SUPPORTING INFORMATION

Unusual Aryl Migration in a Mesomeric Betaine in the Solid and Liquid State: Mechanistic Insights into an Intramolecular S_NAr Reaction

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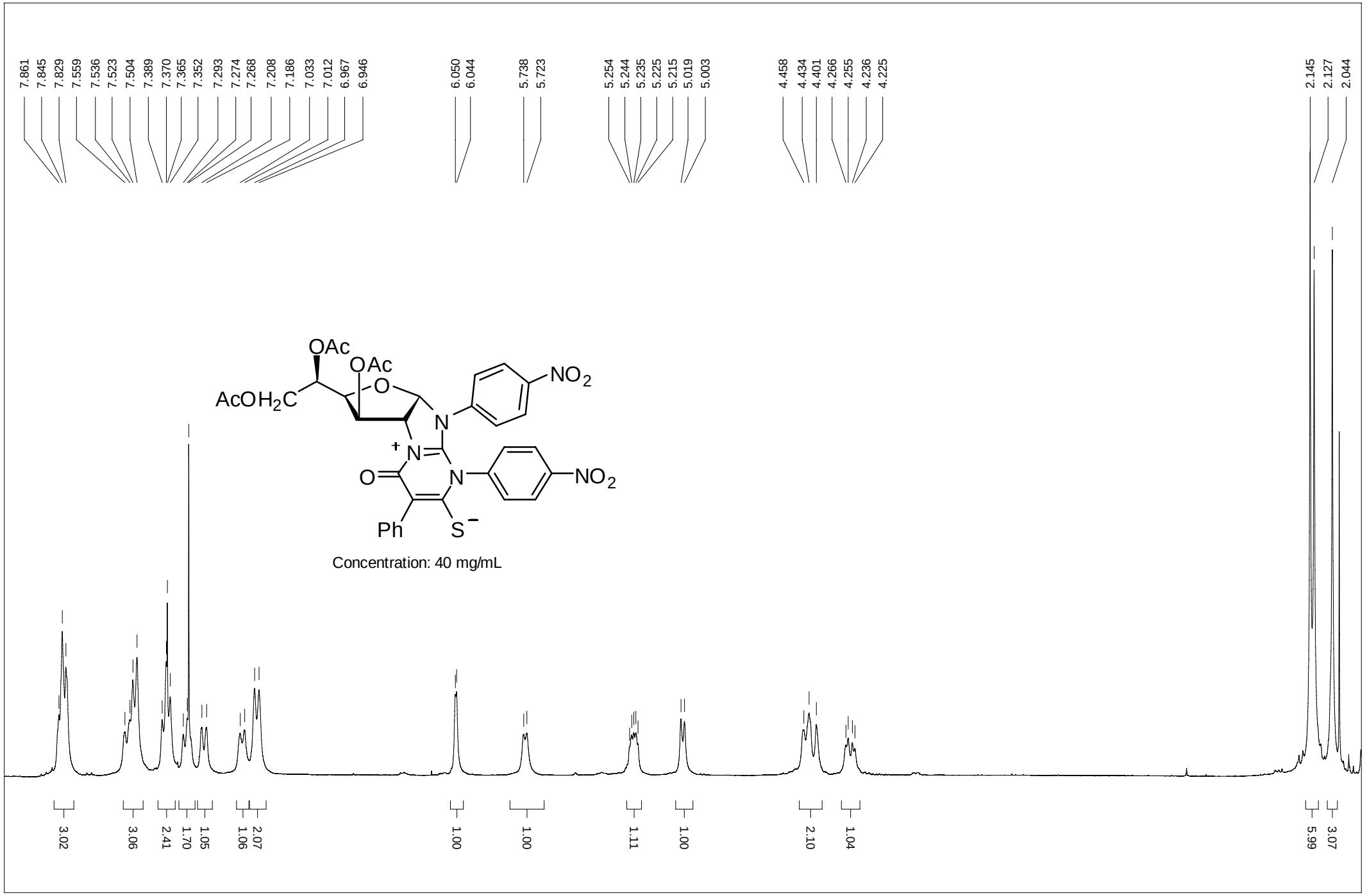
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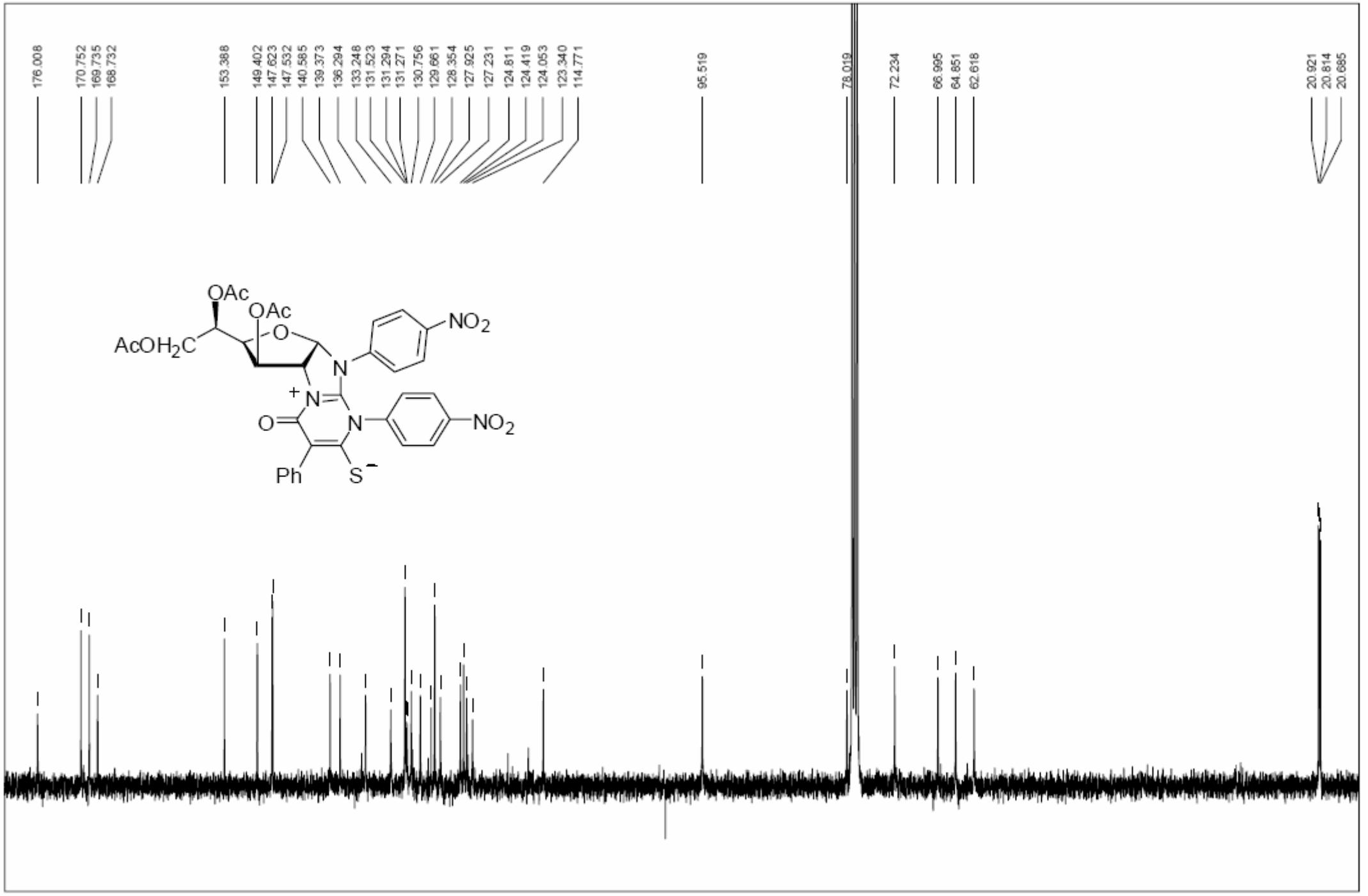
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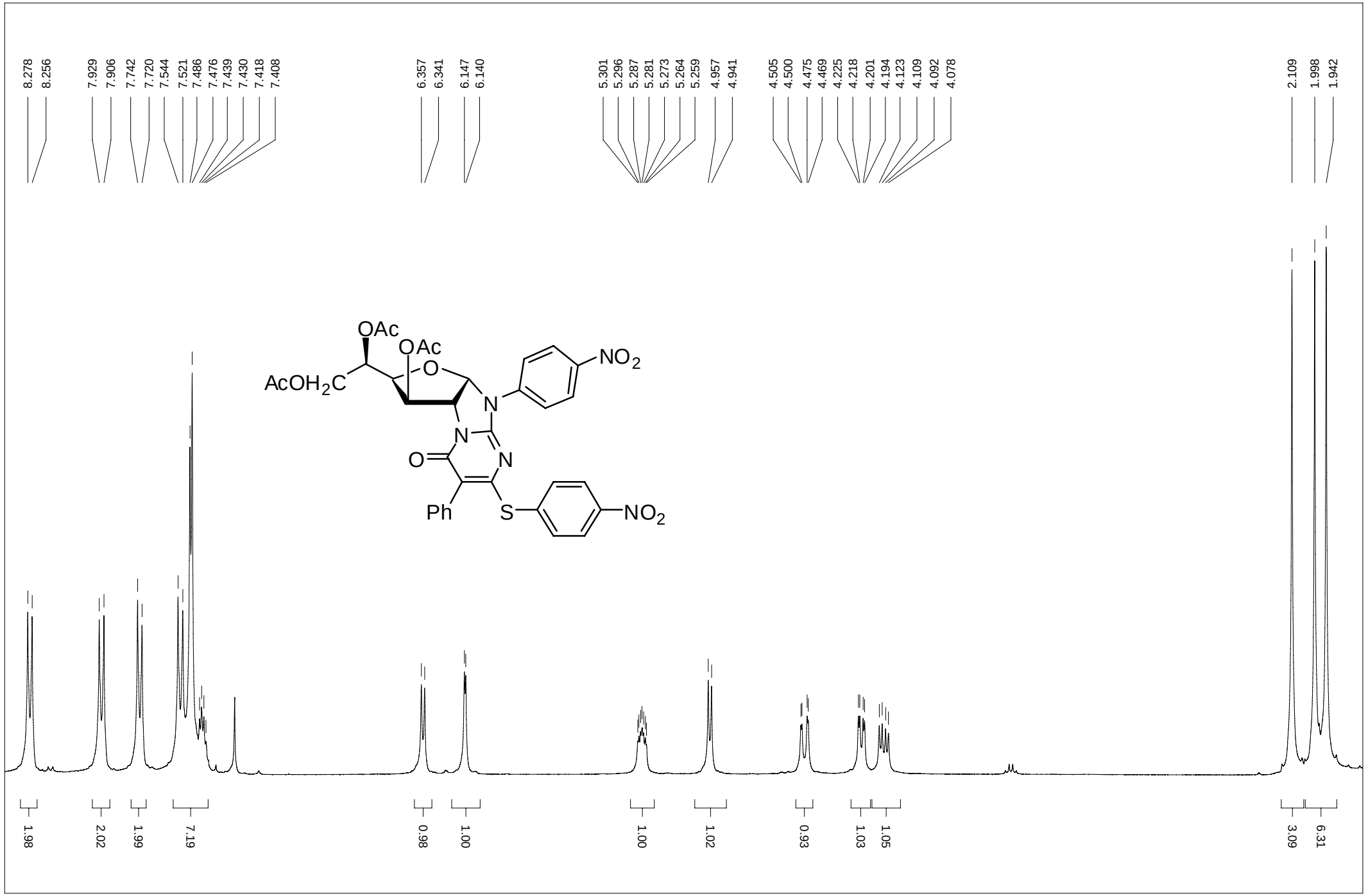
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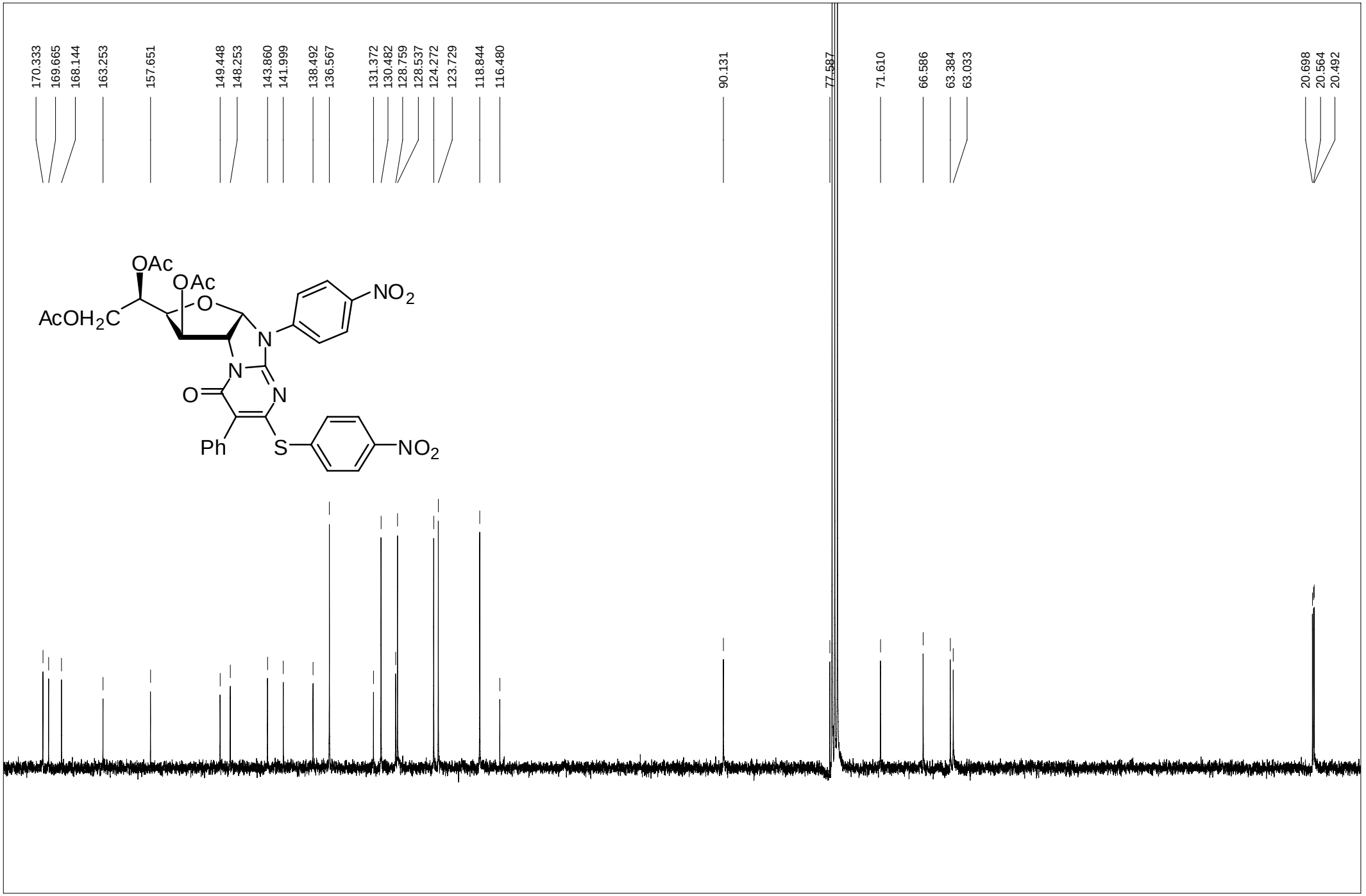
1,6-bis(4-nitrophenyl)-4-oxo-3-phenyl-(3',5',6'-tri-*O*-acetyl-1,2-dideoxy-α-D-glucofurano)[1',2':4,5]-5a*H*,5b*H*-imidazo[2,1-*a*]pyrimidin-5-ylium-2-thiolate



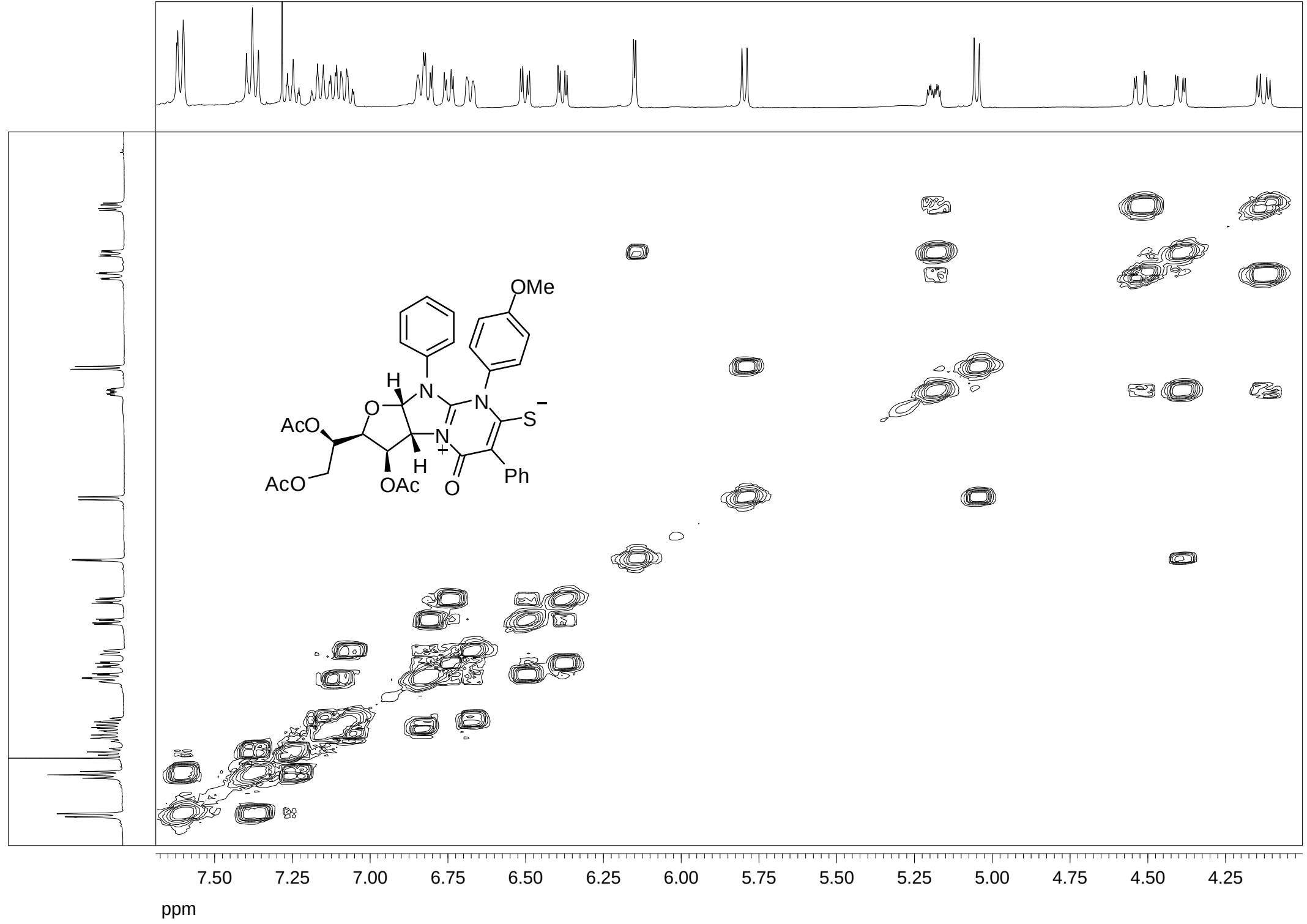
1,6-bis(4-nitrophenyl)-4-oxo-3-phenyl-(3',5',6'-tri-*O*-acetyl-1,2-dideoxy-α-D-glucofurano)[1',2':4,5]-5a*H*,5b*H*-imidazo[2,1-*a*]pyrimidin-5-ylium-2-thiolate

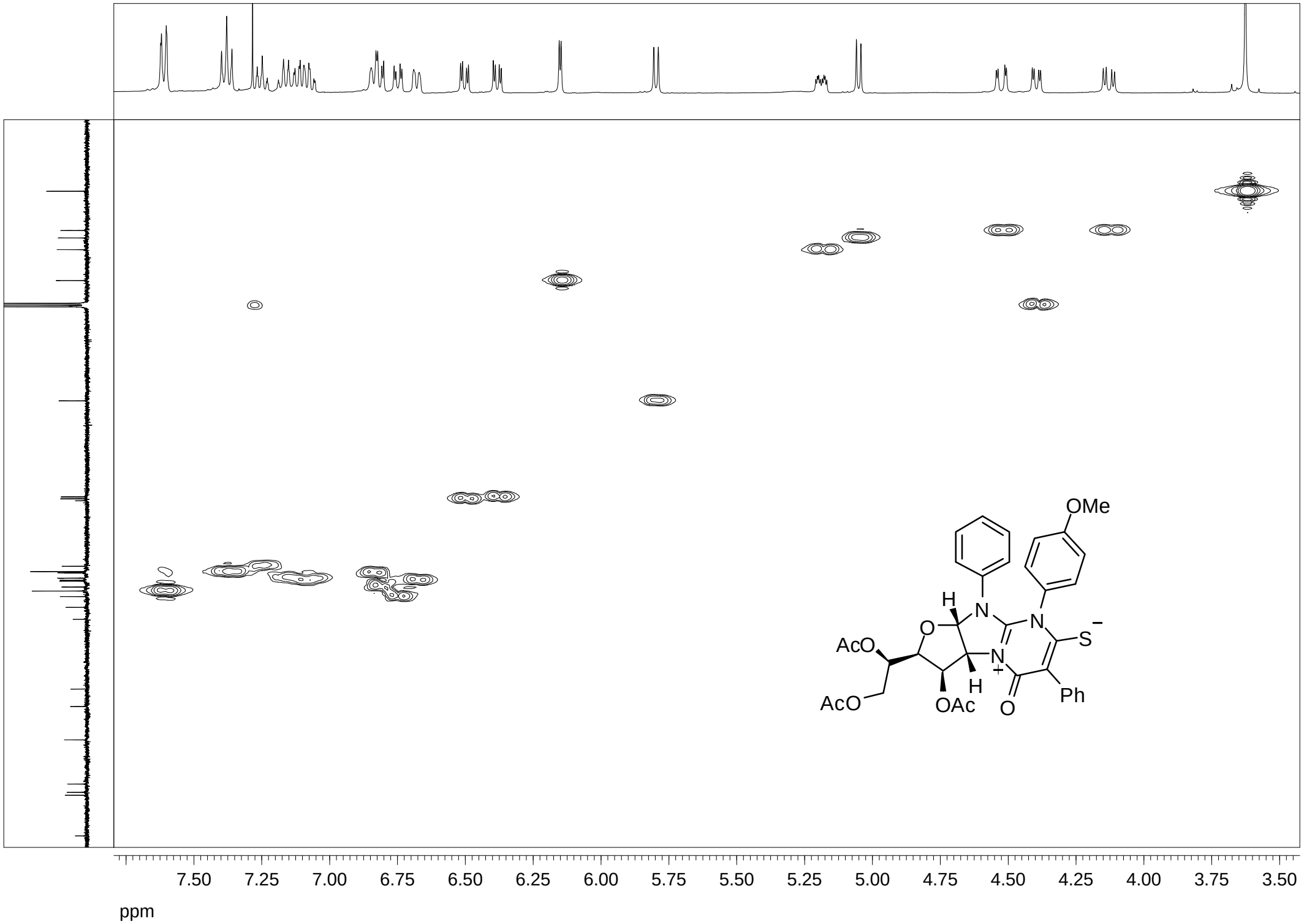


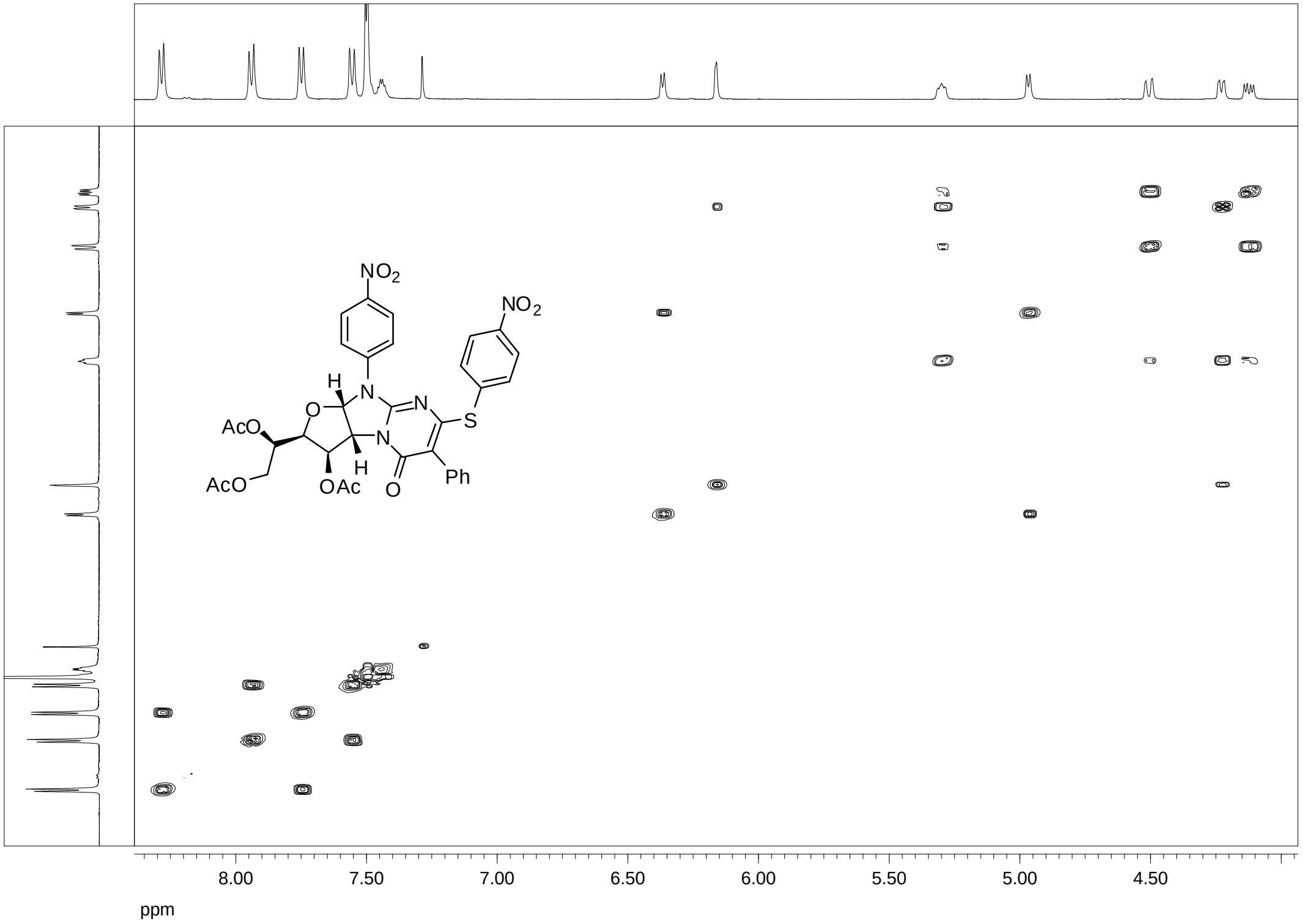
6-(4-nitrophenyl)-2-(4-nitrophenylthio)-3-phenyl-(3',5',6'-tri-*O*-acetyl-1,2-dideoxy-α-D-glucofurano)[1',2':4,5]-5a*H*,5b*H*-imidazo[1,2-*a*]pyrimidin-4-one



6-(4-nitrophenyl)-2-(4-nitrophenylthio)-3-phenyl-(3',5',6'-tri-*O*-acetyl-1,2-dideoxy-α-D-glucofurano)[1',2':4,5]-5a*H*,5b*H*-imidazo[1,2-*a*]pyrimidin-4-one


OMe
H
N
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O
S
AcO
N
H
AcO
OAc
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Ph
7.50
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OMe
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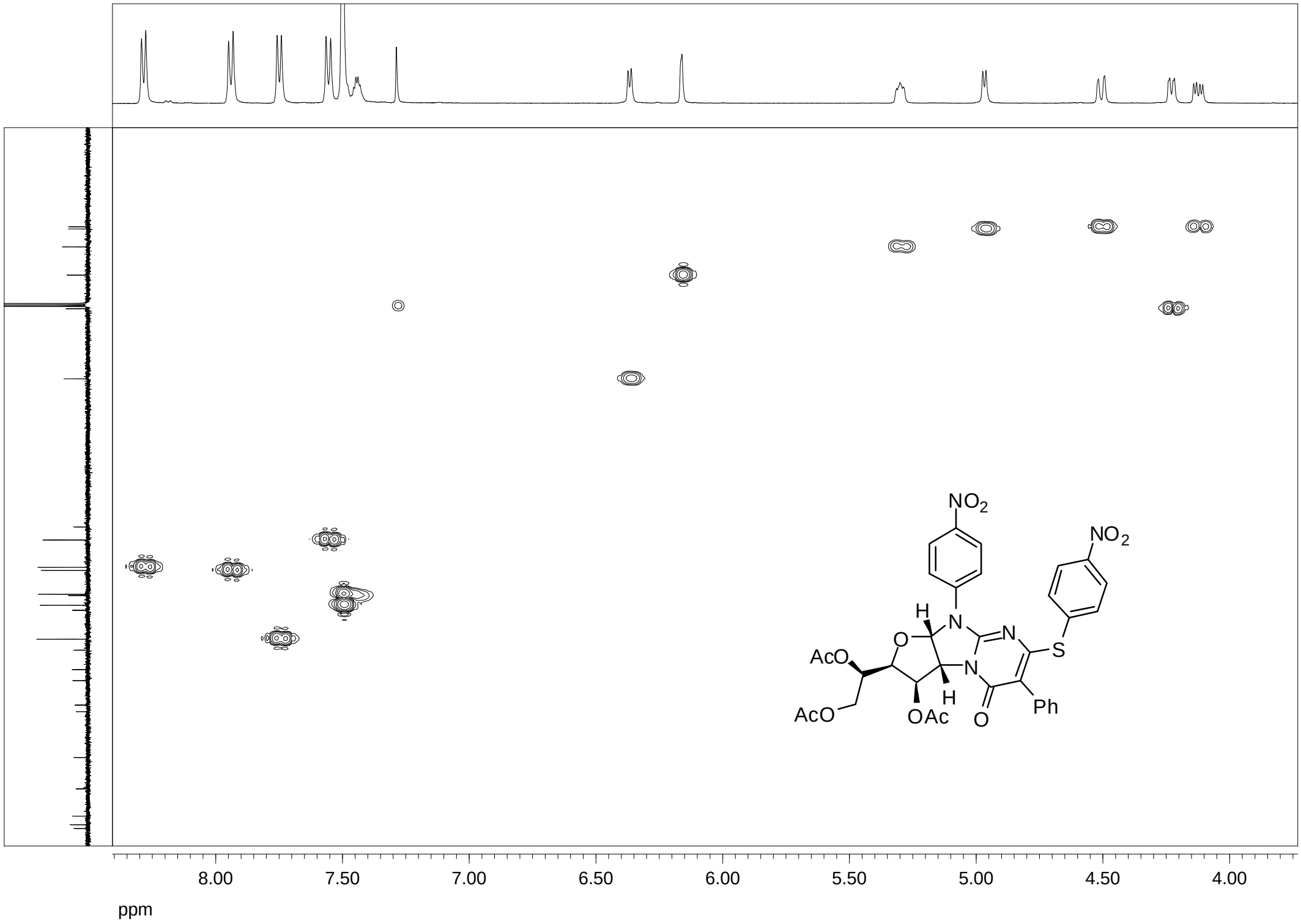
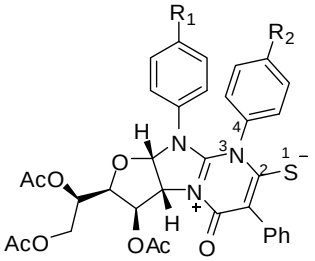

NO2
NO2
H
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O
S
AcO
N
AcO
H
OAc
O
Ph
8.00
7.50
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6.50
6.00
5.50
5.00
4.50
4.00
ppm

Table S1. Bond lengths (Å), angles (º) and bond orders in betaines **3a-i** calculated at the B3LYP/6-31G(d) level



3a $R_1 = R_2 = NO_2$
3b $R_1 = NO_2$; $R_2 = OCH_3$
3c $R_1 = NO_2$; $R_2 = H$
3d $R_1 = H$; $R_2 = NO_2$
3e $R_1 = H$; $R_2 = OCH_3$
3f $R_1 = R_2 = H$
3g $R_1 = OCH_3$; $R_2 = NO_2$
3h $R_1 = R_2 = OCH_3$
3i $R_1 = OCH_3$; $R_2 = H$

Compound	**3a**	**3b**	**3c**	**3d**	**3e**	**3f**	**3g**	**3h**	**3i**
R^1	NO_2	NO_2	NO_2	H	H	H	OCH_3	OCH_3	OCH_3
R^2	NO_2	OCH_3	H	NO_2	OCH_3	H	NO_2	OCH_3	H
D_{S1-C2}	1.675	1.674	1.674	1.677	1.676	1.676	1.677	1.676	1.676
D_{S1-C4}	3.007	3.037	3.032	3.000	3.030	3.022	2.999	3.026	3.020
D_{N3-C4}	1.451	1.453	1.455	1.451	1.451	1.454	1.451	1.451	1.454
$A_{S1-C2-N3}$	116.4	116.5	116.7	116.3	116.7	116.6	116.4	116.6	116.6
$A_{C2-N3-C4}$	119.2	120.2	119.8	119.2	120.1	119.8	119.2	120.0	119.7
$A_{C2-S1-C4}$	57.5	57.1	57.1	57.6	57.1	57.3	57.6	57.2	57.3
OE_{S1-C2}	1.516	1.523	1.523	1.507	1.515	1.515	1.505	1.513	1.513
OE_{S1-C4}	0.009	0.007	0.007	0.010	0.007	0.008	0.010	0.007	0.008
OE_{N3-C4}	0.928	0.923	0.922	0.927	0.924	0.921	0.928	0.924	0.921

Topologies of the orbitals involved in the theoretical rearrangement of betaines 3a-i

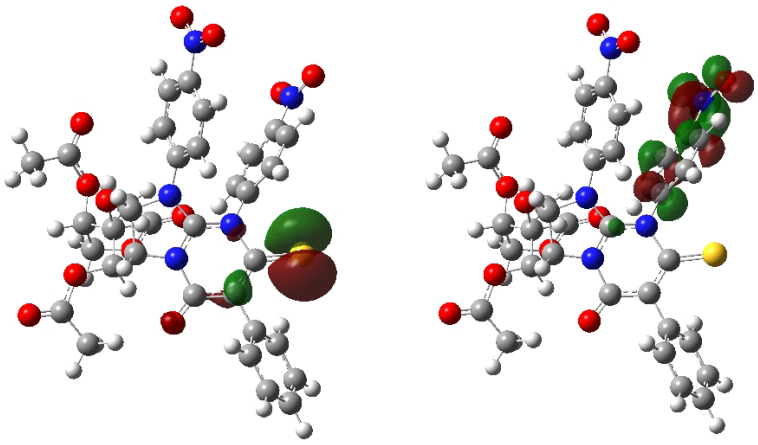


Figure S1. a) HOMO-1 of 3a, b) LUMO+1 of 3a

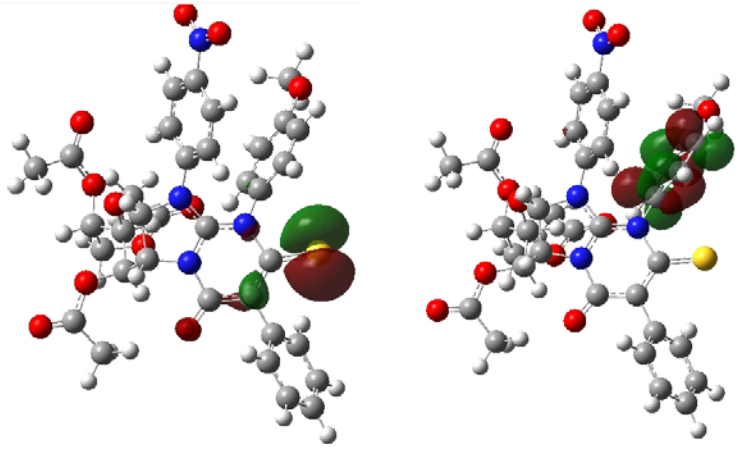


Figure S2. a) HOMO-1 of 3b, b) LUMO+7 of 3b

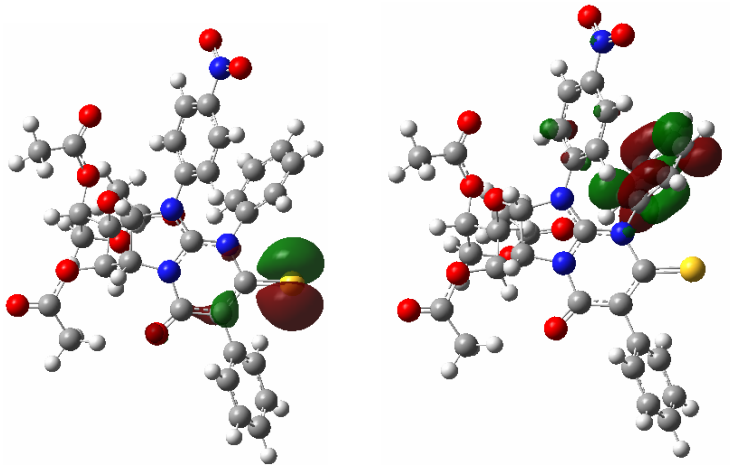


Figure S3. a) HOMO-1 of 3c, b) LUMO+7 of 3c

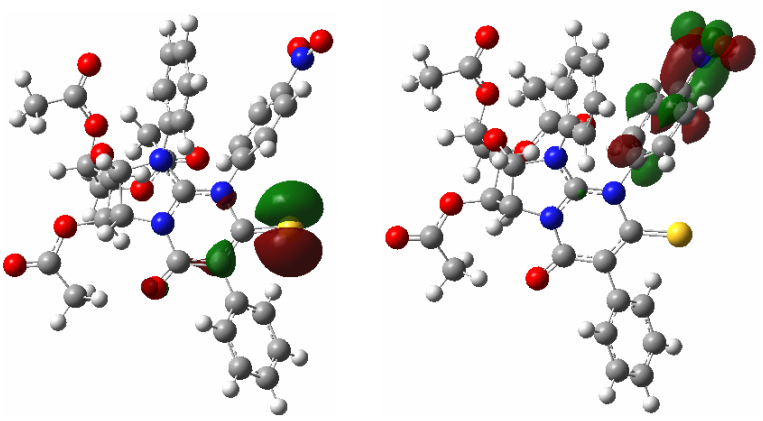


Figure S4. a) HOMO-1 of 3d, b) LUMO of 3d

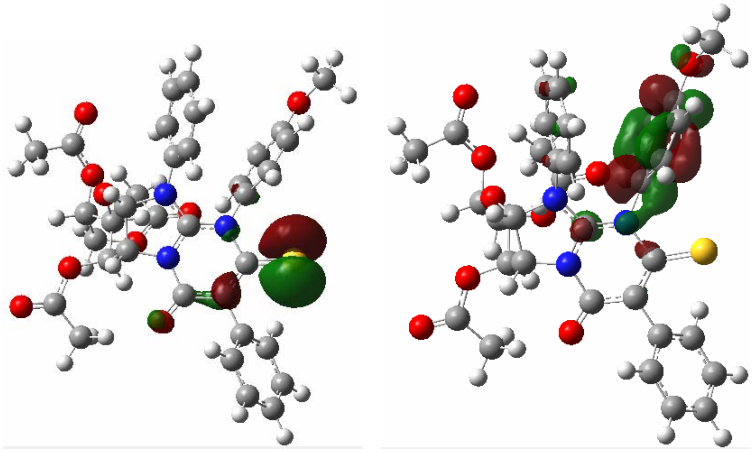


Figure S5. a) HOMO-1 of 3e, b) LUMO+9 of 3e

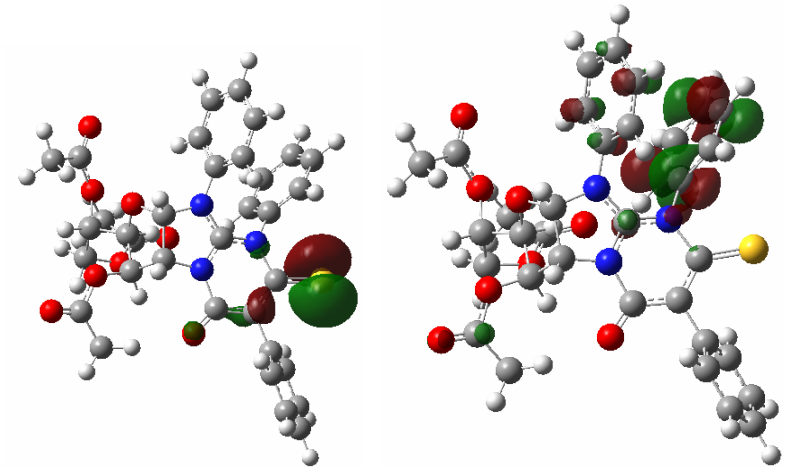


Figure S6. a) HOMO-1 of 3f, b) LUMO+7 of 3f

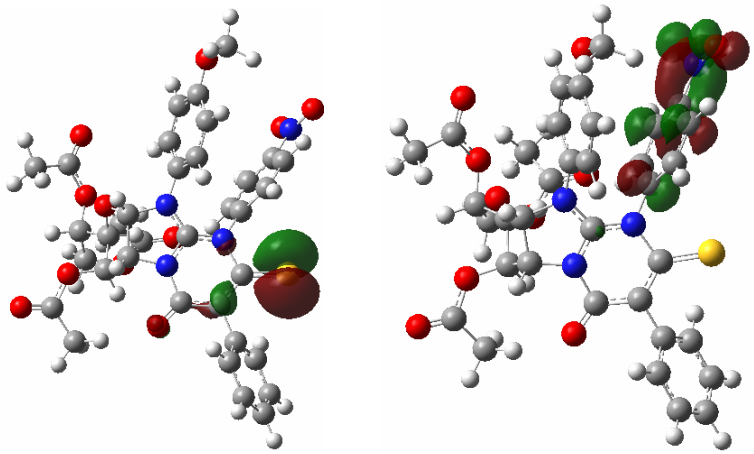


Figure S7. a) HOMO-1 of 3g, b) LUMO of 3g

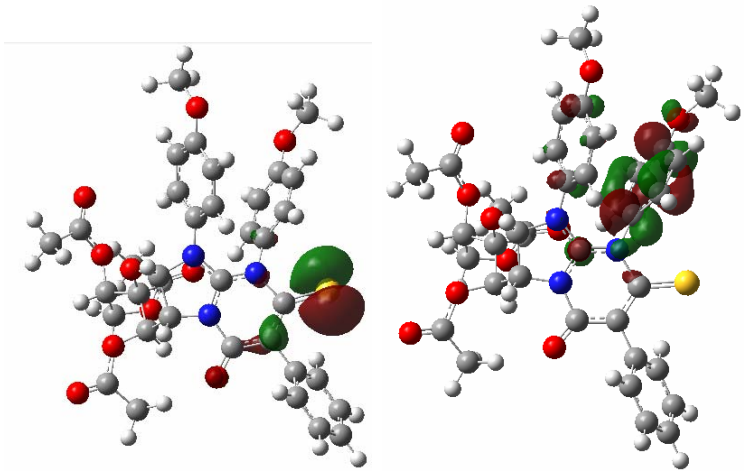


Figure S8. a) HOMO-1 of 3h, b) LUMO+8 of 3h

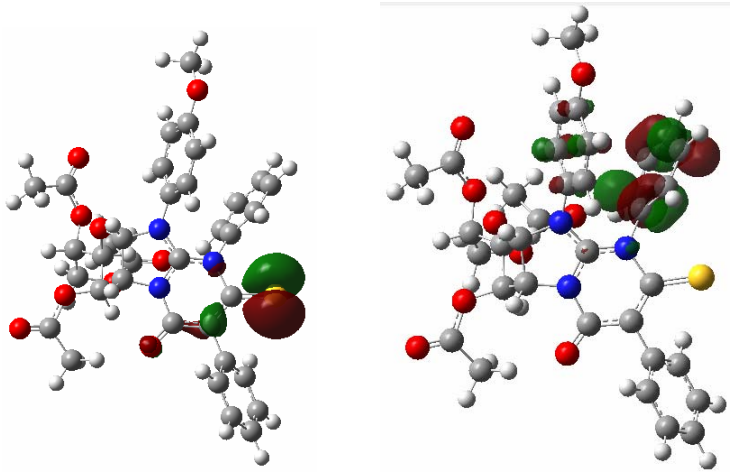
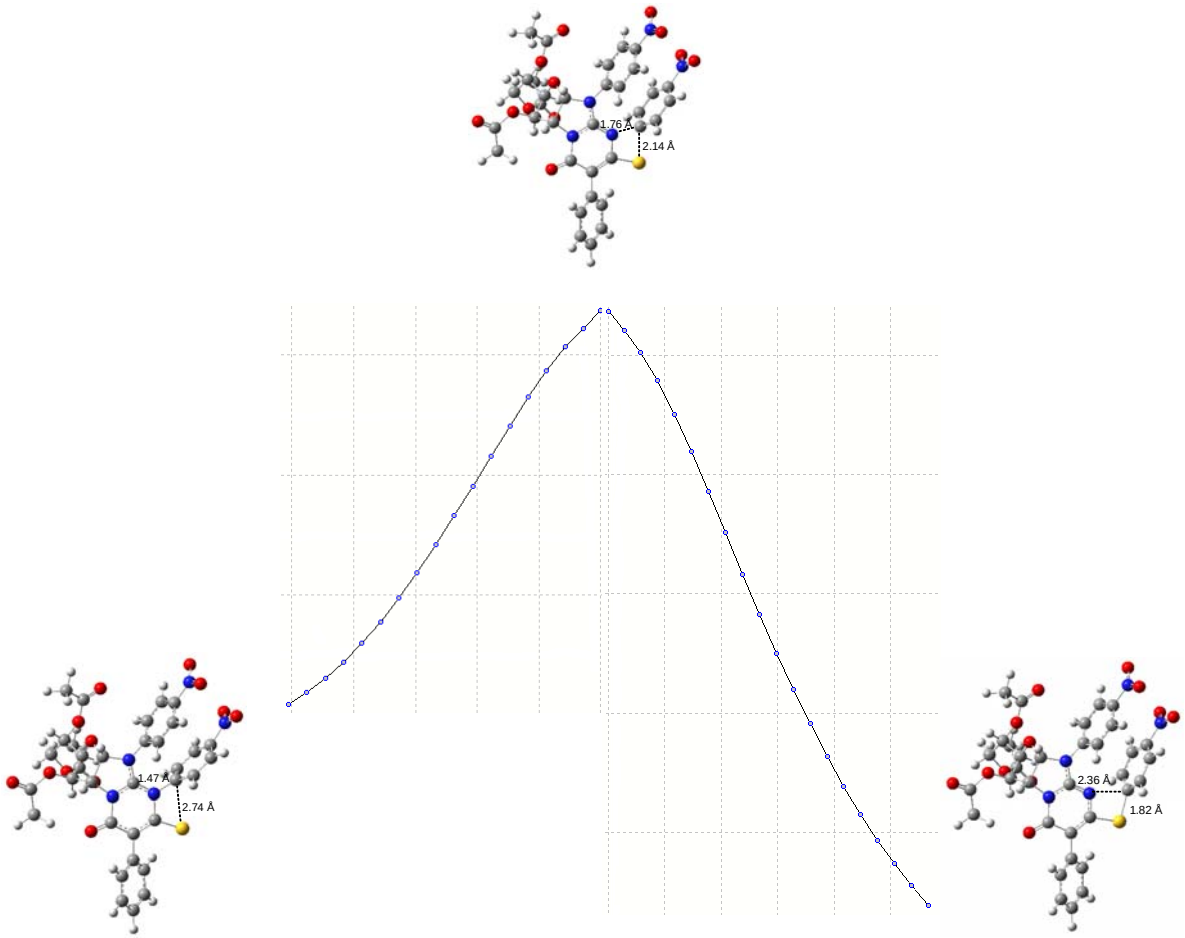


Figure S9. a) HOMO-1 of 3i, b) LUMO+6 of 3i

IRC plot for the $TS_{3a \rightarrow 4a}$



Cartesian coordinates and energies for all optimized geometries

Structure 3a

E (Hartree) = -2887.51951561

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.792612	2.550657	0.063732
2	6	0	2.127441	2.238374	-0.625314
3	6	0	1.675961	1.189814	-1.688065
4	6	0	0.149318	1.461433	-1.827661
5	6	0	-4.486804	-0.414982	-2.310161
6	6	0	0.658736	3.850731	0.856817
7	6	0	4.376162	-3.497885	1.032333
8	6	0	5.565904	-4.198120	1.221214
9	6	0	-3.512669	-1.195710	-2.929270
10	6	0	6.439510	-4.402726	0.150879
11	6	0	0.496145	-0.659082	-0.912960
12	6	0	1.521298	-2.753406	-0.141767
13	6	0	0.373641	2.220073	3.631581
14	6	0	-0.228555	3.325162	4.466551
15	6	0	2.955198	-0.877818	-0.932231
16	6	0	1.505679	3.813292	2.132646
17	6	0	2.786080	-2.201475	-0.432133
18	6	0	6.115497	-3.896693	-1.108178
19	6	0	4.037960	-2.988050	-0.229580
20	6	0	4.926248	-3.191937	-1.294667
21	6	0	-1.077415	-1.401133	1.608395
22	6	0	-2.236534	-1.626056	2.348074
23	6	0	-3.150852	-2.566039	1.882657
24	6	0	-2.942242	-3.294614	0.711764
25	6	0	-0.867438	-2.112527	0.424887
26	6	0	-1.782653	-3.067463	-0.021697
27	6	0	-1.848543	-0.048193	-1.607148
28	6	0	-2.837744	0.732298	-0.999061
29	6	0	3.907098	3.742156	-1.479988
30	6	0	4.956322	2.841599	-0.876265
31	6	0	-2.181150	-1.001056	-2.578993
32	6	0	-4.172104	0.547620	-1.354988
33	6	0	-1.694898	4.521529	0.492647
34	6	0	-1.277804	5.528900	-0.554702
35	1	0	2.563823	3.930699	1.882848
36	1	0	4.918537	2.884012	0.219859
37	1	0	4.826268	1.794010	-1.166279
38	1	0	5.930743	3.205771	-1.202550
39	1	0	-0.706630	5.049687	-1.354778
40	1	0	-3.803769	-1.925259	-3.674695
41	1	0	-0.657601	6.320846	-0.120056
42	1	0	-2.183058	5.969685	-0.972975
43	1	0	-0.813721	2.864249	5.262845
44	1	0	0.542343	3.969524	4.901545
45	1	0	5.810245	-4.586247	2.206684
46	1	0	7.365660	-4.952365	0.298180
47	1	0	0.538126	1.724418	0.736202
48	1	0	2.875669	1.824090	0.049851
49	1	0	2.250936	1.286256	-2.609224
50	1	0	-0.219020	1.666406	-2.832988
51	1	0	0.958891	4.707621	0.248591
52	1	0	3.697091	-3.350642	1.865960
53	1	0	-2.571246	1.478671	-0.259198
54	1	0	-4.960889	1.135029	-0.901688
55	1	0	-0.892377	3.940904	3.852048

56	1	0	-1.400791	-1.583159	-3.059719
57	1	0	6.788463	-4.048702	-1.948185
58	1	0	4.684850	-2.791433	-2.274679
59	1	0	-0.341214	-0.692420	1.976533
60	1	0	-2.423569	-1.089048	3.269252
61	1	0	-3.676405	-4.025947	0.398496
62	1	0	-1.581333	-3.629677	-0.924443
63	1	0	1.211258	4.635474	2.791348
64	7	0	1.718302	-0.173800	-1.180327
65	7	0	0.354833	-1.841969	-0.309687
66	7	0	-0.471955	0.218020	-1.311619
67	8	0	-0.144574	2.574649	-1.028759
68	8	0	2.570001	3.425150	-1.277816
69	8	0	4.132541	4.741275	-2.109489
70	8	0	-0.710581	3.954577	1.275915
71	8	0	-2.835861	4.220287	0.732732
72	8	0	1.399962	2.539022	2.772457
73	8	0	0.047749	1.060200	3.702839
74	8	0	3.985796	-0.261331	-1.210958
75	7	0	-5.899747	-0.610131	-2.690933
76	8	0	-6.736718	0.106775	-2.148544
77	8	0	-6.144684	-1.475882	-3.528916
78	7	0	-4.383966	-2.803787	2.656226
79	8	0	-5.176733	-3.636952	2.220351
80	8	0	-4.544459	-2.150993	3.685850
81	16	0	1.180657	-4.313564	0.362138

Structure 3b

E (Hartree) = -2797.54583946

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.336728	2.545336	-0.020733
2	6	0	1.701767	2.399735	-0.708876
3	6	0	1.406159	1.253327	-1.723637
4	6	0	-0.143844	1.287292	-1.858159
5	6	0	-4.461080	-1.264830	-2.178597
6	6	0	0.020610	3.852527	0.706038
7	6	0	4.780996	-2.909187	1.117782
8	6	0	6.063158	-3.417624	1.315301
9	6	0	-3.390361	-1.945287	-2.755513
10	6	0	6.961622	-3.495458	0.248741
11	6	0	0.520277	-0.720652	-0.865519
12	6	0	1.844622	-2.607474	-0.042300
13	6	0	-0.119336	2.411227	3.619449
14	6	0	-0.862247	3.515417	4.335791
15	6	0	2.982166	-0.567648	-0.905398
16	6	0	0.843298	3.991650	1.990425
17	6	0	3.014976	-1.883197	-0.360820
18	6	0	6.567490	-3.055635	-1.015121
19	6	0	4.371627	-2.467378	-0.148923
20	6	0	5.285037	-2.542559	-1.209965
21	6	0	-0.910254	-1.535722	1.696193
22	6	0	-2.019424	-1.862552	2.477485
23	6	0	-2.821407	-2.951370	2.114035
24	6	0	-2.501209	-3.705042	0.971018
25	6	0	-0.610881	-2.276291	0.555017
26	6	0	-1.398241	-3.375515	0.198594
27	6	0	-1.895136	-0.485135	-1.544432
28	6	0	-2.980852	0.191572	-0.977952
29	6	0	3.240735	4.104639	-1.650149
30	6	0	4.413559	3.389948	-1.025935

31	6	0	-2.097622	-1.543619	-2.439514
32	6	0	-4.277843	-0.201496	-1.298775
33	6	0	-2.393543	4.219436	0.300759
34	6	0	-2.082306	5.192181	-0.814310
35	1	0	1.887801	4.203239	1.744275
36	1	0	4.381014	3.477031	0.067785
37	1	0	4.430206	2.321927	-1.266638
38	1	0	5.322905	3.873387	-1.383781
39	1	0	-1.445121	4.730211	-1.573305
40	1	0	-3.580239	-2.761456	-3.441279
41	1	0	-1.567701	6.081288	-0.432700
42	1	0	-3.027094	5.492110	-1.268286
43	1	0	-1.407312	3.067126	5.166899
44	1	0	-0.179685	4.282147	4.717177
45	1	0	6.360567	-3.755368	2.304856
46	1	0	7.960650	-3.895562	0.402543
47	1	0	0.207863	1.724636	0.693458
48	1	0	2.505719	2.127574	-0.025363
49	1	0	1.954493	1.399902	-2.654544
50	1	0	-0.541575	1.396739	-2.867397
51	1	0	0.217836	4.710248	0.058478
52	1	0	4.084308	-2.860888	1.948299
53	1	0	-2.815250	1.016797	-0.294917
54	1	0	-5.138212	0.300900	-0.874729
55	1	0	-1.577152	3.991074	3.657843
56	1	0	-1.245679	-2.048405	-2.884312
57	1	0	7.258328	-3.110090	-1.852786
58	1	0	4.989032	-2.191486	-2.193793
59	1	0	-0.277226	-0.709595	2.008835
60	1	0	-2.226377	-1.268408	3.359242
61	1	0	-3.127638	-4.554136	0.718510
62	1	0	-1.139226	-3.968421	-0.669914
63	1	0	0.452878	4.821941	2.585738
64	7	0	1.654858	-0.066672	-1.166388
65	7	0	0.556363	-1.883464	-0.215072
66	7	0	-0.569616	-0.009239	-1.288066
67	8	0	-0.597276	2.380180	-1.103521
68	8	0	1.965242	3.611379	-1.412596
69	8	0	3.315497	5.097633	-2.324567
70	8	0	-1.356840	3.802237	1.108366
71	8	0	-3.498780	3.824447	0.571434
72	8	0	0.858604	2.761494	2.718479
73	8	0	-0.294500	1.235012	3.822656
74	8	0	3.908997	0.186766	-1.215337
75	7	0	-5.833608	-1.682665	-2.518093
76	8	0	-6.760826	-1.066143	-1.997198
77	8	0	-5.963425	-2.620883	-3.302749
78	16	0	1.746780	-4.189688	0.495341
79	6	0	-4.284199	-2.658383	3.978980
80	1	0	-5.177100	-3.157110	4.359049
81	1	0	-3.488931	-2.708482	4.733253
82	1	0	-4.517153	-1.607124	3.766390
83	8	0	-3.922897	-3.360354	2.796673

Structure 3c

E (Hartree) = -2683.02160345

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.257083	2.412386	-0.137590
2	6	0	1.040872	2.396284	-0.956588
3	6	0	0.847879	1.101142	-1.802361
4	6	0	-0.691846	0.877222	-1.764925

5	6	0	-4.523600	-2.348964	-1.359647
6	6	0	-0.715162	3.737041	0.471780
7	6	0	5.109843	-2.059349	1.113486
8	6	0	6.472750	-2.319410	1.240444
9	6	0	-3.413876	-2.898531	-1.998988
10	6	0	7.282858	-2.397960	0.105303
11	6	0	0.389046	-0.868641	-0.650144
12	6	0	2.084450	-2.408473	0.220177
13	6	0	-0.193108	2.665528	3.487919
14	6	0	-1.034522	3.692992	4.208705
15	6	0	2.776524	-0.331258	-0.965833
16	6	0	0.222438	4.188492	1.595734
17	6	0	3.080379	-1.547099	-0.289620
18	6	0	6.718552	-2.209411	-1.156463
19	6	0	4.530350	-1.871145	-0.149789
20	6	0	5.354610	-1.944224	-1.281376
21	6	0	-0.645802	-1.615648	2.125888
22	6	0	-1.609226	-2.051415	3.036786
23	6	0	-2.237567	-3.283665	2.852988
24	6	0	-1.899792	-4.086545	1.760242
25	6	0	-0.330509	-2.420400	1.029434
26	6	0	-0.939492	-3.660701	0.843820
27	6	0	-2.082130	-1.101196	-1.088088
28	6	0	-3.207457	-0.557205	-0.459633
29	6	0	2.176911	4.192947	-2.237876
30	6	0	3.503682	3.761746	-1.663743
31	6	0	-2.185558	-2.261062	-1.866837
32	6	0	-4.442044	-1.187199	-0.596768
33	6	0	-3.187487	3.645162	0.384905
34	6	0	-3.198108	4.498727	-0.863279
35	1	0	1.161121	4.557413	1.173009
36	1	0	3.546880	3.974425	-0.587816
37	1	0	3.685278	2.689499	-1.790453
38	1	0	4.282457	4.339337	-2.162256
39	1	0	-2.597414	4.042065	-1.654627
40	1	0	-3.526290	-3.798780	-2.590085
41	1	0	-2.797173	5.499084	-0.664897
42	1	0	-4.231904	4.586296	-1.198322
43	1	0	-1.363472	3.255081	5.151520
44	1	0	-0.471717	4.611119	4.406863
45	1	0	6.902846	-2.462441	2.228505
46	1	0	8.345554	-2.604313	0.204614
47	1	0	-0.176737	1.679950	0.672882
48	1	0	1.938729	2.340569	-0.341878
49	1	0	1.275039	1.213454	-2.799283
50	1	0	-1.194516	0.801105	-2.729387
51	1	0	-0.760640	4.515524	-0.293577
52	1	0	4.483835	-2.009079	1.998486
53	1	0	-3.120340	0.348301	0.129894
54	1	0	-5.330213	-0.792747	-0.119222
55	1	0	-1.914501	3.945589	3.609541
56	1	0	-1.307664	-2.660849	-2.364908
57	1	0	7.339396	-2.267145	-2.047004
58	1	0	4.923915	-1.786945	-2.265617
59	1	0	-0.133828	-0.671228	2.290722
60	1	0	-1.852546	-1.425214	3.889728
61	1	0	-2.376793	-5.052800	1.624876
62	1	0	-0.654958	-4.282575	0.004121
63	1	0	-0.247035	5.001128	2.157655
64	7	0	1.365069	-0.085134	-1.138012
65	7	0	0.680111	-1.926644	0.106766
66	7	0	-0.838981	-0.394052	-1.021496
67	8	0	-1.250014	1.967220	-1.080069
68	8	0	1.030235	3.535921	-1.813697
69	8	0	2.022434	5.089744	-3.024177
70	8	0	-2.000244	3.513439	1.072754
71	8	0	-4.160796	3.112116	0.853214
72	8	0	0.581908	3.085731	2.431012

73	8	0	-0.117292	1.505144	3.807781
74	8	0	3.530474	0.517305	-1.450321
75	16	0	2.308625	-3.910087	0.924891
76	1	0	-2.984554	-3.624192	3.564604
77	7	0	-5.828789	-3.020425	-1.501780
78	8	0	-5.868922	-4.043945	-2.182705
79	8	0	-6.793192	-2.514856	-0.931624

Structure 3d

E (Hartree) = -2683.02426623

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.485029	2.488508	0.032023
2	6	0	0.977864	2.707269	-0.378816
3	6	0	1.120030	1.675442	-1.539095
4	6	0	-0.353610	1.424380	-1.974770
5	6	0	-3.948002	-1.881031	-3.325927
6	6	0	-1.193831	3.593902	0.814014
7	6	0	4.792404	-2.085440	1.475086
8	6	0	6.104679	-2.366386	1.850315
9	6	0	-2.673109	-2.141086	-3.834431
10	6	0	7.152551	-2.166428	0.948909
11	6	0	0.538780	-0.523892	-1.061543
12	6	0	2.075267	-2.217024	-0.167720
13	6	0	-1.387108	1.723635	3.449721
14	6	0	-2.485621	2.487659	4.150363
15	6	0	2.889050	0.090462	-0.622864
16	6	0	-0.624222	3.725638	2.230442
17	6	0	3.106026	-1.255887	-0.206615
18	6	0	6.877021	-1.678560	-0.328776
19	6	0	4.502469	-1.598749	0.192155
20	6	0	5.563310	-1.393784	-0.701277
21	6	0	-1.066708	-1.982368	1.107473
22	6	0	-2.191601	-2.636797	1.604328
23	6	0	-2.656198	-3.763483	0.932230
24	6	0	-2.029607	-4.262933	-0.209626
25	6	0	-0.443222	-2.463827	-0.045629
26	6	0	-0.906554	-3.606273	-0.699912
27	6	0	-1.722618	-0.681245	-2.166200
28	6	0	-2.994653	-0.406138	-1.658428
29	6	0	2.255941	4.786685	-0.823879
30	6	0	3.429001	4.227260	-0.057414
31	6	0	-1.556052	-1.534542	-3.262328
32	6	0	-4.106573	-1.011951	-2.244845
33	6	0	-3.551426	3.539934	0.050042
34	6	0	-3.278941	4.668621	-0.918829
35	1	0	0.357263	4.206638	2.195784
36	1	0	3.190780	4.150691	1.011262
37	1	0	3.714932	3.227296	-0.399851
38	1	0	4.262113	4.920283	-0.176928
39	1	0	-2.459994	4.415703	-1.597415
40	1	0	-2.547382	-2.810053	-4.680770
41	1	0	-3.011176	5.590101	-0.389299
42	1	0	-4.189084	4.839224	-1.494241
43	1	0	-3.007183	1.794767	4.811250
44	1	0	-2.088833	3.324874	4.733817
45	1	0	6.308805	-2.743653	2.849132
46	1	0	8.175687	-2.388975	1.241142
47	1	0	-0.553681	1.566822	0.619912
48	1	0	1.686569	2.505417	0.424068
49	1	0	1.780266	2.047910	-2.322559
50	1	0	-0.585576	1.584223	-3.027833

51	1	0	-1.098534	4.552255	0.298226
52	1	0	3.981834	-2.251506	2.177141
53	1	0	-3.111945	0.272722	-0.820739
54	1	0	-5.096557	-0.802801	-1.851076
55	1	0	-3.195989	2.879085	3.415913
56	1	0	-0.561345	-1.720611	-3.658073
57	1	0	7.684788	-1.517454	-1.038248
58	1	0	5.356715	-1.003692	-1.693384
59	1	0	-0.678521	-1.116542	1.635964
60	1	0	-2.695467	-2.283354	2.494873
61	1	0	-2.420960	-5.150083	-0.690682
62	1	0	-0.388942	-3.974282	-1.576249
63	1	0	-1.292335	4.344411	2.836430
64	7	0	1.545835	0.365534	-1.069479
65	7	0	0.716470	-1.737057	-0.528839
66	7	0	-0.582906	0.006382	-1.622450
67	8	0	-1.157628	2.296829	-1.224536
68	8	0	1.093015	4.032401	-0.891931
69	8	0	2.233436	5.859806	-1.366413
70	8	0	-2.569623	3.210375	0.960625
71	8	0	-4.591520	2.937435	0.119108
72	8	0	-0.400438	2.437968	2.810922
73	8	0	-1.289729	0.520615	3.451941
74	8	0	3.679036	1.035593	-0.685522
75	7	0	-3.855179	-4.452039	1.441523
76	8	0	-4.250703	-5.440631	0.824333
77	8	0	-4.392103	-3.993996	2.449004
78	16	0	2.207698	-3.840416	0.229536
79	1	0	-4.817158	-2.353058	-3.774735

Structure 3e

E (Hartree) = -2593.04791088

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.365039	-2.095698	-0.006838
2	6	0	0.059896	-2.754952	-0.475647
3	6	0	-0.394735	-1.768929	-1.593570
4	6	0	0.914921	-1.011534	-1.958557
5	6	0	3.228897	3.339994	-3.054039
6	6	0	2.385566	-2.964574	0.726645
7	6	0	-5.189030	0.365423	1.421566
8	6	0	-6.522734	0.157276	1.767110
9	6	0	1.949684	3.187224	-3.594118
10	6	0	-7.421096	-0.356318	0.828936
11	6	0	-0.607794	0.470567	-0.999356
12	6	0	-2.651923	1.494409	-0.122029
13	6	0	1.846285	-1.395237	3.520436
14	6	0	3.132581	-1.801663	4.202600
15	6	0	-2.616618	-0.928722	-0.690794
16	6	0	1.860757	-3.407260	2.096019
17	6	0	-3.289411	0.239578	-0.230610
18	6	0	-6.971954	-0.664159	-0.455431
19	6	0	-4.726001	0.063337	0.132454
20	6	0	-5.635115	-0.459383	-0.797966
21	6	0	0.373652	2.290080	1.273743
22	6	0	1.180801	3.269165	1.836192
23	6	0	1.248600	4.544207	1.254624
24	6	0	0.499799	4.827161	0.103696
25	6	0	-0.359426	2.573667	0.116051
26	6	0	-0.307544	3.839166	-0.458359
27	6	0	1.499093	1.430427	-2.003399

28	6	0	2.779234	1.570967	-1.463094
29	6	0	-0.456693	-5.115603	-1.040660
30	6	0	-1.755218	-5.012004	-0.279785
31	6	0	1.083680	2.225339	-3.076972
32	6	0	3.641703	2.530695	-1.994344
33	6	0	4.608550	-2.073975	0.091004
34	6	0	4.748626	-3.142578	-0.970295
35	1	0	1.109714	-4.192044	1.969881
36	1	0	-1.566301	-4.908693	0.796502
37	1	0	-2.353193	-4.148401	-0.589639
38	1	0	-2.309577	-5.935954	-0.446288
39	1	0	3.919225	-3.099645	-1.681266
40	1	0	1.627413	3.810108	-4.423611
41	1	0	4.766143	-4.144787	-0.527246
42	1	0	5.688036	-2.967599	-1.495223
43	1	0	3.372739	-1.039025	4.943907
44	1	0	3.041209	-2.775745	4.694543
45	1	0	-6.861462	0.397880	2.771746
46	1	0	-8.462340	-0.515603	1.098055
47	1	0	1.121053	-1.243834	0.637672
48	1	0	-0.686903	-2.836426	0.313665
49	1	0	-0.868386	-2.301678	-2.418557
50	1	0	1.207109	-1.021778	-3.008936
51	1	0	2.627587	-3.850265	0.134758
52	1	0	-4.497988	0.773609	2.151973
53	1	0	3.094958	0.937216	-0.641779
54	1	0	4.636948	2.642575	-1.574739
55	1	0	3.945095	-1.855206	3.471740
56	1	0	0.091053	2.090898	-3.497930
57	1	0	-7.661350	-1.066280	-1.193744
58	1	0	-5.289215	-0.712771	-1.795516
59	1	0	0.305041	1.316914	1.753009
60	1	0	1.754310	3.067297	2.734517
61	1	0	0.527440	5.808567	-0.354304
62	1	0	-0.900602	4.057043	-1.338042
63	1	0	2.686022	-3.809846	2.690169
64	7	0	-1.251449	-0.707483	-1.090606
65	7	0	-1.198070	1.522579	-0.429702
66	7	0	0.647451	0.375089	-1.526445
67	8	0	1.953355	-1.612751	-1.226566
68	8	0	0.391270	-4.018829	-1.050051
69	8	0	-0.077057	-6.094883	-1.627863
70	8	0	3.551799	-2.161881	0.970511
71	8	0	5.390733	-1.172941	0.255071
72	8	0	1.188106	-2.334246	2.759348
73	8	0	1.331565	-0.310825	3.635643
74	8	0	-3.036438	-2.082145	-0.827057
75	16	0	-3.360218	2.953373	0.299774
76	1	0	3.904262	4.086331	-3.462740
77	8	0	2.065034	5.435261	1.881411
78	6	0	2.136869	6.759545	1.374317
79	1	0	2.821672	7.294519	2.034538
80	1	0	2.532090	6.778649	0.350112
81	1	0	1.155582	7.250798	1.392907

Structure 3f

E (Hartree) = -2478.52444587

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.841836	-1.400664	-0.096088
2	6	0	0.735814	-2.280444	-0.697308
3	6	0	0.070363	-1.289726	-1.698844

4	6	0	1.167374	-0.207537	-1.916662
5	6	0	2.376224	4.672976	-2.401727
6	6	0	3.031509	-2.098667	0.561755
7	6	0	-5.112149	-0.733404	1.388828
8	6	0	-6.362056	-1.287788	1.657006
9	6	0	1.176541	4.286878	-3.004171
10	6	0	-7.105077	-1.877932	0.632016
11	6	0	-0.668631	0.742515	-0.840523
12	6	0	-2.900844	1.138029	0.088005
13	6	0	2.150837	-1.056485	3.511809
14	6	0	3.491540	-1.258016	4.179952
15	6	0	-2.290748	-1.116192	-0.773431
16	6	0	2.613413	-2.816956	1.848279
17	6	0	-3.223116	-0.206935	-0.196126
18	6	0	-6.584240	-1.912800	-0.661655
19	6	0	-4.579437	-0.758363	0.091499
20	6	0	-5.330775	-1.361038	-0.927258
21	6	0	-0.170178	2.434244	1.671779
22	6	0	0.382980	3.505164	2.375441
23	6	0	0.160627	4.813360	1.944622
24	6	0	-0.618681	5.054837	0.810208
25	6	0	-0.935927	2.689888	0.533210
26	6	0	-1.175268	3.992740	0.100005
27	6	0	1.152137	2.290104	-1.651257
28	6	0	2.356156	2.663748	-1.050650
29	6	0	0.802739	-4.601614	-1.573719
30	6	0	-0.492059	-4.906565	-0.862147
31	6	0	0.565028	3.089141	-2.637864
32	6	0	2.964786	3.860254	-1.431332
33	6	0	5.000613	-0.657045	0.126334
34	6	0	5.380592	-1.513288	-1.061167
35	1	0	2.053560	-3.723666	1.602346
36	1	0	-0.345379	-4.907119	0.225661
37	1	0	-1.273823	-4.172797	-1.084531
38	1	0	-0.809848	-5.903563	-1.168345
39	1	0	4.560512	-1.572378	-1.781587
40	1	0	0.719239	4.913240	-3.764648
41	1	0	5.635541	-2.532866	-0.750145
42	1	0	6.250242	-1.057037	-1.534645
43	1	0	3.553296	-0.566408	5.020637
44	1	0	3.615488	-2.284724	4.540118
45	1	0	-6.757122	-1.257840	2.669375
46	1	0	-8.081686	-2.307367	0.841196
47	1	0	1.397354	-0.723331	0.641564
48	1	0	0.021108	-2.638083	0.043289
49	1	0	-0.260458	-1.804390	-2.601303
50	1	0	1.464896	-0.016459	-2.947994
51	1	0	3.474032	-2.824558	-0.124232
52	1	0	-4.543858	-0.268249	2.187670
53	1	0	2.808056	2.026377	-0.298615
54	1	0	3.899975	4.154445	-0.964478
55	1	0	4.299787	-1.035369	3.476834
56	1	0	-0.362577	2.774736	-3.108216
57	1	0	-7.152416	-2.370962	-1.467441
58	1	0	-4.926160	-1.401958	-1.933984
59	1	0	-0.018577	1.417541	2.024767
60	1	0	0.978035	3.306624	3.261770
61	1	0	-0.802186	6.073326	0.480668
62	1	0	-1.793785	4.165820	-0.771987
63	1	0	3.505114	-3.104067	2.412911
64	7	0	-1.014700	-0.531894	-1.096320
65	7	0	-1.495692	1.545701	-0.168701
66	7	0	0.574549	1.012588	-1.332972
67	8	0	2.310384	-0.636250	-1.220174
68	8	0	1.364314	-3.344098	-1.411419
69	8	0	1.412942	-5.378861	-2.260176
70	8	0	3.979719	-1.089727	0.943676
71	8	0	5.564761	0.360016	0.439279

72	8	0	1.719136	-2.009223	2.617623
73	8	0	1.409111	-0.134703	3.745453
74	8	0	-2.424120	-2.308876	-1.064199
75	16	0	-3.932524	2.323996	0.668893
76	1	0	2.853112	5.604907	-2.691857
77	1	0	0.588295	5.646706	2.495451

Structure 3g

E (Hartree) = -2797.54802273

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.767459	2.533561	0.013519
2	6	0	2.119335	2.163616	-0.612650
3	6	0	1.678640	1.116161	-1.678326
4	6	0	0.168125	1.431328	-1.886264
5	6	0	-4.577077	-0.322951	-2.419802
6	6	0	0.663933	3.852159	0.779873
7	6	0	4.110730	-3.637672	1.179727
8	6	0	5.266346	-4.380420	1.413030
9	6	0	-3.582411	-1.062836	-3.075882
10	6	0	6.165660	-4.627863	0.373443
11	6	0	0.403859	-0.674598	-0.922194
12	6	0	1.324301	-2.792417	-0.088028
13	6	0	0.201163	2.286138	3.572548
14	6	0	-0.396541	3.436890	4.347181
15	6	0	2.852634	-0.985088	-0.855543
16	6	0	1.461717	3.796264	2.087343
17	6	0	2.618146	-2.296084	-0.346266
18	6	0	5.901567	-4.121450	-0.899375
19	6	0	3.832036	-3.127188	-0.096459
20	6	0	4.746324	-3.374419	-1.130095
21	6	0	-1.286354	-1.355970	1.555712
22	6	0	-2.483483	-1.534979	2.245712
23	6	0	-3.417471	-2.431884	1.736092
24	6	0	-3.191271	-3.161689	0.568836
25	6	0	-1.057738	-2.069536	0.377288
26	6	0	-1.994065	-2.980938	-0.113601
27	6	0	-1.896388	-0.002321	-1.698133
28	6	0	-2.887700	0.748185	-1.051522
29	6	0	3.988251	3.585533	-1.412664
30	6	0	4.976468	2.652356	-0.757186
31	6	0	-2.245719	-0.888660	-2.717709
32	6	0	-4.217179	0.587617	-1.411594
33	6	0	-1.626611	4.703541	0.360828
34	6	0	-1.107379	5.588529	-0.750081
35	1	0	2.532875	3.856387	1.875389
36	1	0	4.896455	2.710339	0.335963
37	1	0	4.816629	1.606745	-1.039929
38	1	0	5.976746	2.974156	-1.047934
39	1	0	-0.566071	5.004721	-1.499078
40	1	0	-3.833244	-1.763345	-3.863610
41	1	0	-0.429386	6.356660	-0.360382
42	1	0	-1.965303	6.074167	-1.215561
43	1	0	-1.028422	3.020584	5.132270
44	1	0	0.377005	4.069858	4.794150
45	1	0	5.463971	-4.768107	2.409175
46	1	0	7.065333	-5.210393	0.555115
47	1	0	0.458563	1.729120	0.689705
48	1	0	2.821834	1.735075	0.101603
49	1	0	2.295737	1.177783	-2.574937
50	1	0	-0.153139	1.634883	-2.907776
51	1	0	1.031211	4.680907	0.170061

52	1	0	3.411049	-3.457152	1.989332
53	1	0	-2.616592	1.454215	-0.274043
54	1	0	-5.000358	1.155908	-0.921174
55	1	0	-1.013321	4.053016	3.685864
56	1	0	-1.473770	-1.453415	-3.233589
57	1	0	6.595228	-4.306109	-1.715821
58	1	0	4.552021	-2.973800	-2.120452
59	1	0	-0.538463	-0.676652	1.954469
60	1	0	-2.686892	-0.993358	3.160689
61	1	0	-3.943239	-3.857205	0.219067
62	1	0	-1.780507	-3.541675	-1.014320
63	1	0	1.184944	4.644527	2.720177
64	7	0	1.655299	-0.238144	-1.146357
65	7	0	0.201230	-1.845250	-0.308239
66	7	0	-0.513311	0.220210	-1.381901
67	8	0	-0.122855	2.569203	-1.114516
68	8	0	2.634317	3.325472	-1.259716
69	8	0	4.280039	4.566612	-2.044487
70	8	0	-0.710482	4.039191	1.148897
71	8	0	-2.790156	4.574527	0.641579
72	8	0	1.271147	2.541735	2.746654
73	8	0	-0.168189	1.140938	3.666168
74	8	0	3.916662	-0.414641	-1.109154
75	7	0	-4.691984	-2.617089	2.451237
76	8	0	-5.505798	-3.406151	1.971347
77	8	0	-4.868568	-1.968908	3.481558
78	16	0	0.909542	-4.332545	0.430165
79	8	0	-5.903680	-0.407856	-2.686922
80	6	0	-6.343797	-1.329099	-3.677399
81	1	0	-6.072349	-2.359052	-3.413993
82	1	0	-7.430253	-1.237093	-3.705198
83	1	0	-5.932163	-1.082928	-4.664487

Structure 3h

E (Hartree) = -2707.57200026

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.218091	2.557387	0.027948
2	6	0	1.613736	2.429035	-0.599845
3	6	0	1.368758	1.312186	-1.658665
4	6	0	-0.173969	1.334064	-1.854833
5	6	0	-4.549648	-1.166201	-2.305115
6	6	0	-0.125437	3.852924	0.761111
7	6	0	4.684804	-2.928950	1.125274
8	6	0	5.964523	-3.437497	1.338120
9	6	0	-3.456209	-1.713363	-2.997896
10	6	0	6.888369	-3.480365	0.291400
11	6	0	0.462449	-0.690327	-0.893937
12	6	0	1.773350	-2.600633	-0.098609
13	6	0	-0.154294	2.336985	3.631229
14	6	0	-0.962261	3.376413	4.373993
15	6	0	2.925114	-0.532133	-0.865205
16	6	0	0.706052	4.010492	2.038069
17	6	0	2.949093	-1.865476	-0.363442
18	6	0	6.521416	-3.005570	-0.967974
19	6	0	4.302310	-2.452185	-0.137240
20	6	0	5.241140	-2.492750	-1.177843
21	6	0	-1.056653	-1.679134	1.590340
22	6	0	-2.186442	-2.081764	2.288975
23	6	0	-2.964819	-3.147324	1.812575
24	6	0	-2.600006	-3.804529	0.629438
25	6	0	-0.705817	-2.328977	0.402134

26	6	0	-1.465271	-3.394246	-0.069276
27	6	0	-1.942865	-0.431794	-1.618739
28	6	0	-3.025273	0.122505	-0.937497
29	6	0	3.194587	4.156880	-1.420857
30	6	0	4.338823	3.415158	-0.775180
31	6	0	-2.163506	-1.341071	-2.662955
32	6	0	-4.329197	-0.240736	-1.276955
33	6	0	-2.552102	4.204272	0.396669
34	6	0	-2.259131	5.152339	-0.744729
35	1	0	1.733136	4.283583	1.780592
36	1	0	4.263095	3.464104	0.318770
37	1	0	4.360740	2.355904	-1.052302
38	1	0	5.263568	3.906099	-1.079503
39	1	0	-1.652421	4.664203	-1.512074
40	1	0	-3.648585	-2.421074	-3.797617
41	1	0	-1.719357	6.040334	-0.396740
42	1	0	-3.212855	5.459502	-1.174513
43	1	0	-1.479742	2.875042	5.192343
44	1	0	-0.327086	4.173249	4.775188
45	1	0	6.240394	-3.802195	2.324445
46	1	0	7.885780	-3.879991	0.457155
47	1	0	0.064200	1.725137	0.723786
48	1	0	2.382914	2.139700	0.115753
49	1	0	1.954222	1.490795	-2.560943
50	1	0	-0.534493	1.464350	-2.875533
51	1	0	0.046927	4.715459	0.113313
52	1	0	3.968818	-2.907182	1.940336
53	1	0	-2.856697	0.841739	-0.143492
54	1	0	-5.154847	0.202242	-0.733315
55	1	0	-1.703759	3.824671	3.705993
56	1	0	-1.319749	-1.757369	-3.206471
57	1	0	7.232079	-3.031979	-1.790410
58	1	0	4.966510	-2.113677	-2.157464
59	1	0	-0.444503	-0.872776	1.985829
60	1	0	-2.472412	-1.591335	3.213349
61	1	0	-3.179571	-4.637560	0.249955
62	1	0	-1.169639	-3.907427	-0.976088
63	1	0	0.280253	4.806780	2.655494
64	7	0	1.606555	-0.022102	-1.132307
65	7	0	0.488476	-1.879281	-0.288564
66	7	0	-0.612433	0.025606	-1.332485
67	8	0	-0.668707	2.408316	-1.093852
68	8	0	1.910411	3.662419	-1.254184
69	8	0	3.302098	5.173164	-2.056337
70	8	0	-1.499997	3.772733	1.173181
71	8	0	-3.656558	3.837561	0.708281
72	8	0	0.802551	2.770070	2.741933
73	8	0	-0.260261	1.147927	3.801297
74	8	0	3.860331	0.229432	-1.131903
75	16	0	1.671429	-4.200972	0.389778
76	8	0	-4.051679	-3.467377	2.568795
77	6	0	-4.841033	-4.581354	2.179783
78	1	0	-5.624647	-4.669451	2.934338
79	1	0	-5.301984	-4.426334	1.195210
80	1	0	-4.250138	-5.505977	2.159799
81	8	0	-5.774108	-1.594068	-2.711127
82	6	0	-6.925281	-1.070805	-2.060249
83	1	0	-6.997327	0.016954	-2.185370
84	1	0	-7.780364	-1.547940	-2.541386
85	1	0	-6.926560	-1.313744	-0.990138

Structure 3i

E (Hartree) = -2593.04850009

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.772421	2.239498	-0.132422
2	6	0	0.557009	2.483572	-0.860585
3	6	0	0.641893	1.221466	-1.770199
4	6	0	-0.829894	0.721579	-1.831572
5	6	0	-4.136209	-3.107885	-1.646890
6	6	0	-1.485387	3.441284	0.484542
7	6	0	5.290332	-1.328102	1.170684
8	6	0	6.674042	-1.370246	1.328973
9	6	0	-2.961062	-3.337199	-2.382858
10	6	0	7.513532	-1.252627	0.218846
11	6	0	0.482342	-0.846854	-0.717002
12	6	0	2.383935	-2.113176	0.167439
13	6	0	-0.802910	2.412424	3.487197
14	6	0	-1.864460	3.219637	4.198918
15	6	0	2.753941	0.098652	-0.911732
16	6	0	-0.675921	4.039265	1.639398
17	6	0	3.238281	-1.079514	-0.273557
18	6	0	6.956210	-1.087206	-1.049292
19	6	0	4.717650	-1.166817	-0.099520
20	6	0	5.570683	-1.040911	-1.205082
21	6	0	-0.476288	-1.926853	1.999660
22	6	0	-1.379092	-2.575854	2.843298
23	6	0	-1.803924	-3.871395	2.547184
24	6	0	-1.324410	-4.523312	1.407997
25	6	0	-0.015622	-2.585525	0.858772
26	6	0	-0.422369	-3.884221	0.559176
27	6	0	-1.898933	-1.479645	-1.262506
28	6	0	-3.066586	-1.240968	-0.539842
29	6	0	1.449287	4.517346	-1.966203
30	6	0	2.791754	4.276347	-1.320799
31	6	0	-1.854406	-2.522954	-2.198062
32	6	0	-4.186592	-2.051611	-0.727766
33	6	0	-3.915395	2.956506	0.359031
34	6	0	-4.023941	3.763610	-0.915466
35	1	0	0.176028	4.599136	1.243967
36	1	0	2.731684	4.421132	-0.234401
37	1	0	3.160617	3.259765	-1.493059
38	1	0	3.490043	5.007279	-1.729263
39	1	0	-3.336423	3.388769	-1.678223
40	1	0	-2.945310	-4.154947	-3.095845
41	1	0	-3.793180	4.820250	-0.737678
42	1	0	-5.049846	3.679240	-1.274635
43	1	0	-2.115781	2.699753	5.123827
44	1	0	-1.517910	4.232392	4.429920
45	1	0	7.097606	-1.496751	2.322199
46	1	0	8.593066	-1.289058	0.342363
47	1	0	-0.611166	1.500282	0.660141
48	1	0	1.409461	2.545749	-0.185131
49	1	0	1.093037	1.459879	-2.733665
50	1	0	-1.261460	0.596348	-2.824949
51	1	0	-1.655431	4.213136	-0.269459
52	1	0	4.643257	-1.429972	2.035727
53	1	0	-3.106877	-0.421943	0.170014
54	1	0	-5.083065	-1.849547	-0.154238
55	1	0	-2.761578	3.291670	3.576523
56	1	0	-0.949721	-2.695698	-2.774575
57	1	0	7.599308	-0.992897	-1.920849
58	1	0	5.143731	-0.900690	-2.193467
59	1	0	-0.123779	-0.928472	2.245367
60	1	0	-1.736529	-2.064742	3.732235
61	1	0	-1.644969	-5.536314	1.182798
62	1	0	-0.029798	-4.382806	-0.318486
63	1	0	-1.306727	4.725666	2.211423
64	7	0	1.330400	0.114755	-1.125216
65	7	0	0.926765	-1.873972	0.010274

66	7	0	-0.787029	-0.580123	-1.137067
67	8	0	-1.613963	1.668316	-1.148533
68	8	0	0.408108	3.653008	-1.664939
69	8	0	1.195759	5.426525	-2.712577
70	8	0	-2.723171	2.975111	1.046597
71	8	0	-4.822631	2.329903	0.844656
72	8	0	-0.113404	3.009994	2.457144
73	8	0	-0.487102	1.289387	3.792727
74	8	0	3.371644	1.081447	-1.333352
75	16	0	2.834416	-3.583876	0.833355
76	8	0	-5.163407	-3.958747	-1.904041
77	6	0	-6.382789	-3.785785	-1.192528
78	1	0	-6.830645	-2.805037	-1.396682
79	1	0	-7.049818	-4.570486	-1.552427
80	1	0	-6.235116	-3.900267	-0.111312
81	1	0	-2.502654	-4.378127	3.207381

Structure $TS_{3a \rightarrow 4a}$

E (Hartree) = -2887.47632893

Imaginary Frequency (cm^{-1}) = -459.4773

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.239542	-2.420498	-0.095128
2	6	0	-2.391616	-1.839719	-0.924422
3	6	0	-1.652029	-0.791732	-1.801728
4	6	0	-0.174560	-1.281551	-1.794629
5	6	0	4.739291	-0.357506	-1.526150
6	6	0	-1.394174	-3.829144	0.479951
7	6	0	-3.660124	4.242099	1.093857
8	6	0	-4.689409	5.159650	1.301588
9	6	0	4.036464	0.475032	-2.393952
10	6	0	-5.573056	5.470346	0.267579
11	6	0	-0.280458	0.837682	-0.830788
12	6	0	-1.091678	2.869377	0.038298
13	6	0	-2.475290	-2.646820	3.435353
14	6	0	-1.971968	-3.862360	4.180821
15	6	0	-2.676433	1.406960	-1.065156
16	6	0	-2.644049	-3.975357	1.349607
17	6	0	-2.387811	2.658790	-0.388358
18	6	0	-5.423615	4.851573	-0.975145
19	6	0	-3.493650	3.622375	-0.155316
20	6	0	-4.396748	3.933718	-1.185923
21	6	0	1.585241	1.968806	1.845614
22	6	0	2.901849	1.734517	2.192859
23	6	0	3.938953	2.215845	1.383422
24	6	0	3.649839	2.961390	0.233676
25	6	0	1.275300	2.722106	0.679868
26	6	0	2.338196	3.206864	-0.125938
27	6	0	2.007484	-0.151892	-1.245572
28	6	0	2.727081	-0.982615	-0.381085
29	6	0	-4.238516	-2.951629	-2.147465
30	6	0	-5.217205	-1.970224	-1.548671
31	6	0	2.656503	0.572252	-2.252539
32	6	0	4.110142	-1.086052	-0.520954
33	6	0	0.921311	-4.631754	0.838775
34	6	0	0.853830	-5.481312	-0.411242
35	1	0	-3.518758	-4.089666	0.703770
36	1	0	-5.298270	-2.110564	-0.463495
37	1	0	-4.920886	-0.930994	-1.723255
38	1	0	-6.191370	-2.161071	-1.999345
39	1	0	0.634993	-4.866732	-1.288965

40	1	0	4.570664	1.020314	-3.161767
41	1	0	0.079533	-6.252332	-0.331387
42	1	0	1.825556	-5.958640	-0.540153
43	1	0	-1.767064	-3.557848	5.207184
44	1	0	-2.716637	-4.666312	4.187411
45	1	0	-4.802326	5.625928	2.276472
46	1	0	-6.374798	6.185734	0.429431
47	1	0	-1.020277	-1.738532	0.735178
48	1	0	-3.159265	-1.382497	-0.301675
49	1	0	-2.104736	-0.718511	-2.791608
50	1	0	0.256384	-1.522509	-2.767175
51	1	0	-1.454321	-4.553299	-0.335885
52	1	0	-2.991711	3.994151	1.912123
53	1	0	2.213640	-1.553288	0.384470
54	1	0	4.696549	-1.720678	0.131772
55	1	0	-1.054328	-4.246943	3.725578
56	1	0	2.081522	1.203766	-2.922550
57	1	0	-6.108573	5.084514	-1.786042
58	1	0	-4.293714	3.452878	-2.152112
59	1	0	0.780677	1.608925	2.478819
60	1	0	3.146270	1.173962	3.087603
61	1	0	4.467966	3.340804	-0.367262
62	1	0	2.113259	3.801155	-1.005365
63	1	0	-2.552185	-4.873209	1.965558
64	7	0	-1.558449	0.523035	-1.177484
65	7	0	-0.042660	1.986350	-0.223778
66	7	0	0.571718	-0.153709	-1.194314
67	8	0	-0.127020	-2.444153	-1.012185
68	8	0	-2.907028	-2.872298	-1.762771
69	8	0	-4.524788	-3.825834	-2.921452
70	8	0	-0.247043	-4.070434	1.310541
71	8	0	1.922618	-4.451448	1.482315
72	8	0	-2.888456	-2.801861	2.128081
73	8	0	-2.565212	-1.545525	3.911689
74	8	0	-3.746479	1.019425	-1.523378
75	7	0	6.200341	-0.491346	-1.700568
76	8	0	6.790248	-1.265215	-0.952563
77	8	0	6.723646	0.168432	-2.596023
78	7	0	5.311064	1.925270	1.723546
79	8	0	6.194866	2.290835	0.936451
80	8	0	5.534957	1.312946	2.774968
81	16	0	-0.325728	4.116876	0.950552

Structure $TS_{3b \rightarrow 4b}$

E (Hartree) = -2797.48836634

Imaginary Frequency (cm^{-1}) = -501.9355

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.266746	-2.371648	-0.139393
2	6	0	-2.403873	-1.744218	-0.953534
3	6	0	-1.638972	-0.693058	-1.803842
4	6	0	-0.177788	-1.227157	-1.827538
5	6	0	4.760384	-0.647289	-1.033319
6	6	0	-1.452421	-3.790424	0.399180
7	6	0	-3.468815	4.261636	1.300748
8	6	0	-4.488436	5.173706	1.570725
9	6	0	4.234492	0.197991	-2.006815
10	6	0	-5.396489	5.529740	0.572885
11	6	0	-0.205837	0.884175	-0.826090
12	6	0	-0.922545	2.921868	0.099343
13	6	0	-2.458269	-2.777880	3.454166

14	6	0	-1.999987	-4.067668	4.099043
15	6	0	-2.590128	1.500864	-0.967421
16	6	0	-2.694274	-3.936050	1.277718
17	6	0	-2.247477	2.720887	-0.271276
18	6	0	-5.279639	4.960976	-0.696692
19	6	0	-3.335136	3.690107	0.025162
20	6	0	-4.262450	4.047798	-0.968096
21	6	0	2.150307	2.148792	1.556580
22	6	0	3.540321	2.050277	1.700075
23	6	0	4.393110	2.621864	0.751308
24	6	0	3.835522	3.310439	-0.336624
25	6	0	1.618308	2.845027	0.474415
26	6	0	2.457532	3.408574	-0.494045
27	6	0	2.034013	-0.254142	-1.120654
28	6	0	2.578681	-1.117213	-0.161588
29	6	0	-4.265045	-2.770863	-2.228369
30	6	0	-5.219889	-1.766174	-1.630319
31	6	0	2.857697	0.394296	-2.046442
32	6	0	3.955580	-1.310791	-0.109976
33	6	0	0.843373	-4.666148	0.713935
34	6	0	0.742499	-5.474125	-0.561106
35	1	0	-3.581520	-3.965512	0.639243
36	1	0	-5.341356	-1.939075	-0.553445
37	1	0	-4.874817	-0.734900	-1.756435
38	1	0	-6.186620	-1.901204	-2.115974
39	1	0	0.533894	-4.824848	-1.415923
40	1	0	4.899060	0.690949	-2.704908
41	1	0	-0.052875	-6.225129	-0.499620
42	1	0	1.699283	-5.974195	-0.713510
43	1	0	-1.774328	-3.850463	5.143092
44	1	0	-2.777737	-4.838550	4.054775
45	1	0	-4.573907	5.601965	2.565909
46	1	0	-6.190333	6.241653	0.783204
47	1	0	-1.031943	-1.714791	0.706970
48	1	0	-3.162817	-1.282797	-0.323065
49	1	0	-2.097582	-0.576947	-2.787310
50	1	0	0.225546	-1.477937	-2.809717
51	1	0	-1.537925	-4.489314	-0.435962
52	1	0	-2.775737	3.983933	2.087984
53	1	0	1.934116	-1.634891	0.538495
54	1	0	4.402225	-1.966127	0.627258
55	1	0	-1.103558	-4.453764	3.604984
56	1	0	2.420186	1.053289	-2.788675
57	1	0	-5.982389	5.229193	-1.481370
58	1	0	-4.186080	3.604632	-1.954637
59	1	0	1.497819	1.711507	2.304929
60	1	0	3.934078	1.518160	2.559108
61	1	0	4.504050	3.769638	-1.059212
62	1	0	2.040690	3.957988	-1.331470
63	1	0	-2.637914	-4.877504	1.829524
64	7	0	-1.498316	0.596494	-1.142575
65	7	0	0.094034	2.014285	-0.223565
66	7	0	0.609671	-0.131728	-1.232306
67	8	0	-0.156898	-2.404681	-1.057984
68	8	0	-2.941290	-2.748194	-1.815000
69	8	0	-4.567317	-3.620564	-3.024332
70	8	0	-0.301226	-4.083225	1.210694
71	8	0	1.855569	-4.536698	1.354608
72	8	0	-2.869270	-2.809737	2.138641
73	8	0	-2.510591	-1.718543	4.022139
74	8	0	-3.685300	1.144685	-1.400606
75	7	0	6.218842	-0.830088	-0.968499
76	8	0	6.677614	-1.384069	0.031439
77	8	0	6.888732	-0.417047	-1.912950
78	16	0	-0.168170	4.205146	0.948560
79	6	0	6.375102	1.876196	1.862737
80	1	0	7.450987	1.974097	1.707302
81	1	0	6.105876	2.324402	2.828748

82	1	0	6.111201	0.809911	1.870584
83	8	0	5.761889	2.559244	0.781034

Structure 4a

E (Hartree) = -2887.55682478

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.732154	-1.393289	0.047667
2	6	0	-3.267568	-0.298387	-0.884676
3	6	0	-2.036384	-0.005574	-1.776779
4	6	0	-1.186388	-1.307710	-1.688386
5	6	0	3.432345	-3.419154	-1.393969
6	6	0	-3.770659	-2.332464	0.663111
7	6	0	-0.655703	5.152600	0.995278
8	6	0	-0.915804	6.507479	1.201707
9	6	0	3.645142	-2.044167	-1.471196
10	6	0	-1.197363	7.339643	0.117616
11	6	0	0.092518	0.498249	-0.911762
12	6	0	0.797769	2.538206	-0.230183
13	6	0	-3.879068	-0.689389	3.591257
14	6	0	-4.326849	-1.930076	4.331572
15	6	0	-1.464502	2.368958	-1.112196
16	6	0	-4.824595	-1.581464	1.481616
17	6	0	-0.402008	3.165347	-0.525059
18	6	0	-1.222010	6.809948	-1.174382
19	6	0	-0.665675	4.612973	-0.300264
20	6	0	-0.961493	5.456836	-1.382029
21	6	0	3.388892	1.385641	1.670577
22	6	0	4.480674	0.564910	1.930816
23	6	0	5.650151	0.748237	1.193108
24	6	0	5.754554	1.716837	0.198849
25	6	0	3.466835	2.363929	0.668379
26	6	0	4.649730	2.524520	-0.065310
27	6	0	1.263817	-1.692640	-1.229496
28	6	0	1.072118	-3.082000	-1.131201
29	6	0	-5.359237	-0.138907	-2.208024
30	6	0	-5.516834	1.298220	-1.773576
31	6	0	2.562082	-1.177744	-1.392984
32	6	0	2.156061	-3.947040	-1.221175
33	6	0	-2.802821	-4.540680	1.256651
34	6	0	-3.265663	-5.103443	-0.070809
35	1	0	-5.524436	-1.085632	0.803373
36	1	0	-5.746874	1.354900	-0.702021
37	1	0	-4.611248	1.889759	-1.940360
38	1	0	-6.352159	1.721847	-2.331608
39	1	0	-2.893617	-4.511751	-0.911429
40	1	0	4.651742	-1.667503	-1.604307
41	1	0	-4.360205	-5.125829	-0.131130
42	1	0	-2.892487	-6.125336	-0.142011
43	1	0	-4.021865	-1.819059	5.372194
44	1	0	-5.414594	-2.055917	4.289164
45	1	0	-0.905631	6.909044	2.211268
46	1	0	-1.401941	8.394691	0.278508
47	1	0	-2.156252	-0.930111	0.857486
48	1	0	-3.601942	0.586300	-0.344053
49	1	0	-2.341474	0.265033	-2.789766
50	1	0	-1.063561	-1.853057	-2.625233
51	1	0	-4.281233	-2.876530	-0.133466
52	1	0	-0.452931	4.505191	1.843477
53	1	0	0.080900	-3.481356	-0.957693
54	1	0	2.025361	-5.019418	-1.146225
55	1	0	-3.859230	-2.824472	3.909109

56	1	0	2.719394	-0.109982	-1.448345
57	1	0	-1.446843	7.451138	-2.022411
58	1	0	-0.991494	5.045904	-2.386435
59	1	0	2.477095	1.271782	2.246036
60	1	0	4.447345	-0.197692	2.699068
61	1	0	6.682302	1.825220	-0.349341
62	1	0	4.705700	3.283345	-0.838987
63	1	0	-5.385229	-2.297760	2.087285
64	7	0	-1.141807	0.996413	-1.221139
65	7	0	1.064545	1.210855	-0.422146
66	7	0	0.126296	-0.848284	-1.212803
67	8	0	-1.857581	-2.170447	-0.791891
68	8	0	-4.300170	-0.869627	-1.691320
69	8	0	-6.104440	-0.719480	-2.952563
70	8	0	-3.088633	-3.228312	1.553543
71	8	0	-2.214190	-5.179237	2.090261
72	8	0	-4.244965	-0.540476	2.270031
73	8	0	-3.236769	0.200256	4.086006
74	8	0	-2.565751	2.753827	-1.499414
75	7	0	4.578120	-4.331119	-1.498421
76	8	0	4.352631	-5.539776	-1.434181
77	8	0	5.692604	-3.831685	-1.649924
78	7	0	6.817983	-0.101985	1.484919
79	8	0	7.837108	0.084206	0.821694
80	8	0	6.701403	-0.942101	2.375422
81	16	0	2.141875	3.540531	0.402824

Structure 4b

E (Hartree) = -2797.58472202

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.612594	-1.418618	-0.064825
2	6	0	-3.093360	-0.303144	-1.002971
3	6	0	-1.804849	0.032654	-1.792605
4	6	0	-0.943502	-1.261213	-1.681633
5	6	0	3.649485	-3.339244	-0.823260
6	6	0	-3.681266	-2.392316	0.435314
7	6	0	-0.611690	5.111332	1.267511
8	6	0	-0.908853	6.450920	1.519871
9	6	0	3.856127	-1.962808	-0.897928
10	6	0	-1.236508	7.305830	0.467335
11	6	0	0.251915	0.541127	-0.770813
12	6	0	0.881367	2.566939	0.027709
13	6	0	-4.052240	-0.855660	3.410301
14	6	0	-4.510954	-2.141224	4.062729
15	6	0	-1.324807	2.389055	-0.996373
16	6	0	-4.804913	-1.688381	1.200986
17	6	0	-0.317230	3.179554	-0.313068
18	6	0	-1.270009	6.812685	-0.839105
19	6	0	-0.628020	4.608528	-0.042793
20	6	0	-0.972396	5.475374	-1.092309
21	6	0	3.903934	1.552484	1.713598
22	6	0	5.030709	0.732135	1.635329
23	6	0	5.870522	0.813011	0.515908
24	6	0	5.581116	1.732557	-0.506561
25	6	0	3.598798	2.450364	0.688137
26	6	0	4.457592	2.543111	-0.418674
27	6	0	1.460076	-1.638269	-0.999982
28	6	0	1.272453	-3.031101	-0.928560
29	6	0	-5.082277	-0.132294	-2.474574
30	6	0	-5.293266	1.289317	-2.012667
31	6	0	2.764057	-1.110589	-0.994103

32	6	0	2.367155	-3.882767	-0.849277
33	6	0	-2.722258	-4.609778	1.004006
34	6	0	-3.079854	-5.120918	-0.376031
35	1	0	-5.461326	-1.178472	0.490389
36	1	0	-5.610697	1.309700	-0.962313
37	1	0	-4.385132	1.895881	-2.085587
38	1	0	-6.086281	1.720685	-2.624017
39	1	0	-2.656969	-4.489177	-1.161634
40	1	0	4.864702	-1.568877	-0.888512
41	1	0	-4.166708	-5.153401	-0.516806
42	1	0	-2.687117	-6.134282	-0.462599
43	1	0	-4.283475	-2.068124	5.126279
44	1	0	-5.588917	-2.295111	3.938380
45	1	0	-0.891587	6.821939	2.541061
46	1	0	-1.470194	8.348927	0.663305
47	1	0	-2.108410	-0.973326	0.800841
48	1	0	-3.480703	0.561102	-0.464830
49	1	0	-2.040426	0.328773	-2.817128
50	1	0	-0.752921	-1.779831	-2.622591
51	1	0	-4.123233	-2.908054	-0.418894
52	1	0	-0.377782	4.446091	2.093643
53	1	0	0.272234	-3.443024	-0.893306
54	1	0	2.237263	-4.955771	-0.781443
55	1	0	-3.988469	-3.002609	3.636157
56	1	0	2.919922	-0.042581	-1.040961
57	1	0	-1.530497	7.471105	-1.663588
58	1	0	-1.010282	5.093988	-2.107585
59	1	0	3.249664	1.480511	2.576662
60	1	0	5.237170	0.033934	2.438107
61	1	0	6.252635	1.789237	-1.357583
62	1	0	4.238266	3.251287	-1.212018
63	1	0	-5.395912	-2.435797	1.736299
64	7	0	-0.969114	1.028169	-1.143552
65	7	0	1.176230	1.249418	-0.199354
66	7	0	0.326046	-0.799353	-1.108004
67	8	0	-1.664706	-2.157547	-0.856984
68	8	0	-4.055356	-0.864470	-1.900338
69	8	0	-5.761755	-0.699953	-3.289291
70	8	0	-3.055976	-3.318613	1.336993
71	8	0	-2.180222	-5.275910	1.848093
72	8	0	-4.305720	-0.669025	2.068218
73	8	0	-3.491745	0.036145	3.992558
74	8	0	-2.408300	2.768517	-1.440224
75	7	0	4.803139	-4.231992	-0.693978
76	8	0	4.600872	-5.445059	-0.750924
77	8	0	5.912235	-3.717349	-0.528144
78	16	0	2.177007	3.531630	0.805764
79	6	0	7.315671	-0.932645	1.295454
80	1	0	8.229157	-1.405110	0.932580
81	1	0	7.505318	-0.469736	2.271959
82	1	0	6.532667	-1.694000	1.387409
83	8	0	6.974551	0.045553	0.316775