Carboxylate-Assisted C(sp^3)–H Activation in Olefin Metathesis-Relevant Ruthenium Complexes

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Supporting Information

Part 1. Experimental Results

General Procedures. All reactions were carried out using oven-dried glassware under an atmosphere of Ar or N_2 unless otherwise indicated. Ruthenium complex **4b** was obtained from Materia, Inc. and used as received. All solvents were purified by passage through solvent purification columns and further degassed by bubbling argon. Deuterated solvents were obtained from Cambridge Isotope Labs, and used as received except benzene, which was degassed by bubbling argon and dried by passage through a solvent purification column. 1-aminoadamantane-2,2,8,8,9,9-d_6 (Catalog No. D-7085) was purchased from CDN Isotopes, Incorporated (Point Claire, Quebec, CA). The certificate of isotopic analysis reads: 98.1% deuteration at the 2,8,9-positions, 9% deuteration at the 3,5,7-positions, and 17% deuteration at the 4,6,10-positions. Using these percentages, the computed the MW of the supplied compound is 158.39 g/mol. All other commercial reagents were used as received unless otherwise noted. Silica gel chromatography was performed using 230–400 mesh silica gel purchased from Merck. Thin-layer chromatography utilized EMD Sciences silica gel 60 F254 pre-cast glass plates (Cat. No. 1.05714.0001). Microwave-assisted chemistry utilized a Biotage Initiator 2.5 reactor. ^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra were obtained on Varian FT NMR instruments. NMR spectra were reported as δ values in ppm relative to the reported solvent ($CDCl_3$ calibrated to 7.27, C_6D_6 calibrated to 7.16, 1:1 THF-d_8:CD_3OD calibrated to THF signal at 3.58). Splitting patterns are abbreviated as follows: singlet (s), doublet (d), triplet (t), quartet (q), multiplet (m), broad (b), apparent (app) and combinations thereof. High-resolution mass spectra (HRMS) were provided by the California Institute of Technology Mass Spectrometry Facility using a JEOL JMS-600H High Resolution Mass Spectrometer. All HRMS were by positive-ion FAB.

Compounds **3a**, **3b**, **3c**, **3d**, **4c**, **4d**, **5b**, and **6b** were synthesized according to their literature procedures and were confirmed by spectroscopic analysis (NMR).

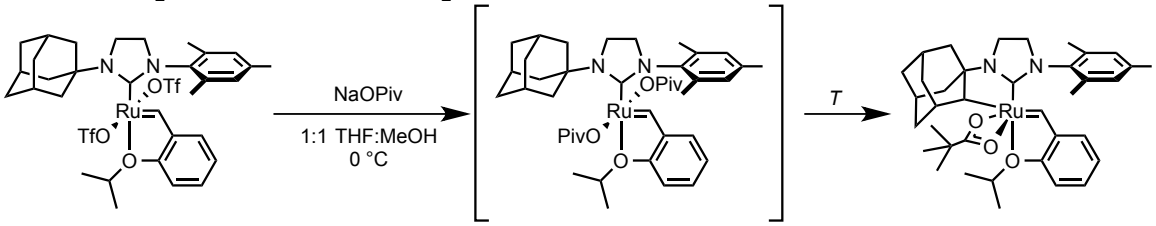
Kinetics Procedures and Data.

General Procedure for Kinetics Experiments.

Three stock solutions were prepared prior to kinetics experiments: (1) 0.05–0.09 M ruthenium bistriflate in THF-d_8; (2) 0.17 M trimethoxybenzene in THF-d_8; (3) 0.28–0.51 M sodium pivalate in CD_3OD.

In a nitrogen filled glovebox, 0.20 mL of a 0.07 M THF-d_8 solution of ruthenium bistriflate **7a** (0.0144 mmol) was added to a J-Young NMR tube followed by 0.05 mL of a 0.17 M THF-d_8 solution of trimethoxybenzene (0.0083 mmol). An additional 0.1 mL of THF-d_8 was added for a total volume of 0.35 mL THF-d_8. The J-Young tube was sealed and removed from the glovebox. The bistriflate solution was then cooled to –78 °C in a dry ice/acetone bath under an argon atmosphere and 0.35 mL of a 0.41 M CD_3OD solution of sodium pivalate (0.144 mmol) was injected. The J-Young tube was sealed, and maintained at –78 °C while preparing the NMR spectrometer. The probe of an NMR spectrometer was cooled to 0 °C. The sample tube was removed from the dry-ice/acetone bath, mixed by inverting multiple times, and allowed to warm to 0 °C inside of the NMR spectrometer. ^{1}H NMR data was collected to ensure full conversion of bistriflate **7a** to dipivalate **6a**. Once full conversion was observed, the sample tube was removed from the spectrometer and returned to the –78 °C dry-ice/acetone bath. The spectrometer probe was then warmed to 40 °C, and the temperature checked by insertion of a thermocouple into the probe. The sample tube was then inserted into the pre-warmed spectrometer, and ^{1}H NMR data was collected periodically (approx. every 5 minutes) until full consumption of the dipivalate complex was observed. Arrayed spectral data was processed using MestReNova 8, and analyzed in Microsoft Excel.

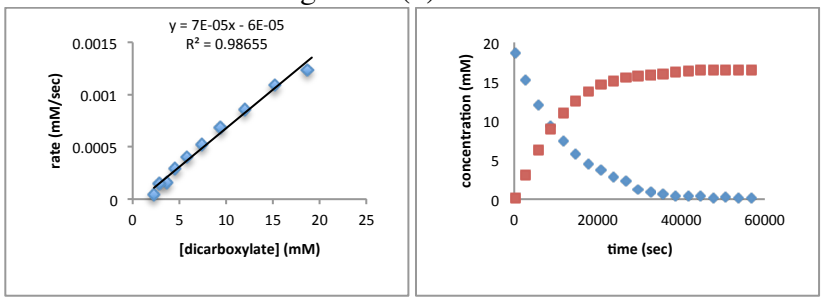
Kinetics Experiments from Complex 7a



287.3 K

run	k (sec^{-1})
1	9.4(1)x10^{-5}
2	9.2(1)x10^{-5}
average	9.3(1)x10^{-5}

1st run:



SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.844137
R Square	0.712567
Adjusted R	0.69888
Standard E	0.000165
Observatic	23

ANOVA

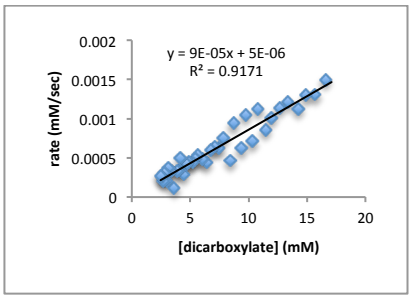
	df	*SS*	*MS*	*F*	*ignificance F*
Regressior	1	1.42E-06	1.42E-06	52.06062	4.14E-07
Residual	21	5.71E-07	2.72E-08		
Total	22	1.99E-06			

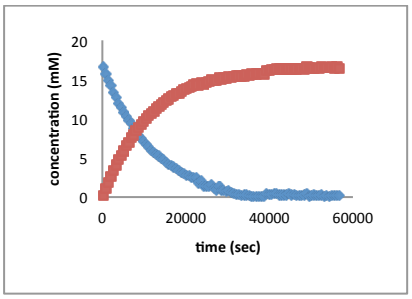
	Coefficients	*tandard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*ower 90.0%*	*Jpper 90.0%*
Intercept	0.001418	8.18E-05	17.32379	6.49E-14	0.001248	0.001588	0.001277	0.001559
X Variable	-7.2E-05	9.97E-06	-7.2153	4.14E-07	-9.3E-05	-5.1E-05	-8.9E-05	-5.5E-05

RESIDUAL OUTPUT

Observatio	*Predicted Y*	*Residuals*	*ıdard Residuals*
1	0.001361	-0.00021	-1.27603
2	0.001289	0.000365	2.266668
3	0.001251	-0.00037	-2.31924
4	0.001197	6.57E-05	0.407876
5	0.001141	0.000146	0.90367
6	0.0011	-0.00014	-0.87858
7	0.001052	6.8E-05	0.42234
8	0.001005	7.8E-05	0.484324
9	0.000962	3.31E-05	0.20521
10	0.000925	-6.6E-05	-0.40898
11	0.000875	0.000274	1.699133
12	0.000843	-9.1E-05	-0.56297
13	0.000815	-0.00018	-1.10258
14	0.000777	0.000119	0.741592
15	0.000742	6.6E-05	0.409774
16	0.000714	-6.3E-05	-0.39091
17	0.000676	0.000186	1.151923
18	0.000651	-6.2E-05	-0.3851
19	0.000629	-0.00011	-0.66086
20	0.000605	-7.2E-05	-0.44605
21	0.00058	4.58E-06	0.028405

2nd run:





SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.884573
R Square	0.78247
Adjusted R	0.772112
Standard E	0.000165
Observatic	23

ANOVA

	df	*SS*	*MS*	*F*	*ignificance F*
Regressior	1	2.05E-06	2.05E-06	75.53851	2.13E-08
Residual	21	5.69E-07	2.71E-08		
Total	22	2.62E-06			

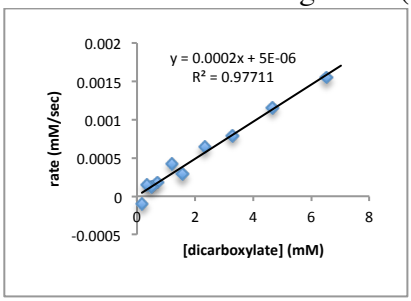
	Coefficients	*tandard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*ower 90.0%*	*Jpper 90.0%*
Intercept	-1.2E-05	0.000105	-0.1139	0.910397	-0.00023	0.000206	-0.00019	0.000168
X Variable	9.23E-05	1.06E-05	8.691289	2.13E-08	7.02E-05	0.000114	7.4E-05	0.000111

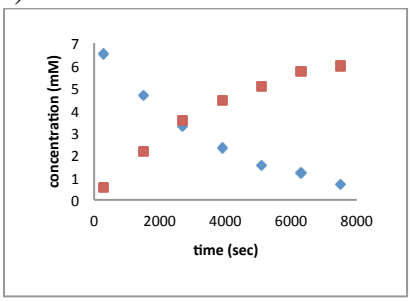
RESIDUAL OUTPUT

Observatio	*Predicted Y*	*Residuals*	*ndard Residuals*
1	0.001434	0.000125	0.775526
2	0.001362	-6.1E-05	-0.37625
3	0.0013	-0.00019	-1.1763
4	0.001221	0.000214	1.329468
5	0.001154	5.7E-05	0.35412
6	0.001092	2.82E-05	0.175358
7	0.001045	-0.00019	-1.20321
8	0.000986	7.6E-05	0.472606
9	0.000941	-0.00013	-0.80967
10	0.000887	8.71E-05	0.541212
11	0.000853	-0.00024	-1.51713
12	0.000792	0.000308	1.91613
13	0.000766	-0.00029	-1.81284
14	0.000711	0.000275	1.706596
15	0.000678	-6.8E-05	-0.42281
16	0.000647	-8.5E-05	-0.52629
17	0.000609	6.7E-05	0.416295
18	0.000578	-1.4E-05	-0.0892
19	0.000542	0.000101	0.625031
20	0.000508	0.00012	0.745749
21	0.00049	-0.00017	-1.08685

298 K	
run	k (sec^{-1})
1	$2.17x10^{-4}$
2	$2.8(3)x10^{-4}$
3	$3.2(3)x10^{-4}$
average	$2.7(3)x10^{-4}$

1st run:





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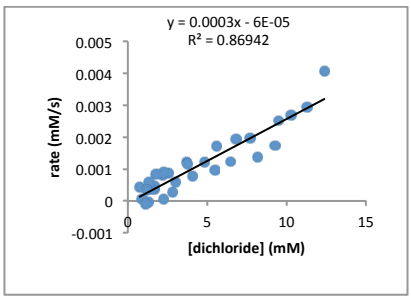
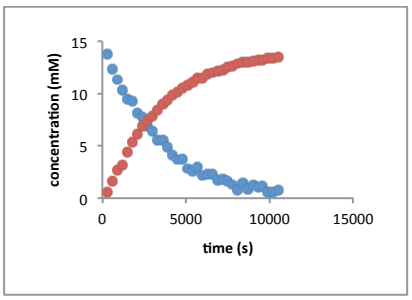




SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.878706
R Square	0.772124
Adjusted R	0.76073
Standard E	0.000507
Observatic	22

ANOVA

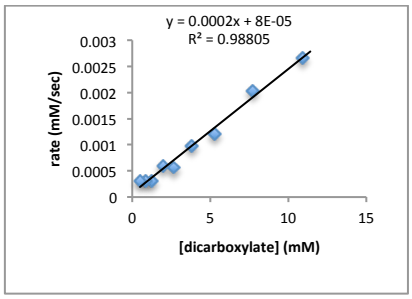
	df	*SS*	*MS*	*F*	*ignificance F*
Regressior	1	1.75E-05	1.75E-05	67.7669	7.47E-08
Residual	20	5.15E-06	2.58E-07		
Total	21	2.26E-05			

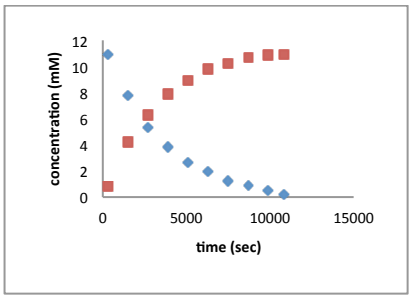
	Coefficients	*tandard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*ower 90.0%*	*pper 90.0%*
Intercept	0.00411	0.000305	13.48442	1.69E-11	0.003474	0.004746	0.003585	0.004636
X Variable	-0.00028	3.41E-05	-8.23207	7.47E-08	-0.00035	-0.00021	-0.00034	-0.00022

RESIDUAL OUTPUT

Observatio	*Predicted Y*	*Residuals*	*ndard Residuals*
1	0.003646	-6.2E-05	-0.12468
2	0.003359	4E-05	0.080757
3	0.003205	-0.00138	-2.77937
4	0.002863	0.001201	2.425862
5	0.002615	0.000323	0.65184
6	0.002388	0.000316	0.638561
7	0.002175	0.00035	0.706562
8	0.00203	-0.00031	-0.61659
9	0.001914	-0.00054	-1.08616
10	0.001749	0.000203	0.409626
11	0.001586	0.000347	0.701085
12	0.001482	-0.00025	-0.50173
13	0.001338	0.000381	0.769977
14	0.001257	-0.0003	-0.6122
15	0.001155	6.44E-05	0.130043
16	0.00109	-0.00032	-0.65101
17	0.000987	0.000231	0.465774
18	0.00089	0.000261	0.527111
19	0.000868	-0.0006	-1.21399
20	0.000795	7.61E-05	0.153759
21	0.000745	-0.00016	-0.32214

3rd run:





SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.907531
R Square	0.823613
Adjusted R	0.814794
Standard E	0.00037
Observatic	22

ANOVA

	df	*SS*	*MS*	*F*	*ignificance F*
Regressior	1	1.28E-05	1.28E-05	93.38725	5.61E-09
Residual	20	2.74E-06	1.37E-07		
Total	21	1.56E-05			

	Coefficient:	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*ower 90.0%*	*Upper 90.0%*
Intercept	0.003611	0.000244	14.82448	2.99E-12	0.003103	0.004119	0.003191	0.004031
X Variable	-0.00032	3.27E-05	-9.66371	5.61E-09	-0.00038	-0.00025	-0.00037	-0.00026

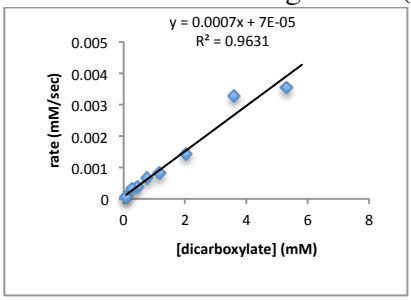
RESIDUAL OUTPUT

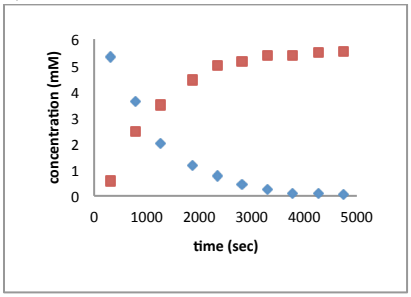
Observatio	*Predicted Y*	*Residuals*	*dard Residuals*
1	0.00303	0.000245	0.67847
2	0.002762	6.36E-05	0.1758
3	0.002539	-0.00019	-0.53352
4	0.002284	0.000406	1.122956
5	0.002134	-0.00056	-1.54423
6	0.001972	-0.00026	-0.72085
7	0.00178	0.000239	0.659942
8	0.001632	-6.8E-05	-0.18737
9	0.001479	0.000133	0.369064
10	0.00135	7.94E-06	0.021955
11	0.001242	-0.00011	-0.29169
12	0.001114	0.000233	0.645841
13	0.001022	-5.4E-05	-0.14972
14	0.000941	-8.2E-05	-0.22632
15	0.000867	-9.1E-05	-0.25284
16	0.000782	0.00011	0.303761
17	0.000796	-0.00094	-2.60168
18	0.000679	0.000549	1.517814
19	0.000576	0.000518	1.432731
20	0.00051	0.000179	0.495324
21	0.000518	-0.0006	-1.66807

307.2 °C

run	k (sec^{-1})
1	$1.0(1)x10^{-3}$
2	$1.04(5)x10^{-3}$
average	$1.0(1)x10^{-3}$

1st run:





SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.894967
R Square	0.800965
Adjusted R	0.789257
Standard E	0.000638
Observatic	19

ANOVA

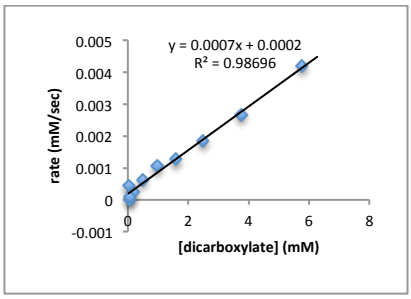
	df	*SS*	*MS*	*F*	*ignificance F*
Regressior	1	2.78E-05	2.78E-05	68.41227	2.31E-07
Residual	17	6.91E-06	4.07E-07		
Total	18	3.47E-05			

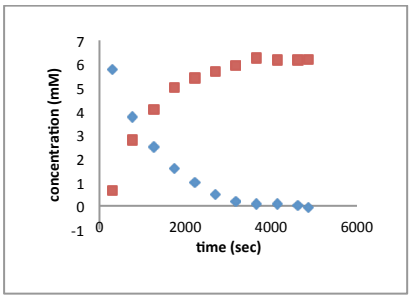
	Coefficient	*tandard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*ower 90.0%*	*Upper 90.0%*
Intercept	0.005594	0.000473	11.82331	1.26E-09	0.004595	0.006592	0.004771	0.006417
X Variable	-0.00101	0.000122	-8.27117	2.31E-07	-0.00126	-0.00075	-0.00122	-0.00079

RESIDUAL OUTPUT

)bservatio	*Predicted Y*	*Residuals*	*ndard Residuals*
1	0.004423	0.000536	0.864541
2	0.004012	-0.0006	-0.97226
3	0.003489	0.000843	1.3602
4	0.003139	-0.00024	-0.38005
5	0.002779	0.0002	0.322662
6	0.002641	-0.00149	-2.40222
7	0.002367	-0.0001	-0.16569
8	0.002098	0.000136	0.218917
9	0.001819	0.000494	0.797502
10	0.001428	0.000192	0.310553
11	0.001275	-4.6E-06	-0.00741
12	0.001134	3.7E-05	0.059721
13	0.001064	-0.00048	-0.78139
14	0.000904	0.000422	0.681398
15	0.000708	0.000915	1.476529
16	0.000587	0.000418	0.675122
17	0.000637	-0.00106	-1.70519
18	0.000535	0.000317	0.51117
19	0.000535	-0.00054	-0.86412

2nd run:





SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.990229
R Square	0.980552
Adjusted R	0.977774
Standard E	0.000206
Observatic	9

ANOVA

	df	*SS*	*MS*	*F*	*ignificance F*
Regressior	1	1.5E-05	1.5E-05	352.9432	3.01E-07
Residual	7	2.98E-07	4.25E-08		
Total	8	1.53E-05			

	Coefficient:	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*ower 90.0%*	*pper 90.0%*
Intercept	0.000209	9.1E-05	2.302708	0.054772	-5.6E-06	0.000425	3.71E-05	0.000382
X Variable	0.001045	5.56E-05	18.78678	3.01E-07	0.000913	0.001176	0.000939	0.00115

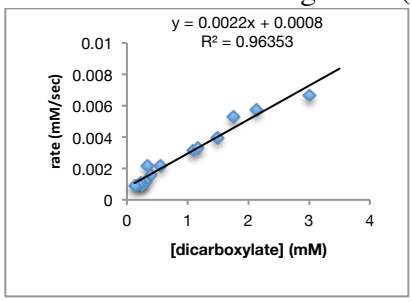
RESIDUAL OUTPUT

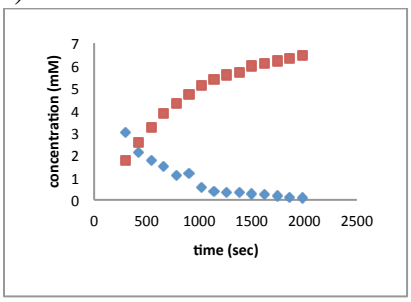
Observatio	*Predicted Y*	*Residuals*	*dard Residuals*
1	0.004136	5.56E-05	0.288279
2	0.002805	-0.00015	-0.78301
3	0.001877	-2.7E-05	-0.14119
4	0.00124	3.09E-05	0.160118
5	0.000712	0.000341	1.76552
6	0.0004	0.000222	1.151764
7	0.000278	-3.3E-05	-0.17262
8	0.000279	-0.00028	-1.45919
9	0.000238	-0.00016	-0.80967

312.1 K

run	k (sec^{-1})
1	$1.9(1)x10^{-3}$
2	$1.6(1)x10^{-3}$
3	$1.4(1)x10^{-3}$
average	$1.6(1)x10^{-3}$

1st run:





SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.974511
R Square	0.949672
Adjusted R	0.944639
Standard E	0.000441
Observatic	12

ANOVA

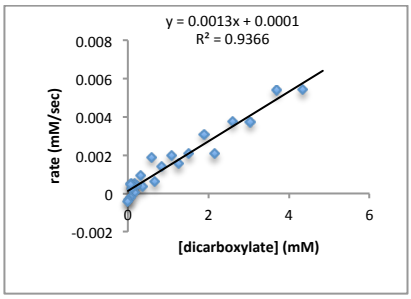
	df	*SS*	*MS*	*F*	*ignificance F*
Regressior	1	3.68E-05	3.68E-05	188.6961	8.12E-08
Residual	10	1.95E-06	1.95E-07		
Total	11	3.87E-05			

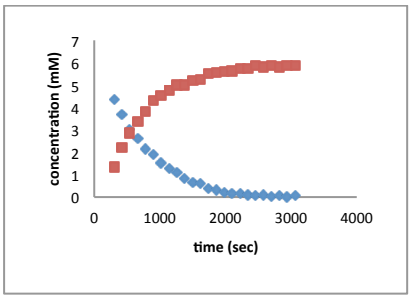
	Coefficient:	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*ower 90.0%*	*Jpper 90.0%*
Intercept	0.013403	0.000887	15.11595	3.25E-08	0.011427	0.015378	0.011796	0.01501
X Variable	-0.00185	0.000135	-13.7367	8.12E-08	-0.00215	-0.00155	-0.0021	-0.00161

RESIDUAL OUTPUT

Observatio	*Predicted Y*	*Residuals*	*ndard Residuals*
1	0.005862	6.86E-05	0.162916
2	0.003819	-0.00014	-0.33152
3	0.002456	-2.7E-06	-0.00651
4	0.001398	0.000506	1.202467
5	0.000948	-0.00014	-0.32715
6	0.000744	-0.00038	-0.89333
7	0.000276	0.000567	1.347584
8	-2.2E-05	0.000557	1.323592
9	0.000132	-0.00041	-0.96791
10	0.000333	-0.0007	-1.65329
11	8.39E-05	0.000365	0.866615
12	0.000163	-0.0003	-0.72346

2nd run:





SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.975551
R Square	0.951699
Adjusted R	0.946869
Standard E	0.000446
Observatic	12

ANOVA

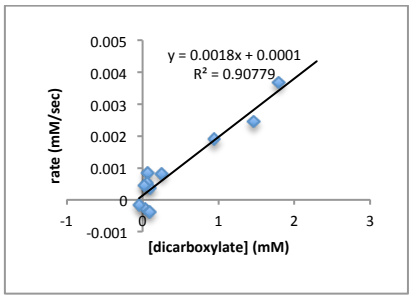
	df	*SS*	*MS*	*F*	*ignificance F*
Regressior	1	3.92E-05	3.92E-05	197.0345	6.6E-08
Residual	10	1.99E-06	1.99E-07		
Total	11	4.12E-05			

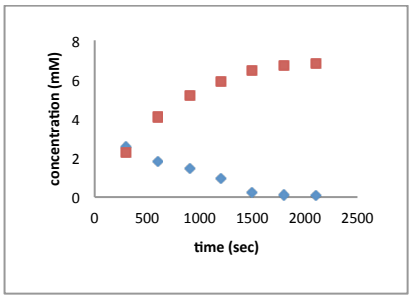
	Coefficient:	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*ower 90.0%*	*Upper 90.0%*
Intercept	0.010892	0.000569	19.13469	3.31E-09	0.009624	0.012161	0.00986	0.011924
X Variable	-0.00159	0.000113	-14.0369	6.6E-08	-0.00185	-0.00134	-0.0018	-0.00139

RESIDUAL OUTPUT

Observatio	*Predicted Y*	*Residuals*	*dard Residuals*
1	0.006856	-0.00021	-0.48218
2	0.005762	-4E-05	-0.09412
3	0.004755	0.000513	1.206718
4	0.003994	-1.1E-05	-0.02511
5	0.003389	-0.00022	-0.5211
6	0.002757	0.000549	1.291723
7	0.002343	-0.00018	-0.41815
8	0.002034	-0.00042	-0.98081
9	0.001812	-0.00065	-1.5226
10	0.001394	0.00079	1.856794
11	0.001212	-0.00026	-0.60864
12	0.000997	0.000126	0.297471

3rd run:





SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.95171
R Square	0.905752
Adjusted R	0.899469
Standard E	0.000533
Observatic	17

ANOVA

	df	*SS*	*MS*	*F*	*ignificance F*
Regressior	1	4.1E-05	4.1E-05	144.1547	4.29E-09
Residual	15	4.26E-06	2.84E-07		
Total	16	4.52E-05			

	Coefficient:	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*ower 90.0%*	*Upper 90.0%*
Intercept	0.000325	0.000195	1.667081	0.116236	-9.1E-05	0.000742	-1.7E-05	0.000668
X Variable	0.001446	0.00012	12.00644	4.29E-09	0.001189	0.001703	0.001235	0.001657

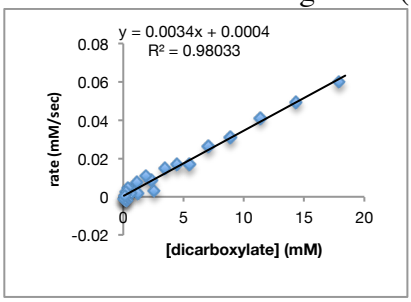
RESIDUAL OUTPUT

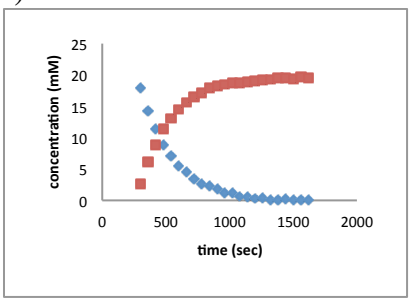
Observatio	*Predicted Y*	*Residuals*	*dard Residuals*
1	0.005661	-0.00024	-0.45612
2	0.004724	0.000672	1.301855
3	0.004077	-0.00035	-0.67551
4	0.003422	0.000354	0.685446
5	0.003057	-0.00095	-1.84208
6	0.002518	0.000586	1.13451
7	0.002154	-6E-05	-0.11545
8	0.001885	-0.00033	-0.64623
9	0.001542	0.000435	0.842984
10	0.001298	0.000109	0.210914
11	0.001189	-0.00056	-1.08521
12	0.000859	0.001042	2.01774
13	0.000797	-0.00044	-0.85503
14	0.000637	0.000289	0.560012
15	0.000562	-0.00013	-0.25432
16	0.000552	-0.0005	-0.96272
17	0.00046	7.19E-05	0.13922

322.0 K

run	k (sec^{-1})
1	$4.4(3)x10^{-3}$
2	$4.2(2)x10^{-3}$
average	$4.3(3)x10^{-3}$

1st run:





SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.959754
R Square	0.921128
Adjusted R	0.91587
Standard E	0.005068
Observatic	17

ANOVA

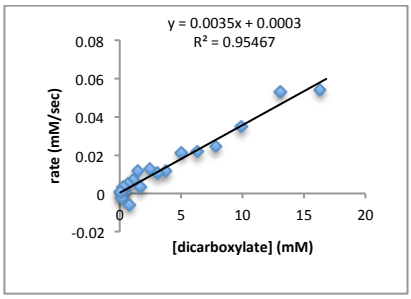
	df	*SS*	*MS*	*F*	*ignificance F*
Regressior	1	0.0045	0.0045	175.1821	1.12E-09
Residual	15	0.000385	2.57E-05		
Total	16	0.004885			

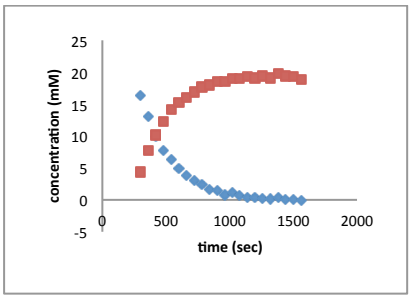
	Coefficient:	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*ower 90.0%*	*pper 90.0%*
Intercept	0.000807	0.001674	0.482261	0.636582	-0.00276	0.004374	-0.00213	0.003741
X Variable	0.0044	0.000332	13.23564	1.12E-09	0.003692	0.005109	0.003817	0.004983

RESIDUAL OUTPUT

)bservatio	*Predicted Y*	*Residuals*	*ndard Residuals*
1	0.058318	-0.00429	-0.87438
2	0.044318	0.008712	1.775411
3	0.035093	-0.00015	-0.03089
4	0.028574	-0.00388	-0.79127
5	0.022832	-0.00108	-0.2208
6	0.017252	0.003885	0.791776
7	0.014228	-0.00277	-0.56526
8	0.011481	-0.00107	-0.21888
9	0.008092	0.004745	0.967037
10	0.007242	-0.00402	-0.81963
11	0.004134	0.007635	1.555911
12	0.005655	-0.01142	-2.32625
13	0.003754	0.003445	0.702107
14	0.002454	0.002472	0.503843
15	0.002247	-0.00147	-0.29874
16	0.002113	-0.0016	-0.32666
17	0.00149	0.000867	0.176665

2nd run:





SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.983535
R Square	0.967341
Adjusted R	0.9653
Standard E	0.003363
Observatic	18

ANOVA

	df	*SS*	*MS*	*F*	*ignificance F*
Regressior	1	0.005358	0.005358	473.9153	2.58E-13
Residual	16	0.000181	1.13E-05		
Total	17	0.005539			

	Coefficient:	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*ower 90.0%*	*Jpper 90.0%*
Intercept	0.000952	0.001067	0.892544	0.385329	-0.00131	0.003213	-0.00091	0.002814
X Variable	0.004222	0.000194	21.76959	2.58E-13	0.003811	0.004634	0.003884	0.004561

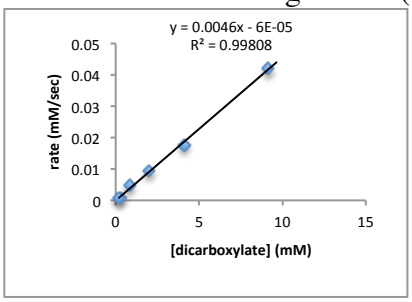
RESIDUAL OUTPUT

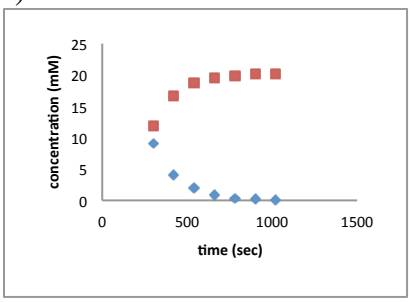
Observatio	*Predicted Y*	*Residuals*	*ndard Residuals*
1	0.061439	-0.00158	-0.48393
2	0.048933	0.000429	0.13143
3	0.038523	0.00257	0.787705
4	0.030729	3.72E-05	0.011399
5	0.024101	0.002058	0.630883
6	0.019804	-0.00284	-0.87166
7	0.015554	0.001222	0.374506
8	0.011762	0.003207	0.983119
9	0.01094	-0.00769	-2.35855
10	0.00876	-0.00015	-0.04723
11	0.006039	0.004699	1.440474
12	0.0056	-0.00387	-1.18574
13	0.003729	0.003657	1.121089
14	0.003286	-0.00153	-0.47047
15	0.002188	0.002144	0.657275
16	0.002649	-0.00447	-1.37037
17	0.001478	0.003147	0.964567
18	0.001386	-0.00103	-0.31449

326.6 K

run	k (sec^{-1})
1	$1.00(6)x10^{-2}$
2	$8.1(4)x10^{-3}$
average	$9.1(5)x10^{-3}$

1st run:





SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.994588
R Square	0.989205
Adjusted R	0.985607
Standard E	0.00197
Observatic	5

ANOVA

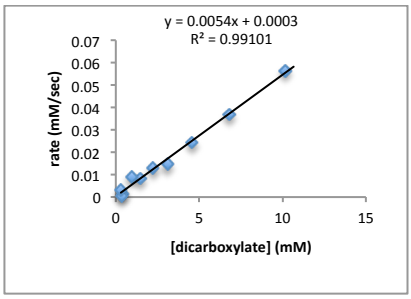
	df	*SS*	*MS*	*F*	*ignificance F*
Regressior	1	0.001067	0.001067	274.9173	0.000478
Residual	3	1.16E-05	3.88E-06		
Total	4	0.001078			

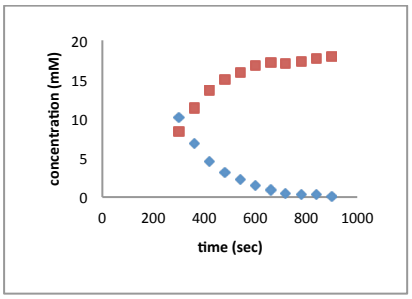
	Coefficient:	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*ower 90.0%*	*pper 90.0%*
Intercept	-9.9E-06	0.001259	-0.00783	0.994247	-0.00402	0.003998	-0.00297	0.002954
X Variable	0.010047	0.000606	16.58063	0.000478	0.008118	0.011975	0.008621	0.011473

RESIDUAL OUTPUT

)bservatio	*Predicted Y*	*Residuals*	*ndard Residuals*
1	0.041168	0.000896	0.525325
2	0.019958	-0.00237	-1.3865
3	0.008575	0.000867	0.508275
4	0.002921	0.001769	1.036984
5	0.001962	-0.00117	-0.68408

2nd run:





SUMMARY OUTPUT

Regression Statistics	
Multiple R	0.990135
R Square	0.980367
Adjusted R	0.977562
Standard E	0.002734
Observatic	9

ANOVA

	df	*SS*	*MS*	*F*	*ignificance F*
Regressior	1	0.002614	0.002614	349.5429	3.11E-07
Residual	7	5.23E-05	7.48E-06		
Total	8	0.002666			

	Coefficient:	*andard Err*	*t Stat*	*P-value*	*Lower 95%*	*Upper 95%*	*ower 90.0%*	*Upper 90.0%*
Intercept	0.000164	0.00133	0.123102	0.905486	-0.00298	0.003309	-0.00236	0.002684
X Variable	0.008097	0.000433	18.69607	3.11E-07	0.007073	0.009121	0.007276	0.008917

RESIDUAL OUTPUT

Observatio	*Predicted Y*	*Residuals*	*ıdard Residuals*
1	0.055092	0.001303	0.509544
2	0.03716	-0.00025	-0.09607
3	0.025317	-0.00094	-0.36682
4	0.018212	-0.00359	-1.40285
5	0.01192	0.001033	0.403944
6	0.007817	0.000627	0.245196
7	0.003505	0.005371	2.099732
8	0.002845	-0.00149	-0.58089
9	0.002594	-0.00208	-0.81178

Eyring Analysis

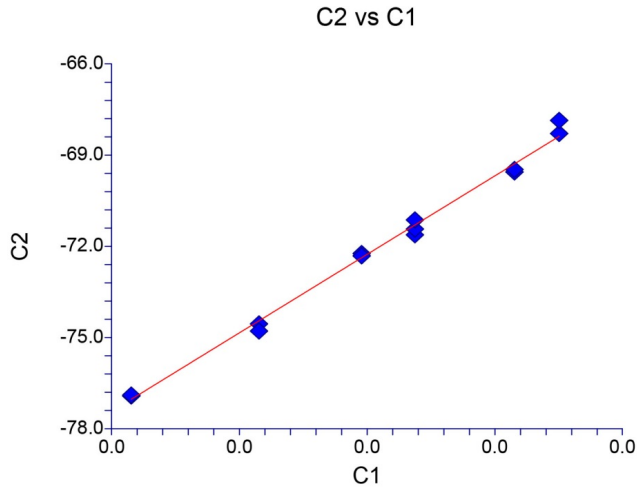
Table 1. Tabulated rate data as a function of temperature (see attached Excel file for data):

temp (K)	neg 1/T	RIn(hk/kBT)
326.6	-0.0030618494	-68.2901688827
326.6	-0.0030618494	-67.8613232983
322	-0.0031055901	-69.5557529645
322	-0.0031055901	-69.4737954858
312.2	-0.0032030750	-71.6235085262
312.2	-0.0032030750	-71.4321573220
312.2	-0.0032030750	-71.1330364216
307.2	-0.0032552083	-72.2376779070
307.2	-0.0032552083	-72.3144970478
298	-0.0033557047	-74.5509030726
298	-0.0033557047	-74.7880520115
287.3	-0.0034806822	-76.9156093209
287.3	-0.0034806822	-76.9264083158
287.3	-0.0034806822	-76.8924307364

Linear Regression Report

Page/Date/Time 1 2/23/2014 1:51:08 PM
Database
Y = C2 X = C1

Linear Regression Plot Section



Regression Estimation Section

Parameter	Intercept B(0)	Slope B(1)
Regression Coefficients	-5.181496	20642.318390
Lower 90% Confidence Limit	-7.796209	19840.506075
Upper 90% Confidence Limit	-2.566784	21444.130705
Standard Error	1.467054	449.878199
Standardized Coefficient	0.000000	0.997162
T Value	-3.531905	45.884238
Prob Level (T Test)	0.004132	0.000000
Reject H0 (Alpha = 0.100000)	Yes	Yes
Power (Alpha = 0.100000)	0.953354	1.000000
Regression of Y on X	-5.181496	20642.318390
Inverse Regression from X on Y	-4.798208	20759.974008
Orthogonal Regression of Y and X	-4.798208	20759.974008

Estimated Model

(-5.18149623023439) + (20642.3183897598) * (C1)

Figure 2. NCSS output (part 1), including Eyring plot of data in Table 1.

Linear Regression Report

Page/Date/Time 2 2/23/2014 1:51:08 PM
Database
Y = C2 X = C1

Correlation and R-Squared Section

Parameter	Pearson Correlation Coefficient	R-Squared	Spearman Rank Correlation Coefficient
Estimated Value	0.997162	0.994333	0.986725
Lower 90% Conf. Limit (r dist'n)	0.991852		
Upper 90% Conf. Limit (r dist'n)	0.998797		
Lower 90% Conf. Limit (Fisher's z)	0.992367		0.964605
Upper 90% Conf. Limit (Fisher's z)	0.998947		0.995056
Adjusted (Rbar)		0.993860	
T-Value for H0: Rho = 0	45.884238	45.884238	21.047565
Prob Level for H0: Rho = 0	0.000000	0.000000	0.000000

Analysis of Variance Section

Source	DF	Sum of Squares	Mean Square	F-Ratio	Prob Level	Power (10%)
Intercept	1	73441.89	73441.89			
Slope	1	127.9709	127.9709	2105.363307	0.000000	1.000000
Error	12	0.7293993	6.078327E-02			
Adj. Total	13	128.7003	9.900021			
Total	14	73570.59				

s = Square Root(6.078327E-02) = 0.2465426

Summary Matrices

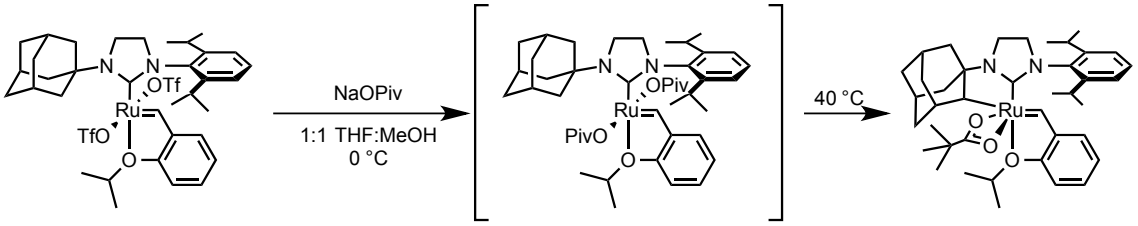
Index	X'X 0	X'X 1	X'Y 2	X'X Inverse 0	X'X Inverse 1
0	14	-4.560798E-02	-1013.995	35.40857	10847.22
1	-4.560798E-02	1.48878E-04	3.309505	10847.22	3329705
2 (Y'Y)			73570.59		
Determinant		4.204576E-06			237836.1

Variance - Covariance Matrix of Regression Coefficients

Index	VC(b) 0	VC(b) 1
0	2.152248	659.3297
1	659.3297	202390.4

Figure 3. NCSS output (part 2) for Eyring plot shown in Figure 1.

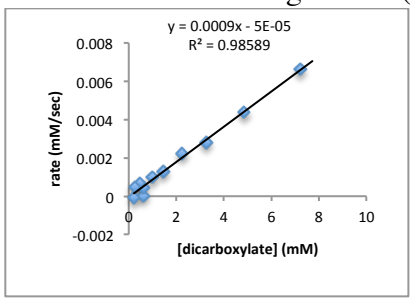
Kinetics Experiments from Complex 7d

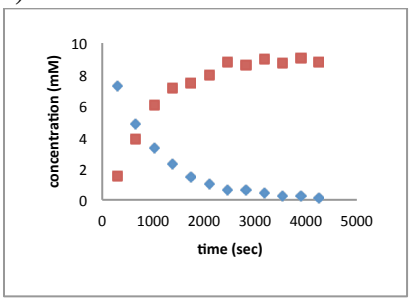


312.1 K

run	k (sec^{-1})
1	$1.36(8)x10^{-3}$
2	$1.3(3)x10^{-3}$
3	$1.6(2)x10^{-3}$
average	$1.4(2)x10^{-3}$

1st run:





Linear Regression

Regression Statistics

R	0.98413
R Square	0.96852
Adjusted R Square	0.96502
S	0.00039
Total number of observations	11

0.01524042644447 =- 0.0001 + 0.0014 * 7.22025185495953

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00004	0.00004	276.90811	0.
Residual	9.	0.	0.		
Total	10.	0.00004			

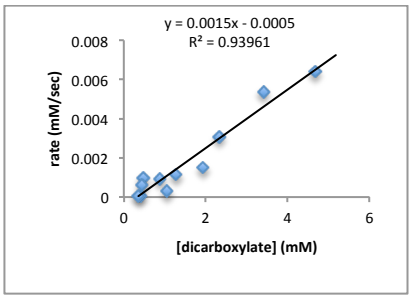
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	-0.00006	0.00016	-0.00036	0.00024	-0.38187
7.22025185495953	0.00136	0.00008	0.00121	0.00151	16.64056
T (10%)	1.83311				

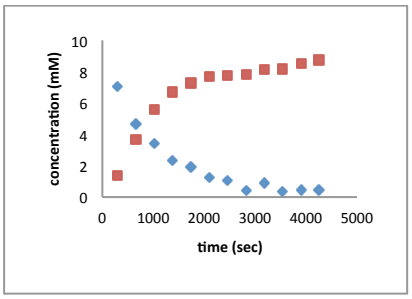
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.00653	0.00009	0.25217
2	0.00438	0.	-0.00669
3	0.003	-0.0002	-0.53734
4	0.00192	0.00029	0.78446
5	0.0013	-0.00003	-0.06913
6	0.0008	0.0002	0.53547
7	0.0008	-0.0008	-2.16074
8	0.00058	-0.00013	-0.34113
9	0.00024	0.00046	1.2561
10	0.00027	-0.00035	-0.93749
11	0.00003	0.00045	1.22431

2nd run:





Linear Regression

Regression Statistics

R	0.86152
R Square	0.74222
Adjusted R Square	0.71358
S	0.00115
Total number of observations	11

0.01580850735852 =- 0.0004 + 0.0013 * 7.04954354034568

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00003	0.00003	25.91416	0.00065
Residual	9.	0.00001	0.		
Total	10.	0.00005			

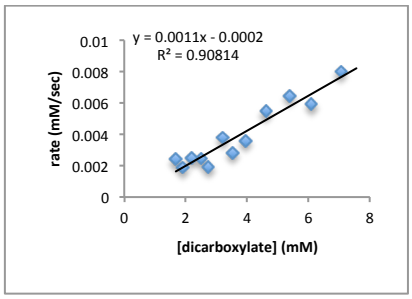
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	-0.0004	0.00053	-0.00137	0.00058	-0.74131
7.04954354034568	0.00132	0.00026	0.00084	0.00179	5.0906
T (10%)	1.83311				

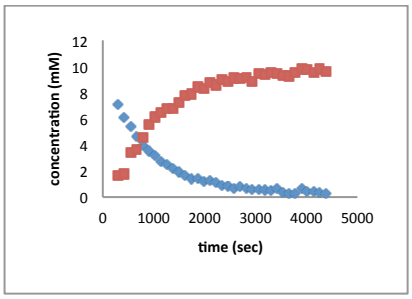
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.00576	0.00083	0.75918
2	0.00409	-0.00057	-0.52114
3	0.00267	0.00033	0.30149
4	0.00215	-0.00104	-0.95227
5	0.00129	0.00052	0.47886
6	0.00099	-0.00035	-0.3198
7	0.00014	0.00164	1.49912
8	0.00077	-0.0021	-1.91764
9	0.00007	0.0014	1.27993
10	0.00022	-0.00054	-0.49773
11	0.00019	-0.00012	-0.11

3rd run:





Linear Regression

Regression Statistics

R	0.88703
R Square	0.78683
Adjusted R Square	0.78037
S	0.00154
Total number of observations	35

=- 0.0008 + 0.0016 * 11.8

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00029	0.00029	121.80636	1.29452E-12
Residual	33.	0.00008	0.		
Total	34.	0.00037			

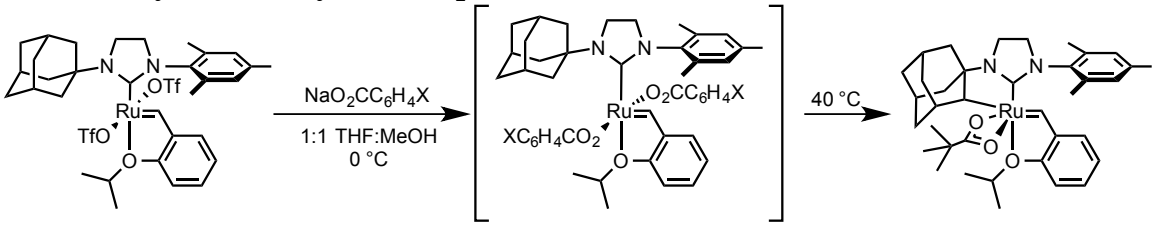
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	-0.00078	0.00037	-0.0014	-0.00016	-2.14262
11.8	0.00163	0.00015	0.00138	0.00188	11.03659
T (10%)	1.69236				

LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.01074	0.00502	3.30856
2	0.00917	-0.00116	-0.762
3	0.00801	-0.0021	-1.38359
4	0.00675	-0.00028	-0.1846
5	0.00567	-0.00019	-0.12816
6	0.00497	-0.00138	-0.90924
7	0.00442	-0.00162	-1.06649
8	0.00368	0.00012	0.07857
9	0.0033	-0.00135	-0.89121
10	0.00281	-0.00034	-0.22667
11	0.00232	0.00018	0.11815
12	0.00196	-0.00008	-0.05087
13	0.00148	0.00092	0.60905
14	0.00151	-0.00164	-1.0821
15	0.00112	0.00086	0.56584
16	0.0013	-0.00218	-1.43878
17	0.00104	0.00024	0.15784
18	0.00063	0.00149	0.98149
19	0.0006	-0.00045	-0.29853
20	0.0003	0.00124	0.8161
21	0.00051	-0.00161	-1.06212
22	0.00029	0.00083	0.54543
23	0.00016	0.00051	0.3385
24	0.00017	-0.00019	-0.12718
25	0.0001	0.00027	0.17814
26	0.	0.00047	0.30985
27	0.00028	-0.00167	-1.0997
28	-0.00021	0.00272	1.78836
29	-0.00031	0.0008	0.52475
30	-0.00028	0.00012	0.07708
31	0.00024	-0.00288	-1.89596
32	-0.00013	0.002	1.31554

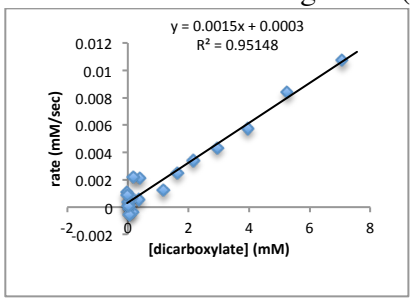
Hammett Study of Carboxylate Complexes 8a–e

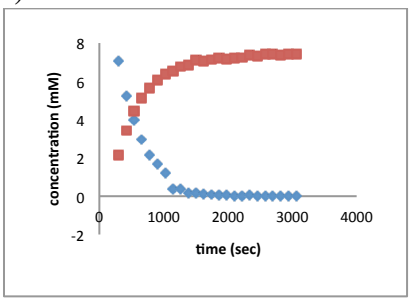


X = OMe (8e)

run	k (sec^{-1})
1	$2.0(2)x10^{-3}$
2	$1.9(3)x10^{-3}$
3	$1.9(4)x10^{-3}$
average	$1.9(3)x10^{-3}$

1st run:





Linear Regression

Regression Statistics

R	0.91263
R Square	0.8329
Adjusted R Square	0.8253
S	0.00128
Total number of observations	24

= 0.0152 - 0.0020 * 0

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00018	0.00018	109.6559	0.
Residual	22.	0.00004	0.		
Total	23.	0.00021			

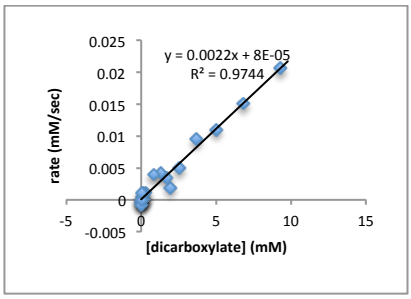
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	0.01515	0.00127	0.01297	0.01734	11.92069
0	-0.00201	0.00019	-0.00234	-0.00168	-10.47167
T (10%)	1.71714				

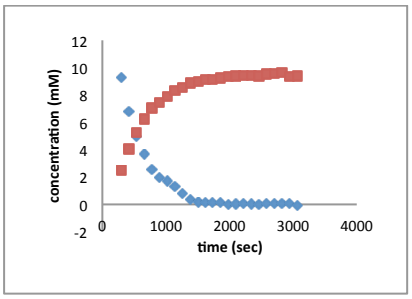
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.01083	-0.00368	-2.94769
2	0.00823	0.00254	2.03481
3	0.00619	0.00223	1.78939
4	0.0048	0.00094	0.74929
5	0.00375	0.0006	0.47811
6	0.00293	0.00049	0.38964
7	0.00232	0.0002	0.16098
8	0.00202	-0.00079	-0.63175
9	0.0015	0.00065	0.52322
10	0.00137	-0.00085	-0.68432
11	0.00085	0.00131	1.04789
12	0.00094	-0.00128	-1.02537
13	0.00077	-0.00008	-0.06459
14	0.00067	-0.00028	-0.22603
15	0.0007	-0.00082	-0.65776
16	0.00066	-0.00049	-0.39254
17	0.00058	-0.00023	-0.18703
18	0.00031	0.00079	0.6356
19	0.00044	-0.00098	-0.78701
20	0.00023	0.00066	0.53244
21	0.0002	-0.00011	-0.08513
22	0.00031	-0.00073	-0.58658
23	0.00015	0.0005	0.3991
24	0.00023	-0.00058	-0.46468

2nd run:





Linear Regression

Regression Statistics

R	0.82597
R Square	0.68223
Adjusted R Square	0.66779
S	0.00319
Total number of observations	24

= 0.0009 + 0.0019 * 11.8

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00048	0.00048	47.23333	0.
Residual	22.	0.00022	0.00001		
Total	23.	0.0007			

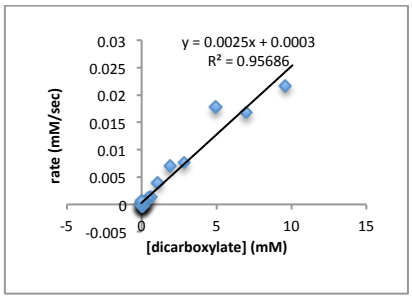
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	0.00093	0.00076	-0.00037	0.00223	1.22656
11.8	0.00186	0.00027	0.0014	0.00233	6.87265
T (10%)	1.71714				

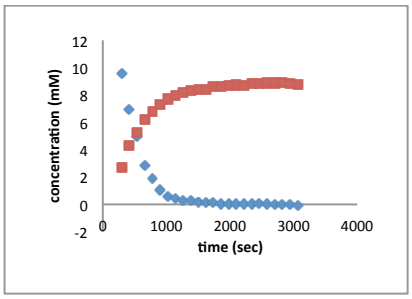
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.01824	-0.00988	-3.17114
2	0.01362	0.00703	2.25706
3	0.01025	0.00483	1.55053
4	0.00779	0.0032	1.02686
5	0.00567	0.00383	1.22857
6	0.00456	0.00039	0.12424
7	0.00415	-0.00232	-0.74519
8	0.00337	0.00013	0.04211
9	0.00244	0.00171	0.54868
10	0.00155	0.00242	0.77569
11	0.00128	-0.00009	-0.02899
12	0.00116	-0.00059	-0.18868
13	0.00116	-0.00115	-0.36965
14	0.00115	-0.00114	-0.36673
15	0.00093	0.00009	0.02747
16	0.00098	-0.00123	-0.39347
17	0.00104	-0.00131	-0.42117
18	0.00102	-0.00095	-0.30353
19	0.00092	-0.00043	-0.13778
20	0.00109	-0.00185	-0.59295
21	0.00104	-0.00086	-0.27513
22	0.00103	-0.00097	-0.31187
23	0.00104	-0.0011	-0.35234
24	0.00081	0.00024	0.07741

3rd run:





Linear Regression

Regression Statistics

R	0.75258
R Square	0.56637
Adjusted R Square	0.54666
S	0.00428
Total number of observations	24

= 0.0013 + 0.0019 * 11.8

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00053	0.00053	28.73478	0.00002
Residual	22.	0.0004	0.00002		
Total	23.	0.00093			

	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	0.0013	0.00098	-0.00038	0.00298	1.33257
11.8	0.00192	0.00036	0.00131	0.00254	5.36048
T (10%)	1.71714				

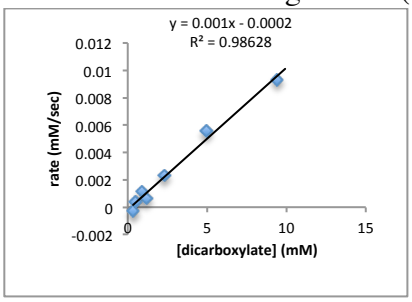
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

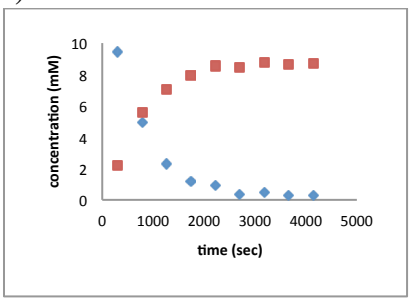
Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.01971	-0.01229	-2.93885
2	0.0147	0.00703	1.68016
3	0.01082	0.00599	1.43122
4	0.00674	0.01095	2.61836
5	0.00498	0.00265	0.6336
6	0.00337	0.00357	0.85419
7	0.00247	0.00144	0.34494
8	0.00216	-0.00079	-0.18982
9	0.00188	-0.00067	-0.15951
10	0.00177	-0.00131	-0.3122
11	0.00163	-0.00105	-0.24996
12	0.00151	-0.00097	-0.23214
13	0.00151	-0.00151	-0.3605
14	0.0014	-0.00093	-0.22311
15	0.00134	-0.00105	-0.25189
16	0.0014	-0.00168	-0.40261
17	0.00132	-0.00095	-0.22793
18	0.00138	-0.00168	-0.40099
19	0.00146	-0.00176	-0.4215
20	0.00133	-0.00077	-0.18471
21	0.0013	-0.00117	-0.28042
22	0.00127	-0.00114	-0.27286
23	0.0013	-0.00142	-0.33833
24	0.00114	-0.00048	-0.11513

X = Me (8d)	
run	k (sec^{-1})
1	$1.6(2)x10^{-3}$
2	$1.24(5)x10^{-3}$
3	$1.45(9)x10^{-3}$
average	$1.4(1)x10^{-3}$

1st run:





Linear Regression

Regression Statistics

R	0.85126
R Square	0.72464
Adjusted R Square	0.71515
S	0.00202
Total number of observations	31

0.00792019092161 =- 0.0002 + 0.0016 * 9.41998262884835

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00031	0.00031	76.31823	0.
Residual	29.	0.00012	0.		
Total	30.	0.00043			

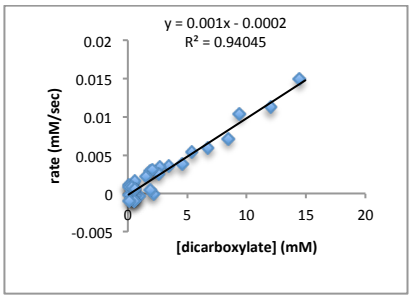
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	-0.00017	0.00048	-0.00098	0.00064	-0.35707
9.41998262884835	0.00158	0.00018	0.00127	0.00188	8.73603
T (10%)	1.69913				

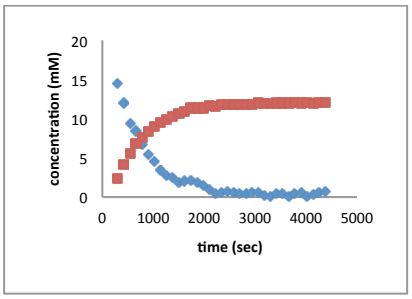
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.01183	0.00329	1.65485
2	0.00997	-0.00015	-0.07706
3	0.00868	-0.00189	-0.9487
4	0.00765	-0.0022	-1.10488
5	0.00648	-0.00028	-0.14236
6	0.00512	0.00208	1.04557
7	0.00406	0.00151	0.7587
8	0.00346	-0.00031	-0.15828
9	0.00344	-0.00333	-1.67282
10	0.00245	0.00278	1.39817
11	0.00235	-0.00179	-0.90263
12	0.0017	0.00169	0.85161
13	0.00183	-0.00251	-1.26246
14	0.00147	0.00044	0.21933
15	0.00184	-0.00378	-1.89943
16	0.00123	0.002	1.00681
17	0.00136	-0.00204	-1.02486
18	0.00084	0.00186	0.93776
19	0.00033	0.0024	1.20646
20	0.00036	-0.00055	-0.27703
21	0.0005	-0.00122	-0.61446
22	0.	0.00263	1.32459
23	0.0003	-0.0019	-0.95353
24	0.00059	-0.00214	-1.07511
25	0.00032	0.00113	0.56617
26	0.00032	-0.00031	-0.15593
27	0.00002	0.00157	0.78774
28	0.00028	-0.00163	-0.81916
29	-0.00015	0.00238	1.1951
30	-0.00006	-0.00037	-0.18792
31	-0.00016	0.00064	0.32373

2nd run:





Linear Regression

Regression Statistics

R	0.97778
R Square	0.95605
Adjusted R Square	0.95467
S	0.0008
Total number of observations	34

0.00798742281566 =- 0.0003 + 0.0012 * 14.4421610342286

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00044	0.00044	696.05742	0.E+0
Residual	32.	0.00002	0.		
Total	33.	0.00046			

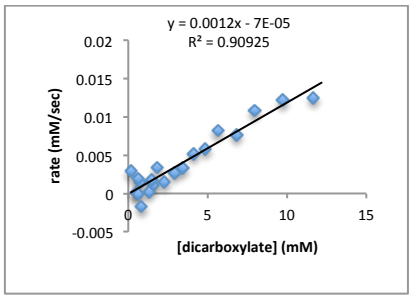
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	-0.00032	0.00017	-0.00061	-0.00003	-1.8575
14.4421610342286	0.00124	0.00005	0.00116	0.00132	26.3829
T (10%)	1.69389				

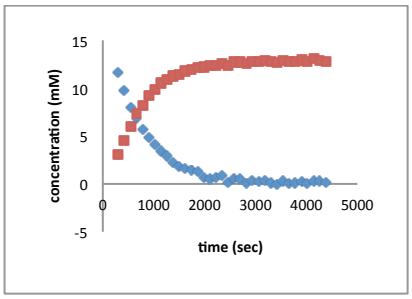
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.01458	0.00035	0.45251
2	0.01128	-0.00008	-0.09761
3	0.01014	0.00029	0.37178
4	0.00801	-0.0009	-1.14437
5	0.00639	-0.00039	-0.49174
6	0.00537	-0.00002	-0.01954
7	0.00397	-0.00017	-0.2203
8	0.00303	0.00057	0.733
9	0.00287	0.00064	0.81442
10	0.00205	0.00048	0.60725
11	0.00222	0.00075	0.95409
12	0.00233	0.00077	0.98798
13	0.002	-0.00205	-2.62056
14	0.00153	-0.00103	-1.3172
15	0.00088	0.00132	1.68799
16	0.00022	-0.00061	-0.77879
17	0.00039	0.0009	1.14455
18	0.00051	-0.00054	-0.68676
19	0.00036	-0.00058	-0.73998
20	0.00033	0.0002	0.26093
21	0.00022	0.00016	0.20837
22	0.00041	-0.00036	-0.4565
23	0.00037	0.00124	1.58116
24	-0.00014	-0.00085	-1.07998
25	-0.00024	0.00006	0.07405
26	0.00018	0.00092	1.17729
27	0.00031	-0.00085	-1.07951
28	-0.00021	0.00049	0.62632
29	0.00034	0.00054	0.68896
30	0.00038	-0.00133	-1.70274
31	-0.00017	0.00071	0.9042
32	0.00008	-0.00103	-1.30942

3rd run:





Linear Regression

Regression Statistics

R	0.96813
R Square	0.93727
Adjusted R Square	0.93378
S	0.00108
Total number of observations	20

0.01010936698823 =- 0.0002 + 0.0015 * 11.6801091192353

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00031	0.00031	268.92646	2.87359E-12
Residual	18.	0.00002	0.		
Total	19.	0.00033			

	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	-0.00015	0.00035	-0.00076	0.00046	-0.42957
11.6801091192353	0.00145	0.00009	0.0013	0.00161	16.39898
T (10%)	1.73406				

LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

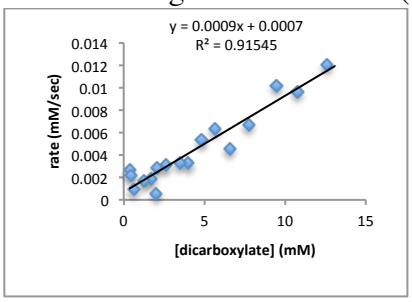
Residuals

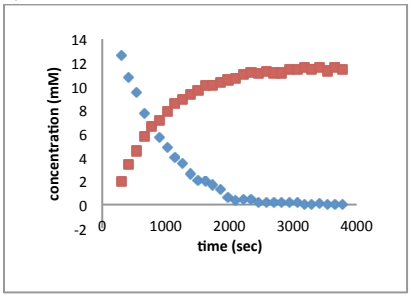
Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.01398	-0.00152	-1.44741
2	0.01144	0.00074	0.70378
3	0.0098	0.00101	0.96588
4	0.00809	-0.00045	-0.42838
5	0.00689	0.00136	1.29885
6	0.00582	0.	-0.00272
7	0.00484	0.00031	0.2938
8	0.0041	-0.00079	-0.75075
9	0.00312	-0.00039	-0.37091
10	0.00248	-0.00093	-0.8851
11	0.00213	0.00122	1.1666
12	0.00197	-0.00086	-0.81661
13	0.00174	-0.00003	-0.03215
14	0.00089	-0.00067	-0.6405
15	0.00056	0.00093	0.88266
16	0.00075	-0.0006	-0.57484
17	0.00103	0.00092	0.88042
18	0.0001	-0.00185	-1.76418
19	0.00072	0.00217	2.07259
20	0.00053	-0.00058	-0.55103

X = H (8a)

run	k (sec^{-1})
1	$1.2(1)x10^{-3}$
2	$1.37(5)x10^{-3}$
3	$0.9(2)x10^{-3}$
average	$1.2(1)x10^{-3}$

1st run:





Linear Regression

Regression Statistics

R	0.86252
R Square	0.74394
Adjusted R Square	0.73479
S	0.00183
Total number of observations	30

= 0.0139 - 0.0012 * 0

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00027	0.00027	81.34771	0.
Residual	28.	0.00009	0.		
Total	29.	0.00037			

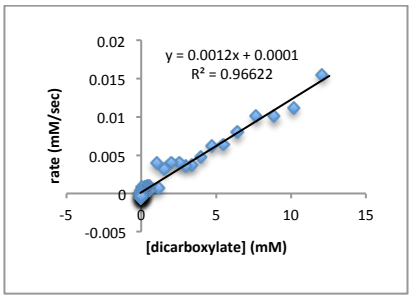
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	0.01386	0.00127	0.0117	0.01601	10.94791
0	-0.00116	0.00013	-0.00138	-0.00094	-9.0193
T (10%)	1.70113				

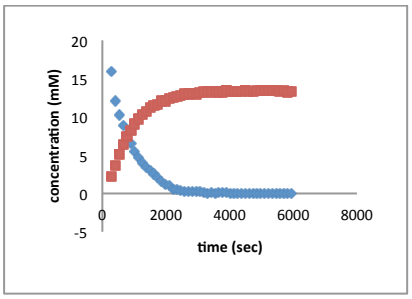
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.01159	-0.00508	-2.8251
2	0.0099	0.00214	1.19141
3	0.00855	0.00113	0.62776
4	0.00713	0.00308	1.71251
5	0.0062	0.00047	0.26073
6	0.00556	-0.00097	-0.53789
7	0.00467	0.00166	0.92462
8	0.00393	0.0014	0.7766
9	0.00348	-0.00024	-0.13382
10	0.00302	0.00029	0.16067
11	0.00259	0.00048	0.26864
12	0.00219	0.00071	0.39306
13	0.00212	-0.00162	-0.89803
14	0.00185	0.00006	0.03561
15	0.00162	0.00005	0.0263
16	0.00149	-0.00057	-0.31908
17	0.00112	0.00154	0.85581
18	0.00081	0.00138	0.76953
19	0.00097	-0.00208	-1.15694
20	0.00077	0.00067	0.37096
21	0.00092	-0.00205	-1.14173
22	0.0009	-0.00076	-0.42325
23	0.00057	0.00183	1.01709
24	0.0006	-0.00078	-0.43563
25	0.00034	0.00153	0.84967
26	0.00054	-0.00198	-1.10203
27	0.00037	0.00085	0.47161
28	0.00069	-0.00297	-1.6535
29	0.00035	0.00208	1.15565
30	0.00058	-0.00223	-1.24121

2nd run:





Linear Regression

Regression Statistics

R	0.96822
R Square	0.93746
Adjusted R Square	0.936
S	0.00079
Total number of observations	45

0.0155353789407 = 0.0002 + 0.0014 * 10.1970900546371

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.0004	0.0004	644.54418	0.E+0
Residual	43.	0.00003	0.		
Total	44.	0.00043			

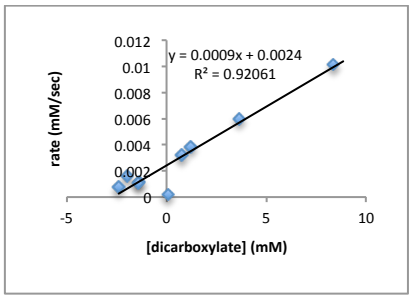
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	0.0002	0.00013	-0.00002	0.00043	1.49759
10.1970900546371	0.00137	0.00005	0.00127	0.00146	25.38787
T (10%)	1.68107				

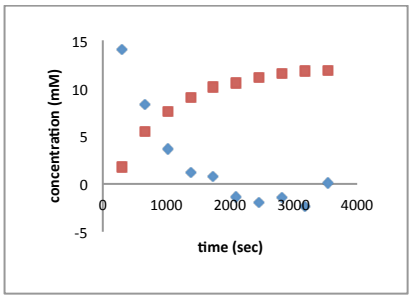
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.0123	-0.00115	-1.46815
2	0.01065	-0.00058	-0.74745
3	0.009	0.00107	1.36998
4	0.0077	0.00026	0.33305
5	0.00665	-0.00028	-0.3531
6	0.00563	0.00062	0.79075
7	0.00483	0.00001	0.01525
8	0.00423	-0.00052	-0.66794
9	0.00364	-0.00004	-0.0488
10	0.00297	0.00113	1.44562
11	0.0023	0.00175	2.24094
12	0.00177	0.00148	1.90191
13	0.00165	-0.00091	-1.17211
14	0.001	0.00296	3.79889
15	0.00092	-0.00043	-0.55527
16	0.00077	0.00018	0.23055
17	0.00061	0.00033	0.42248
18	0.00046	0.00045	0.57994
19	0.00049	-0.00066	-0.84178
20	0.00049	-0.00049	-0.62389
21	0.00051	-0.00064	-0.81402
22	0.00037	0.00048	0.61898
23	0.00027	0.00033	0.41838
24	0.00034	-0.00072	-0.92816
25	0.00028	0.00008	0.10253
26	0.00033	-0.00068	-0.87528
27	0.00036	-0.00049	-0.625
28	0.00034	-0.00025	-0.32571
29	0.00025	0.00031	0.39633
30	0.00029	-0.00051	-0.64838
31	0.00022	0.00016	0.20384
32	0.0003	-0.00078	-1.00571

3rd run:





Linear Regression

Regression Statistics

R	0.74971
R Square	0.56206
Adjusted R Square	0.54522
S	0.00242
Total number of observations	28

= 0.0117 - 0.0009 * 0

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00019	0.00019	33.3692	0.
Residual	26.	0.00015	0.00001		
Total	27.	0.00035			

	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	0.01172	0.00154	0.00909	0.01435	7.60057
0	-0.00092	0.00016	-0.00119	-0.00065	-5.77661
T (10%)	1.70562				

LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

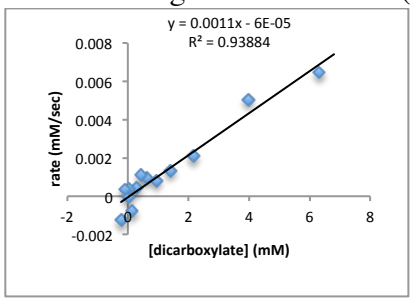
Residuals

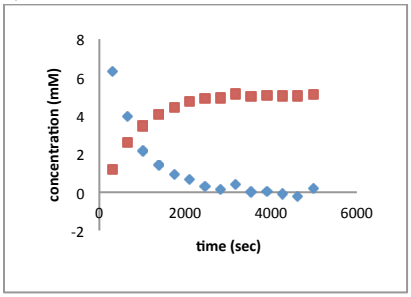
Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.01007	-0.00412	-1.739
2	0.00925	-0.00182	-0.76872
3	0.00791	0.0042	1.77284
4	0.00671	0.00415	1.75098
5	0.00645	-0.00408	-1.72217
6	0.00551	0.00304	1.28323
7	0.00473	0.00233	0.98507
8	0.00419	0.00074	0.31263
9	0.00379	-0.00016	-0.06924
10	0.00346	-0.00052	-0.2197
11	0.00309	0.00024	0.10221
12	0.00245	0.0034	1.43575
13	0.00241	-0.00206	-0.86827
14	0.00214	0.00031	0.13204
15	0.00182	0.00108	0.4562
16	0.00202	-0.00384	-1.61931
17	0.00165	0.00169	0.7111
18	0.00145	0.00033	0.1377
19	0.00148	-0.00175	-0.73769
20	0.00138	-0.00044	-0.18509
21	0.00113	0.00112	0.47434
22	0.00112	-0.00105	-0.44226
23	0.00134	-0.00335	-1.41311
24	0.00102	0.00189	0.79694
25	0.00088	0.00043	0.18047
26	0.00072	0.00073	0.31011
27	0.00093	-0.00287	-1.20892
28	0.0008	0.00036	0.15188

X = Cl (8c)

run	k (sec^{-1})
1	$1.1(1)x10^{-3}$
2	$1.08(8)x10^{-3}$
3	$1.4(1)x10^{-3}$
average	$1.2(1)x10^{-3}$

1st run:





Linear Regression

Regression Statistics

R	0.96894
R Square	0.93884
Adjusted R Square	0.93328
S	0.00056
Total number of observations	13

0.0182933434491 =- 0.0001 + 0.0011 * 11.8

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00005	0.00005	168.85032	0.
Residual	11.	0.	0.		
Total	12.	0.00006			

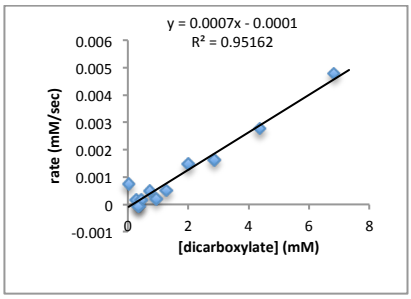
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	-0.00006	0.00019	-0.00039	0.00028	-0.29795
11.8	0.0011	0.00008	0.00095	0.00125	12.99424
T (10%)	1.79588				

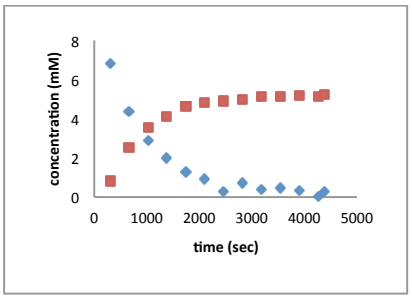
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.00687	-0.0004	-0.75323
2	0.00431	0.00071	1.3293
3	0.00232	-0.00023	-0.43656
4	0.0015	-0.00016	-0.30089
5	0.00097	-0.00014	-0.26406
6	0.00064	0.0003	0.56213
7	0.00027	0.00014	0.2588
8	0.00011	-0.00088	-1.63753
9	0.00041	0.00072	1.33439
10	-0.00003	-0.00001	-0.0169
11	-0.00002	0.00039	0.72751
12	-0.00016	0.00051	0.94347
13	-0.0003	-0.00094	-1.74643

2nd run:





Linear Regression

Regression Statistics

R	0.97537
R Square	0.95135
Adjusted R Square	0.94648
S	0.00033
Total number of observations	12

0.00269742022416 =- 0.0002 + 0.0011 * 6.82558667805555

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00002	0.00002	195.5336	0.
Residual	10.	0.	0.		
Total	11.	0.00002			

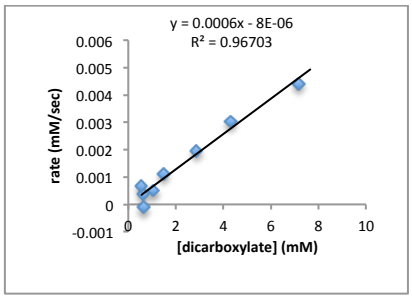
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	-0.0002	0.00013	-0.00043	0.00004	-1.48132
6.82558667805555	0.00108	0.00008	0.00094	0.00122	13.98333
T (10%)	1.81246				

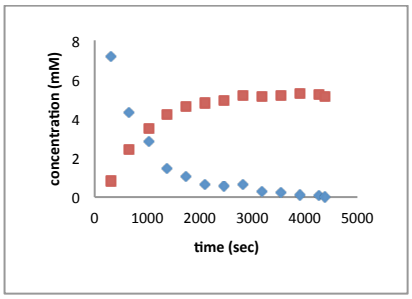
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.00452	0.00027	0.83642
2	0.00291	-0.00015	-0.46616
3	0.00196	-0.00032	-0.99613
4	0.00119	0.00028	0.87156
5	0.00081	-0.00031	-0.97048
6	0.00011	0.0001	0.30621
7	0.0006	-0.00043	-1.35872
8	0.00023	0.00025	0.78112
9	0.0003	-0.00035	-1.09174
10	0.00017	-0.00002	-0.05018
11	-0.00017	0.00008	0.24467
12	0.00013	0.0006	1.89342

3rd run:





Linear Regression

Regression Statistics

R	0.90939
R Square	0.82699
Adjusted R Square	0.81947
S	0.00069
Total number of observations	25

0.00273404633315 = 0.0072 - 0.0014 * 0.82158092284047

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00005	0.00005	109.94138	0.
Residual	23.	0.00001	0.		
Total	24.	0.00006			

	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	0.00721	0.00057	0.00623	0.00819	12.61944
0.82158092284047	-0.00138	0.00013	-0.00161	-0.00116	-10.48529
T (10%)	1.71387				

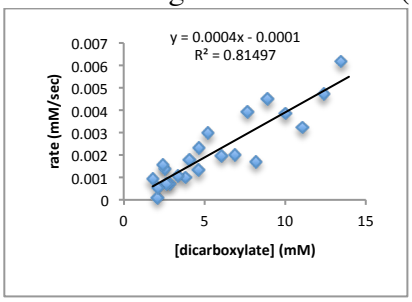
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

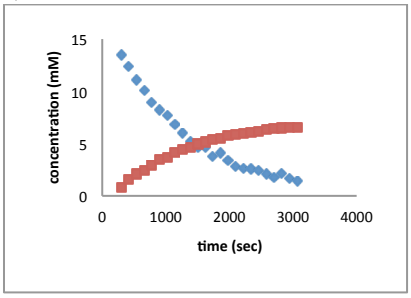
Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.00524	-0.00016	-0.22976
2	0.00454	-0.0003	-0.44848
3	0.00388	0.00004	0.06479
4	0.00322	0.00078	1.14939
5	0.00284	-0.00052	-0.76521
6	0.00238	0.0004	0.58965
7	0.00212	-0.00056	-0.82421
8	0.00171	0.00074	1.08954
9	0.0014	0.00047	0.69425
10	0.00106	0.00103	1.52226
11	0.00108	-0.00122	-1.79426
12	0.00085	0.00055	0.81538
13	0.00077	-0.00033	-0.48703
14	0.00061	0.00038	0.56091
15	0.00059	-0.00049	-0.71918
16	0.00062	-0.00076	-1.12187
17	0.00047	0.0004	0.58204
18	0.00039	0.00008	0.11839
19	0.00025	0.00063	0.92592
20	0.00028	-0.00044	-0.64739
21	0.00006	0.00122	1.78874
22	0.00017	-0.00078	-1.14863
23	0.00007	0.00053	0.78361
24	0.00012	-0.00044	-0.64706
25	0.00028	-0.00126	-1.85179

X = NO_2 (8b)	
run	k (sec^{-1})
1	$7.6(7)x10^{-4}$
2	$8.8(5)x10^{-4}$
3	$7.2(6)x10^{-4}$
average	$7.9(6)x10^{-4}$

1st run:





Linear Regression

Regression Statistics

R	0.83531
R Square	0.69774
Adjusted R Square	0.69144
S	0.00087
Total number of observations	50

= 0.0057 - 0.0008 * 0

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00008	0.00008	110.80289	4.59632E-14
Residual	48.	0.00004	0.		
Total	49.	0.00012			

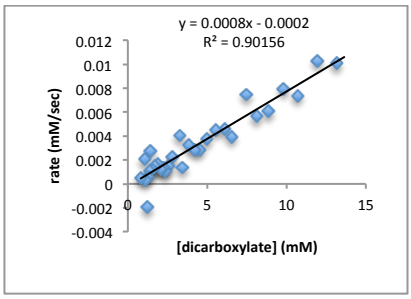
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	0.00571	0.00045	0.00495	0.00647	12.62217
0	-0.00076	0.00007	-0.00089	-0.00064	-10.5263
T (10%)	1.67722				

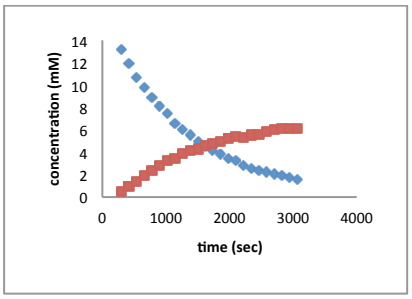
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.00511	-0.00252	-2.92737
2	0.00455	0.00162	1.87595
3	0.00411	0.00061	0.71236
4	0.00382	-0.00059	-0.6901
5	0.00346	0.0004	0.465
6	0.00305	0.00145	1.67968
7	0.0029	-0.00121	-1.40067
8	0.00254	0.00137	1.58578
9	0.00236	-0.00035	-0.40509
10	0.00217	-0.00018	-0.21259
11	0.0019	0.00108	1.25104
12	0.00178	-0.00047	-0.5461
13	0.00157	0.00076	0.88202
14	0.00148	-0.00048	-0.5516
15	0.00131	0.00045	0.52106
16	0.00122	-0.00016	-0.19062
17	0.00115	-0.00042	-0.48995
18	0.00108	-0.00036	-0.4178
19	0.00096	0.00042	0.49317
20	0.00082	0.00073	0.85111
21	0.00081	-0.00072	-0.83526
22	0.00072	0.0002	0.22941
23	0.00067	-0.00015	-0.16929
24	0.00071	-0.00113	-1.30619
25	0.0006	0.00068	0.79092
26	0.0005	0.0005	0.57927
27	0.00046	0.	0.00196
28	0.00037	0.0006	0.69675
29	0.00042	-0.00091	-1.05878
30	0.00025	0.00155	1.80135
31	0.00029	-0.00072	-0.8386
32	0.00032	-0.00064	-0.7376

2nd run:





Linear Regression

Regression Statistics

R	0.92561
R Square	0.85675
Adjusted R Square	0.85371
S	0.0011
Total number of observations	49

-0.00444431177816 =- 0.0003 + 0.0009 * 13.1355156888928

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00034	0.00034	281.10522	0.E+0
Residual	47.	0.00006	0.		
Total	48.	0.0004			

	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	-0.00028	0.00021	-0.00064	0.00008	-1.31894
13.1355156888928	0.00088	0.00005	0.00079	0.00097	16.76619

T (10%) 1.67793

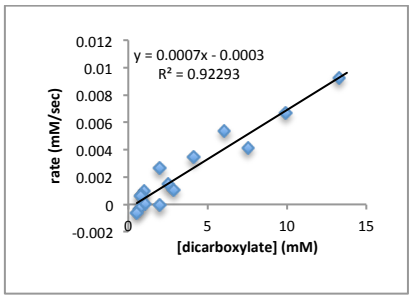
LCL - Lower value of a reliable interval (LCL)

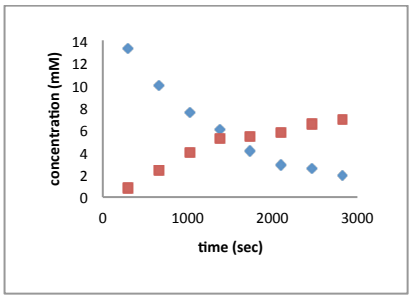
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.01019	-0.00013	-0.11892
2	0.00911	0.00119	1.08996
3	0.00833	-0.00095	-0.8676
4	0.00749	0.00043	0.39636
5	0.00686	-0.0008	-0.72934
6	0.00626	-0.0006	-0.55048
7	0.00547	0.00198	1.81026
8	0.00506	-0.0011	-1.01133
9	0.00457	0.00002	0.02085
10	0.00409	0.00045	0.41229
11	0.0037	0.00005	0.04179
12	0.0034	-0.00051	-0.46842
13	0.00309	-0.00022	-0.19991
14	0.00275	0.0005	0.45336
15	0.0026	-0.00121	-1.11264
16	0.00218	0.00184	1.68573
17	0.00194	0.0003	0.27209
18	0.00179	-0.0003	-0.2758
19	0.00168	-0.00064	-0.58213
20	0.00153	-0.00016	-0.14736
21	0.0014	-0.00014	-0.12475
22	0.00122	0.00046	0.42248
23	0.00107	0.00042	0.38559
24	0.00094	0.00024	0.21996
25	0.00083	0.00023	0.21391
26	0.00077	-0.0002	-0.18748
27	0.00098	-0.00295	-2.69798
28	0.00069	0.00206	1.88524
29	0.00065	-0.00029	-0.26518
30	0.00043	0.00163	1.49338
31	0.00038	0.00012	0.11432
32	0.00041	-0.0007	-0.64326

3rd run:





Linear Regression

Regression Statistics

R	0.96069
R Square	0.92293
Adjusted R Square	0.917
S	0.00083
Total number of observations	15

-0.00492232160507 =- 0.0003 + 0.0007 * 11.8

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00011	0.00011	155.67583	0.
Residual	13.	0.00001	0.		
Total	14.	0.00012			

	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	-0.00029	0.0003	-0.00083	0.00025	-0.95933
11.8	0.00072	0.00006	0.00062	0.00082	12.47701
T (10%)	1.77093				

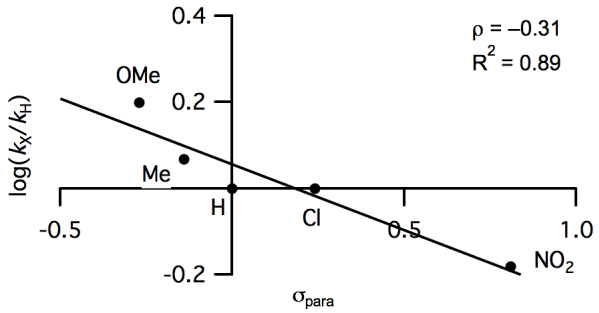
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.00927	-0.00001	-0.01607
2	0.00687	-0.00017	-0.21525
3	0.00513	-0.00101	-1.25661
4	0.00407	0.00132	1.63568
5	0.00267	0.00078	0.96912
6	0.00178	-0.00074	-0.91784
7	0.00151	-0.00004	-0.04685
8	0.00113	-0.00117	-1.45439
9	0.00114	0.00149	1.84824
10	0.00046	-0.00041	-0.51047
11	0.00045	0.00051	0.62868
12	0.0002	-0.00053	-0.65761
13	0.00028	0.00042	0.52237
14	0.0001	-0.00075	-0.92886
15	0.00027	0.00032	0.39987

Hammett Plots

Benzoate	σ	σ+	k (sec^{-1})	log (k_X/k_H)
NO2	0.81	0.79	0.00079	-0.181
H	0	0	0.0012	0
Cl	0.24	0.11	0.0012	0
OMe	-0.27	-0.78	0.0019	0.200
Me	-0.14	-0.31	0.0014	0.067



Linear Regression

Regression Statistics

R	0.94384
R Square	0.89083
Adjusted R Square	0.85444
S	0.05253
Total number of observations	5

log (kX/kH) = 0.0561 - 0.3054 * ?

ANOVA

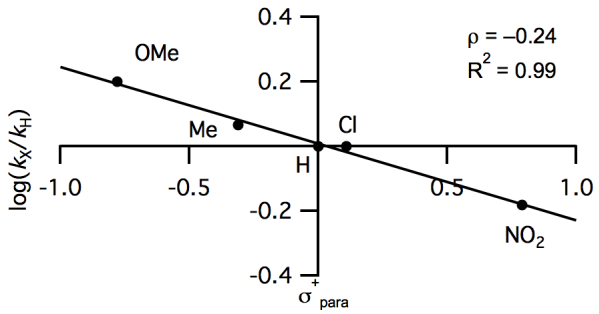
	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.06755	0.06755	24.47983	0.01584
Residual	3.	0.00828	0.00276		
Total	4.	0.07583			

	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	0.05608	0.02479	-0.00225	0.11441	2.26278
?	-0.30539	0.06172	-0.45066	-0.16013	-4.94771
T (10%)	2.35336				

LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	-0.19129	0.00973	0.21393
2	0.05608	-0.05608	-1.2328
3	-0.01721	0.01721	0.37833
4	0.13854	0.06103	1.34158
5	0.09884	-0.03189	-0.70104



Linear Regression

Regression Statistics

R	0.99569
R Square	0.99141
Adjusted R Square	0.98854
S	0.01474
Total number of observations	5

log (kX/kH) = 0.0080 - 0.2374 * ?+

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.07518	0.07518	346.09479	0.00034
Residual	3.	0.00065	0.00022		
Total	4.	0.07583			

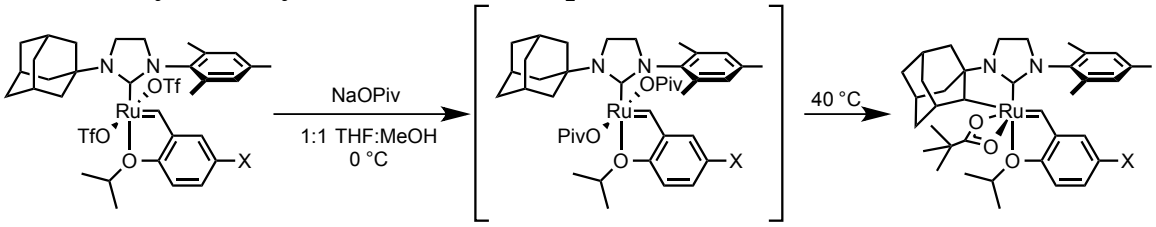
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	0.00797	0.00661	-0.00758	0.02352	1.20599
?+	-0.23744	0.01276	-0.26747	-0.2074	-18.60362
T (10%)	2.35336				

LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

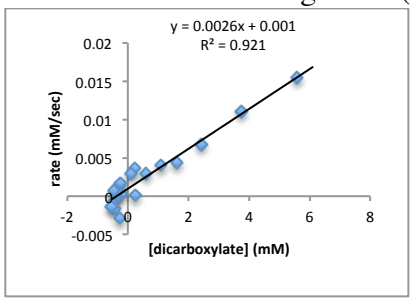
Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	-0.17961	-0.00195	-0.15265
2	0.00797	-0.00797	-0.62445
3	-0.01815	0.01815	1.42183
4	0.19317	0.0064	0.50144
5	0.08158	-0.01463	-1.14617

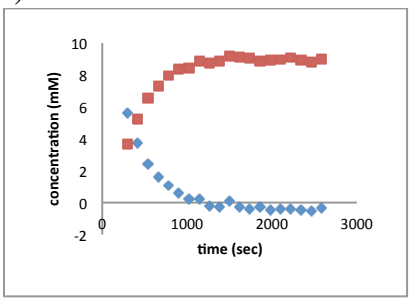
Hammett Study of Benzylidene Chelate Complexes 10a–d



X = OMe (S1)

run	k (sec^{-1})
1	$2.6(2)x10^{-3}$
2	$2.7(2)x10^{-3}$
3	$3.0(5)x10^{-3}$
average	$2.8(3)x10^{-3}$





1st run:

Linear Regression

Regression Statistics

R	0.95969
R Square	0.921
Adjusted R Square	0.91635
S	0.0013
Total number of observations	19

0.02064533295452 = 0.0010 + 0.0026 * 11.8

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00033	0.00033	198.19501	8.43341E-11
Residual	17.	0.00003	0.		
Total	18.	0.00036			

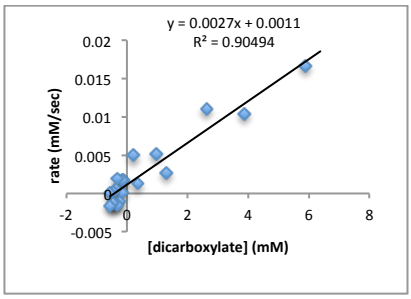
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	0.00097	0.00032	0.00041	0.00153	3.03034
11.8	0.00261	0.00019	0.00228	0.00293	14.07817
T (10%)	1.73961				

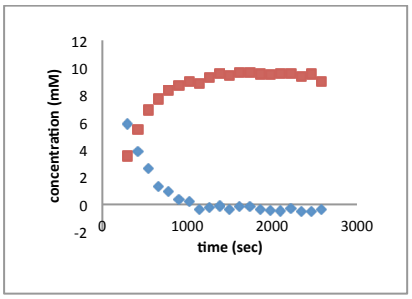
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.01555	-0.00009	-0.07152
2	0.01072	0.00033	0.26045
3	0.00726	-0.00053	-0.41947
4	0.00516	-0.00076	-0.60311
5	0.00378	0.00026	0.20363
6	0.00252	0.00048	0.37836
7	0.00158	-0.00143	-1.13383
8	0.00153	0.00212	1.67986
9	0.00039	-0.00007	-0.05337
10	0.00029	-0.00319	-2.53089
11	0.0012	0.00176	1.39702
12	0.00027	0.00114	0.90654
13	-0.00017	-0.00145	-1.14882
14	0.00034	0.00136	1.07457
15	-0.00019	-0.00043	-0.33967
16	0.	0.00002	0.01977
17	-0.00001	0.00058	0.46183
18	-0.00019	0.00089	0.70317
19	-0.00041	-0.00099	-0.78453

2nd run:





Linear Regression

Regression Statistics

R	0.95128
R Square	0.90494
Adjusted R Square	0.89935
S	0.00158
Total number of observations	19

0.01970239185308 = 0.0011 + 0.0027 * 11.8

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00041	0.00041	161.83309	0.
Residual	17.	0.00004	0.		
Total	18.	0.00045			

	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	0.00115	0.00038	0.00048	0.00181	2.98512
11.8	0.00273	0.00021	0.00236	0.0031	12.72136

T (10%) 1.73961

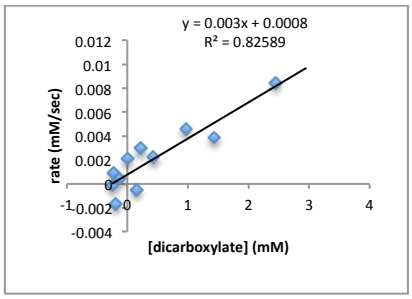
LCL - Lower value of a reliable interval (LCL)

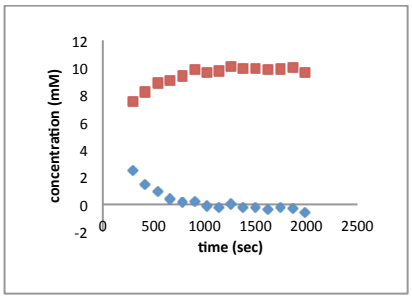
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.01719	-0.0005	-0.32393
2	0.01173	-0.0013	-0.8426
3	0.00831	0.0028	1.82115
4	0.00467	-0.00198	-1.2856
5	0.00379	0.00135	0.87992
6	0.0021	-0.00082	-0.53599
7	0.00169	0.00332	2.15811
8	0.00005	-0.00134	-0.87118
9	0.00047	-0.00154	-1.00295
10	0.00082	0.00089	0.57951
11	0.00026	-0.0017	-1.10406
12	0.00073	-0.00063	-0.41146
13	0.0007	0.00099	0.64111
14	0.00015	0.0005	0.3271
15	-0.00007	0.0003	0.19399
16	-0.00014	-0.00114	-0.74253
17	0.00028	0.00167	1.08786
18	-0.00036	0.00037	0.24293
19	-0.00037	-0.00125	-0.81138

3rd run:





Linear Regression

Regression Statistics

R	0.90878
R Square	0.82589
Adjusted R Square	0.80654
S	0.00124
Total number of observations	11

0.03113158475814 = 0.0008 + 0.0030 * 11.8

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00007	0.00007	42.69093	0.00011
Residual	9.	0.00001	0.		
Total	10.	0.00008			

	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	0.00078	0.00043	-0.00001	0.00156	1.8163
11.8	0.00302	0.00046	0.00217	0.00386	6.53383
T (10%)	1.83311				

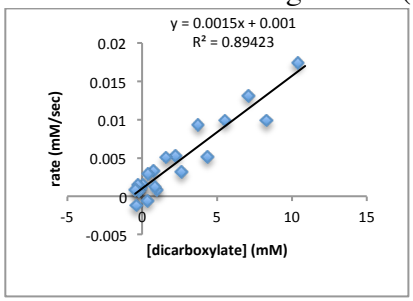
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

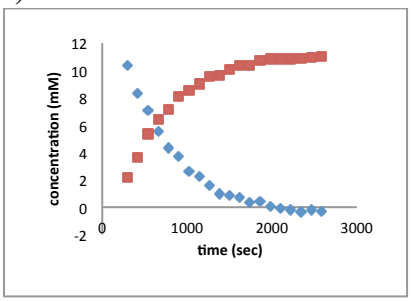
Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.00815	0.00026	0.219
2	0.00511	-0.00125	-1.05974
3	0.00371	0.00085	0.71817
4	0.00206	0.00018	0.14905
5	0.00125	-0.00177	-1.49942
6	0.00144	0.00151	1.2802
7	0.00037	0.00011	0.09369
8	0.0002	-0.0019	-1.60634
9	0.00081	0.00132	1.12209
10	0.00004	-0.00017	-0.14741
11	0.00009	0.00086	0.7307

X = Me (S2)	
run	k (sec^{-1})
1	$1.4(1)x10^{-3}$
2	$1.28(7)x10^{-3}$
3	$1.2(1)x10^{-3}$
average	$1.3(1)x10^{-3}$

1st run:





Linear Regression

Regression Statistics

R	0.94564
R Square	0.89423
Adjusted R Square	0.88866
S	0.00164
Total number of observations	21

0.00470653635742 = 0.0010 + 0.0015 * 11.8

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00043	0.00043	160.63649	0.
Residual	19.	0.00005	0.		
Total	20.	0.00048			

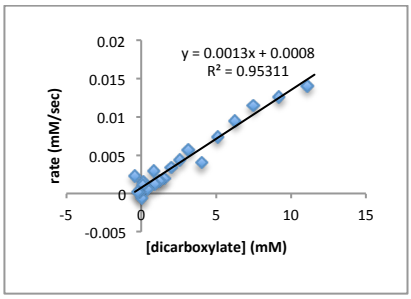
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	0.00101	0.00044	0.00024	0.00178	2.27422
11.8	0.00147	0.00012	0.00127	0.00167	12.67425
T (10%)	1.72913				

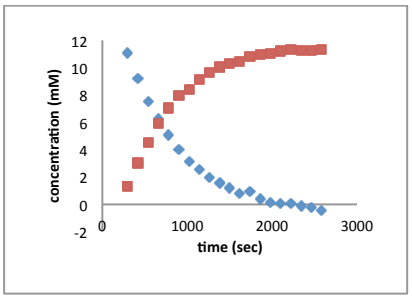
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.01627	0.00119	0.74156
2	0.01319	-0.00332	-2.07509
3	0.01145	0.0016	0.99916
4	0.00915	0.00075	0.467
5	0.00741	-0.00225	-1.40847
6	0.0065	0.00283	1.77057
7	0.00485	-0.00161	-1.00452
8	0.00428	0.00102	0.63743
9	0.00335	0.0017	1.06642
10	0.00245	-0.00167	-1.04197
11	0.00232	-0.00112	-0.70293
12	0.00211	0.00123	0.77203
13	0.00152	-0.00212	-1.3242
14	0.00162	0.0013	0.81148
15	0.00111	0.00035	0.21836
16	0.00085	0.00007	0.04377
17	0.00069	0.00045	0.28246
18	0.00049	-0.00171	-1.07011
19	0.0007	-0.00004	-0.0271
20	0.00059	0.00089	0.55799
21	0.00033	0.00046	0.28616

2nd run:





Linear Regression

Regression Statistics

R	0.97628
R Square	0.95311
Adjusted R Square	0.95051
S	0.00099
Total number of observations	20

0.00441477332771 = 0.0008 + 0.0013 * 11.8

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00036	0.00036	365.90819	2.07501E-13
Residual	18.	0.00002	0.		
Total	19.	0.00037			

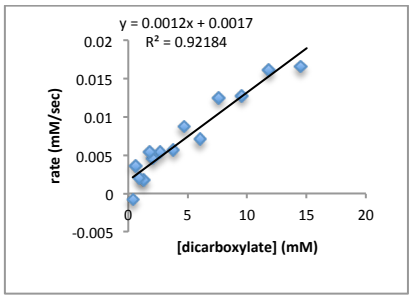
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	0.00075	0.00029	0.00025	0.00125	2.61122
11.8	0.00128	0.00007	0.00116	0.00139	19.12873
T (10%)	1.73406				

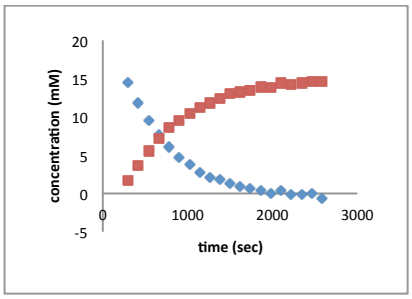
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.01487	-0.00081	-0.84372
2	0.01248	0.00012	0.12139
3	0.01033	0.00113	1.17758
4	0.00874	0.00078	0.80978
5	0.00724	0.00012	0.13015
6	0.00587	-0.00184	-1.91516
7	0.00476	0.00092	0.95968
8	0.00401	0.00036	0.37498
9	0.00331	0.00006	0.06515
10	0.00275	-0.00078	-0.81209
11	0.00227	-0.00063	-0.65345
12	0.00179	0.0012	1.24848
13	0.00189	-0.0007	-0.73341
14	0.00125	-0.00066	-0.69102
15	0.00091	0.00058	0.60106
16	0.00087	0.00022	0.22834
17	0.00085	-0.00148	-1.54239
18	0.00058	-0.00047	-0.49463
19	0.00044	-0.0002	-0.20776
20	0.00021	0.00209	2.17705

3rd run:





Linear Regression

Regression Statistics

R	0.96012
R Square	0.92184
Adjusted R Square	0.91532
S	0.00157
Total number of observations	14

0.00556450964153 = 0.0017 + 0.0012 * 11.8

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00035	0.00035	141.52606	0.
Residual	12.	0.00003	0.		
Total	13.	0.00038			

	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	0.00168	0.00063	0.00056	0.0028	2.67304
11.8	0.00115	0.0001	0.00098	0.00132	11.89647
T (10%)	1.78229				

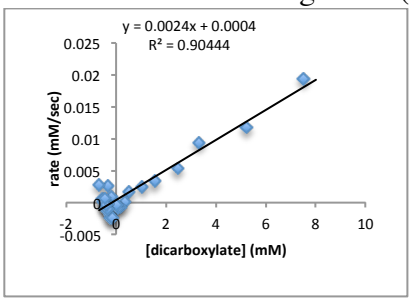
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

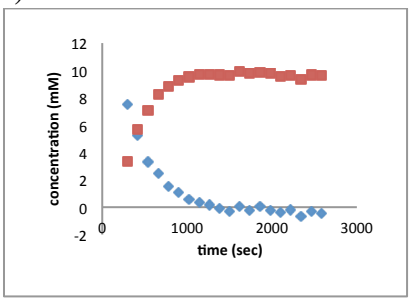
Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.01839	-0.00181	-1.20212
2	0.01527	0.00085	0.56481
3	0.01268	0.00009	0.06158
4	0.01046	0.00205	1.35836
5	0.00865	-0.00162	-1.07465
6	0.00709	0.00168	1.11263
7	0.00601	-0.00031	-0.20658
8	0.00477	0.0006	0.397
9	0.00403	0.00049	0.32557
10	0.00371	0.00171	1.13319
11	0.00318	-0.00143	-0.95079
12	0.00272	-0.00067	-0.44538
13	0.00238	0.00125	0.82794
14	0.00211	-0.00286	-1.90155

X = Cl (S3)	
run	k (sec^{-1})
1	$2.4(2)x10^{-3}$
2	$2.4(2)x10^{-3}$
3	$2.2(2)x10^{-3}$
average	$2.3(2)x10^{-3}$

1st run:





Linear Regression

Regression Statistics

R	0.95102
R Square	0.90444
Adjusted R Square	0.90091
S	0.00146
Total number of observations	29

0.01113203615226 = 0.0004 + 0.0024 * 11.8

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00054	0.00054	255.55869	2.77556E-15
Residual	27.	0.00006	0.		
Total	28.	0.0006			

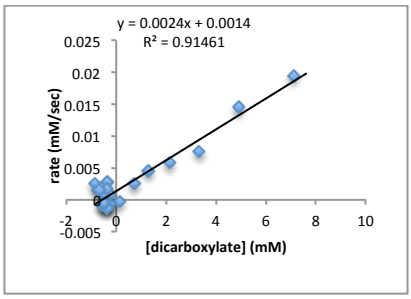
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	0.00041	0.00028	-0.00008	0.00089	1.4361
11.8	0.00235	0.00015	0.0021	0.0026	15.9862
T (10%)	1.70329				

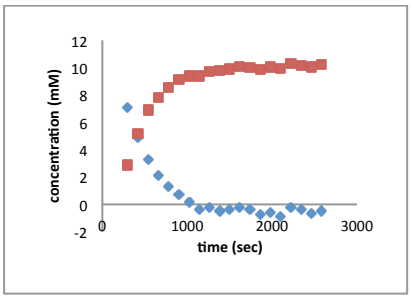
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.01807	0.00133	0.92871
2	0.0127	-0.00093	-0.65023
3	0.00822	0.00113	0.78664
4	0.00619	-0.00086	-0.60297
5	0.00402	-0.00067	-0.47025
6	0.00284	-0.0004	-0.27557
7	0.00166	-0.00006	-0.04071
8	0.00124	-0.00121	-0.84513
9	0.00077	-0.00149	-1.03998
10	0.00016	-0.00054	-0.37928
11	-0.00034	0.00285	1.98804
12	0.00056	-0.00137	-0.95737
13	-0.0002	0.00064	0.44302
14	0.00042	-0.00073	-0.51053
15	-0.00017	-0.00179	-1.2507
16	-0.00049	0.00083	0.58068
17	-0.00008	-0.00232	-1.61652
18	-0.00119	0.00394	2.74702
19	-0.00034	0.00012	0.08028
20	-0.00063	-0.00036	-0.25393
21	-0.00053	0.00001	0.00565
22	-0.00007	0.00106	0.73689
23	-0.00034	0.00006	0.0389
24	0.00004	-0.00254	-1.77257
25	-0.00088	0.00142	0.9924
26	-0.00042	-0.0005	-0.34895
27	-0.00078	0.00092	0.64406
28	-0.00054	0.00021	0.14356
29	-0.00064	0.00129	0.89884

2nd run:





Linear Regression

Regression Statistics

R	0.95635
R Square	0.91461
Adjusted R Square	0.91012
S	0.00159
Total number of observations	21

0.00953817430763 = 0.0014 + 0.0024 * 11.8

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00051	0.00051	203.51798	1.32591E-11
Residual	19.	0.00005	0.		
Total	20.	0.00056			

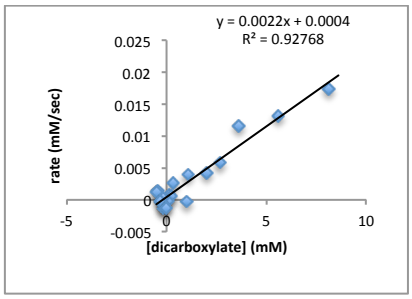
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	0.00136	0.00036	0.00074	0.00199	3.76511
11.8	0.00242	0.00017	0.00213	0.00271	14.26597
T (10%)	1.72913				

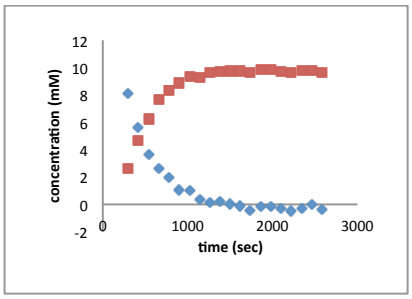
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.01857	0.00084	0.54036
2	0.01321	0.00123	0.79317
3	0.00938	-0.00177	-1.14557
4	0.00655	-0.00065	-0.42068
5	0.00447	0.0001	0.06428
6	0.00315	-0.0006	-0.38886
7	0.00172	-0.00199	-1.2875
8	0.00051	0.00228	1.46974
9	0.00081	0.00002	0.01585
10	0.00013	0.00071	0.4613
11	0.00048	0.00124	0.80063
12	0.00077	-0.00165	-1.06344
13	0.0004	-0.00167	-1.07885
14	-0.00042	0.00201	1.29909
15	-0.00002	-0.00083	-0.5335
16	-0.00074	0.00333	2.1484
17	0.0007	-0.00132	-0.85493
18	0.0005	-0.00178	-1.15176
19	-0.00031	0.00186	1.20034
20	0.00021	-0.00075	-0.48239
21	0.00015	-0.0006	-0.38567

3rd run:





Linear Regression

Regression Statistics

R	0.96316
R Square	0.92768
Adjusted R Square	0.92343
S	0.00148
Total number of observations	19

0.00862176160748 = 0.0004 + 0.0022 * 11.8

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00048	0.00048	218.07088	3.96728E-11
Residual	17.	0.00004	0.		
Total	18.	0.00051			

	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	0.00044	0.00038	-0.00023	0.00111	1.14285
11.8	0.00221	0.00015	0.00195	0.00247	14.76722
T (10%)	1.73961				

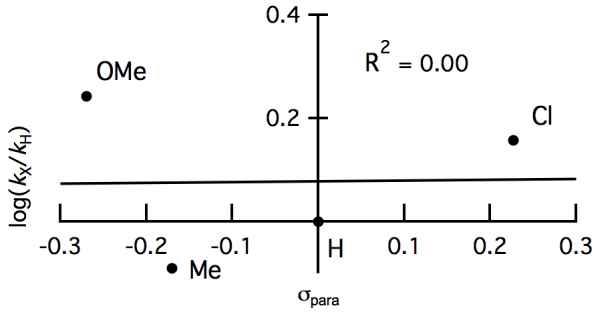
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.0184	-0.00097	-0.67782
2	0.01285	0.00031	0.21885
3	0.00843	0.00313	2.17882
4	0.00634	-0.00044	-0.30826
5	0.00489	-0.00061	-0.42653
6	0.00281	0.00116	0.80453
7	0.00263	-0.00291	-2.02758
8	0.00121	0.0014	0.97277
9	0.00074	0.00009	0.06391
10	0.00096	-0.00045	-0.31498
11	0.00051	-0.00067	-0.46775
12	0.00017	-0.00099	-0.69098
13	-0.00054	0.00196	1.3628
14	0.00004	0.00019	0.13515
15	0.00006	-0.00139	-0.96912
16	-0.00024	-0.0001	-0.07024
17	-0.00069	0.00194	1.34813
18	-0.00022	0.00003	0.02017
19	0.00039	-0.00165	-1.15186

Hammett Plots

Benzoate	σ-para	σ-meta	k (exp.)	log (kX/kH)
Cl	0.227	0.373	0.0023	0.158
H	0	0	0.0016	0
OMe	-0.27	0.115	0.0028	0.243
Me	-0.17	-0.069	0.0013	-0.0901



Linear Regression

Regression Statistics

R	0.68908
R Square	0.47483
Adjusted R Square	0.21224
S	0.13357
Total number of observations	4

log (kX/kH) = 0.0217 + 0.5338 * ?-meta

ANOVA

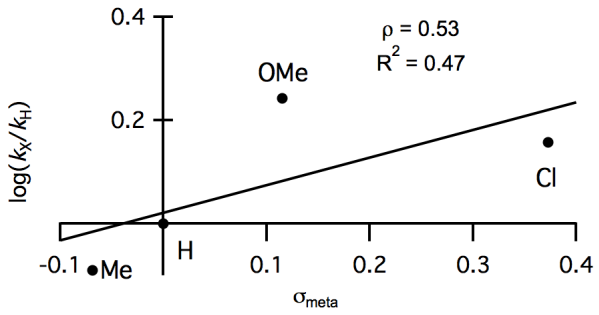
	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.03226	0.03226	1.80828	0.31092
Residual	2.	0.03568	0.01784		
Total	3.	0.06794			

	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	0.0217	0.07867	-0.20801	0.25142	0.27588
?-meta	0.53378	0.39695	-0.6253	1.69287	1.34472
T (10%)	2.91999				

LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.22081	-0.0632	-0.57948
2	0.0217	-0.0217	-0.19901
3	0.08309	0.15995	1.46664
4	-0.01513	-0.07505	-0.68815



Linear Regression

Regression Statistics

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ANOVA

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Regression	1.	0.03226	0.03226	1.80828	0.31092
Residual	2.	0.03568	0.01784		
Total	3.	0.06794			

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Intercept	0.0217	0.07867	-0.20801	0.25142	0.27588
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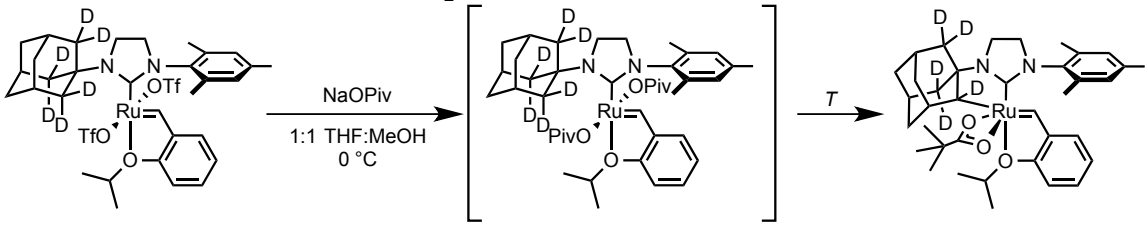
T (10%)	2.91999				

LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.22081	-0.0632	-0.57948
2	0.0217	-0.0217	-0.19901
3	0.08309	0.15995	1.46664
4	-0.01513	-0.07505	-0.68815

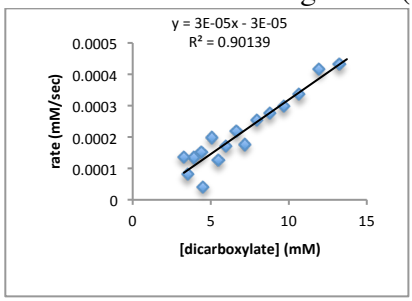
Cyclometalation of Deuterated Complex 7a-d_6

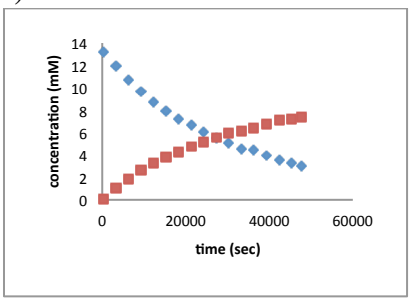


25 °C

run	k (sec^{-1})
1	$3.4(1)x10^{-5}$
2	$3.2(1)x10^{-5}$
3	$4.0(1)x10^{-5}$
average	$3.5(1)x10^{-5}$

1st run:





Linear Regression

Regression Statistics

R	0.96708
R Square	0.93524
Adjusted R Square	0.93062
S	0.00002
Total number of observations	16

0.00023539141253 = 0.0003 - 0.0000 * 0

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.	0.	202.19673	0.
Residual	14.	0.	0.		
Total	15.	0.			

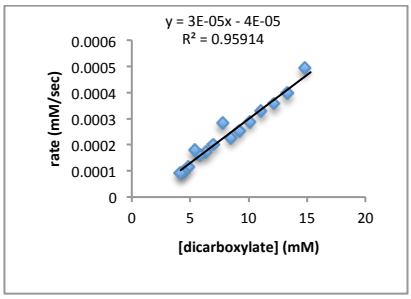
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	0.00031	0.00001	0.00029	0.00033	25.47977
0	-0.00003	0.	-0.00004	-0.00003	-14.21959
T (10%)	1.76131				

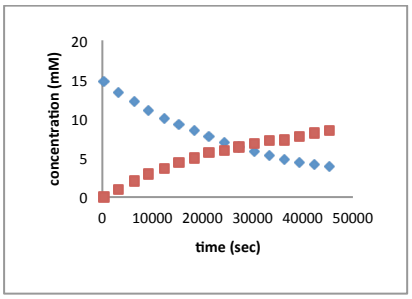
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.00031	0.00002	0.90409
2	0.00027	0.	-0.21394
3	0.00024	0.00001	0.65107
4	0.00022	-0.00001	-0.40677
5	0.0002	-0.00002	-1.21645
6	0.00018	0.	-0.16116
7	0.00016	-0.00001	-0.65971
8	0.00014	0.	-0.0603
9	0.00013	0.	0.23918
10	0.00012	0.00002	1.00067
11	0.0001	-0.00005	-2.43082
12	0.0001	0.	0.24139
13	0.00009	0.00001	0.56114
14	0.00008	0.00004	1.97055
15	0.00006	-0.00001	-0.59125
16	0.00006	0.	0.17233

2nd run:





Linear Regression

Regression Statistics

R	0.97936
R Square	0.95914
Adjusted R Square	0.956
S	0.00002
Total number of observations	15

-0.00135064484445 =- 0.0000 + 0.0000 * 14.4

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.	0.	305.18577	0.
Residual	13.	0.	0.		
Total	14.	0.			

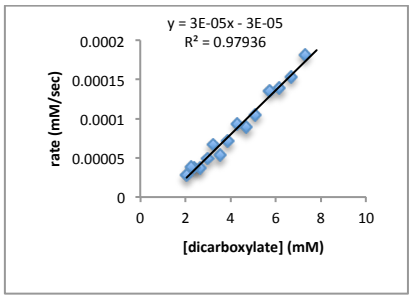
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	-0.00004	0.00002	-0.00007	-0.00001	-2.21616
14.4	0.00003	0.	0.00003	0.00004	17.46957
T (10%)	1.77093				

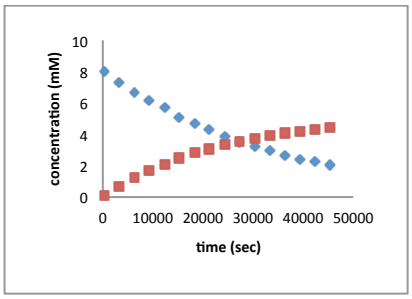
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.00046	0.00003	1.30148
2	0.00041	-0.00002	-0.64689
3	0.00037	-0.00001	-0.57125
4	0.00033	-0.00001	-0.3042
5	0.0003	-0.00001	-0.63754
6	0.00027	-0.00002	-0.84015
7	0.00025	-0.00002	-0.92853
8	0.00022	0.00006	2.41643
9	0.0002	0.00001	0.24409
10	0.00018	0.	-0.15521
11	0.00016	0.	0.13973
12	0.00014	0.00004	1.61325
13	0.00012	-0.00001	-0.39152
14	0.00011	-0.00002	-0.73763
15	0.0001	-0.00001	-0.50205

3rd run:





Linear Regression

Regression Statistics

R	0.99108
R Square	0.98225
Adjusted R Square	0.98088
S	0.00001
Total number of observations	15

0.00019583957553 = 0.0002 - 0.0000 * 0.08232110580365

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.	0.	719.2411	9.12825E-13
Residual	13.	0.	4.45975E-11		
Total	14.	0.			

	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	0.00021	0.	0.0002	0.00022	42.49205
0.08232110580365	-0.00004	0.	-0.00004	-0.00004	-26.81867
T (10%)	1.77093				

LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

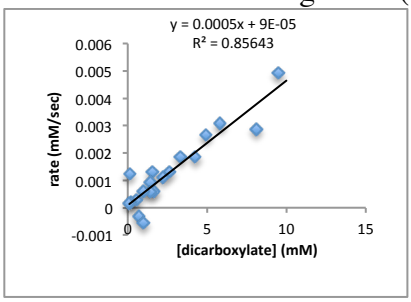
Residuals

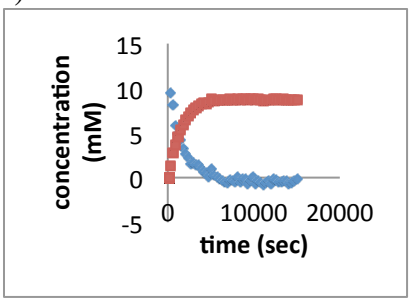
Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.00018	0.	0.02686
2	0.00016	-0.00001	-0.83522
3	0.00014	0.	-0.26884
4	0.00012	0.00001	1.89604
5	0.00011	0.	-0.41895
6	0.00009	-0.00001	-0.86704
7	0.00008	0.00001	1.45192
8	0.00007	0.	-0.22005
9	0.00006	-0.00001	-1.61337
10	0.00006	0.00001	1.52614
11	0.00005	0.	-0.01331
12	0.00004	-0.00001	-1.01294
13	0.00004	0.	-0.12537
14	0.00003	0.	0.71886
15	0.00003	0.	-0.24473

50 °C

run	k (sec^{-1})
1	$5.8(4)x10^{-4}$
2	$4.6(4)x10^{-4}$
average	$5.2(4)x10^{-4}$

1st run:





Linear Regression

Regression Statistics

R	0.95071
R Square	0.90385
Adjusted R Square	0.89948
S	0.00065
Total number of observations	24

0.00785104262657 =- 0.0001 + 0.0006 * 14.4

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00009	0.00009	206.81299	1.14342E-12
Residual	22.	0.00001	0.		
Total	23.	0.0001			

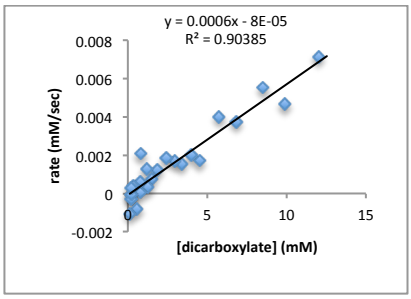
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	-0.00008	0.00018	-0.00039	0.00022	-0.47302
14.4	0.00058	0.00004	0.00051	0.00065	14.38099
T (10%)	1.71714				

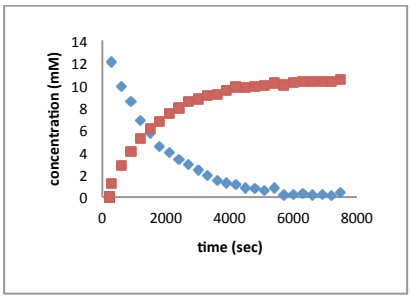
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.00688	0.00027	0.4224
2	0.00564	-0.00098	-1.54085
3	0.00483	0.00069	1.07884
4	0.00387	-0.00016	-0.24603
5	0.00323	0.00077	1.2029
6	0.00254	-0.0008	-1.26284
7	0.00224	-0.00021	-0.33646
8	0.00188	-0.00034	-0.53136
9	0.00162	0.00007	0.11325
10	0.00132	0.00055	0.85657
11	0.001	0.00023	0.35808
12	0.00079	-0.00003	-0.04276
13	0.00065	-0.00033	-0.51269
14	0.0006	0.0007	1.09768
15	0.00037	-0.00031	-0.48915
16	0.00036	0.00026	0.41307
17	0.00025	-0.00106	-1.6562
18	0.00039	0.00169	2.64769
19	0.00003	-0.00012	-0.18138
20	0.00005	-0.00033	-0.51725
21	0.0001	0.00028	0.44468
22	0.00003	-0.00007	-0.10831
23	0.00004	0.00026	0.4041
24	-0.00001	-0.00103	-1.61399

2nd run:





Linear Regression

Regression Statistics

R	0.96834
R Square	0.93768
Adjusted R Square	0.93145
S	0.00036
Total number of observations	12

0.01631089658008 = 0.0001 + 0.0005 * 14.4

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	0.00002	0.00002	150.46546	0.
Residual	10.	0.	0.		
Total	11.	0.00002			

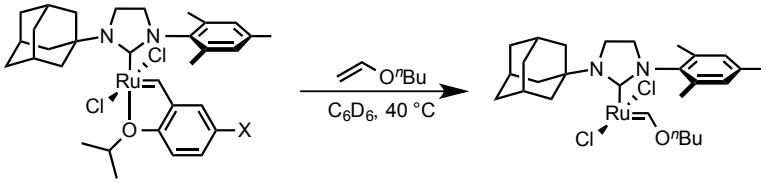
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	0.00012	0.00011	-0.00009	0.00033	1.04386
14.4	0.00046	0.00004	0.00039	0.00052	12.26644
T (10%)	1.81246				

LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.00445	-0.00006	-0.16259
2	0.00205	0.0002	0.58434
3	0.00082	-0.00036	-1.05117
4	0.00057	-0.00057	-1.64347
5	0.00057	0.00053	1.55025
6	-0.00003	0.00005	0.14151
7	-0.00004	-0.00012	-0.33998
8	0.00004	-0.00021	-0.60628
9	0.00013	0.00059	1.71864
10	-0.00026	-0.00029	-0.85405
11	0.00004	0.00015	0.42338
12	-0.00006	0.00008	0.23941

Initiation rate measurements of complexes 4a, and S1–S3



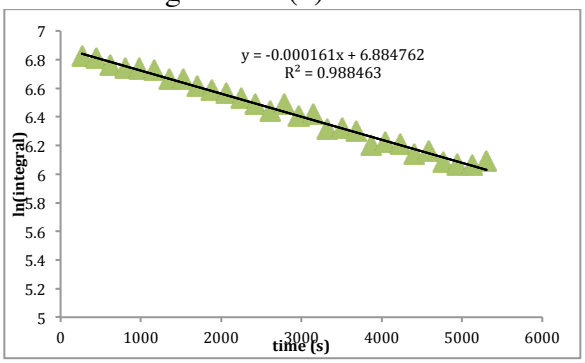
Typical procedure

A 0.25 mL 0.12 M C_6D_6 solution of dichloride **4a** (0.0031 mmol) was added to an NMR tube followed by an additional 0.45 mL of C_6D_6. To this green solution was added 12 μL (0.093 mmol) of *n*-butylvinylether, the reaction was mixed by inverting multiple times, then inserted into the NMR. ^{1}H NMR data was collected periodically over ~3 h.

X = Me (S2)

run	k (sec^{-1})
1	1.58(2)x10^{-4}
2	1.71(2)x10^{-4}
3	1.62(3)x10^{-4}
average	1.64(2)x10^{-4}

1st run:



Linear Regression

Regression Statistics

R	0.99352
R Square	0.98708
Adjusted R Square	0.98683
S	0.05264
Total number of observations	55

ln conc = 1.1624 - 0.0002 * Time (s)

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	11.21657	11.21657	4,047.90515	0.E+0
Residual	53.	0.14686	0.00277		
Total	54.	11.36343			

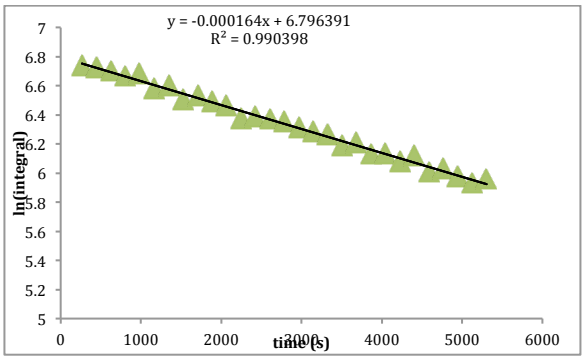
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	1.1624	0.01458	1.138	1.18681	79.74351
Time (s)	-0.000158	0.00000248	-0.00016	-0.00015	-63.62315

T (10%) 1.67412
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	1.12052	-0.00867	-0.16617
2	1.092	0.00424	0.08126
3	1.06355	-0.01483	-0.28442
4	1.0351	-0.00531	-0.10174
5	1.00665	0.01729	0.33162
6	0.97821	0.03208	0.61513
7	0.94976	-0.00192	-0.03672
8	0.92131	0.03	0.57531
9	0.89286	0.01084	0.2078
10	0.86442	0.00752	0.14416
11	0.83597	0.01908	0.36589
12	0.80752	0.00934	0.17907
13	0.77907	-0.00685	-0.13132
14	0.75062	-0.02232	-0.4279
15	0.72218	0.05533	1.06095
16	0.69373	-0.00087	-0.01669
17	0.66528	0.04234	0.81183
18	0.63683	-0.03874	-0.74288
19	0.60839	0.00134	0.02572
20	0.57994	0.00516	0.09889
21	0.55149	-0.06133	-1.17612
22	0.52304	-0.01159	-0.22218
23	0.4946	0.00082	0.01579
24	0.46615	-0.03446	-0.66069
25	0.4377	0.01181	0.22654
26	0.40925	-0.03842	-0.73672
27	0.38081	-0.02492	-0.47791
28	0.35236	-0.00155	-0.02972
29	0.32391	0.05594	1.07271
30	0.29546	-0.01311	-0.25137
31	0.26702	-0.00676	-0.12958
32	0.23857	-0.03379	-0.64803

2nd run:



Linear Regression

Regression Statistics

R	0.99631
R Square	0.99264
Adjusted R Square	0.99247
S	0.03511
Total number of observations	45

ln conc = 1.1842 - 0.0002 * Time (s)

ANOVA

	d.f.	*SS*	*MS*
Regression	1.	7.1475	7.1475
Residual	43.	0.05301	0.00123
Total	44.	7.20051	

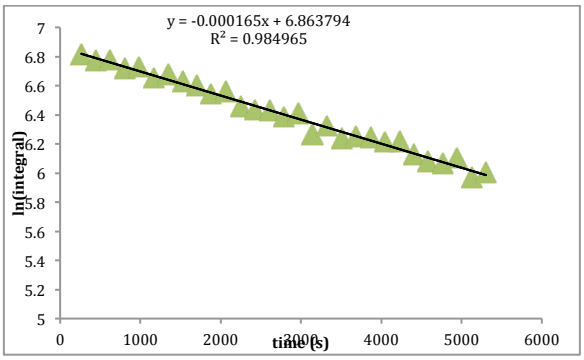
	Coefficients	*Standard Error*	*LCL*
Intercept	1.18418	0.01081	1.166
Time (s)	-0.0001705	0.00000224	-0.00017
T (10%)	1.68107		

LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	1.139	-0.02714	-0.78188
2	1.10823	-0.00895	-0.25782
3	1.07754	-0.00254	-0.07316
4	1.04685	-0.00582	-0.16777
5	1.01616	0.04198	1.2093
6	0.98548	-0.0279	-0.80385
7	0.95479	0.01813	0.5222
8	0.9241	-0.04394	-1.26591
9	0.89342	0.01041	0.29998
10	0.86273	0.00166	0.04784
11	0.83204	0.00475	0.13683
12	0.80136	-0.05115	-1.47368
13	0.77067	-0.00654	-0.18841
14	0.73998	0.00745	0.21471
15	0.7093	0.01924	0.55437
16	0.67861	0.00486	0.14006
17	0.64792	0.00905	0.2606
18	0.61724	0.02166	0.62398
19	0.58655	-0.01893	-0.54528
20	0.55586	0.02567	0.73955
21	0.52517	-0.02283	-0.65777
22	0.49449	0.0163	0.46947
23	0.4638	-0.01307	-0.37663
24	0.43311	0.06361	1.83247
25	0.40243	-0.02023	-0.58271
26	0.37174	0.03492	1.00608
27	0.34105	0.00718	0.20696
28	0.31037	-0.00276	-0.07961
29	0.27968	0.05243	1.51037
30	0.24899	0.02098	0.60452
31	0.21831	0.01573	0.45316
32	0.18762	-0.02152	-0.61995

3rd run:



Linear Regression

Regression Statistics

R	0.99053
R Square	0.98115
Adjusted R Square	0.98071
S	0.05356
Total number of observations	45

ln conc = 1.1507 - 0.0002 * Time (s)

ANOVA

	d.f.	*SS*	*MS*	*F*
Regression	1.	6.42058	6.42058	2,238.40593
Residual	43.	0.12334	0.00287	
Total	44.	6.54392		

	Coefficients	*Standard Error*	*LCL*	*UCL*
Intercept	1.15075	0.01649	1.12302	1.17847
Time (s)	-0.000162	0.00000342	-0.00017	-0.00016
T (10%)	1.68107			

LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

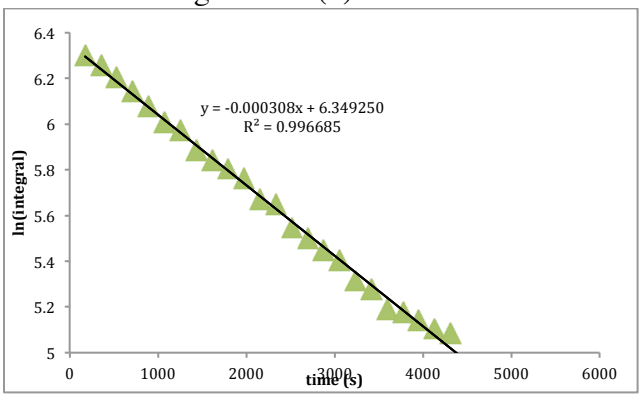
Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	1.10793	0.00393	0.0742
2	1.07876	-0.01196	-0.22594
3	1.04968	0.02307	0.43568
4	1.02059	-0.00561	-0.10598
5	0.99151	0.03203	0.60505
6	0.96243	-0.01049	-0.19815
7	0.93334	0.03828	0.72295
8	0.90426	0.01796	0.33926
9	0.87517	0.02275	0.42974
10	0.84609	-0.00727	-0.13727
11	0.817	0.04108	0.77598
12	0.78792	-0.03456	-0.65266
13	0.75883	-0.02915	-0.55059
14	0.72975	-0.00621	-0.11731
15	0.70066	-0.01957	-0.36968
16	0.67158	0.03526	0.66599
17	0.64249	-0.0812	-1.53361
18	0.61341	0.00634	0.11981
19	0.58433	-0.05439	-1.02721
20	0.55524	-0.01188	-0.22432
21	0.52616	0.01273	0.24041
22	0.49707	0.01289	0.24347
23	0.46799	0.04654	0.87895
24	0.4389	-0.01738	-0.3282
25	0.40982	-0.0306	-0.57791
26	0.38073	-0.01944	-0.36712
27	0.35165	0.04743	0.89587
28	0.32256	-0.05268	-0.99503
29	0.29348	0.00696	0.13153
30	0.2644	-0.06844	-1.29268
31	0.23531	0.01218	0.23002
32	0.20623	0.02231	0.42143

X = OMe (S1)

run	k (sec^{-1})
1	$2.86(3)x10^{-4}$
2	$2.98(3)x10^{-4}$
3	$2.49(6)x10^{-4}$
average	$2.78(4)x10^{-4}$

1st run:



Linear Regression

Regression Statistics

R	0.99631
R Square	0.99263
Adjusted R Square	0.99249
S	0.07434
Total number of observations	57

ln conc = 1.0176 - 0.0003 * Time (s)

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	40.91962	40.91962	7,404.41718	0.E+0
Residual	55.	0.30395	0.00553		
Total	56.	41.22357			

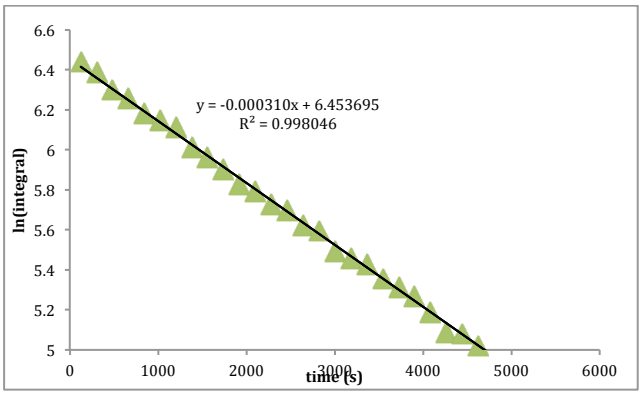
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	1.01765	0.01979	0.98453	1.05077	51.41032
Time (s)	-0.000286	0.00000332	-0.00029	-0.00028	-86.04892
T (10%)	1.67303				

LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.98217	0.05811	0.78869
2	0.93053	0.06503	0.88266
3	0.87903	0.06438	0.87381
4	0.82753	0.05474	0.74298
5	0.77603	0.03985	0.54084
6	0.72453	0.02345	0.31835
7	0.67303	0.03857	0.5236
8	0.62153	0.00121	0.01649
9	0.57003	0.00951	0.12911
10	0.51853	0.02454	0.33315
11	0.46703	0.0329	0.44657
12	0.41553	-0.00595	-0.08077
13	0.36403	0.02401	0.32588
14	0.31253	-0.02803	-0.38053
15	0.26103	-0.02274	-0.30869
16	0.20953	-0.0231	-0.31354
17	0.15803	-0.01501	-0.20369
18	0.10653	-0.05271	-0.71548
19	0.05503	-0.03824	-0.51903
20	0.00352	-0.07326	-0.99442
21	-0.04798	-0.03691	-0.50103
22	-0.09948	-0.02242	-0.30433
23	-0.15098	-0.00553	-0.07508
24	-0.20248	0.0265	0.35974
25	-0.25398	-0.02488	-0.33775
26	-0.30548	-0.03368	-0.45722
27	-0.35698	-0.08823	-1.19763
28	-0.40848	-0.09604	-1.30366
29	-0.45998	-0.00149	-0.02024
30	-0.51148	0.04023	0.54611
31	-0.56298	-0.04945	-0.6712
32	-0.61448	-0.04778	-0.64859

2nd run:



Linear Regression

Regression Statistics

R	0.99783
R Square	0.99567
Adjusted R Square	0.99557
S	0.046
Total number of observations	44

ln conc = 1.0286 - 0.0003 * Time (s)

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	20.42662	20.42662	9,655.30861	0.E+0
Residual	42.	0.08885	0.00212		
Total	43.	20.51547			

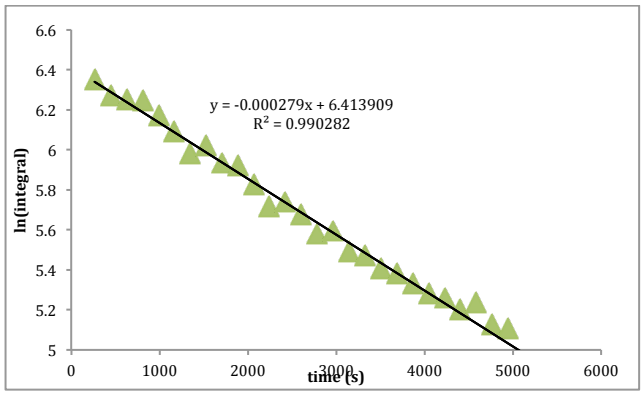
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	1.02859	0.01396	1.0051	1.05207	73.67317
Time (s)	-0.000298	0.000003	-0.0003	-0.00029	-98.26143

T (10%) 1.68195
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.99162	0.04865	1.07032
2	0.93782	0.04886	1.07491
3	0.88416	0.0172	0.37827
4	0.83051	0.02834	0.62333
5	0.77685	0.0073	0.1607
6	0.72319	0.02479	0.54538
7	0.66954	0.0411	0.90407
8	0.61588	-0.00262	-0.05767
9	0.56223	0.00236	0.05201
10	0.50857	-0.0063	-0.13869
11	0.45491	-0.02695	-0.59284
12	0.40126	-0.00773	-0.17002
13	0.3476	-0.02145	-0.47182
14	0.29395	0.00516	0.11353
15	0.24029	-0.01614	-0.35511
16	0.18663	0.00906	0.19929
17	0.13298	-0.03755	-0.82599
18	0.07932	-0.0192	-0.42235
19	0.02567	0.00036	0.00801
20	-0.02799	-0.01674	-0.36821
21	-0.08165	-0.00499	-0.10988
22	-0.1353	0.00599	0.13179
23	-0.18896	-0.02135	-0.46971
24	-0.24261	-0.06903	-1.51856
25	-0.29627	-0.02374	-0.52221
26	-0.34993	-0.03001	-0.66017
27	-0.40358	-0.04599	-1.01179
28	-0.45724	0.01959	0.43085
29	-0.51089	-0.00447	-0.09824
30	-0.56455	-0.03402	-0.74844
31	-0.61821	0.0078	0.17158
32	-0.67186	-0.04909	-1.07981

3rd run:



Linear Regression

Regression Statistics

R	0.98969
R Square	0.97948
Adjusted R Square	0.97895
S	0.07874
Total number of observations	41

ln conc = 1.0351 - 0.0002 * Time (s)

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	11.54258	11.54258	1,861.62326	0.E+0
Residual	39.	0.24181	0.0062		
Total	40.	11.78439			

	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	1.03508	0.02548	0.99215	1.07802	40.61892
Time (s)	-0.000249	0.000006	-0.00026	-0.00024	-43.14653
T (10%)	1.68488				

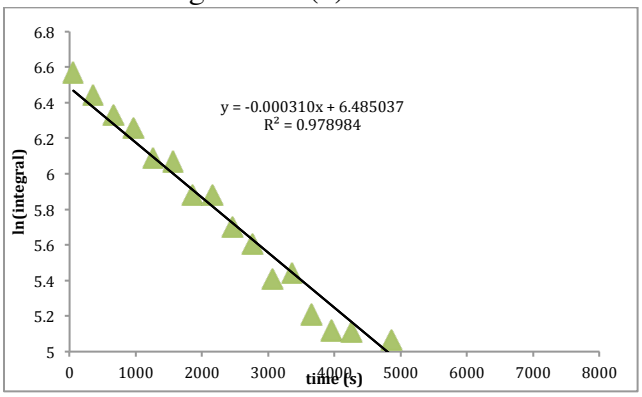
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.96906	0.07121	0.91592
2	0.9241	0.03615	0.46491
3	0.87925	0.06061	0.77953
4	0.83441	0.10294	1.32402
5	0.78957	0.07018	0.90262
6	0.74472	0.03566	0.4586
7	0.69988	-0.02774	-0.35672
8	0.65504	0.05467	0.70313
9	0.6102	0.01353	0.17406
10	0.56535	0.04585	0.58976
11	0.52051	-0.00683	-0.08784
12	0.47567	-0.06978	-0.89753
13	0.43083	-0.0027	-0.03478
14	0.38598	-0.01896	-0.24382
15	0.34114	-0.07228	-0.92961
16	0.2963	-0.01251	-0.16091
17	0.25146	-0.06795	-0.87391
18	0.20661	-0.04327	-0.55651
19	0.16177	-0.06474	-0.83268
20	0.11693	-0.04783	-0.61522
21	0.07209	-0.0502	-0.64562
22	0.02724	-0.05573	-0.71676
23	-0.0176	-0.03349	-0.43071
24	-0.06244	-0.04693	-0.60353
25	-0.10729	0.03191	0.41038
26	-0.15213	-0.02939	-0.37797
27	-0.19697	-0.00435	-0.05596
28	-0.24181	-0.16557	-2.12948
29	-0.28666	-0.14863	-1.91165
30	-0.3315	0.06954	0.89435
31	-0.37634	-0.113	-1.45341
32	-0.42118	0.07007	0.90124

X = H (4a)	
run	k (sec^{-1})
1	$3.1(1)x10^{-4}$
2	$2.9(1)x10^{-4}$
3	$3.06(9)x10^{-4}$
average	$3.0(1)x10^{-4}$

1st run:



Linear Regression

Regression Statistics

R	0.98944
R Square	0.97899
Adjusted R Square	0.97807
S	0.10231
Total number of observations	25

ln conc = 1.0496 - 0.0003 * Time (s)

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	11.21667	11.21667	1,071.56389	0.E+0
Residual	23.	0.24075	0.01047		
Total	24.	11.45743			

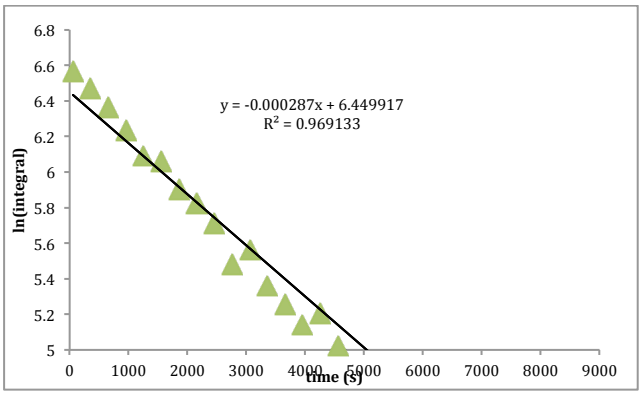
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	1.04956	0.0402	0.98067	1.11845	26.11042
Time (s)	-0.0003096	0.0000095	-0.00033	-0.00029	-32.73475
T (10%)	1.71387				

LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	1.03176	0.10287	1.02704
2	0.93872	0.06908	0.68968
3	0.84583	0.05065	0.50568
4	0.75294	0.06681	0.66702
5	0.66006	-0.00517	-0.05161
6	0.56717	0.06479	0.64685
7	0.47428	-0.03052	-0.30476
8	0.3814	0.06011	0.60015
9	0.28851	-0.0233	-0.23263
10	0.19562	-0.02756	-0.27517
11	0.10274	-0.1267	-1.26504
12	0.00985	-0.00484	-0.0483
13	-0.08304	-0.14527	-1.45045
14	-0.17592	-0.14045	-1.40231
15	-0.26881	-0.05389	-0.53804
16	-0.3617	-0.09091	-0.90771
17	-0.45458	0.08484	0.84705
18	-0.54747	-0.11692	-1.16735
19	-0.64036	-0.15567	-1.55425
20	-0.73325	-0.00995	-0.09937
21	-0.82613	0.03095	0.30906
22	-0.91902	-0.07757	-0.77447
23	-1.01191	0.08305	0.82919
24	-1.10479	0.15968	1.59433
25	-1.19768	0.23591	2.35542

2nd run:



Linear Regression

Regression Statistics

R	0.98445
R Square	0.96914
Adjusted R Square	0.96795
S	0.12896
Total number of observations	28

ln conc = 1.0200 - 0.0003 * Time (s)

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	13.578	13.578	816.38741	0.E+0
Residual	26.	0.43243	0.01663		
Total	27.	14.01043			

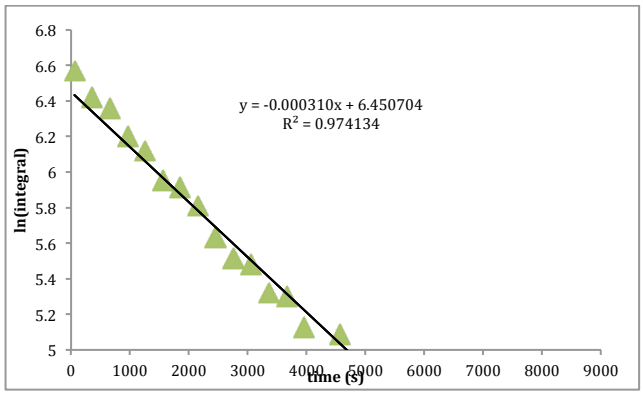
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	1.02001	0.04797	0.9382	1.10183	21.26467
Time (s)	-0.000287	0.0000101	-0.0003	-0.00027	-28.57249

T (10%) 1.70562
LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	1.00349	0.13113	1.03618
2	0.91714	0.12519	0.98923
3	0.83093	0.10234	0.80868
4	0.74472	0.06066	0.47931
5	0.65852	0.00224	0.01772
6	0.57231	0.05384	0.42539
7	0.4861	-0.0118	-0.09327
8	0.3999	-0.00592	-0.04679
9	0.31369	-0.03013	-0.23806
10	0.22748	-0.17406	-1.37535
11	0.14127	-0.01075	-0.08491
12	0.05507	-0.12579	-0.99395
13	-0.03114	-0.14453	-1.14208
14	-0.11735	-0.17113	-1.35223
15	-0.20355	-0.0228	-0.18015
16	-0.28976	-0.11802	-0.93257
17	-0.37597	-0.07448	-0.58855
18	-0.46218	0.00508	0.04014
19	-0.54838	0.02306	0.18219
20	-0.63459	-0.05052	-0.39917
21	-0.7208	0.02661	0.21031
22	-0.807	0.19073	1.50708
23	-0.89321	-0.12572	-0.9934
24	-0.97942	-0.09796	-0.77407
25	-1.06563	0.41054	3.24402
26	-1.15183	-0.10865	-0.85854
27	-1.23804	0.13806	1.09092
28	-1.32425	0.00278	0.02195

3rd run:



Linear Regression

Regression Statistics

R	0.98743
R Square	0.97503
Adjusted R Square	0.97416
S	0.13574
Total number of observations	31

ln conc = 1.0055 - 0.0003 * Time (s)

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	20.86028	20.86028	1,132.2149	0.E+0
Residual	29.	0.5343	0.01842		
Total	30.	21.39458			

	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	1.00551	0.04805	0.92386	1.08716	20.92456
Time (s)	-0.000306	0.000009	-0.00032	-0.00029	-33.6484
T (10%)	1.69913				

LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

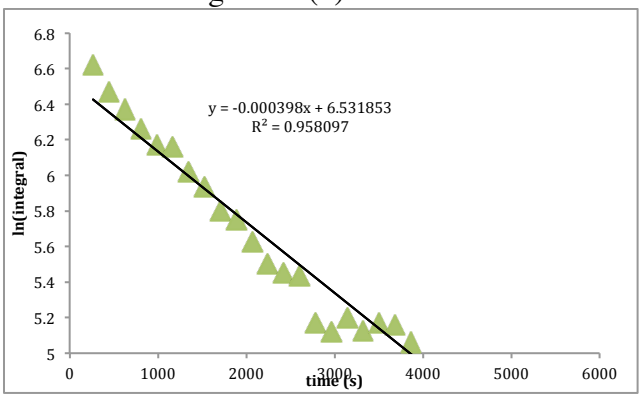
Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.98794	0.14669	1.09915
2	0.89607	0.09158	0.68625
3	0.80436	0.11907	0.89218
4	0.71264	0.05061	0.37922
5	0.62093	0.06618	0.49589
6	0.52922	-0.00981	-0.07351
7	0.43751	0.04331	0.32452
8	0.34579	0.03045	0.22815
9	0.25408	-0.05585	-0.41852
10	0.16237	-0.08277	-0.62024
11	0.07066	-0.02437	-0.1826
12	-0.02106	-0.09179	-0.68778
13	-0.11277	-0.0172	-0.12889
14	-0.20448	-0.105	-0.78681
15	-0.2962	-0.17451	-1.30767
16	-0.38791	0.04149	0.31085
17	-0.47962	-0.21333	-1.59851
18	-0.57133	-0.16742	-1.25448
19	-0.66305	-0.01444	-0.10823
20	-0.75476	-0.12805	-0.95953
21	-0.84647	-0.06604	-0.49482
22	-0.93818	-0.02578	-0.19319
23	-1.0299	-0.04517	-0.33846
24	-1.12161	0.02796	0.20948
25	-1.21332	0.21156	1.58525
26	-1.30504	0.21813	1.63445
27	-1.39675	-0.01732	-0.12982
28	-1.48846	-0.27638	-2.07096
29	-1.58017	0.29429	2.20513
30	-1.67189	0.24374	1.82639
31	-1.7636	-0.06978	-0.52291

X = Cl (S3)

run	k (sec^{-1})
1	$3.3(2)x10^{-4}$
2	$3.3(2)x10^{-4}$
average	$3.3(2)x10^{-4}$

1st run:



Linear Regression

Regression Statistics

R	0.96102
R Square	0.92357
Adjusted R Square	0.9215
S	0.19691
Total number of observations	39

ln conc = 0.8723 - 0.0003 * Time (s)

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	17.3346	17.3346	447.07251	0.E+0
Residual	37.	1.43462	0.03877		
Total	38.	18.76923			

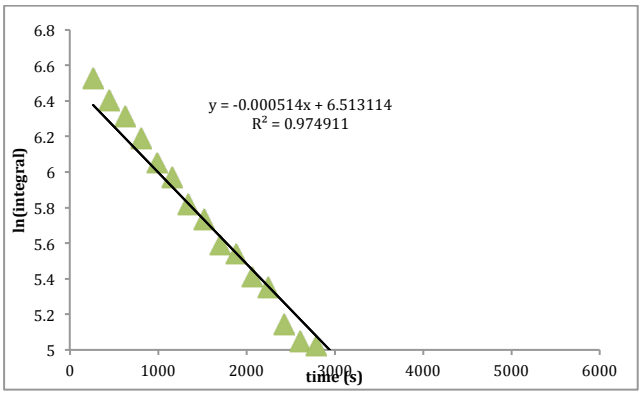
	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	0.87231	0.06546	0.76188	0.98274	13.32652
Time (s)	-0.000329	0.00002	-0.00036	-0.0003	-21.14409
T (10%)	1.68709				

LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.7851	0.32676	1.6817
2	0.7257	0.23753	1.22249
3	0.66646	0.19546	1.00598
4	0.60723	0.14163	0.72894
5	0.54799	0.11222	0.57754
6	0.48875	0.1645	0.84664
7	0.42952	0.07974	0.41039
8	0.37028	0.05552	0.28572
9	0.31104	-0.02069	-0.10649
10	0.25181	-0.01408	-0.07245
11	0.19257	-0.07594	-0.39085
12	0.13333	-0.13836	-0.71207
13	0.0741	-0.12996	-0.66885
14	0.01486	-0.08931	-0.45963
15	-0.04438	-0.29447	-1.51551
16	-0.10361	-0.28756	-1.47999
17	-0.16285	-0.14975	-0.77072
18	-0.22208	-0.1604	-0.82555
19	-0.28132	-0.06048	-0.31126
20	-0.34056	-0.00951	-0.04892
21	-0.39979	-0.04993	-0.25699
22	-0.45903	-0.25826	-1.32919
23	-0.51827	-0.0991	-0.51005
24	-0.5775	-0.24462	-1.25899
25	-0.63674	-0.05132	-0.26413
26	-0.69598	-0.349	-1.79617
27	-0.75521	-0.02296	-0.11814
28	-0.81445	0.05705	0.29363
29	-0.87369	-0.0541	-0.27844
30	-0.93292	0.12682	0.65271
31	-0.99216	0.11295	0.5813
32	-1.05139	-0.00814	-0.04188

2nd run:



Linear Regression

Regression Statistics

R	0.96102
R Square	0.92357
Adjusted R Square	0.9215
S	0.19691
Total number of observations	39

ln conc = 0.8723 - 0.0003 * Time (s)

ANOVA

	d.f.	*SS*	*MS*	*F*	*p-level*
Regression	1.	17.3346	17.3346	447.07251	0.E+0
Residual	37.	1.43462	0.03877		
Total	38.	18.76923			

	Coefficients	*Standard Error*	*LCL*	*UCL*	*t Stat*
Intercept	0.87231	0.06546	0.76188	0.98274	13.32652
Time (s)	-0.0003291	0.000016	-0.00036	-0.0003	-21.14409
T (10%)	1.68709				

LCL - Lower value of a reliable interval (LCL)
UCL - Upper value of a reliable interval (UCL)

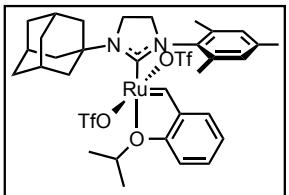
Residuals

Observation	*Predicted Y*	*Residual*	*Standard Residuals*
1	0.7851	0.32676	1.6817
2	0.7257	0.23753	1.22249
3	0.66646	0.19546	1.00598
4	0.60723	0.14163	0.72894
5	0.54799	0.11222	0.57754
6	0.48875	0.1645	0.84664
7	0.42952	0.07974	0.41039
8	0.37028	0.05552	0.28572
9	0.31104	-0.02069	-0.10649
10	0.25181	-0.01408	-0.07245
11	0.19257	-0.07594	-0.39085
12	0.13333	-0.13836	-0.71207
13	0.0741	-0.12996	-0.66885
14	0.01486	-0.08931	-0.45963
15	-0.04438	-0.29447	-1.51551
16	-0.10361	-0.28756	-1.47999
17	-0.16285	-0.14975	-0.77072
18	-0.22208	-0.1604	-0.82555
19	-0.28132	-0.06048	-0.31126
20	-0.34056	-0.00951	-0.04892
21	-0.39979	-0.04993	-0.25699
22	-0.45903	-0.25826	-1.32919
23	-0.51827	-0.0991	-0.51005
24	-0.5775	-0.24462	-1.25899
25	-0.63674	-0.05132	-0.26413
26	-0.69598	-0.349	-1.79617
27	-0.75521	-0.02296	-0.11814
28	-0.81445	0.05705	0.29363
29	-0.87369	-0.0541	-0.27844
30	-0.93292	0.12682	0.65271
31	-0.99216	0.11295	0.5813
32	-1.05139	-0.00814	-0.04188

Synthesis and Characterization of New Compounds.

General Procedure for Preparation of ruthenium bistriflates.

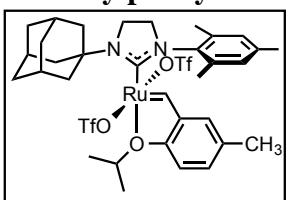
(1-(1-adamantyl)-3-(2,4,6-trimethylphenyl)-2-imidazolidinylidene)bistriflato(*o*-isopropoxyphenylmethylidene)ruthenium (7a)



7a: $C_{34}H_{42}F_6N_2O_7RuS_2$
Exact Mass: 870.1381

In a nitrogen filled glovebox, ruthenium dichloride (**4a**, 50 mg, 0.0778 mmol) and silver trifluoromethanesulfonate (80 mg, 0.311 mmol) were added to a 20 mL vial equipped with a stirbar. The reagents were suspended in benzene (2.6 mL) and stirred at ambient temperature for 24 h. Upon completion (^{1}H NMR), the reaction mixture was filtered through Celite with benzene (2 mL), concentrated, filtered through silica gel with dichloromethane (4 mL), and concentrated again to provide 45 mg (67%) of bistriflato complex **7a** as a green solid. ^{1}H NMR (500 MHz, C_6D_6) δ 18.89 (s, 1H), 7.15–7.08 (m, 2H), 6.86 (s, 2H), 6.70 (td, *J* = 7.5, 0.8 Hz, 1H), 6.54 (d, *J* = 8.4 Hz, 1H), 4.70 (hept, *J* = 6.1 Hz, 1H), 3.23–3.12 (m, 4H), 3.01 (s, 6H), 2.38 (s, 3H), 2.21 (s, 6H), 2.21 (s, 3H), 1.96 (d, *J* = 11.8 Hz, 3H), 1.76 (d, *J* = 12.9 Hz, 3H), 1.40 (d, *J* = 6.1 Hz, 6H); ^{13}C NMR (126 MHz, C_6D_6) δ 202.0, 138.7, 138.4, 137.6, 133.5, 129.8, 127.9, 127.8, 127.8, 127.6, 127.6, 127.5, 122.8, 122.5, 119.2, 116.7, 114.3, 75.7, 57.3, 51.2, 44.0, 41.2, 35.8, 29.8, 21.2, 20.6, 17.7; HRMS (EI) m/z calculated for $C_{34}H_{42}RuS_2N_2F_6O_7$ (M^+) 870.1381, found 870.1350.

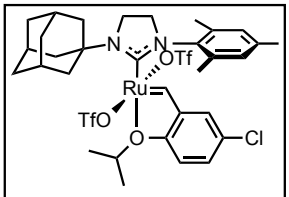
(1-(1-adamantyl)-3-(2,4,6-trimethylphenyl)-2-imidazolidinylidene)bistriflato(*o*-isopropoxy-*m*-methylphenylmethylidene)ruthenium (S4)



S4: $C_{35}H_{44}F_6N_2O_7RuS_2$
Exact Mass: 884.1538

Following the general procedure, 36 mg (54%) of bistriflato complex **S4** was synthesized from dichloride complex **S2** (50 mg, 0.0761 mmol) and silver trifluoromethanesulfonate (78 mg, 0.304 mmol) in benzene (2.5 mL); ^{1}H NMR (400 MHz, C_6D_6) δ 18.81 (s, 1H), 6.99 (dd, *J* = 8.6, 2.4 Hz, 1H), 6.88 (s, 2H), 6.87 (s, 1H), 6.51 (d, *J* = 8.5 Hz, 1H), 4.70 (hept, *J* = 6.2 Hz, 1H), 3.30–3.13 (m, 4H), 3.02 (s, 6H), 2.39 (s, 3H), 2.26 (s, 3H), 2.22 (s, 6H), 2.06 (s, 3H), 1.97 (d, *J* = 12.5 Hz, 3H), 1.76 (d, *J* = 12.6 Hz, 3H), 1.43 (d, *J* = 6.1 Hz, 6H); ^{13}C NMR (101 MHz, C_6D_6) δ 202.8, 153.1, 147.1, 139.2, 138.7, 138.1, 134.5, 132.3, 130.3, 123.6, 120.0, 116.8, 114.5, 76.0, 57.8, 51.6, 44.4, 41.6, 36.2, 30.2, 21.6, 21.1, 20.0, 18.1; HRMS (EI) m/z calculated for $C_{34}H_{44}RuSN_2F_3O_4$ ($[M–Otf^–]^+$) 735.2018, found 735.1983.

(1-(1-adamantyl)-3-(2,4,6-trimethylphenyl)-2-imidazolidinylidene)bistriflato(*o*-isopropoxy-*m*-chlorophenylmethylidene)ruthenium (S5)

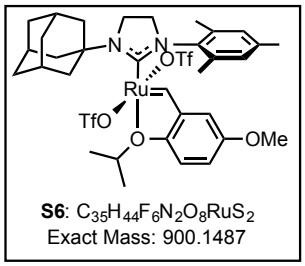


S5: $C_{34}H_{41}ClF_6N_2O_7RuS_2$
Exact Mass: 904.0991

Following the general procedure, 36 mg (54%) of bistriflato complex **S5** was synthesized from dichloride complex **S3** (50 mg, 0.0739 mmol) and silver trifluoromethanesulfonate (76 mg, 0.295 mmol) in benzene (2.5 mL); ^{1}H NMR (400 MHz, C_6D_6) δ 18.67 (s, 1H), 7.14 (d, *J* = 9.2 Hz, 2H), 6.76 (s, 2H), 6.31 (d, *J* = 8.7 Hz, 1H), 4.57 (hept, *J* = 5.9 Hz, 1H), 3.24–3.07 (m, 4H), 2.98 (s, 4H), 2.37 (s, 3H), 2.22 (s, 3H), 2.14 (s, 6H), 1.94 (d, *J* = 12.6 Hz, 3H), 1.75 (d, *J* = 12.6 Hz, 3H), 1.34 (d, *J* = 6.1 Hz, 6H); ^{13}C NMR (101 MHz, C_6D_6) δ 200.6, 152.9, 147.4, 139.1, 138.7,

137.9, 132.6, 130.4, 128.6, 122.3, 119.9, 116.8, 116.0, 76.8, 57.8, 51.4, 44.4, 41.6, 36.2, 30.2, 21.5, 20.9, 17.9. HRMS (EI) m/z calculated for $C_{33}H_{41}RuClSN_2F_3O_4$ ([M–Otf$^-$]$^+$) 755.1472, found 755.1455.

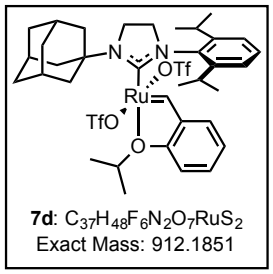
(1-(1-adamantyl)-3-(2,4,6-trimethylphenyl)-2-imidazolidinylidene)bistriflato(*o*-isopropoxy-*m*-methoxyphenylmethylidene)ruthenium (S6)



S6: $C_{35}H_{44}F_6N_2O_8RuS_2$
Exact Mass: 900.1487

Following the general procedure, 27 mg (40%) of bistriflato complex **S6** was synthesized from dichloride complex **S1** (50 mg, 0.0743 mmol) and silver trifluoromethanesulfonate (76 mg, 0.297 mmol) in benzene (2.5 mL); ^{1}H NMR (500 MHz, C_6D_6) δ 18.72 (d, *J* = 0.8 Hz, 1H), 6.90 (dd, *J* = 9.0, 3.1 Hz, 1H), 6.84 (s, 2H), 6.59 (d, *J* = 3.1 Hz, 1H), 6.52–6.48 (m, 1H), 4.67 (hept, *J* = 6.3 Hz, 1H), 3.30 (s, 3H), 3.25–3.13 (m, 4H), 3.02 (s, 6H), 2.40 (s, 3H), 2.21 (s, 6H), 2.17 (s, 3H), 1.98 (d, *J* = 12.3 Hz, 3H), 1.76 (d, *J* = 12.5 Hz, 3H), 1.40 (d, *J* = 6.1 Hz, 6H); ^{13}C NMR (126 MHz, C_6D_6) δ 202.4, 155.4, 142.8, 139.0, 138.7, 138.1, 130.2, 119.4, 115.3, 106.9, 76.0, 57.8, 55.2, 51.4, 44.4, 41.5, 36.2, 30.2, 21.6, 21.0, 18.1; HRMS (EI) m/z calculated for $C_{35}H_{44}RuSN_2F_3O_5$ ([M–Otf$^-$]$^+$) 751.1967, found 751.2002.

(1-(1-adamantyl)-3-(2,6-diisopropylphenyl)-2-imidazolidinylidene)bistriflato(*o*-isopropoxyphenylmethylidene)ruthenium (7d)



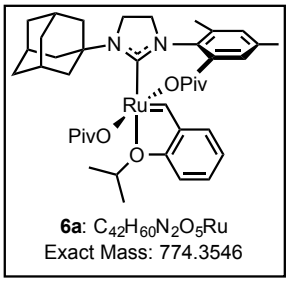
7d: $C_{37}H_{48}F_6N_2O_7RuS_2$
Exact Mass: 912.1851

Following the general procedure, 51 mg (77%) of bistriflato complex **7d** was synthesized from dichloride complex **4d** (50 mg, 0.0729 mmol) and silver trifluoromethanesulfonate (75 mg, 0.292 mmol) in benzene (2.5 mL); ^{1}H NMR (500 MHz, C_6D_6) δ 19.27 (d, *J* = 0.8 Hz, 1H), 7.36 (dd, *J* = 8.4, 7.0 Hz, 1H), 7.28 (d, *J* = 7.4 Hz, 2H), 7.08 (ddd, *J* = 8.7, 7.3, 1.7 Hz, 1H), 7.02 (dd, *J* = 7.5, 1.7 Hz, 1H), 6.60 (t, *J* = 7.4 Hz, 1H), 6.51 (d, *J* = 8.5 Hz, 1H), 4.68 (hept, *J* = 6.4 Hz, 1H), 3.50 (dd, *J* = 10.9, 8.7 Hz, 2H), 3.20 (dd, *J* = 10.9, 8.7 Hz, 2H), 3.16–3.06 (m, 8H), 2.44 (s, 3H), 2.06 (d, *J* = 11.7 Hz, 3H), 1.77 (d, *J* = 12.7 Hz, 3H), 1.45 (d, *J* = 6.1 Hz, 6H), 1.24 (d, *J* = 6.6 Hz, 6H), 1.09 (d, *J* = 6.8 Hz, 6H); ^{13}C NMR (126 MHz, c_6d6) ? 202.6, 155.1, 148.4, 142.9, 139.7, 134.0, 129.9, 125.7, 123.1, 123.0, 115.3, 77.0, 67.8, 58.3, 55.0, 44.0, 41.4, 36.1, 30.3, 28.1, 26.2, 23.9, 21.3; HRMS (FAB) m/z calculated for $C_{33}H_{41}RuClSN_2F_3O_4$ ([M+H$^+$]$^+$) 913.1929, found 913.1910.

Characterization data for dipivalate complexes

The ready conversion of ruthenium dicarboxylates to cyclometalated complexes precludes their isolation and full characterization. For this reason, only the ^{1}H NMR spectrum for these compounds is reported, and was obtained as a solution in THF-d_8/CD_3OD, in the presence of excess sodium carboxylate and trimethoxybenzene. For most pivalates HRMS data could also be obtained to further support the structural assignment.

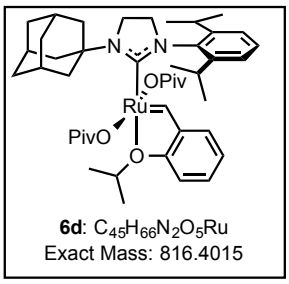
(1-(1-adamantyl)-3-(2,4,6-trimethylphenyl)-2-imidazolidinylidene)bispivalato(*o*-isopropoxyphenylmethylidene)ruthenium (6a)



6a: $C_{42}H_{60}N_2O_5Ru$
Exact Mass: 774.3546

Bispivalato complex **6a** was observed while conducting kinetics experiments described above; ^{1}H NMR (500 MHz, 1:1 THF-d_8:CD_3OD, 0 °C) δ 17.38 (s, 1H), 7.70 (dq, *J* = 9.6, 5.1 Hz, 1H), 7.39 (s, 2H), 7.29 (d, *J* = 8.3 Hz, 1H), 7.21 (d, *J* = 4.4 Hz, 2H), 5.26 (d, *J* = 9.8 Hz, 1H), 4.30 (dd, *J* = 11.2, 8.6 Hz, 2H), 4.09–4.00 (m, 3H), 3.39 (s, 6H), 2.84–2.69 (m, 7H), 2.30 (d, *J* = 25.1 Hz, 14H), 1.65 (d, *J* = 6.2 Hz, 7H), 1.16 (s, 18H); HRMS (FAB) m/z calculated for $C_{42}H_{60}RuN_2O_5Na$ ([M+Na$^+$]$^+$) 797.3444, found 797.3429.

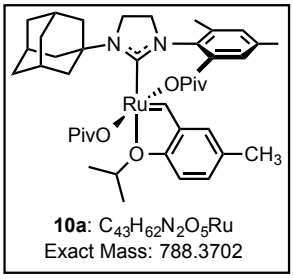
(1-(1-adamantyl)-3-(2,6-diisopropylphenyl)-2-imidazolidinylidene)bispivalato(*o*-isopropoxyphenylmethylidene)ruthenium (6d)



6d: $C_{45}H_{66}N_2O_5Ru$
Exact Mass: 816.4015

Bispivalato complex **6d** was observed while conducting kinetics experiments described above; ^{1}H NMR (500 MHz, 1:1 THF-d_8:CD_3OD, 0 °C) δ 17.56 (s, 1H), 7.87 (t, *J* = 7.9 Hz, 1H), 7.79–7.70 (m, 1H), 7.69 (d, *J* = 7.7 Hz, 1H), 7.42–7.35 (m, 1H), 7.32 (d, *J* = 8.5 Hz, 1H), 7.17 (dt, *J* = 7.5, 3.2 Hz, 1H), 7.11–7.03 (m, 1H), 5.23 (p, *J* = 6.1 Hz, 1H), 4.87 (p, *J* = 6.0 Hz, 1H), 4.32 (dd, *J* = 10.7, 8.4 Hz, 2H), 4.19–4.07 (m, 2H), 3.95 (s, 4H), 3.41–3.26 (m, 6H), 2.74 (s, 3H), 2.54 (s, 3H), 2.28 (q, *J* = 14.0, 13.1 Hz, 6H), 1.69 (d, *J* = 6.1 Hz, 6H), 1.60 (t, *J* = 6.0 Hz, 6H), 1.22 (s, 18H), 1.09 (d, *J* = 6.7 Hz, 6H).

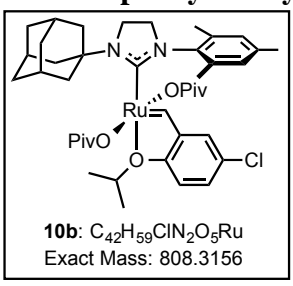
(1-(1-adamantyl)-3-(2,4,6-trimethylphenyl)-2-imidazolidinylidene)bispivalato(*o*-isopropoxy-*m*-methylphenylmethylidene)ruthenium (10a)



10a: $C_{43}H_{62}N_2O_5Ru$
Exact Mass: 788.3702

Bispivalato complex **10a** was observed while conducting kinetics experiments described above; ^{1}H NMR (500 MHz, 1:1 THF-d_8:CD_3OD, 0 °C) δ 17.33 (s, 1H), 7.58–7.50 (m, 1H), 7.41 (s, 2H), 7.17 (d, *J* = 8.4 Hz, 1H), 7.03 (s, 1H), 5.23 (s, 1H), 4.32 (t, *J* = 9.8 Hz, 2H), 4.08 (t, *J* = 10.9 Hz, 2H), 3.97 (s, 6H), 3.41 (s, 6H), 2.66 (s, 4H), 2.40–2.27 (m, 13H), 2.12 (s, 6H), 1.66 (d, *J* = 6.1 Hz, 6H), 1.19 (s, 18H); HRMS (FAB) m/z calculated for $C_{43}H_{62}RuN_2O_5Na$ ([M+Na$^+$]$^+$) 811.3600, found 811.3590.

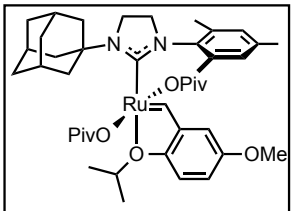
(1-(1-adamantyl)-3-(2,4,6-trimethylphenyl)-2-imidazolidinylidene)bispivalato(*o*-isopropoxy-*m*-chlorophenylmethylidene)ruthenium (10b)



10b: $C_{42}H_{59}ClN_2O_5Ru$
Exact Mass: 808.3156

Bispivalato complex **10b** was observed while conducting kinetics experiments described above; ^{1}H NMR (500 MHz, 1:1 THF-d_8:CD_3OD, 0 °C) δ 17.21 (s, 1H), 7.75–7.69 (m, 1H), 7.48–7.36 (m, 2H), 7.29 (dd, *J* = 13.5, 6.4 Hz, 1H), 7.22 (d, *J* = 8.1 Hz, 1H), 5.24 (s, 1H), 4.35 (t, *J* = 9.9 Hz, 2H), 4.09 (d, *J* = 10.2 Hz, 2H), 3.97 (s, 6H), 3.49–3.36 (m, 6H), 2.34 (q, *J* = 13.0 Hz, 8H), 1.66 (d, *J* = 6.2 Hz, 6H), 1.22 (s, 18H); HRMS (FAB) m/z calculated for $C_{42}H_{59}RuClN_2O_5Na$ ([M+Na$^+$]$^+$) 831.3054, found 831.3055.

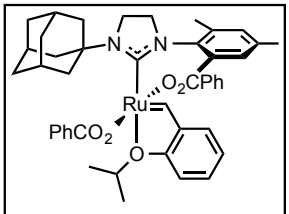
(1-(1-adamantyl)-3-(2,4,6-trimethylphenyl)-2-imidazolidinylidene)bispivalato(*o*-isopropoxy-*m*-methoxyphenylmethylidene)ruthenium (10c)



10c: $C_{43}H_{62}N_2O_6Ru$
Exact Mass: 804.3651

Bispivalato complex **10c** was observed while conducting kinetics experiments described above; ^{1}H NMR (500 MHz, 1:1 THF-d_8:CD_3OD, 0 °C) δ 17.21 (s, 1H), 7.40 (s, 2H), 7.28 (dd, J = 9.0, 3.1 Hz, 1H), 7.17 (d, J = 7.9 Hz, 1H), 6.76 (s, 1H), 5.23–5.09 (m, 1H), 4.31 (dd, J = 11.0, 8.6 Hz, 2H), 4.11–4.04 (m, 2H), 3.95 (s, 6H), 3.44–3.33 (m, 6H), 2.77 (q, J = 5.9, 5.2 Hz, 6H), 2.38–2.20 (m, 14H), 2.09 (s, 7H), 1.61 (d, J = 6.2 Hz, 6H), 1.17 (s, 18H); HRMS (FAB) m/z calculated for $C_{43}H_{62}RuN_2O_6Na$ ([M+Na$^+$]$^+$) 827.3550, found 827.3571.

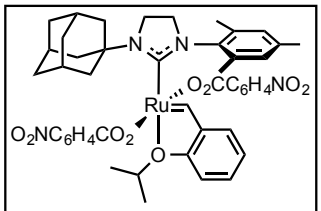
(1-(1-adamantyl)-3-(2,4,6-trimethylphenyl)-2-imidazolidinylidene)70isbenzoate(*o*-isopropoxy-phenylmethylidene)ruthenium (8a)



8a: $C_{46}H_{52}N_2O_5Ru$
Exact Mass: 814.2920

Dibenzoate complex **8a** was observed while conducting kinetics experiments described above; ^{1}H NMR (500 MHz, 1:1 THF-d_8:CD_3OD, 0 °C) δ 17.86 (s, 1H), 7.99 (d, J = 7.5 Hz, 4H), 7.76–7.65 (m, 3H), 7.55 (t, J = 7.5 Hz, 4H), 7.39 (d, J = 8.5 Hz, 3H), 7.29 (dd, J = 12.8, 7.5 Hz, 2H), 5.30 (p, J = 6.4 Hz, 1H), 4.29 (dd, J = 11.5, 8.2 Hz, 2H), 4.06 (dd, J = 11.3, 8.7 Hz, 2H), 3.95 (d, J = 3.2 Hz, 3H), 3.45 (s, 6H), 2.75 (s, 3H), 2.43 (d, J = 12.6 Hz, 3H), 2.39–2.30 (m, 9H), 2.09 (s, 3H), 1.63 (d, J = 6.0 Hz, 6H).

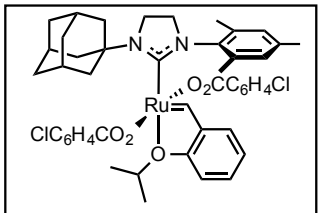
(1-(1-adamantyl)-3-(2,4,6-trimethylphenyl)-2-imidazolidinylidene)bis-*p*-nitrobenzoato(*o*-isopropoxy-phenylmethylidene)ruthenium (8b)



8b: $C_{46}H_{50}N_4O_9Ru$
Exact Mass: 904.2621

Dibenzoate complex **8b** was observed while conducting kinetics experiments described above; ^{1}H NMR (500 MHz, 1:1 THF-d_8:CD_3OD, 0 °C) δ 17.89 (s, 1H), 8.14 (d, J = 8.3 Hz, 4H), 7.76 (t, J = 7.7 Hz, 1H), 7.48–7.28 (m, 6H), 5.34 (s, 1H), 4.31 (t, J = 9.7 Hz, 2H), 4.09 (t, J = 10.4 Hz, 2H), 3.96 (d, J = 16.8 Hz, 8H), 3.45 (s, 7H), 2.88 (s, 3H), 2.78 (d, J = 17.3 Hz, 3H), 2.51–2.26 (m, 15H), 2.11 (d, J = 20.7 Hz, 8H).

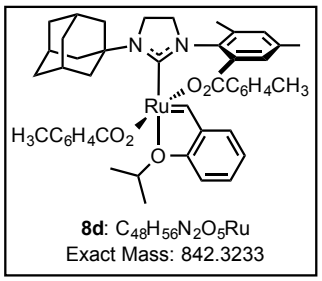
(1-(1-adamantyl)-3-(2,4,6-trimethylphenyl)-2-imidazolidinylidene)bis-*p*-chlorobenzoato(*o*-isopropoxy-phenylmethylidene)ruthenium (8c)



8c: $C_{46}H_{50}Cl_2N_2O_5Ru$
Exact Mass: 882.2140

Dibenzoate complex **8c** was observed while conducting kinetics experiments described above; ^{1}H NMR (500 MHz, 1:1 THF-d_8:CD_3OD, 0 °C) δ 17.86 (s, 1H), 7.94 (d, J = 8.1 Hz, 4H), 7.74 (t, J = 7.8 Hz, 1H), 7.57 (d, J = 8.5 Hz, 4H), 7.43–7.34 (m, 3H), 7.34–7.25 (m, 2H), 5.36–5.24 (m, 1H), 4.29 (t, J = 9.8 Hz, 2H), 4.07 (dd, J = 11.5, 8.8 Hz, 2H), 3.95 (s, 4H), 3.44 (s, 6H), 2.86 (d, J = 5.0 Hz, 4H), 2.75 (s, 3H), 2.45–2.38 (m, 3H), 2.36 (d, J = 13.1 Hz, 3H), 2.32 (s, 6H), 2.09 (s, 5H), 1.61 (t, J = 5.8 Hz, 6H).

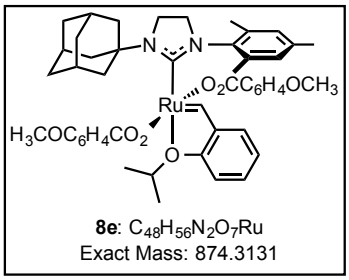
(1-(1-adamantyl)-3-(2,4,6-trimethylphenyl)-2-imidazolidinylidene)bis-*p*-methylbenzoato(*o*-isopropoxy-phenylmethylidene)ruthenium (8d)



8d: $C_{48}H_{56}N_2O_5Ru$
Exact Mass: 842.3233

Dibenzoate complex **8d** was observed while conducting kinetics experiments described above; ^{1}H NMR (500 MHz, 1:1 THF-d_8:CD_3OD, 0 °C) δ 17.85 (s, 1H), 7.88 (d, J = 7.7 Hz, 4H), 7.76–7.67 (m, 1H), 7.36 (t, J = 6.1 Hz, 7H), 7.26 (dd, J = 11.0, 7.9 Hz, 2H), 5.34–5.22 (m, 1H), 4.28 (dd, J = 11.3, 8.3 Hz, 2H), 4.05 (dd, J = 11.0, 8.3 Hz, 2H), 3.95 (s, 3H), 3.45 (s, 6H), 2.85 (s, 3H), 2.74 (s, 3H), 2.65 (s, 6H), 2.59 (s, 6H), 2.47–2.39 (m, 3H), 2.35 (d, J = 12.6 Hz, 3H), 2.08 (s, 3H), 1.62 (dd, J = 9.5, 6.1 Hz, 6H).

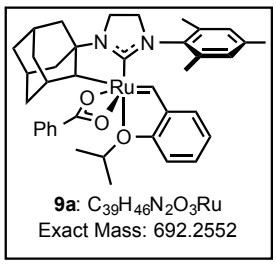
(1-(1-adamantyl)-3-(2,4,6-trimethylphenyl)-2-imidazolidinylidene)bis-*p*-methoxybenzoato(*o*-isopropoxy-phenylmethylidene)ruthenium (8e)



8e: $C_{48}H_{56}N_2O_7Ru$
Exact Mass: 874.3131

Dibenzoate complex **8e** was observed while conducting kinetics experiments described above; ^{1}H NMR (500 MHz, 1:1 THF-d_8:CD_3OD, 0 °C) δ 17.85 (s, 1H), 7.93 (d, J = 8.3 Hz, 4H), 7.72 (t, J = 7.7 Hz, 1H), 7.37 (d, J = 8.0 Hz, 3H), 7.31–7.23 (m, 2H), 7.07 (d, J = 8.4 Hz, 4H), 5.34–5.23 (m, 1H), 4.28 (t, J = 9.9 Hz, 2H), 4.09–4.04 (m, 5H), 3.95 (s, 3H), 3.44 (s, 6H), 2.85 (s, 3H), 2.74 (s, 3H), 2.43 (d, J = 9.8 Hz, 4H), 2.35 (d, J = 12.9 Hz, 9H), 2.09 (s, 4H), 1.62 (d, J = 6.1 Hz, 6H).

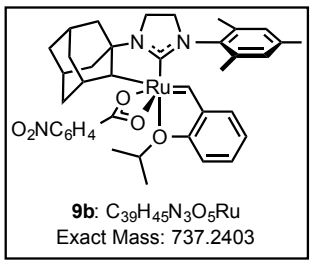
Cyclometalated Benzoate (9a)



9a: $C_{39}H_{46}N_2O_3Ru$
Exact Mass: 692.2552

Cyclometalated complex **9a** was isolated from kinetics experiments by concentrating the reaction mixture, filtering through Celite with benzene to remove excess sodium pivalate and concentrating. The crude solid was then triturated with pentanes to remove pivalic acid; ^{1}H NMR (500 MHz, C_6D_6) δ 15.07 (s, 1H), 8.09 (dd, J = 6.6, 3.0 Hz, 2H), 7.49 (dd, J = 7.5, 1.7 Hz, 1H), 7.23 (ddd, J = 8.6, 7.4, 1.7 Hz, 1H), 7.20–7.15 (m, 3H), 6.88 (td, J = 7.4, 0.9 Hz, 1H), 6.78 (d, J = 1.6 Hz, 2H), 6.59 (d, J = 8.3 Hz, 1H), 6.16 (d, J = 2.0 Hz, 1H), 4.69 (hept, J = 6.3 Hz, 1H), 4.25 (s, 1H), 3.39–3.19 (m, 4H), 2.50 (s, 3H), 2.47 (s, 1H), 2.21–2.14 (m, 2H), 2.11 (s, 1H), 2.09 (s, 4H), 2.06–1.98 (m, 1H), 1.87 (dq, J = 11.8, 2.3 Hz, 1H), 1.72 (dd, J = 6.4, 3.2 Hz, 1H), 1.63–1.46 (m, 6H), 1.39–1.15 (m, 5H), 0.92 (d, J = 6.2 Hz, 3H), 0.88 (t, J = 7.1 Hz, 1H), 0.76 (dd, J = 12.9, 3.4 Hz, 1H); ^{13}C NMR (126 MHz, C_6D_6) δ 215.5, 154.7, 143.9, 137.5, 137.2, 136.4, 136.2, 130.4, 130.0, 129.7, 129.2, 128.6, 127.7, 127.5, 125.7, 123.3, 123.2, 112.9, 74.2, 68.9, 62.9, 51.4, 43.4, 41.7, 40.6, 38.2, 38.0, 37.7, 33.6, 31.2, 30.0, 22.7, 21.3, 21.1, 20.7, 18.8, 18.4; HRMS (FAB) m/z calculated for $C_{39}H_{45}RuN_2O_3$ ($[M+H^+–H_2]^+$) 691.2474, found 691.2464.

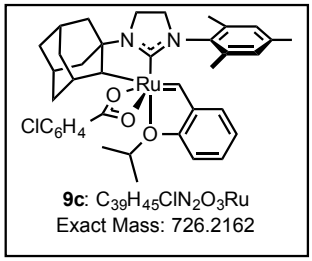
Cyclometalated *p*-Nitrobenzoate (9b)



9b: $C_{39}H_{45}N_3O_5Ru$
Exact Mass: 737.2403

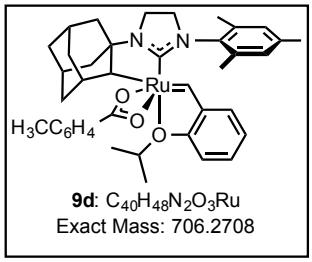
Cyclometalated complex **9b** was not stable enough to be isolated. Complex **9b** has a ^{1}H NMR (500 MHz, 1:1 THF-d_8:CD_3OD) peak associated with the benzylidene proton at δ 15.33 ppm.

Cyclometalated *p*-chlorobenzoate (9c)



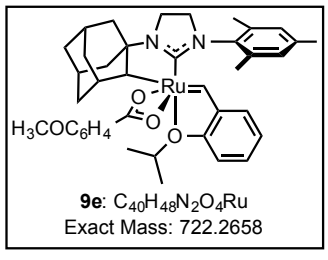
Cyclometalated complex **9c** was isolated from kinetics experiments by concentrating the reaction mixture, filtering through Celite with benzene to remove excess sodium pivalate and concentrating. The crude solid was then triturated with pentanes to remove pivalic acid; ^{1}H NMR (500 MHz, C_6D_6) δ 15.06 (s, 1H), 7.85 (d, *J* = 8.4 Hz, 2H), 7.48 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.24 (ddd, *J* = 8.3, 7.4, 1.7 Hz, 1H), 7.12 (d, *J* = 8.8 Hz, 1H), 6.87 (td, *J* = 7.4, 0.9 Hz, 1H), 6.73 (s, 1H), 6.60 (d, *J* = 8.3 Hz, 1H), 6.07 (s, 1H), 4.68 (hept, *J* = 6.4 Hz, 1H), 4.20 (s, 1H), 3.37–3.16 (m, 4H), 2.47 (s, 3H), 2.44 (q, *J* = 2.9 Hz, 1H), 2.17 (t, *J* = 3.3 Hz, 1H), 2.13 (dt, *J* = 11.5, 3.0 Hz, 1H), 2.10–2.04 (m, 4H), 2.04–1.95 (m, 4H), 1.87 (dq, *J* = 12.0, 2.5 Hz, 1H), 1.73–1.65 (m, 1H), 1.61–1.45 (m, 7H), 1.30–1.16 (m, 3H), 0.93–0.85 (m, 4H), 0.77–0.70 (m, 1H); ^{13}C NMR (126 MHz, C_6D_6) δ 215.1, 154.7, 143.8, 137.4, 137.0, 136.5, 136.2, 134.3, 131.1, 129.9, 129.2, 127.7, 127.7, 125.8, 123.3, 112.9, 74.1, 69.1, 62.9, 51.4, 43.4, 41.6, 40.6, 38.2, 38.0, 37.7, 33.6, 31.2, 30.0, 22.7, 21.3, 21.0, 20.7, 18.8, 18.3, 14.3. HRMS (FAB) m/z calculated for $C_{39}H_{44}RuN_2O_3Cl$ ($[M+H^+–H_2]^+$) 725.2084, found 725.2066.

Cyclometalated *p*-methylbenzoate (9d)



Cyclometalated complex **9d** was isolated from kinetics experiments by concentrating the reaction mixture, filtering through Celite with benzene to remove excess sodium pivalate and concentrating. The crude solid was then triturated with pentanes to remove pivalic acid; ^{1}H NMR (500 MHz, C_6D_6) δ 15.05 (s, 1H), 8.01 (d, *J* = 7.7 Hz, 2H), 7.50 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.23 (ddd, *J* = 8.5, 7.4, 1.7 Hz, 1H), 6.99 (dd, *J* = 7.8, 1.2 Hz, 2H), 6.88 (td, *J* = 7.5, 0.9 Hz, 1H), 6.78 (s, 1H), 6.60 (d, *J* = 8.3 Hz, 1H), 6.23 (s, 1H), 4.71 (hept, *J* = 6.4 Hz, 1H), 4.27 (s, 1H), 3.39–3.20 (m, 4H), 2.51 (s, 3H), 2.47 (q, *J* = 2.9 Hz, 1H), 2.22–2.16 (m, 2H), 2.16–2.01 (m, 12H), 1.94–1.84 (m, 1H), 1.72 (s, 1H), 1.63–1.57 (m, 4H), 1.57–1.47 (m, 2H), 1.32–1.24 (m, 1H), 1.24–1.16 (m, 1H), 0.93 (d, *J* = 6.2 Hz, 3H), 0.87 (t, *J* = 7.1 Hz, 1H), 0.78 (d, *J* = 12.1 Hz, 1H); ^{13}C NMR (126 MHz, C_6D_6) δ 215.8, 175.3, 154.7, 143.9, 140.2, 137.5, 137.3, 136.3, 136.1, 133.6, 130.0, 129.8, 129.2, 128.1, 125.6, 123.3, 123.2, 112.9, 74.2, 68.9, 62.9, 51.4, 43.5, 41.7, 40.7, 38.3, 38.0, 37.7, 33.6, 31.2, 30.0, 21.4, 21.3, 21.1, 20.7, 18.8, 18.4. HRMS (FAB) m/z calculated for $C_{40}H_{47}RuN_2O_3$ ($[M+H^+–H_2]^+$) 705.2631, found 705.2659.

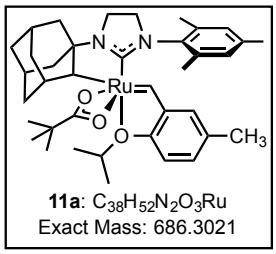
Cyclometalated *p*-methoxybenzoate (9e)



Cyclometalated complex **9e** was isolated from kinetics experiments by concentrating the reaction mixture, filtering through Celite with benzene to remove excess sodium pivalate and concentrating. The crude solid was then triturated with pentanes to remove pivalic acid; ^{1}H NMR (500 MHz, C_6D_6) δ 15.06 (s, 1H), 8.05 (d, *J* = 8.2 Hz, 3H), 7.49 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.24 (ddd, *J* = 8.2, 7.3, 1.7 Hz, 1H), 6.88 (td, *J* = 7.4, 0.9 Hz, 1H), 6.81–6.74 (m, 3H), 6.62 (dd, *J* = 8.3, 1.1 Hz, 2H), 6.25 (s, 1H), 4.73 (hept, *J* = 6.3 Hz, 1H), 4.27 (s, 1H), 3.40–3.21 (m, 9H), 2.51 (s, 4H), 2.48 (s, 2H), 2.22–2.17 (m, 3H), 2.16 (s, 5H), 2.13–2.01 (m, 5H), 1.94–1.84 (m, 2H), 1.76–1.69 (m, 2H), 1.61 (d, *J* = 6.4 Hz, 4H), 1.60–1.53 (m, 1H), 1.53–1.47 (m, 2H), 1.31–1.24 (m, 1H), 1.24–1.16 (m, 1H), 0.97 (d, *J* = 6.2 Hz, 4H), 0.78 (d, *J* = 12.1

Hz, 2H); ^{13}C NMR (125 MHz, C_6D_6) δ 215.9, 175.2, 162.0, 154.7, 143.9, 137.3, 136.3, 136.1, 131.4, 130.0, 129.2, 129.1, 125.6, 123.3, 123.2, 112.9, 112.8, 74.2, 68.9, 62.9, 51.5, 43.5, 41.7, 40.7, 38.3, 38.0, 37.8, 33.6, 31.3, 30.1, 25.8, 21.3, 21.1, 20.7, 18.8, 18.4; HRMS (FAB) m/z calculated for $C_{40}H_{47}RuN_2O_4$ ([M+H$^+$–H$_2$]$^+$) 721.2580, found 721.2614.

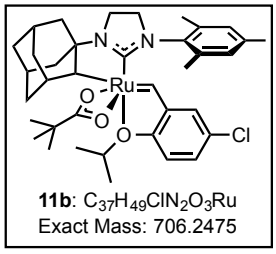
Methylbenzylidene cyclometalated complex (11a)



11a: $C_{38}H_{52}N_2O_3Ru$
Exact Mass: 686.3021

Cyclometalated complex **11a** was isolated from kinetics experiments by concentrating the reaction mixture, filtering through Celite with benzene to remove excess sodium pivalate and concentrating. The crude solid was then triturated with pentanes to remove pivalic acid; ^{1}H NMR (500 MHz, C_6D_6) δ 14.88 (s, 1H), 7.33 (d, *J* = 2.2 Hz, 1H), 7.11 (ddd, *J* = 8.3, 2.3, 0.9 Hz, 1H), 6.83 (s, 1H), 6.75 (s, 1H), 6.65 (d, *J* = 8.3 Hz, 1H), 4.80 (hept, *J* = 6.5 Hz, 1H), 4.22 (s, 1H), 3.49–3.36 (m, 2H), 3.32–3.13 (m, 3H), 2.57 (s, 1H), 2.46 (s, 3H), 2.28 (d, *J* = 4.0 Hz, 6H), 2.20 (s, 3H), 2.16–2.09 (m, 3H), 2.04 (dd, *J* = 11.1, 2.8 Hz, 1H), 1.96 (dt, *J* = 11.2, 3.0 Hz, 1H), 1.88–1.81 (m, 1H), 1.68 (s, 1H), 1.58–1.46 (m, 5H), 1.45–1.39 (m, 1H), 1.26 (s, 9H), 1.22–1.18 (m, 4H), 0.75 (d, *J* = 12.0 Hz, 1H); ^{13}C NMR (126 MHz, C_6D_6) δ 215.9, 152.4, 143.8, 138.0, 137.1, 136.7, 136.4, 132.1, 129.8, 129.6, 127.7, 125.8, 123.6, 113.6, 93.5, 74.1, 68.5, 65.9, 62.7, 54.9, 51.7, 43.4, 41.3, 40.6, 38.2, 38.1, 36.9, 33.8, 31.1, 30.0, 28.6, 21.6, 21.2, 21.0, 20.3, 19.2, 19.0; HRMS (EI) m/z calculated for $C_{38}H_{51}RuN_2O_3$ ([M+H$^+$–H$_2$]$^+$) 685.2944, found 685.2950.

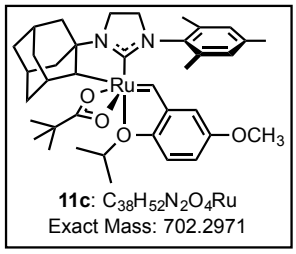
Chlorobenzylidene cyclometalated complex (11b)



11b: $C_{37}H_{49}ClN_2O_3Ru$
Exact Mass: 706.2475

Cyclometalated complex **11b** was isolated from kinetics experiments by concentrating the reaction mixture, filtering through Celite with benzene to remove excess sodium pivalate and concentrating. The crude solid was then triturated with pentanes to remove pivalic acid; ^{1}H NMR (500 MHz, C_6D_6) δ 14.66 (s, 1H), 7.55 (d, *J* = 2.6 Hz, 1H), 7.26 (dd, *J* = 8.7, 2.6 Hz, 1H), 6.80 (s, 1H), 6.73 (s, 1H), 6.40 (d, *J* = 8.8 Hz, 1H), 4.63 (hept, *J* = 6.7 Hz, 1H), 4.23 (s, 1H), 3.45–3.33 (m, 2H), 3.31 (s, 1H), 3.30–3.19 (m, 2H), 3.13 (dt, *J* = 11.5, 9.5 Hz, 1H), 2.48 (s, 1H), 2.35 (s, 3H), 2.24 (s, 3H), 2.18 (s, 3H), 2.09 (d, *J* = 14.6, 3.3, 2.4 Hz, 2H), 2.00 (d, 1H), 1.92 (d, 1H), 1.83 (d, 1H), 1.62 (s, 1H), 1.55 (d, 1H), 1.49 (t, *J* = 2.7 Hz, 1H), 1.45 (d, *J* = 6.6 Hz, 3H), 1.34 (d, 1H), 1.24 (s, 13H), 1.09 (d, *J* = 6.3 Hz, 3H), 0.59 (d, *J* = 12.2 Hz, 1H); ^{13}C NMR (126 MHz, C_6D_6) δ 214.7, 152.5, 144.9, 142.8, 137.7, 136.9, 136.7, 136.6, 129.8, 129.7, 128.6, 128.5, 124.2, 122.1, 114.7, 93.5, 74.9, 69.6, 65.9, 62.7, 51.7, 43.2, 41.3, 40.5, 39.6, 38.1, 38.1, 36.9, 33.8, 31.0, 29.8, 28.5, 21.5, 21.0, 19.2, 18.9; HRMS (EI) m/z calculated for $C_{37}H_{48}RuClN_2O_3$ ([M+H$^+$–H$_2$]$^+$) 705.2398, found 705.2428.

Methoxybenzylidene cyclometalated complex (11c)

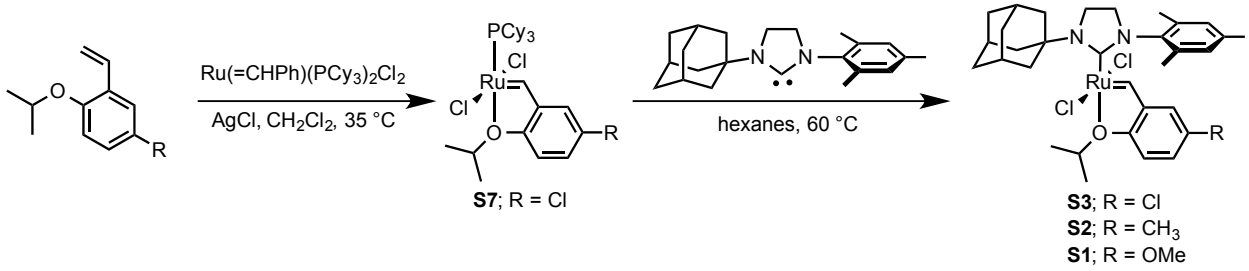


11c: $C_{38}H_{52}N_2O_4Ru$
Exact Mass: 702.2971

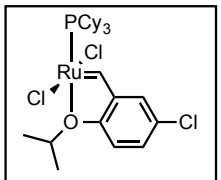
Cyclometalated complex **11c** was isolated from kinetics experiments by concentrating the reaction mixture, filtering through Celite with benzene to remove excess sodium pivalate and concentrating. The crude solid was then triturated with pentanes to remove pivalic acid; ^{1}H NMR (500 MHz, C_6D_6) δ 14.85 (s, 1H), 7.18 (d, *J* = 3.0 Hz, 1H), 6.95 (dd, *J* = 8.9, 3.0 Hz, 1H), 6.82 (s, 1H), 6.75 (s, 1H), 6.62 (d, *J* = 8.5 Hz, 1H), 4.76 (hept, *J* = 6.4 Hz, 1H), 4.23 (s, 1H), 3.47–3.33 (m, 5H), 3.32–3.22 (m, 2H), 3.17 (dt, *J* = 11.5, 9.6 Hz, 1H), 2.58 (s, 1H), 2.43 (s, 3H), 2.27 (s, 3H), 2.20 (s,

3H), 2.12 (d, *J* = 8.7 Hz, 3H), 2.03 (dt, *J* = 11.1, 1.9 Hz, 1H), 1.95 (dq, *J* = 10.6, 2.2 Hz, 1H), 1.89–1.82 (m, 1H), 1.71–1.64 (m, 1H), 1.60–1.54 (m, 1H), 1.52 (d, *J* = 6.6 Hz, 5H), 1.39 (dq, *J* = 11.3, 2.0 Hz, 1H), 1.25 (s, 12H), 1.20 (d, *J* = 6.3 Hz, 4H), 1.05 (dq, *J* = 10.4, 2.6 Hz, 1H), 0.79–0.70 (m, 1H); ^{13}C NMR (126 MHz, C_6D_6) δ 215.2, 155.9, 148.0, 144.0, 137.6, 136.6, 136.3, 136.0, 129.4, 129.2, 113.6, 109.8, 107.4, 73.8, 68.6, 62.3, 55.0, 51.3, 42.9, 40.9, 40.2, 39.1, 37.8, 37.6, 36.5, 33.4, 30.7, 29.6, 28.1, 21.2, 20.9, 20.6, 18.8, 18.6; HRMS (FAB) m/z calculated for $C_{38}H_{51}RuN_2O_4$ ([M+H$^+$–H$_2$]$^+$) 701.2893, found 701.2923.

Synthesis of New Benzylidene Chelates

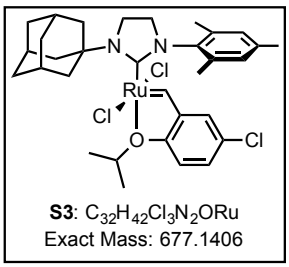


tricyclohexylphosphinedichloro(*o*-isopropoxy-*m*-chlorophenylmethylidene)ruthenium (S7)



Following the analogous reported procedure,[1] in a nitrogen filled glovebox, benzylidenebis(tricyclohexylphosphine)ruthenium dichloride (200 mg, 0.243 mmol), silver(I) chloride (70 mg, 0.487 mmol) and 2-isopropoxy-5-chlorostyrene (96 mg, 0.487 mmol) were weighed into a 20 mL vial. The reagents were suspended in dichloromethane (8 mL), the vial was sealed, removed from the glovebox and heated to 35 °C. Silica gel was added to the reaction mixture, and the residual solvent was removed under reduced pressure. The product-laden silica gel was loaded onto a silica gel column and eluted with 3:1 hexanes:CH_2Cl_2 to provide 95 mg (62%) of **S7** as a brown powder; ^{1}H NMR (500 MHz, C_6D_6) δ 17.04 (d, *J* = 4.6 Hz, 1H), 7.35 (d, *J* = 2.5 Hz, 1H), 7.18 (dd, *J* = 8.8, 2.5 Hz, 1H), 6.24 (d, *J* = 8.8 Hz, 1H), 4.56 (heptd, *J* = 6.2, 1.8 Hz, 1H), 2.39 (qt, *J* = 12.2, 2.7 Hz, 3H), 2.16 (d, *J* = 12.9 Hz, 6H), 1.91 (q, *J* = 12.4 Hz, 3H), 1.73 (dq, *J* = 11.4, 3.9 Hz, 6H), 1.67 (d, *J* = 6.1 Hz, 6H), 1.58 (s, 3H), 1.26 ? 1.13 (m, 9H); ^{13}C NMR (126 MHz, C_6D_6) δ 266.4, 151.4, 144.9, 142.8, 128.4, 121.9, 114.4, 76.3, 36.1 (d, *J* = 24.4 Hz), 30.5, 28.1 (d, *J* = 10.5 Hz), 26.6, 22.1; ^{31}P NMR (121 MHz, C_6D_6) δ 59.6; HRMS (FAB) m/z calculated for $C_{28}H_{44}RuPOCl_2{}^{37}Cl$ ([M]$^+$) 636.1210, found 636.1218.

(1-(1-adamantyl)-3-(2,4,6-trimethylphenyl)-2-imidazolidinylidene)dichloro(*o*-isopropoxy-*m*-chlorophenylmethylidene)ruthenium (S3)

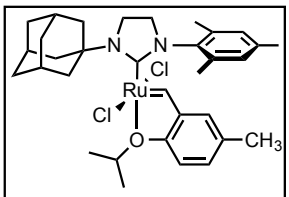


In a nitrogen filled glovebox, ruthenium complex **S7** (95 mg, 0.150 mmol) and 1-(1-adamantyl)-3-(2,4,6-trimethylphenyl)imidazolinylidene (48 mg, 0.150 mmol) were weighed into a 20 mL vial. The reagents were suspended in hexanes (3.7 mL), sealed, removed from the glovebox, and heated to 60 °C. The solution was stirred until the brown color disappeared and was replaced by a green precipitate. The mixture was filtered through Celite with extra hexanes (2 mL) to collect a green

[1] Van Veldhuizen, J. J.; Gillingham, D. G.; Garber, S. B.; Kataoka, O.; Hoveyda, A. H. *J. Am. Chem. Soc.* **2003**, *125*, 12502–12508.

solid. The solid was eluted with dichloromethane (2 mL) into a clean flask to provide 96 mg (95%) of ruthenium NHC complex **S3** as a green solid. ^{1}H NMR (500 MHz, C_6D_6) δ 16.88 (s, 1H), 7.18 (dd, *J* = 8.6, 2.6 Hz, 1H), 7.11 (d, *J* = 2.6 Hz, 1H), 6.78 (s, 2H), 6.15 (d, *J* = 8.6 Hz, 1H), 4.40 (hept, *J* = 6.2 Hz, 1H), 3.30–3.24 (m, 4H), 2.92 (s, 6H), 2.31 (s, 6H), 2.29 (s, 3H), 2.25 (s, 3H), 1.88 (d, *J* = 12.3 Hz, 3H), 1.68 (d, *J* = 12.8 Hz, 3H), 1.50 (d, *J* = 6.1 Hz, 6H); ^{13}C NMR (126 MHz, C_6D_6) δ 208.4, 150.8, 147.0, 140.0, 138.6, 138.4, 130.0, 128.6, 128.4, 122.6, 114.5, 74.8, 57.2, 50.9, 44.4, 42.2, 36.4, 30.5, 22.4, 21.0, 18.5; HRMS (FAB) m/z calculated for $C_{32}H_{41}RuON_2Cl_2{}^{37}Cl$ ([M]$^+$) 678.1299, found 678.1290.

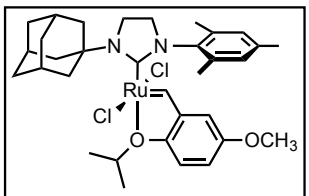
(1-(1-adamantyl)-3-(2,4,6-trimethylphenyl)-2-imidazolidinylidene)dichloro(*o*-isopropoxy-*m*-methylphenylmethylidene)ruthenium (S2)



S2: $C_{33}H_{45}Cl_2N_2ORu$
Exact Mass: 657.1952

In a nitrogen filled glovebox, ruthenium complex (120 mg, 0.195 mmol) and 1-(1-adamantyl)-3-(2,4,6-trimethylphenyl)imidazolinylidene (63 mg, 0.195 mmol) were weighed into a 20 mL vial. The reagents were suspended in hexanes (4.9 mL), sealed, removed from the glovebox, and heated to 60 °C. The solution was stirred until the brown color disappeared and was replaced by a green precipitate. The mixture was filtered through Celite with extra hexanes (2 mL) to collect a green solid. The solid was eluted with dichloromethane (2 mL) into a clean flask to provide 120 mg (94%) of ruthenium NHC complex **S2** as a green solid. ^{1}H NMR (500 MHz, C_6D_6) δ 17.03 (s, 1H), 7.04 (ddd, *J* = 8.3, 2.3, 0.9 Hz, 1H), 6.86 (s, 2H), 6.85 (d, *J* = 2.2 Hz, 1H), 6.41 (d, *J* = 8.3 Hz, 1H), 4.59 (hept, *J* = 7.0 Hz, 1H), 3.34–3.27 (m, 4H), 2.96 (s, 6H), 2.37 (s, 6H), 2.34–2.29 (m, 4H), 2.28 (s, 3H), 2.22 (s, 3H), 1.91 (d, *J* = 12.1 Hz, 3H), 1.69 (dt, *J* = 12.5, 3.1 Hz, 3H), 1.59 (d, *J* = 6.1 Hz, 6H); ^{13}C NMR (126 MHz, C_6D_6) δ 210.0, 150.5, 146.0, 140.0, 138.1, 137.8, 130.9, 129.9, 129.5, 127.9, 127.6, 123.6, 112.8, 73.6, 56.8, 50.6, 44.0, 41.8, 36.0, 30.1, 22.1, 20.7, 19.7, 18.3; HRMS (FAB) m/z calculated for $C_{33}H_{44}RuON_2Cl_2$ ([M]$^+$) 656.1875, found 656.1861.

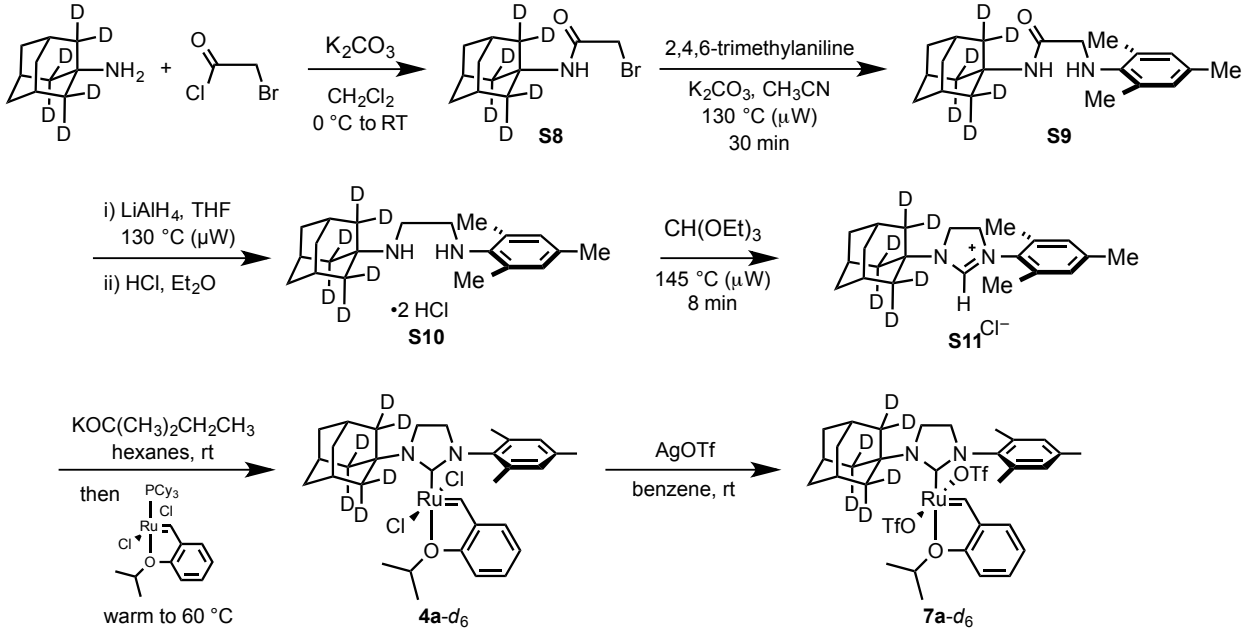
(1-(1-adamantyl)-3-(2,4,6-trimethylphenyl)-2-imidazolidinylidene)dichloro(*o*-isopropoxy-*m*-methoxyphenylmethylidene)ruthenium (S1)



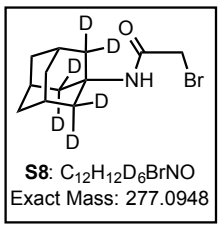
S1: $C_{33}H_{45}Cl_2N_2O_2Ru$
Exact Mass: 673.1902

In a nitrogen filled glovebox, ruthenium complex (135 mg, 0.214 mmol) and 1-(1-adamantyl)-3-(2,4,6-trimethylphenyl)imidazolinylidene (72 mg, 0.225 mmol) were weighed into a 20 mL vial. The reagents were suspended in hexanes (5.4 mL), sealed, removed from the glovebox, and heated to 60 °C. The solution was stirred until the brown color disappeared and was replaced by a green precipitate. The mixture was filtered through Celite with extra hexanes (2 mL) to collect a green solid. The solid was eluted with dichloromethane (2 mL) into a clean flask to provide 136 mg (94%) of ruthenium NHC complex **S1** as a green solid. ^{1}H NMR (500 MHz, C_6D_6) δ 16.92 (s, 1H), 6.95 (dd, *J* = 8.9, 3.1 Hz, 1H), 6.84 (s, 2H), 6.62 (d, *J* = 3.0 Hz, 1H), 6.38 (dt, *J* = 8.9, 0.9 Hz, 1H), 4.54 (hept, *J* = 6.2 Hz, 1H), 3.43 (s, 3H), 3.33–3.29 (m, 4H), 2.96 (s, 6H), 2.36 (s, 6H), 2.31 (s, 3H), 2.20 (s, 3H), 1.91 (d, *J* = 12.1 Hz, 3H), 1.69 (d, *J* = 12.4 Hz, 3H), 1.58 (d, *J* = 6.1 Hz, 6H); ^{13}C NMR (126 MHz, C_6D_6) δ 210.1, 155.5, 138.6, 138.2, 129.9, 128.6, 128.1, 127.7, 115.4, 113.7, 107.5, 74.1, 65.9, 57.2, 55.3, 50.9, 44.4, 42.2, 36.4, 30.5, 22.5, 21.1, 18.7; HRMS (FAB) m/z calculated for $C_{33}H_{44}RuO_2N_2Cl_2$ ([M]$^+$) 672.1824, found 672.1807.

Synthesis of Deuterated Complexes



N-(adamantan-1-yl-2,2,8,8,9,9-d_6)-2-bromoacetamide (S8)



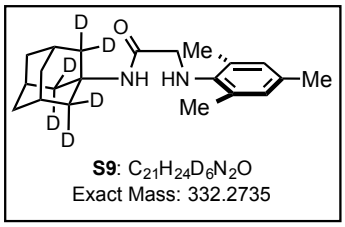
1-aminoadamantane-d_6 (500 mg, 3.16 mmol) was transferred to a 20 mL scintillation vial equipped with a stir bar and suspended in dichloromethane (6.6 mL). Solid K_2CO_3 (872 mg, 6.4 mmol) was added to the vial, which was capped with a septum and attached to a nitrogen bubbler and cooled by immersion in an ice bath. Bromoacetyl chloride (0.350 mL, 3.63 mmol) was then added drop-wise via syringe. The slurry immediately thickened and after five minutes the vial was warmed to room temperature and gently stirred for two hours. The reaction was diluted with chloroform (7 mL) and an additional quantity of bromoacetyl chloride (0.1 mL) was added to ensure complete consumption of starting material. This homogenous solution was stirred at room temperature for 10 minutes. The vial contents were transferred to a 50 mL round bottom flask containing water (6.6 mL) and vigorously stirred for 75 minutes at room temperature. A very mild exotherm was noted at the beginning of the quenching process. The flask contents were then transferred to a 125 mL separatory funnel and vigorously shaken. The organic layer was drawn off and dried by slow passage through a plug of magnesium sulfate (3 g). Additional chloroform (15 mL) was used for a second aqueous extraction and used to rinse the magnesium salts. The organic solvents were removed with rotary evaporation and the residue was pumped overnight on the vacuum manifold (60 mTorr) to provide the amide (**S8**) as a white powder (818 mg, 93% yield). This preparation is based upon that reported for the analogous *t*-butyl amide;[2] ^{1}H NMR[3] (400 MHz, $CDCl_3$) δ 1.64–1.72 (m,

[2] Mani, T.; Tircso, G.; Zhao, P.; Sherry, A. D.; Woods, M., *Inorg. Chem.* **2009**, *48*, 10338-10345.

[3] Literature NMR characterization of the unlabeled compound: Battistini, E.; Gianolo, E.; Gref, R.; Couvreur, P.; Fuzerova, S.; Othman, M.; Aime, S.; Badet, B.; Durand, P., *Chem. Eur. J.* **2008**, *14*, 4551-4561. ^{1}H NMR (300 MHz , $CDCl_3$): δ=1.66–1.71 (m, 6H; $3CH_2$ Ad), 1.99–2.03 (m, 6H; $3CH_2$ Ad), 2.06–2.13 (m, 3H; 3CH Ad), 3.77 (s, 2H; CH_2Br), 6.11 ppm (sl, 1H; NH); ^{13}C

5.9H), 2.06–2.10 (m, 3H), 3.78 (s, 2H), 6.14 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 29.14(m), 29.93, 36.10(m), 40.21(quintet, $^1J_{CD}$ = 19.7 Hz), 52.15, 164.10; HRMS (FAB) m/z calculated for $C_{12}H_{13}ON^2H_6{}^{81}Br$ ([M+H$^+$]$^+$) 280.1006, found 280.0999.

***N*-(adamantan-1-yl-2,2,8,8,9,9-d_6)-2-(2,4,6-trimethylphenyl)amino)acetamide (S9)**

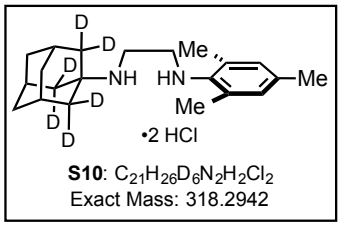


S9: $C_{21}H_{24}D_6N_2O$
Exact Mass: 332.2735

The α-bromo amide (**S8**, 360 mg, 1.29 mmol) and K_2CO_3 (285 mg, 2.06 mmol) were transferred into a 2-5 mL microwave vial containing a magnetic stir bar. Acetonitrile (2.4 mL) was added via syringe and used to wash the sidewalls free of any particulate matter. 2,4,6-trimethyl aniline (1.8 mL, 12.82 mmol) was added to the vial, which was sealed with a septum and stirred for five minutes at room temperature. The vial was transferred to a microwave reactor and heated to 130 °C for 30 minutes. At the midpoint of the run, the average microwave power was 70 W and the average internal pressure was 4 bar. Upon cooling, the vial was opened and the heterogeneous mixture was stirred briefly with chloroform (4 mL). The inorganic salts were removed with paper/gravity filtration and additional chloroform (10 mL) was used to rinse the microwave vial and filter cake. The organic solvents were combined in a 100 mL flask and removed with rotary evaporation, leaving behind a viscous oily residue consisting of reaction products and excess 2,4,6-trimethyl aniline. The bulk 2,4,6-trimethyl aniline was removed by overnight evacuation (60 mTorr) on the vacuum manifold), after which a buff-colored waxy solid, still contaminated with residual 2,4,6-trimethyl aniline, remained in the flask. The residue was purified by silica gel column chromatography in the following manner: silica gel (40 g) was dispersed in chloroform containing 0.5% diethylamine (80 mL) and the slurry was transferred to a flash silica gel column (Chem Glass Part No. CG-1197-13) to provide a settled column dimension of 1 x 6 in. The residue was dissolved in chloroform/0.5% diethylamine (6 mL), loaded onto the column, and gravity-eluted with 150 mL chloroform/0.5% diethylamine, followed with 200 mL of chloroform/0.5% diethylamine/0.5% methanol. After approximately 100 mL solvent had exited the column, fractions (8 mL) were collected in 13 x 100 mm culture tubes. TLC (5% methanol in dichloromethane) with UV visualization was used to detect the desired product (R_f = 0.4) which was found in tubes 17-25. Other components eluting off the column included 2,4,6-trimethyl aniline (R_f = 0.5, tubes 2-10) and the dialkylation product (Rf = 0.38, tubes 26-27). Fractions containing the desired product were combined and the solvent removed using rotary evaporation. Residual solvents were removed by overnight evacuation (60 mTorr) using a vacuum manifold to provide a hard and waxy buff-colored solid (**S9**, 336 mg, 78% yield); ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.64–1.72 (m, 5.6H), 2.06–2.10 (m, 3H), 2.23 (s, 3H), 2.25 (s, 6H), 3.47 (s, 2H), 6.82 (s, 2H), 6.90 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 18.32, 20.52, 29.22(m), 36.23, 40.74(quintet, $^1J_{CD}$ = 19.7 Hz), 51.15, 52.68, 129.55, 129.66, 132.18, 142.73, 170.06; HRMS (FAB) m/z calculated for $C_{21}H_{25}ON_2{}^2H_6$ ([M+H$^+$]$^+$) 333.2813, found 333.2812.

NMR (75 MHz , $CDCl_3$): δ=29.26(3) (CH Ad), 29.83 (CH_2Br), 36.12(3) (CH_2 Ad), 41.06(3) (CH_2 Ad), 52.43 (CAdNH), 164.07 ppm (C=O).

N^1-(adamantan-1-yl-2,2,8,8,9,9-d_6)-N^2-(2,4,6-trimethylphenyl)ethane-1,2-diammonium dichloride (S10)



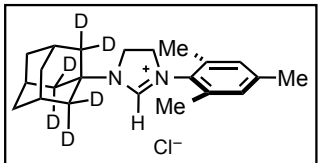
S10: $C_{21}H_{26}D_6N_2H_2Cl_2$
Exact Mass: 318.2942

$LiAlH_4$ (161 mg, 4.2 mmol) was weighed into an oven-dried 2-5 mL microwave vial containing a stir bar. This vessel was fit with a 14/20 septum, attached to a dry nitrogen source via a needle connection, and cooled in an ice bath. Anhydrous THF (2.5 mL) was added via syringe to the vial, washing the sidewalls to remove any particulate lithium aluminum hydride. In a separate 10 mL conical flask, the starting amide (**S9**, 140 mg, 0.420 mmol) was mostly dissolved in THF (1.5 mL) and transferred via syringe with drop-wise addition to the 0 °C stirring suspension of lithium aluminum hydride. Additional THF (0.6 mL and 0.2 mL, respectively) was used to transfer all of the amide (**S9**) from the conical flask to the microwave vial. The microwave vial was then warmed to room temperature and its contents stirred under nitrogen for 30 min. The vial was then sealed with a septum, transferred to a microwave reactor, and heated to 130 °C for 60 minutes. At the midpoint of the run, the average microwave power was 100 W and the average internal pressure was 8 bar. After cooling to room temperature, the vial was opened and its contents were transferred via Pasteur pipet to a 50 mL pear-shaped flask equipped with a stir bar. The flask contents were cooled to 0 °C and the excess lithium aluminum hydride was quenched by slow and drop-wise successive additions of water (0.161 mL, **warning**: vigorous reaction), 15% aqueous NaOH (0.161 mL), and water (0.483 mL). Ethyl acetate (16 mL) was used in aliquots to rinse the microwave vial and this solution was transferred to the 50 mL flask and used to disperse and render granular the forming aluminum salts. After stirring overnight, the insoluble material was removed by gravity filtration through fluted filter paper and the filter cake was rinsed with additional ethyl acetate (25 mL). The volatile solvents were removed with rotary evaporation, and a hard white solid formed after overnight evacuation (60 mTorr) on the vacuum manifold. The residue was purified by silica gel column chromatography in the following manner: silica gel (15.6 g) was dispersed in chloroform containing 0.5% diethylamine/0.5% methanol (80 mL) and the slurry was transferred to a flash silica gel column (Chem Glass Part No. CG-1197-13) to provide a settled column dimension of 1 x 2.5 in. The residue was dissolved in chloroform/0.5% diethylamine/0.5% methanol (6 mL), loaded onto the column, and gravity-eluted with chloroform/0.5% diethylamine/0.5% methanol (100 mL), chloroform/0.5% diethylamine/1% methanol (100 mL), and chloroform/0.5% diethylamine/2% methanol (50 mL). After collecting an approximate 60 mL forecut, fractions (8 mL) were collected in 13 x 100 mm culture tubes. TLC (10% methanol in dichloromethane) with UV visualization was used to detect the desired product (R_f = 0.2), which was found in tubes 8-20. Fractions containing the desired product were combined and the solvent removed using rotary evaporation. Residual solvents were removed by overnight evacuation (60 mTorr) using a vacuum manifold to provide a hard white solid (127 mg, 94% yield). This material was not characterized.

To form the bis-HCl salt, the diamine was transferred to a pre-weighed 0.5-2 mL conical microwave vial using aliquots of diethyl ether (7 mL total). 2 M HCl in diethyl ether (1.5 mL, 3 mmol) was added to the vigorously stirred diamine solution and a white precipitate immediately formed. This suspension was stirred for 60 min, after which the diamine bis-HCl salt was separated by brief centrifugation. The salt was washed three times by re-suspension/pelleting using fresh diethyl ether (3 x 3 mL). After the final wash, the vial/pellet was allowed to air dry

for 8 h before being placed overnight on the vacuum manifold for removal of trace solvents (60 mTorr). A white powder was obtained (**S10**, 153 mg, 93% yield over two steps); ^{1}H NMR[4] (400 MHz, DMSO-d_6) δ 1.55–1.70 (m, 5.4H), 2.13 (m, 2.9H), 2.23 (s, 3H), 2.44 (s, 6H), 3.37 (br m, 2H), 3.61 (br m, 2H), 6.98 (s, 2H), 9.72 (br s, 2H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 17.89, 20.15, 28.11 (m), 34.95 (m), 35.83 (br), 36.15 (m), 45.94, 56.22, 130.15, 131.33, 133.33 (br), 137.17 (br); HRMS (FAB) m/z calculated for $C_{21}H_{27}N_2D_6$ ([M–Cl$^-$–HCl]$^+$) 319.3020, found 319.3009.

1-(adamantan-1-yl-2,2,8,8,9,9-d_6)-3-(2,4,6-trimethylphenyl)-4,5-dihydro-1*H*-imidazol-3-ium chloride (S11)



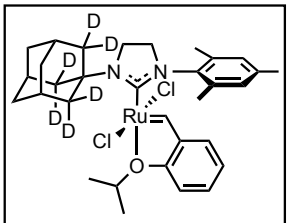
S11: $C_{22}H_{25}D_6ClN_2$
Exact Mass: 364.2552

The diamine bis-HCl salt (**S10**, 116 mg, 0.296 mmol) was suspended in triethyl orthoformate (3 mL) in a 0.5-2 mL conical microwave vial equipped with a stir bar. The vial was sealed with a septum, transferred to a microwave reactor, and heated to 145 °C for 8 minutes. At the midpoint of the run, the average microwave power was 60 W and the average internal pressure was 1 bar. The suspension was cooled to room temperature and anhydrous ether (3 mL) was added via syringe to the septum-sealed vial. This suspension was stirred for 30 min, after which the insoluble material was separated by centrifugation. The supernatant was removed via syringe, and the product was washed three times by re-suspension/pelleting using fresh anhydrous diethyl ether (3 x 3 mL) delivered and removed from the septum-sealed vial via syringe. After removing the final wash solvent, the pellet was dried for 35 min with a gentle flow of nitrogen gas delivered via a needle inlet. The septum was removed and the vial was placed in a vacuum chamber (60 mTorr) for 12 hours. A white powder was obtained (**S11**, 87 mg, 80% yield). This preparation is based upon that reported for the analogous 1,3-diarylimidazolinium chlorides;[5] ^{1}H NMR (400 MHz, $CDCl_3$) δ1.72 (m, 5.2H), 2.26 (m, 3.5H), 2.30 (s, 6H), 4.24 (app t, J = 11.1 Hz, 2H), 4.39 (app t, J = 11.1 Hz, 2H), 6.90 ppm (s, 2H), 9.09 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ=18.17, 21.03, 28.99(m), 29.93, 35.32(m), 40.11(quintet, $^{1}J_{CD}$ = 19.9 Hz), 45.22, 50.85, 57.65, 129.88, 131.03, 135.30, 140.01, 156.71; HRMS (FAB) m/z calculated for $C_{22}H_{24}N_2D_7$ ([M]$^+$) 330.2927, found 330.2938.

[4] Literature NMR characterization of the unlabeled compound: Dinger, M.B.; Nieczypor, P.; Mol., J. C. *Organometallics*, **2003**, *22*, 5291. ^{1}H NMR (DMSO-d_6): δ 9.90 (br s, 2 H, N*H*), 6.98 (s, 2 H, C6*H*2Me3), 3.69 (br s, 2 H, C*H*2NHMes), 3.42 (br s, 2 H, AdNHC*H*2), 2.47 (s, 6 H, *o*-C*H*3), 2.22 (s, 3 H, *p*-CH3), 2.13 (br s, 3 H, *H*-Ad), 1.94 (s, 6 H, *H*-Ad), 1.63 (pseudo q, *J*H,H ~ 11.5 Hz, 6 H, *H*-Ad). ^{13}C NMR (DMSO-d_6): δ 138.0 (*i*-*C*6H2Me3), 133.4 (*p*-*C*6H2Me3), 131.5 (*m*-*C*6H2Me3), 130.2 (*o*-*C*6H2Me3), 56.6 (*C*-1 Ad), 50.0 (MesN*C*H2), 46.0 (AdN*C*H2), 37.5 (*C*-2 Ad), 35.1 (*C*-4 Ad), 28.4 (*C*H-3 Ad), 20.2 (*p*-*C*H3), 18.1 (*o*-*C*H3).

[5] Aidouni, A.; Demonceau, A.; Delaude, L. *Synlett*, **2006**, 493-495. See also Hans, M.; Delaude, L. *Org. Synth.* **2010**, *87*, 77-87.

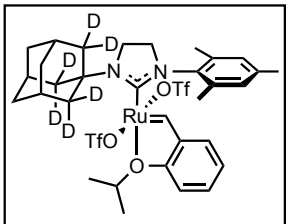
(1-(adamant-1-yl-2,2,8,8,9,9-d_6)-3-(2,4,6-trimethylphenyl)-2-imidazolidinylidene)dichloro(*o*-isopropoxyphenylmethylidene)ruthenium (4a-d_6)



4a-d_6: $C_{32}H_{36}D_6Cl_2N_2ORu$
Exact Mass: 648.2094

In a nitrogen filled glovebox, imidazolinium chloride (**S14**, 86 mg, 0.237 mmol) was weighed into a 20 mL vial with a stir bar. Potassium *tert*-amyloxide (31 mg, 0.249 mmol) was added and the solids were suspended in hexanes (5.7 mL). The mixture was stirred at ambient temperature until all of the solids had dissolved, indicating complete deprotonation of the imidazolinium. To this solution was added dichloro(*o*-isopropoxyphenylmethylene)(tricyclohexylphosphine)ruthenium(II) (136 mg, 0.226 mmol). The brown mixture was sealed, removed from the glovebox, and warmed to 60 °C. The solution was stirred until the brown color disappeared and was replaced by a green precipitate. The mixture was filtered through Celite with extra hexanes (2 mL) to collect a green solid. The solid was eluted with dichloromethane (2 mL) into a clean flask to provide 140 mg (95%) of ruthenium NHC complex **4a-d_6** as a green solid. ^{1}H NMR (500 MHz, C_6D_6) δ 17.11 (s, 1H), 7.20 (ddd, *J* = 8.6, 7.4, 1.7 Hz, 1H), 7.12 (dd, *J* = 7.6, 1.7 Hz, 1H), 6.85 (s, 2H), 6.73 (dd, *J* = 7.8, 7.0 Hz, 1H), 6.48 (d, *J* = 8.3 Hz, 1H), 4.59 (hept, *J* = 6.2 Hz, 1H), 3.36–3.25 (m, 4H), 2.34 (s, 6H), 2.29 (s, 3H), 2.24 (s, 3H), 1.89 (dt, *J* = 13.3, 3.6 Hz, 3H), 1.67 (d, *J* = 12.8 Hz, 3H), 1.57 (d, *J* = 6.1 Hz, 6H); ^{13}C NMR (126 MHz, C_6D_6) δ 209.7, 152.8, 146.4, 140.3, 138.5, 138.3, 130.0, 129.9, 127.9, 123.3, 122.5, 113.6, 74.2, 56.7, 51.1, 44.5, 41.3, 36.3, 36.3, 30.3, 30.2, 22.5, 21.2, 18.6; HRMS (FAB) m/z calculated for $C_{32}H_{37}RuON_2Cl_2D_6$ ([M+H$^+$]$^+$) 649.2193, found 649.2193.

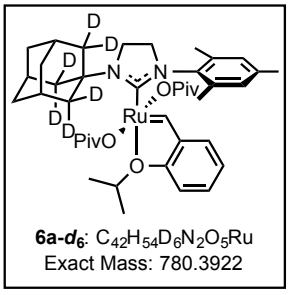
(1-(adamant-1-yl-2,2,8,8,9,9-d_6)-3-(2,4,6-trimethylphenyl)-2-imidazolidinylidene)bistriflato(*o*-isopropoxyphenylmethylidene)ruthenium (7a-d_6)



7a-d_6: $C_{34}H_{36}D_6F_6N_2O_7RuS_2$
Exact Mass: 876.1758

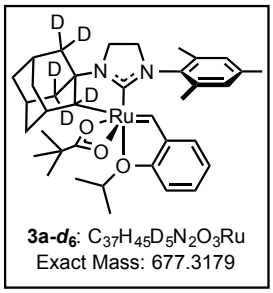
In a nitrogen filled glovebox, ruthenium dichloride **4a-d_6** (50 mg, 0.0771 mmol) and silver trifluoromethanesulfonate (79 mg, 0.308 mmol) were weighed into a 20 mL vial equipped with a stirbar. The reagents were suspended in benzene (2.6 mL) and stirred at ambient temperature for 24 hours. The reaction progress was followed by ^{1}H NMR spectroscopy. Upon completion, the reaction mixture was filtered through Celite with benzene (2 mL), concentrated, filtered through silica gel with dichloromethane (2 mL), and concentrated again to provide 45 mg (67%) of bistriflato complex **7a-d_6** as a green solid. ^{1}H NMR (500 MHz, C_6D_6) δ 18.89 (d, *J* = 0.8 Hz, 1H), 7.12 (ddd, *J* = 8.5, 7.3, 1.7 Hz, 1H), 7.09 (dd, *J* = 7.6, 1.7 Hz, 1H), 6.86 (s, 2H), 6.70 (td, *J* = 7.5, 0.8 Hz, 1H), 6.54 (d, *J* = 8.4 Hz, 1H), 4.69 (hept, *J* = 6.2 Hz, 1H), 3.23–3.11 (m, 4H), 2.37 (s, 3H), 2.21 (d, *J* = 2.6 Hz, 9H), 1.95 (d, *J* = 13.0 Hz, 3H), 1.80–1.70 (m, 3H), 1.40 (d, *J* = 6.1 Hz, 6H); ^{13}C NMR (126 MHz, C_6D_6) δ 202.3, 154.8, 147.1, 139.1, 138.8, 138.0, 133.9, 130.3, 123.2, 122.9, 117.1, 114.7, 76.1, 51.6, 44.4, 36.1, 30.0, 29.9, 21.6, 21.0, 18.1; HRMS (FAB) m/z calculated for $C_{34}H_{37}RuO_7N_2S_2F_6D_6$ ([M+H$^+$]$^+$) 877.1836, found 877.1805.

(1-(adamant-1-yl-2,2,8,8,9,9-*d*$_6$)-3-(2,4,6-trimethylphenyl)-2-imidazolidinylidene)bispivalato(*o*-isopropoxyphenylmethylidene)ruthenium (6a-*d*$_6$)



Bispivalato complex **6a-*d*$_6$** was observed while conducting kinetics experiments described above; ^{1}H NMR matched that of d_0-complex **6a**. HRMS (FAB) m/z calculated for $C_{42}H_{54}RuO_5N_2D_6Na$ ([M+Na$^+$]$^+$) 803.3820, found 803.3789.

***d*$_6$-Cyclometalated Pivalate (3a-*d*$_6$)**



Cyclometalated complex **3a-*d*$_6$** was isolated from kinetics experiments by concentrating the reaction mixture, filtering through Celite with benzene to remove excess sodium pivalate and concentrating. The crude solid was then triturated with pentanes to remove pivalic acid; ^{1}H NMR (500 MHz, C_6D_6) δ 14.86 (s, 1H), 7.47 (dd, *J* = 7.5, 1.7 Hz, 1H), 7.26 (ddd, *J* = 8.3, 7.4, 1.7 Hz, 1H), 6.90 (td, *J* = 7.4, 0.9 Hz, 1H), 6.82 (s, 1H), 6.74 (s, 1H), 6.70 (d, *J* = 8.3 Hz, 1H), 4.80 (hept, *J* = 6.5 Hz, 1H), 4.18 (s, 0H), 3.48–3.34 (m, 2H), 3.31–3.22 (m, 1H), 3.21–3.12 (m, 1H), 2.53 (s, 1H), 2.43 (s, 3H), 2.27 (s, 3H), 2.20 (s, 3H), 2.10 (s, 2H), 1.88–1.77 (m, 1H), 1.64 (s, 1H), 1.58–1.44 (m, 5H), 1.24 (s, 11H), 1.22–1.15 (m, 5H), 0.91–0.84 (m, 1H), 0.66 (d, *J* = 12.4 Hz, 1H); ^{13}C NMR (126 MHz, C_6D_6) δ 154.2, 143.8, 138.0, 137.0, 136.7, 136.4, 129.8, 129.7, 128.1, 127.7, 125.5, 123.2, 123.1, 113.9, 74.4, 51.7, 41.3, 39.5, 38.0, 30.9, 29.8, 28.4, 22.7, 21.6, 21.2, 21.0, 19.2, 18.9, 14.3; LRMS (FAB) m/z calculated for $C_{37}H_{45}RuO_3N_2D_6$ ([M–OPiv$^-$]$^+$) 576.26, found 576.30.

Part 2. Computational Results

Complete Reference of Gaussian 09

Gaussian 09, Revision B.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

Details of Computations of Rate Constants in Table 2

The rate constants *k* were calculated from transition state theory,

$$k = A\frac{k_B T}{h} e^{\frac{-\Delta G^{\ddagger}}{RT}} \quad (A = 1)$$

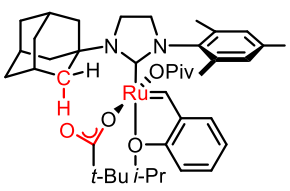
whereas $\Delta G^{\ddagger}$ at 313K were used (see below).

entry	**4**	$\Delta G^{\ddagger}_{313K}$ from **6** (kcal/mol)	calculated *k* from **6** (sec^{-1})
1	**4a**	23.5	2.7×10^{-4}
2	**4b**	25.6	8.4×10^{-6}
3	**4c**	15.2	165
4	**4d**	23.5	2.6×10^{-4}

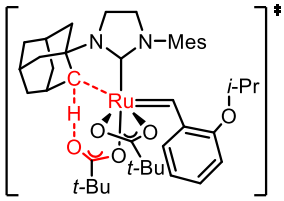
Charge Analysis of 6a and 12a-TS

Charge analysis shows polarization of the C-H bond and increased positive charge on the carboxylate carbon, as in Table S1.

Table S1. NPA charges of dicarboxylate **6a** and C-H activation transition state structure **12a-TS**



6a



12a-TS

	6a	**12a-TS**
Ru	+0.19	+0.03
C	-0.38	-0.47
H	+0.23	+0.46
O	-0.72	-0.75
C(C=O)	+0.85	+0.89

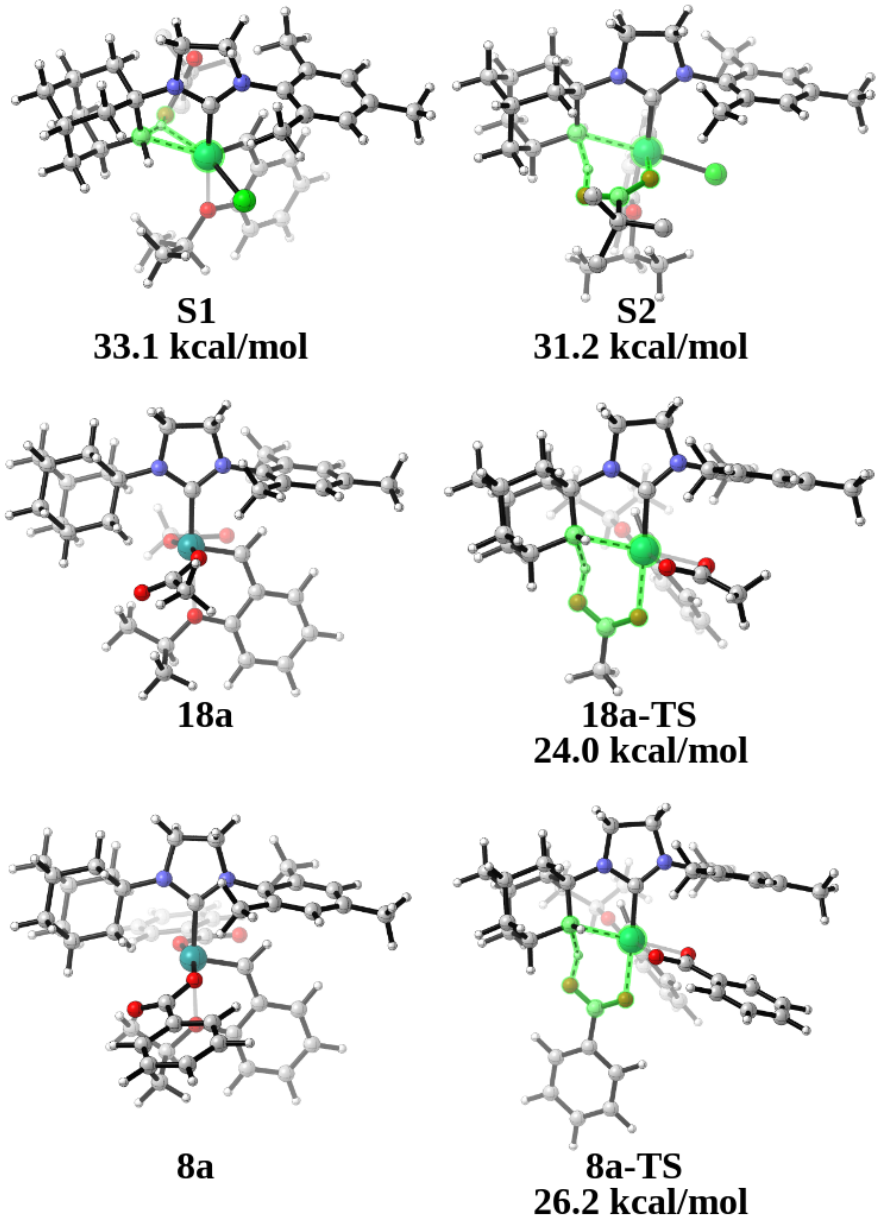


Figure S1. Four-membered (**S1**) and six-membered (**S2**), side-attack C-H activation transition state for monochloro, monopivalate substrate, diacetate **18a** and the corresponding C-H activation transition state **18a-TS**, dibenzoate **8a** and the corresponding C-H activation transition state **8a-TS**.

Data sheet for Complexes and Transition State Geometries

Table S2. Energies in solvation, E(Solv), and thermal corrections to enthalpy (TCH) and Gibbs free energies (TCG) at 298K

	E(Solv)	TCH	TCG
03a-epi	-1869.37864600	0.851700	0.732280
03a	-1869.38476169	0.851373	0.732382
04a	-2444.14717697	0.725122	0.615594
05a	-2330.23014205	0.868057	0.741943
06a	-2216.31832920	1.011048	0.869425
06b	-2175.80908361	0.952833	0.805210
06b-TS	-2175.76144430	0.946573	0.798423
06c	-1984.15813308	0.897619	0.760840
06c-TS	-1984.12548578	0.891037	0.752465
06d	-2334.18729189	1.101439	0.954810
06d-TS	-2334.14417225	1.095097	0.949076
08a	-2363.83909020	0.945826	0.805915
08a-ts	-2363.79182503	0.939171	0.800348
12a-ts	-2216.29801603	1.009455	0.870100
13a	-2216.30417093	1.010139	0.865891
14a-tsA	-2216.27388006	1.004554	0.862389
14a-tsB	-2216.26807284	1.005471	0.867582
14a-tsC	-2216.25046870	1.004130	0.861255
14a-tsD	-2216.26446321	1.004492	0.864077
14a-tsE	-2216.27110069	1.004503	0.862999
14a-tsF	-2216.26590497	1.004704	0.861097
15a	-2216.30518822	1.010013	0.866241
16a-ts	-2330.17657440	0.860968	0.733686
17a	-2330.20989960	0.866698	0.738169
18a	-1980.56126095	0.833411	0.708765
18a-ts	-1980.51528189	0.826316	0.701062
19	-1869.37741863	0.851780	0.733992
s1	-2330.17125327	0.861045	0.735743
s2	-2330.17575035	0.861844	0.737290

The Cartesian Coordinates (Å) for Complexes and Transition State Geometries

3a-epi

Ru	-0.39513	0.27672	-0.12367
O	-1.23657	2.59841	0.45421
O	-0.24126	-0.58334	2.15327
O	1.34998	0.67141	1.28422
N	-0.73977	-2.25821	-1.42969
N	1.40499	-1.78624	-1.53683
C	0.20343	-1.34974	-1.06045
C	-0.15959	-3.49662	-1.95056
H	-0.71694	-3.87128	-2.81362
H	-0.14877	-4.28215	-1.18075
C	1.25920	-3.03272	-2.31879
H	2.03338	-3.75547	-2.04797
H	1.35507	-2.81725	-3.39192
C	-2.06751	-2.12341	-0.81643
C	-2.09841	-2.81758	0.56988
H	-1.28389	-2.43073	1.18928
H	-1.94770	-3.90071	0.44476
C	-3.45156	-2.55142	1.25584
H	-3.46311	-3.04683	2.23592
C	-4.59047	-3.10807	0.37899
H	-4.48288	-4.19640	0.26371
H	-5.56267	-2.93280	0.86046
C	-4.55537	-2.41829	-1.00034
H	-5.36454	-2.81027	-1.63131
C	-3.19801	-2.71367	-1.68703
H	-3.16752	-2.26455	-2.68887
H	-3.08170	-3.80156	-1.81023
C	-4.74606	-0.89797	-0.79760
H	-4.77336	-0.38439	-1.76829
H	-5.71523	-0.71427	-0.31067
C	-3.58828	-0.33068	0.06791
H	-3.73381	0.75024	0.19325
C	-2.27847	-0.59469	-0.70138
H	-2.45005	-0.24295	-1.72384
C	-3.61182	-1.02869	1.44380
H	-2.80010	-0.65532	2.07571
H	-4.56064	-0.81228	1.95672
C	-0.27607	1.24392	-1.70846
H	0.03185	0.82295	-2.67247
C	-0.61408	2.65317	-1.81009
C	-1.08125	3.36358	-0.67505
C	0.87538	0.00801	2.26238
C	-1.47613	3.25680	1.73469
H	-2.19589	4.06322	1.55902
C	1.63899	-0.05062	3.60597
C	1.65303	-1.50463	4.12033
H	2.10566	-1.54573	5.11885
H	0.63641	-1.90261	4.17968
H	2.23614	-2.15756	3.46317
C	0.87512	0.81571	4.63371
H	0.84517	1.86846	4.33282
H	-0.15345	0.46169	4.75640
H	1.37450	0.76243	5.60909
C	3.07285	0.47844	3.44532
H	3.60420	0.42129	4.40393
H	3.63124	-0.10299	2.70503
H	3.07558	1.51945	3.10935
C	-2.13277	2.23509	2.65046
H	-3.09860	1.92194	2.24339
H	-1.51011	1.34644	2.77602
H	-2.30475	2.68851	3.63321
C	-0.15940	3.82185	2.26066
H	0.58469	3.02363	2.32744
H	0.23429	4.59628	1.59463
H	-0.30562	4.26555	3.25193
C	-0.48390	3.35741	-3.02412
C	-1.36615	4.72871	-0.76022
H	-0.13435	2.81156	-3.89743
H	-1.70318	5.29025	0.10197
C	-0.78111	4.71331	-3.11938
C	-1.21628	5.39379	-1.98125
H	-1.44516	6.45486	-2.03269
H	-0.66972	5.23661	-4.06454
C	2.71457	-1.25796	-1.27921
C	3.42487	-1.76557	-0.17098
C	3.31909	-0.35074	-2.16374
C	4.72276	-1.30995	0.06102
C	4.62442	0.08001	-1.88786
C	5.33773	-0.37332	-0.77925
H	5.27187	-1.70016	0.91574
H	5.09403	0.78645	-2.56995
C	2.63098	0.17034	-3.40306
H	2.25153	1.18604	-3.24082
H	3.33376	0.21438	-4.24280
H	1.78247	-0.45111	-3.69910
C	2.81346	-2.80994	0.73225
H	1.83495	-2.50055	1.11117

H	2.66892	-3.76478	0.20885
H	3.46606	-3.00729	1.58765
C	6.73084	0.13212	-0.48501
H	7.37478	-0.66583	-0.09809
H	7.20498	0.54677	-1.38071
H	6.70986	0.92643	0.27279

3a

Ru	0.37617	0.14022	-0.12421
O	1.37393	2.41322	-0.14100
O	-0.94384	0.46691	-2.15291
O	-1.58436	1.25836	-0.19672
N	0.73299	-2.70390	0.11320
N	-1.33301	-2.28172	0.73007
C	-0.18882	-1.71665	0.25230
C	0.30356	-3.98726	0.66946
H	0.83638	-4.20664	1.60445
H	0.49215	-4.81088	-0.02663
C	-1.19745	-3.74407	0.90944
H	-1.82413	-4.27749	0.18563
H	-1.52338	-4.03650	1.91282
C	2.11802	-2.33167	-0.17982
C	2.81091	-3.32962	-1.13751
H	2.21857	-3.42595	-2.05695
H	2.88176	-4.33148	-0.68673
C	4.23209	-2.80619	-1.45860
H	4.71737	-3.49944	-2.15859
C	5.05683	-2.71973	-0.15802
H	5.15008	-3.71439	0.30117
H	6.07560	-2.37561	-0.38357
C	4.36943	-1.74688	0.82099
H	4.94523	-1.69377	1.75486
C	2.94897	-2.25697	1.12634
H	3.00126	-3.25238	1.59104
H	2.45092	-1.58683	1.83321
C	4.26229	-0.34321	0.19131
H	5.26749	0.04984	-0.01938
H	3.78260	0.34646	0.89615
C	3.44397	-0.42409	-1.11195
H	3.40075	0.56694	-1.57590
C	2.01627	-0.95048	-0.86808
H	1.56631	-1.12954	-1.86433
C	4.15301	-1.39945	-2.08930
H	3.60446	-1.43887	-3.04020
H	5.16789	-1.04275	-2.31915
C	-2.66049	-1.73124	0.74792
C	-3.46360	-1.84596	-0.40397
C	-4.79776	-1.43491	-0.32419
H	-5.42778	-1.53020	-1.20633
C	-5.34359	-0.90982	0.85244
C	-4.51569	-0.80351	1.97224
H	-4.92115	-0.39919	2.89753
C	-3.17681	-1.20915	1.94509
C	-2.90811	-2.37130	-1.70856
H	-2.10974	-1.71983	-2.08107
H	-3.69377	-2.41337	-2.46904
H	-2.49274	-3.38163	-1.61317
C	-6.78138	-0.44655	0.90006
H	-7.18692	-0.49985	1.91605
H	-7.42018	-1.05100	0.24668
H	-6.87127	0.59624	0.56750
C	-2.32031	-1.06285	3.17915
H	-1.70867	-1.95217	3.36702
H	-2.94051	-0.88231	4.06280
H	-1.63246	-0.21646	3.07099
C	0.82054	0.43541	1.65347
H	0.68602	-0.27621	2.47849
C	1.15053	1.77783	2.11319
C	1.17437	2.10820	3.48182
H	1.00424	1.31318	4.20415
C	1.38451	3.41425	3.91564
H	1.39364	3.64614	4.97666
C	1.56473	4.42413	2.96992
H	1.71047	5.45267	3.28872
C	1.56333	4.13275	1.60169
H	1.70291	4.93848	0.89189
C	1.37900	2.81660	1.17429
C	1.82299	3.34102	-1.17709
H	1.22910	4.25643	-1.06231
C	3.31572	3.64660	-1.03313
H	3.90044	2.73029	-1.15966
H	3.56928	4.08103	-0.06370
H	3.61632	4.35496	-1.81343
C	1.51206	2.71652	-2.53030
H	2.16898	1.86533	-2.73107
H	1.67884	3.46634	-3.31210
H	0.48299	2.36349	-2.59213
C	-1.74596	1.15996	-1.45377
C	-2.88839	1.94727	-2.13322
C	-3.53799	1.08190	-3.22878
H	-4.04676	0.21439	-2.79472
H	-2.78484	0.71824	-3.93300

H	-4.28413	1.66671	-3.78159
C	-3.93839	2.38234	-1.09744
H	-4.74347	2.94127	-1.59220
H	-3.49331	3.02099	-0.32929
H	-4.37651	1.51601	-0.59283
C	-2.26785	3.20278	-2.78895
H	-3.05591	3.81281	-3.24774
H	-1.55292	2.92836	-3.57139
H	-1.75198	3.82371	-2.04667

4a

Ru	-0.08023	0.58100	0.01346
O	-0.70564	2.94347	-0.06441
N	1.66139	-1.83467	0.20683
N	-0.44582	-2.45764	0.13623
C	0.37964	-1.37200	0.10900
C	1.71345	-3.29884	0.39886
H	2.02745	-3.53292	1.42204
H	2.42408	-3.76206	-0.29066
C	0.27892	-3.73709	0.13231
H	0.15982	-4.23793	-0.83690
H	-0.11382	-4.40196	0.90719
C	2.96439	-1.12727	0.04837
C	3.49881	-1.33774	-1.39405
H	2.77499	-0.91896	-2.10178
H	3.58823	-2.41187	-1.60783
C	4.87749	-0.66255	-1.55846
H	5.23510	-0.83037	-2.58256
C	5.87639	-1.26727	-0.55108
H	5.99718	-2.34410	-0.73624
H	6.86697	-0.80968	-0.67805
C	5.36641	-1.02997	0.88597
H	6.06754	-1.47265	1.60557
C	3.99084	-1.70767	1.06041
H	3.61678	-1.56036	2.08224
H	4.11636	-2.78574	0.90915
C	5.23457	0.48114	1.14602
H	4.89521	0.66200	2.17490
H	6.21124	0.97243	1.03762
C	4.22882	1.07154	0.14142
H	4.10623	2.14516	0.32970
C	2.85535	0.38376	0.32430
H	2.47644	0.55345	1.33628
C	4.73588	0.85032	-1.29768
H	4.03532	1.29219	-2.01766
H	5.70413	1.35112	-1.43583
C	-1.87669	-2.54286	0.09090
C	-2.52286	-2.66570	-1.15372
C	-3.91441	-2.81725	-1.16010
H	-4.42622	-2.90036	-2.11662
C	-4.66131	-2.86047	0.02219
C	-3.98193	-2.74496	1.23999
H	-4.54643	-2.77296	2.16974
C	-2.59255	-2.59472	1.30190
C	-1.75715	-2.58181	-2.45323
H	-1.03280	-3.39986	-2.55572
H	-1.19568	-1.64350	-2.53193
H	-2.44113	-2.64338	-3.30511
C	-6.15954	-3.05865	-0.01177
H	-6.65417	-2.51960	0.80357
H	-6.42131	-4.11984	0.09667
H	-6.58904	-2.71335	-0.95806
C	-1.89232	-2.46417	2.63313
H	-1.14891	-3.25864	2.77956
H	-2.61271	-2.53129	3.45408
H	-1.36140	-1.50900	2.71699
C	-1.92144	0.54236	-0.15742
H	-2.51035	-0.36949	-0.20753
C	-2.69982	1.75327	-0.26516
C	-4.09851	1.71241	-0.43500
H	-4.58270	0.74027	-0.48147
C	-4.84324	2.88114	-0.54178
H	-5.92031	2.83862	-0.67189
C	-4.18800	4.11430	-0.47750
H	-4.75821	5.03596	-0.55751
C	-2.80271	4.19323	-0.30816
H	-2.32944	5.16558	-0.25701
C	-2.05929	3.01545	-0.20668
C	0.07673	4.15687	0.15371
H	-0.30010	4.90777	-0.54998
C	1.51399	3.82482	-0.21221
H	1.93529	3.11747	0.50751
H	2.11508	4.74069	-0.18844
H	1.56568	3.38846	-1.21373
C	-0.08083	4.62327	1.59851
H	-1.11929	4.87321	1.83566
H	0.53280	5.51546	1.76859
H	0.24303	3.82837	2.27710
H	2.16813	0.84696	-0.39885
Cl	0.07821	0.82000	2.42783
Cl	0.42961	0.71011	-2.37073

5a

Ru	-0.09315	0.29768	-0.43993
O	-0.60075	2.63928	-1.14913
O	1.45104	2.46251	1.33450
O	0.00562	0.75818	1.61711
N	1.45500	-2.23265	-0.09847
N	-0.69375	-2.66996	0.05442
C	0.21131	-1.65831	-0.09453
C	1.36178	-3.70082	-0.23006
H	2.11597	-4.21159	0.36858
H	1.49300	-3.99149	-1.28021
C	-0.05082	-3.97800	0.25393
H	-0.56099	-4.75399	-0.32220
H	-0.08450	-4.25815	1.31613
C	2.79553	-1.60709	-0.26337
C	3.37916	-1.89352	-1.67206
H	2.69807	-1.48850	-2.42875
H	3.45364	-2.97673	-1.83729
C	4.78454	-1.26439	-1.80064
H	5.17611	-1.48066	-2.80300
C	5.72272	-1.86632	-0.73444
H	5.81600	-2.95194	-0.88019
H	6.73160	-1.44370	-0.83626
C	5.16478	-1.56448	0.67228
H	5.82095	-2.00604	1.43394
C	3.75975	-2.18811	0.80954
H	3.34668	-1.99439	1.80826
H	3.85192	-3.27518	0.70015
C	5.07418	-0.04127	0.87639
H	4.69751	0.18716	1.88264
H	6.07083	0.41351	0.79544
C	4.13265	0.55031	-0.18834
H	4.02683	1.62939	-0.03276
C	2.73424	-0.08812	-0.04528
H	2.32879	0.13510	0.94202
C	4.68868	0.26097	-1.59648
H	4.03551	0.70307	-2.35988
H	5.67953	0.72125	-1.71312
C	-2.10806	-2.61900	0.28670
C	-2.97363	-2.91944	-0.78129
C	-4.35020	-2.93687	-0.53021
H	-5.02938	-3.15636	-1.35140
C	-4.87334	-2.67604	0.74103
C	-3.98049	-2.38523	1.77861
H	-4.37034	-2.17425	2.77235
C	-2.59597	-2.35796	1.58096
C	-2.44079	-3.16831	-2.17271
H	-1.85467	-4.09544	-2.22495
H	-1.78374	-2.35568	-2.50359
H	-3.26353	-3.26221	-2.88800
C	-6.36204	-2.73585	0.99624
H	-6.66866	-2.00817	1.75543
H	-6.66162	-3.72818	1.35941
H	-6.93436	-2.53763	0.08396
C	-1.66575	-2.01167	2.71902
H	-0.91406	-2.79365	2.88524
H	-2.22859	-1.89371	3.65029
H	-1.12457	-1.07881	2.52080
C	-1.94253	0.36530	-0.52082
H	-2.59160	-0.46973	-0.26907
C	-2.65565	1.54497	-0.94197
C	-4.06311	1.53936	-1.04323
H	-4.59282	0.63044	-0.76916
C	-4.75733	2.65465	-1.49375
H	-5.84019	2.63775	-1.57092
C	-4.03998	3.80015	-1.85215
H	-4.56802	4.68032	-2.20946
C	-2.64703	3.84617	-1.75750
H	-2.12981	4.75510	-2.03495
C	-1.95027	2.72370	-1.29731
C	0.24247	3.75538	-1.59987
H	-0.20855	4.12012	-2.52939
C	1.62091	3.19351	-1.90572
H	2.07308	2.81515	-0.98621
H	2.25060	3.99748	-2.30477
H	1.55596	2.39158	-2.64568
C	0.27407	4.84762	-0.53349
H	-0.72723	5.21723	-0.29099
H	0.86820	5.69413	-0.89773
H	0.73642	4.45212	0.37438
C	0.68170	1.79052	2.03303
C	0.47977	2.11136	3.53790
C	1.02223	0.92732	4.36731
H	2.09153	0.77044	4.17727
H	0.49335	0.00072	4.12615
H	0.90010	1.12632	5.43956
C	1.24465	3.39227	3.90591
H	2.31140	3.29293	3.68533
H	1.12733	3.60708	4.97563
H	0.87231	4.25291	3.34085
C	-1.02499	2.29689	3.82150
H	-1.18808	2.51984	4.88373

H	-1.58810	1.39561	3.56458
H	-1.43555	3.13033	3.23827
H	2.09725	0.38191	-0.81273
Cl	0.24662	-0.15120	-2.82372

6a

Ru	0.03286	0.25428	0.22681
O	0.52313	1.64096	2.23171
O	-1.29696	3.12914	-0.00297
O	0.29596	1.92736	-1.04651
N	-1.44942	-1.33763	-1.80829
N	0.71069	-1.70549	-2.04530
C	-0.21072	-0.99738	-1.31927
C	-1.37288	-2.47940	-2.74049
H	-2.02145	-2.33960	-3.60503
H	-1.66968	-3.40669	-2.23222
C	0.09592	-2.48773	-3.12902
H	0.52485	-3.49208	-3.17595
H	0.27425	-1.99625	-4.09507
C	-2.79452	-0.93996	-1.30627
C	-3.36619	-1.99486	-0.32530
H	-2.68220	-2.08673	0.52448
H	-3.42425	-2.97614	-0.81607
C	-4.77657	-1.57144	0.14643
H	-5.16067	-2.33085	0.84005
C	-5.71883	-1.45286	-1.06889
H	-5.80302	-2.42168	-1.58161
H	-6.72975	-1.17884	-0.73804
C	-5.17358	-0.38470	-2.03939
H	-5.83000	-0.31218	-2.91653
C	-3.76636	-0.80294	-2.51291
H	-3.36243	-0.06860	-3.22298
H	-3.85793	-1.75682	-3.04450
C	-5.09574	0.97700	-1.32782
H	-4.72792	1.74748	-2.01885
H	-6.09486	1.29217	-0.99752
C	-4.15132	0.85181	-0.11918
H	-4.05368	1.82131	0.38165
C	-2.74699	0.42549	-0.60083
H	-2.32706	1.18435	-1.26332
C	-4.69638	-0.20653	0.86077
H	-4.04426	-0.27793	1.74054
H	-5.69158	0.08926	1.22002
C	2.14300	-1.58489	-2.12751
C	2.93822	-2.60806	-1.57450
C	4.32589	-2.53023	-1.74026
H	4.94630	-3.31301	-1.30892
C	4.93221	-1.48260	-2.44013
C	4.10841	-0.50426	-3.00524
H	4.55803	0.30581	-3.57583
C	2.71582	-0.53821	-2.87559
C	2.33678	-3.74045	-0.77664
H	1.53314	-4.25170	-1.31979
H	1.91581	-3.37077	0.16569
H	3.10170	-4.48632	-0.53860
C	6.43532	-1.40398	-2.57703
H	6.87331	-0.77398	-1.79130
H	6.72784	-0.96889	-3.53896
H	6.89804	-2.39326	-2.49648
C	1.86886	0.52856	-3.52508
H	1.12089	0.09712	-4.20287
H	2.49539	1.20404	-4.11621
H	1.33023	1.11930	-2.77627
C	1.82679	-0.07202	0.57405
H	2.44117	-0.76810	0.01291
C	2.54500	0.63290	1.61518
C	3.92639	0.43568	1.80055
H	4.43975	-0.25138	1.13300
C	4.61826	1.08686	2.81586
H	5.68421	0.92728	2.94740
C	3.92008	1.94092	3.67250
H	4.44384	2.45181	4.47618
C	2.54764	2.15864	3.51936
H	2.04162	2.83033	4.20027
C	1.86051	1.51435	2.48651
C	-0.32533	2.35599	3.19034
H	0.04903	2.08677	4.18523
C	-1.73947	1.82154	3.02350
H	-2.12621	2.11307	2.04410
H	-2.38124	2.25219	3.80086
H	-1.75441	0.73232	3.11227
C	-0.24336	3.86387	2.96319
H	0.78280	4.23731	3.02926
H	-0.84088	4.37798	3.72554
H	-0.64551	4.10215	1.97556
C	-0.37749	3.01694	-0.82697
C	0.02486	4.21247	-1.73254
C	-0.45719	3.90481	-3.16794
H	-1.54637	3.77604	-3.19643
H	0.00550	2.99208	-3.55518
H	-0.20080	4.73224	-3.84175
C	-0.65121	5.49867	-1.23159

H	-1.73865	5.38847	-1.20261
H	-0.40058	6.33835	-1.89225
H	-0.31953	5.75234	-0.21893
C	1.55628	4.38782	-1.72425
H	1.84664	5.22839	-2.36760
H	2.06058	3.48635	-2.08100
H	1.92289	4.59944	-0.71233
H	-2.13001	0.37419	0.31005
O	-0.66627	-1.16749	1.59108
C	0.09315	-2.03944	2.18925
O	1.30283	-2.19310	1.98264
C	-0.62306	-2.97050	3.20700
C	-1.92978	-2.36281	3.74113
H	-2.39768	-3.05125	4.45647
H	-1.74340	-1.41655	4.26158
H	-2.64589	-2.16679	2.93874
C	-0.92579	-4.29388	2.46692
H	-1.39864	-5.01171	3.14878
H	-1.60739	-4.13159	1.62343
H	-0.00367	-4.74220	2.08215
C	0.33587	-3.25179	4.37939
H	1.28079	-3.66221	4.01629
H	0.56158	-2.33278	4.93344
H	-0.11786	-3.96495	5.07906

6b-TS

Ru	0.56407	0.12606	0.01509
O	-3.61685	1.29745	-1.53486
O	2.60601	-0.26462	1.21917
O	0.59543	-0.29601	2.12251
N	-0.41065	-2.76306	-0.64973
N	1.65970	-2.31741	-1.22772
C	0.55308	-1.80550	-0.61489
C	0.07225	-4.03014	-1.23270
H	-0.65911	-4.44204	-1.93303
H	0.23908	-4.76865	-0.43727
C	1.37503	-3.59738	-1.90712
H	2.18020	-4.32000	-1.76872
H	1.25061	-3.42136	-2.98456
C	2.78417	-1.52273	-1.63010
C	4.08711	-2.01047	-1.44278
C	5.16012	-1.22905	-1.88870
H	6.17216	-1.60148	-1.74295
C	4.96951	0.02083	-2.48091
C	3.66103	0.49546	-2.61410
H	3.48951	1.47931	-3.04619
C	2.55265	-0.25230	-2.20110
C	4.36599	-3.31477	-0.73185
H	5.36721	-3.29819	-0.29016
H	4.33126	-4.18150	-1.40708
H	3.64557	-3.48816	0.07417
C	6.14176	0.83919	-2.97117
H	6.01743	1.90086	-2.72963
H	6.25156	0.76737	-4.06190
H	7.08192	0.49900	-2.52442
C	1.17462	0.32460	-2.29424
H	0.41719	-0.39982	-2.60000
H	1.16173	1.08323	-3.09098
H	0.93863	1.51316	-1.56871
C	-1.24959	0.41687	-0.39033
H	-1.64746	0.08715	-1.35479
C	-2.22612	1.16560	0.38023
C	-2.00006	1.49426	1.73655
H	-1.07944	1.14933	2.19158
C	-2.92921	2.21439	2.47831
H	-2.73526	2.44550	3.52157
C	-4.11491	2.63213	1.87083
H	-4.85101	3.19634	2.43843
C	-4.37933	2.33250	0.53314
H	-5.31031	2.66841	0.09300
C	-3.44904	1.60474	-0.21951
C	-4.73972	1.79949	-2.28463
H	-4.95497	2.82254	-1.95115
C	-5.96564	0.90801	-2.08053
H	-5.75637	-0.10565	-2.44012
H	-6.82119	1.30206	-2.64087
H	-6.24692	0.84267	-1.02539
C	-4.28158	1.84224	-3.73889
H	-3.40064	2.48225	-3.84555
H	-5.07999	2.23552	-4.37760
H	-4.02188	0.83724	-4.08938
C	1.87919	-0.31964	2.24180
C	2.51046	-0.42155	3.63913
C	3.31088	-1.74133	3.69739
H	4.05506	-1.77529	2.89629
H	2.65076	-2.61115	3.59044
H	3.82806	-1.82902	4.66083
C	3.47610	0.77136	3.80586
H	4.22689	0.77303	3.01107
H	3.98641	0.71231	4.77530
H	2.93399	1.72340	3.76358
C	1.44404	-0.39647	4.74500

H	1.92477	-0.46188	5.72922
H	0.74551	-1.23397	4.65051
H	0.85928	0.52820	4.71045
O	0.86677	2.16254	0.73082
C	1.00494	3.06210	-0.14203
O	0.98991	2.81768	-1.39605
C	1.20498	4.52311	0.29096
C	1.14515	4.65255	1.82043
H	1.27983	5.70170	2.11140
H	0.18218	4.30666	2.20867
H	1.92878	4.05793	2.29991
C	2.58277	4.98718	-0.23131
H	2.75164	6.03730	0.03642
H	3.39188	4.39191	0.20839
H	2.63943	4.89094	-1.31945
C	0.09182	5.37417	-0.35830
H	0.11651	5.28322	-1.44788
H	-0.89907	5.05898	-0.01006
H	0.22354	6.42990	-0.09158
C	-1.72691	-2.72411	-0.07637
C	-1.90576	-2.98062	1.29661
C	-2.83156	-2.54022	-0.93012
C	-3.20849	-2.98772	1.80357
C	-4.11447	-2.55434	-0.37313
C	-4.32470	-2.76286	0.99200
H	-3.35262	-3.17814	2.86503
H	-4.97029	-2.39998	-1.02728
C	-2.66940	-2.36519	-2.42257
H	-2.62254	-3.33576	-2.93661
H	-3.51932	-1.81848	-2.84178
H	-1.75730	-1.81885	-2.67705
C	-0.73614	-3.23875	2.21326
H	-0.03215	-3.96329	1.78679
H	-0.18568	-2.31014	2.39555
H	-1.08249	-3.63337	3.17374
C	-5.71621	-2.73012	1.57967
H	-5.80408	-3.40124	2.44097
H	-5.97181	-1.72046	1.92789
H	-6.47190	-3.02225	0.84250

6b

Ru	-0.12906	0.11926	0.22928
O	-0.15742	0.54563	2.60844
O	-1.91037	2.42639	0.60372
O	0.19029	2.19338	-0.11729
N	-1.09221	-0.35104	-2.50792
N	1.09487	-0.29438	-2.58581
C	0.02980	-0.23933	-1.73504
C	-0.82126	-0.37205	-3.95382
H	-1.19748	0.54560	-4.42247
H	-1.32107	-1.22294	-4.42783
C	0.70676	-0.47186	-4.00003
H	1.05655	-1.44327	-4.36930
H	1.16674	0.30616	-4.61746
C	2.50612	-0.28241	-2.31366
C	3.18712	-1.50300	-2.14271
C	4.57432	-1.46377	-1.95474
H	5.10654	-2.40151	-1.80961
C	5.28804	-0.26194	-1.94185
C	4.57936	0.92967	-2.12982
H	5.11670	1.87588	-2.12587
C	3.19565	0.94487	-2.32966
C	2.45777	-2.82412	-2.08496
H	1.70943	-2.92474	-2.87847
H	1.93849	-2.93427	-1.12487
H	3.16355	-3.65487	-2.18377
C	6.78904	-0.24956	-1.76468
H	7.11630	0.61656	-1.17897
H	7.30266	-0.19676	-2.73412
H	7.14081	-1.15457	-1.25861
C	2.46628	2.24932	-2.53548
H	1.94280	2.27279	-3.50058
H	3.16991	3.08777	-2.52320
H	1.71674	2.40796	-1.75299
C	1.60903	-0.27359	0.71846
H	2.38483	-0.63727	0.05142
C	2.05159	-0.03137	2.07957
C	3.39399	-0.22094	2.45471
H	4.09726	-0.55159	1.69503
C	3.81398	-0.00499	3.76354
H	4.85334	-0.15449	4.04007
C	2.88021	0.39921	4.71986
H	3.19217	0.56776	5.74720
C	1.53754	0.59708	4.38256
H	0.84144	0.91799	5.14682
C	1.12476	0.38874	3.06469
C	-1.25463	0.73053	3.56591
H	-1.00100	0.11650	4.43784
C	-2.52457	0.19322	2.92273
H	-2.80598	0.81019	2.06557
H	-3.33439	0.22112	3.66150
H	-2.38268	-0.83530	2.58587

C	-1.37701	2.20222	3.95209
H	-0.44174	2.60733	4.35042
H	-2.15129	2.31487	4.72012
H	-1.67090	2.78124	3.07335
C	-0.81507	2.91183	0.27269
C	-0.56345	4.44163	0.30402
C	-0.25139	4.93753	-1.12442
H	-1.08946	4.74710	-1.80521
H	0.63741	4.44666	-1.53011
H	-0.07004	6.01971	-1.11434
C	-1.80504	5.17303	0.83864
H	-2.68601	4.96382	0.22429
H	-1.63119	6.25652	0.83788
H	-2.04090	4.86747	1.86278
C	0.65034	4.72670	1.21420
H	0.85552	5.80435	1.24686
H	1.54262	4.21203	0.84732
H	0.46405	4.39033	2.24106
O	-0.86179	-1.75353	0.76765
C	-0.10619	-2.75500	1.11240
O	1.12822	-2.78983	1.01128
C	-0.83022	-3.99062	1.71650
C	-2.35718	-3.83366	1.76649
H	-2.81258	-4.75506	2.15219
H	-2.65550	-3.01211	2.42457
H	-2.77817	-3.63060	0.77828
C	-0.45326	-5.22210	0.86509
H	-0.87021	-6.13435	1.30978
H	-0.84705	-5.13831	-0.15516
H	0.63345	-5.32693	0.80395
C	-0.28103	-4.18217	3.14760
H	0.80635	-4.29501	3.13153
H	-0.52523	-3.32144	3.78274
H	-0.72261	-5.07512	3.60774
C	-2.45744	-0.38900	-2.05976
C	-3.05063	-1.64566	-1.81522
C	-3.21563	0.79359	-2.00706
C	-4.39121	-1.68397	-1.43104
C	-4.55552	0.70344	-1.60836
C	-5.15655	-0.51767	-1.30161
H	-4.85336	-2.64940	-1.23550
H	-5.14152	1.61777	-1.54438
C	-6.59338	-0.58545	-0.83934
H	-7.10112	-1.47259	-1.23445
H	-6.65253	-0.63973	0.25576
H	-7.15824	0.29846	-1.15330
C	-2.65643	2.12698	-2.43941
H	-1.57412	2.18031	-2.31045
H	-2.88223	2.31173	-3.49960
H	-3.10450	2.93614	-1.85826
C	-2.27272	-2.92372	-2.01000
H	-1.92602	-3.03159	-3.04616
H	-1.39378	-2.95011	-1.36247
H	-2.89585	-3.79363	-1.78159

6c-TS

Ru	-0.00376	0.25701	-0.76142
O	3.25967	-2.07841	1.41355
O	-1.77545	1.66332	-1.52124
O	-1.36726	1.18577	0.59011
N	-0.42597	-2.28130	-2.10763
N	-1.98654	-2.13581	-0.57706
C	-0.94396	-1.48135	-1.14853
C	-1.08419	-3.58920	-2.20752
H	-0.38204	-4.40028	-1.97893
H	-1.47682	-3.76036	-3.21513
C	-2.20582	-3.47583	-1.15704
H	-3.20508	-3.54344	-1.60101
H	-2.13542	-4.24296	-0.37781
C	0.71570	-1.87305	-2.94775
C	0.40381	-2.21975	-4.42040
H	-0.54061	-1.76321	-4.73695
H	0.34424	-3.30165	-4.59152
C	1.99855	-2.61285	-2.51398
H	2.29283	-2.34009	-1.49758
H	1.86528	-3.70088	-2.55994
C	0.88485	-0.35055	-2.80535
C	1.09703	-0.69556	0.43127
H	1.22797	-1.77672	0.31459
C	1.84813	-0.18838	1.56949
C	2.96076	-0.92732	2.07854
C	-1.97189	1.89351	-0.29508
O	1.08615	2.16048	-0.50901
C	2.24802	2.18278	-1.00410
O	2.73303	1.20988	-1.67488
H	1.71715	0.35781	-1.90614
C	3.13809	3.42356	-0.81600
C	4.37119	-2.90569	1.80780
H	4.40910	-2.95006	2.90406
C	-2.85884	3.06282	0.15352
C	-4.13763	3.09637	-0.70416
H	-4.72868	3.98917	-0.46544

H	-3.89013	3.11461	-1.76893
H	-4.76324	2.21713	-0.51221
C	-2.03737	4.35066	-0.09561
H	-1.09537	4.32812	0.46303
H	-1.79841	4.45815	-1.15829
H	-2.61041	5.22961	0.22508
C	-3.21435	2.94854	1.64479
H	-3.84926	3.79247	1.94292
H	-3.75458	2.01902	1.85180
H	-2.31538	2.95555	2.26756
C	3.43812	4.00672	-2.21470
H	3.92213	3.26084	-2.85177
H	2.51754	4.33705	-2.71101
H	4.10261	4.87478	-2.12527
C	2.43793	4.47581	0.05670
H	2.20918	4.07531	1.04908
H	3.08806	5.35097	0.17889
H	1.49694	4.80460	-0.39439
C	4.45685	2.97494	-0.14914
H	5.12711	3.83519	-0.03036
H	4.27096	2.54971	0.84403
H	4.96304	2.21913	-0.75622
C	4.05907	-4.29854	1.27021
H	3.11651	-4.67013	1.68428
H	3.97289	-4.27578	0.17836
H	4.85816	-4.99743	1.53997
C	5.67908	-2.34116	1.25218
H	5.64295	-2.32109	0.15763
H	5.85956	-1.32142	1.60426
H	6.52500	-2.96617	1.56046
C	1.49062	1.00882	2.22723
C	3.67435	-0.45328	3.18510
H	0.62819	1.54848	1.85622
H	4.53259	-0.99292	3.56685
C	2.19208	1.46521	3.33901
C	3.28562	0.73496	3.80814
H	3.84839	1.08584	4.66959
H	1.88822	2.38066	3.83807
C	-2.96294	-1.62458	0.34395
C	-4.12122	-1.00938	-0.16677
C	-2.80066	-1.84526	1.72165
C	-5.11605	-0.61959	0.73602
C	-3.82112	-1.43345	2.58493
C	-4.98506	-0.81900	2.11459
H	-6.01916	-0.15151	0.34942
H	-3.70215	-1.60153	3.65339
C	-1.55489	-2.49398	2.27441
H	-0.69358	-1.82324	2.18160
H	-1.68191	-2.73540	3.33425
H	-1.30015	-3.41999	1.74578
C	-4.28786	-0.74506	-1.64565
H	-3.54099	-0.02404	-1.99641
H	-4.17600	-1.65533	-2.24732
H	-5.28073	-0.33417	-1.85288
C	-6.06212	-0.36097	3.07083
H	-6.09961	-0.99177	3.96558
H	-5.88013	0.66875	3.40629
H	-7.05121	-0.37907	2.60050
H	0.04979	0.18126	-3.28057
H	2.82309	-2.35353	-3.18761
H	1.20020	-1.83120	-5.06301
H	1.75215	-0.09171	-3.43130

6c

Ru	0.49872	0.25315	-0.24208
O	1.82404	1.08912	1.64497
O	3.48960	-0.72939	-0.57288
O	1.47482	-1.62821	-0.13523
N	-0.34226	-0.39708	-3.02226
N	-1.78116	-1.29022	-1.61442
C	-0.66613	-0.50499	-1.69250
C	-1.34562	-1.03304	-3.89739
H	-0.86881	-1.67897	-4.63726
H	-1.92673	-0.27227	-4.43473
C	-2.20339	-1.82485	-2.91800
H	-3.27737	-1.67585	-3.06494
H	-2.00282	-2.90248	-2.96442
C	0.60234	0.56634	-3.66756
C	-0.13860	1.88634	-3.96789
H	-0.48554	2.33662	-3.03444
H	-0.99648	1.73305	-4.63263
C	1.12404	-0.05946	-4.97870
H	1.59385	-1.03134	-4.79014
H	0.33924	-0.18761	-5.73093
C	1.81324	0.84669	-2.77398
H	2.30833	-0.06168	-2.42525
C	-2.55311	-1.74178	-0.48755
C	-3.70812	-1.01811	-0.13169
C	-4.50095	-1.50879	0.91218
H	-5.38632	-0.94695	1.20218
C	-4.18641	-2.69014	1.59027
C	-3.04546	-3.39487	1.19300

H	-2.78620	-4.32093	1.70216
C	-2.22355	-2.95244	0.15122
C	-4.06723	0.28629	-0.80089
H	-3.96403	0.23746	-1.89062
H	-3.41362	1.08929	-0.43982
H	-5.10163	0.56221	-0.57254
C	-5.07514	-3.21335	2.69530
H	-4.49503	-3.73964	3.46103
H	-5.81661	-3.92386	2.30551
H	-5.62681	-2.40315	3.18344
C	-1.01119	-3.75467	-0.25168
H	-1.10374	-4.14054	-1.27604
H	-0.88889	-4.61873	0.40908
H	-0.10053	-3.14849	-0.20859
C	-0.63012	0.01971	1.20855
H	-1.64731	-0.35172	1.14581
C	-0.18637	0.30944	2.55692
C	-1.01653	0.05450	3.66447
H	-1.99924	-0.37166	3.48115
C	-0.60101	0.34823	4.95880
H	-1.25005	0.14584	5.80542
C	0.66011	0.91565	5.15497
H	0.99760	1.15570	6.15980
C	1.51057	1.18377	4.07803
H	2.48354	1.61758	4.26897
C	1.09225	0.87493	2.78103
C	3.07435	1.85230	1.72604
H	2.89762	2.64361	2.46388
C	3.30994	2.48421	0.36279
H	3.52816	1.70789	-0.37464
H	4.16898	3.16223	0.42658
H	2.43201	3.05254	0.04532
C	4.22464	0.94596	2.15682
H	4.02675	0.45304	3.11347
H	5.13718	1.54409	2.26560
H	4.39079	0.18426	1.39092
C	2.76552	-1.68780	-0.26354
C	3.37493	-3.09778	-0.03846
C	2.94609	-3.99657	-1.21988
H	3.31452	-3.59384	-2.17160
H	1.85692	-4.07768	-1.28208
H	3.36022	-5.00577	-1.10074
C	4.90873	-3.00380	0.00028
H	5.30148	-2.56029	-0.91870
H	5.34425	-4.00372	0.12232
H	5.24704	-2.38167	0.83585
C	2.85494	-3.69178	1.28560
H	3.27989	-4.69098	1.44619
H	1.76531	-3.77408	1.28489
H	3.14441	-3.06531	2.13818
H	1.55629	1.48707	-1.92351
O	-0.04211	2.25334	-0.53575
C	-1.05544	2.83650	0.03572
O	-1.88978	2.27594	0.75661
C	-1.21170	4.35713	-0.24238
C	-0.01520	4.95530	-0.99721
H	-0.18431	6.02514	-1.17525
H	0.91151	4.85349	-0.42258
H	0.13870	4.47004	-1.96529
C	-2.50043	4.53688	-1.07540
H	-2.69552	5.60208	-1.25175
H	-2.41486	4.04667	-2.05344
H	-3.35969	4.10776	-0.55143
C	-1.38191	5.06961	1.11531
H	-2.21541	4.63683	1.67409
H	-0.47683	4.97268	1.72769
H	-1.57214	6.13946	0.96337
H	1.87985	0.60296	-5.41152
H	0.53794	2.59184	-4.46389
H	2.55335	1.42076	-3.34320

6d-TS

Ru	0.06345	-0.10643	-0.56640
O	-3.06271	-0.42799	2.75377
O	1.77784	-0.38690	-2.23269
O	1.51584	-1.65988	-0.45537
N	0.32393	2.50131	0.65424
N	2.05005	1.32951	1.33976
C	0.96005	1.31715	0.52019
C	1.02144	3.43449	1.55440
H	0.33457	3.87056	2.28606
H	1.48075	4.25371	0.98964
C	2.07548	2.52727	2.20175
H	3.07134	2.97746	2.21561
H	1.81229	2.25070	3.23098
C	-0.80007	2.91254	-0.20699
C	-0.44108	4.28736	-0.84444
H	0.48708	4.18193	-1.42251
H	-0.25491	5.03489	-0.06138
C	-1.58458	4.78995	-1.73989
H	-1.29607	5.75250	-2.18324
C	-2.84745	4.97204	-0.87376

H	-2.66036	5.71799	-0.08770
H	-3.67527	5.35426	-1.48638
C	-3.23736	3.61734	-0.25012
H	-4.13715	3.74128	0.36774
C	-2.08973	3.08697	0.63352
H	-2.36876	2.12565	1.08024
H	-1.89906	3.78816	1.45901
C	-3.50773	2.59725	-1.36961
H	-3.83729	1.64382	-0.94838
H	-4.31802	2.95884	-2.01881
C	-2.22805	2.40134	-2.21148
H	-2.42689	1.68220	-3.00975
C	-1.02526	1.86837	-1.34184
C	-1.84638	3.75591	-2.84642
H	-0.95497	3.64232	-3.47818
H	-2.66135	4.09816	-3.50030
C	-0.97058	-0.46211	0.96632
H	-1.12280	0.32498	1.71305
C	-1.65028	-1.69253	1.34043
C	-2.72071	-1.66110	2.28746
C	2.04964	-1.44699	-1.60623
O	-0.96475	-1.60773	-1.83463
C	-2.17157	-1.34394	-2.06539
O	-2.72024	-0.24951	-1.68255
H	-1.79452	0.55732	-1.28196
C	-3.05631	-2.33073	-2.84302
C	-4.13997	-0.25231	3.69426
H	-4.09890	-1.06082	4.43554
C	2.93729	-2.53328	-2.23171
C	4.19754	-1.88838	-2.83854
H	4.79393	-2.64877	-3.35785
H	3.92855	-1.10825	-3.55588
H	4.82434	-1.43841	-2.06073
C	2.10025	-3.18377	-3.35895
H	1.17230	-3.60956	-2.96209
H	1.83547	-2.44377	-4.12044
H	2.67477	-3.98747	-3.83617
C	3.33112	-3.59672	-1.19380
H	3.96144	-4.36127	-1.66555
H	3.89081	-3.15441	-0.36356
H	2.44812	-4.08945	-0.77643
C	-3.51359	-1.63167	-4.14295
H	-4.06476	-0.71344	-3.91981
H	-2.65668	-1.37363	-4.77692
H	-4.16749	-2.29913	-4.71711
C	-2.27858	-3.61217	-3.17856
H	-1.93778	-4.11702	-2.26943
H	-2.92310	-4.30336	-3.73517
H	-1.39717	-3.39479	-3.78924
C	-4.28963	-2.66883	-1.97692
H	-4.95345	-3.34902	-2.52443
H	-3.99313	-3.16120	-1.04382
H	-4.84956	-1.76402	-1.72426
C	-3.86213	1.07318	4.39564
H	-2.88966	1.04797	4.89710
H	-3.85681	1.89457	3.67086
H	-4.63582	1.27624	5.14390
C	-5.48629	-0.26266	2.96951
H	-5.52694	0.55716	2.24417
H	-5.64661	-1.20094	2.43058
H	-6.30565	-0.13344	3.68585
C	-1.25791	-2.94828	0.82762
C	-3.35444	-2.84795	2.67424
H	-0.42935	-2.96931	0.13057
H	-4.17777	-2.83567	3.37832
C	-1.88087	-4.12656	1.22721
C	-2.93027	-4.06953	2.14641
H	-3.43065	-4.98146	2.46245
H	-1.54878	-5.08181	0.83137
C	3.20924	0.47860	1.30537
C	4.29645	0.86611	0.48674
C	3.29012	-0.63946	2.16086
C	5.45688	0.08250	0.51940
C	4.47691	-1.38311	2.16239
C	5.54964	-1.03288	1.34759
H	6.30337	0.35799	-0.10393
H	4.56130	-2.24970	2.81178
C	2.15242	-1.03279	3.09494
H	1.27051	-0.45647	2.80027
C	4.27446	2.12424	-0.38013
H	3.29276	2.59427	-0.27094
H	-0.15973	1.90629	-2.01906
C	4.44888	1.81413	-1.87889
H	4.40604	2.74410	-2.45973
H	5.41939	1.34500	-2.08148
H	3.66005	1.14542	-2.23377
C	5.33250	3.14332	0.09338
H	5.21508	3.39311	1.15474
H	6.34867	2.75431	-0.04067
H	5.25435	4.07135	-0.48571
C	1.78533	-2.52250	2.96926
H	1.58714	-2.78167	1.92652

H	2.58813	-3.17065	3.34179
H	0.88742	-2.74088	3.55896
C	2.48916	-0.67311	4.55711
H	3.36545	-1.23151	4.90852
H	2.71075	0.39442	4.67390
H	1.64842	-0.91971	5.21706
H	6.46128	-1.62481	1.36333

6d

Ru	-0.01127	0.39946	0.34233
O	0.49300	1.89939	2.25367
O	-1.32203	3.21889	-0.12059
O	0.33937	1.99523	-1.02081
N	-1.42362	-0.88613	-1.93226
N	0.72093	-1.40207	-2.03466
C	-0.22274	-0.76651	-1.26954
C	-1.30870	-1.74386	-3.12845
H	-1.81773	-1.30093	-3.98512
H	-1.74860	-2.73280	-2.93913
C	0.19327	-1.81666	-3.34336
H	0.54584	-2.81623	-3.60630
H	0.53242	-1.11831	-4.11937
C	-2.79708	-0.68369	-1.37829
C	-3.24313	-1.92826	-0.56861
H	-2.54572	-2.06663	0.26396
H	-3.19623	-2.82691	-1.19900
C	-4.68402	-1.73497	-0.04376
H	-4.97925	-2.62815	0.52251
C	-5.64828	-1.52772	-1.23007
H	-5.63842	-2.40852	-1.88782
H	-6.67792	-1.41432	-0.86466
C	-5.22757	-0.27139	-2.01999
H	-5.89979	-0.13159	-2.87674
C	-3.79214	-0.46553	-2.55111
H	-3.47854	0.40721	-3.14015
H	-3.79341	-1.33156	-3.22267
C	-5.28072	0.96419	-1.10493
H	-5.00415	1.86658	-1.66661
H	-6.30265	1.11734	-0.73211
C	-4.31057	0.75082	0.07092
H	-4.31184	1.63384	0.72076
C	-2.87662	0.55670	-0.47282
H	-2.55368	1.45115	-1.00728
C	-4.73170	-0.49630	0.87327
H	-4.05934	-0.63682	1.72868
H	-5.74546	-0.36241	1.27510
C	2.10928	-1.71077	-1.79978
C	2.43030	-2.97338	-1.24225
C	3.78296	-3.31280	-1.11449
H	4.05108	-4.27187	-0.68166
C	4.78872	-2.45078	-1.54016
C	4.45323	-1.22803	-2.11222
H	5.24264	-0.56679	-2.45718
C	3.11700	-0.83283	-2.25961
C	1.37285	-3.99125	-0.82022
H	0.40204	-3.48661	-0.81690
C	2.80891	0.50642	-2.91981
H	1.74554	0.71801	-2.78118
C	1.74927	0.00265	0.77730
H	2.32461	-0.80094	0.32857
C	2.48906	0.78505	1.74789
C	3.86239	0.56545	1.96089
H	4.35810	-0.19904	1.36836
C	4.57047	1.29569	2.90980
H	5.63108	1.11963	3.06185
C	3.89497	2.24905	3.67422
H	4.43057	2.82143	4.42705
C	2.52920	2.48819	3.49347
H	2.04005	3.23515	4.10483
C	1.82764	1.76597	2.52427
C	-0.33379	2.74599	3.11955
H	0.01792	2.56561	4.14257
C	-1.76820	2.25816	2.98643
H	-2.12854	2.45513	1.97422
H	-2.39930	2.79897	3.70131
H	-1.83405	1.18833	3.19579
C	-0.18496	4.21800	2.74074
H	0.85661	4.55095	2.77069
H	-0.75772	4.83270	3.44541
H	-0.57951	4.37285	1.73367
C	-0.39576	3.06105	-0.93154
C	-0.03708	4.19510	-1.93023
C	0.16134	3.61791	-3.34474
H	-0.75670	3.13749	-3.70622
H	0.95887	2.87207	-3.35974
H	0.41842	4.41834	-4.05034
C	-1.16358	5.24148	-1.95551
H	-2.10941	4.79739	-2.28475
H	-0.90783	6.05445	-2.64709
H	-1.33131	5.66765	-0.96304
C	1.27127	4.85726	-1.44461
H	1.57048	5.66101	-2.12961

H	2.08522	4.12915	-1.38943
H	1.14026	5.29774	-0.44889
H	-2.23389	0.43468	0.41025
O	-0.81965	-0.93531	1.74269
C	-0.09862	-1.66552	2.54561
O	1.13227	-1.76739	2.49964
C	-0.90431	-2.46095	3.61242
C	-1.91721	-1.53612	4.31304
H	-2.48220	-2.09685	5.06849
H	-1.41099	-0.70808	4.82389
H	-2.62730	-1.11133	3.59846
C	-1.66124	-3.60708	2.90708
H	-2.20980	-4.20596	3.64502
H	-2.38263	-3.22166	2.18028
H	-0.96845	-4.27480	2.38231
C	0.06228	-3.05038	4.65373
H	0.79303	-3.71528	4.18585
H	0.62037	-2.26021	5.16664
H	-0.49807	-3.62005	5.40575
C	1.60853	-4.53621	0.60084
H	0.78936	-5.21196	0.87638
H	2.53703	-5.11614	0.66464
H	1.65138	-3.72677	1.33435
C	1.29982	-5.15740	-1.83027
H	1.10334	-4.81221	-2.85191
H	2.24220	-5.71793	-1.85029
H	0.50188	-5.85551	-1.55008
C	3.57820	1.66578	-2.26021
H	4.66378	1.54743	-2.35933
H	3.30839	2.61290	-2.73899
H	3.33331	1.74463	-1.19742
C	3.11052	0.45622	-4.43312
H	4.18027	0.29943	-4.61817
H	2.56951	-0.35556	-4.93293
H	2.82300	1.39993	-4.91179
H	5.83224	-2.73651	-1.43537

8a-ts

Ru	-0.06233	-0.06392	-0.45684
O	2.84835	-0.36962	3.06951
O	-1.82828	0.36630	-2.03183
O	-1.91803	0.80718	0.13174
N	0.37402	-2.92423	-0.63065
N	-1.55183	-2.64368	0.38253
C	-0.51722	-1.99940	-0.21795
C	-0.06885	-4.30558	-0.38000
H	0.70447	-4.88423	0.13569
H	-0.30383	-4.81756	-1.31978
C	-1.32483	-4.09727	0.48197
H	-2.19101	-4.65233	0.10911
H	-1.16729	-4.38454	1.52948
C	1.56662	-2.59030	-1.42986
C	1.59921	-3.53505	-2.66530
H	0.67745	-3.39670	-3.24663
H	1.62524	-4.58393	-2.33957
C	2.83599	-3.25606	-3.53424
H	2.82427	-3.92834	-4.40273
C	4.10336	-3.51095	-2.69292
H	4.13511	-4.56110	-2.36821
H	5.00201	-3.33727	-3.30033
C	4.10413	-2.56869	-1.47388
H	5.00436	-2.74700	-0.87028
C	2.85607	-2.82571	-0.60294
H	2.85805	-2.15991	0.26763
H	2.86867	-3.85849	-0.22498
C	4.07886	-1.10803	-1.95730
H	4.13630	-0.42188	-1.10783
H	4.95557	-0.90909	-2.59027
C	2.79227	-0.85481	-2.77228
H	2.78295	0.18098	-3.12039
C	1.49590	-1.11044	-1.91180
C	2.79509	-1.79148	-3.99924
H	1.90299	-1.61355	-4.61483
H	3.66887	-1.56861	-4.62817
C	0.84567	-0.15360	1.18975
H	1.26406	-1.10771	1.52860
C	1.08392	0.91048	2.15152
C	2.09910	0.76558	3.14818
C	-2.41813	0.89575	-1.04907
O	0.46106	2.04343	-0.84716
C	1.69565	2.23674	-1.00269
O	2.54462	1.27503	-1.05215
H	1.88498	0.17011	-1.16303
C	3.85041	-0.67767	4.05757
H	4.42178	0.23326	4.27749
C	3.20193	-1.21766	5.33289
H	2.50435	-0.49575	5.76761
H	2.64873	-2.13716	5.11160
H	3.96829	-1.44743	6.08186
C	4.77820	-1.69107	3.39610
H	4.22596	-2.59933	3.13098
H	5.21464	-1.27395	2.48353

H	5.58989	-1.96561	4.07850
C	0.30247	2.08754	2.16834
C	2.29677	1.76982	4.10241
H	-0.48260	2.18081	1.42799
H	3.06452	1.67498	4.86083
C	0.50035	3.07919	3.12278
C	1.50060	2.91711	4.08270
H	1.66840	3.68623	4.83256
H	-0.12156	3.96939	3.12243
C	-2.80768	-2.10274	0.82096
C	-3.87941	-2.06738	-0.09251
C	-2.97475	-1.70327	2.15568
C	-5.11775	-1.60404	0.35704
C	-4.23479	-1.24507	2.55847
C	-5.31510	-1.18056	1.67597
H	-5.94754	-1.56259	-0.34552
H	-4.36991	-0.92650	3.59011
C	-1.82986	-1.73236	3.13918
H	-1.08050	-0.97414	2.88754
H	-2.18672	-1.52943	4.15380
H	-1.31730	-2.70149	3.15263
C	-3.70176	-2.48379	-1.53481
H	-3.03629	-1.78958	-2.06009
H	-3.27100	-3.48837	-1.62747
H	-4.66556	-2.48780	-2.05315
C	-6.65745	-0.64520	2.11682
H	-7.47709	-1.30041	1.79859
H	-6.71113	-0.54059	3.20534
H	-6.84537	0.34275	1.67650
H	0.66554	-1.02372	-2.62768
C	2.21132	3.63158	-1.13619
C	1.32279	4.71239	-1.05301
C	3.57666	3.86889	-1.34501
C	1.79673	6.01712	-1.17676
H	0.26891	4.51064	-0.89401
C	4.04798	5.17510	-1.46759
H	4.25265	3.02307	-1.40867
C	3.15928	6.25035	-1.38363
H	1.10482	6.85276	-1.11292
H	5.10743	5.35567	-1.62943
H	3.52780	7.26856	-1.47996
C	-3.70312	1.63650	-1.22781
C	-4.24613	1.78285	-2.51076
C	-4.36630	2.19372	-0.12579
C	-5.44165	2.47783	-2.69042
H	-3.71536	1.34921	-3.35198
C	-5.56113	2.88915	-0.30773
H	-3.93561	2.06840	0.86180
C	-6.10091	3.03178	-1.58975
H	-5.85841	2.59079	-3.68798
H	-6.07081	3.32442	0.54833
H	-7.03170	3.57579	-1.73034

8a

Ru	0.07509	-0.00935	0.26910
O	0.44276	-0.16987	2.69203
O	0.99530	2.86746	1.30917
O	1.84571	1.13768	0.13424
N	-1.17767	0.69712	-2.34672
N	0.26673	-0.93668	-2.65566
C	-0.24579	-0.08448	-1.71169
C	-1.50548	0.15512	-3.67984
H	-1.68235	0.94332	-4.41099
H	-2.40467	-0.47247	-3.61898
C	-0.26982	-0.66583	-3.99974
H	-0.49342	-1.59669	-4.52623
H	0.46416	-0.10200	-4.59227
C	-2.02340	1.79662	-1.80771
C	-3.48696	1.32822	-1.60903
H	-3.49733	0.48836	-0.90635
H	-3.90236	0.96891	-2.56032
C	-4.35022	2.49897	-1.08598
H	-5.38082	2.14565	-0.95143
C	-4.32638	3.65637	-2.10582
H	-4.73956	3.32261	-3.06822
H	-4.96131	4.48121	-1.75514
C	-2.87638	4.15036	-2.29221
H	-2.85368	4.96177	-3.03148
C	-2.00578	2.98608	-2.81074
H	-0.96898	3.31528	-2.96040
H	-2.39426	2.67694	-3.78788
C	-2.31969	4.64924	-0.94728
H	-1.29436	5.02183	-1.07244
H	-2.92324	5.48765	-0.57332
C	-2.34113	3.48754	0.06130
H	-1.91401	3.81517	1.01548
C	-1.47632	2.32295	-0.47137
H	-0.44158	2.65503	-0.57742
C	-3.78913	2.99762	0.26096
H	-3.81506	2.19021	1.00486
H	-4.41400	3.81291	0.65075
C	1.44476	-1.76260	-2.62038

C	1.28404	-3.16251	-2.62626
C	2.43286	-3.96026	-2.67695
H	2.31702	-5.04212	-2.67349
C	3.71648	-3.40850	-2.73575
C	3.83447	-2.01581	-2.76992
H	4.82286	-1.56713	-2.84677
C	2.71902	-1.17186	-2.72618
C	-0.08207	-3.80344	-2.54815
H	-0.71803	-3.51954	-3.39635
H	-0.60975	-3.51474	-1.63203
H	0.00879	-4.89408	-2.56002
C	4.94324	-4.29099	-2.75680
H	5.36279	-4.41167	-1.74906
H	5.73309	-3.86494	-3.38533
H	4.71079	-5.29197	-3.13525
C	2.90015	0.32510	-2.80112
H	2.29756	0.76885	-3.60338
H	3.94719	0.57251	-3.00216
H	2.60646	0.80571	-1.86231
C	0.92904	-1.64253	0.47160
H	1.13309	-2.33290	-0.34003
C	1.41958	-2.08176	1.76020
C	2.14162	-3.28290	1.89372
H	2.32449	-3.87361	1.00005
C	2.60183	-3.71208	3.13360
H	3.15899	-4.63957	3.22426
C	2.33111	-2.93714	4.26398
H	2.68117	-3.26075	5.24064
C	1.61445	-1.74048	4.16945
H	1.42972	-1.16245	5.06556
C	1.16223	-1.31042	2.91950
C	-0.05874	0.60790	3.82982
H	-0.35110	-0.12317	4.59226
C	-1.29469	1.35259	3.34981
H	-1.00782	2.09979	2.60529
H	-1.76045	1.86360	4.20028
H	-2.01688	0.65811	2.91240
C	1.02596	1.54622	4.35285
H	1.93296	1.00736	4.64292
H	0.65094	2.07888	5.23484
H	1.28003	2.27694	3.58072
C	1.93803	2.26739	0.76513
H	-1.52151	1.53834	0.29751
O	-1.83388	-0.76490	0.63291
C	-2.13207	-2.03212	0.68064
O	-1.35347	-2.96674	0.45322
C	3.32725	2.85811	0.80755
C	4.45196	2.12386	0.40762
C	3.49429	4.16849	1.27514
C	5.72374	2.69391	0.47251
H	4.31619	1.10706	0.05580
C	4.76421	4.74096	1.33202
H	2.61361	4.71916	1.58916
C	5.88225	4.00416	0.93124
H	6.59241	2.11604	0.16661
H	4.88432	5.76016	1.69087
H	6.87338	4.44860	0.97887
C	-3.56491	-2.32950	1.05506
C	-4.00466	-3.66007	1.03241
C	-4.46101	-1.31982	1.43136
C	-5.31933	-3.97547	1.37201
H	-3.29584	-4.43041	0.74774
C	-5.77578	-1.63562	1.77563
H	-4.11674	-0.29166	1.45508
C	-6.20852	-2.96357	1.74466
H	-5.65138	-5.01034	1.34889
H	-6.46286	-0.84589	2.06922
H	-7.23333	-3.20904	2.01186

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Ru	-0.26327	-0.07900	0.64712
O	0.71012	2.95388	-1.71857
O	-0.39407	-1.96593	2.12904
O	-2.12985	-0.82063	1.40493
N	0.41722	-1.93471	-1.76880
N	-1.56804	-1.01739	-2.00819
C	-0.48179	-1.08656	-1.17798
C	0.00512	-2.29190	-3.14594
H	0.15537	-3.35198	-3.34810
H	0.58983	-1.71448	-3.87539
C	-1.46434	-1.91404	-3.16782
H	-1.76899	-1.40269	-4.08536
H	-2.11854	-2.78478	-3.02919
C	1.85059	-2.18416	-1.40421
C	2.73331	-0.97701	-1.80885
H	2.39217	-0.08393	-1.27878
H	2.62613	-0.79163	-2.88814
C	4.21347	-1.26672	-1.47096
H	4.81960	-0.39569	-1.75399
C	4.69610	-2.51008	-2.24263
H	4.61952	-2.34185	-3.32644
H	5.75479	-2.70516	-2.02364

C	3.84031	-3.72558	-1.83247
H	4.15792	-4.61065	-2.39969
C	2.36179	-3.43803	-2.17030
H	1.73942	-4.30619	-1.91321
H	2.28886	-3.28891	-3.25360
C	3.99126	-3.98657	-0.32356
H	3.41050	-4.87238	-0.03142
H	5.04177	-4.19544	-0.07865
C	3.49579	-2.74667	0.44060
H	3.57590	-2.91766	1.52156
C	2.01255	-2.48077	0.10064
H	1.39020	-3.34047	0.37473
C	4.34625	-1.52143	0.04425
H	4.00511	-0.63831	0.59392
H	5.39956	-1.69429	0.30612
C	-2.87721	-0.46326	-1.77921
C	-3.21289	0.75781	-2.39865
C	-4.50686	1.25849	-2.22574
H	-4.76523	2.21055	-2.68459
C	-5.47525	0.56740	-1.49039
C	-5.13148	-0.67710	-0.95802
H	-5.88228	-1.25038	-0.41778
C	-3.85055	-1.22093	-1.10345
C	-2.22618	1.50381	-3.26792
H	-2.02931	0.95966	-4.20207
H	-1.26282	1.65622	-2.77433
H	-2.62528	2.48520	-3.54303
C	-6.85234	1.15110	-1.27657
H	-6.89619	1.72489	-0.34133
H	-7.61521	0.36761	-1.21149
H	-7.13110	1.83103	-2.08878
C	-3.58157	-2.62489	-0.61737
H	-3.82955	-3.35667	-1.39962
H	-4.20578	-2.85982	0.24868
H	-2.54009	-2.77254	-0.33069
C	-0.91410	1.52497	0.00825
H	-1.84574	1.50182	-0.56610
C	-0.45268	2.89852	0.32841
C	-0.87572	3.52838	1.50567
H	-1.49577	2.96720	2.19749
C	-0.50131	4.84119	1.80193
H	-0.84364	5.30889	2.72061
C	0.31539	5.53673	0.91359
H	0.62026	6.55723	1.13004
C	0.75391	4.93034	-0.26696
H	1.38921	5.48960	-0.94368
C	0.37016	3.61777	-0.56833
C	1.68026	3.50792	-2.62561
H	1.44313	4.56695	-2.79680
C	1.50108	2.75225	-3.93842
H	1.67903	1.68200	-3.78701
H	2.21119	3.12015	-4.68698
H	0.48678	2.88390	-4.32756
C	3.09589	3.36881	-2.06403
H	3.20237	3.88258	-1.10481
H	3.82480	3.79386	-2.76388
H	3.33345	2.31148	-1.90786
C	-1.61731	-1.68078	2.21252
C	-2.48626	-2.32191	3.30618
H	1.67061	-1.63866	0.70091
O	1.76969	0.71639	0.83778
C	1.54758	1.05865	2.05584
O	0.38790	0.86828	2.52980
C	2.66644	1.63815	2.92599
C	-3.91696	-1.76194	3.29528
H	-4.50813	-2.23297	4.09067
H	-3.91815	-0.68008	3.46015
H	-4.41820	-1.94759	2.34079
C	-2.49959	-3.84966	3.08305
H	-1.47972	-4.24513	3.06262
H	-3.04963	-4.34493	3.89266
H	-2.98717	-4.11223	2.13655
C	-1.81537	-2.01252	4.66350
H	-1.76902	-0.93209	4.84198
H	-2.38913	-2.46978	5.47922
H	-0.79456	-2.40297	4.68821
C	3.64996	2.44410	2.05856
H	4.46055	2.83875	2.68333
H	4.08932	1.82511	1.27160
H	3.14548	3.29089	1.57994
C	3.39607	0.44738	3.59351
H	4.18913	0.82017	4.25319
H	2.70166	-0.14881	4.19530
H	3.85597	-0.21012	2.84854
C	2.05900	2.53981	4.01658
H	2.85649	2.92927	4.66116
H	1.52784	3.38998	3.57599
H	1.34959	1.98491	4.63610

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Ru	-0.08251	-0.04293	-0.60947
O	1.89875	1.41987	3.32059

O	-1.68040	-0.52716	-2.32314
O	-1.96223	0.84448	-0.62267
N	0.51360	-2.76863	0.45800
N	-1.50103	-2.22879	1.13137
C	-0.44517	-1.80412	0.39481
C	0.11023	-3.93529	1.26471
H	0.84178	-4.14021	2.05338
H	0.02988	-4.82964	0.63811
C	-1.25232	-3.50663	1.82373
H	-2.04621	-4.22687	1.60304
H	-1.23509	-3.35018	2.90926
C	1.83475	-2.74175	-0.20491
C	2.11376	-4.11172	-0.88085
H	1.31171	-4.33288	-1.59825
H	2.11023	-4.91217	-0.13029
C	3.48552	-4.09822	-1.58715
H	3.65146	-5.08006	-2.04944
C	4.58919	-3.81918	-0.54592
H	4.59954	-4.61328	0.21442
H	5.57404	-3.82916	-1.03159
C	4.33898	-2.44765	0.11326
H	5.11899	-2.24821	0.85974
C	2.96509	-2.45723	0.81950
H	2.78286	-1.49102	1.30403
H	2.95288	-3.22364	1.60693
C	4.35108	-1.34608	-0.96554
H	4.18382	-0.35674	-0.52695
H	5.33036	-1.31999	-1.46275
C	3.25054	-1.63375	-2.00318
H	3.23219	-0.83277	-2.74736
C	1.86718	-1.66387	-1.30517
C	3.49925	-3.00040	-2.66849
H	2.73029	-3.20390	-3.42652
H	4.46713	-2.99310	-3.18749
C	0.66659	0.70288	0.95445
H	1.32903	0.08698	1.57146
C	0.52043	2.03860	1.49312
C	1.19457	2.40682	2.70296
C	-2.34669	0.38553	-1.76539
O	0.40505	1.61309	-1.86238
C	1.63947	1.98893	-1.96389
O	2.60275	1.44764	-1.39344
H	1.79130	-0.62317	-0.88136
C	1.91518	3.21653	-2.87505
C	2.74501	1.69226	4.45481
H	2.20404	2.34308	5.15403
C	-3.55737	1.02610	-2.45530
C	-4.40302	-0.06720	-3.13432
H	-5.21219	0.39203	-3.71528
H	-3.78909	-0.67164	-3.80748
H	-4.85770	-0.73390	-2.39306
C	-2.98535	1.97637	-3.53487
H	-2.33625	2.73453	-3.08588
H	-2.39517	1.41971	-4.26929
H	-3.80629	2.48369	-4.05666
C	-4.41131	1.82637	-1.45777
H	-5.26084	2.28377	-1.98027
H	-4.80138	1.18249	-0.66303
H	-3.82796	2.62214	-0.98620
C	2.87363	2.75779	-3.99432
H	3.77914	2.31911	-3.56511
H	2.39855	2.00529	-4.63656
H	3.16038	3.60654	-4.62857
C	0.63164	3.79360	-3.48823
H	-0.06191	4.12999	-2.71067
H	0.87160	4.65372	-4.12739
H	0.11045	3.04787	-4.09567
C	2.61488	4.28848	-2.01283
H	2.88458	5.15861	-2.62542
H	1.95824	4.63428	-1.20501
H	3.52308	3.88123	-1.55971
C	2.97573	0.34095	5.12298
H	2.02399	-0.10886	5.42254
H	3.48137	-0.34427	4.43379
H	3.60141	0.46039	6.01388
C	4.04598	2.35864	4.00732
H	4.59277	1.69605	3.32778
H	3.85656	3.30006	3.48374
H	4.68238	2.56962	4.87421
C	-0.25934	3.02520	0.84446
C	1.08637	3.71110	3.19936
H	-0.77069	2.74184	-0.06585
H	1.59816	4.00570	4.10762
C	-0.36557	4.31630	1.34677
C	0.31034	4.65295	2.52186
H	0.23723	5.66039	2.92414
H	-0.96752	5.05689	0.82880
C	-2.80750	-1.64423	1.25414
C	-3.81615	-2.06937	0.36890
C	-3.09095	-0.77658	2.32174
C	-5.11538	-1.59143	0.56656
C	-4.40527	-0.32165	2.47431

C	-5.43006	-0.71204	1.60858
H	-5.90266	-1.92024	-0.10885
H	-4.63238	0.35256	3.29752
C	-2.02046	-0.32819	3.28677
H	-1.33710	0.38250	2.81101
H	-2.46688	0.16518	4.15581
H	-1.41281	-1.16450	3.65079
C	-3.51331	-3.00933	-0.77539
H	-2.82242	-2.54550	-1.48781
H	-3.05538	-3.94565	-0.43224
H	-4.43118	-3.27041	-1.31088
C	-6.83606	-0.18512	1.78036
H	-7.58257	-0.91765	1.45447
H	-7.04404	0.07108	2.82467
H	-6.99165	0.72411	1.18460
H	1.09242	-1.86068	-2.05268

14a-tsA

Ru	0.18862	0.08449	-0.51613
O	-2.58815	-1.17206	2.89098
O	1.81408	0.37983	-2.24449
O	2.01156	-1.02845	-0.56150
N	-0.10961	2.71935	0.64832
N	1.81554	1.93594	1.35023
C	0.74519	1.67949	0.55339
C	0.39279	3.80723	1.50286
H	-0.34386	4.08743	2.26301
H	0.62055	4.69878	0.90853
C	1.66286	3.18970	2.11151
H	2.54363	3.82763	1.98883
H	1.55315	2.97159	3.18137
C	-1.33743	2.82768	-0.15897
C	-1.35038	4.22856	-0.83666
H	-0.45094	4.33450	-1.45830
H	-1.31585	5.01920	-0.07454
C	-2.62031	4.41387	-1.68277
H	-2.59436	5.40445	-2.15649
C	-3.85220	4.30833	-0.76158
H	-3.82122	5.10098	0.00002
H	-4.77261	4.45902	-1.34202
C	-3.87380	2.91872	-0.09486
H	-4.74888	2.83916	0.56432
C	-2.59307	2.71114	0.74222
H	-2.60752	1.72420	1.21902
H	-2.54315	3.46265	1.54344
C	-3.93647	1.83298	-1.18344
H	-4.00819	0.83969	-0.73277
H	-4.83715	1.97223	-1.79835
C	-2.68512	1.92797	-2.08092
H	-2.73690	1.15920	-2.85559
C	-1.35764	1.72412	-1.25707
C	-2.66667	3.31558	-2.75752
H	-1.79888	3.40146	-3.42545
H	-3.56501	3.43254	-3.38043
C	-0.63564	-0.56465	1.04713
H	-0.97688	0.13591	1.81747
C	-0.90811	-1.94506	1.41943
C	-1.91032	-2.24354	2.39391
C	2.39819	-0.60453	-1.71060
O	-0.48065	-1.61242	-1.77776
C	-1.72784	-1.67060	-1.92368
O	-2.51306	-0.75315	-1.49161
H	-1.78861	0.26746	-1.13548
C	-2.37758	-2.86020	-2.64787
C	-3.62744	-1.33197	3.87548
H	-3.31516	-2.09580	4.59955
C	3.51308	-1.35332	-2.45418
C	4.50903	-0.33564	-3.04257
H	5.25083	-0.85061	-3.66540
H	3.98957	0.40430	-3.65762
H	5.04686	0.19426	-2.24799
C	2.82688	-2.12543	-3.60640
H	2.07356	-2.81962	-3.21810
H	2.32852	-1.43426	-4.29313
H	3.57252	-2.70117	-4.16877
C	4.23822	-2.33849	-1.52346
H	5.02949	-2.86077	-2.07624
H	4.69360	-1.81924	-0.67412
H	3.54695	-3.08572	-1.12301
C	-3.10166	-2.31594	-3.89933
H	-3.85945	-1.57794	-3.62055
H	-2.39563	-1.84038	-4.59081
H	-3.59450	-3.13676	-4.43428
C	-1.31708	-3.89366	-3.05706
H	-0.78728	-4.28346	-2.18253
H	-1.79635	-4.73438	-3.57349
H	-0.57261	-3.45581	-3.72896
C	-3.40865	-3.50565	-1.69581
H	-3.90701	-4.34346	-2.19884
H	-2.92403	-3.89198	-0.79205
H	-4.16865	-2.77941	-1.39408
C	-3.72879	0.01185	4.58993

H	-2.77324	0.27555	5.05380
H	-3.99901	0.80179	3.88065
H	-4.49609	-0.03013	5.37048
C	-4.93925	-1.73963	3.20368
H	-5.25230	-0.96556	2.49470
H	-4.83610	-2.68030	2.65504
H	-5.72893	-1.86381	3.95348
C	-0.16901	-3.01970	0.87783
C	-2.14998	-3.56914	2.77412
H	0.60964	-2.78478	0.16211
H	-2.92035	-3.81036	3.49663
C	-0.39889	-4.33397	1.27380
C	-1.39348	-4.60255	2.21611
H	-1.58956	-5.62541	2.52800
H	0.19384	-5.14211	0.85538
C	3.05342	1.21557	1.45217
C	4.10956	1.57460	0.59356
C	3.23147	0.25979	2.46566
C	5.34774	0.94865	0.76650
C	4.48795	-0.34185	2.59714
C	5.55699	-0.01571	1.75865
H	6.17127	1.22633	0.11150
H	4.63255	-1.08349	3.38017
C	2.10551	-0.13465	3.39048
H	1.34931	-0.72019	2.85670
H	2.48125	-0.74490	4.21768
H	1.59516	0.73526	3.81956
C	3.91616	2.59746	-0.50218
H	3.19320	2.24081	-1.24422
H	3.54517	3.55435	-0.11420
H	4.86219	2.79451	-1.01579
C	6.89739	-0.69847	1.90517
H	7.72065	-0.03016	1.62974
H	7.06472	-1.03832	2.93281
H	6.96446	-1.58105	1.25510
H	-0.55160	1.93815	-1.97354

14a-tsB

Ru	-0.16200	0.29628	-0.01470
O	-0.66092	2.58974	0.84618
O	1.77348	0.61571	0.69780
O	2.46778	1.90741	-1.01646
N	-1.02727	-1.91057	-1.69113
N	1.16278	-2.01105	-1.53783
C	0.06004	-1.32212	-1.12227
C	-0.67136	-2.96967	-2.64414
H	-0.81199	-2.62190	-3.67573
H	-1.28620	-3.86317	-2.50241
C	0.80421	-3.20912	-2.32226
H	0.96098	-4.11365	-1.71937
H	1.43212	-3.28661	-3.21436
C	-2.42151	-1.46089	-1.52393
C	-3.24642	-2.57610	-0.82765
H	-2.81140	-2.78709	0.15622
H	-3.19248	-3.50590	-1.41166
C	-4.72310	-2.14974	-0.68126
H	-5.28502	-2.96501	-0.20554
C	-5.32121	-1.85004	-2.06973
H	-5.29311	-2.74741	-2.70475
H	-6.37695	-1.56380	-1.96813
C	-4.52068	-0.70926	-2.72950
H	-4.94715	-0.48141	-3.71581
C	-3.06103	-1.17698	-2.91248
H	-2.46813	-0.41025	-3.42966
H	-3.05556	-2.07545	-3.54718
C	-4.57771	0.54909	-1.83685
H	-4.04185	1.37898	-2.31707
H	-5.62377	0.86824	-1.71843
C	-3.95039	0.23475	-0.45394
H	-3.99030	1.13482	0.17310
C	-2.44719	-0.15726	-0.69390
H	-2.13797	0.63225	-1.37815
C	-4.80193	-0.88250	0.19014
H	-4.47014	-1.10034	1.20641
H	-5.84658	-0.54557	0.25723
C	0.11973	1.43292	-1.49021
H	0.47034	1.11218	-2.47522
C	-0.27820	2.83113	-1.45956
C	-0.72618	3.41646	-0.24852
C	2.60699	1.41593	0.11696
O	-0.23472	-0.93089	1.98133
C	-1.33555	-1.10779	2.52534
O	-2.44865	-0.71442	1.97088
H	-2.25099	-0.40255	0.90728
C	-1.47889	-1.81569	3.87950
C	-0.97403	3.11465	2.16997
H	-0.66387	4.16455	2.17959
C	-0.09814	-2.01255	4.52475
H	-0.20988	-2.51706	5.49161
H	0.55592	-2.61907	3.89236
H	0.40382	-1.05453	4.69445
C	-2.38460	-0.97356	4.80315

H	-3.37167	-0.82110	4.35865
H	-2.51036	-1.48501	5.76462
H	-1.94400	0.01023	5.00299
C	-2.14287	-3.18862	3.62029
H	-1.52547	-3.80871	2.95969
H	-2.26557	-3.72602	4.56806
H	-3.12918	-3.07060	3.16121
C	3.84388	1.83921	0.95866
C	5.09945	1.80539	0.06665
H	5.96719	2.18560	0.62104
H	5.32217	0.78514	-0.26092
H	4.95387	2.42259	-0.82391
C	3.60070	3.29988	1.40403
H	2.72008	3.38282	2.05159
H	4.46550	3.67181	1.96808
H	3.44776	3.94787	0.53529
C	4.04038	0.93951	2.18840
H	4.19785	-0.10264	1.89306
H	4.91685	1.27207	2.76042
H	3.16774	0.96520	2.84712
C	2.54296	-1.92035	-1.14450
C	3.46188	-1.34277	-2.04052
C	2.98048	-2.58245	0.01806
C	4.82723	-1.45283	-1.75570
C	4.35554	-2.65382	0.26494
C	5.29591	-2.10286	-0.61044
H	5.54180	-1.01715	-2.45120
H	4.69898	-3.16962	1.15945
C	2.00785	-3.20394	0.98992
H	1.41124	-2.43329	1.48811
H	1.30669	-3.88748	0.49512
H	2.54409	-3.77613	1.75392
C	6.77580	-2.18417	-0.31544
H	7.13019	-1.27039	0.18009
H	7.00734	-3.02518	0.34678
H	7.36264	-2.30199	-1.23326
C	3.01319	-0.58716	-3.26813
H	2.17314	-1.07118	-3.77734
H	2.69253	0.41960	-2.97602
H	3.83536	-0.48808	-3.98410
C	-0.12141	2.35995	3.17971
H	-0.37353	1.29864	3.20414
H	0.93803	2.44093	2.92830
H	-0.28338	2.78474	4.17709
C	-2.47334	2.99613	2.43066
H	-2.71794	3.41838	3.41227
H	-3.05525	3.53227	1.67415
H	-2.77546	1.94433	2.41909
C	-0.27978	3.62431	-2.62113
C	-1.18373	4.73580	-0.22456
C	-1.18199	5.48856	-1.40356
C	-0.72923	4.94159	-2.60473
H	-1.55227	5.19004	0.68663
H	-1.54277	6.51319	-1.37185
H	-0.72751	5.53551	-3.51384
H	0.08234	3.17993	-3.54476

14a-tsC

Ru	-0.03649	0.40419	-0.06029
O	2.35481	-3.08127	1.75923
O	-1.67837	2.06161	-0.57432
O	-1.94502	0.43867	0.88646
N	0.59044	-0.91347	-2.49214
N	-1.37618	-1.68608	-1.88531
C	-0.39024	-0.81096	-1.56390
C	0.33897	-1.95845	-3.49330
H	1.09889	-2.74700	-3.43645
H	0.35638	-1.54824	-4.50796
C	-1.05933	-2.46976	-3.09629
H	-1.80652	-2.28997	-3.87636
H	-1.07044	-3.54098	-2.86560
C	1.87250	-0.20103	-2.36238
C	2.35751	0.22389	-3.77609
H	1.59787	0.86438	-4.24376
H	2.47657	-0.66136	-4.41631
C	2.95264	-1.13294	-1.75340
H	2.63896	-1.47449	-0.76412
H	3.06021	-2.02367	-2.38900
C	1.66586	1.09080	-1.50242
C	0.75456	-1.03515	0.86548
H	0.90829	-1.99303	0.36048
C	1.13172	-1.11590	2.26558
C	1.92028	-2.21877	2.72425
C	-2.35951	1.52964	0.35245
O	-0.19381	2.95043	2.49583
C	0.63428	3.10559	1.60860
O	1.24428	2.05521	1.05189
H	1.42885	1.59759	-0.11173
C	1.07524	4.51605	1.15814
C	3.06953	-4.28555	2.09634
H	3.82081	-4.04894	2.86065
C	-3.65200	2.18458	0.86277

C	2.10840	-5.35741	2.61205
H	1.56565	-5.01796	3.49903
H	1.37525	-5.60725	1.83709
H	2.65824	-6.26842	2.87432
C	3.78726	-4.70789	0.81869
H	3.06267	-4.91789	0.02418
H	4.45865	-3.91560	0.47363
H	4.37778	-5.61311	0.99639
C	0.70447	-0.16511	3.22027
C	2.23572	-2.34514	4.08094
H	0.11148	0.67989	2.88929
H	2.82955	-3.17685	4.44052
C	1.02175	-0.29785	4.56729
C	1.78557	-1.38639	4.99152
H	2.03974	-1.50003	6.04255
H	0.67344	0.44310	5.28025
C	-2.70278	-1.78659	-1.34334
C	-3.73080	-1.02501	-1.93220
C	-2.97478	-2.71969	-0.33042
C	-5.04088	-1.22730	-1.48961
C	-4.30147	-2.87786	0.08680
C	-5.34767	-2.14519	-0.47824
H	-5.84295	-0.65126	-1.94671
H	-4.51992	-3.59822	0.87235
C	-1.87802	-3.52643	0.32054
H	-1.30551	-2.90611	1.01943
H	-2.29669	-4.36726	0.88242
H	-1.16718	-3.92603	-0.41120
C	-3.43280	0.00877	-2.99420
H	-2.78325	0.79728	-2.59784
H	-2.92941	-0.42208	-3.86842
H	-4.35722	0.47649	-3.34576
C	-6.76973	-2.31855	0.00282
H	-7.04006	-1.53477	0.72263
H	-7.48476	-2.25744	-0.82532
H	-6.90942	-3.28301	0.50202
H	1.01832	1.75988	-2.08870
C	3.70709	0.96190	-3.68442
C	4.30088	-0.39689	-1.65200
C	3.06984	1.78496	-1.39316
C	4.76462	0.02976	-3.05875
H	4.91284	-0.85596	-3.69290
H	5.73198	0.54677	-3.00038
H	4.02194	1.25601	-4.69443
C	3.54278	2.20876	-2.80009
H	4.49875	2.74617	-2.72404
H	2.81944	2.90391	-3.24721
C	4.11075	0.84305	-0.75884
H	5.04495	-1.06920	-1.20427
H	3.78410	0.54426	0.24485
H	5.06459	1.37640	-0.64344
H	2.98871	2.68007	-0.77278
C	2.58644	4.68166	1.43179
H	3.18097	3.92127	0.91845
H	2.92394	5.66921	1.09347
H	2.79884	4.60384	2.50472
C	0.77031	4.70213	-0.34419
H	-0.28534	4.50547	-0.55810
H	1.00034	5.73200	-0.64439
H	1.36536	4.03272	-0.97081
C	0.29874	5.57103	1.96480
H	0.46120	5.44480	3.03910
H	0.62943	6.57693	1.67719
H	-0.77724	5.49642	1.78344
C	-3.28006	3.54619	1.49247
H	-2.83553	4.20827	0.74243
H	-4.18447	4.02800	1.88485
H	-2.55987	3.42717	2.30617
C	-4.33869	1.29339	1.91074
H	-5.26186	1.77431	2.25809
H	-4.59357	0.31344	1.49488
H	-3.68844	1.13008	2.77505
C	-4.59605	2.43088	-0.33235
H	-4.93281	1.48725	-0.77394
H	-5.48310	2.98200	0.00356
H	-4.09612	3.01880	-1.10783

14a-tsD

Ru	-0.15401	-0.46568	0.34930
O	-0.08259	0.00548	2.75308
O	-1.04405	-2.84606	0.69774
O	-2.17225	-0.94599	0.76605
N	0.91312	-1.08066	-2.27708
N	-1.00135	-0.04391	-2.57366
C	-0.13671	-0.51806	-1.63686
C	0.87824	-0.83225	-3.72607
H	1.13981	-1.72974	-4.29415
H	1.58116	-0.03247	-3.98202
C	-0.57241	-0.39181	-3.94096
H	-0.66025	0.47181	-4.60541
H	-1.20179	-1.19931	-4.33794
C	2.13103	-1.54334	-1.59321

C	3.38184	-0.84109	-2.18318
H	3.26386	0.24296	-2.10320
H	3.46556	-1.08668	-3.25097
C	2.29963	-3.07639	-1.77811
H	1.40825	-3.58428	-1.38896
H	2.37768	-3.32353	-2.84717
C	1.98804	-1.25511	-0.07839
C	-2.28792	0.56110	-2.38288
C	-2.40946	1.95957	-2.49268
C	-3.67870	2.52695	-2.32631
H	-3.77919	3.60858	-2.39444
C	-4.81504	1.74900	-2.09132
C	-4.66734	0.35854	-2.06136
H	-5.54661	-0.26709	-1.92100
C	-3.42197	-0.25588	-2.21624
C	-1.23849	2.84709	-2.85539
H	-1.15404	2.93788	-3.94818
H	-0.27578	2.48013	-2.48944
H	-1.38856	3.86132	-2.46978
C	-6.16563	2.39004	-1.87147
H	-6.97668	1.75763	-2.24894
H	-6.23410	3.36351	-2.36869
H	-6.35454	2.55539	-0.80233
C	-3.32512	-1.76160	-2.28146
H	-3.22869	-2.10241	-3.32183
H	-4.23088	-2.22370	-1.87851
H	-2.46730	-2.15186	-1.72981
C	-0.46835	1.35396	0.42550
H	-0.52180	2.00691	-0.44427
C	-0.75757	1.99351	1.69227
C	-1.26209	3.30729	1.75743
H	-1.40871	3.84877	0.82676
C	-1.57773	3.90046	2.97554
H	-1.96773	4.91323	3.00935
C	-1.38623	3.17765	4.15510
H	-1.62760	3.62722	5.11444
C	-0.88104	1.87416	4.12810
H	-0.73909	1.34304	5.06139
C	-0.57018	1.28291	2.90270
C	0.56939	-0.64159	3.89386
H	-0.12798	-0.57822	4.73700
C	1.87894	0.07199	4.22254
H	2.53484	0.08020	3.34669
H	2.38801	-0.44836	5.04153
H	1.71366	1.10859	4.52844
C	0.76275	-2.10889	3.54522
H	-0.17526	-2.57794	3.24418
H	1.14994	-2.63292	4.42630
H	1.48209	-2.23267	2.73258
C	-2.10297	-2.22026	0.94483
C	-3.33483	-2.94375	1.52416
H	2.04219	0.14554	0.15681
O	2.58644	1.30207	0.44719
C	2.48121	2.23799	-0.44740
O	1.95477	2.10392	-1.56411
C	3.11183	3.60724	-0.07120
C	3.31787	-1.67480	0.63070
C	4.65701	-1.32625	-1.46566
C	3.57150	-3.55388	-1.04219
H	3.66696	-4.64121	-1.16258
C	4.80340	-2.85031	-1.64672
H	5.71916	-3.20331	-1.15277
H	4.89745	-3.10138	-2.71294
H	5.52467	-0.81704	-1.90570
C	4.56054	-0.98784	0.03206
C	3.47549	-3.20720	0.45941
H	4.38256	-3.55026	0.97718
H	2.62577	-3.73379	0.91544
H	3.24830	-1.42721	1.69617
H	5.45787	-1.34765	0.55571
H	4.50104	0.09230	0.18082
C	-3.56548	-4.25364	0.74478
H	-2.66254	-4.87008	0.74698
H	-4.38270	-4.82421	1.20268
H	-3.83728	-4.05607	-0.29799
C	-4.58728	-2.05344	1.47371
H	-5.44656	-2.59650	1.88682
H	-4.44521	-1.13665	2.05281
H	-4.82938	-1.75734	0.44860
C	-3.01019	-3.28781	2.99669
H	-2.80888	-2.38118	3.57998
H	-3.86253	-3.80162	3.45768
H	-2.13813	-3.94627	3.06261
C	2.09276	4.71919	-0.38823
H	1.21024	4.63964	0.25888
H	2.53920	5.70821	-0.22423
H	1.76167	4.65006	-1.42795
C	4.35418	3.78590	-0.97230
H	4.82108	4.76337	-0.79604
H	5.10593	3.01351	-0.76697
H	4.07407	3.71824	-2.02817
C	3.52205	3.67454	1.40755

H	3.96216	4.65473	1.63382
H	2.65824	3.52879	2.06485
H	4.25703	2.90237	1.65269
H	1.28522	-2.01803	0.31446

14a-tsE

Ru	-0.11665	-0.41042	0.27860
O	-1.29306	3.42060	-2.00342
O	0.76565	-2.11066	1.70660
O	1.72265	-0.15502	1.37124
N	-0.18184	-2.01336	-2.13887
N	1.85001	-1.20113	-1.99544
C	0.63380	-1.23557	-1.39316
C	0.54491	-2.74012	-3.19103
H	-0.00340	-2.73995	-4.13588
H	0.71944	-3.78340	-2.89337
C	1.85255	-1.94126	-3.27180
H	2.74093	-2.57318	-3.35616
H	1.85440	-1.23616	-4.11438
C	-1.45253	-2.47775	-1.55714
C	-1.20473	-3.67369	-0.60112
H	-0.52891	-3.36753	0.20251
H	-0.71368	-4.48626	-1.15694
C	-2.54231	-4.17361	-0.02396
H	-2.34926	-5.00827	0.66281
C	-3.45642	-4.64531	-1.17340
H	-2.98856	-5.48392	-1.70899
H	-4.41067	-5.01509	-0.77329
C	-3.71442	-3.47218	-2.14107
H	-4.34961	-3.80850	-2.97181
C	-2.37623	-2.96198	-2.70538
H	-2.54647	-2.13903	-3.41324
H	-1.88673	-3.77460	-3.26049
C	-4.39493	-2.32559	-1.38005
H	-4.61550	-1.49204	-2.06119
H	-5.35659	-2.66369	-0.96754
C	-3.48073	-1.84342	-0.23354
H	-4.00279	-1.05139	0.30306
C	-2.13442	-1.28154	-0.81529
H	-2.38685	-0.54710	-1.59395
C	-3.21114	-3.01217	0.73443
H	-2.56578	-2.67933	1.55760
H	-4.15818	-3.34754	1.18074
C	-0.32355	1.22585	-0.63514
H	-0.69098	1.22301	-1.66743
C	-0.12365	2.57095	-0.12826
C	-0.64104	3.69889	-0.84327
C	1.61908	-1.24191	2.04403
O	-0.93265	0.35031	2.18151
C	-2.12244	0.75638	2.09328
O	-2.82179	0.57816	1.03721
H	-2.11917	-0.24948	0.26888
C	-2.78918	1.48670	3.26899
C	-1.93690	4.45225	-2.77649
H	-1.27551	5.32753	-2.82202
C	2.47849	-1.43644	3.30238
C	2.94667	-2.90090	3.39206
H	3.46986	-3.07140	4.34103
H	2.09551	-3.58429	3.33283
H	3.63858	-3.14952	2.57898
C	1.56022	-1.11908	4.50753
H	1.17079	-0.09760	4.44439
H	0.70752	-1.80480	4.53712
H	2.12272	-1.22044	5.44413
C	3.68416	-0.48239	3.30296
H	4.28497	-0.64058	4.20731
H	4.32497	-0.64766	2.43040
H	3.36094	0.56202	3.27992
C	-3.96466	0.61389	3.76275
H	-4.68462	0.43583	2.95850
H	-3.61036	-0.35736	4.12835
H	-4.48302	1.11553	4.58891
C	-1.78544	1.71691	4.40886
H	-0.93981	2.32454	4.07180
H	-2.27720	2.23989	5.23815
H	-1.38647	0.77045	4.78545
C	-3.32925	2.83982	2.75653
H	-3.83443	3.37275	3.57134
H	-2.51520	3.47534	2.38896
H	-4.04214	2.69176	1.94061
C	-2.08708	3.87521	-4.18016
H	-1.11008	3.60569	-4.59317
H	-2.71311	2.97664	-4.15815
H	-2.55654	4.60908	-4.84404
C	-3.27905	4.83096	-2.15009
H	-3.93966	3.95760	-2.12451
H	-3.15779	5.19509	-1.12579
H	-3.76477	5.61737	-2.73899
C	0.58521	2.81616	1.07071
C	-0.45979	4.99356	-0.34108
H	1.00121	1.96332	1.59378
H	-0.86116	5.85351	-0.86357

C	0.77400	4.10589	1.55496
C	0.24453	5.18848	0.84856
H	0.37867	6.20150	1.21991
H	1.33082	4.26898	2.47295
C	3.02351	-0.47351	-1.60639
C	4.01526	-1.16034	-0.87508
C	3.22493	0.84638	-2.03599
C	5.19165	-0.48548	-0.55149
C	4.42115	1.48560	-1.67860
C	5.40994	0.84519	-0.93406
H	5.95985	-1.00994	0.01362
H	4.57945	2.51292	-2.00194
C	2.22234	1.59487	-2.88384
H	1.84611	2.47753	-2.35530
H	2.68812	1.94545	-3.81351
H	1.35856	0.98079	-3.14541
C	3.82176	-2.60121	-0.46496
H	2.87591	-2.75002	0.06447
H	3.81433	-3.27327	-1.33400
H	4.63685	-2.92782	0.18807
C	6.68051	1.56159	-0.53918
H	7.56206	0.92632	-0.68496
H	6.82252	2.47682	-1.12295
H	6.66038	1.84628	0.52093

14a-tsF

Ru	0.58305	0.05179	-0.04770
O	-2.06347	3.42925	-1.73617
O	1.80602	-1.59753	1.20441
O	-0.11899	-0.72141	1.82469
N	-1.41790	-1.99491	-1.49569
N	0.74131	-2.20104	-1.91764
C	-0.17537	-1.50060	-1.18639
C	-1.30627	-3.12957	-2.44702
H	-2.05126	-3.05409	-3.23995
H	-1.45135	-4.08370	-1.92313
C	0.11233	-2.99825	-2.97627
H	0.60630	-3.96006	-3.11845
H	0.15398	-2.44609	-3.92617
C	-2.64268	-2.00671	-0.61957
C	-2.44306	-3.00668	0.55046
H	-1.59222	-2.67239	1.15215
H	-2.20681	-4.00666	0.16079
C	-3.71753	-3.07657	1.42045
H	-3.55146	-3.79290	2.23598
C	-4.91008	-3.53746	0.55973
H	-4.71893	-4.53916	0.14895
H	-5.81570	-3.61356	1.17677
C	-5.13697	-2.52826	-0.58570
H	-5.97351	-2.86305	-1.21341
C	-3.86691	-2.45890	-1.46110
H	-4.01514	-1.75931	-2.29556
H	-3.70185	-3.45195	-1.89305
C	-5.44332	-1.13901	0.00101
H	-5.63198	-0.41907	-0.80756
H	-6.35368	-1.17878	0.61494
C	-4.24172	-0.68639	0.84756
H	-4.42613	0.31607	1.25422
C	-2.96952	-0.62375	-0.02576
H	-3.10203	0.10189	-0.83817
C	-4.01469	-1.68053	2.00411
H	-3.17540	-1.34541	2.62623
H	-4.90377	-1.72253	2.64870
C	2.15804	-1.97785	-1.94493
C	3.03570	-3.06233	-1.77566
C	4.41173	-2.81848	-1.85719
H	5.09735	-3.65292	-1.72298
C	4.92679	-1.53732	-2.07173
C	4.02709	-0.47421	-2.18663
H	4.40404	0.53793	-2.31845
C	2.64209	-0.66929	-2.12531
C	2.54935	-4.45696	-1.45583
H	3.32223	-5.01079	-0.91390
H	2.31338	-5.04126	-2.35667
H	1.65301	-4.42987	-0.82803
C	6.41651	-1.30746	-2.18294
H	6.74405	-1.30964	-3.23174
H	6.98209	-2.08882	-1.66396
H	6.70537	-0.34059	-1.75649
C	1.69584	0.47991	-2.14527
H	0.76897	0.27106	-2.68019
H	2.14786	1.32312	-2.68793
H	1.89480	1.41841	-1.11168
C	-0.69008	1.33403	-0.56226
H	-1.00097	1.38906	-1.61125
C	-1.28137	2.38983	0.24177
C	-1.19702	2.38096	1.65330
H	-0.68775	1.54767	2.12246
C	-1.76377	3.38871	2.42527
H	-1.69126	3.35519	3.50831
C	-2.42948	4.44221	1.79413
H	-2.87272	5.24021	2.38475

C	-2.54077	4.49016	0.40358
H	-3.06087	5.32257	-0.05471
C	-1.98251	3.47181	-0.37959
C	-2.66700	4.49744	-2.49198
H	-3.59100	4.81067	-1.98851
C	-3.02510	3.88819	-3.84340
H	-2.12308	3.52988	-4.35108
H	-3.50816	4.63642	-4.48095
H	-3.70915	3.04340	-3.71664
C	-1.70223	5.67707	-2.61625
H	-1.41659	6.07018	-1.63621
H	-2.16560	6.48815	-3.18940
H	-0.79077	5.36193	-3.13575
C	0.91412	-1.45067	2.07650
C	1.05770	-2.11892	3.45257
C	1.24053	-3.63608	3.23514
H	2.09041	-3.83041	2.57495
H	0.34636	-4.08372	2.78332
H	1.41829	-4.13786	4.19429
C	2.32982	-1.53814	4.10987
H	3.20435	-1.71449	3.47731
H	2.49935	-2.00826	5.08658
H	2.23305	-0.45701	4.26288
C	-0.16385	-1.85139	4.34493
H	-0.02374	-2.32746	5.32353
H	-1.08118	-2.25259	3.90123
H	-0.31298	-0.77890	4.50301
H	-2.13865	-0.28995	0.59078
O	1.64922	1.43342	1.25242
C	2.36768	2.32010	0.71640
O	2.49607	2.43028	-0.54995
C	3.11137	3.33664	1.59642
C	2.97967	2.97112	3.08285
H	3.50843	3.71077	3.69652
H	1.93114	2.94887	3.39352
H	3.40800	1.98463	3.28778
C	4.59727	3.35592	1.18058
H	5.14284	4.10038	1.77309
H	5.06788	2.38002	1.34978
H	4.70331	3.60591	0.12145
C	2.48020	4.72356	1.33478
H	2.56031	4.99604	0.27814
H	1.41983	4.73160	1.61321
H	2.99442	5.48674	1.93166

15a

Ru	-0.17418	-0.06317	-0.47393
O	2.87538	-0.00436	2.86154
O	-1.79151	0.29487	-2.18725
O	-1.98580	1.25996	-0.21580
N	-0.20819	-2.95413	-0.37239
N	-1.94243	-2.27350	0.78279
C	-0.88533	-1.85749	0.03344
C	-0.72711	-4.21157	0.16909
H	0.00271	-4.68027	0.84071
H	-0.95386	-4.92537	-0.63039
C	-1.98943	-3.74473	0.92185
H	-2.90901	-4.14397	0.48137
H	-1.97984	-4.02445	1.98124
C	1.06007	-2.79887	-1.08195
C	1.18816	-3.78961	-2.26579
H	0.33386	-3.66017	-2.94286
H	1.17454	-4.83304	-1.91501
C	2.51817	-3.51649	-3.00655
H	2.59317	-4.19511	-3.86678
C	3.69567	-3.76776	-2.04355
H	3.68925	-4.81106	-1.69663
H	4.64934	-3.61013	-2.56595
C	3.58316	-2.80729	-0.84404
H	4.41405	-2.98650	-0.14763
C	2.24765	-3.03875	-0.11482
H	2.16497	-2.35858	0.73929
H	2.20620	-4.06615	0.27564
C	3.61458	-1.34589	-1.32765
H	3.57866	-0.68488	-0.45399
H	4.56196	-1.13506	-1.84337
C	2.43143	-1.08643	-2.28559
H	2.47815	-0.05536	-2.65597
C	1.05242	-1.35537	-1.63905
C	2.57350	-2.05221	-3.49433
H	1.76981	-1.86123	-4.21754
H	3.52502	-1.87577	-4.01736
C	0.69381	0.01089	1.19225
H	0.87728	-0.89311	1.78518
C	1.08341	1.21536	1.94267
C	2.19574	1.18183	2.83170
C	-2.35093	1.14541	-1.43059
O	0.60809	1.97157	-1.30379
C	1.75769	2.40329	-1.25860
O	2.73660	1.73270	-0.65419
H	2.32539	0.91463	-0.28325
C	2.21212	3.71774	-1.88777

C	4.00593	-0.19246	3.73187
H	3.79912	0.29704	4.69274
C	-3.43300	2.08413	-1.99870
C	-4.41632	1.27744	-2.86762
H	-5.13382	1.95249	-3.35090
H	-3.88337	0.71929	-3.64215
H	-4.98492	0.56294	-2.26213
C	-2.70869	3.12137	-2.88657
H	-1.98796	3.70168	-2.30111
H	-2.16798	2.62596	-3.69947
H	-3.43514	3.81776	-3.32432
C	-4.18620	2.80175	-0.86701
H	-4.95029	3.46847	-1.28706
H	-4.68019	2.08297	-0.20505
H	-3.50382	3.39839	-0.25497
C	3.20174	3.38119	-3.02904
H	4.07526	2.84127	-2.65199
H	2.72304	2.76889	-3.80202
H	3.54547	4.30947	-3.49954
C	0.99793	4.47377	-2.44592
H	0.28670	4.72244	-1.65204
H	1.33075	5.40726	-2.91358
H	0.46659	3.88003	-3.19465
C	2.92496	4.56770	-0.81136
H	3.23087	5.52564	-1.24748
H	2.26049	4.77278	0.03511
H	3.81486	4.06079	-0.42859
C	4.11028	-1.69741	3.95831
H	3.18951	-2.08453	4.40552
H	4.27736	-2.21596	3.00780
H	4.94659	-1.92467	4.62834
C	5.26943	0.39349	3.09972
H	5.48300	-0.11336	2.15212
H	5.15885	1.46251	2.89585
H	6.12889	0.25771	3.76626
C	0.34595	2.41248	1.85122
C	2.53865	2.31077	3.58235
H	-0.52012	2.42544	1.19670
H	3.39307	2.29835	4.24898
C	0.68367	3.53402	2.60866
C	1.78022	3.47980	3.46908
H	2.05594	4.34766	4.06281
H	0.08597	4.43854	2.53695
C	-3.09468	-1.51642	1.18682
C	-4.19635	-1.44156	0.31096
C	-3.15018	-0.96164	2.47496
C	-5.34858	-0.78461	0.75051
C	-4.32470	-0.30813	2.86686
C	-5.43070	-0.20326	2.02134
H	-6.20592	-0.72703	0.08263
H	-4.37349	0.12610	3.86347
C	-1.98064	-1.04237	3.42590
H	-1.21132	-0.30897	3.15981
H	-2.30120	-0.83513	4.45194
H	-1.50258	-2.02767	3.40971
C	-4.14116	-2.03771	-1.07729
H	-3.35829	-1.56368	-1.67930
H	-3.93575	-3.11510	-1.05974
H	-5.09658	-1.89922	-1.59255
C	-6.67773	0.53165	2.45600
H	-7.58494	0.03424	2.09448
H	-6.74148	0.60316	3.54686
H	-6.69047	1.55561	2.05944
H	0.32407	-1.34527	-2.46996

16a-ts

Ru	0.12198	0.28682	-0.98117
O	-0.83490	-2.23955	2.65000
N	0.49698	2.52623	0.81980
N	2.45232	1.54369	0.66923
C	1.17474	1.52607	0.20832
C	1.28983	3.21490	1.85062
H	0.92404	2.95781	2.85258
H	1.24103	4.30127	1.74204
C	2.69932	2.66659	1.59424
H	3.35711	3.40714	1.12246
H	3.19354	2.31225	2.50386
C	-0.93240	2.79722	0.60496
C	-1.08965	4.31176	0.28340
H	-0.49692	4.54834	-0.61039
H	-0.68820	4.91650	1.10766
C	-2.56770	4.67493	0.07068
H	-2.64570	5.74562	-0.16046
C	-3.35082	4.36145	1.36178
H	-2.95951	4.96296	2.19489
H	-4.40739	4.63544	1.23954
C	-3.23341	2.85717	1.67985
H	-3.78810	2.62996	2.60000
C	-1.75174	2.47446	1.88189
H	-1.65829	1.40498	2.10947
H	-1.34312	3.02962	2.73727
C	-3.80560	2.04203	0.50813

H	-3.78421	0.97260	0.73220
H	-4.85717	2.31434	0.34057
C	-2.99220	2.33876	-0.76928
H	-3.39795	1.75767	-1.60080
C	-1.47509	1.95862	-0.58615
C	-3.11825	3.84189	-1.09828
H	-2.57208	4.07826	-2.02185
H	-4.17391	4.08917	-1.27857
C	0.08438	-0.92129	0.43578
H	0.21131	-0.53727	1.45182
C	-0.12413	-2.35825	0.39829
C	-0.57572	-3.03462	1.57479
O	-1.19494	-0.93339	-2.27894
C	-2.36243	-1.07321	-1.82966
O	-2.78760	-0.42505	-0.80688
H	-1.91361	0.52753	-0.57235
C	-3.35057	-2.03068	-2.51433
C	-1.26261	-2.79575	3.90822
H	-0.70710	-3.72471	4.09153
C	-4.51035	-1.18218	-3.08291
H	-5.00634	-0.61482	-2.28955
H	-4.15045	-0.47554	-3.84073
H	-5.25274	-1.83390	-3.55925
C	-2.65998	-2.80776	-3.64537
H	-1.83180	-3.41021	-3.26064
H	-3.38089	-3.47879	-4.12842
H	-2.25197	-2.13260	-4.40315
C	-3.90077	-3.00900	-1.45364
H	-4.63129	-3.68464	-1.91502
H	-3.09766	-3.61912	-1.02535
H	-4.39121	-2.46748	-0.63983
C	-0.87016	-1.76972	4.96642
H	0.20990	-1.59347	4.95108
H	-1.37965	-0.81757	4.78185
H	-1.15149	-2.12511	5.96354
C	-2.76677	-3.07000	3.88640
H	-3.31492	-2.13657	3.71891
H	-3.03821	-3.76997	3.09096
H	-3.08981	-3.49543	4.84343
C	0.17114	-3.13514	-0.74308
C	-0.73077	-4.42499	1.57075
H	0.54350	-2.62295	-1.62223
H	-1.08986	-4.94729	2.44926
C	0.03061	-4.51979	-0.73419
C	-0.42591	-5.15740	0.42045
H	-0.54800	-6.23754	0.43702
H	0.28001	-5.09697	-1.61950
C	3.60018	0.79100	0.23634
C	4.35916	1.25957	-0.85329
C	4.01920	-0.31692	0.99081
C	5.53499	0.58287	-1.18134
C	5.20320	-0.96477	0.61896
C	5.97096	-0.53684	-0.46522
H	6.12132	0.93534	-2.02752
H	5.53137	-1.82633	1.19711
C	3.22721	-0.83841	2.16709
H	2.42520	-1.50700	1.83292
H	3.87218	-1.40899	2.84341
H	2.75475	-0.03656	2.74351
C	3.90524	2.43070	-1.69033
H	3.03974	2.13869	-2.29607
H	3.61328	3.29764	-1.08620
H	4.70164	2.75044	-2.36933
C	7.22829	-1.27074	-0.86974
H	8.00990	-0.57740	-1.20061
H	7.63005	-1.86601	-0.04299
H	7.03125	-1.95755	-1.70340
H	-0.99383	2.32372	-1.51428
Cl	1.88123	-0.46096	-2.40376

17a

Ru	0.27546	0.13042	-0.87505
O	-1.77892	-0.92707	2.91970
N	1.13058	2.73803	0.01966
N	2.84889	1.40644	0.33160
C	1.56849	1.45692	-0.11661
C	2.07735	3.60601	0.72500
H	1.71025	3.84994	1.73052
H	2.23656	4.54608	0.18742
C	3.34097	2.72927	0.77188
H	4.12011	3.09005	0.09125
H	3.77724	2.65703	1.77328
C	-0.30366	3.00610	-0.09598
C	-0.59390	4.38048	-0.74543
H	-0.10138	4.43232	-1.72530
H	-0.18797	5.19926	-0.13236
C	-2.12380	4.55539	-0.89346
H	-2.32750	5.51851	-1.37981
C	-2.78124	4.52782	0.50161
H	-2.39339	5.34799	1.12235
H	-3.86498	4.68224	0.40856
C	-2.49212	3.17202	1.17325

H	-2.94825	3.15026	2.17269
C	-0.97121	2.97534	1.30479
H	-0.75854	2.01587	1.78734
H	-0.54662	3.76851	1.93626
C	-3.05540	2.02031	0.31958
H	-2.85606	1.07159	0.83316
H	-4.14603	2.11304	0.22263
C	-2.40049	2.04208	-1.07679
H	-2.82675	1.24597	-1.69723
C	-0.86831	1.88935	-0.99975
C	-2.71065	3.40927	-1.74434
H	-2.28796	3.43202	-2.75774
H	-3.79700	3.54404	-1.84765
C	-0.05533	-0.54255	0.82553
H	0.23762	0.00651	1.72535
C	-0.58386	-1.88270	1.13248
C	-1.43912	-2.07463	2.25322
O	-1.24973	-1.17306	-2.03197
C	-2.40127	-1.53875	-1.82614
O	-3.05677	-1.23265	-0.70127
H	-2.43070	-0.73350	-0.13328
C	-3.21740	-2.37101	-2.81078
C	-2.60877	-0.97191	4.09544
H	-2.32647	-1.84803	4.69374
C	-4.46462	-1.55666	-3.22710
H	-5.09063	-1.31261	-2.36378
H	-4.18028	-0.62174	-3.72409
H	-5.06356	-2.14309	-3.93309
C	-3.65678	-3.67513	-2.10527
H	-4.21970	-4.29765	-2.81012
H	-2.79060	-4.24901	-1.75847
H	-4.29392	-3.46688	-1.24105
C	-2.28053	0.29044	4.88643
H	-1.21890	0.31487	5.15090
H	-2.50972	1.18326	4.29414
H	-2.87125	0.32606	5.80823
C	-4.08573	-1.05148	3.70515
H	-4.37294	-0.15951	3.13728
H	-4.29151	-1.92935	3.08577
H	-4.71535	-1.10785	4.60054
C	-0.21124	-3.01456	0.38288
C	-1.88773	-3.35450	2.59296
H	0.46205	-2.86964	-0.45754
H	-2.54858	-3.50662	3.43836
C	-0.65763	-4.29139	0.72425
C	-1.49324	-4.45691	1.82831
H	-1.84673	-5.44641	2.10641
H	-0.33983	-5.15098	0.14091
C	3.78998	0.31782	0.29681
C	4.66210	0.19450	-0.80512
C	3.91192	-0.52408	1.41452
C	5.62700	-0.81315	-0.77487
C	4.89494	-1.52224	1.39349
C	5.75392	-1.69058	0.30821
H	6.29460	-0.92055	-1.62728
H	4.98911	-2.17966	2.25574
C	3.02520	-0.39837	2.63164
H	2.15020	-1.05384	2.54873
H	3.56987	-0.69070	3.53594
H	2.65088	0.61983	2.77128
C	4.55899	1.10048	-2.00847
H	3.59077	0.96334	-2.50015
H	4.66619	2.16092	-1.74840
H	5.34245	0.86023	-2.73357
C	6.78802	-2.79219	0.29246
H	7.75463	-2.43168	-0.07852
H	6.94368	-3.21066	1.29233
H	6.47731	-3.61491	-0.36469
H	-0.48074	2.07853	-2.02566
Cl	1.82300	-1.04334	-2.34886
C	-2.35511	-2.69336	-4.04130
H	-1.45739	-3.25259	-3.76282
H	-2.93760	-3.29499	-4.74831
H	-2.02724	-1.78153	-4.54893

18a-ts

Ru	0.17229	-0.30239	0.92941
O	-2.12345	2.92217	-1.36715
O	1.61465	-1.68889	2.23741
O	2.11456	0.34032	1.52827
N	-0.31798	-1.90551	-1.43093
N	1.74086	-1.16617	-1.59674
C	0.63610	-1.18629	-0.80384
C	0.14273	-2.49837	-2.69678
H	-0.55392	-2.28588	-3.51424
H	0.23661	-3.58635	-2.60696
C	1.51071	-1.82626	-2.89534
H	2.30720	-2.54399	-3.11406
H	1.49963	-1.08126	-3.70152
C	-1.61786	-2.23014	-0.81509
C	-1.84978	-3.76295	-0.95024
H	-1.03030	-4.29538	-0.44852

H	-1.83121	-4.05768	-2.00846
C	-3.20605	-4.16456	-0.34808
H	-3.33505	-5.25080	-0.44729
C	-4.32785	-3.43364	-1.11303
H	-4.31573	-3.72881	-2.17230
H	-5.30900	-3.72195	-0.71184
C	-4.13123	-1.91062	-0.97499
H	-4.92645	-1.38483	-1.52065
C	-2.76331	-1.49642	-1.55726
H	-2.62349	-0.41361	-1.45957
H	-2.72278	-1.73698	-2.62959
C	-4.17216	-1.52316	0.51360
H	-4.08759	-0.43944	0.63146
H	-5.13641	-1.81936	0.95075
C	-3.02896	-2.23768	1.26479
H	-3.06699	-1.96645	2.32264
C	-1.61464	-1.84041	0.69270
C	-3.22982	-3.76291	1.13518
H	-2.44430	-4.29760	1.68624
H	-4.19022	-4.04685	1.58901
C	-0.43652	1.17102	-0.07169
H	-0.78521	1.02733	-1.10054
C	-0.51824	2.56733	0.33186
C	-1.36952	3.47266	-0.37464
C	2.38527	-0.69187	2.24291
O	-0.39410	0.56459	2.88284
C	-1.63285	0.73966	3.00728
O	-2.48825	0.30707	2.15822
H	-1.86520	-0.48296	1.33468
C	-2.15395	1.53312	4.18498
C	-2.95824	3.73443	-2.21427
H	-3.49136	4.46373	-1.59092
C	3.64106	-0.66379	3.08536
C	-2.11763	4.45345	-3.27026
H	-1.36163	5.09852	-2.81303
H	-1.60444	3.72061	-3.90282
H	-2.75690	5.07355	-3.90883
C	-3.97482	2.77612	-2.82583
H	-3.46803	2.01392	-3.42781
H	-4.54732	2.27181	-2.04155
H	-4.67089	3.32190	-3.47190
C	0.26044	3.08159	1.39247
C	-1.42123	4.82246	-0.00818
H	0.92720	2.39873	1.90494
H	-2.06601	5.51767	-0.53232
C	0.20799	4.42544	1.74916
C	-0.63711	5.28858	1.04962
H	-0.68892	6.34068	1.31886
H	0.82739	4.79956	2.55903
C	3.05262	-0.66468	-1.29688
C	3.99456	-1.54479	-0.73118
C	3.40673	0.64636	-1.65623
C	5.29681	-1.07952	-0.52242
C	4.72102	1.06627	-1.42667
C	5.67931	0.22360	-0.85733
H	6.03089	-1.75601	-0.08882
H	5.00090	2.08120	-1.70200
C	2.40270	1.60194	-2.25354
H	1.68973	1.93878	-1.49320
H	2.90413	2.48580	-2.66018
H	1.82047	1.14322	-3.06050
C	3.61766	-2.95381	-0.33316
H	2.88107	-2.94732	0.47789
H	3.18189	-3.51778	-1.16722
H	4.49893	-3.50399	0.01120
C	7.08476	0.71286	-0.59318
H	7.80912	-0.10813	-0.62688
H	7.39169	1.46693	-1.32613
H	7.16308	1.17556	0.39979
H	-0.91002	-2.50313	1.21571
H	4.50391	-0.41932	2.45802
H	3.79361	-1.62840	3.57375
H	3.55088	0.11931	3.84641
H	-1.48850	1.41701	5.04352
H	-3.17105	1.22875	4.44172
H	-2.16975	2.59432	3.90838

18a

Ru	-0.00840	0.47979	0.08197
O	-0.57791	2.87244	-0.04835
O	1.36008	1.99509	2.52809
O	-0.31981	0.53060	2.16777
N	1.56357	-2.04958	0.25627
N	-0.58569	-2.53206	0.18679
C	0.30850	-1.49827	0.16068
C	1.52861	-3.52426	0.18647
H	2.14370	-3.97354	0.96733
H	1.90306	-3.87041	-0.78593
C	0.05256	-3.84206	0.37971
H	-0.33143	-4.56904	-0.34216
H	-0.16442	-4.22010	1.38683
C	2.88537	-1.38933	0.05116

C	3.27727	-1.39103	-1.45001
H	2.51848	-0.83466	-2.00855
H	3.29473	-2.42091	-1.83305
C	4.66873	-0.74624	-1.63717
H	4.92479	-0.75806	-2.70478
C	5.72458	-1.53848	-0.84045
H	5.77639	-2.57479	-1.20363
H	6.72022	-1.09887	-0.98970
C	5.35849	-1.51879	0.65802
H	6.09531	-2.10107	1.22690
C	3.97053	-2.16517	0.84882
H	3.69814	-2.18485	1.91297
H	4.03014	-3.20437	0.50599
C	5.32968	-0.06700	1.16765
H	5.09314	-0.04321	2.23990
H	6.31714	0.39883	1.04549
C	4.26966	0.71525	0.37284
H	4.21298	1.74572	0.74209
C	2.88513	0.05897	0.57278
H	2.59855	0.09340	1.62614
C	4.63003	0.70887	-1.12712
H	3.88836	1.28499	-1.69478
H	5.60542	1.19050	-1.28219
C	-2.02344	-2.54535	0.23710
C	-2.73240	-2.80953	-0.95169
C	-4.12637	-2.90991	-0.88325
H	-4.68117	-3.09942	-1.79982
C	-4.82014	-2.77123	0.32308
C	-4.08093	-2.53433	1.48602
H	-4.60197	-2.43329	2.43590
C	-2.68508	-2.43220	1.47497
C	-2.03132	-2.92321	-2.28474
H	-1.17613	-3.60791	-2.24690
H	-1.65799	-1.94529	-2.61240
H	-2.72210	-3.29417	-3.04838
C	-6.32377	-2.91596	0.37544
H	-6.75867	-2.29877	1.16889
H	-6.61530	-3.95583	0.57618
H	-6.78803	-2.62676	-0.57339
C	-1.93402	-2.19638	2.76315
H	-1.19667	-2.98714	2.95361
H	-2.62786	-2.18669	3.60985
H	-1.39497	-1.24283	2.74103
C	-1.79364	0.47948	-0.41923
H	-2.36866	-0.41131	-0.64718
C	-2.55564	1.70842	-0.50379
C	-3.93354	1.69058	-0.78960
H	-4.41293	0.72737	-0.94265
C	-4.66489	2.86983	-0.88474
H	-5.72796	2.84296	-1.10429
C	-4.01150	4.09080	-0.70323
H	-4.56759	5.02149	-0.77955
C	-2.64321	4.14618	-0.42048
H	-2.17119	5.10989	-0.27997
C	-1.91700	2.95726	-0.31379
C	0.23283	4.09330	-0.03267
H	-0.16222	4.73100	-0.83227
C	1.65822	3.68640	-0.37278
H	2.06417	3.07063	0.43377
H	2.27549	4.58640	-0.47587
H	1.68603	3.12511	-1.31090
C	0.12908	4.78617	1.32405
H	-0.90599	5.02513	1.58647
H	0.69729	5.72369	1.29812
H	0.55157	4.13812	2.09628
C	0.39451	1.31957	2.91139
C	-0.06695	1.37304	4.36610
H	2.17822	0.68029	0.00550
O	0.71338	0.67793	-1.86403
C	-0.01484	0.56053	-2.93956
O	-1.21360	0.27009	-2.97665
C	0.76633	0.79790	-4.22997
H	-1.02261	1.90745	4.42649
H	0.67195	1.89318	4.97933
H	-0.23481	0.36432	4.75689
H	1.43294	1.65953	-4.12851
H	1.39192	-0.07748	-4.44388
H	0.07913	0.94938	-5.06482

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Ru	0.52067	0.56825	-0.37274
O	1.42454	2.74915	0.19631
O	1.52466	-0.67504	1.43930
O	-0.38436	0.39145	1.72660
N	-1.58843	-1.35106	-1.54749
N	0.52011	-2.06628	-1.59752
C	-0.29509	-1.05106	-1.15551
C	-1.60697	-2.64933	-2.26466
H	-2.25225	-2.60678	-3.14381
H	-1.96710	-3.45116	-1.60579
C	-0.14683	-2.86746	-2.62656
H	0.14504	-3.91739	-2.59684

H	0.09591	-2.46918	-3.62273
C	-2.83476	-1.04714	-0.74662
C	-2.78641	-1.82059	0.59714
H	-1.92216	-1.46877	1.16802
H	-2.65360	-2.89546	0.41085
C	-4.08206	-1.58869	1.40356
H	-4.02217	-2.15285	2.34385
C	-5.29600	-2.07022	0.58531
H	-5.21049	-3.14583	0.37451
H	-6.22139	-1.93049	1.16062
C	-5.37345	-1.27429	-0.73440
H	-6.22672	-1.62686	-1.32910
C	-4.08170	-1.50801	-1.54953
H	-4.12642	-0.96058	-2.50141
H	-4.02511	-2.57486	-1.79023
C	-5.53381	0.22413	-0.42387
H	-5.62175	0.79801	-1.35701
H	-6.45672	0.39585	0.14717
C	-4.30793	0.69388	0.37799
H	-4.38742	1.76890	0.58538
C	-3.02064	0.45546	-0.44301
H	-3.07591	1.01141	-1.38693
C	-4.22416	-0.08377	1.70610
H	-3.36197	0.26523	2.28734
H	-5.12487	0.09855	2.30878
C	1.93865	-2.13383	-1.40407
C	2.53601	-3.34203	-1.00881
C	3.92626	-3.36431	-0.82691
H	4.39457	-4.29757	-0.52002
C	4.71601	-2.22526	-0.98832
C	4.08085	-1.02795	-1.33610
H	4.67122	-0.12049	-1.45017
C	2.70220	-0.95801	-1.55367
C	1.73942	-4.59274	-0.71448
H	2.28186	-5.22912	-0.00815
H	1.55600	-5.20073	-1.61183
H	0.76697	-4.35234	-0.27143
C	6.21357	-2.27784	-0.78984
H	6.74908	-2.18367	-1.74414
H	6.52362	-3.22253	-0.33093
H	6.56102	-1.46135	-0.14550
C	2.00042	0.31337	-1.88012
H	1.53137	0.25411	-2.86905
H	2.68812	1.16710	-1.88133
C	-0.39004	1.72707	-1.50921
H	-1.08553	1.42220	-2.30107
C	-0.20068	3.16646	-1.43708
C	-0.92386	4.06663	-2.24274
H	-1.63149	3.65868	-2.96061
C	-0.75493	5.44362	-2.12725
H	-1.32476	6.12264	-2.75466
C	0.15018	5.94181	-1.18859
H	0.28645	7.01429	-1.07851
C	0.89426	5.07991	-0.37552
H	1.58083	5.50193	0.34772
C	0.73014	3.70004	-0.50845
C	2.37695	3.14725	1.23058
H	2.86453	4.06355	0.88199
C	3.42926	2.05180	1.32718
H	2.98782	1.08869	1.59651
H	4.16678	2.33175	2.08833
H	3.95026	1.93551	0.37182
C	1.62319	3.40414	2.53233
H	0.90202	4.22035	2.42073
H	2.32649	3.67425	3.32817
H	1.07378	2.50648	2.83004
C	0.55284	-0.35159	2.17807
C	0.49536	-0.87993	3.62593
C	0.29558	-2.41078	3.55240
H	1.09827	-2.87670	2.97307
H	-0.66097	-2.66432	3.07926
H	0.29488	-2.84249	4.56111
C	1.84299	-0.57999	4.31435
H	2.67203	-1.01313	3.74834
H	1.85218	-0.99840	5.32843
H	2.01438	0.50032	4.39798
C	-0.65507	-0.23632	4.41495
H	-0.67201	-0.62709	5.44028
H	-1.62395	-0.44614	3.95244
H	-0.54451	0.85199	4.46716
H	-2.16454	0.83181	0.11592

S1

Ru	0.05166	-0.03195	-0.99224
O	-0.23272	2.21710	-1.89029
N	-0.75511	-2.49912	0.28883
N	1.42860	-2.36187	0.49535
C	0.32906	-1.73964	-0.00204
C	-0.42871	-3.61060	1.19427
H	-0.92037	-4.53784	0.88620
H	-0.74375	-3.36369	2.21418
C	1.09622	-3.67769	1.07502

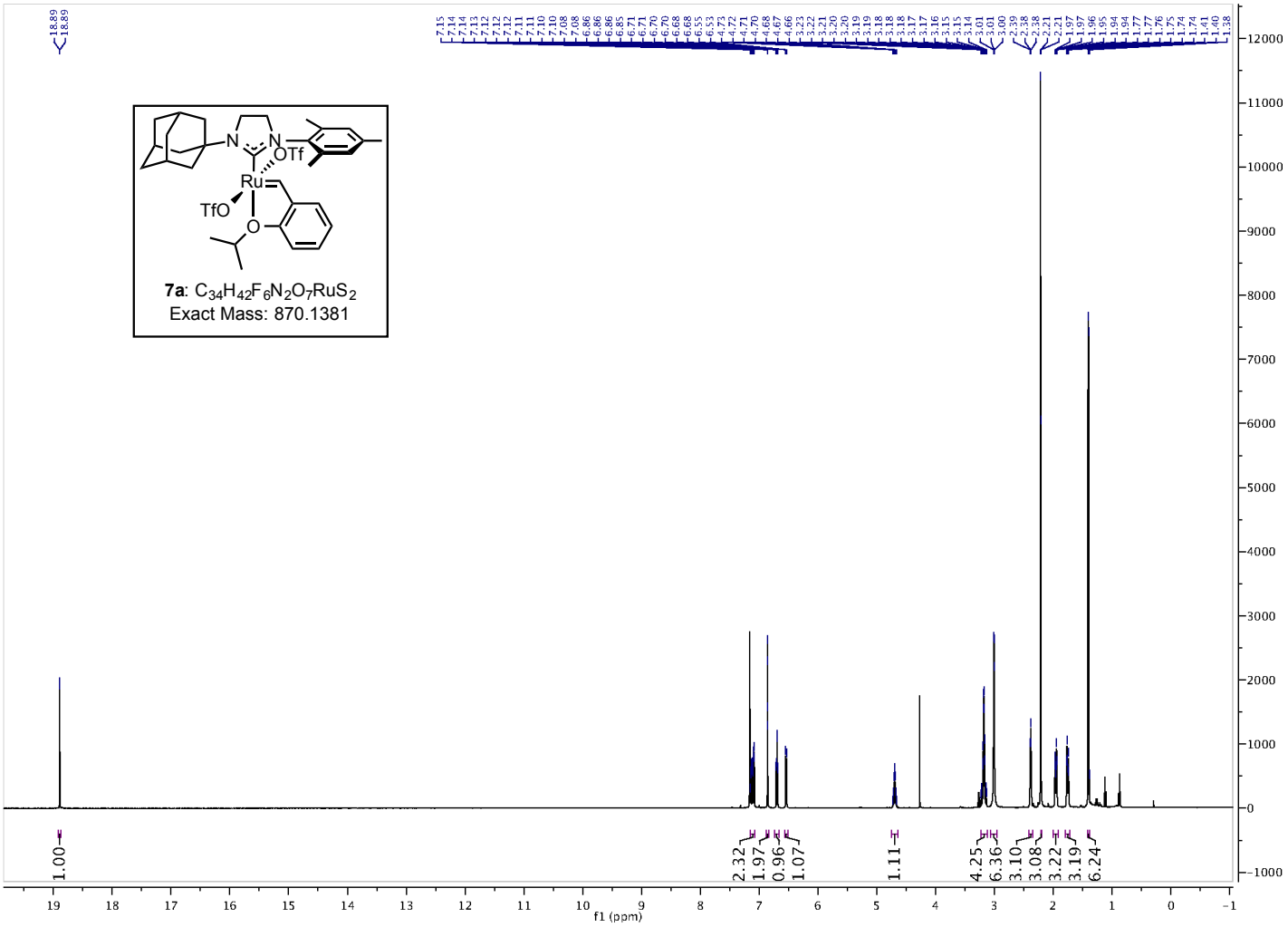
H	1.59283	-3.81079	2.03941
H	1.42896	-4.47635	0.39949
C	-2.14009	-2.07760	0.03906
C	-2.96356	-2.06795	1.35337
H	-2.47433	-1.41415	2.08067
H	-2.98157	-3.08184	1.77600
C	-2.82042	-3.05709	-0.95788
H	-2.23231	-3.09559	-1.88440
H	-2.82947	-4.07311	-0.53812
C	-2.12309	-0.67204	-0.60098
C	2.80951	-1.96883	0.42364
C	3.38033	-1.30210	1.52633
C	4.72926	-0.93672	1.45082
H	5.17409	-0.40705	2.29107
C	5.51954	-1.24334	0.33957
C	4.93893	-1.97598	-0.69975
H	5.54700	-2.25905	-1.55638
C	3.59587	-2.36425	-0.67578
C	2.60540	-1.03861	2.79980
H	2.59177	-1.93824	3.43227
H	1.56227	-0.75274	2.63692
H	3.08937	-0.25103	3.38692
C	6.96000	-0.79383	0.26078
H	7.04721	0.15527	-0.28474
H	7.58149	-1.52657	-0.26567
H	7.38758	-0.63838	1.25706
C	3.05129	-3.24940	-1.77182
H	3.02553	-4.29901	-1.44541
H	3.68950	-3.19963	-2.65863
H	2.04554	-2.95627	-2.07527
C	1.15371	0.99271	0.07934
H	1.68662	0.58827	0.93800
C	1.35566	2.39812	-0.17866
C	2.27703	3.15890	0.56866
H	2.82279	2.66604	1.36875
C	2.49993	4.50199	0.28540
H	3.21528	5.07534	0.86697
C	1.79281	5.10419	-0.75763
H	1.95528	6.15298	-0.99054
C	0.86549	4.38207	-1.51555
H	0.33036	4.88548	-2.31045
C	0.64611	3.03371	-1.22806
C	-1.03025	2.75486	-2.99067
H	-0.36626	3.40118	-3.57485
C	-2.21108	3.54846	-2.43569
H	-2.86427	2.89406	-1.85014
H	-2.79332	3.97286	-3.26146
H	-1.88749	4.36668	-1.78678
C	-1.45699	1.58801	-3.86908
H	-0.59005	1.00819	-4.19463
H	-1.97947	1.97759	-4.75008
H	-2.14564	0.92528	-3.33527
H	-1.71478	0.28662	0.31900
O	-1.81595	1.25635	1.24287
C	-1.25541	1.00896	2.38703
O	-0.72587	-0.07025	2.70215
C	-1.30871	2.15616	3.43381
C	-3.59008	-0.20098	-0.83231
C	-4.41336	-1.62303	1.06845
C	-4.26693	-2.59983	-1.24401
H	-4.72567	-3.29322	-1.96119
C	-5.06948	-2.60080	0.07286
H	-6.10944	-2.30403	-0.12013
H	-5.09916	-3.61490	0.49577
H	-4.97340	-1.62618	2.01260
C	-4.40954	-0.20319	0.47329
C	-4.25644	-1.17476	-1.83573
H	-5.28493	-0.84835	-2.04336
H	-3.71891	-1.16726	-2.79484
H	-3.57227	0.81119	-1.25292
H	-5.43855	0.11403	0.25284
H	-3.98507	0.51291	1.18024
C	0.09545	2.33045	4.04453
H	0.81101	2.68063	3.29034
H	0.07355	3.07173	4.85353
H	0.45920	1.38095	4.44635
C	-2.28943	1.70378	4.53880
H	-2.33428	2.44991	5.34232
H	-3.30413	1.57901	4.14039
H	-1.96988	0.74857	4.96715
C	-1.78523	3.48172	2.82068
H	-1.81952	4.26345	3.59105
H	-1.11005	3.81614	2.02584
H	-2.78381	3.38210	2.38564
H	-1.75804	-0.80012	-1.65231
Cl	1.48853	-0.41288	-2.84688

S2

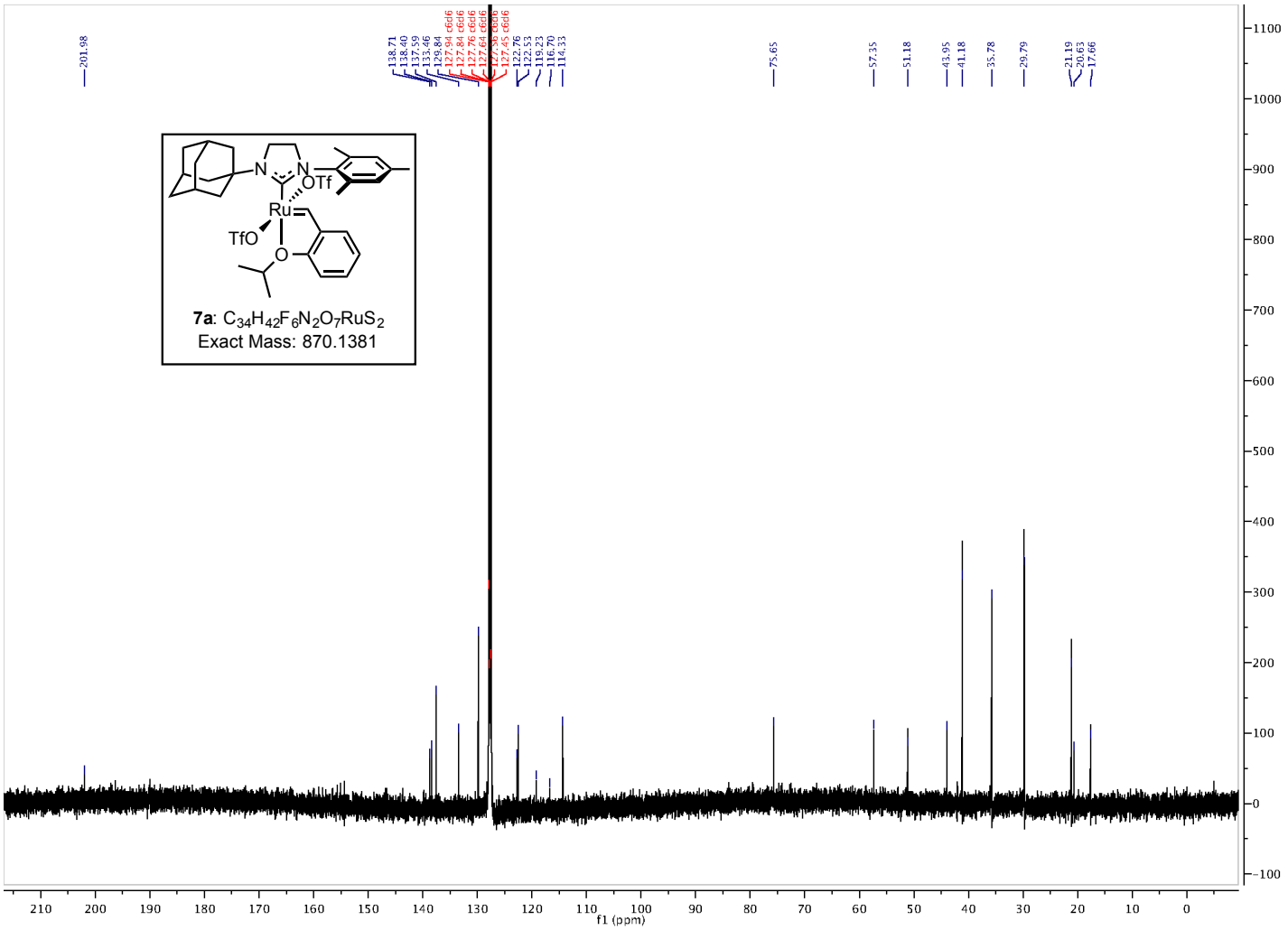
Ru	0.09259	0.50484	0.13689
O	-1.01323	2.44253	1.34368
N	-0.01275	-1.43841	-2.00491
N	2.10809	-1.07526	-1.54472

C	0.83310	-0.75416	-1.19142
C	0.68949	-2.19454	-3.05182
H	0.54477	-1.72122	-4.03078
H	0.32324	-3.22317	-3.11838
C	2.14771	-2.11603	-2.59021
H	2.50630	-3.06187	-2.16547
H	2.83500	-1.82633	-3.39071
C	-1.48594	-1.37434	-1.95591
C	-2.05594	-2.76277	-1.56255
H	-1.68427	-3.03649	-0.56802
H	-1.69856	-3.52933	-2.26416
C	-3.59980	-2.74003	-1.57283
H	-3.97254	-3.73987	-1.31272
C	-4.11064	-2.34536	-2.97189
H	-3.78122	-3.07638	-3.72428
H	-5.20900	-2.34795	-2.98282
C	-3.57774	-0.94272	-3.32847
H	-3.94458	-0.64855	-4.32105
C	-2.03682	-0.99714	-3.36028
H	-1.61850	-0.02594	-3.65861
H	-1.72480	-1.73141	-4.11674
C	-4.05239	0.08028	-2.27499
H	-3.70439	1.08755	-2.54148
H	-5.15150	0.11373	-2.26071
C	-3.51413	-0.32270	-0.88014
H	-3.85051	0.40945	-0.13535
C	-1.94134	-0.29489	-0.94519
H	-1.76658	0.66676	-1.42719
C	-4.09877	-1.71183	-0.54164
H	-3.82298	-2.01841	0.46843
H	-5.19654	-1.65745	-0.57497
C	0.21518	1.95270	-1.04167
H	0.71771	1.90648	-2.01629
C	-0.35689	3.24884	-0.76536
C	-1.02527	3.48809	0.46772
O	0.05221	-1.21936	1.73438
C	-1.06680	-1.55908	2.15504
O	-2.16283	-1.12408	1.60617
H	-1.88876	-0.65765	0.56292
C	-1.22857	-2.53826	3.32850
C	-1.49445	2.63639	2.71231
H	-1.34179	3.69171	2.95640
C	0.11532	-2.72666	4.04989
H	-0.01138	-3.41241	4.89609
H	0.87318	-3.14126	3.37955
H	0.49957	-1.77526	4.43106
C	-2.29160	-2.00147	4.30906
H	-3.24989	-1.84406	3.80691
H	-2.43910	-2.71919	5.12470
H	-1.97788	-1.05021	4.75402
C	-1.70691	-3.88733	2.74162
H	-0.97710	-4.28973	2.02915
H	-1.82928	-4.62039	3.54772
H	-2.66762	-3.77814	2.22843
C	3.36697	-0.76135	-0.91940
C	4.16746	0.25087	-1.47253
C	3.83453	-1.56598	0.13572
C	5.44455	0.45524	-0.94140
C	5.11744	-1.32338	0.63202
C	5.93599	-0.31536	0.11435
H	6.06799	1.24093	-1.36382
H	5.48392	-1.93644	1.45289
C	2.97350	-2.63710	0.75877
H	2.12341	-2.18925	1.28438
H	2.56763	-3.33551	0.01611
H	3.55390	-3.22308	1.47876
C	7.30501	-0.05218	0.69737
H	7.98051	0.38765	-0.04454
H	7.24519	0.64910	1.54027
H	7.76595	-0.97234	1.07336
C	3.67055	1.14030	-2.58654
H	4.50562	1.64652	-3.08125
H	3.10845	0.58826	-3.34773
H	3.00246	1.91314	-2.18744
C	-0.62183	1.80643	3.64086
H	-0.74406	0.73922	3.44806
H	0.43382	2.04959	3.50310
H	-0.91433	2.00980	4.67796
C	-2.97537	2.27440	2.77516
H	-3.35741	2.43503	3.78992
H	-3.56884	2.88455	2.08592
H	-3.11155	1.22002	2.51489
C	-0.30689	4.29388	-1.71267
C	-1.64250	4.72106	0.70356
C	-1.57639	5.72636	-0.26452
C	-0.90553	5.52444	-1.47365
H	-2.18670	4.91163	1.61979
H	-2.06193	6.67785	-0.06457
H	-0.85834	6.31561	-2.21576
H	0.21409	4.10987	-2.64926
Cl	2.07901	1.14570	1.37307

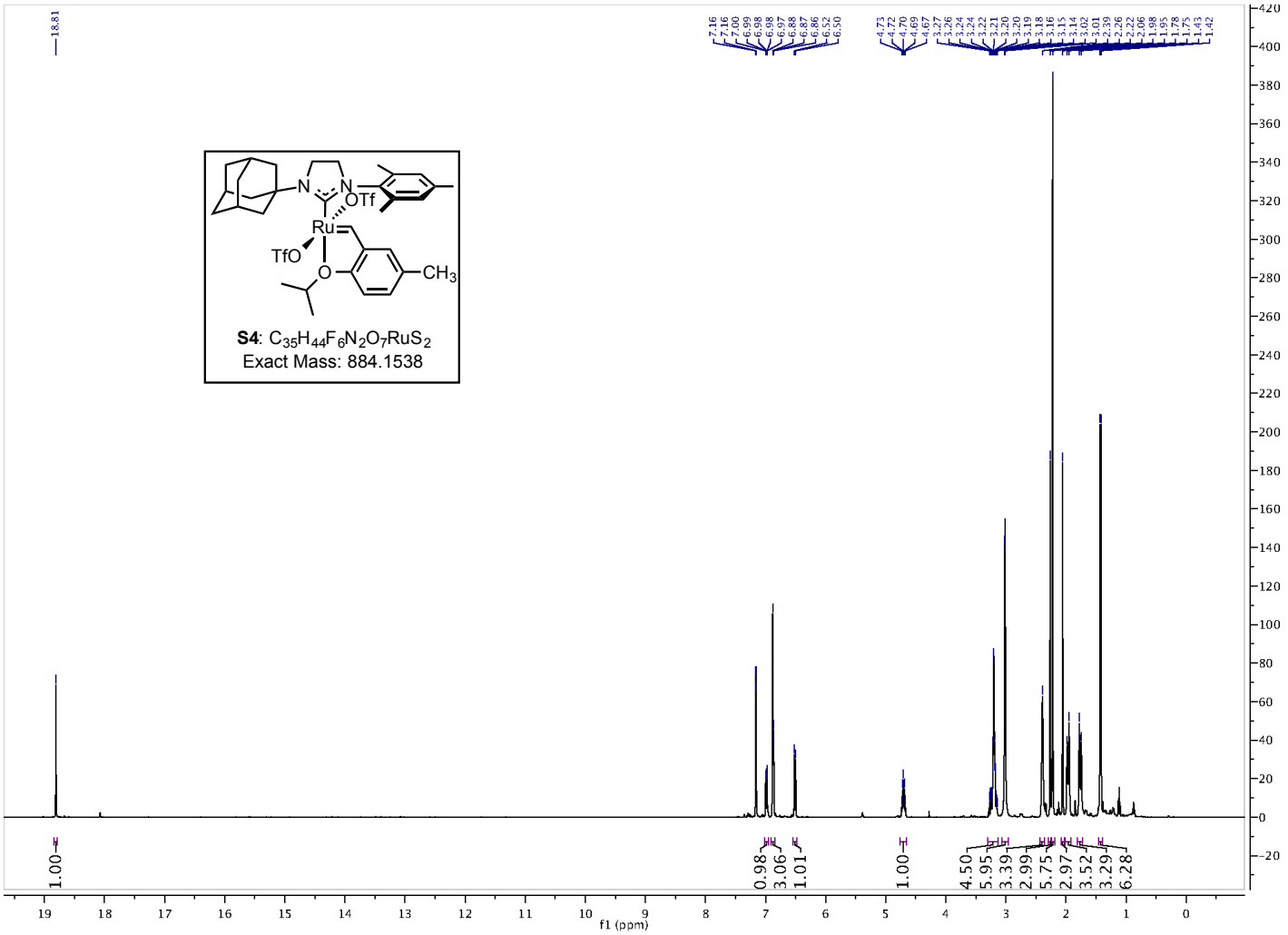
Part 3. NMR Spectra: ^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **7a**.



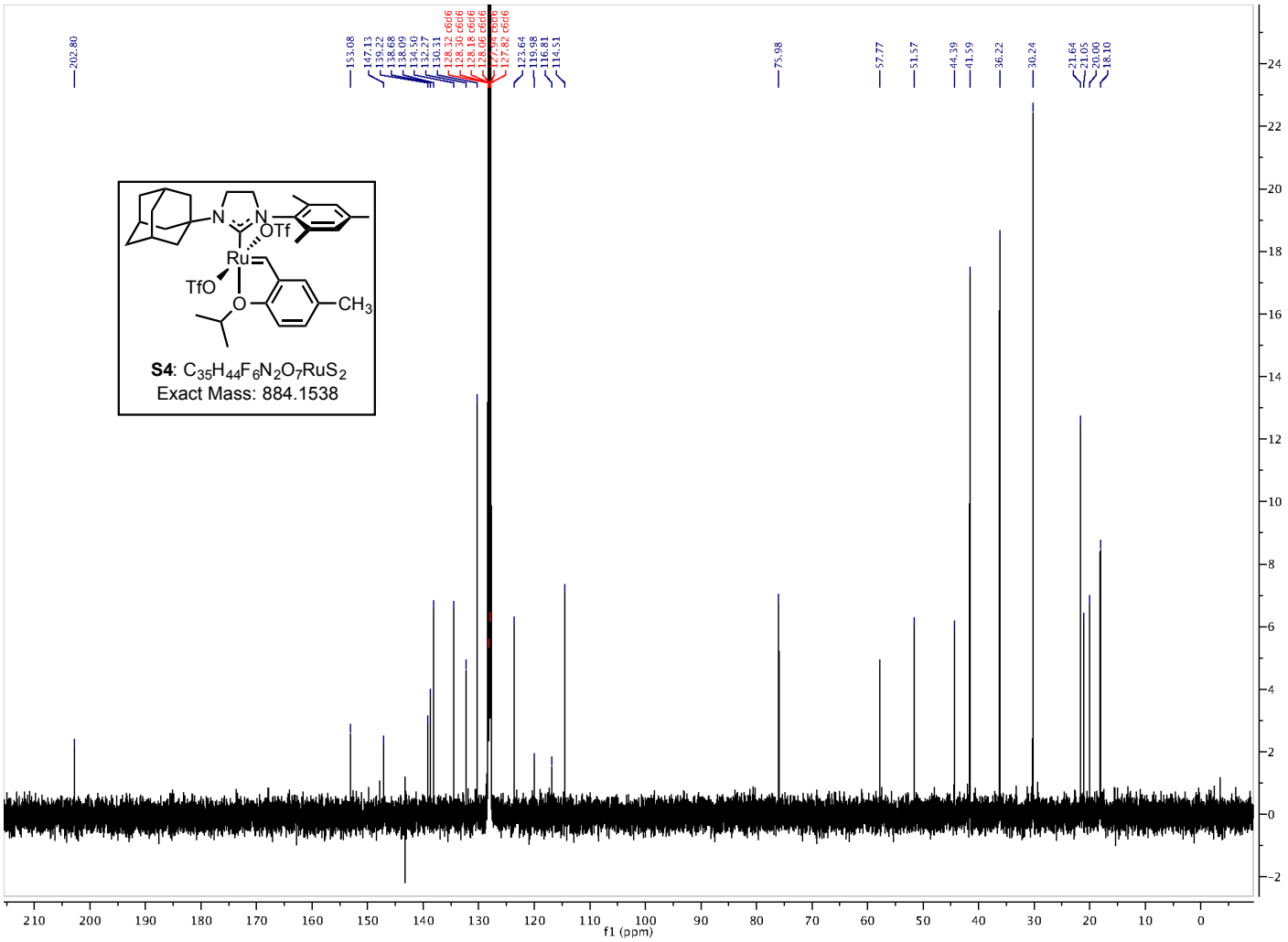
^{13}C NMR (126 MHz, C_6D_6) spectrum of compound **7a**.



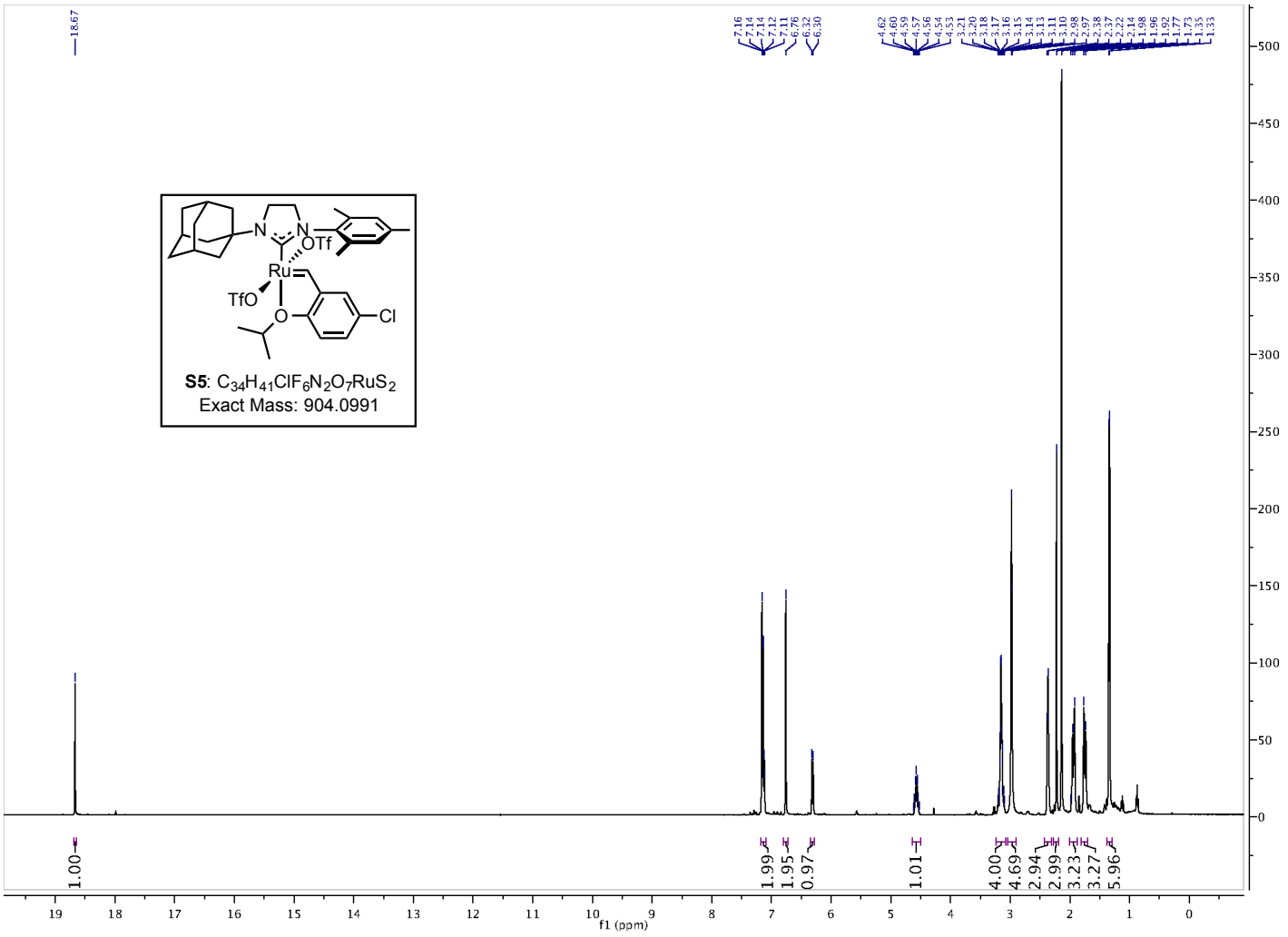
^{1}H NMR (400 MHz, C_6D_6) spectrum of compound **S4**.



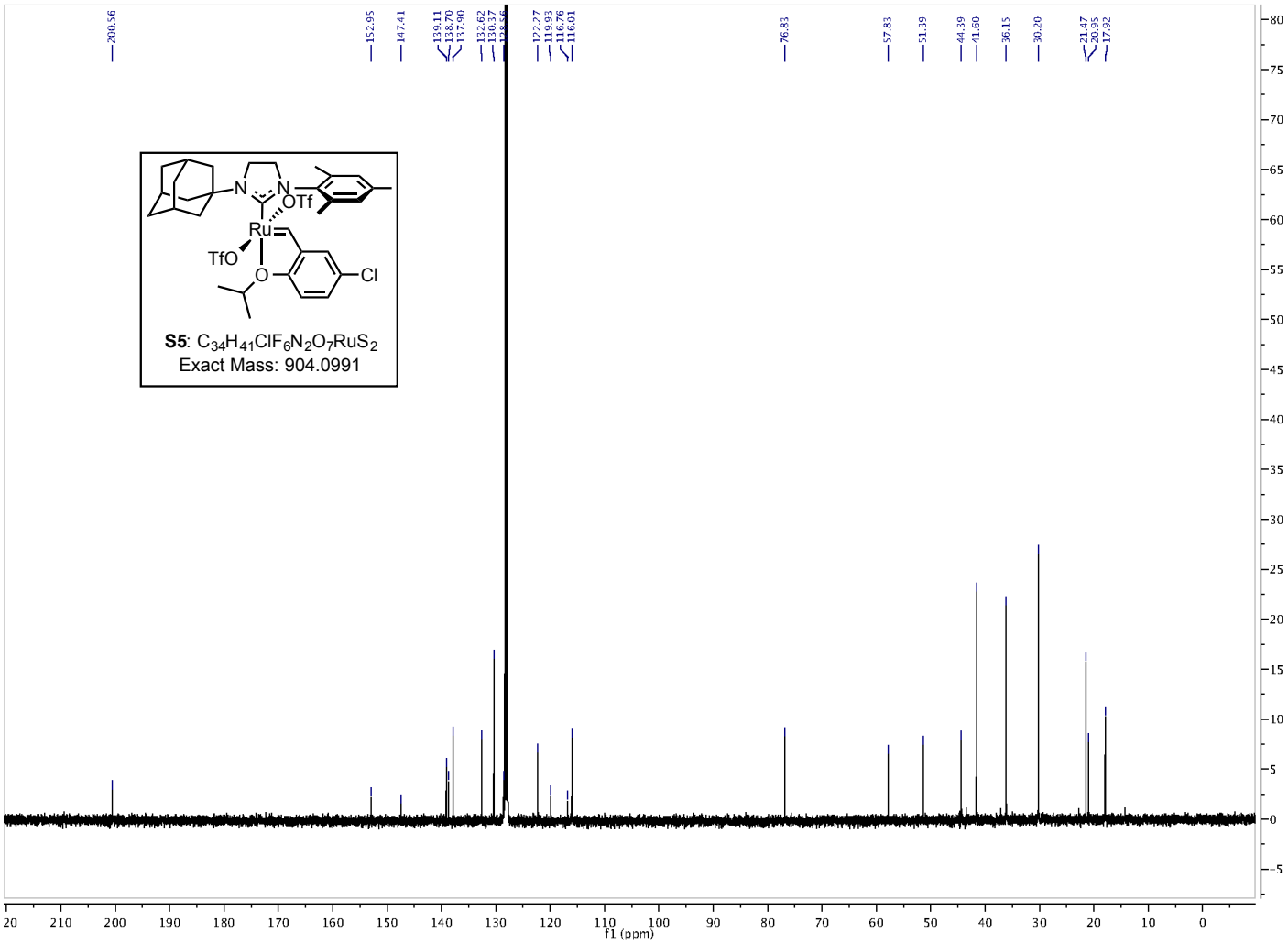
^{13}C NMR (101 MHz, C_6D_6) spectrum of compound **S4**.



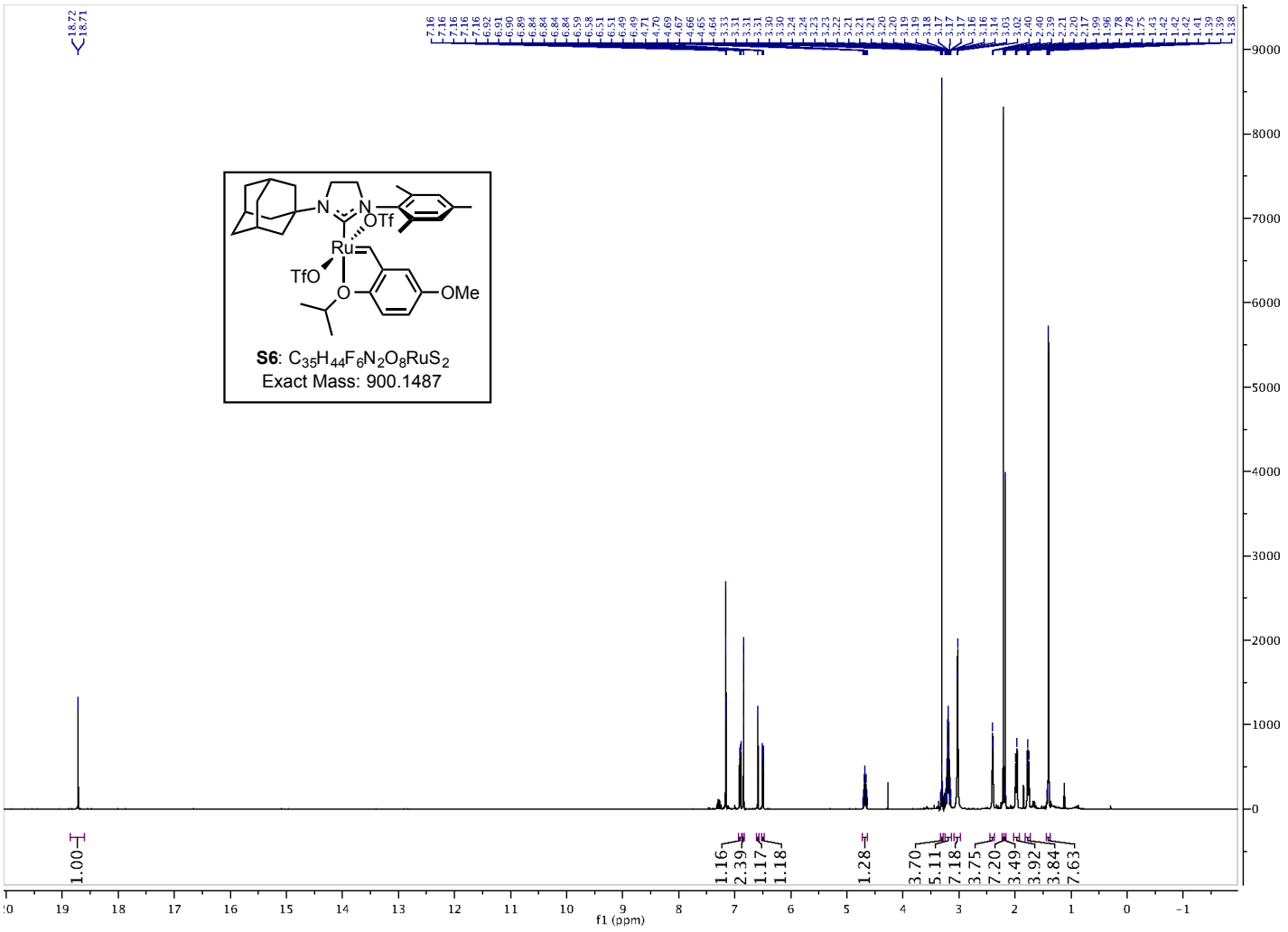
^{1}H NMR (400 MHz, C_6D_6) spectrum of compound **S5**.



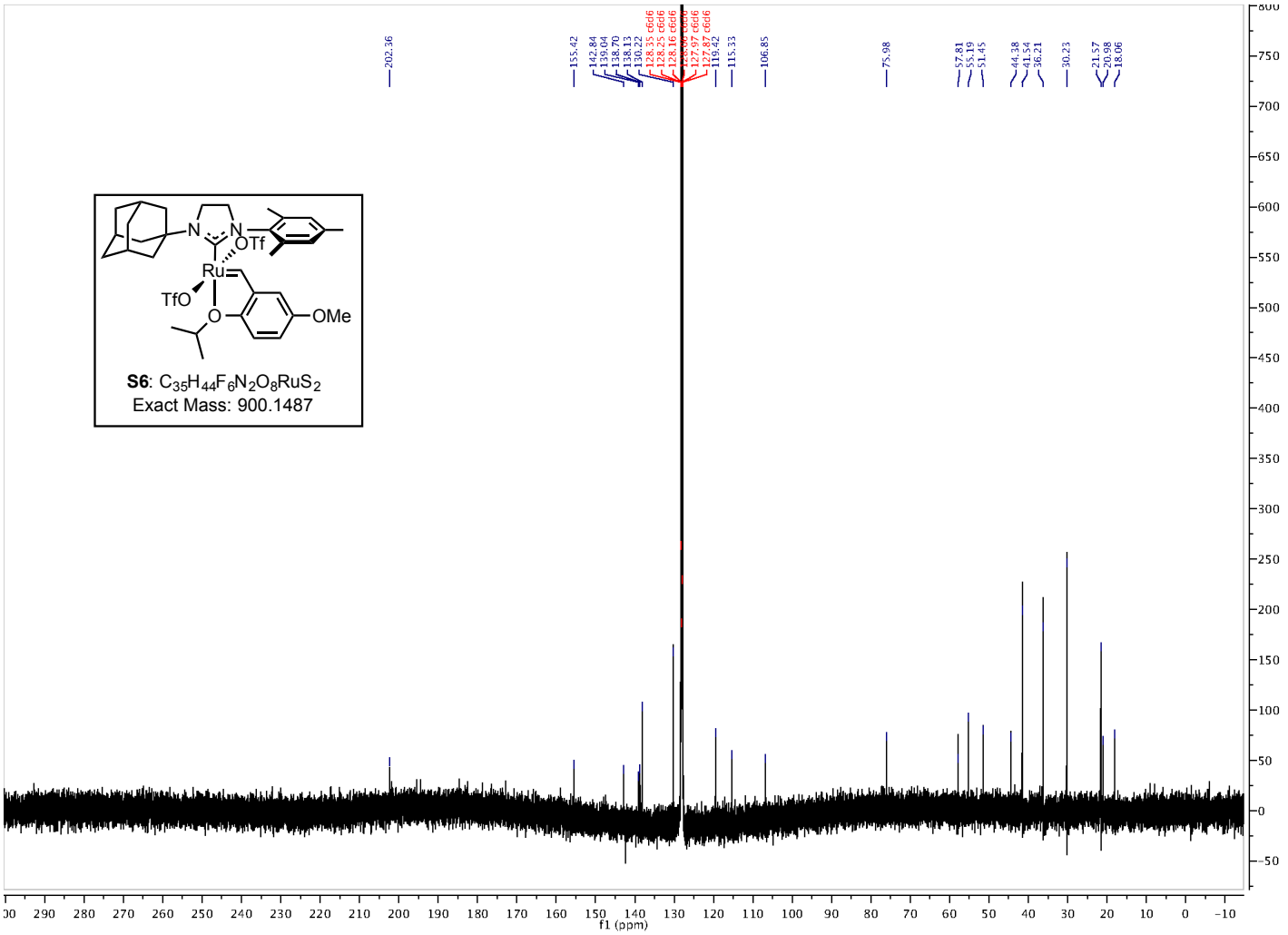
^{13}C NMR (101 MHz, C_6D_6) spectrum of compound **S5**.



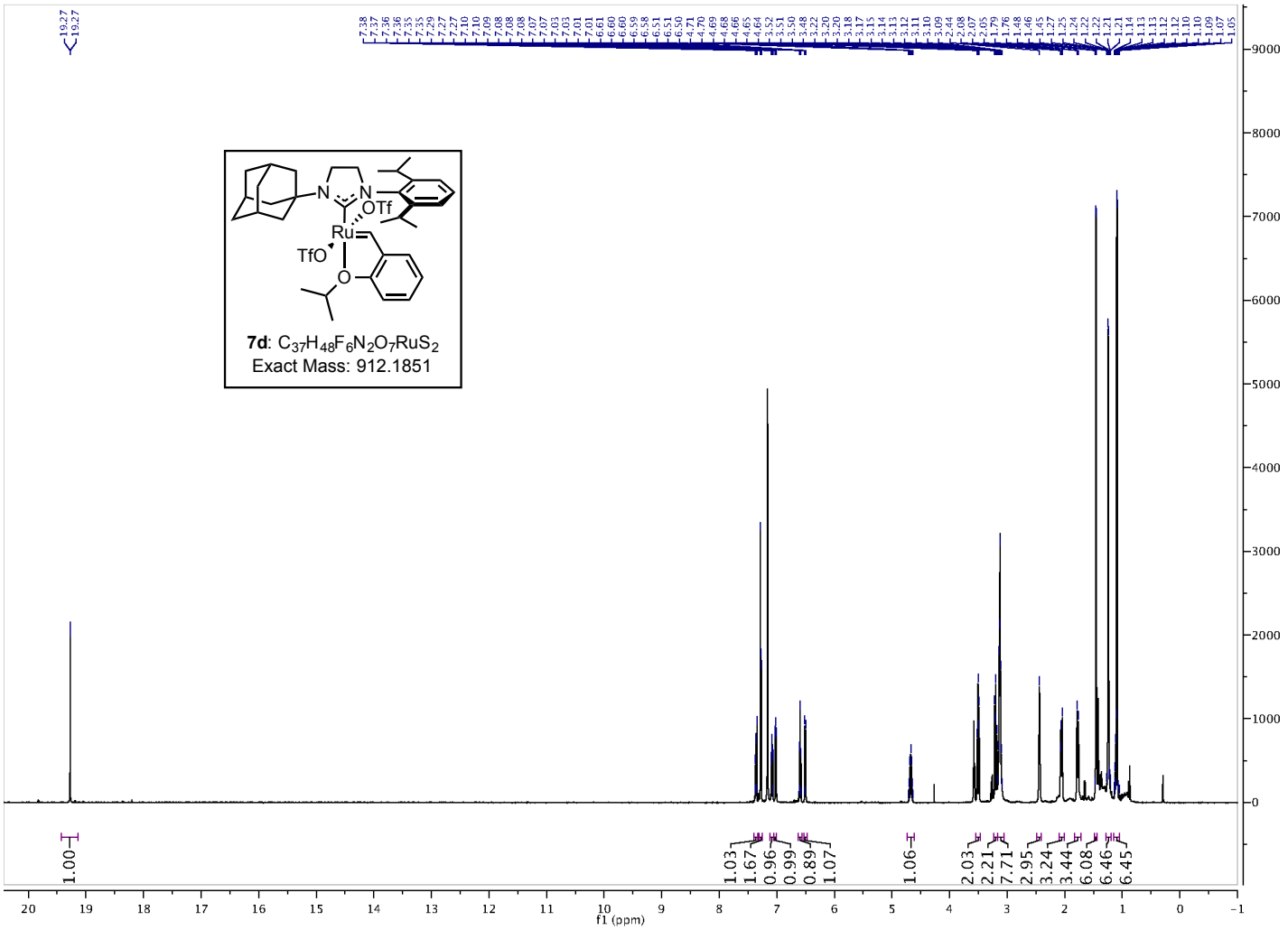
^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **S6**.



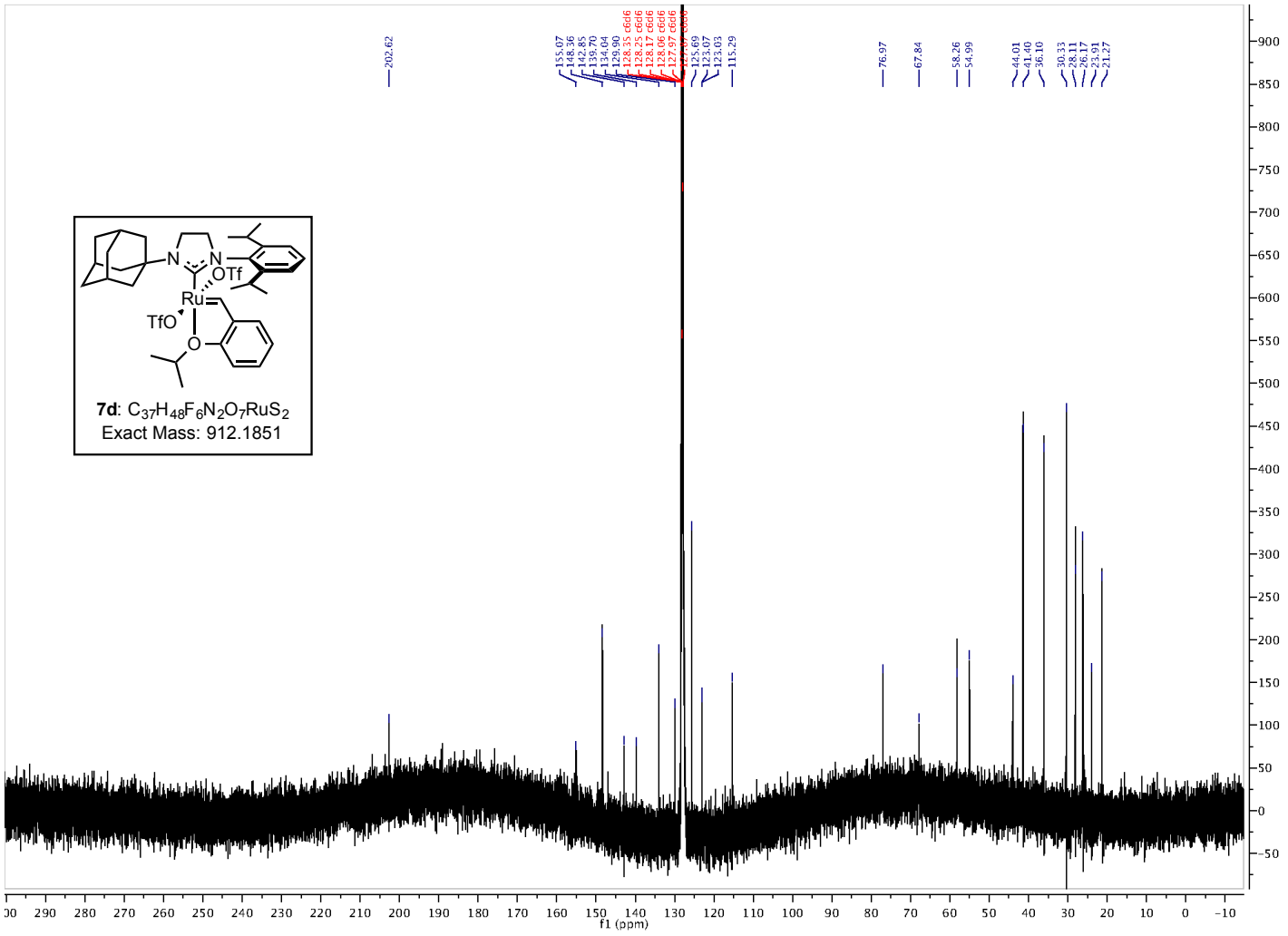
^{13}C NMR (126 MHz, C_6D_6) spectrum of compound **S6**.



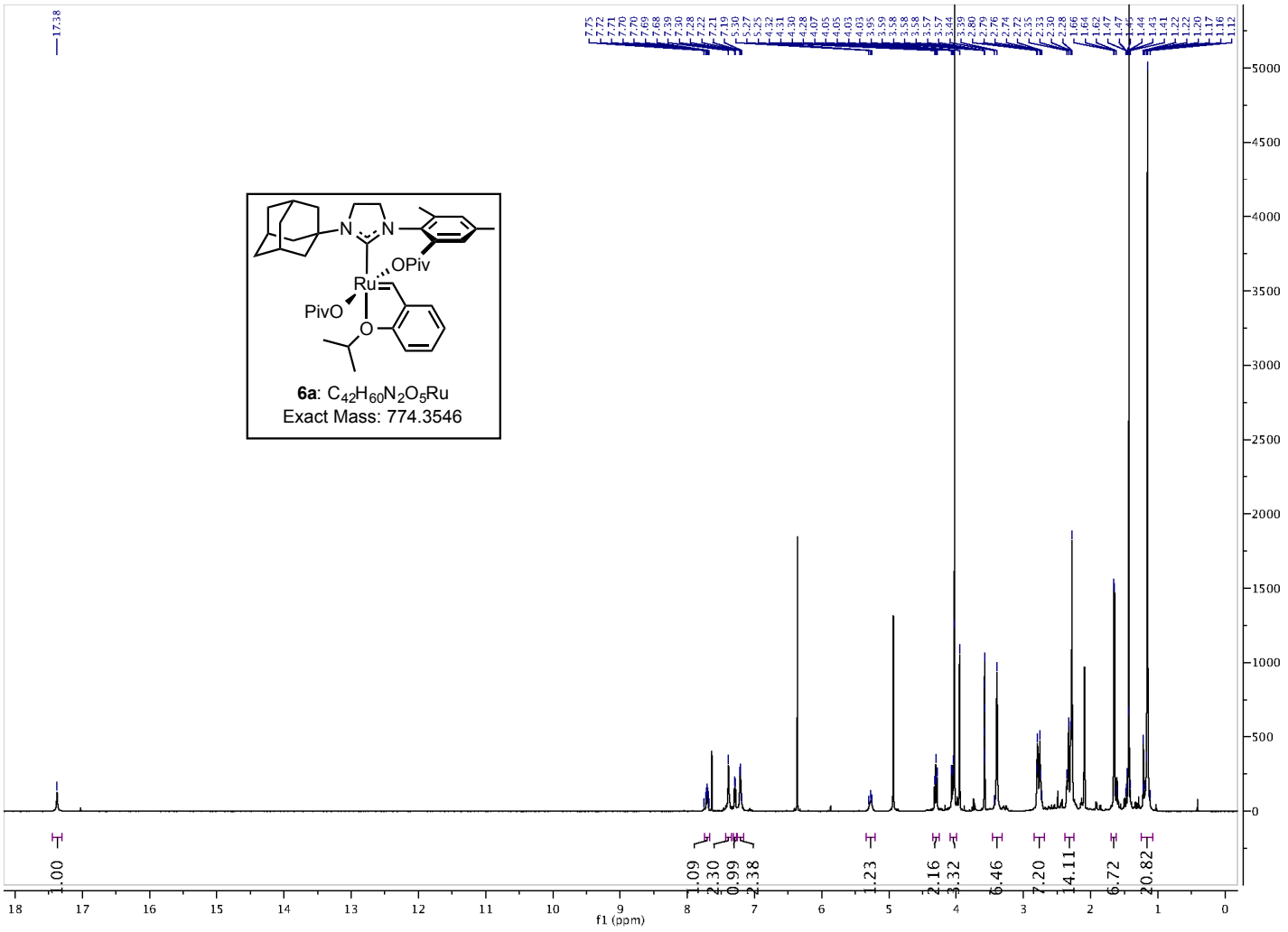
^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **7d**.



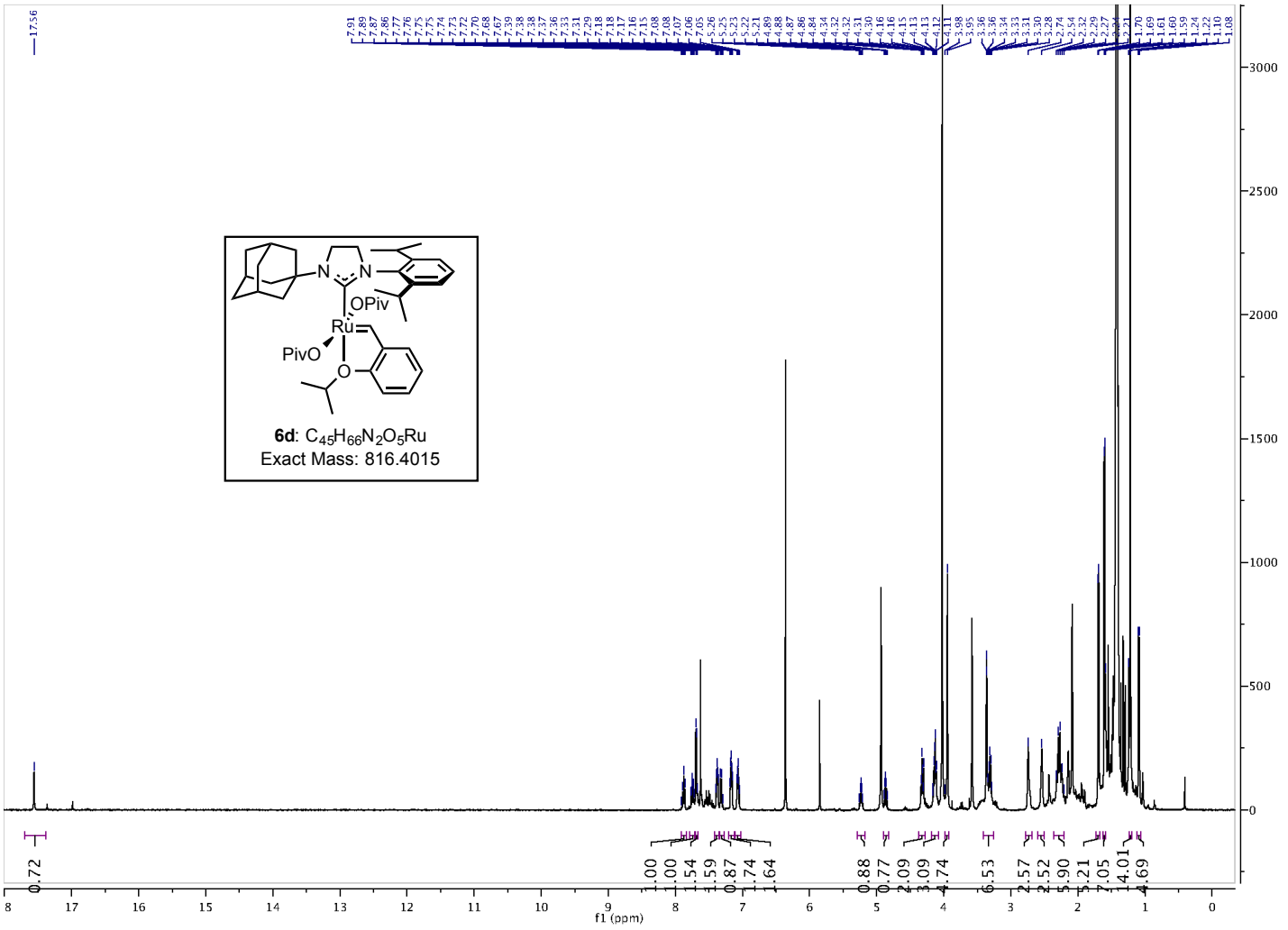
^{13}C NMR (126 MHz, C_6D_6) spectrum of compound **7d**.



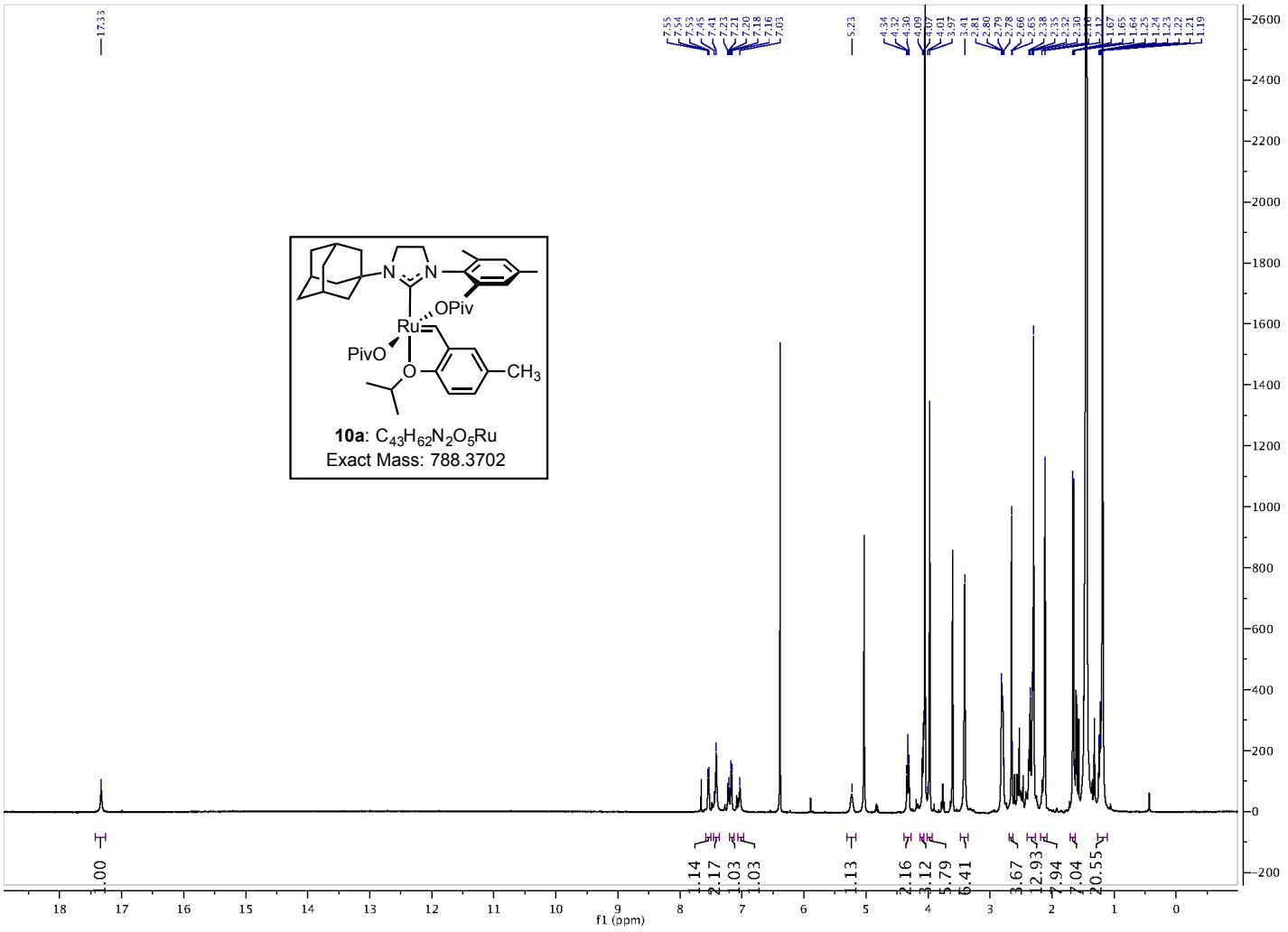
^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **6a**.



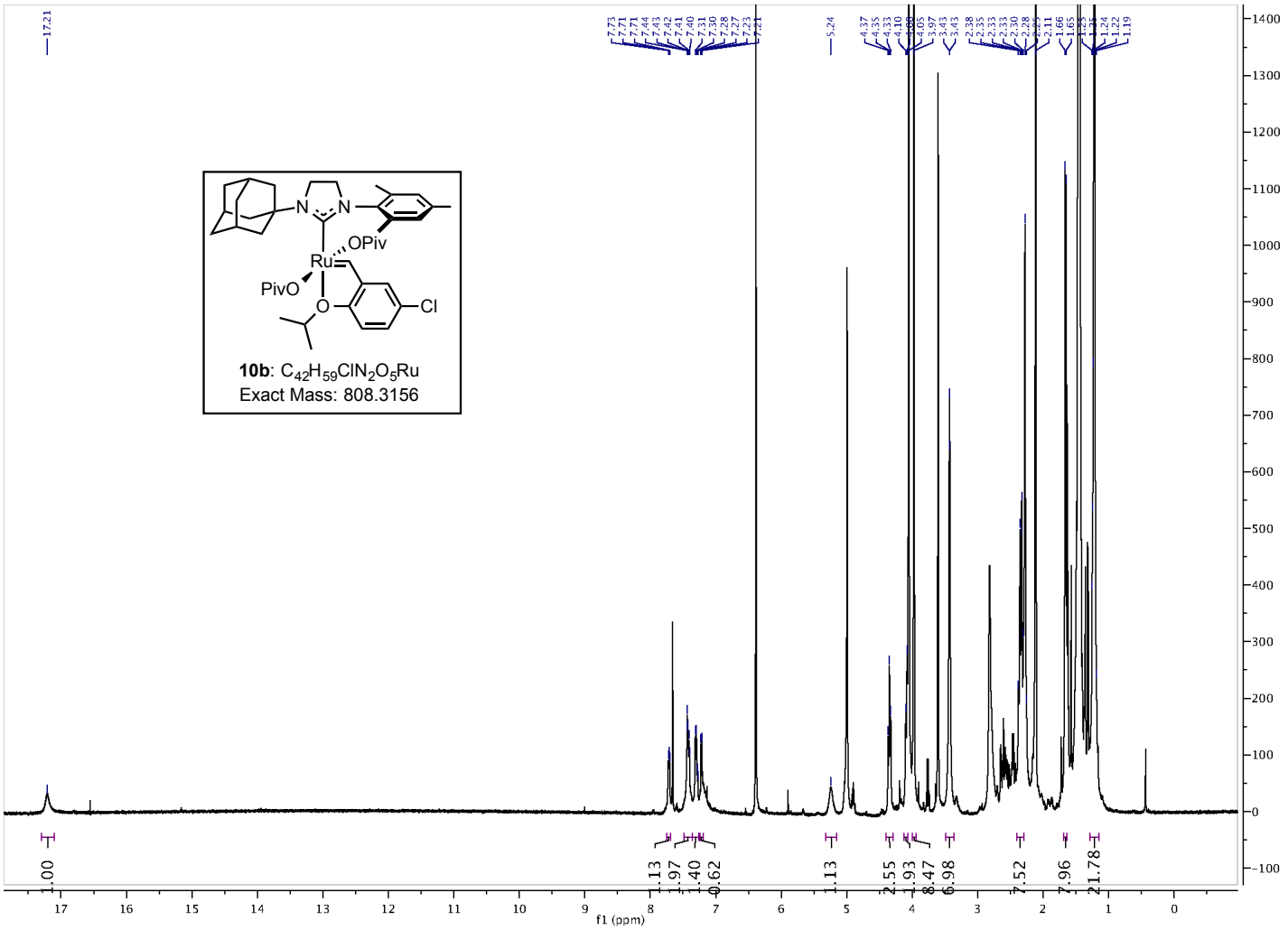
^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **6d**.



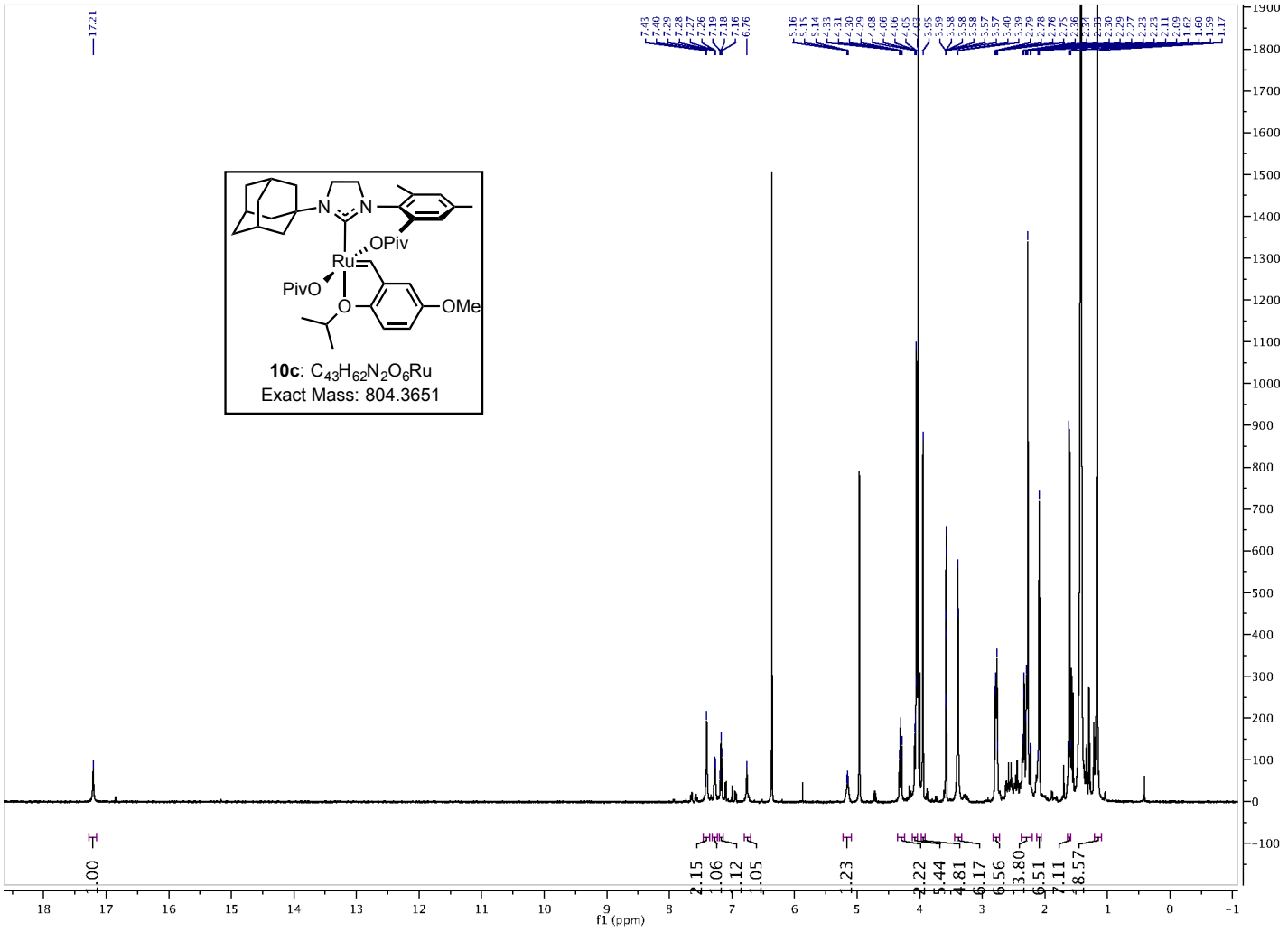
^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **10a**.



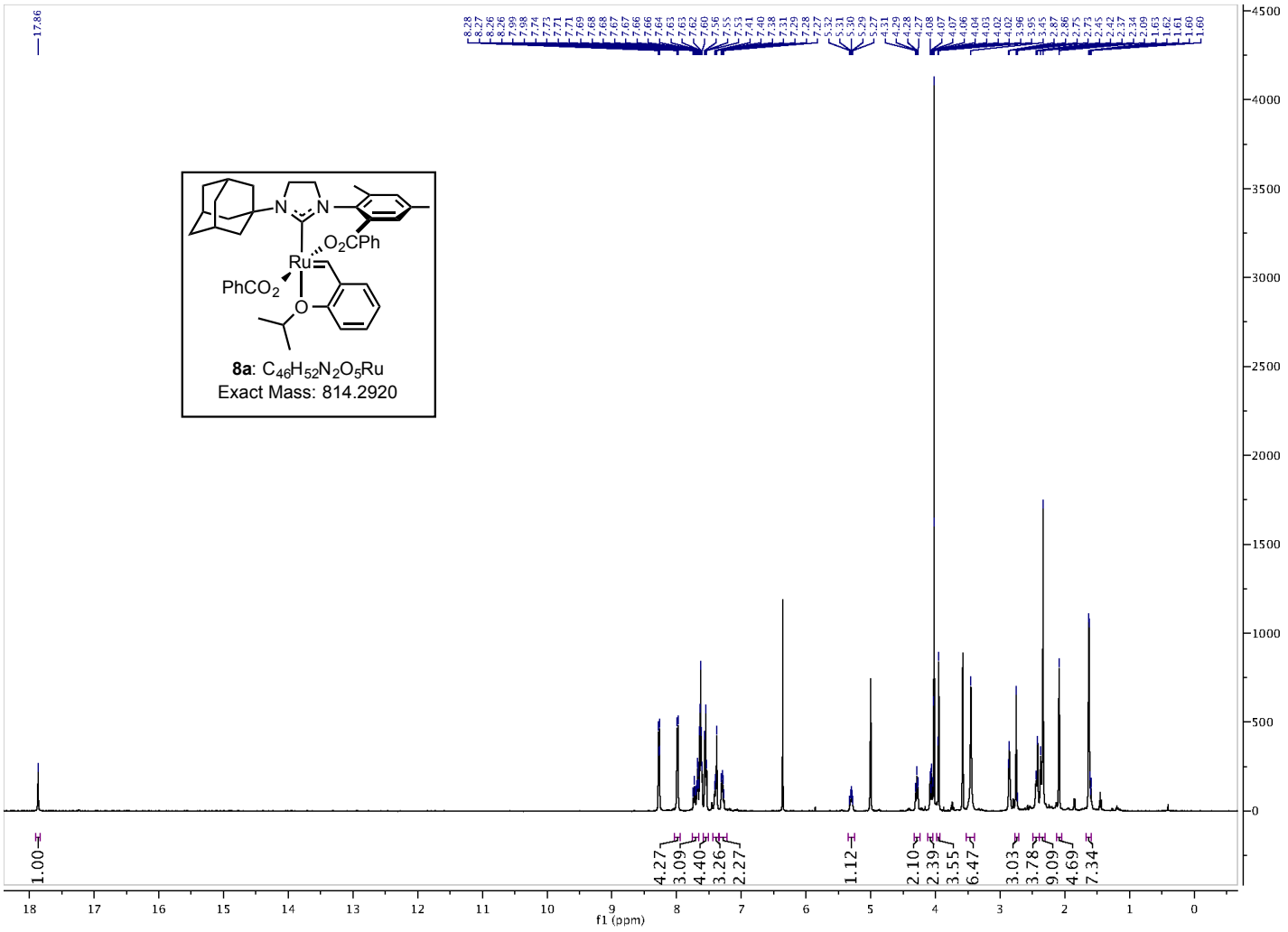
^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **10b**.



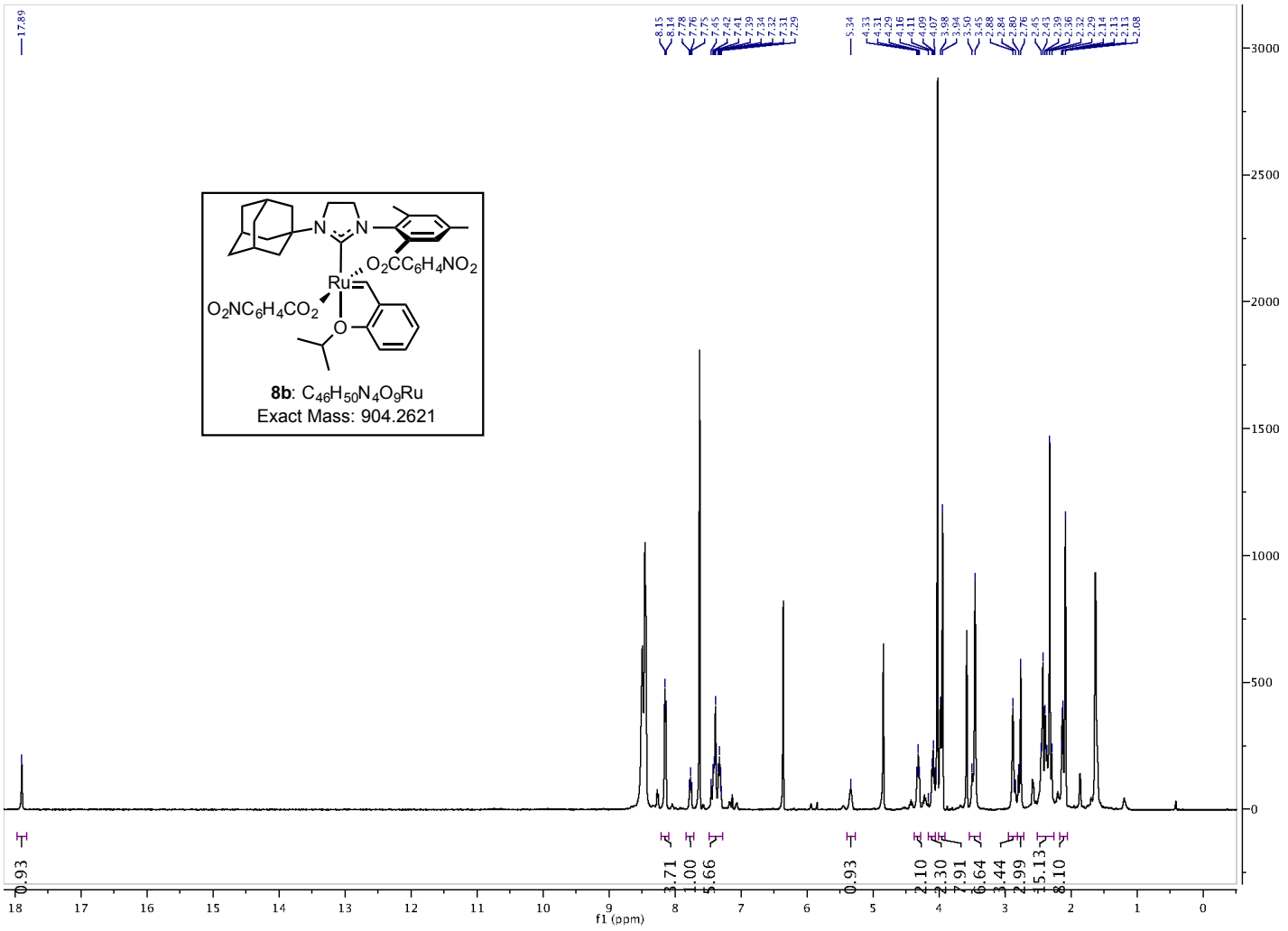
^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **10c**.



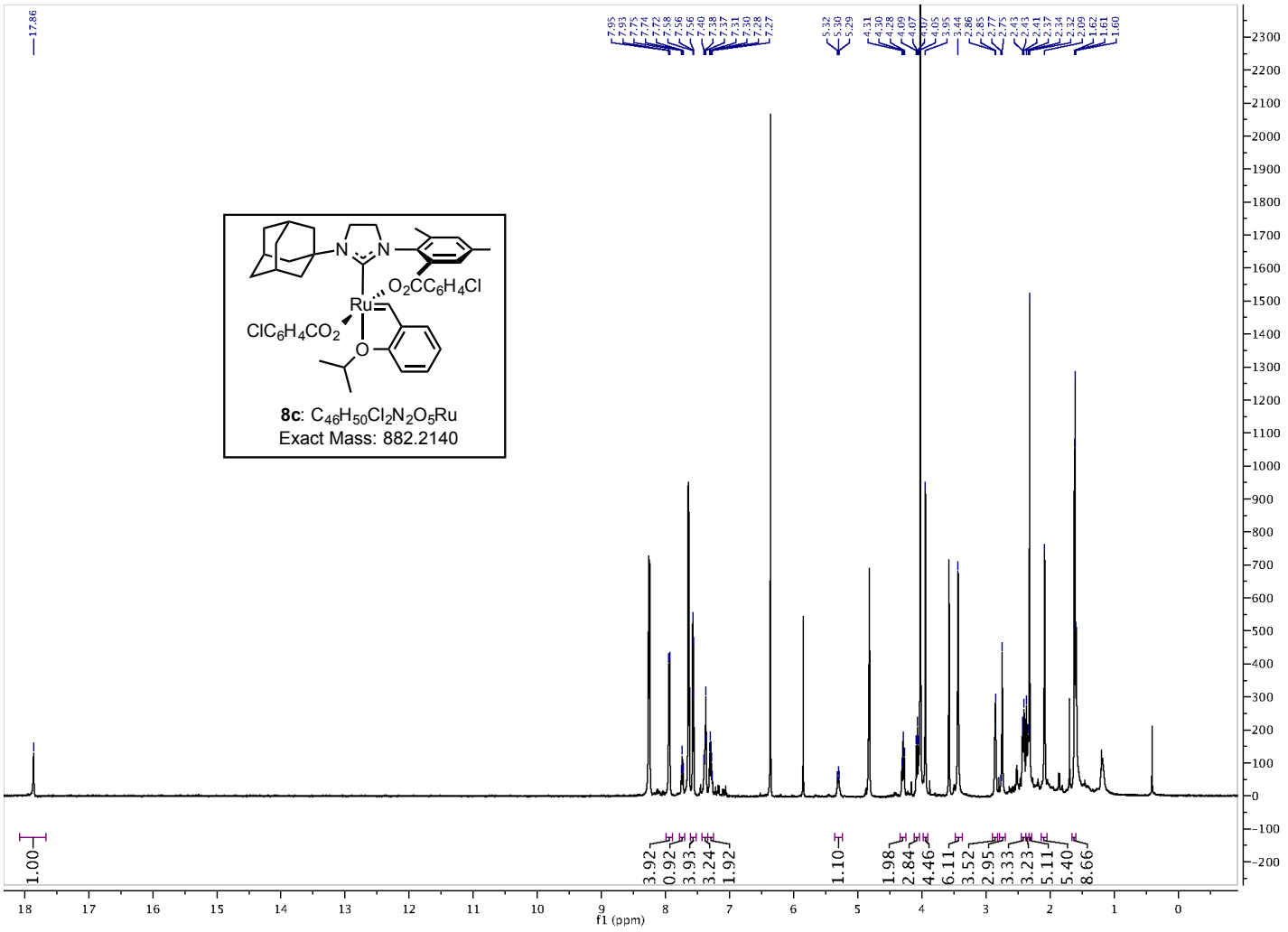
^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **8a**.



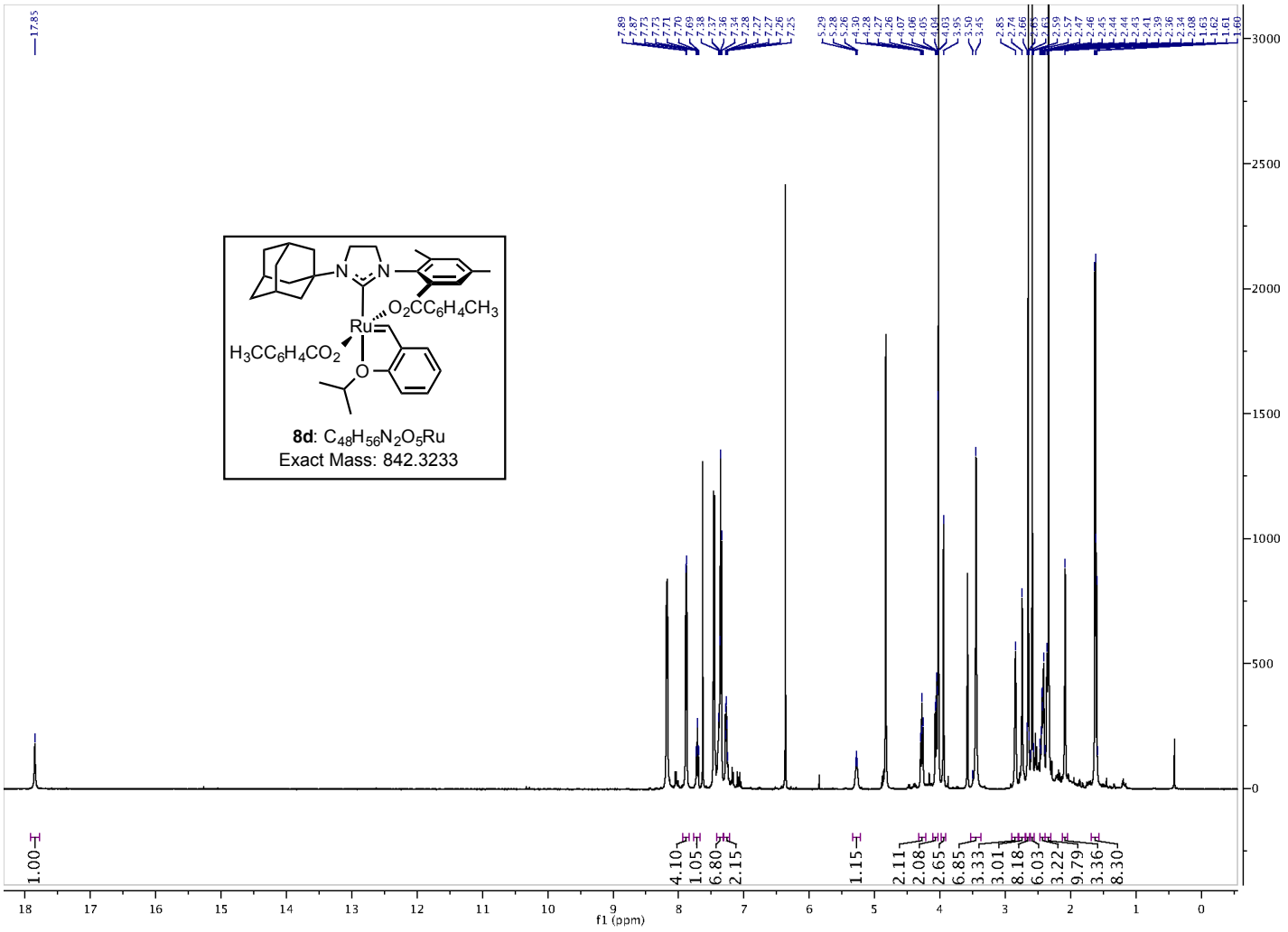
^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **8b**.



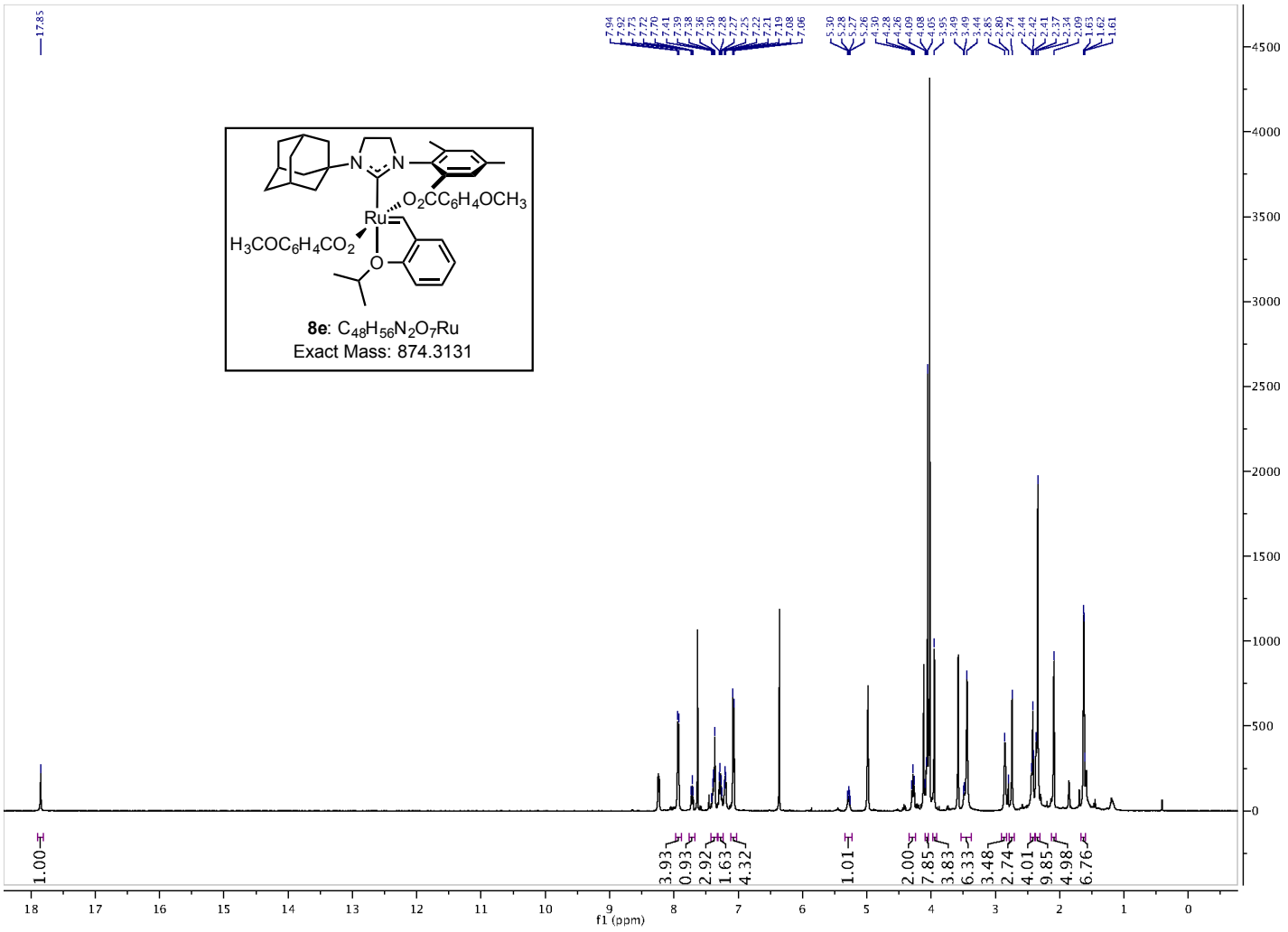
^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **8c**.



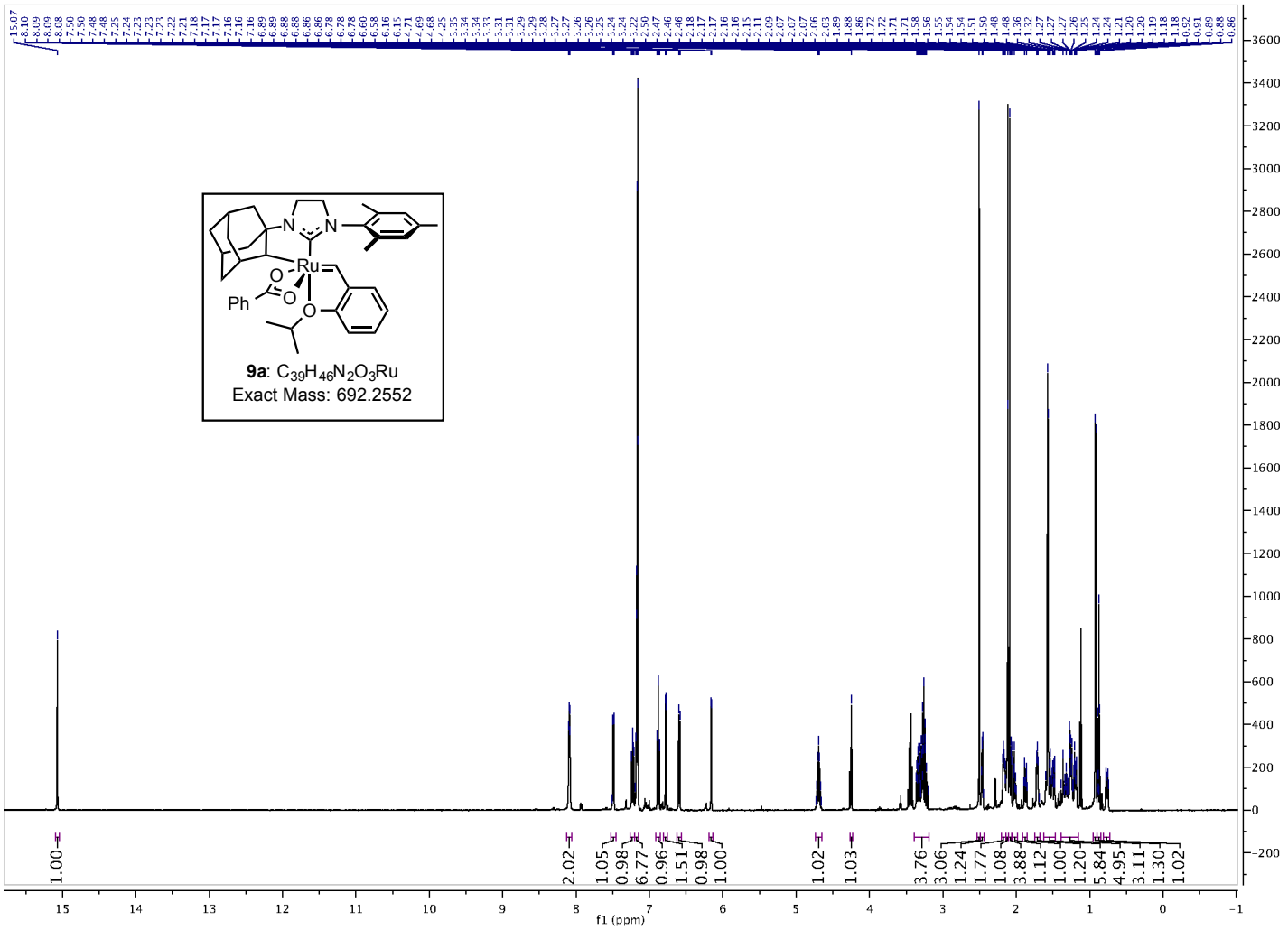
^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **8d**.



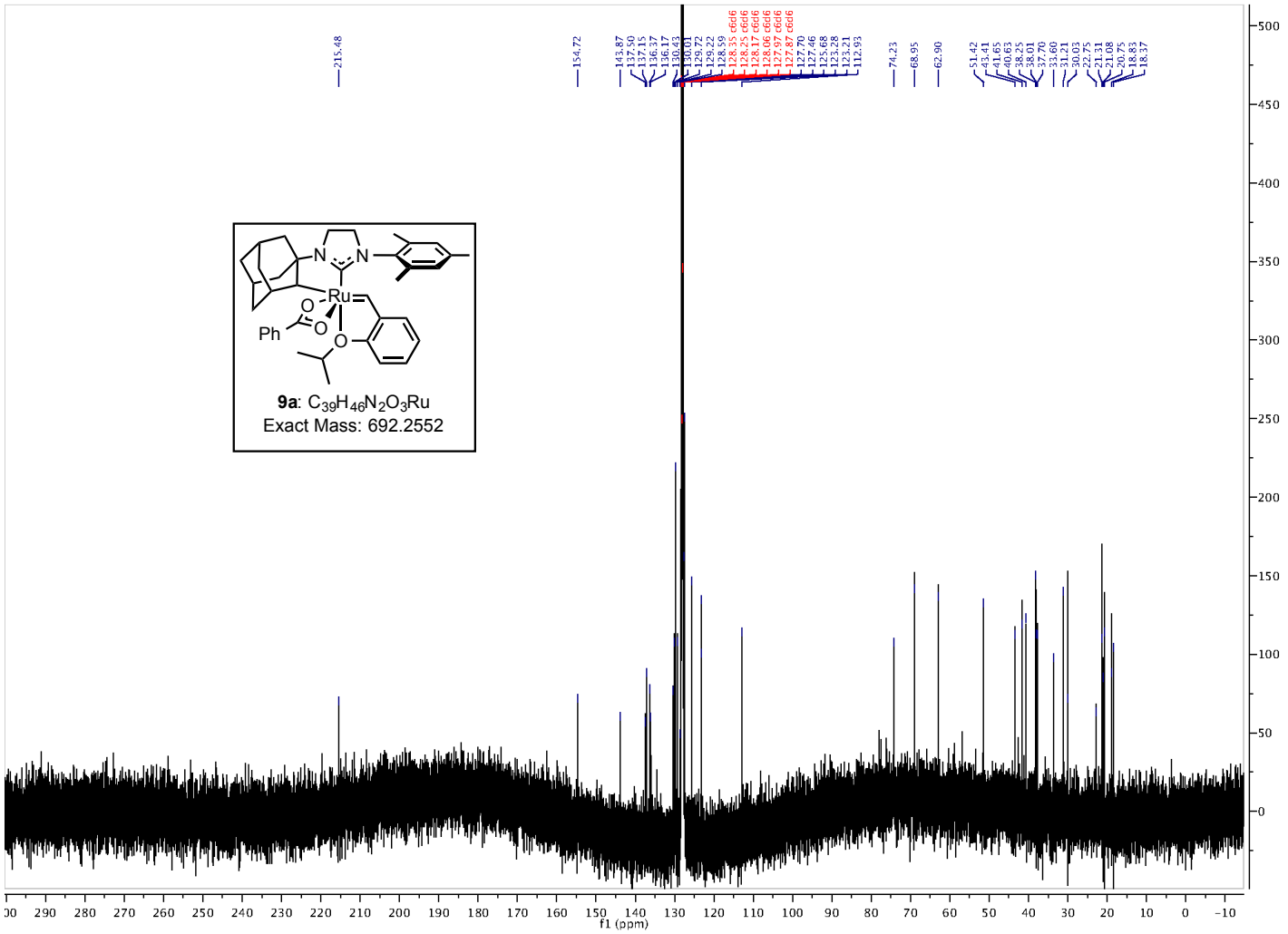
^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **8e**.



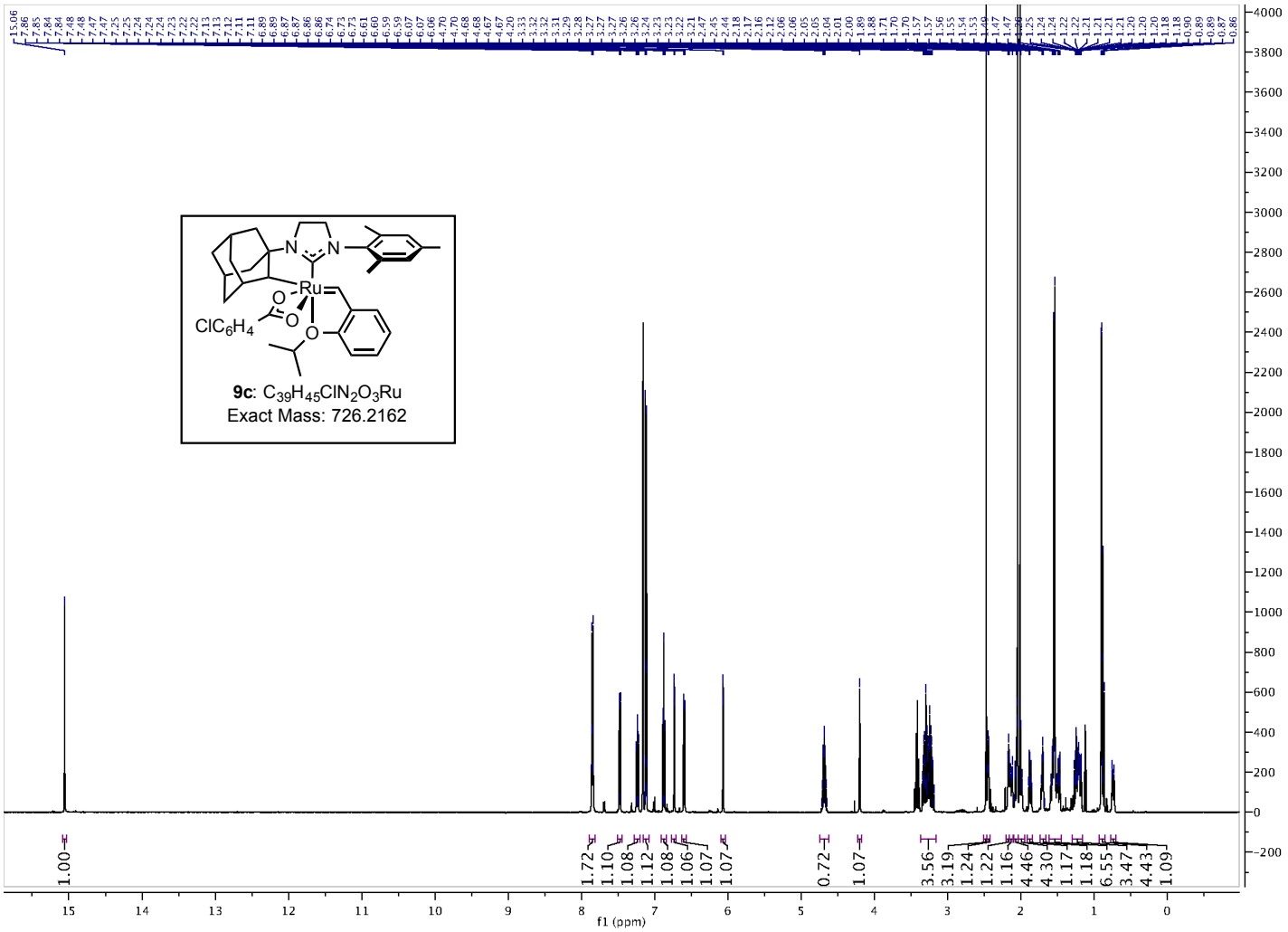
^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **9a**.



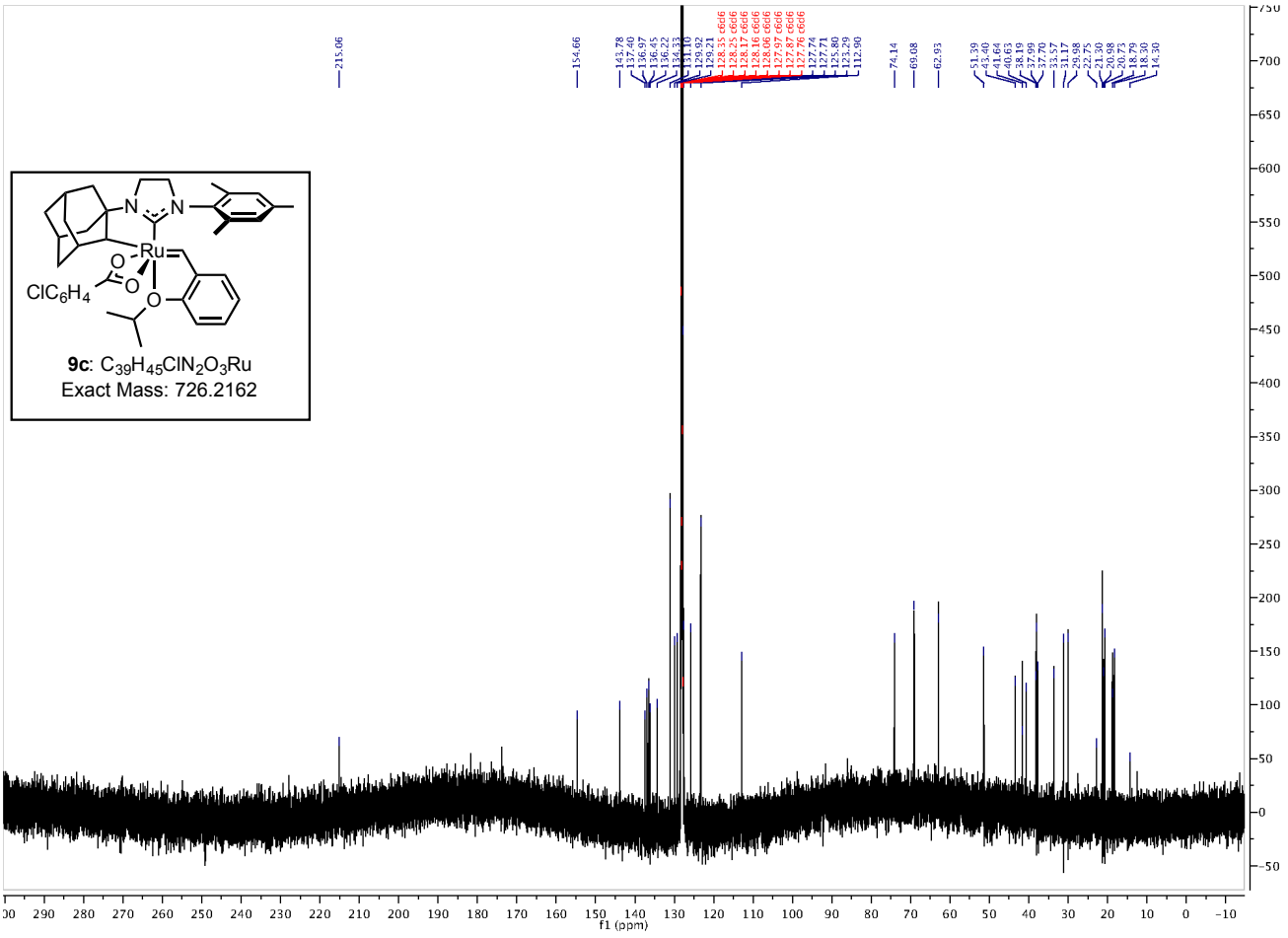
^{13}C NMR (126 MHz, C_6D_6) spectrum of compound **9a**.



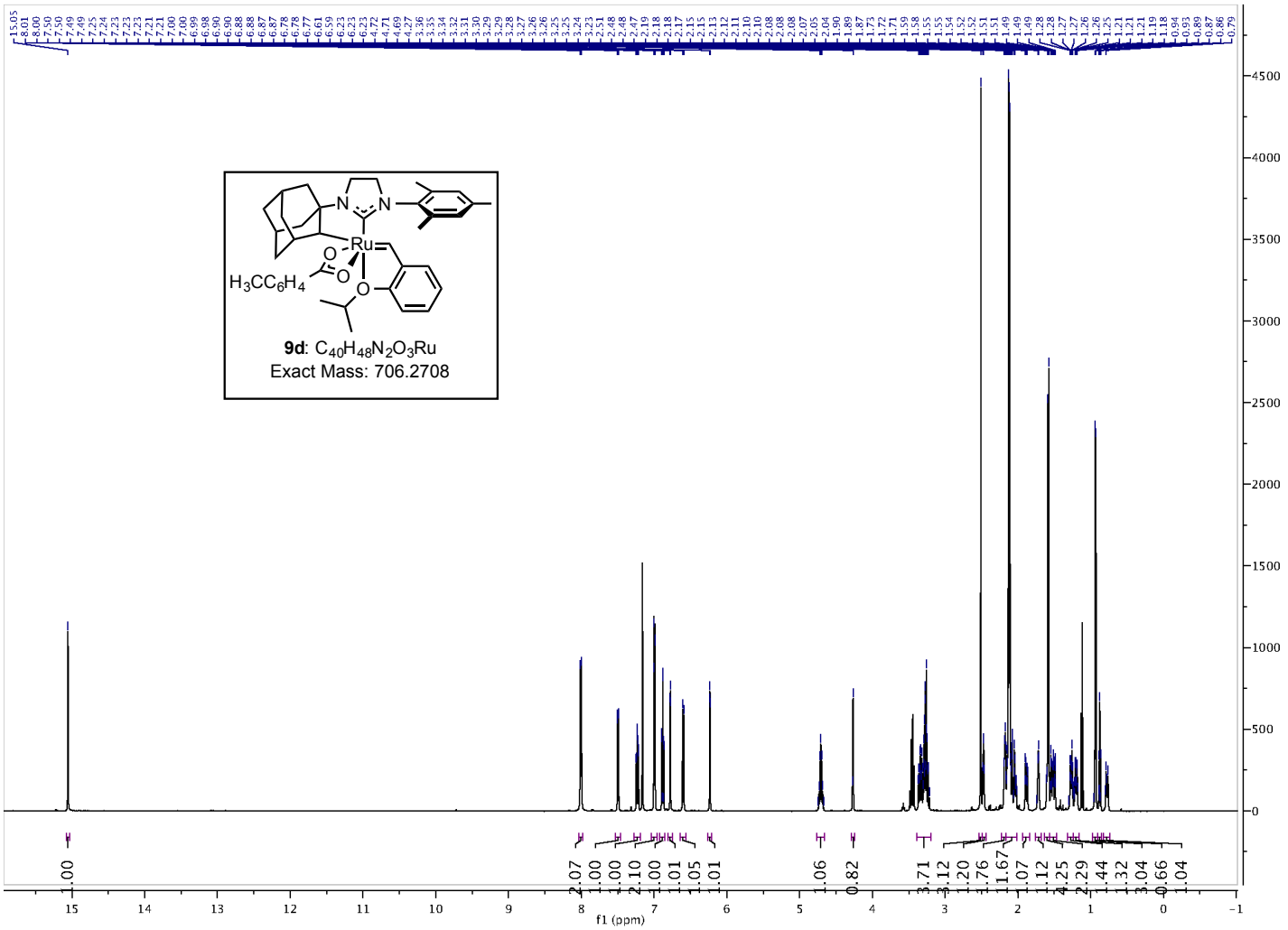
^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **9c**.



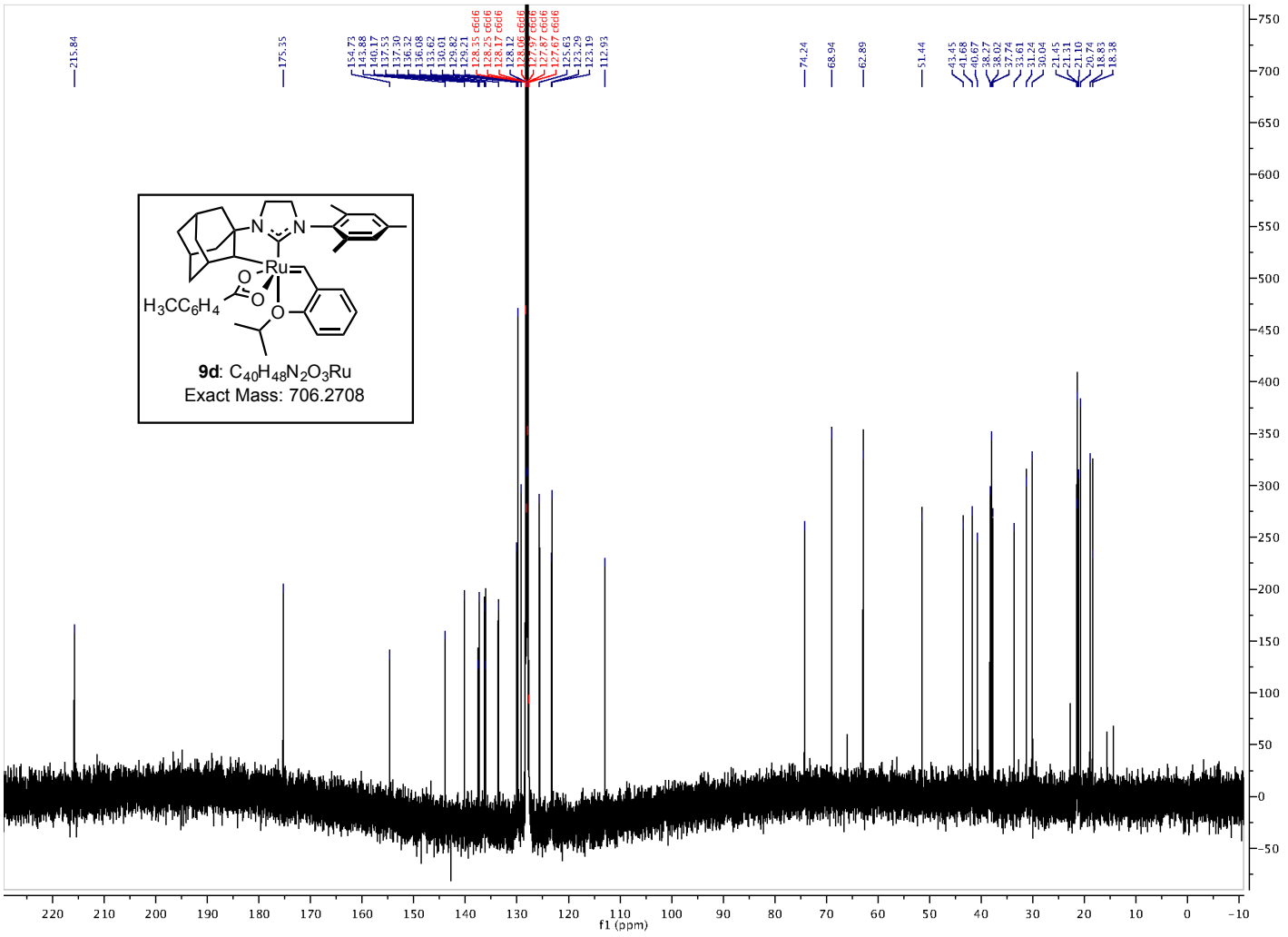
^{13}C NMR (126 MHz, C_6D_6) spectrum of compound **9c**.



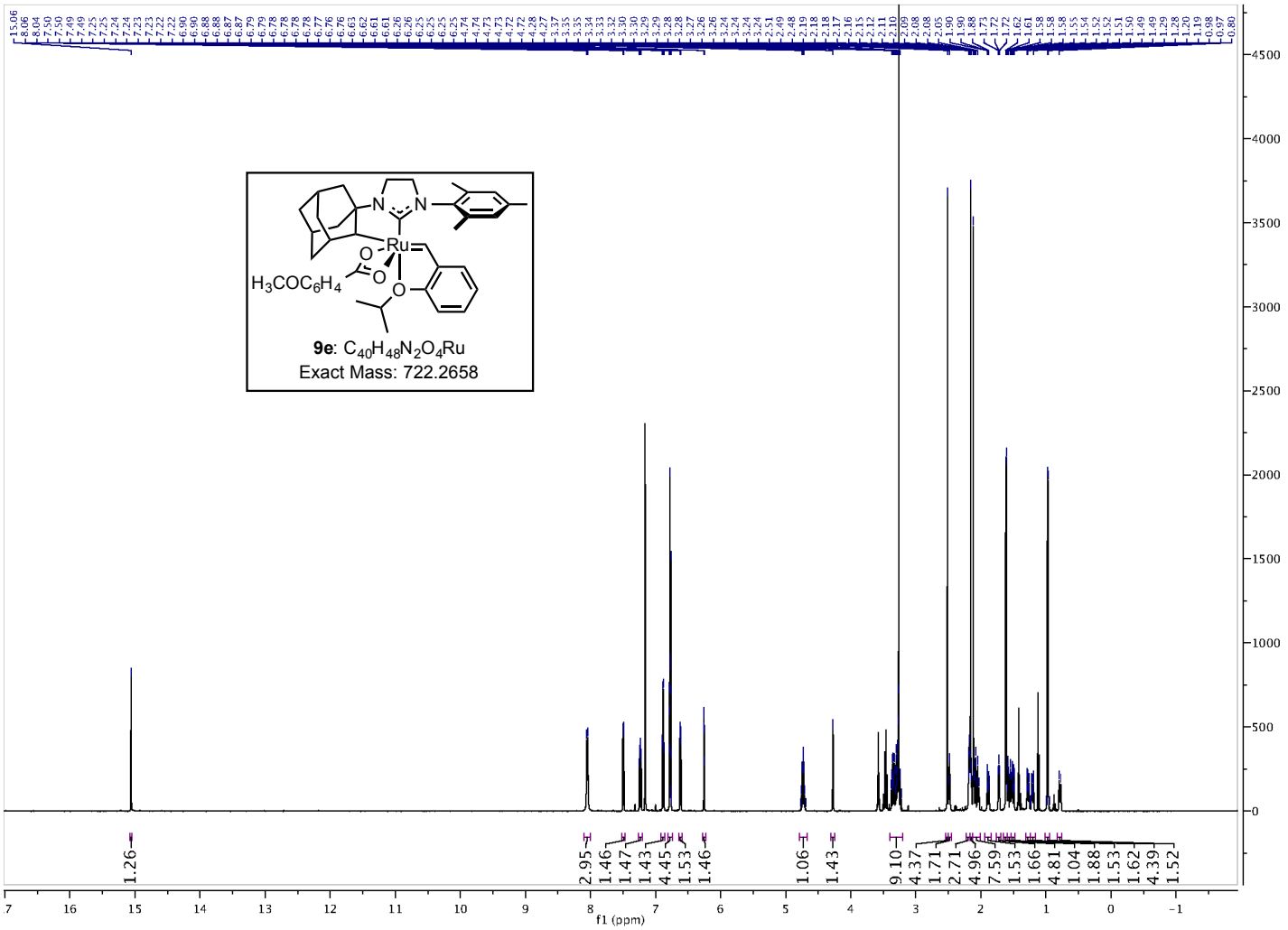
^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **9d**.



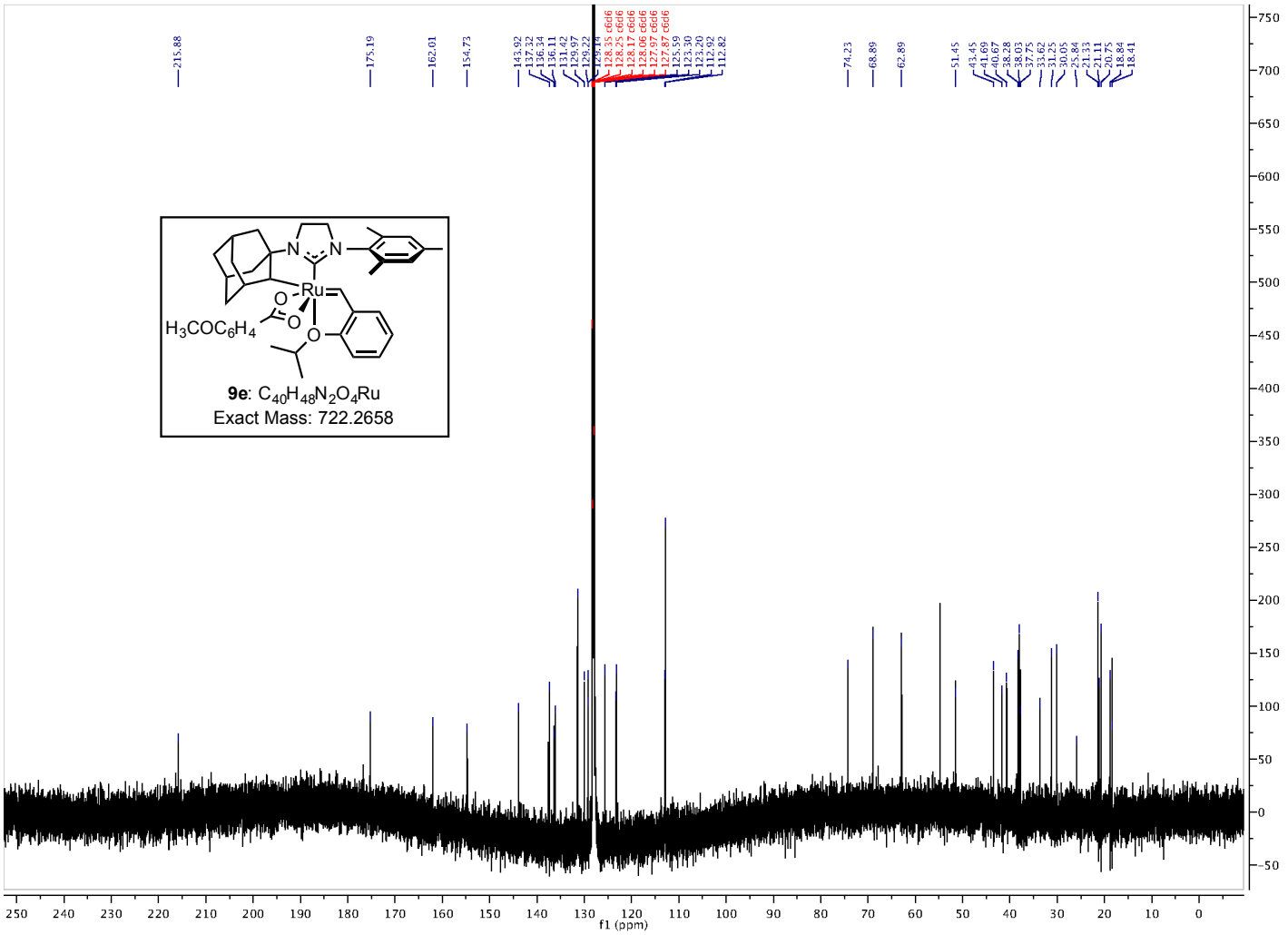
^{13}C NMR (126 MHz, C_6D_6) spectrum of compound **9d**.



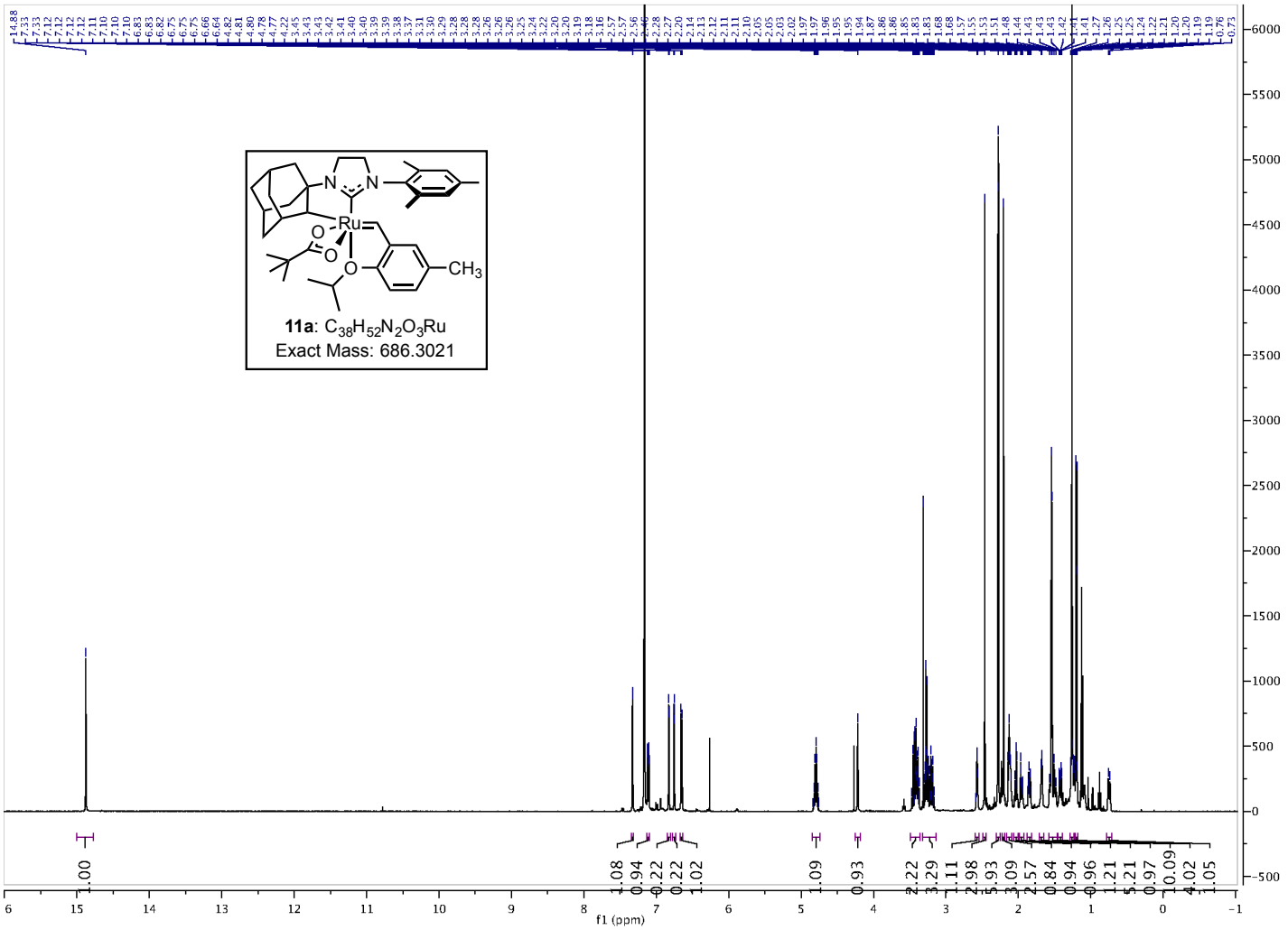
^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **9e**.



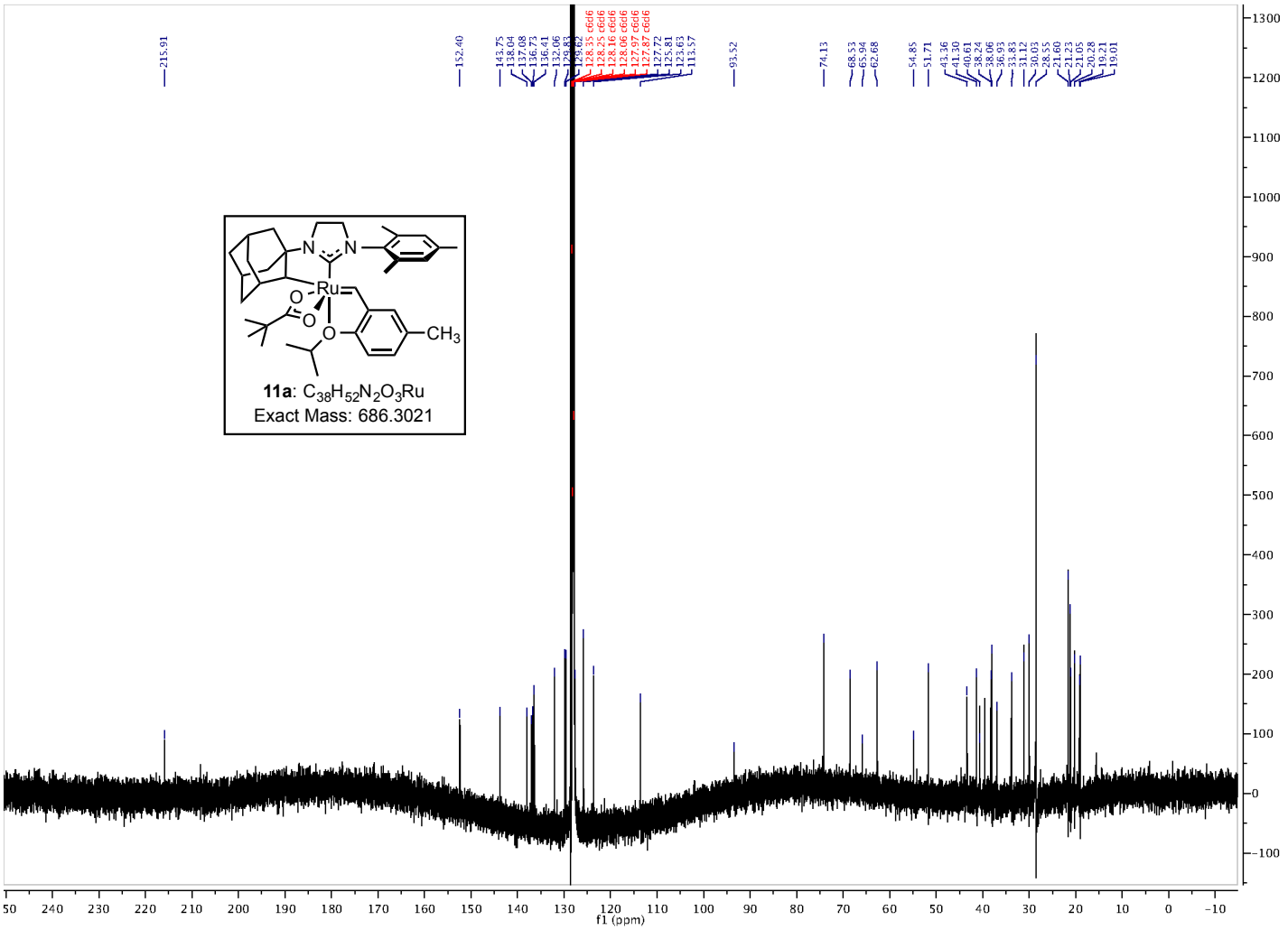
^{13}C NMR (126 MHz, C_6D_6) spectrum of compound **9e**.



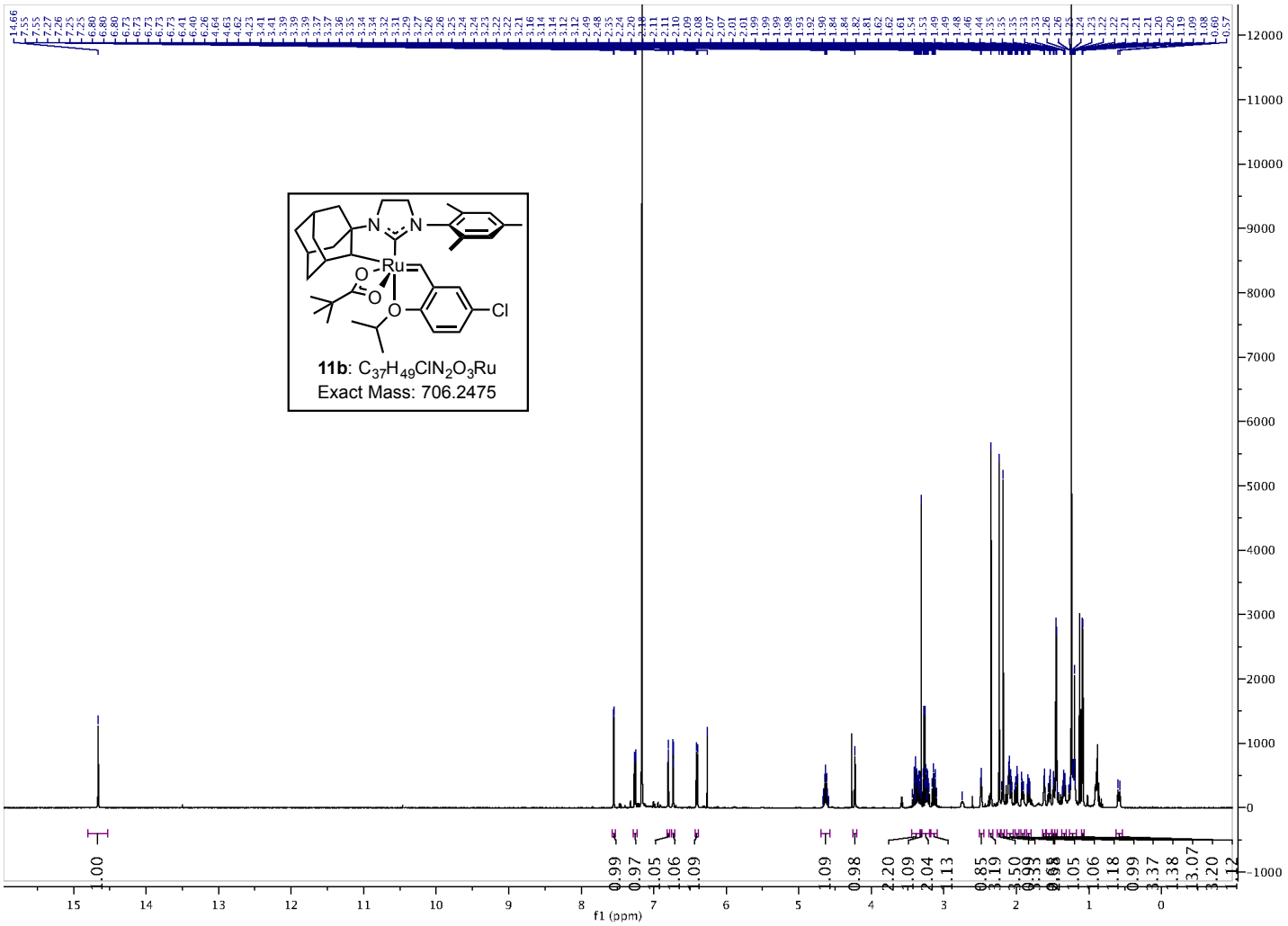
^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **11a**.



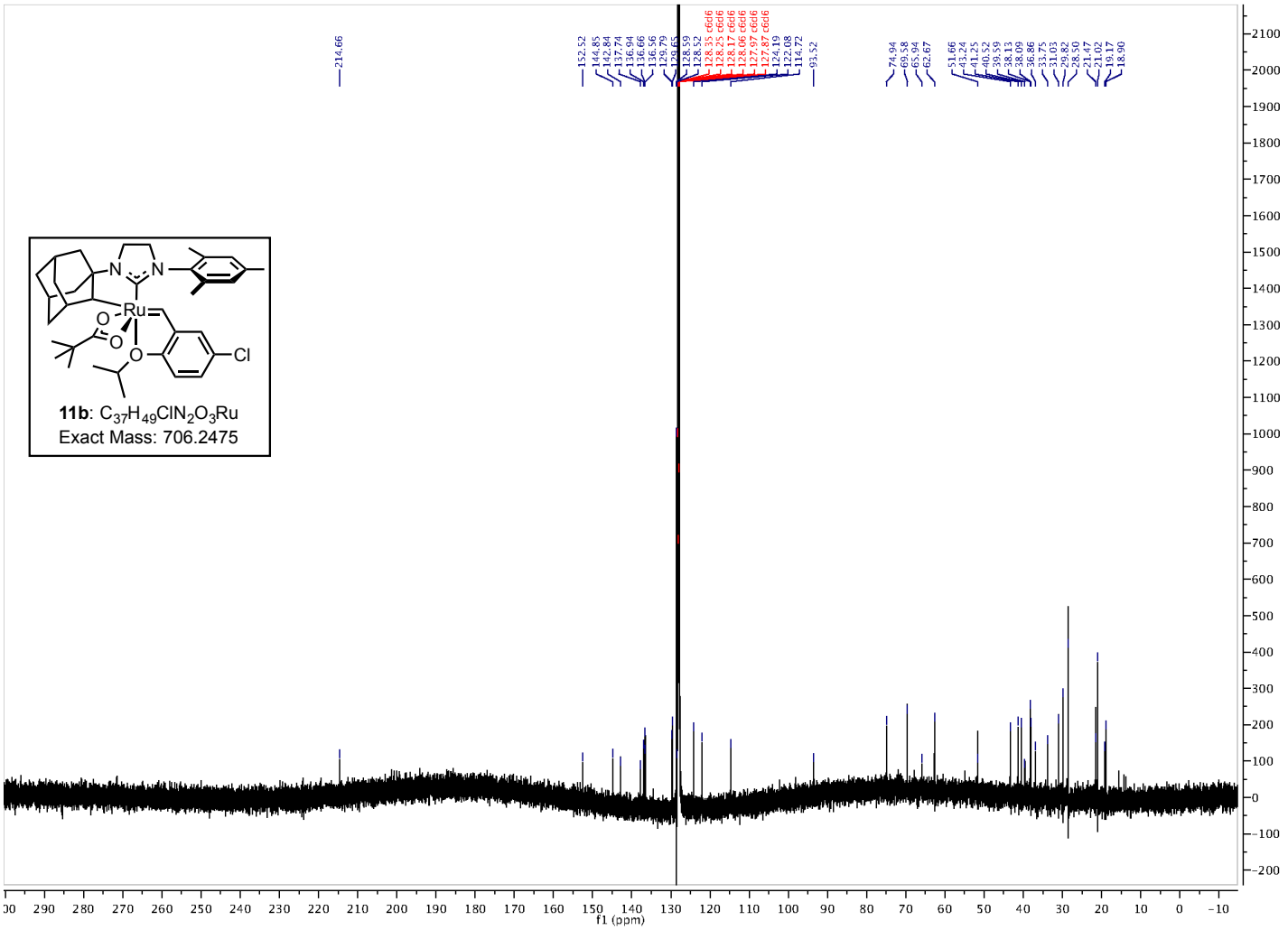
^{13}C NMR (126 MHz, C_6D_6) spectrum of compound **11a**.



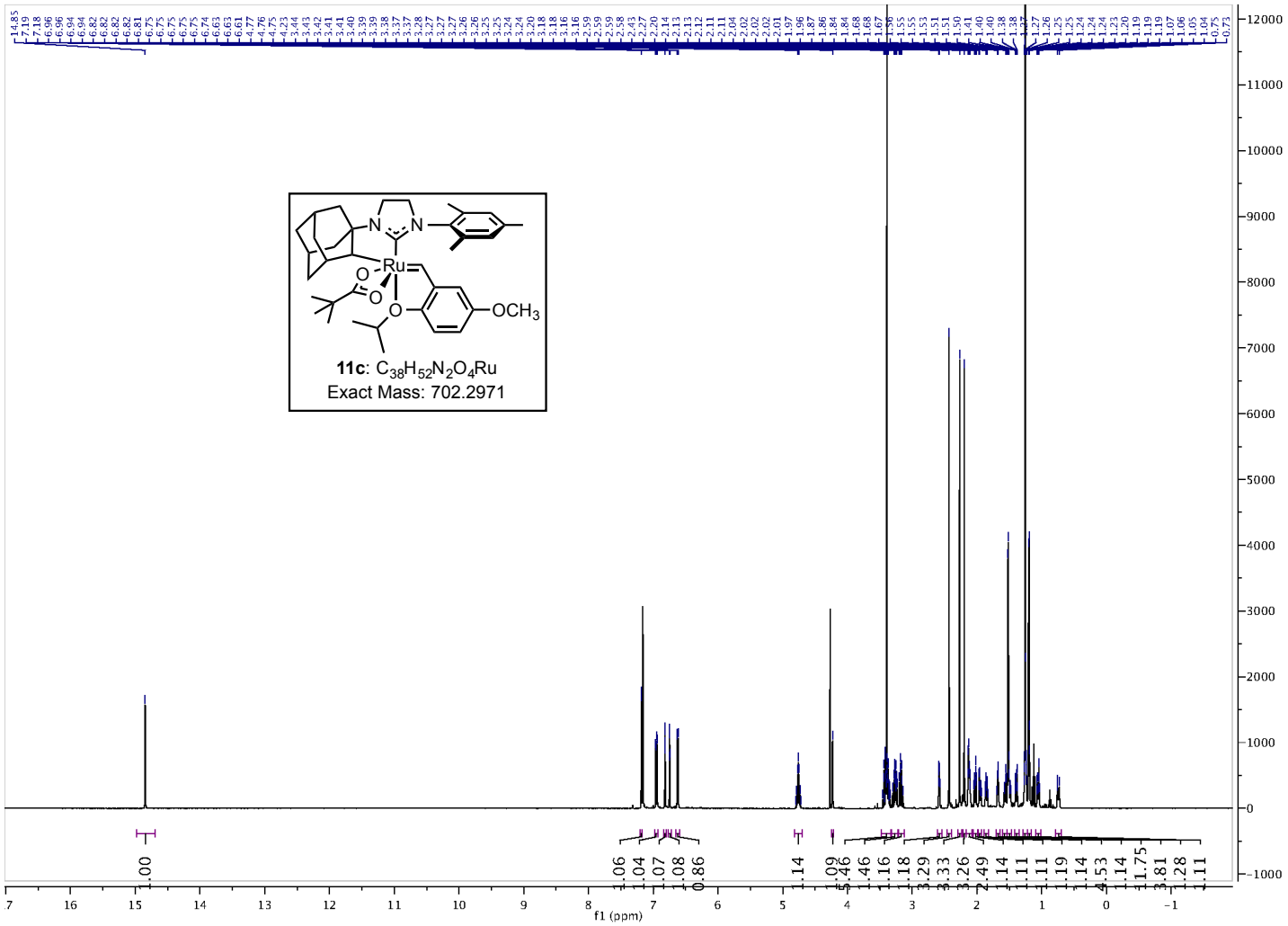
^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **11b**.



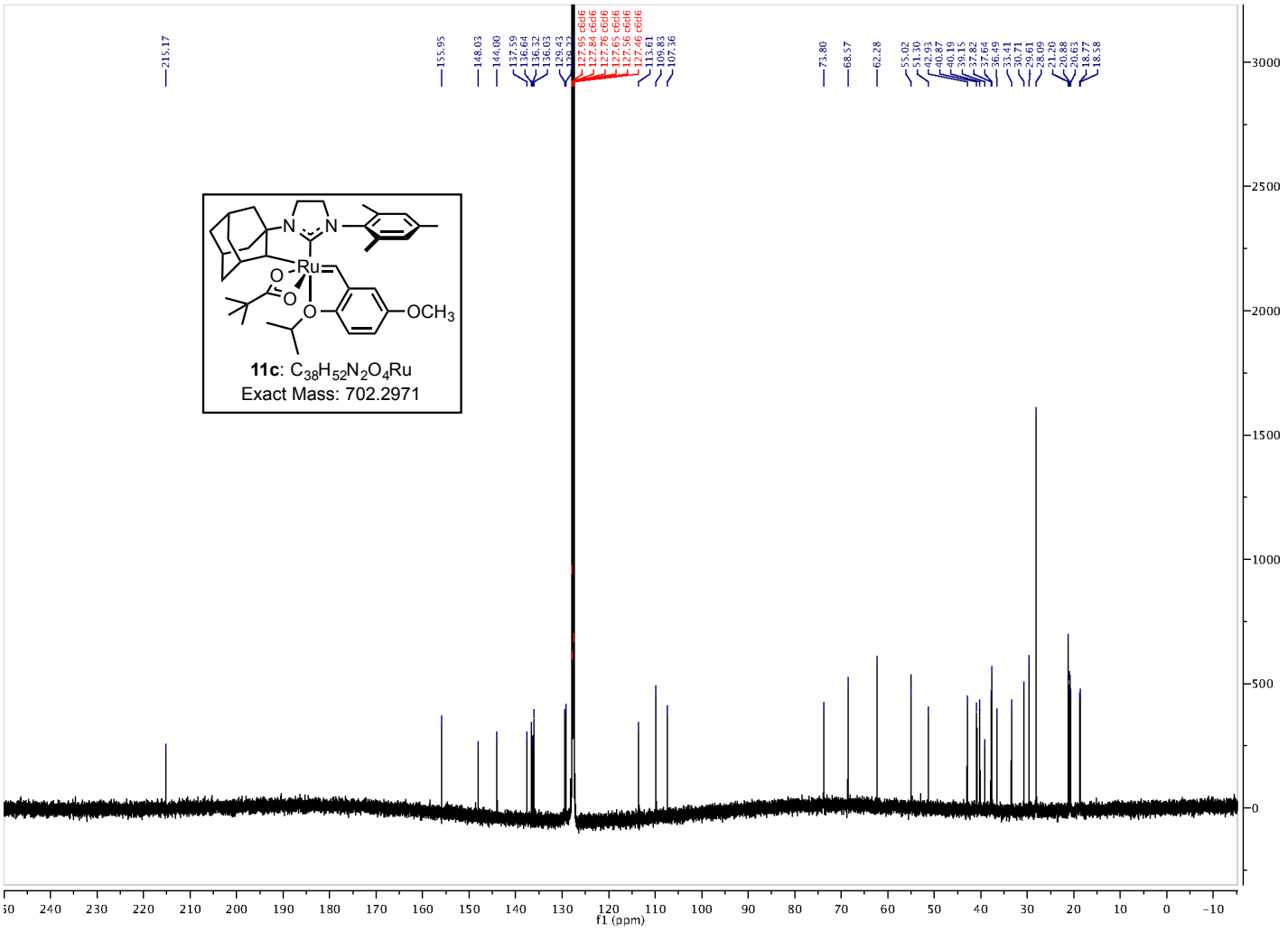
^{13}C NMR (126 MHz, C_6D_6) spectrum of compound **11b**.



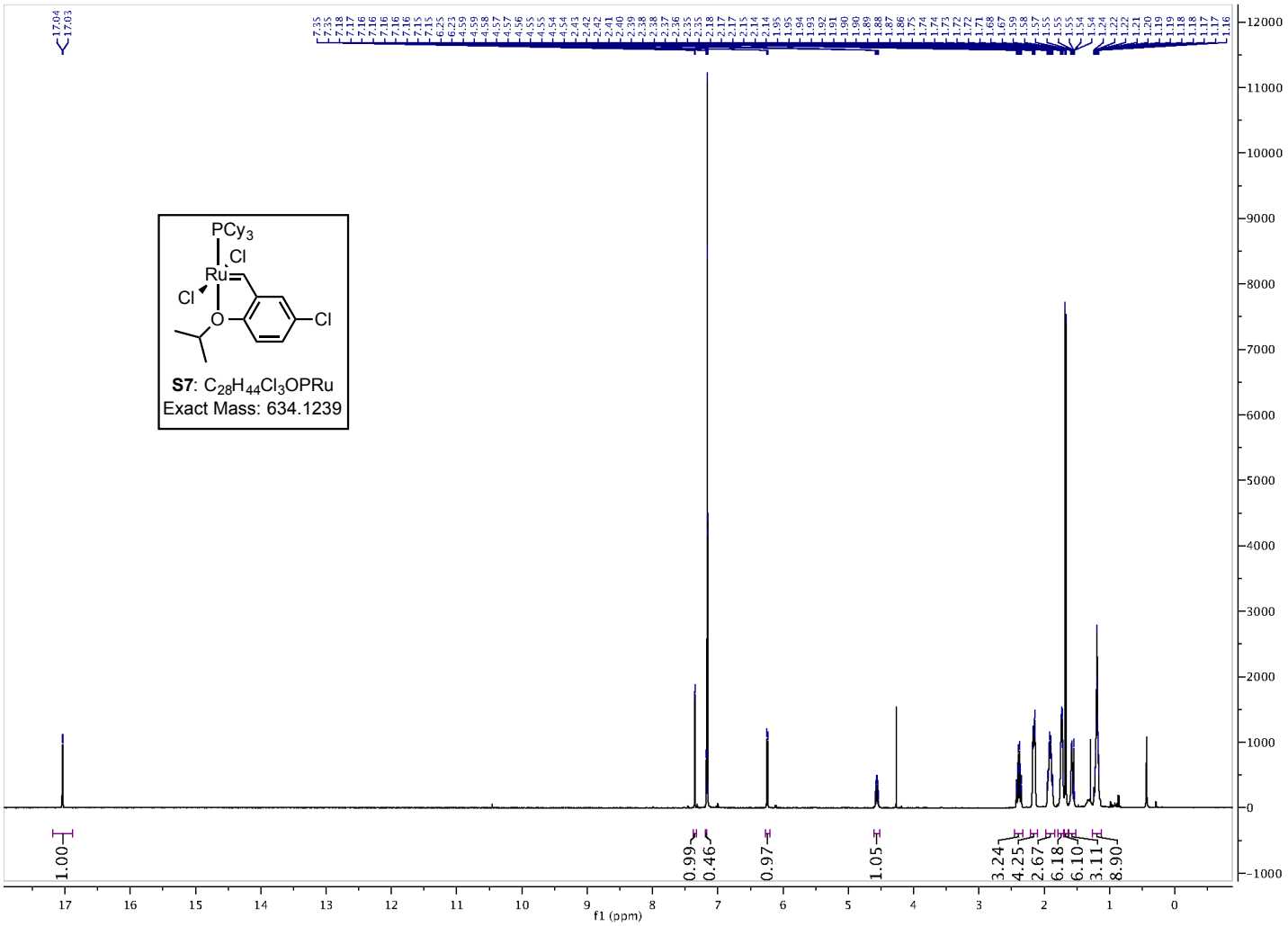
^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **11c**.



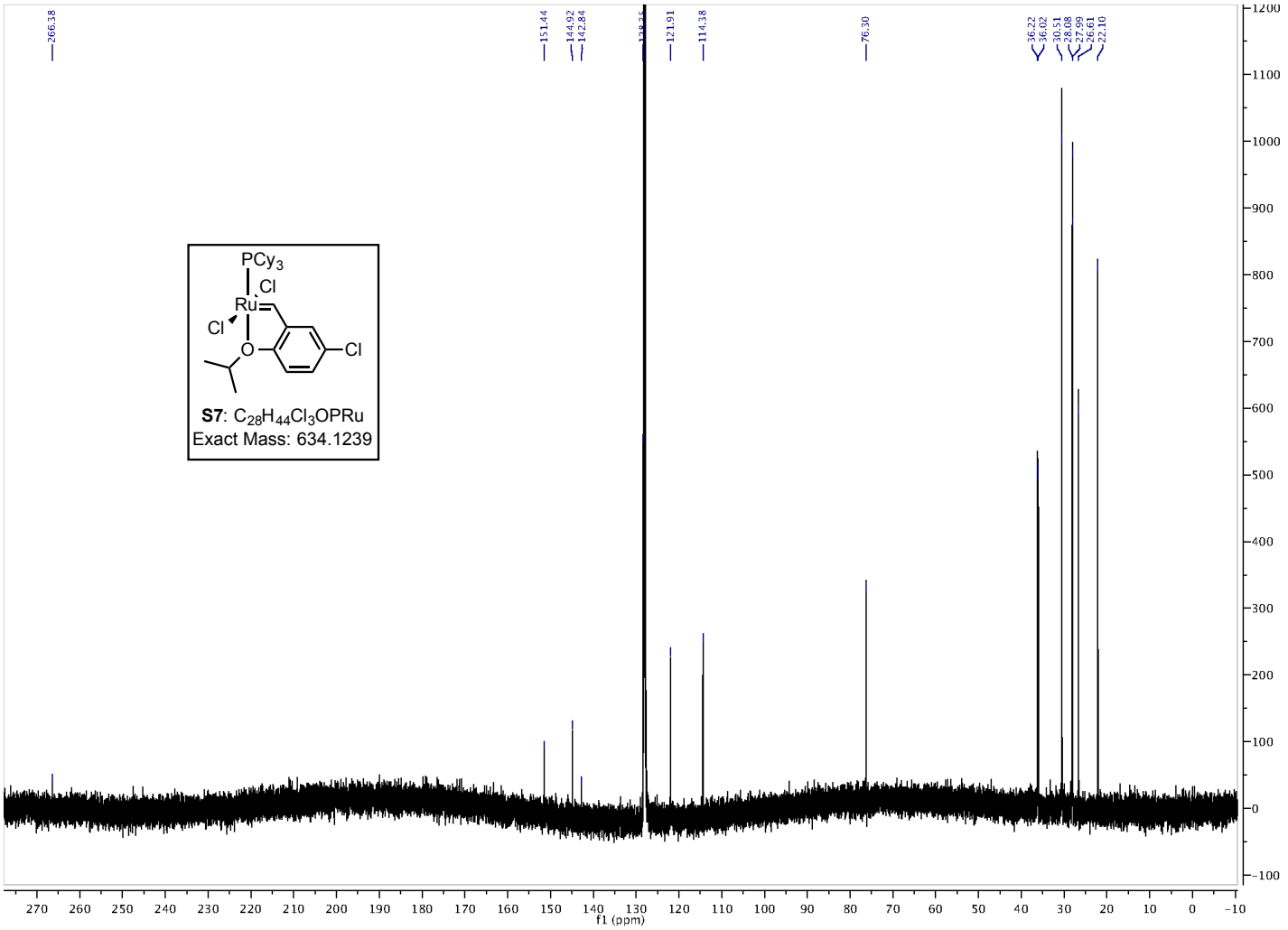
^{13}C NMR (126 MHz, C_6D_6) spectrum of compound **11c**.



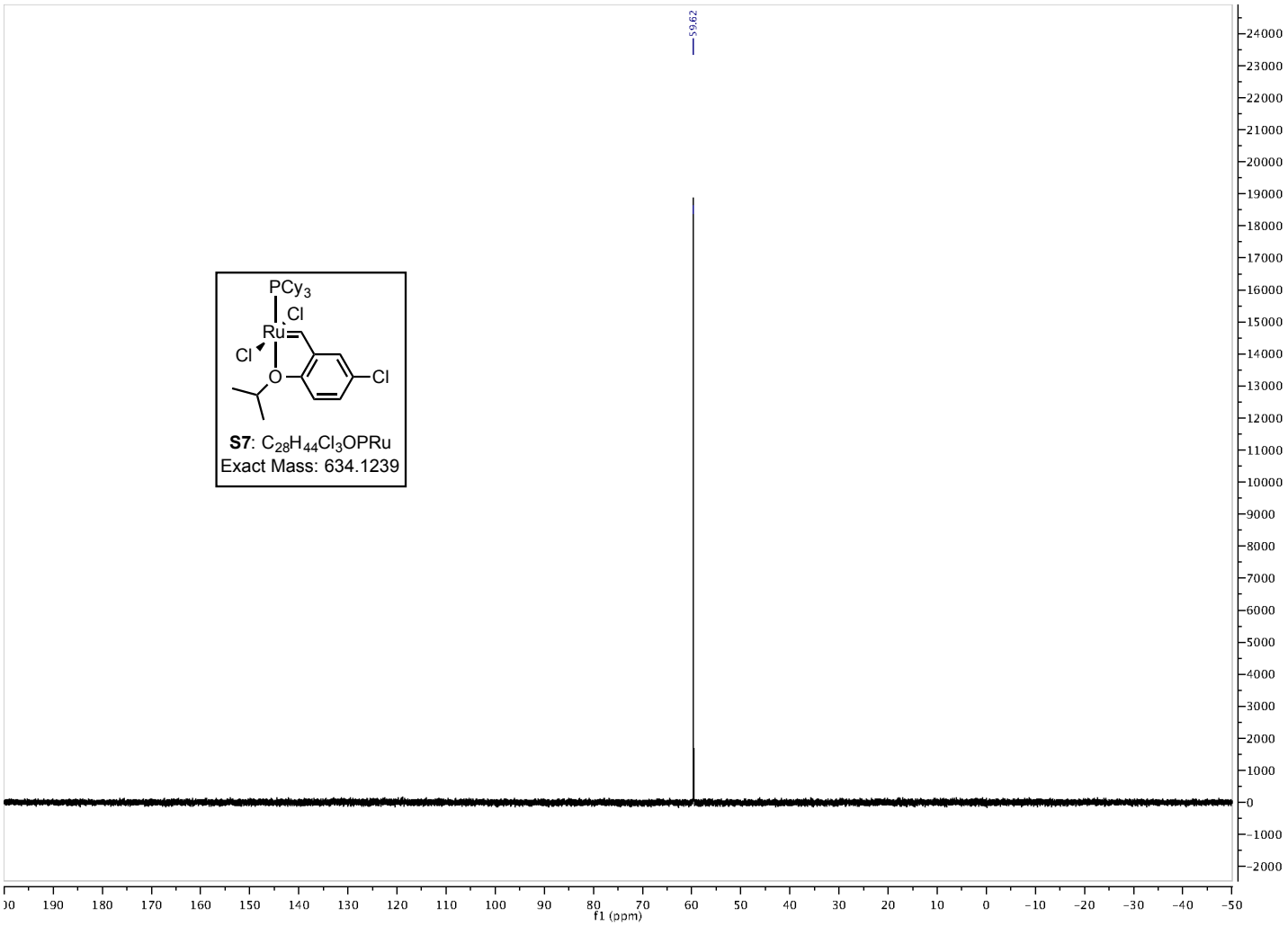
^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **S7**.



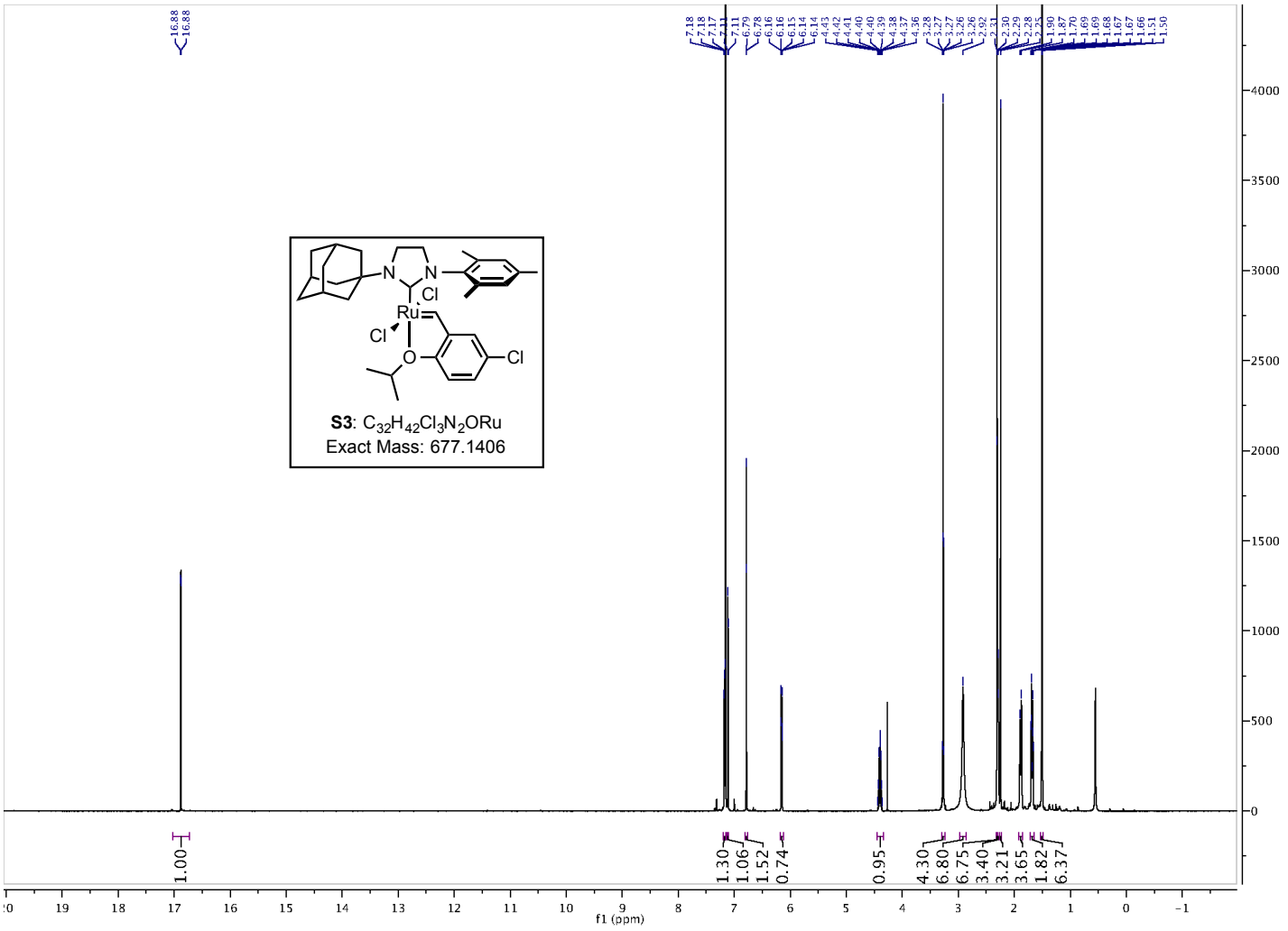
^{13}C NMR (126 MHz, C_6D_6) spectrum of compound **S7**.



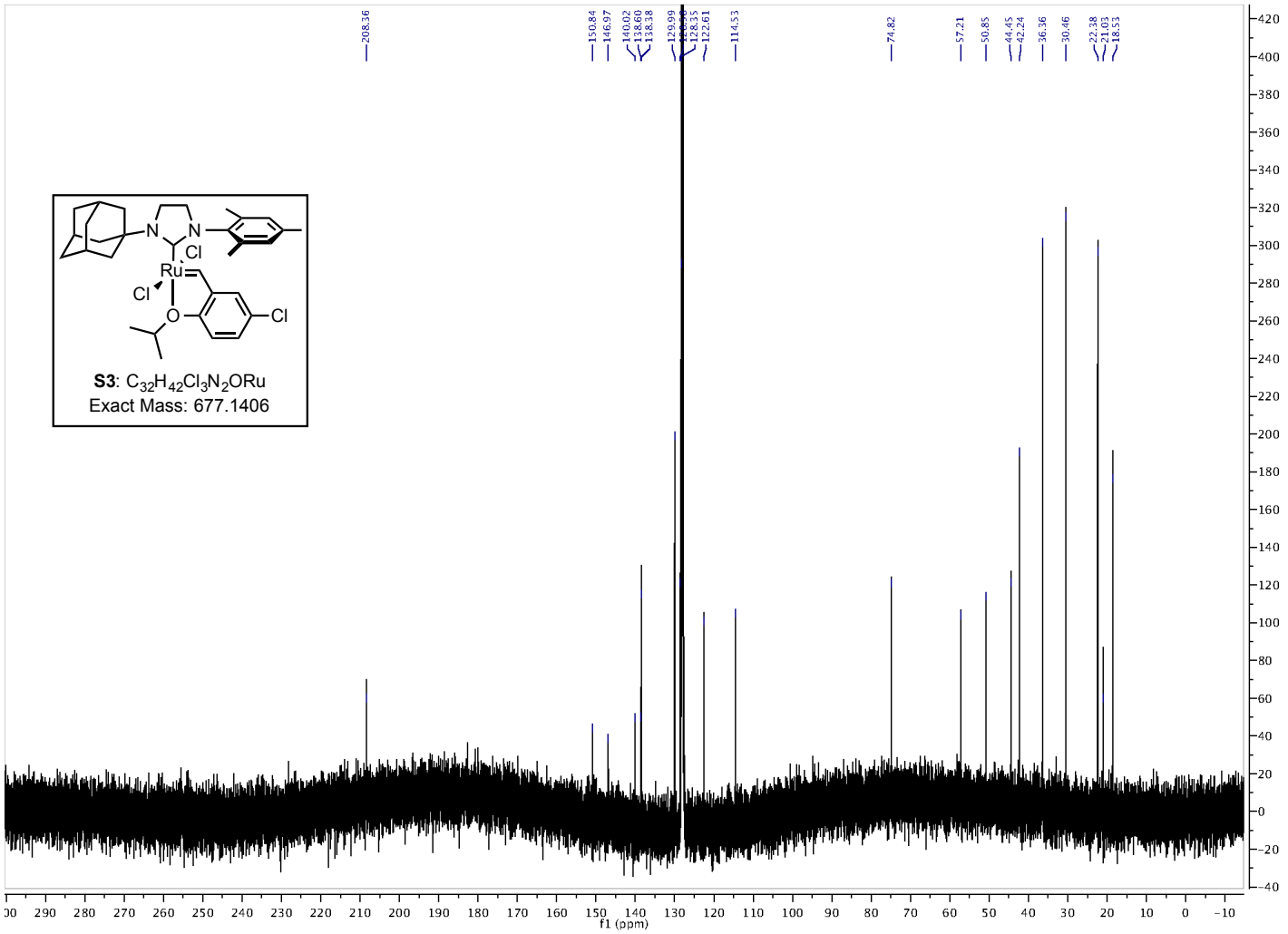
^{31}P NMR (121 MHz, C_6D_6) spectrum of compound **S7**.



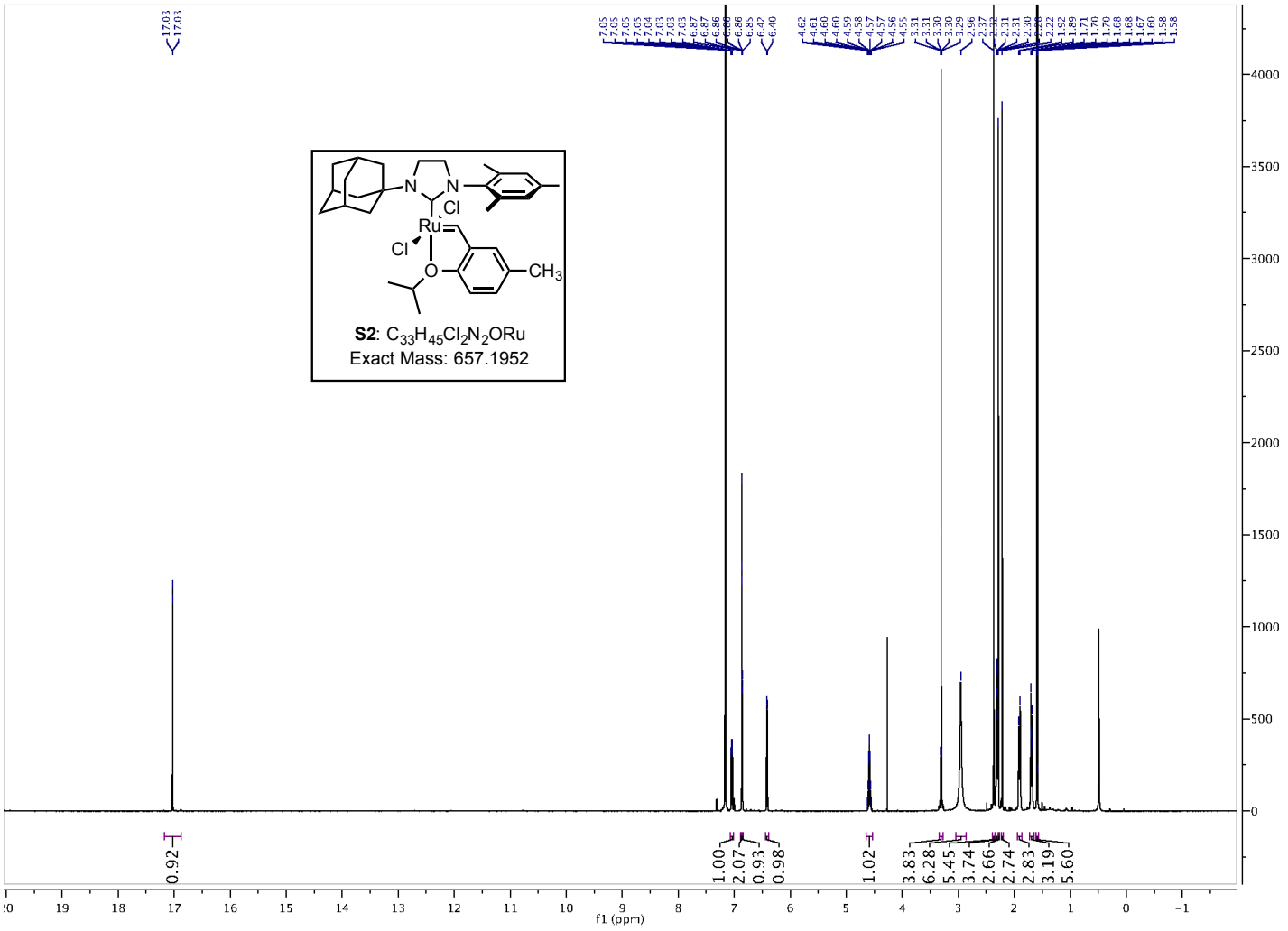
^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **S3**.



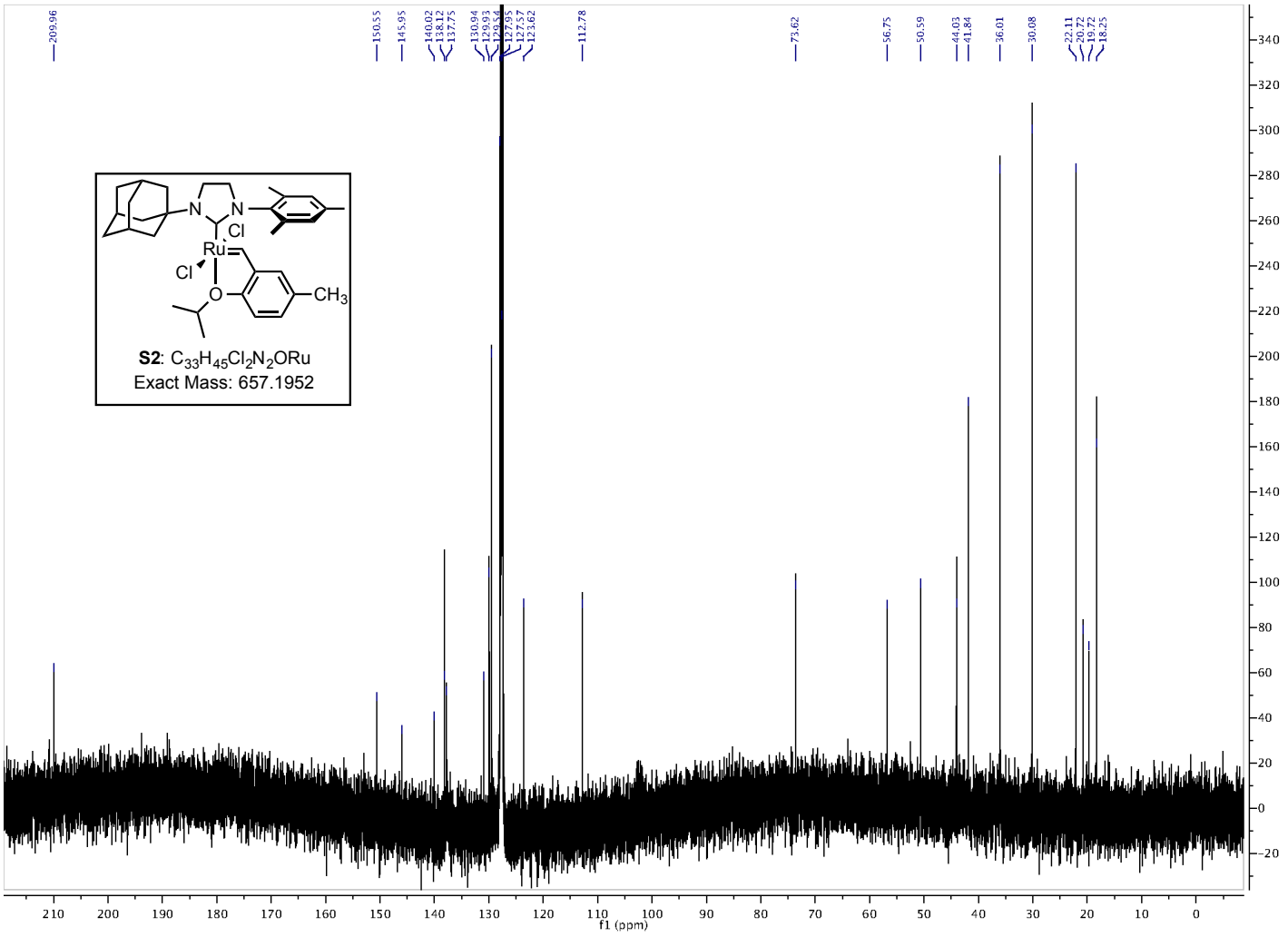
^{13}C NMR (126 MHz, C_6D_6) spectrum of compound **S3**.



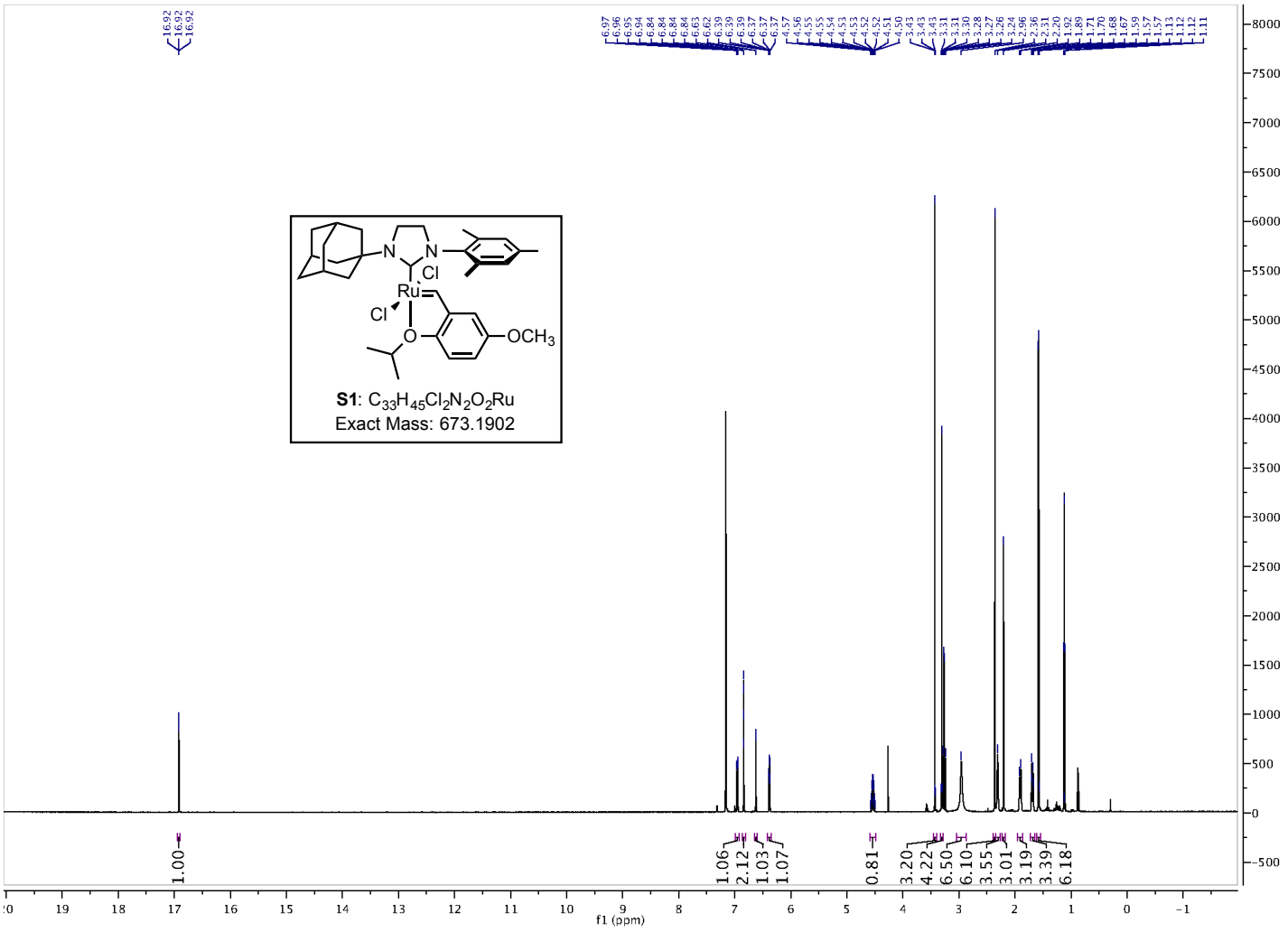
^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **S2**.



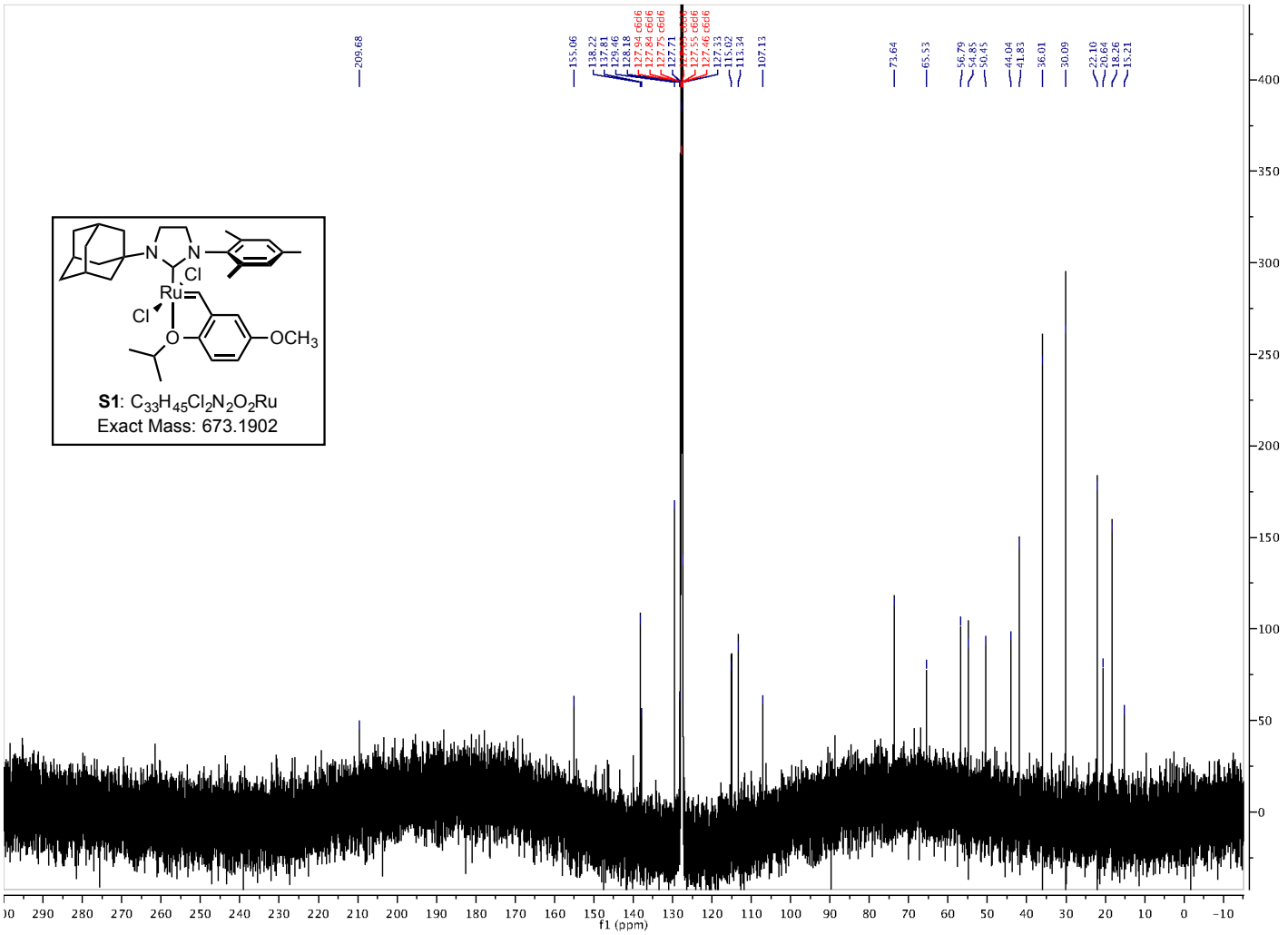
^{13}C NMR (126 MHz, C_6D_6) spectrum of compound **S2**.



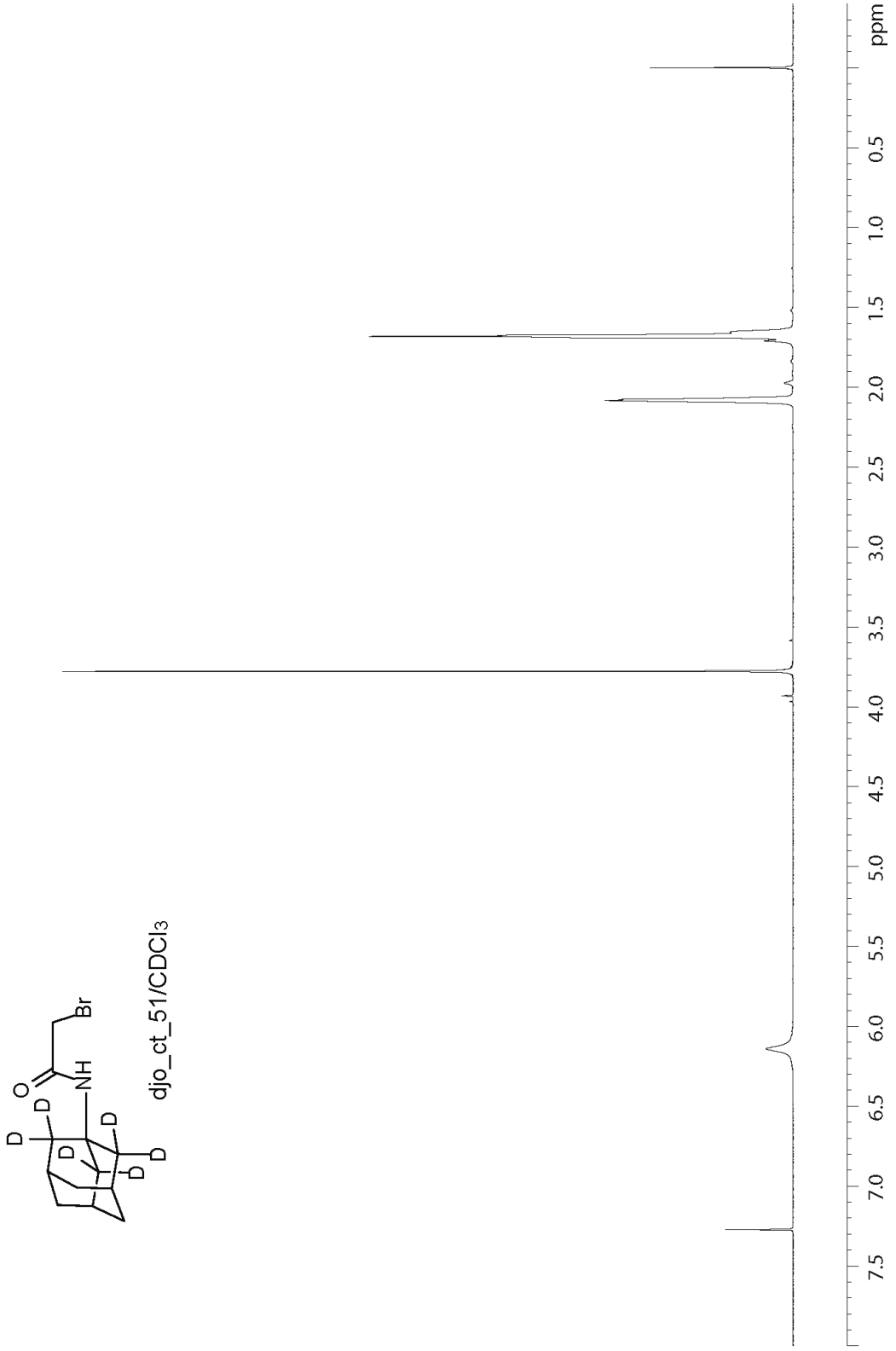
^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **S1**.



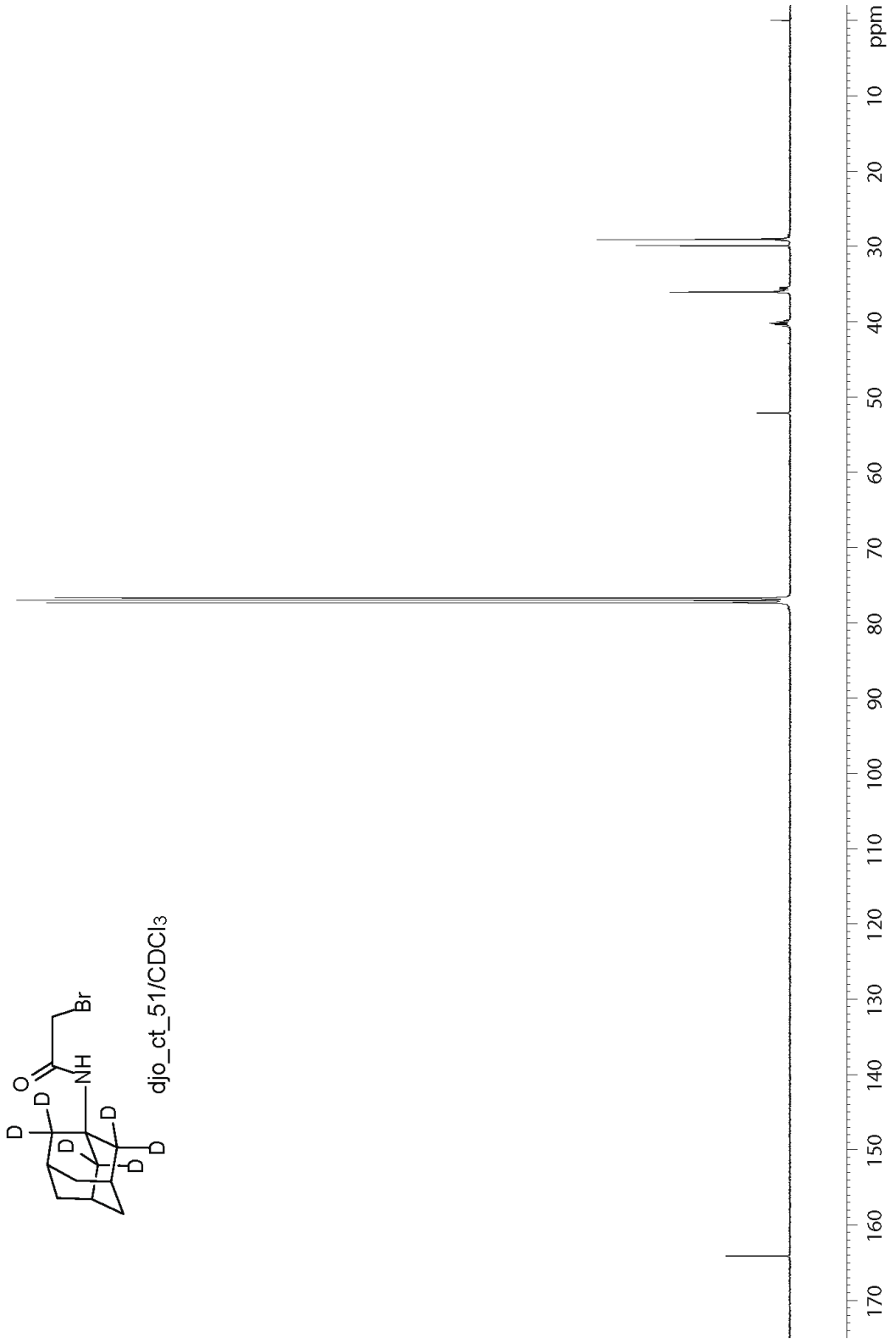
^{13}C NMR (126 MHz, C_6D_6) spectrum of compound **S1**.



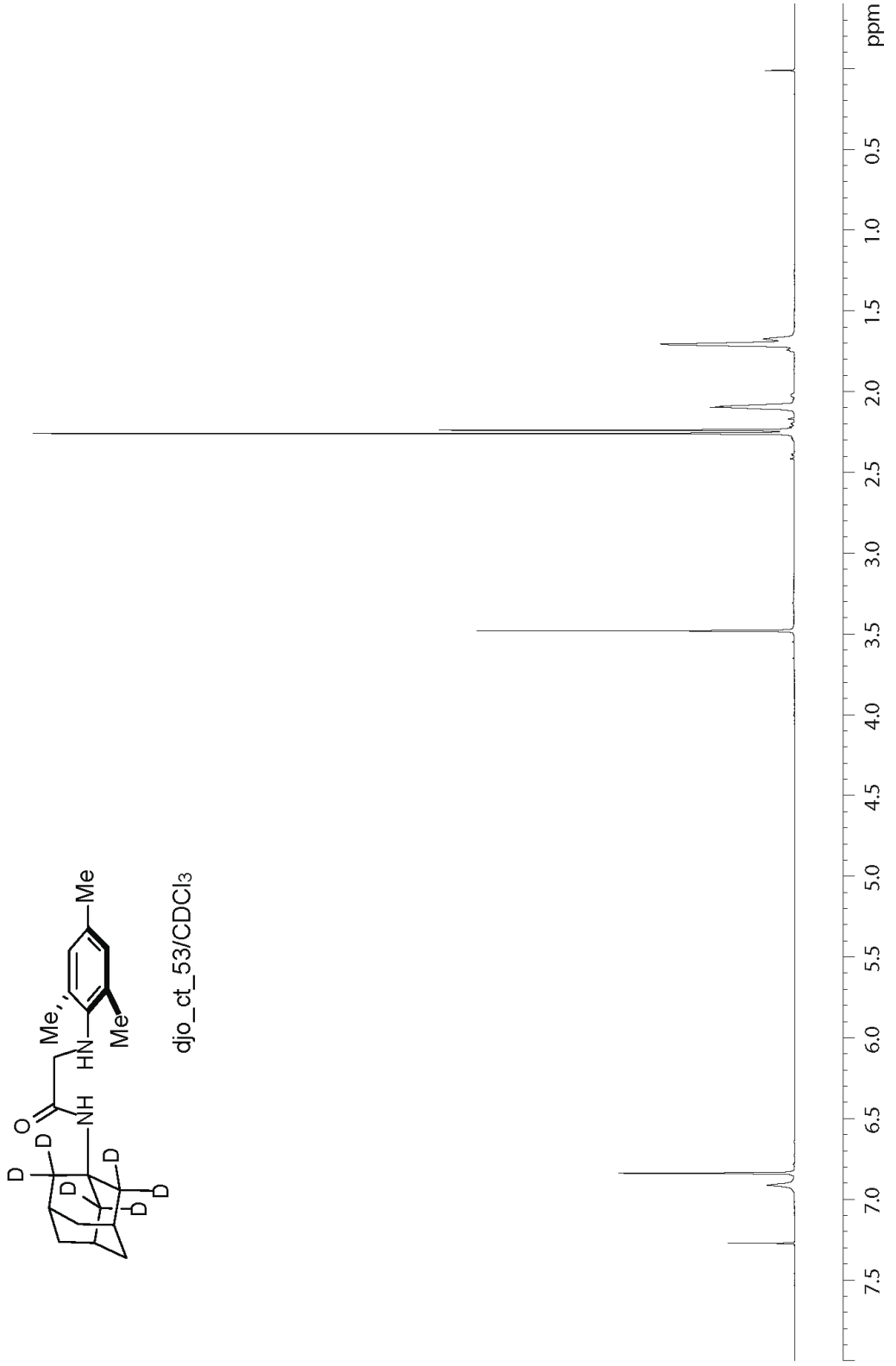
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **S8**.



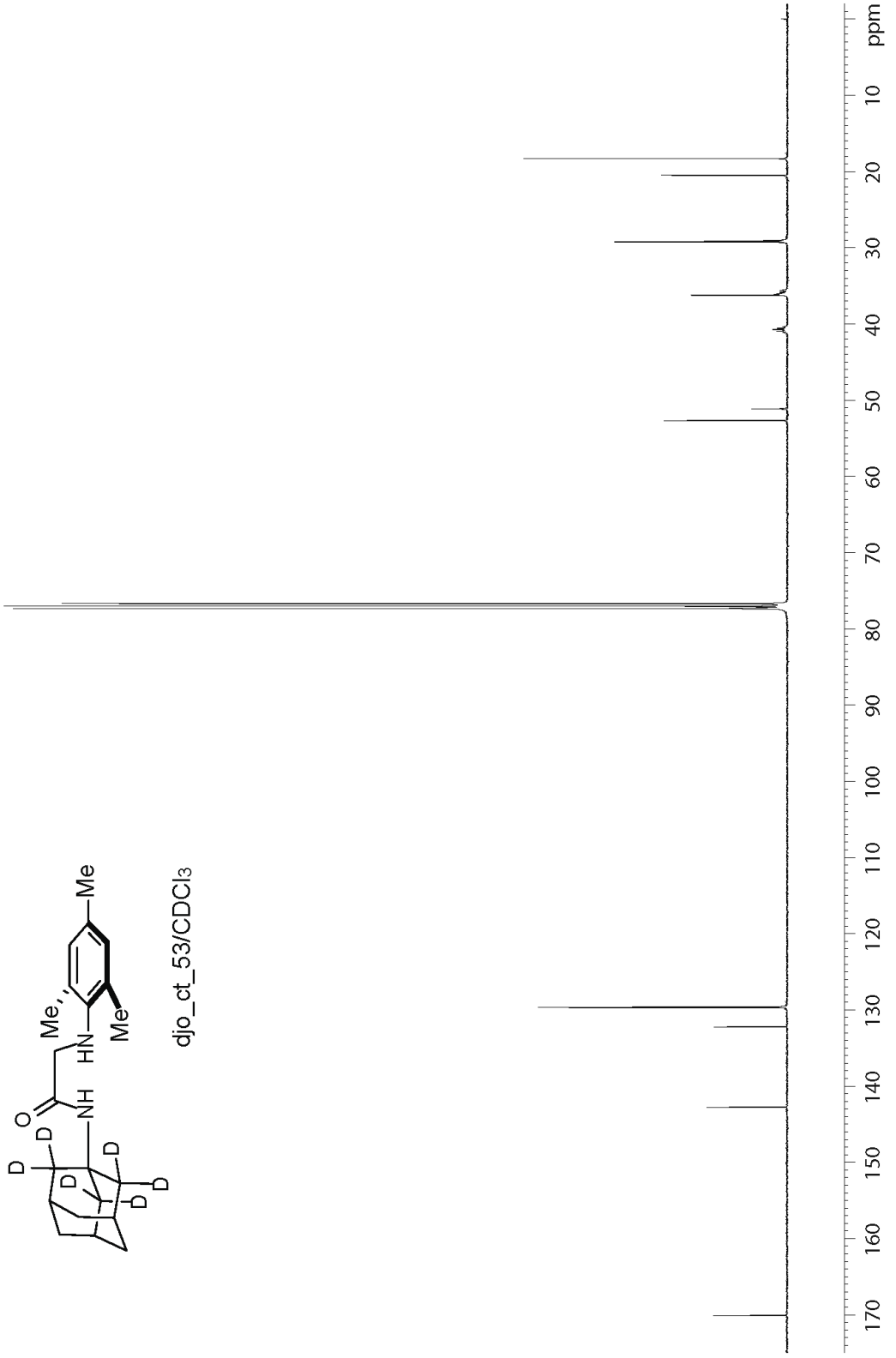
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **S8**.



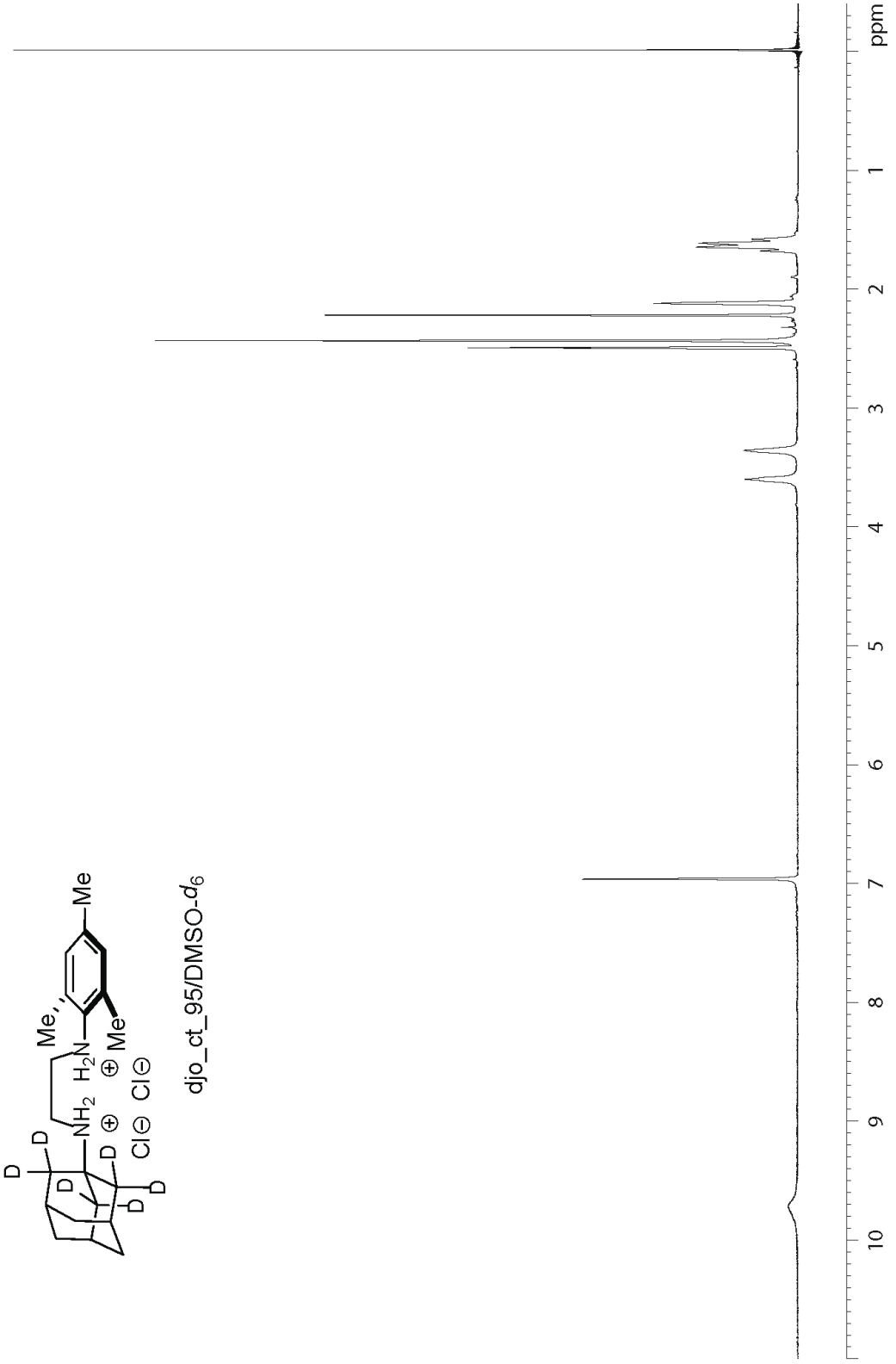
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **S9**.



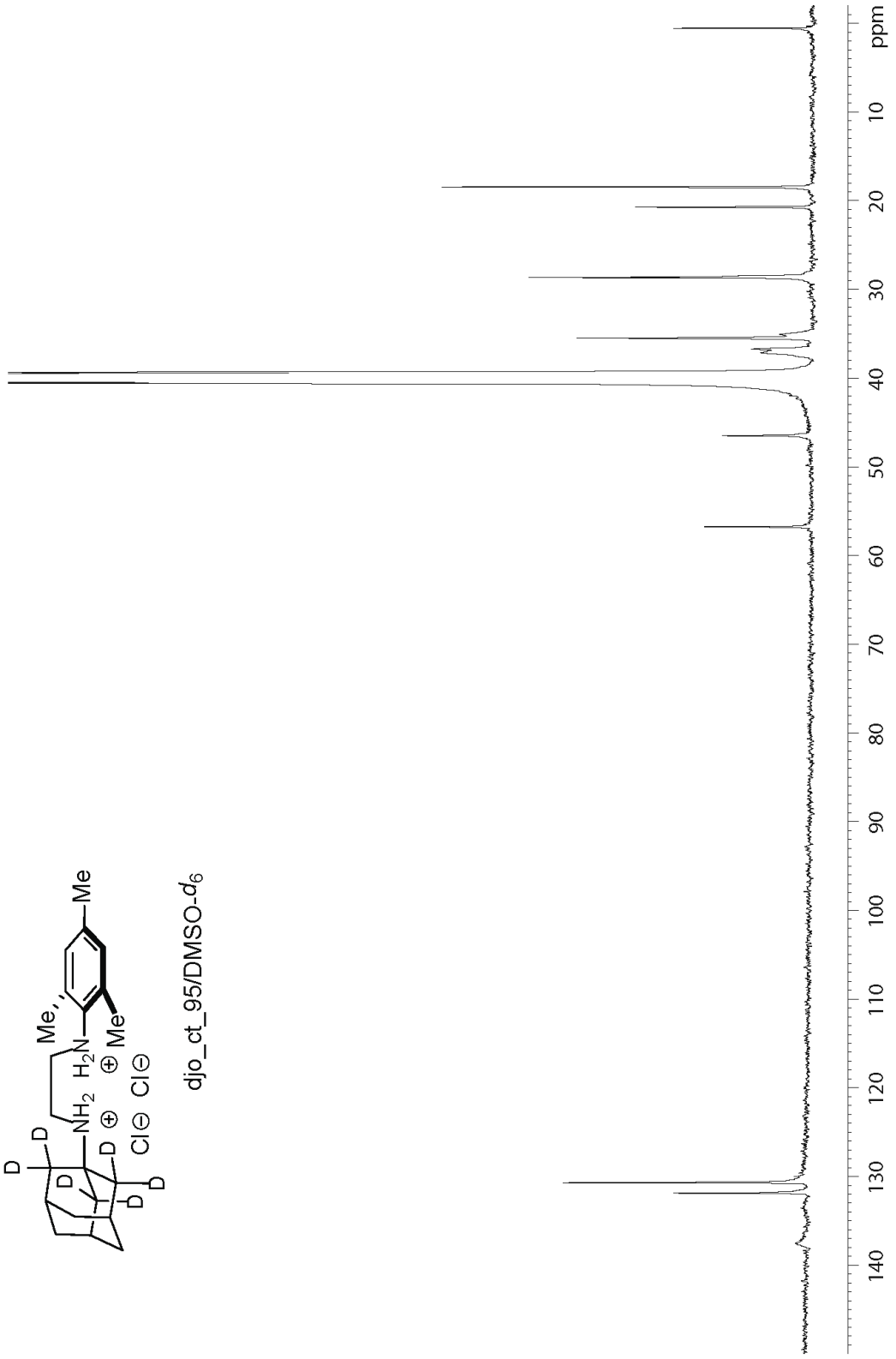
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **S9**.



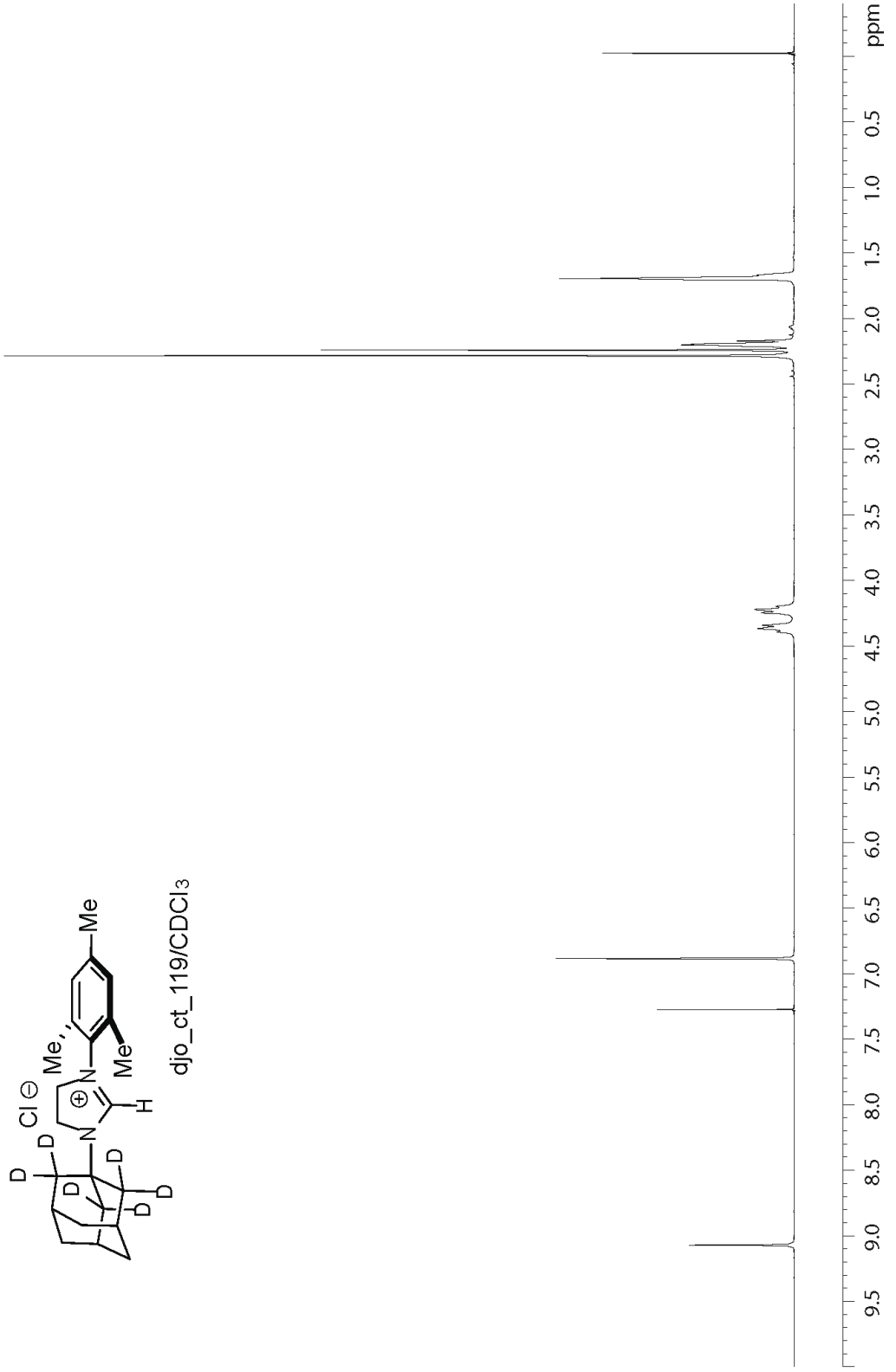
^{1}H NMR (400 MHz, DMSO-d_6) spectrum of compound **S10**.



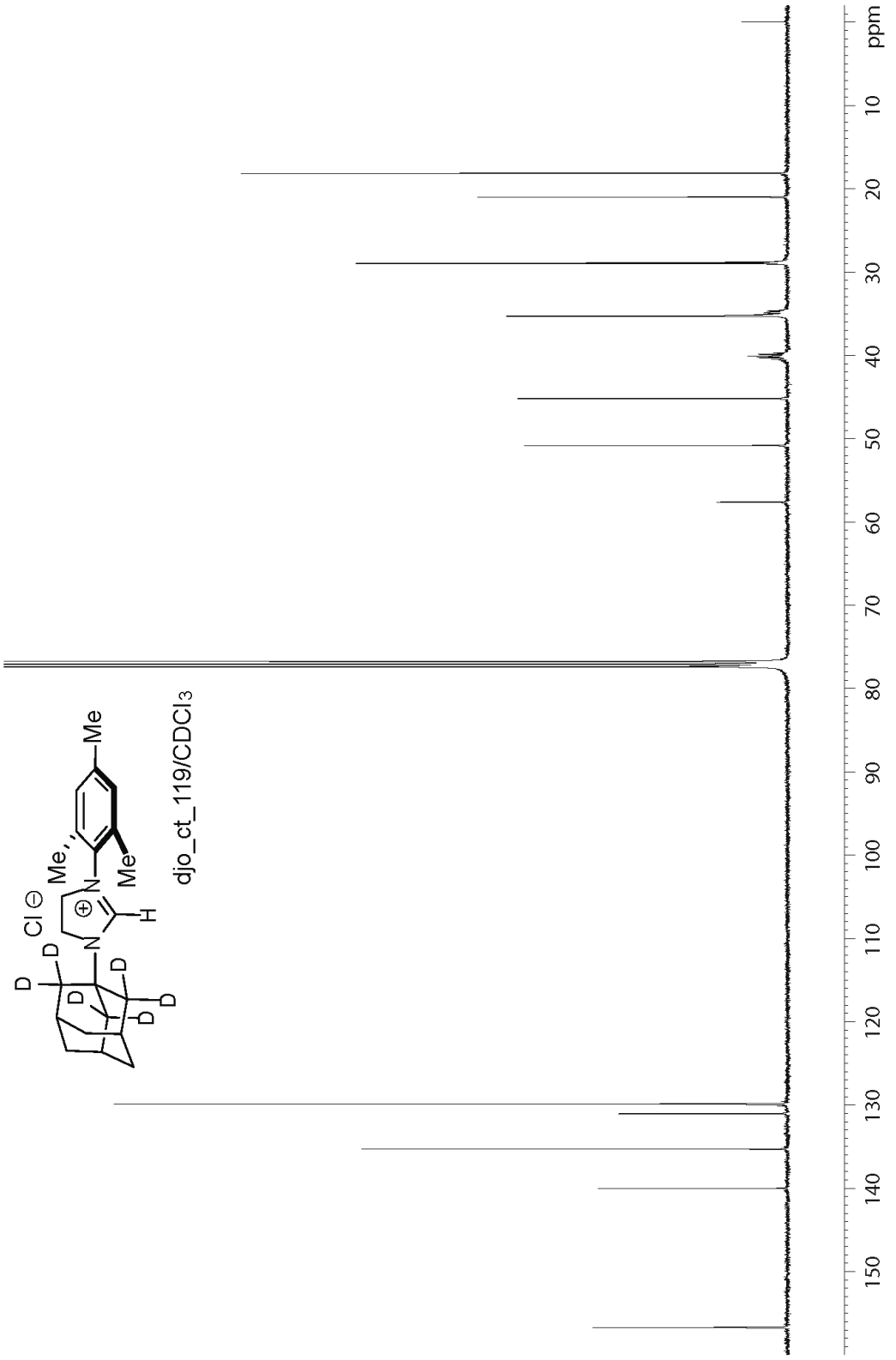
^{13}C NMR (100 MHz, DMSO-d_6) spectrum of compound **S10**.



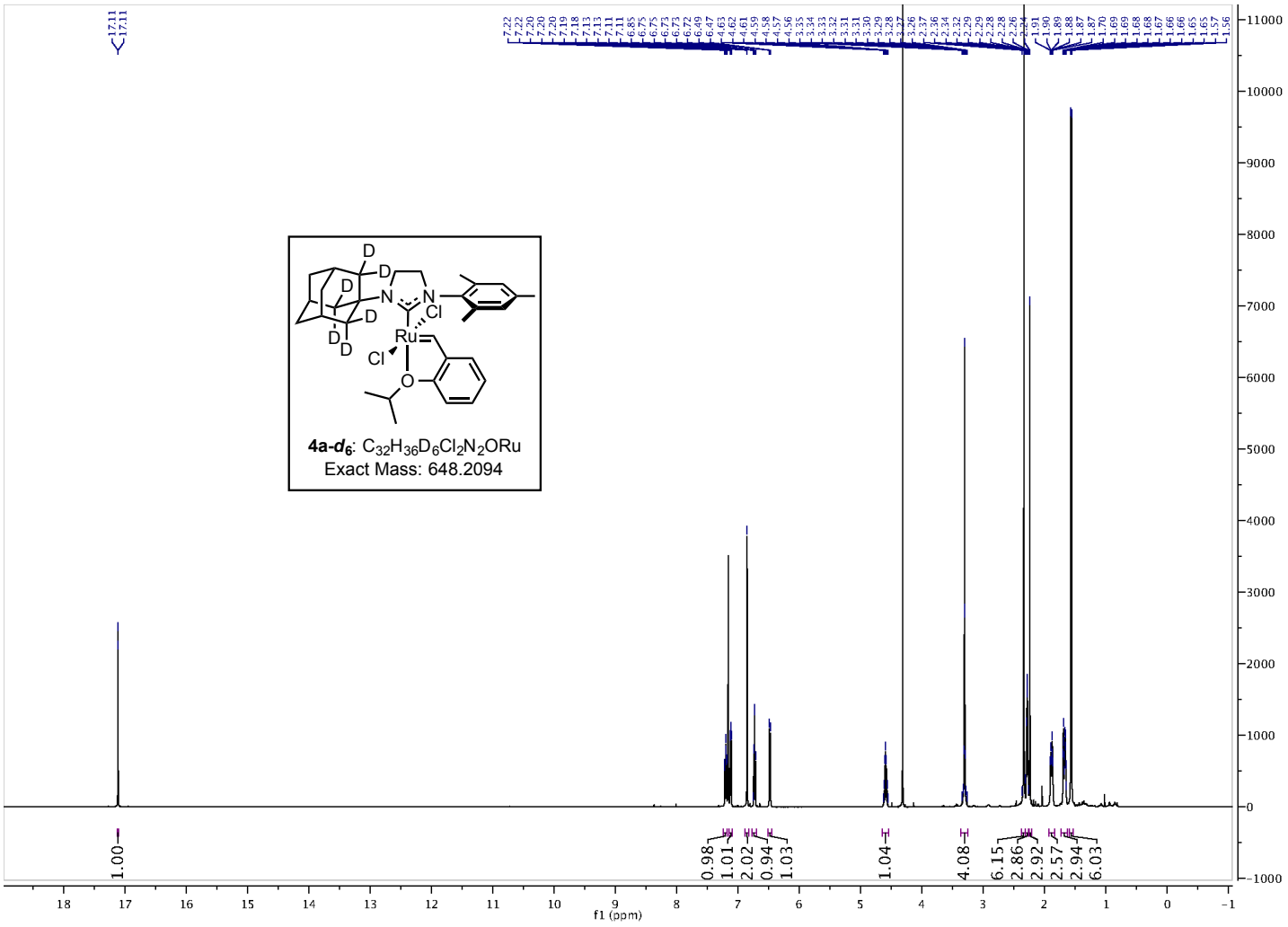
^{1}H NMR (400 MHz, $CDCl_3$) spectrum of compound **S11**.



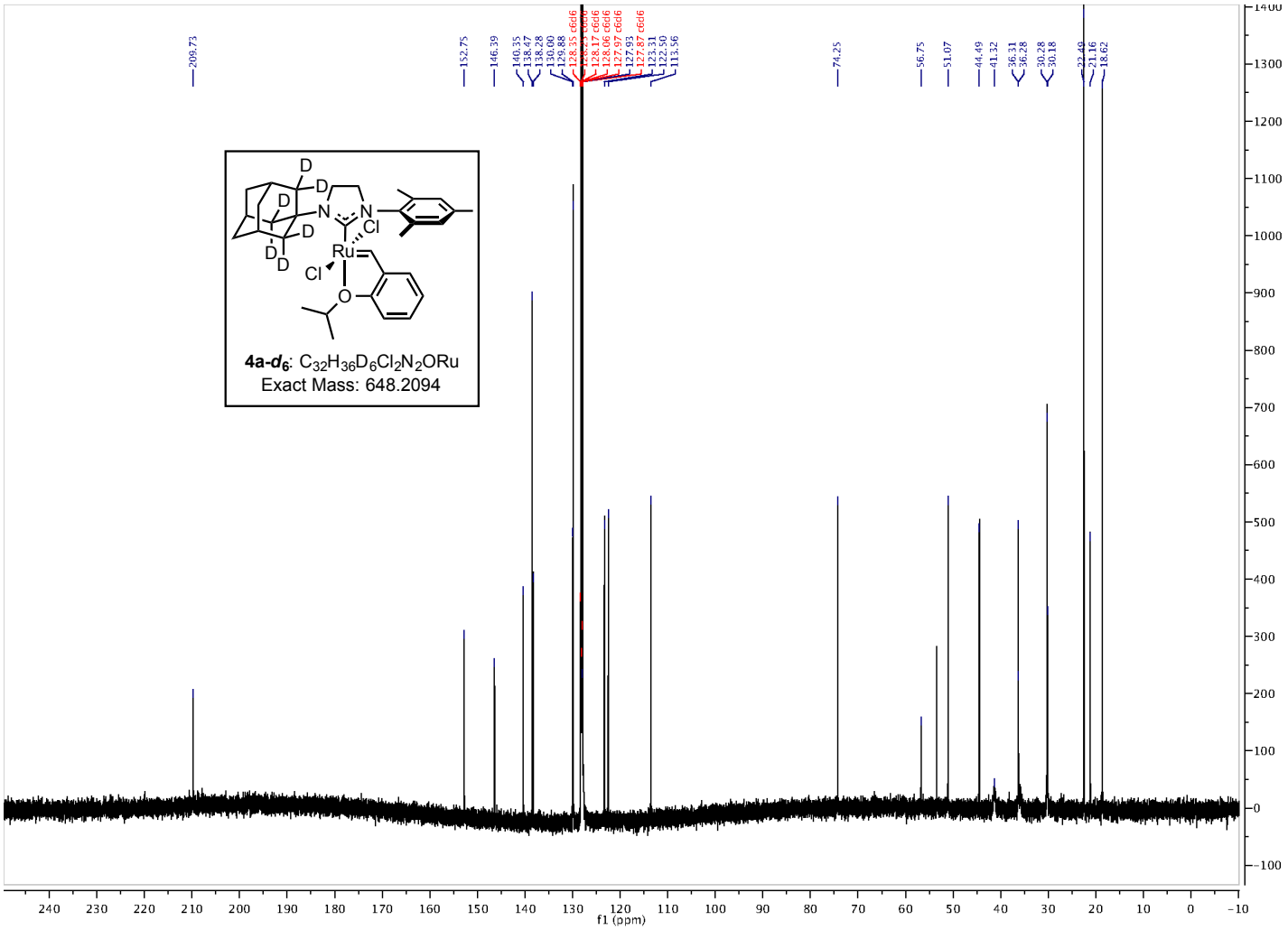
^{13}C NMR (100 MHz, $CDCl_3$) spectrum of compound **S11**.



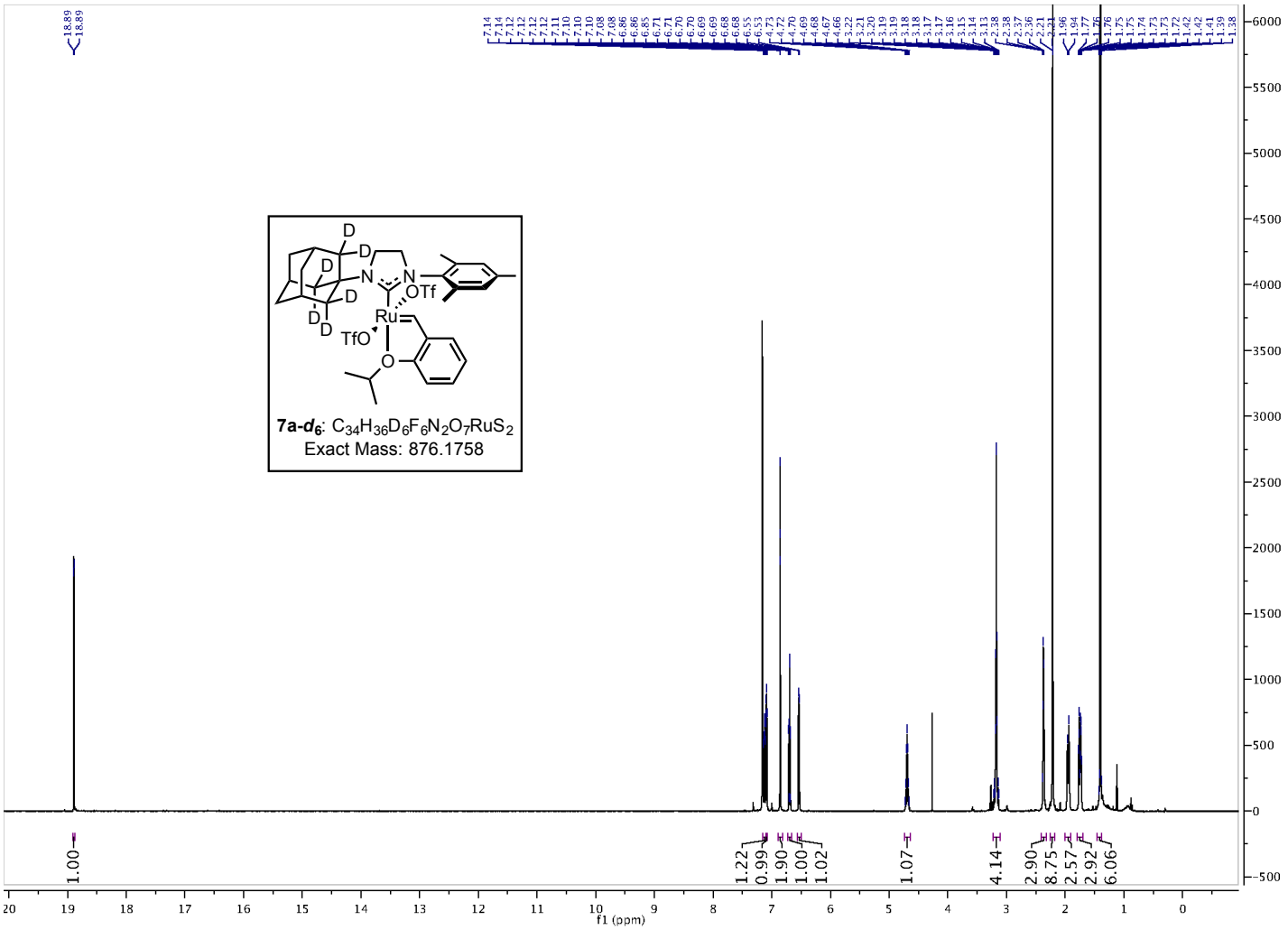
^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **4a-*d*$_6$**.



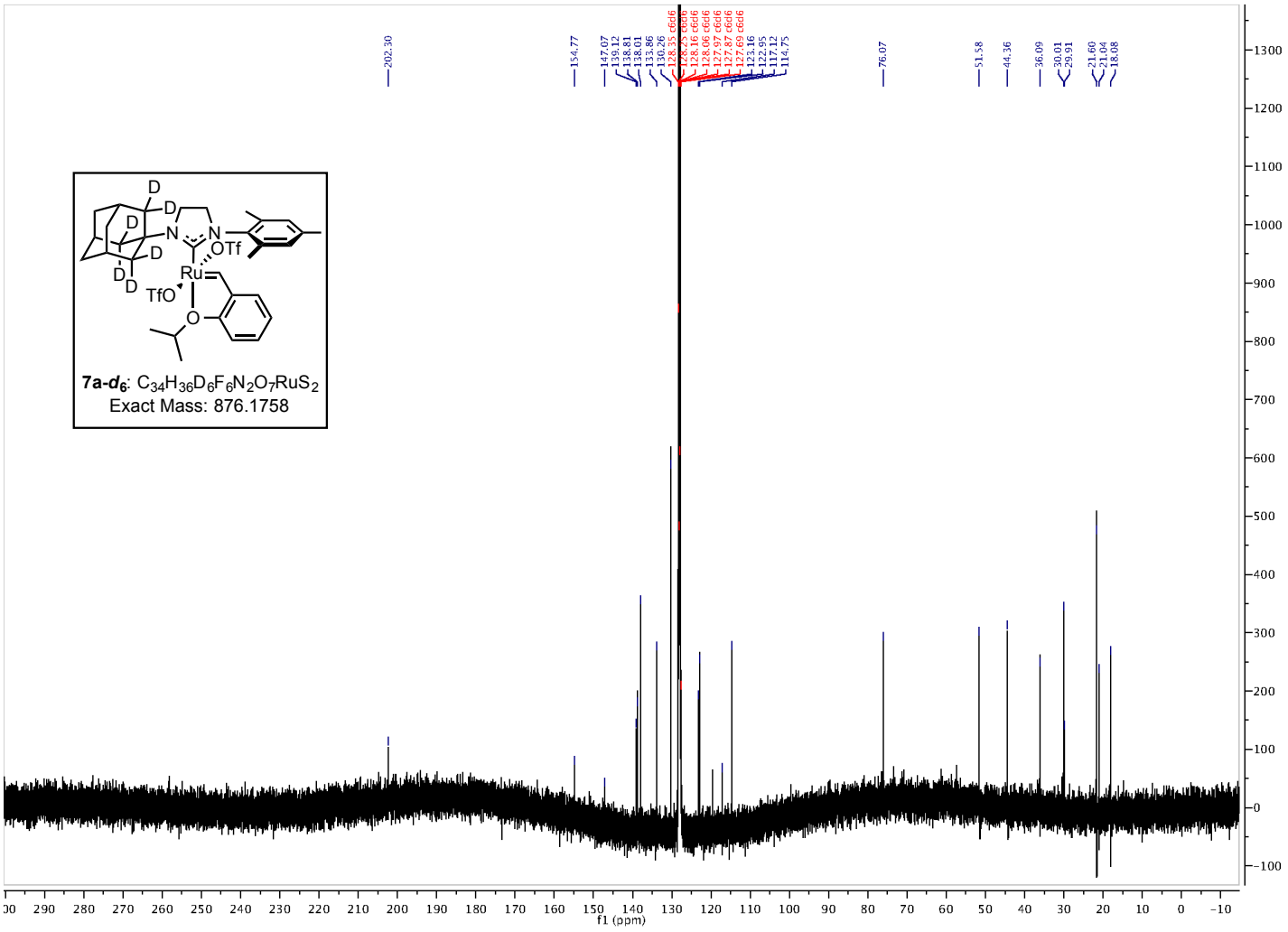
^{13}C NMR (126 MHz, C_6D_6) spectrum of compound **4a-*d*$_6$**.



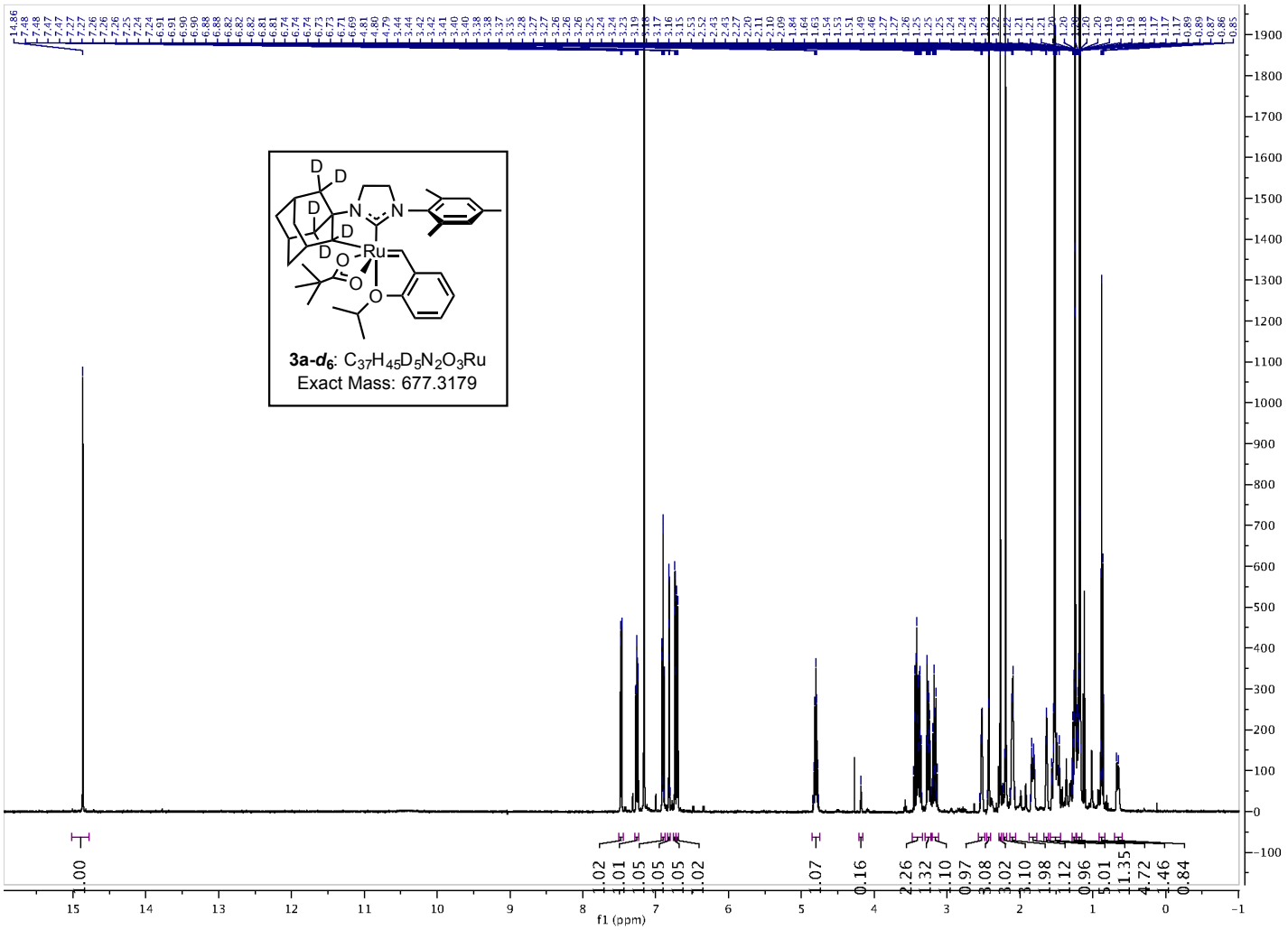
^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **7a-*d*$_6$**.



^{13}C NMR (126 MHz, C_6D_6) spectrum of compound **7a-*d*$_6$**.



^{1}H NMR (500 MHz, C_6D_6) spectrum of compound **3a-*d*$_6$**.



^{13}C NMR (126 MHz, C_6D_6) spectrum of compound **3a-*d*$_6$**.