Supplementary Material (ESI) for New Journal of Chemistry

Electronic Supplementary Information: Gaywood, Hill, Imam, McNab, Neumajer, O'Neill and Mátyus.

Cyclisation reactions of some pyridazinylimidoylketenes

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Supporting Information

5-(Methoxymethylene)-2,2-dimethyl-1,3-dioxane-4,6-dione 3

This compound was synthesized according to the literature procedure for the ethoxy-analogue[1] with slight modification as follows:

2,2-Dimethyl-1,3-dioxane-4,6-dione (Meldrum's acid) (3.75 mmol) was reacted with trimethyl orthoformate (4.6 cm^3) at 50 °C for 3 h, then at room temperature overnight. The reaction mixture was concentrated under reduced pressure to provide a yellow-orange oil, which was used in the following step without further purification.

Alternatively, the literature method[2] was used.

3-Aminothiophene-2-methanol

To a suspension of $LiAlH_4$ (1.0 g, 27 mmol) in dry THF (20 cm^3) was added dropwise a solution of methyl 3-aminothiophene-2-carboxylate (1.0 g, 6.4 mmol) in dry THF (8 cm^3) at 0 °C under a nitrogen atmosphere. The mixture was stirred for 1.5 h at 0 °C, quenched with water until hydrogen evolution ceased, dried ($MgSO_4$), filtered and the solvent removed by rotary evaporation to yield 3-aminothiophene-2-methanol (730 mg, 88%); mp 71-73 °C; (Found: M^+ 129.0249. C_5H_7NOS requires *M* 129.0248); δ_H (d_6-DMSO) 7.10 (1H, d, ^3J 5.2, thiophene-H), 6.52 (1H, d, ^3J 5.2, thiophene-H), 4.95 (1H, t, ^3J 5.5, OH), 4.66 (2H, br s, NH_2) and 4.43 (2H, d, ^3J 5.5, CH_2); δ_C (d_6-DMSO) 143.5 (quat), 122.5, 121.9, 114.2 (quat) and 55.5 (CH_2); *m/z* 129 (M^+, 58%), 113 (60), 112 (100), 111 (46), 70 (15) and 67 (16). *m/z* 125 (M^+, 48%), 113 (57) and 112 (100).

3-Aminothiophene-2-carboxaldehyde

To a solution of 3-aminothiophene-2-methanol (695 mg, 5.4 mmol) in toluene (45 cm^3) was added activated manganese dioxide (6.0 g, 69 mmol) and the mixture heated under reflux for 3 h. The mixture was then cooled to room temperature, filtered through celite and the solvent removed to yield 3-aminothiophene-2-carboxaldehyde (252 mg, 37%); δ_H 9.56 (1H, d, ^4J 0.8, aldehyde), 7.46 (1H, d, ^3J 5.3, thiophene-H), 6.53 (1H, dd, ^3J 5.3 and ^4J 0.8, thiophene-H) and 6.15 (2H, br s, NH_2), consistent with reported data;[3] δ_C 182.9, 154.7 (quat), 136.6, 120.0 and 113.7 (quat).

Structure determination of compound 24

The ^{1}H NMR spectrum of the unknown compound showed 4 protons in the aromatic region, along with the *N*-methyl group (Figure 1). Accurate mass measurement of the molecular ion at *m/z* 133 supported the formula $C_7H_7N_3$.

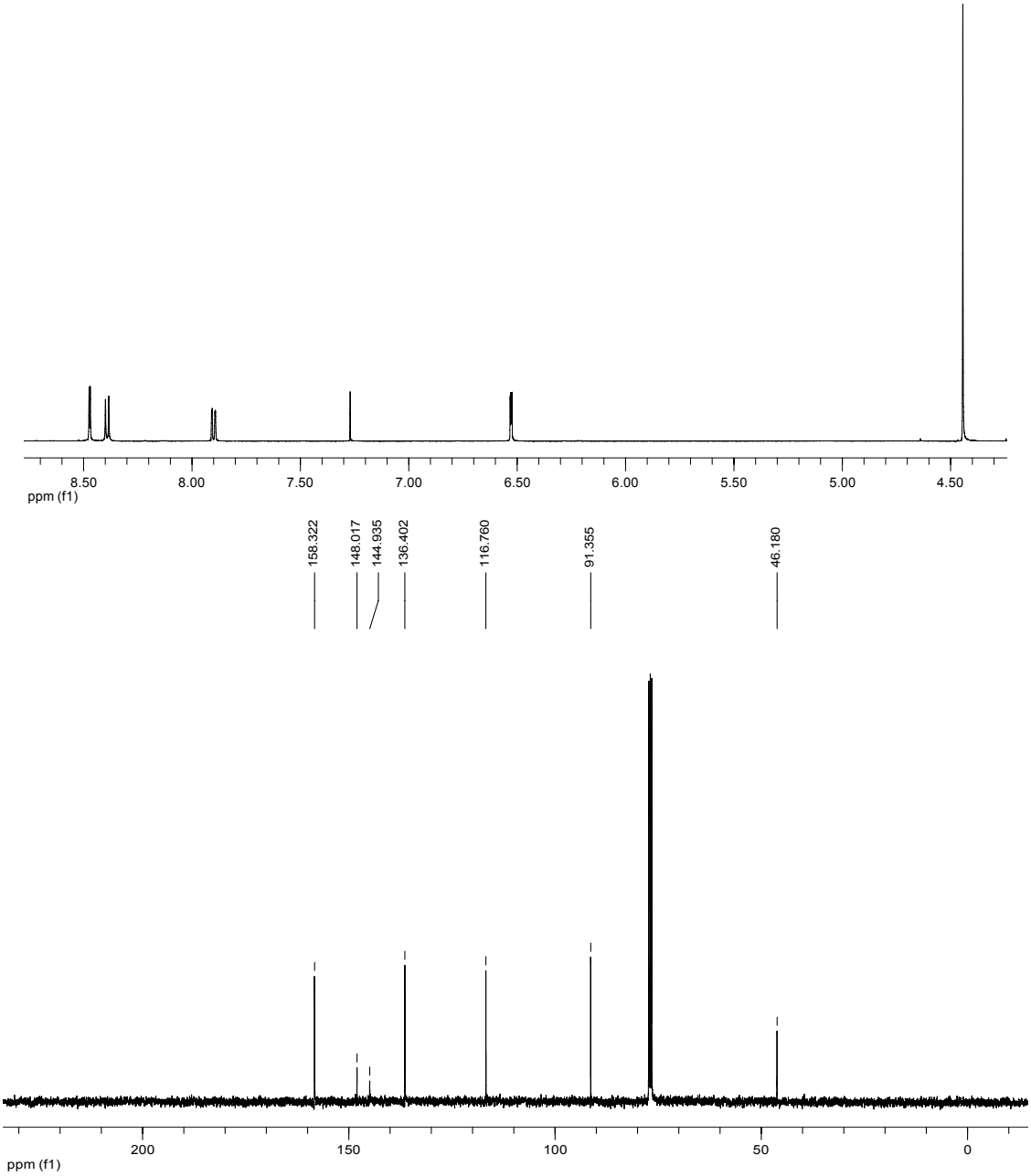


Figure 1. ^{1}H and ^{13}C NMR spectrum of the unknown compound **24**

The protons at δ_H = 8.4 and δ_H = 7.9 ppm had coupling constants of *ca.* 5 Hz, typical of a pyridazine ring.[4] The coupling constants of the remaining two protons, at δ_H = 8.5 and δ_H = 6.5 ppm, were 2.2 Hz; small coupling constants of this magnitude in aromatic systems are typically associated with pyrrole type protons.[4] The ^{13}C NMR spectrum showed the expected 7 carbon atoms: 4 CHs, 2 quaternary carbons and the *N*-methyl group. No carbonyl signals were observed, with the highest quaternary carbon at δ_C = 148 ppm (Figure 1). The proton/carbon connectivity was obtained from a HSQC experiment (Figure 2 and Table 1).

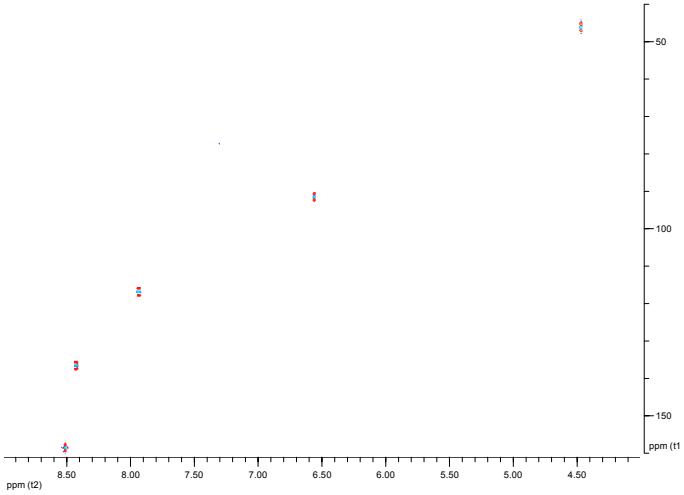


Figure 2. HSQC spectrum of the unknown compound **24**

^{13}C signals	^{1}H signals
158.3	8.47
136.4	8.39
116.8	7.90
91.3	6.52
46.2	4.42
148.0	Quaternary
144.9	Quaternary

Table 1. HSQC Data of compound **24**

The results of a NOESY experiment are shown in Figure 3.

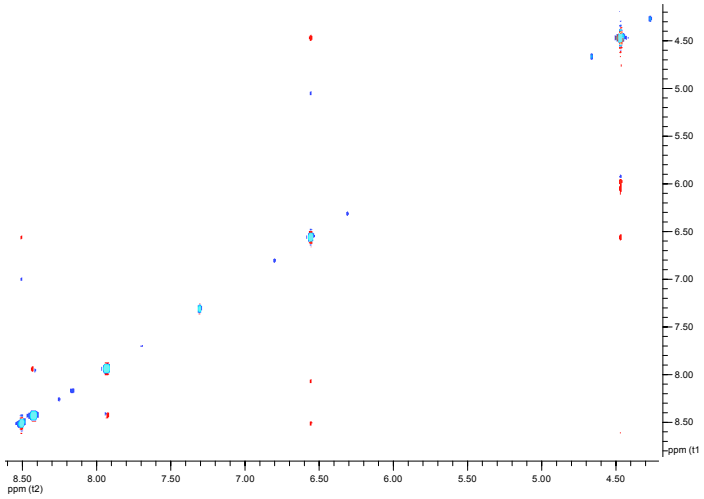


Figure 3. NOESY Spectrum of compound **24**

The proton at δ_H = 6.5 ppm shows a NOESY interaction with the methyl group at δ_H = 4.6 ppm. A further NOE signal to the proton at δ_H = 8.5 ppm identifies it as being next to the doublet at δ_H = 6.5 ppm. These data give the sub-structure shown in Figure 4 which has the formula $C_7H_7N_2$'RX'.

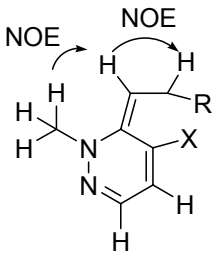
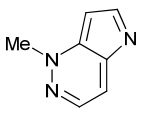
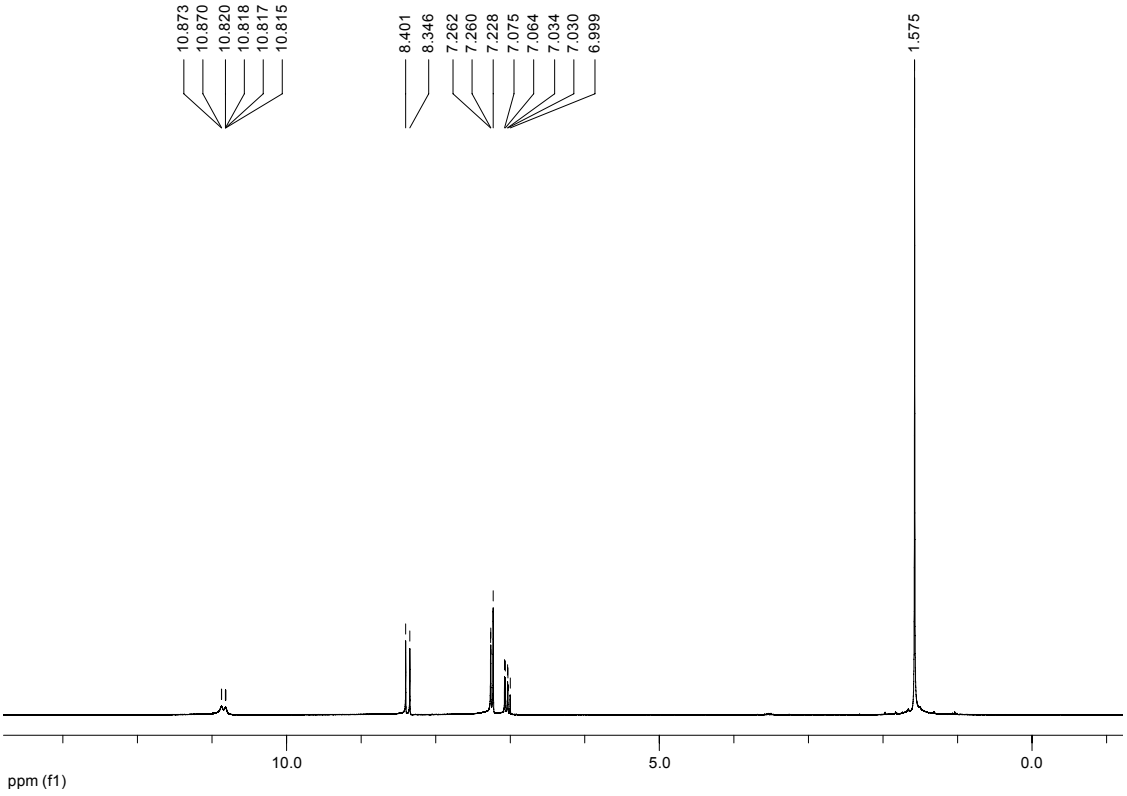


Figure 4. NOE Interactions in compound **24**

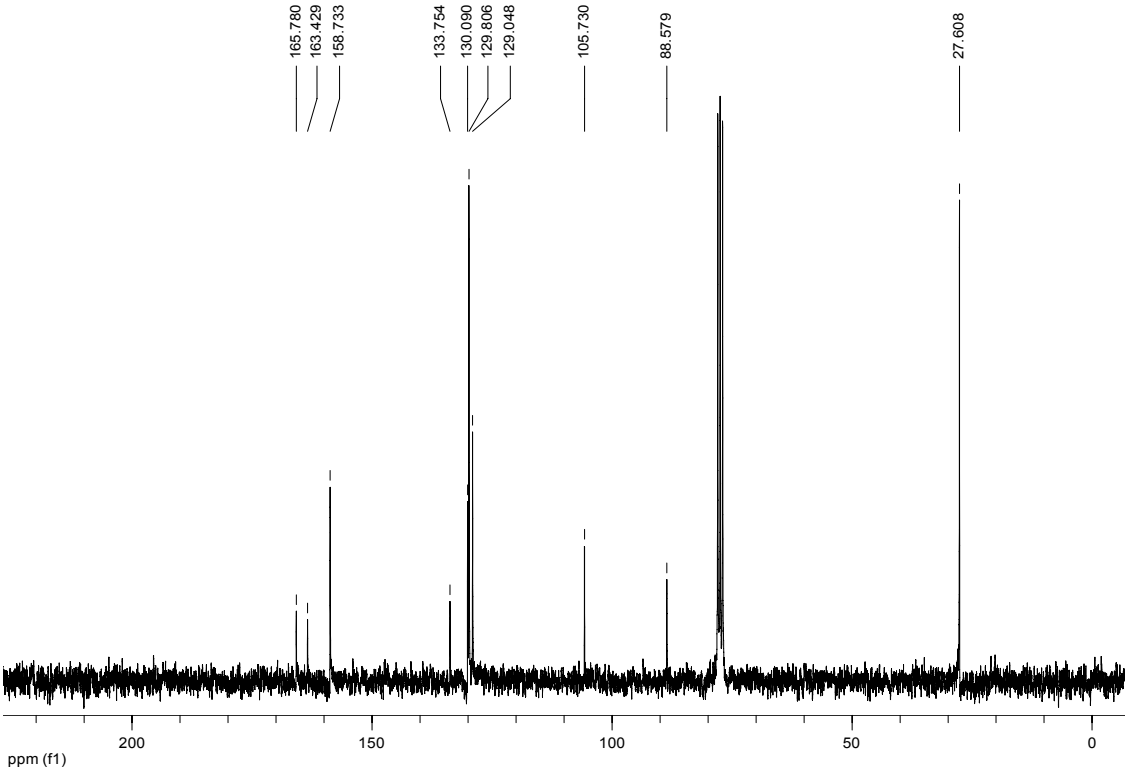
To match the overall formula $C_7H_7N_3$ the group 'RX' must be N. This generates the pyrrolopyridazine structure **24**.



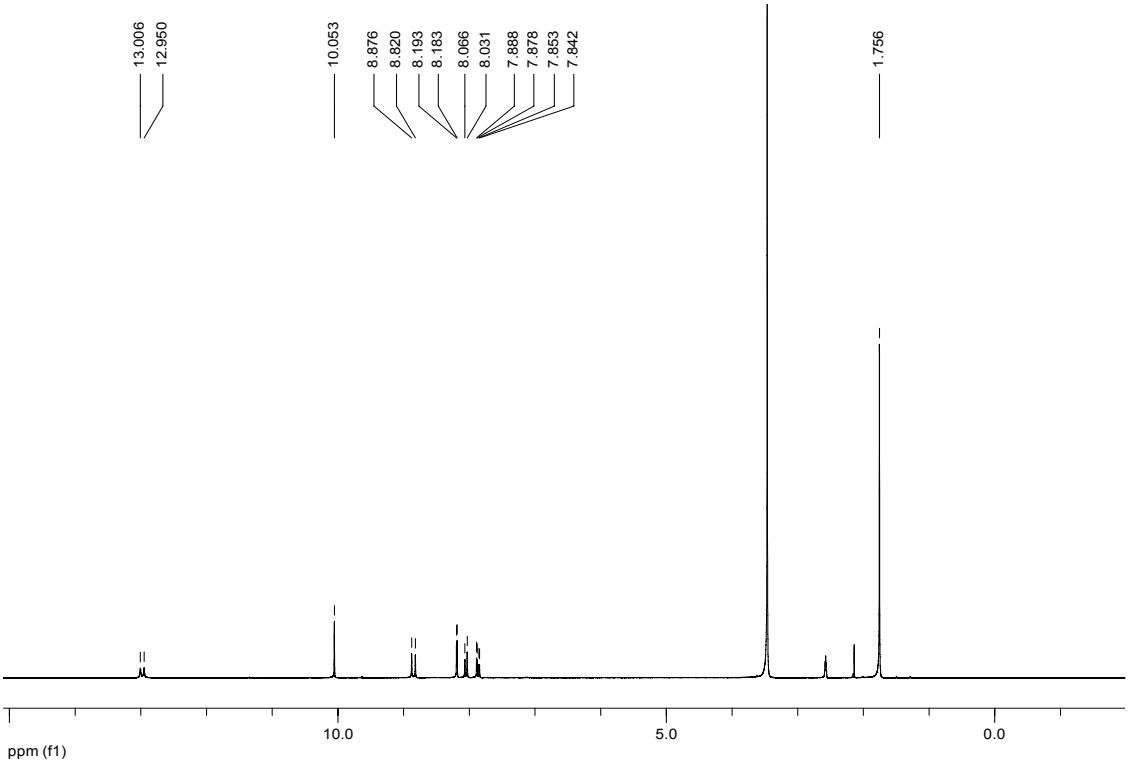
24



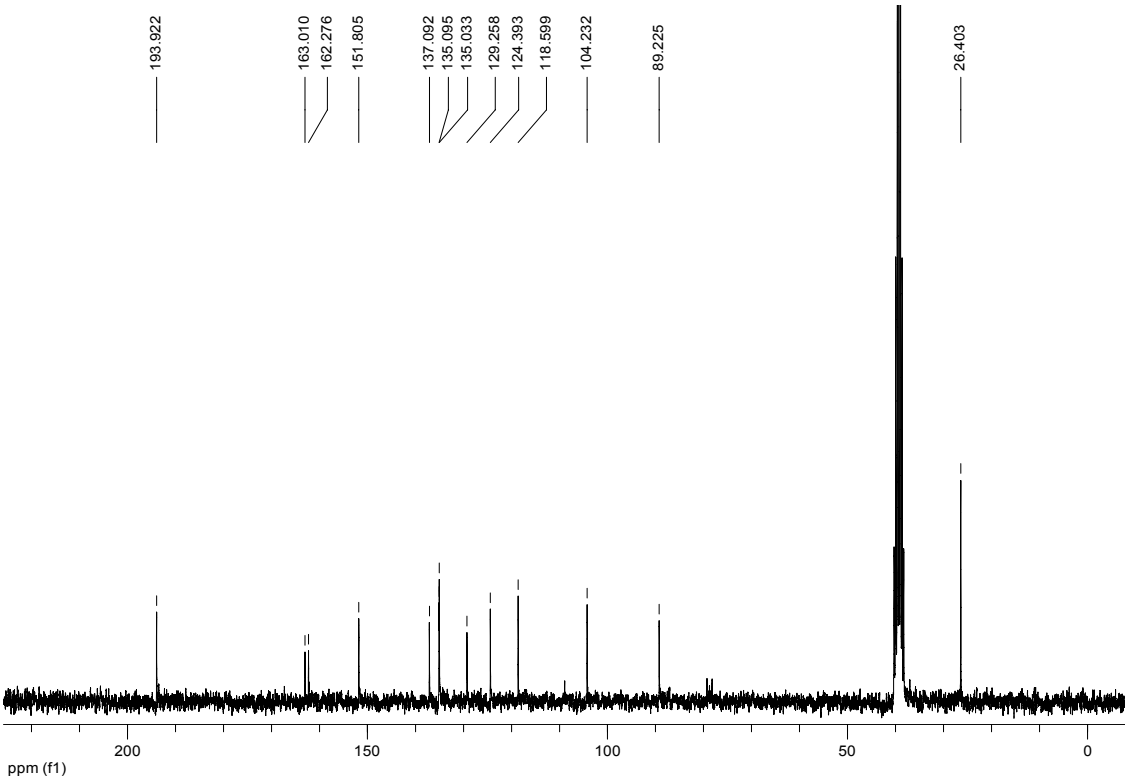
^{1}H NMR spectrum of compound **14**



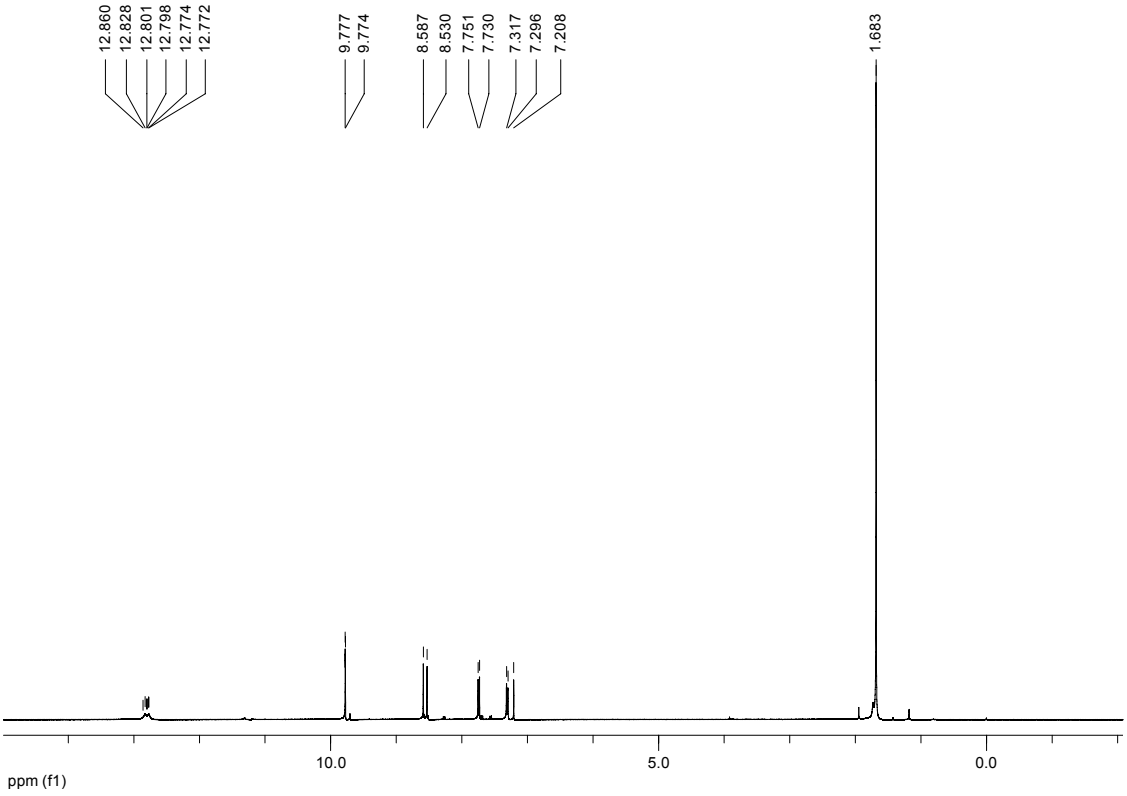
^{13}C NMR spectrum of compound **14**



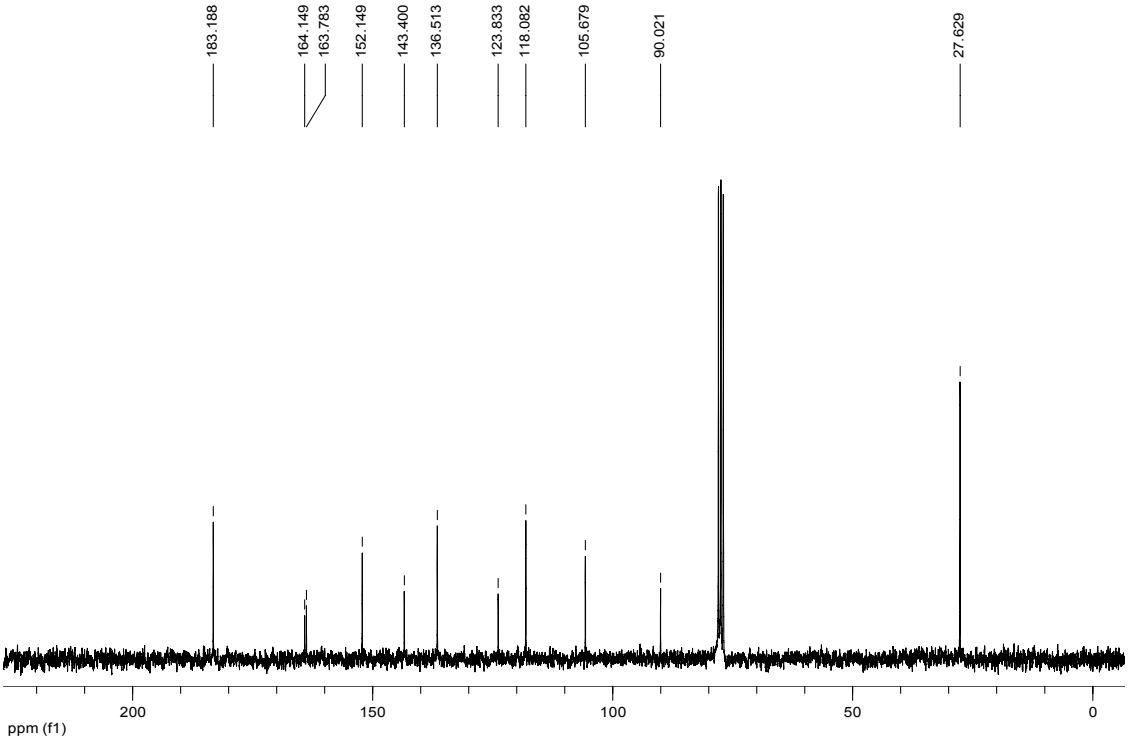
^{1}H NMR spectrum (d_6-DMSO) of compound **15**



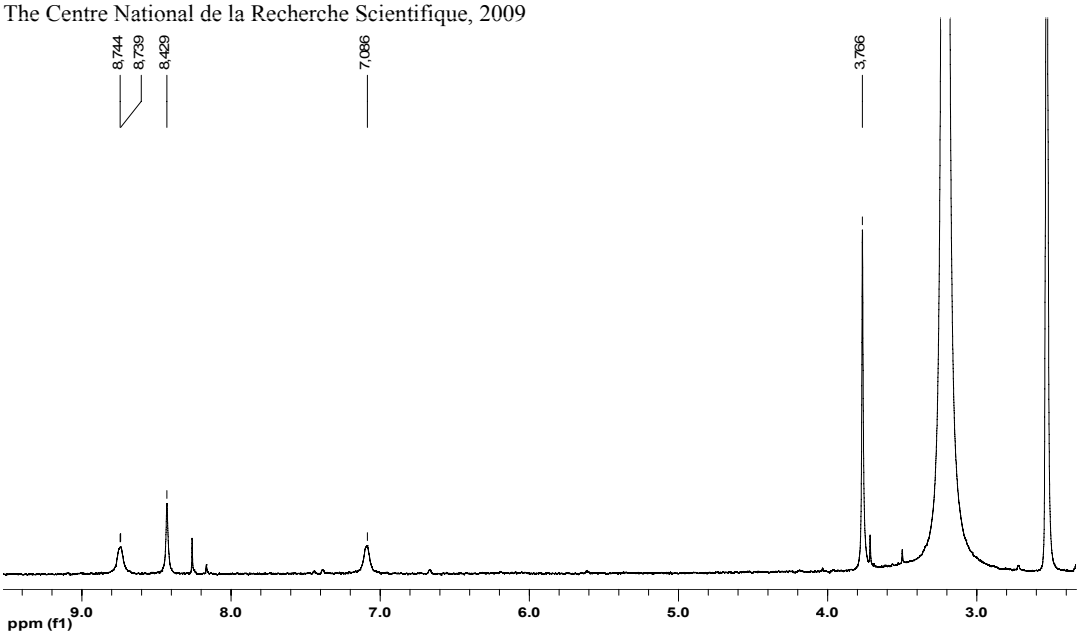
^{13}C NMR spectrum (d_6-DMSO) of compound **15**



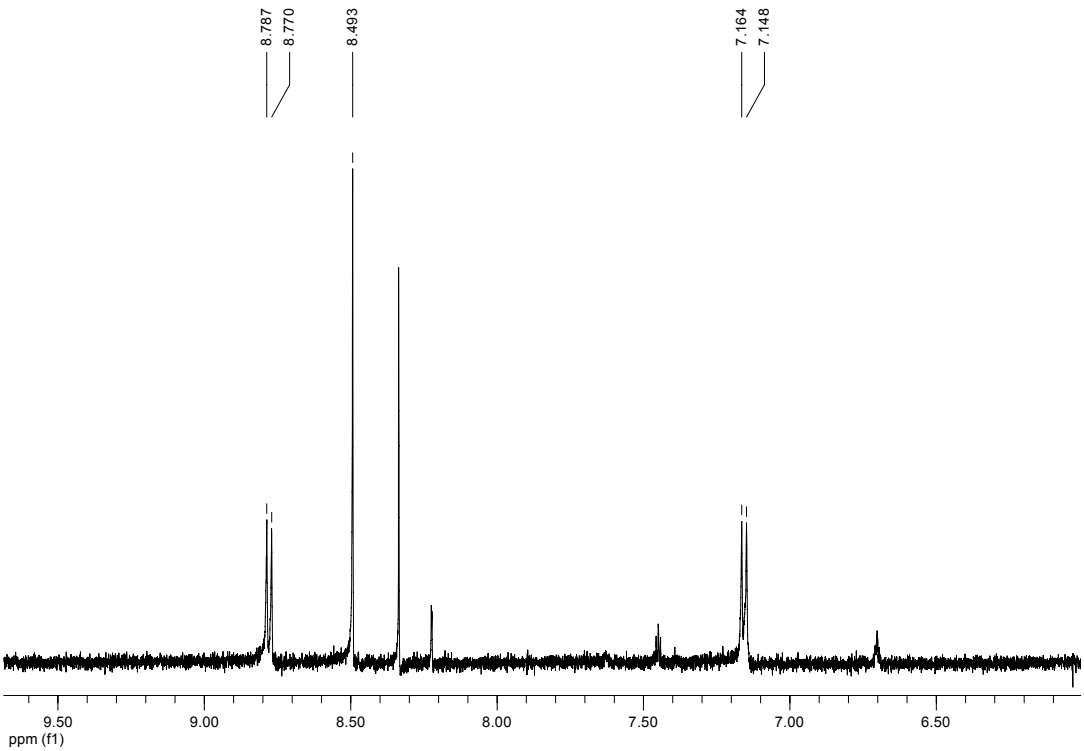
^{1}H NMR spectrum ($CDCl_3$) of compound **16**



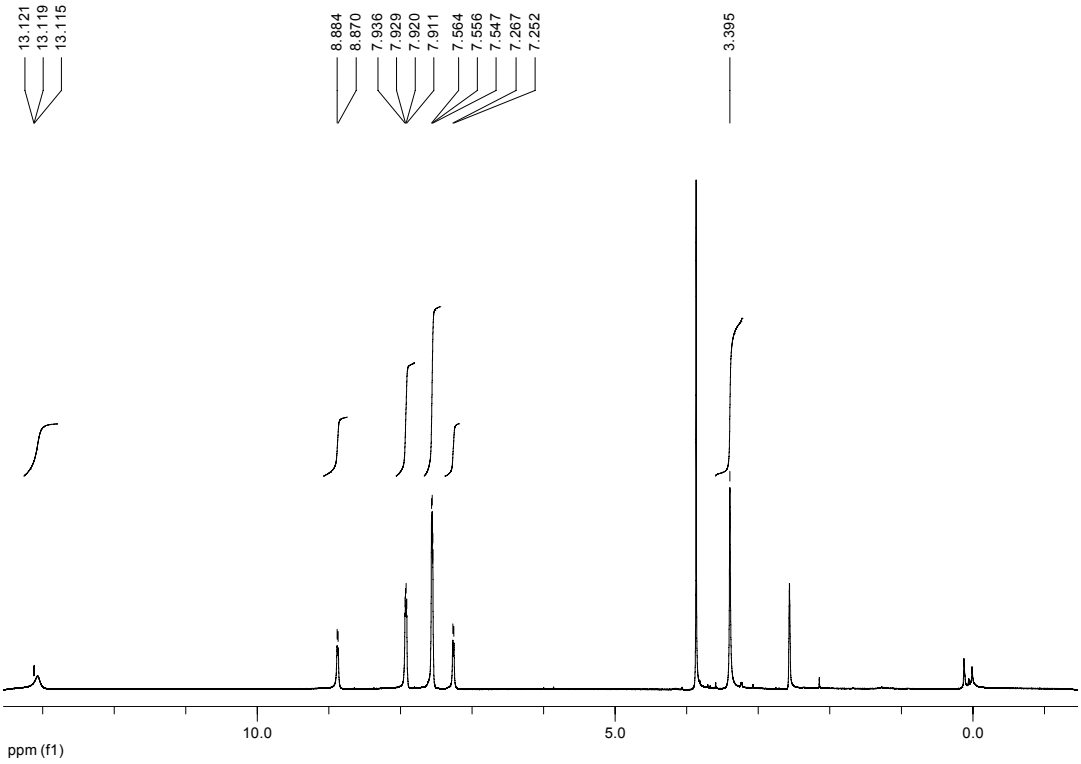
^{13}C NMR spectrum ($CDCl_3$) of compound **16**



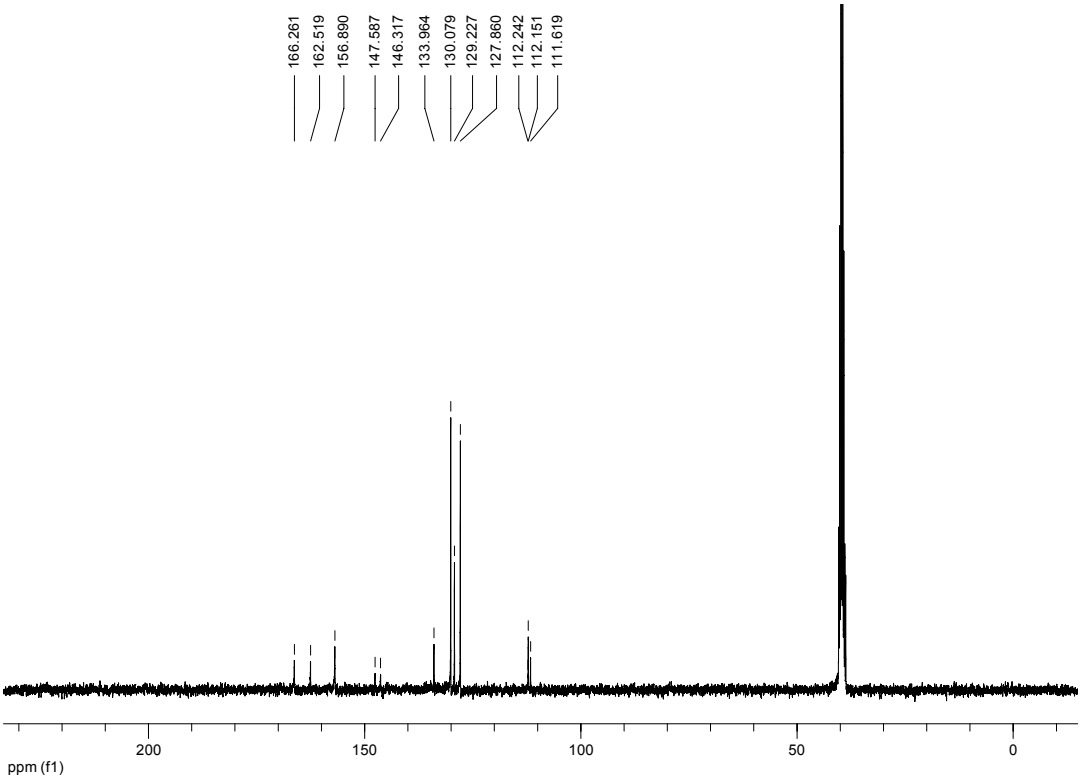
^{1}H NMR spectrum (360 MHz) of compound **17**.



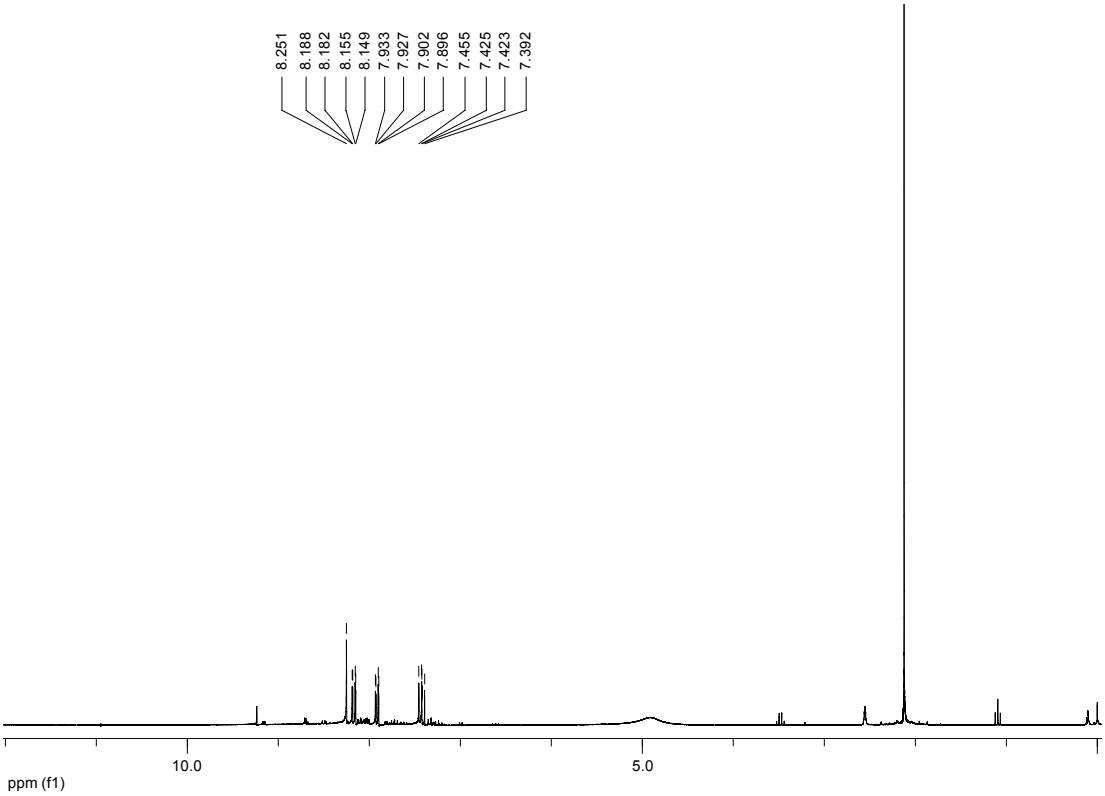
^{1}H NMR spectrum (d_6-DMSO/TFA, 360 MHz) of compound **17**



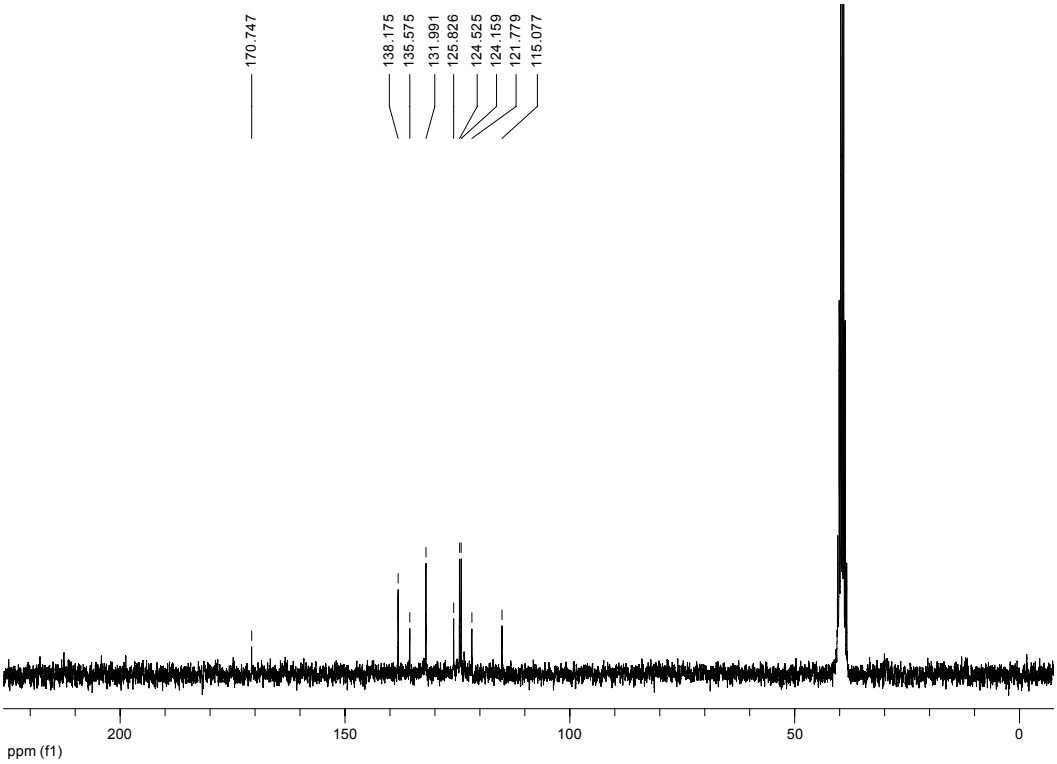
^{1}H NMR spectrum (d_6-DMSO) of compound **19**



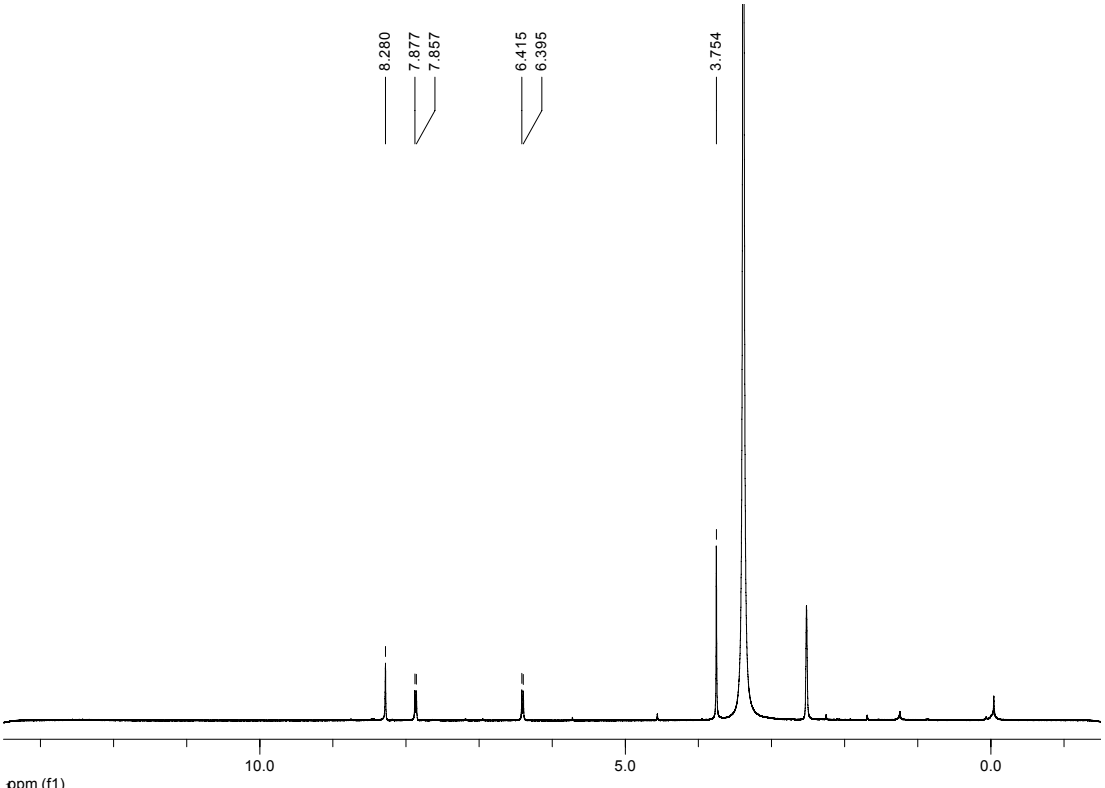
^{13}C NMR spectrum (d_6-DMSO) of compound **19**



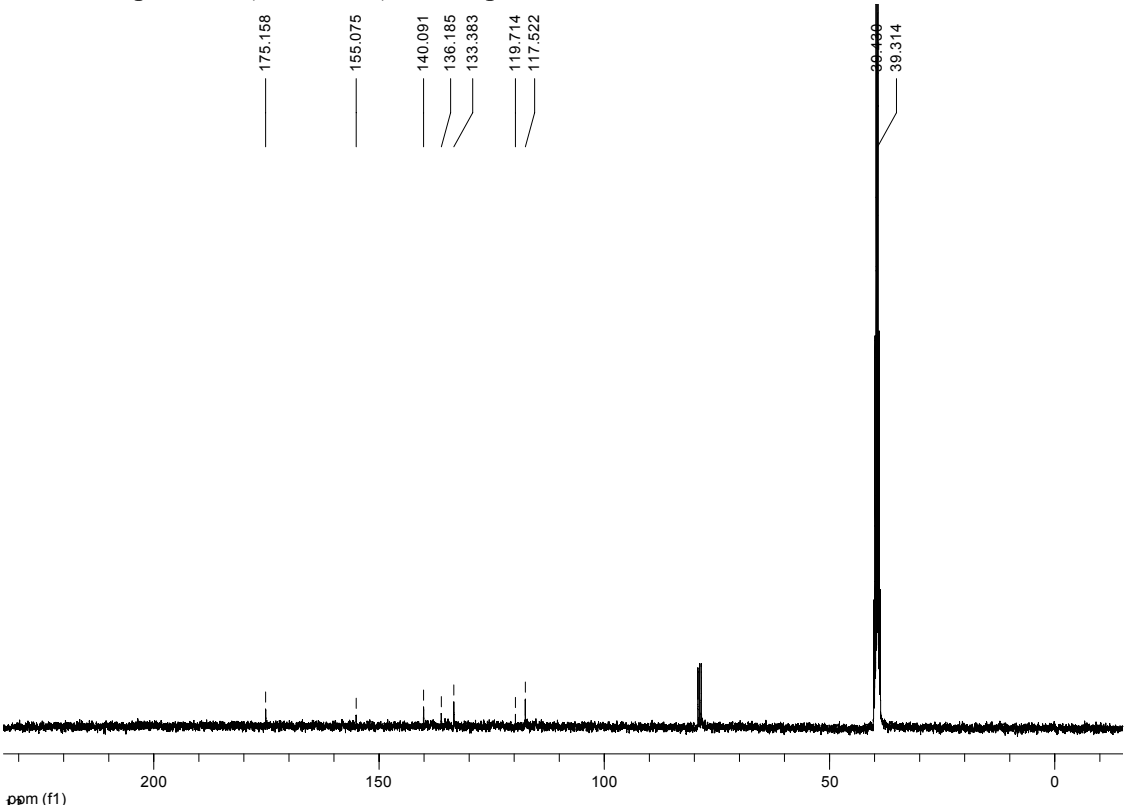
^{1}H NMR spectrum (d_6-DMSO) of compound **21**



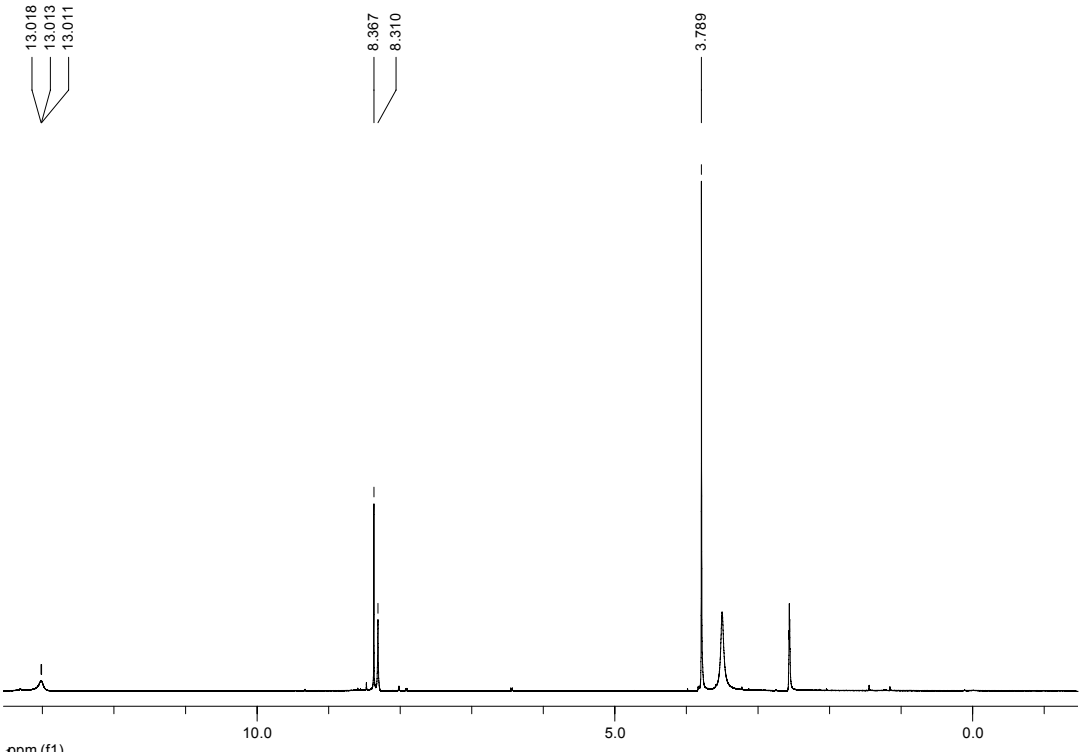
^{13}C NMR spectrum (d_6-DMSO) of compound **21**



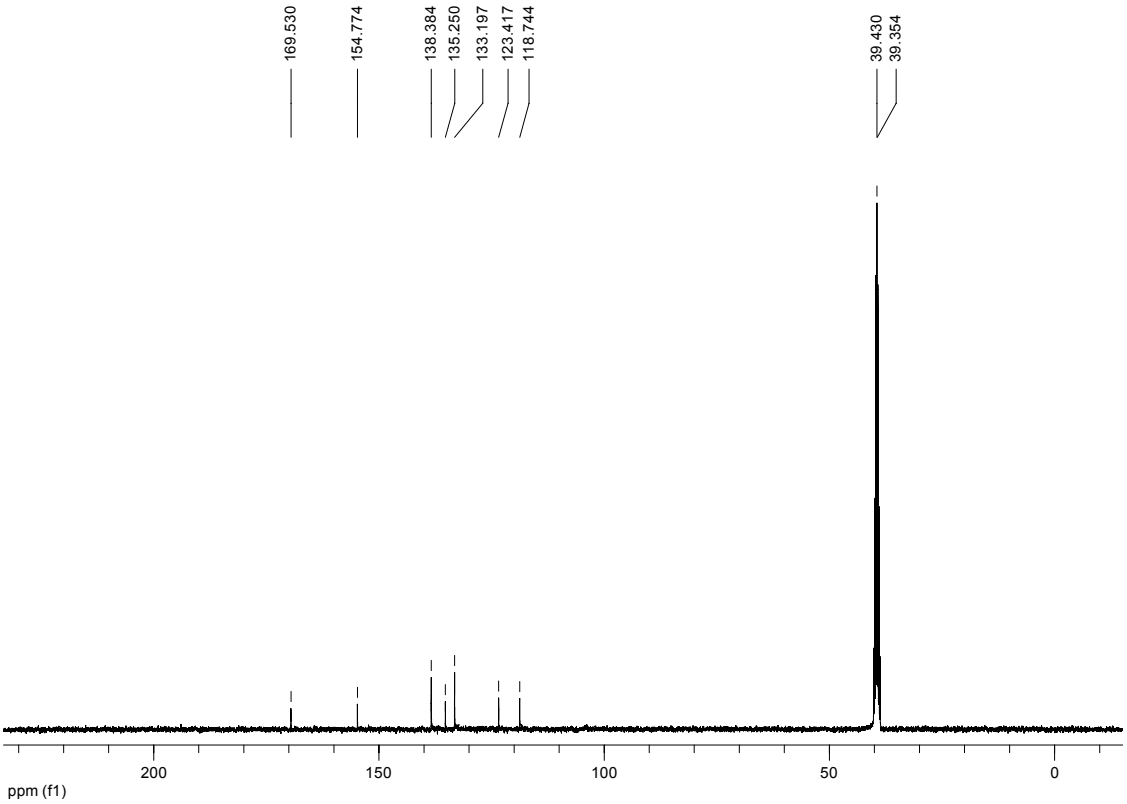
^{1}H NMR spectrum (d_6-DMSO) of compound **22**



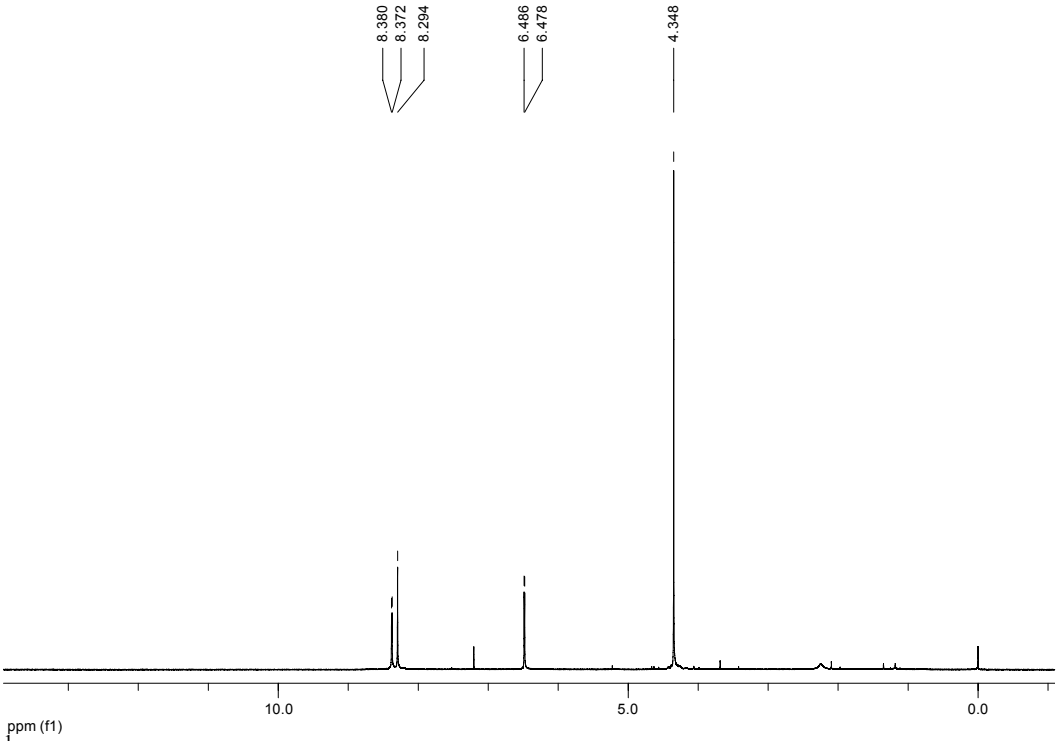
^{13}C NMR spectrum (d_6-DMSO) of compound **22**



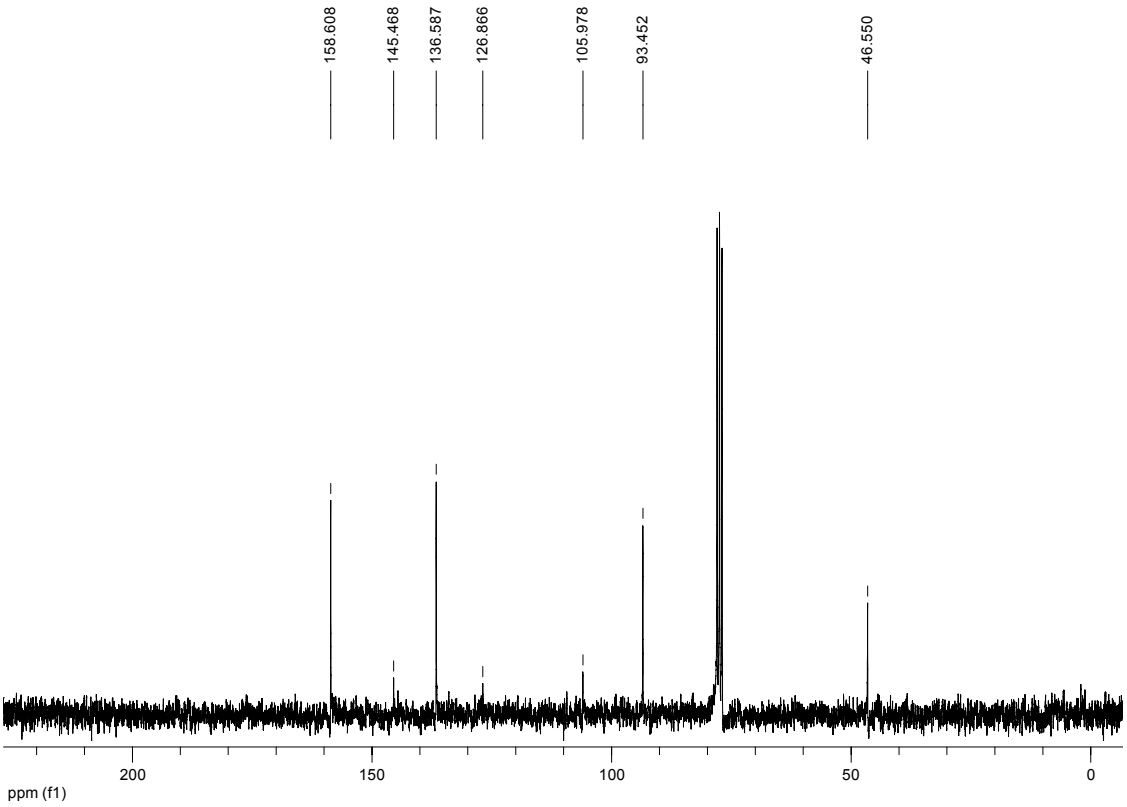
^{1}H NMR spectrum (d_6-DMSO) of compound **23**



^{13}C NMR spectrum (d_6-DMSO) of compound **23**



^{1}H NMR spectrum ($CDCl_3$) of compound **25**



^{13}C NMR spectrum ($CDCl_3$) of compound **25**

DFT calculations[5]

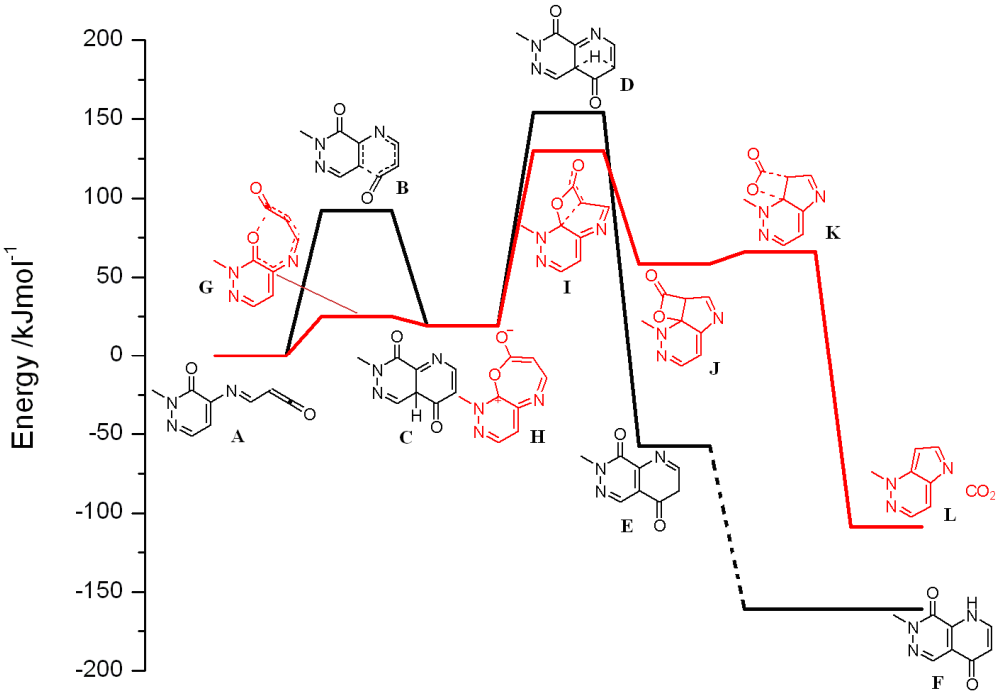
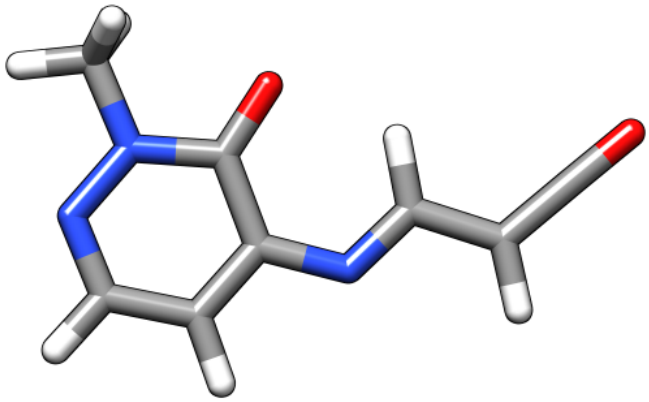


Figure 1. Energy surface for the formation of compounds **22** and **24**

Imidoylketene A

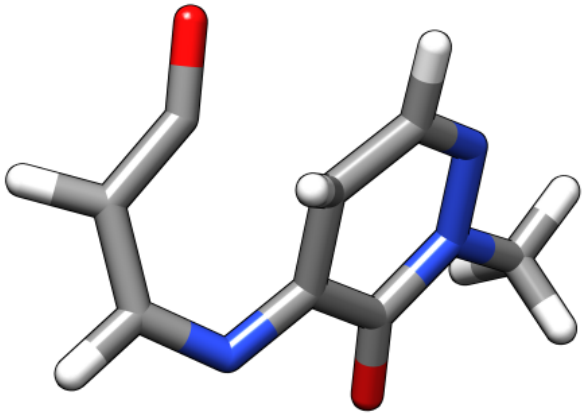


Energy = -623.7170819 Ha

Cartesian Coordinates

C	-0.986418	0.563358	0.000025
C	-0.468073	-0.814614	-0.000088
C	-1.386580	-1.840768	0.000298
N	-2.385670	0.659259	-0.000249
N	-3.271112	-0.352536	0.000241
C	-2.772991	-1.565995	0.000539
C	-2.957395	2.006658	-0.000422
O	-0.314382	1.600660	0.000243
N	0.876386	-1.157721	-0.000605
C	1.813822	-0.263144	0.000049
C	3.190831	-0.702774	-0.000788
C	4.211338	0.150886	0.000059
O	5.110873	0.890998	0.000667
H	-1.023056	-2.862989	0.000342
H	-3.506732	-2.365430	0.000926
H	-4.039590	1.895989	-0.002482
H	-2.620611	2.555097	-0.883126
H	-2.624013	2.554101	0.884224
H	1.609227	0.807522	0.001154
H	3.428423	-1.762207	-0.002052

Electrocyclisation transition state B



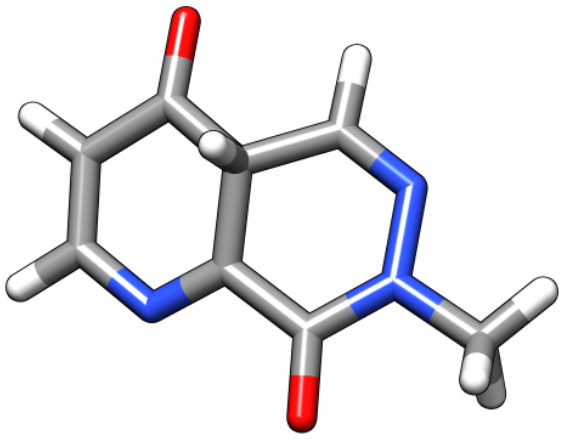
Energy = -623.681967 Ha

Cartesian Coordinates

C	2.274545	-0.757478	-0.382763
C	2.806530	0.526837	-0.380390
C	2.140934	1.671407	0.096458
N	0.854586	1.798953	0.399018
C	0.097830	0.701637	0.420645
C	0.589474	-0.584180	0.735667
O	2.522730	-1.893219	-0.614357
C	-1.325787	0.839875	-0.003230
N	-2.017813	-0.370218	-0.075770
N	-1.541081	-1.612115	0.220725
C	-0.313885	-1.705355	0.628538
O	-1.871680	1.898285	-0.277691
C	-3.412569	-0.315633	-0.510296
H	3.727672	0.648057	-0.942969
H	2.719887	2.593177	0.130478
H	0.026225	-2.708628	0.864540
H	1.367588	-0.649123	1.499166
H	-3.479559	0.157644	-1.492845
H	-4.003293	0.278501	0.191918
H	-3.779188	-1.339149	-0.549494

Negative Frequency = -511.5050 cm^{-1}

Cyclised intermediate C

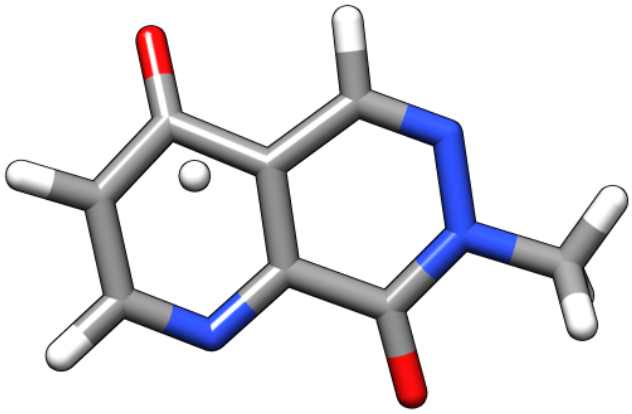


Energy = -623.7097197 Ha

Cartesian Coordinates

C	-1.414397	0.815219	0.090522
C	0.089653	0.750558	0.120188
C	0.707965	-0.583475	0.434205
N	-2.043005	-0.418695	-0.011663
N	-1.425727	-1.642981	-0.185439
C	-0.163033	-1.728114	0.009034
C	-3.497191	-0.427924	-0.161188
O	-2.052594	1.854566	0.123811
N	0.754501	1.828279	-0.105830
C	2.149149	1.728757	-0.160462
C	2.864652	0.577875	-0.119010
C	2.186063	-0.709358	0.035654
O	2.725685	-1.797711	-0.077123
H	0.759514	-0.618619	1.544017
H	0.297633	-2.701299	-0.128899
H	-3.804747	-1.466989	-0.259188
H	-3.796824	0.143128	-1.044649
H	-3.966780	0.027472	0.713721
H	2.650477	2.683066	-0.298692
H	3.938438	0.570952	-0.272952

1,5-Hydrogen shift transition state D



Energy = -623.6582916 Ha

Cartesian Coordinates

C	-1.380102	0.806933	-0.116739
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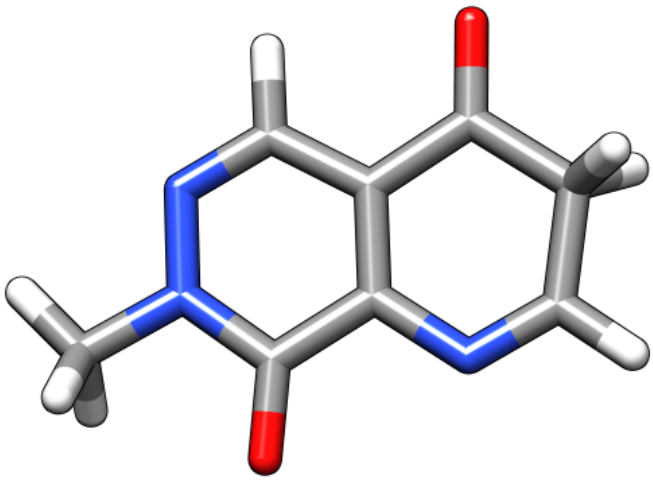
C	0.695981	-0.580507	0.131024
N	-2.043714	-0.414786	0.063586
N	-1.477029	-1.638034	0.209547
C	-0.183879	-1.724961	0.220852
C	-3.506163	-0.392270	0.026369
O	-2.008460	1.836554	-0.298518
N	0.807559	1.842787	-0.094221
C	2.109017	1.721570	0.172105
C	2.774069	0.490056	0.359607
C	2.159653	-0.743199	-0.195511
O	2.709240	-1.755264	-0.572714
H	1.607207	-0.155520	1.210481
H	0.234597	-2.722136	0.305377
H	-3.850012	-1.403541	0.232882
H	-3.854975	-0.061353	-0.955391
H	-3.885428	0.306888	0.774782
H	2.662031	2.649107	0.307412
H	3.834010	0.482189	0.601089

Negative Frequency = -1581.4506 cm^{-1}

1,5-Hydrogen shift product E



Energy = -623.7389376 Ha

Cartesian Coordinates

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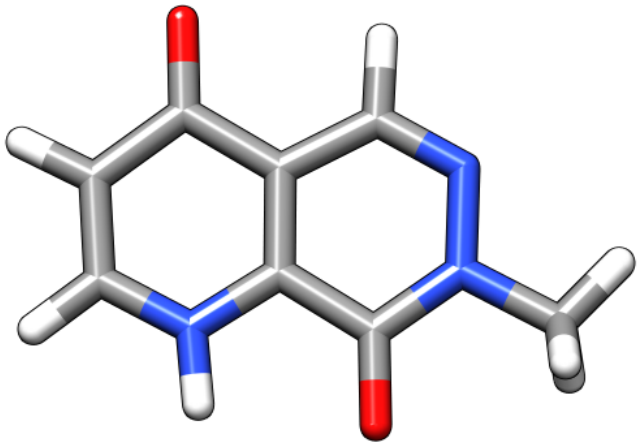
C	0.624398	-0.610527	0.000123
C	-0.243174	-1.740291	0.000238
N	-1.546108	-1.640963	0.000487
N	-2.073517	-0.403814	0.000290
N	0.831871	1.848558	0.000126
C	2.111336	1.757598	0.000446
C	2.913655	0.487318	0.000730
C	2.096239	-0.796271	-0.000195
C	-3.533746	-0.327815	0.000427
O	2.620185	-1.897637	-0.001226
O	-1.987522	1.880273	-0.001092
H	0.168743	-2.742699	0.000309
H	2.672035	2.694975	0.000675
H	3.588253	0.474773	-0.867277
H	-3.877246	0.215780	0.883865
H	-3.911736	-1.347865	0.000685
H	-3.877399	0.215468	-0.883130
H	3.586436	0.474487	0.870180

Final dione F



Energy = -623.7783223 Ha

Cartesian Coordinates

C	1.362412	0.775827	-0.000211
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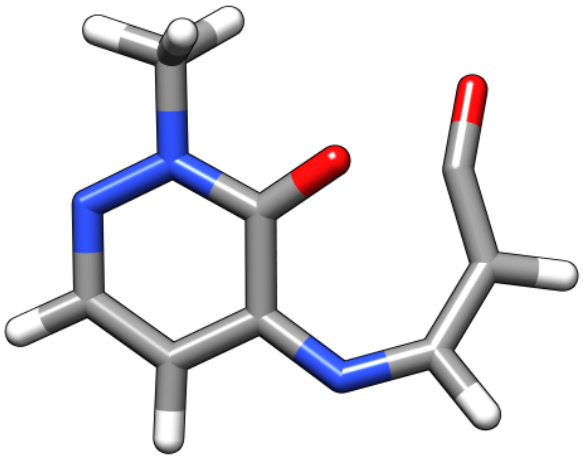
C	-0.673575	-0.635551	0.000048
C	0.207324	-1.758608	0.000100
N	1.509639	-1.669512	0.000060
N	2.054579	-0.420722	-0.000330
N	-0.827563	1.755176	-0.000122
C	-2.196246	1.695459	-0.000036
C	-2.855882	0.505901	0.000080
C	-2.149810	-0.777138	-0.000184
C	3.515601	-0.361251	-0.000022
O	-2.708170	-1.874529	0.000100
O	1.915802	1.879939	0.000379
H	-0.208147	-2.760349	0.000390
H	-0.306027	2.624643	-0.000072
H	-2.707398	2.651691	-0.000031
H	-3.939098	0.485234	0.000224
H	3.867736	0.179090	-0.882137
H	3.879005	-1.386527	-0.006338
H	3.868394	0.167896	0.888700

8π-Electrocyclisation transition state G



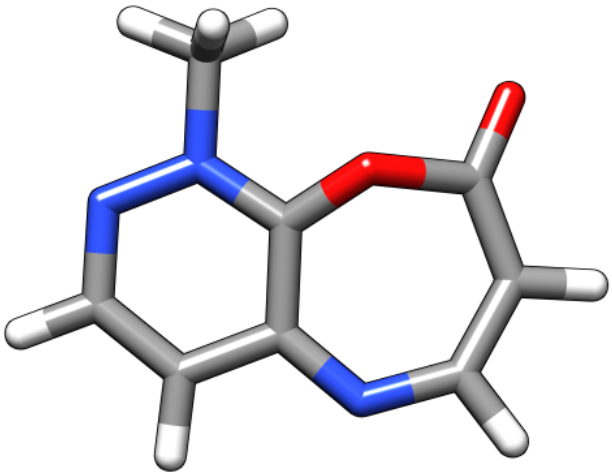
Energy = -623.707429 Ha

Cartesian Coordinates

C	-0.355855	0.222896	0.299673
C	-0.349869	-1.216038	0.102700
C	-1.560645	-1.792074	-0.251132
N	-1.542541	0.881306	0.081272
N	-2.715611	0.318769	-0.274129
C	-2.698762	-0.987000	-0.438872
O	0.640149	0.896537	0.695153
C	-1.574171	2.335128	0.282786
N	0.734112	-2.019350	0.331070
C	2.321987	0.784074	-0.291774
O	2.531079	1.885704	-0.634744
C	2.705550	-0.520635	-0.173861
C	1.992692	-1.679357	0.239133
H	-1.612910	-2.868475	-0.371236
H	-3.651404	-1.419571	-0.727393
H	-1.388211	2.570803	1.333016
H	-2.562445	2.674244	-0.018743
H	-0.794710	2.805754	-0.317921
H	3.757021	-0.654429	-0.417816
H	2.665560	-2.513288	0.457413

Negative Frequency = -109.3769 cm^{-1}

7-Membered ring intermediate H

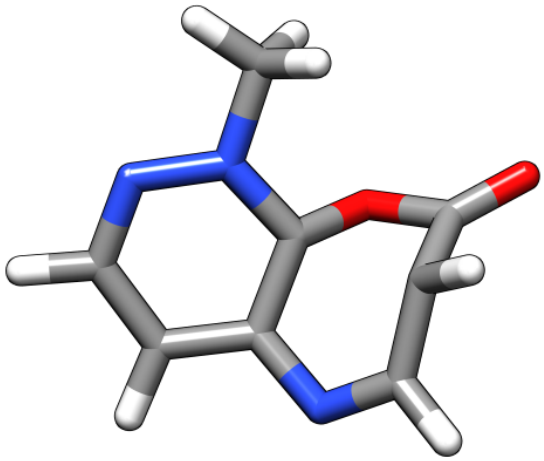


Energy = -623.709672 Ha

Cartesian Coordinates

C	-0.316125	0.189519	0.200792
C	-0.377908	-1.249279	0.088533
C	-1.677651	-1.745711	-0.116826
N	-1.432785	0.926740	0.015118
N	-2.672830	0.445913	-0.204029
C	-2.756410	-0.877579	-0.258688
O	0.742132	0.876011	0.578719
C	-1.357967	2.395345	0.129595
N	0.652227	-2.107457	0.206700
C	2.110799	0.747061	-0.120174
O	2.576584	1.813349	-0.403719
C	2.601541	-0.572862	-0.189272
C	1.936739	-1.763428	0.080451
H	-1.812161	-2.820406	-0.156980
H	-3.760732	-1.252765	-0.427681
H	-1.233699	2.678712	1.176930
H	-2.295924	2.781253	-0.261650
H	-0.503412	2.763230	-0.436388
H	3.654594	-0.628321	-0.442053
H	2.597216	-2.631359	0.136839

Ring contraction transition state I



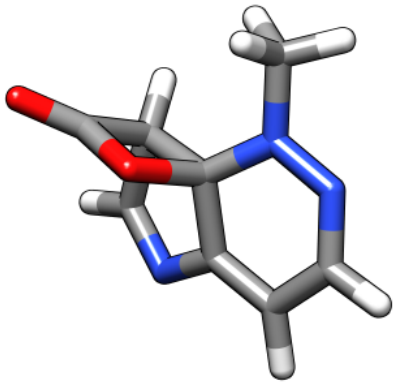
Energy = -623.667537 Ha

Cartesian Coordinates

C	-1.981708	-1.388843	-0.368436
C	-0.620725	-1.225894	-0.252052
C	-0.101047	0.127920	-0.092834
N	-1.027268	1.109903	0.183788
N	-2.350595	0.922260	0.218882
C	-2.805612	-0.273167	-0.114063
N	0.255010	-2.259870	-0.059429
C	1.321292	-1.860754	0.599225
C	1.629269	-0.474973	0.899359
C	-0.572478	2.476558	0.457209
O	0.900841	0.565600	-0.990081
C	2.049715	0.404034	-0.216646
O	3.083754	0.956202	-0.461851
H	-2.403379	-2.372087	-0.548319
H	-3.887042	-0.355307	-0.121682
H	1.944687	-2.649292	1.022940
H	0.168000	2.458317	1.261586
H	-1.446332	3.051001	0.756723
H	-0.119019	2.906221	-0.438044
H	2.214063	-0.328618	1.809001

Negative Frequency = -411.0689 cm^{-1}

Tricyclic lactone intermediate J

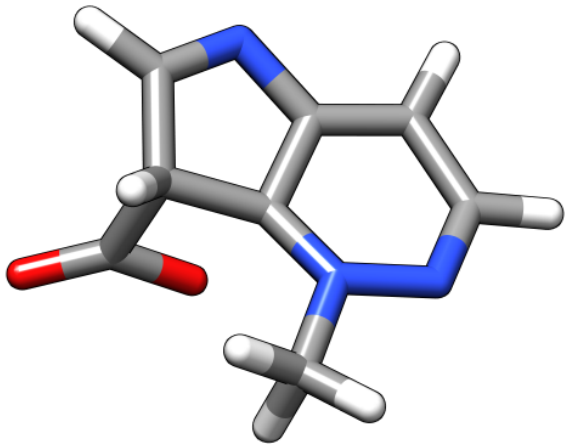


Energy = -623.69475 Ha

Cartesian Coordinates

C	1.825492	1.500341	-0.443254
C	0.544102	1.295936	-0.066315
C	0.027356	-0.089891	0.086890
N	1.040994	-1.001474	0.399451
N	2.310812	-0.840871	-0.071976
C	2.667893	0.336354	-0.503329
N	-0.412280	2.242680	0.329421
C	-1.402667	1.608287	0.861356
C	-1.314874	0.095105	0.840803
C	0.708955	-2.380679	0.748020
O	-0.816085	-0.544210	-1.150854
C	-1.966802	-0.481086	-0.432229
O	-3.077672	-0.776997	-0.762442
H	2.228971	2.494580	-0.598935
H	3.697286	0.408496	-0.838970
H	-2.253513	2.141480	1.277001
H	-0.059218	-2.389657	1.524805
H	1.612061	-2.854462	1.130240
H	0.346032	-2.934963	-0.123939
H	-1.534981	-0.404365	1.786250

Decarboxylation transition state K



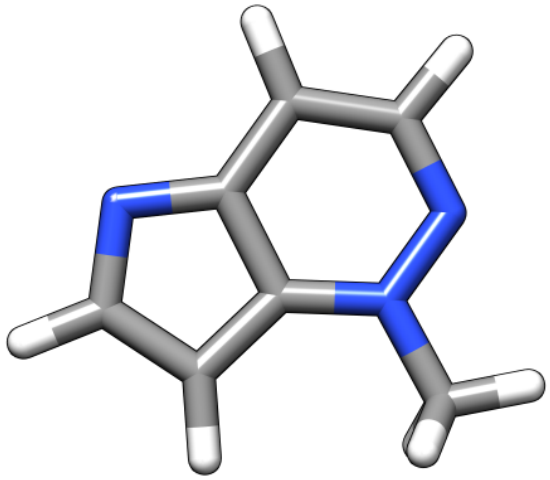
Energy = -623.691848 Ha

Cartesian Coordinates

C	1.903870	1.454439	-0.432727
C	0.617908	1.291737	-0.026851
C	0.105138	-0.048921	0.201383
N	1.027804	-1.025063	0.384732
N	2.305996	-0.911112	-0.075896
C	2.699851	0.267262	-0.485349
N	-0.341241	2.262620	0.304715
C	-1.353567	1.633705	0.808572
C	-1.270202	0.127089	0.821412
C	0.629895	-2.393218	0.717727
O	-0.968630	-0.538041	-1.277655
C	-1.983028	-0.446966	-0.455726
O	-3.152144	-0.708670	-0.603086
H	2.329198	2.428482	-0.643593
H	3.730758	0.304269	-0.822742
H	-2.230513	2.173879	1.155508
H	0.186961	-2.870558	-0.160635
H	-0.099381	-2.377398	1.529336
H	1.522181	-2.932450	1.030220
H	-1.520114	-0.348421	1.772314

Negative Frequency = -280.2592 cm^{-1}

Pyrrolopyrazine L



Energy = -435.1775273 Ha

Cartesian Coordinates

C	-0.061889	1.929588	-0.000006
C	-0.865057	0.808913	-0.000003
C	-0.198808	-0.498448	-0.000007
N	1.154990	-0.547506	-0.000015
N	1.936966	0.538880	0.000009
C	1.332433	1.722154	0.000007
N	-2.212671	0.659621	0.000005
C	-2.392931	-0.676423	0.000005
C	-1.209083	-1.455773	0.000002
C	1.854447	-1.831395	0.000003
H	-0.475144	2.932400	-0.000016
H	2.019267	2.562063	0.000000
H	-3.400785	-1.081278	0.000004
H	-1.130882	-2.532728	-0.000016
H	1.577667	-2.402405	-0.890770
H	1.577780	-2.402316	0.890866
H	2.922441	-1.624390	-0.000074

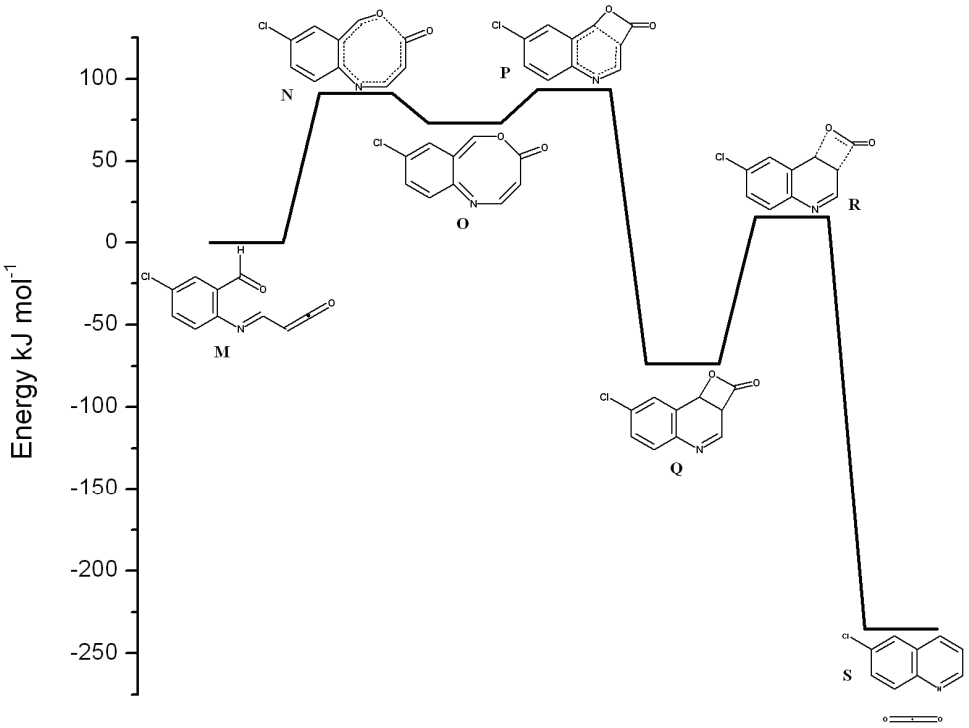
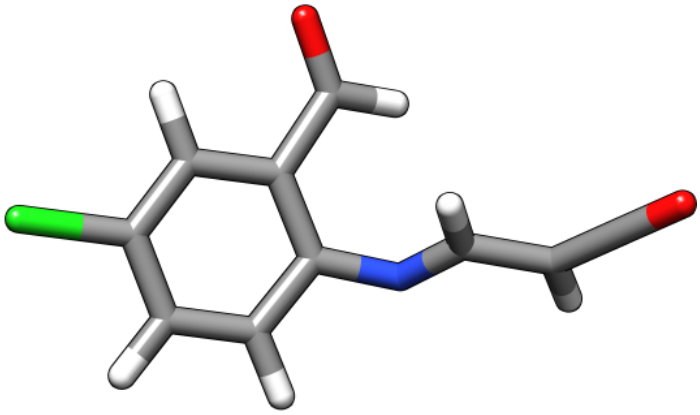


Figure 2 Energy surface for the formation of 6-chloroquinoline **30** from the arylimidoylketene

Imidoylketene M

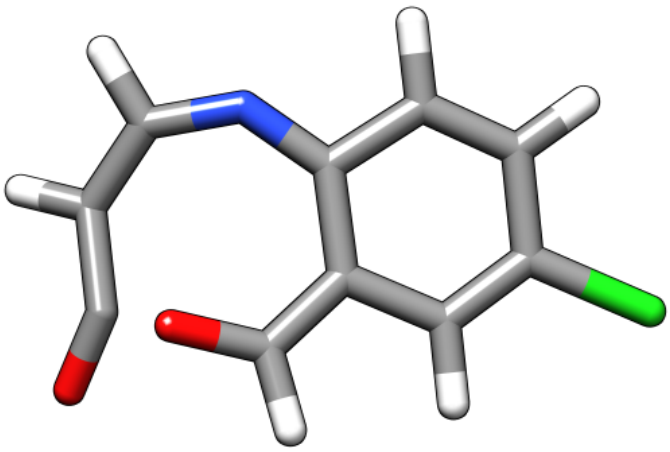


Energy = -1050.0269399 Ha

Cartesian Coordinates

C	-1.839200	0.810900	0.016200
C	-0.478200	0.634900	-0.292700
C	0.043700	-0.673300	-0.452300
C	-2.669900	-0.286800	0.150000
C	-2.176500	-1.584000	-0.044200
C	-0.837900	-1.766500	-0.356600
CL	-4.368400	-0.062500	0.542200
N	1.382500	-0.956800	-0.744000
C	2.318700	-0.469600	-0.013200
C	3.710900	-0.710000	-0.329000
C	4.704500	-0.244800	0.422400
O	5.580000	0.161600	1.072800
C	0.321400	1.859200	-0.540200
O	-0.067800	2.985300	-0.284600
H	-2.210600	1.823200	0.129400
H	-2.842200	-2.435300	0.045800
H	-0.439000	-2.763200	-0.511800
H	3.977700	-1.291400	-1.205800
H	2.108500	0.130900	0.882800
H	1.307400	1.702100	-1.018200

Electrocyclisation transition state N



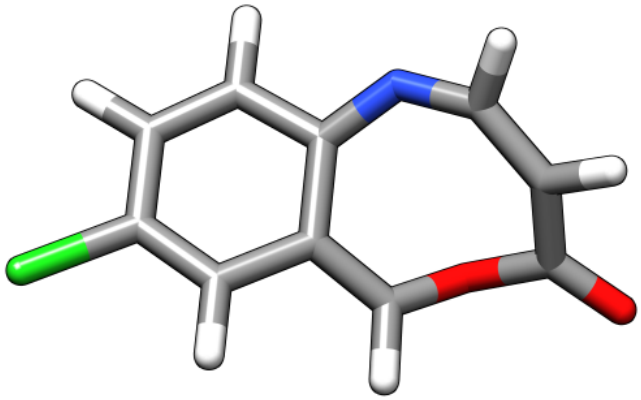
Energy = -1049.9921324 Ha

Cartesian Coordinates

C	1.400700	-0.902800	0.112600
C	0.086500	-0.342900	0.287400
C	-0.104600	1.102600	0.207200
C	2.487000	-0.101700	-0.073200
C	2.341900	1.313200	-0.066300
C	1.103700	1.874100	0.094200
N	-1.205200	1.867400	0.220300
C	-0.891600	-1.249900	0.692900
C	-2.475700	1.651600	-0.122300
O	-2.117400	-0.956300	0.999600
C	-3.056200	-0.803800	-0.316700
C	-3.220000	0.567100	-0.576000
O	-3.503600	-1.828900	-0.716500
CL	4.085500	-0.789700	-0.288200
H	1.515000	-1.981100	0.150600
H	3.219700	1.938200	-0.190200
H	0.977800	2.950600	0.092600
H	-0.590600	-2.297800	0.816500
H	-3.038100	2.589200	-0.146800
H	-4.162500	0.791700	-1.068000

Negative Frequency = -226.4167 cm^{-1}

8-Membered ring intermediate O

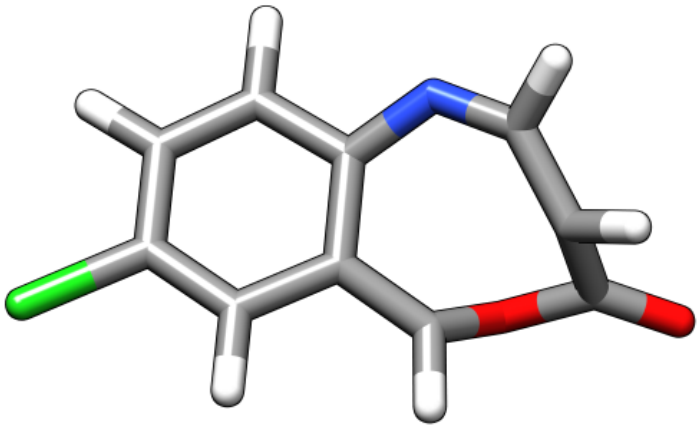


Energy = -1049.9990827 Ha

Cartesian Coordinates

C	-1.421300	-0.909200	0.351400
C	-0.104400	-0.386900	0.048300
C	0.041400	1.051000	-0.233400
C	-2.505900	-0.157600	0.037900
C	-2.372900	1.149200	-0.561500
C	-1.148800	1.719600	-0.719600
N	1.072100	1.802400	0.063100
C	0.940500	-1.239000	-0.136500
C	2.187500	1.496300	0.785100
O	2.036000	-0.892300	-0.862500
C	3.206300	-0.663800	-0.093100
C	3.080900	0.459500	0.820500
O	4.189000	-1.328100	-0.287100
CL	-4.128200	-0.770500	0.302100
H	-1.525100	-1.923200	0.722600
H	-3.274100	1.681600	-0.845100
H	-1.038000	2.733500	-1.088300
H	0.883200	-2.290600	0.147100
H	2.456900	2.331900	1.435500
H	3.952200	0.596900	1.452400

Ring contraction transition state P



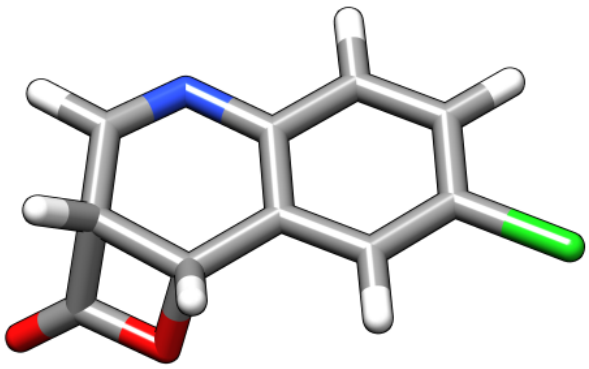
Energy = -1049.9912997 Ha

Cartesian Coordinates

C	-1.384900	-0.872200	0.351500
C	-0.089800	-0.328300	0.104100
C	0.042900	1.068100	-0.230800
C	-2.488700	-0.134400	0.010200
C	-2.368400	1.172000	-0.541800
C	-1.133700	1.758400	-0.653600
N	1.107500	1.827300	0.104900
C	1.052000	-1.129100	0.153500
C	2.157700	1.416400	0.801200
O	1.987600	-1.005500	-0.863800
C	3.159000	-0.681500	-0.201500
C	2.810100	0.169400	0.953100
O	4.245400	-1.050200	-0.551400
CL	-4.093800	-0.815500	0.202100
H	-1.485500	-1.894800	0.698600
H	-3.266800	1.709300	-0.824300
H	-1.026600	2.787900	-0.977300
H	1.053200	-2.098200	0.648600
H	2.600400	2.222400	1.394000
H	3.566800	0.157300	1.736800

Negative Frequency = -360.1380 cm^{-1}

Lactone Q

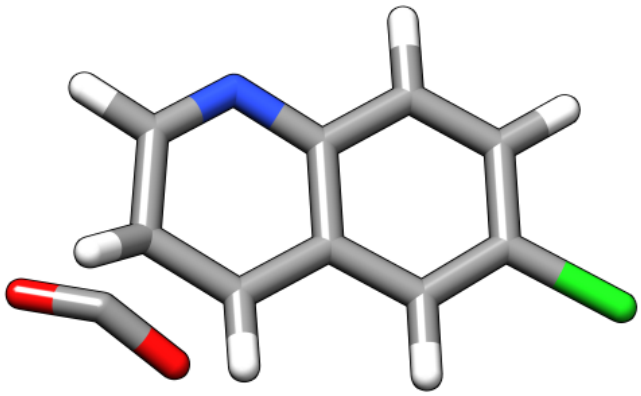


Energy = -1050.0550069 Ha

Cartesian Coordinates

C	1.266100	-0.782600	0.342500
C	0.040200	-0.117400	0.340800
C	-0.023300	1.244500	-0.019300
C	1.152300	1.908300	-0.391400
C	2.374900	1.244200	-0.406600
C	2.421800	-0.100200	-0.034800
C	-1.218000	-0.832900	0.718000
C	-2.480900	0.042900	0.817000
C	-2.301900	1.476800	0.397400
N	-1.208900	2.010600	0.002800
CL	3.958500	-0.947600	-0.039100
C	-2.995100	-0.871400	-0.321300
O	-3.998300	-1.002500	-0.951900
O	-1.826500	-1.578900	-0.417300
H	1.322000	-1.829000	0.624700
H	1.083500	2.956000	-0.663700
H	3.283800	1.759400	-0.695700
H	-1.067700	-1.533800	1.542000
H	-3.196400	2.101400	0.406500
H	-3.075700	-0.041000	1.730900

Decarboxylation transition state R



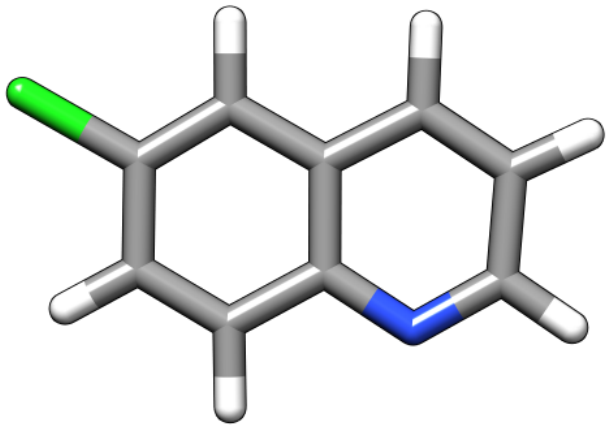
Energy = -1050.020789 Ha

Cartesian Coordinates

C	1.305100	-0.778200	0.402500
C	0.062700	-0.107500	0.408400
C	-0.026300	1.250200	-0.021000
C	1.146300	1.892100	-0.455900
C	2.361300	1.225700	-0.462300
C	2.435700	-0.110600	-0.027100
C	-1.124500	-0.741800	0.876500
C	-2.364200	0.021600	0.902700
C	-2.268100	1.414300	0.462800
N	-1.204200	1.989400	-0.003300
CL	3.984900	-0.930400	-0.042500
C	-2.984800	-0.941000	-0.420800
O	-4.101700	-0.766000	-0.814200
O	-2.021000	-1.715400	-0.686800
H	1.362500	-1.813900	0.720400
H	1.072100	2.923800	-0.781400
H	3.262700	1.727000	-0.797700
H	-1.046300	-1.673300	1.424400
H	-3.186000	2.002100	0.472100
H	-3.056800	-0.171400	1.721500

Negative Frequency = -757.4332 cm^{-1}

6-Chloroquinolinone S



Energy = -861.5355698 Ha

Cartesian Coordinates

C	1.205500	0.135600	0.000000
C	0.000000	0.883800	0.000000
C	-1.257100	0.198900	0.000000
C	-1.262900	-1.221200	0.000000
C	-0.085800	-1.932100	0.000000
C	1.148400	-1.237800	0.000000
C	-0.028700	2.302200	0.000000
C	-1.241600	2.947700	0.000000
C	-2.429100	2.172200	0.000000
N	-2.453600	0.854500	0.000000
CL	2.637000	-2.173500	0.000000
H	2.161200	0.649100	0.000000
H	-2.225000	-1.722300	0.000000
H	-0.086600	-3.016200	0.000000
H	0.905600	2.857500	0.000000
H	-1.304600	4.031100	0.000000
H	-3.396000	2.673700	0.000000

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