

Supplementary Material

A cascade reaction of imidazo[1,2-*a*]pyridines with maleic anhydride: Formation of cross-conjugated mesomeric betaines

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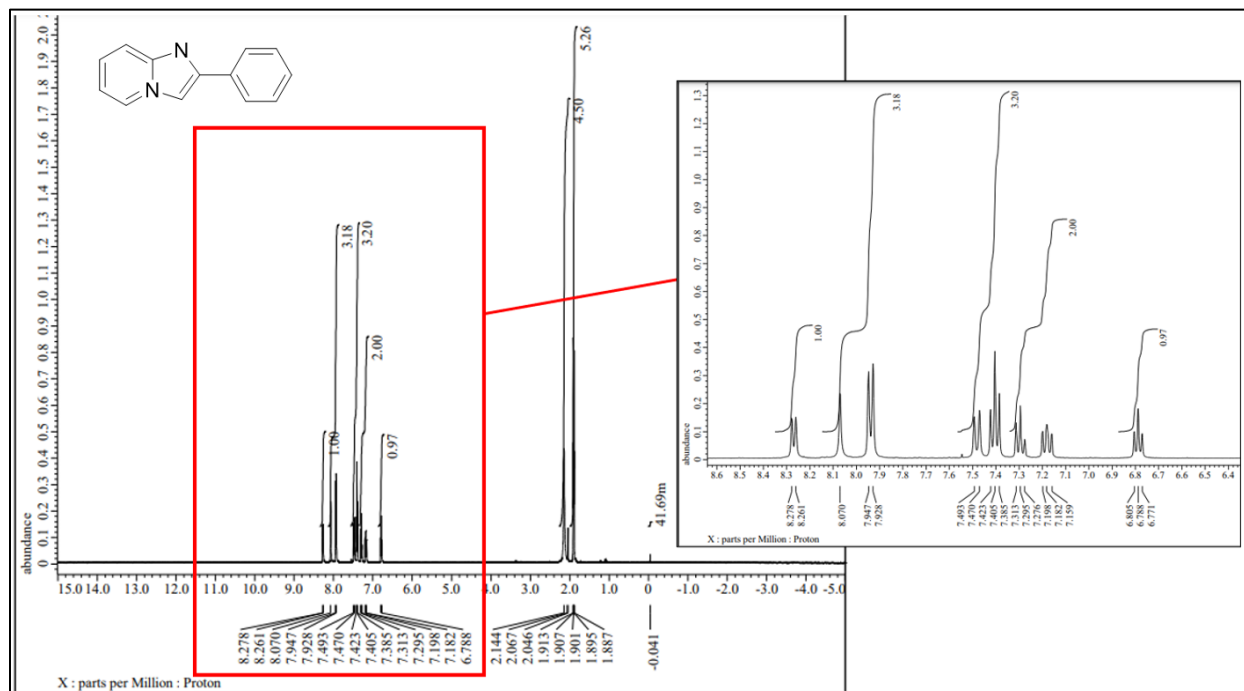
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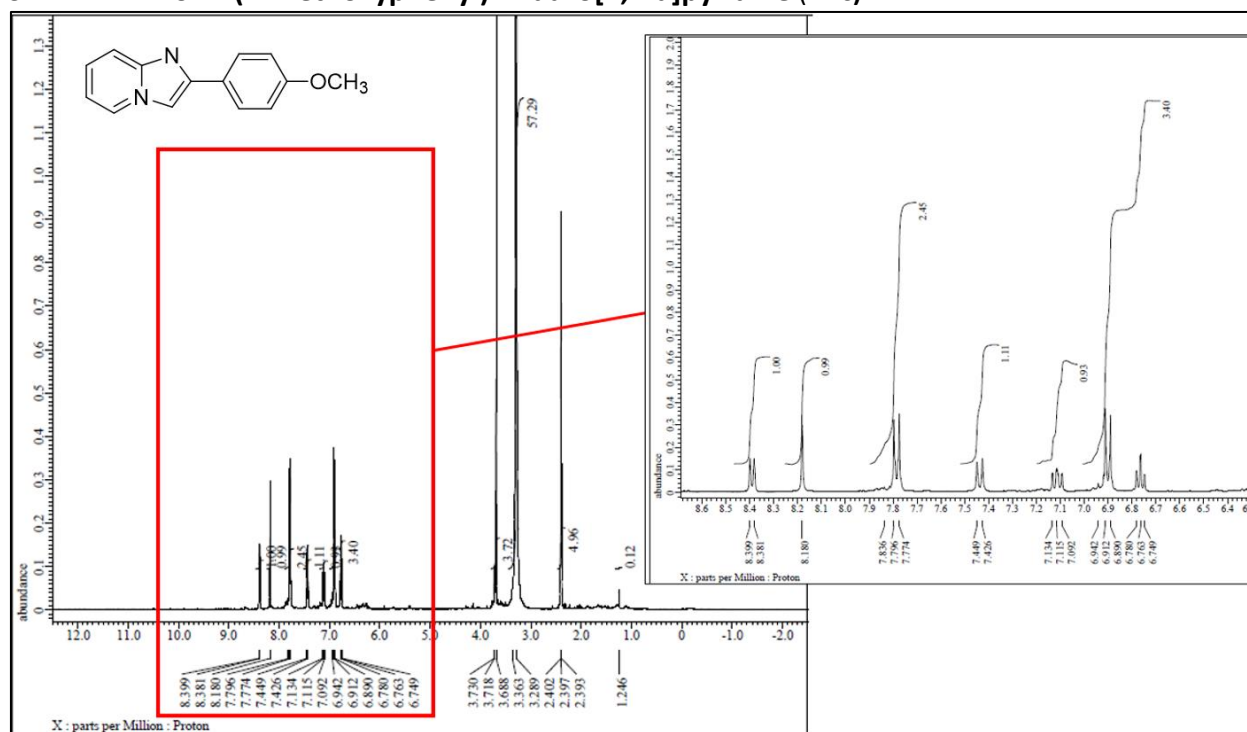
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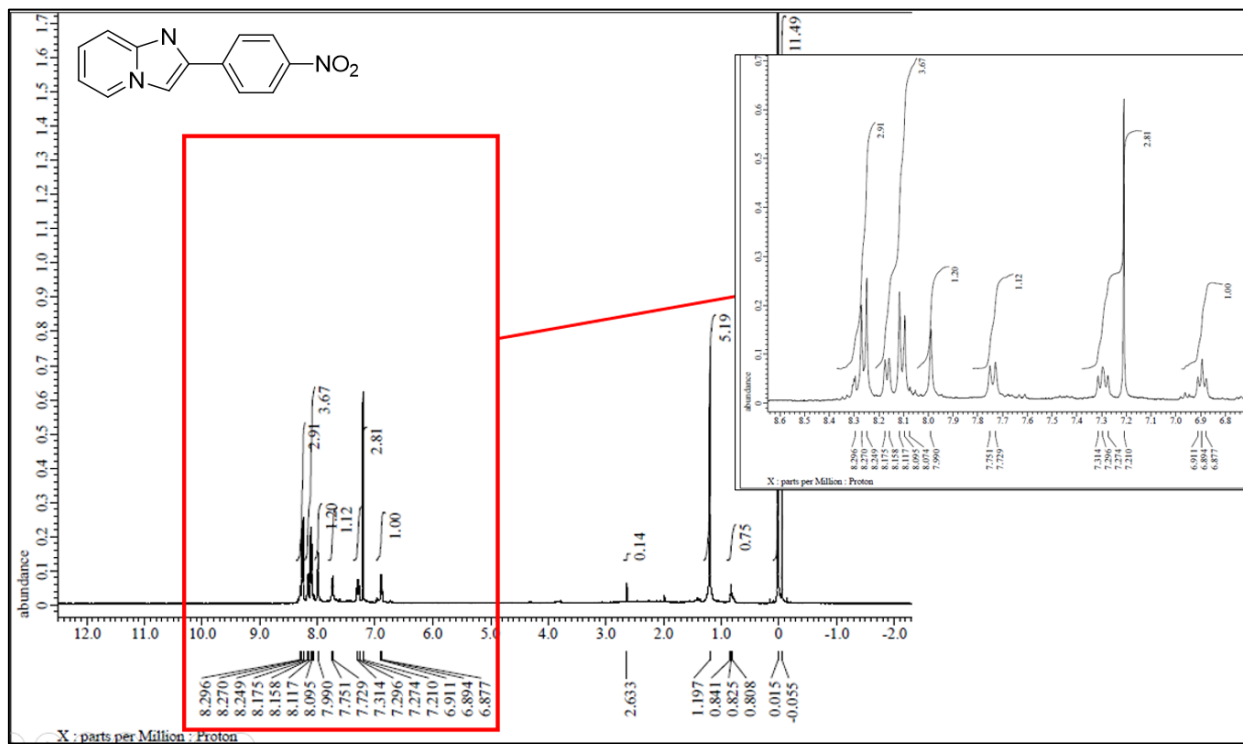
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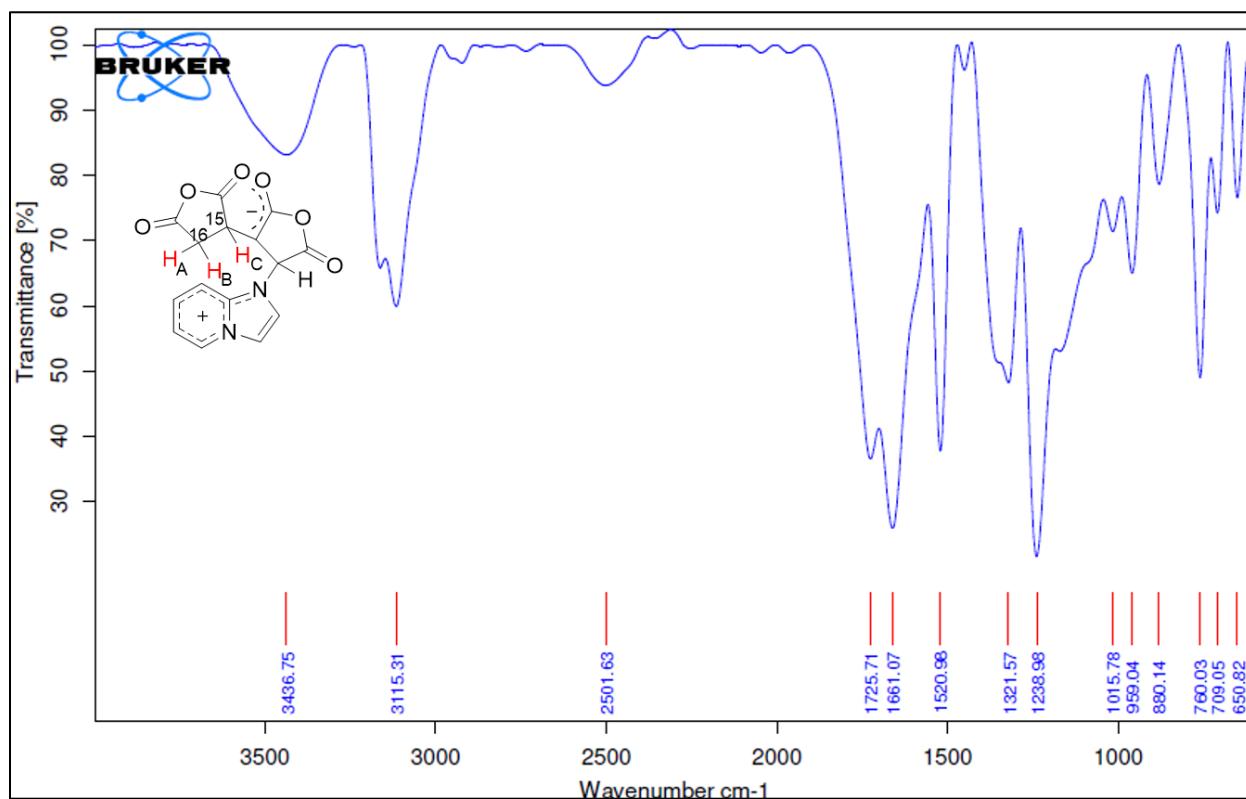
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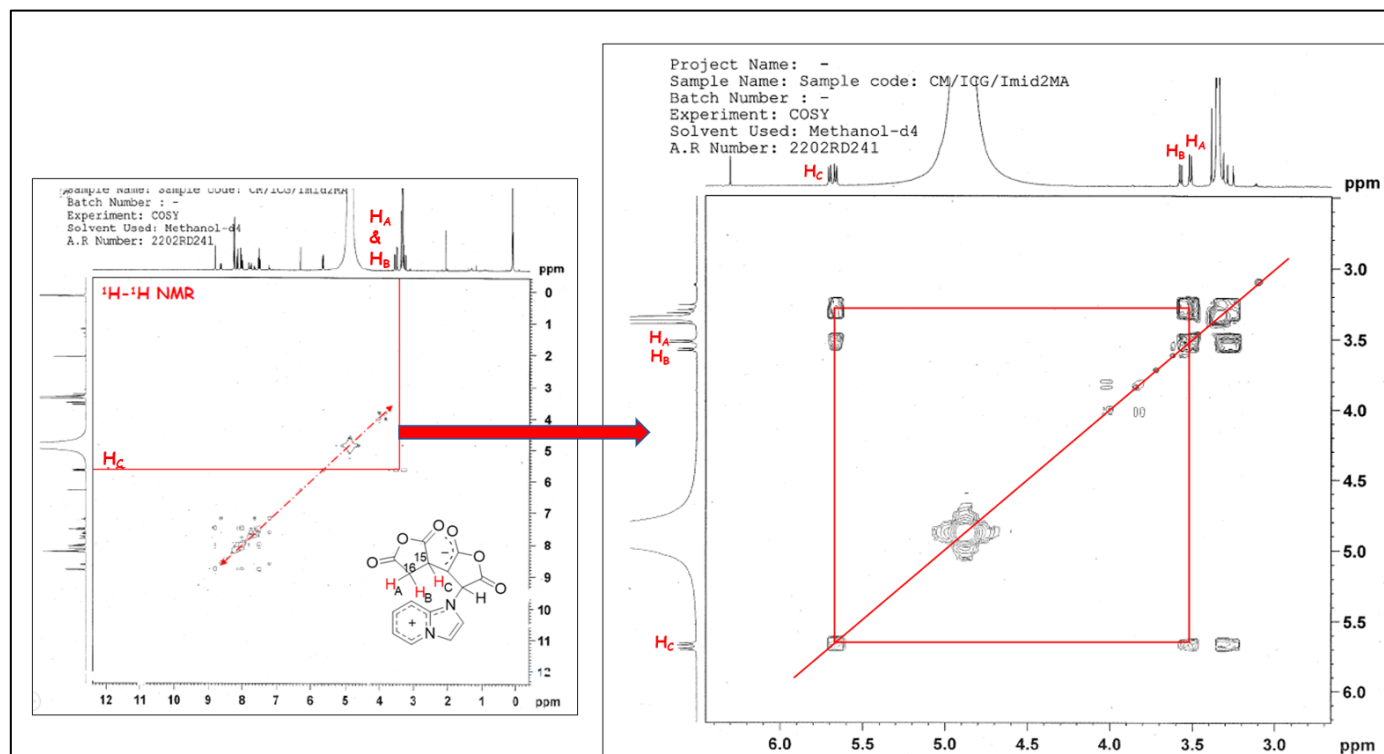
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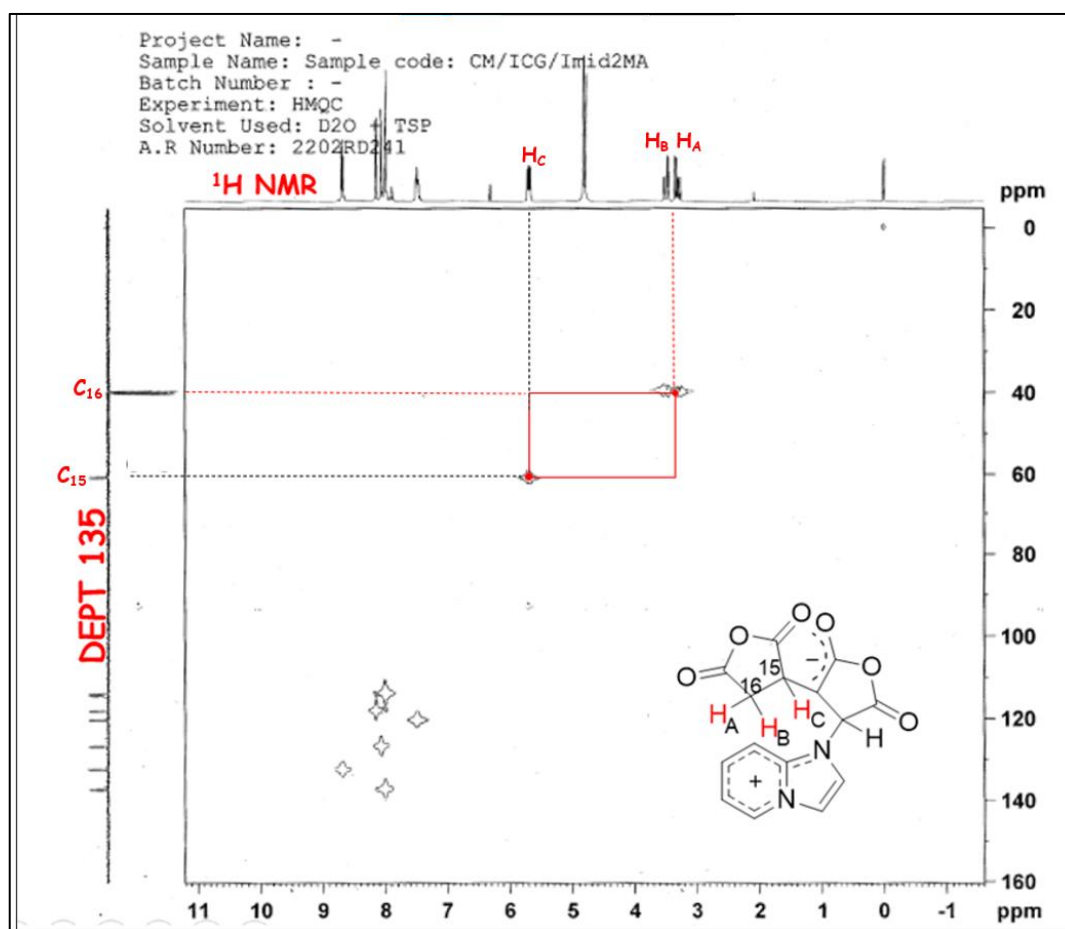
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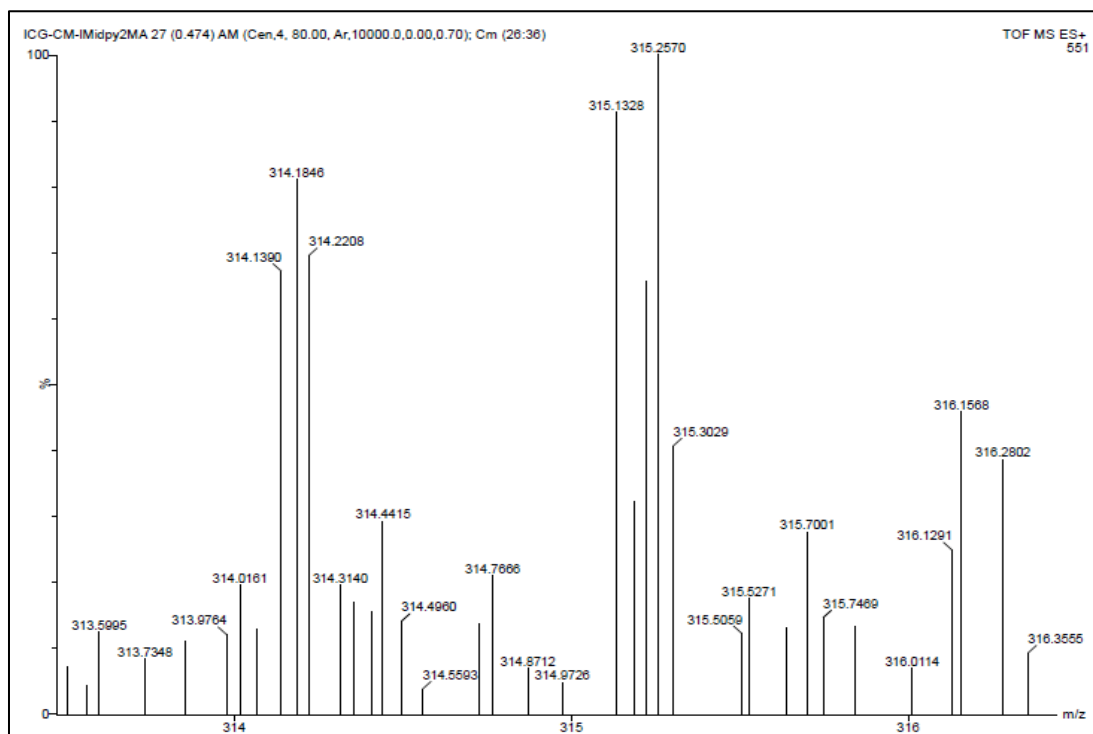
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HMQC

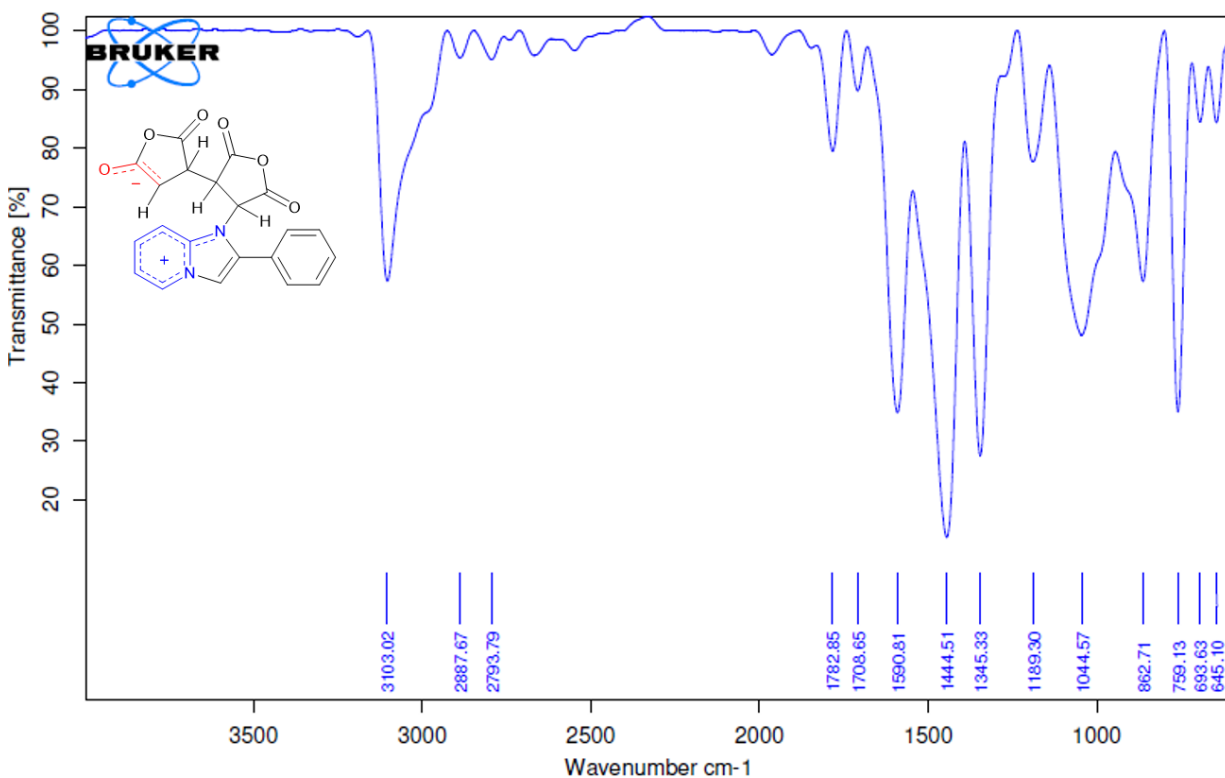
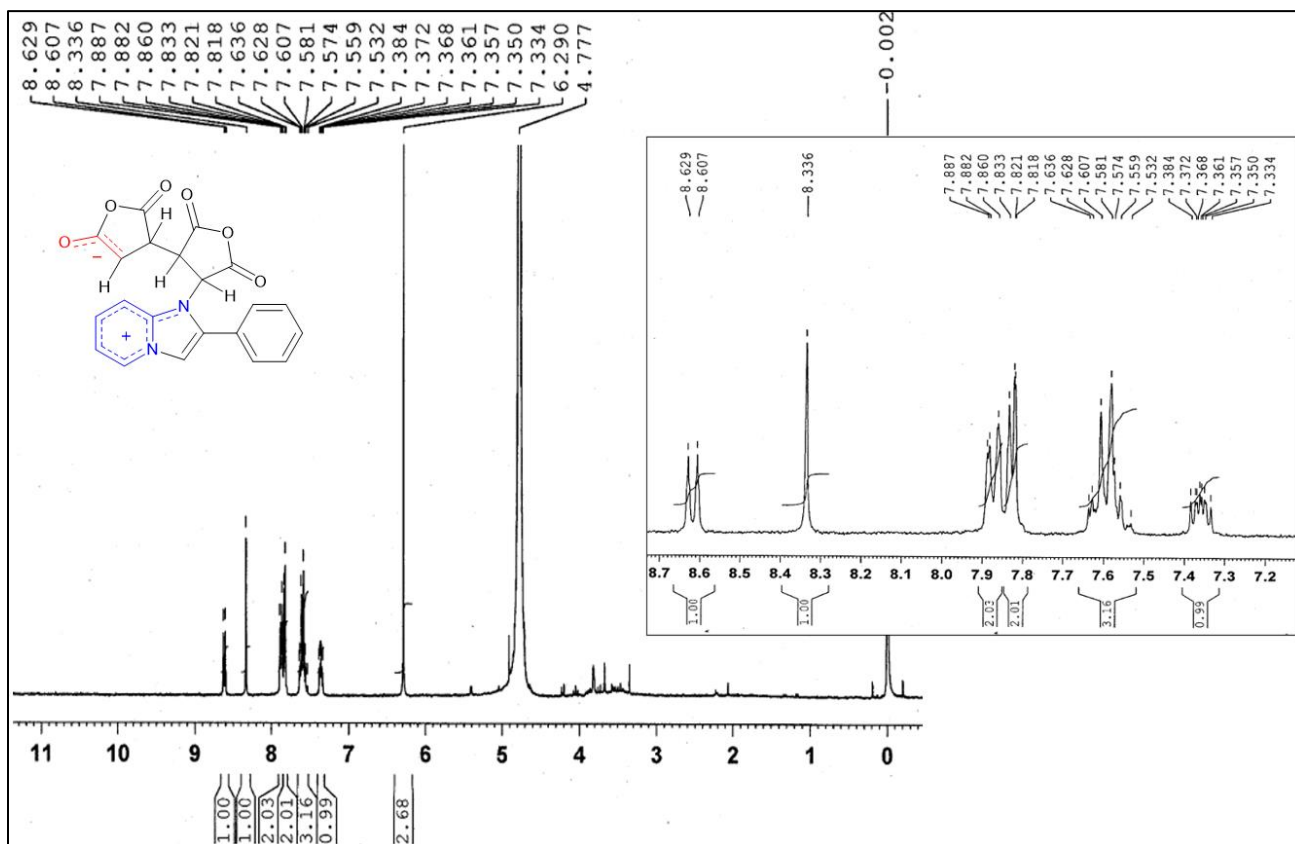


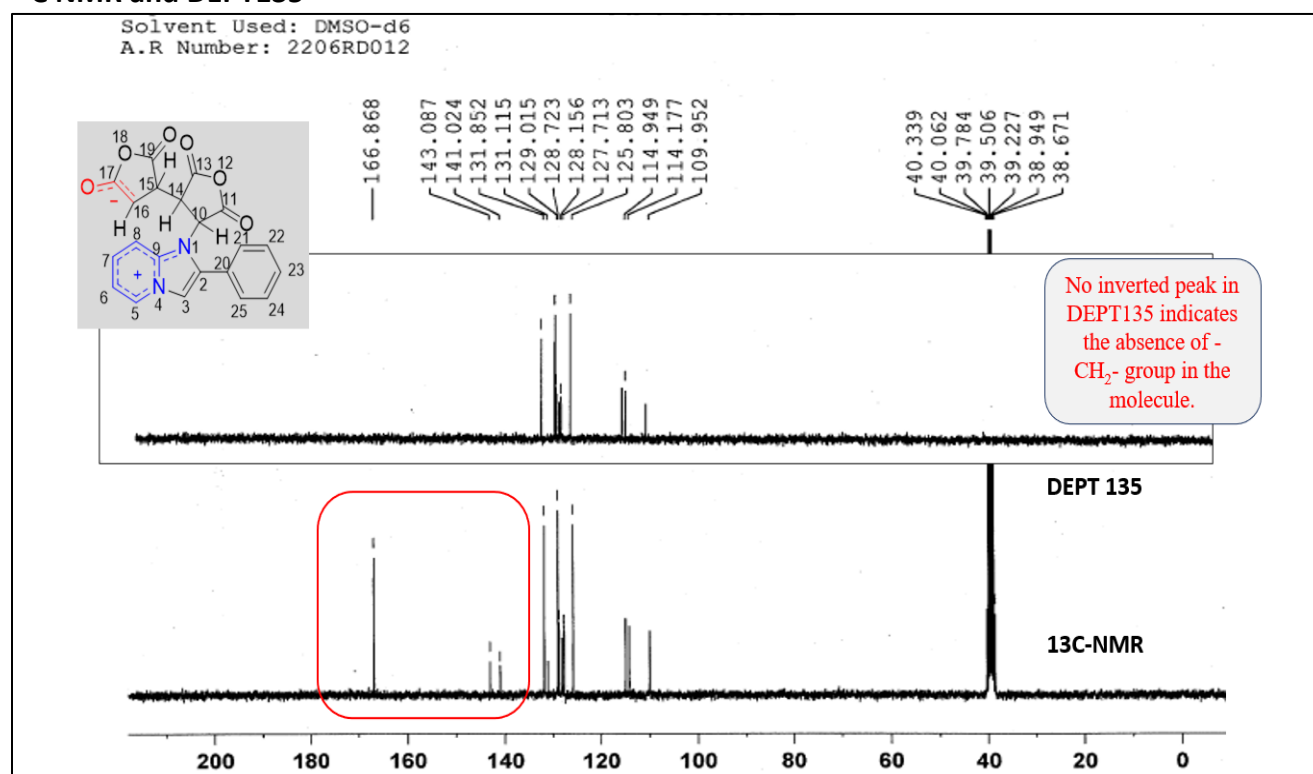
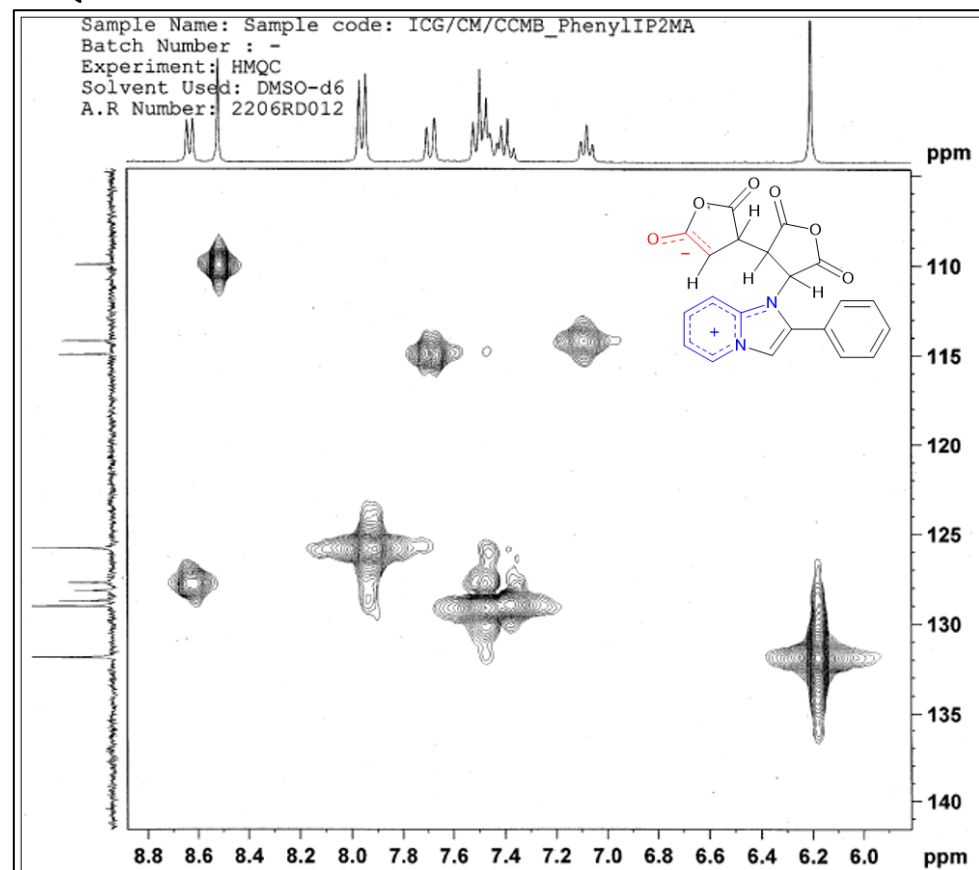
HRMS



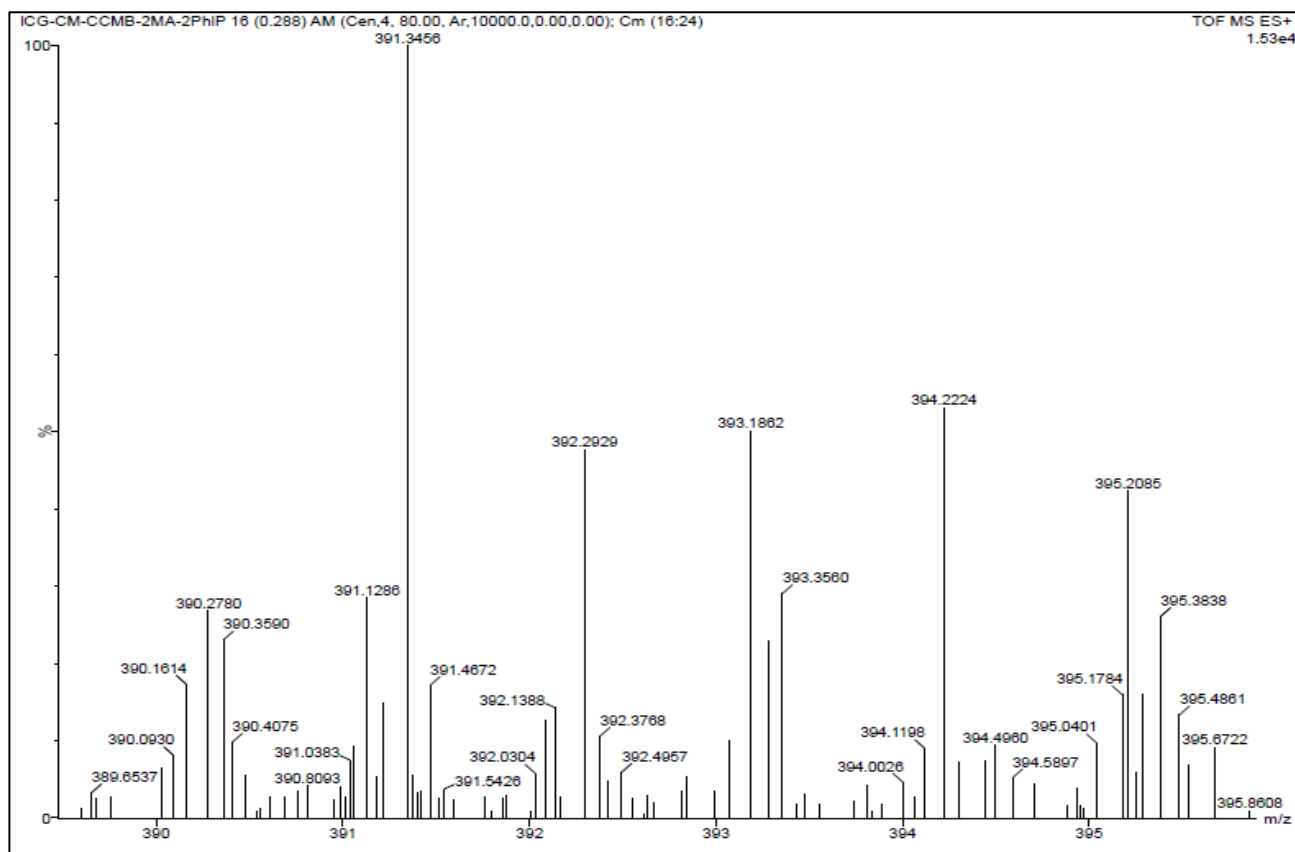
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IR

¹H NMR

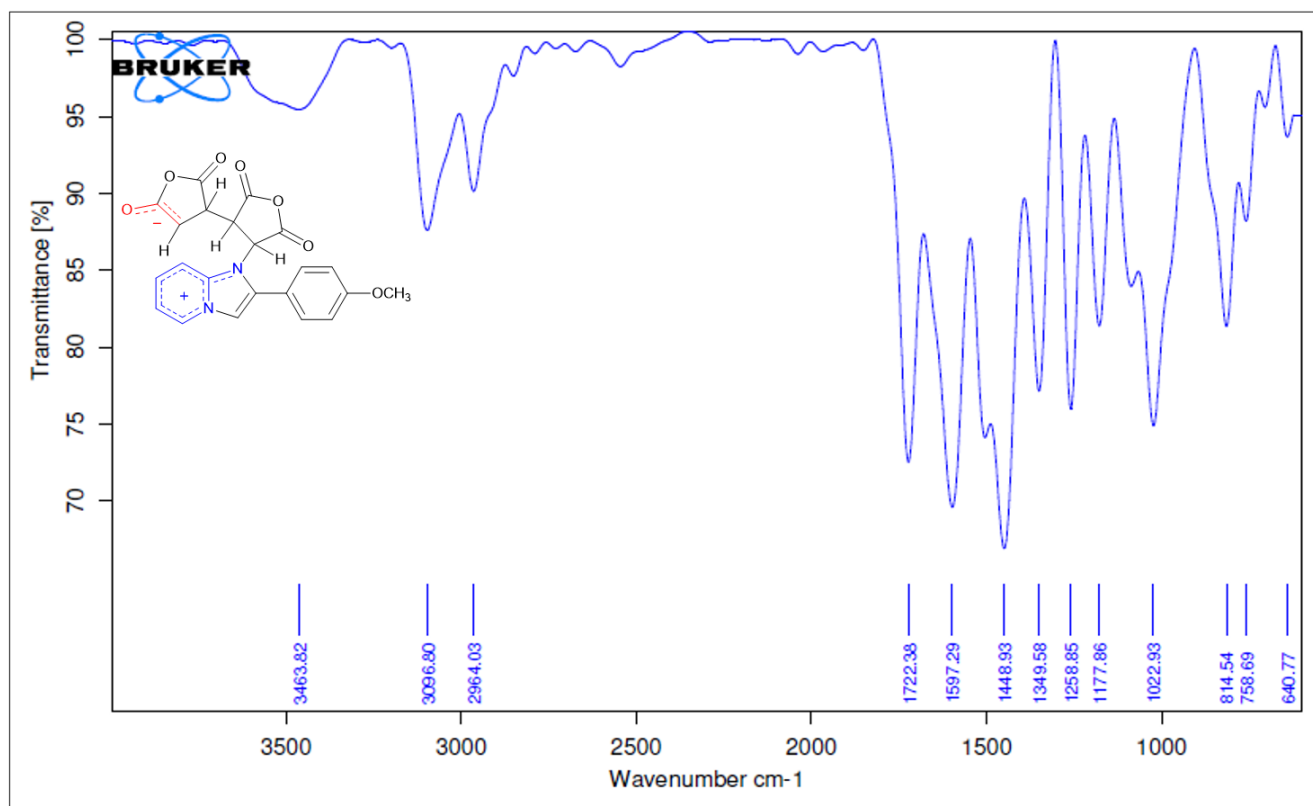
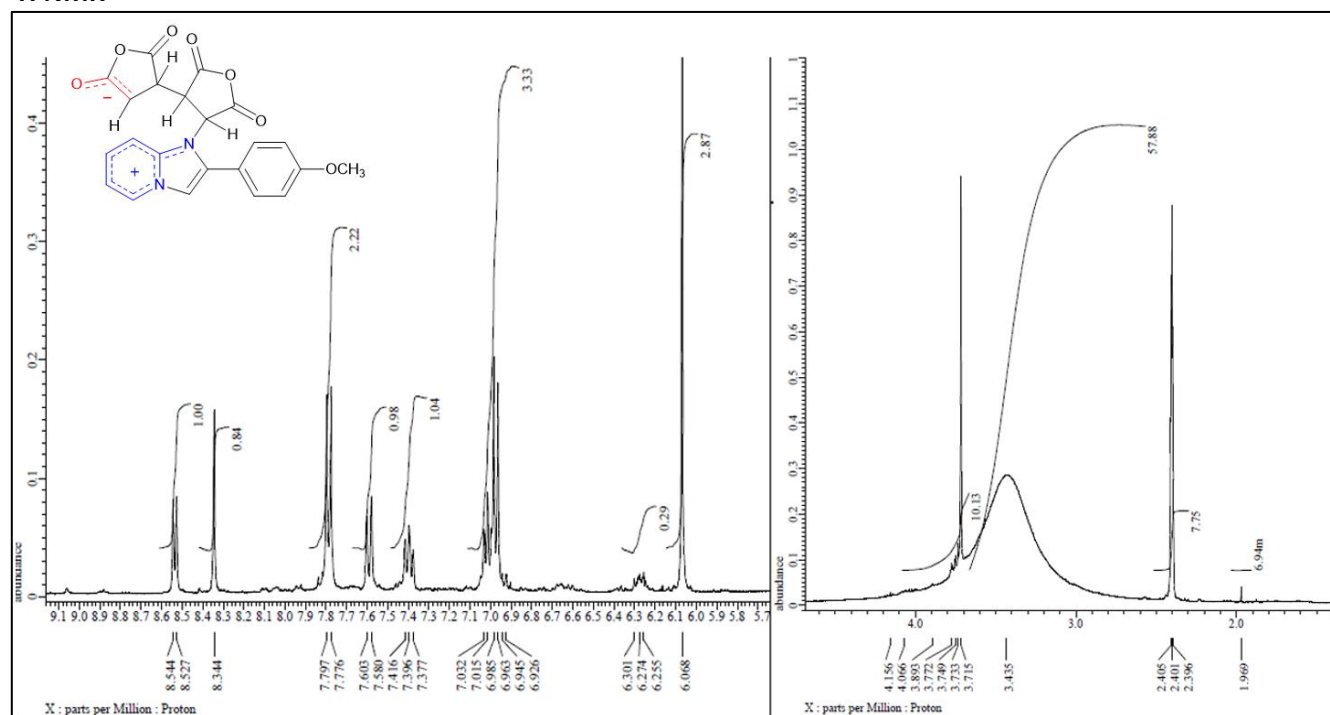
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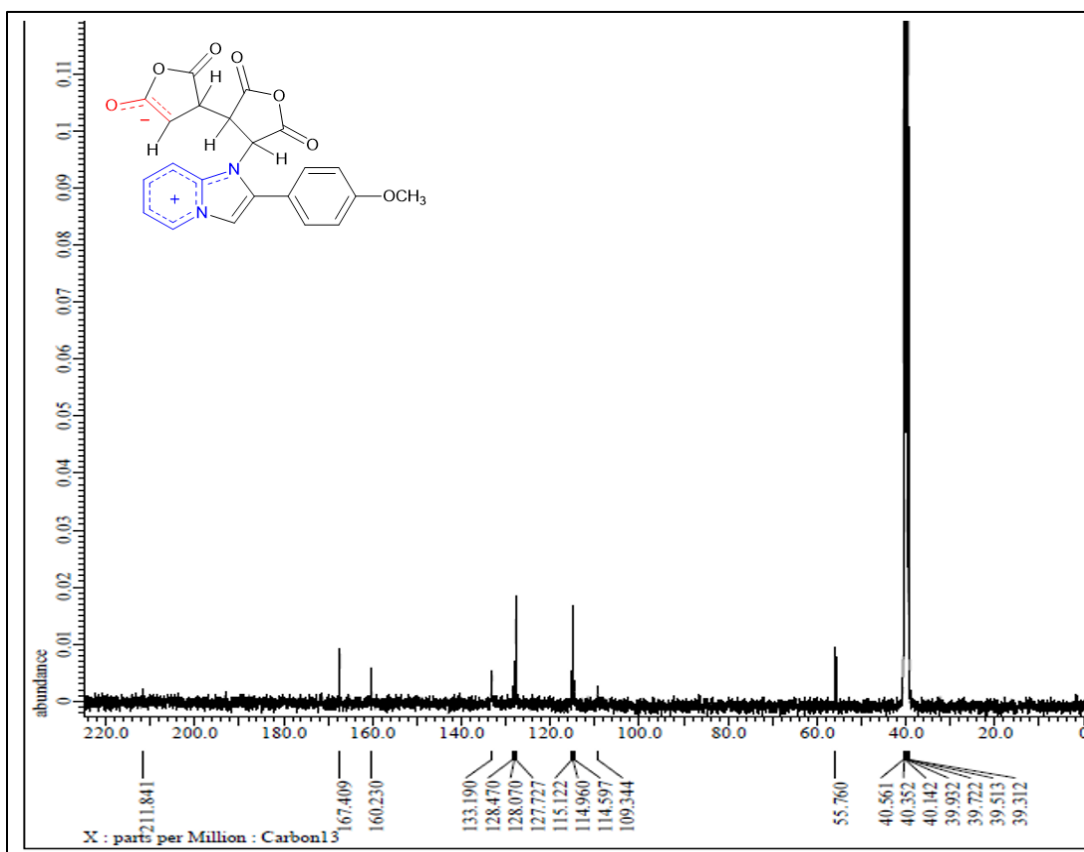
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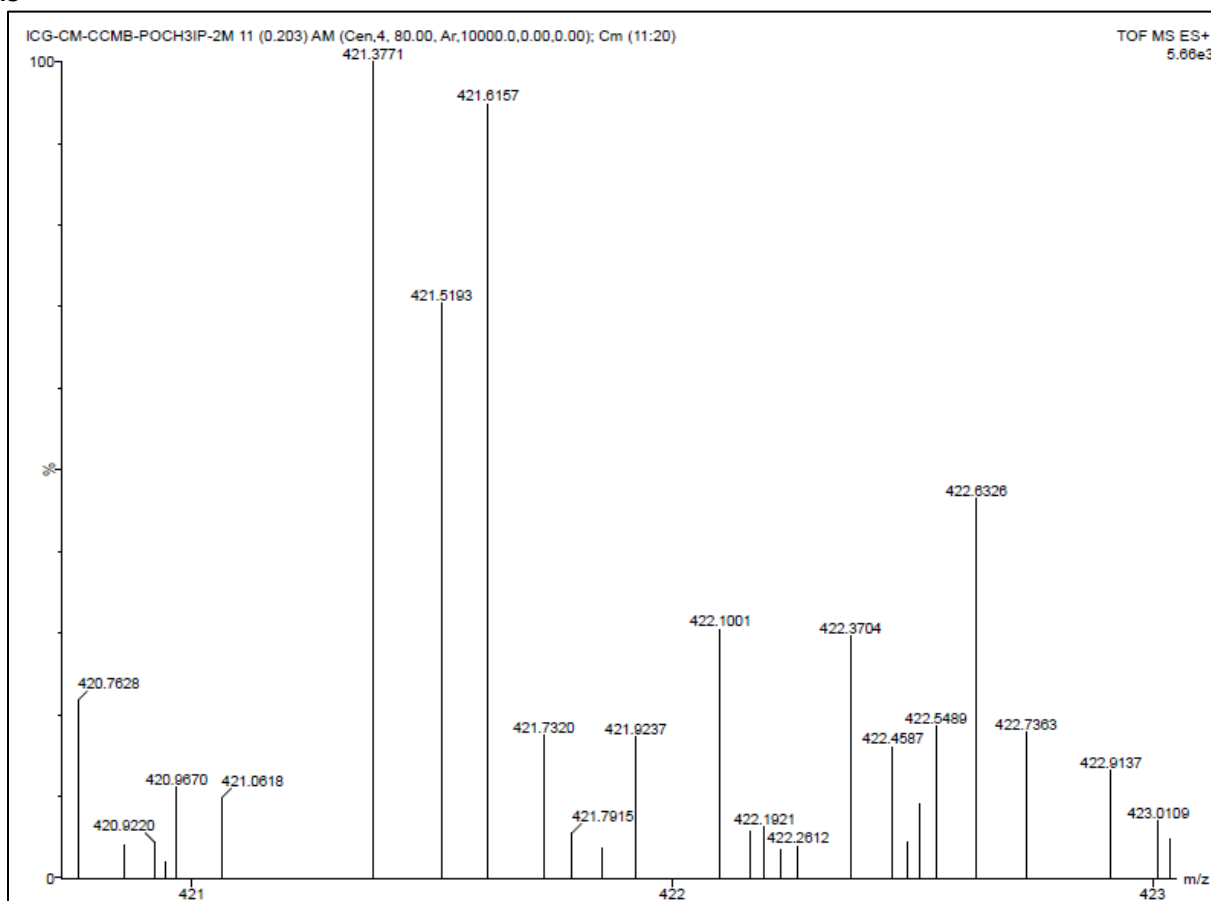
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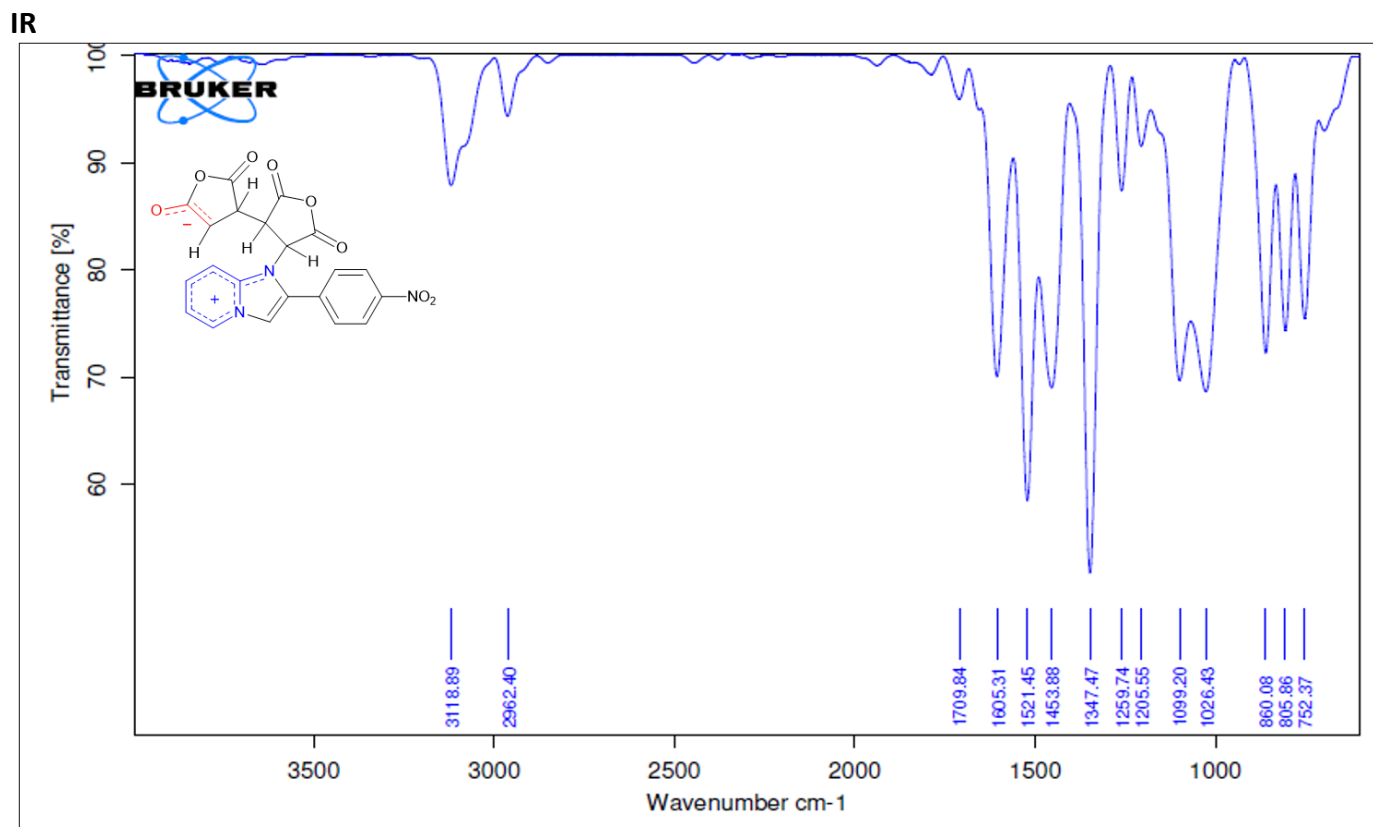
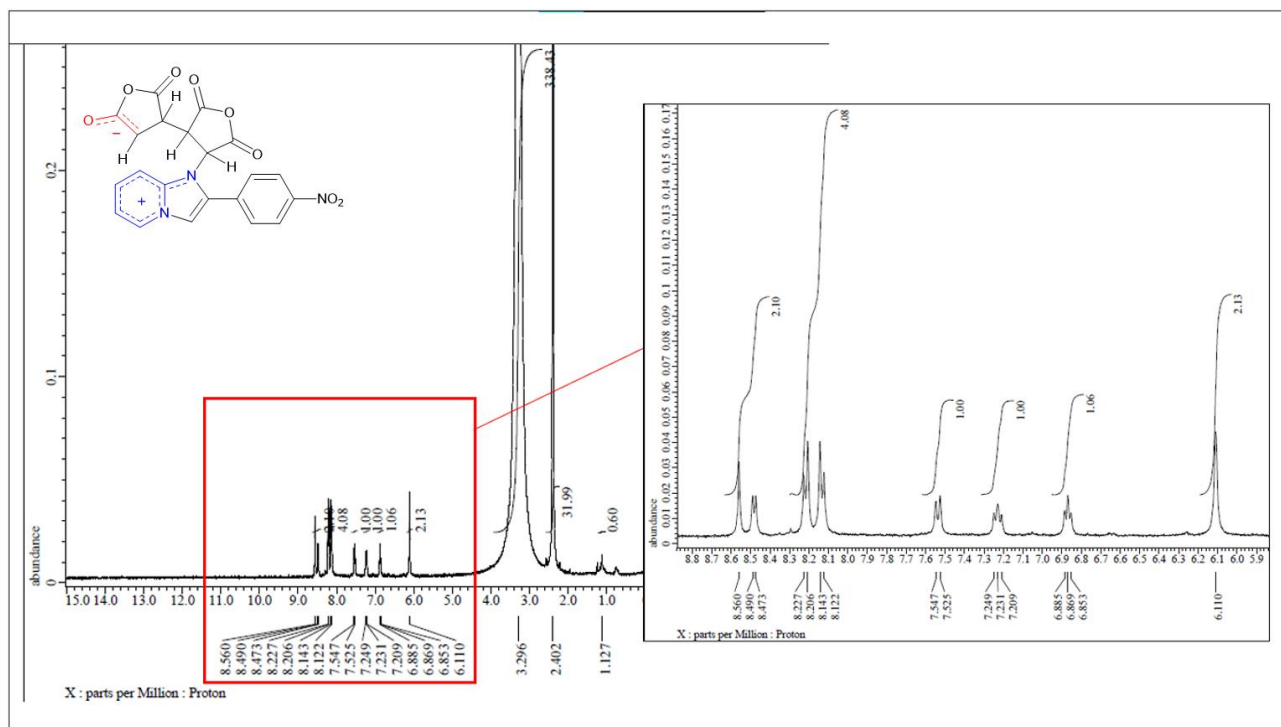
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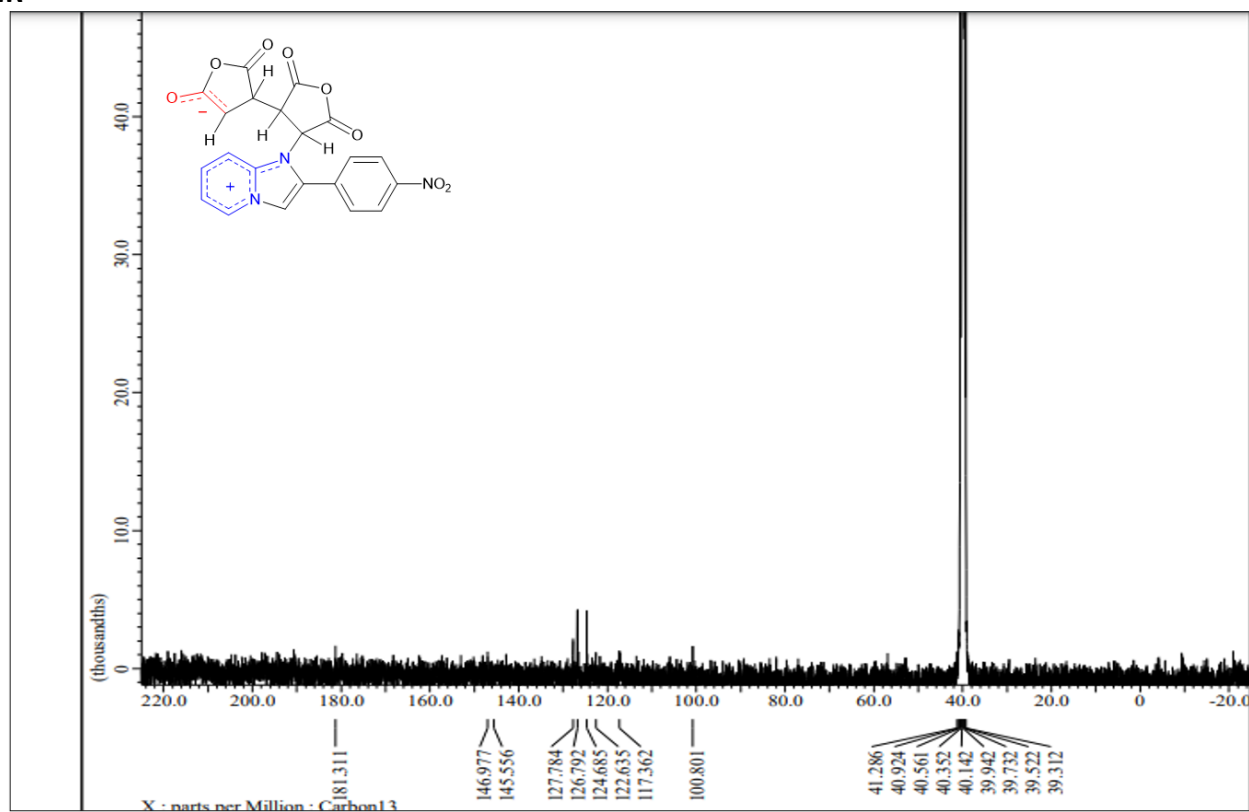
¹H NMR

¹³C NMR

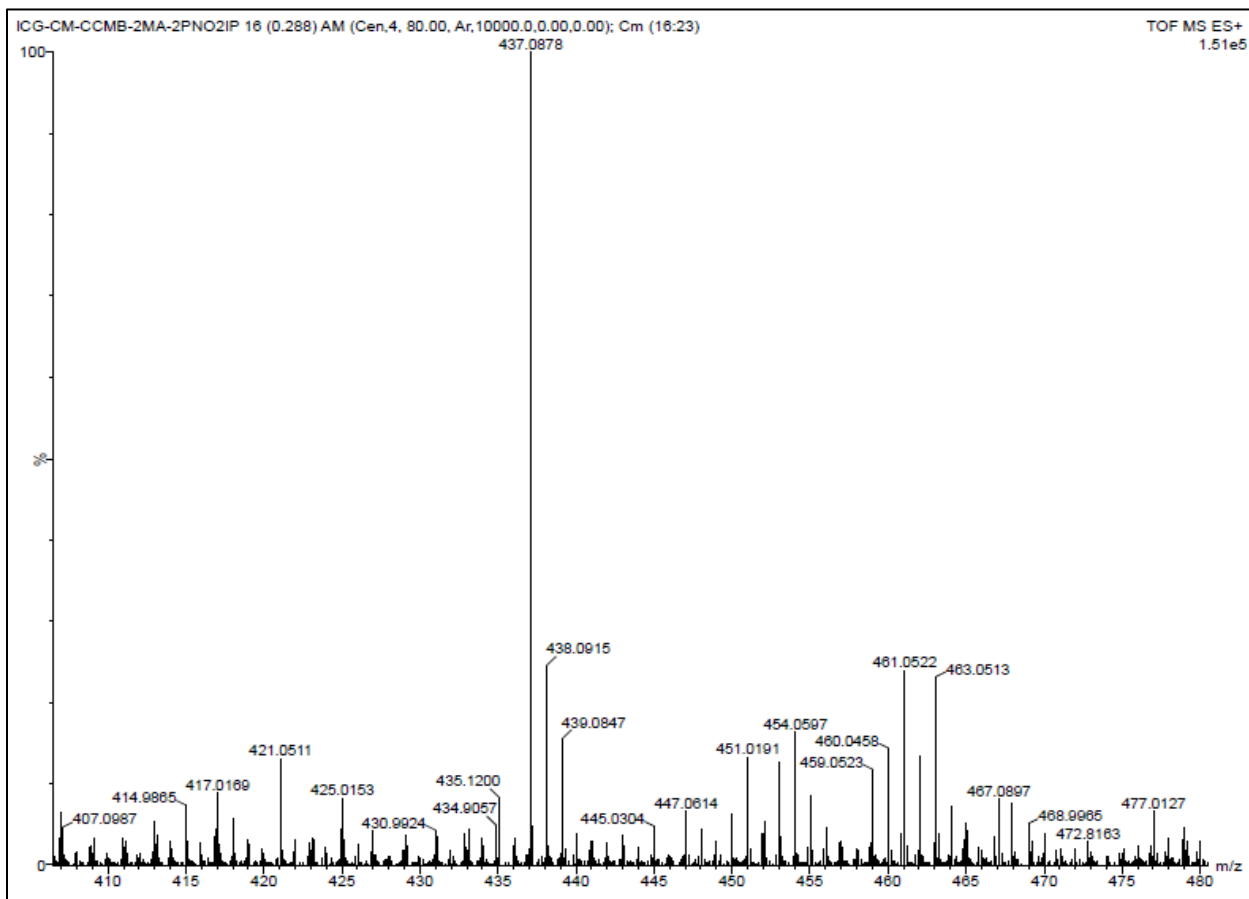
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S7. Spectra of 4-(4-(2-(4-Nitrophenyl)-1H-imidazo[1,2-a]pyridin-4-ium-1-yl)-2,5-dioxotetrahydrofuran-3-yl)-2,5-dioxotetrahydrofuran-3-ide (15d)**¹H NMR**

^{13}C NMR

HRMS



S8. Thermodynamic data of the species involved in the formation of 3-(2,5-Dioxotetrahydrofuran-3-yl)-4(1H-imidazo[1,2-a]pyridin-4-ium-1-yl)-5-oxo-4,5-dihydrofuran-2-olate (16)**Calculation of Enthalpy and Free Energy**

Total enthalpy (H) was calculated by adding thermal correction to the sum of the electronic and thermal enthalpy. The free energy (G) was calculated at temperature 298.15 K as follows:

$$\Delta G = \Delta H - T\Delta S$$

where

ΔH = relative enthalpy in kCal mol⁻¹

ΔS = relative entropy in kCal mol⁻¹ K⁻¹

T = 298.15 K

Table S1. Thermodynamic data of the species involved in the formation of 16

Basis set used: B3LYP/6-31+G(d)

Species	Total Enthalpy H (a. u.)	Entropy S (Cal K ⁻¹ mol ⁻¹)	Activation Enthalpy $\Delta H^\#$ (kcal mol ⁻¹)	Activation Entropy S (kcal K ⁻¹ mol ⁻¹)	Activation Free Energy $\Delta G^\#$ (kcal mol ⁻¹)	Standard Enthalpy ΔH° (kcal mol ⁻¹)	Standard Free Energy ΔG° (kcal mol ⁻¹)
Imidazo[1,2-a]pyridine	-379.615016	77.988	-	-	-	-	-
Maleic Anhydride	-379.182706	74.116	-	-	-	-	-
TS1	-758.765294	111.424	20.35	-0.04	32.48	-	-
Int1	-758.763749	112.461	-	-	-	21.32	33.14
TS2	-1137.93815	141.048	5.21	-0.05	18.79	-	-
Int2	-1137.930838	139.640	-	-	-	31.12	56.93
TS3	-1137.910121	140.773	12.99	0.001	12.66	-	-
Product	-1137.977761	143.725	-	-	-	1.67	26.27

S9. Cartesian coordinates of the optimized geometries of relevant structures.

NOTE: All geometries have been optimized at B3LYP/6-31+G(d,p) level unless mentioned otherwise.

A. Species involved in the formation of 16**Imidazo[1,2-*a*]pyridine**

7	-1.898925342	-0.490884848	0.000000000
6	-0.567734564	-0.555058229	0.000000000
6	0.303937908	-1.669773501	0.000000000
6	1.664478210	-1.468349870	0.000000000
6	2.196627403	-0.144938143	0.000000000
6	1.360123105	0.937153508	0.000000000
7	0.000000000	0.736429328	0.000000000
1	-0.137470416	-2.660649158	0.000000000
1	2.342789657	-2.316222281	0.000000000
1	3.269027133	0.019011260	0.000000000
1	1.697242113	1.967559510	0.000000000
6	-1.056133636	1.625510708	0.000000000
6	-2.193645494	0.840651375	0.000000000
1	-3.219862206	1.185558480	0.000000000
1	-0.905166485	2.694755785	0.000000000

Maleic Anhydride

6	1.132191404	-0.158169453	-0.000073242
8	0.000000000	-0.972375477	-0.000259134
6	-1.132191637	-0.158169903	-0.000116822
6	-0.668707520	1.258936256	-0.000034089
6	0.668706748	1.258936599	-0.000068401
1	-1.362649244	2.089976702	0.000197985
1	1.362648186	2.089977295	0.000128133
8	2.246806328	-0.600634260	0.000217134
8	-2.246805445	-0.600634641	0.000220650

TS1

7	-0.196697430	-0.909122762	-0.562195840
6	-1.084435957	0.058560290	-0.250772880
6	-0.972420076	1.461894887	-0.139387309
6	-2.094192441	2.180616219	0.207433718
6	-3.335177480	1.528740800	0.446590486
6	-3.428537719	0.169262676	0.340114424
7	-2.310278123	-0.554435932	-0.002261822
1	-0.013776800	1.927475810	-0.326214942
1	-2.028956671	3.259629061	0.303983509
1	-4.216715555	2.097936211	0.720288681
1	-4.332967705	-0.401677343	0.512645076

6	-2.147939540	-1.924589291	-0.156691047
6	-0.837243653	-2.116695243	-0.493980164
1	-0.305538720	-3.039606146	-0.674655970
1	-2.962295356	-2.616659616	-0.007962012
6	2.632748705	1.129077826	-0.158468142
8	2.648758577	0.121940804	0.974288210
6	2.069475799	-1.001530953	0.546553123
6	1.478613988	-0.763094019	-0.854108929
6	1.957392449	0.522348529	-1.232186309
1	1.560486064	-1.621190950	-1.523945110
1	1.889628545	0.979178241	-2.210365474
8	1.992382177	-2.036083799	1.175245863
8	3.175016821	2.188177400	0.053821936

Int 1

7	0.198084535	-0.912357554	0.579502524
6	1.049486397	0.087848124	0.240533968
6	0.874123952	1.473777901	0.047479535
6	1.975233416	2.223715631	-0.302731614
6	3.250862695	1.618835698	-0.464287564
6	3.400007434	0.272642256	-0.279190014
7	2.303219105	-0.481880922	0.065000946
1	-0.112480068	1.895878049	0.188063346
1	1.864674001	3.291737610	-0.460356442
1	4.115701460	2.212028620	-0.740281236
1	4.333052924	-0.266314147	-0.390218404
6	2.202982102	-1.850024872	0.284641880
6	0.896380957	-2.093907468	0.588356924
1	0.400336092	-3.028859117	0.800468316
1	3.054409494	-2.506749475	0.199307218
6	-2.728763298	1.004964620	0.283422273
8	-2.681812692	0.064381426	-0.967329375
6	-1.928018952	-0.979916137	-0.686280555
6	-1.338066675	-0.834545177	0.745547057
6	-1.892080313	0.423773496	1.229262594
1	-1.532993152	-1.742516883	1.332960173
1	-1.850619212	0.775788976	2.252017444
8	-1.679915956	-1.913912965	-1.426373504
8	-3.432533018	1.980242952	0.166951424

TS2

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6	-1.904988497	0.337073583	-1.374772870

6	-2.768773188	-0.370442272	-2.181982401
6	-3.633359784	-1.354046584	-1.637201075
6	-3.627348034	-1.597383255	-0.292028448
7	-2.774573685	-0.885601712	0.512973151
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1	-2.787782727	-0.170190134	-3.248276563
1	-4.304251716	-1.918519580	-2.274666203
1	-4.252531477	-2.327895016	0.206248192
6	-2.590301631	-0.973522839	1.886421927
6	-1.608179730	-0.091659423	2.199462898
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1	-3.149279587	-1.664988987	2.496203047
6	1.973433213	2.091860695	0.009987763
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6	-0.267010946	2.666029890	0.081735193
6	-0.043900747	1.474439737	1.032920689
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6	2.886381503	-0.721668738	-1.029806142
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Int 2

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6	-1.915263071	0.170963737	-0.062628003
6	-1.850665372	0.204165903	-1.465900314
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7	-2.880023873	-0.588407418	0.563064972
1	-1.135590262	0.838775166	-1.968714408
1	-2.700973681	-0.576597738	-3.258958530
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6	-1.719303703	0.407694312	2.142247947
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1	-3.393939004	-0.964723627	2.631234523
6	2.227670099	1.968450539	0.104610832
8	1.351429088	2.865951891	-0.591413732
6	0.052444217	2.588695917	-0.310902306
6	0.037194450	1.551472117	0.815214920
6	1.406765974	0.824040998	0.666094364
1	0.084890088	2.143464081	1.738100725
1	1.825773134	0.524765818	1.629023710
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6	1.492936636	-0.421370765	-0.325996934
6	2.861959645	-0.809876040	-0.726823025
6	0.951194819	-1.701873864	0.370992494
1	0.819662776	-0.181487853	-1.170331923
6	3.198920355	-2.092557770	-0.362922451
1	3.553691874	-0.186553766	-1.277183351
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TS 3

7	-0.817605282	-0.054677782	1.053280736
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6	-2.051878391	0.566832931	-1.071546670
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1	-1.431968405	1.406169305	-1.356760591
1	-3.354862921	0.721955404	-2.752344409
1	-4.768408121	-1.240600872	-2.076754537
1	-4.210408074	-2.470995858	0.043845314
6	-2.114036111	-1.768838070	1.645207564
6	-1.025771727	-1.037114689	1.997612386
1	-0.364258668	-1.148361452	2.843210504
1	-2.576637248	-2.626810199	2.106182809
6	0.862191169	2.255459387	-0.780752013
8	0.175899317	3.073224936	0.221185507
6	-0.135438976	2.322930550	1.297887707
6	0.350570654	0.866960274	1.074114063
6	1.192845012	0.986582061	-0.171864559
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6	3.249902863	-0.054420389	-0.673613967
6	1.392721122	-1.558350077	-0.560064642
1	1.496311649	-0.046098737	-2.097270014
6	3.666703004	-1.272532893	-0.065682748
1	3.955959655	0.504564902	-1.279564950
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8	4.684477900	-1.725133993	0.390603032
8	0.306399352	-2.098289426	-0.684664183

16

6	-3.011649030	0.147965430	1.423502680
6	-1.743469043	-0.400416460	0.740131521
6	-2.295651209	-1.484599909	-0.185793619
8	-3.669517428	-1.466207358	-0.198977279
6	-4.167948119	-0.525088702	0.718787495
6	-0.964776270	0.603956207	-0.085947653
6	-0.027675626	0.244790195	-1.164086774
6	0.466612187	1.615409916	-1.689594565
8	-0.093220601	2.591175504	-0.980457443
6	-1.021579378	1.986799246	0.066616005
7	1.187016363	-0.573761602	-0.745988815
6	2.155335808	-0.197149454	0.124421432
7	3.062715862	-1.239736435	0.206623728
6	2.632890562	-2.266661890	-0.627771427
6	1.475464097	-1.835557737	-1.205364875
6	2.355353081	0.980276797	0.870273225
6	3.472658422	1.052380441	1.673408695
6	4.390404164	-0.029776479	1.743666516
6	4.176248645	-1.163011851	1.008420883
8	-1.588472397	2.786395441	0.787948353
8	1.273090710	1.764716832	-2.581784026
8	-1.674052460	-2.269774214	-0.861029101
8	-5.346788720	-0.375461931	0.855465041
1	5.269759283	0.030265221	2.375150528
1	3.654127001	1.948791604	2.257304686
1	1.645624185	1.794718510	0.799657357
1	4.828978765	-2.027425306	1.002502549
1	0.809355075	-2.340485476	-1.888053131
1	3.176567024	-3.193525313	-0.720318040
1	-3.106236690	1.234759115	1.351738117

1	-0.422727271	-0.348474560	-1.996974886
1	-3.065534996	-0.110854886	2.487069304
1	-1.099660481	-0.915931331	1.474137566

16 (GS at wB97XD/6-311+G(d,p))

6	2.920637480	0.075861571	-1.461808599
6	1.652869320	-0.424171904	-0.763724650
6	2.183041650	-1.514252165	0.154163004
8	3.542082207	-1.481802519	0.207618796
6	4.055313805	-0.544631627	-0.688587111
6	0.957645485	0.603780467	0.090818671
6	0.047582222	0.272103991	1.194607474
6	-0.428361602	1.654171287	1.685256693
8	0.131145871	2.598235527	0.951806389
6	1.006537647	1.975755391	-0.097093725
7	-1.153024546	-0.538742387	0.807281389
6	-2.083802019	-0.186094299	-0.097053932
7	-2.983445449	-1.215455401	-0.179087598
6	-2.588716539	-2.220628385	0.691788295
6	-1.454722889	-1.783198025	1.288310668
6	-2.248509702	0.970292260	-0.880447361
6	-3.329890306	1.020519589	-1.714020159
6	-4.249400907	-0.056242797	-1.783724371
6	-4.066966220	-1.159439423	-1.014929604
8	1.534060556	2.745942497	-0.861326044
8	-1.222926717	1.831477516	2.566441796
8	1.552125889	-2.299295197	0.801084368
8	5.222869881	-0.363578374	-0.767809296
1	-5.104321202	-0.009953141	-2.444153104
1	-3.487309536	1.897134966	-2.329388317
1	-1.537873934	1.781257214	-0.810639891
1	-4.721671271	-2.019221153	-1.005273368
1	-0.810968177	-2.271852176	1.999579258
1	-3.138423902	-3.139668971	0.790695397
1	3.016829358	1.161455498	-1.471478673
1	0.462807357	-0.289643348	2.037376262
1	2.996097653	-0.274358671	-2.494298696
1	0.965717591	-0.906556908	-1.473635192

16 (ES at wB97XD/6-311+G(d,p))

6	3.011649331	0.147964659	-1.423502141
6	1.743468863	-0.400416416	-0.740131875
6	2.295651241	-1.484600136	0.185793052
8	3.669517487	-1.466207623	0.198976708

6	4.167948061	-0.525088655	-0.718787061
6	0.964776074	0.603956032	0.085947753
6	0.027675555	0.244790462	1.164086118
6	-0.466612108	1.615409958	1.689593988
8	0.093221057	2.591175514	0.980457559
6	1.021579378	1.986799252	-0.066615392
7	-1.187016511	-0.573761681	0.745989254
6	-2.155335744	-0.197149476	-0.124421261
7	-3.062716052	-1.239736456	-0.206623681
6	-2.632890710	-2.266661646	0.627770882
6	-1.475464171	-1.835557759	1.205365219
6	-2.355353124	0.980276877	-0.870272674
6	-3.472658084	1.052380822	-1.673409367
6	-4.390403656	-0.029776637	-1.743666457
6	-4.176248693	-1.163011412	-1.008420692
8	1.588472598	2.786395632	-0.787948316
8	-1.273090609	1.764716604	2.581783888
8	1.674051894	-2.269774240	0.861029520
8	5.346788509	-0.375461770	-0.855464956
1	-5.269759595	0.030265247	-2.375150952
1	-3.654126673	1.948791636	-2.257304697
1	-1.645624312	1.794718441	-0.799657781
1	-4.828978675	-2.027424840	-1.002502374
1	-0.809355615	-2.340485227	1.888053316
1	-3.176567268	-3.193525007	0.720317828
1	3.106236351	1.234759200	-1.351738197
1	0.422727120	-0.348474608	1.996974531
1	3.065534959	-0.110855033	-2.487069230
1	1.099660672	-0.915931283	-1.474137228

B. 15b

7	-0.719814956	0.880967733	0.460600744
6	-0.095843829	2.063711032	0.197682799
6	1.040877006	2.692495838	0.734829874
6	1.413126816	3.916939897	0.219864102
6	0.662767458	4.529157588	-0.814375946
6	-0.455207446	3.909725915	-1.301667625
7	-0.825231917	2.694053276	-0.786040230
1	1.596288657	2.232910409	1.539438552
1	2.291446266	4.416430377	0.615367994
1	0.960713892	5.486576764	-1.226300836
1	-1.087529876	4.304101806	-2.087368007
6	-1.900322259	1.890182064	-1.135261341
6	-1.830117467	0.762807676	-0.379832087

1	-2.595745828	2.169020686	-1.910721397
6	1.376496881	-1.708418961	2.107274782
8	1.124620232	-0.722574415	3.115984924
6	0.269977844	0.230744276	2.662577384
6	-0.246157697	-0.216091846	1.294013526
6	0.838948615	-1.209018976	0.780120763
1	-1.141565334	-0.810367466	1.510759405
1	0.393535214	-2.052542926	0.248587018
8	-0.024880494	1.218890116	3.283020077
8	1.945636660	-2.713336251	2.396121484
6	2.029209337	-0.641673569	-0.114102657
6	3.209239618	-1.526948355	-0.234035957
6	1.546204856	-0.490221340	-1.583656354
1	2.256779293	0.365410890	0.278775129
6	3.478538000	-1.923101705	-1.520774418
1	3.839326587	-1.841716133	0.586944889
8	2.277447564	-1.182117849	-2.397173261
8	4.236949811	-2.569018730	-2.194701261
8	0.573181660	0.196887856	-1.913226543
6	-2.688698081	-0.440273918	-0.434183863
6	-3.727667256	-0.629074690	0.491736063
6	-2.459885474	-1.395094355	-1.438922175
6	-4.531340560	-1.768493692	0.413227150
1	-3.910389181	0.117028367	1.261410582
6	-3.269726266	-2.531010469	-1.510220374
1	-1.647060991	-1.240235978	-2.143566038
6	-4.302061510	-2.719022367	-0.586412309
1	-5.336163317	-1.910958960	1.129104898
1	-3.089929241	-3.269311957	-2.286689724
1	-4.928173008	-3.605258996	-0.645157381

15b (GS at wB97XD/6-311+G(d,p))

7	-0.665601456	0.966433134	0.472205112
6	0.056292657	2.079446324	0.210301896
6	1.247117542	2.594867197	0.743406964
6	1.732740397	3.759768698	0.217956730
6	1.047329947	4.432032131	-0.819658352
6	-0.116902222	3.923834934	-1.297189547
7	-0.601302663	2.760434858	-0.771031186
1	1.757406534	2.085036452	1.544845638
1	2.656354540	4.172330273	0.603363978
1	1.438504347	5.347527663	-1.240840203
1	-0.704162539	4.367386436	-2.088283097
6	-1.731897947	2.050427170	-1.137387512

6	-1.757048953	0.931723007	-0.384881715
1	-2.379643931	2.372938832	-1.932622942
6	1.158012666	-1.801177399	2.091127330
8	1.032053934	-0.800435714	3.089026110
6	0.277011204	0.226048428	2.653620758
6	-0.300747664	-0.162416034	1.299721920
6	0.670451720	-1.239871470	0.772392505
1	-1.244927489	-0.663339626	1.537547998
1	0.151332272	-2.031006857	0.231048786
8	0.093106854	1.228251267	3.270635191
8	1.595188577	-2.857427734	2.374236152
6	1.902657317	-0.772455853	-0.088099495
6	2.974324560	-1.782309801	-0.223348429
6	1.460245288	-0.535378032	-1.550289845
1	2.242345994	0.190032918	0.324296137
6	3.178313066	-2.195163757	-1.509067990
1	3.557783086	-2.185177764	0.588786420
8	2.084243877	-1.308058240	-2.359979652
8	3.832130755	-2.917094887	-2.193929519
8	0.604800107	0.280537718	-1.875339955
6	-2.655420818	-0.234552054	-0.459603994
6	-3.775536635	-0.336575918	0.364410840
6	-2.339901794	-1.257507747	-1.355571747
6	-4.580185859	-1.466865094	0.293373033
1	-4.013106713	0.464903824	1.055721063
6	-3.149828603	-2.384186182	-1.418728041
1	-1.463967219	-1.154873872	-1.988114823
6	-4.265397470	-2.489524057	-0.594939619
1	-5.452046785	-1.548831459	0.931694098
1	-2.906488456	-3.180372190	-2.112254895
1	-4.893018044	-3.371796736	-0.645866410

15b (ES at wB97XD/6-311+G(d,p))

7	-0.719815263	0.880967765	0.460600348
6	-0.095844066	2.063711037	0.197682512
6	1.040876202	2.692495907	0.734829953
6	1.413126446	3.916940040	0.219864501
6	0.662767072	4.529158191	-0.814375978
6	-0.455207965	3.909726079	-1.301667932
7	-0.825232044	2.694052784	-0.786040182
1	1.596288588	2.232910478	1.539438563
1	2.291445996	4.416430403	0.615368152
1	0.960713390	5.486576447	-1.226300296
1	-1.087530659	4.304101599	-2.087367705

6	-1.900322693	1.890181715	-1.135261780
6	-1.830117467	0.762807449	-0.379831644
1	-2.595745542	2.169020765	-1.910721651
6	1.376497342	-1.708418337	2.107274517
8	1.124620243	-0.722574605	3.115984759
6	0.269977651	0.230744494	2.662577411
6	-0.246158012	-0.216092368	1.294013733
6	0.838948847	-1.209018389	0.780121207
1	-1.141565165	-0.810367058	1.510759146
1	0.393535258	-2.052543371	0.248586893
8	-0.024880654	1.218890048	3.283020156
8	1.945636739	-2.713336569	2.396121690
6	2.029209056	-0.641673522	-0.114102959
6	3.209239523	-1.526947720	-0.234036208
6	1.546204607	-0.490221241	-1.583655905
1	2.256778795	0.365411377	0.278775180
6	3.478538333	-1.923101075	-1.520774243
1	3.839326841	-1.841716281	0.586944539
8	2.277448263	-1.182117843	-2.397173028
8	4.236949769	-2.569018132	-2.194701467
8	0.573181703	0.196887942	-1.913226421
6	-2.688697822	-0.440274389	-0.434183623
6	-3.727666912	-0.629074891	0.491736234
6	-2.459885072	-1.395095001	-1.438922080
6	-4.531339973	-1.768493808	0.413226910
1	-3.910388768	0.117027673	1.261411154
6	-3.269725816	-2.531010601	-1.510220602
1	-1.647061065	-1.240236343	-2.143566324
6	-4.302061066	-2.719022780	-0.586412647
1	-5.336162735	-1.910959230	1.129104877
1	-3.089928701	-3.269312121	-2.286689936
1	-4.928172876	-3.605259663	-0.645157508

C. 15c (Ground State)

7	-0.281888664	-1.093081390	0.160167963
6	-1.336815573	-1.833761472	-0.269246752
6	-2.655718999	-1.976502076	0.193529936
6	-3.496407940	-2.837162103	-0.484059700
6	-3.035805759	-3.555626350	-1.614557184
6	-1.741193850	-3.410724395	-2.036658454
7	-0.905425406	-2.560407715	-1.359036810
1	-3.002501333	-1.432341009	1.062252375
1	-4.520458602	-2.959047478	-0.146978389
1	-3.696271323	-4.224593596	-2.154392369

1	-1.308676922	-3.923861187	-2.886687987
6	0.433224261	-2.274287148	-1.584516585
1	0.988829254	-2.733206307	-2.386567676
6	-2.280979606	0.738415981	2.296828051
8	-1.594672438	-0.168830304	3.156911709
6	-0.462572599	-0.652548934	2.570429909
6	-0.297908173	-0.031353714	1.169832464
6	-1.384886611	1.082931559	1.114264313
1	0.697684362	0.409152295	1.114066946
1	-0.871691981	2.006493631	1.418865257
8	0.255136530	-1.462384614	3.091750892
8	-3.386251302	1.081145162	2.580466496
6	-2.184249164	1.470237482	-0.177360179
6	-2.908729135	2.765560188	-0.042424172
6	-1.228861541	1.708584488	-1.376799349
1	-2.833846760	0.618144057	-0.436149083
6	-2.504547188	3.728924438	-0.926764055
1	-3.719212951	2.945228151	0.650682807
8	-1.299183202	2.921737211	-1.811475976
8	-2.678009421	4.860144013	-1.293058668
8	-0.507509648	0.815964155	-1.842004662
6	0.824769797	-1.360071479	-0.652705999
6	2.144224530	-0.729203709	-0.491305249
6	2.941292142	-0.995103862	0.631773922
6	2.635006324	0.128455295	-1.496231293
6	4.212090408	-0.429598265	0.755957667
6	3.898339328	0.690109988	-1.379148684
1	1.995846278	0.381132844	-2.336592711
6	4.697258123	0.413439238	-0.255714962
1	4.807068112	-0.654996120	1.633414717
1	4.282435294	1.363525720	-2.138996989
1	2.573348691	-1.651165719	1.416679734
8	5.916328170	1.011921613	-0.237854110
6	6.774060672	0.802900415	0.881171921
1	7.038310570	-0.256928322	0.985620567
1	6.310670262	1.163691426	1.807858282
1	7.673419209	1.383924085	0.673347632

15c (GS at wB97XD/6-311+G(d,p))

7	-0.314130703	-1.105303998	0.156060657
6	-1.411198277	-1.767764147	-0.260552010
6	-2.723157749	-1.833309036	0.230442902
6	-3.623153506	-2.610539163	-0.446423878
6	-3.234237496	-3.330759432	-1.598858585

6	-1.949780297	-3.266528268	-2.036863573
7	-1.051367755	-2.492302402	-1.359614757
1	-3.015124576	-1.285982028	1.114804555
1	-4.645034832	-2.671607096	-0.094776235
1	-3.947395308	-3.937393424	-2.139276839
1	-1.569010718	-3.787226584	-2.903835320
6	0.294418471	-2.285947199	-1.612582305
1	0.800516974	-2.748978191	-2.440529472
6	-2.182099656	0.773895575	2.301529230
8	-1.522381619	-0.142177214	3.148198176
6	-0.427381412	-0.669283773	2.552639239
6	-0.253952599	-0.054036582	1.159595636
6	-1.288504156	1.090592971	1.118289505
1	0.758619323	0.339849455	1.091203959
1	-0.746547456	1.994373757	1.423124313
8	0.251798619	-1.507577250	3.051986359
8	-3.268053912	1.142623176	2.580692629
6	-2.082673935	1.503913571	-0.153044170
6	-2.708896692	2.844515757	-0.012938264
6	-1.147025639	1.672870405	-1.367581589
1	-2.791269518	0.701106212	-0.395068357
6	-2.215475474	3.773075029	-0.880670325
1	-3.488606438	3.087846405	0.690237912
8	-1.105408092	2.887885637	-1.766015084
8	-2.282816152	4.908884164	-1.228587713
8	-0.539703722	0.733080948	-1.872752659
6	0.748245057	-1.416201902	-0.682379164
6	2.083043755	-0.824560693	-0.532664659
6	2.903182061	-1.183351657	0.533187185
6	2.526378972	0.124546071	-1.461530972
6	4.165265926	-0.619763144	0.674709967
6	3.780307634	0.684980504	-1.327147071
1	1.856269560	0.441738411	-2.252643497
6	4.609170553	0.315345370	-0.262341810
1	4.783703682	-0.915609528	1.511179355
1	4.137058921	1.429210471	-2.028255511
1	2.553863697	-1.902383283	1.266886017
8	5.812592019	0.920628409	-0.219877504
6	6.689458936	0.616993790	0.847088885
1	6.964472246	-0.443201492	0.846885321
1	6.247110518	0.882943972	1.813017750
1	7.580039216	1.219670415	0.681346152

15c (ES at wB97XD/6-311+G(d,p))

7	-0.281888349	-1.093081305	0.160168221
6	-1.336815414	-1.833761498	-0.269246753
6	-2.655719258	-1.976501902	0.193529667
6	-3.496408045	-2.837162135	-0.484060259
6	-3.035806061	-3.555625726	-1.614557104
6	-1.741194295	-3.410724120	-2.036658623
7	-0.905425453	-2.560408027	-1.359037324
1	-3.002501868	-1.432341094	1.062251936
1	-4.520458729	-2.959046906	-0.146978171
1	-3.696271334	-4.224592903	-2.154392406
1	-1.308677033	-3.923861160	-2.886687818
6	0.433223944	-2.274286762	-1.584516384
1	0.988829143	-2.733206032	-2.386567961
6	-2.280979568	0.738415431	2.296827676
8	-1.594672872	-0.168830099	3.156911878
6	-0.462572133	-0.652548966	2.570430141
6	-0.297908055	-0.031353293	1.169832687
6	-1.384886733	1.082931262	1.114264498
1	0.697684108	0.409151829	1.114067078
1	-0.871692124	2.006493260	1.418865066
8	0.255136294	-1.462384254	3.091750712
8	-3.386251202	1.081144908	2.580466914
6	-2.184249068	1.470237186	-0.177359924
6	-2.908729098	2.765559929	-0.042423785
6	-1.228861599	1.708585144	-1.376799216
1	-2.833846739	0.618143618	-0.436149536
6	-2.504547113	3.728924576	-0.926763806
1	-3.719213157	2.945227956	0.650682394
8	-1.299182630	2.921737301	-1.811476188
8	-2.678008955	4.860144172	-1.293058912
8	-0.507509905	0.815963970	-1.842004730
6	0.824770152	-1.360071632	-0.652705687
6	2.144224456	-0.729203471	-0.491305711
6	2.941291787	-0.995103741	0.631773938
6	2.635006128	0.128455542	-1.496230870
6	4.212090831	-0.429598762	0.755957635
6	3.898339365	0.690110078	-1.379148806
1	1.995846119	0.381132675	-2.336592515
6	4.697258388	0.413438679	-0.255715094
1	4.807068456	-0.654996591	1.633414822
1	4.282434940	1.363525668	-2.138996709
1	2.573348390	-1.651165682	1.416679961
8	5.916327853	1.011921052	-0.237854207
6	6.774060884	0.802900452	0.881171911

1	7.038310941	-0.256928518	0.985620588
1	6.310670315	1.163691320	1.807858859
1	7.673419262	1.383923836	0.673347632

D. 15d

7	-0.511961454	-1.105779543	0.124650992
6	-1.576194490	-1.792798723	-0.369148461
6	-2.920126988	-1.891576219	0.030588248
6	-3.761307895	-2.702335694	-0.704649292
6	-3.279885247	-3.413323365	-1.831684859
6	-1.963894349	-3.310398342	-2.193954131
7	-1.127329397	-2.509072606	-1.458741117
1	-3.286468005	-1.353380863	0.894700840
1	-4.803345297	-2.790786385	-0.415649293
1	-3.941650057	-4.043128256	-2.415184338
1	-1.513801132	-3.820390799	-3.036746430
6	0.229664397	-2.267515431	-1.623857887
1	0.800918381	-2.724806692	-2.415960778
6	-2.533513218	0.690808603	2.245194010
8	-1.915367620	-0.275946845	3.093890233
6	-0.768725915	-0.763044779	2.541852945
6	-0.521765050	-0.084604235	1.179267520
6	-1.564112267	1.069654380	1.132476652
1	0.489899739	0.318863539	1.181202975
1	-1.036986215	1.954070163	1.519495058
8	-0.096370771	-1.615924990	3.054187208
8	-3.644434607	1.046624475	2.485433284
6	-2.261922795	1.548771763	-0.183163808
6	-2.993832590	2.836330908	-0.019713418
6	-1.207547609	1.845371758	-1.285345672
1	-2.896819832	0.723568818	-0.545602625
6	-2.555395623	3.856591746	-0.813316756
1	-3.850704803	2.972652482	0.626501936
8	-1.246484821	3.065307989	-1.678191790
8	-2.693638491	4.997748863	-1.144125356
8	-0.439038645	0.964216929	-1.707043412
6	0.610673837	-1.395530096	-0.650755071
6	1.959109190	-0.839822027	-0.409144886
6	2.711009279	-1.267080156	0.699591654
6	2.498189869	0.085159823	-1.318197297
6	4.004026433	-0.785552651	0.893408833
6	3.794155266	0.565800553	-1.131306403
1	1.880694895	0.453792412	-2.130829562
6	4.524988666	0.117854266	-0.032326792

1	4.603925576	-1.102677580	1.737973500
1	4.229968201	1.284153128	-1.815491511
1	2.286868798	-1.973638513	1.407423900
7	5.902901091	0.620470442	0.164079705
8	6.514014664	0.230275153	1.158726616
8	6.352654074	1.393424426	-0.679958220

15d (GS at wB97XD/6-311+G(d,p))

7	-0.544562427	-1.119306282	0.137143265
6	-1.651879050	-1.722821806	-0.340932754
6	-2.985687319	-1.738603665	0.092184056
6	-3.887958389	-2.462055604	-0.638989566
6	-3.482153561	-3.176762074	-1.789192148
6	-2.179096226	-3.160603726	-2.172117267
7	-1.278374846	-2.438996054	-1.440762146
1	-3.293247305	-1.196516312	0.974243388
1	-4.925643599	-2.484770215	-0.331799313
1	-4.197369935	-3.741161239	-2.371019363
1	-1.784064193	-3.680640718	-3.033095049
6	0.084296721	-2.284940460	-1.636462190
1	0.604259399	-2.750887119	-2.454254198
6	-2.424911383	0.765747653	2.250666597
8	-1.839072284	-0.200762644	3.097134593
6	-0.735790458	-0.746884743	2.537867288
6	-0.477200352	-0.097244561	1.172960479
6	-1.460458001	1.090283148	1.126039946
1	0.551745283	0.255613397	1.158093582
1	-0.898219853	1.957108503	1.495473078
8	-0.107535441	-1.623752289	3.037084469
8	-3.511026625	1.161654009	2.486819527
6	-2.159148810	1.578997108	-0.172217819
6	-2.768701553	2.924436899	-0.009505914
6	-1.131621364	1.769028468	-1.310077342
1	-2.870493819	0.808307532	-0.496031447
6	-2.223976309	3.893775544	-0.790638505
1	-3.590862919	3.147037558	0.651568808
8	-1.030211804	2.985122517	-1.664115257
8	-2.233396718	5.033767624	-1.108476304
8	-0.509798245	0.818098708	-1.787759093
6	0.531124817	-1.457973509	-0.666928606
6	1.893365267	-0.943459285	-0.444376597
6	2.650660297	-1.421957996	0.626921505
6	2.405573113	0.024165415	-1.308405195
6	3.936285686	-0.945571734	0.828624509

6	3.695034392	0.499607550	-1.113320986
1	1.770368022	0.424920187	-2.090094947
6	4.434155650	0.001153630	-0.053312694
1	4.548508907	-1.295171070	1.648565141
1	4.120930139	1.252820782	-1.762243854
1	2.230726129	-2.156477053	1.304886674
7	5.811053754	0.505767305	0.154806336
8	6.413500673	0.098605323	1.126791087
8	6.248174165	1.289474688	-0.660644706

15d (ES at wB97XD/6-311+G(d,p))

7	-0.511961113	-1.105779458	0.124651376
6	-1.576194415	-1.792798586	-0.369148254
6	-2.920126803	-1.891576436	0.030588397
6	-3.761307768	-2.702336090	-0.704649625
6	-3.279884908	-3.413323270	-1.831685329
6	-1.963894322	-3.310398363	-2.193954052
7	-1.127329382	-2.509072362	-1.458741218
1	-3.286468339	-1.353380541	0.894700703
1	-4.803345112	-2.790786014	-0.415648985
1	-3.941650533	-4.043128489	-2.415184126
1	-1.513801587	-3.820390757	-3.036746314
6	0.229664311	-2.267515923	-1.623858305
1	0.800918445	-2.724806809	-2.415960868
6	-2.533513154	0.690808317	2.245194290
8	-1.915367377	-0.275946537	3.093889905
6	-0.768726174	-0.763045023	2.541852623
6	-0.521765432	-0.084604085	1.179267377
6	-1.564111891	1.069654321	1.132476197
1	0.489899241	0.318863533	1.181203510
1	-1.036986061	1.954070676	1.519495550
8	-0.096371467	-1.615925229	3.054187546
8	-3.644434903	1.046624538	2.485433327
6	-2.261922599	1.548771493	-0.183163501
6	-2.993832674	2.836331316	-0.019713761
6	-1.207547710	1.845372176	-1.285345391
1	-2.896819339	0.723569114	-0.545602154
6	-2.555395565	3.856591328	-0.813317131
1	-3.850705332	2.972652302	0.626501994
8	-1.246485027	3.065307677	-1.678191557
8	-2.693638274	4.997749265	-1.144125441
8	-0.439038927	0.964217104	-1.707042957
6	0.610674048	-1.395530228	-0.650755283
6	1.959108893	-0.839822344	-0.409145053

6	2.711009644	-1.267079812	0.699591929
6	2.498190091	0.085160166	-1.318197106
6	4.004026222	-0.785552857	0.893408489
6	3.794155218	0.565801035	-1.131306731
1	1.880695334	0.453792684	-2.130829398
6	4.524988036	0.117853980	-0.032326510
1	4.603925978	-1.102677606	1.737974077
1	4.229968365	1.284152509	-1.815491299
1	2.286868835	-1.973638259	1.407424164
7	5.902901356	0.620470204	0.164080205
8	6.514014770	0.230275104	1.158726526