ACS Catalysis

Supporting Information

Exploring Rhodium(I) Complexes [RhCl(COD)(PR_3)] (COD = 1,5-Cyclooctadiene) as Catalysts for Nitrile Hydration Reactions in Water: The Aminophosphines Make the Difference

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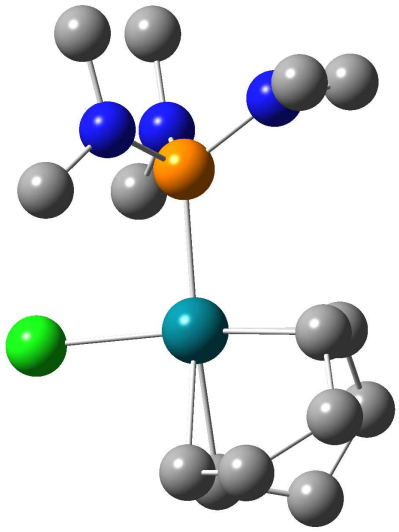
Theoretical Calculations: Equilibrium Geometries of Complexes 3h-k.

All the theoretical calculations were performed using the Gaussian09 program.[1] Geometry optimizations were carried out using the B3LYP hybrid density functional theory (DFT) functional. We used the LANL2DZ effective core potential for the Rh atom along with its associated basis set, augmented by a shell of f polarization basis functions. For the non-metal atoms, C, N, P, Cl and H, we used the 6-31G* basis set. Analytical frequency calculations were performed to determine whether the optimized geometries were minima on the potential energy surface.

Figure S1. Optimized Structure of Complex [RhCl(COD){$P(NMe_2)_3$}] (**3h**) and Cartesian Coordinates.

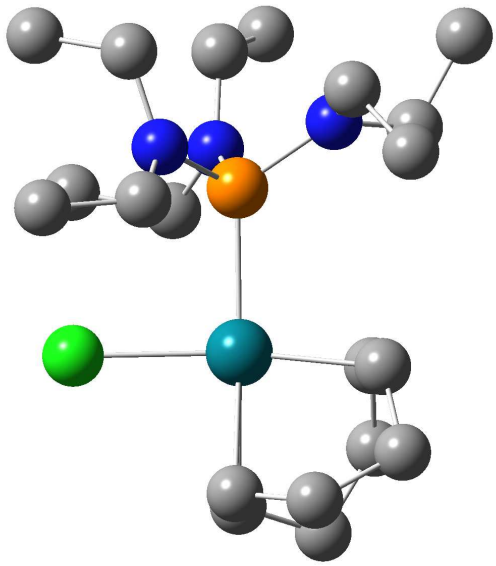


C	-1.340478	1.592582	0.746668
C	-1.424981	1.605753	-0.662097
C	-2.728918	1.598922	-1.458296
C	-3.209035	0.174904	-1.820589
H	-2.582422	2.166242	-2.384834
H	-3.505888	2.136082	-0.903066
C	-2.498731	1.507834	1.722661
C	-3.600884	0.510788	1.298870

H	-2.933999	2.506758	1.890693
H	-2.088605	1.190583	2.689339
C	-2.893646	-0.862563	-0.762970
H	-2.712808	-0.140982	-2.745456
H	-4.288255	0.181112	-2.042032
C	-3.034593	-0.715608	0.604717
Rh	-0.846341	-0.364197	0.033360
H	-0.581078	2.042261	-1.190016
H	-0.451485	2.040199	1.186563
H	-2.722303	-1.871631	-1.130961
H	-4.332068	1.003537	0.649961
H	-4.154322	0.191125	2.189318
H	-2.933152	-1.615918	1.206045
Cl	-0.431435	-2.752399	0.226499
P	1.494770	0.088608	-0.012401
N	2.247591	-0.624003	-1.362802
N	2.232802	-0.286608	1.476557
N	2.131502	1.692820	-0.200377
C	1.563168	-1.584324	-2.226419
C	3.688295	-0.583707	-1.590889
C	1.552562	-1.100815	2.483188
C	3.667857	-0.174366	1.717714
C	2.157006	2.646338	0.901959
C	2.157911	2.349466	-1.501449
H	2.056210	2.126599	1.855396
H	1.351090	3.393244	0.819379
H	3.111353	3.193834	0.906003
H	2.057656	1.613850	-2.300152
H	3.111636	2.880679	-1.637309
H	1.351076	3.093190	-1.604292
H	4.114792	0.569548	1.056990
H	4.186305	-1.134934	1.575742
H	3.839581	0.149282	2.753464
H	0.479462	-1.120560	2.294082

H	1.735593	-0.667496	3.477160
H	1.910039	-2.139431	2.483190
H	4.140628	0.256997	-1.063782
H	3.886745	-0.452607	-2.663787
H	4.181385	-1.513827	-1.269764
H	0.484631	-1.521026	-2.087320
H	1.866141	-2.617833	-2.013332
H	1.803799	-1.355024	-3.274940

Figure S2. Optimized Structure of Complex [RhCl(COD){$P(NEt_2)_3$}] (**3i**) and Cartesian Coordinates.

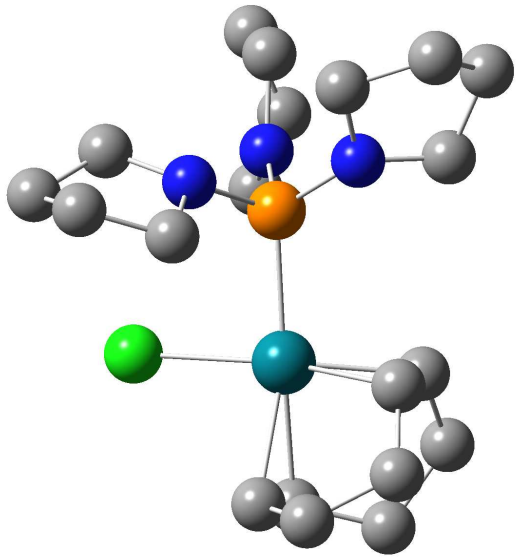


C	-3.428053	-0.901844	-0.490780
C	-3.474891	-0.726032	0.881635
C	-4.022849	0.502915	1.585012
C	-2.916296	1.532814	1.903177
H	-4.502981	0.193674	2.520572
H	-4.810023	0.962721	0.979041
C	-3.856668	0.100240	-1.542861
C	-3.383178	1.543148	-1.252773
H	-4.950368	0.075329	-1.673741
H	-3.430516	-0.227179	-2.498317
C	-1.835202	1.616368	0.841873
H	-2.429832	1.249144	2.844462
H	-3.358861	2.527434	2.077676
C	-2.023775	1.596417	-0.556325
Rh	-1.349893	-0.344235	0.139216
H	-3.311748	-1.608945	1.494455
H	-3.265575	-1.916757	-0.846789
H	-0.925942	2.089450	1.206742

H	-4.129044	2.078460	-0.654377
H	-3.318295	2.089406	-2.201299
H	-1.230499	2.035691	-1.153228
Cl	-0.896954	-2.709732	0.459347
P	1.012468	0.089767	-0.129957
N	1.706401	-1.035888	-1.209030
N	1.797153	0.076437	1.384696
N	1.633541	1.603925	-0.749760
C	0.882682	-1.567396	-2.309125
C	3.160388	-1.213925	-1.347159
C	1.018453	-3.070910	-2.551611
H	0.763117	-3.625570	-1.645785
H	2.027207	-3.347497	-2.878415
H	0.325664	-3.368417	-3.348376
H	1.125177	-1.029151	-3.243161
H	-0.162145	-1.343812	-2.071926
C	3.727096	-2.431162	-0.606560
H	3.284566	-3.362461	-0.968107
H	3.525226	-2.365178	0.465919
H	4.813721	-2.486337	-0.751550
H	3.391705	-1.297479	-2.419144
H	3.673382	-0.309906	-1.004080
C	1.142034	-0.584575	2.529903
C	3.206778	0.449786	1.580620
C	1.729497	-1.942515	2.921076
H	1.188076	-2.337836	3.788576
H	2.789072	-1.874934	3.196136
H	1.614239	-2.656495	2.101422
H	1.177504	0.101224	3.386913
H	0.087425	-0.717724	2.274926
C	3.463317	1.312450	2.822181
H	3.285190	0.766420	3.753825
H	2.833129	2.208488	2.827758
H	4.511448	1.633801	2.828174

H	3.839621	-0.447478	1.640218
H	3.521263	1.005063	0.695302
C	1.407189	2.840303	0.015068
C	2.582661	3.825937	-0.014828
H	2.744022	4.253680	-1.009665
H	3.514484	3.347783	0.304656
H	2.375954	4.659765	0.666143
H	0.502533	3.363879	-0.330317
H	1.224262	2.549266	1.052009
C	1.900509	1.789597	-2.182285
C	0.748801	2.343377	-3.034099
H	-0.100609	1.652661	-3.052108
H	1.089073	2.485863	-4.067012
H	0.393394	3.313857	-2.669892
H	2.215151	0.831486	-2.595600
H	2.766585	2.456858	-2.280482

Figure S3. Optimized Structure of Complex [RhCl(COD){P(*N*-pyrrolidinyl)$_3$}] (**3j**) and Cartesian Coordinates.

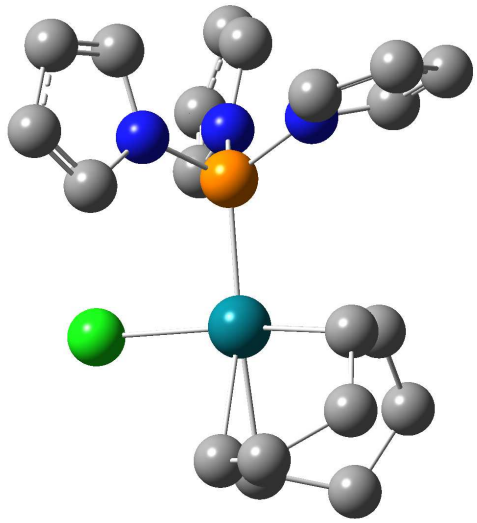


C	1.841579	-1.886972	0.246792
C	1.931100	-1.411085	-1.080683
C	3.244559	-1.144834	-1.814430
C	3.741995	0.310979	-1.657072
H	3.106325	-1.354910	-2.881510
H	4.009970	-1.849462	-1.470251
C	2.999809	-2.154794	1.190798
C	4.105666	-1.075014	1.152814
H	3.434168	-3.148985	0.993775
H	2.588571	-2.202555	2.206772
C	3.418523	0.926025	-0.310113
H	3.263470	0.932840	-2.422311
H	4.824624	0.366909	-1.854089
C	3.548230	0.318535	0.924117
Rh	1.355362	0.190395	0.241643
H	1.081163	-1.614286	-1.729008
H	0.951757	-2.454982	0.507870
H	3.245882	1.999673	-0.313250

H	4.843378	-1.313394	0.379807
H	4.650380	-1.089513	2.103979
H	3.441110	0.955194	1.799208
Cl	0.915343	2.388756	1.194983
P	-0.977949	-0.022565	-0.099918
N	-1.571955	-1.308788	-1.074019
N	-1.629585	1.287395	-0.989842
N	-1.855879	-0.092517	1.337669
C	-1.403302	-2.715322	-0.641273
C	-2.739429	-1.184789	-1.978481
C	-0.888651	1.739791	-2.188071
C	-2.268302	2.445714	-0.315439
C	-1.263555	0.077644	2.682965
C	-3.306049	-0.355687	1.419678
C	-3.629102	-0.219861	2.918678
H	-3.534945	-1.367912	1.057770
H	-3.883128	0.349376	0.808877
C	-2.300222	-0.576243	3.603165
H	-4.464727	-0.858550	3.222358
H	-3.899440	0.817403	3.149914
C	-1.794471	3.672662	-1.109608
H	-1.977482	2.510506	0.735000
H	-3.363064	2.341654	-0.367372
C	-1.508075	3.105484	-2.506628
C	-2.985292	-2.625016	-2.445450
H	-2.523949	-0.510609	-2.811111
H	-3.625936	-0.791045	-1.461222
C	-2.632131	-3.451061	-1.202387
H	-1.345866	-2.795581	0.451653
H	-0.480813	-3.142135	-1.055580
H	-2.162399	-1.664979	3.619441
H	-2.234640	-0.210398	4.632556
H	-1.126544	1.138431	2.925588
H	-0.276850	-0.392527	2.728318

H	-1.000204	1.022901	-3.010995
H	0.185851	1.841892	-1.973838
H	-0.869783	4.053451	-0.664350
H	-2.537231	4.477224	-1.112315
H	-2.440578	2.976183	-3.070834
H	-0.837446	3.733780	-3.101653
H	-2.306380	-2.874636	-3.270250
H	-4.011446	-2.778537	-2.794675
H	-3.458877	-3.416626	-0.482066
H	-2.423145	-4.503514	-1.418990

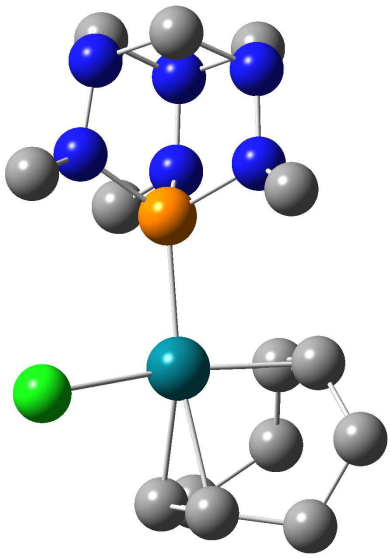
Figure S4. Optimized Structure of Complex [RhCl(COD){P(*N*-pyrrolyl)$_3$}] (**3k**) and Cartesian Coordinates.



C	1.798903	1.392392	-1.019878
C	1.845897	1.610650	0.370032
C	3.123604	1.679251	1.204404
C	3.546755	0.313389	1.790175
C	3.254403	-0.860933	0.881191
C	3.438105	-0.915922	-0.486434
C	4.044531	0.185256	-1.336265
C	2.971787	1.117252	-1.941427
Rh	1.226117	-0.449086	-0.048781
P	-1.042907	-0.012966	-0.034145
N	-1.586099	1.647954	0.034541
N	-1.950105	-0.508478	-1.411511
N	-1.884421	-0.627556	1.334205
C	-1.749026	2.369636	1.217416
C	-1.554952	2.557441	-1.023538
C	-1.854114	3.700564	0.901809
C	-1.733059	3.819682	-0.516347
C	-3.212352	-0.065814	-1.832817
C	-1.555215	-1.554667	-2.255037

C	-3.583124	-0.807669	-2.920578
C	-2.538735	-1.749260	-3.185145
C	-3.258077	-0.570486	1.592512
C	-1.250833	-1.144779	2.470586
C	-3.475438	-1.042079	2.857532
C	-2.205914	-1.402443	3.414135
Cl	0.759895	-2.805584	0.118081
H	-2.022060	4.502428	1.608318
H	-1.802190	1.860007	2.167528
H	-1.792620	4.729159	-1.099274
H	-1.454536	2.212116	-2.041484
H	-4.502709	-0.685288	-3.477818
H	-3.698881	0.762144	-1.342311
H	-2.518348	-2.489399	-3.973621
H	-0.630892	-2.079347	-2.066203
H	-4.442073	-1.135434	3.334872
H	-3.945950	-0.209865	0.844598
H	-2.024462	-1.826455	4.392508
H	-0.186843	-1.320503	2.459523
H	3.325287	-1.890826	-0.955318
H	4.762666	0.761000	-0.744768
H	4.618052	-0.271876	-2.150429
H	3.430277	2.066826	-2.261650
H	2.571811	0.653513	-2.851170
H	0.932321	1.797206	-1.539526
H	0.996254	2.135483	0.800691
H	3.042999	-1.802622	1.382459
H	2.966294	2.380665	2.031282
H	3.933407	2.105752	0.602553
H	3.002806	0.144245	2.726205
H	4.614995	0.327118	2.058388

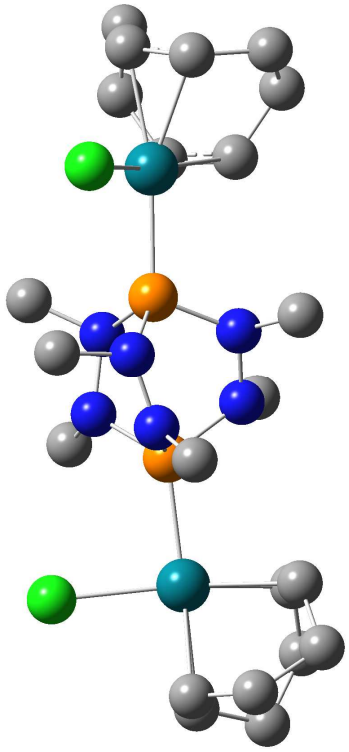
Figure S5. Optimized Structure of Complex [RhCl(COD)(THPA)] (**3l**) and Cartesian Coordinates.



C	-3.343140	0.555642	-0.868127
C	-3.490599	0.594377	0.507509
C	-3.529617	-0.649485	-1.764755
C	-3.940662	-0.570341	1.372429
C	-2.916421	-1.948741	-1.196651
C	-2.751400	-1.374711	1.942088
H	-4.540657	-0.182417	2.203525
H	-4.604984	-1.224645	0.799145
C	-1.635738	-1.712609	-0.398530
H	-2.693500	-2.625622	-2.029500
H	-3.646754	-2.476611	-0.573370
C	-1.577027	-1.490097	0.989523
H	-3.085372	-2.376820	2.256888
H	-2.392296	-0.877641	2.851721
H	-3.050917	-0.419119	-2.723317
H	-4.598564	-0.795779	-1.987213
Rh	-1.268364	0.415233	0.004114
H	-3.273838	1.512592	-1.378868

H	-0.732450	-2.121064	-0.845513
H	-3.497020	1.578438	0.970001
H	-0.646702	-1.782114	1.471876
P	1.065774	0.126403	0.000293
N	1.547871	-1.006841	-1.228788
N	1.681057	-0.794135	1.344143
N	2.276016	1.343460	-0.261417
N	2.956268	-1.353990	-1.222915
N	3.089813	-1.134008	1.225436
N	3.627969	0.793432	-0.232852
C	1.065244	-0.771559	-2.589044
H	1.283002	-1.662441	-3.185129
H	1.518842	0.103995	-3.076629
H	-0.015210	-0.609164	-2.550322
C	1.347283	-0.382936	2.705643
H	1.909752	0.495559	3.056640
H	1.554563	-1.216693	3.383642
H	0.283195	-0.134663	2.746713
C	2.234804	2.684830	0.317655
H	2.921747	3.321230	-0.248550
H	1.218419	3.070002	0.227935
H	2.536409	2.707814	1.376974
C	3.246884	-2.016221	0.057626
H	4.287341	-2.357683	0.031759
H	2.573728	-2.866480	0.171495
C	3.788794	-0.137891	-1.350239
H	3.538634	0.381226	-2.276059
H	4.837559	-0.452880	-1.389853
C	3.902669	0.085722	1.028218
H	3.740908	0.767613	1.865213
H	4.957491	-0.209980	1.027702
Cl	-1.173703	2.808264	-0.250104

Figure S6. Optimized Structure of Complex [{RhCl(COD)}$_2$(μ-THDP)] (**3m**) and Cartesian Coordinates.



C	-3.972416	1.491318	-1.225362
C	-4.050991	2.008364	0.081455
C	-5.159171	1.320151	-2.172833
C	-5.304691	2.433920	0.821657
C	-5.840377	-0.062796	-2.060533
H	-4.812306	1.458416	-3.203203
H	-5.886933	2.119906	-1.996014
C	-6.506891	1.487900	0.610353
H	-5.578784	3.465137	0.545440
H	-5.060860	2.462607	1.890768
C	-5.821764	-0.643661	-0.662459
H	-5.321236	-0.771596	-2.715342
H	-6.874903	-0.008913	-2.434658
C	-6.084795	0.032826	0.514839
H	-7.066009	1.774503	-0.286110

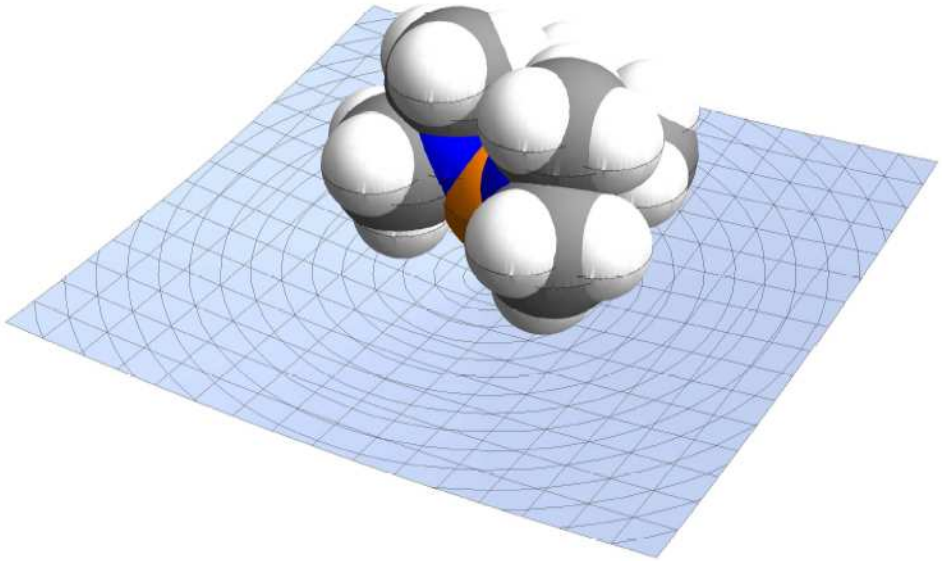
H	-7.202414	1.600939	1.449678
Rh	-3.819531	-0.131924	0.232533
H	-3.150817	2.489833	0.453433
H	-3.006380	1.598815	-1.714054
H	-5.785052	-1.728807	-0.605344
H	-6.203308	-0.572036	1.410891
Cl	-3.837762	-2.313799	1.247836
P	-1.478575	-0.187449	0.238074
N	-0.871984	-1.035396	-1.098784
N	-0.570916	-0.953591	1.504896
N	-0.613539	1.336604	0.054844
C	-1.499951	-1.001858	-2.414263
H	-2.580401	-0.913019	-2.275800
H	-1.297464	-1.945548	-2.930219
H	-1.139040	-0.176965	-3.043345
C	-0.583916	2.250073	1.209078
H	-1.572858	2.279128	1.675460
H	-0.335808	3.260048	0.864844
H	0.151811	1.936136	1.957128
C	-1.107366	-0.809394	2.866395
H	-0.855553	0.159183	3.320399
H	-0.716071	-1.608977	3.501882
H	-2.189369	-0.938556	2.814626
N	0.518070	-1.397952	-1.122249
N	0.877688	-0.628232	1.474201
N	0.718818	1.155955	-0.461773
C	0.912510	1.763505	-1.779985
H	0.665939	2.828060	-1.715511
H	0.296204	1.303330	-2.561221
H	1.965882	1.660400	-2.059101
C	0.697482	-2.857062	-1.012207
H	0.247524	-3.333570	-1.889096
H	0.218680	-3.254742	-0.110562
H	1.767307	-3.072857	-1.025171

C	1.621413	-1.667617	2.215091
H	1.268523	-2.676957	1.972012
H	1.518049	-1.504466	3.292208
H	2.680520	-1.587281	1.956675
P	1.490195	-0.347333	-0.140229
Rh	3.832269	-0.186681	-0.267022
Cl	4.038364	-2.147858	-1.641727
C	5.838676	0.445374	-1.079799
C	6.083834	-0.230024	0.102980
C	5.782287	1.945512	-1.271248
C	6.418166	0.422157	1.433449
C	5.033291	2.687641	-0.142790
C	5.167276	0.647131	2.311857
H	6.941307	1.368351	1.263465
H	7.122432	-0.220087	1.974296
C	3.858278	1.891240	0.421512
C	3.925052	1.021410	1.526150
H	5.374939	1.407164	3.082512
H	4.946928	-0.279623	2.855730
H	4.658070	3.639474	-0.536073
H	5.723580	2.953184	0.665429
H	2.999681	0.883960	2.084504
H	2.877023	2.309786	0.213171
H	5.270875	2.133307	-2.222091
H	6.799175	2.352498	-1.388930
H	5.876507	-0.142004	-1.993789
H	6.264308	-1.299423	0.023585

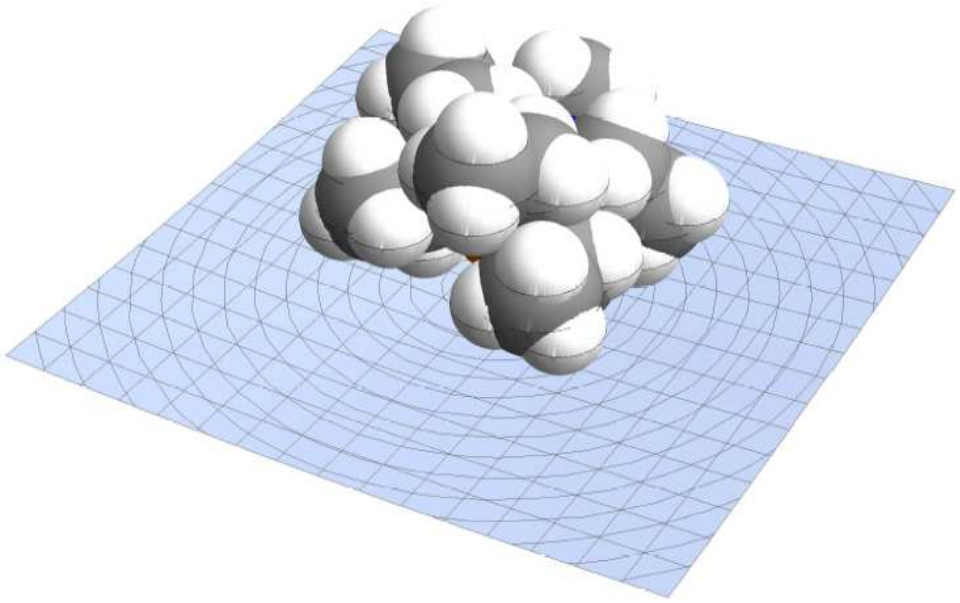
Calculation of the cone angles of ligands $P(NMe_2)_3$, $P(NEt_2)_3$, $P(N\text{-pyrrolidinyl})_3$, $P(N\text{-pyrrolyl})_3$, THPA and THDP in complexes 3h-m.

The cone angles of ligands **2h-m** have been calculated from the DFT-optimized structures of the Rh(I) complexes **3h-m** (Figures S1-S6) following the procedure described by Allen and coworkers.[2] The Mathematica[3] package FindConeAngle was used to compute the cone angles and visualize the solutions (copies are included below). This package is freely available at www.psicode.org and www.ccqc.uga.edu. The adopted van der Waals radii were r = 1.80 Å, 1.20 Å, 1.70 Å, 1.55 Å, 1.52 Å, 1.47 Å, 1.80 Å and 1.75 Å for P, H, C, N, O, F, S and Cl, respectively.[4]

```
[RhCl(COD){P(NMe2)3}](3h)
Ligand = 1   Ligand atoms forming cone = {13, 21, 27}
Cone angle (deg) = 167.893   Cone axis = {0.989427, -0.144398, 0.0135539}
```



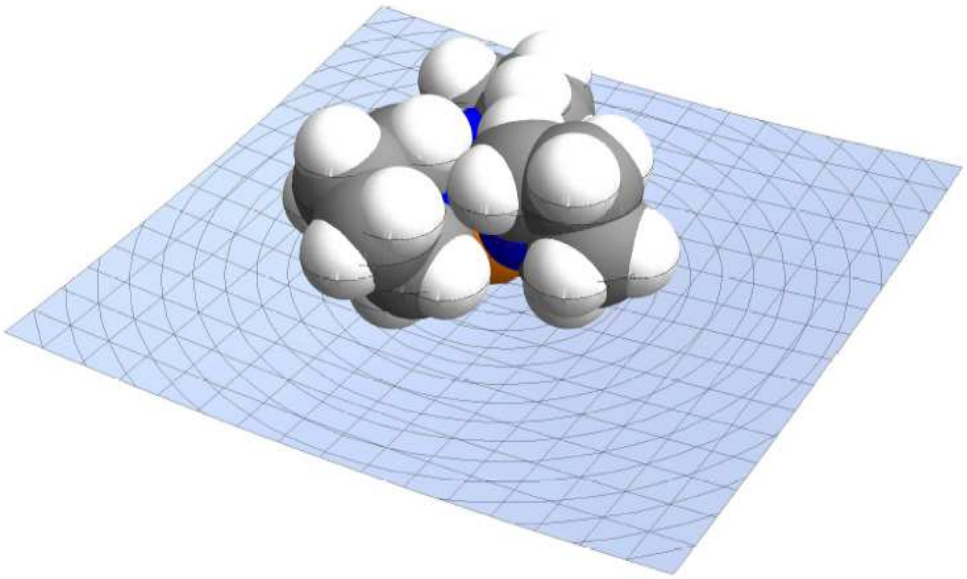
```
[RhCl(COD){P(NEt2)3}](3i)
Ligand = 1   Ligand atoms forming cone = {13, 27, 43}
Cone angle (deg) = 173.966   Cone axis = {0.998288, -0.0150942, -0.056505}
```



[RhCl(COD){P(N-pyrrolidinyl)3}](3j)

Ligand = 1 Ligand atoms forming cone = {27, 31, 33}

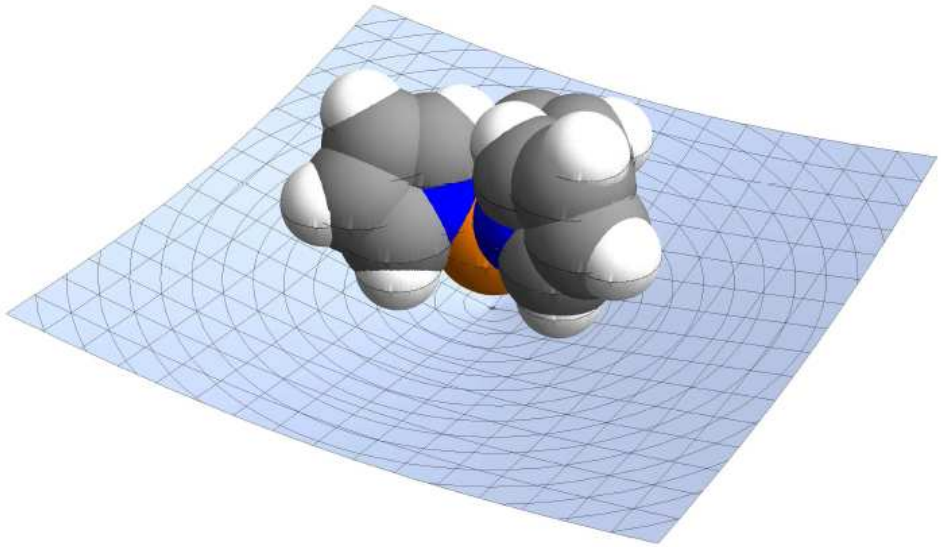
Cone angle (deg) = 169.803 Cone axis = {-0.993368, 0.10478, -0.0473308}



[RhCl(COD){P(N-pyrrolyl)3}](3k)

Ligand = 1 Ligand atoms forming cone = {9, 25, 29}

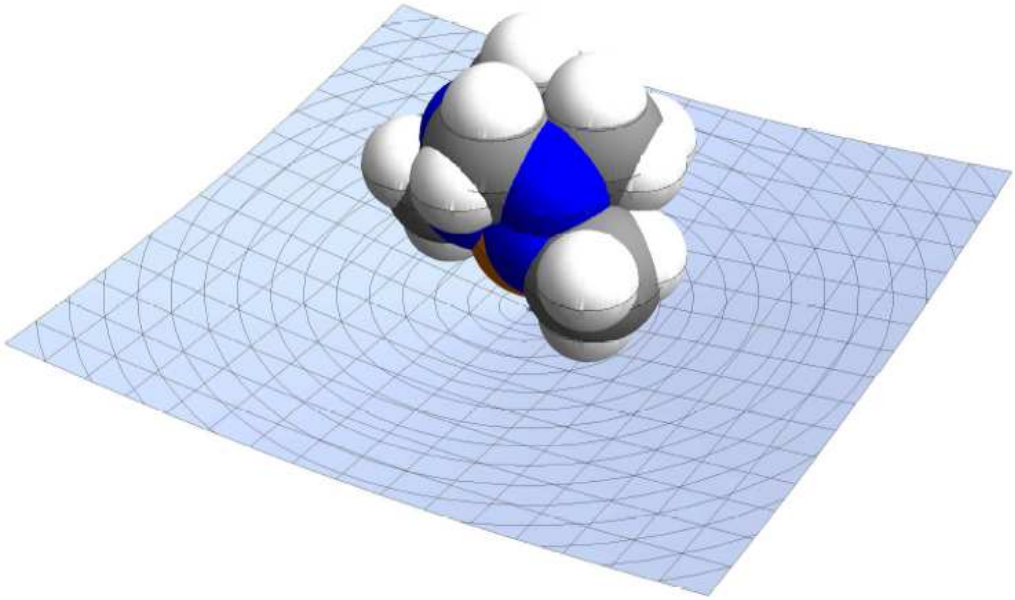
Cone angle (deg) = 157.778 Cone axis = {-0.992948, -0.0640536, 0.0997528}



[RhCl(COD)(THPA)](3l)

Ligand = 1 Ligand atoms forming cone = {12, 16, 19}

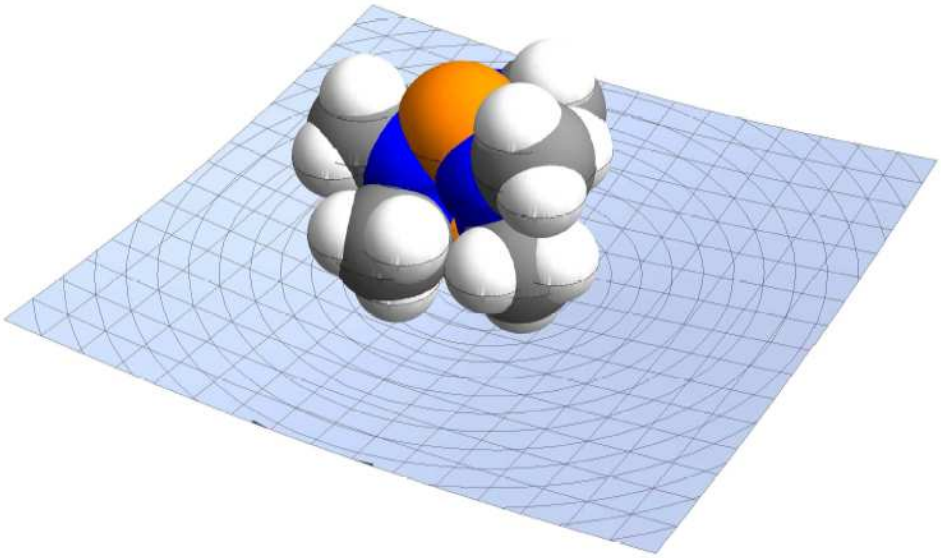
Cone angle (deg) = 165.022 Cone axis = {0.959736, -0.279847, -0.0243404}



[{RhCl(COD)}2(n-THDP)](3m)

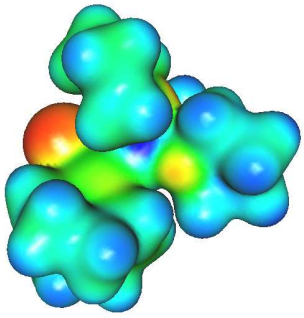
Ligand = 1 Ligand atoms forming cone = {24, 28, 32}

Cone angle (deg) = 165.899 Cone axis = {-0.971236, 0.0774635, 0.225168}

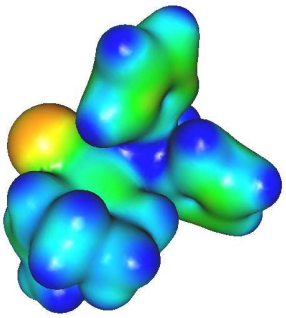


Electrostatic Properties of Complexes [RhCl(COD){P(N-pyrrolidinyl)$_3$}] (3j) and [RhCl(COD){P(N-pyrrolyl)$_3$}] (3k).

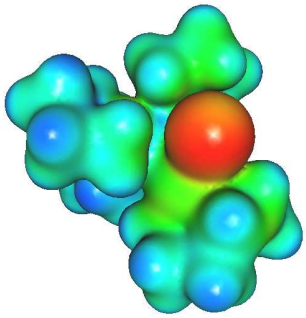
B3LYP/6-31G* (LANL2DZ-*f* for Rh) electrostatic potential mapped onto the charge density surface for the [RhCl(COD){P(N-pyrrolidinyl)$_3$}] (**3j**) and [RhCl(COD){P(N-pyrrolyl)$_3$}] (**3k**) complexes. Red indicates negative electrostatic potential and blue is positive potential. Molecular graphics were generated with the GABEDIT program. Note that the nitrogen atoms of the pyrrole moieties of **3k** show a more concentrated positive potential than the pyrrolidine ones in **3j**.



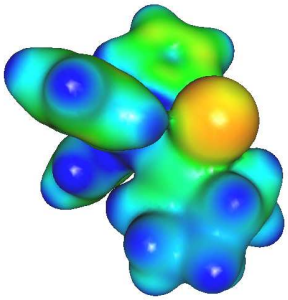
3j (front-view)



3k (front-view)



3j (rear view)



3k (rear view)

Relative Basicity of the N-atoms of the Pyrrolidine/Pyrrole Fragments in Complexes [RhCl(COD){P(N-pyrrolidinyl)$_3$}] (3j) and [RhCl(COD){P(N-pyrrolyl)$_3$}] (3k).

The molecular geometries and electronic energies in aqueous solution for **3j/3j-H$^+$** and **3k/3k-H$^+$** pairs were calculated. The initial geometries of the protonated complexes were built from the corresponding neutral forms by attaching on proton to the N atom bearing the more negative electrostatic potential in **3j/3k**. The SMD solvent model[5] included in the program Gaussian was employed to take into account continuum solvent effects on molecular geometries and energies from the outset. Geometry optimizations were carried out at the SMD-B3LYP/6-31G*(LANL2DZ for Rh) level of theory using the Gaussian09 program. Analytical frequency calculations were also performed to characterize the stationary points found as minima as well as to compute the thermal free energy corrections (G^{therm}). To further improve the quality of the calculated energy difference, we used the M06 DFT functional that has been reported to yield better thermochemical properties for organometallic systems by means of single-point SMD-M06/6-31+G**(LANL2DZ for Rh) calculations on the SMD-B3LYP geometries. To take into account the dispersion interactions, we computed the atom-pair wise DFT-D dispersion correction (E^{disp}) developed by Grimme and co-workers,[6] which was thereby added to the SMD-M06 energies. The single-point DFT-D calculations were done on the SMD-M06 geometries and using the zero damping option. The free energy in aqueous solution of the optimized structures was estimated by means of the following composite approximation:

$$G_{sol} = E_{\text{SMD-M06}} + G^{\text{therm}}{}_{\text{SMD-B3LYP}} + E^{\text{disp}}{}_{\text{DFT-m06}}$$

To assess the relative basicity of the N atoms of the pyrrolidine and pyrrole fragments in the **3j/3k** rhodium complexes, we computed the Gibbs reaction energy for the following acid-base exchange equilibrium:

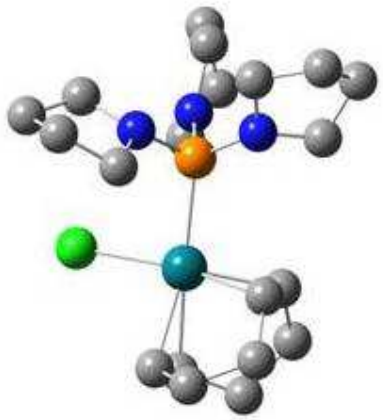
$$\mathbf{3j_{(aq)} + 3k\text{-}H^+_{(aq)} \rightleftharpoons 3j\text{-}H^+_{(aq)} + 3k_{(aq)}}$$

The resulting free energy difference, -37.12 kcal/mol, strongly favors the protonation of the pyrrolidine N atom in **3j** with respect to the pyrrole moiety in **3k**.

Inspection of the optimized geometries of **3j-H$^+$/3k-H$^+$** shows that P-N bond of the protonated heterocycle is significantly elongated by ~0.3 Å. The protonated N atom of the pyrrole fragment acquires a tetrahedral geometry what implies the loss of the aromatic stabilization characteristic of the pyrrole compounds.

$$\Delta G = (3j\text{-}H^+ + 3k) - (3j + 3k\text{-}H^+) = -37{,}12 \text{ Kcal/mol}$$

- Figure S7. Optimized Structure of Complex [RhCl(COD){P(*N*-pyrrolidinyl)$_3$}] (**3j**), Energy Data and Cartesian Coordinates.



$E_{SMD\text{-}m06}$ = - 1858,51017020

$G^{therm}_{SMD\text{-}B3LYP}$ = 0,488619

$E^{disp}_{DFT\text{-}m06}$ = - 0,01619009

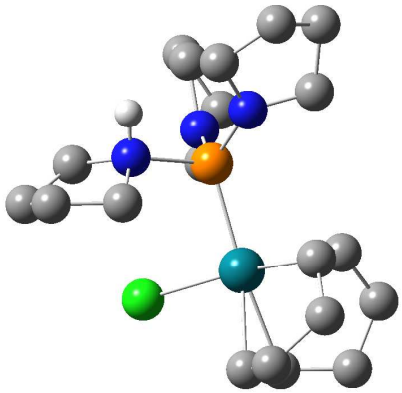
G_{sol} = - 1858,03774129

C	1.817335	-1.882586	0.084645
C	1.887867	-1.311796	-1.206176
C	3.188240	-1.017965	-1.952078
C	3.718413	0.411986	-1.702157
H	3.017176	-1.144761	-3.026871
H	3.946110	-1.760279	-1.679827
C	2.989145	-2.242674	0.978401
C	4.122519	-1.191620	0.988306
H	3.390890	-3.229317	0.696986
H	2.600651	-2.355549	1.997852
C	3.445452	0.927849	-0.303791
H	3.232644	1.098494	-2.404928
H	4.795826	0.463067	-1.923611
C	3.596568	0.227489	0.876951
Rh	1.369347	0.197775	0.245929

H	1.019759	-1.450337	-1.846943
H	0.920589	-2.447810	0.326237
H	3.306379	2.003851	-0.224225
H	4.832856	-1.389852	0.180067
H	4.688477	-1.288844	1.921408
H	3.536876	0.797294	1.801523
Cl	1.000386	2.352186	1.433613
P	-0.977450	0.003208	-0.077205
N	-1.571800	-1.185801	-1.159581
N	-1.625607	1.395019	-0.831667
N	-1.835410	-0.182875	1.360333
C	-1.412235	-2.631374	-0.857175
C	-2.744053	-0.975401	-2.048005
C	-0.938393	1.957164	-2.011391
C	-2.307852	2.467606	-0.067860
C	-1.217725	-0.201956	2.702318
C	-3.274518	-0.521394	1.433364
C	-3.553889	-0.663982	2.940941
H	-3.473127	-1.462209	0.905266
H	-3.897328	0.254922	0.972916
C	-2.187907	-1.056024	3.525053
H	-4.341843	-1.395283	3.144553
H	-3.874050	0.299012	3.355981
C	-1.964105	3.762796	-0.823661
H	-1.970789	2.500661	0.971037
H	-3.393055	2.290366	-0.067980
C	-1.668598	3.283240	-2.252084
C	-3.002855	-2.367493	-2.635588
H	-2.524537	-0.235741	-2.821573
H	-3.622990	-0.621770	-1.492424
C	-2.653408	-3.300831	-1.470561
H	-1.343624	-2.811257	0.222439
H	-0.500021	-3.025607	-1.321523
H	-1.991730	-2.121515	3.352653

H	-2.107208	-0.862745	4.599154
H	-1.143312	0.812378	3.117190
H	-0.204986	-0.612720	2.653006
H	-1.006942	1.277222	-2.868332
H	0.130072	2.133588	-1.811332
H	-1.065175	4.215397	-0.390780
H	-2.773462	4.497806	-0.772496
H	-2.602743	3.104226	-2.798469
H	-1.065934	3.989357	-2.831786
H	-2.329263	-2.549871	-3.481871
H	-4.032011	-2.479084	-2.990629
H	-3.474930	-3.319003	-0.744413
H	-2.454965	-4.331836	-1.778752

- Figure S8. Optimized Structure of Complex [RhCl(COD){P(*NH*-pyrrolidinyl)(*N*-pyrrolidinyl)$_2$}] (**3j-H$^+$**), Energy Data and Cartesian Coordinates.



$E_{SMD\text{-}m06}$ = - 1858,9531660

$G^{therm}_{SMD\text{-}B3LYP}$ = 0,5051790

$E^{disp}_{DFT\text{-}m06}$ = - 0,01656792

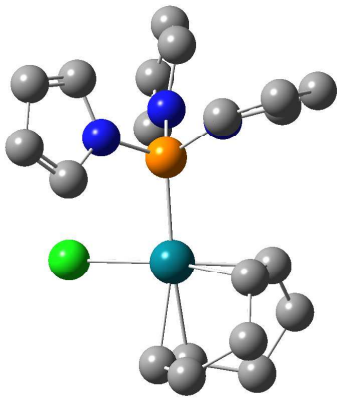
G_{sol} = - 1858,46455492

C	1.764441	-1.968549	0.286906
C	1.870171	-1.493916	-1.035296
C	3.185775	-1.264599	-1.774370
C	3.726098	0.174647	-1.622005
H	3.030694	-1.469163	-2.838810
H	3.928592	-1.992325	-1.432602
C	2.904147	-2.262029	1.241481
C	4.049278	-1.227756	1.191376
H	3.295465	-3.273911	1.053391
H	2.486085	-2.283446	2.254596
C	3.432112	0.796788	-0.273890
H	3.267191	0.812059	-2.385501
H	4.809109	0.198020	-1.816748
C	3.540878	0.183186	0.960736
Rh	1.338770	0.145966	0.298606
H	1.010407	-1.657699	-1.681376
H	0.852733	-2.498027	0.553227

H	3.310469	1.877577	-0.276598
H	4.772439	-1.493640	0.415171
H	4.594138	-1.255224	2.140882
H	3.469079	0.823702	1.836897
Cl	1.017767	2.381418	1.275944
P	-0.979308	-0.098739	-0.033071
N	-1.633364	-1.283520	-1.050585
N	-1.588440	1.386530	-1.115534
N	-1.940526	-0.040631	1.316070
C	-1.538728	-2.709929	-0.609075
C	-2.657701	-1.146343	-2.122584
C	-0.604054	1.834239	-2.180615
C	-2.009396	2.644551	-0.347445
C	-1.430455	0.213168	2.692277
C	-3.399360	-0.339769	1.341081
C	-3.790268	-0.185711	2.821112
H	-3.573368	-1.360048	0.984635
H	-3.958599	0.345467	0.695264
C	-2.481412	-0.464791	3.574866
H	-4.602981	-0.863209	3.096233
H	-4.123745	0.839622	3.015277
C	-1.477296	3.830542	-1.175558
H	-1.570538	2.602676	0.646320
H	-3.096848	2.624199	-0.269612
C	-1.090423	3.234467	-2.540731
C	-2.918029	-2.591442	-2.566814
H	-2.285787	-0.541498	-2.955912
H	-3.587821	-0.698726	-1.742699
C	-2.741719	-3.392052	-1.272693
H	-1.565386	-2.791216	0.482614
H	-0.602712	-3.151792	-0.966416
H	-2.290849	-1.543087	3.627115
H	-2.479608	-0.065608	4.592920
H	-1.381171	1.289376	2.889569

H	-0.426495	-0.201354	2.805112
H	-0.609590	1.112575	-2.998935
H	0.384191	1.848928	-1.715732
H	-0.594382	4.247321	-0.683279
H	-2.227144	4.620369	-1.261621
H	-1.957274	3.176422	-3.208704
H	-0.310449	3.807914	-3.048176
H	-2.169808	-2.893315	-3.307889
H	-3.908694	-2.699650	-3.016186
H	-3.632258	-3.298131	-0.640860
H	-2.558814	-4.456192	-1.444605
H	-2.421387	1.064701	-1.611403

- Figure S9. Optimized Structure of Complex [RhCl(COD){P(*N*-pyrrolyl)$_3$}] (**3k**), Energy Data and Cartesian Coordinates.



$E_{SMD\text{-}m06}$ = - 1851,25606060

$G^{therm}_{SMD\text{-}B3LYP}$ = 0,3482650

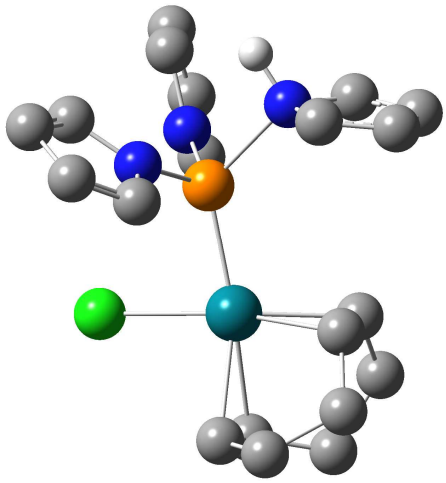
$E^{disp}_{DFT\text{-}m06}$ = - 0,01278236

G_{sol} = - 1850,92057796

C	1.780372	1.400745	-1.025718
C	1.828580	1.611607	0.366413
C	3.105264	1.694893	1.200255
C	3.547779	0.333518	1.779673
C	3.275862	-0.839727	0.864104
C	3.459203	-0.884288	-0.502814
C	4.043405	0.230556	-1.349185
C	2.952993	1.142978	-1.950634
Rh	1.225720	-0.448554	-0.057874
P	-1.033709	0.005606	-0.036006
N	-1.605229	1.650968	0.050374
N	-1.955741	-0.507547	-1.397691
N	-1.843148	-0.650248	1.339240
C	-1.796456	2.358635	1.238877
C	-1.604928	2.567631	-1.003761
C	-1.947692	3.686826	0.930681

C	-1.828034	3.819086	-0.487778
C	-3.246369	-0.113395	-1.778456
C	-1.517189	-1.482197	-2.302705
C	-3.598013	-0.822994	-2.894603
C	-2.506360	-1.688765	-3.225409
C	-3.217914	-0.776928	1.561355
C	-1.179331	-0.994861	2.522510
C	-3.406587	-1.202826	2.848550
C	-2.117296	-1.336135	3.458920
Cl	0.758021	-2.855536	0.103047
H	-2.142499	4.478254	1.642232
H	-1.825532	1.844064	2.187400
H	-1.916800	4.729824	-1.065144
H	-1.488108	2.235617	-2.024415
H	-4.534387	-0.726866	-3.428462
H	-3.770947	0.658767	-1.238241
H	-2.457411	-2.381211	-4.055240
H	-0.551037	-1.944286	-2.171763
H	-4.364852	-1.410184	3.306659
H	-3.927138	-0.569293	0.775987
H	-1.908946	-1.659090	4.470235
H	-0.100970	-0.973764	2.563736
H	3.366061	-1.857542	-0.979946
H	4.750490	0.816765	-0.756066
H	4.621949	-0.214469	-2.165607
H	3.392706	2.101297	-2.268098
H	2.557648	0.676028	-2.860509
H	0.906989	1.793707	-1.543311
H	0.971873	2.119079	0.804110
H	3.082336	-1.786090	1.364237
H	2.935478	2.387995	2.030758
H	3.906766	2.135975	0.599126
H	3.007682	0.150689	2.714951
H	4.615629	0.361341	2.044862

- **Figure S10.** Optimized Structure of Complex [RhCl(COD){P(*NH*-pyrrolyl)(*N*-pyrrolyl)$_2$}] (**3k-H$^+$**), Energy Data and Cartesian Coordinates.



$E_{SMD\text{-}m06}$ = - 1851,63450040

$G^{therm}_{SMD\text{-}B3LYP}$ = 0,3597720

$E^{disp}_{DFT\text{-}m06}$ = - 0,01350035

G_{sol} = - 1851,28822875

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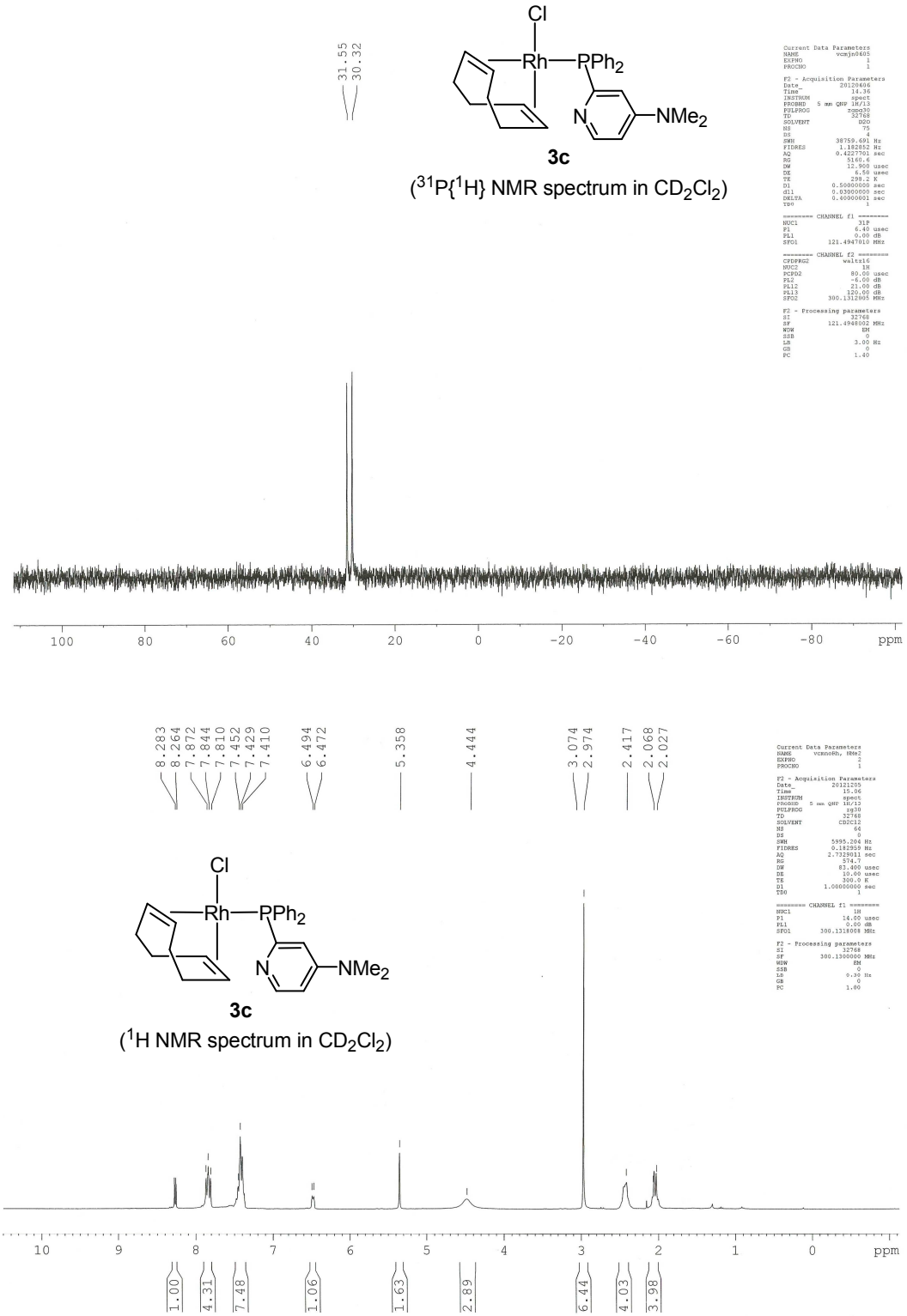
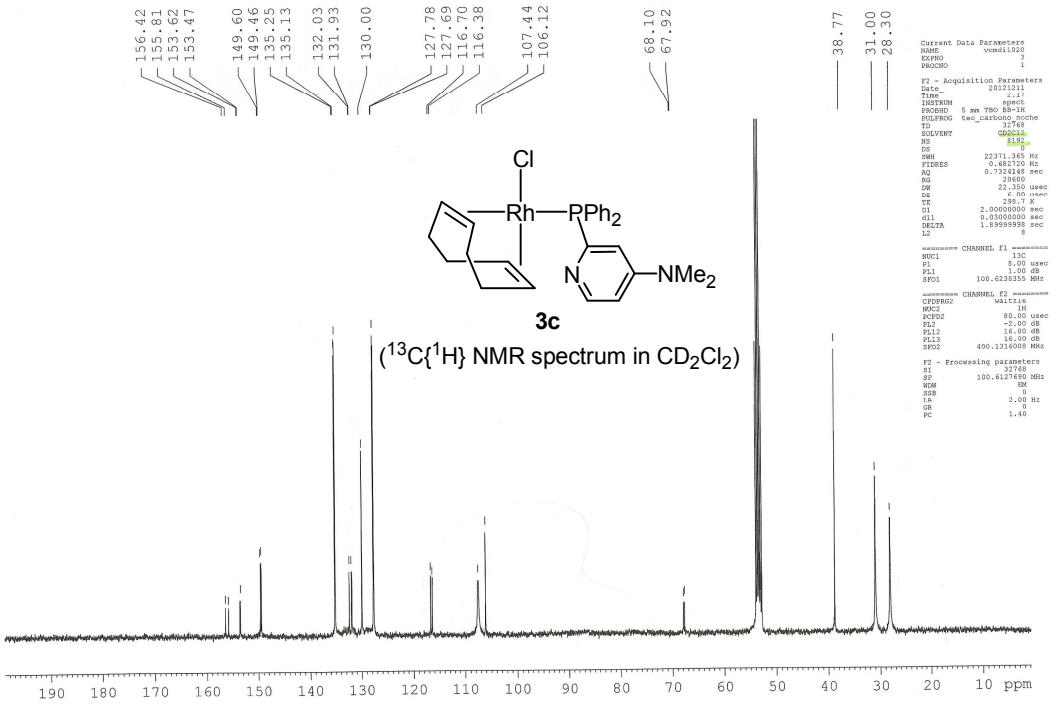
C	-2.133412	0.943056	-1.153691
C	-3.427310	0.332997	-1.682328
C	-3.603303	-1.150093	-1.295311
C	-3.085444	-1.486804	0.084060
C	-3.208818	-0.719904	1.230720
C	-3.965339	0.590180	1.345140
C	-3.051971	1.816663	1.129695
Rh	-1.131021	-0.363441	0.325577
P	1.094094	-0.012096	-0.040886
N	1.872673	1.581234	-1.159050
N	2.135953	0.302074	1.263411
N	1.864370	-1.236122	-0.930046
C	1.374614	1.667322	-2.520930
C	1.562380	2.861338	-0.544489

C	0.769933	2.859905	-2.681086
C	0.886360	3.610605	-1.435985
C	3.525483	0.546494	1.282823
C	1.624832	0.645086	2.532031
C	3.859012	0.999757	2.526060
C	2.661947	1.059134	3.314192
C	3.027491	-1.982599	-0.663142
C	1.274538	-1.759991	-2.099015
C	3.160114	-2.922573	-1.643208
C	2.058574	-2.780446	-2.551273
Cl	-0.265246	-2.285111	1.588141
H	0.287215	3.207185	-3.584525
H	1.542336	0.841057	-3.194582
H	0.501571	4.606156	-1.260949
H	1.880357	3.049088	0.469921
H	4.858813	1.258884	2.847278
H	4.146172	0.362674	0.419209
H	2.584133	1.368630	4.347254
H	0.572436	0.530194	2.740569
H	3.955359	-3.653414	-1.701826
H	3.616361	-1.798259	0.219534
H	1.866262	-3.375899	-3.433266
H	0.345030	-1.358659	-2.474386
H	-2.922231	-1.195940	2.166024
H	-4.800175	0.600739	0.639437
H	-4.405759	0.650229	2.345444
H	-3.656784	2.703881	0.888384
H	-2.536424	2.047385	2.068774
H	-1.172345	2.333612	0.138203
H	-1.393577	1.164215	-1.917294
H	-2.743484	-2.510877	0.217176
H	-3.425788	0.410452	-2.774045
H	-4.279181	0.926587	-1.337816
H	-3.061334	-1.775782	-2.012096

H	-4.661038	-1.443497	-1.372783
H	2.880946	1.387715	-1.142573

Figure S11. Copies of the $^{31}P\{^{1}H\}$, ^{1}H and $^{13}C\{^{1}H\}$ NMR spectra of the Rh(I) complexes **3c-k**.





3c

($^{13}C\{^{1}H\}$ NMR spectrum in CD_2Cl_2)

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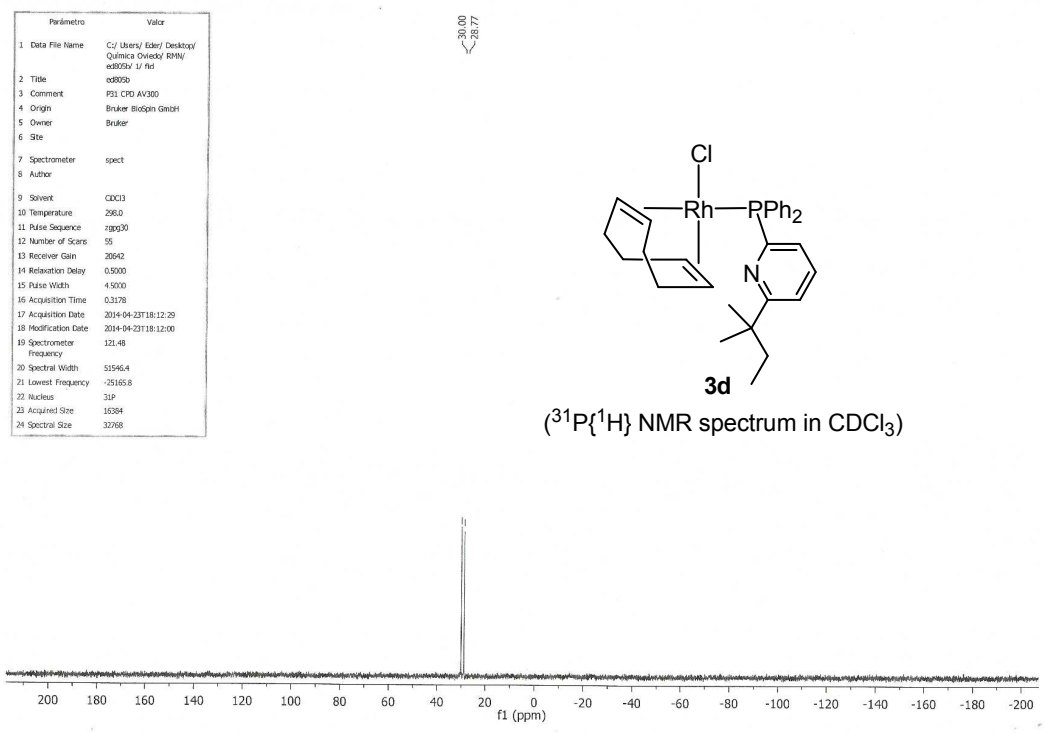
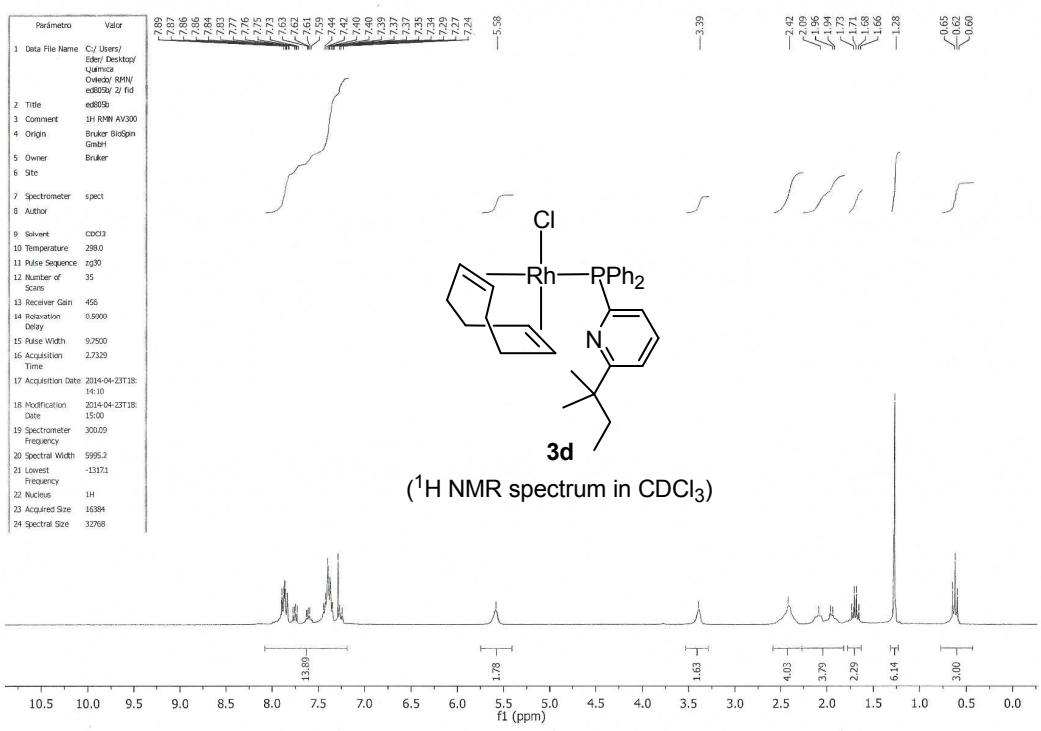
3 Comment	P31 CPD AV300
4 Origin	Bruker BioSpin GmbH
5 Owner	Bruker
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.0
11 Pulse Sequence	zgpg30
12 Number of Scans	55
13 Receiver Gain	20642
14 Relaxation Delay	0.5000
15 Pulse Width	4.5000
16 Acquisition Time	0.3178
17 Acquisition Date	2014-04-23T18:12:29
18 Modification Date	2014-04-23T18:12:00
19 Spectrometer Frequency	121.48
20 Spectral Width	51546.4
21 Lowest Frequency	-25165.8
22 Nucleus	31P
23 Acquired Size	16384
24 Spectral Size	32768

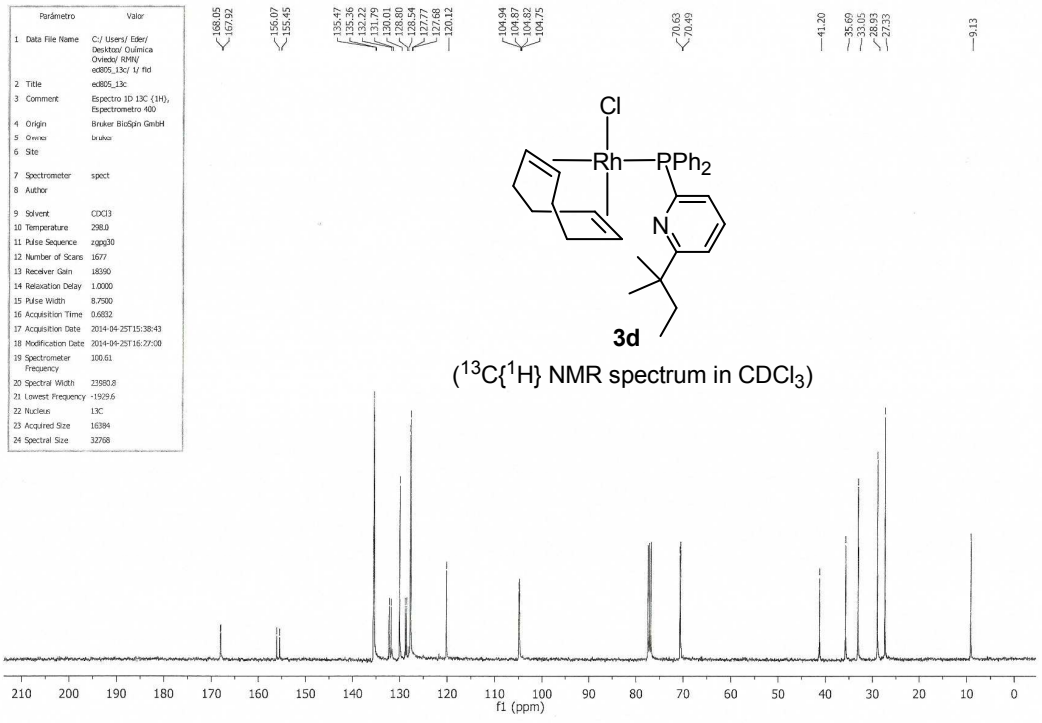


3d

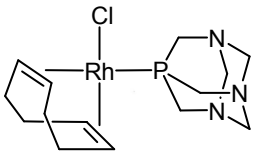
($^{31}P\{^{1}H\}$ NMR spectrum in $CDCl_3$)



(^{1}H NMR spectrum in $CDCl_3$)

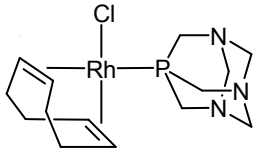


($^{13}C\{^1H\}$ NMR spectrum in $CDCl_3$)



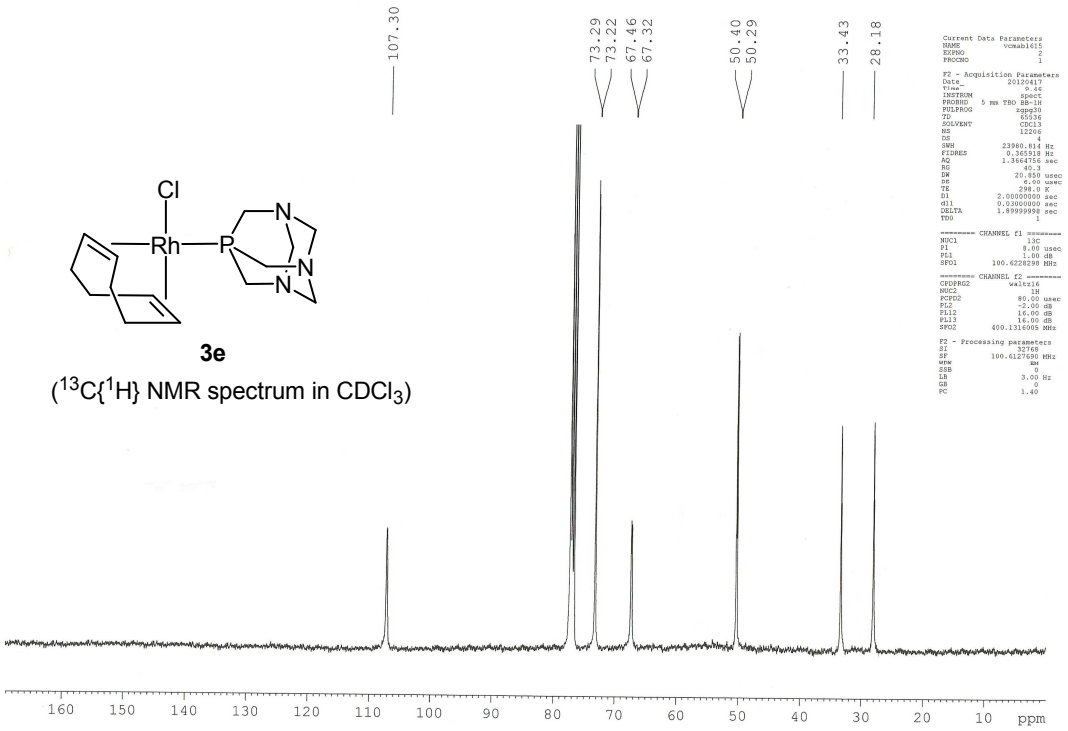
3e

($^{31}P\{^{1}H\}$ NMR spectrum in $CDCl_3$)



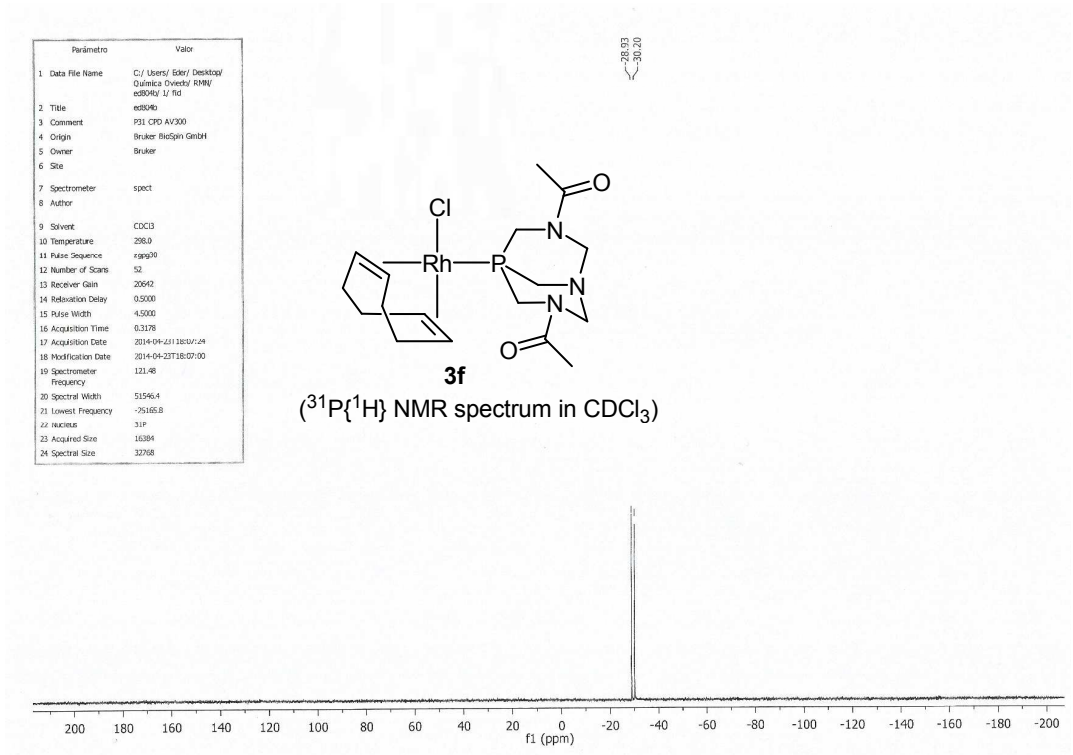
3e

(^{1}H NMR spectrum in $CDCl_3$)



3e

($^{13}C\{^{1}H\}$ NMR spectrum in $CDCl_3$)



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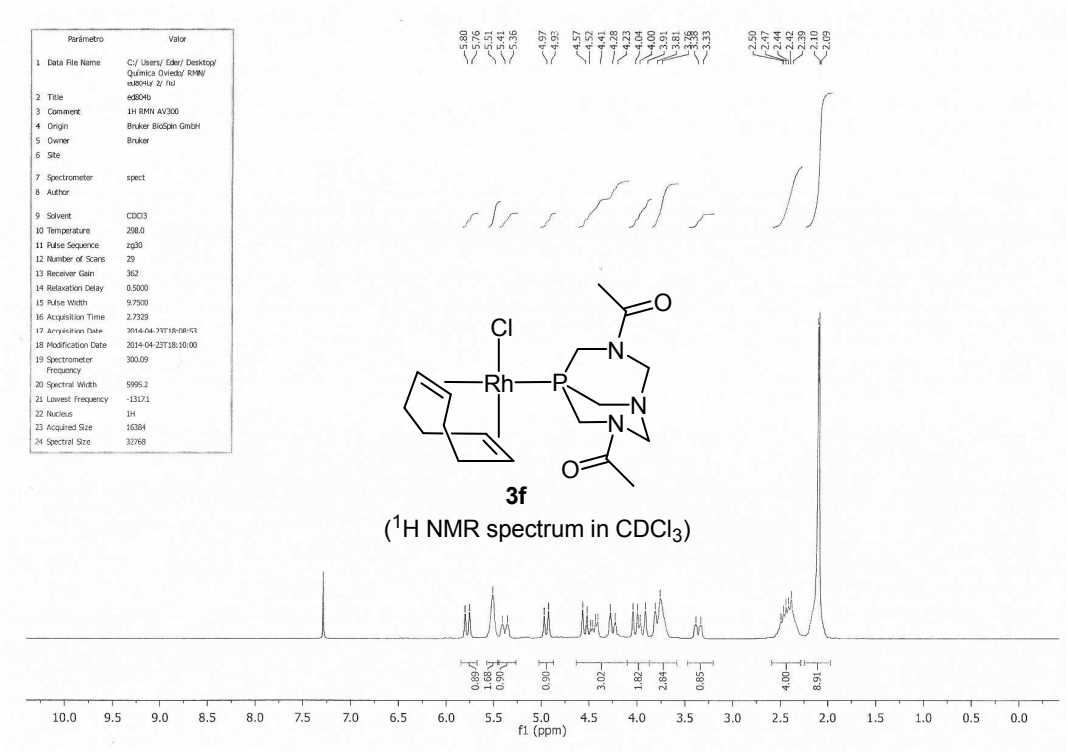
5	Owner	Bruker
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zgpg30
12	Number of Scans	52
13	Receiver Gain	20642
14	Relaxation Delay	0.5000
15	Pulse Width	4.5000
16	Acquisition Time	0.3178
17	Acquisition Date	2014-04-[illegible]
18	Modification Date	2014-04-23T18:07:00
19	Spectrometer Frequency	121.48
20	Spectral Width	51546.4
21	Lowest Frequency	-2516[illegible]
22	nucleus	31P
23	Acquired Size	16384
24	Spectral Size	32768

3f

($^{31}P\{^{1}H\}$ NMR spectrum in $CDCl_3$)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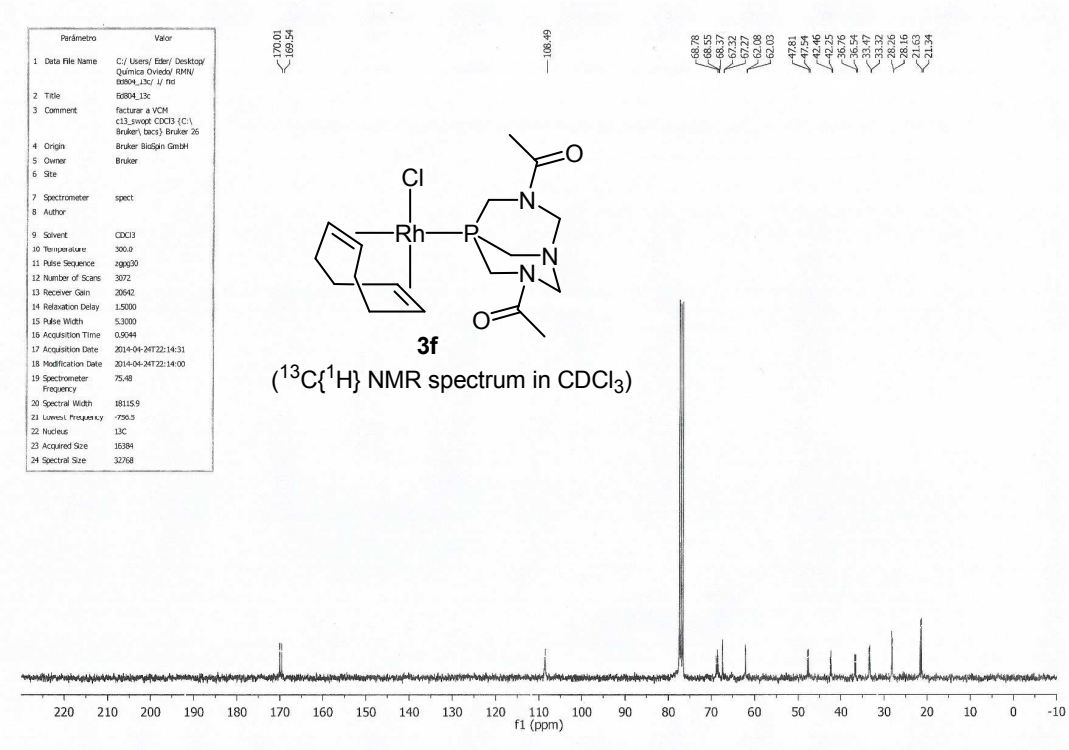
3 Comment 1H RMN AV300
4 Origin Bruker BioSpin GmbH
5 Owner Bruker
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 298.0
11 Pulse Sequence zg30
12 Number of Scans 29
13 Receiver Gain 362
14 Relaxation Delay 0.5000
15 Pulse Width 9.7500
16 Acquisition Time 2.7329
17 Acquisition Date 2014-04-23T18:08:53
18 Modification Date 2014-04-23T18:10:00
19 Spectrometer Frequency 300.09
20 Spectral Width 5995.2
21 Lowest Frequency -1317.1
22 Nucleus 1H
23 Acquired Size 16384
24 Spectral Size 32768
5.80 5.76 5.51 5.41 5.36 4.97 4.93 4.57 4.52 4.41 4.28 4.23 4.04 4.00 3.91 3.81 3.38 3.33 2.50 2.47 2.44 2.42 2.39 2.10 2.09
Cl Rh P N N N O O
3f
(1H NMR spectrum in CDCl3)
0.89 1.65 0.90 0.90 3.02 1.82 2.84 0.85 4.00 8.91
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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4 Origin Bruker BioSpin GmbH
5 Owner Bruker
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
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11 Pulse Sequence zgpg30
12 Number of Scans 3072
13 Receiver Gain 20642
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15 Pulse Width 5.3000
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17 Acquisition Date 2014-04-24T22:14:31
18 Modification Date 2014-04-24T22:14:00
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20 Spectral Width 18115.9
21 Lowest Frequency -756.5
22 Nucleus 13C
23 Acquired Size 16384
24 Spectral Size 32768
170.01 169.54 108.49 68.78 68.55 68.37 67.32 67.27 62.08 62.03 47.81 47.54 42.46 42.25 36.76 36.54 33.47 33.32 28.26 28.16 21.63 21.34
Cl Rh P N N N O O
3f
(13C{1H} NMR spectrum in CDCl3)
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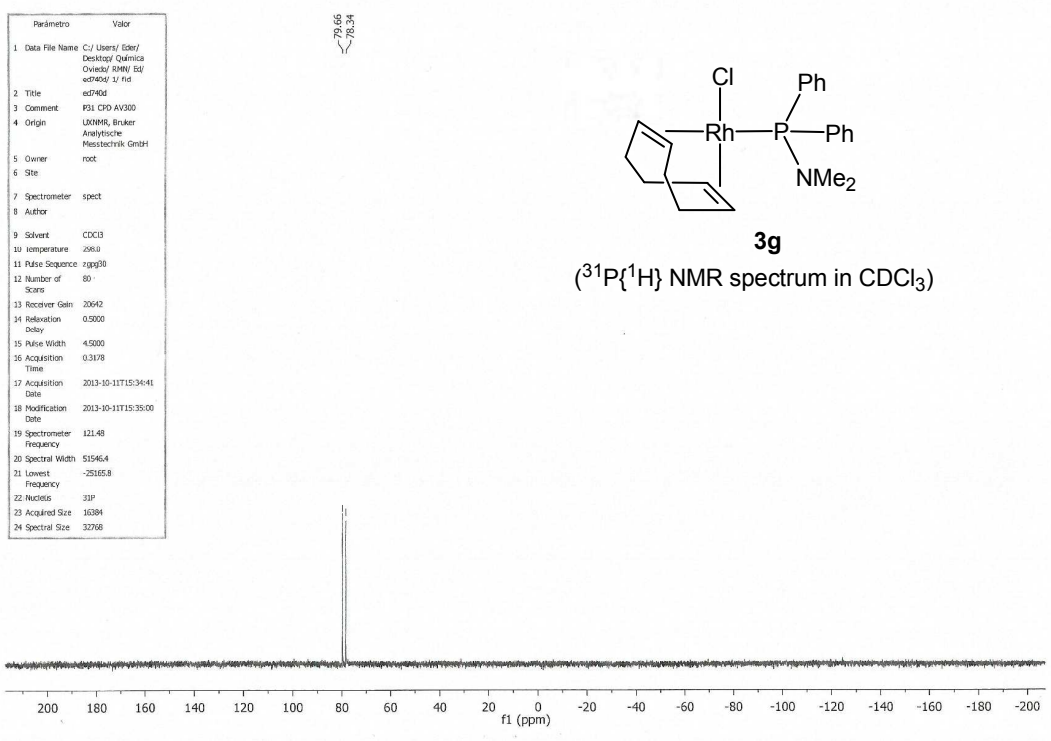
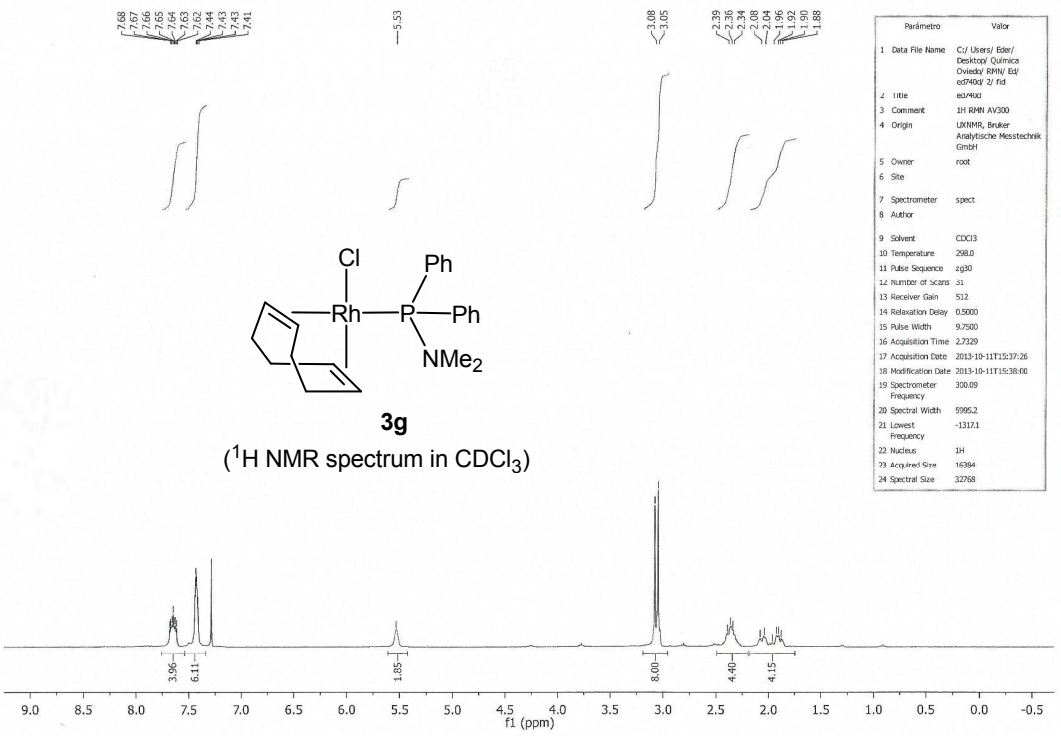
f1 (ppm)



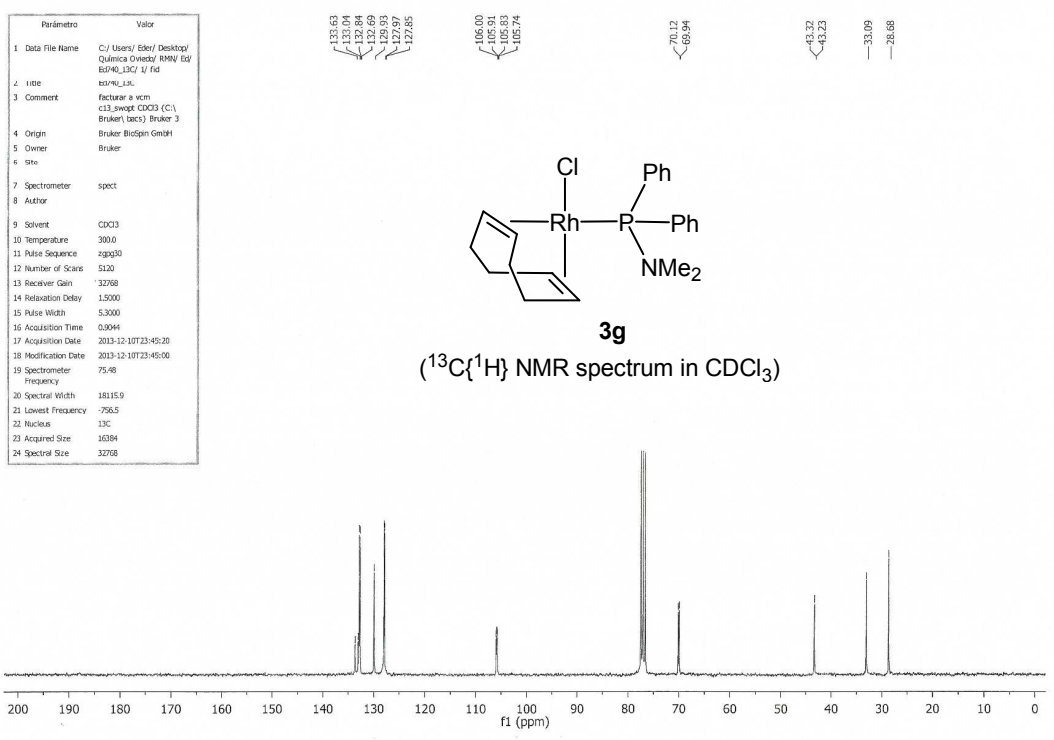
3g

($^{31}P\{^{1}H\}$ NMR spectrum in $CDCl_3$)



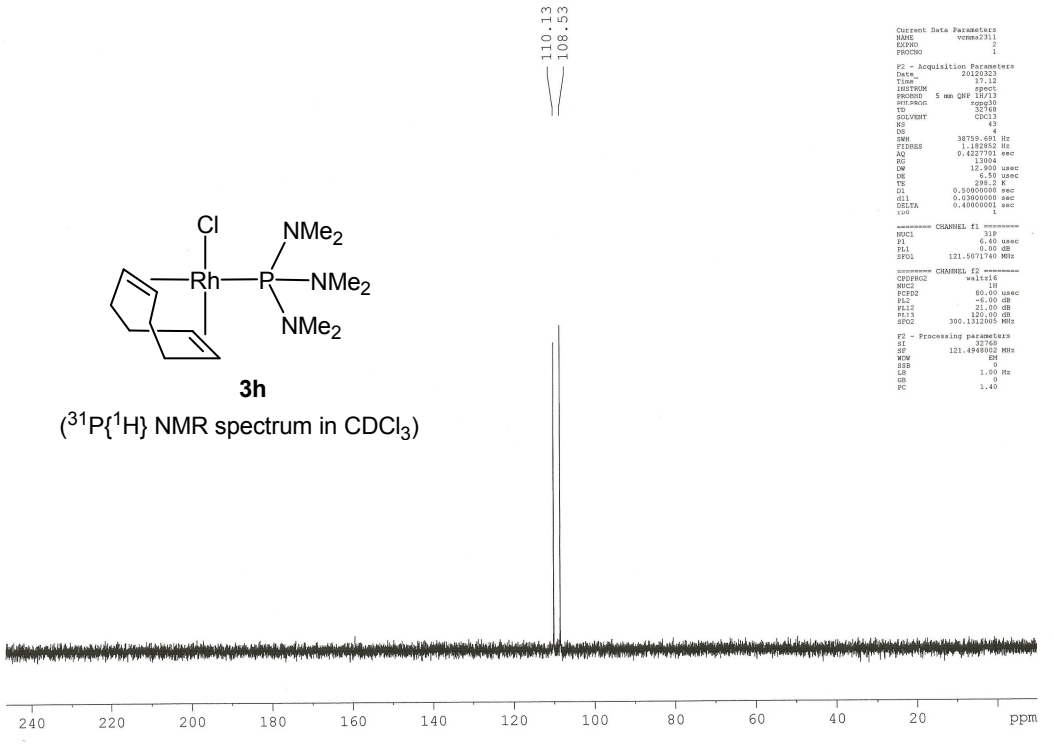
3g

(^{1}H NMR spectrum in $CDCl_3$)



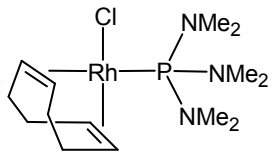
3g

($^{13}C\{^1H\}$ NMR spectrum in $CDCl_3$)



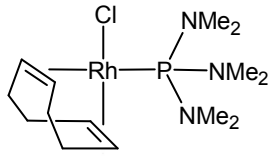
3h

($^{31}P\{^1H\}$ NMR spectrum in $CDCl_3$)



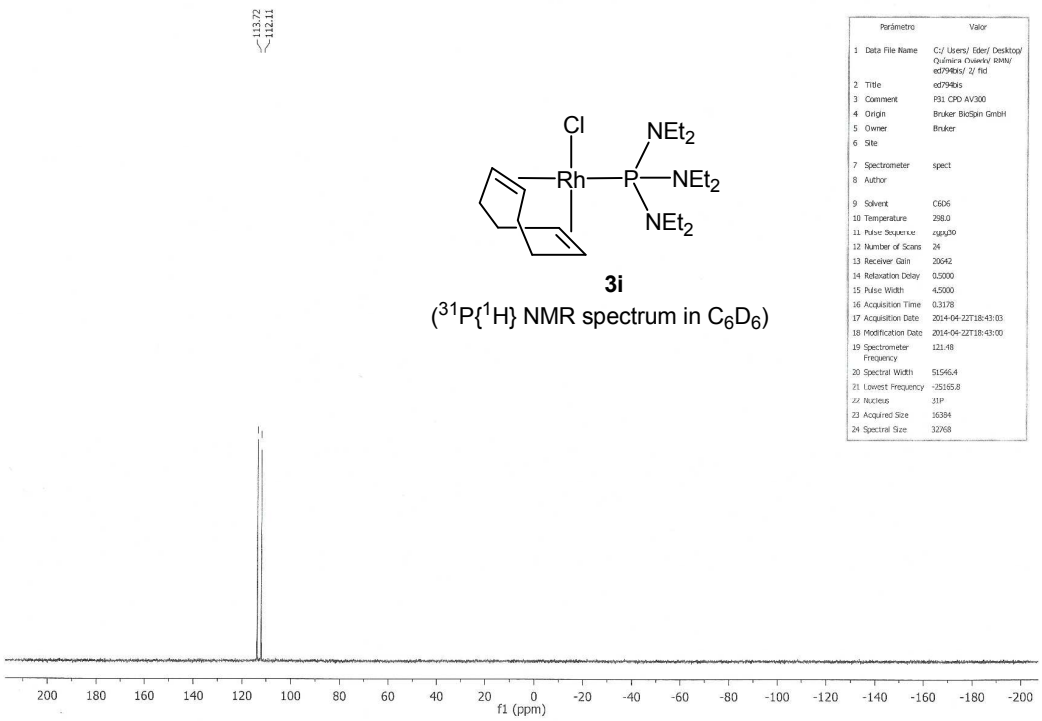
3h

(^{1}H NMR spectrum in $CDCl_3$)



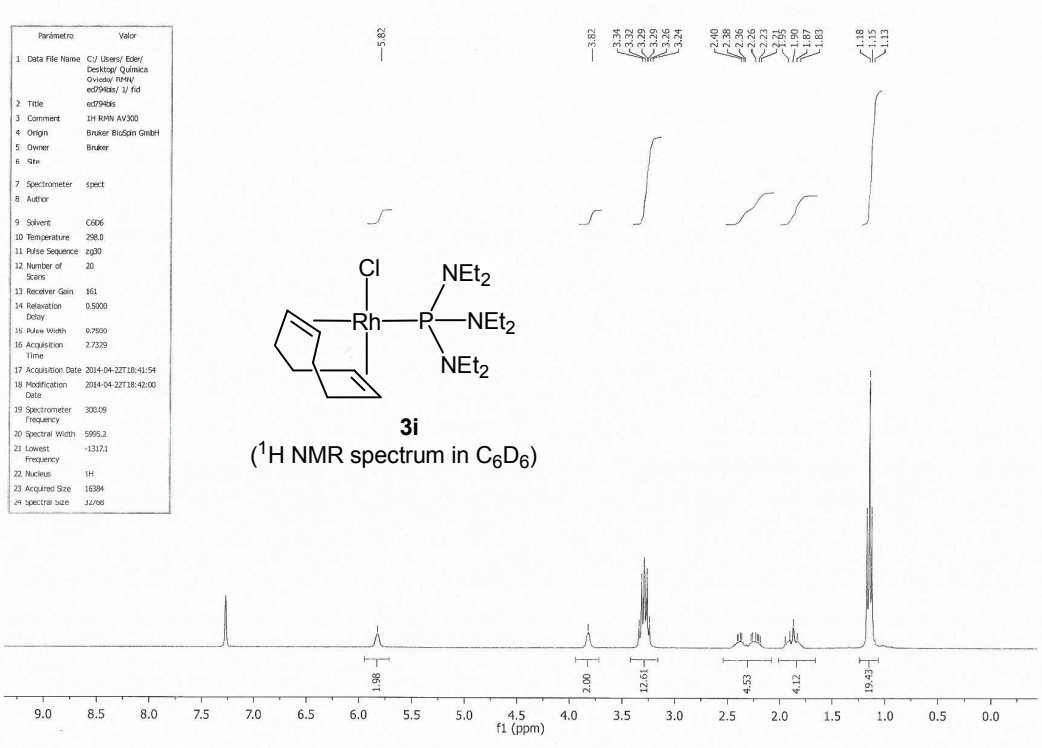
3h

($^{13}C\{^1H\}$ NMR spectrum in $CDCl_3$)



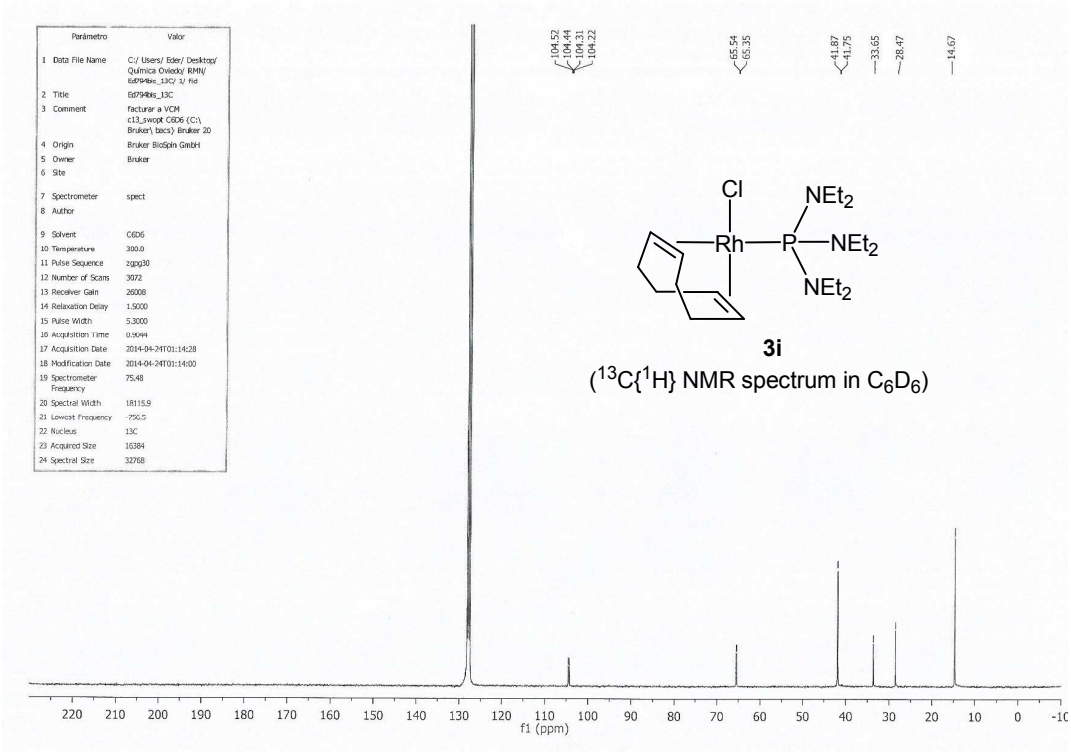
3i

($^{31}P\{^{1}H\}$ NMR spectrum in C_6D_6)



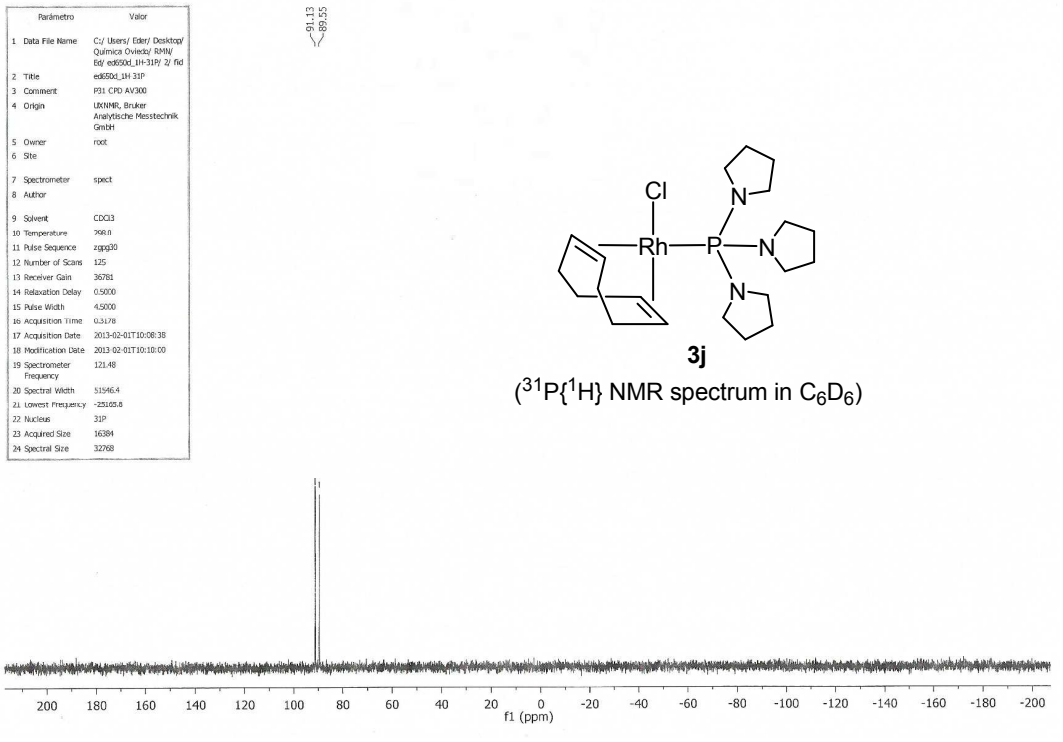
3i

(^{1}H NMR spectrum in C_6D_6)



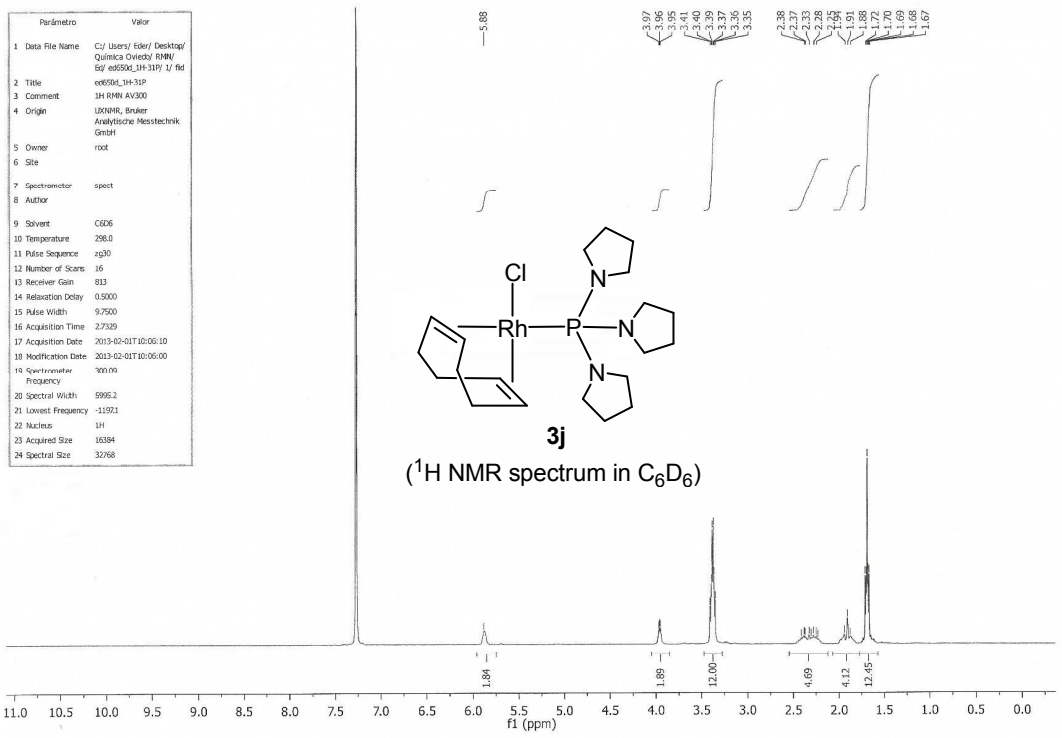
3i

($^{13}C\{^1H\}$ NMR spectrum in C_6D_6)



3j

($^{31}P\{^1H\}$ NMR spectrum in C_6D_6)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3 Comment 1H RMN AV300
4 Origin UXNMR, Bruker Analytische Messtechnik GmbH
5 Owner root
6 Site
7 Spectrometer spect
8 Author
9 Solvent C6D6
10 Temperature 298.0
11 Pulse Sequence zg30
12 Number of Scans 16
13 Receiver Gain 813
14 Relaxation Delay 0.5000
15 Pulse Width 9.7500
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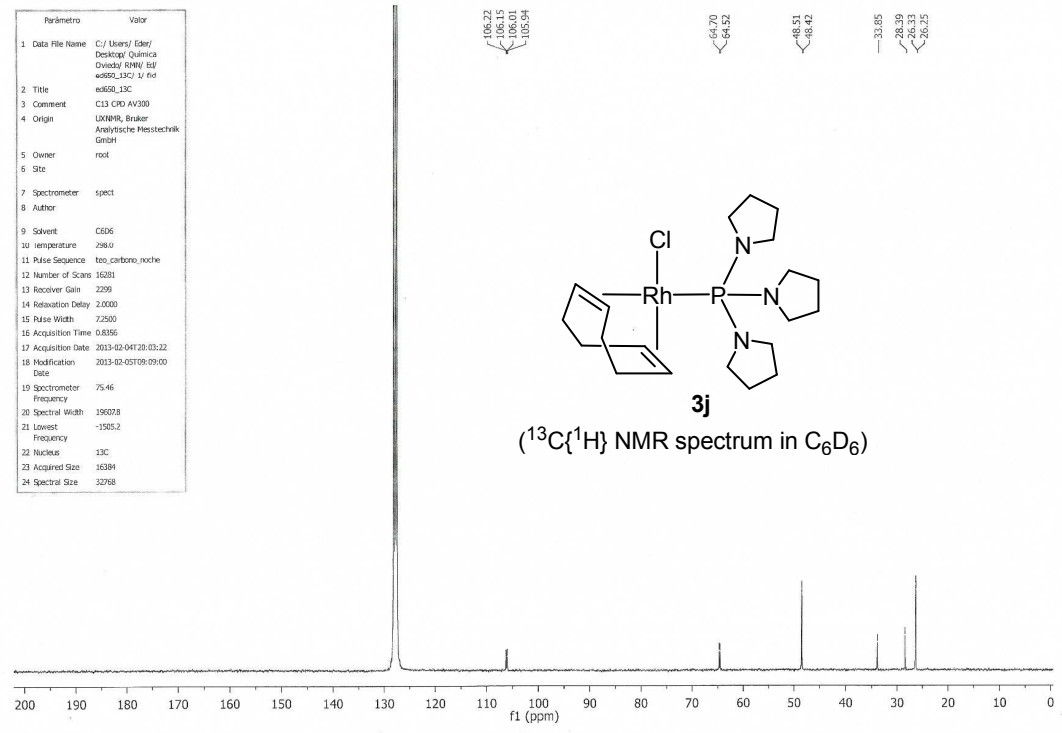
17 Acquisition Date 2013-02-01T10:06:10
18 Modification Date 2013-02-01T10:06:00
19 Spectrometer Frequency 300.09
20 Spectral Width 5995.2
21 Lowest Frequency -1197.1
22 Nucleus 1H
23 Acquired Size 16384
24 Spectral Size 32768
5.88
3.97 3.96 3.95 3.41 3.40 3.39 3.37 3.36 3.35
2.38 2.37 2.33 2.28 2.25 2.24 1.91 1.88 1.72 1.70 1.69 1.68 1.67
Cl
Rh
P
N
N
N
3j
(1H NMR spectrum in C6D6)
1.84 1.89 12.00 4.69 4.12 12.45
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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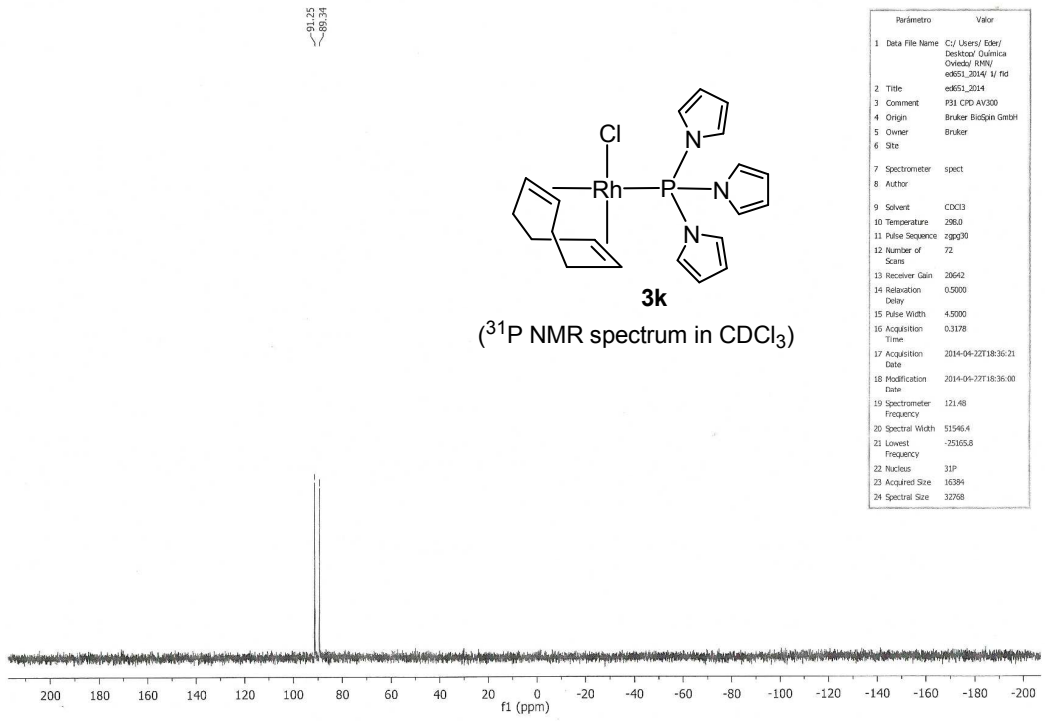
5 Owner root
6 Site
7 Spectrometer spect
8 Author
9 Solvent C6D6
10 Temperature 298.0
11 Pulse Sequence teo_carbono_noche
12 Number of Scans 16281
13 Receiver Gain 2299
14 Relaxation Delay 2.0000
15 Pulse Width 7.2500
16 Acquisition Time 0.8356
17 Acquisition Date 2013-02-04T20:03:22
18 Modification Date 2013-02-05T09:09:00
19 Spectrometer Frequency 75.46
20 Spectral Width 19607.8
21 Lowest Frequency -1505.2
22 Nucleus 13C
23 Acquired Size 16384
24 Spectral Size 32768
106.22 106.15 106.01 105.94
64.70 64.52
48.51 48.42
33.85
28.39 26.33 26.25
Cl
Rh
P
N
N
N
3j
(13C{1H} NMR spectrum in C6D6)
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)



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5	Owner	Bruker
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zgpg30
12	Number of Scans	72
13	Receiver Gain	20642
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15	Pulse Width	4.5000
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21	Lowest Frequency	-25165.8
22	Nucleus	31P
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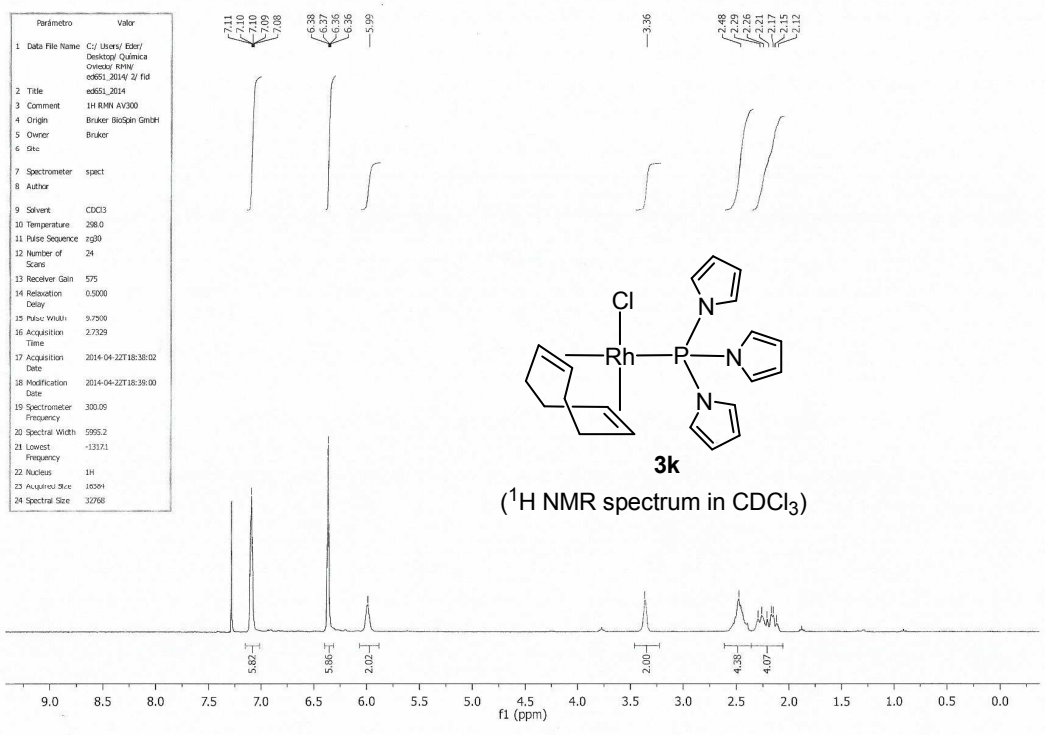

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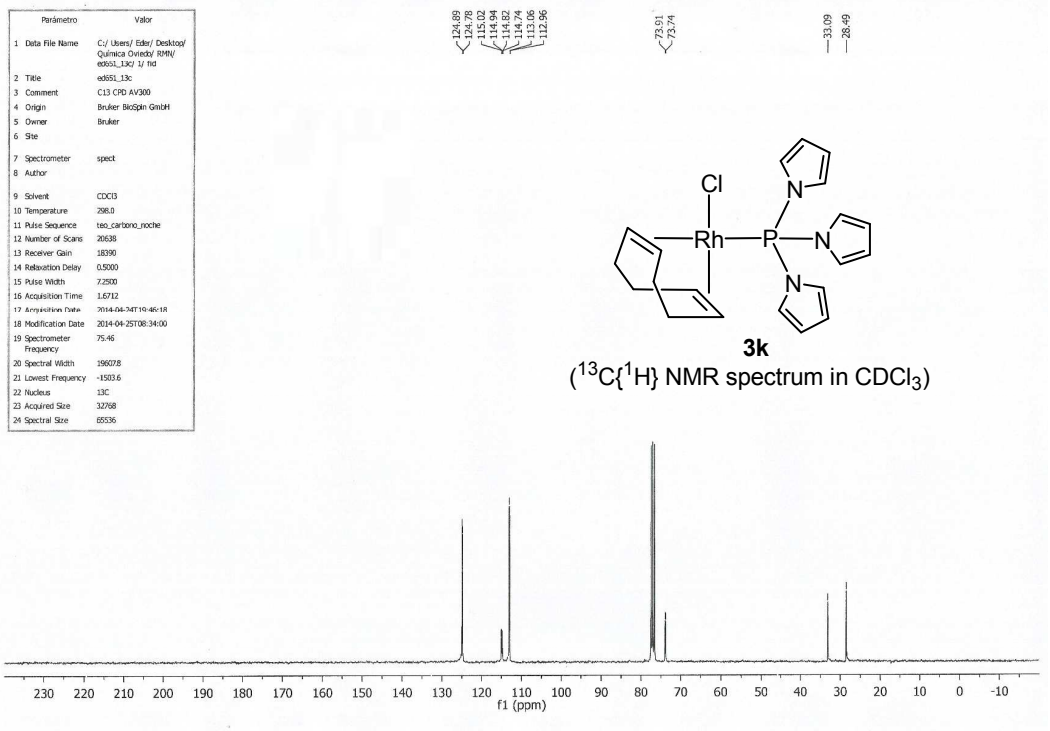
5	Owner	Bruker
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	zg30
12	Number of Scans	24
13	Receiver Gain	575
14	Relaxation Delay	0.5000
15	Pulse Width	9.7500
16	Acquisition Time	2.7329
17	Acquisition Date	2014-04-22T18:38:02
18	Modification Date	2014-04-22T18:39:00
19	Spectrometer Frequency	300.09
20	Spectral Width	5995.2
21	Lowest Frequency	-1317.1
22	Nucleus	1H
23	Acquired Size	16384
24	Spectral Size	32768

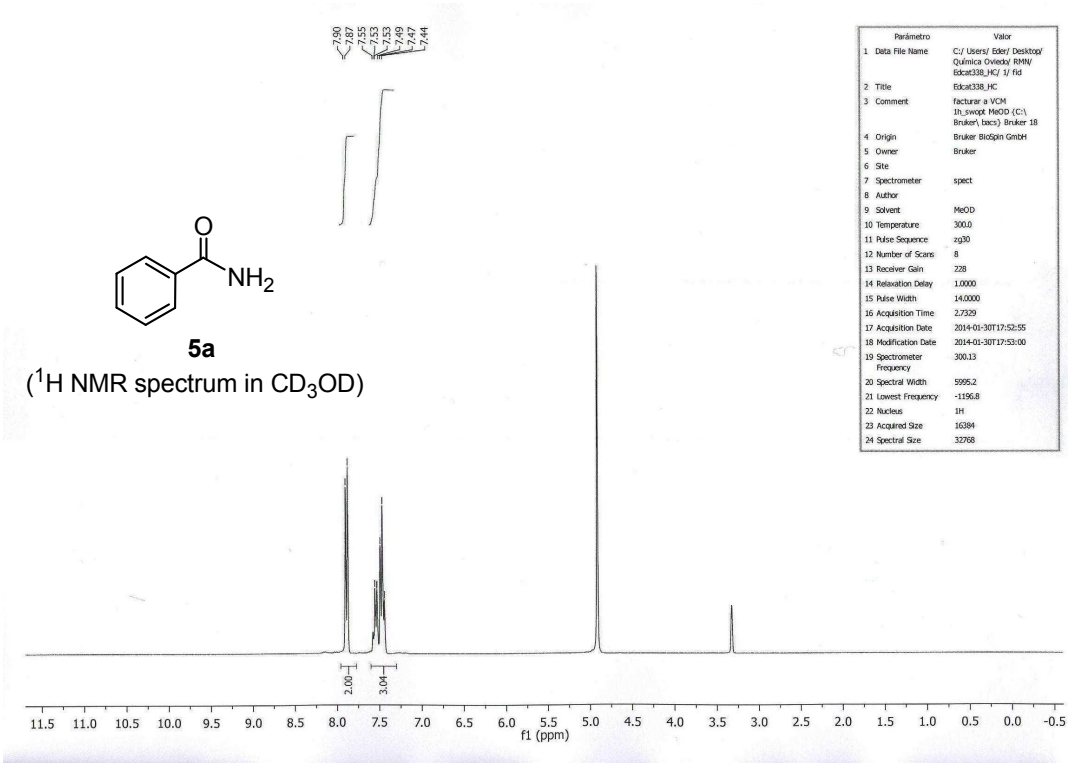
	Parámetro	Valor
1	Data File Name	C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ ed651_13C/ 1/ fid
2	Title	ed651_13c
3	Comment	C13 CPD AV300
4	Origin	Bruker BioSpin GmbH
5	Owner	Bruker
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	298.0
11	Pulse Sequence	teo_carbono_noche
12	Number of Scans	20638
13	Receiver Gain	18390
14	Relaxation Delay	0.5000
15	Pulse Width	7.2500
16	Acquisition Time	1.6712
17	Acquisition Date	2014-04-24T19:46:18
18	Modification Date	2014-04-25T08:34:00
19	Spectrometer Frequency	75.46
20	Spectral Width	19607.8
21	Lowest Frequency	-1503.6
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

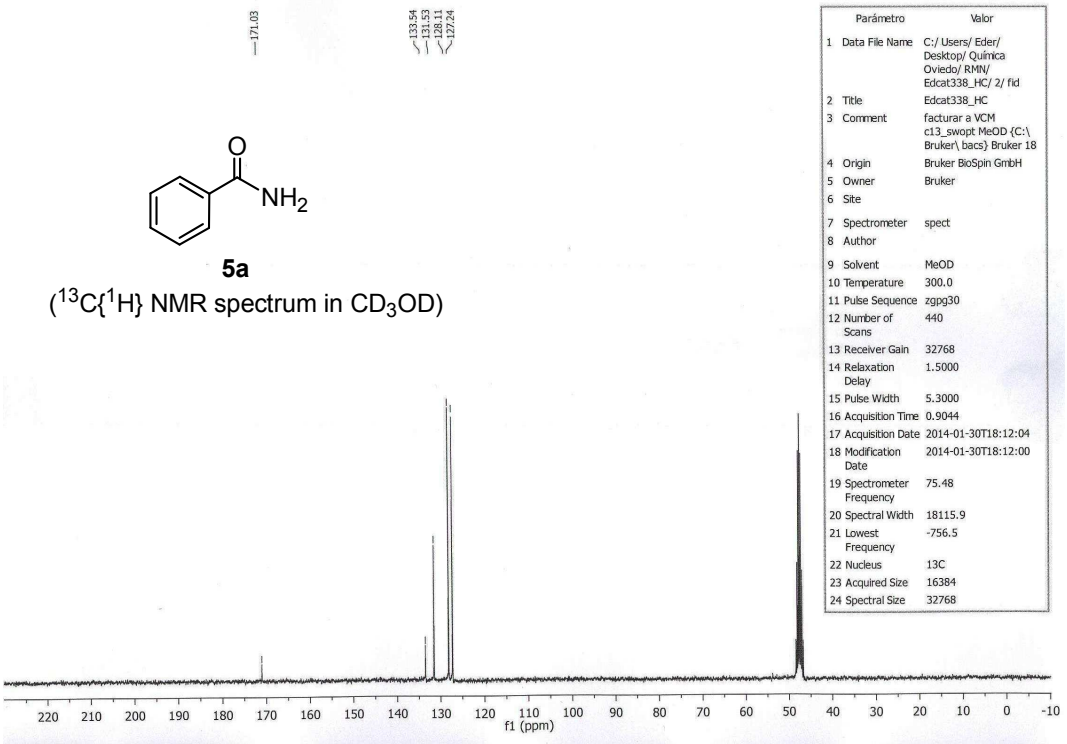


3k

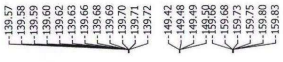
($^{13}C\{^{1}H\}$ NMR spectrum in $CDCl_3$)

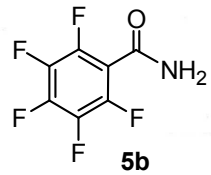
Figure S12. Copies of the ^{1}H, $^{13}C\{^{1}H\}$ and/or ^{19}F NMR spectra of the amides **5a-z**.





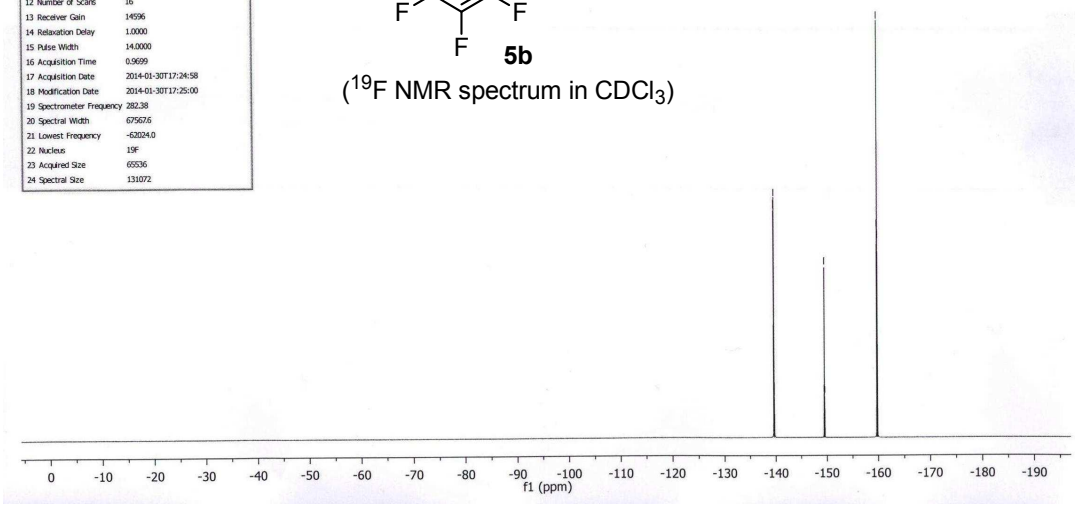
Parámetro	Valor
1 Data File Name	C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ Edcat348b_H-F/ 2/ fid
2 Title	Edcat348b_H-F
3 Comment	facturar a VCM F19CPD CDCl3 (C:\ Bruker\ bacs) Bruker 16
4 Origin	Bruker BioSpin GmbH
5 Owner	Bruker
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.0
11 Pulse Sequence	zgfhigqn
12 Number of Scans	16
13 Receiver Gain	14596
14 Relaxation Delay	1.0000
15 Pulse Width	14.0000
16 Acquisition Time	0.9699
17 Acquisition Date	2014-01-30T17:24:58
18 Modification Date	2014-01-30T17:25:00
19 Spectrometer Frequency	282.38
20 Spectral Width	67567.6
21 Lowest Frequency	-62024.0
22 Nucleus	19F
23 Acquired Size	65536
24 Spectral Size	131072



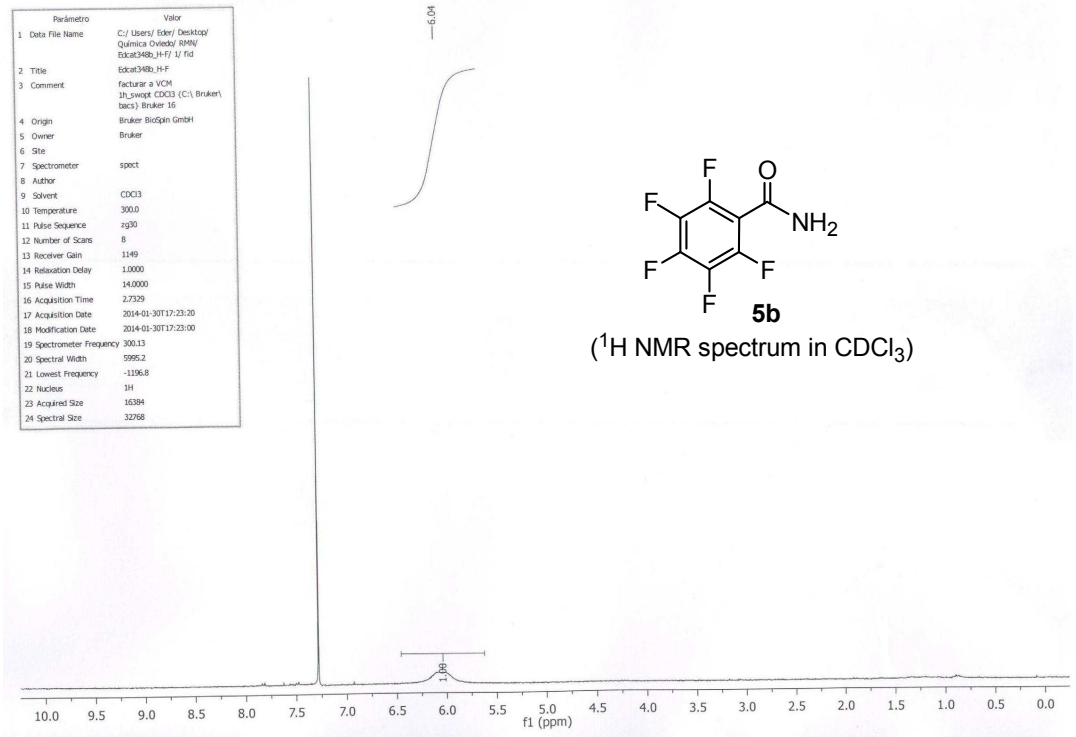


5b

(^{19}F NMR spectrum in $CDCl_3$)



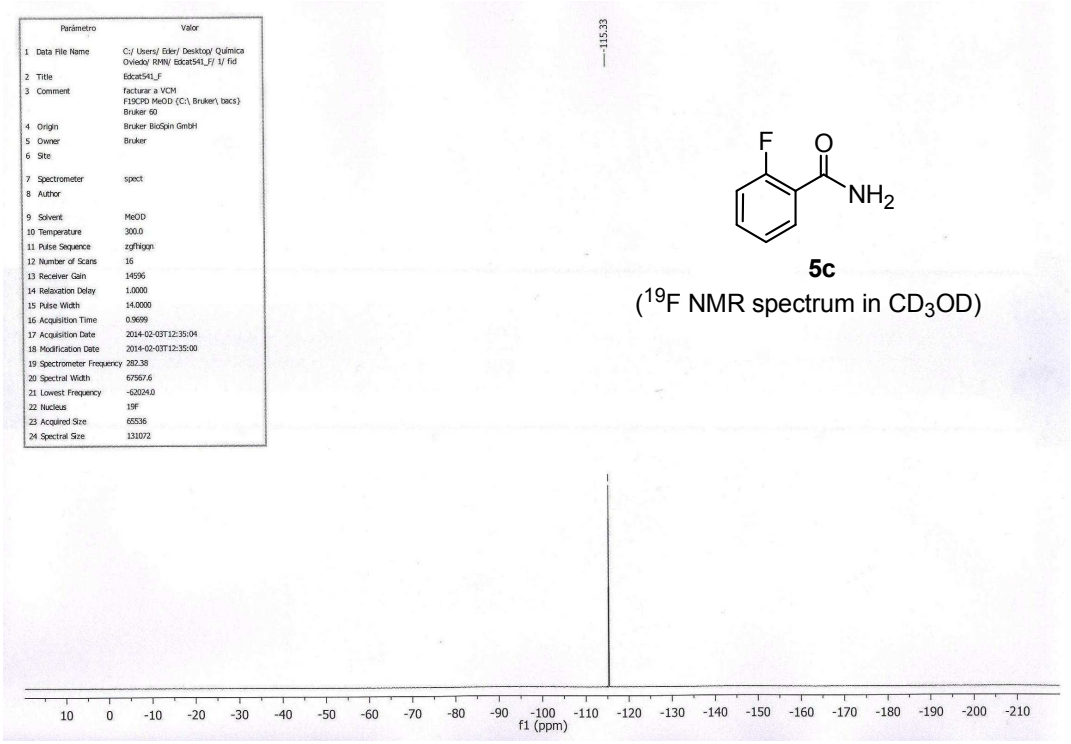
Parámetro	Valor
1 Data File Name	C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ Edcat348b_H-F/ 1/ fid
2 Title	Edcat348b_H-F
3 Comment	facturar a VCM 1h_swopt CDCl3 (C:\ Bruker\ bacs) Bruker 16
4 Origin	Bruker BioSpin GmbH
5 Owner	Bruker
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.0
11 Pulse Sequence	zg30
12 Number of Scans	8
13 Receiver Gain	1149
14 Relaxation Delay	1.0000
15 Pulse Width	14.0000
16 Acquisition Time	2.7329
17 Acquisition Date	2014-01-30T17:23:20
18 Modification Date	2014-01-30T17:23:00
19 Spectrometer Frequency	300.13
20 Spectral Width	5995.2
21 Lowest Frequency	-1196.8
22 Nucleus	1H
23 Acquired Size	16384
24 Spectral Size	32768



5b

(^{1}H NMR spectrum in $CDCl_3$)

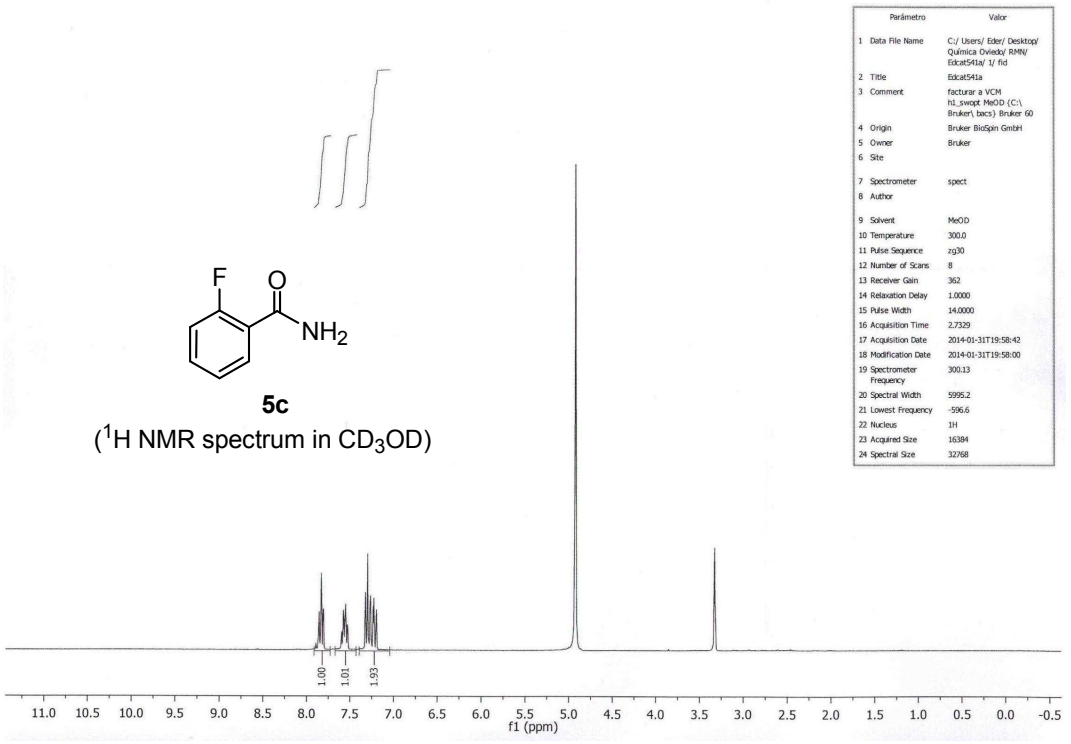
	Parámetro	Valor
1	Data File Name	C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ Edcat541_F/ 1/ fid
2	Title	Edcat541_F
3	Comment	facturar a VCM F19CPD MeOD {C:\ Bruker\ bacs} Bruker 60
4	Origin	Bruker BioSpin GmbH
5	Owner	Bruker
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	MeOD
10	Temperature	300.0
11	Pulse Sequence	zgfhigqn
12	Number of Scans	16
13	Receiver Gain	14596
14	Relaxation Delay	1.0000
15	Pulse Width	14.0000
16	Acquisition Time	0.9699
17	Acquisition Date	2014-02-03T12:35:04
18	Modification Date	2014-02-03T12:35:00
19	Spectrometer Frequency	282.38
20	Spectral Width	67567.6
21	Lowest Frequency	-62024.0
22	Nucleus	19F
23	Acquired Size	65536
24	Spectral Size	131072



5c

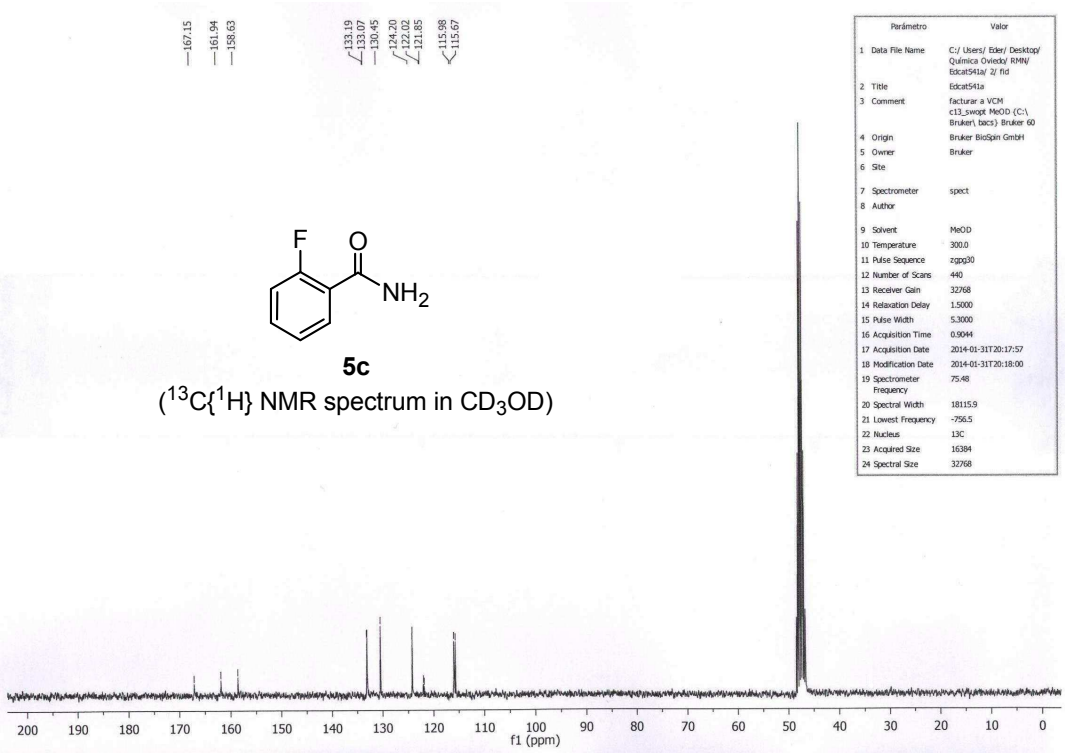
(^{19}F NMR spectrum in CD_3OD)

	Parámetro	Valor
1	Data File Name	C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ Edcat541a/ 1/ fid
2	Title	Edcat541a
3	Comment	facturar a VCM h1_swopt MeOD {C:\ Bruker\ bacs} Bruker 60
4	Origin	Bruker BioSpin GmbH
5	Owner	Bruker
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	MeOD
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	8
13	Receiver Gain	362
14	Relaxation Delay	1.0000
15	Pulse Width	14.0000
16	Acquisition Time	2.7329
17	Acquisition Date	2014-01-31T19:58:42
18	Modification Date	2014-01-31T19:58:00
19	Spectrometer Frequency	300.13
20	Spectral Width	5995.2
21	Lowest Frequency	-596.6
22	Nucleus	1H
23	Acquired Size	16384
24	Spectral Size	32768



5c

(^{1}H NMR spectrum in CD_3OD)

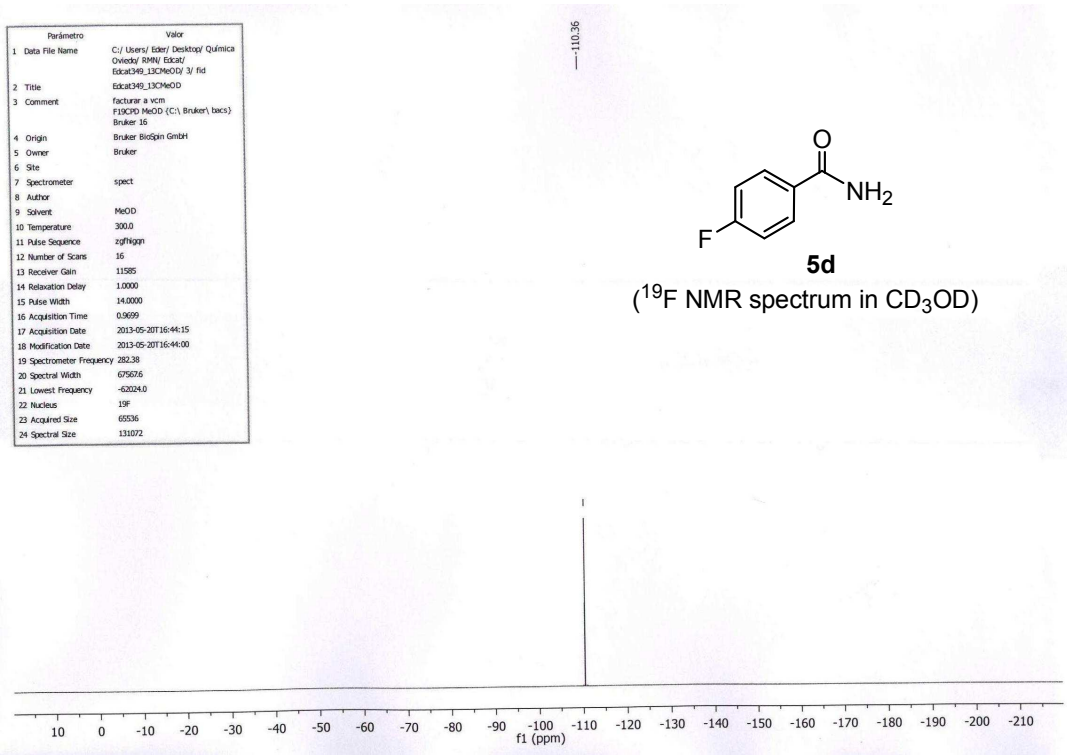


Parámetro	Valor
1 Data File Name	C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ Edcat541a/ 2/ fid
2 Title	Edcat541a
3 Comment	facturar a VCM c13_swopt MeOD {C:\ Bruker\ bacs} Bruker 60
4 Origin	Bruker BioSpin GmbH
5 Owner	Bruker
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	MeOD
10 Temperature	300.0
11 Pulse Sequence	zgpg30
12 Number of Scans	440
13 Receiver Gain	32768
14 Relaxation Delay	1.5000
15 Pulse Width	5.3000
16 Acquisition Time	0.9044
17 Acquisition Date	2014-01-31T20:17:57
18 Modification Date	2014-01-31T20:18:00
19 Spectrometer Frequency	75.48
20 Spectral Width	18115.9
21 Lowest Frequency	-756.5
22 Nucleus	13C
23 Acquired Size	16384
24 Spectral Size	32768

5c

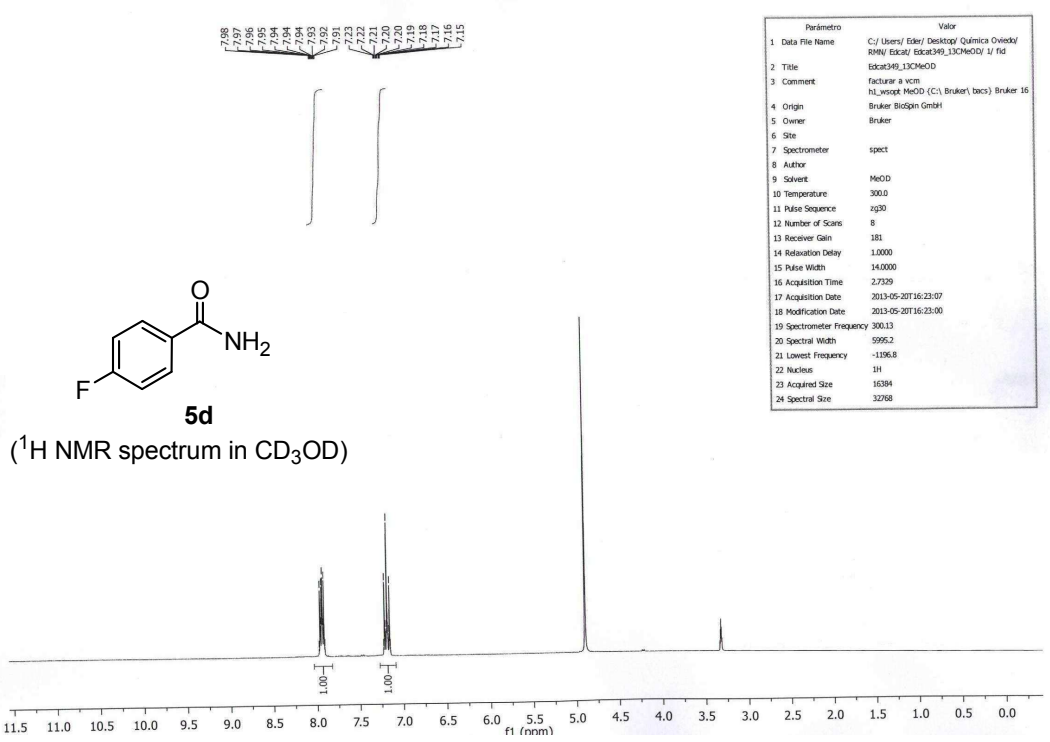
($^{13}C\{^{1}H\}$ NMR spectrum in CD_3OD)

Parámetro	Valor
1 Data File Name	C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ Edcat/ Edcat349_13CMeOD/ 3/ fid
2 Title	Edcat349_13CMeOD
3 Comment	facturar a vcm F19CPD MeOD {C:\ Bruker\ bacs} Bruker 16
4 Origin	Bruker BioSpin GmbH
5 Owner	Bruker
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	MeOD
10 Temperature	300.0
11 Pulse Sequence	zgfhigqn
12 Number of Scans	16
13 Receiver Gain	11585
14 Relaxation Delay	1.0000
15 Pulse Width	14.0000
16 Acquisition Time	0.9699
17 Acquisition Date	2013-05-20T16:44:15
18 Modification Date	2013-05-20T16:44:00
19 Spectrometer Frequency	282.38
20 Spectral Width	67567.6
21 Lowest Frequency	-62024.0
22 Nucleus	19F
23 Acquired Size	65536
24 Spectral Size	131072



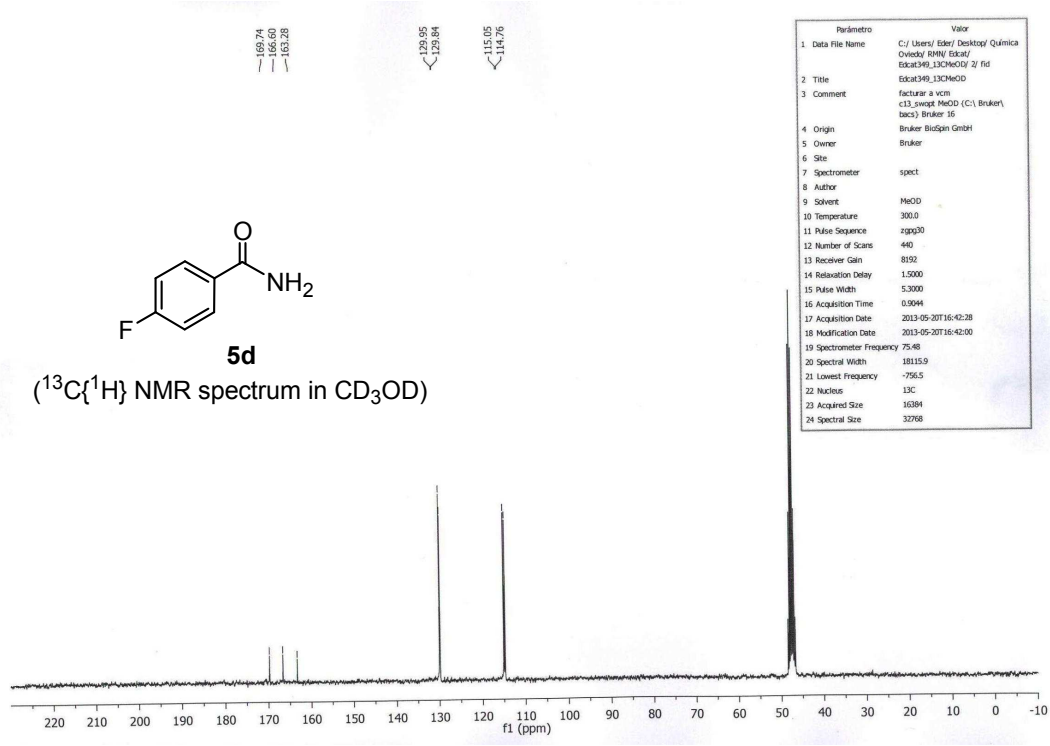
5d

(^{19}F NMR spectrum in CD_3OD)



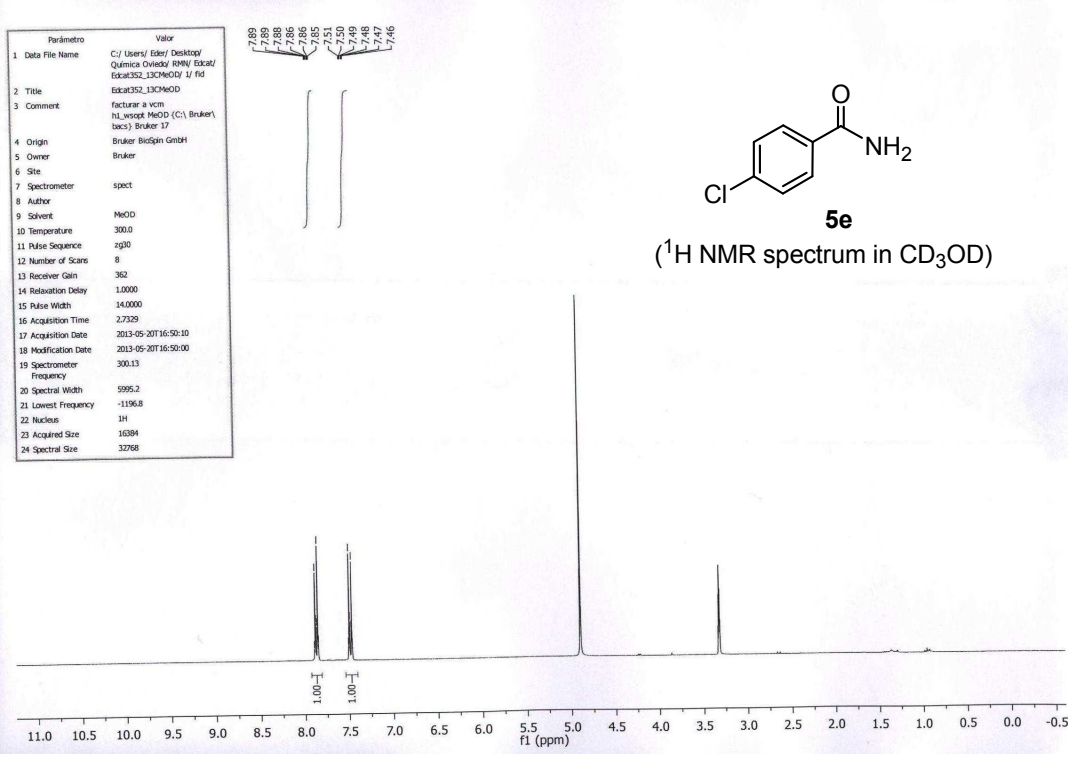
5d

(^{1}H NMR spectrum in CD_3OD)



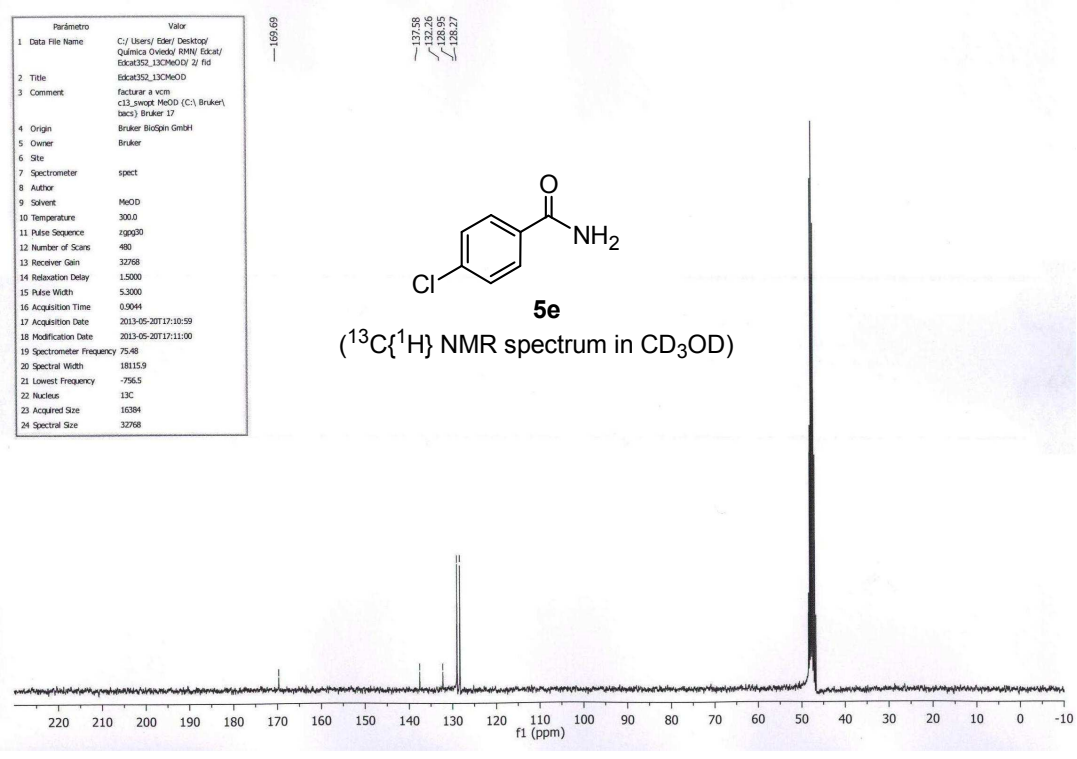
5d

($^{13}C\{^1H\}$ NMR spectrum in CD_3OD)



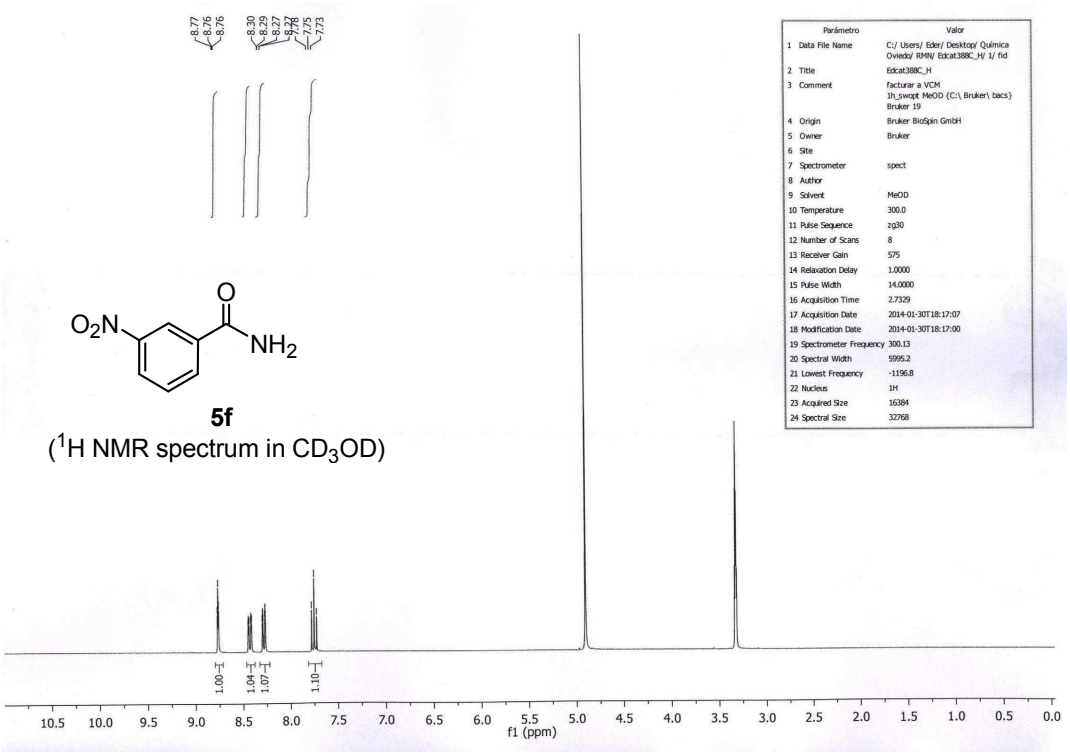
5e

(^{1}H NMR spectrum in CD_3OD)



5e

($^{13}C\{^1H\}$ NMR spectrum in CD_3OD)



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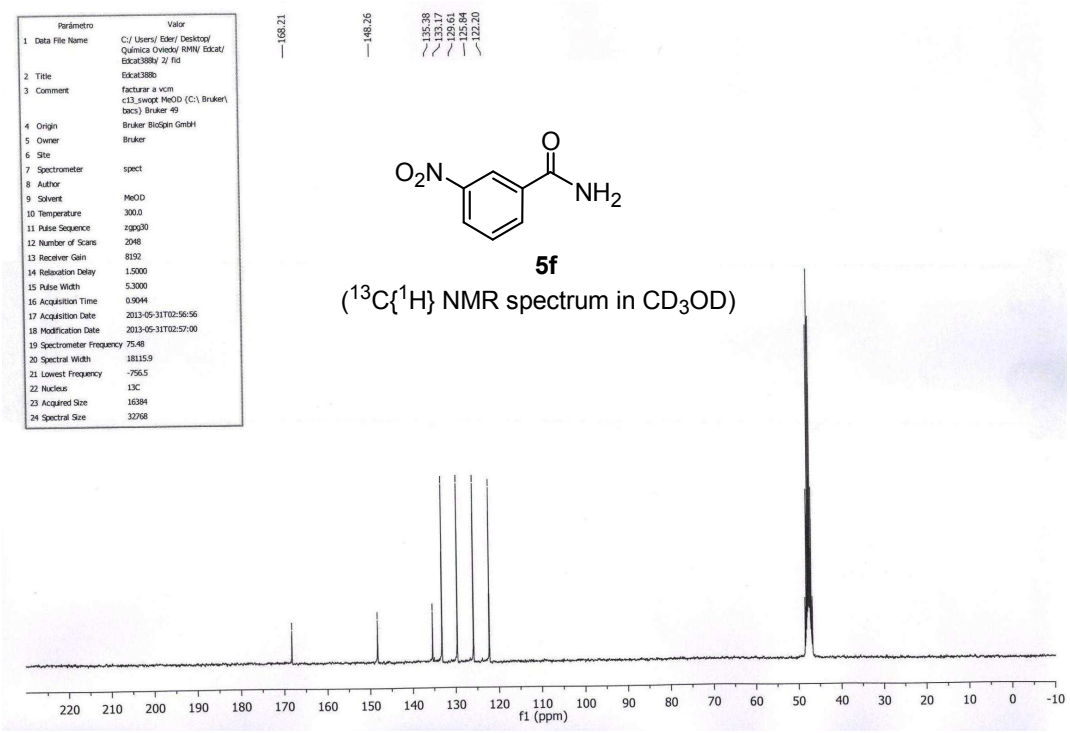
4 Origin	Bruker BioSpin GmbH
5 Owner	Bruker
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	MeOD
10 Temperature	300.0
11 Pulse Sequence	zg30
12 Number of Scans	8
13 Receiver Gain	575
14 Relaxation Delay	1.0000
15 Pulse Width	14.0000
16 Acquisition Time	2.7329
17 Acquisition Date	2014-01-30T18:17:07
18 Modification Date	2014-01-30T18:17:00
19 Spectrometer Frequency	300.13
20 Spectral Width	5995.2
21 Lowest Frequency	-1196.8
22 Nucleus	1H
23 Acquired Size	16384
24 Spectral Size	32768

5f

(^{1}H NMR spectrum in CD_3OD)



Parámetro	Valor
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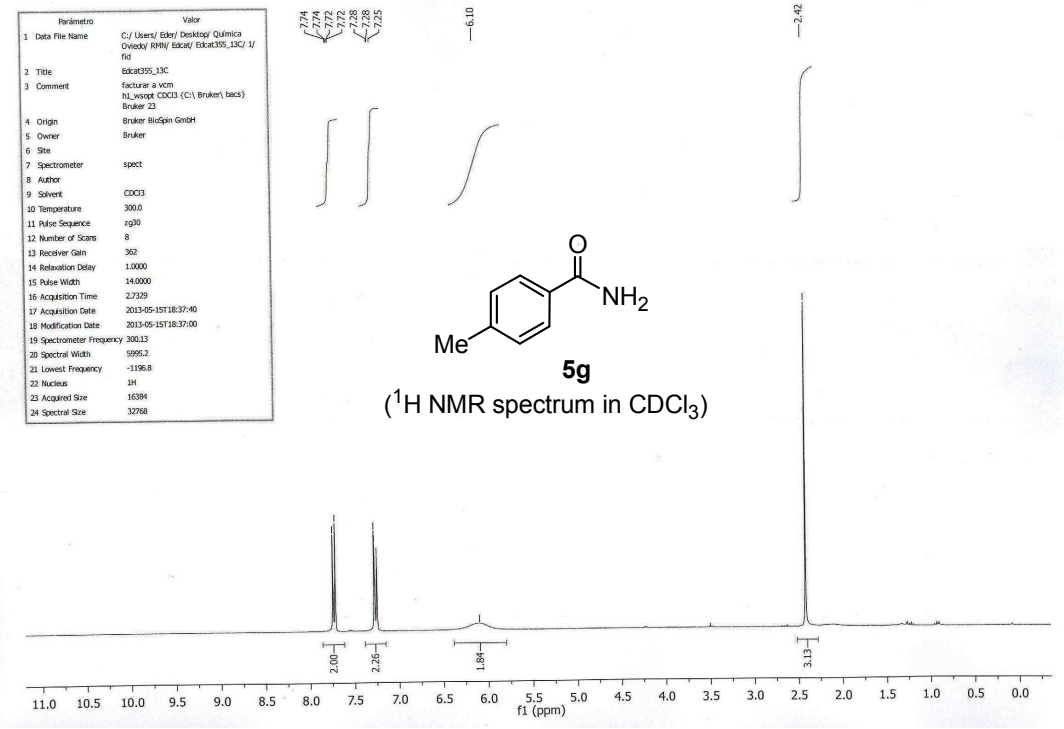
2 Title	Edcat388b
3 Comment	facturar a vcm c13_swopt MeOD {C:\ Bruker\ bacs} Bruker 49
4 Origin	Bruker BioSpin GmbH
5 Owner	Bruker
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	MeOD
10 Temperature	300.0
11 Pulse Sequence	zgpg30
12 Number of Scans	2048
13 Receiver Gain	8192
14 Relaxation Delay	1.5000
15 Pulse Width	5.3000
16 Acquisition Time	0.9044
17 Acquisition Date	2013-05-31T02:56:56
18 Modification Date	2013-05-31T02:57:00
19 Spectrometer Frequency	75.48
20 Spectral Width	18115.9
21 Lowest Frequency	-756.5
22 Nucleus	13C
23 Acquired Size	16384
24 Spectral Size	32768

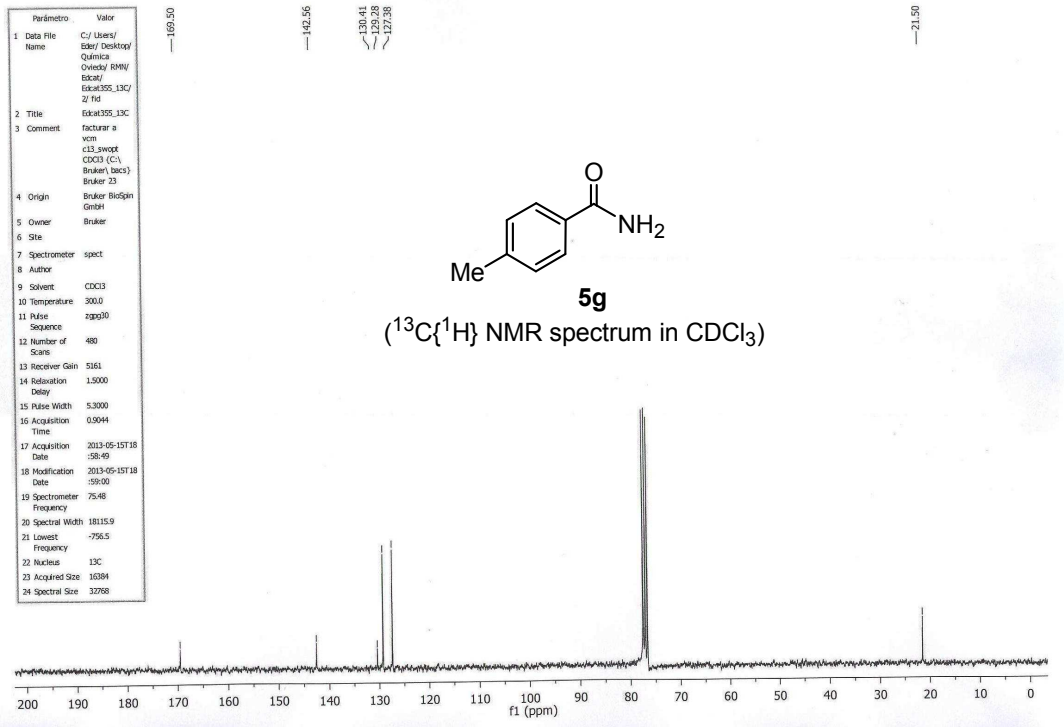
5f

($^{13}C\{^1H\}$ NMR spectrum in CD_3OD)



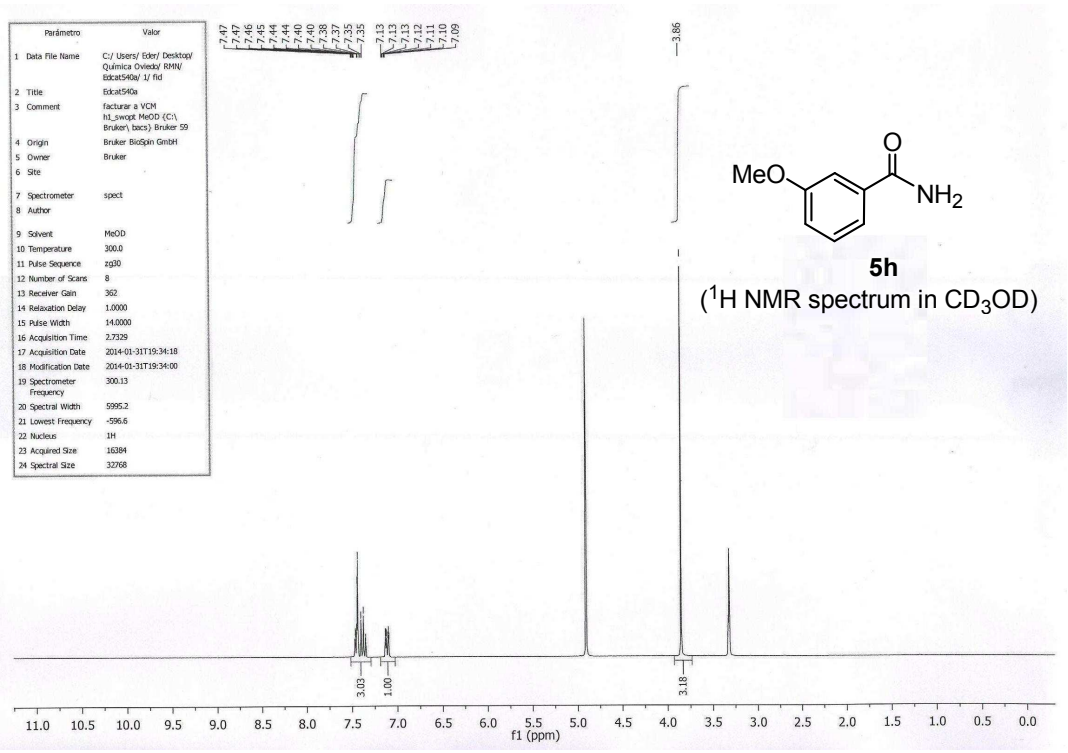
5g

(^{1}H NMR spectrum in $CDCl_3$)



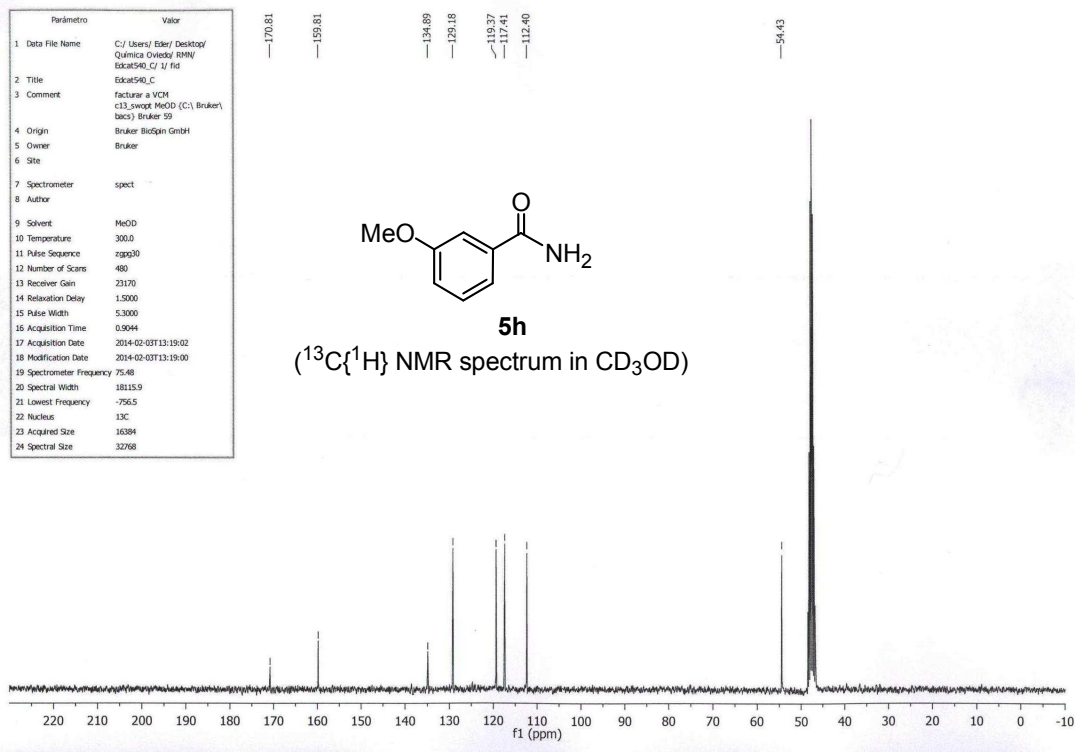
5g

($^{13}C\{^1H\}$ NMR spectrum in $CDCl_3$)



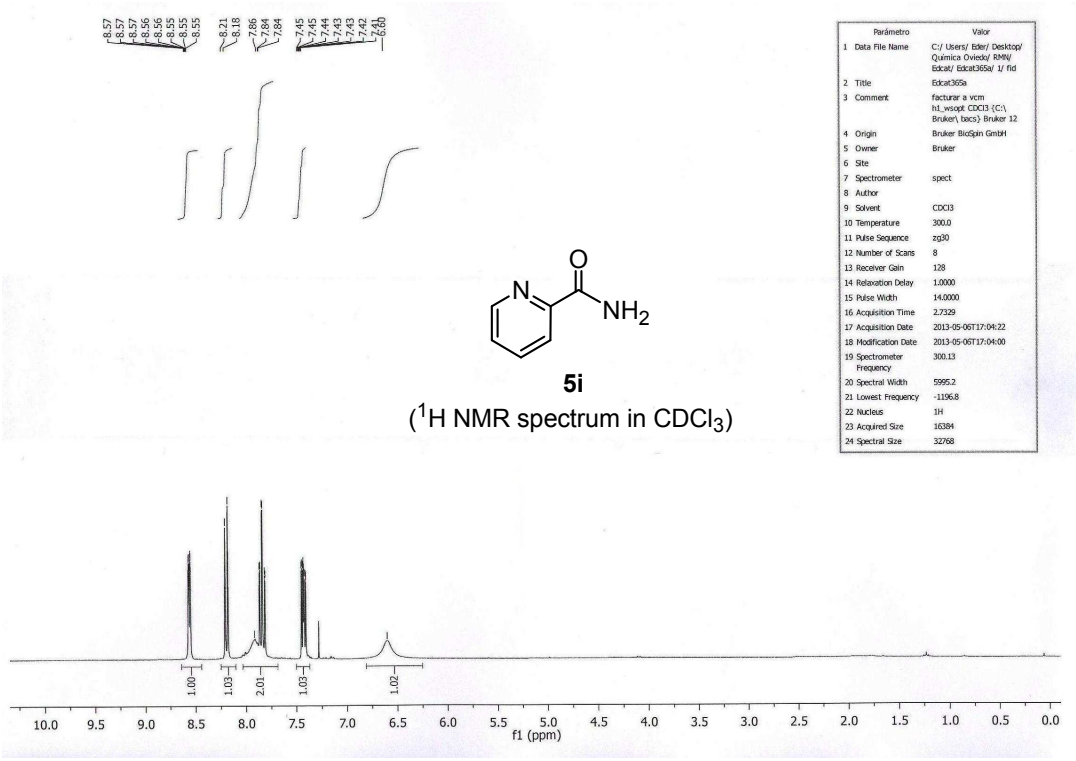
5h

(^{1}H NMR spectrum in CD_3OD)



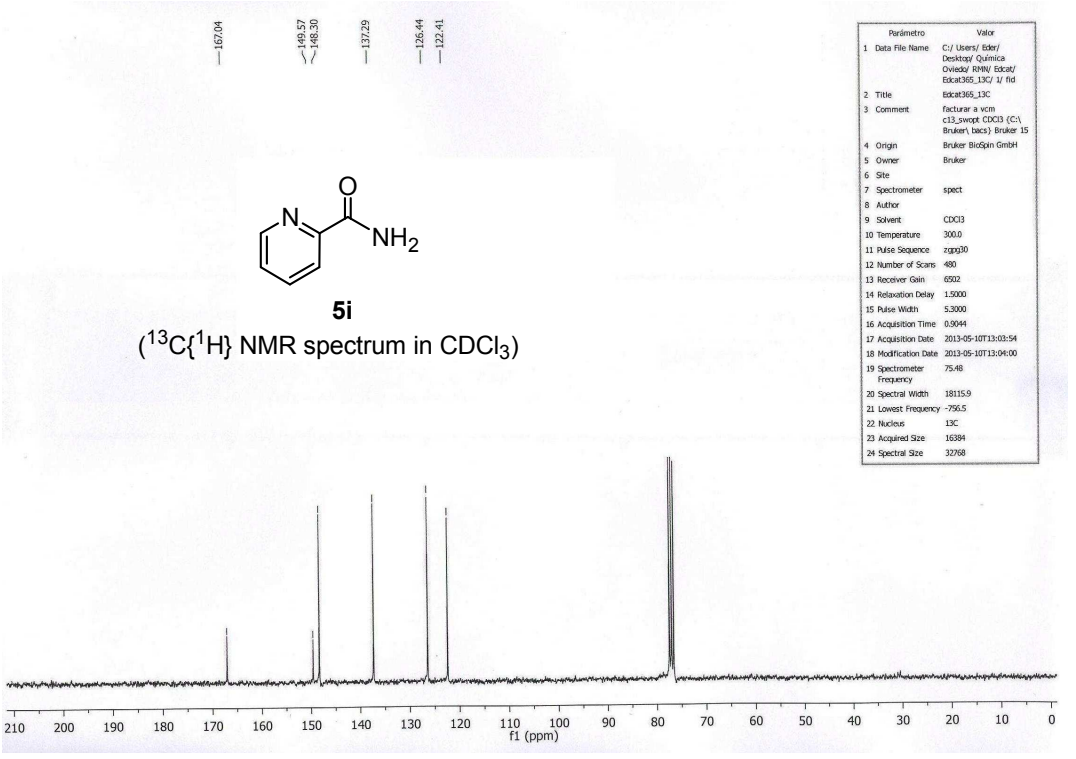
5h

($^{13}C\{^1H\}$ NMR spectrum in CD_3OD)



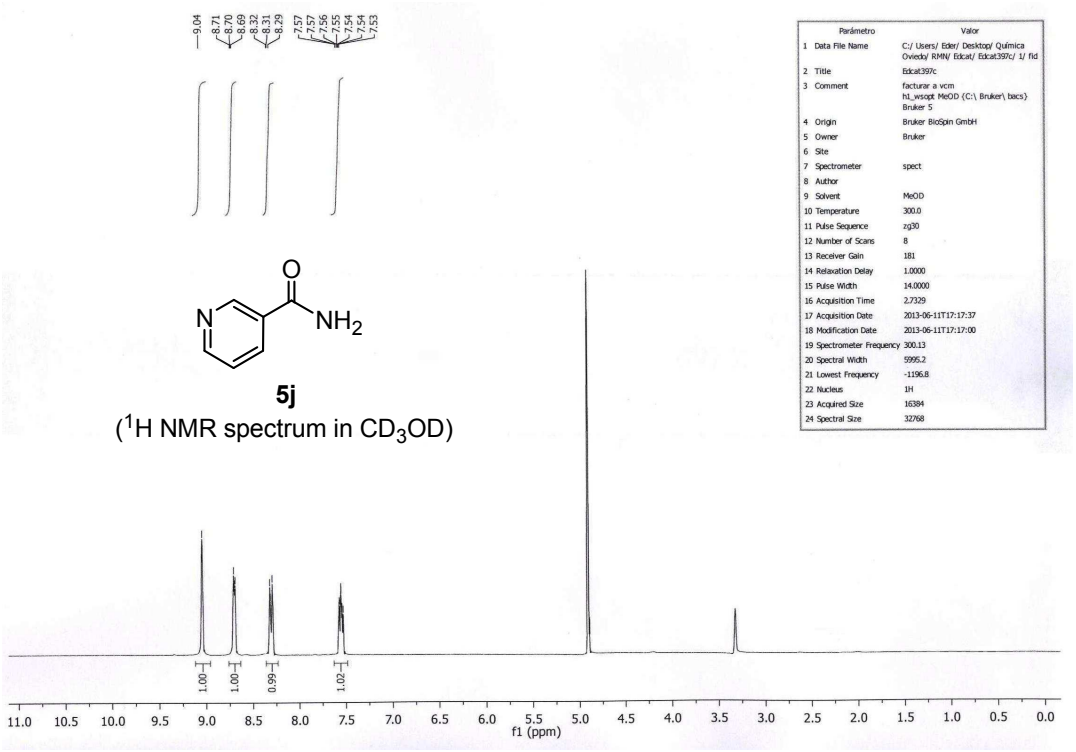
5i

(^{1}H NMR spectrum in $CDCl_3$)



5i

($^{13}C\{^1H\}$ NMR spectrum in $CDCl_3$)



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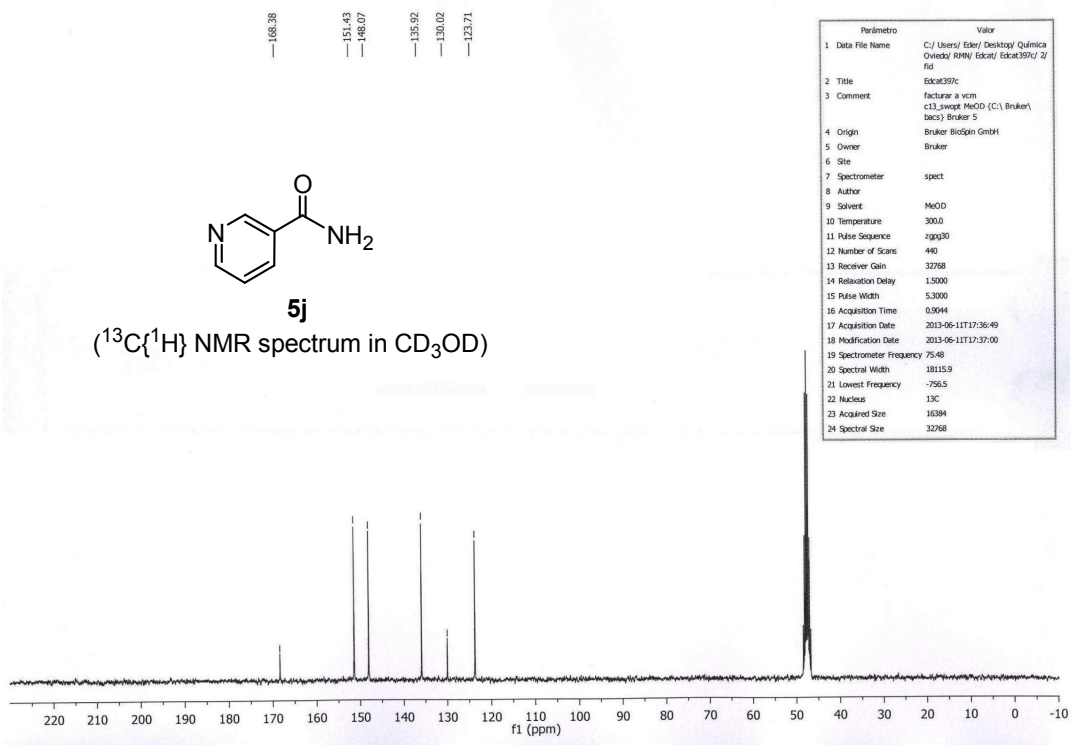
2	Title	Edcat397c
3	Comment	facturar a vcm h1_wsopt MeOD {C:\ Bruker\ bacs} Bruker 5
4	Origin	Bruker BioSpin GmbH
5	Owner	Bruker
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	MeOD
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	8
13	Receiver Gain	181
14	Relaxation Delay	1.0000
15	Pulse Width	14.0000
16	Acquisition Time	2.7329
17	Acquisition Date	2013-06-11T17:17:37
18	Modification Date	2013-06-11T17:17:00
19	Spectrometer Frequency	300.13
20	Spectral Width	5995.2
21	Lowest Frequency	-1196.8
22	Nucleus	1H
23	Acquired Size	16384
24	Spectral Size	32768

5j

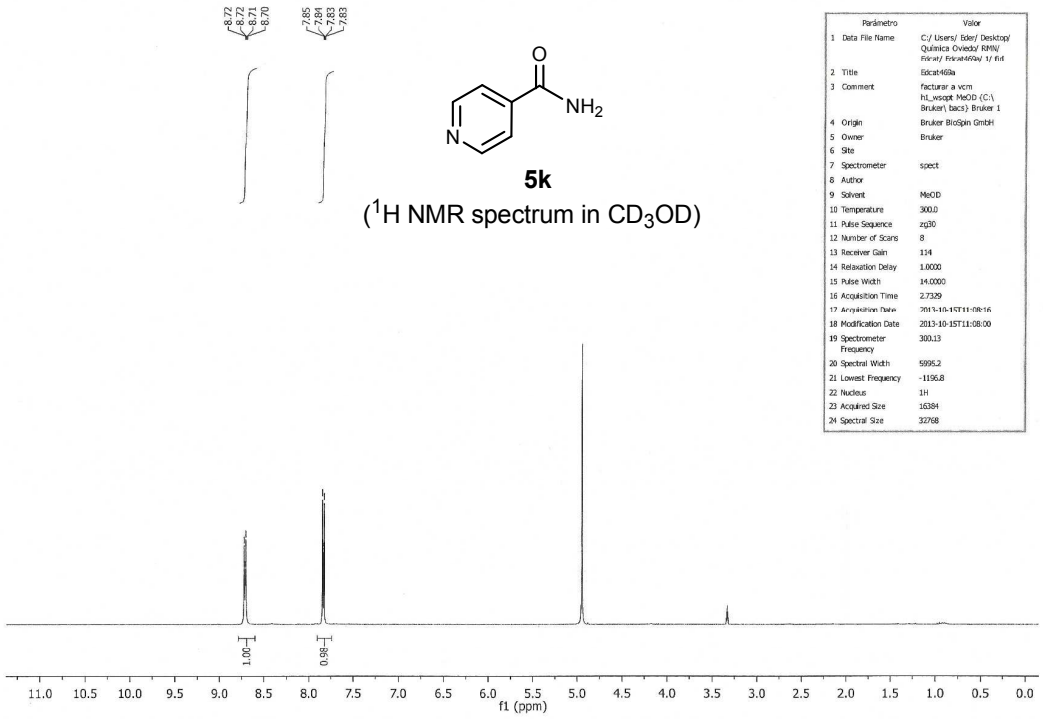
(^{1}H NMR spectrum in CD_3OD)



Parámetro		Valor
1	Data File Name	C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ Edcat/ Edcat397c/ 2/ fid
2	Title	Edcat397c
3	Comment	facturar a vcm c13_swopt MeOD {C:\ Bruker\ bacs} Bruker 5
4	Origin	Bruker BioSpin GmbH
5	Owner	Bruker
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	MeOD
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Number of Scans	440
13	Receiver Gain	32768
14	Relaxation Delay	1.5000
15	Pulse Width	5.3000
16	Acquisition Time	0.9044
17	Acquisition Date	2013-06-11T17:36:49
18	Modification Date	2013-06-11T17:37:00
19	Spectrometer Frequency	75.48
20	Spectral Width	18115.9
21	Lowest Frequency	-756.5
22	Nucleus	13C
23	Acquired Size	16384
24	Spectral Size	32768

5j

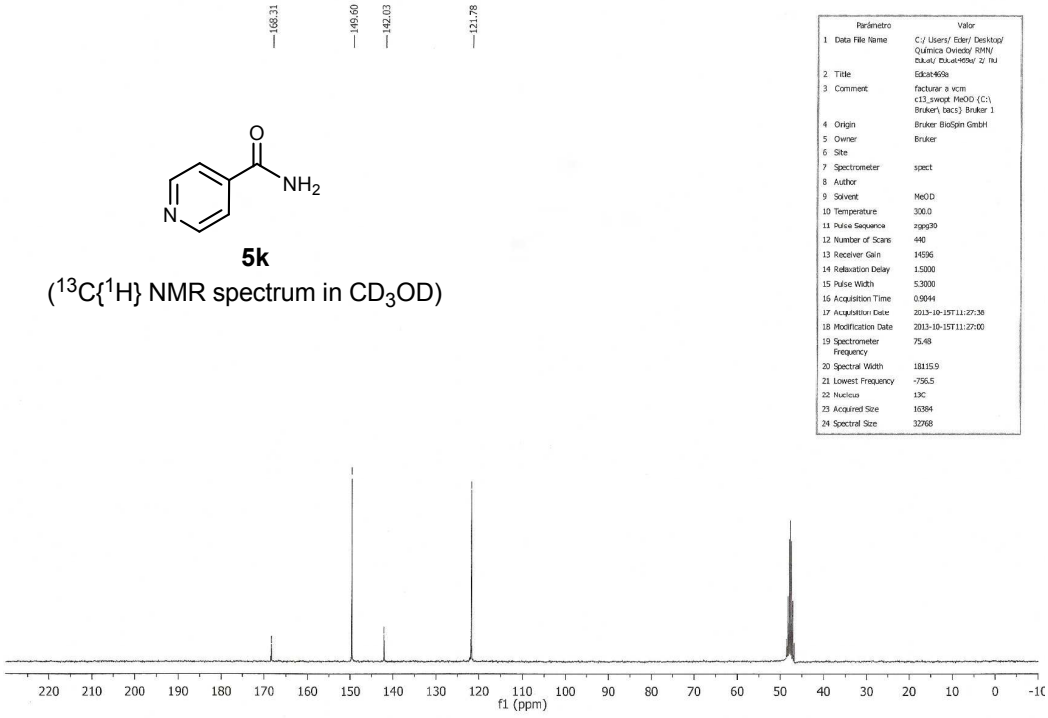
($^{13}C\{^1H\}$ NMR spectrum in CD_3OD)



Parámetro	Valor
1 Data File Name	C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ Eder/ Edcat469a/ 1/ fid
2 Title	Edcat469a
3 Comment	facturar a vcm h1_wsopt MeOD {C:\ Bruker\ bacs} Bruker 1
4 Origin	Bruker BioSpin GmbH
5 Owner	Bruker
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	MeOD
10 Temperature	300.0
11 Pulse Sequence	zg30
12 Number of Scans	8
13 Receiver Gain	114
14 Relaxation Delay	1.0000
15 Pulse Width	14.0000
16 Acquisition Time	2.7329
17 Acquisition Date	2013-10-15T11:08:16
18 Modification Date	2013-10-15T11:08:00
19 Spectrometer Frequency	300.13
20 Spectral Width	5995.2
21 Lowest Frequency	-1196.8
22 Nucleus	1H
23 Acquired Size	16384
24 Spectral Size	32768

5k

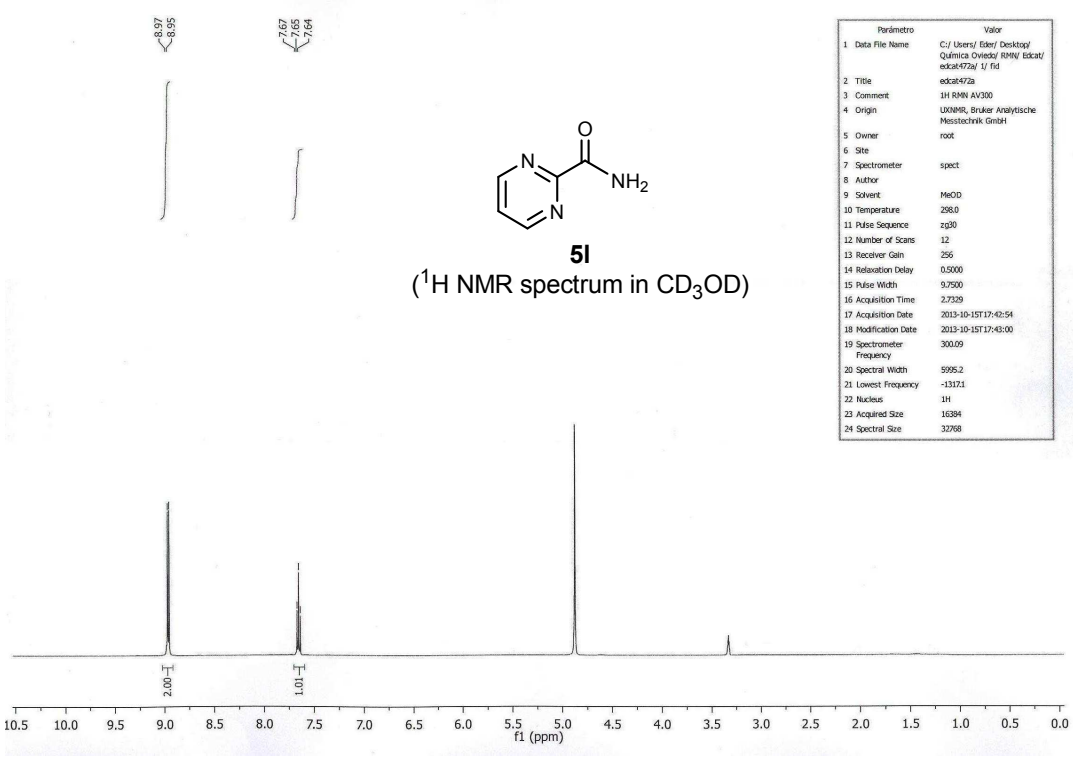
(^{1}H NMR spectrum in CD_3OD)



Parámetro	Valor
1 Data File Name	C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ Eder/ Edcat469a/ 2/ fid
2 Title	Edcat469a
3 Comment	facturar a vcm c13_swopt MeOD {C:\ Bruker\ bacs} Bruker 1
4 Origin	Bruker BioSpin GmbH
5 Owner	Bruker
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	MeOD
10 Temperature	300.0
11 Pulse Sequence	zgpg30
12 Number of Scans	440
13 Receiver Gain	14596
14 Relaxation Delay	1.5000
15 Pulse Width	5.3000
16 Acquisition Time	0.9044
17 Acquisition Date	2013-10-15T11:27:38
18 Modification Date	2013-10-15T11:27:00
19 Spectrometer Frequency	75.48
20 Spectral Width	18115.9
21 Lowest Frequency	-756.5
22 Nucleus	13C
23 Acquired Size	16384
24 Spectral Size	32768

5k

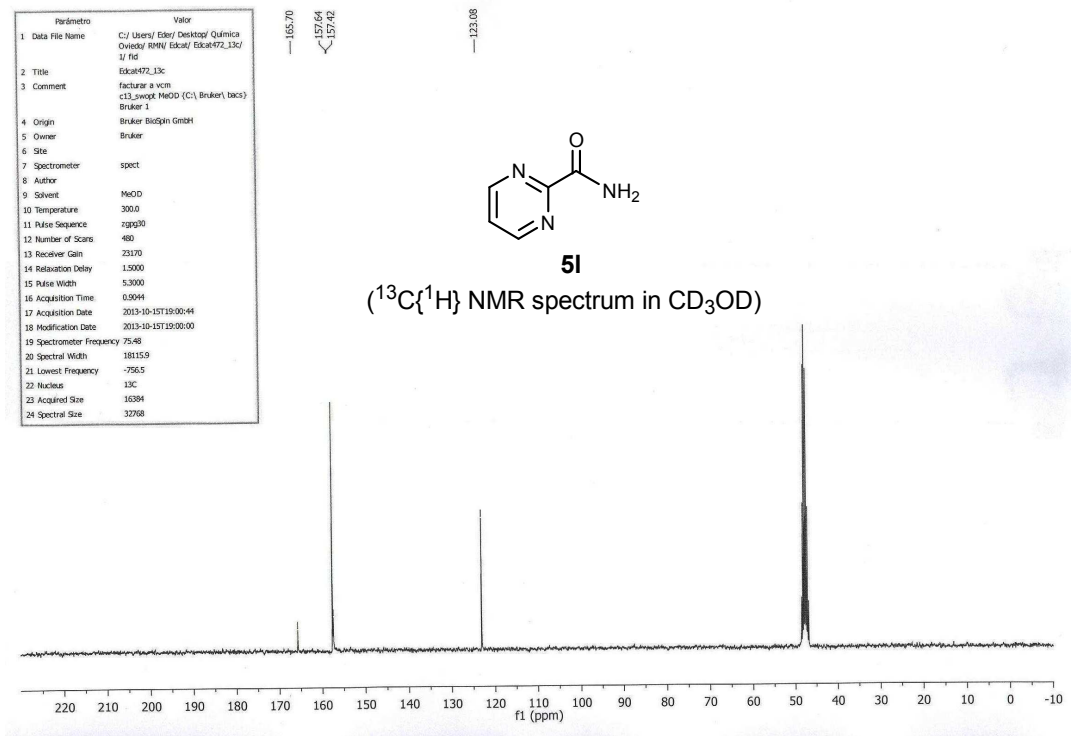
($^{13}C\{^1H\}$ NMR spectrum in CD_3OD)



	Parámetro	Valor
1	Data File Name	C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ Edcat/ edcat472a/ 1/ fid
2	Title	edcat472a
3	Comment	1H RMN AV300
4	Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	MeOD
10	Temperature	298.0
11	Pulse Sequence	zg30
12	Number of Scans	12
13	Receiver Gain	256
14	Relaxation Delay	0.5000
15	Pulse Width	9.7500
16	Acquisition Time	2.7329
17	Acquisition Date	2013-10-15T17:42:54
18	Modification Date	2013-10-15T17:43:00
19	Spectrometer Frequency	300.09
20	Spectral Width	5995.2
21	Lowest Frequency	-1317.1
22	Nucleus	1H
23	Acquired Size	16384
24	Spectral Size	32768

5l

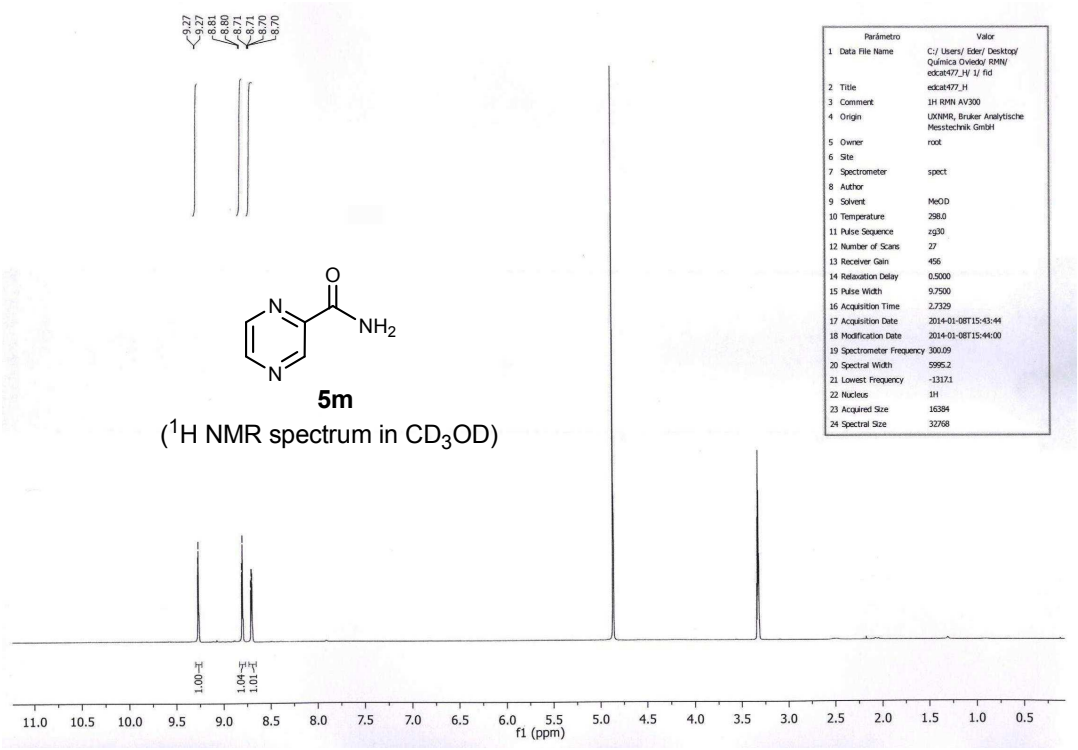
(^{1}H NMR spectrum in CD_3OD)



	Parámetro	Valor
1	Data File Name	C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ Edcat/ Edcat472_13c/ 1/ fid
2	Title	Edcat472_13c
3	Comment	facturar a vcm c13_swopt MeOD (C:\ Bruker\ bacs) Bruker 1
4	Origin	Bruker BioSpin GmbH
5	Owner	Bruker
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	MeOD
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Number of Scans	480
13	Receiver Gain	23170
14	Relaxation Delay	1.5000
15	Pulse Width	5.3000
16	Acquisition Time	0.9044
17	Acquisition Date	2013-10-15T19:00:44
18	Modification Date	2013-10-15T19:00:00
19	Spectrometer Frequency	75.48
20	Spectral Width	18115.9
21	Lowest Frequency	-756.5
22	Nucleus	13C
23	Acquired Size	16384
24	Spectral Size	32768

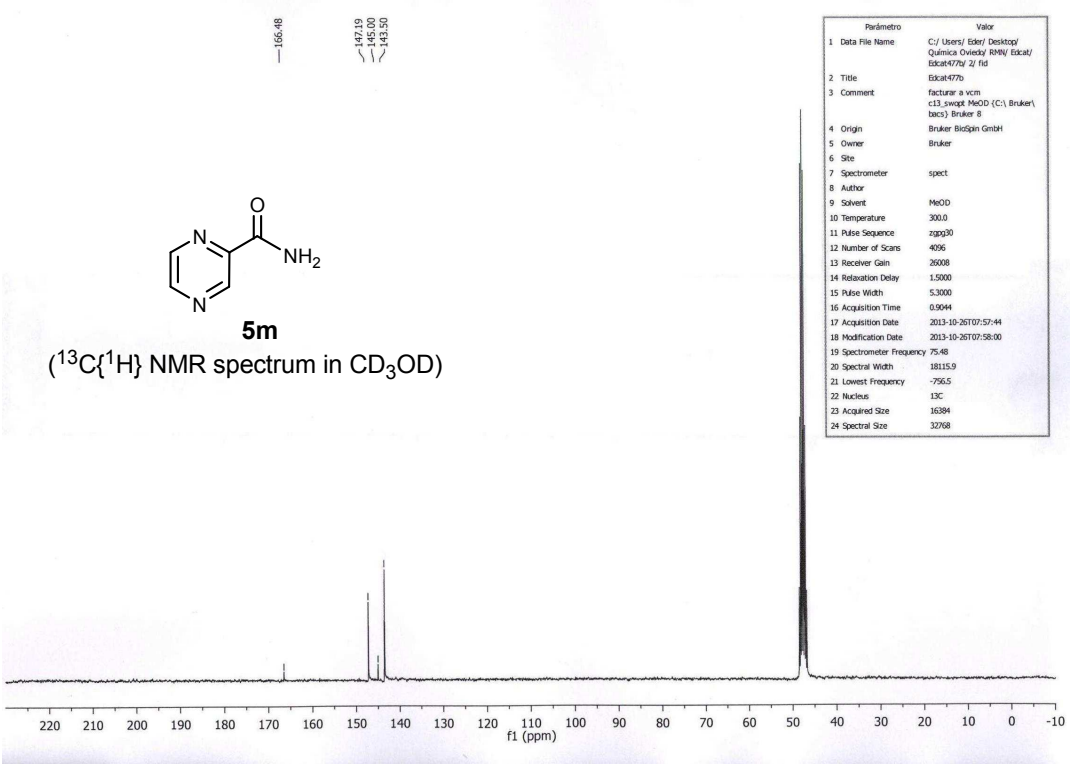
5l

($^{13}C\{^{1}H\}$ NMR spectrum in CD_3OD)



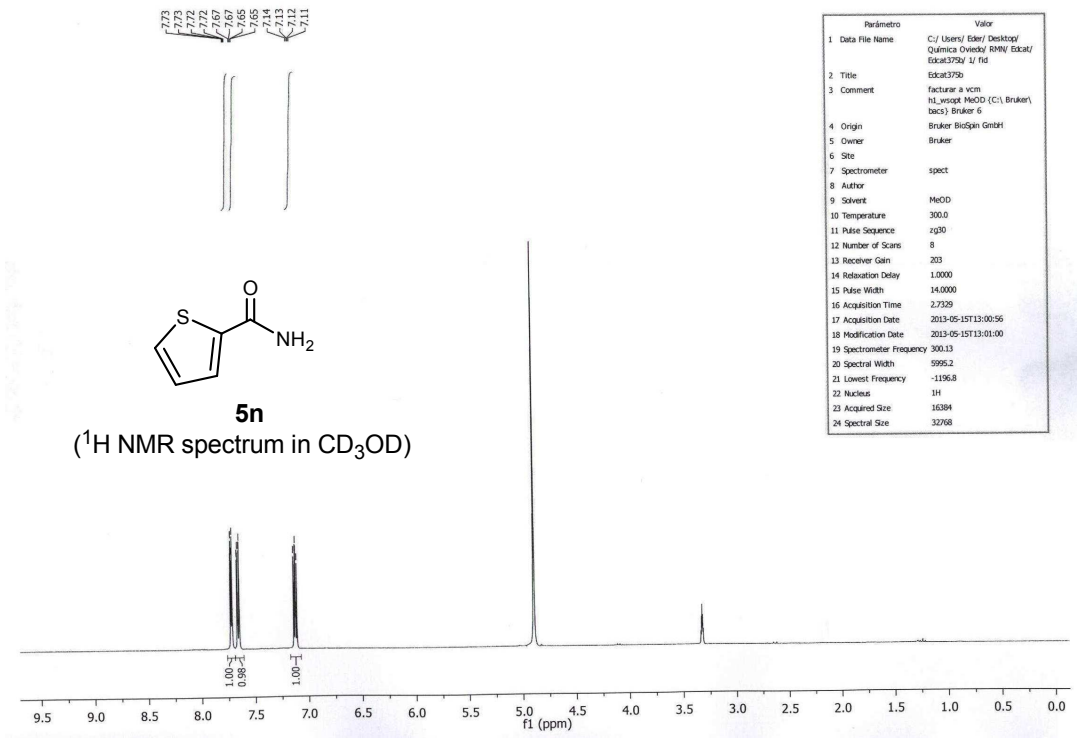
5m

(^{1}H NMR spectrum in CD_3OD)



5m

($^{13}C\{^{1}H\}$ NMR spectrum in CD_3OD)



Parámetro	Valor
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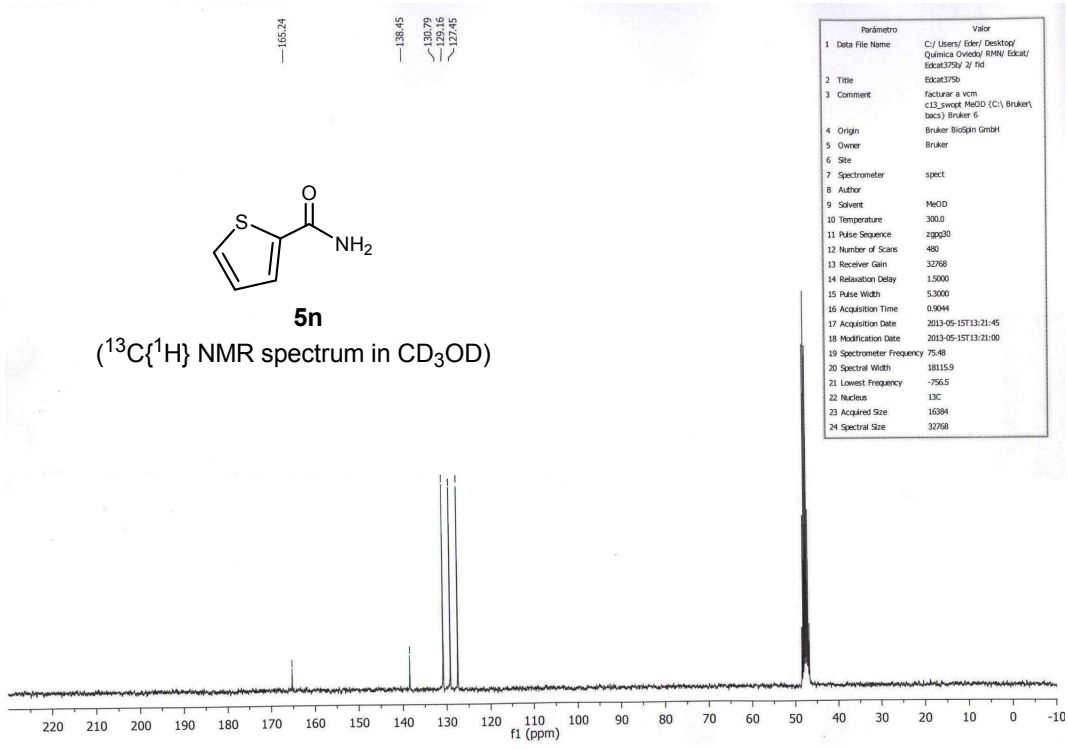
2 Title	Edcat375b
3 Comment	facturar a vcm h1_wsopt MeOD {C:\ Bruker\ bacs} Bruker 6
4 Origin	Bruker BioSpin GmbH
5 Owner	Bruker
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	MeOD
10 Temperature	300.0
11 Pulse Sequence	zg30
12 Number of Scans	8
13 Receiver Gain	203
14 Relaxation Delay	1.0000
15 Pulse Width	14.0000
16 Acquisition Time	2.7329
17 Acquisition Date	2013-05-15T13:00:56
18 Modification Date	2013-05-15T13:01:00
19 Spectrometer Frequency	300.13
20 Spectral Width	5995.2
21 Lowest Frequency	-1196.8
22 Nucleus	1H
23 Acquired Size	16384
24 Spectral Size	32768

5n

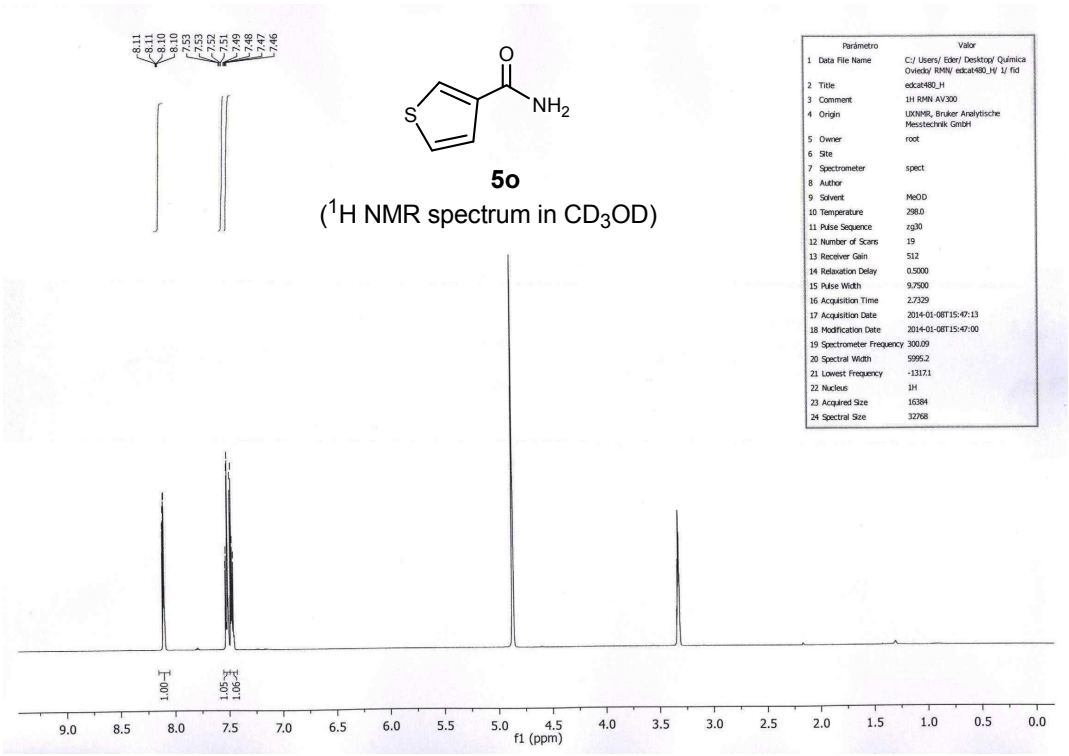
(^{1}H NMR spectrum in CD_3OD)

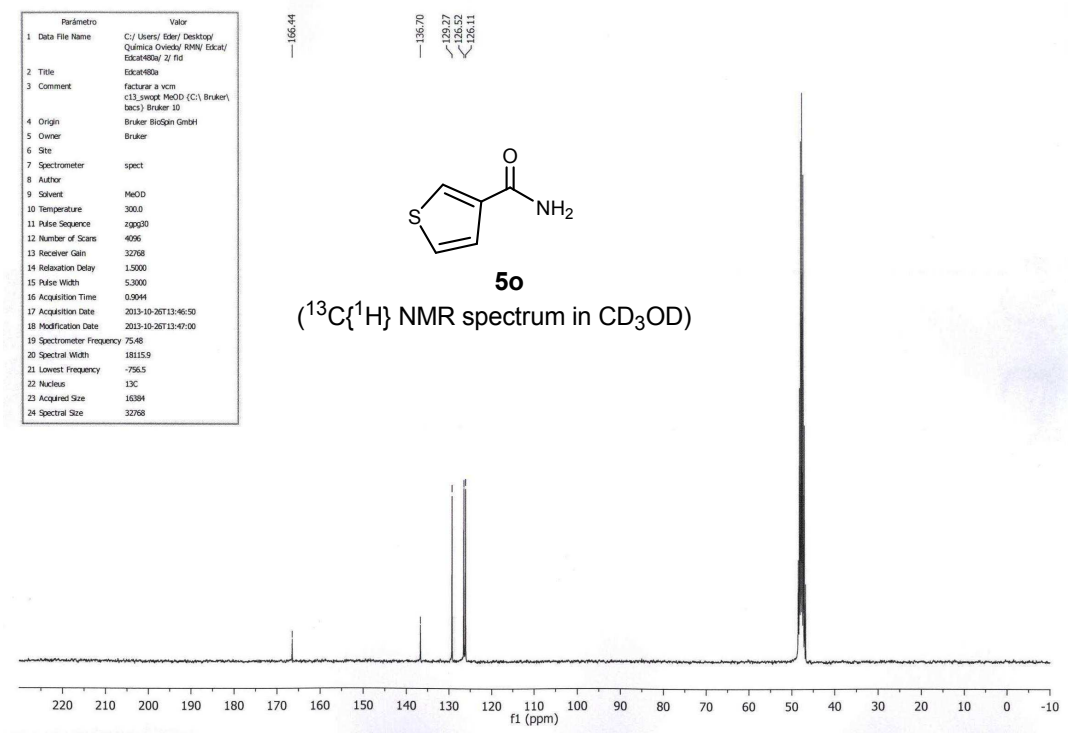


Parámetro	Valor
1 Data File Name	C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ Edcat/ Edcat375b/ 2/ fid
2 Title	Edcat375b
3 Comment	facturar a vcm c13_swopt MeOD {C:\ Bruker\ bacs} Bruker 6
4 Origin	Bruker BioSpin GmbH
5 Owner	Bruker
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	MeOD
10 Temperature	300.0
11 Pulse Sequence	zgpg30
12 Number of Scans	480
13 Receiver Gain	32768
14 Relaxation Delay	1.5000
15 Pulse Width	5.3000
16 Acquisition Time	0.9044
17 Acquisition Date	2013-05-15T13:21:45
18 Modification Date	2013-05-15T13:21:00
19 Spectrometer Frequency	75.48
20 Spectral Width	18115.9
21 Lowest Frequency	-756.5
22 Nucleus	13C
23 Acquired Size	16384
24 Spectral Size	32768

5n

($^{13}C\{^1H\}$ NMR spectrum in CD_3OD)


8.11
8.11
8.10
8.10
7.53
7.53
7.52
7.51
7.49
7.48
7.47
7.46
O
NH2
S
5o
(1H NMR spectrum in CD3OD)
Parámetro Valor
1 Data File Name C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ edcat480_H/ 1/ fid
2 Title edcat480_H
3 Comment 1H RMN AV300
4 Origin UXNMR, Bruker Analytische Messtechnik GmbH
5 Owner root
6 Site
7 Spectrometer spect
8 Author
9 Solvent MeOD
10 Temperature 298.0
11 Pulse Sequence zg30
12 Number of Scans 19
13 Receiver Gain 512
14 Relaxation Delay 0.5000
15 Pulse Width 9.7500
16 Acquisition Time 2.7329
17 Acquisition Date 2014-01-08T15:47:13
18 Modification Date 2014-01-08T15:47:00
19 Spectrometer Frequency 300.09
20 Spectral Width 5995.2
21 Lowest Frequency -1317.1
22 Nucleus 1H
23 Acquired Size 16384
24 Spectral Size 32768
1.00
1.05
1.06
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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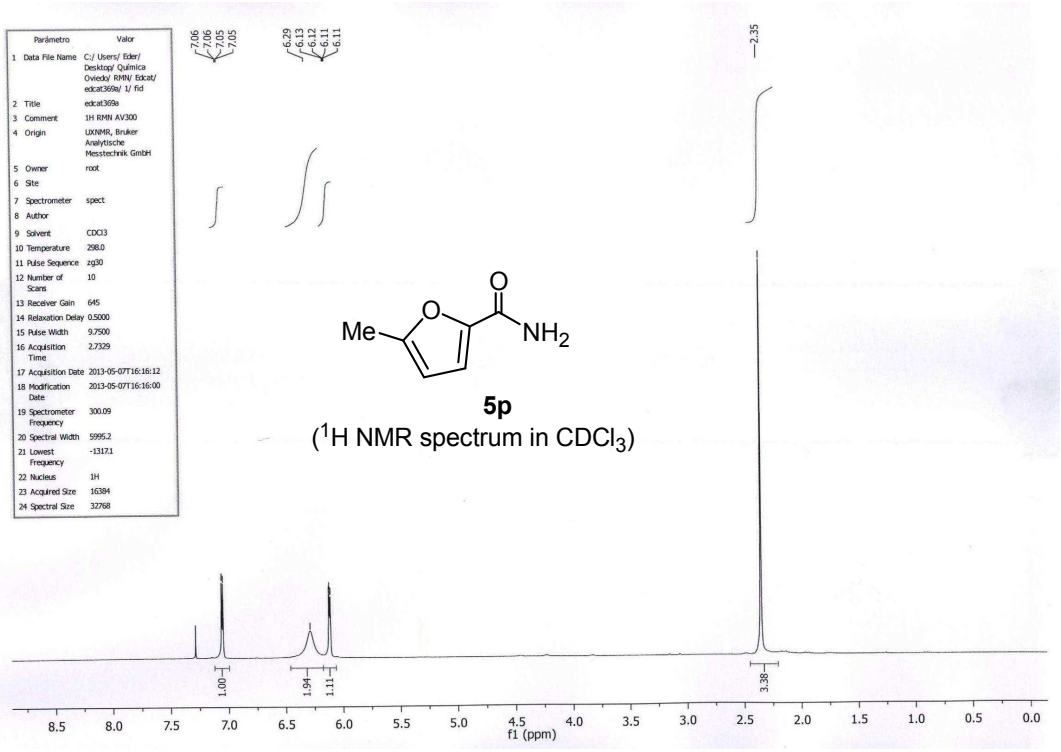
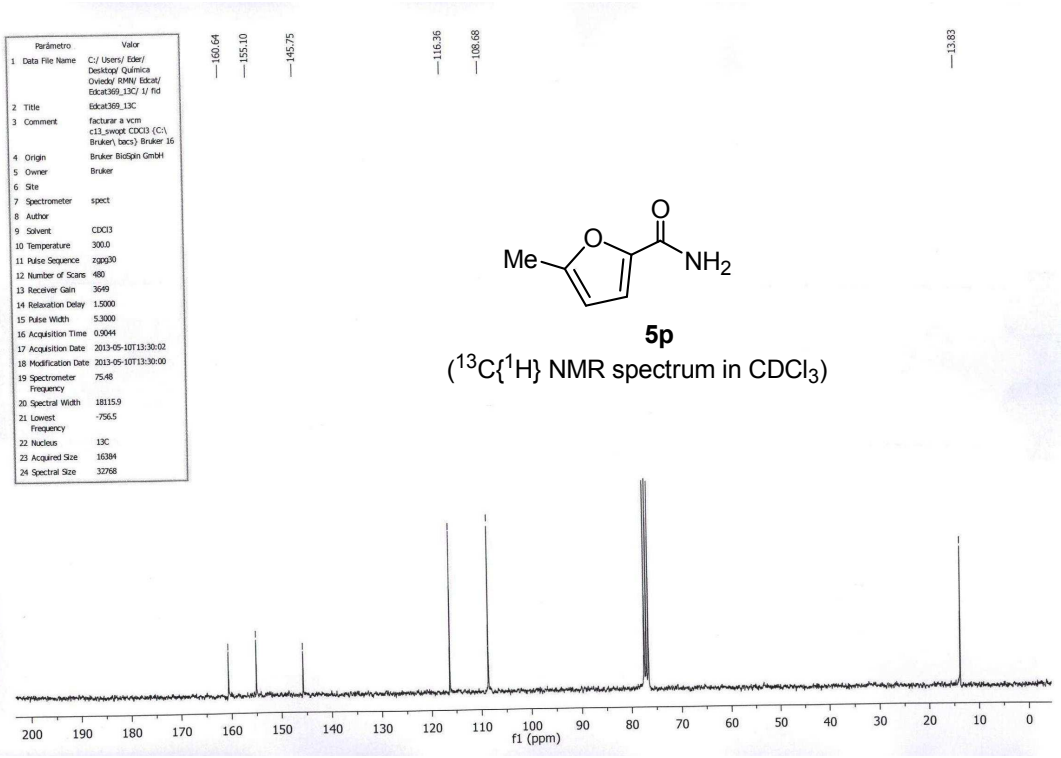
1 Data File Name C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ Edcat/ Edcat480a/ 2/ fid
2 Title Edcat480a
3 Comment facturar a vcm c13_swopt MeOD {C:\ Bruker\ bacs} Bruker 10
4 Origin Bruker BioSpin GmbH
5 Owner Bruker
6 Site
7 Spectrometer spect
8 Author
9 Solvent MeOD
10 Temperature 300.0
11 Pulse Sequence zgpg30
12 Number of Scans 4096
13 Receiver Gain 32768
14 Relaxation Delay 1.5000
15 Pulse Width 5.3000
16 Acquisition Time 0.9044
17 Acquisition Date 2013-10-26T13:46:50
18 Modification Date 2013-10-26T13:47:00
19 Spectrometer Frequency 75.48
20 Spectral Width 18115.9
21 Lowest Frequency -756.5
22 Nucleus 13C
23 Acquired Size 16384
24 Spectral Size 32768
166.44
136.70
129.27
126.52
126.11
O
NH2
S
5o
(13C{1H} NMR spectrum in CD3OD)
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)



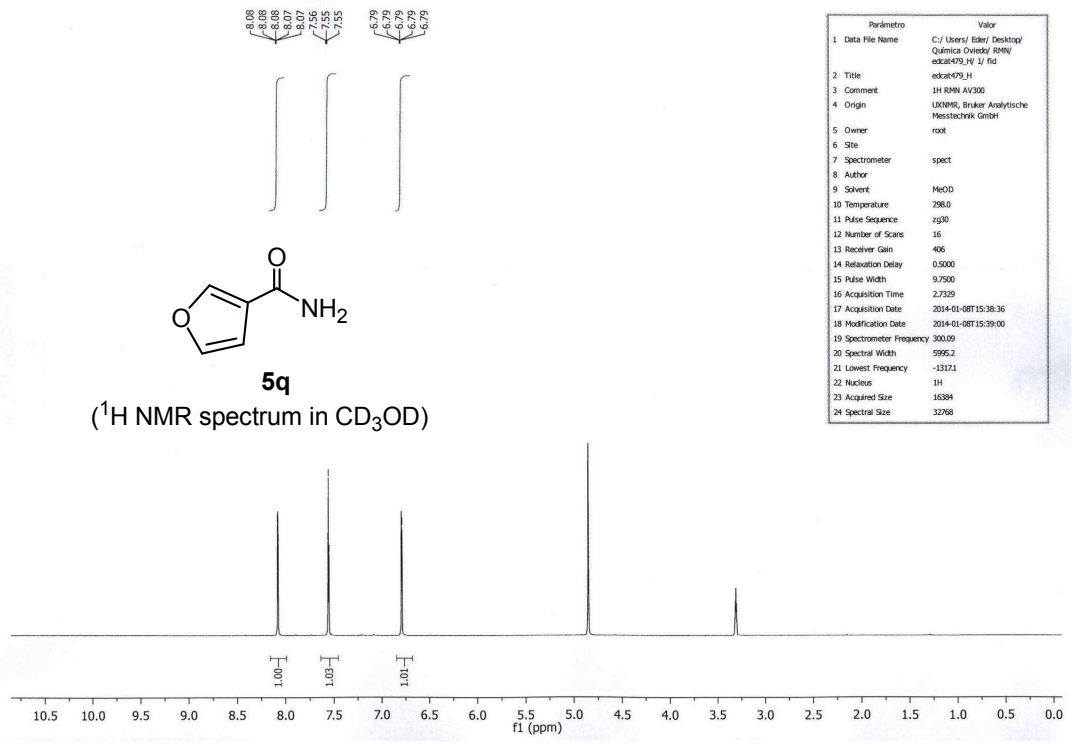
5p

(^{1}H NMR spectrum in $CDCl_3$)



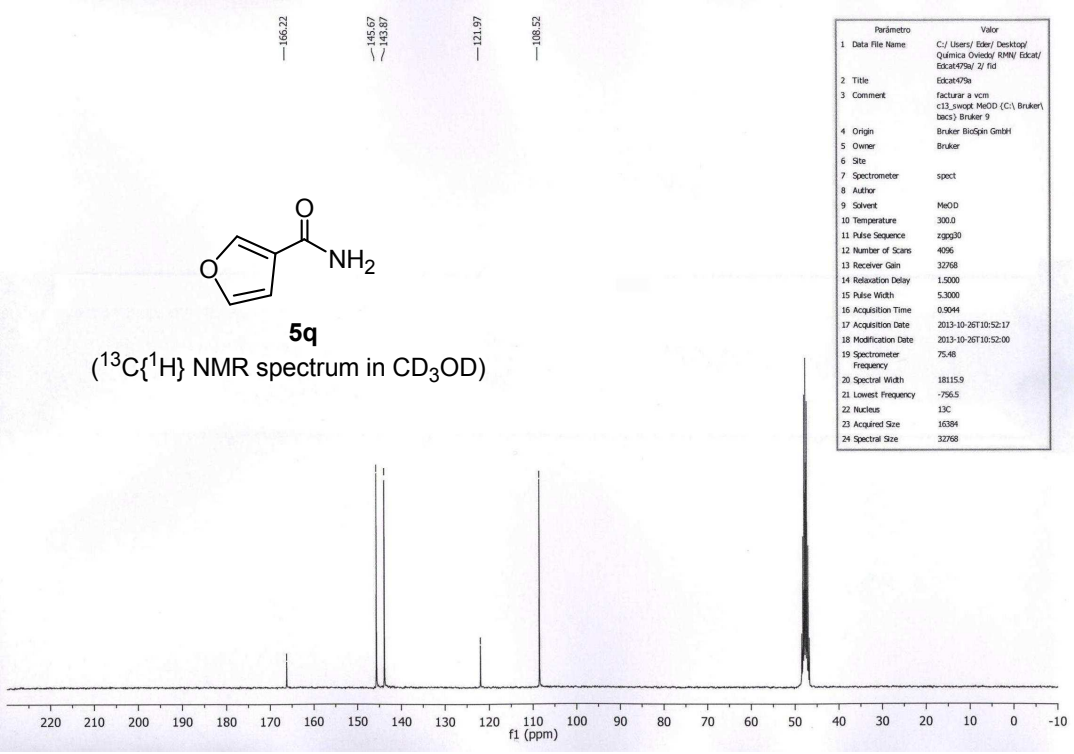
5p

($^{13}C\{^{1}H\}$ NMR spectrum in $CDCl_3$)



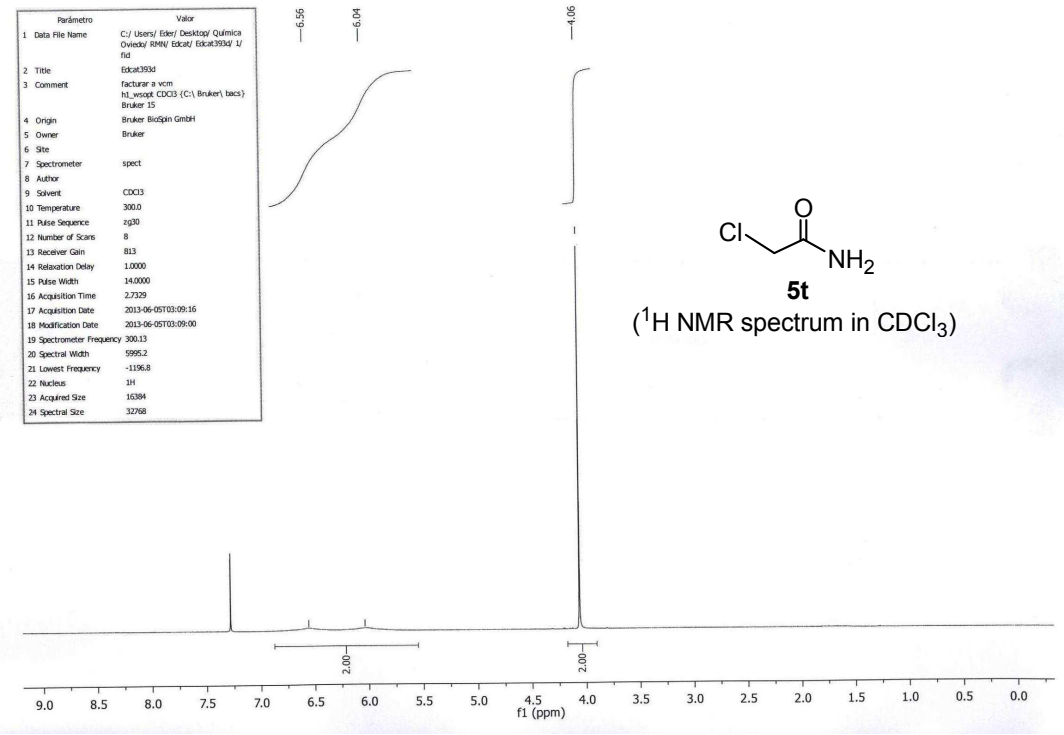
5q

(^{1}H NMR spectrum in CD_3OD)



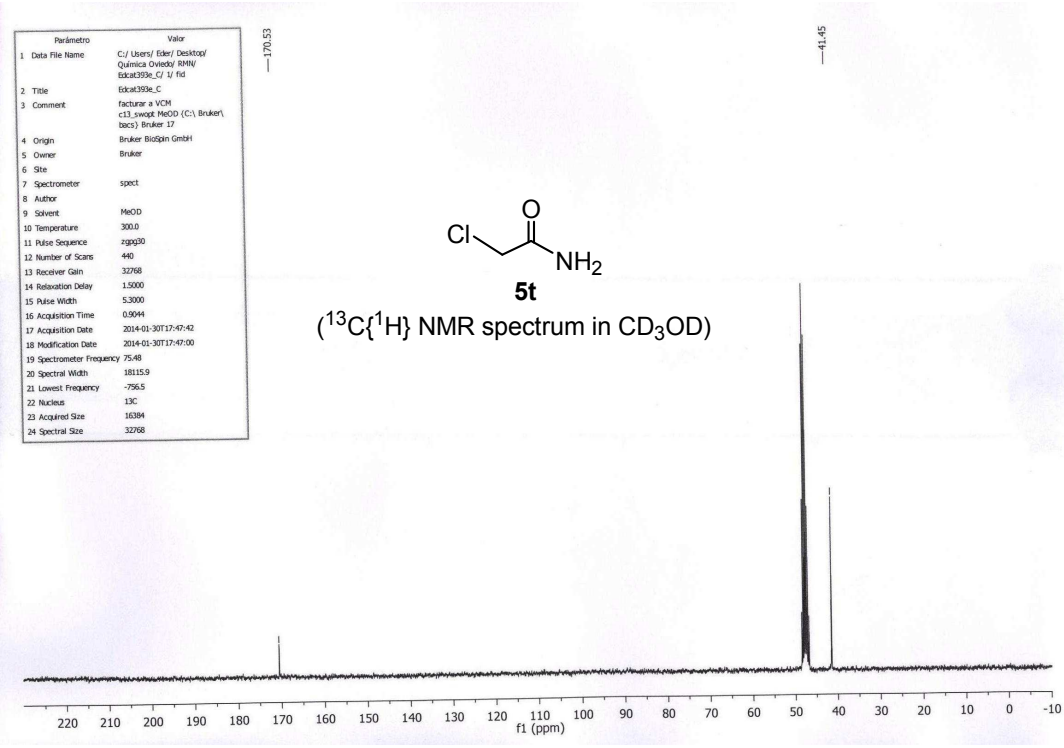
5q

($^{13}C\{^1H\}$ NMR spectrum in CD_3OD)



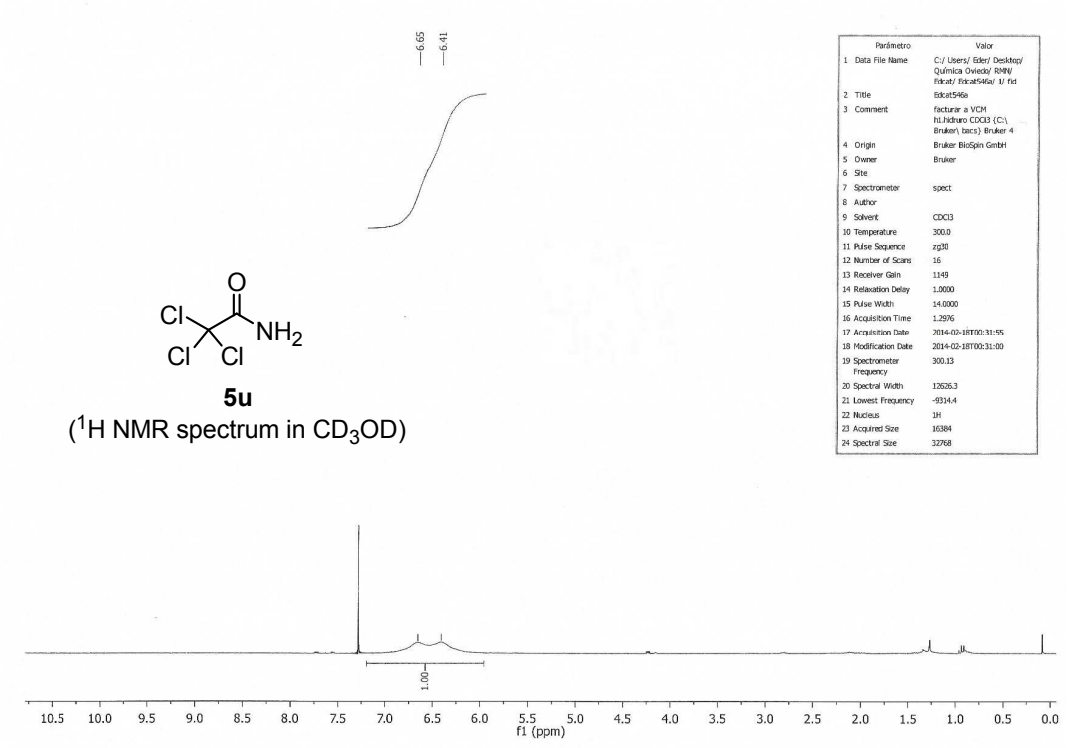
5t

(^{1}H NMR spectrum in $CDCl_3$)



5t

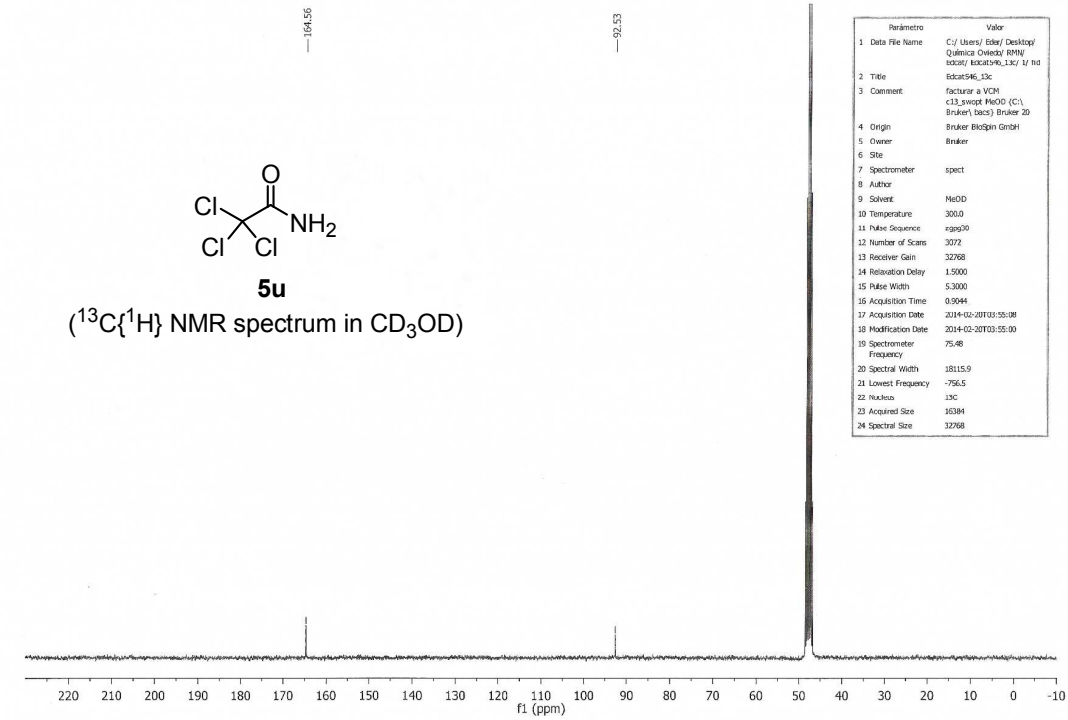
($^{13}C\{^1H\}$ NMR spectrum in CD_3OD)



	Parámetro	Valor
1	Data File Name	C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ fidcat/ fidcat546a/ 1/ fid
2	Title	fidcat546a
3	Comment	facturar a VCM h1.hidruro CDCl3 (C:\ Bruker\ bacs) Bruker 4
4	Origin	Bruker BioSpin GmbH
5	Owner	Bruker
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	1149
14	Relaxation Delay	1.0000
15	Pulse Width	14.0000
16	Acquisition Time	1.2976
17	Acquisition Date	2014-02-18T00:31:55
18	Modification Date	2014-02-18T00:31:00
19	Spectrometer Frequency	300.13
20	Spectral Width	12626.3
21	Lowest Frequency	-9314.4
22	Nucleus	1H
23	Acquired Size	16384
24	Spectral Size	32768

5u

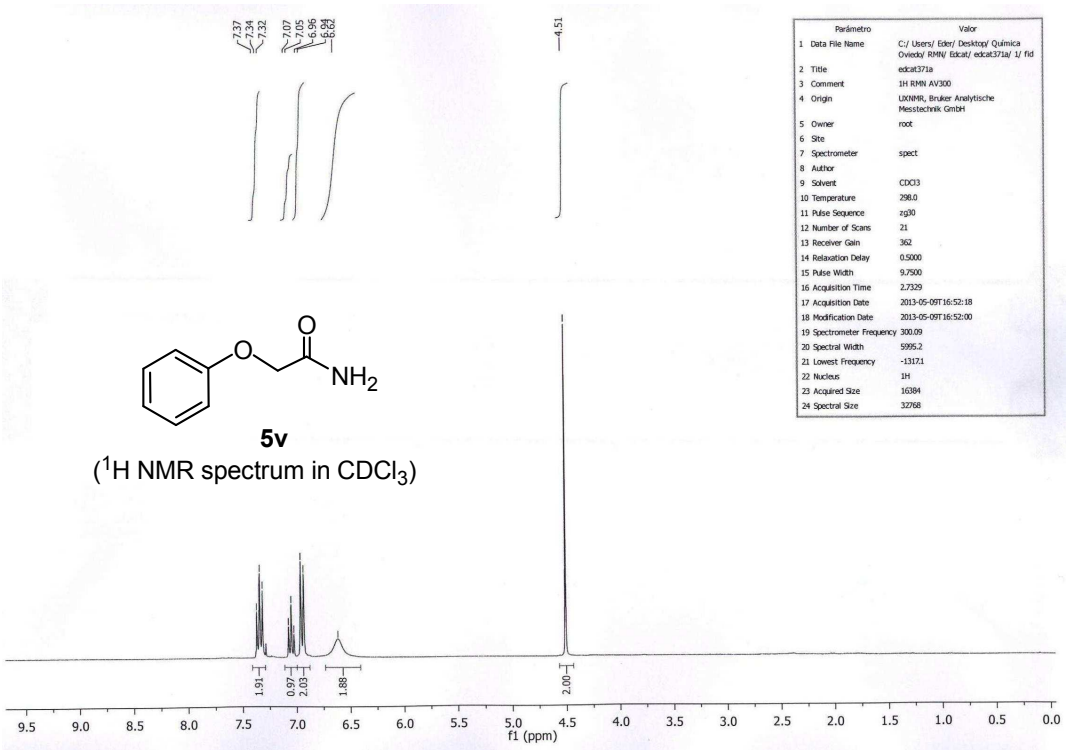
(^{1}H NMR spectrum in CD_3OD)



	Parámetro	Valor
1	Data File Name	C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ fidcat/ fidcat546_13c/ 1/ fid
2	Title	fidcat546_13c
3	Comment	facturar a VCM c13_swopt MeOD (C:\ Bruker\ bacs) Bruker 20
4	Origin	Bruker BioSpin GmbH
5	Owner	Bruker
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	MeOD
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Number of Scans	3072
13	Receiver Gain	32768
14	Relaxation Delay	1.5000
15	Pulse Width	5.3000
16	Acquisition Time	0.9044
17	Acquisition Date	2014-02-20T03:55:08
18	Modification Date	2014-02-20T03:55:00
19	Spectrometer Frequency	75.48
20	Spectral Width	18115.9
21	Lowest Frequency	-756.5
22	Nucleus	13C
23	Acquired Size	16384
24	Spectral Size	32768

5u

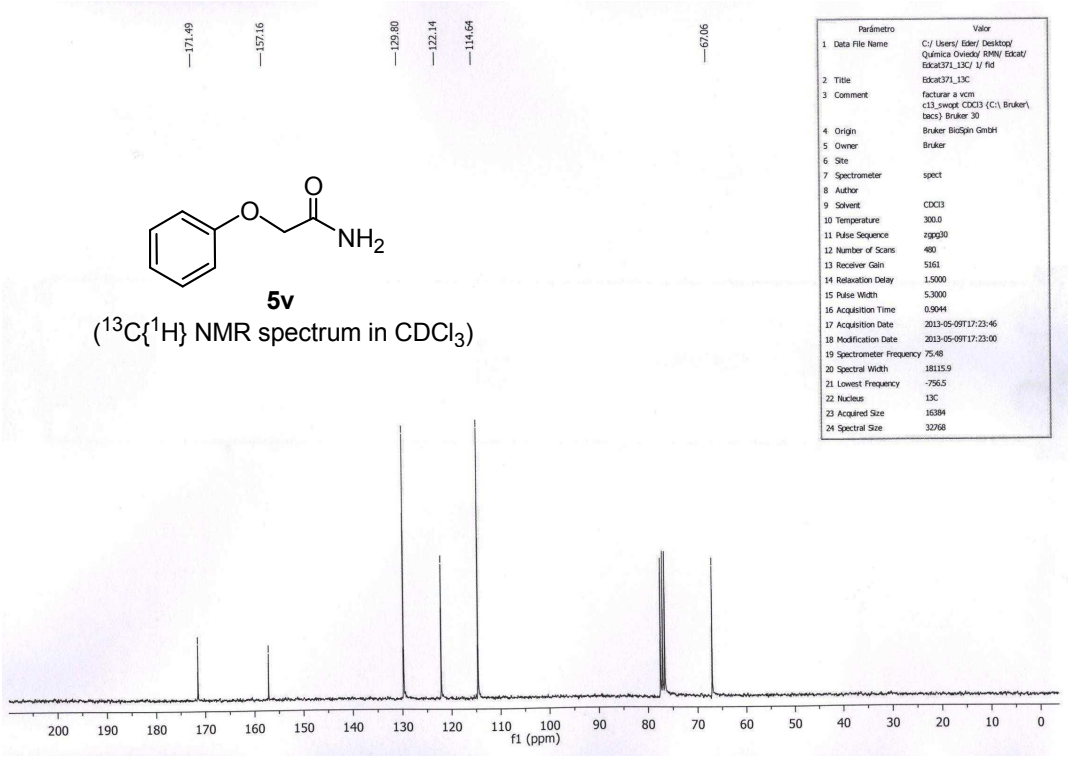
($^{13}C\{^1H\}$ NMR spectrum in CD_3OD)



Parámetro	Valor
1 Data File Name	C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ Edcat/ edcat371a/ 1/ fid
2 Title	edcat371a
3 Comment	1H RMN AV300
4 Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.0
11 Pulse Sequence	zg30
12 Number of Scans	21
13 Receiver Gain	362
14 Relaxation Delay	0.5000
15 Pulse Width	9.7500
16 Acquisition Time	2.7329
17 Acquisition Date	2013-05-09T16:52:18
18 Modification Date	2013-05-09T16:52:00
19 Spectrometer Frequency	300.09
20 Spectral Width	5995.2
21 Lowest Frequency	-1317.1
22 Nucleus	1H
23 Acquired Size	16384
24 Spectral Size	32768

5v

(^{1}H NMR spectrum in $CDCl_3$)

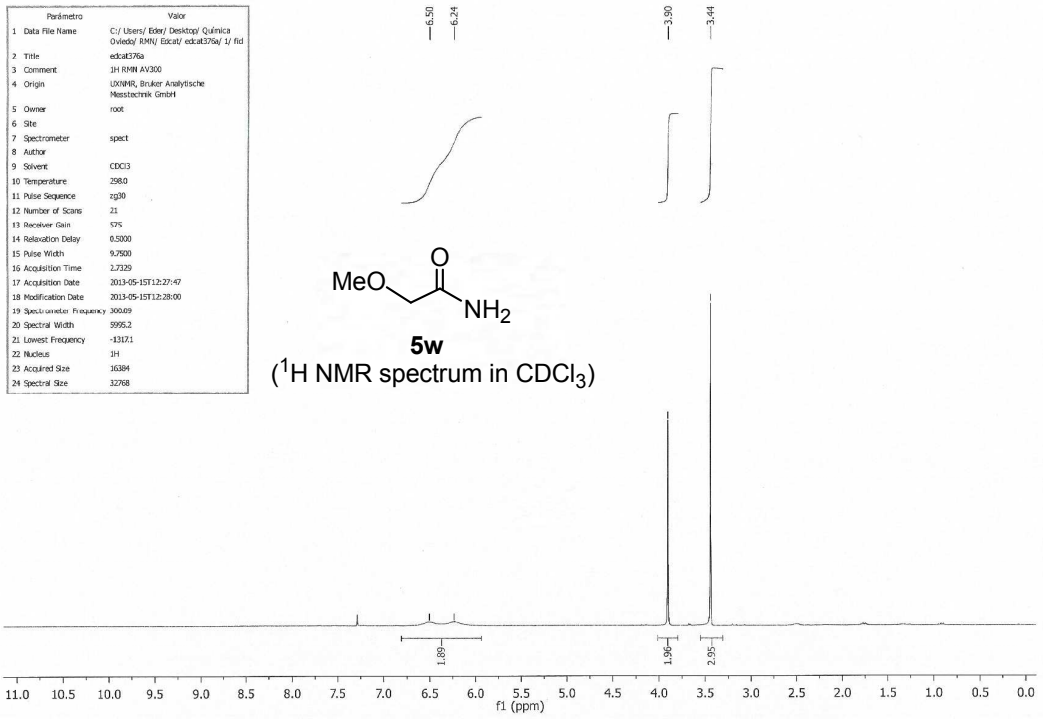


Parámetro	Valor
1 Data File Name	C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ Edcat/ Edcat371_13C/ 1/ fid
2 Title	Edcat371_13C
3 Comment	facturar a vcm c13_swopt CDCl3 {C:\ Bruker\ bacs} Bruker 30
4 Origin	Bruker BioSpin GmbH
5 Owner	Bruker
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.0
11 Pulse Sequence	zgpg30
12 Number of Scans	480
13 Receiver Gain	5161
14 Relaxation Delay	1.5000
15 Pulse Width	5.3000
16 Acquisition Time	0.9044
17 Acquisition Date	2013-05-09T17:23:46
18 Modification Date	2013-05-09T17:23:00
19 Spectrometer Frequency	75.48
20 Spectral Width	18115.9
21 Lowest Frequency	-756.5
22 Nucleus	13C
23 Acquired Size	16384
24 Spectral Size	32768

5v

(^{13}C{^{1}H} NMR spectrum in $CDCl_3$)

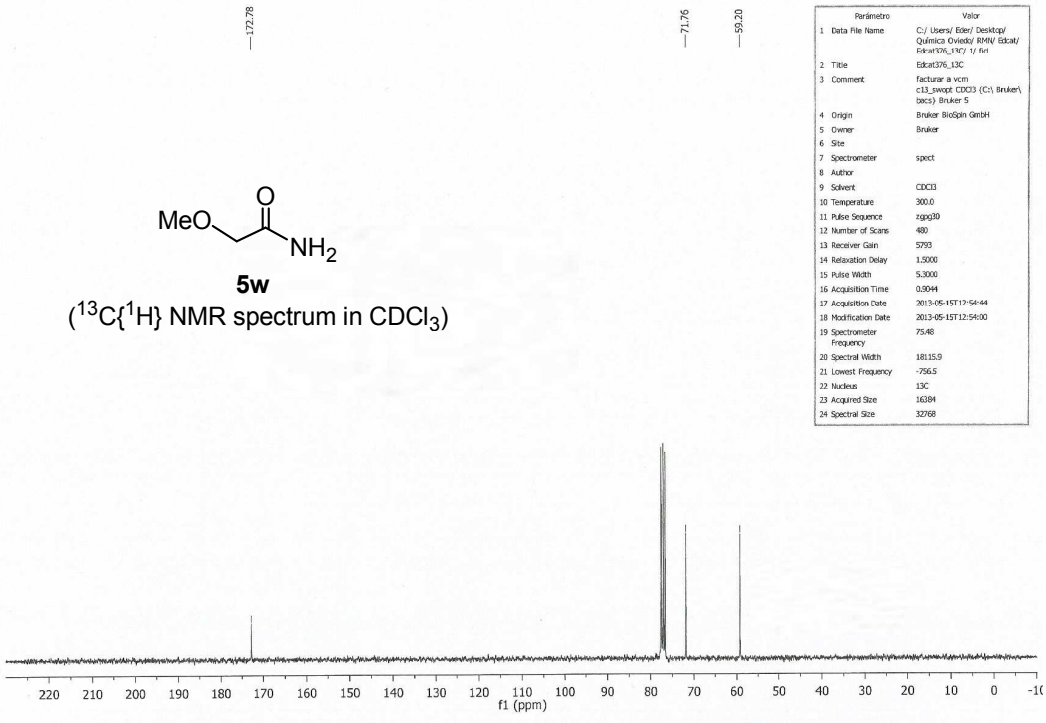
Parámetro	Valor
1 Data File Name	C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ Edcat/ edcat376a/ 1/ fid
2 Title	edcat376a
3 Comment	1H RMN AV300
4 Origin	LOXNMR, Bruker Analytische Messtechnik GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	298.0
11 Pulse Sequence	zg30
12 Number of Scans	21
13 Receiver Gain	575
14 Relaxation Delay	0.5000
15 Pulse Width	9.7500
16 Acquisition Time	2.7329
17 Acquisition Date	2013-05-15T12:27:47
18 Modification Date	2013-05-15T12:28:00
19 Spectrometer Frequency	300.09
20 Spectral Width	5995.2
21 Lowest Frequency	-1317.1
22 Nucleus	1H
23 Acquired Size	16384
24 Spectral Size	32768



5w

(^{1}H NMR spectrum in $CDCl_3$)

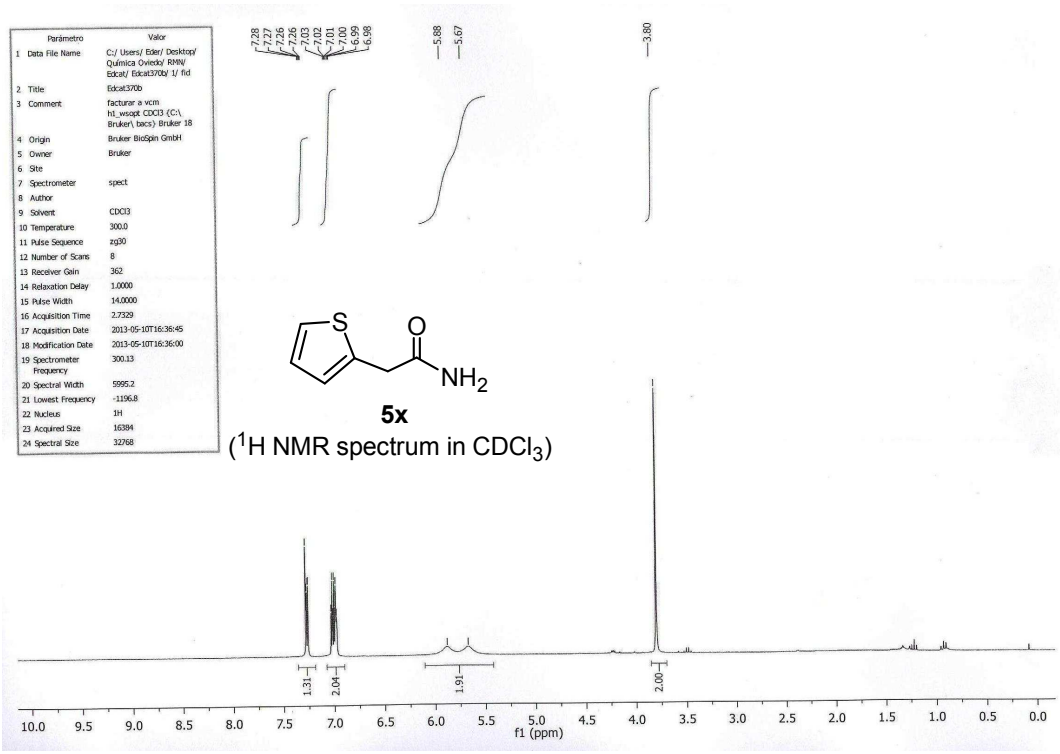
Parámetro	Valor
1 Data File Name	C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ Edcat/ Edcat376_13C/ 1/ fid
2 Title	Edcat376_13C
3 Comment	facturar a vcm c13_swopt CDCl3 (C:\ Bruker\ data) Bruker 5
4 Origin	Bruker BioSpin GmbH
5 Owner	Bruker
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	CDCl3
10 Temperature	300.0
11 Pulse Sequence	zgpg30
12 Number of Scans	480
13 Receiver Gain	5793
14 Relaxation Delay	1.5000
15 Pulse Width	5.3000
16 Acquisition Time	0.9044
17 Acquisition Date	2013-05-15T12:54:44
18 Modification Date	2013-05-15T12:54:00
19 Spectrometer Frequency	75.48
20 Spectral Width	18115.9
21 Lowest Frequency	-756.5
22 Nucleus	13C
23 Acquired Size	16384
24 Spectral Size	32768



5w

($^{13}C\{^1H\}$ NMR spectrum in $CDCl_3$)

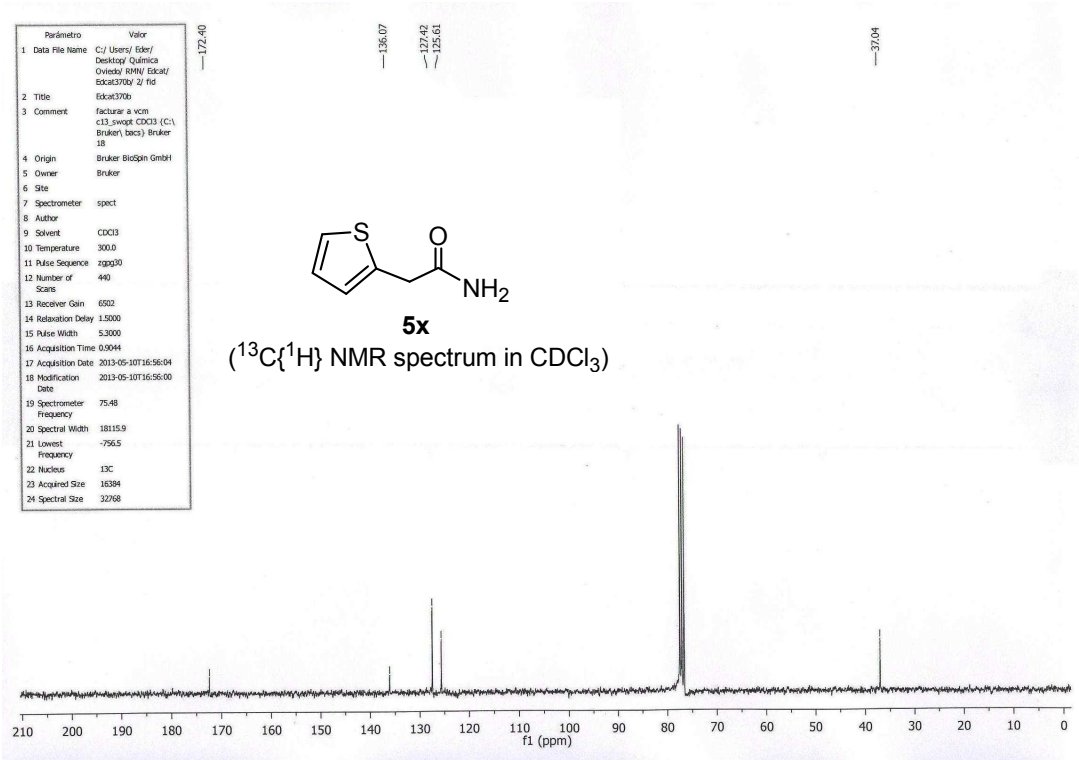
	Parámetro	Valor
1	Data File Name	C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ Edcat/ Edcat370b/ 1/ fid
2	Title	Edcat370b
3	Comment	facturar a vcm ht_wsqpt CDCl3 (C:\ Bruker\ bacs) Bruker 18
4	Origin	Bruker BioSpin GmbH
5	Owner	Bruker
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	8
13	Receiver Gain	362
14	Relaxation Delay	1.0000
15	Pulse Width	14.0000
16	Acquisition Time	2.7329
17	Acquisition Date	2013-05-10T16:36:45
18	Modification Date	2013-05-10T16:36:00
19	Spectrometer Frequency	300.13
20	Spectral Width	5995.2
21	Lowest Frequency	-1196.8
22	Nucleus	1H
23	Acquired Size	16384
24	Spectral Size	32768



5x

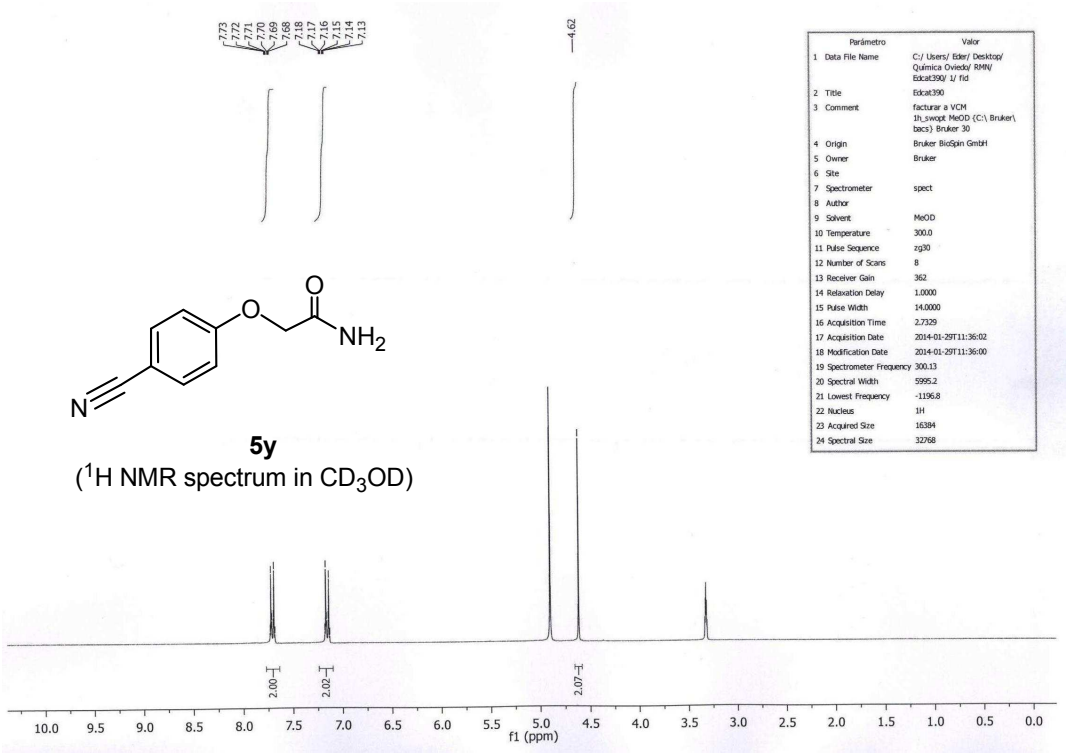
(^{1}H NMR spectrum in $CDCl_3$)

	Parámetro	Valor
1	Data File Name	C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ Edcat/ Edcat370b/ 2/ fid
2	Title	Edcat370b
3	Comment	facturar a vcm c13_swqpt CDCl3 (C:\ Bruker\ bacs) Bruker 18
4	Origin	Bruker BioSpin GmbH
5	Owner	Bruker
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Number of Scans	440
13	Receiver Gain	6502
14	Relaxation Delay	1.5000
15	Pulse Width	5.3000
16	Acquisition Time	0.9044
17	Acquisition Date	2013-05-10T16:56:04
18	Modification Date	2013-05-10T16:56:00
19	Spectrometer Frequency	75.48
20	Spectral Width	18115.9
21	Lowest Frequency	-756.5
22	Nucleus	13C
23	Acquired Size	16384
24	Spectral Size	32768



5x

($^{13}C\{^{1}H\}$ NMR spectrum in $CDCl_3$)

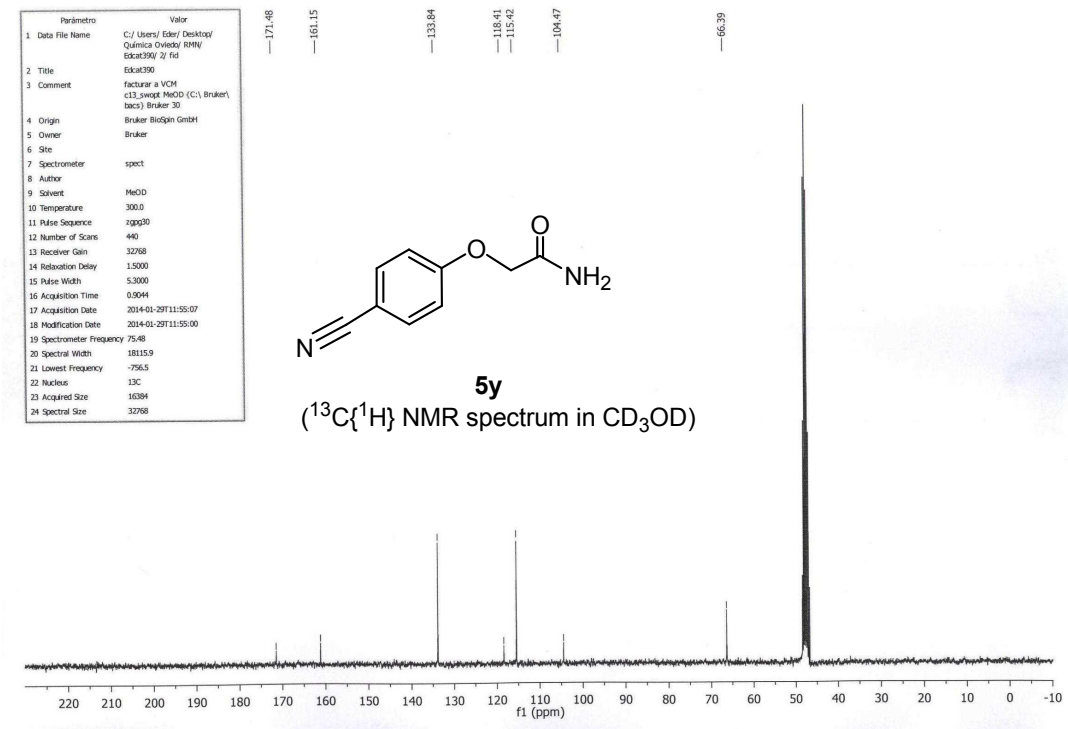


Parámetro		Valor
1	Data File Name	C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ Edcat390/ 1/ fid
2	Title	Edcat390
3	Comment	facturar a VCM 1h_swopt MeOD (C:\ Bruker\ bacs) Bruker 30
4	Origin	Bruker BioSpin GmbH
5	Owner	Bruker
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	MeOD
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	8
13	Receiver Gain	362
14	Relaxation Delay	1.0000
15	Pulse Width	14.0000
16	Acquisition Time	2.7329
17	Acquisition Date	2014-01-29T11:36:02
18	Modification Date	2014-01-29T11:36:00
19	Spectrometer Frequency	300.13
20	Spectral Width	5995.2
21	Lowest Frequency	-1196.8
22	Nucleus	1H
23	Acquired Size	16384
24	Spectral Size	32768

5y

(^{1}H NMR spectrum in CD_3OD)

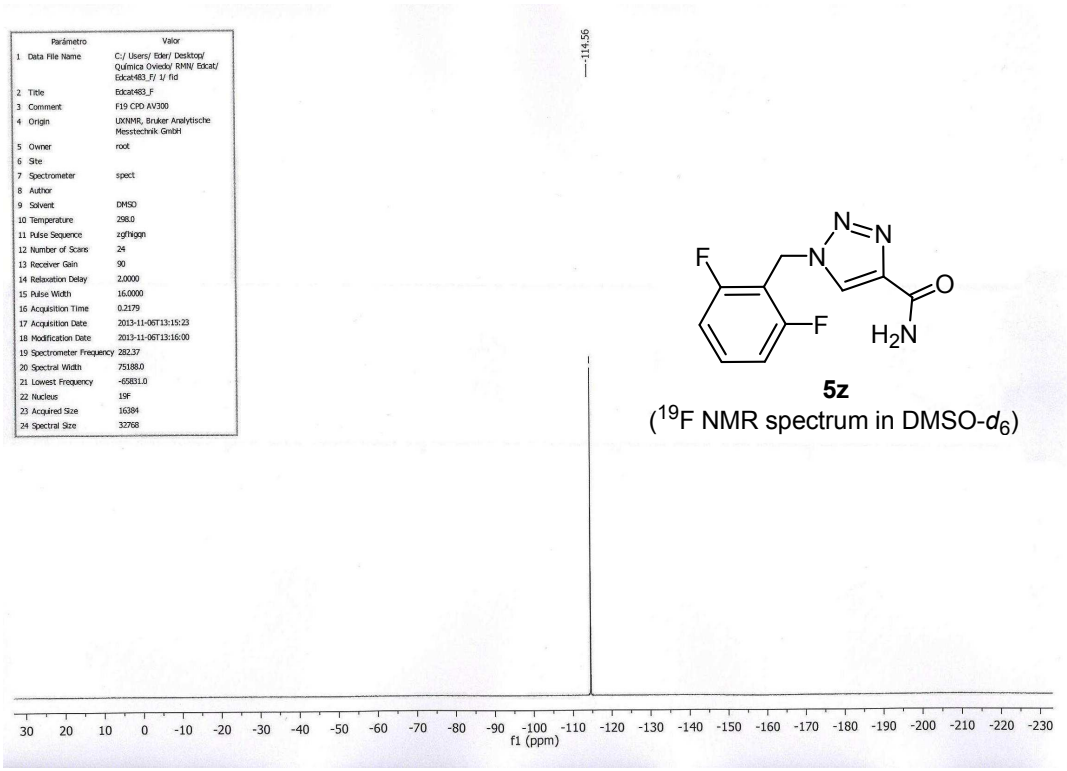
Parámetro		Valor
1	Data File Name	C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ Edcat390/ 2/ fid
2	Title	Edcat390
3	Comment	facturar a VCM c13_swopt MeOD (C:\ Bruker\ bacs) Bruker 30
4	Origin	Bruker BioSpin GmbH
5	Owner	Bruker
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	MeOD
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Number of Scans	440
13	Receiver Gain	32768
14	Relaxation Delay	1.5000
15	Pulse Width	5.3000
16	Acquisition Time	0.9044
17	Acquisition Date	2014-01-29T11:55:07
18	Modification Date	2014-01-29T11:55:00
19	Spectrometer Frequency	75.48
20	Spectral Width	18115.9
21	Lowest Frequency	-756.5
22	Nucleus	13C
23	Acquired Size	16384
24	Spectral Size	32768



5y

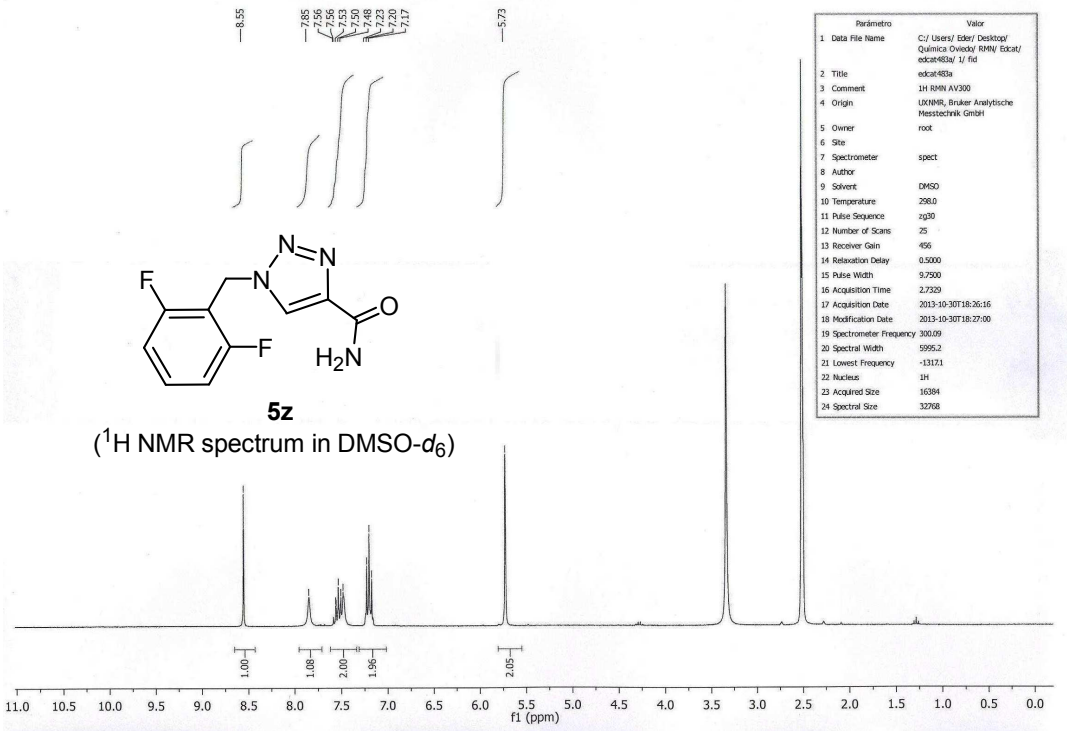
($^{13}C\{^1H\}$ NMR spectrum in CD_3OD)

Parámetro	Valor
1 Data File Name	C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ Edcat/ Edcat483_F/ 1/ fid
2 Title	Edcat483_F
3 Comment	F19 CPD AV300
4 Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.0
11 Pulse Sequence	zgfhigqn
12 Number of Scans	24
13 Receiver Gain	90
14 Relaxation Delay	2.0000
15 Pulse Width	16.0000
16 Acquisition Time	0.2179
17 Acquisition Date	2013-11-06T13:15:23
18 Modification Date	2013-11-06T13:16:00
19 Spectrometer Frequency	282.37
20 Spectral Width	75188.0
21 Lowest Frequency	-65831.0
22 Nucleus	19F
23 Acquired Size	16384
24 Spectral Size	32768



5z

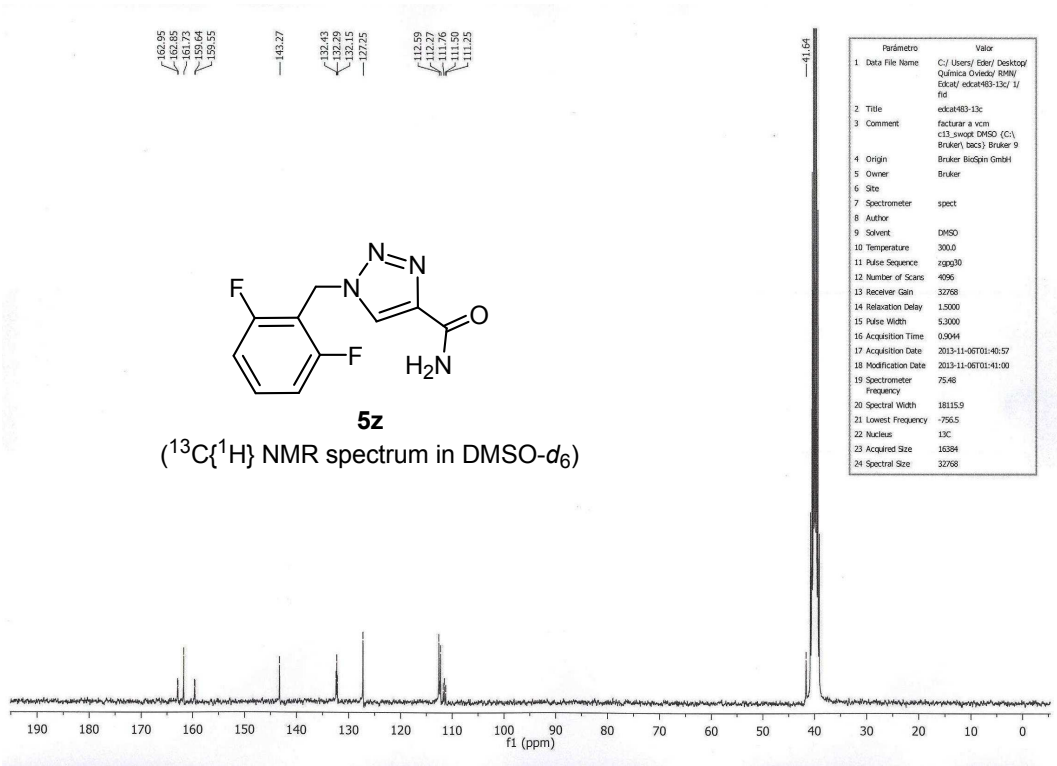
(^{19}F NMR spectrum in DMSO-d_6)



Parámetro	Valor
1 Data File Name	C:/ Users/ Eder/ Desktop/ Química Oviedo/ RMN/ Edcat/ edcat483a/ 1/ fid
2 Title	edcat483a
3 Comment	1H RMN AV300
4 Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5 Owner	root
6 Site	
7 Spectrometer	spect
8 Author	
9 Solvent	DMSO
10 Temperature	298.0
11 Pulse Sequence	zg30
12 Number of Scans	25
13 Receiver Gain	456
14 Relaxation Delay	0.5000
15 Pulse Width	9.7500
16 Acquisition Time	2.7329
17 Acquisition Date	2013-10-30T18:26:16
18 Modification Date	2013-10-30T18:27:00
19 Spectrometer Frequency	300.09
20 Spectral Width	5995.2
21 Lowest Frequency	-1317.1
22 Nucleus	1H
23 Acquired Size	16384
24 Spectral Size	32768

5z

(^{1}H NMR spectrum in DMSO-d_6)



5z

($^{13}C\{^{1}H\}$ NMR spectrum in DMSO-d_6)

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