Supporting information for

Efficient Synthesis of 1*H*-Benzo[4,5]imidazo[1,2-*c*][1,3]oxazin-1-one Derivatives Using Ag_2CO_3/TFA-Catalyzed 6-*endo*-*dig* Cyclization: Reaction Scope and Mechanistic study.

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mohamed.abarbri@univ-tours.fr (M.A.)

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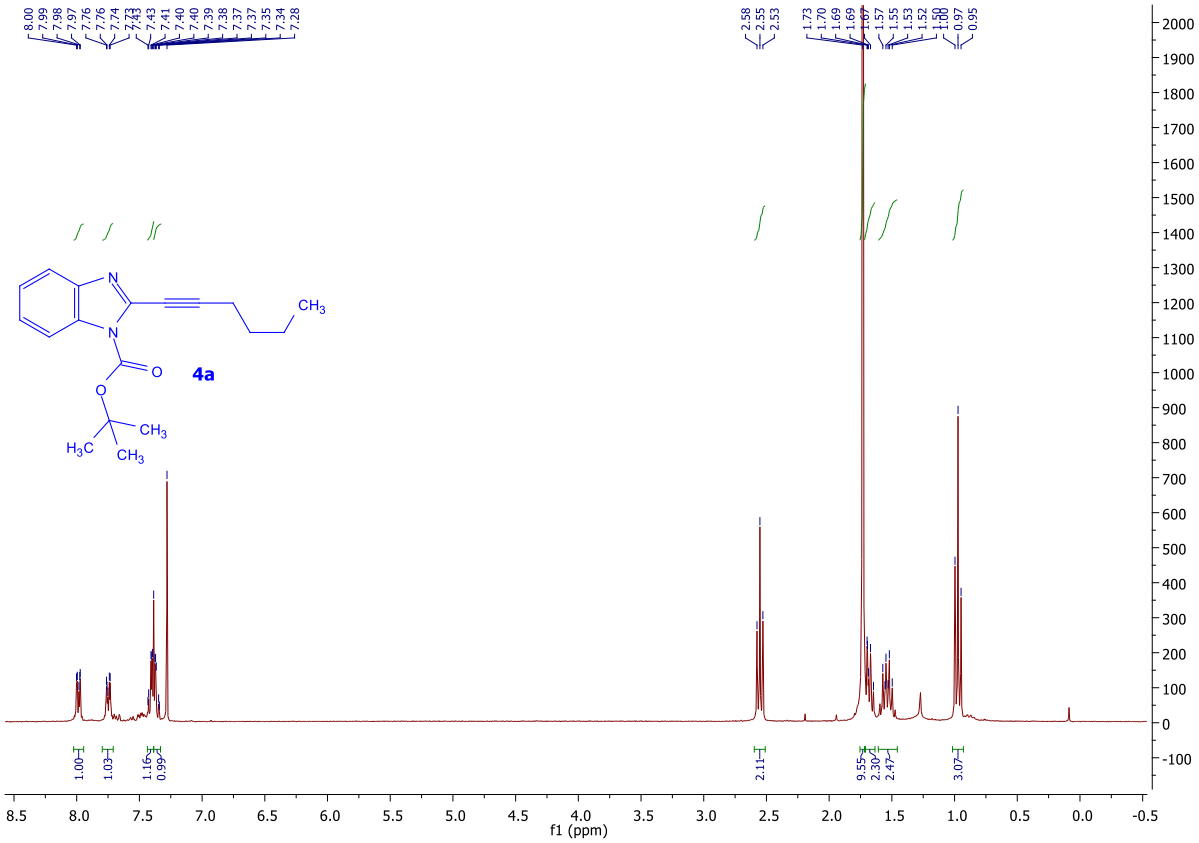
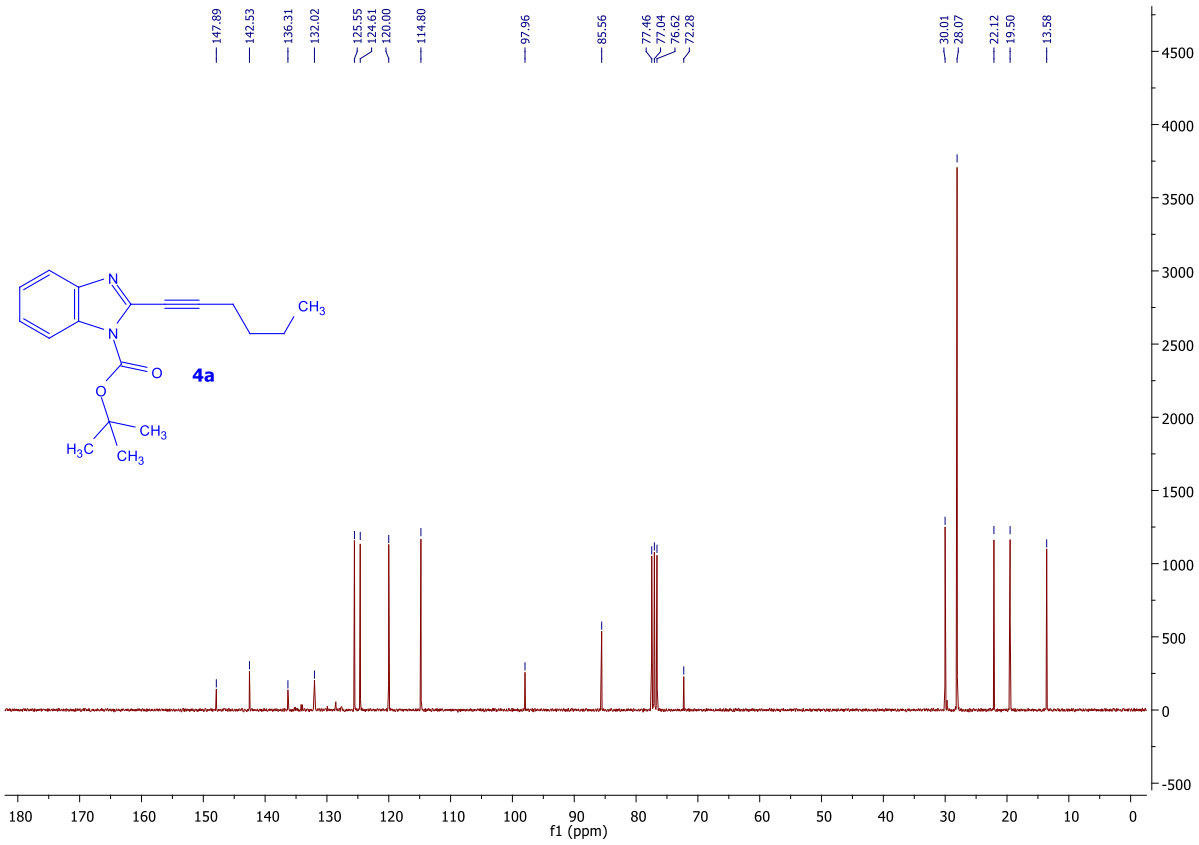
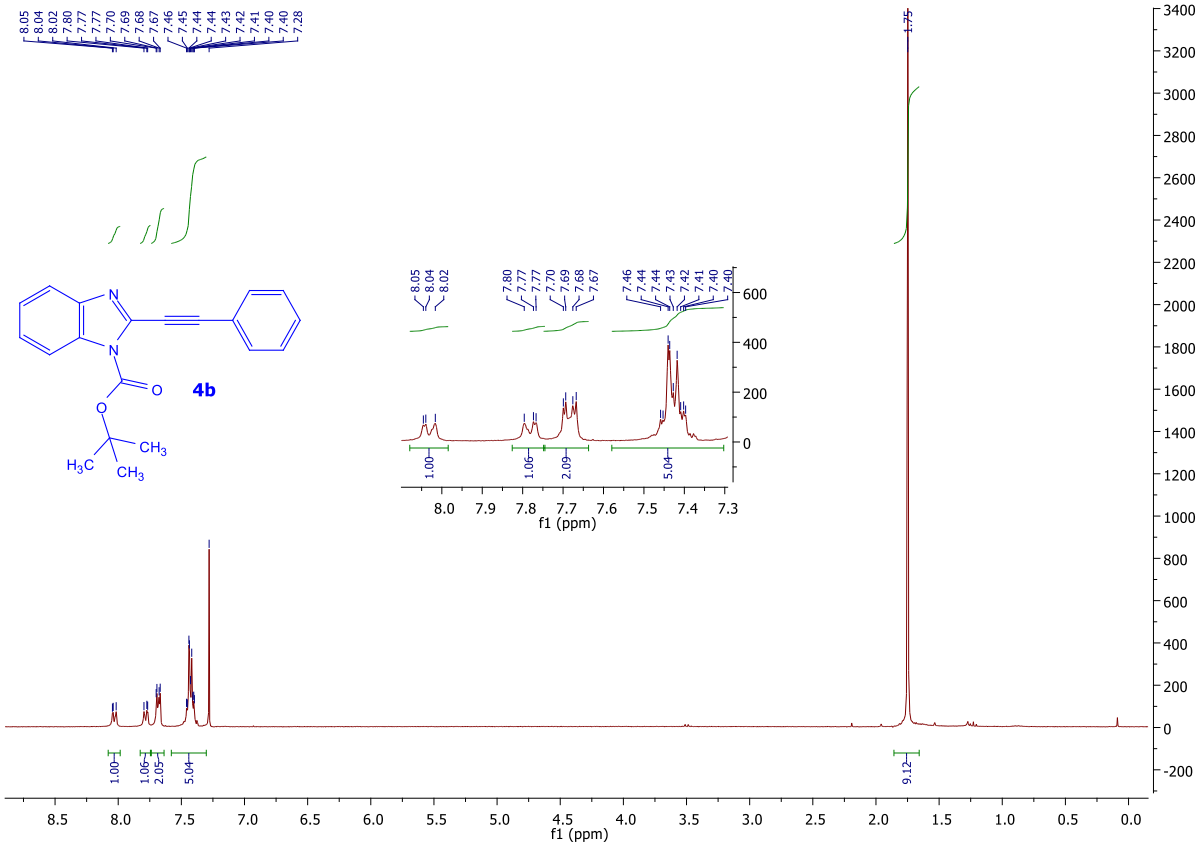
^{1}H NMR (300 MHz, $CDCl_3$) of **4a**



^{13}C NMR (75 MHz, $CDCl_3$) of **4a**



^{1}H NMR (300 MHz, $CDCl_3$) of **4b**



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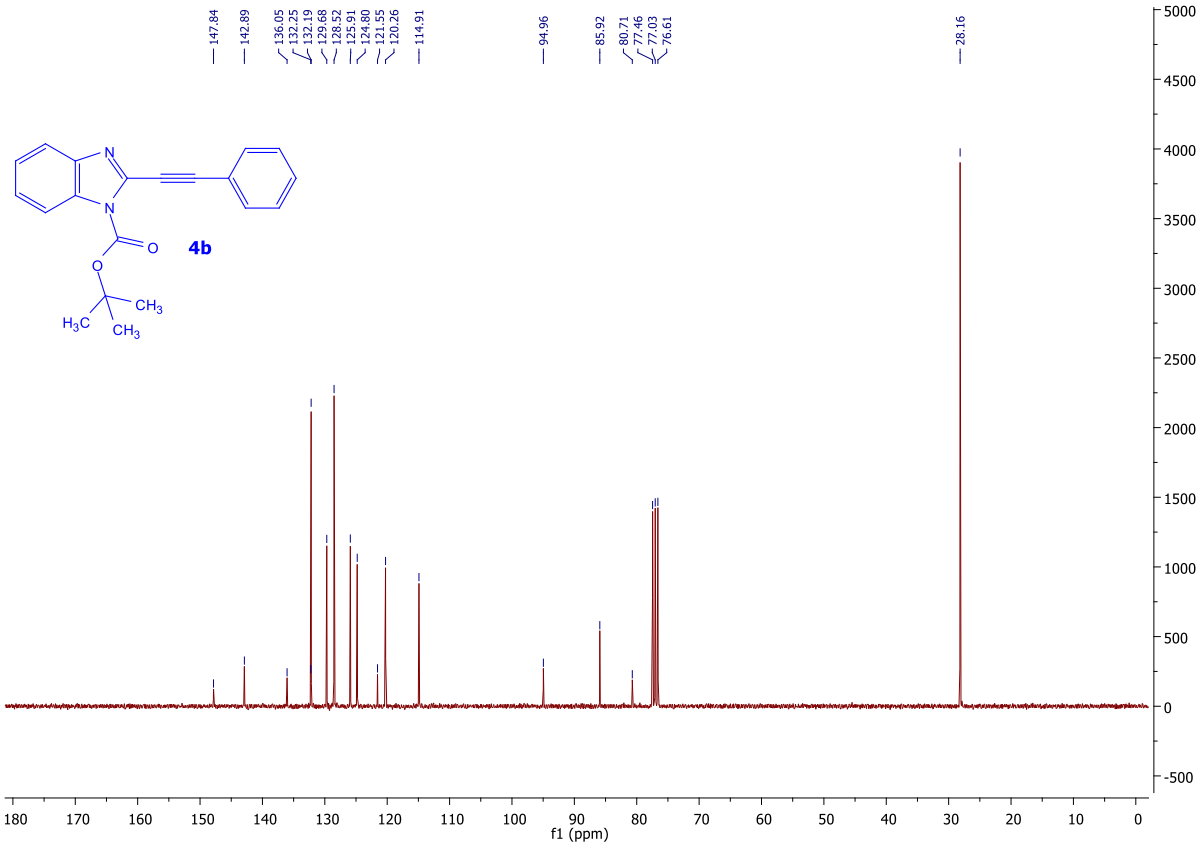
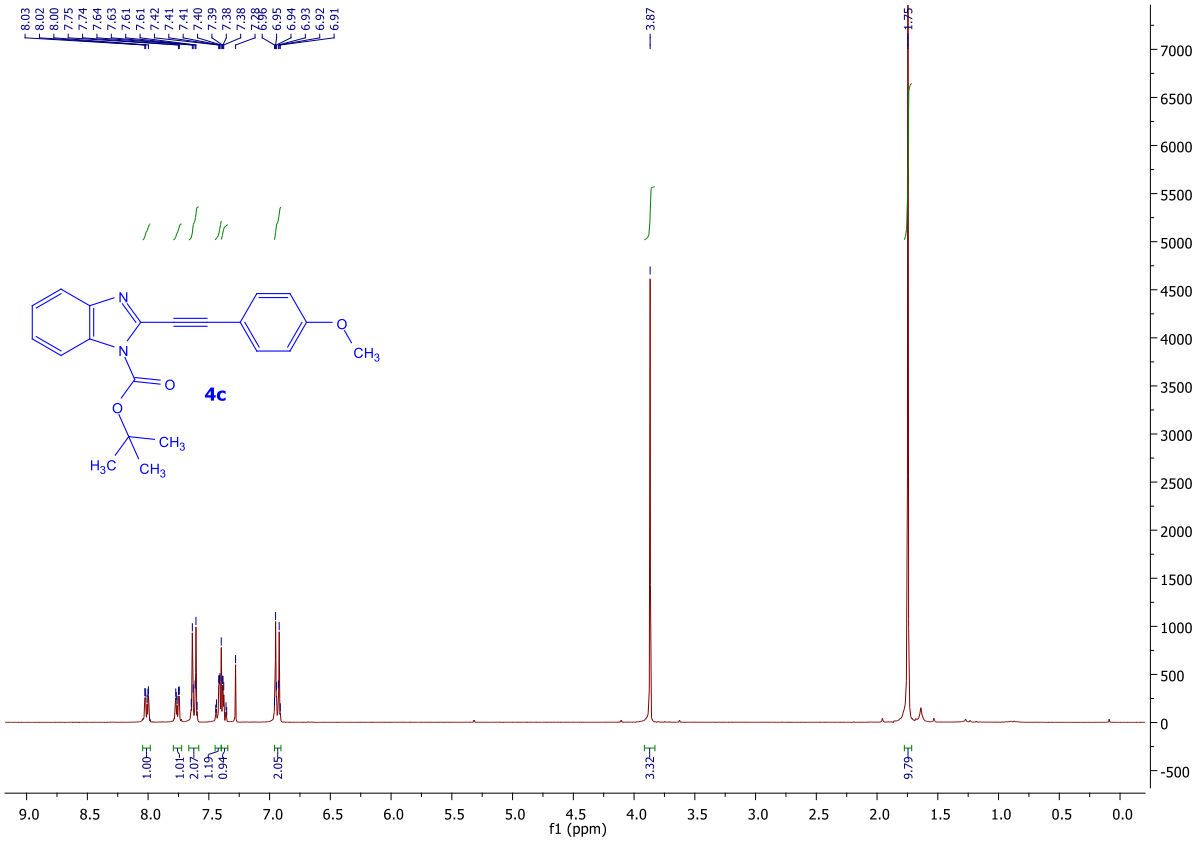


^{1}H NMR (300 MHz, $CDCl_3$) of **4c**



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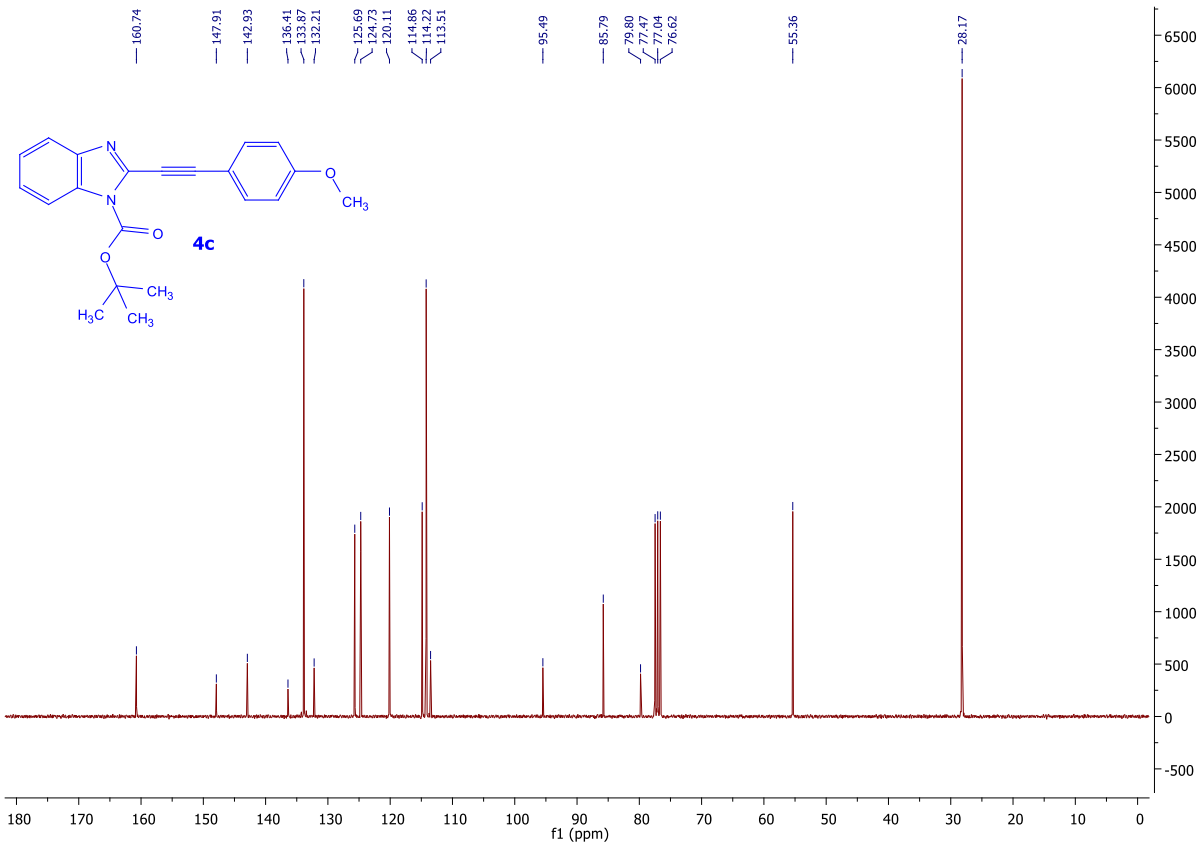

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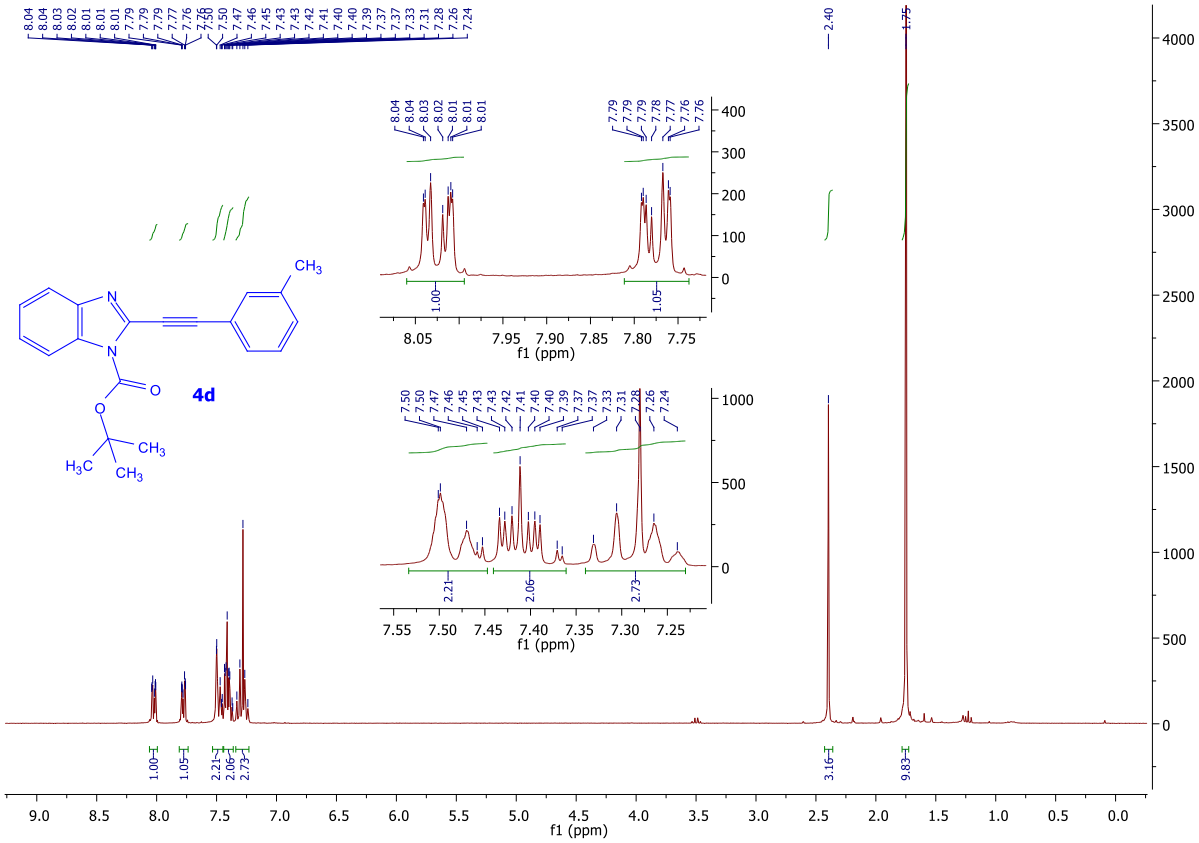
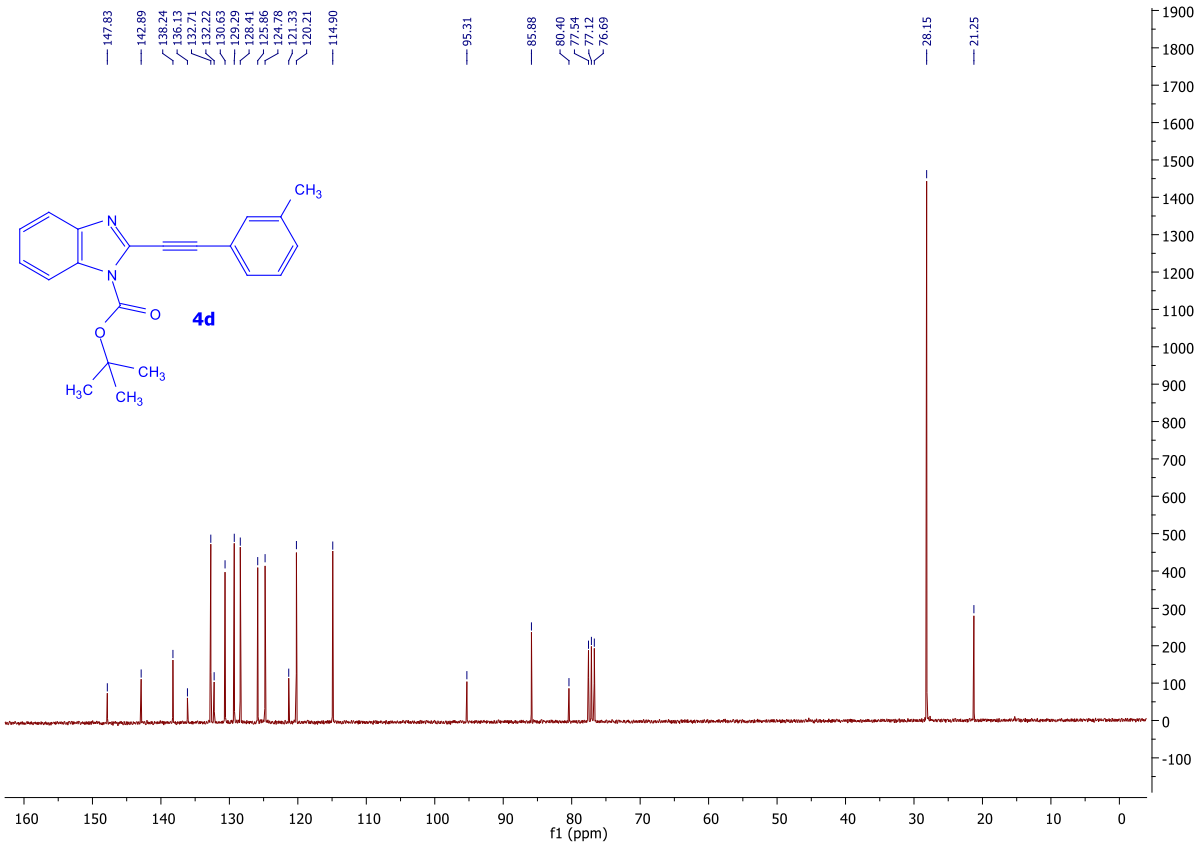


^{13}C NMR (75 MHz, $CDCl_3$) of **4d**



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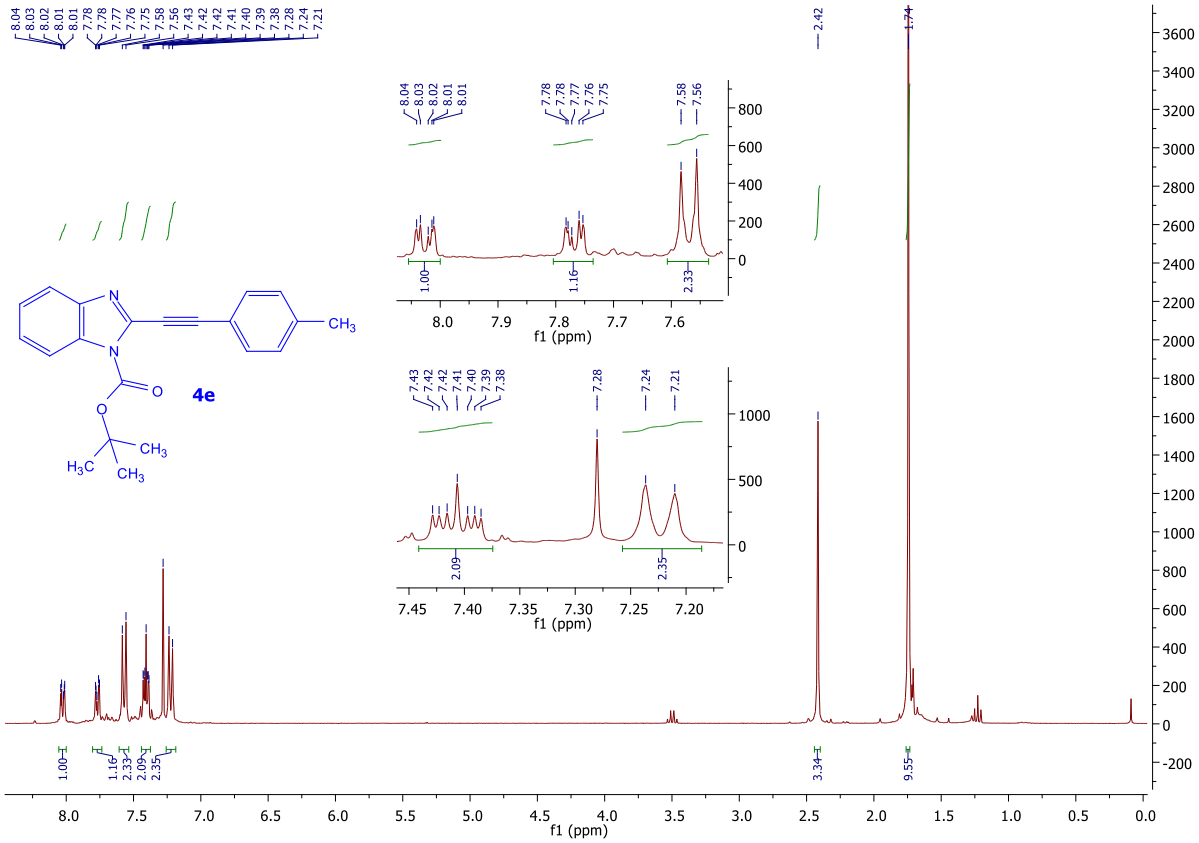
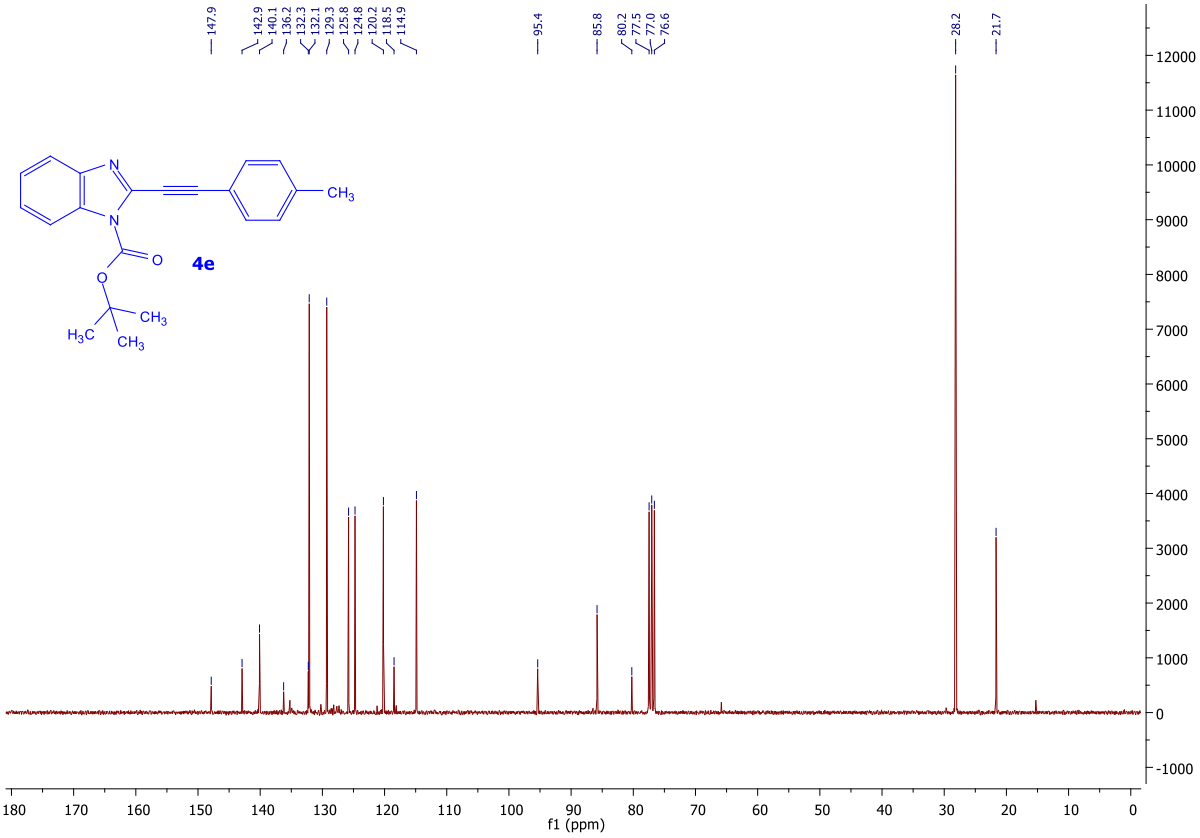


^{13}C NMR (75 MHz, $CDCl_3$) of **4e**



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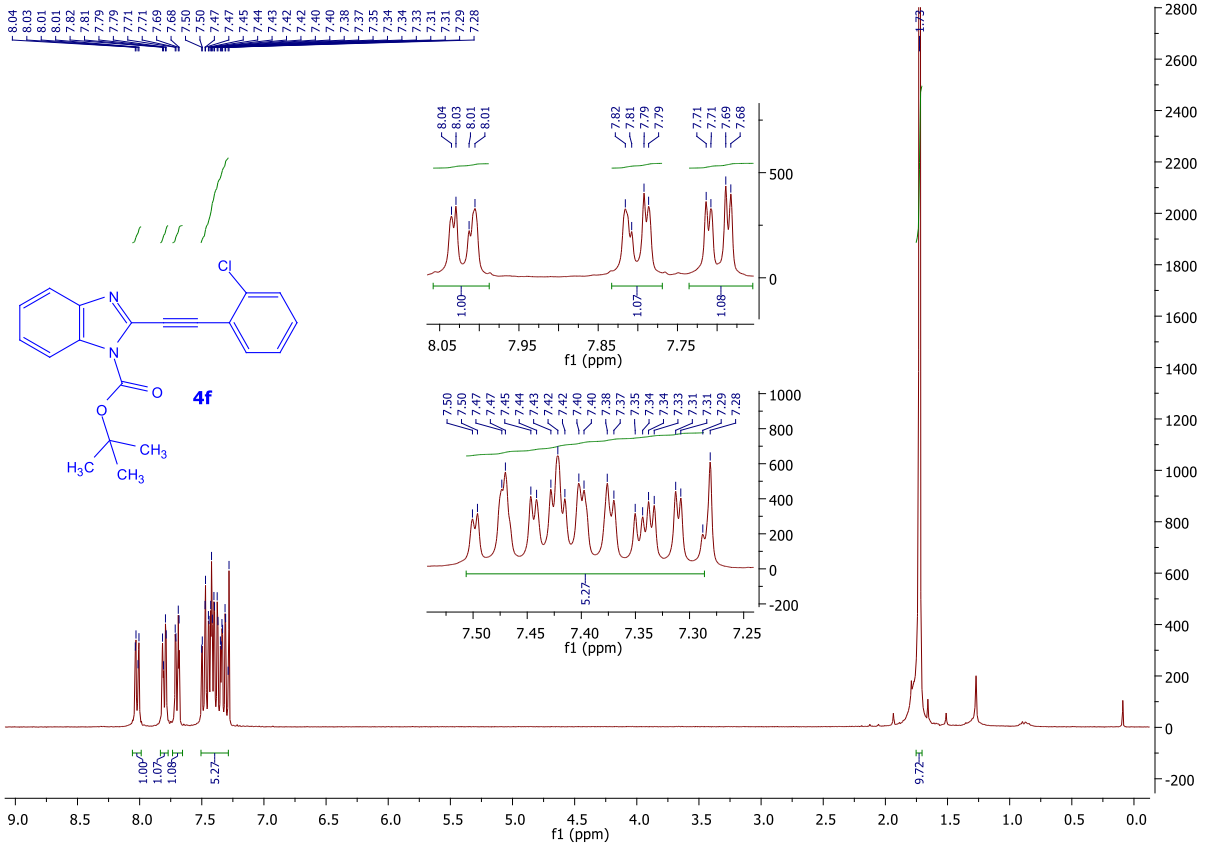

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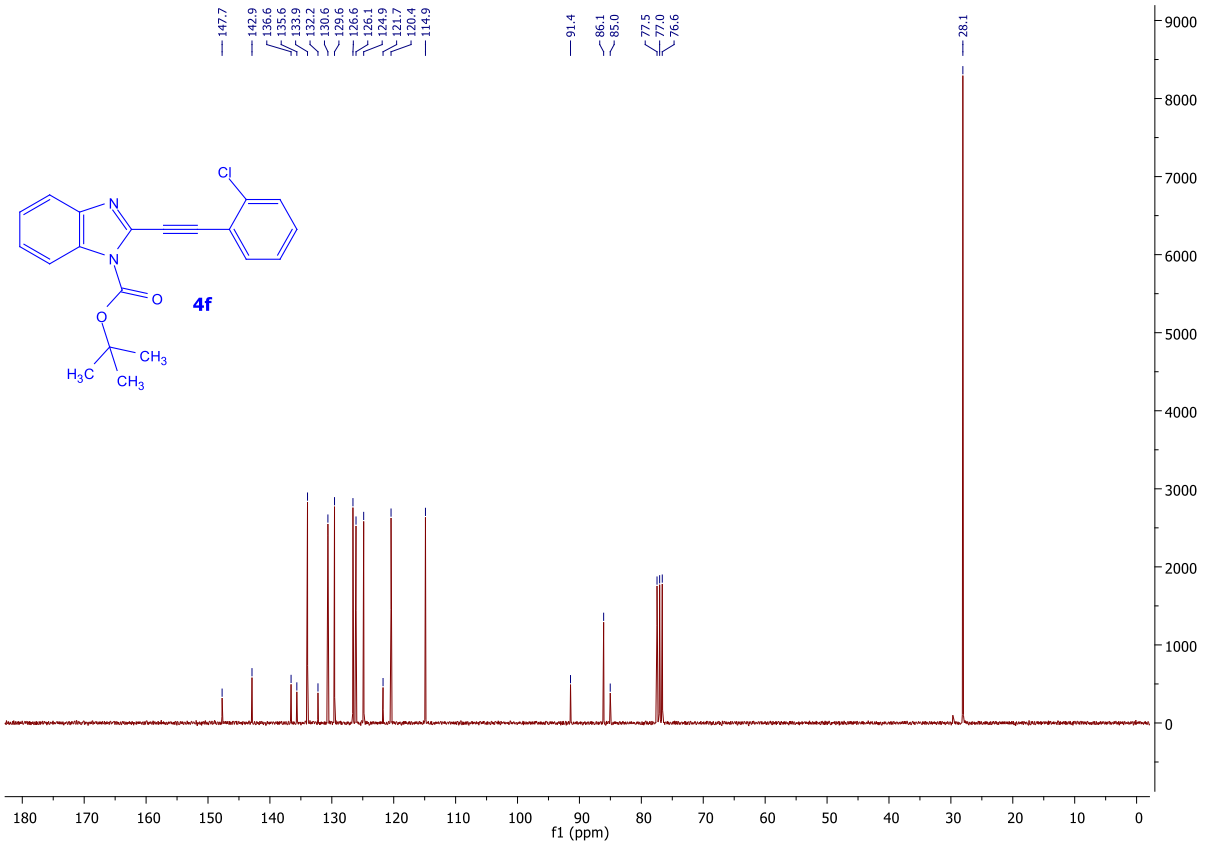

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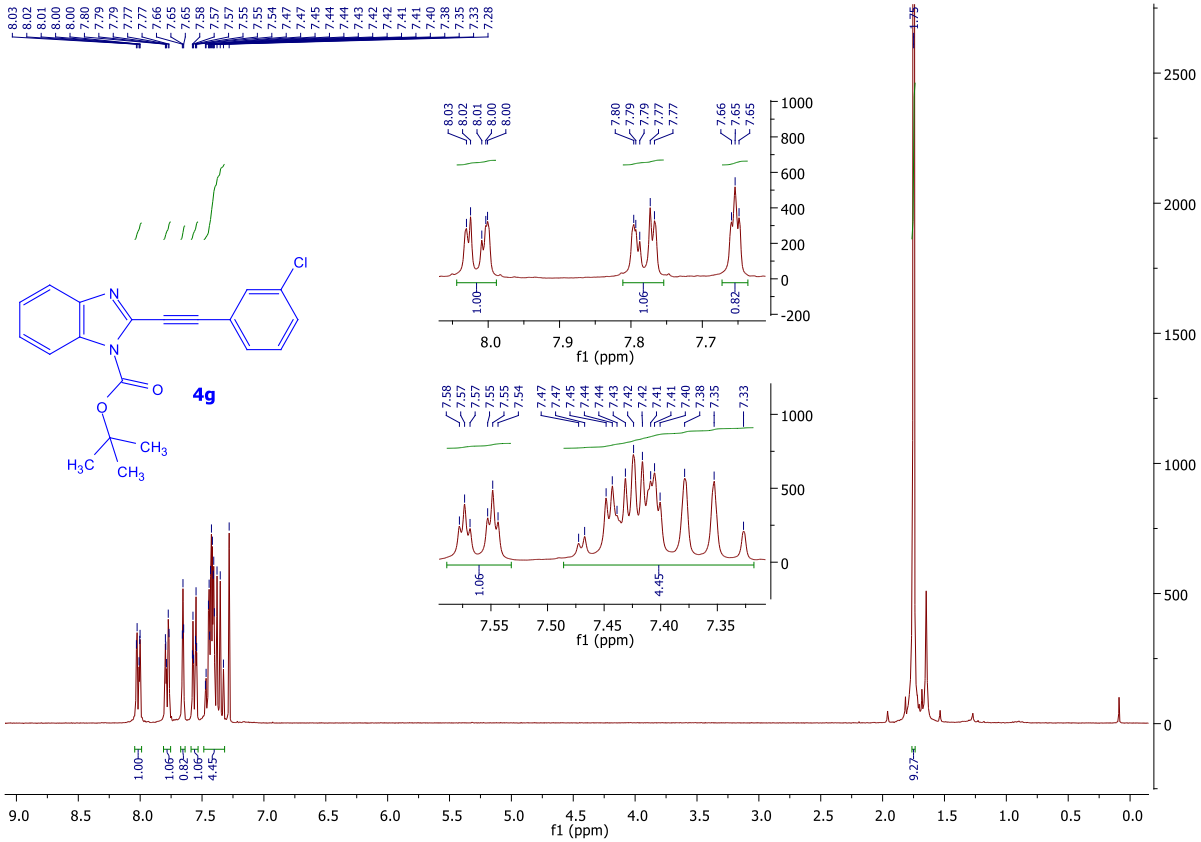

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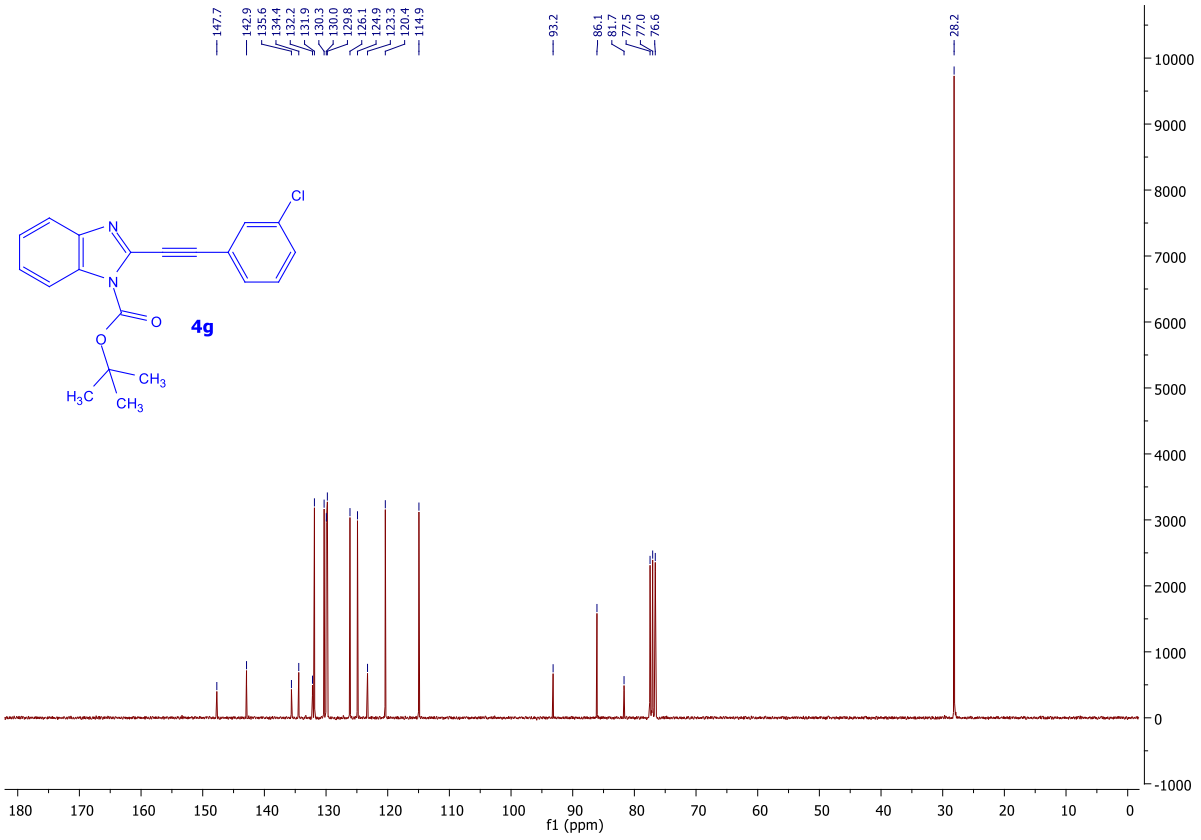

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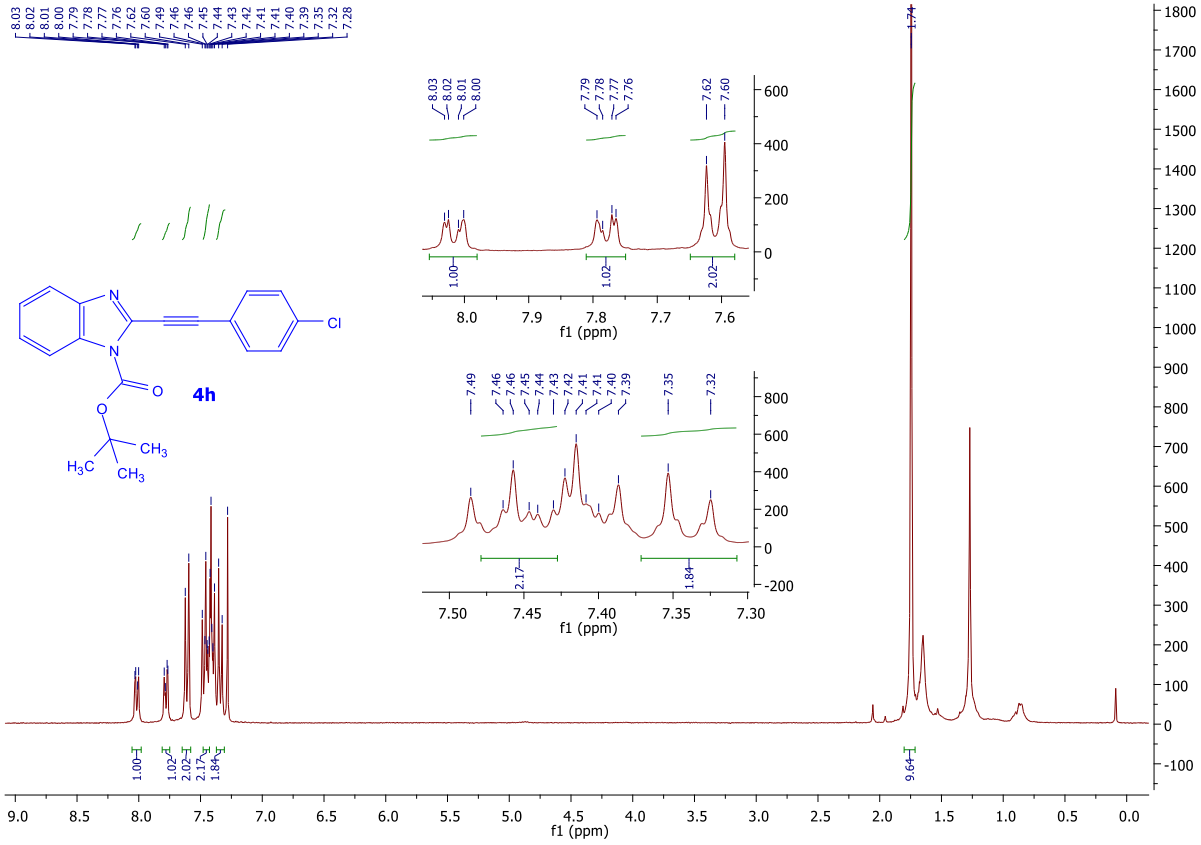
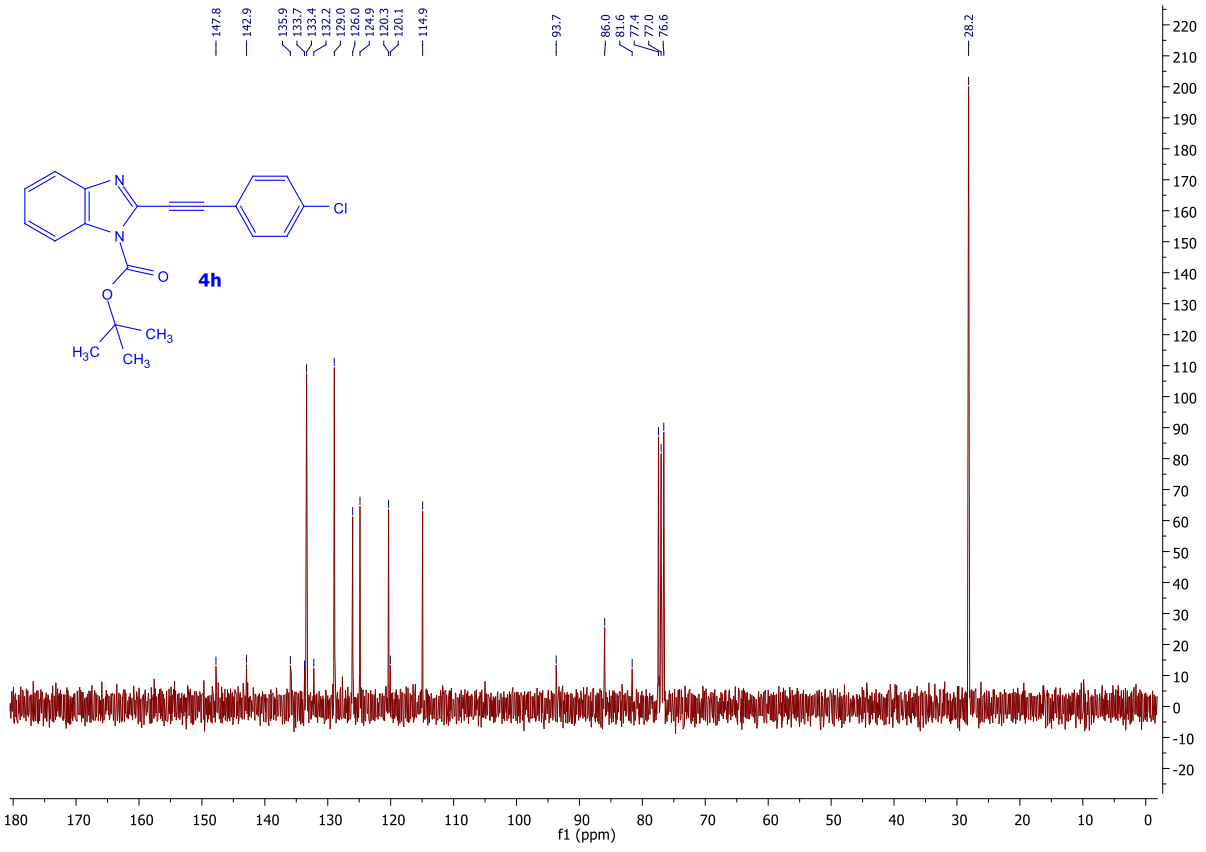


^{13}C NMR (75 MHz, $CDCl_3$) of **4h**



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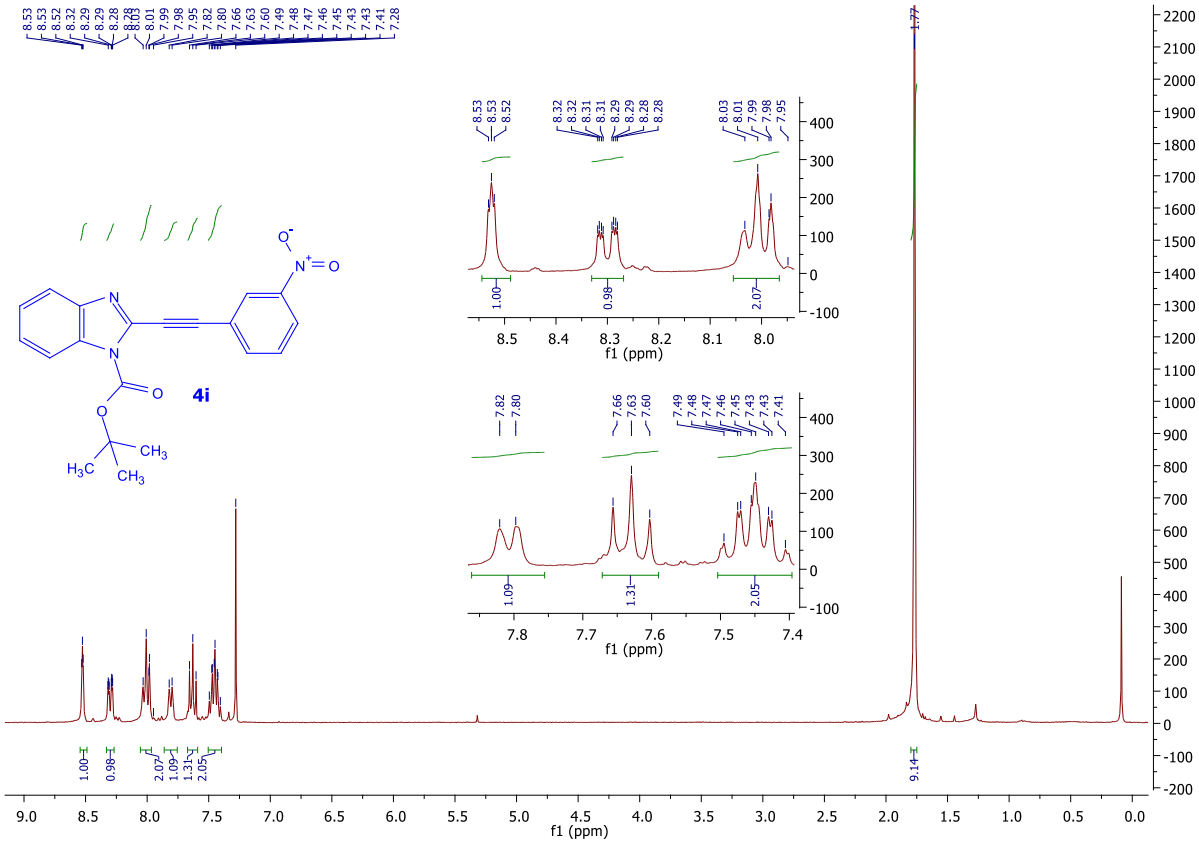

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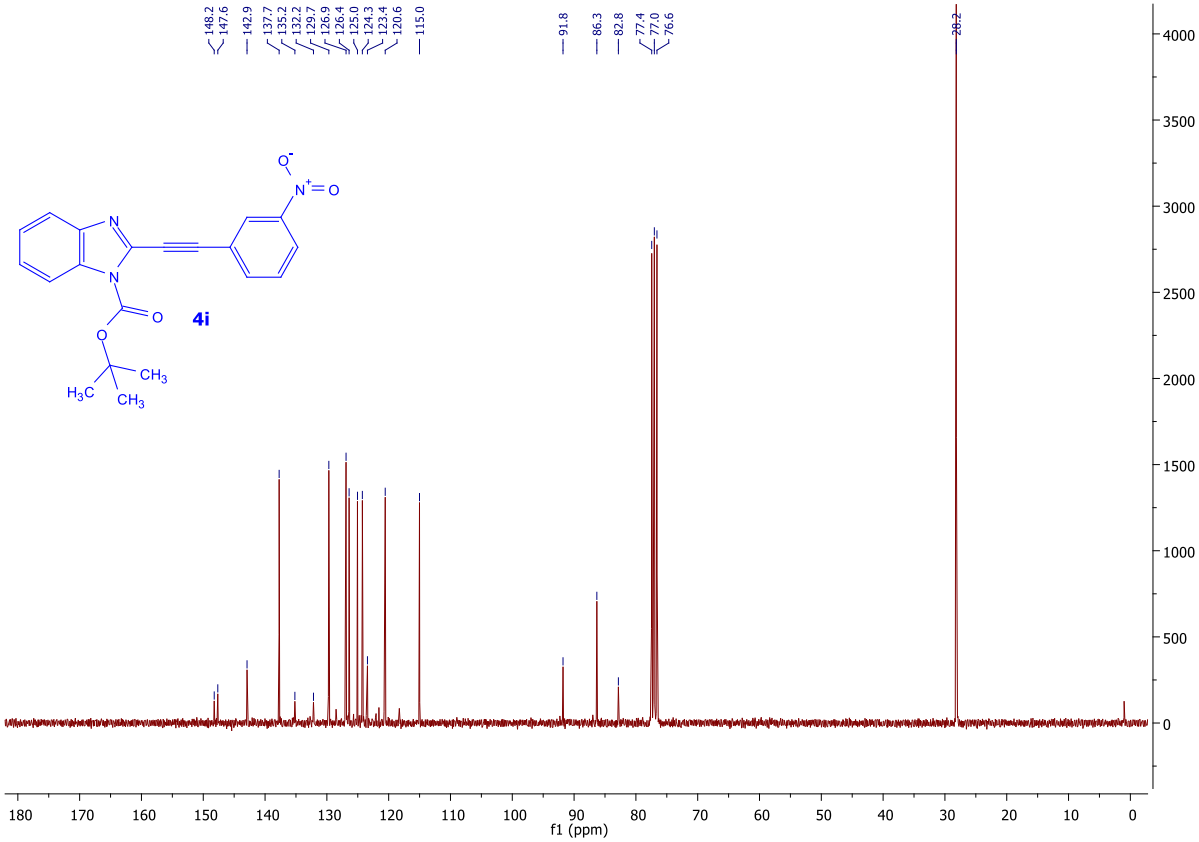

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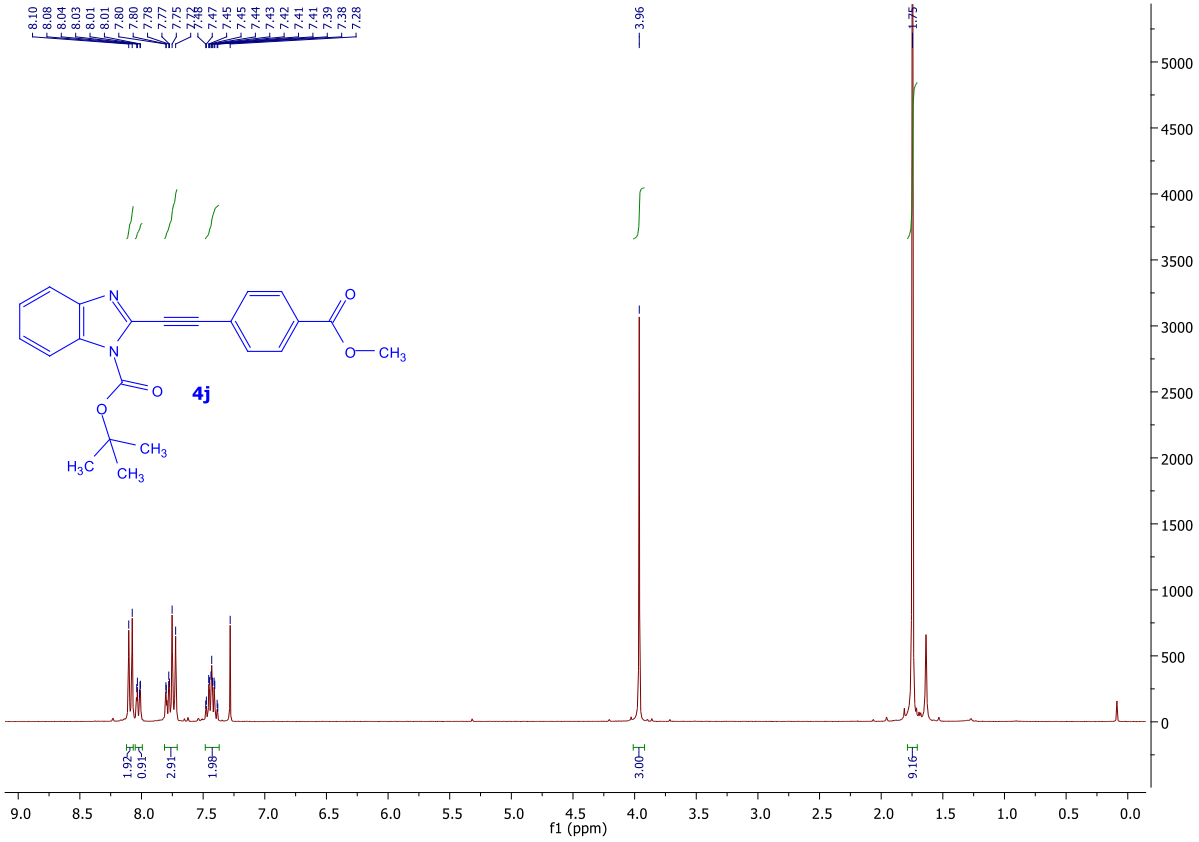

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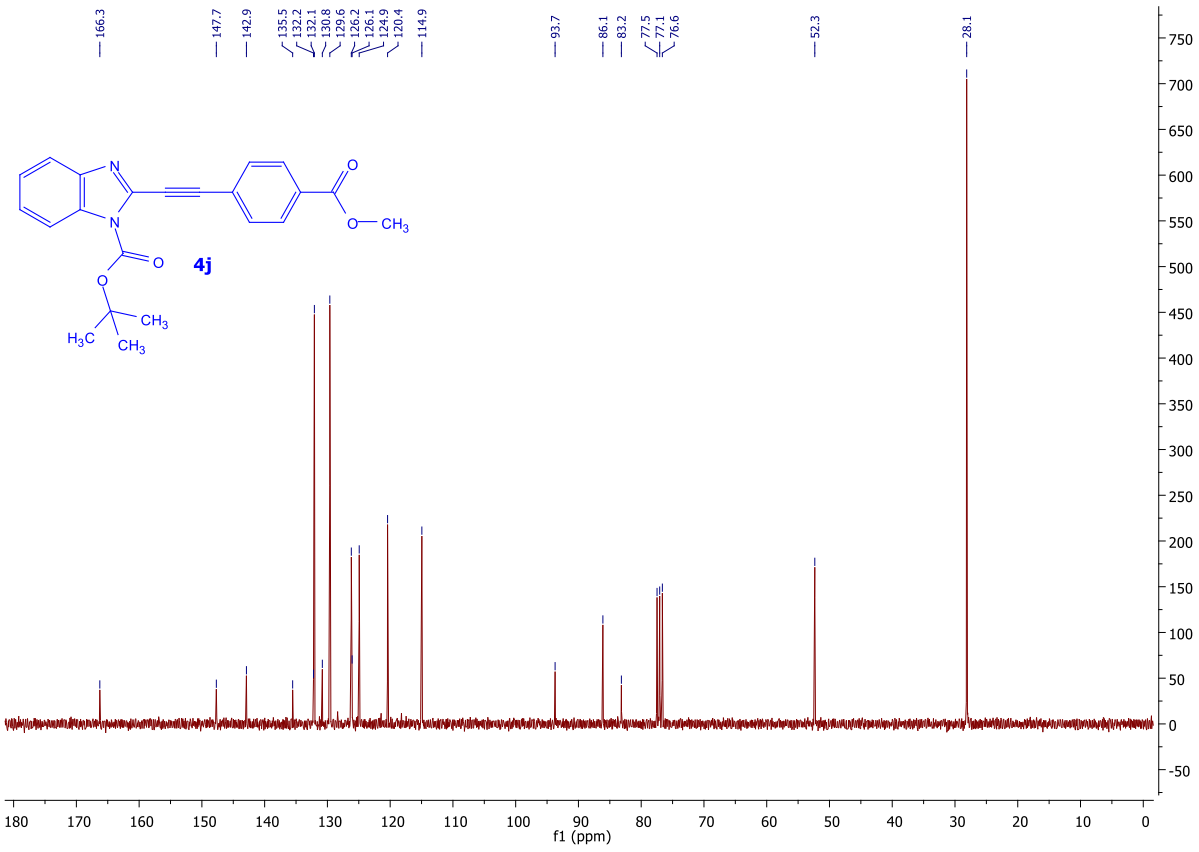
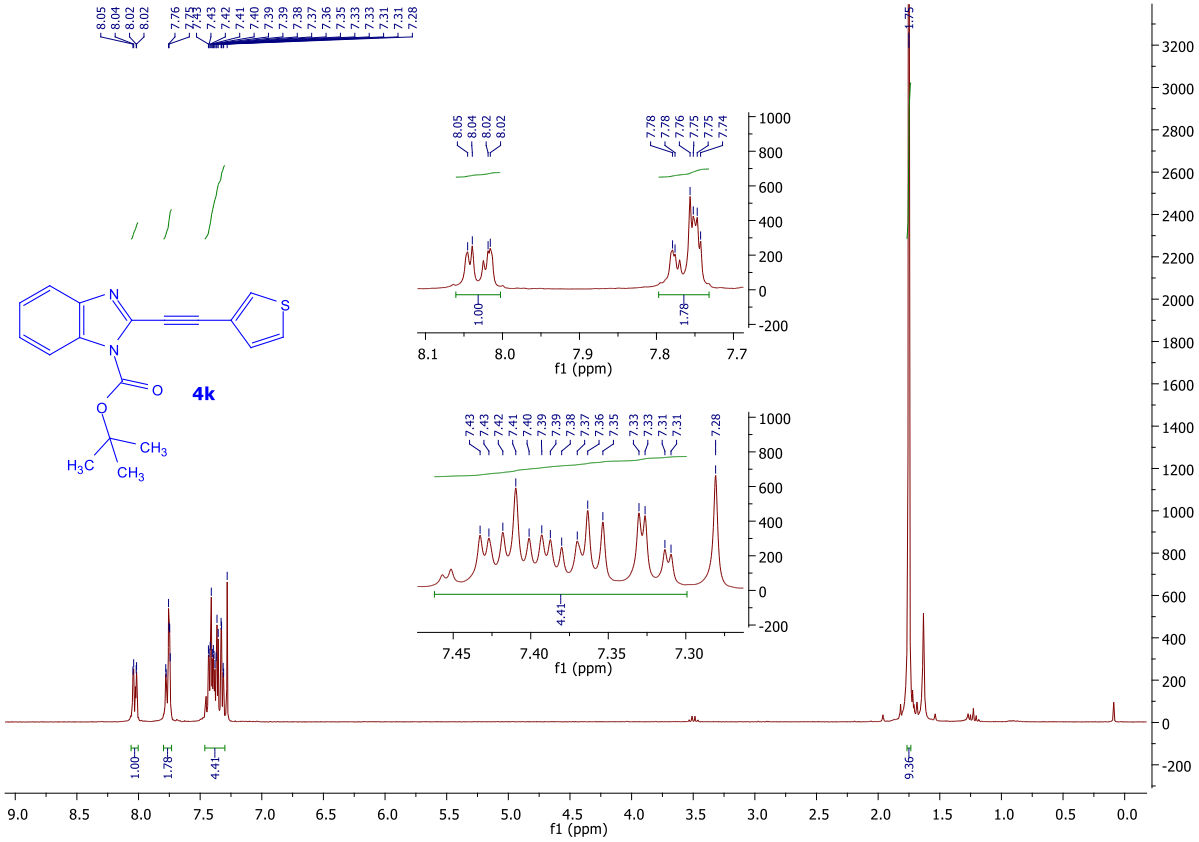
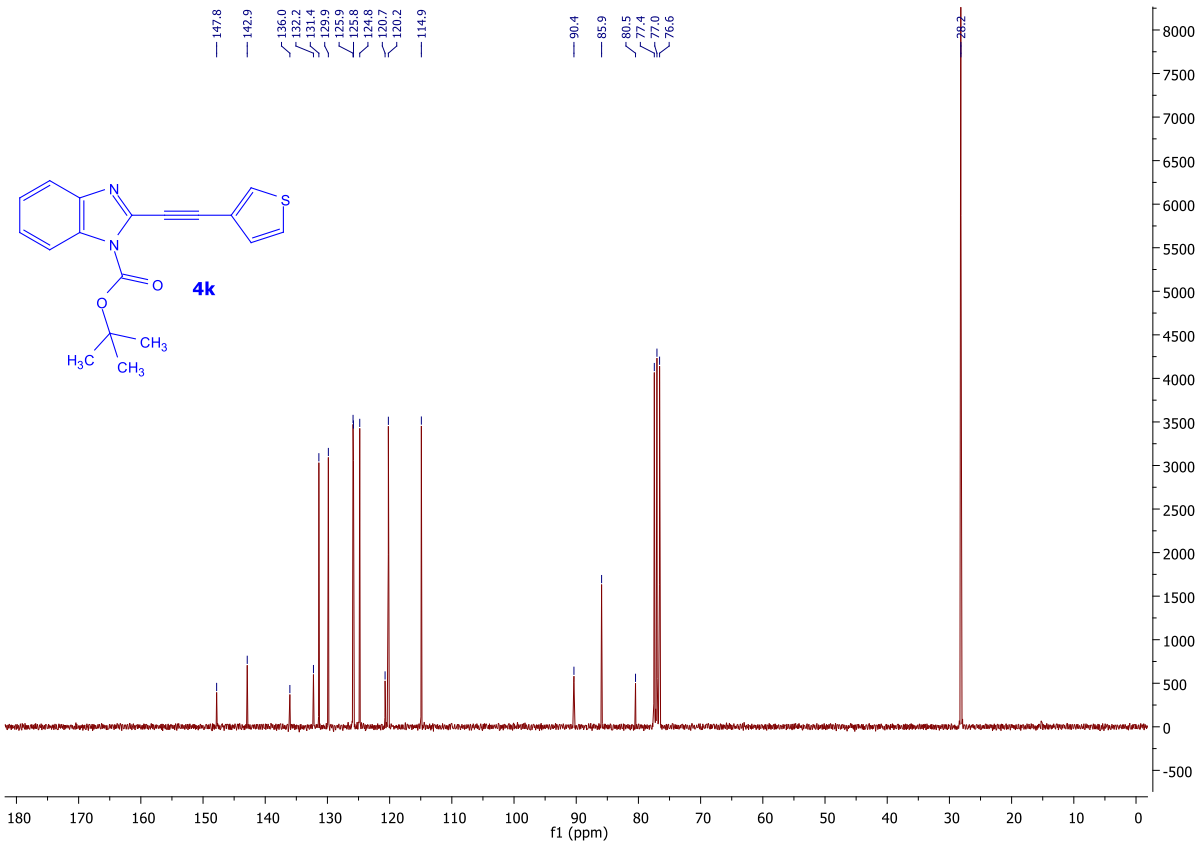


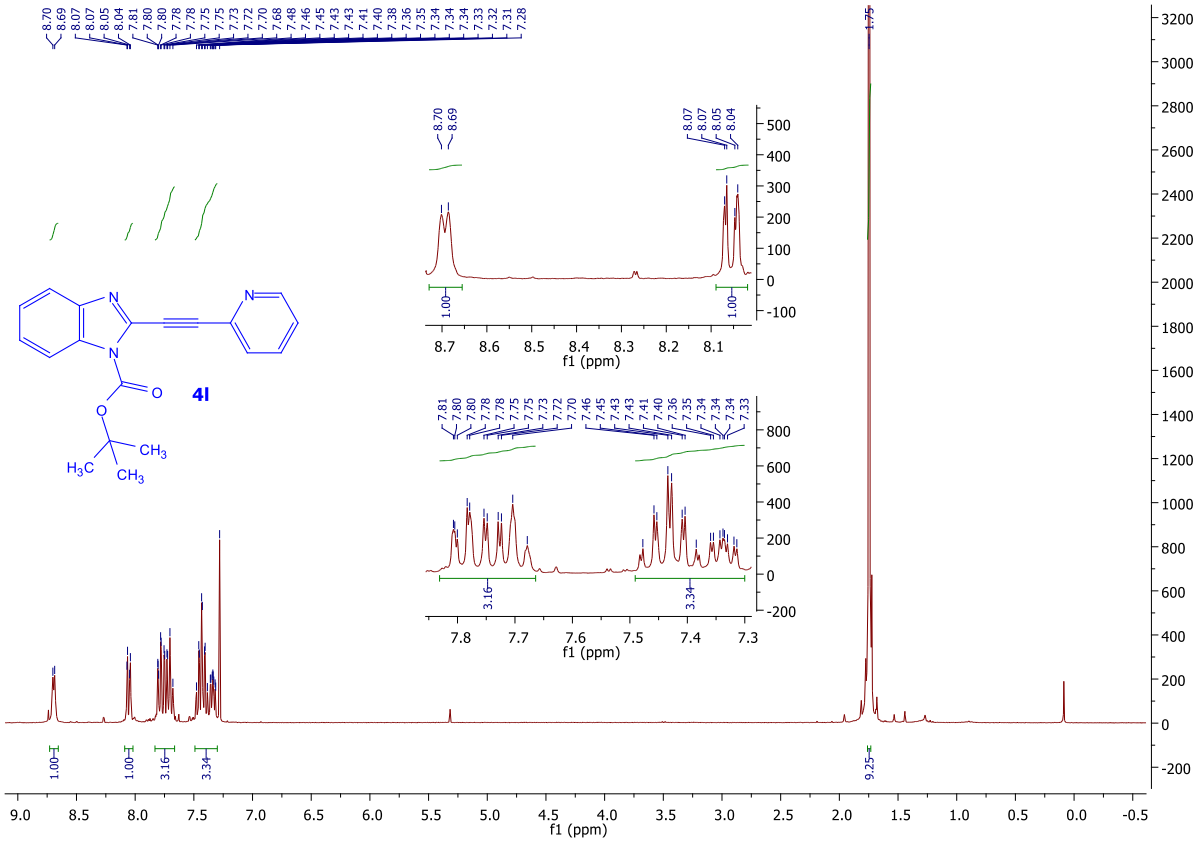
^{1}H NMR (300 MHz, $CDCl_3$) of **4k**



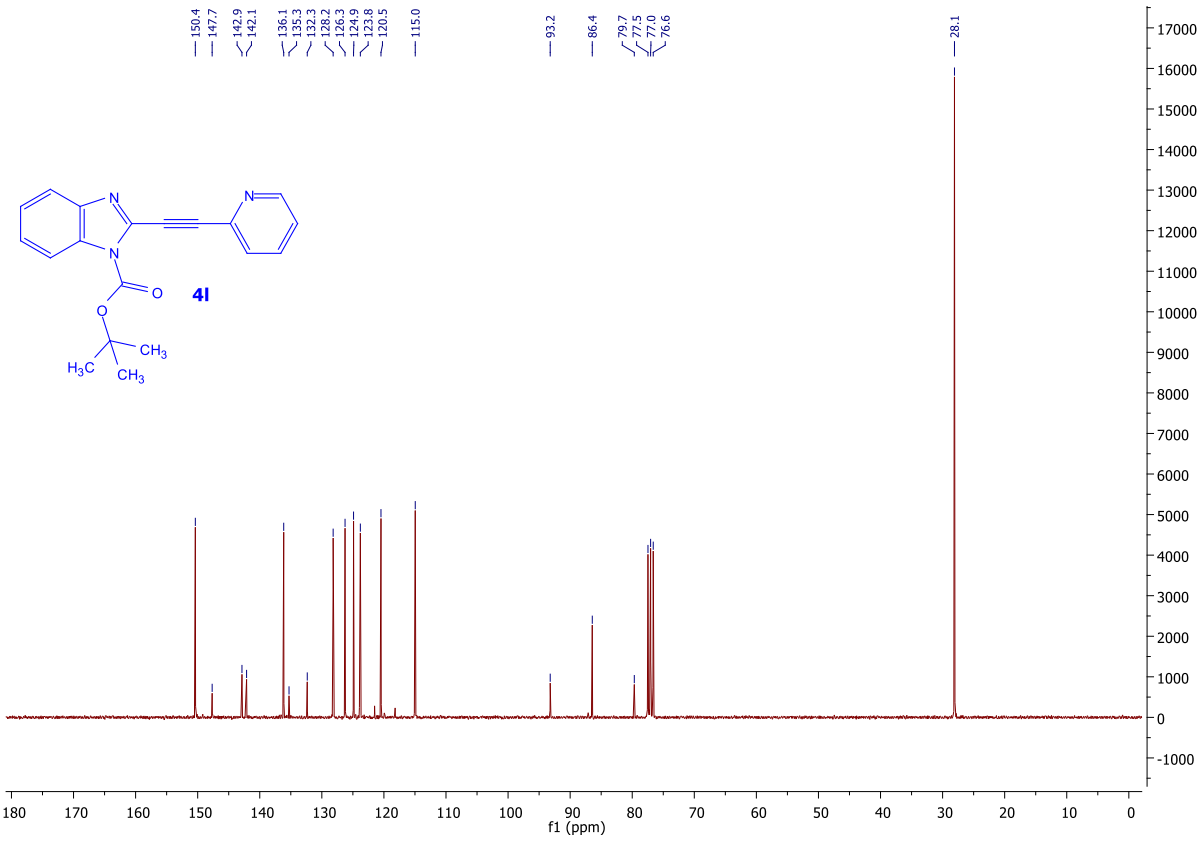
^{13}C NMR (75 MHz, $CDCl_3$) of **4k**



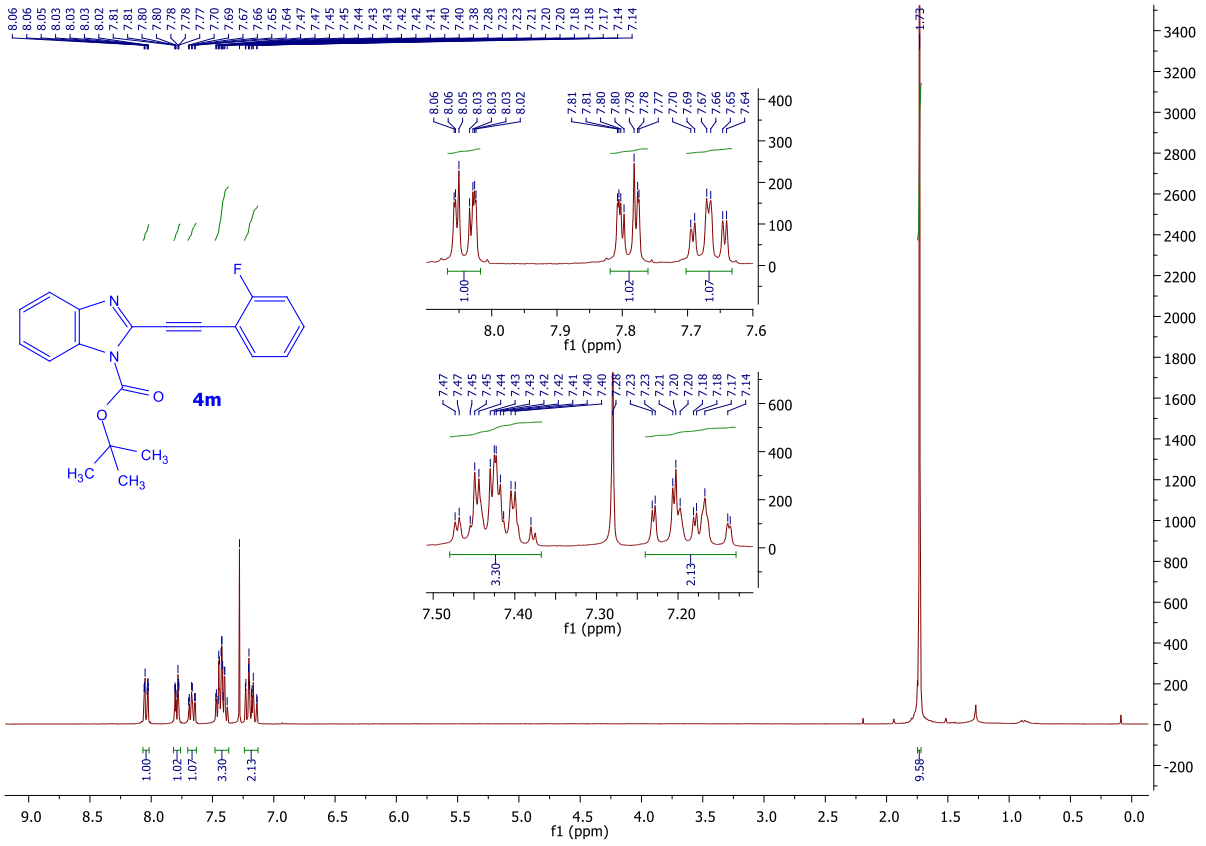
^{1}H NMR (300 MHz, $CDCl_3$) of **4l**



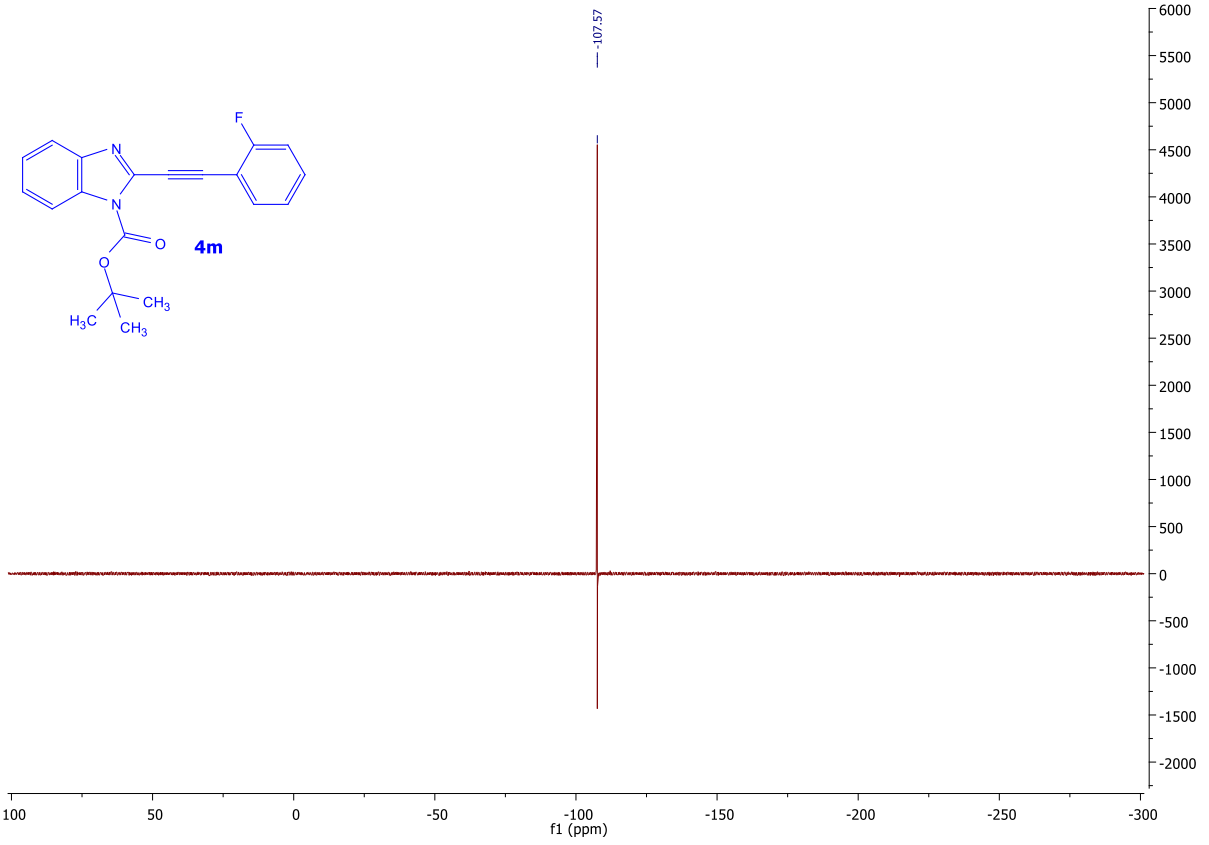
^{13}C NMR (75 MHz, $CDCl_3$) of **4l**



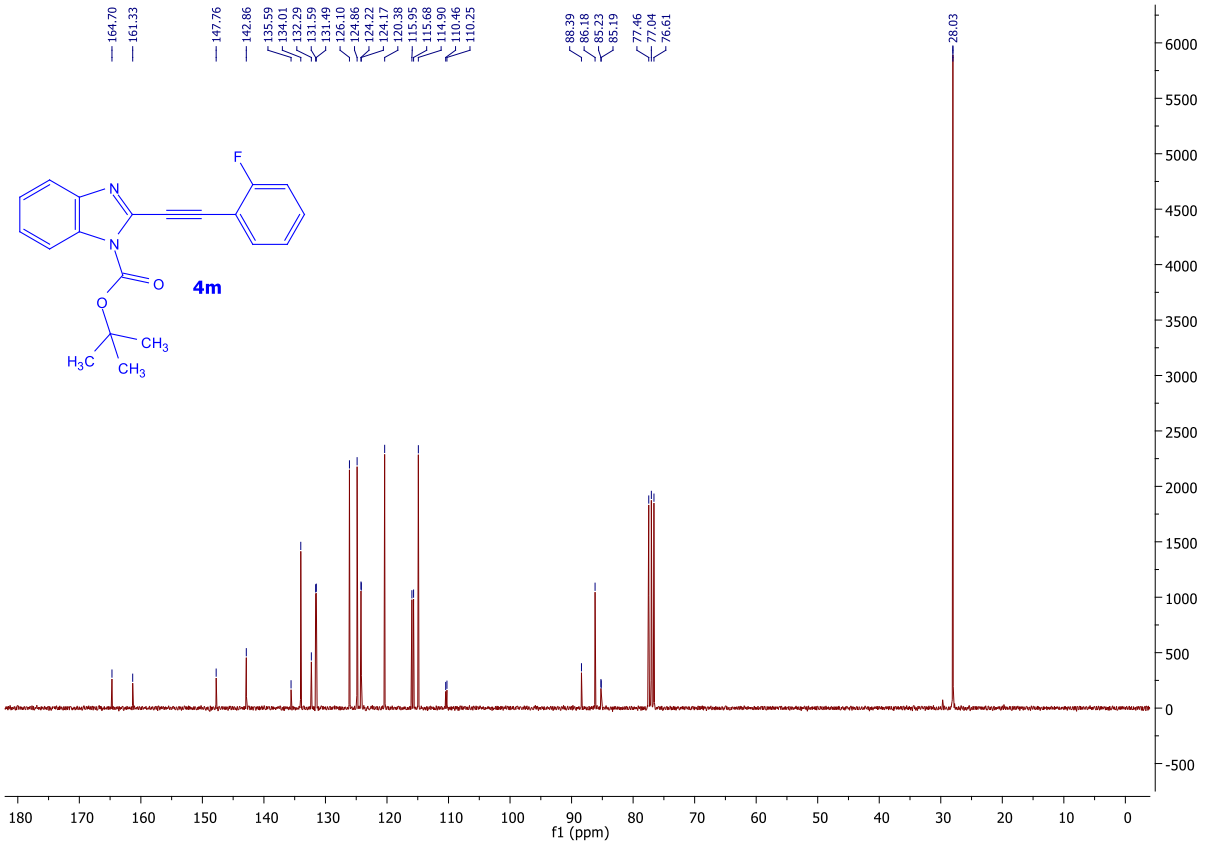
^{1}H NMR (300 MHz, $CDCl_3$) of **4m**



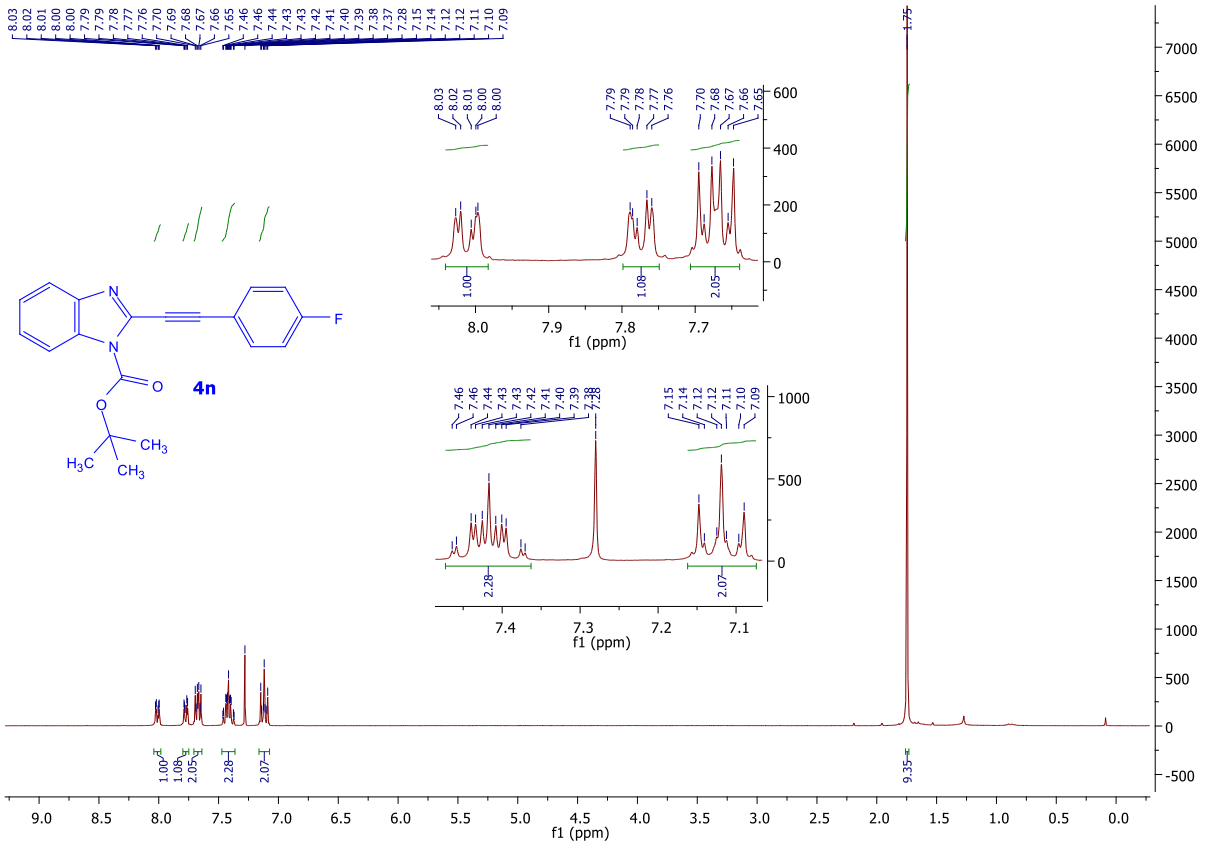
^{19}F NMR (282 MHz, $CDCl_3$) of **4m**



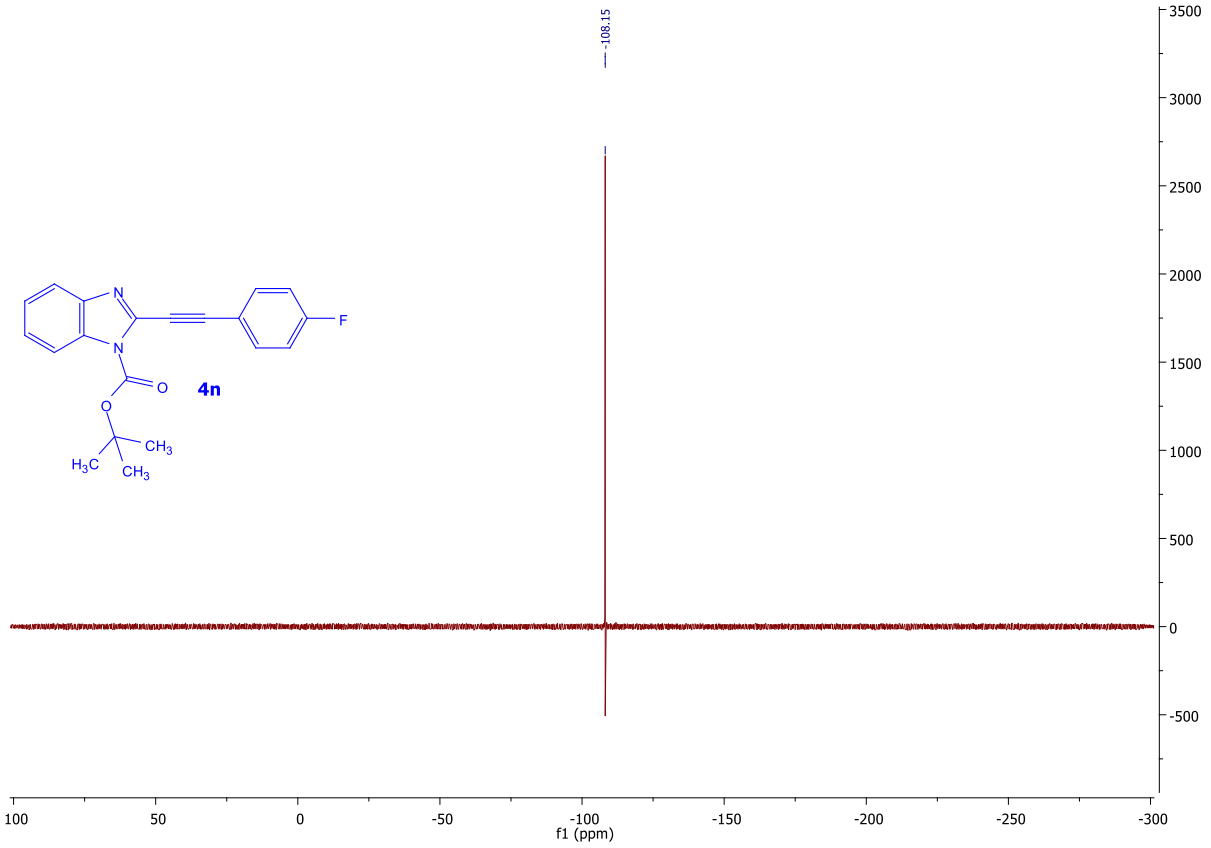
^{13}C NMR (75 MHz, $CDCl_3$) of **4m**



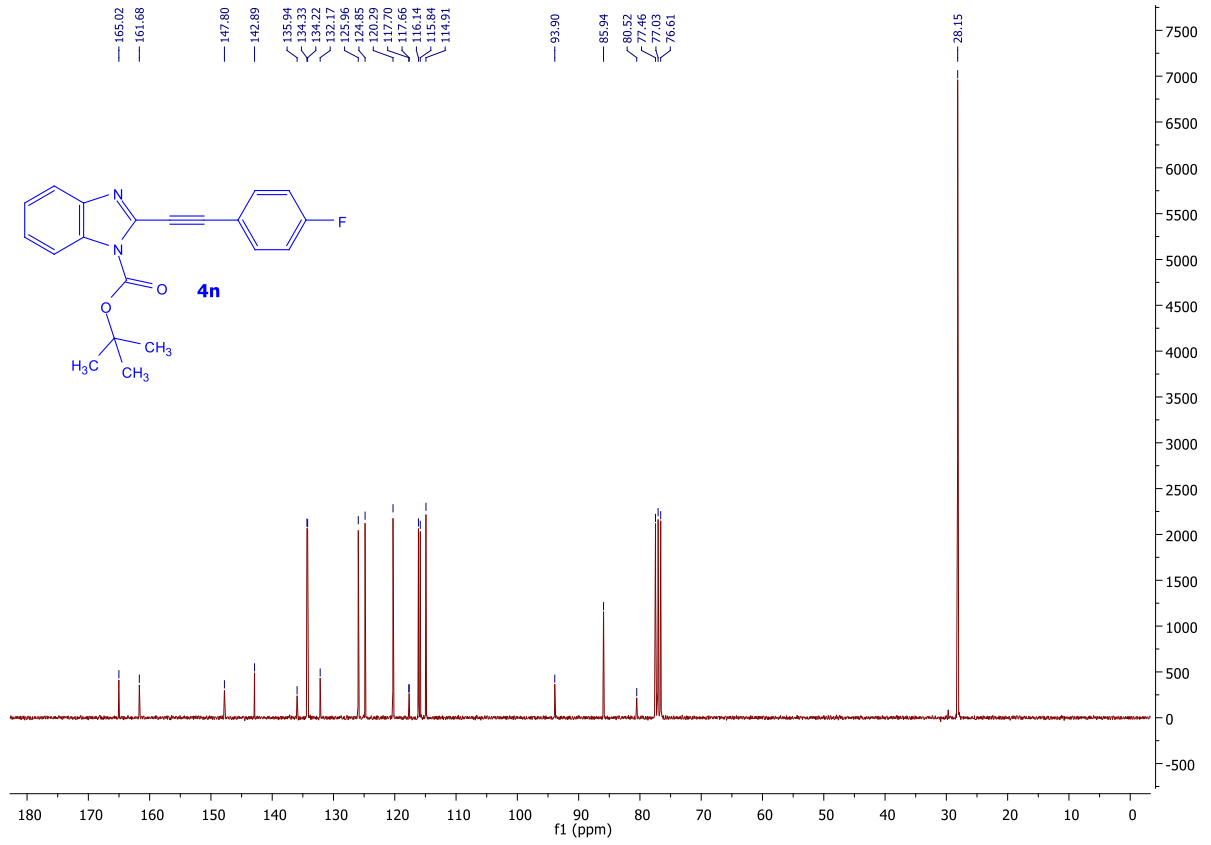
^{1}H NMR (300 MHz, $CDCl_3$) of **4n**



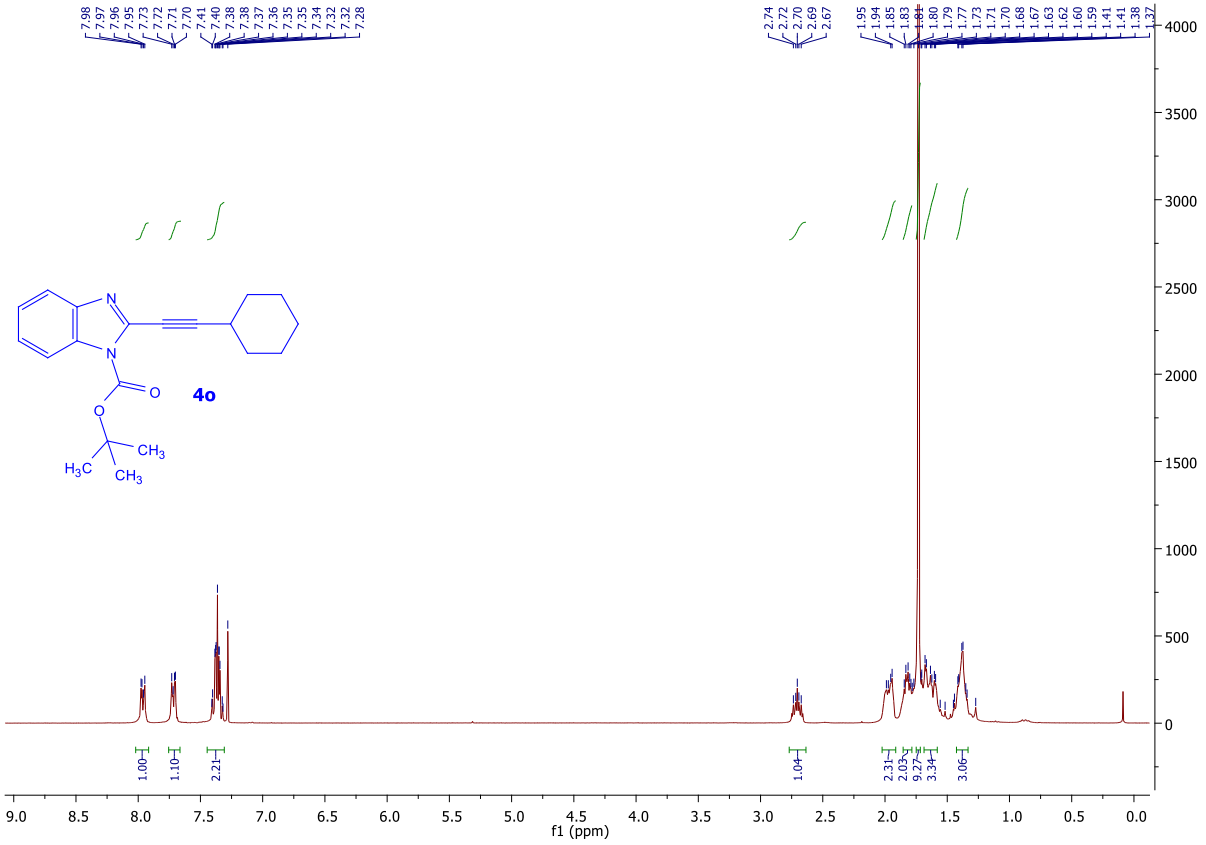
^{19}F NMR (282 MHz, $CDCl_3$) of **4n**



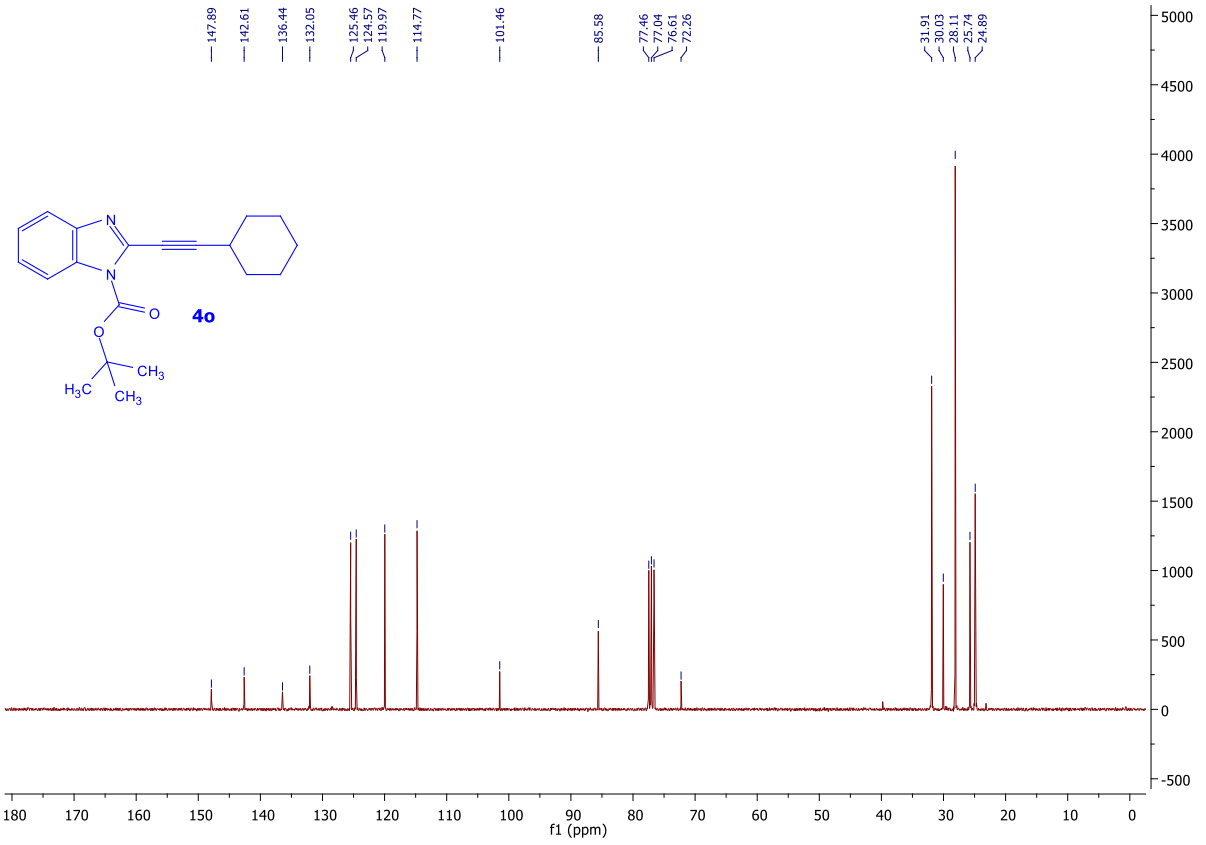
^{13}C NMR (75 MHz, $CDCl_3$) of **4n**



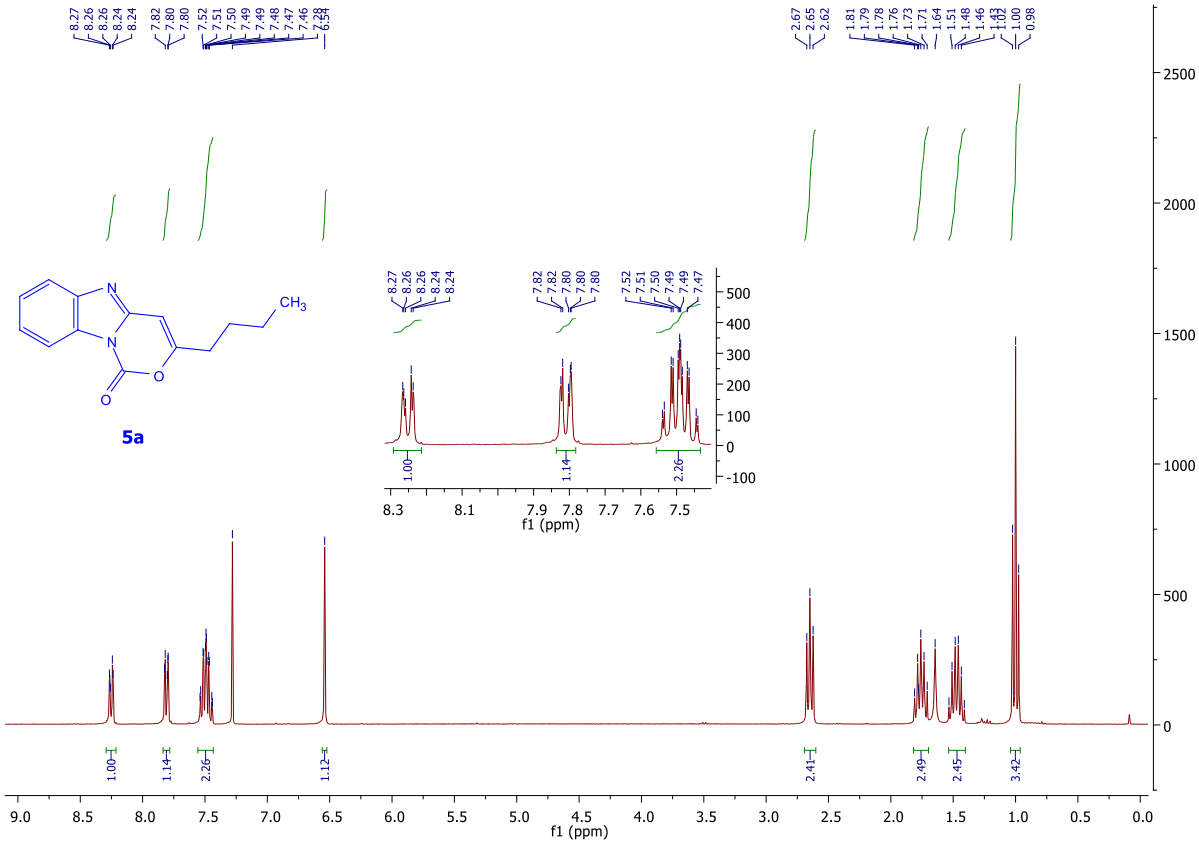
^{1}H NMR (300 MHz, $CDCl_3$) of **4o**



^{13}C NMR (75 MHz, $CDCl_3$) of **4o**



^{1}H NMR (300 MHz, $CDCl_3$) of **5a**



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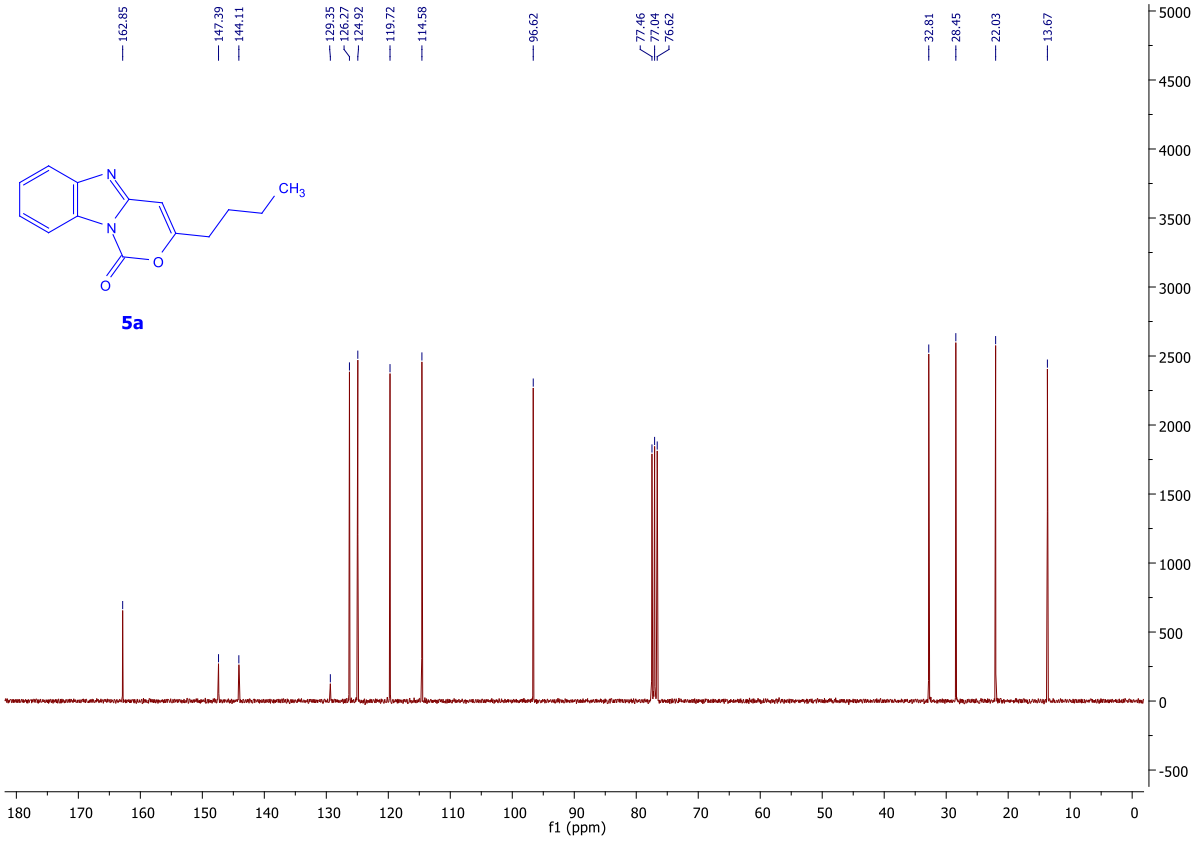

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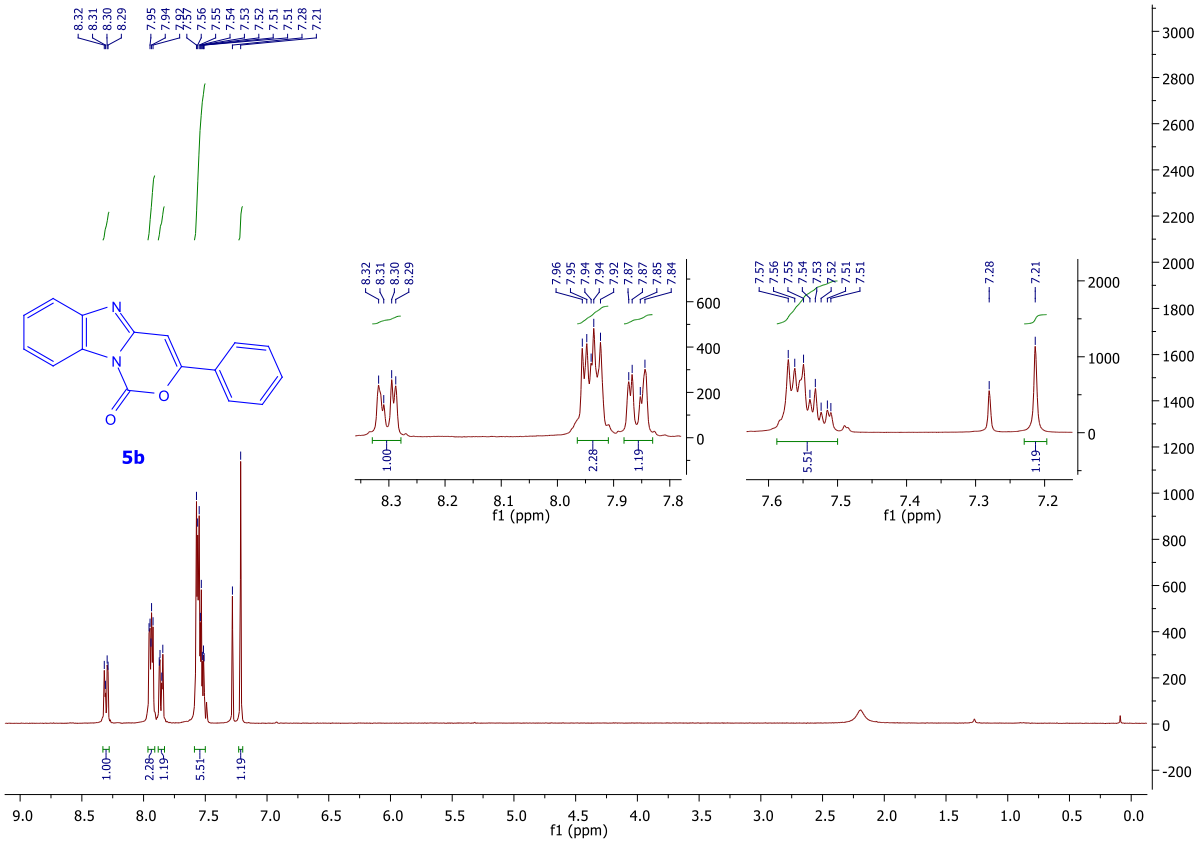
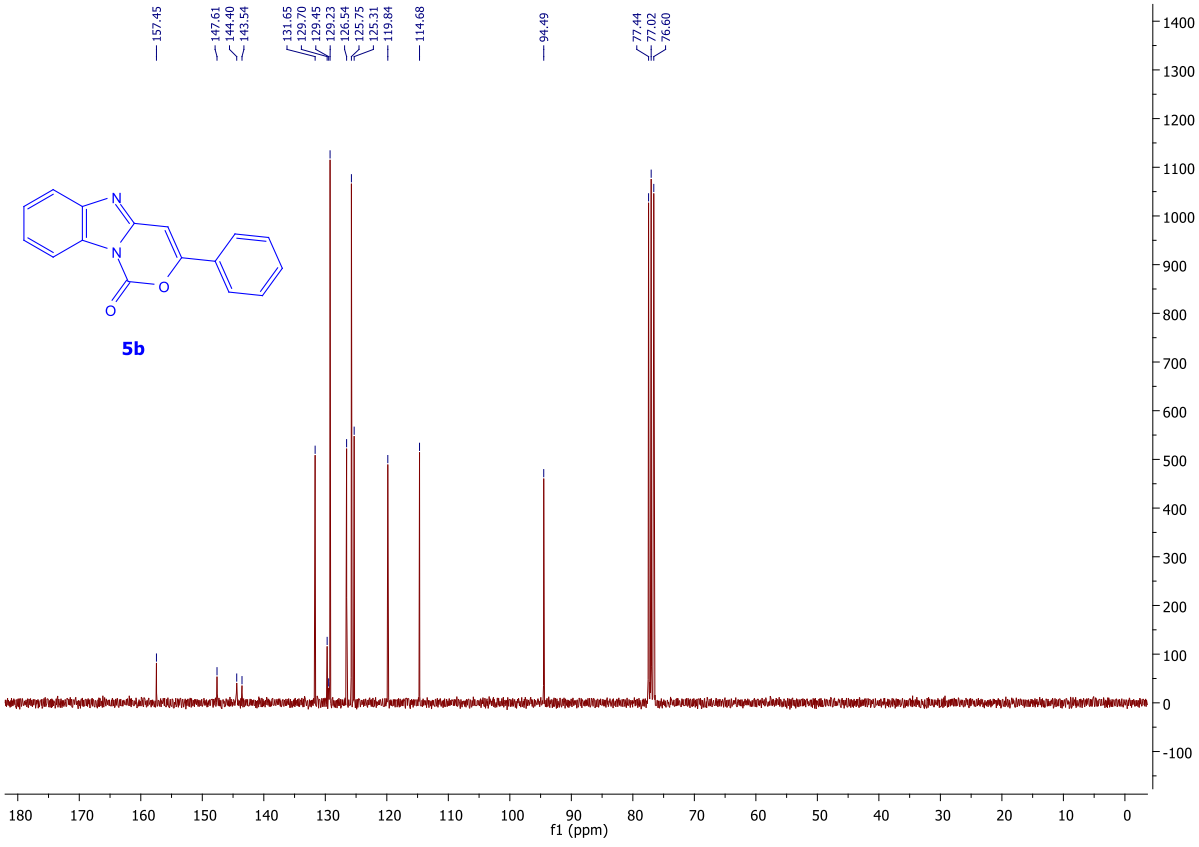


^{13}C NMR (75 MHz, $CDCl_3$) of **5b**



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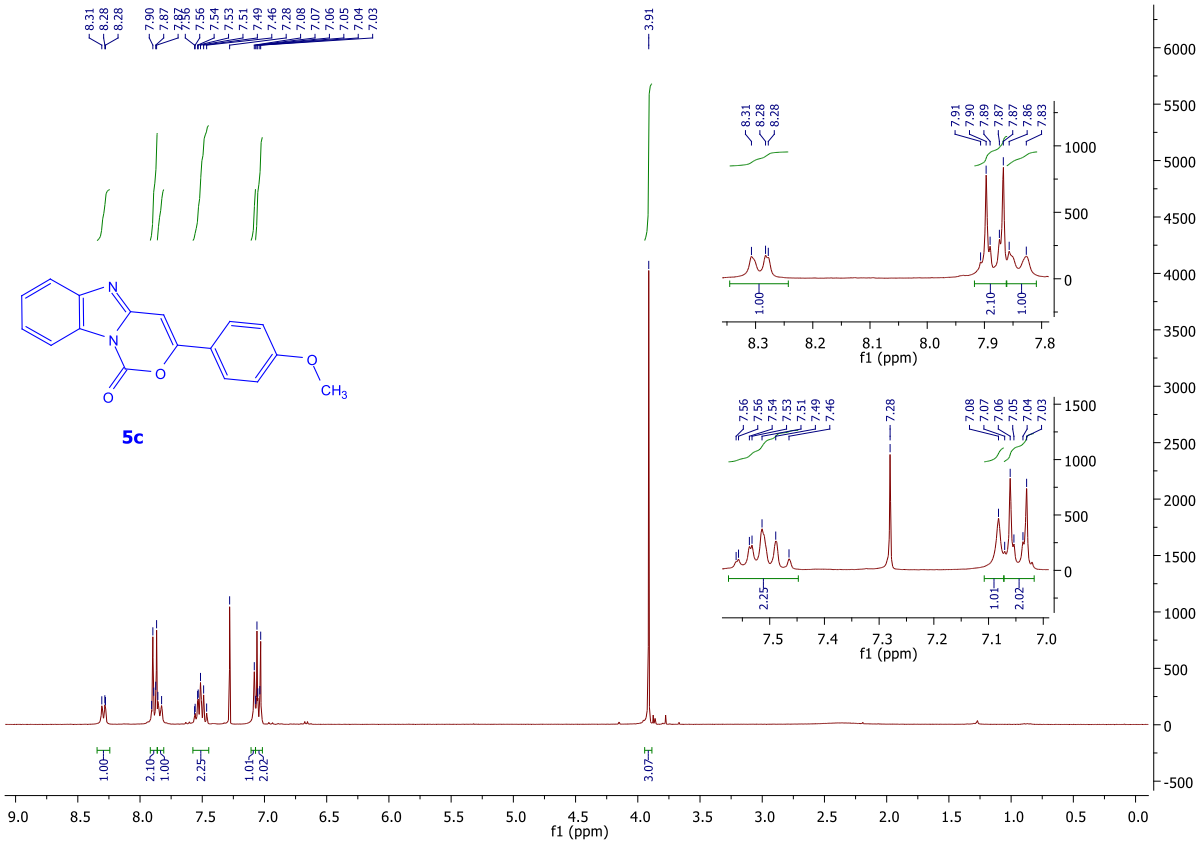

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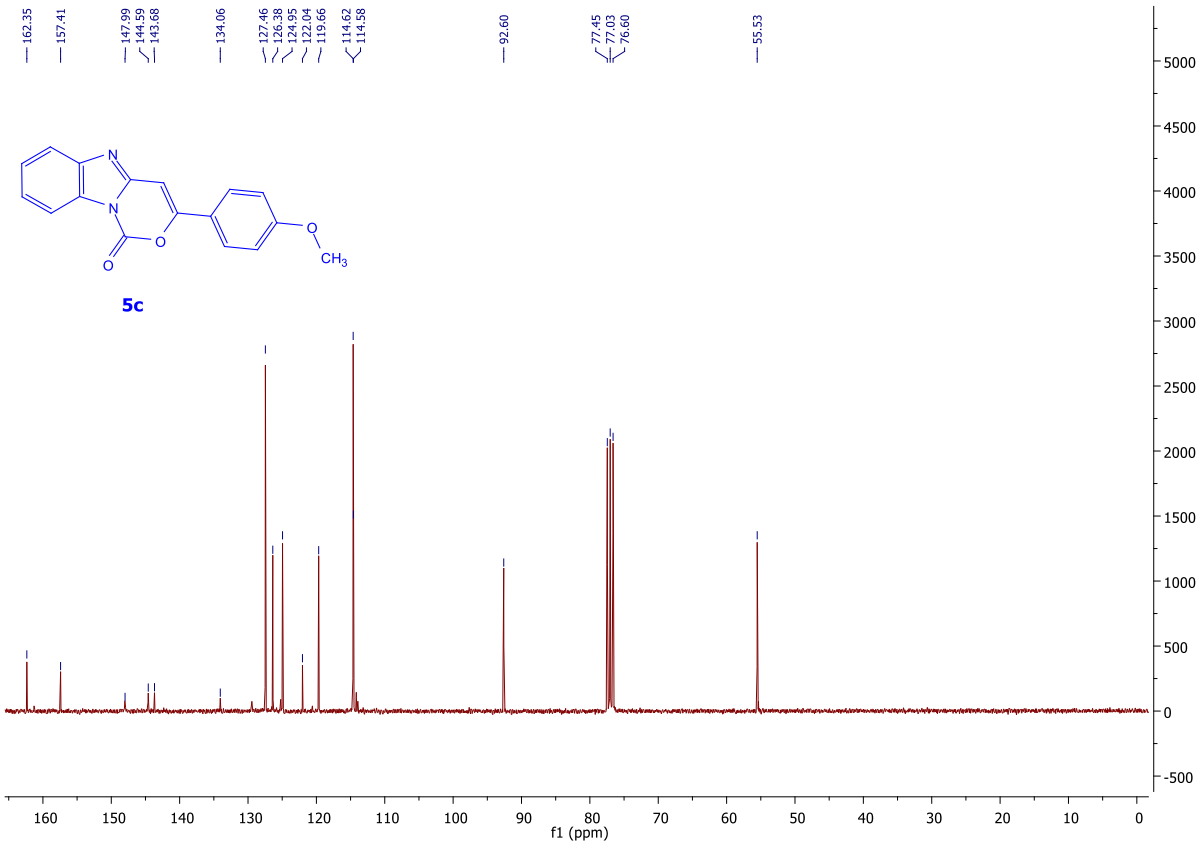

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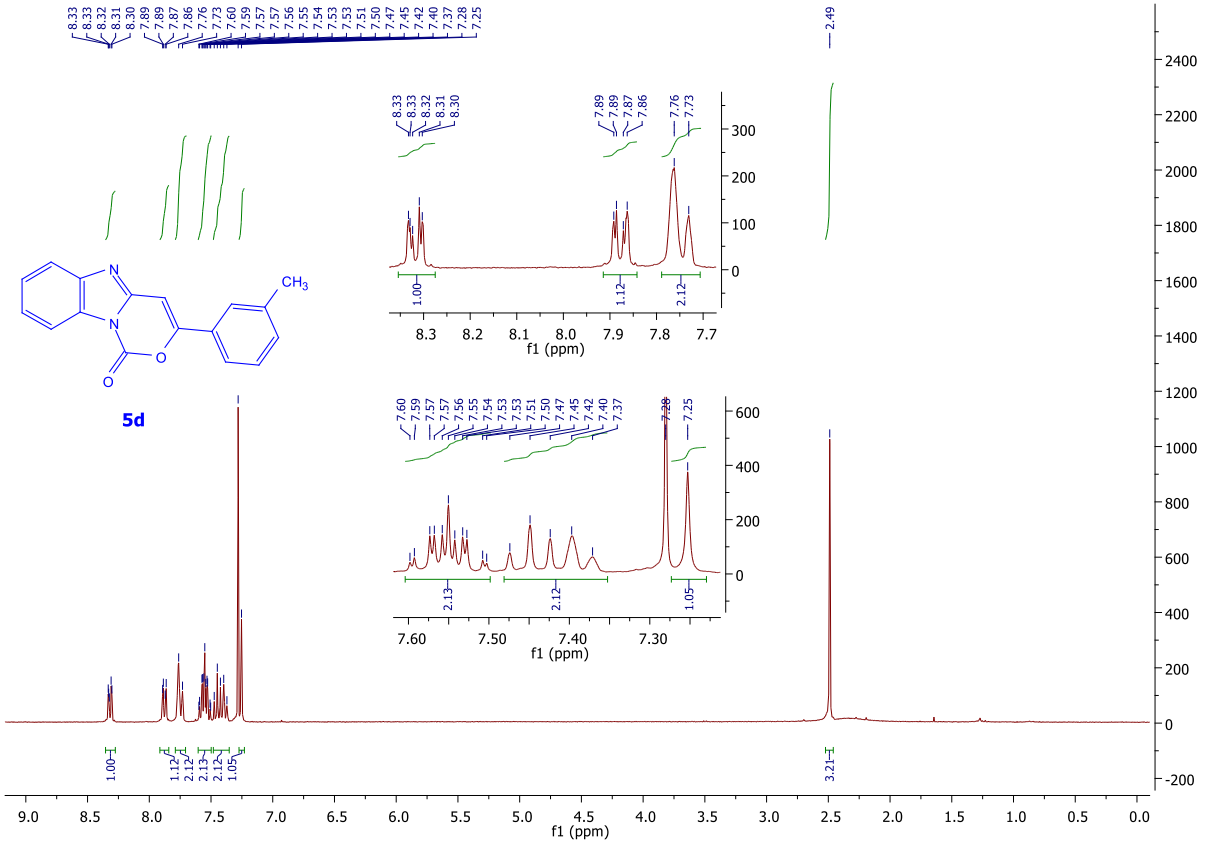

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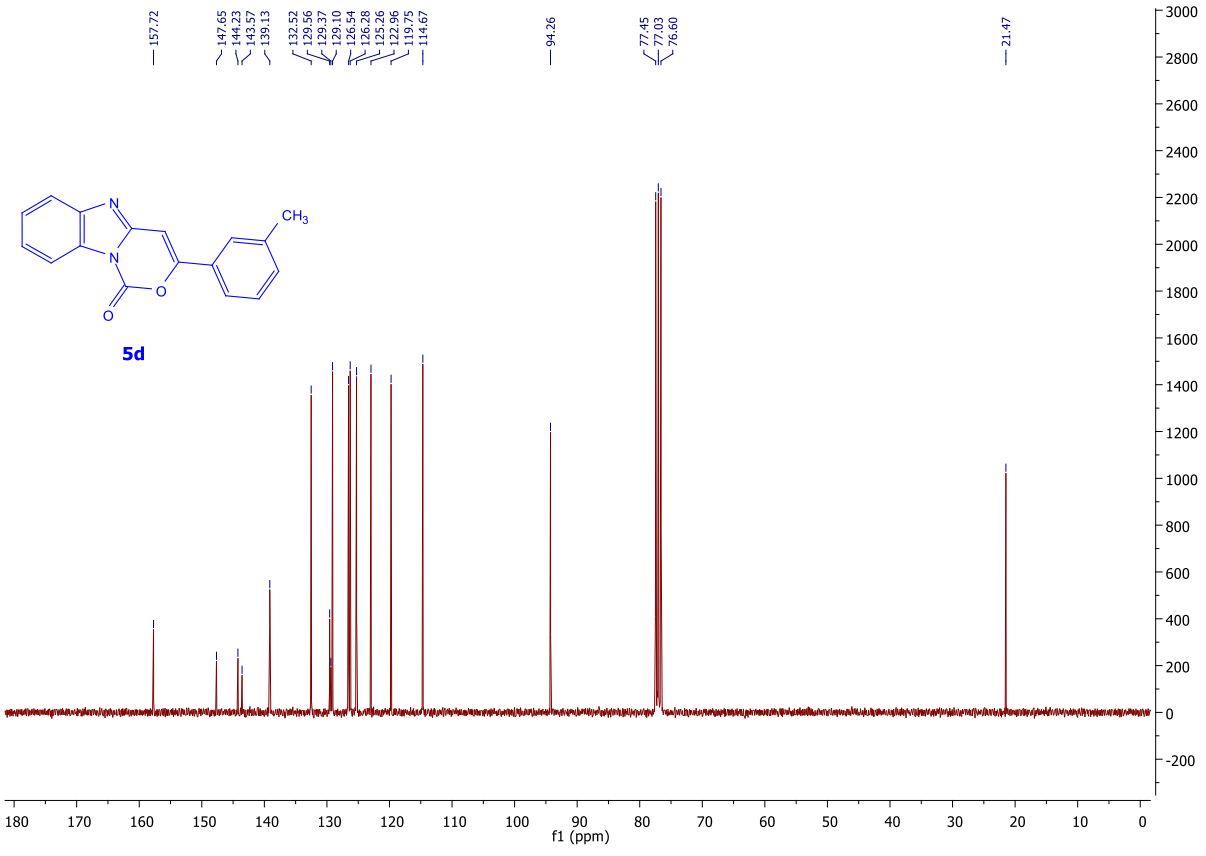

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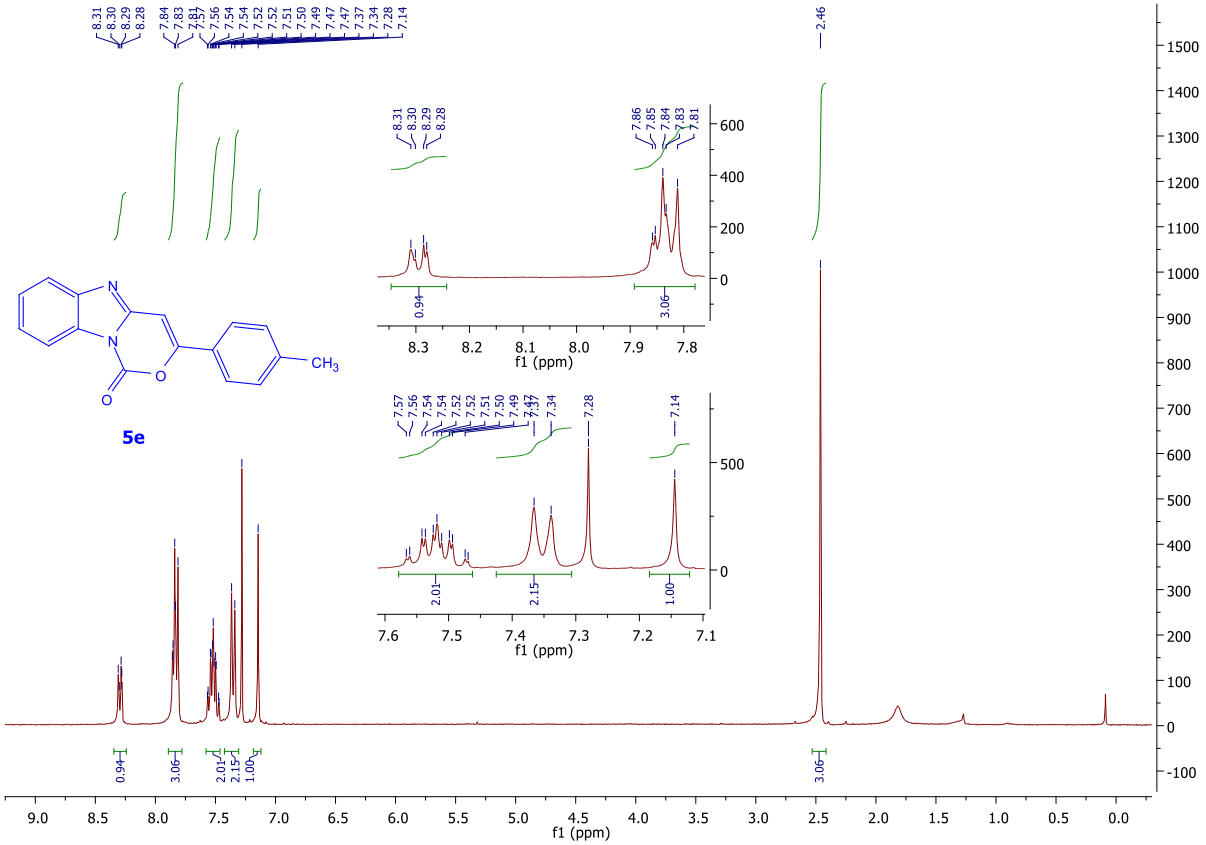

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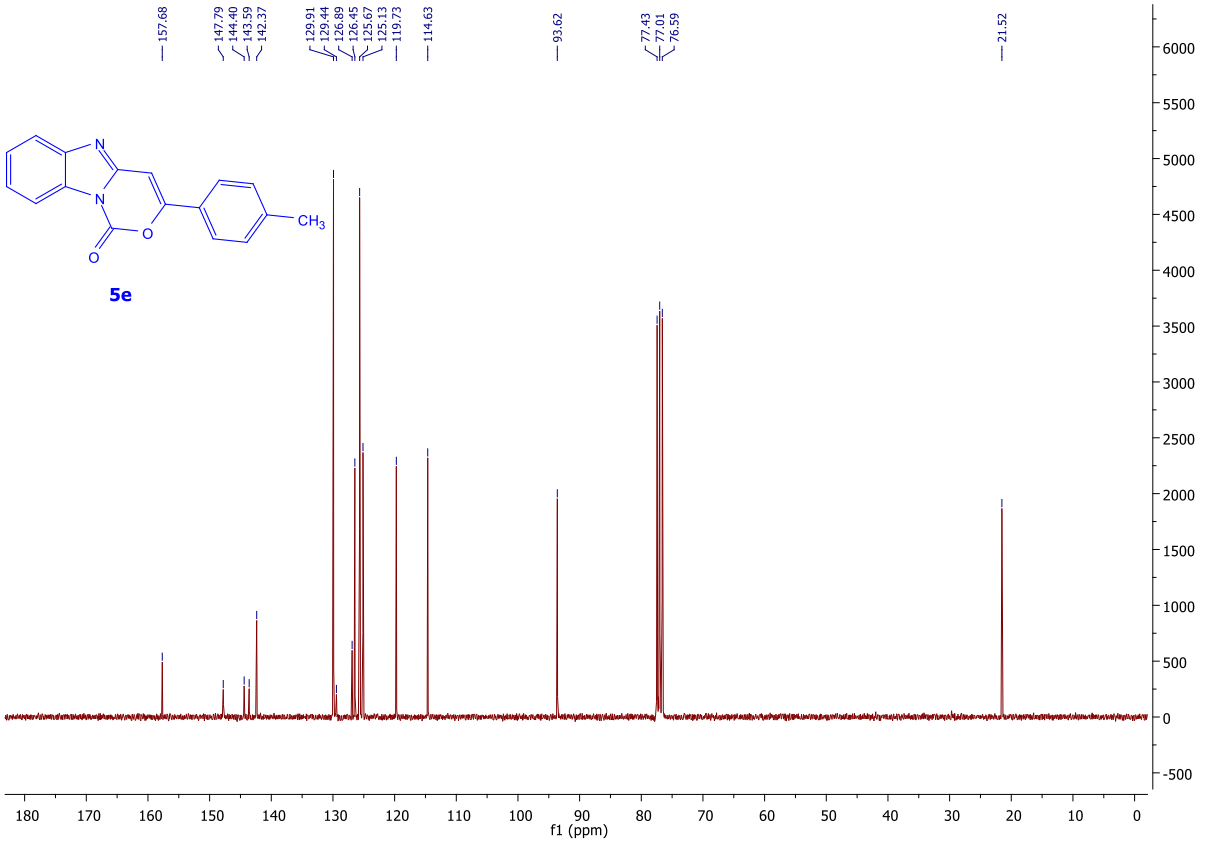
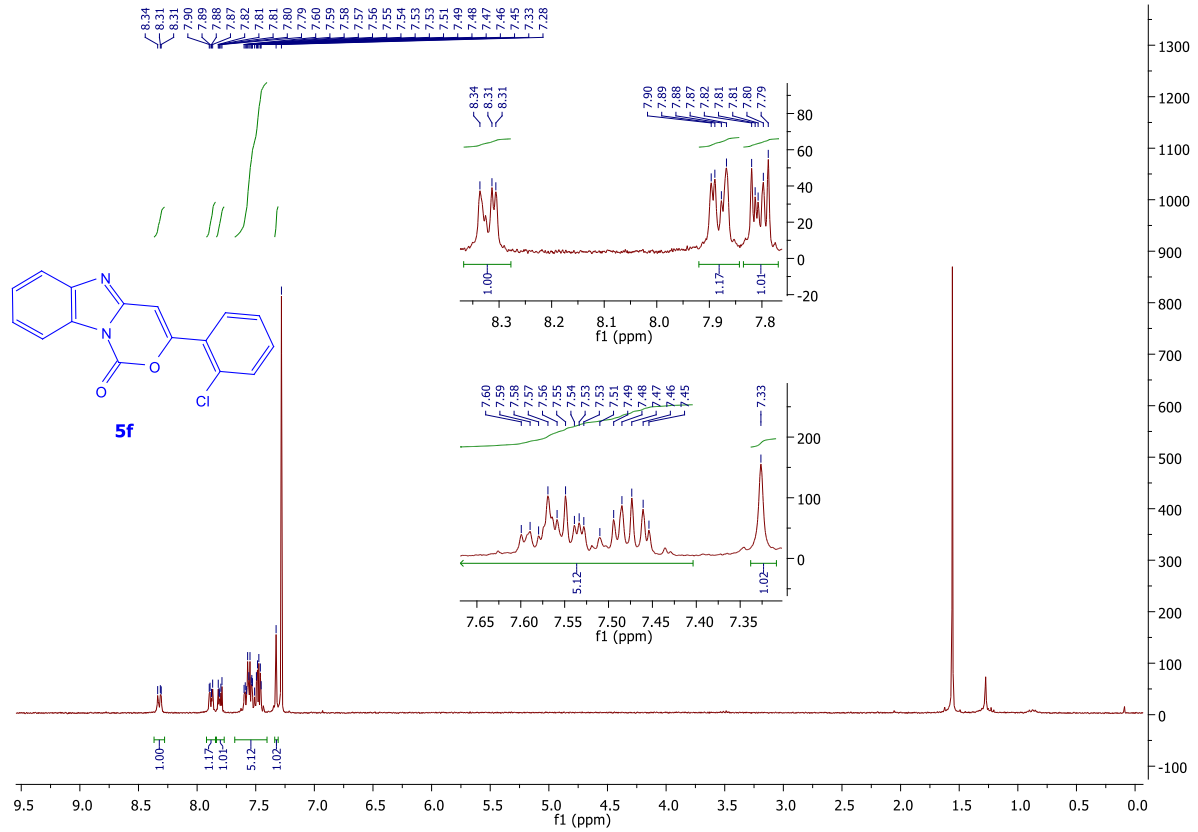
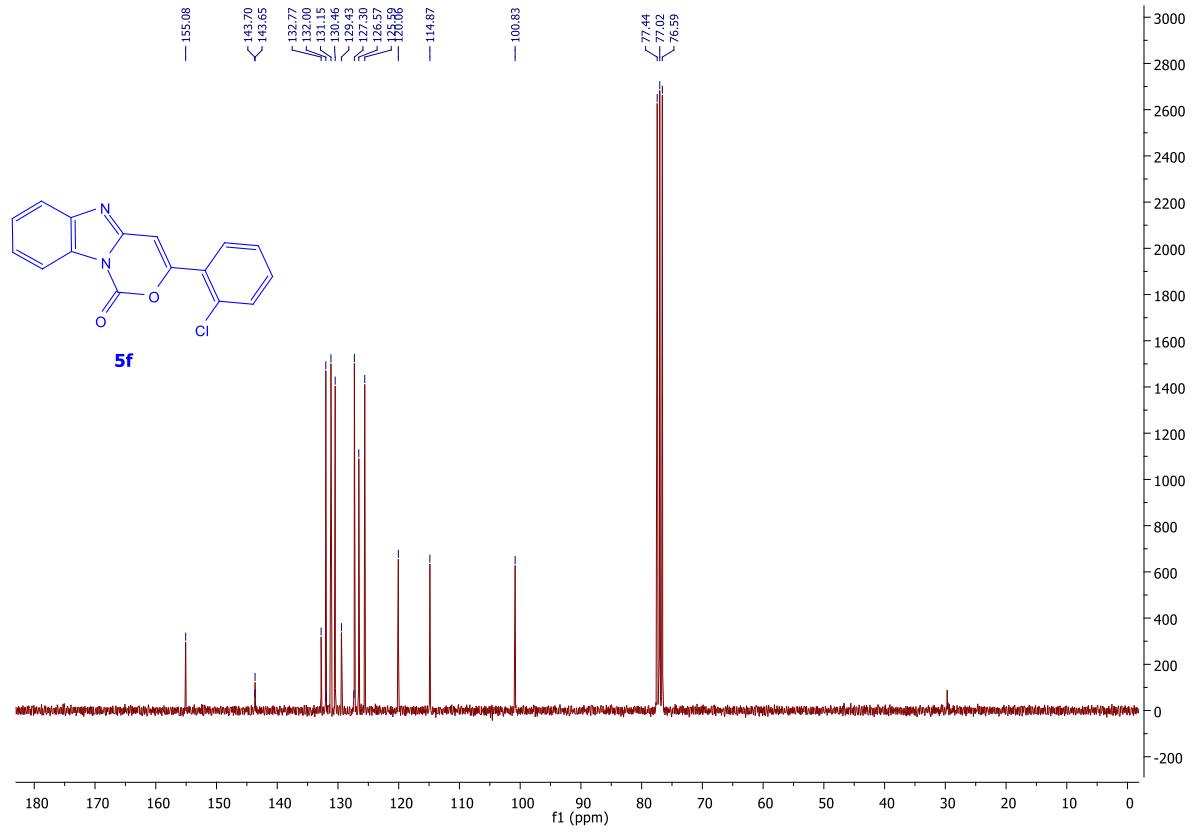


^{1}H NMR (300 MHz, $CDCl_3$) of **5f**



^{13}C NMR (75 MHz, $CDCl_3$) of **5f**



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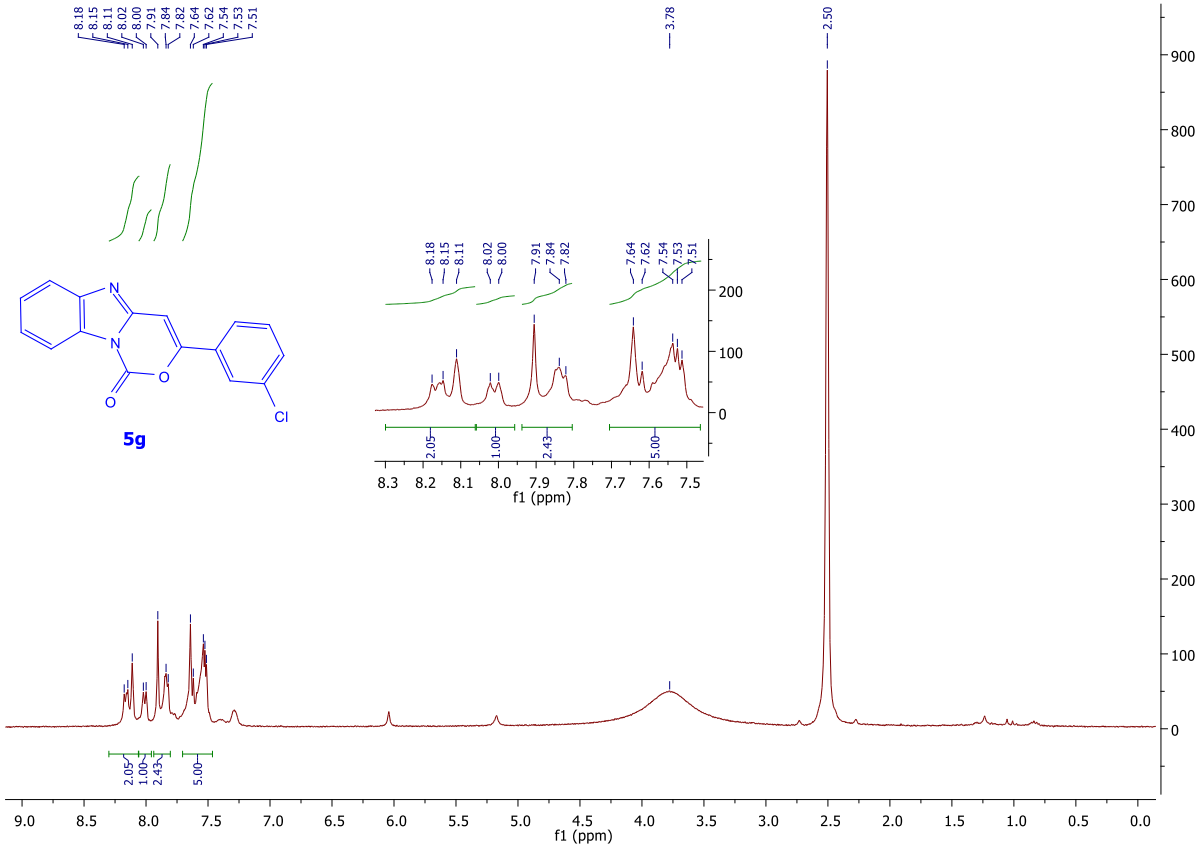
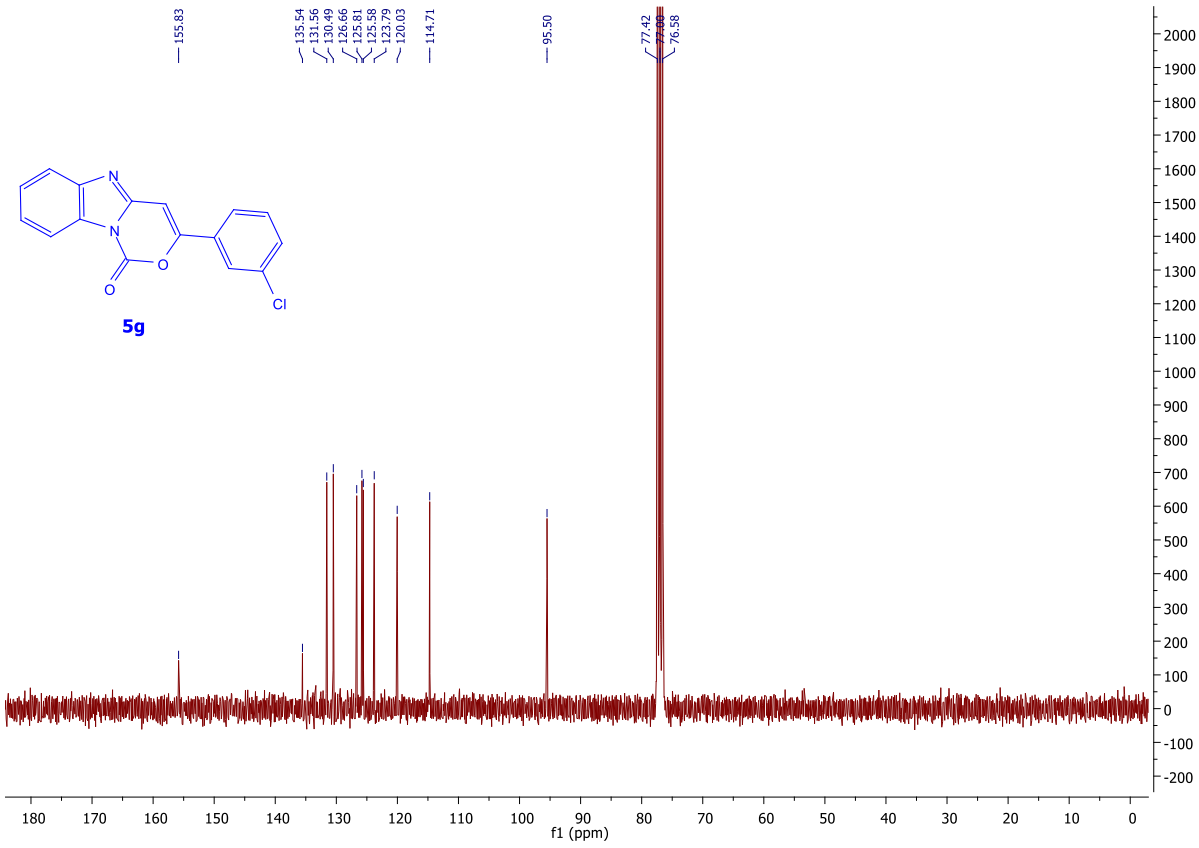
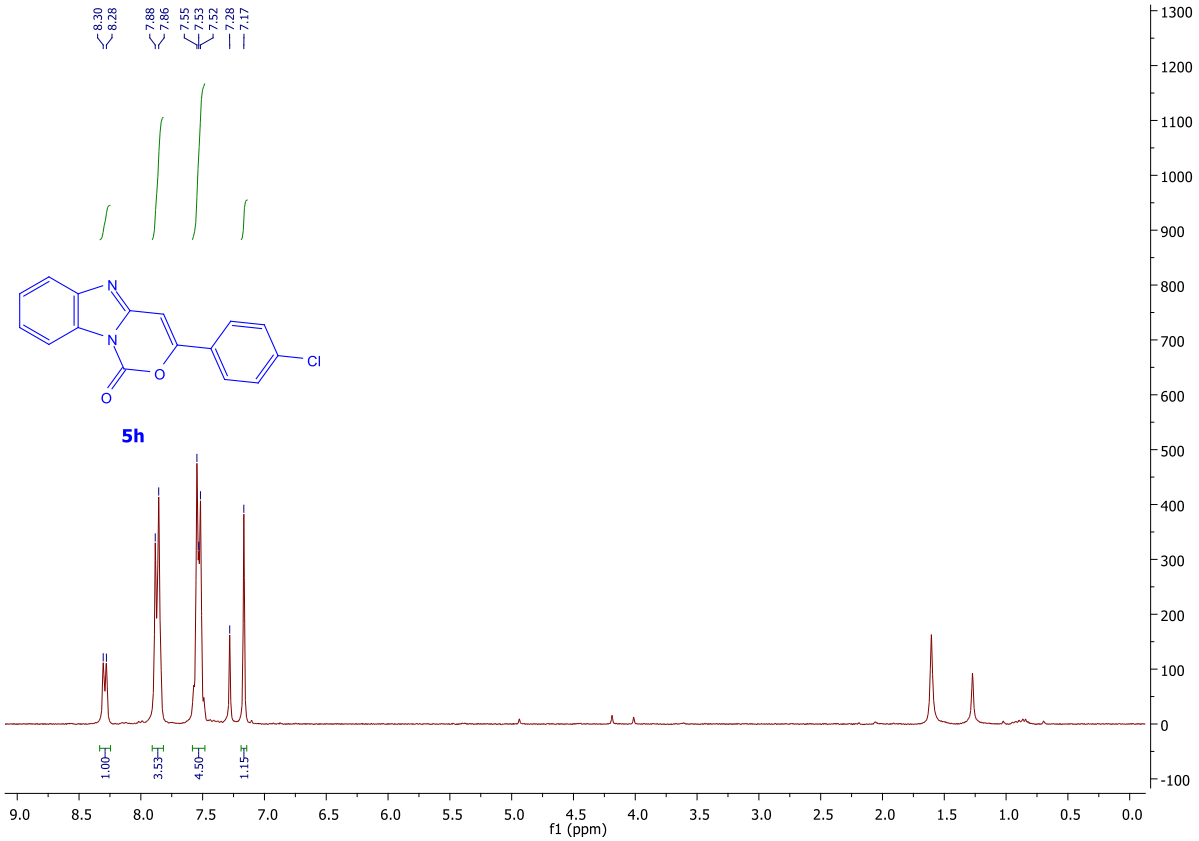


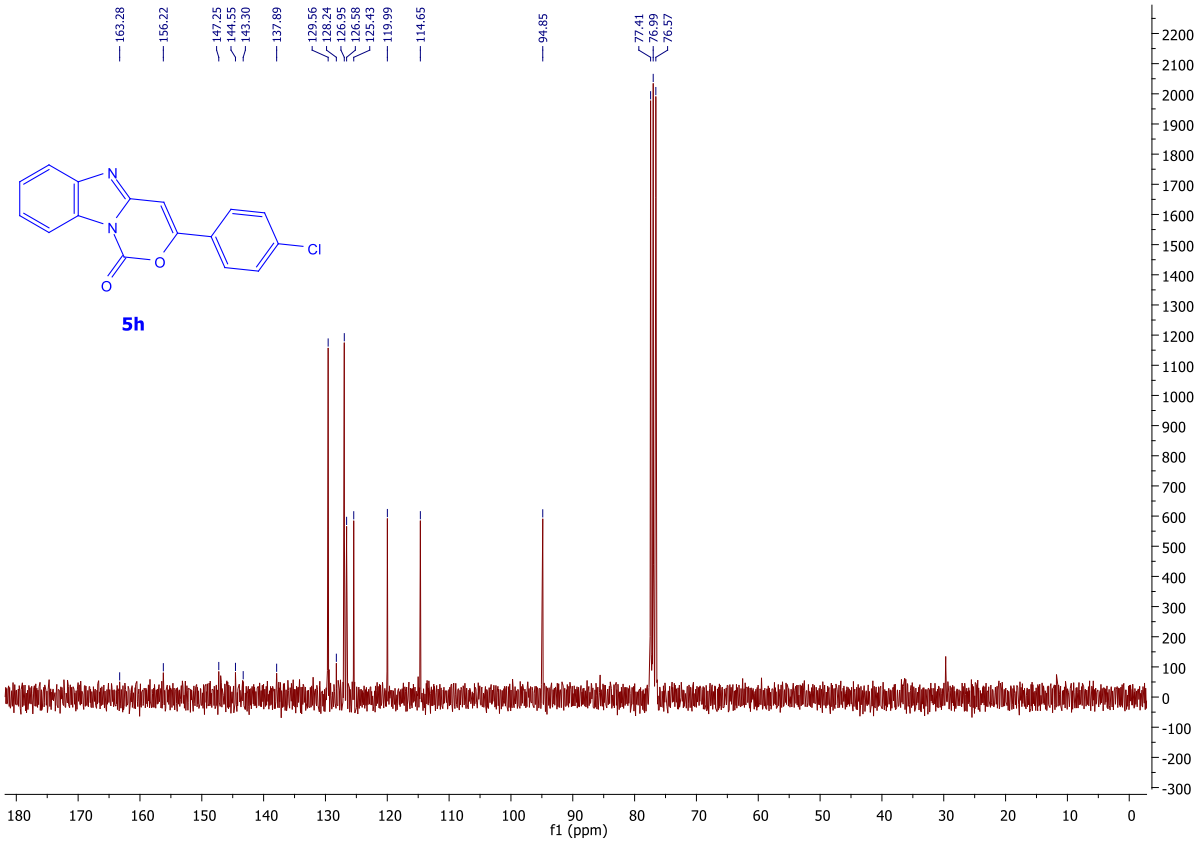
^{13}C NMR (75 MHz, $CDCl_3$) of **5g**



^{1}H NMR (300 MHz, $CDCl_3$) of **5h**



^{13}C NMR (75 MHz, $CDCl_3$) of **5h**



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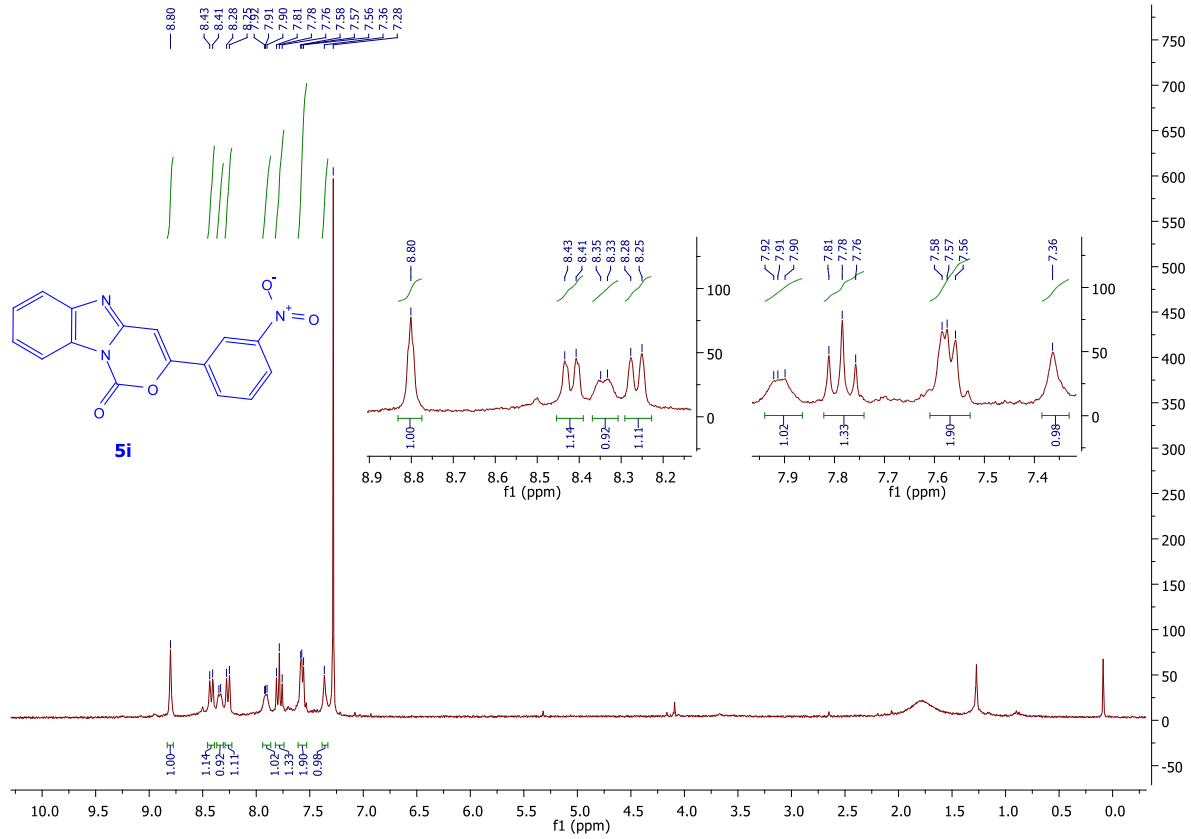
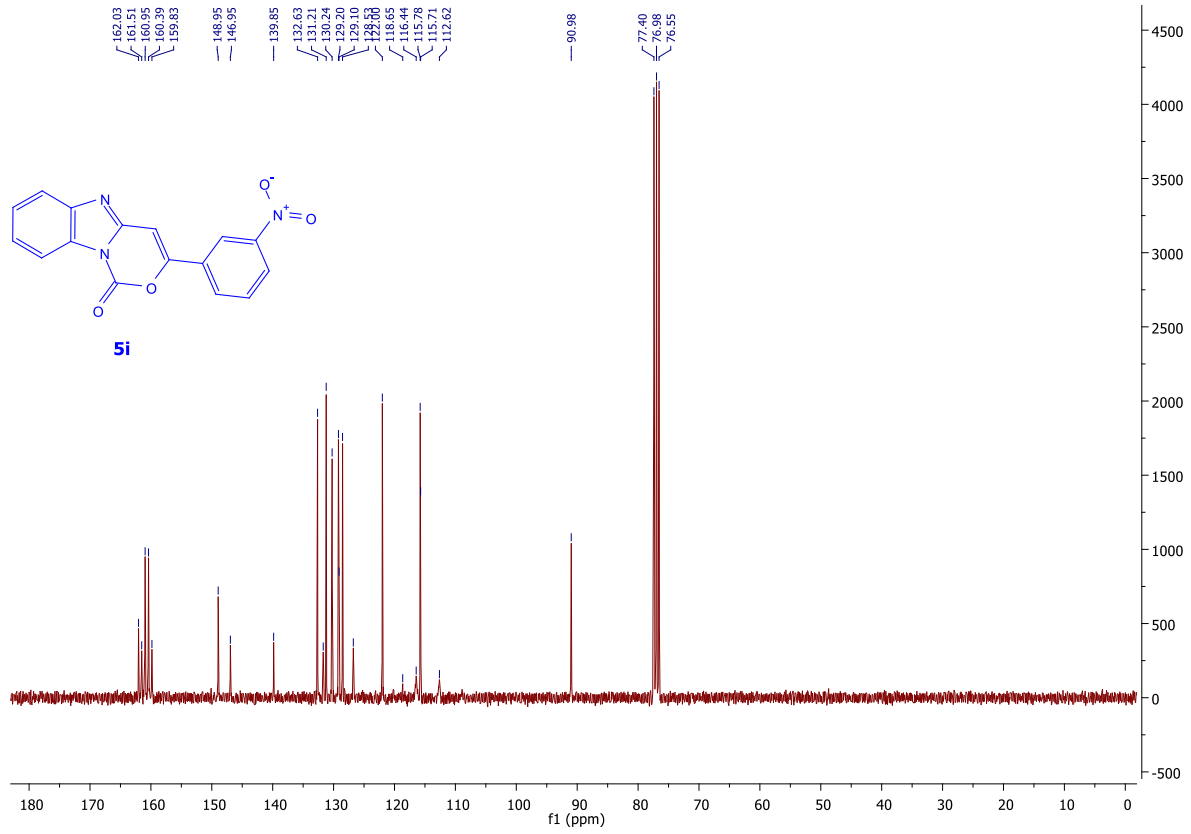
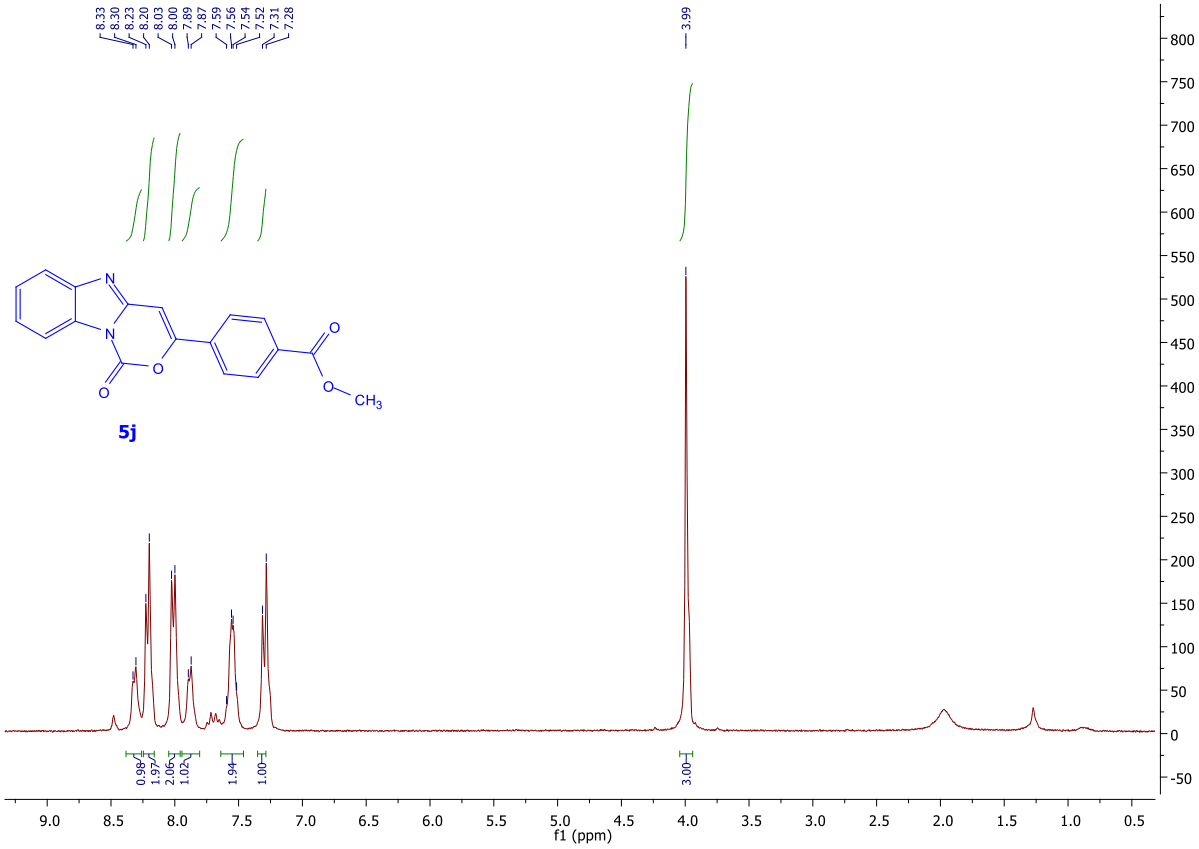


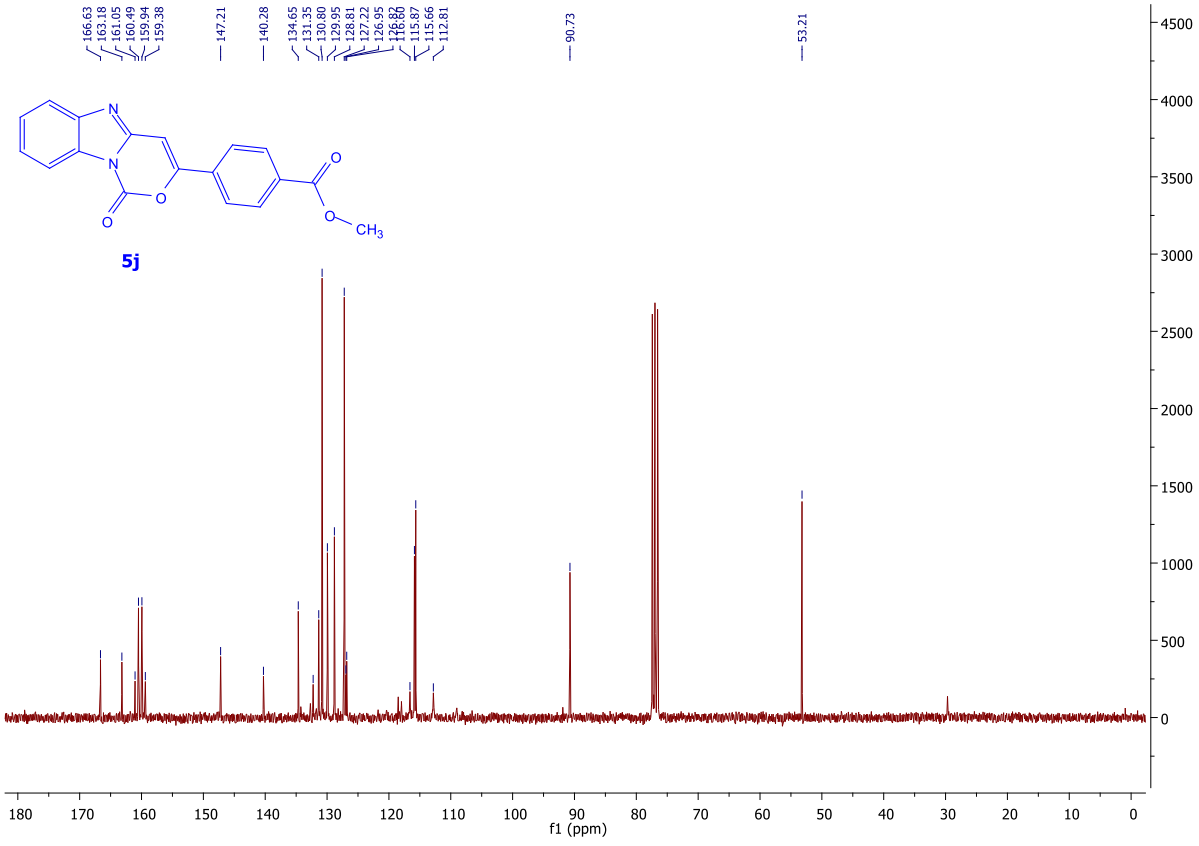
^{13}C NMR (75 MHz, $CDCl_3$/TFA-d_1) of **5i**



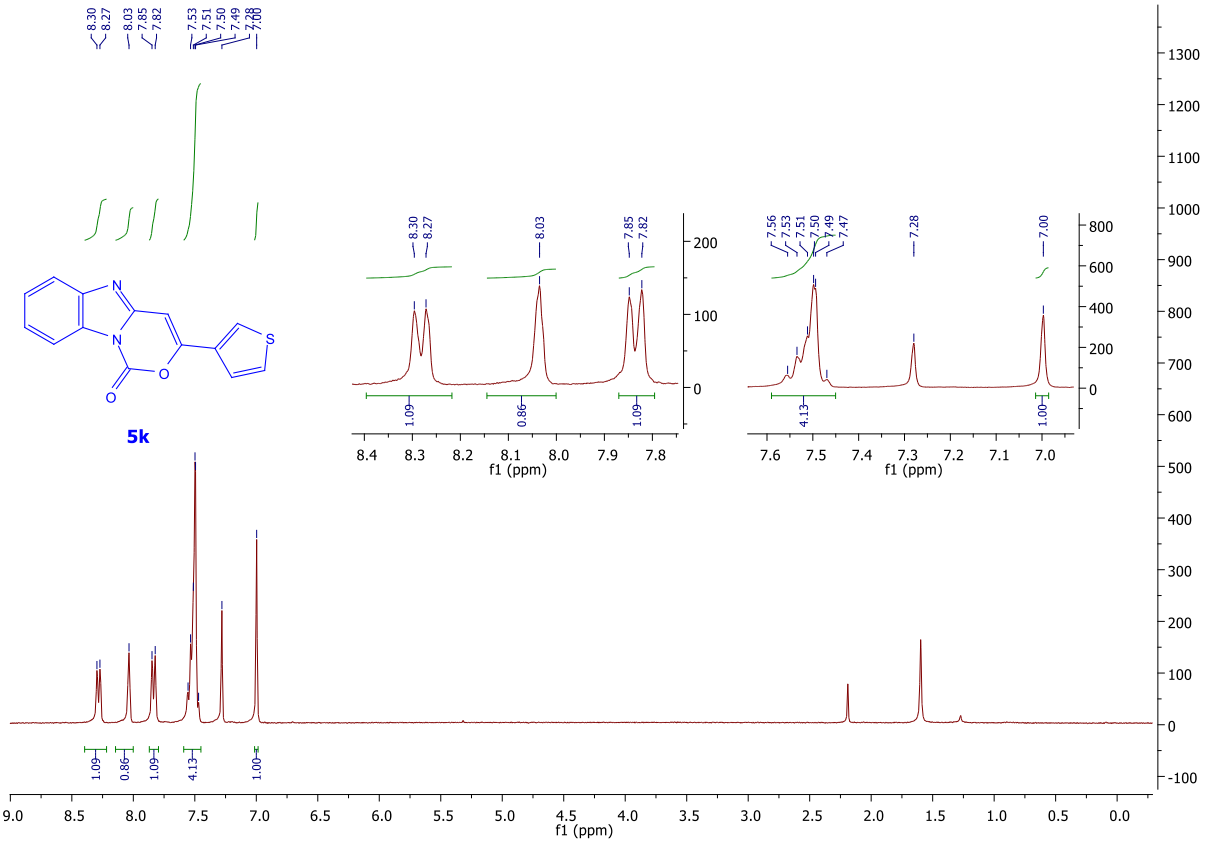
^{1}H NMR (300 MHz, $CDCl_3$) of **5j**



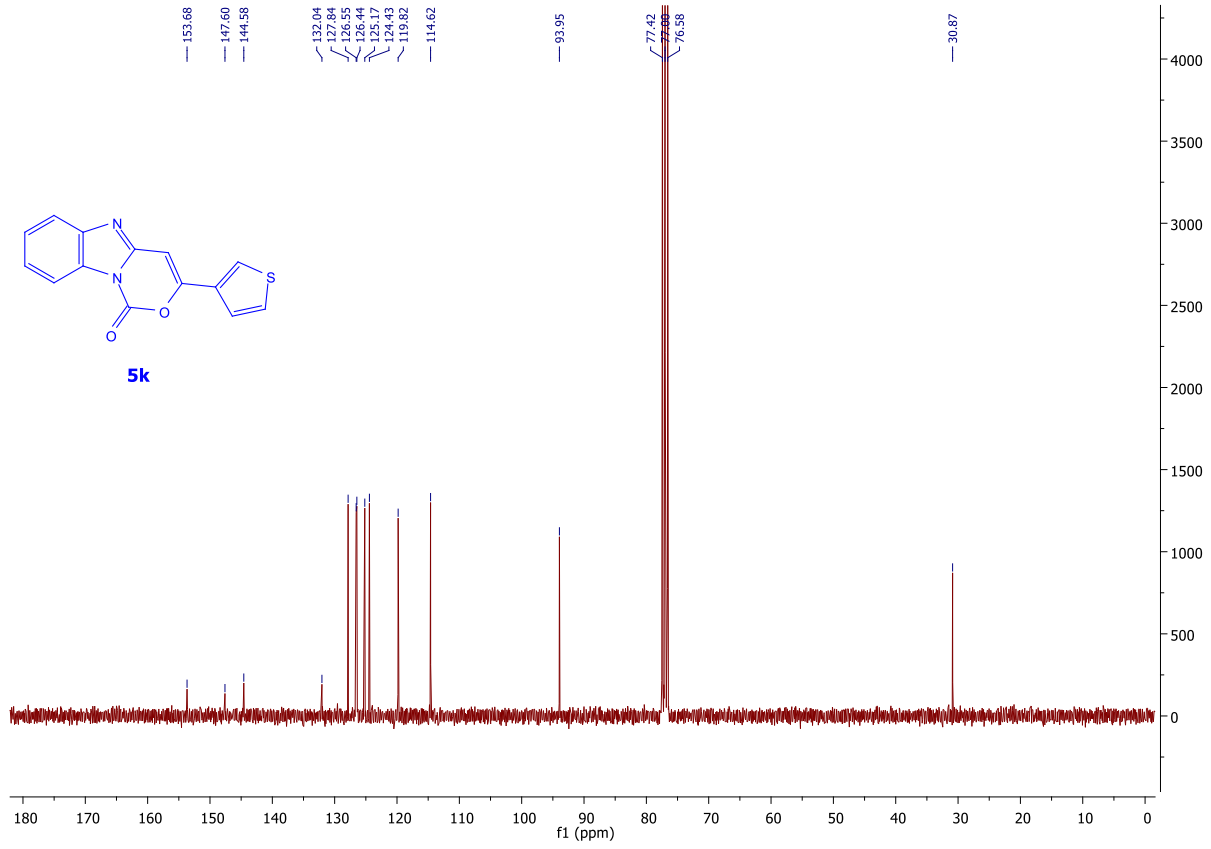
^{13}C NMR (75 MHz, $CDCl_3$/TFA-d_1) of **5j**



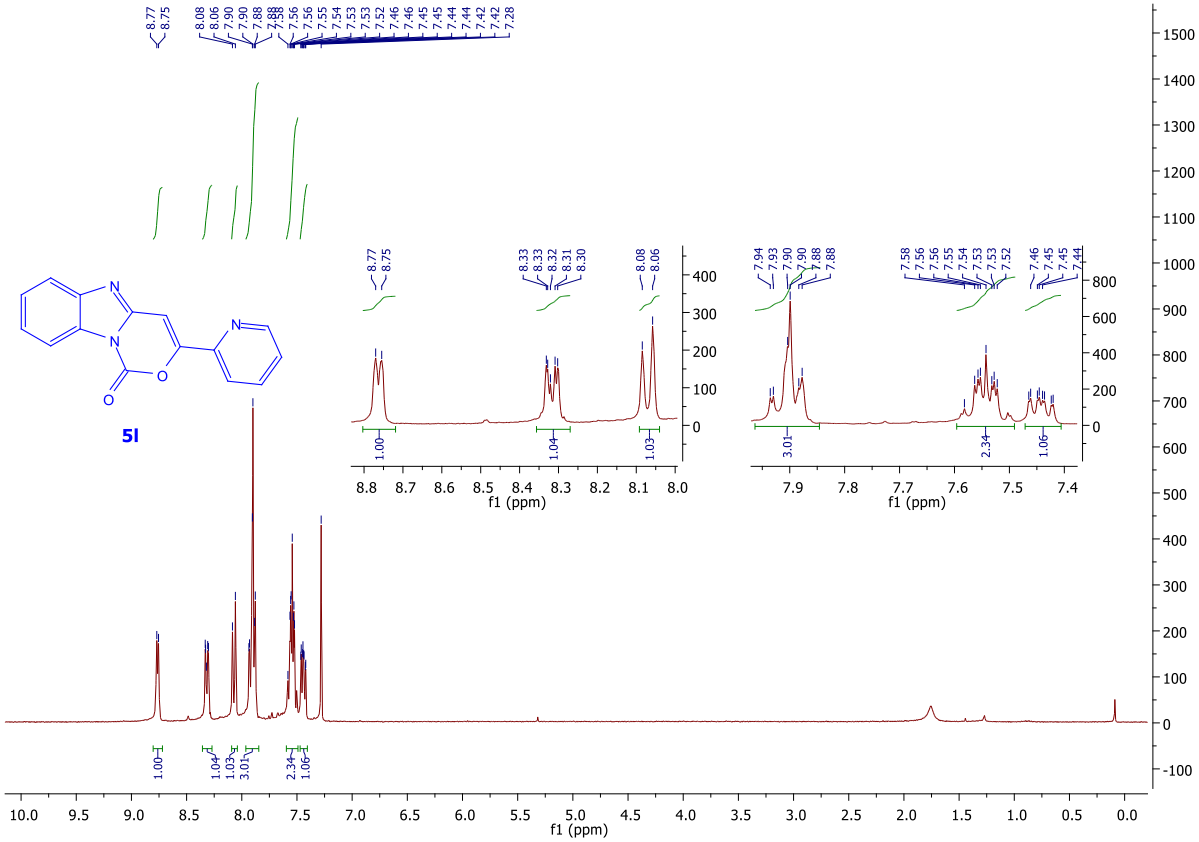
^{1}H NMR (300 MHz, $CDCl_3$) of **5k**



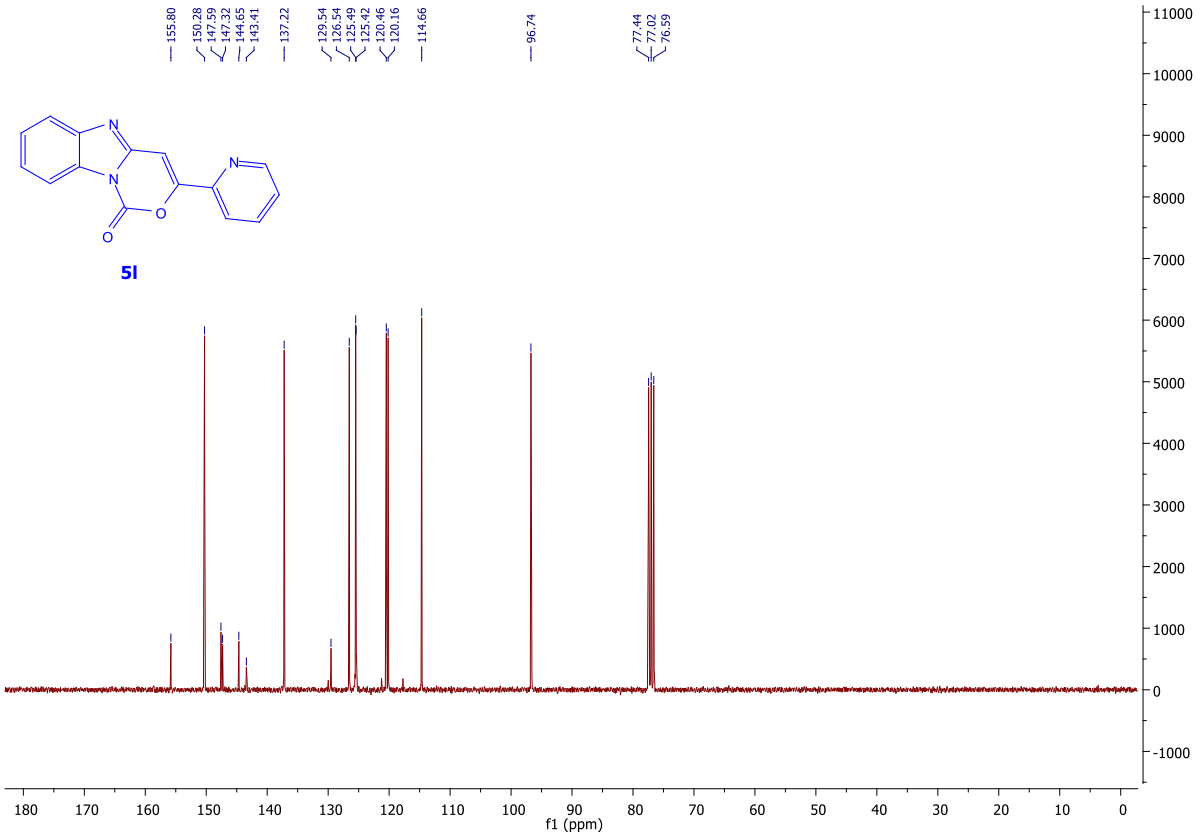
^{13}C NMR (75 MHz, $CDCl_3$) of **5k**



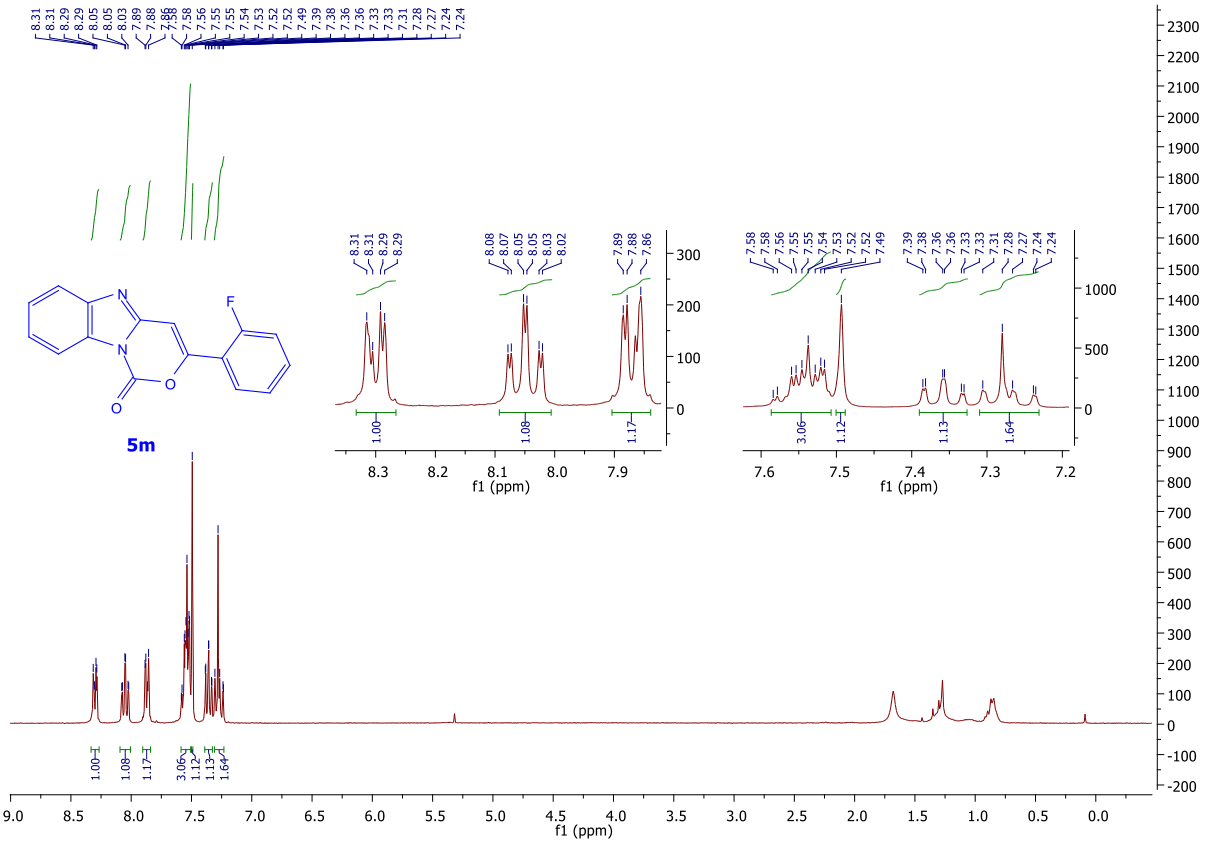
^{1}H NMR (300 MHz, $CDCl_3$) of **5l**



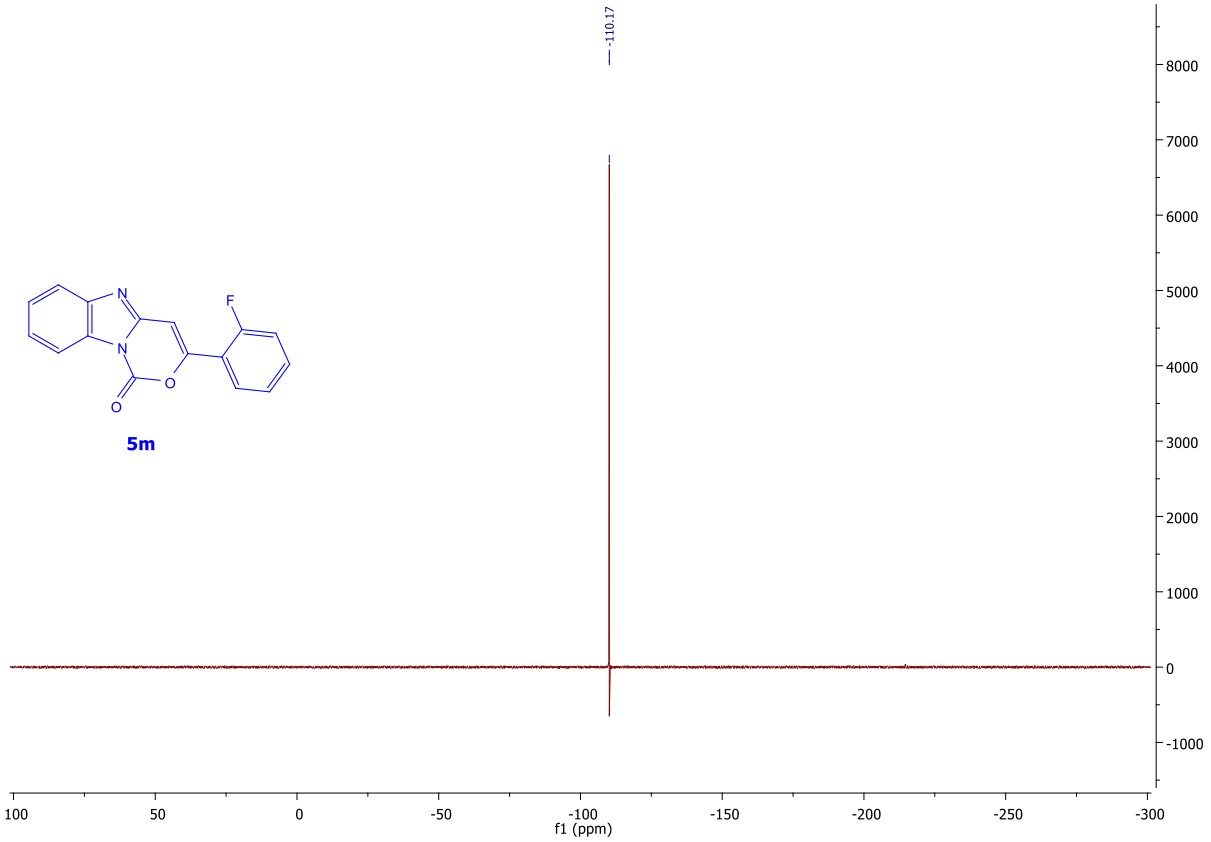
^{13}C NMR (75 MHz, $CDCl_3$) of **5l**



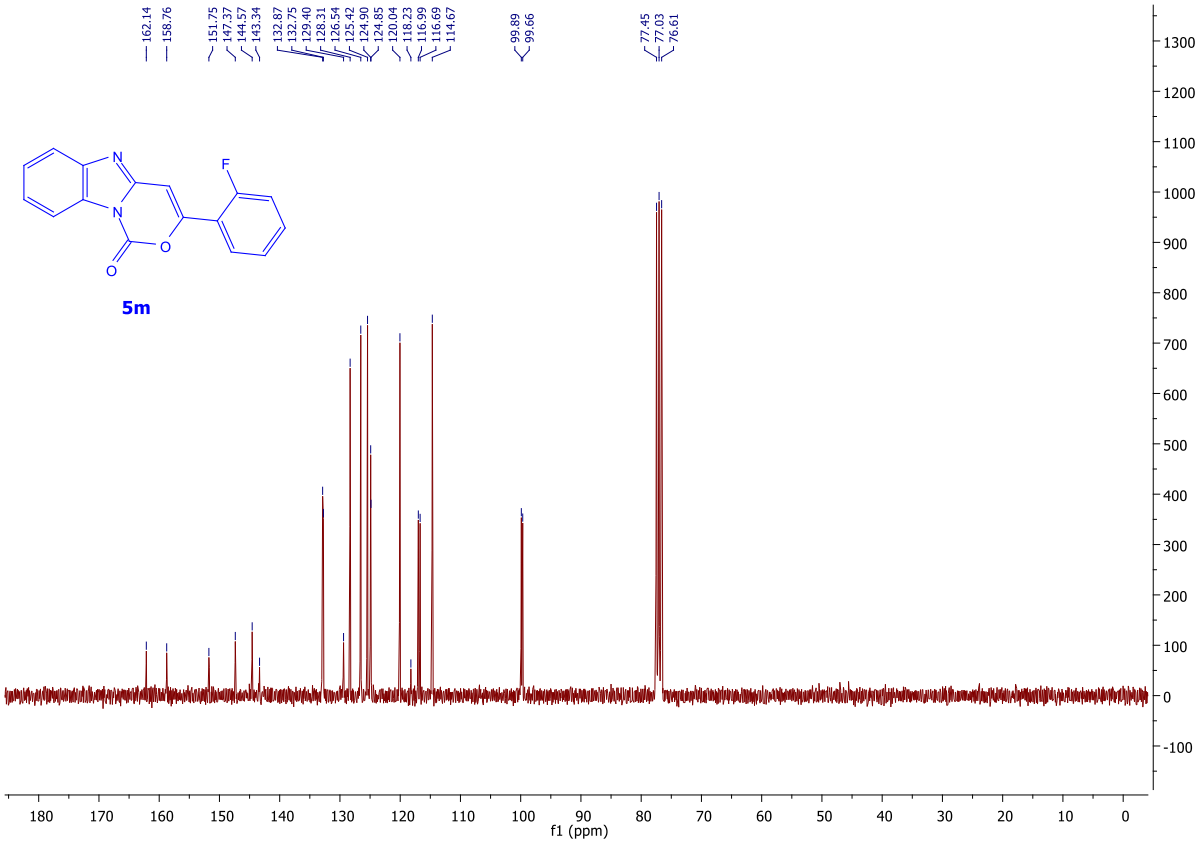
^{1}H NMR (300 MHz, $CDCl_3$) of **5m**



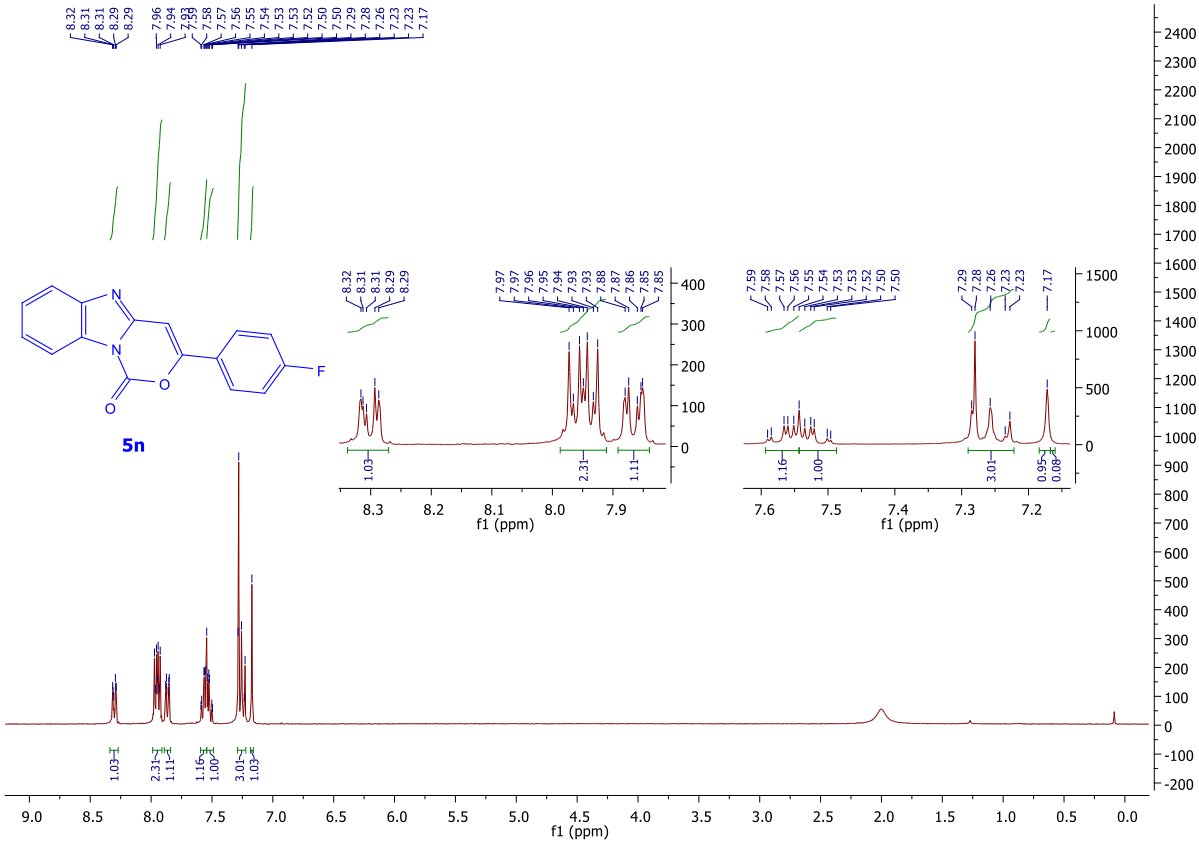
^{19}F NMR (282 MHz, $CDCl_3$) of **5m**



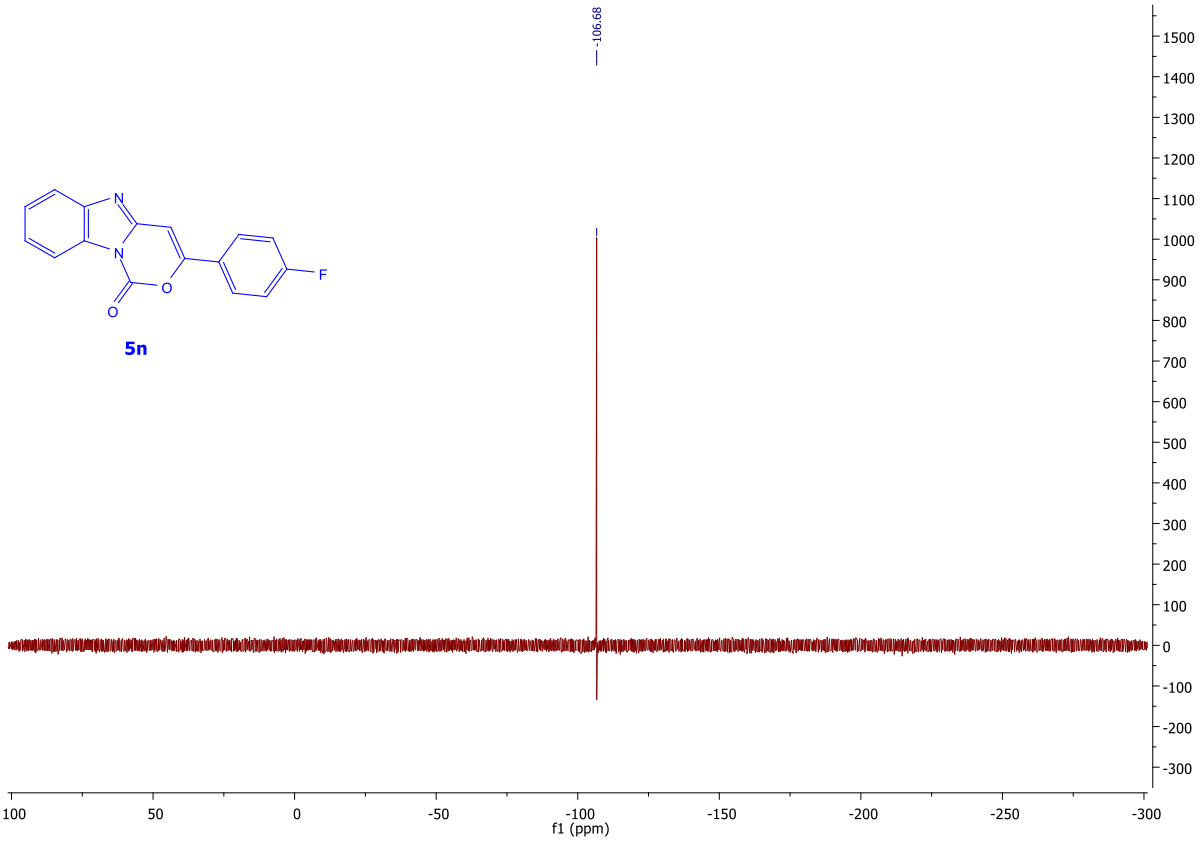
^{13}C NMR (75 MHz, $CDCl_3$) of **5m**



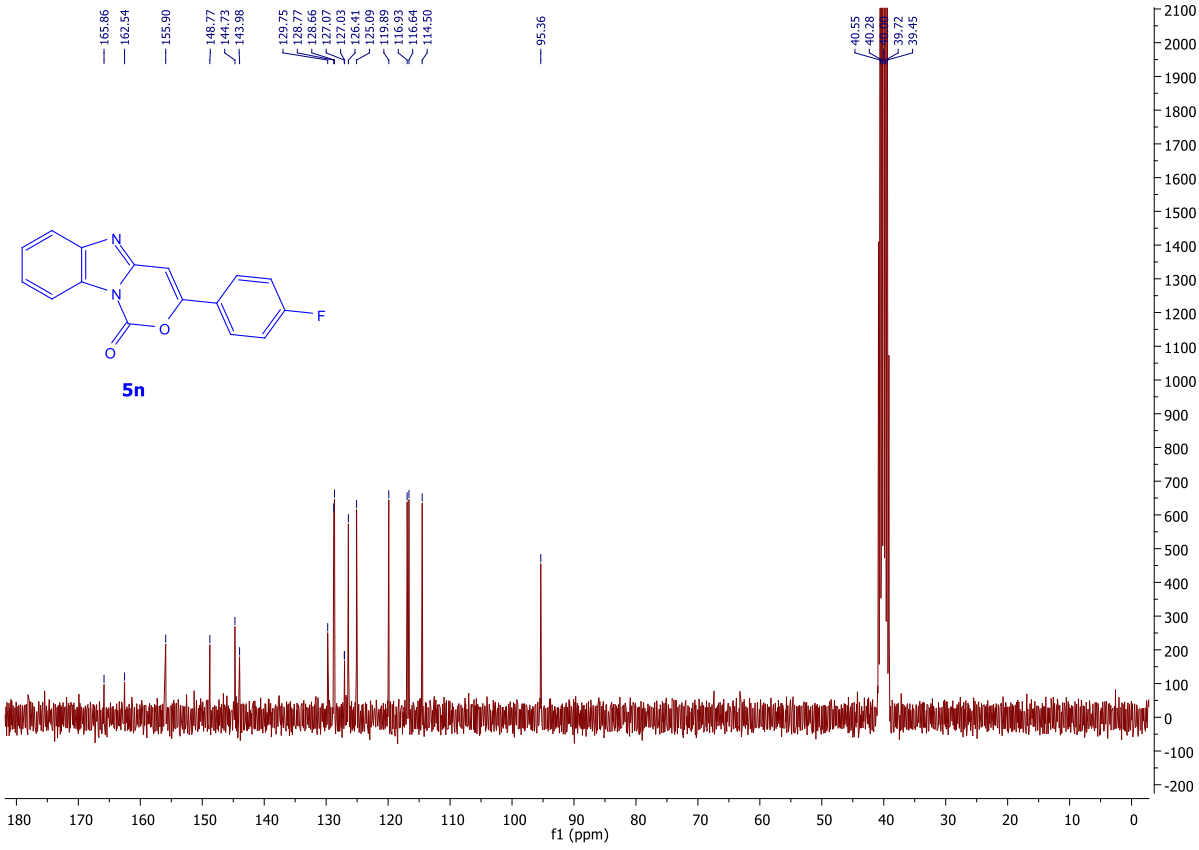
^{1}H NMR (300 MHz, $CDCl_3$) of **5n**



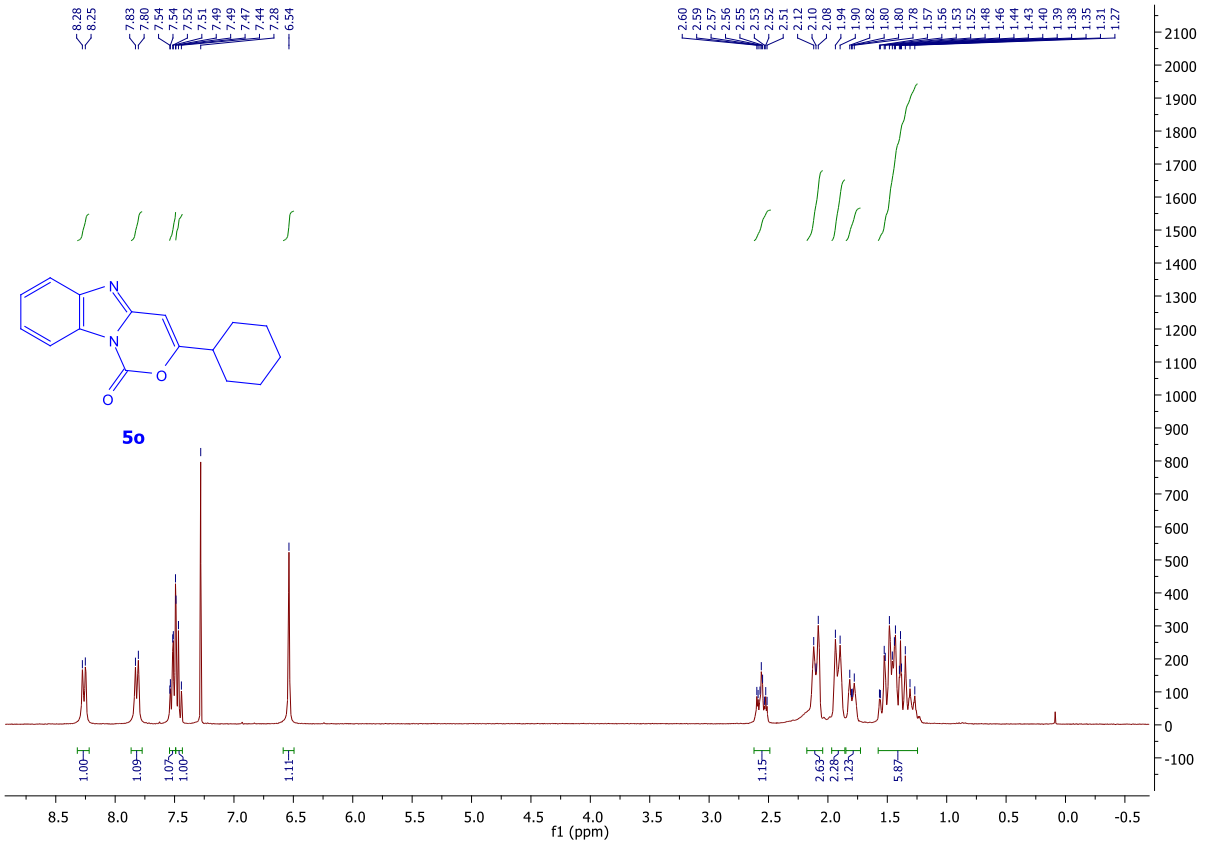
^{19}F NMR (282 MHz, $CDCl_3$) of **5n**



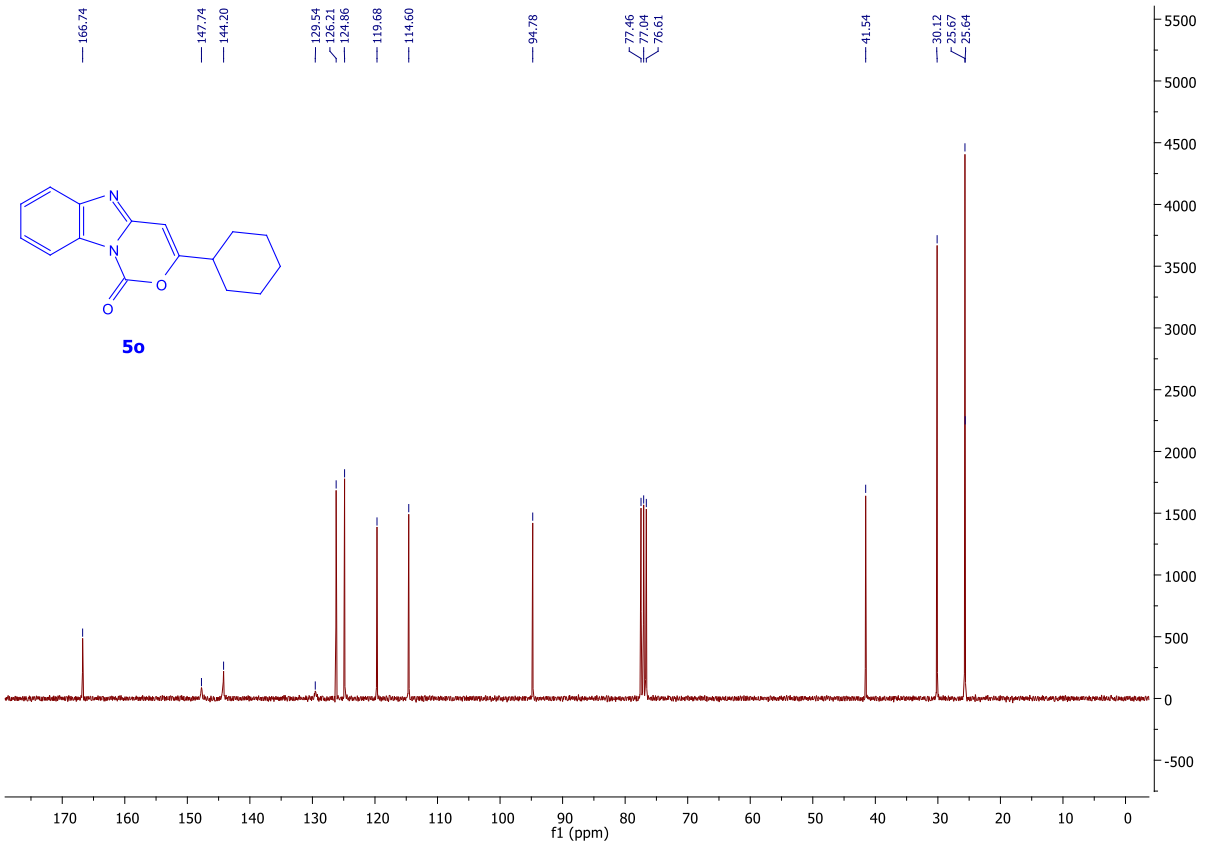
^{13}C NMR (75 MHz, DMSO-d_6) of **5n**



^{1}H NMR (300 MHz, $CDCl_3$) of **5o**



^{13}C NMR (75 MHz, $CDCl_3$) of **5o**



2. Details of DFT calculations

The structure of each studied species was optimized by using the Turbomole 7.4 program package.[1] Before their visualization using TmoleX (version 4.5.3), the structure of each individual species was optimized in the gas phase, with a convergence criterion of 10^{-8} Hartree, using the hybrid functional B3LYP and the triplet-ζ basis set 6-311+G*,[2] to collect its more stable 3D conformer. The stability of each structure was then investigated during further DFT calculations. During this step, the energy of each species was then minimized again using DFT calculations combining the Resolution of Identity (RI) approximation,[3,4] within the Turbomole 7.4 program package using the B3LYP function with the def2-TZVP basis set.[5–7] All minimum energy structures were obtained with full optimization, without constraints. Corrections for long range non-bonding interactions were given using the Grimme D3 dispersion model.[8] An implicit solvent model was additionally undertaken, using the COSMO Model implemented in Turbomole to determine thermodynamic and charge population properties in DCE. Analytical frequencies were then run on each structure at 1 atm and 298.15 K to calculate finally each energy.

2.1. Cartesian coordinates of the molecule 4a

	x	y	z
C	4.091520	1.523016	0.754366
C	2.956604	0.792659	0.407099
C	2.988477	-0.110663	-0.671854
C	4.137255	-0.312627	-1.428727
C	5.260214	0.424315	-1.068024
C	5.241390	1.327762	0.004462
N	1.695647	-0.655372	-0.729930
C	0.966147	-0.038203	0.325675
N	1.701268	0.809746	0.993133
C	-0.385864	-0.303908	0.625094
C	-1.534063	-0.480419	0.940105
C	-2.935651	-0.689389	1.261382
C	-3.884481	0.135883	0.373102
C	-5.354845	-0.105450	0.709541
H	4.057884	2.215499	1.584911
H	4.151533	-1.006951	-2.253229
H	6.174151	0.294175	-1.633919
H	6.140369	1.879924	0.247977
H	-3.108204	-0.437213	2.312810
H	-3.173066	-1.753770	1.155229
H	-3.644485	1.196516	0.486554
H	-3.697496	-0.113713	-0.675298
H	-5.529843	0.143055	1.761746
H	-5.578496	-1.172788	0.605694
O	0.021447	-1.944073	-1.497134
C	-0.654648	-2.927201	-2.373961
C	0.037946	-4.281244	-2.262373
C	-0.687234	-2.400891	-3.805087
C	-2.056105	-2.978844	-1.777459

C	1.290810	-1.608549	-1.680621
O	2.042781	-2.027959	-2.526666
H	1.038465	-4.251408	-2.686662
H	0.102041	-4.589000	-1.217204
H	-0.549126	-5.027333	-2.801422
H	0.310307	-2.360690	-4.236651
H	-1.305354	-3.062397	-4.415017
H	-1.128249	-1.402949	-3.830747
H	-2.670218	-3.682707	-2.340678
H	-2.524495	-1.995276	-1.816677
H	-2.015309	-3.302448	-0.737212
C	-6.302915	0.704828	-0.172705
H	-6.173142	0.449533	-1.227702
H	-7.346494	0.518840	0.089107
H	-6.118265	1.776906	-0.066648

2.2. Cartesian coordinates of the molecule 4b

	x	y	z
C	4.075269	1.367095	0.919766
C	2.929473	0.687216	0.509631
C	2.947603	-0.116076	-0.646577
C	4.093579	-0.266862	-1.419865
C	5.226831	0.418042	-0.995557
C	5.221424	1.222759	0.153565
N	1.646922	-0.632345	-0.752978
C	0.927960	-0.103106	0.353976
N	1.675535	0.669086	1.096837
C	-0.428476	-0.365457	0.629550
C	-1.581964	-0.528925	0.942842
H	4.051792	1.983114	1.808790
H	4.098391	-0.886921	-2.301665
H	6.138998	0.325566	-1.571547
H	6.128677	1.737395	0.443869
O	-0.035812	-1.856035	-1.603794
C	-0.694243	-2.843695	-2.494679
C	-0.001318	-4.194938	-2.357384
C	-0.691573	-2.324895	-3.928679
C	-2.108533	-2.893207	-1.932408
C	1.240824	-1.534632	-1.753614
O	2.000732	-1.926525	-2.605276
H	1.012138	-4.164290	-2.750185
H	0.028919	-4.500623	-1.310117
H	-0.568523	-4.943615	-2.913650
H	0.314289	-2.295399	-4.340989
H	-1.304421	-2.984161	-4.546385
H	-1.123464	-1.323425	-3.968796

H	-2.701170	-3.617096	-2.493294
H	-2.586626	-1.917371	-2.010429
H	-2.097183	-3.185379	-0.882671
C	-2.940861	-0.748595	1.291583
C	-3.281598	-1.186030	2.580879
C	-4.609247	-1.412275	2.913404
C	-5.614505	-1.203877	1.973122
C	-5.286016	-0.763724	0.693960
C	-3.961180	-0.536268	0.351871
H	-2.496726	-1.344722	3.308641
H	-4.861219	-1.751067	3.910586
H	-6.649620	-1.380983	2.236979
H	-6.065546	-0.594592	-0.038549
H	-3.701968	-0.186293	-0.638336

2.3. Cartesian coordinates of the molecule 4c

	x	y	z
C	4.119786	1.350593	0.872779
C	2.962328	0.690994	0.462349
C	2.982946	-0.161817	-0.657593
C	4.141786	-0.382167	-1.393691
C	5.286856	0.283345	-0.969483
C	5.279542	1.136375	0.143936
N	1.667442	-0.636005	-0.779540
C	0.937946	-0.037207	0.285362
N	1.694130	0.739832	1.015709
C	-0.425937	-0.260904	0.552505
C	-1.582916	-0.378359	0.876782
H	4.094779	2.005273	1.733726
H	4.148686	-1.042494	-2.245785
H	6.209634	0.135532	-1.516332
H	6.195890	1.633549	0.436276
O	-0.048676	-1.773550	-1.683548
C	-0.709918	-2.797353	-2.529839
C	-0.136329	-4.172145	-2.204618
C	-0.557554	-2.430695	-4.002194
C	-2.163010	-2.691754	-2.088365
C	1.258742	-1.565921	-1.751651
O	2.040690	-2.070087	-2.520731
H	0.904090	-4.252605	-2.511524
H	-0.210682	-4.369382	-1.133847
H	-0.714336	-4.933214	-2.732089
H	0.475596	-2.516140	-4.329529
H	-1.173593	-3.104169	-4.601402
H	-0.903067	-1.410029	-4.176070
H	-2.764998	-3.426092	-2.625226

H	-2.553809	-1.697531	-2.305044
H	-2.257323	-2.873476	-1.018093
C	-2.940168	-0.536910	1.254563
C	-3.288268	-0.748521	2.594018
C	-4.613103	-0.915181	2.974963
C	-5.622539	-0.867096	2.011268
C	-5.289485	-0.648962	0.669770
C	-3.971017	-0.486175	0.298256
H	-2.507436	-0.783897	3.342277
H	-4.844604	-1.078464	4.017325
H	-6.086316	-0.607648	-0.061118
H	-3.720957	-0.309521	-0.738720
C	-7.349291	-1.227141	3.623453
O	-6.947053	-1.017891	2.275567
H	-8.432766	-1.312932	3.599424
H	-7.065498	-0.382841	4.258725
H	-6.920570	-2.148675	4.028213

2.4. Cartesian coordinates of the molecule 4d

	x	y	z
C	4.074175	1.372341	0.921998
C	2.927906	0.693990	0.510767
C	2.943858	-0.102256	-0.650351
C	4.088011	-0.247411	-1.427350
C	5.221832	0.435965	-1.001892
C	5.218578	1.233739	0.151995
N	1.644094	-0.621196	-0.755062
C	0.927019	-0.098664	0.356613
N	1.675501	0.671142	1.101156
C	-0.430483	-0.358139	0.628634
C	-1.586356	-0.518546	0.934933
H	4.052462	1.982939	1.814815
H	4.090677	-0.861181	-2.313554
H	6.132481	0.348105	-1.581007
H	6.126038	1.747613	0.443052
O	-0.026867	-1.876307	-1.582425
C	-0.683991	-2.864343	-2.473325
C	0.038848	-4.203124	-2.369802
C	-0.721640	-2.325837	-3.899655
C	-2.084895	-2.950652	-1.882444
C	1.238444	-1.523679	-1.755639
O	1.989996	-1.891751	-2.625310
H	1.042974	-4.146418	-2.783194
H	0.097388	-4.522116	-1.327731
H	-0.525020	-4.955513	-2.924415
H	0.274844	-2.269047	-4.331405

H	-1.332623	-2.989677	-4.514271
H	-1.175672	-1.333557	-3.916831
H	-2.674240	-3.679105	-2.440941
H	-2.584609	-1.984287	-1.935597
H	-2.045016	-3.257038	-0.837353
C	-2.948026	-0.735925	1.274583
C	-3.293564	-1.170845	2.563060
C	-4.619366	-1.401369	2.915351
C	-5.612163	-1.181565	1.956553
C	-5.284721	-0.744928	0.677908
C	-3.960934	-0.521063	0.329806
H	-2.505733	-1.326218	3.289761
H	-6.651013	-1.349592	2.216944
H	-6.067875	-0.572369	-0.050133
H	-3.700478	-0.170346	-0.659616
C	-4.975473	-1.899002	4.291725
H	-4.182259	-1.685024	5.008807
H	-5.895954	-1.437549	4.653587
H	-5.132936	-2.981559	4.285041

2.5. Cartesian coordinates of the molecule 4e

	x	y	z
C	4.058620	1.383565	0.912879
C	2.916792	0.698344	0.500550
C	2.948653	-0.125789	-0.640494
C	4.103876	-0.291877	-1.396509
C	5.233096	0.398565	-0.970226
C	5.214389	1.223533	0.164236
N	1.646861	-0.636536	-0.758358
C	0.914224	-0.087764	0.330348
N	1.655143	0.693253	1.071195
C	-0.439582	-0.361020	0.606184
C	-1.589093	-0.533554	0.930475
H	4.024954	2.015749	1.790156
H	4.119850	-0.930724	-2.264728
H	6.152673	0.293314	-1.532089
H	6.118900	1.741497	0.457258
O	-0.050546	-1.788369	-1.678613
C	-0.699186	-2.799801	-2.549691
C	-0.094688	-4.171399	-2.271233
C	-0.567478	-2.385362	-4.011231
C	-2.149884	-2.737101	-2.092269
C	1.250990	-1.549766	-1.752244
O	2.037499	-2.014327	-2.541041
H	0.944602	-4.220647	-2.588262
H	-0.156280	-4.402990	-1.206563

H	-0.660978	-4.928000	-2.817599
H	0.464101	-2.439904	-4.350116
H	-1.175417	-3.052394	-4.625666
H	-0.934759	-1.366991	-4.150630
H	-2.742602	-3.463730	-2.649580
H	-2.562193	-1.743654	-2.269259
H	-2.231126	-2.958120	-1.028432
C	-2.940536	-0.761453	1.299336
C	-3.269700	-1.132564	2.611921
C	-4.589517	-1.362429	2.965131
C	-5.623583	-1.230436	2.034537
C	-5.291686	-0.850313	0.732447
C	-3.975604	-0.619125	0.364124
H	-2.480514	-1.235049	3.345260
H	-4.823659	-1.646749	3.984749
H	-6.078005	-0.729310	-0.003935
H	-3.736968	-0.316404	-0.646486
C	-7.050288	-1.513679	2.419966
H	-7.246298	-1.229017	3.454960
H	-7.749420	-0.974981	1.778972
H	-7.273560	-2.580936	2.326796

2.6. Cartesian coordinates of the molecule 4f

	x	y	z
C	3.932539	1.821925	0.484632
C	2.833411	1.002294	0.230839
C	2.945391	-0.091965	-0.649177
C	4.136683	-0.399421	-1.297033
C	5.220915	0.428793	-1.031688
C	5.124157	1.521328	-0.155977
N	1.667763	-0.666276	-0.680834
C	0.871576	0.109875	0.198697
N	1.547788	1.090335	0.737635
C	-0.463389	-0.193812	0.529663
C	-1.590442	-0.435062	0.882356
H	3.840064	2.660295	1.162159
H	4.212245	-1.245626	-1.961352
H	6.168034	0.220137	-1.513101
H	5.997322	2.136752	0.020354
O	-0.012061	-1.832389	-1.606265
C	-0.667818	-2.922472	-2.374236
C	-0.289872	-4.268820	-1.768404
C	-0.285700	-2.809804	-3.846032
C	-2.146355	-2.620693	-2.166517
C	1.305382	-1.740797	-1.518847
O	2.132730	-2.424670	-2.069180

H	0.765958	-4.487929	-1.911553
H	-0.520313	-4.279802	-0.702435
H	-0.876663	-5.052624	-2.251123
H	0.768868	-3.023711	-4.002524
H	-0.877350	-3.524313	-4.421392
H	-0.506295	-1.808058	-4.219231
H	-2.747623	-3.348818	-2.713008
H	-2.389013	-1.622570	-2.532278
H	-2.404711	-2.677464	-1.111076
C	-2.925493	-0.714275	1.261593
C	-3.333691	-1.996094	1.665179
C	-4.647966	-2.258808	2.019565
C	-5.587213	-1.235327	1.981311
C	-5.208829	0.046420	1.591607
C	-3.894950	0.303090	1.237160
H	-4.927098	-3.257232	2.326710
H	-6.612507	-1.442195	2.260160
H	-5.938400	0.845386	1.564888
H	-3.588720	1.294932	0.932823
Cl	-2.161786	-3.304556	1.741047

2.7. Cartesian coordinates of the molecule 4g

	x	y	z
C	4.079047	1.366391	0.919592
C	2.932364	0.687790	0.509438
C	2.948098	-0.112878	-0.648771
C	4.092760	-0.262591	-1.424345
C	5.226634	0.420835	-0.999948
C	5.223530	1.223182	0.151112
N	1.647818	-0.630170	-0.753026
C	0.932058	-0.103700	0.355971
N	1.679695	0.667676	1.099169
C	-0.425752	-0.361827	0.631251
C	-1.580003	-0.522016	0.941718
H	4.057374	1.979997	1.810292
H	4.095716	-0.879718	-2.308208
H	6.137942	0.329324	-1.577400
H	6.131512	1.736783	0.440794
O	-0.031478	-1.869640	-1.586556
C	-0.694037	-2.854500	-2.478380
C	0.014215	-4.200105	-2.366221
C	-0.718020	-2.319810	-3.906294
C	-2.099029	-2.924147	-1.895052
C	1.238701	-1.531569	-1.753944
O	1.991186	-1.908847	-2.618208
H	1.020981	-4.155312	-2.774517

H	0.063868	-4.516576	-1.322936
H	-0.554341	-4.948416	-2.921509
H	0.281320	-2.275073	-4.332811
H	-1.332504	-2.978988	-4.522376
H	-1.161225	-1.322747	-3.929238
H	-2.693217	-3.647251	-2.455212
H	-2.587740	-1.952278	-1.954196
H	-2.068309	-3.229431	-0.849327
C	-2.941194	-0.738881	1.281833
C	-3.279116	-1.199262	2.563394
C	-4.610205	-1.419482	2.873930
C	-5.622794	-1.193194	1.950185
C	-5.282536	-0.731181	0.682889
C	-3.957411	-0.503207	0.344118
H	-2.505899	-1.379619	3.296303
H	-6.654029	-1.373118	2.220344
H	-6.063923	-0.546039	-0.043270
H	-3.695554	-0.136536	-0.638699
Cl	-5.028818	-2.001970	4.483271

2.8. Cartesian coordinates of the molecule 4h

	x	y	z
C	4.070763	1.361151	0.927179
C	2.925848	0.681815	0.513319
C	2.945787	-0.118127	-0.645260
C	4.092821	-0.266118	-1.417604
C	5.224921	0.418127	-0.989618
C	5.217729	1.219527	0.162004
N	1.645340	-0.634137	-0.755401
C	0.925293	-0.108684	0.351709
N	1.671173	0.661302	1.098596
C	-0.431064	-0.372262	0.627149
C	-1.583673	-0.533870	0.944261
H	4.045859	1.974534	1.817956
H	4.099378	-0.883813	-2.301037
H	6.137927	0.327859	-1.564582
H	6.124432	1.733614	0.454856
O	-0.038398	-1.849536	-1.616851
C	-0.693372	-2.839076	-2.509188
C	-0.006799	-4.192088	-2.359548
C	-0.677366	-2.327117	-3.945452
C	-2.112399	-2.880516	-1.958442
C	1.241016	-1.534691	-1.758630
O	2.004229	-1.930058	-2.605312
H	1.010098	-4.166976	-2.743742
H	0.013280	-4.493344	-1.310754

H	-0.571677	-4.941232	-2.917495
H	0.331533	-2.304857	-4.350586
H	-1.289132	-2.986168	-4.564433
H	-1.103628	-1.323585	-3.993795
H	-2.702871	-3.606128	-2.519230
H	-2.586267	-1.903482	-2.048520
H	-2.110662	-3.165791	-0.906728
C	-2.940248	-0.750891	1.298833
C	-3.281396	-1.158142	2.597590
C	-4.604411	-1.385192	2.943407
C	-5.597329	-1.201823	1.989137
C	-5.288872	-0.791533	0.698240
C	-3.964268	-0.567036	0.357704
H	-2.499498	-1.296338	3.332336
H	-4.865739	-1.701009	3.943959
H	-6.077028	-0.647869	-0.027966
H	-3.713177	-0.239857	-0.641943
Cl	-7.277526	-1.492112	2.423766

2.9. Cartesian coordinates of the molecule 4i

	x	y	z
C	4.068324	1.420249	0.890798
C	2.926498	0.727372	0.490689
C	2.947754	-0.090802	-0.655240
C	4.093466	-0.244650	-1.428557
C	5.222013	0.453341	-1.014505
C	5.213450	1.273075	0.124514
N	1.651091	-0.618261	-0.751997
C	0.932846	-0.080496	0.348679
N	1.673974	0.707166	1.080633
C	-0.423602	-0.343468	0.629112
C	-1.575883	-0.508137	0.943000
H	4.042400	2.046862	1.772221
H	4.101223	-0.875588	-2.302593
H	6.134017	0.359666	-1.590462
H	6.118077	1.796725	0.406387
O	-0.023846	-1.873889	-1.569447
C	-0.682791	-2.873862	-2.447737
C	0.029155	-4.215517	-2.315471
C	-0.707529	-2.359856	-3.883080
C	-2.088039	-2.939080	-1.864121
C	1.246042	-1.535168	-1.740758
O	2.000164	-1.922041	-2.598696
H	1.035813	-4.173720	-2.724276
H	0.079717	-4.516831	-1.267776
H	-0.536798	-4.973577	-2.860042

H	0.291941	-2.318248	-4.309529
H	-1.319227	-3.029869	-4.490129
H	-1.153731	-1.364554	-3.921118
H	-2.680203	-3.671192	-2.414465
H	-2.579001	-1.969055	-1.937978
H	-2.056467	-3.230643	-0.814456
C	-2.936933	-0.729519	1.279533
C	-3.283504	-1.209337	2.548807
C	-4.619130	-1.428401	2.837606
C	-5.632927	-1.188704	1.920174
C	-5.283851	-0.707505	0.664491
C	-3.953435	-0.478407	0.343492
H	-2.527972	-1.408760	3.293589
H	-6.660152	-1.376042	2.195387
H	-6.056377	-0.507706	-0.066514
H	-3.684631	-0.097214	-0.632286
N	-4.979475	-1.944015	4.181100
O	-4.070182	-2.148734	4.973100
O	-6.165800	-2.134221	4.414057

2.10. Cartesian coordinates of the molecule 4j

	x	y	z
C	4.116985	1.353315	0.879088
C	2.957949	0.689616	0.479111
C	2.957966	-0.125265	-0.669399
C	4.098821	-0.305098	-1.444128
C	5.244915	0.364071	-1.030019
C	5.257523	1.180705	0.110927
N	1.649803	-0.623997	-0.763478
C	0.944985	-0.071354	0.339284
N	1.706578	0.697748	1.071276
C	-0.420027	-0.289660	0.610746
C	-1.581098	-0.409520	0.915680
H	4.107368	1.978294	1.762074
H	4.089127	-0.931840	-2.321173
H	6.153289	0.250476	-1.608182
H	6.174659	1.682265	0.392755
O	-0.029061	-1.904878	-1.532936
C	-0.703197	-2.902767	-2.402333
C	0.029974	-4.236497	-2.308014
C	-0.778613	-2.372773	-3.830157
C	-2.088515	-2.993262	-1.776652
C	1.227892	-1.543192	-1.743251
O	1.962351	-1.916299	-2.624596
H	1.023285	-4.176864	-2.746325
H	0.115717	-4.548825	-1.265832

H	-0.542918	-4.995407	-2.844066
H	0.206510	-2.313530	-4.286818
H	-1.400816	-3.043577	-4.425529
H	-1.238652	-1.383168	-3.842484
H	-2.685900	-3.731331	-2.313322
H	-2.597124	-2.031600	-1.827910
H	-2.020718	-3.290098	-0.730085
C	-2.947819	-0.581083	1.252908
C	-3.318745	-0.932161	2.560684
C	-4.652131	-1.115688	2.884588
C	-5.641894	-0.950781	1.912317
C	-5.278971	-0.593543	0.611624
C	-3.948724	-0.408885	0.282734
H	-2.550150	-1.059021	3.311288
H	-4.934306	-1.388078	3.891517
H	-6.056953	-0.463327	-0.128652
H	-3.667740	-0.123158	-0.721810
O	-7.310621	-1.470062	3.496761
C	-7.086859	-1.140062	2.207561
O	-7.972365	-1.015837	1.392892
C	-8.687590	-1.669731	3.859913
H	-8.674630	-1.921318	4.916726
H	-9.262518	-0.760131	3.687846
H	-9.121553	-2.481388	3.276320

2.11. Cartesian coordinates of the molecule 4k

	x	y	z
C	1.293667	0.427785	2.268154
C	0.175244	-0.308555	1.880241
C	0.244620	-1.195324	0.788839
C	1.414489	-1.374600	0.059050
C	2.520054	-0.632974	0.460753
C	2.464118	0.254417	1.545905
N	-1.042590	-1.744747	0.682562
C	-1.804582	-1.153956	1.727303
N	-1.094140	-0.312662	2.432382
C	-3.150802	-1.449218	2.014541
C	-4.291522	-1.615966	2.372169
H	1.231277	1.107947	3.107089
H	1.459211	-2.060983	-0.771042
H	3.450399	-0.747055	-0.081273
H	3.351268	0.810644	1.821299
O	-2.702810	-2.971128	-0.207596
C	-3.317149	-4.027910	-1.049167
C	-2.698893	-5.377630	-0.702251
C	-3.162255	-3.672029	-2.523911

C	-4.777566	-3.968255	-0.623733
C	-1.403955	-2.712934	-0.270652
O	-0.596008	-3.201422	-1.022242
H	-1.653498	-5.424664	-0.998818
H	-2.776224	-5.565271	0.370022
H	-3.244544	-6.164782	-1.225994
H	-2.123346	-3.723991	-2.839565
H	-3.746955	-4.374015	-3.121696
H	-3.542268	-2.666477	-2.713268
H	-5.350045	-4.722189	-1.165597
H	-5.195598	-2.986205	-0.847071
H	-4.876165	-4.152789	0.445779
S	-7.701246	-2.087451	4.306449
C	-7.909822	-2.214157	2.581947
C	-6.736121	-2.052497	1.918618
C	-5.623217	-1.819115	2.798614
C	-6.005196	-1.809697	4.120475
H	-8.889451	-2.394959	2.170526
H	-6.641501	-2.085199	0.844240
H	-5.374104	-1.654636	4.979846

2.12. Cartesian coordinates of the molecule 4l

	x	y	z
C	1.183627	-0.028749	2.532911
C	0.025350	-0.665759	2.086653
C	0.007181	-1.325994	0.841367
C	1.123728	-1.373465	0.013649
C	2.267151	-0.732768	0.475098
C	2.299757	-0.070476	1.713102
N	-1.281072	-1.860722	0.731773
C	-1.966215	-1.470234	1.907193
N	-1.206053	-0.766824	2.708487
C	-3.332691	-1.708055	2.142938
C	-4.506763	-1.834004	2.386064
H	1.191903	0.476482	3.489493
H	1.092865	-1.871382	-0.942616
H	3.156841	-0.741787	-0.141818
H	3.214426	0.415581	2.028183
O	-2.800424	-3.338237	-0.002021
C	-3.557800	-4.155991	-0.989427
C	-2.664681	-5.270457	-1.524272
C	-4.084417	-3.241783	-2.089108
C	-4.694647	-4.716315	-0.146558
C	-1.721033	-2.658397	-0.347481
O	-1.128385	-2.684370	-1.397697
H	-1.854558	-4.879319	-2.135018

H	-2.243414	-5.846508	-0.698488
H	-3.270236	-5.944670	-2.132898
H	-3.274304	-2.825637	-2.684848
H	-4.737484	-3.817515	-2.747493
H	-4.669958	-2.430129	-1.654528
H	-5.320230	-5.359429	-0.768283
H	-5.310803	-3.917202	0.264610
H	-4.298802	-5.312740	0.676971
C	-5.889596	-1.971708	2.689596
C	-6.369151	-1.609230	3.956454
C	-7.721885	-1.750302	4.221344
C	-8.554394	-2.243696	3.223802
C	-7.988225	-2.576828	1.996314
N	-6.692975	-2.450440	1.720100
H	-5.682293	-1.227792	4.699479
H	-8.119963	-1.478491	5.190945
H	-9.616643	-2.369147	3.387333
H	-8.606885	-2.964745	1.193690

2.13. Cartesian coordinates of the molecule 4m

	x	y	z
C	4.144966	1.160227	1.047838
C	2.973233	0.543506	0.609677
C	2.934624	-0.113006	-0.636566
C	4.043060	-0.177043	-1.473425
C	5.200970	0.443685	-1.019929
C	5.254023	1.102364	0.218766
N	1.636379	-0.627761	-0.736246
C	0.966792	-0.227041	0.445628
N	1.744251	0.461457	1.241375
C	-0.404188	-0.439359	0.684799
C	-1.580800	-0.538283	0.928857
H	4.169104	1.663328	2.005283
H	3.996376	-0.672335	-2.430491
H	6.085213	0.421781	-1.644308
H	6.178786	1.573035	0.527696
O	0.117731	-2.128775	-1.425330
C	-0.628153	-2.984166	-2.385363
C	0.279600	-4.097114	-2.898686
C	-1.183994	-2.111165	-3.504104
C	-1.744767	-3.548969	-1.517203
C	1.188142	-1.443743	-1.795677
O	1.765910	-1.485638	-2.853491
H	1.074503	-3.707327	-3.529722
H	0.722223	-4.641022	-2.062345
H	-0.319124	-4.799803	-3.481368

H	-0.386407	-1.696656	-4.117417
H	-1.830559	-2.717347	-4.141281
H	-1.780752	-1.298856	-3.087159
H	-2.366128	-4.218827	-2.113304
H	-2.369206	-2.747987	-1.128298
H	-1.330874	-4.110542	-0.679005
C	-2.960697	-0.663322	1.215647
C	-3.429470	-0.794065	2.534218
C	-4.784163	-0.919421	2.798667
C	-5.705167	-0.915125	1.753715
C	-5.270049	-0.782725	0.439147
C	-3.917032	-0.658511	0.194092
H	-2.706341	-0.794602	3.338540
H	-5.123778	-1.019915	3.821143
H	-6.763491	-1.012235	1.958655
H	-5.961449	-0.770867	-0.392749
F	-3.499847	-0.525408	-1.084245

2.14. Cartesian coordinates of the molecule 4n

	x	y	z
C	4.124816	1.274748	0.997250
C	2.962537	0.668159	0.523139
C	2.983198	-0.093237	-0.661038
C	4.147003	-0.272789	-1.400786
C	5.296424	0.338149	-0.912353
C	5.289136	1.100253	0.265625
N	1.662517	-0.534578	-0.834534
C	0.931833	-0.014442	0.268062
N	1.689125	0.689878	1.066681
C	-0.435583	-0.252753	0.509392
C	-1.592967	-0.410332	0.810828
H	4.099967	1.858888	1.907483
H	4.154127	-0.863998	-2.302217
H	6.223479	0.219168	-1.458905
H	6.209793	1.556989	0.606188
O	-0.070329	-1.521347	-1.873844
C	-0.748816	-2.436644	-2.825997
C	-0.239319	-3.857746	-2.614462
C	-0.541617	-1.943778	-4.253812
C	-2.208107	-2.310707	-2.410689
C	1.245451	-1.362275	-1.893107
O	2.028525	-1.827845	-2.684286
H	0.805064	-3.954110	-2.902578
H	-0.351135	-4.148042	-1.568359
H	-0.832278	-4.543078	-3.222935
H	0.495882	-2.042310	-4.562981

H	-1.166954	-2.533242	-4.927154
H	-0.841533	-0.897884	-4.341136
H	-2.825077	-2.960110	-3.033287
H	-2.550723	-1.283264	-2.534907
H	-2.340243	-2.595706	-1.367342
C	-2.953363	-0.629088	1.151577
C	-3.298589	-1.098009	2.429151
C	-4.623553	-1.335639	2.761221
C	-5.601050	-1.098068	1.809010
C	-5.300538	-0.625949	0.542140
C	-3.973255	-0.391412	0.217216
H	-2.517505	-1.276341	3.155865
H	-4.904440	-1.699525	3.740372
H	-6.097087	-0.446652	-0.167463
H	-3.715360	-0.018250	-0.763952
F	-6.892492	-1.333853	2.127035

2.15. Cartesian coordinates of the molecule 4o

	x	y	z
C	1.222609	0.634467	2.338269
C	0.078624	-0.070334	1.968754
C	0.086051	-0.903544	0.834313
C	1.218754	-1.059750	0.043241
C	2.351265	-0.349469	0.427100
C	2.356681	0.484582	1.554449
N	-1.209868	-1.439752	0.767157
C	-1.916212	-0.889596	1.874332
N	-1.164723	-0.088131	2.580039
C	-3.261609	-1.173910	2.185482
C	-4.403817	-1.373010	2.510159
H	1.207947	1.273388	3.211246
H	1.214259	-1.701090	-0.823264
H	3.253416	-0.445657	-0.163925
H	3.262139	1.018463	1.814192
O	-2.911095	-2.654042	-0.056763
C	-3.612920	-3.575118	-0.978864
C	-2.941211	-4.944045	-0.950441
C	-3.651880	-2.969697	-2.378323
C	-5.008618	-3.637270	-0.369559
C	-1.638907	-2.327198	-0.235105
O	-0.903037	-2.704478	-1.114598
H	-1.944805	-4.906309	-1.383966
H	-2.871060	-5.309895	0.075472
H	-3.545854	-5.649998	-1.522991
H	-2.658217	-2.920944	-2.817786
H	-4.286715	-3.586946	-3.016789

H	-4.077209	-1.965243	-2.344020
H	-5.642250	-4.293871	-0.967292
H	-5.458243	-2.644536	-0.342170
H	-4.962565	-4.024953	0.648304
C	-8.193494	-0.858580	2.555812
C	-6.735183	-0.614211	2.163394
C	-5.790416	-1.601105	2.884084
C	-5.987515	-1.524856	4.413039
C	-7.449625	-1.764339	4.794577
C	-8.387349	-0.793117	4.072948
H	-8.503879	-1.845780	2.193904
H	-6.441591	0.404793	2.433056
H	-6.061528	-2.614955	2.561217
H	-5.669563	-0.534958	4.753607
H	-7.726548	-2.793195	4.536260
H	-8.183323	0.227107	4.417484
H	-8.836041	-0.127785	2.058012
H	-6.603949	-0.706104	1.082972
H	-5.335387	-2.251928	4.901164
H	-7.567239	-1.672819	5.877422
H	-9.427386	-1.009548	4.330481

2.16. Cartesian coordinates of Ag^+ (charge +1)

	x	y	z
Ag	0	0	0

2.17. Cartesian coordinates of TS1 (charge +1)

	x	y	z
C	3.662499	1.593233	0.892982
C	2.583750	0.828237	0.447794
C	2.742327	-0.112656	-0.588684
C	3.966630	-0.322143	-1.211081
C	5.029403	0.449303	-0.755684
C	4.884525	1.390811	0.276612
N	1.460031	-0.670891	-0.781756
C	0.630557	-0.040899	0.186502
N	1.276111	0.839290	0.896989
H	3.530279	2.310761	1.691017
H	4.092533	-1.053276	-1.993015
H	6.002080	0.313446	-1.210288
H	5.746631	1.962340	0.593948
O	-0.131368	-1.762644	-2.009155
C	-0.613631	-2.813227	-2.980986
C	-0.210898	-4.190798	-2.474602
C	-0.090010	-2.499152	-4.374493
C	-2.126908	-2.641733	-2.917571

C	1.194757	-1.631358	-1.766535
O	2.063921	-2.227642	-2.335418
H	0.865031	-4.332860	-2.526146
H	-0.543543	-4.336929	-1.445540
H	-0.687004	-4.949563	-3.097279
H	0.985118	-2.639017	-4.438015
H	-0.569191	-3.168705	-5.090606
H	-0.332475	-1.472839	-4.657906
H	-2.618773	-3.336930	-3.598092
H	-2.425766	-1.637707	-3.274399
H	-2.512766	-2.836994	-1.914573
C	-0.731798	-0.340783	0.427389
C	-1.811597	-0.575121	0.960331
C	-3.014306	-0.885989	1.643994
C	-3.567129	-2.175685	1.554937
C	-4.732284	-2.472743	2.241314
C	-5.351754	-1.497284	3.020898
C	-4.804597	-0.219950	3.116965
C	-3.642526	0.094202	2.430791
Ag	-2.038452	-0.198044	-1.509400
H	-3.068302	-2.933682	0.964424
H	-5.156076	-3.466474	2.178430
H	-6.260316	-1.735621	3.558654
H	-5.284963	0.531309	3.729858
H	-3.207224	1.082107	2.502537

2.18. Cartesian coordinates of TSIIa$_{endo}$ (charge +1)

	x	y	z
C	3.029894	0.064291	0.384387
C	3.302187	-0.560462	-0.849603
C	4.618440	-0.817103	-1.218991
C	5.622499	-0.439491	-0.337404
C	5.330944	0.179860	0.885466
C	4.021776	0.445845	1.273829
N	2.128094	-0.840461	-1.548771
C	1.141461	-0.424168	-0.823682
N	1.624193	0.158201	0.417536
C	0.789775	0.647496	1.329172
O	-0.492913	0.606234	1.119616
C	-1.064325	0.061039	-0.101761
C	-0.262835	-0.458632	-1.041527
C	-2.518277	0.197373	-0.058938
C	-3.230356	-0.028912	1.124958
C	-4.614678	0.067541	1.138599
C	-5.305038	0.399488	-0.023209
C	-4.603752	0.640438	-1.201000

C	-3.219781	0.543251	-1.220380
H	4.837856	-1.295220	-2.163646
H	6.655896	-0.626789	-0.597911
H	6.142000	0.458844	1.544895
H	3.796560	0.923027	2.215059
Ag	-0.898085	-1.416820	-2.817994
H	-2.703565	-0.309692	2.026799
H	-5.157262	-0.124368	2.055287
H	-6.384449	0.476394	-0.009326
H	-5.135254	0.919728	-2.101584
H	-2.672383	0.769846	-2.126425
C	0.465526	1.827287	3.536824
C	-0.384888	0.756886	4.193670
C	-0.331132	2.977555	2.948558
C	1.586789	2.306550	4.439075
H	-0.845665	1.184849	5.085173
H	0.314187	3.646534	2.378167
H	2.193665	1.470556	4.786299
H	-0.755947	3.550160	3.774482
H	-1.181525	0.410586	3.539490
H	0.226221	-0.090601	4.505300
H	2.225040	3.023087	3.922286
H	-1.150185	2.637328	2.319301
H	1.153142	2.799772	5.309536
O	1.274395	1.156176	2.399288

2.19. Cartesian coordinates of TSII'a_{endo} (charge +1)

	x	y	z
C	2.955389	0.057893	0.340510
C	3.204469	-0.595966	-0.883291
C	4.513818	-0.856049	-1.274240
C	5.534531	-0.452693	-0.423732
C	5.265976	0.195189	0.789588
C	3.964070	0.465223	1.199077
N	2.017146	-0.897993	-1.550260
C	1.044153	-0.468057	-0.814784
N	1.550285	0.146767	0.401244
C	0.733048	0.655756	1.317627
O	-0.553571	0.604182	1.136314
C	-1.148125	0.025829	-0.058482
C	-0.364299	-0.513694	-1.001888
C	-2.601467	0.157041	0.011928
C	-3.287237	-0.044790	1.215575
C	-4.671323	0.046866	1.256522
C	-5.387492	0.349696	0.102408
C	-4.712437	0.565841	-1.095324

C	-3.328812	0.473326	-1.141978
H	4.715394	-1.356309	-2.211369
H	6.563052	-0.641946	-0.701525
H	6.089473	0.493558	1.424653
H	3.756611	0.964290	2.133013
Ag	-1.032581	-1.518582	-2.739996
H	-2.740259	-0.303158	2.112079
H	-5.193582	-0.126100	2.188673
H	-6.466674	0.423087	0.137579
H	-5.264148	0.822266	-1.990529
H	-2.801623	0.680706	-2.064459
C	0.449583	1.892494	3.499239
C	-0.388036	0.839138	4.198995
C	-0.358571	3.027070	2.896460
C	1.587121	2.394598	4.368141
H	-0.830529	1.289325	5.088784
H	0.275926	3.682113	2.298411
H	2.200398	1.567623	4.725657
H	-0.769881	3.619798	3.714972
H	-1.197813	0.477676	3.569673
H	0.228923	-0.000922	4.519063
H	2.215626	3.097212	3.821289
H	-1.188005	2.670321	2.290302
H	1.169475	2.910287	5.233401
O	1.237659	1.193329	2.364161

2.20. Cartesian coordinates of TSIIb$_{exo}$ (charge +1)

	x	y	z
C	3.391689	-0.319611	0.161007
C	3.319653	0.995250	0.684490
C	4.487954	1.637192	1.073059
C	5.687149	0.946923	0.926393
C	5.732905	-0.351889	0.406836
C	4.574393	-1.016746	0.010833
N	1.990329	1.461274	0.726436
C	1.280009	0.489964	0.255191
N	2.047648	-0.636086	-0.112297
C	1.241577	-1.582874	-0.608752
O	-0.008444	-1.201156	-0.595521
C	-0.089576	0.200655	-0.033394
C	-1.193641	0.933667	0.088054
C	-2.564482	0.600618	-0.228735
C	-2.999270	-0.722973	-0.449584
C	-4.322419	-0.992066	-0.754821
C	-5.245850	0.046726	-0.859641
C	-4.839537	1.359311	-0.641336

C	-3.519693	1.628818	-0.316992
H	4.457214	2.640438	1.475234
H	6.611189	1.426052	1.221876
H	6.687195	-0.851911	0.310285
H	4.602689	-2.019900	-0.390856
Ag	-0.556453	2.850465	0.891265
H	-2.297760	-1.538719	-0.364734
H	-4.641603	-2.014953	-0.909567
H	-6.278906	-0.168667	-1.100899
H	-5.554192	2.168860	-0.712770
H	-3.205381	2.649203	-0.133149
C	0.773916	-3.830385	-1.620093
C	0.059399	-3.274050	-2.837132
C	-0.153401	-4.293801	-0.513065
C	1.814952	-4.870742	-1.980759
H	-0.458505	-4.098636	-3.329609
H	0.410706	-4.588891	0.372211
H	2.514877	-4.484166	-2.721148
H	-0.698239	-5.169387	-0.869983
H	-0.679959	-2.520201	-2.576206
H	0.770984	-2.855451	-3.549395
H	2.367649	-5.193485	-1.098878
H	-0.882851	-3.533768	-0.241546
H	1.310572	-5.738855	-2.406574
O	1.674202	-2.700484	-1.034344

2.21. Cartesian coordinates of TSII'b_{exo} (charge +1)

	x	y	z
C	3.347991	-0.280019	0.168407
C	3.267352	1.024034	0.717039
C	4.431501	1.666317	1.117273
C	5.635264	0.987157	0.956810
C	5.689544	-0.301055	0.412342
C	4.535320	-0.966012	0.004173
N	1.934928	1.480173	0.768162
C	1.230963	0.513235	0.278449
N	2.005980	-0.600155	-0.110813
C	1.205750	-1.543749	-0.622635
O	-0.046716	-1.170683	-0.602057
C	-0.136988	0.220310	-0.013465
C	-1.245513	0.943225	0.126957
C	-2.615919	0.611924	-0.192671
C	-3.041449	-0.703586	-0.473008
C	-4.365059	-0.969843	-0.778461
C	-5.298891	0.064054	-0.823461
C	-4.902111	1.368307	-0.546165

C	-3.581176	1.634235	-0.223344
H	4.394249	2.661503	1.538501
H	6.556206	1.466849	1.260937
H	6.647151	-0.792593	0.305653
H	4.570174	-1.961008	-0.416843
Ag	-0.613345	2.845572	0.970748
H	-2.332043	-1.515970	-0.435943
H	-4.676565	-1.986861	-0.980377
H	-6.332322	-0.149140	-1.065079
H	-5.624487	2.173718	-0.571723
H	-3.273753	2.647680	0.005098
C	0.752324	-3.778317	-1.668432
C	0.032917	-3.208794	-2.876462
C	-0.170611	-4.264531	-0.567592
C	1.799856	-4.806145	-2.045746
H	-0.480711	-4.029227	-3.380227
H	0.396535	-4.569616	0.312335
H	2.496403	-4.403813	-2.780968
H	-0.710224	-5.138038	-0.937285
H	-0.710586	-2.463145	-2.603952
H	0.741033	-2.775524	-3.583378
H	2.355688	-5.138369	-1.169399
H	-0.904613	-3.513589	-0.283197
H	1.300844	-5.671119	-2.484075
O	1.645579	-2.651231	-1.067006

2.22. Cartesian coordinates of the species Ia_{endo}

	x	y	z
C	2.810065	0.138288	0.489350
C	3.074663	-0.028864	-0.887678
C	4.393619	-0.054222	-1.337842
C	5.404447	0.087020	-0.396858
C	5.119184	0.251499	0.966824
C	3.810921	0.280492	1.438856
N	1.892133	-0.149698	-1.609612
C	0.922500	-0.057813	-0.736053
N	1.415095	0.119900	0.577529
C	0.622606	0.221662	1.703294
O	-0.713739	0.172072	1.446536
C	-1.264201	-0.004877	0.167281
C	-0.487755	-0.136013	-0.924616
C	-2.729782	-0.051317	0.252223
C	-3.354338	-0.562854	1.396597
C	-4.738802	-0.643350	1.466287
C	-5.523628	-0.201361	0.406137
C	-4.912440	0.334241	-0.724020

C	-3.529010	0.412282	-0.798995
O	1.033628	0.348910	2.823365
H	4.608807	-0.180701	-2.390627
H	6.437830	0.070340	-0.719815
H	5.935398	0.358430	1.669868
H	3.576435	0.406219	2.485432
Ag	-1.058523	-0.568718	-2.897419
H	-2.747860	-0.901483	2.224850
H	-5.206138	-1.052267	2.353503
H	-6.603216	-0.260829	0.464953
H	-5.516092	0.707332	-1.542265
H	-3.059206	0.865334	-1.661947

2.23. Cartesian coordinates of the species Ib_{exo}

	x	y	z
C	3.344634	-0.346807	0.199153
C	3.269086	1.016880	0.593201
C	4.435201	1.690046	0.944817
C	5.634051	0.988312	0.894009
C	5.684577	-0.356595	0.502691
C	4.533301	-1.052823	0.145714
N	1.944764	1.476251	0.557307
C	1.257001	0.440156	0.161455
N	2.020200	-0.683103	-0.073276
C	1.227747	-1.754984	-0.488823
O	-0.059648	-1.281661	-0.513588
C	-0.113711	0.099292	-0.112609
C	-1.194318	0.881754	-0.014865
C	-2.580859	0.541659	-0.287936
C	-2.987537	-0.733978	-0.732380
C	-4.324772	-1.006355	-0.978419
C	-5.295153	-0.025285	-0.791282
C	-4.915319	1.239386	-0.353414
C	-3.578723	1.514593	-0.107338
H	4.399173	2.728101	1.247547
H	6.553841	1.491782	1.163452
H	6.639167	-0.866055	0.477260
H	4.559341	-2.090115	-0.157879
Ag	-0.502328	2.815697	0.648684
H	-2.250213	-1.507540	-0.882675
H	-4.612495	-1.993501	-1.319231
H	-6.337658	-0.245292	-0.985609
H	-5.660740	2.010880	-0.204305
H	-3.280365	2.499230	0.233102
O	1.563437	-2.864889	-0.772297

2.24. Cartesian coordinates of the molecule 5b

	x	y	z
C	2.823770	0.100132	0.494606
C	3.071521	0.050439	-0.894704
C	4.383955	0.067599	-1.362614
C	5.405612	0.133170	-0.425262
C	5.137006	0.181403	0.950890
C	3.835139	0.165794	1.440739
N	1.880524	-0.011475	-1.612999
C	0.929520	0.001308	-0.722759
N	1.428608	0.068205	0.599023
C	0.651342	0.084485	1.736149
O	-0.698651	0.052295	1.489405
C	-1.261615	-0.018006	0.229251
C	-0.482942	-0.055769	-0.871850
C	-2.723576	-0.064056	0.276880
C	-3.384124	-0.377581	1.471417
C	-4.770653	-0.440931	1.509472
C	-5.517551	-0.188807	0.364111
C	-4.868402	0.133678	-0.825305
C	-3.484734	0.199330	-0.870144
O	1.062427	0.127386	2.859397
H	4.584680	0.030388	-2.424928
H	6.434849	0.147574	-0.760827
H	5.961862	0.231746	1.649978
H	3.615201	0.202237	2.497363
H	-0.900711	-0.142413	-1.860898
H	-2.806187	-0.572715	2.363274
H	-5.268290	-0.688423	2.438647
H	-6.598683	-0.236344	0.397265
H	-5.443546	0.344082	-1.718119
H	-2.996349	0.475269	-1.795177

2.25. Cartesian coordinates of the molecule 6b

	x	y	z
C	3.050333	-0.545297	0.000000
C	3.066852	0.874887	0.000000
C	4.288376	1.542784	0.000000
C	5.448188	0.778234	0.000000
C	5.406622	-0.623542	0.000000
C	4.199776	-1.316074	0.000000
N	1.767851	1.400804	0.000000
C	1.001392	0.353311	0.000000
N	1.693386	-0.853113	0.000000
C	0.835269	-1.940631	0.000000

O	-0.442756	-1.402451	0.000000
C	-0.399116	0.001020	0.000000
C	-1.477460	0.795160	0.000000
C	-2.888931	0.459064	0.000000
C	-3.380931	-0.858392	0.000000
C	-4.747225	-1.094849	0.000000
C	-5.651334	-0.035262	0.000000
C	-5.178826	1.273683	0.000000
C	-3.813979	1.516996	0.000000
O	1.077122	-3.106944	0.000000
H	4.319143	2.624023	0.000000
H	6.410222	1.274807	0.000000
H	6.334411	-1.180932	0.000000
H	4.157089	-2.396274	0.000000
H	-1.233096	1.851805	0.000000
H	-2.692318	-1.689458	0.000000
H	-5.110533	-2.114962	0.000000
H	-6.716680	-0.229345	0.000000
H	-5.874107	2.103758	0.000000
H	-3.448740	2.537191	0.000000

2.26. Cartesian coordinates of isobutylene

	x	y	z
C	0.122978	0.176824	-0.018765
C	0.885152	1.273422	-0.133786
C	0.715720	-1.201552	0.112027
C	-1.381621	0.243514	-0.010912
H	0.444060	2.267571	-0.227493
H	1.975078	1.212669	-0.138022
H	0.392222	-1.680483	1.051174
H	1.813170	-1.177772	0.097545
H	0.372778	-1.856137	-0.706437
H	-1.745464	1.274427	-0.110691
H	-1.805607	-0.354556	-0.834525
H	-1.788492	-0.178465	0.922940

2.27. Cartesian coordinates of TFA

	x	y	z
C	-0.800793	-0.026695	0.018073
C	0.591474	0.691616	0.075917
O	1.454308	0.198451	0.988300
O	0.840180	1.608467	-0.658531
F	-0.972238	-0.619115	-1.177811
F	-0.901609	-1.000643	0.985780
F	-1.794384	0.854922	0.217189
H	1.035667	-0.539001	1.479018

2.28. Cartesian coordinates of anion TFA (Charge -1)

	x	y	z
C	-0.593034	0.038451	0.000000
C	1.004796	-0.035012	0.000000

O	1.581054	1.074563	0.000000
O	1.420749	-1.215737	0.000000
F	-1.118262	1.308332	0.000000
F	-1.147652	-0.585298	1.100062
F	-1.147652	-0.585298	-1.100062

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