname
46	C46	5.844908581	1.630583453	0.631112751	C.ar	1	noname
47	C47	4.420469188	3.534827041	0.385300953	C.ar	1	noname
48	C48	5.514432664	4.384995909	0.515666811	C.ar	1	noname
49	C49	6.941913056	2.460382888	0.763459223	C.ar	1	noname
50	H50	3.440624496	3.969100467	0.212512588	H	1	noname
51	H51	5.363384156	5.455823903	0.457786461	H	1	noname
52	H52	7.936962948	2.059379281	0.922548352	H	1	noname
53	H53	5.983882088	0.556303947	0.702484045	H	1	noname
54	O54	7.920304304	4.578241191	0.845877993	O.3	1	noname
55	C55	7.815847557	5.984872096	0.804465596	C.3	1	noname
56	H56	7.175253394	6.364641253	1.609501919	H	1	noname
57	H57	8.827717063	6.367486955	0.939854166	H	1	noname
58	H58	7.424915988	6.331342396	-0.159793033	H	1	noname

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9	9	12	ar
10	12	13	ar
11	10	13	ar
12	10	14	ar
13	11	14	ar
14	9	11	ar

15	7	9	1
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52	44	46	ar
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No imaginary frequencies
mol2 file:

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59 63
SMALL
NO_CHARGES


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      3     C3          -1.465491468      -3.214742358      -0.433674743       C.2     1    noname
      4     N4          -0.144988095      -2.758903613      -0.353972789       N.am    1    noname
      5     C5          -0.178410979      -1.379304223      -0.179679823       C.2     1    noname
      6     O6          -1.773906665      -4.383337752      -0.551554686       O.2     1    noname
      7     C7          -3.609345358      -1.818016364      -0.470380727       C.2     1    noname
      8     C8           0.956422340      -3.691358794      -0.247084057       C.3     1    noname
      9     C9          -4.249737193      -0.481646473      -0.537271824       C.ar    1    noname
     10     C10         -5.525903638       2.013358828      -0.646123629       C.ar    1    noname
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11	C11	-3.670319531	0.588526602	-1.229711740	C.ar	1	noname
12	C12	-5.486025525	-0.278164378	0.089135417	C.ar	1	noname
13	C13	-6.111996964	0.959724646	0.045998633	C.ar	1	noname
14	C14	-4.307102157	1.820375691	-1.287160528	C.ar	1	noname
15	C15	-4.519000899	-2.990801413	-0.537820749	C.ar	1	noname
16	C16	-6.299628526	-5.145108174	-0.667391699	C.ar	1	noname
17	C17	-5.467184190	-3.072240547	-1.562968576	C.ar	1	noname
18	C18	-4.487085341	-3.998341467	0.428272429	C.ar	1	noname
19	C19	-5.374536969	-5.063589627	0.367157688	C.ar	1	noname
20	C20	-6.341637952	-4.147623158	-1.635367052	C.ar	1	noname
21	H21	-7.061324108	-4.203119930	-2.446231370	H	1	noname
22	H22	-5.510218273	-2.286961847	-2.310916559	H	1	noname
23	H23	-5.339657896	-5.835567826	1.129428562	H	1	noname
24	H24	-3.763483818	-3.941877064	1.233082211	H	1	noname
25	H25	-5.952426010	-1.098604016	0.623742198	H	1	noname
26	H26	-7.062959367	1.099157584	0.550795562	H	1	noname
27	H27	-6.018862754	2.979794175	-0.689389395	H	1	noname
28	H28	-3.847134390	2.635058227	-1.838064735	H	1	noname
29	H29	-2.716822965	0.447647665	-1.720976662	H	1	noname
30	H30	0.518840390	-4.666546136	-0.027676665	H	1	noname
31	H31	1.635204122	-3.399286467	0.556448713	H	1	noname
32	H32	-6.989265997	-5.982188657	-0.717115160	H	1	noname
33	C33	1.012028340	-0.536001882	0.005946314	C.ar	1	noname
34	C34	3.200143874	1.200098374	0.382622450	C.ar	1	noname
35	C35	0.866341604	0.649821028	0.732696146	C.ar	1	noname
36	C36	2.260374677	-0.834996540	-0.542756112	C.ar	1	noname
37	C37	3.335585798	0.021969709	-0.355515082	C.ar	1	noname
38	C38	1.942752718	1.499206028	0.919419151	C.ar	1	noname
39	H39	1.516361244	-3.770602066	-1.183668408	H	1	noname
40	H40	2.395955754	-1.721281718	-1.150630559	H	1	noname
41	H41	-0.106517877	0.885174453	1.148469417	H	1	noname
42	H42	4.288920193	-0.214046824	-0.817120345	H	1	noname
43	H43	1.814482866	2.397858041	1.514161836	H	1	noname
44	C44	4.353643693	2.107867053	0.585600785	C.ar	1	noname
45	C45	6.544723437	3.831203339	0.968233921	C.ar	1	noname
46	C46	5.641671413	1.598177064	0.788778120	C.ar	1	noname
47	C47	4.183918767	3.495158770	0.578223190	C.ar	1	noname
48	C48	5.263944924	4.345844246	0.767226744	C.ar	1	noname
49	C49	6.719291375	2.446188685	0.977011604	C.ar	1	noname
50	H50	3.198784369	3.912988174	0.397818179	H	1	noname
51	H51	5.099526270	5.418034955	0.749060324	H	1	noname
52	H52	7.717618460	2.056649993	1.142486973	H	1	noname
53	H53	5.791512103	0.523784212	0.823575558	H	1	noname
54	C54	7.746105926	4.697384701	1.176951481	C.2	1	noname
55	C55	7.575158370	6.200395375	1.157595369	C.3	1	noname
56	O56	8.839957669	4.199305015	1.359567935	O.2	1	noname
57	H57	8.550148422	6.663138746	1.309998674	H	1	noname
58	H58	6.889432180	6.526962429	1.946139375	H	1	noname
59	H59	7.160327116	6.535858592	0.201450709	H	1	noname

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9	9	12	ar
10	12	13	ar
11	10	13	ar
12	10	14	ar
13	11	14	ar
14	9	11	ar
15	7	9	1
16	15	18	ar
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23	20	21	1

24	17	22	1
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51 55
SMALL
NO_CHARGES

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3	C3	0.334549709	0.212854911	2.429772001	C.2	1	noname
4	N4	-0.983506405	0.223853559	1.961966412	N.am	1	noname
5	C5	-0.948687382	0.065412725	0.579923418	C.2	1	noname
6	O6	0.638950315	0.293379215	3.602716414	O.2	1	noname
7	C7	2.490020270	0.131886190	1.054493968	C.2	1	noname
8	C8	-2.096911498	0.172935455	2.884752886	C.3	1	noname
9	C9	3.150951512	0.170811220	-0.272652746	C.ar	1	noname
10	C10	4.465767986	0.219558862	-2.749839138	C.ar	1	noname
11	C11	2.625084002	0.898436273	-1.347494133	C.ar	1	noname
12	C12	4.353906973	-0.521595485	-0.462628100	C.ar	1	noname
13	C13	4.998594073	-0.507737383	-1.691514634	C.ar	1	noname
14	C14	3.281109460	0.925469598	-2.570237617	C.ar	1	noname
15	C15	3.388053045	0.130198768	2.238399243	C.ar	1	noname
16	C16	5.149974889	0.122742400	4.412187785	C.ar	1	noname
17	C17	4.395648999	1.094686347	2.343732084	C.ar	1	noname
18	C18	3.287023668	-0.845561563	3.231835630	C.ar	1	noname

19	C19	4.164751745	-0.852624363	4.306815299	C.ar	1	noname
20	C20	5.261254903	1.099651983	3.428811776	C.ar	1	noname
21	H21	6.028138299	1.864500512	3.502654202	H	1	noname
22	H22	4.492795399	1.848610209	1.568978216	H	1	noname
23	H23	4.075241074	-1.621542074	5.067756501	H	1	noname
24	H24	2.516515559	-1.604109833	3.156808340	H	1	noname
25	H25	4.778687411	-1.084299683	0.361550087	H	1	noname
26	H26	5.922436128	-1.063257705	-1.820249585	H	1	noname
27	H27	4.973500849	0.239587870	-3.709399468	H	1	noname
28	H28	2.862904439	1.503582921	-3.388588491	H	1	noname
29	H29	1.697567803	1.439667415	-1.217571574	H	1	noname
30	H30	-1.682066491	-0.089799056	3.859248697	H	1	noname
31	H31	-2.823555497	-0.580375816	2.574752309	H	1	noname
32	H32	5.832269348	0.119287647	5.256757193	H	1	noname
33	C33	-2.139950337	-0.032378839	-0.275132478	C.ar	1	noname
34	C34	-4.325847298	-0.242507204	-2.034020848	C.ar	1	noname
35	C35	-2.025374631	-0.739594815	-1.478141617	C.ar	1	noname
36	C36	-3.357749681	0.581374522	0.024540192	C.ar	1	noname
37	C37	-4.435164646	0.478579104	-0.842420203	C.ar	1	noname
38	C38	-3.099729964	-0.846218006	-2.340012285	C.ar	1	noname
39	H39	-2.596270537	1.142119731	2.975933598	H	1	noname
40	H40	-3.468724573	1.170725115	0.926510237	H	1	noname
41	H41	-1.073048956	-1.197747823	-1.718702588	H	1	noname
42	H42	-5.372347066	0.965965167	-0.600418952	H	1	noname
43	H43	-2.988511554	-1.406034878	-3.262850566	H	1	noname
44	C44	-5.458927048	-0.361007504	-2.942025469	C.2	1	noname
45	C45	-7.530567955	0.024158340	-3.546026821	C.2	1	noname
46	C46	-6.990433761	-0.730603573	-4.533142154	C.2	1	noname
47	C47	-5.641462423	-0.982562696	-4.141915558	C.2	1	noname
48	O48	-6.616998613	0.257583194	-2.573855432	O.3	1	noname
49	H49	-7.486661178	-1.068882968	-5.430835771	H	1	noname
50	H50	-8.505562720	0.457901022	-3.388584541	H	1	noname
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51 55
SMALL
NO_CHARGES

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3	C3	0.412664528	0.011947458	2.475895889	C.2	1	noname
4	N4	-0.921687855	0.049599388	2.057895184	N.am	1	noname
5	C5	-0.935981273	0.007264865	0.667356336	C.2	1	noname
6	O6	0.758953667	-0.000370595	3.639856700	O.2	1	noname
7	C7	2.516912969	0.064500476	1.021228740	C.2	1	noname
8	C8	-2.001481354	-0.084919993	3.011831896	C.3	1	noname
9	C9	3.126772129	0.222487228	-0.321789296	C.ar	1	noname
10	C10	4.346667065	0.495943963	-2.832785468	C.ar	1	noname
11	C11	2.557240918	1.035848982	-1.309207970	C.ar	1	noname
12	C12	4.325221888	-0.440768455	-0.615550454	C.ar	1	noname
13	C13	4.922724671	-0.315523594	-1.861985100	C.ar	1	noname
14	C14	3.166271532	1.173975601	-2.548762882	C.ar	1	noname
15	C15	3.458655994	-0.029445974	2.166996237	C.ar	1	noname
16	C16	5.299750874	-0.204608676	4.267010096	C.ar	1	noname
17	C17	4.464867594	0.930699036	2.315898411	C.ar	1	noname
18	C18	3.398897230	-1.085342862	3.078615103	C.ar	1	noname
19	C19	4.315963980	-1.175318673	4.116485809	C.ar	1	noname
20	C20	5.369915427	0.851753928	3.365316628	C.ar	1	noname
21	H21	6.135314984	1.613791708	3.474957107	H	1	noname
22	H22	4.529852935	1.747732463	1.604359239	H	1	noname
23	H23	4.258189885	-2.005704954	4.813179715	H	1	noname
24	H24	2.629882708	-1.841127225	2.968603573	H	1	noname
25	H25	4.784188784	-1.068676859	0.140416995	H	1	noname
26	H26	5.843820800	-0.850136105	-2.072774219	H	1	noname
27	H27	4.817722285	0.602837691	-3.805190268	H	1	noname
28	H28	2.714591073	1.817300875	-3.297700688	H	1	noname
29	H29	1.632988066	1.556773642	-1.098133274	H	1	noname
30	H30	-1.550758598	-0.422001277	3.946644178	H	1	noname
31	H31	-2.734583497	-0.816857262	2.667576934	H	1	noname
32	H32	6.012797620	-0.273138663	5.082902205	H	1	noname
33	C33	-2.156693971	-0.029624179	-0.150794971	C.ar	1	noname
34	C34	-4.407280532	-0.113168079	-1.846980472	C.ar	1	noname
35	C35	-3.366720189	0.545274498	0.241716865	C.ar	1	noname
36	C36	-2.082476054	-0.636149056	-1.409747773	C.ar	1	noname
37	C37	-3.189448827	-0.686196638	-2.236398279	C.ar	1	noname
38	C38	-4.471351247	0.507520327	-0.596382318	C.ar	1	noname
39	H39	-2.502447115	0.869671575	3.198443595	H	1	noname
40	H40	-1.139631130	-1.072820893	-1.718190619	H	1	noname
41	H41	-3.448543018	1.061243506	1.190494024	H	1	noname
42	H42	-3.120149313	-1.195072983	-3.191903166	H	1	noname

43	H43	-5.391451285	0.990013003	-0.281837130	H	1	noname
44	C44	-5.568882233	-0.162027938	-2.742342425	C.2	1	noname
45	C45	-7.861659390	-0.218637177	-3.714591715	C.2	1	noname
46	C46	-6.888825910	-0.263391391	-4.664834571	C.2	1	noname
47	C47	-5.579166674	-0.232065511	-4.108784072	C.2	1	noname
48	S48	-7.196765812	-0.138370256	-2.127262410	S.3	1	noname
49	H49	-7.091919317	-0.311150514	-5.727982797	H	1	noname
50	H50	-8.933488418	-0.231010523	-3.854050859	H	1	noname
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9	9	12	ar
10	12	13	ar
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13	11	14	ar
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35	33	36	ar
36	36	37	ar
37	34	37	ar
38	34	38	ar
39	35	38	ar
40	33	35	ar
41	5	33	1
42	8	39	1
43	36	40	1
44	35	41	1
45	37	42	1
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mol2 file:
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File Created by: Spartan '18 Export
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M0003
57 62
SMALL
NO_CHARGES

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3	C3	-1.320801197	-0.293229821	2.973528878	C.2	1	noname
4	N4	-0.011533251	-0.399354424	2.491944250	N.am	1	noname
5	C5	-0.038452004	-0.154562549	1.122725188	C.2	1	noname
6	O6	-1.625551999	-0.416595287	4.142583094	O.2	1	noname
7	C7	-3.465713982	0.071316351	1.626539750	C.2	1	noname
8	C8	1.105885311	-0.512815132	3.404407004	C.3	1	noname
9	C9	-4.130204603	0.170381089	0.304311617	C.ar	1	noname
10	C10	-5.448706876	0.384997594	-2.161633248	C.ar	1	noname
11	C11	-3.680895649	-0.546234322	-0.811809318	C.ar	1	noname
12	C12	-5.259527361	0.986914428	0.161101531	C.ar	1	noname
13	C13	-5.904933433	1.102997316	-1.061946729	C.ar	1	noname
14	C14	-4.339044302	-0.442734850	-2.029292158	C.ar	1	noname
15	C15	-4.356722322	0.088168228	2.815124318	C.ar	1	noname
16	C16	-6.107481875	0.134781053	4.997304758	C.ar	1	noname
17	C17	-5.456434957	-0.774978402	2.866577378	C.ar	1	noname
18	C18	-4.157063693	0.983840836	3.867466469	C.ar	1	noname
19	C19	-5.029026298	1.010913003	4.946772763	C.ar	1	noname
20	C20	-6.317216965	-0.761870645	3.955307684	C.ar	1	noname
21	H21	-7.157143510	-1.448945548	3.986362473	H	1	noname
22	H22	-5.629773408	-1.464587744	2.046605218	H	1	noname
23	H23	-4.862162515	1.717307531	5.753872919	H	1	noname
24	H24	-3.314475337	1.664643469	3.834921240	H	1	noname
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26	H26	-6.769875399	1.752629454	-1.153989287	H	1	noname
27	H27	-5.958247785	0.466775908	-3.116937316	H	1	noname
28	H28	-3.981910658	-1.014292531	-2.880484676	H	1	noname
29	H29	-2.811341460	-1.182800032	-0.717746686	H	1	noname
30	H30	0.721484334	-0.276758265	4.398019097	H	1	noname
31	H31	1.898806406	0.188111805	3.136744040	H	1	noname
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33	C33	1.151437485	-0.117201460	0.260164354	C.ar	1	noname
34	C34	3.333731598	-0.005479375	-1.508538760	C.ar	1	noname
35	C35	1.093109540	0.666591098	-0.898969456	C.ar	1	noname
36	C36	2.309303894	-0.855812746	0.510474390	C.ar	1	noname
37	C37	3.386026446	-0.801405098	-0.362126157	C.ar	1	noname
38	C38	2.166529008	0.724526443	-1.766072227	C.ar	1	noname
39	H39	1.512303519	-1.528311035	3.427608384	H	1	noname
40	H40	2.371529531	-1.503846755	1.375964856	H	1	noname
41	H41	0.184911452	1.222424555	-1.100801660	H	1	noname
42	H42	4.276711368	-1.384519822	-0.160849398	H	1	noname
43	H43	2.100944510	1.344555992	-2.653972759	H	1	noname
44	C44	6.820897215	0.726604256	-5.105273090	C.ar	1	noname
45	C45	7.759912259	-1.061047423	-3.101429383	C.ar	1	noname
46	C46	6.005174363	0.391519568	-4.019261866	C.ar	1	noname
47	C47	8.086115553	0.167969702	-5.175336260	C.ar	1	noname
48	C48	8.550587039	-0.714317076	-4.187023663	C.ar	1	noname
49	C49	6.498407747	-0.490641185	-3.051714642	C.ar	1	noname
50	C50	4.679961639	0.732882825	-3.580797380	C.2	1	noname
51	C51	4.468569867	0.059531677	-2.420782986	C.2	1	noname
52	O52	5.566380161	-0.693065196	-2.080325581	O.3	1	noname
53	H53	3.982930228	1.394979133	-4.072925306	H	1	noname
54	H54	6.470609947	1.407742614	-5.874243338	H	1	noname
55	H55	8.734453482	0.415000364	-6.009889644	H	1	noname
56	H56	9.547770796	-1.133435106	-4.273877659	H	1	noname
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6	3	6	2

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13	11	14	ar
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53 57
SMALL
NO_CHARGES


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3	C3	0.499389549	0.328683289	2.579227286	C.2	1	noname
4	N4	-0.805357447	0.232389471	2.082771891	N.am	1	noname
5	C5	-0.725550522	0.038961079	0.707815379	C.2	1	noname
6	O6	0.768288376	0.463655702	3.755724241	O.2	1	noname
7	C7	2.686129236	0.369981253	1.249794393	C.2	1	noname
8	C8	-1.934838790	0.135101812	2.982036003	C.3	1	noname
9	C9	3.365054778	0.430003786	-0.067553674	C.ar	1	noname
10	C10	4.712576383	0.527552073	-2.524378711	C.ar	1	noname
11	C11	2.811212679	1.108273436	-1.160225196	C.ar	1	noname
12	C12	4.612203077	-0.187574318	-0.228492198	C.ar	1	noname
13	C13	5.273658018	-0.150306926	-1.447816847	C.ar	1	noname
14	C14	3.483337766	1.160305303	-2.373240205	C.ar	1	noname
15	C15	3.560225878	0.461129187	2.446804541	C.ar	1	noname
16	C16	5.277500872	0.635274653	4.648876560	C.ar	1	noname
17	C17	4.507746276	1.486809755	2.533645329	C.ar	1	noname
18	C18	3.497396242	-0.483284765	3.473423634	C.ar	1	noname
19	C19	4.353519093	-0.400170855	4.562539864	C.ar	1	noname
20	C20	5.350421834	1.581592365	3.632470067	C.ar	1	noname
21	H21	6.069795216	2.392456759	3.691431151	H	1	noname
22	H22	4.575136701	2.217281188	1.733803057	H	1	noname
23	H23	4.295100613	-1.145749301	5.349236704	H	1	noname
24	H24	2.774993250	-1.288748425	3.412533370	H	1	noname
25	H25	5.058197489	-0.710627192	0.610496578	H	1	noname
26	H26	6.232500313	-0.647946016	-1.554993889	H	1	noname
27	H27	5.233249675	0.566384378	-3.476377270	H	1	noname
28	H28	3.043089040	1.699951943	-3.206114478	H	1	noname
29	H29	1.850227917	1.593044609	-1.051422993	H	1	noname
30	H30	-1.526442864	-0.063772024	3.974174676	H	1	noname
31	H31	-2.599469475	-0.678303946	2.684673138	H	1	noname
32	H32	5.942483361	0.702279155	5.504497393	H	1	noname
33	C33	-1.886318377	-0.167579450	-0.172538816	C.ar	1	noname
34	C34	-4.008610891	-0.577877487	-1.975580208	C.ar	1	noname
35	C35	-3.146942924	0.378581928	0.076870173	C.ar	1	noname
36	C36	-1.695244261	-0.909581197	-1.342536562	C.ar	1	noname
37	C37	-2.740133060	-1.112125992	-2.226602488	C.ar	1	noname
38	C38	-4.191274755	0.173718786	-0.813208113	C.ar	1	noname
39	H39	-2.502587989	1.069294907	3.027261912	H	1	noname
40	H40	-0.712488119	-1.322197702	-1.538872776	H	1	noname
41	H41	-3.315013484	0.997113512	0.950088748	H	1	noname
42	H42	-2.578551536	-1.714768420	-3.114589231	H	1	noname
43	H43	-5.155537043	0.631092124	-0.616538053	H	1	noname
44	C44	-5.127883125	-0.797150366	-2.921156648	C.ar	1	noname
45	N45	-7.256723400	-1.211283753	-4.719633240	N.ar	1	noname
46	C46	-4.925426957	-0.810717957	-4.302028688	C.ar	1	noname
47	C47	-6.434346132	-0.998763933	-2.473119927	C.ar	1	noname
48	C48	-7.447795892	-1.198581416	-3.400966853	C.ar	1	noname
49	C49	-6.008698858	-1.018572338	-5.145378038	C.ar	1	noname
50	H50	-6.658920605	-1.024219588	-1.412043662	H	1	noname
51	H51	-8.469002168	-1.362865135	-3.063996194	H	1	noname
52	H52	-5.864843715	-1.025022042	-6.223622924	H	1	noname
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M0003
52 56
SMALL
NO_CHARGES

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3	C3	-0.374836609	-2.496984302	-0.321584680	C.2	1	noname
4	N4	0.930326433	-1.999425467	-0.225667619	N.am	1	noname
5	C5	0.849842908	-0.626918415	-0.018301231	C.2	1	noname
6	O6	-0.642559947	-3.672307937	-0.467127393	O.2	1	noname
7	C7	-2.562366444	-1.170509840	-0.345769647	C.2	1	noname
8	C8	2.060506390	-2.899130989	-0.139969082	C.3	1	noname
9	C9	-3.245121652	0.145057710	-0.395135373	C.ar	1	noname
10	C10	-4.600820476	2.597994801	-0.475598837	C.ar	1	noname
11	C11	-2.694285804	1.244758664	-1.064406692	C.ar	1	noname
12	C12	-4.493667814	0.297165891	0.222006210	C.ar	1	noname
13	C13	-5.159225155	1.514280453	0.193008586	C.ar	1	noname
14	C14	-3.370178108	2.455892506	-1.107657813	C.ar	1	noname
15	C15	-3.431561438	-2.370358422	-0.444691894	C.ar	1	noname
16	C16	-5.135817877	-4.580824682	-0.634804685	C.ar	1	noname
17	C17	-4.374343666	-2.458052956	-1.474566531	C.ar	1	noname
18	C18	-3.367290737	-3.400046411	0.496002534	C.ar	1	noname
19	C19	-4.216896124	-4.493452687	0.405085508	C.ar	1	noname
20	C20	-5.210563525	-3.561002895	-1.577142167	C.ar	1	noname
21	H21	-5.926224222	-3.620531318	-2.391206935	H	1	noname
22	H22	-4.443050016	-1.655997736	-2.202546767	H	1	noname

23	H23	-4.157030975	-5.282879739	1.147642727	H	1	noname
24	H24	-2.649144927	-3.337646321	1.305317201	H	1	noname
25	H25	-4.937680302	-0.546884070	0.738557739	H	1	noname
26	H26	-6.119331845	1.613969152	0.689700118	H	1	noname
27	H27	-5.124691786	3.548479216	-0.507989983	H	1	noname
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30	H30	1.652168518	-3.893846838	0.045681088	H	1	noname
31	H31	2.724957274	-2.612732652	0.677518575	H	1	noname
32	H32	-5.795574997	-5.439950361	-0.708245466	H	1	noname
33	C33	2.010128429	0.254535719	0.187763789	C.ar	1	noname
34	C34	4.130917993	2.057873385	0.598709053	C.ar	1	noname
35	C35	3.269369605	0.008520982	-0.362716012	C.ar	1	noname
36	C36	1.819557065	1.421794004	0.934175626	C.ar	1	noname
37	C37	2.864258765	2.305158812	1.139828422	C.ar	1	noname
38	C38	4.312810863	0.900071590	-0.160295135	C.ar	1	noname
39	H39	2.628324806	-2.932270676	-1.074578125	H	1	noname
40	H40	0.837522362	1.615737525	1.349520180	H	1	noname
41	H41	3.437117430	-0.862682298	-0.983902740	H	1	noname
42	H42	2.702802497	3.189104119	1.748812522	H	1	noname
43	H43	5.274841520	0.706427273	-0.624045603	H	1	noname
44	C44	5.247707642	3.000310438	0.818719523	C.ar	1	noname
45	C45	7.271732422	4.706129390	1.213192083	C.ar	1	noname
46	C46	5.073650688	4.384911937	0.814011651	C.ar	1	noname
47	C47	6.556361176	2.572462201	1.045605256	C.ar	1	noname
48	N48	7.570643365	3.409863596	1.238641751	N.ar	1	noname
49	N49	6.070443244	5.241841686	1.012595502	N.ar	1	noname
50	H50	6.789940442	1.510319047	1.089095905	H	1	noname
51	H51	8.093947114	5.399106657	1.372942990	H	1	noname
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8	4	8	1
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11	10	13	ar
12	10	14	ar
13	11	14	ar
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36	36	37	ar
37	34	37	ar
38	34	38	ar
39	35	38	ar
40	33	35	ar
41	5	33	1
42	8	39	1

43	36	40	1
44	35	41	1
45	37	42	1
46	38	43	1
47	44	47	ar
48	47	48	ar
49	45	48	ar
50	45	49	ar
51	46	49	ar
52	44	46	ar
53	34	44	1
54	47	50	1
55	45	51	1
56	46	52	1

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E = -1071.436857 hartrees
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mol2 file
#
File Created by: Spartan '18 Export
#

@<TRIPOS>MOLECULE
M0004
44 47
SMALL
NO_CHARGES

@<TRIPOS>ATOM

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3	C3	0.827164255	-1.748532846	-0.126667746	C.2	1	noname
4	N4	2.124206923	-1.235401211	-0.023397940	N.am	1	noname
5	C5	2.026330348	0.138474087	0.173159982	C.2	1	noname
6	O6	0.573406590	-2.928123187	-0.265203427	O.2	1	noname
7	C7	-1.377080335	-0.450188917	-0.168406537	C.2	1	noname
8	C8	3.264978226	-2.119201491	0.083226838	C.3	1	noname
9	C9	-2.079026175	0.855493487	-0.219519777	C.ar	1	noname
10	C10	-3.470999911	3.289113823	-0.299208789	C.ar	1	noname
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13	C13	-4.017480138	2.194215258	0.360802618	C.ar	1	noname
14	C14	-2.233915718	3.167794068	-0.922682129	C.ar	1	noname
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16	C16	-3.912919046	-3.890312935	-0.456221453	C.ar	1	noname
17	C17	-3.165788135	-1.765389785	-1.303938033	C.ar	1	noname
18	C18	-2.163239511	-2.685472276	0.678859818	C.ar	1	noname
19	C19	-3.001514757	-3.787851482	0.588775439	C.ar	1	noname
20	C20	-3.990808210	-2.876981747	-1.405416884	C.ar	1	noname
21	H21	-4.700271686	-2.948426807	-2.224018024	H	1	noname
22	H22	-3.237604508	-0.967931896	-2.036687087	H	1	noname
23	H23	-2.938969771	-4.572201701	1.336537042	H	1	noname
24	H24	-1.450052442	-2.612279653	1.491622983	H	1	noname
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28	H28	-1.804011882	4.015121615	-1.448030044	H	1	noname
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31	H31	3.926626362	-1.802618229	0.891615982	H	1	noname
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34	C34	5.269239059	2.831217417	0.818766444	C.ar	1	noname
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36	C36	2.975331459	2.181578473	1.155967425	C.ar	1	noname
37	C37	4.014928653	3.072698332	1.371946547	C.ar	1	noname
38	C38	5.474466565	1.697449368	0.042058924	C.ar	1	noname
39	H39	3.832563485	-2.167829919	-0.850862730	H	1	noname
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35	33	36	ar
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