Supporting Information

Synthesis, characterization and catalytic activity of novel ruthenium complexes bearing NNN click based ligands

Roberto Sole,[a] Marco Bortoluzzi,[b] Anke Spannenberg,[b] Sergey Tin,[b] Valentina Beghetto *[a] and Johannes G. de Vries *[b]

[a] Dipartimento di Scienze Molecolari e Nanosistemi,Università Ca´Foscari Venezia, Via Torino 155, 30170, Venezia Mestre, Italy

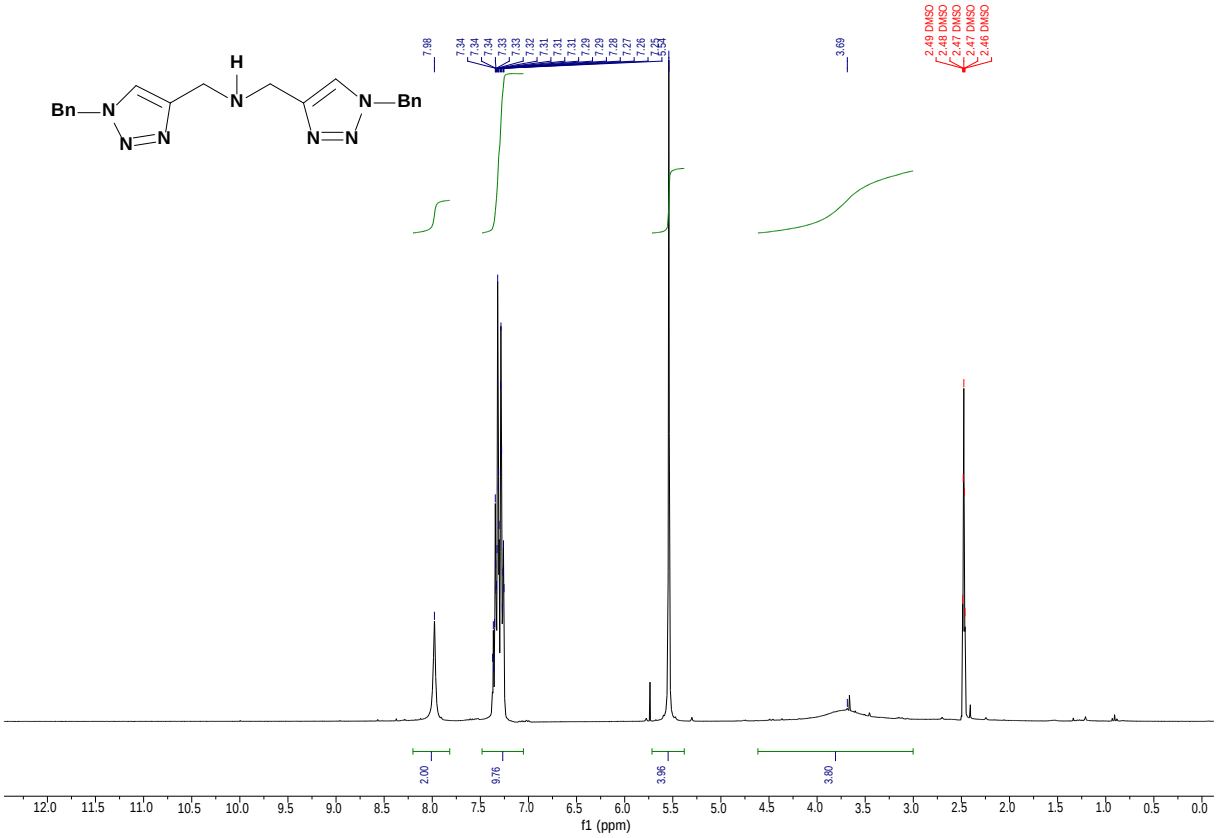
[b] Leibniz Institute für Katalyse e.V. an der Universität Rostock, Albert-Einstein-Straße 29a, 18055, Rostock, Germany.

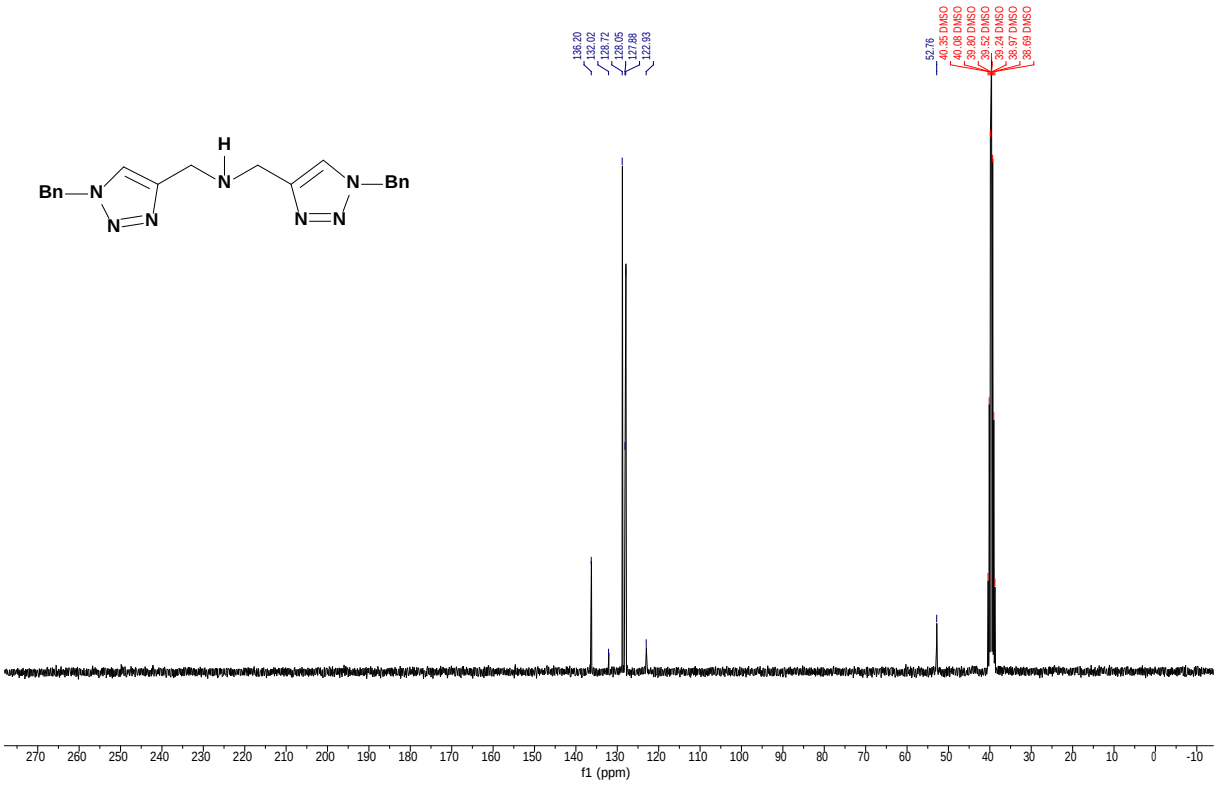
Table of Contents

1. Characterization data of ligands and complexes

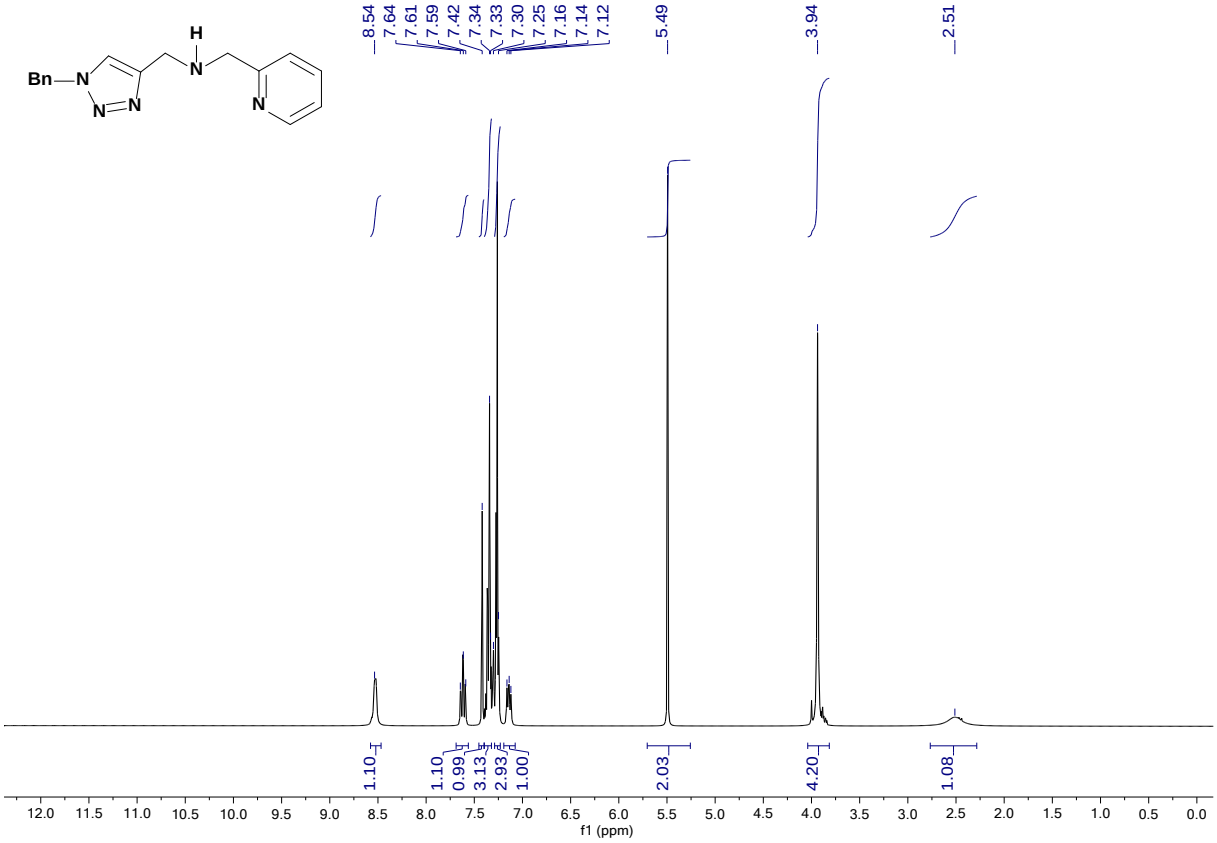
a. NMR spectra

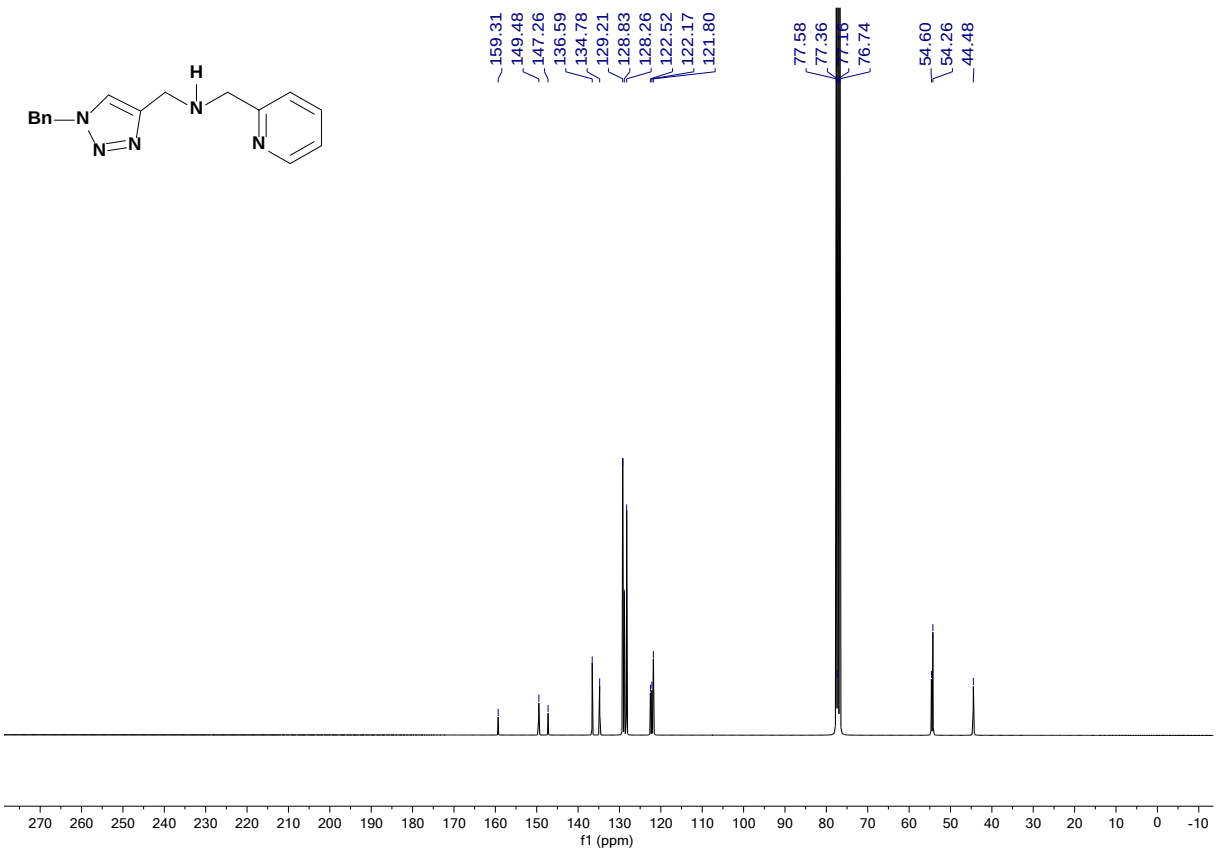
bis((1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)amine (L1)



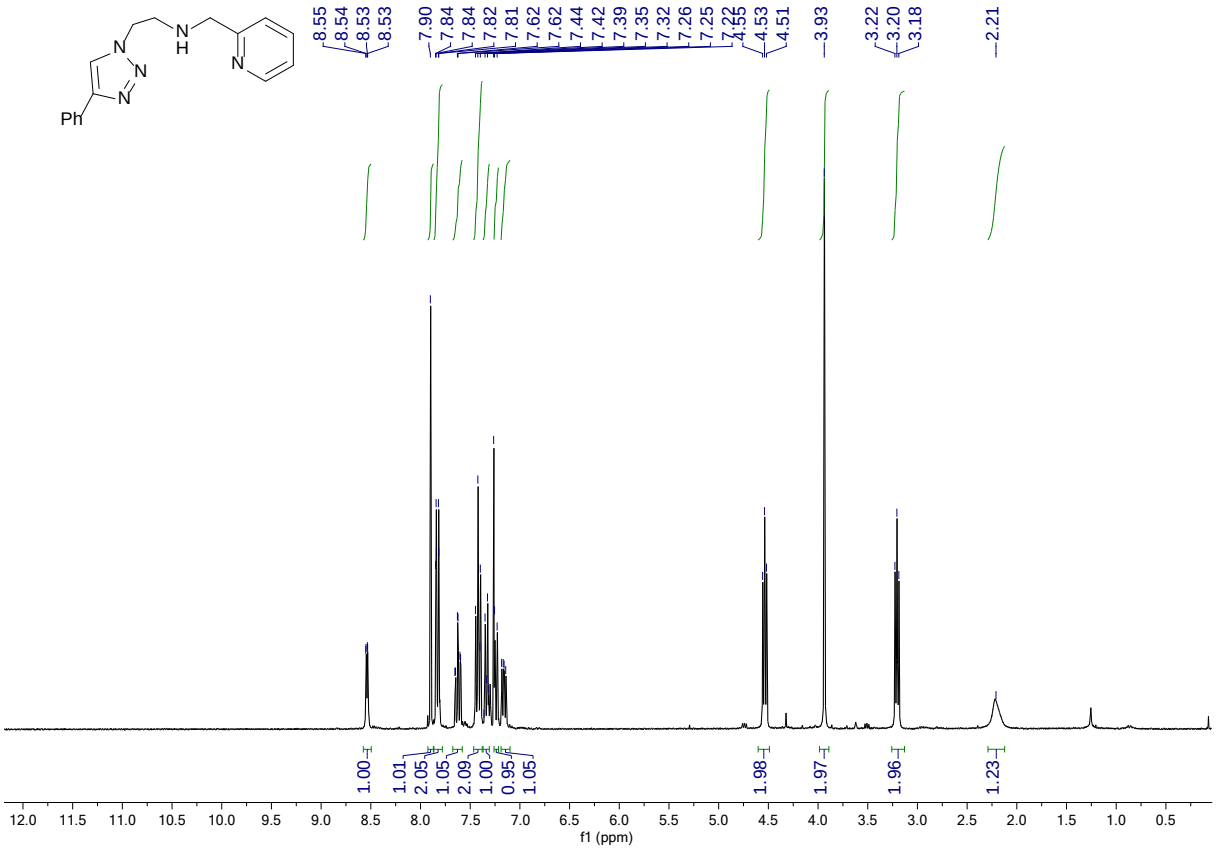


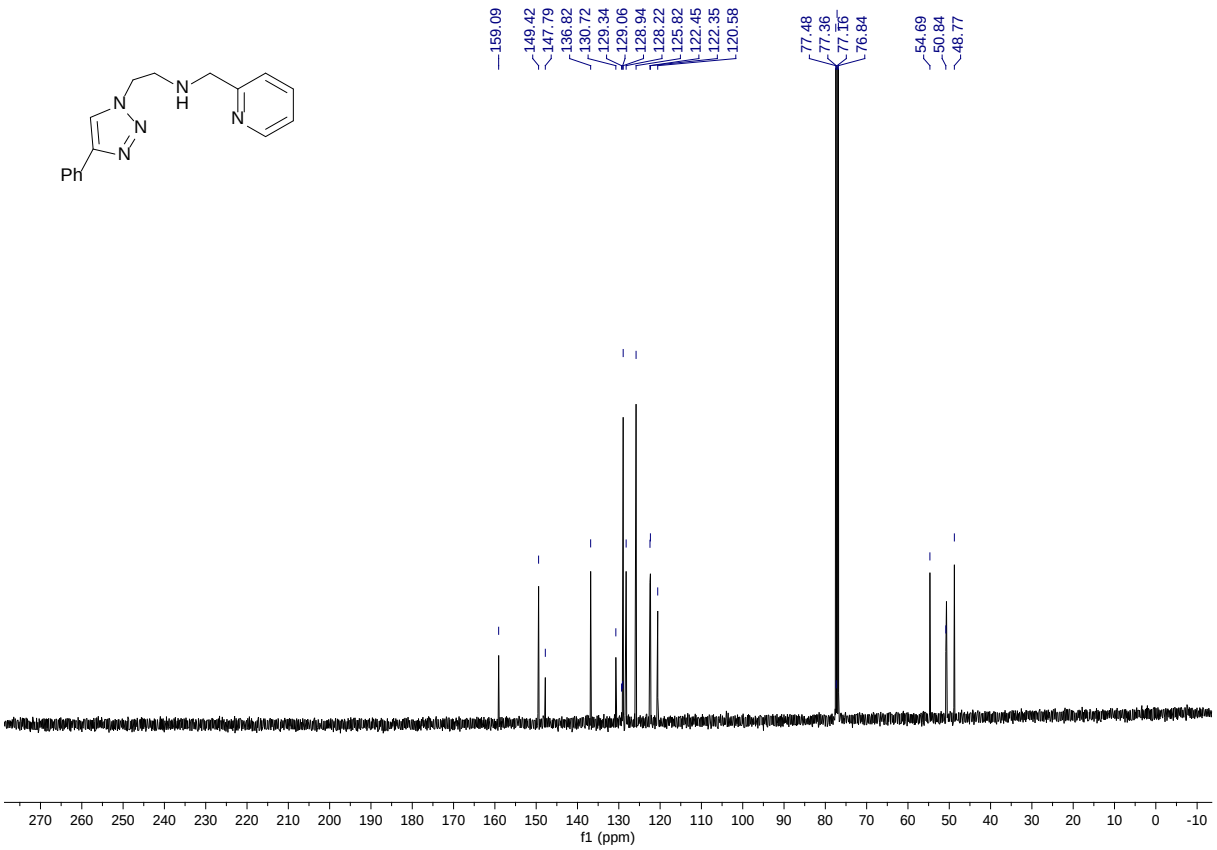
1-(1-benzyl-1*H*-1,2,3-triazol-4-yl)-N-(pyridin-2-ylmethyl)methanamine (L2)



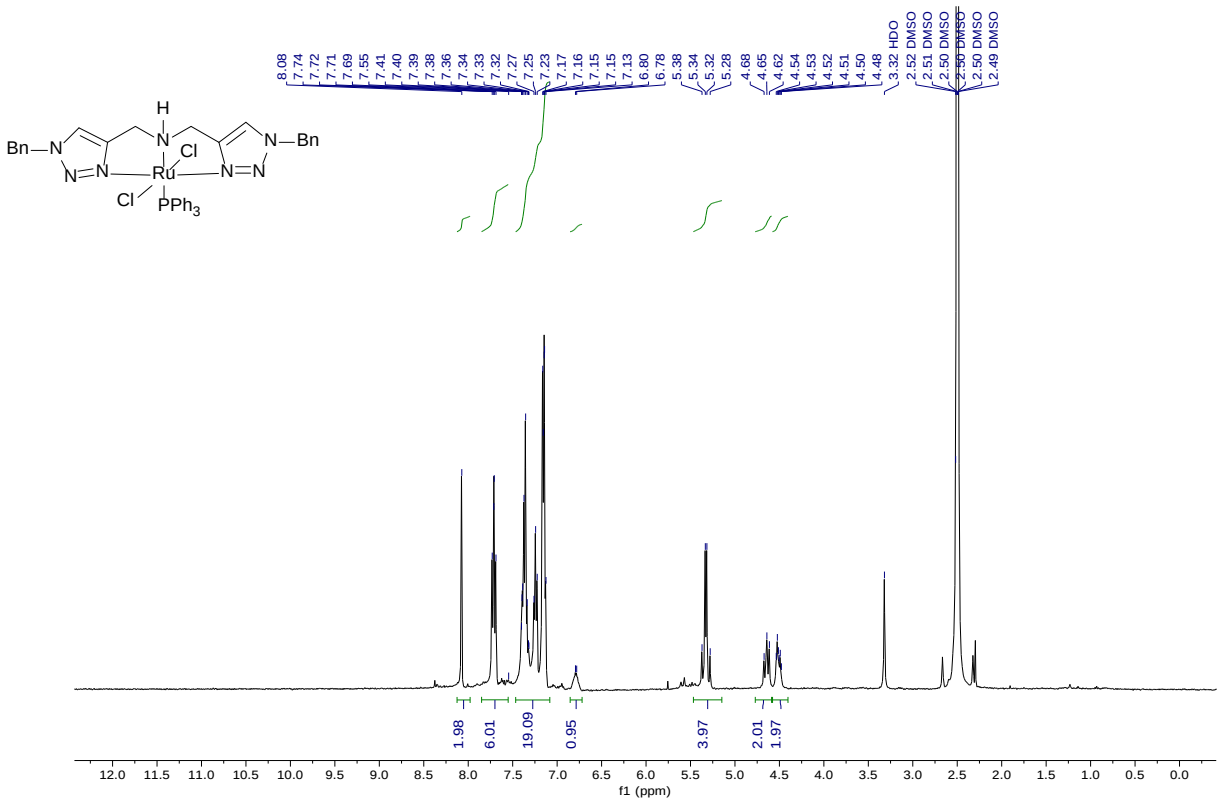


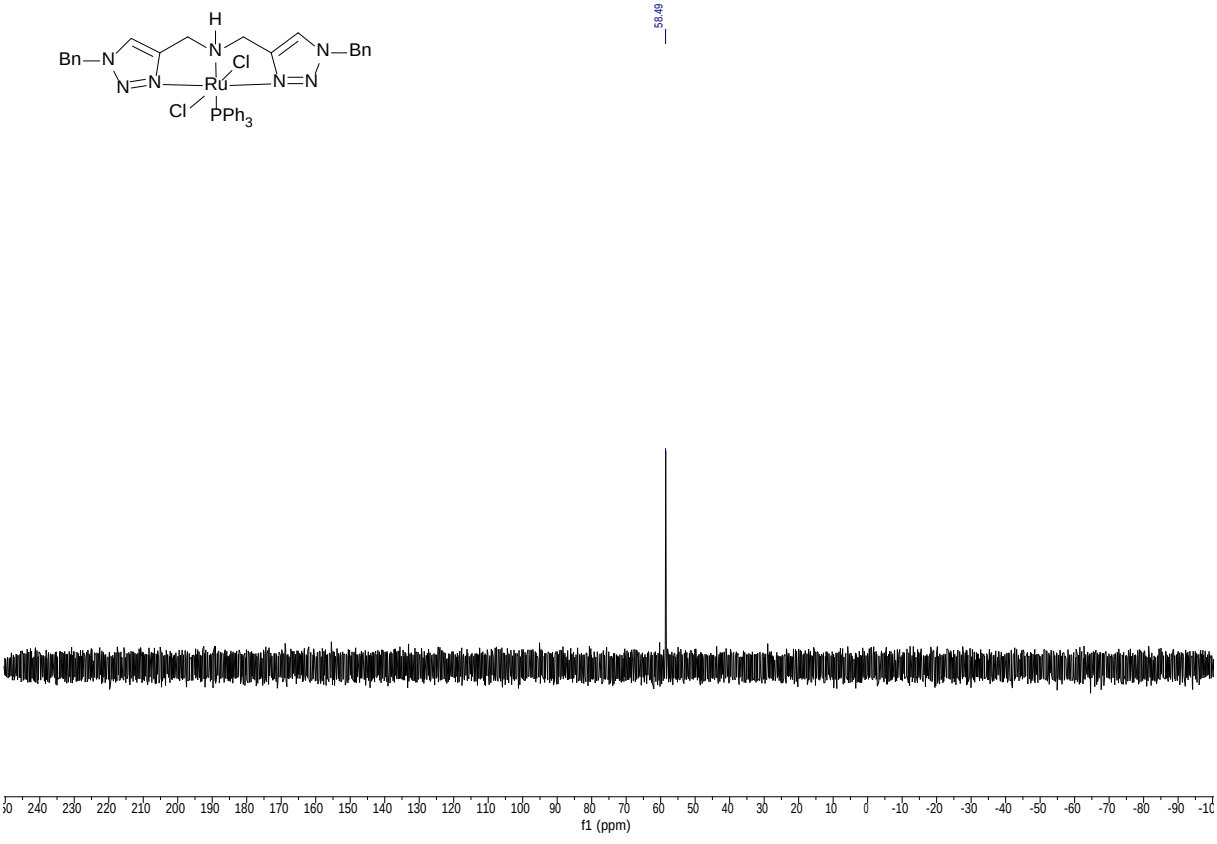
2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)-N-(pyridin-2-ylmethyl)ethan-1-amine (L3)



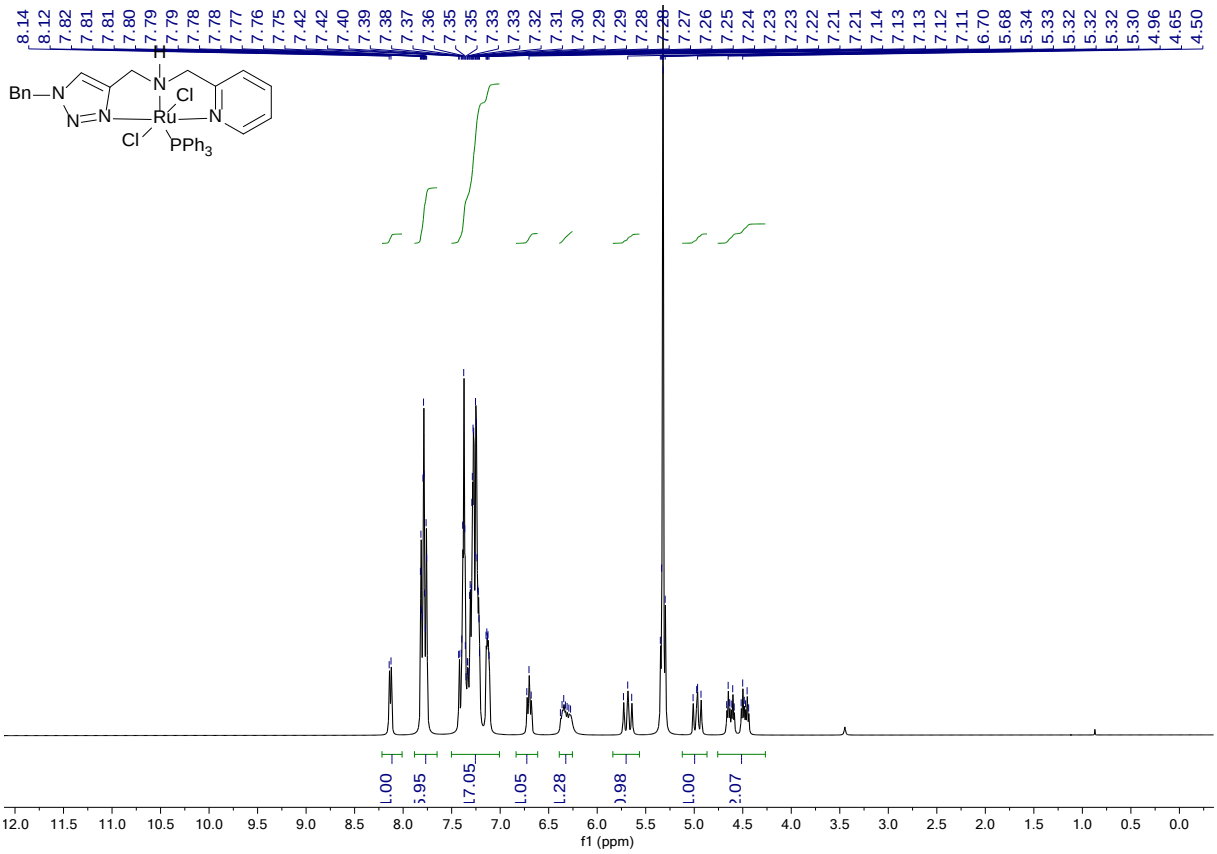


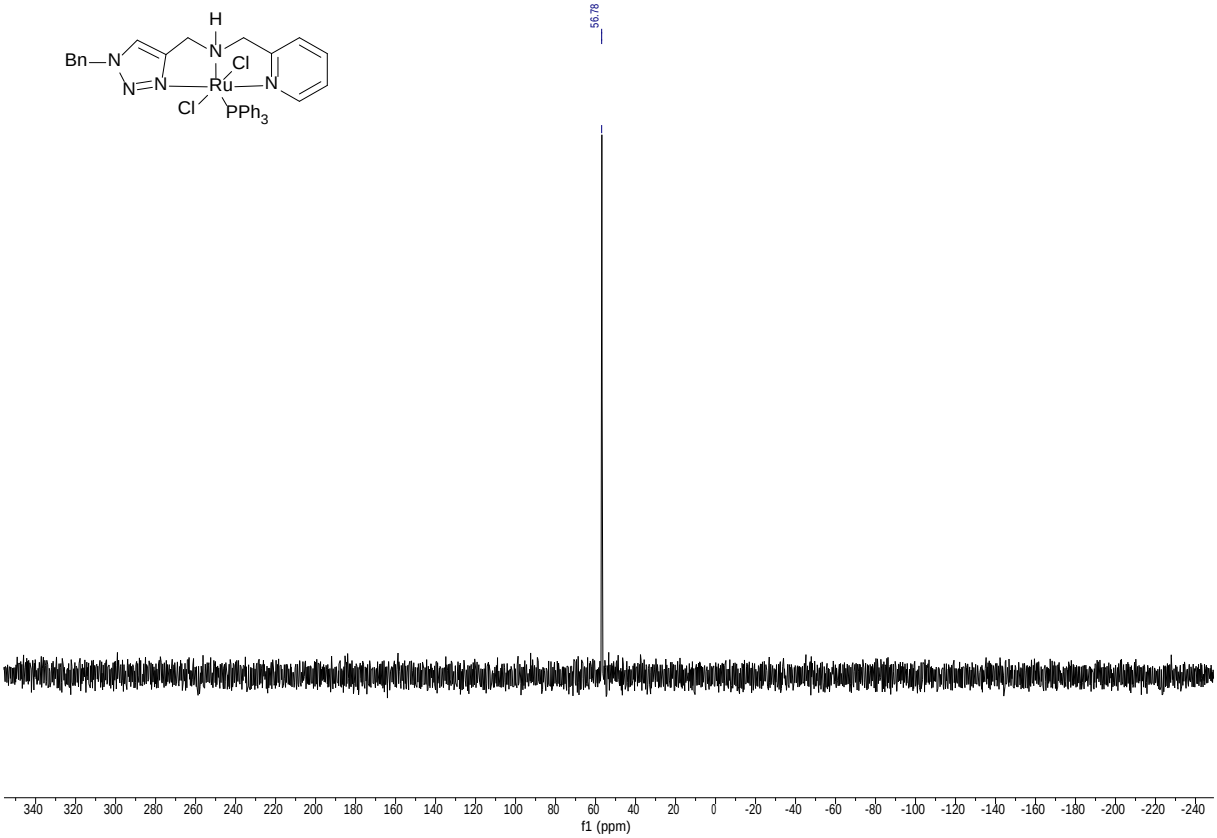
$Ru(NNN_{L1})(PPh_3)Cl_2$ (1)



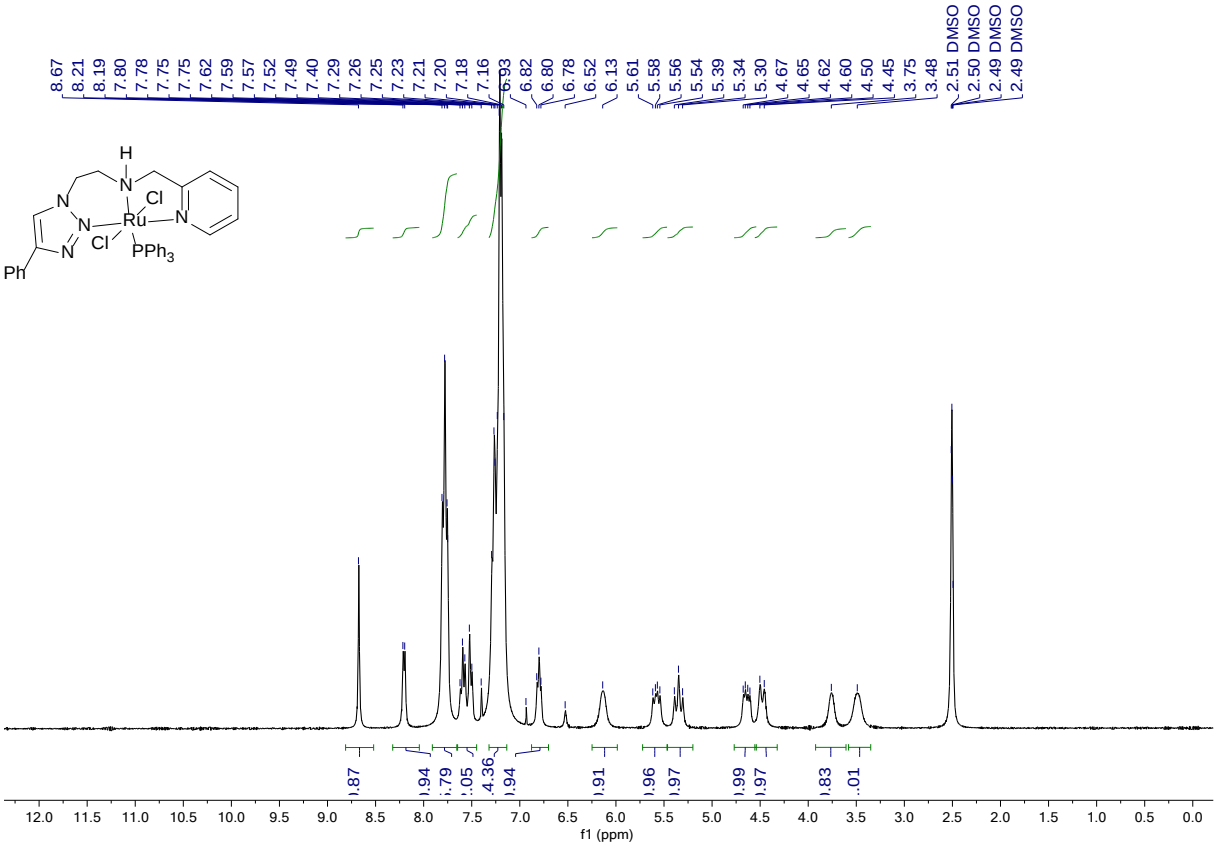


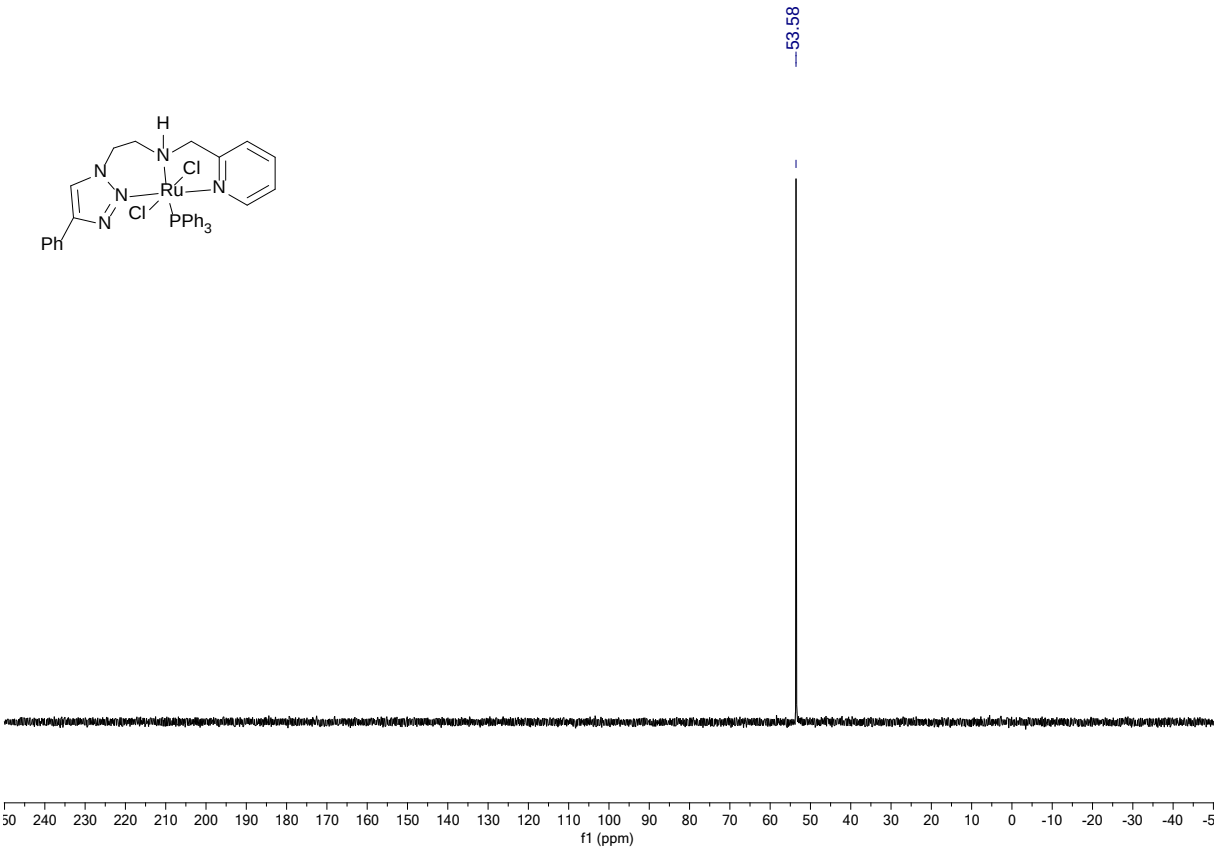
$Ru(NNN_{L2})(PPh_3)Cl_2$ (2)





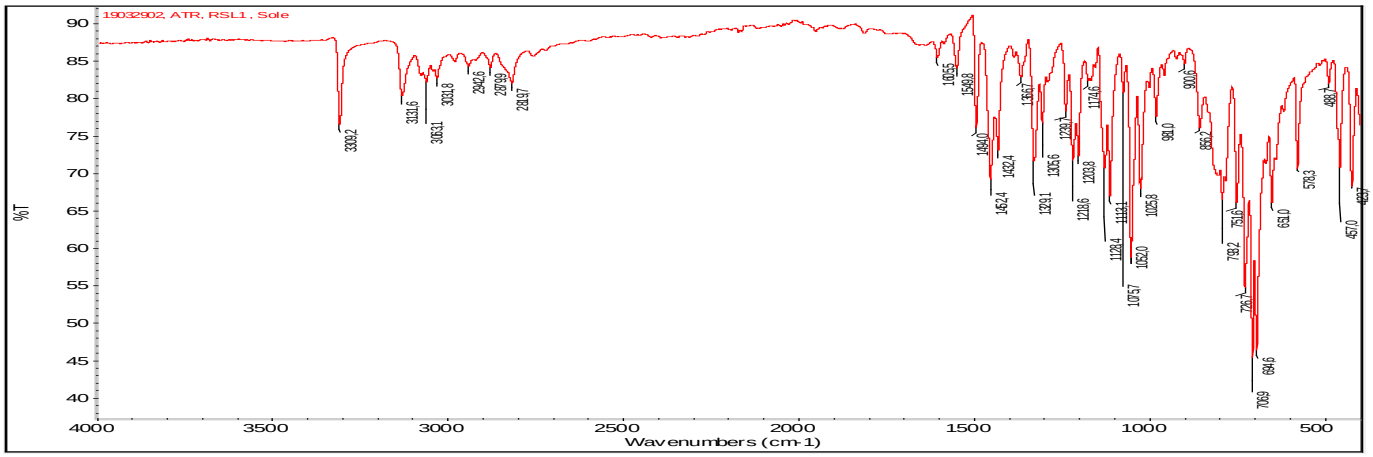
Ru(NNN$_{L3}$)(PPh$_3$)Cl$_2$ (3)



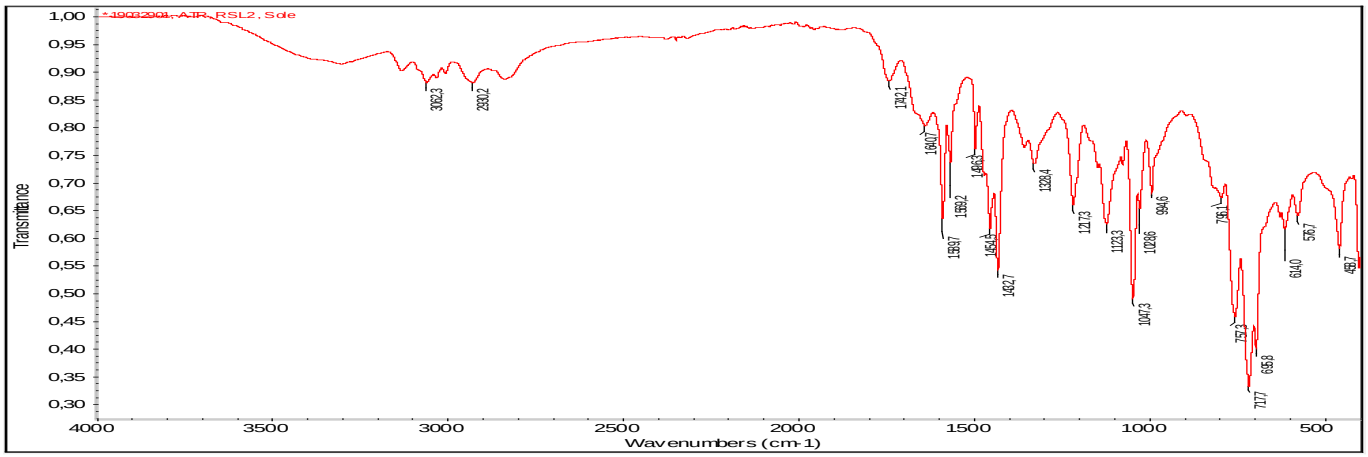


b. ATR-IR spectra complexes

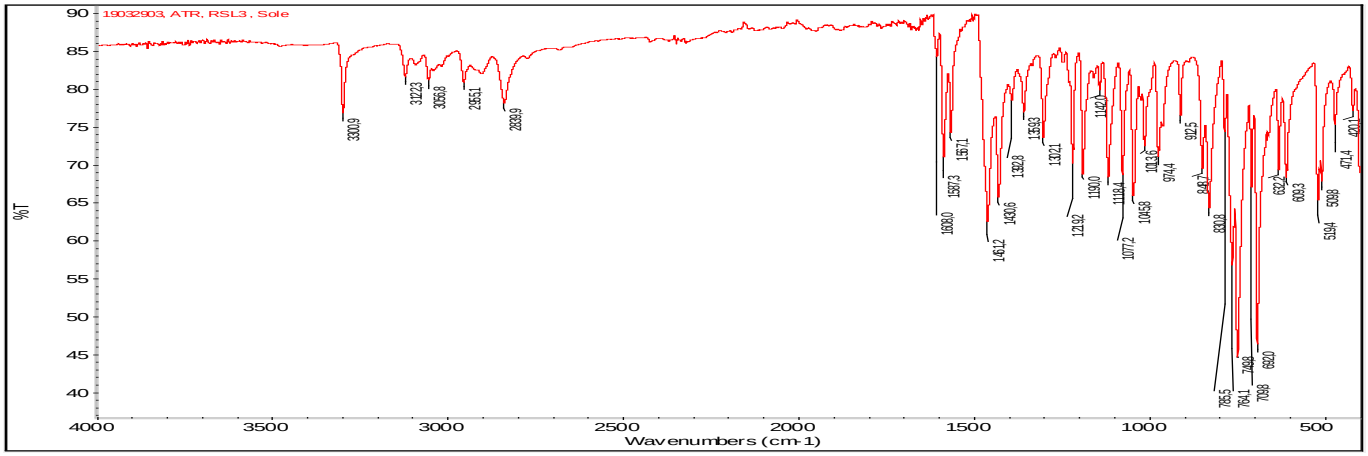
bis((1-benzyl-1H-1,2,3-triazol-4-yl)methyl)amine (L1)



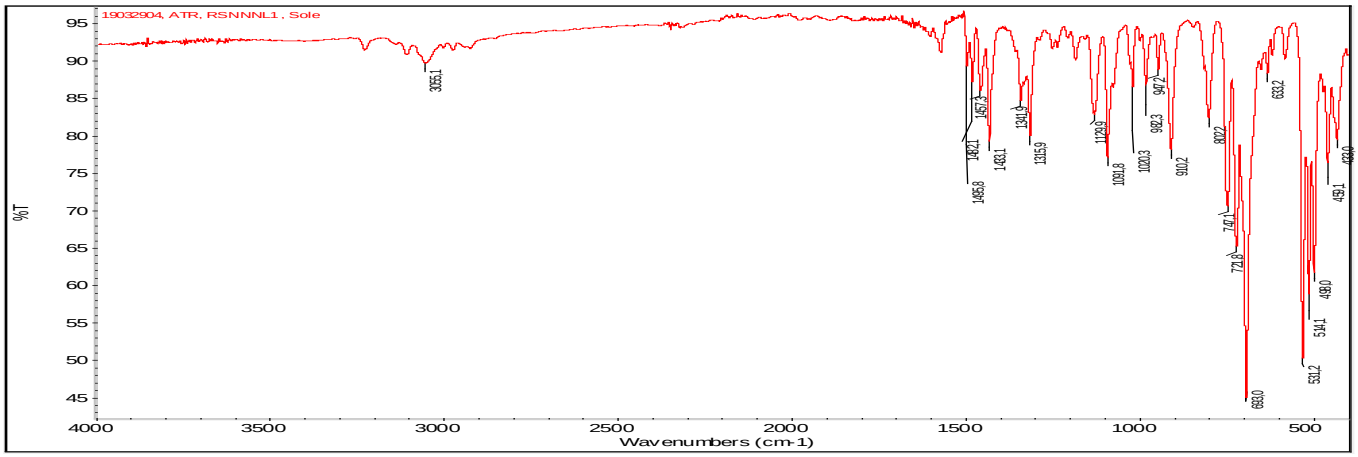
1-(1-benzyl-1H-1,2,3-triazol-4-yl)-N-(pyridin-2-ylmethyl)methanamine (L2)



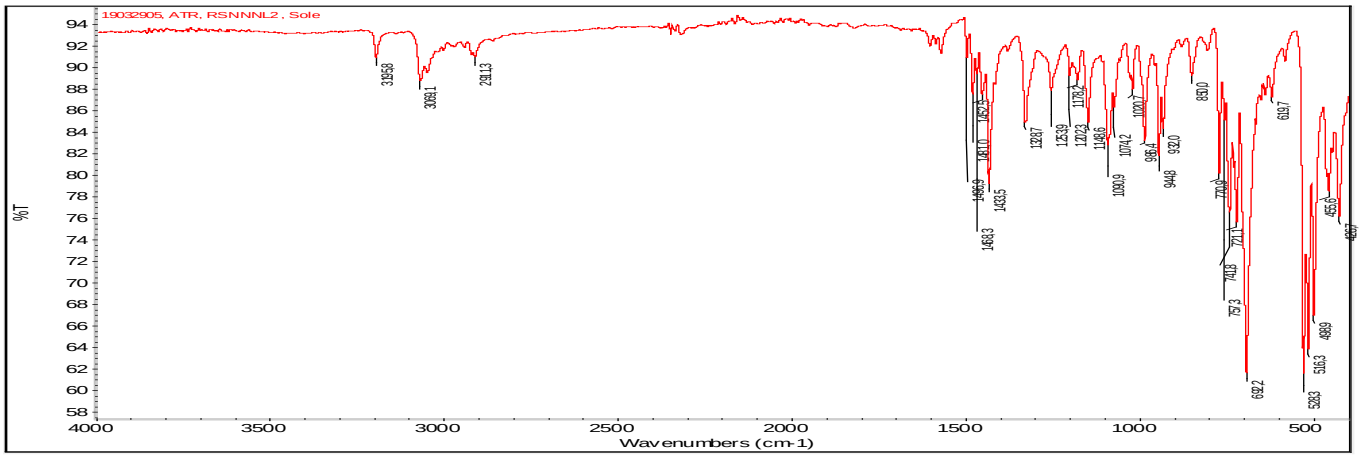
2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)-N-(pyridin-2-ylmethyl)ethan-1-amine (L3)



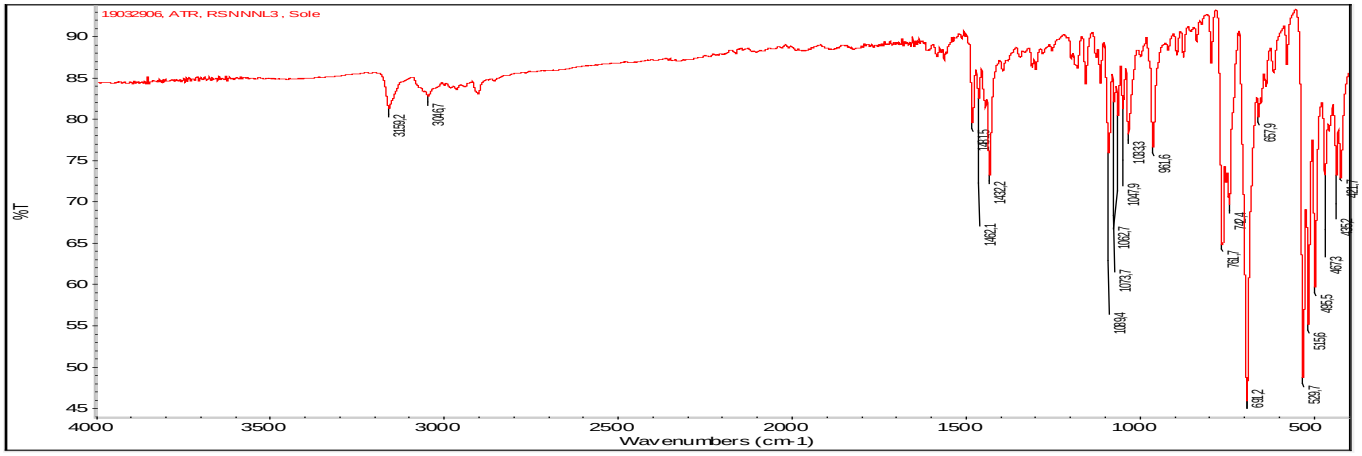
$Ru(NNN_{L1})(PPh_3)Cl_2$ (1)



$Ru(NNN_{L2})(PPh_3)Cl_2$ (2)

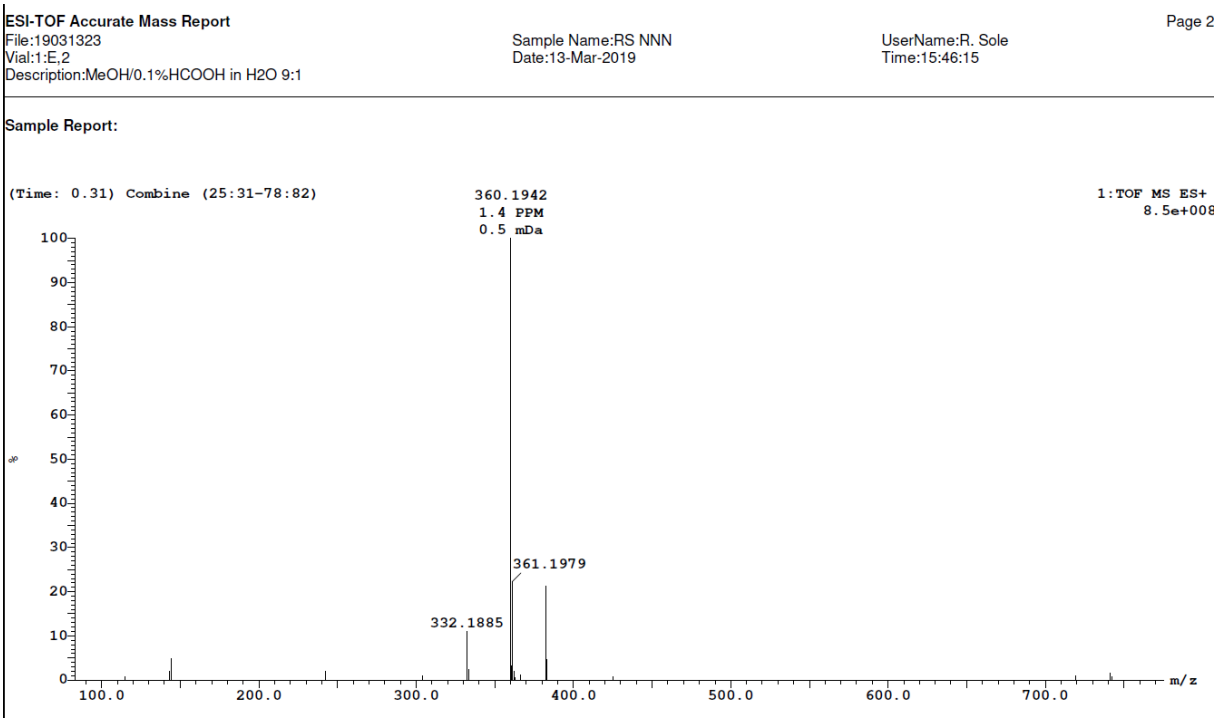


$Ru(NNN_{L3})(PPh_3)Cl_2$ (3)

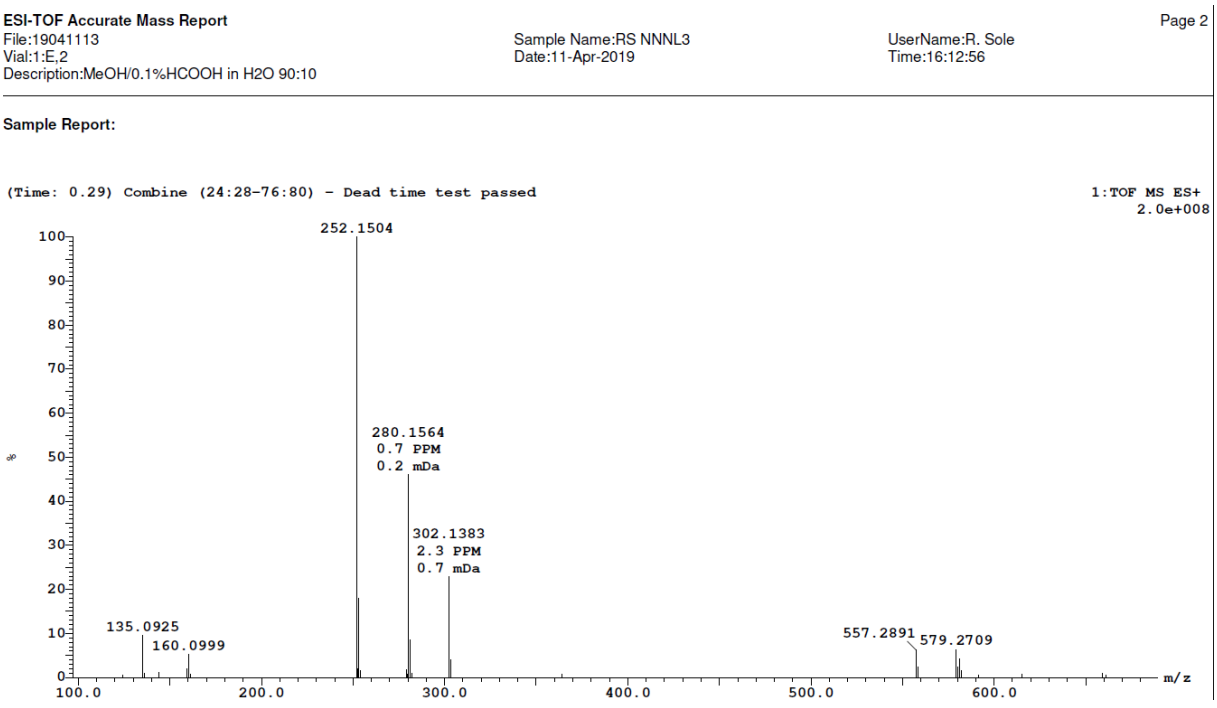


c. ESI-HRMS spectra complexes

bis((1-benzyl-1*H*-1,2,3-triazol-4-yl)methyl)amine (L1)



1-(1-benzyl-1*H*-1,2,3-triazol-4-yl)-N-(pyridin-2-ylmethyl)methanamine (L2)

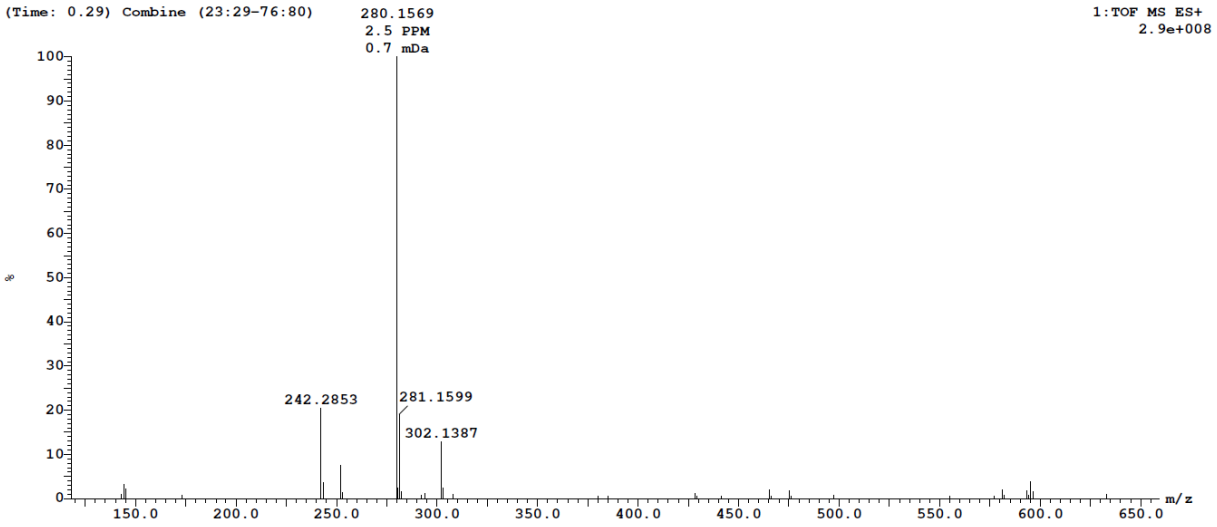


2-(4-phenyl-1*H*-1,2,3-triazol-1-yl)-N-(pyridin-2-ylmethyl)ethan-1-amine (L3)

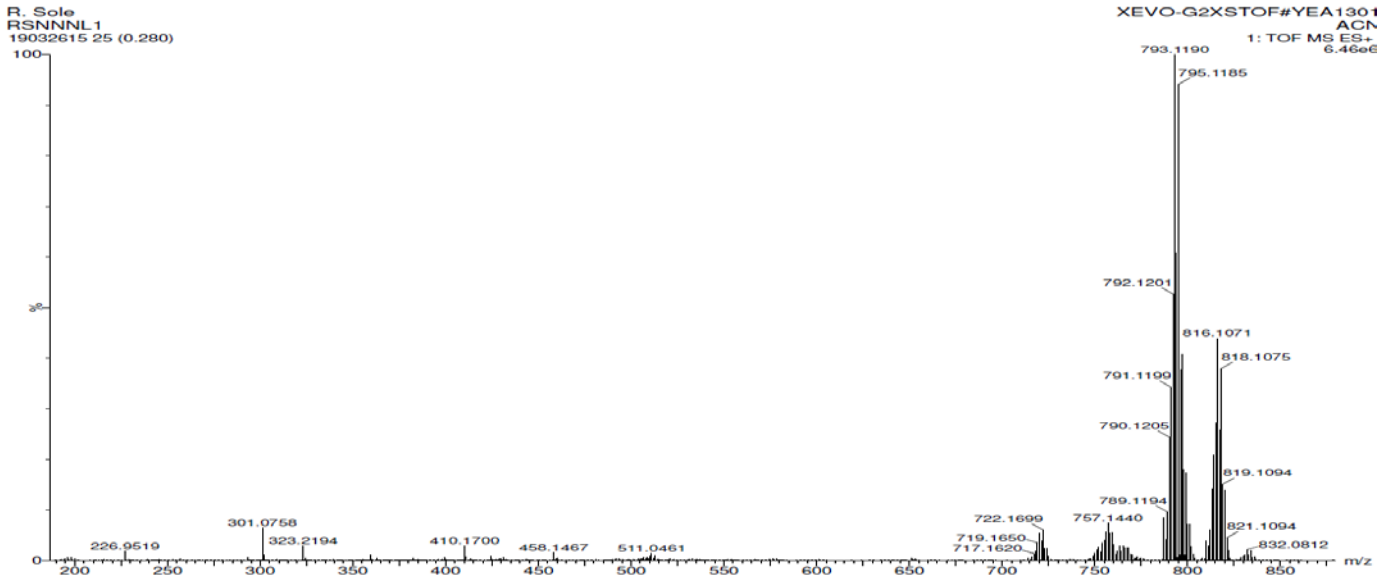
ESI-TOF Accurate Mass Report Page 2

File:19041114 Sample Name:RS ? UserName:R. Sole
Vial:1:E,3 Date:11-Apr-2019 Time:16:15:32
Description:MeOH/0.1%HCOOH in H2O 90:10

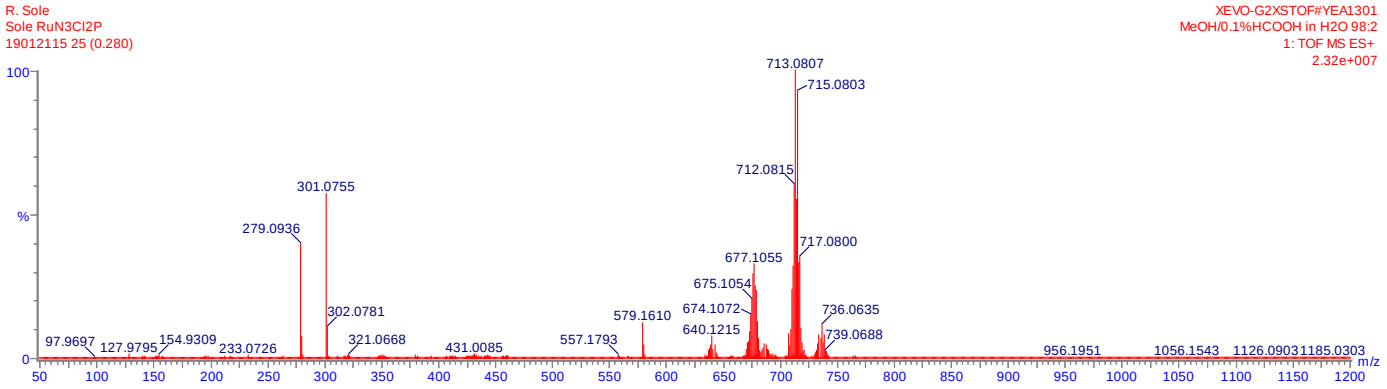
Sample Report:



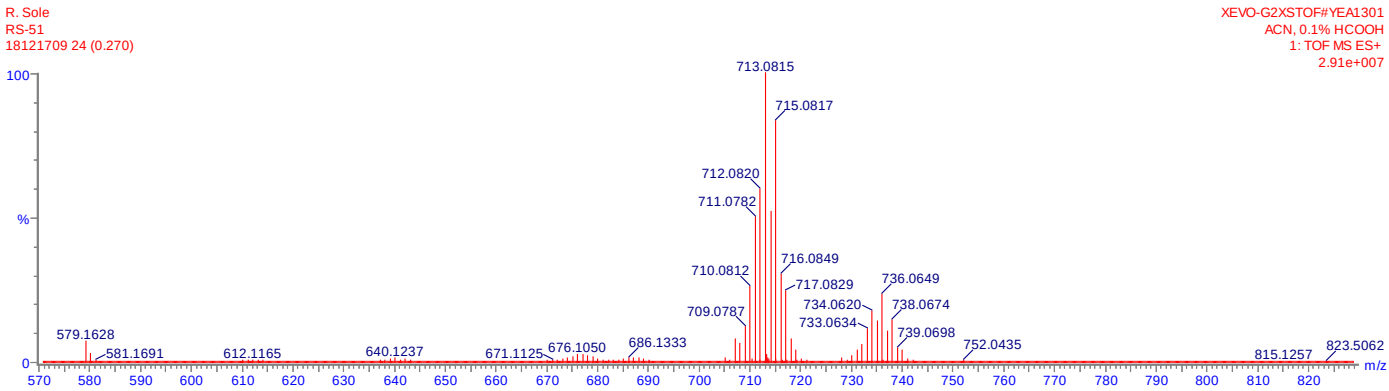
$Ru(NNN_{L1})(PPh_3)Cl_2$ (1)



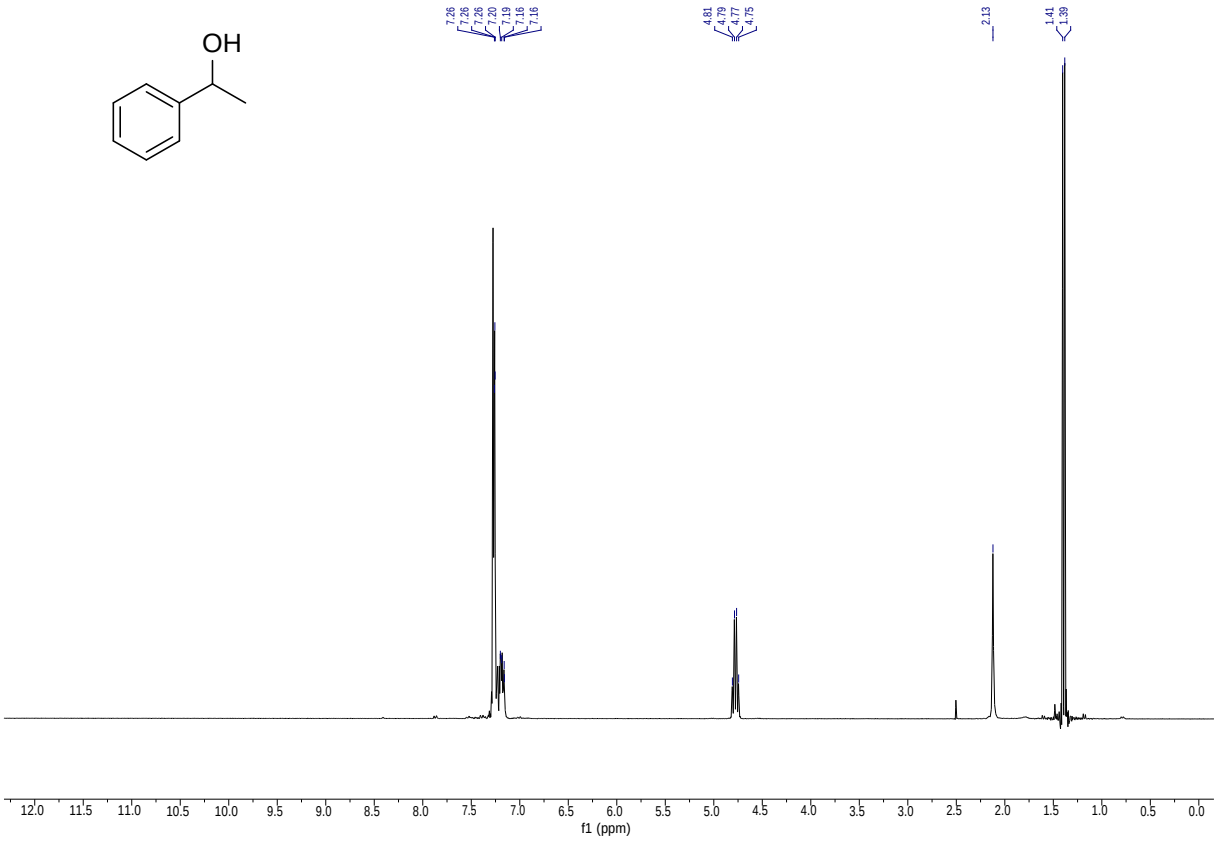
$Ru(NNN_{L2})(PPh_3)Cl_2$ (2)

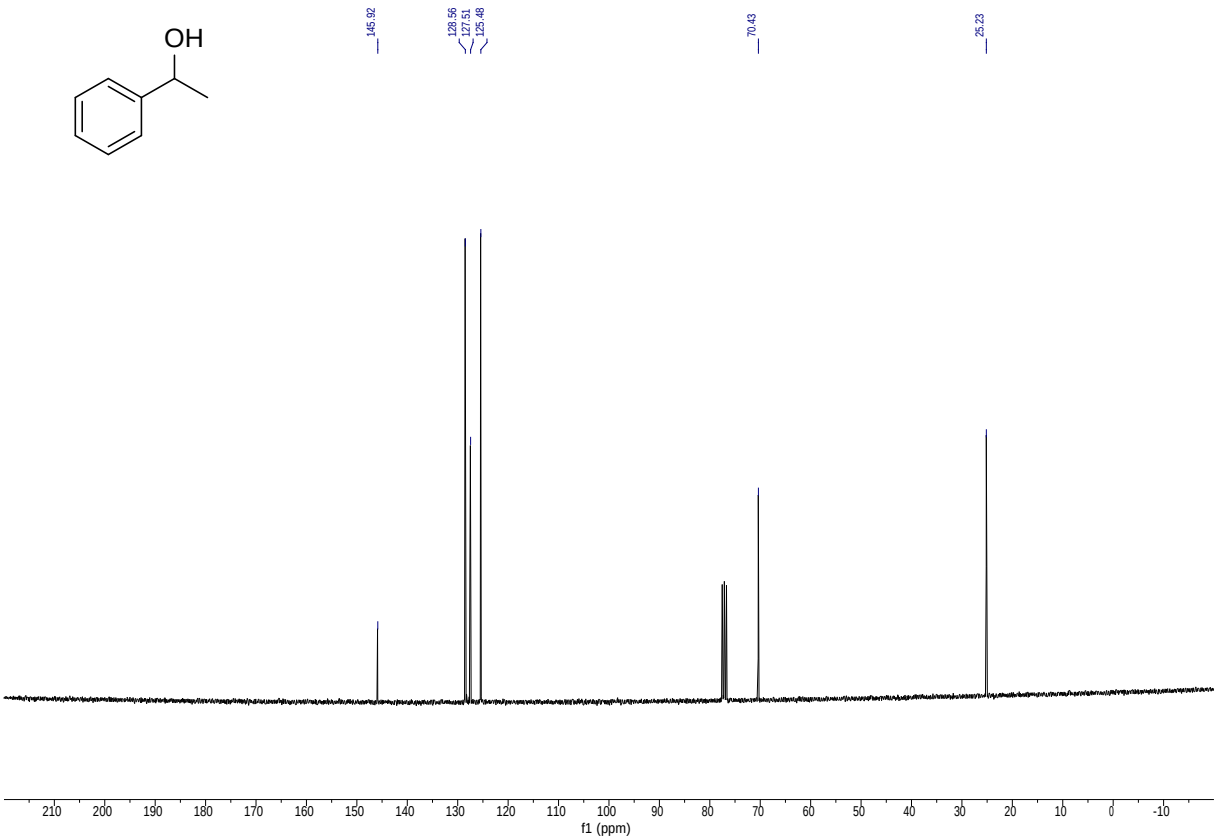


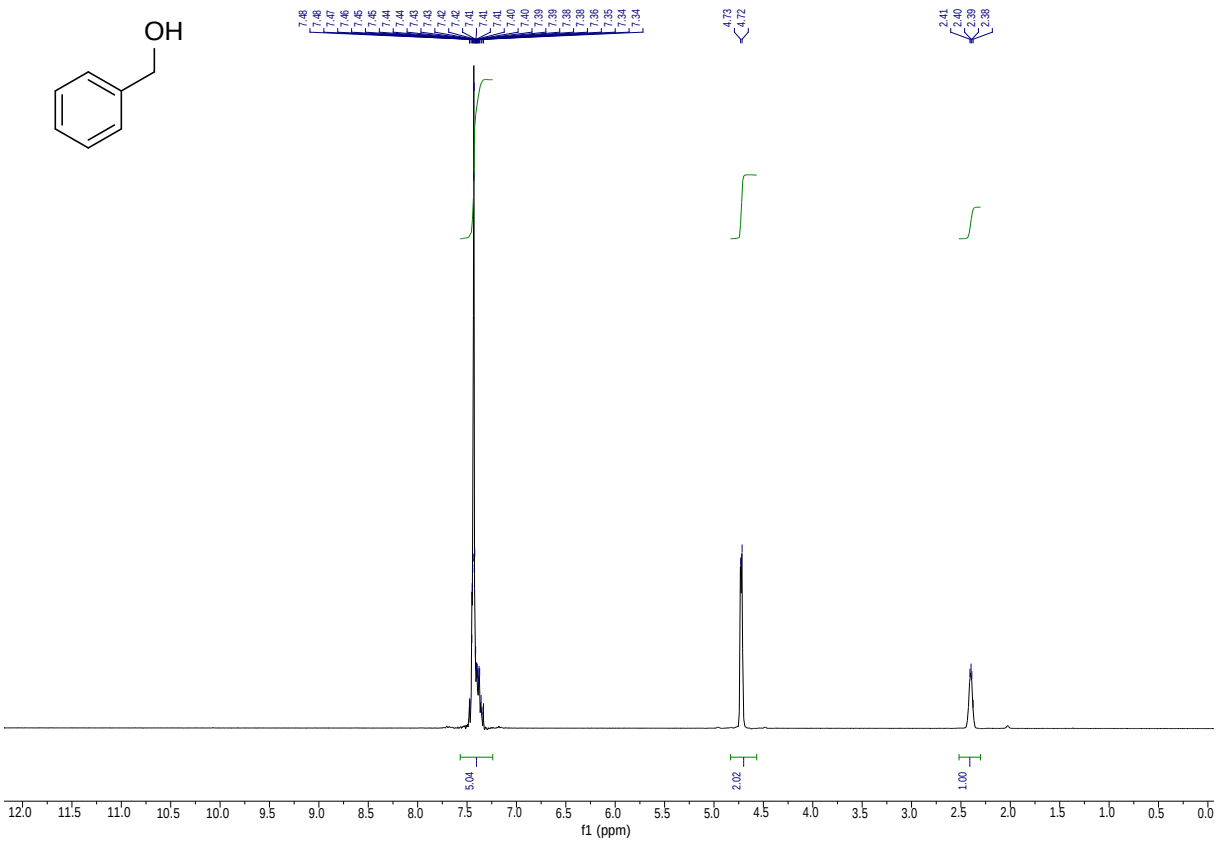
$Ru(NNN_{L3})(PPh_3)Cl_2$ (3)

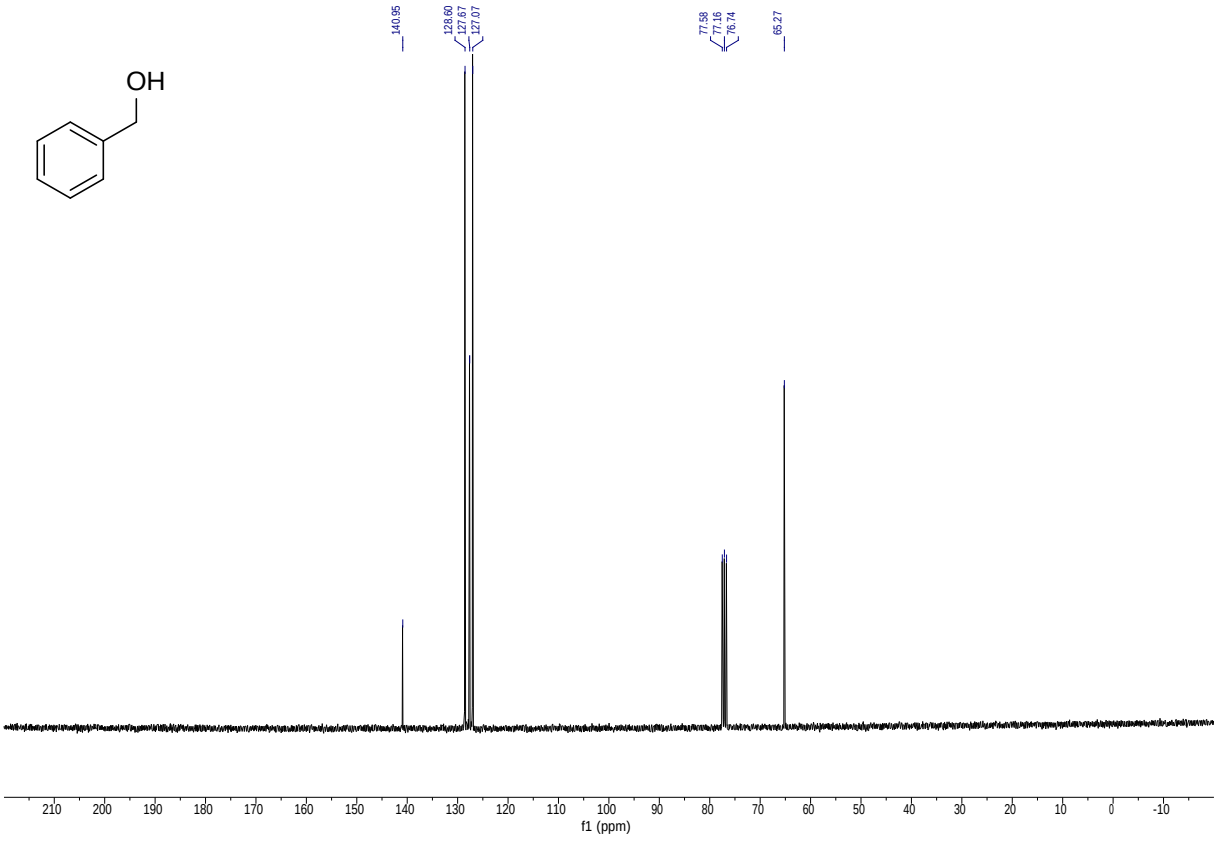


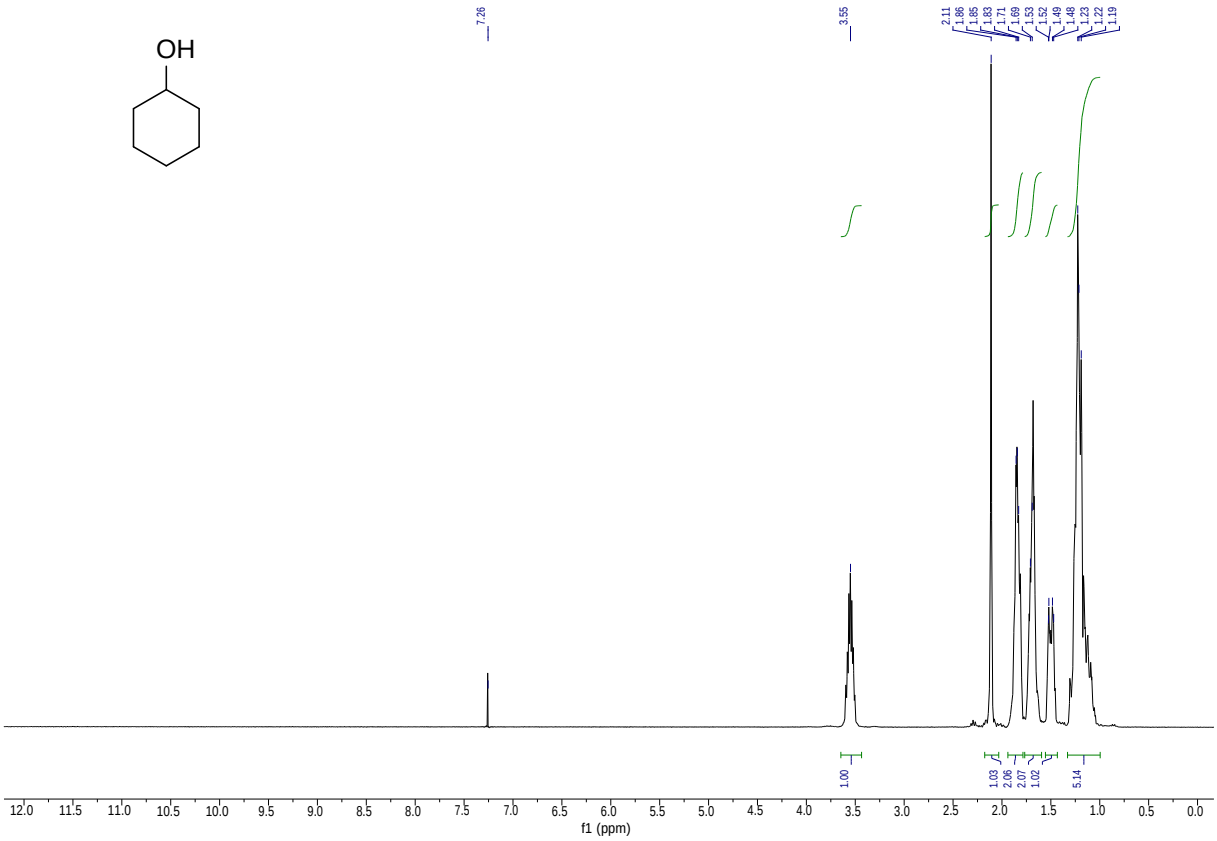
2. ^{1}H-^{13}C NMR spectra hydrogenation products

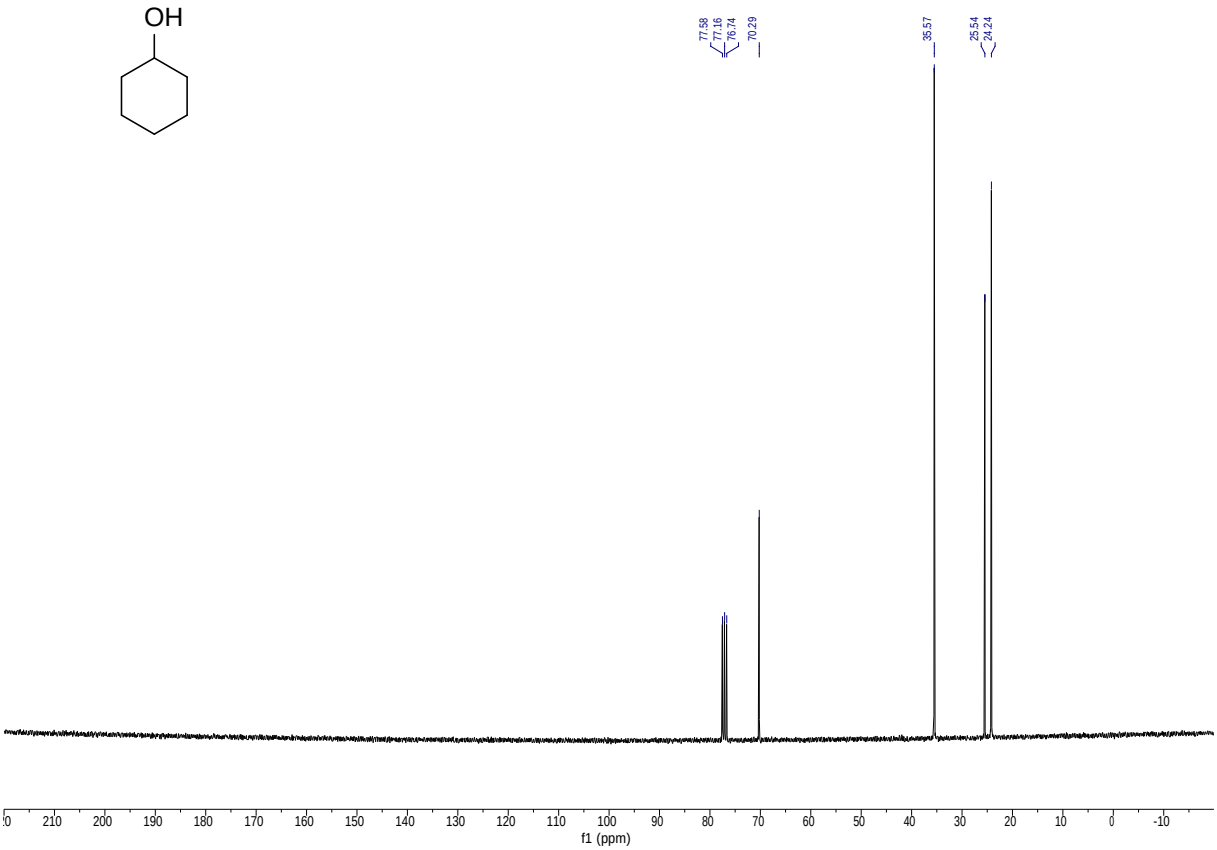


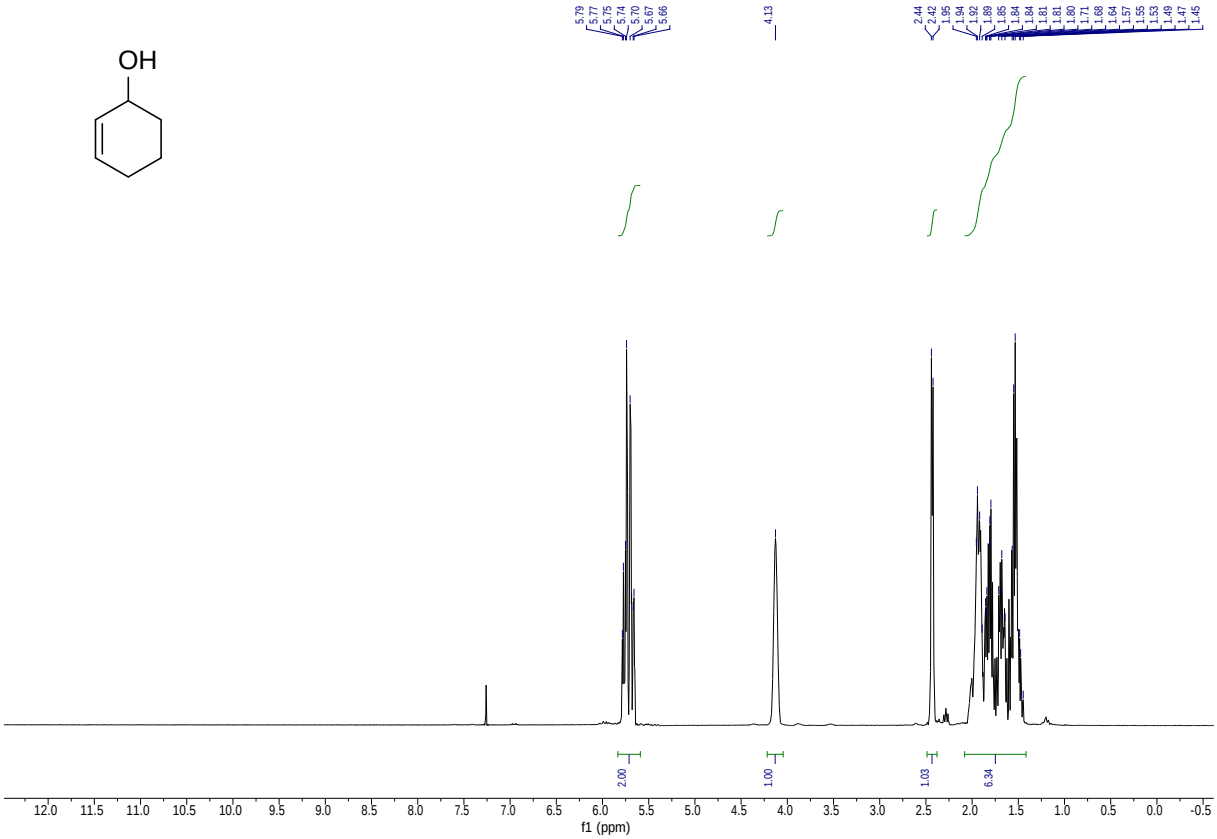


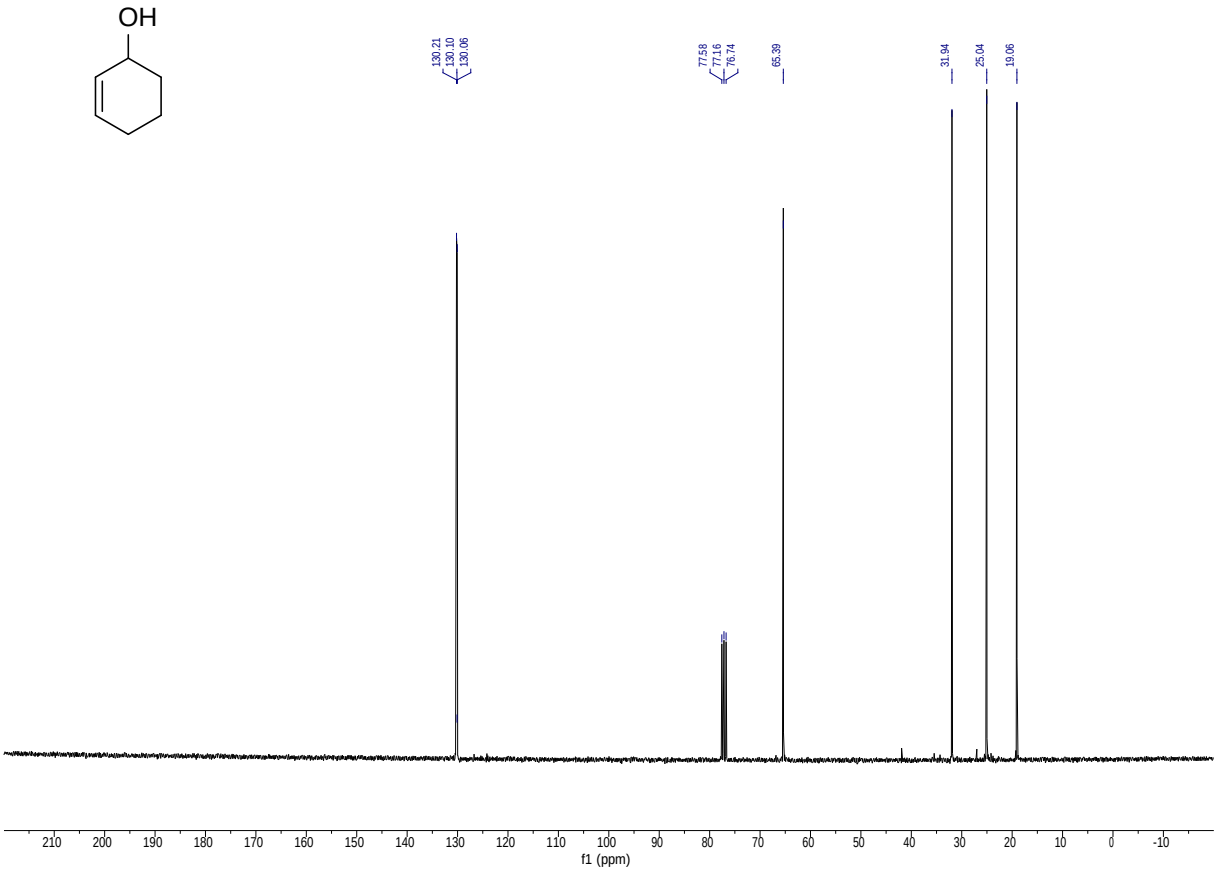

OH
7.48
7.48
7.47
7.46
7.45
7.45
7.44
7.44
7.43
7.43
7.42
7.42
7.41
7.41
7.41
7.40
7.40
7.39
7.39
7.38
7.38
7.36
7.35
7.34
7.34
4.73
4.72
2.41
2.40
2.39
2.38
5.04
2.02
1.00
f1 (ppm)

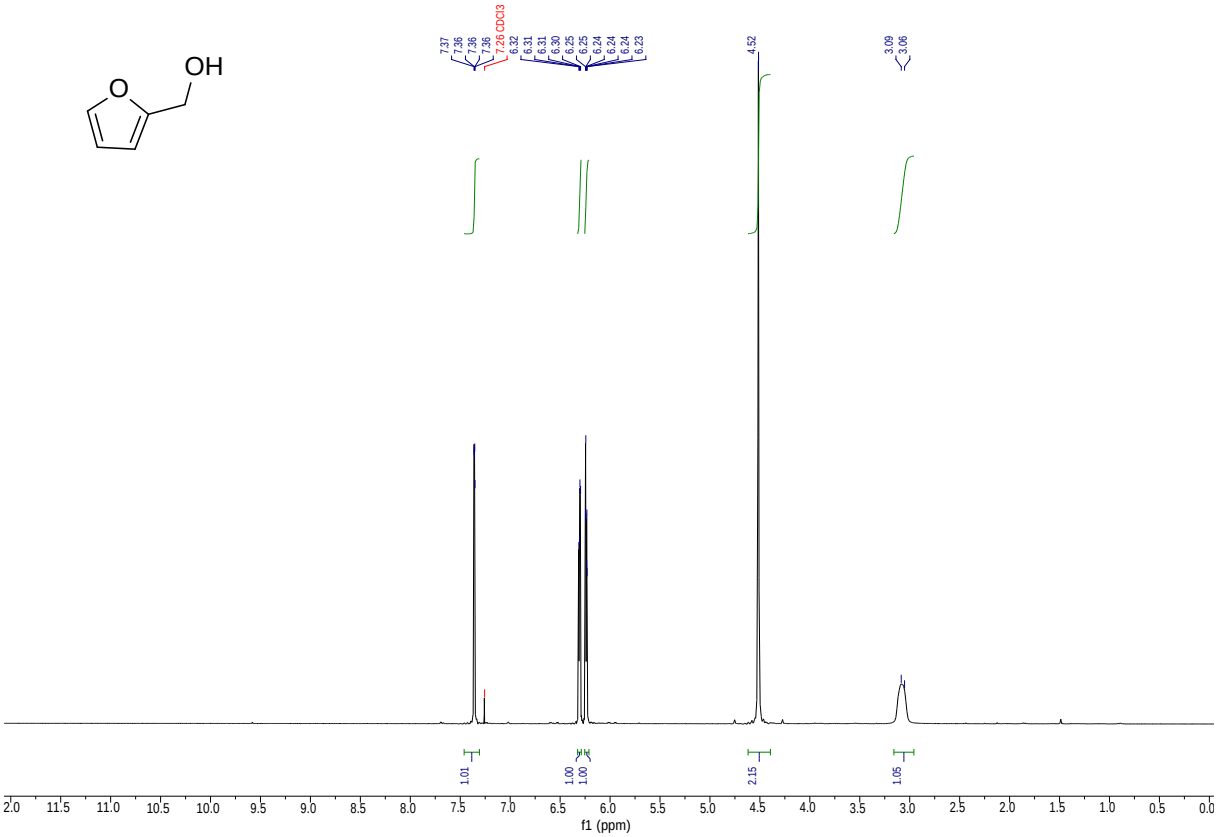

OH
140.95
128.60
127.67
127.07
77.58
77.16
76.74
65.27
f1 (ppm)

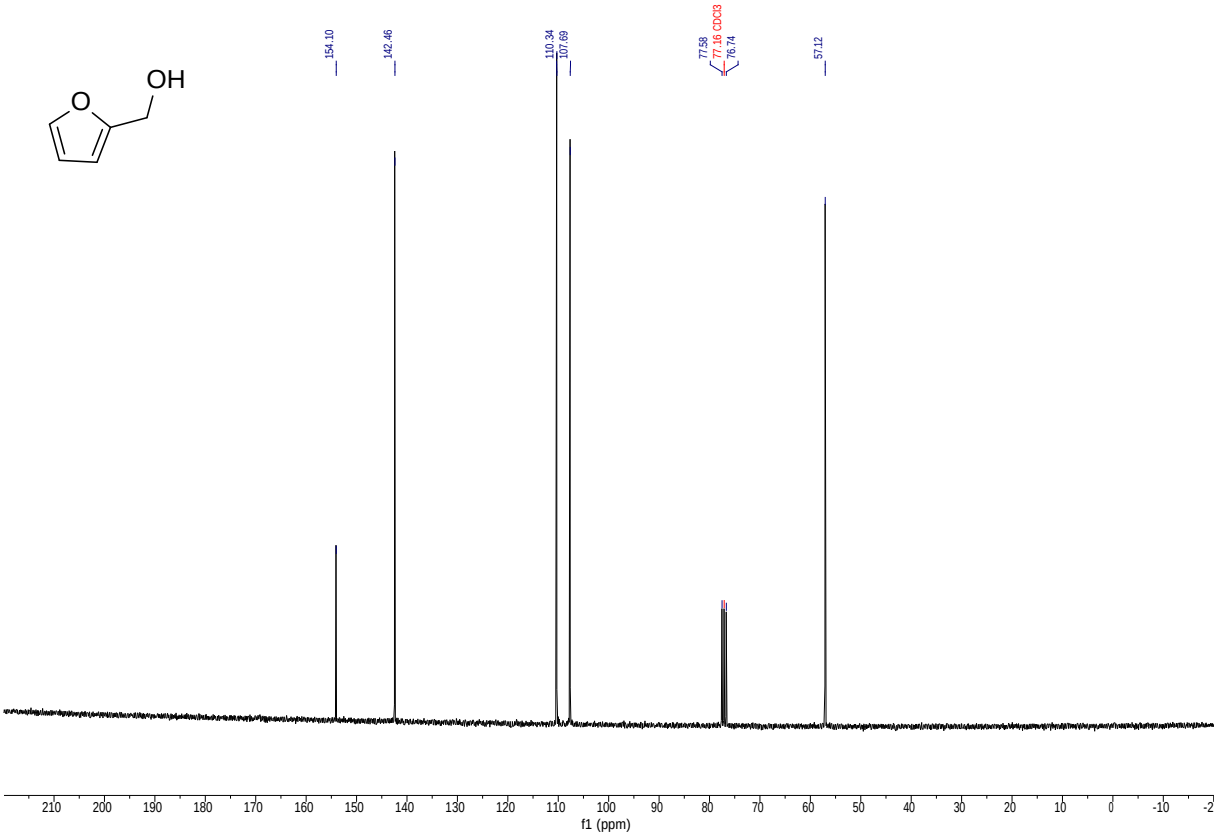

OH
7.26
3.55
2.11
1.86
1.85
1.83
1.71
1.69
1.53
1.52
1.49
1.48
1.23
1.22
1.19
1.00
1.03
2.06
2.07
1.02
5.14
f1 (ppm)

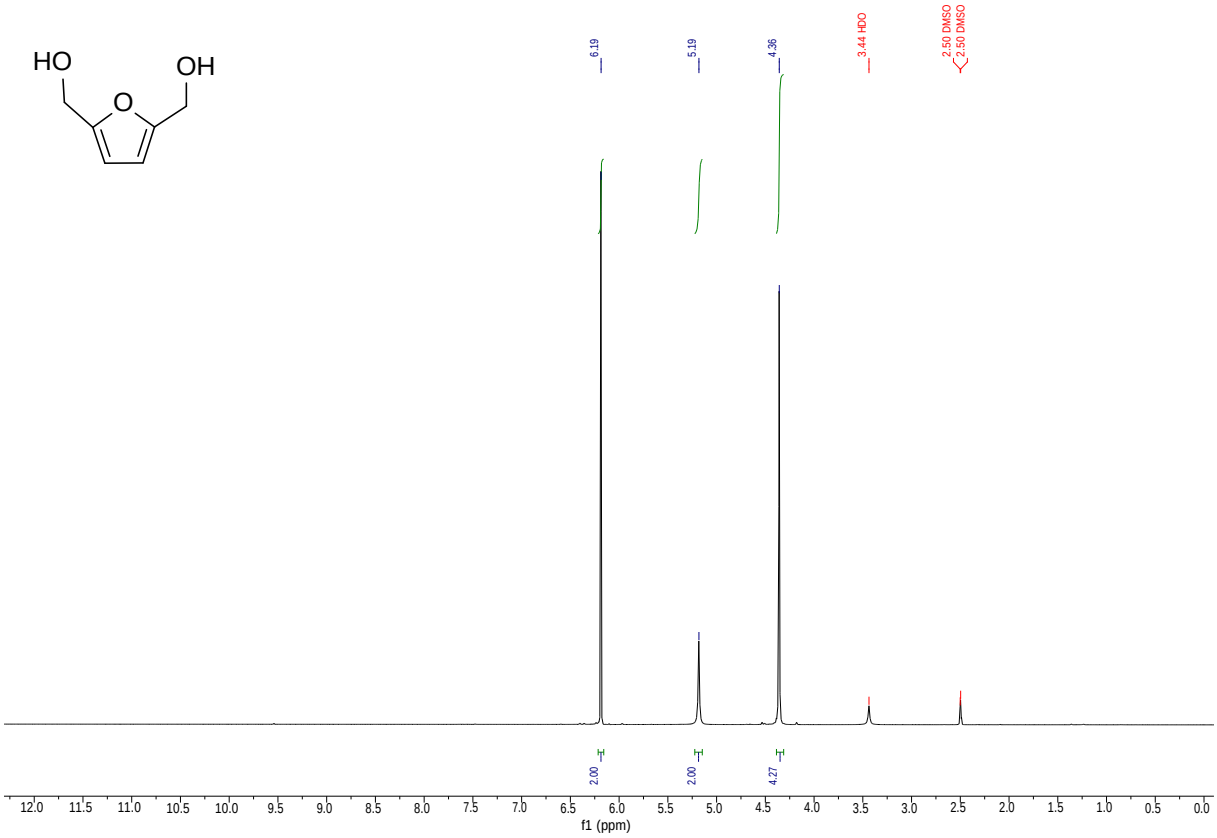

OH
77.58
77.16
76.74
70.29
35.57
25.54
24.24
f1 (ppm)

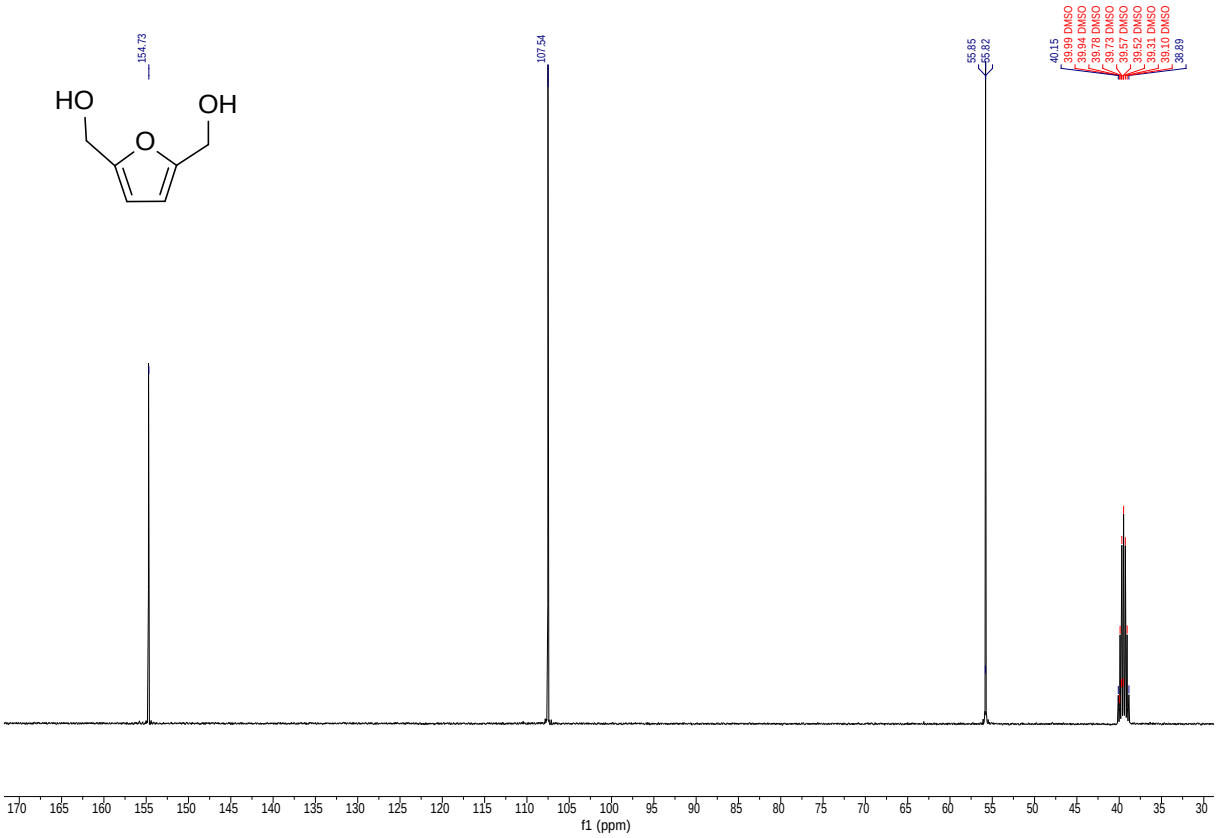

OH
5.79
5.77
5.75
5.74
5.70
5.67
5.66
4.13
2.44
2.42
1.95
1.94
1.92
1.89
1.85
1.84
1.84
1.81
1.81
1.80
1.71
1.68
1.64
1.57
1.55
1.53
1.49
1.47
1.45
2.00
1.00
1.03
6.34
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

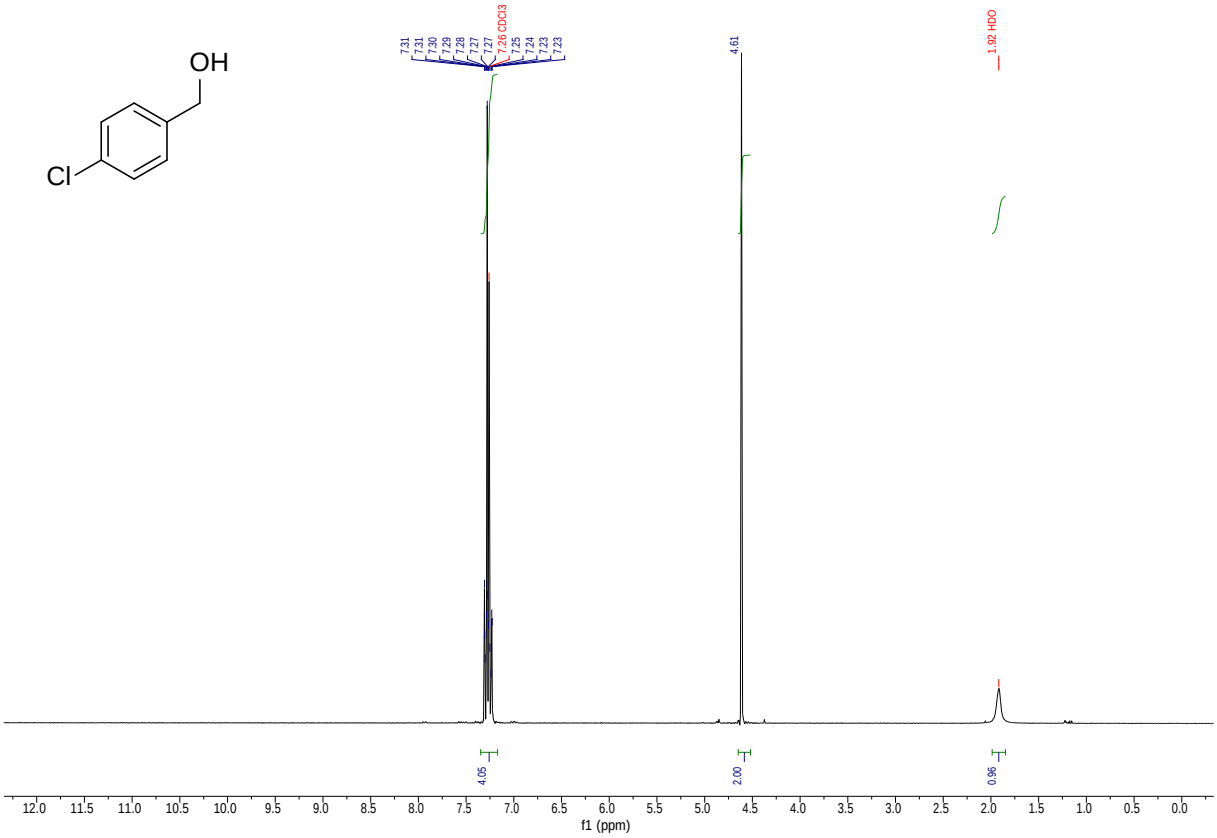

OH
130.21
130.10
130.06
77.58
77.16
76.74
65.39
31.94
25.04
19.06
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

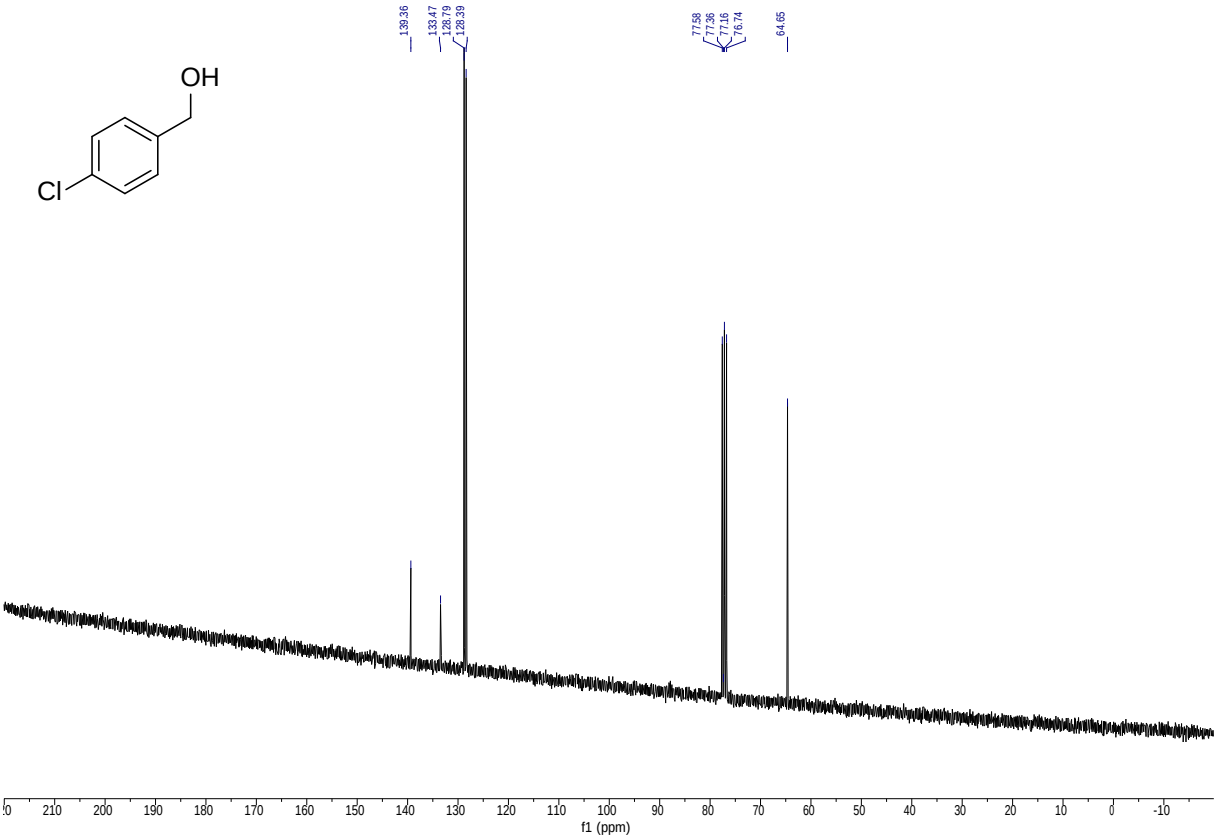

OH
O
7.37
7.36
7.36
7.36
7.26 CDCl3
6.32
6.31
6.31
6.30
6.25
6.24
6.24
6.24
6.23
4.52
3.09
3.06
1.01
1.00
1.00
2.15
1.05
f1 (ppm)

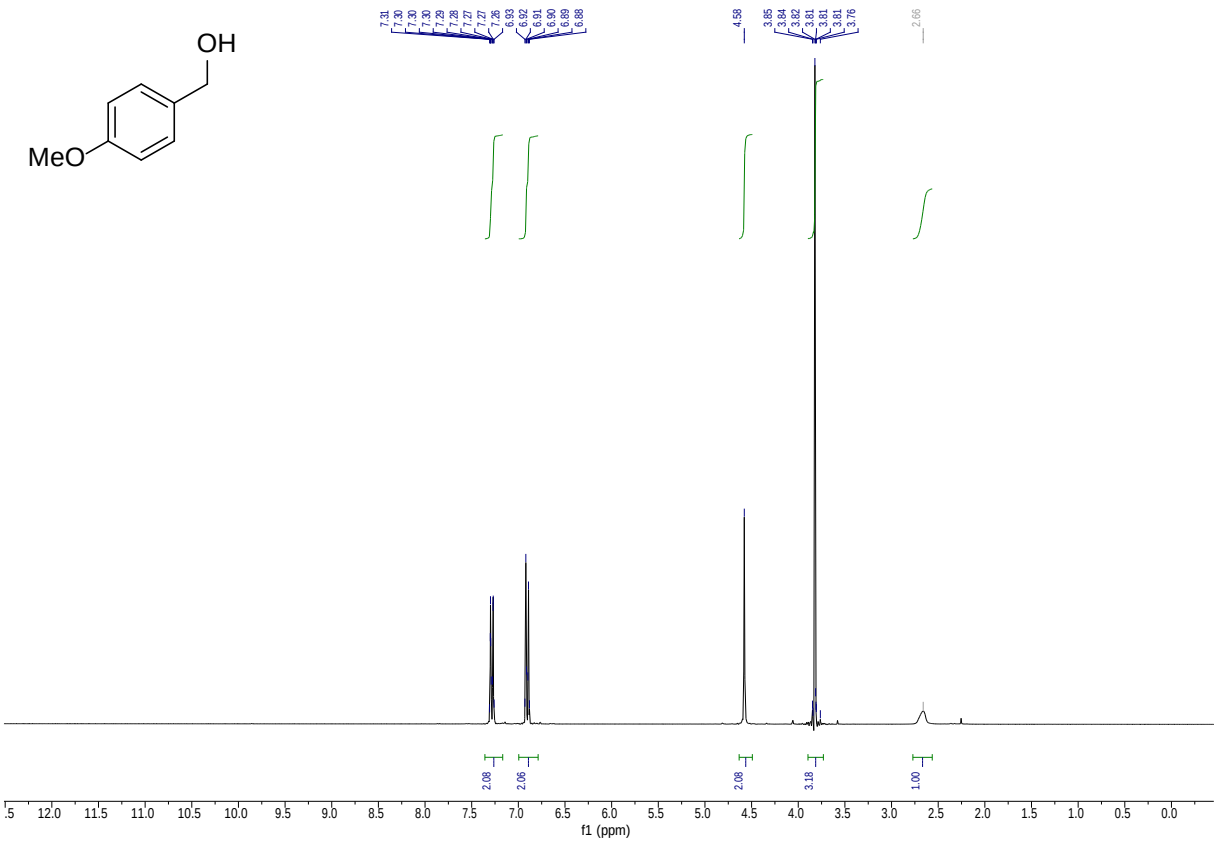

OH
O
154.10
142.46
110.34
107.69
77.58
77.16 CDCl3
76.74
57.12
f1 (ppm)

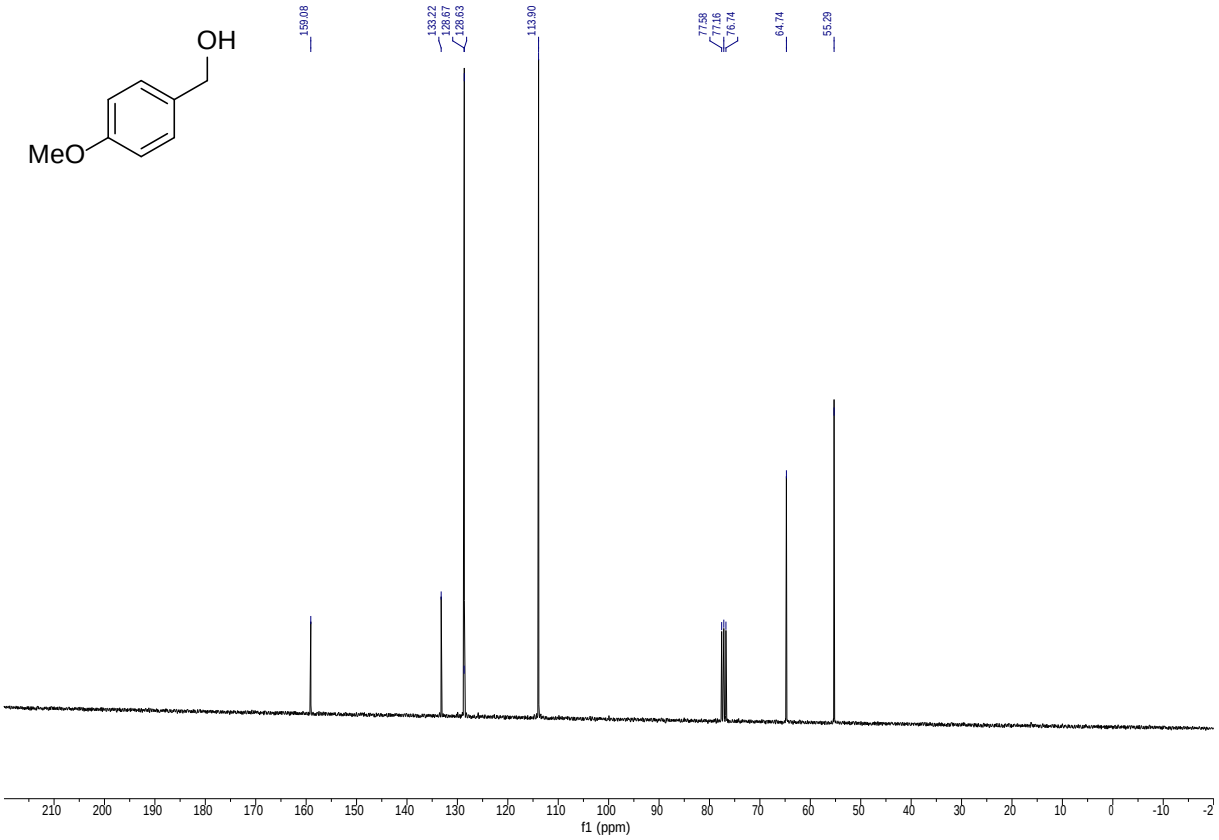

HO
OH
O
6.19
5.19
4.36
3.44 HDO
2.50 DMSO
2.50 DMSO
2.00
2.00
4.27
f1 (ppm)

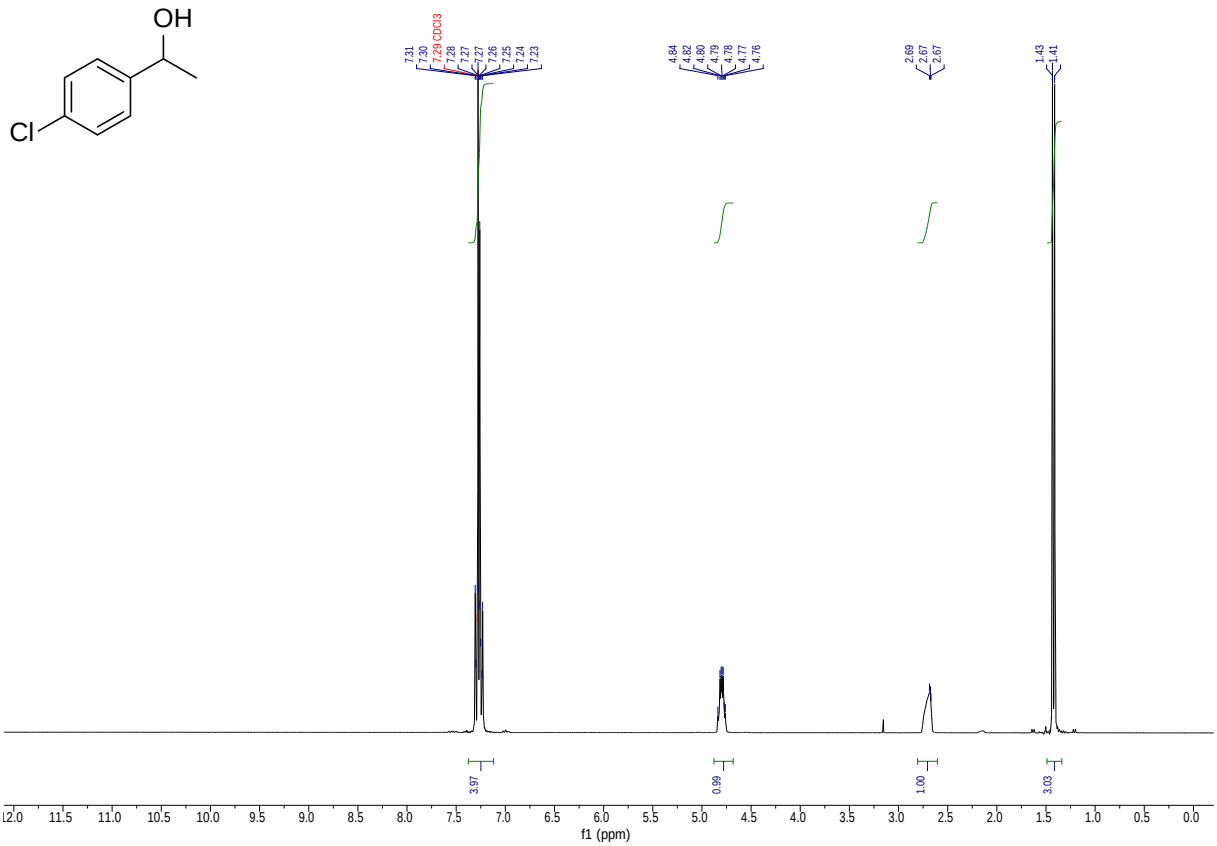

HO
OH
O
154.73
107.54
55.85
55.82
40.15
39.99 DMSO
39.94 DMSO
39.78 DMSO
39.73 DMSO
39.57 DMSO
39.52 DMSO
39.31 DMSO
39.10 DMSO
38.89
f1 (ppm)

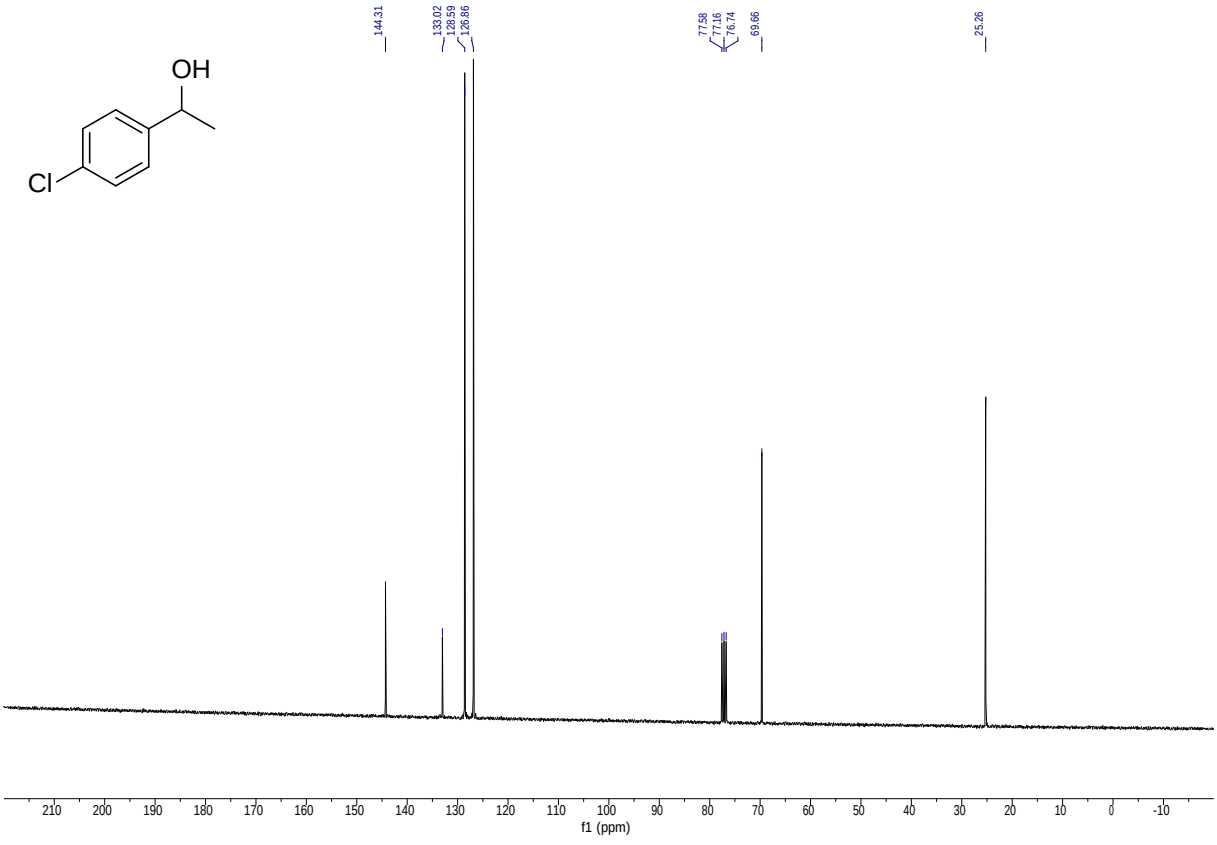

OH
Cl
7.31
7.31
7.30
7.29
7.28
7.27
7.27
7.26 CDCl3
7.25
7.24
7.23
7.23
4.61
1.92 HDO
4.05
2.00
0.96
f1 (ppm)

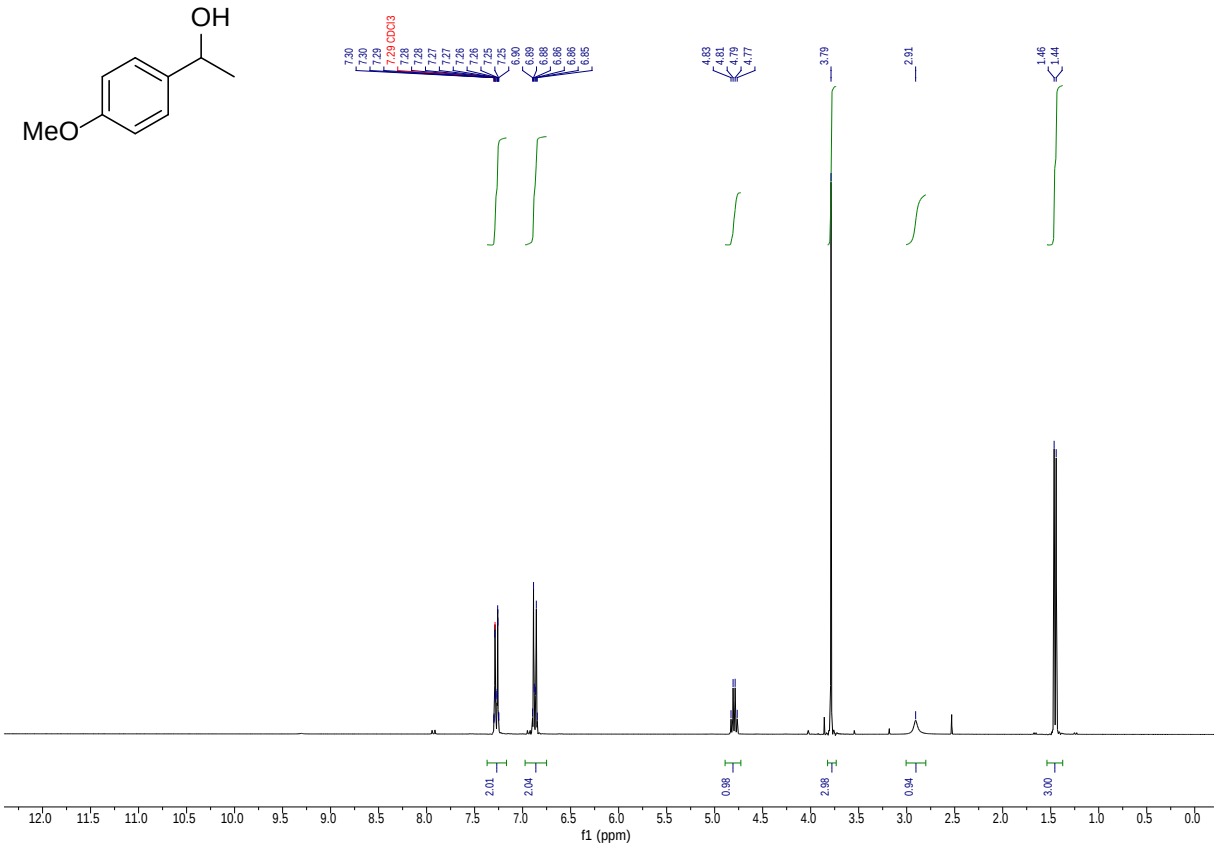

OH
Cl
139.36
133.47
128.79
128.39
77.58
77.36
77.16
76.74
64.65
f1 (ppm)

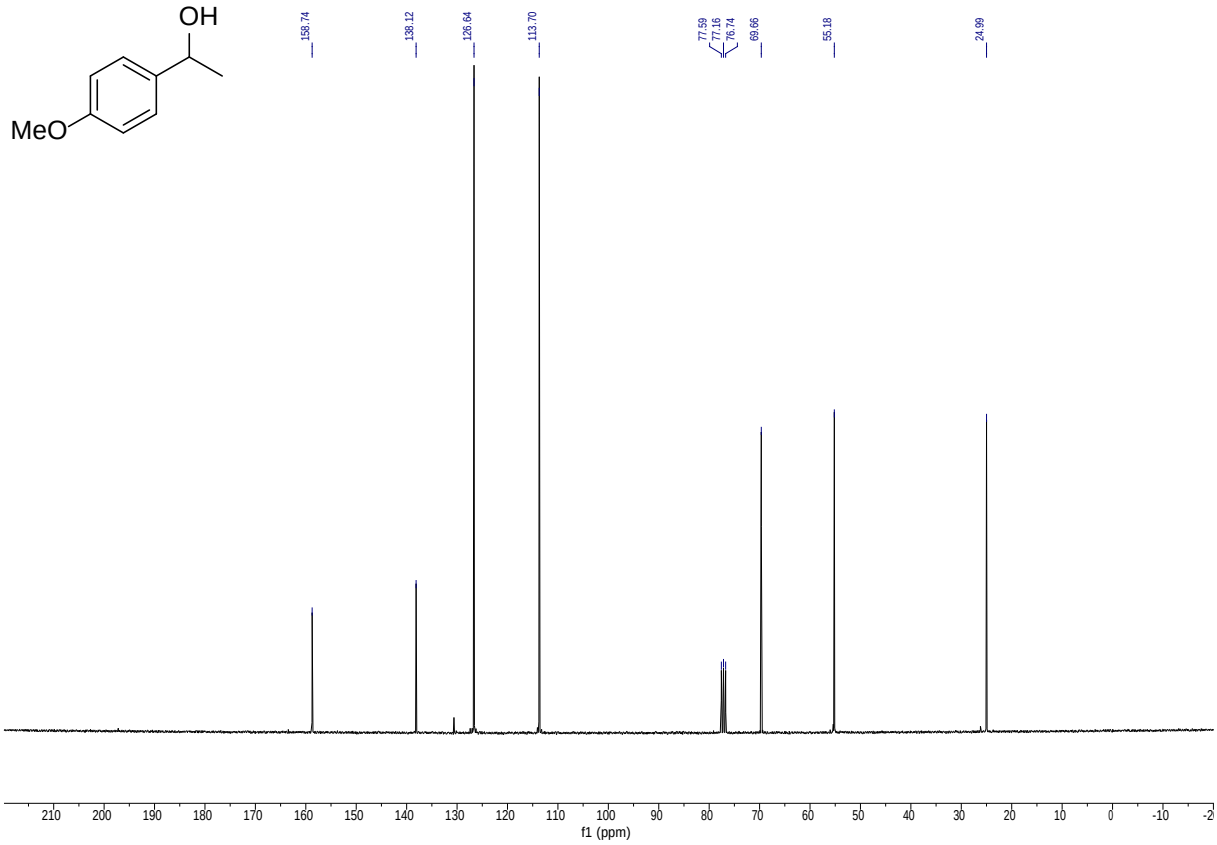

OH
MeO
7.31
7.30
7.30
7.30
7.29
7.28
7.27
7.27
7.26
6.93
6.92
6.91
6.90
6.89
6.88
4.58
3.85
3.84
3.82
3.81
3.81
3.81
3.76
2.66
2.08
2.06
2.08
3.18
1.00
f1 (ppm)

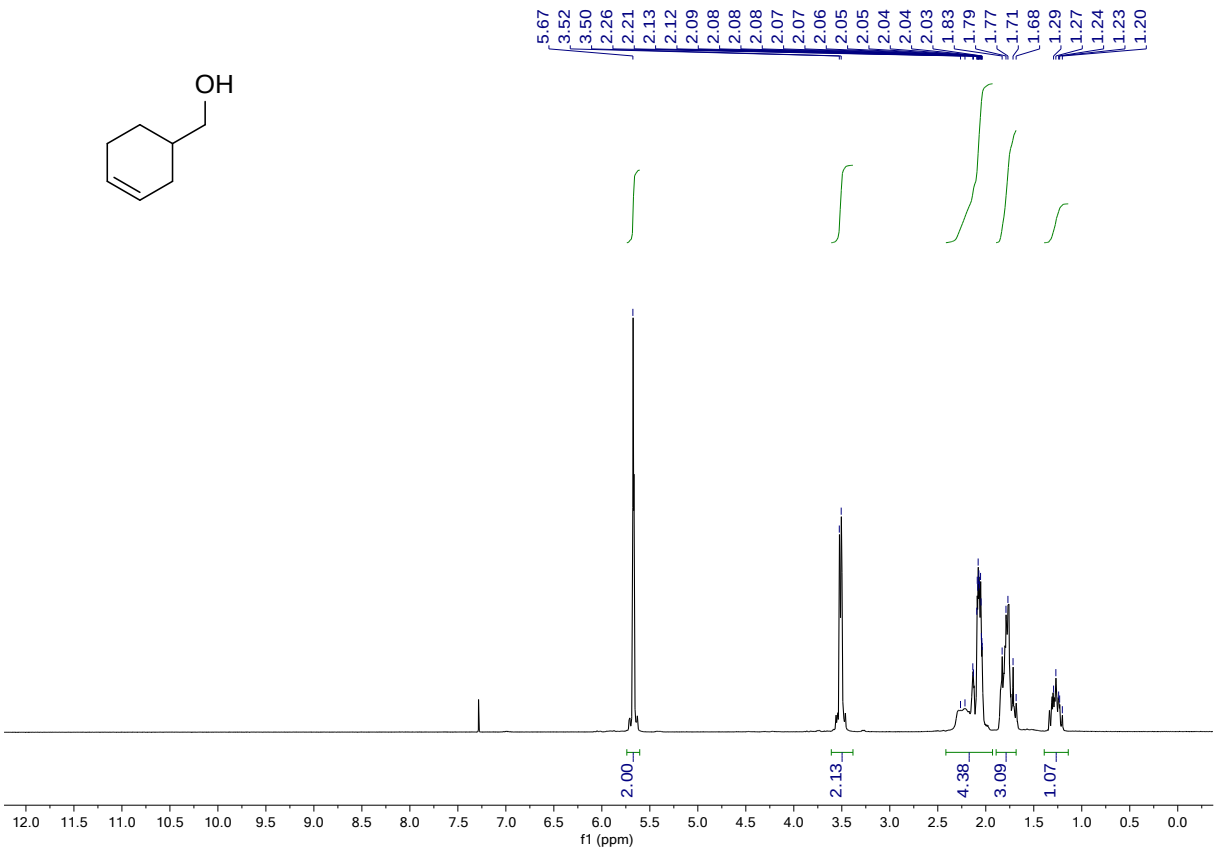

OH
MeO
159.08
133.22
128.67
128.63
113.90
77.58
77.16
76.74
64.74
55.29
f1 (ppm)

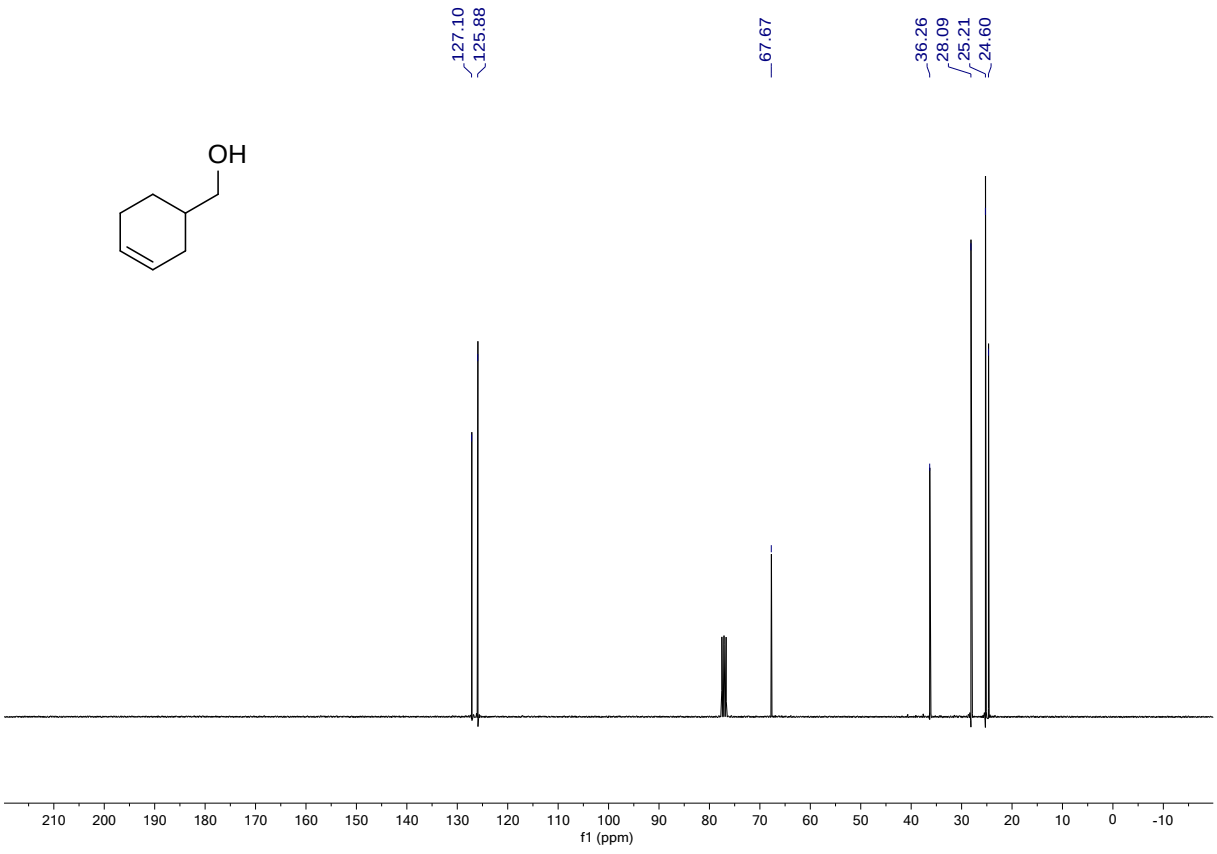

OH
Cl
7.31
7.30
7.29 CDCl3
7.28
7.27
7.27
7.26
7.25
7.24
7.23
4.84
4.82
4.80
4.79
4.78
4.77
4.76
2.69
2.67
2.67
1.43
1.41
3.97
0.99
1.00
3.03
f1 (ppm)

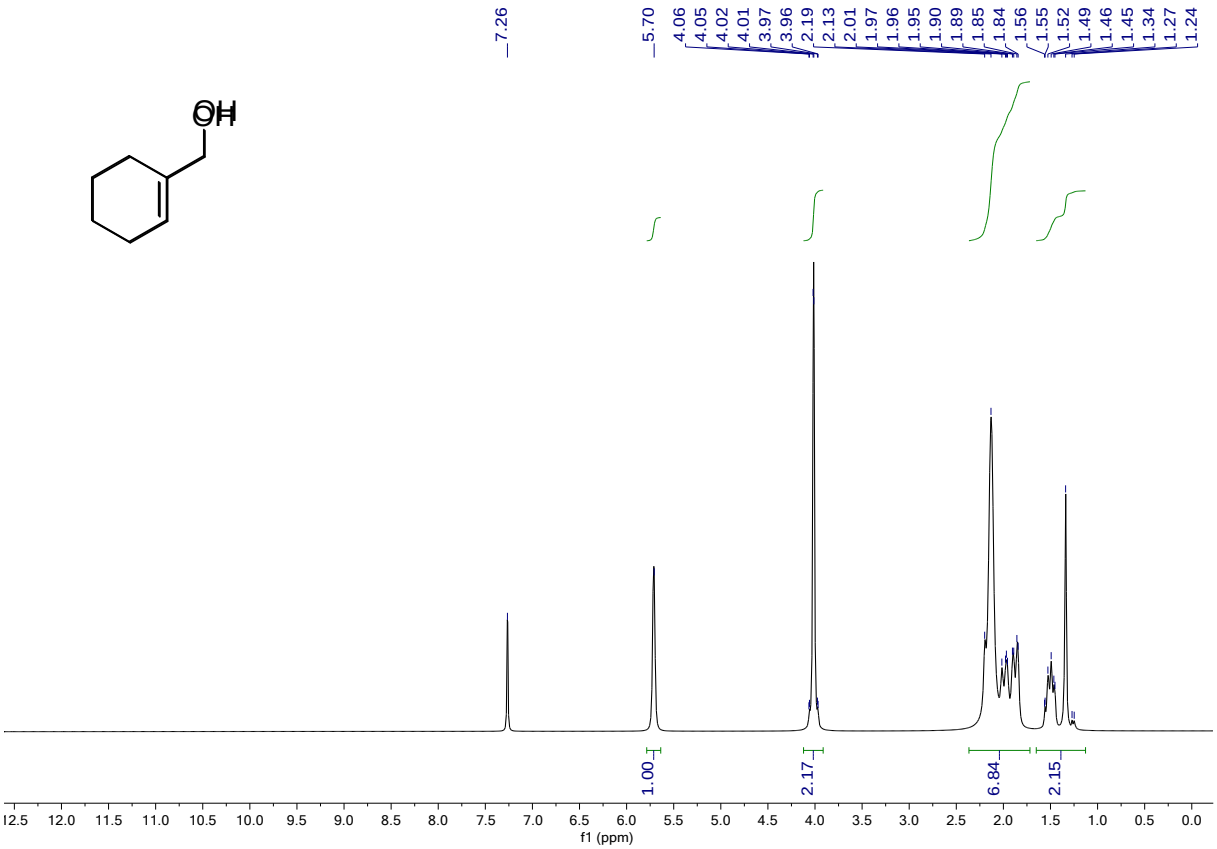

OH
Cl
144.31
133.02
128.59
126.86
77.58
77.16
76.74
69.66
25.26
f1 (ppm)

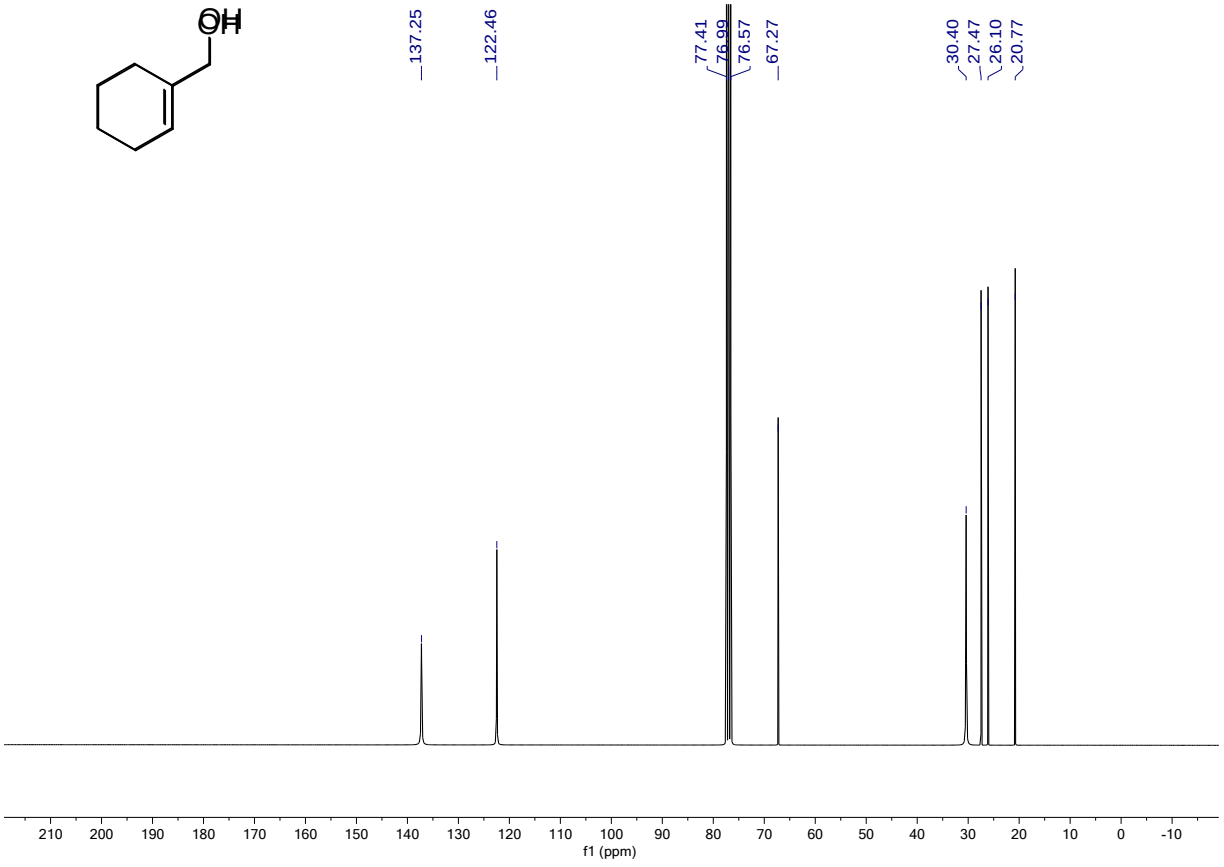

OH
MeO
7.30
7.30
7.29
7.29 CDCl3
7.28
7.28
7.27
7.27
7.26
7.26
7.25
7.25
6.90
6.89
6.88
6.86
6.86
6.85
4.83
4.81
4.79
4.77
3.79
2.91
1.46
1.44
2.01
2.04
0.98
2.98
0.94
3.00
f1 (ppm)


OH
MeO
158.74
138.12
126.64
113.70
77.59
77.16
76.74
69.66
55.18
24.99
f1 (ppm)


OH
5.67
3.52
3.50
2.26
2.21
2.13
2.12
2.09
2.08
2.08
2.08
2.07
2.07
2.06
2.05
2.05
2.04
2.04
2.03
1.83
1.79
1.77
1.71
1.68
1.29
1.27
1.24
1.23
1.20
2.00
2.13
4.38
3.09
1.07
f1 (ppm)


OH
127.10
125.88
67.67
36.26
28.09
25.21
24.60
f1 (ppm)


7.26
5.70
4.06
4.05
4.02
4.01
3.97
3.96
2.19
2.13
2.01
1.97
1.96
1.95
1.90
1.89
1.85
1.84
1.56
1.55
1.52
1.49
1.46
1.45
1.34
1.27
1.24
OH
1.00
2.17
6.84
2.15
f1 (ppm)


OH
137.25
122.46
77.41
76.99
76.57
67.27
30.40
27.47
26.10
20.77
f1 (ppm)

3. Crystallographic data

$Ru(NNN_{L3})(PPh_3)Cl_2$ (3)

Chemical formula	$C_{34}H_{32}Cl_2N_5PRu$
Formula weight	713.58
Crystal color & shape	brown needle
Crystal size	0.16 x 0.05 x 0.03
Crystal system	triclinic
Space group	$P\bar{1}$
a (Å)	9.8760(3)
b (Å)	10.6624(4)
c (Å)	15.3841(5)
$a(^o)$	78.8256(14)
$\beta(^o)$	80.6086(13)
$\gamma(^o)$	81.4425(14)
V ($Å^3$)	1556.43(9)
Z	2
T (K)	150(2)
D_c ($g \cdot cm^{-3}$)	1.523
μ (mm^{-1})	6.400
Reflections collected	21508
Independent reflections	5494 [R_{int} = 0.03]
Reflections observed [$I>2\sigma(I)$]	5124
Parameters	392
Final *R* indices [$I>2\sigma(I)$]	R_1 = 0.0237
	wR_2 = 0.0588
R indices (all data)	R_1 = 0.0262
	wR_2 = 0.0604
Goodness-of-fit on F^2	1.042
Largest diff. peak and hole ($e \cdot Å^{-3}$)	0.50 and -0.34

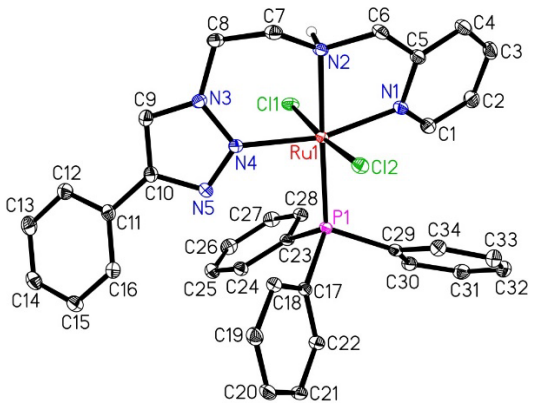


Fig. 1. Molecular structure of **Ru(NNNL$_3$)(PPh$_3$)Cl$_2$ (3)** with atom labelling and displacement ellipsoids drawn at the 30% probability level. Hydrogen atoms except the N-bound are omitted for clarity. Selected bond lengths (Å) and angles (°):Cl1-Ru1 2.3958(5), Cl2-Ru1 2.4340(5), N1-Ru1 2.0972(17), N2-Ru1 2.1296(16), N4-Ru1 2.0759(16), P1-Ru1 2.3099(5); N4-Ru1-N1 165.11(7), N4-Ru1-N2 90.39(6), N1-Ru1-N2 77.24(7), N4-Ru1-P1 90.80(5), N1-Ru1-P1 101.69(5), N2-Ru1-P1 178.58(5), N4-Ru1-Cl1 84.18(5), N1-Ru1-Cl1 86.63(5), N2-Ru1-Cl1 85.73(5), P1-Ru1-Cl1 95.165(17), N4-Ru1-Cl2 96.35(5), N1-Ru1-Cl2 91.63(5), N2-Ru1-Cl2 88.44(5), P1-Ru1-Cl2 90.657(17), Cl1-Ru1-Cl2 174.149(16).

4. DFT cartesian coordinates

Dihydride-is1-EDF2

C	-3.431000000	-2.983000000	0.339000000
H	-4.328000000	-3.512000000	0.674000000
C	-2.554000000	-3.939000000	-0.474000000
H	-2.617000000	-4.952000000	-0.053000000
H	-2.929000000	-3.993000000	-1.499000000
N	-1.143000000	-3.511000000	-0.533000000
C	-0.307000000	-4.160000000	0.479000000
H	-0.493000000	-3.672000000	1.439000000
H	-0.559000000	-5.230000000	0.566000000
C	1.161000000	-4.104000000	0.114000000
H	1.291000000	-4.478000000	-0.912000000
H	1.712000000	-4.776000000	0.776000000
N	1.806000000	-2.810000000	0.219000000
N	1.204000000	-1.627000000	-0.071000000
N	2.133000000	-0.716000000	-0.141000000
C	3.347000000	-1.285000000	0.090000000
C	3.149000000	-2.626000000	0.311000000
H	3.823000000	-3.446000000	0.491000000
C	4.584000000	-0.510000000	0.057000000
C	6.952000000	0.982000000	-0.037000000
C	4.617000000	0.730000000	-0.590000000
C	5.752000000	-0.990000000	0.658000000
C	6.927000000	-0.252000000	0.608000000
C	5.792000000	1.469000000	-0.633000000
H	3.714000000	1.096000000	-1.065000000
H	5.735000000	-1.939000000	1.186000000
H	7.824000000	-0.636000000	1.082000000
H	5.802000000	2.427000000	-1.141000000
H	7.869000000	1.560000000	-0.072000000
H	-0.780000000	-3.731000000	-1.456000000
Ru	-0.806000000	-1.298000000	-0.388000000
H	-0.457000000	-1.295000000	-2.062000000
P	-0.518000000	0.921000000	0.102000000
C	0.195000000	2.082000000	-1.159000000
C	1.294000000	3.713000000	-3.159000000
C	0.513000000	1.554000000	-2.412000000
C	0.446000000	3.440000000	-0.918000000
C	0.987000000	4.250000000	-1.911000000
C	1.058000000	2.365000000	-3.406000000
H	0.328000000	0.494000000	-2.580000000
H	0.229000000	3.866000000	0.056000000
H	1.174000000	5.299000000	-1.708000000
H	1.301000000	1.938000000	-4.374000000
H	1.719000000	4.345000000	-3.932000000
C	-2.116000000	1.761000000	0.582000000
C	-4.566000000	2.895000000	1.387000000
C	-2.560000000	2.974000000	0.047000000
C	-2.946000000	1.111000000	1.506000000
C	-4.149000000	1.675000000	1.912000000
C	-3.770000000	3.535000000	0.446000000
H	-1.967000000	3.490000000	-0.698000000
H	-2.652000000	0.134000000	1.877000000
H	-4.768000000	1.152000000	2.634000000
H	-4.089000000	4.479000000	0.014000000
H	-5.507000000	3.334000000	1.701000000
C	0.533000000	1.283000000	1.600000000
C	2.092000000	1.719000000	3.901000000
C	1.758000000	1.950000000	1.524000000
C	0.117000000	0.817000000	2.852000000
C	0.883000000	1.038000000	3.990000000
C	2.530000000	2.167000000	2.661000000
H	2.127000000	2.292000000	0.567000000
H	-0.803000000	0.253000000	2.933000000
H	0.532000000	0.670000000	4.950000000
H	3.481000000	2.681000000	2.570000000
H	2.693000000	1.889000000	4.789000000
H	-1.205000000	-1.441000000	1.278000000
N	-2.824000000	-1.010000000	-0.944000000
C	-5.487000000	-0.536000000	-1.685000000
C	-3.157000000	-0.024000000	-1.804000000
C	-3.823000000	-1.800000000	-0.484000000
C	-5.153000000	-1.575000000	-0.832000000
C	-4.456000000	0.247000000	-2.192000000
H	-2.324000000	0.549000000	-2.187000000
H	-5.917000000	-2.230000000	-0.428000000
H	-4.646000000	1.063000000	-2.878000000
H	-6.520000000	-0.349000000	-1.957000000
H	-2.851000000	-2.643000000	1.207000000

Dihydride-is2-EDF2

C	2.839000000	-0.935000000	-2.482000000
H	3.754000000	-0.702000000	-3.035000000
C	1.652000000	-0.781000000	-3.438000000
H	1.503000000	0.286000000	-3.626000000
H	1.875000000	-1.254000000	-4.407000000
N	0.420000000	-1.321000000	-2.868000000
C	-0.798000000	-0.845000000	-3.507000000
H	-0.860000000	0.241000000	-3.385000000
H	-0.806000000	-1.058000000	-4.589000000
C	-2.023000000	-1.513000000	-2.888000000
H	-1.815000000	-2.573000000	-2.709000000
H	-2.873000000	-1.425000000	-3.567000000
N	-2.450000000	-0.927000000	-1.633000000
N	-1.656000000	-0.886000000	-0.534000000
N	-2.339000000	-0.337000000	0.431000000
C	-3.583000000	-0.018000000	-0.020000000
C	-3.662000000	-0.397000000	-1.341000000
H	-4.447000000	-0.338000000	-2.076000000
C	-4.563000000	0.634000000	0.846000000
C	-6.407000000	1.912000000	2.525000000
C	-4.210000000	0.981000000	2.155000000
C	-5.851000000	0.936000000	0.391000000
C	-6.764000000	1.569000000	1.224000000
C	-5.127000000	1.614000000	2.984000000
H	-3.213000000	0.749000000	2.511000000
H	-6.146000000	0.672000000	-0.620000000
H	-7.760000000	1.795000000	0.855000000
H	-4.836000000	1.878000000	3.996000000
H	-7.121000000	2.406000000	3.175000000
H	0.442000000	-2.334000000	-2.945000000
Ru	0.282000000	-1.585000000	-0.551000000
H	-0.373000000	-3.051000000	-0.961000000
P	1.011000000	0.483000000	0.415000000
C	0.312000000	0.959000000	2.073000000
C	-0.634000000	1.596000000	4.633000000
C	-0.303000000	-0.013000000	2.863000000
C	0.450000000	2.254000000	2.584000000
C	-0.024000000	2.573000000	3.851000000
C	-0.769000000	0.304000000	4.137000000
H	-0.423000000	-1.011000000	2.455000000
H	0.928000000	3.025000000	1.989000000
H	0.089000000	3.584000000	4.230000000
H	-1.243000000	-0.465000000	4.739000000
H	-1.000000000	1.842000000	5.625000000
C	2.805000000	0.759000000	0.811000000
C	5.499000000	0.988000000	1.565000000
C	3.525000000	-0.358000000	1.249000000
C	3.458000000	1.996000000	0.766000000
C	4.795000000	2.108000000	1.134000000
C	4.858000000	-0.245000000	1.627000000
H	3.023000000	-1.318000000	1.294000000
H	2.921000000	2.880000000	0.440000000
H	5.285000000	3.075000000	1.090000000
H	5.397000000	-1.123000000	1.969000000
H	6.542000000	1.078000000	1.853000000
C	0.562000000	1.961000000	-0.611000000
C	-0.324000000	3.932000000	-2.421000000
C	-0.709000000	2.538000000	-0.487000000
C	1.378000000	2.399000000	-1.663000000
C	0.945000000	3.375000000	-2.554000000
C	-1.147000000	3.509000000	-1.382000000
H	-1.364000000	2.222000000	0.317000000
H	2.373000000	1.984000000	-1.782000000
H	1.605000000	3.707000000	-3.350000000
H	-2.135000000	3.940000000	-1.260000000
H	-0.663000000	4.694000000	-3.115000000
H	0.140000000	-2.152000000	0.936000000
N	2.109000000	-2.601000000	-0.835000000
C	4.272000000	-4.283000000	-1.436000000
C	2.319000000	-3.755000000	-0.162000000
C	3.001000000	-2.264000000	-1.804000000
C	4.075000000	-3.096000000	-2.121000000
C	3.374000000	-4.609000000	-0.424000000
H	1.580000000	-3.969000000	0.597000000
H	4.761000000	-2.787000000	-2.902000000
H	3.478000000	-5.517000000	0.157000000
H	5.108000000	-4.932000000	-1.675000000
H	2.733000000	-0.189000000	-1.690000000

Dihydride-is3-EDF2

C	1.782000000	-2.063000000	1.398000000
H	2.546000000	-2.779000000	1.715000000
C	0.625000000	-2.106000000	2.397000000
H	-0.083000000	-2.887000000	2.104000000
H	1.012000000	-2.380000000	3.391000000
N	-0.103000000	-0.834000000	2.443000000
C	-1.310000000	-0.903000000	3.279000000
H	-1.613000000	-1.951000000	3.371000000
H	-1.118000000	-0.540000000	4.298000000
C	-2.480000000	-0.109000000	2.707000000
H	-2.159000000	0.910000000	2.470000000
H	-3.307000000	-0.094000000	3.420000000
N	-2.984000000	-0.683000000	1.476000000
N	-2.244000000	-0.646000000	0.348000000
N	-2.925000000	-1.214000000	-0.606000000
C	-4.126000000	-1.623000000	-0.110000000
C	-4.168000000	-1.286000000	1.227000000
H	-4.921000000	-1.401000000	1.989000000
C	-5.125000000	-2.281000000	-0.949000000
C	-7.033000000	-3.521000000	-2.583000000
C	-4.921000000	-2.382000000	-2.329000000
C	-6.297000000	-2.813000000	-0.400000000
C	-7.243000000	-3.425000000	-1.211000000
C	-5.867000000	-2.998000000	-3.137000000
H	-4.013000000	-1.968000000	-2.752000000
H	-6.469000000	-2.753000000	0.670000000
H	-8.146000000	-3.832000000	-0.769000000
H	-5.696000000	-3.066000000	-4.206000000
H	-7.772000000	-3.999000000	-3.216000000
H	0.520000000	-0.120000000	2.810000000
Ru	-0.342000000	0.253000000	0.306000000
H	-1.019000000	1.582000000	0.980000000
H	-0.701000000	0.875000000	-1.116000000
N	0.503000000	-1.562000000	-0.629000000
C	1.514000000	-3.804000000	-1.955000000
C	0.118000000	-1.868000000	-1.880000000
C	1.385000000	-2.379000000	-0.017000000
C	1.906000000	-3.502000000	-0.658000000
C	0.594000000	-2.968000000	-2.575000000
H	-0.604000000	-1.188000000	-2.313000000
H	2.617000000	-4.130000000	-0.134000000
H	0.247000000	-3.156000000	-3.584000000
H	1.916000000	-4.672000000	-2.466000000
H	2.230000000	-1.064000000	1.445000000
P	1.443000000	1.628000000	0.135000000
C	2.398000000	1.954000000	1.704000000
C	3.621000000	2.425000000	4.195000000
C	3.789000000	2.040000000	1.815000000
C	1.632000000	2.128000000	2.866000000
C	2.234000000	2.363000000	4.097000000
C	4.394000000	2.267000000	3.050000000
H	4.410000000	1.932000000	0.933000000
H	0.548000000	2.099000000	2.775000000
H	1.619000000	2.506000000	4.981000000
H	5.476000000	2.327000000	3.114000000
H	4.095000000	2.602000000	5.154000000
C	1.114000000	3.383000000	-0.380000000
C	0.607000000	6.018000000	-1.179000000
C	2.122000000	4.351000000	-0.325000000
C	-0.152000000	3.752000000	-0.837000000
C	-0.401000000	5.063000000	-1.237000000
C	1.872000000	5.659000000	-0.721000000
H	3.110000000	4.081000000	0.035000000
H	-0.927000000	2.995000000	-0.865000000
H	-1.391000000	5.336000000	-1.591000000
H	2.664000000	6.400000000	-0.670000000
H	0.410000000	7.040000000	-1.487000000
C	2.760000000	1.166000000	-1.087000000
C	4.555000000	0.270000000	-3.062000000
C	3.704000000	0.170000000	-0.809000000
C	2.728000000	1.693000000	-2.383000000
C	3.614000000	1.250000000	-3.360000000
C	4.597000000	-0.268000000	-1.781000000
H	3.759000000	-0.264000000	0.183000000
H	2.002000000	2.458000000	-2.631000000
H	3.569000000	1.677000000	-4.356000000
H	5.327000000	-1.033000000	-1.535000000
H	5.250000000	-0.072000000	-3.823000000

Dihydride-is4-EDF2

C	-2.874000000	3.378000000	-0.287000000
H	-3.541000000	4.167000000	-0.648000000
C	-2.139000000	3.905000000	0.950000000
H	-1.356000000	4.600000000	0.630000000
H	-2.838000000	4.481000000	1.573000000
N	-1.500000000	2.839000000	1.741000000
C	-0.431000000	3.347000000	2.607000000
H	0.164000000	4.062000000	2.032000000
H	-0.834000000	3.889000000	3.476000000
C	0.494000000	2.243000000	3.114000000
H	-0.100000000	1.387000000	3.449000000
H	1.105000000	2.619000000	3.937000000
N	1.405000000	1.770000000	2.091000000
N	0.940000000	1.095000000	1.020000000
N	1.955000000	0.810000000	0.251000000
C	3.095000000	1.301000000	0.815000000
C	2.748000000	1.924000000	1.995000000
H	3.320000000	2.432000000	2.753000000
C	4.401000000	1.139000000	0.180000000
C	6.889000000	0.817000000	-1.069000000
C	4.513000000	0.407000000	-1.008000000
C	5.555000000	1.706000000	0.731000000
C	6.787000000	1.546000000	0.112000000
C	5.746000000	0.249000000	-1.625000000
H	3.619000000	-0.033000000	-1.433000000
H	5.490000000	2.282000000	1.649000000
H	7.672000000	1.993000000	0.554000000
H	5.815000000	-0.322000000	-2.545000000
H	7.852000000	0.693000000	-1.553000000
H	-2.205000000	2.381000000	2.313000000
Ru	-1.178000000	0.807000000	0.749000000
H	-1.395000000	0.150000000	2.230000000
N	-1.092000000	1.951000000	-1.163000000
C	-1.025000000	3.332000000	-3.593000000
C	-0.193000000	1.652000000	-2.114000000
C	-1.941000000	2.977000000	-1.391000000
C	-1.929000000	3.676000000	-2.597000000
C	-0.129000000	2.303000000	-3.336000000
H	0.505000000	0.864000000	-1.868000000
H	-2.634000000	4.487000000	-2.744000000
H	0.610000000	1.996000000	-4.066000000
H	-1.015000000	3.862000000	-4.539000000
H	-3.479000000	2.513000000	0.006000000
P	-1.153000000	-1.333000000	0.068000000
H	-2.796000000	0.711000000	0.647000000
C	-2.636000000	-2.386000000	0.463000000
C	-4.821000000	-3.988000000	1.183000000
C	-2.843000000	-3.628000000	-0.146000000
C	-3.538000000	-1.960000000	1.439000000
C	-4.621000000	-2.758000000	1.799000000
C	-3.928000000	-4.422000000	0.207000000
H	-2.156000000	-3.979000000	-0.909000000
H	-3.374000000	-0.992000000	1.897000000
H	-5.313000000	-2.412000000	2.560000000
H	-4.076000000	-5.380000000	-0.281000000
H	-5.668000000	-4.607000000	1.460000000
C	0.173000000	-2.436000000	0.773000000
C	2.098000000	-4.071000000	2.003000000
C	0.710000000	-2.100000000	2.018000000
C	0.612000000	-3.614000000	0.159000000
C	1.569000000	-4.422000000	0.765000000
C	1.662000000	-2.910000000	2.629000000
H	0.359000000	-1.194000000	2.499000000
H	0.216000000	-3.902000000	-0.808000000
H	1.900000000	-5.328000000	0.268000000
H	2.065000000	-2.630000000	3.598000000
H	2.845000000	-4.701000000	2.476000000
C	-0.975000000	-1.616000000	-1.753000000
C	-0.718000000	-1.738000000	-4.552000000
C	-2.102000000	-1.563000000	-2.582000000
C	0.285000000	-1.710000000	-2.357000000
C	0.412000000	-1.778000000	-3.742000000
C	-1.975000000	-1.624000000	-3.965000000
H	-3.090000000	-1.485000000	-2.141000000
H	1.175000000	-1.735000000	-1.738000000
H	1.398000000	-1.866000000	-4.187000000
H	-2.865000000	-1.589000000	-4.587000000
H	-0.621000000	-1.794000000	-5.631000000

Dihydride-is5-EDF2

C	0.724000000	-0.160000000	2.588000000
H	1.162000000	0.180000000	3.529000000
C	0.134000000	-1.554000000	2.772000000
H	0.958000000	-2.271000000	2.834000000
H	-0.388000000	-1.580000000	3.740000000
N	-0.737000000	-1.953000000	1.664000000
C	-0.919000000	-3.409000000	1.589000000
H	0.034000000	-3.881000000	1.846000000
H	-1.651000000	-3.755000000	2.334000000
C	-1.346000000	-3.890000000	0.199000000
H	-2.142000000	-3.235000000	-0.170000000
H	-1.743000000	-4.906000000	0.294000000
H	-1.648000000	-1.513000000	1.785000000
Ru	-0.445000000	-0.838000000	-0.431000000
H	-0.056000000	0.544000000	2.290000000
C	-0.228000000	-3.894000000	-0.801000000
C	1.848000000	-3.866000000	-2.599000000
C	0.221000000	-5.090000000	-1.360000000
N	0.336000000	-2.712000000	-1.133000000
C	1.358000000	-2.712000000	-2.008000000
C	1.266000000	-5.084000000	-2.273000000
H	-0.258000000	-6.018000000	-1.072000000
H	1.783000000	-1.740000000	-2.219000000
H	1.617000000	-6.009000000	-2.718000000
H	2.671000000	-3.799000000	-3.301000000
N	1.782000000	-0.116000000	1.597000000
N	1.521000000	-0.293000000	0.283000000
N	2.652000000	-0.202000000	-0.364000000
C	3.660000000	0.036000000	0.523000000
C	3.106000000	0.091000000	1.784000000
H	3.522000000	0.275000000	2.760000000
C	5.046000000	0.206000000	0.093000000
C	7.694000000	0.542000000	-0.758000000
C	5.352000000	0.270000000	-1.271000000
C	6.086000000	0.311000000	1.023000000
C	7.398000000	0.479000000	0.601000000
C	6.665000000	0.436000000	-1.690000000
H	4.545000000	0.193000000	-1.990000000
H	5.871000000	0.252000000	2.085000000
H	8.192000000	0.558000000	1.336000000
H	6.886000000	0.486000000	-2.751000000
H	8.719000000	0.673000000	-1.087000000
H	-0.179000000	-0.230000000	-1.881000000
H	-1.875000000	-1.353000000	-1.003000000
P	-1.689000000	1.012000000	-0.114000000
C	-3.035000000	1.326000000	-1.353000000
C	-4.975000000	1.850000000	-3.308000000
C	-4.244000000	1.941000000	-1.013000000
C	-2.816000000	0.969000000	-2.686000000
C	-3.775000000	1.236000000	-3.656000000
C	-5.209000000	2.197000000	-1.983000000
H	-4.447000000	2.206000000	0.019000000
H	-1.893000000	0.460000000	-2.941000000
H	-3.588000000	0.953000000	-4.687000000
H	-6.146000000	2.667000000	-1.699000000
H	-5.726000000	2.049000000	-4.066000000
C	-0.908000000	2.700000000	-0.073000000
C	0.374000000	5.194000000	-0.113000000
C	0.450000000	2.798000000	-0.384000000
C	-1.620000000	3.875000000	0.199000000
C	-0.983000000	5.111000000	0.186000000
C	1.087000000	4.036000000	-0.404000000
H	0.996000000	1.894000000	-0.628000000
H	-2.682000000	3.828000000	0.412000000
H	-1.550000000	6.012000000	0.401000000
H	2.142000000	4.094000000	-0.653000000
H	0.870000000	6.159000000	-0.128000000
C	-2.673000000	0.966000000	1.463000000
C	-4.008000000	0.524000000	3.905000000
C	-3.611000000	-0.071000000	1.599000000
C	-2.422000000	1.773000000	2.578000000
C	-3.082000000	1.553000000	3.786000000
C	-4.273000000	-0.287000000	2.803000000
H	-3.821000000	-0.707000000	0.744000000
H	-1.711000000	2.589000000	2.503000000
H	-2.872000000	2.196000000	4.635000000
H	-5.003000000	-1.087000000	2.879000000
H	-4.525000000	0.356000000	4.844000000

Dihydride-is4-acetophenone-out-wB97X

C	-0.475997000	-3.021383000	-3.362720000
H	-0.548760000	-3.825695000	-4.110381000
C	-0.623168000	-1.680955000	-4.083934000
H	0.304969000	-1.482291000	-4.645233000
H	-1.429670000	-1.755723000	-4.835759000
N	-0.870966000	-0.538062000	-3.187701000
C	-0.416451000	0.717700000	-3.796132000
H	0.597229000	0.566061000	-4.202184000
H	-1.068797000	0.999548000	-4.642291000
C	-0.379457000	1.884286000	-2.819819000
H	-1.286341000	1.887072000	-2.198701000
H	-0.314725000	2.832821000	-3.369927000
N	0.781692000	1.832960000	-1.943990000
N	0.974375000	0.803082000	-1.127649000
N	2.084403000	0.982873000	-0.487139000
C	2.636035000	2.160280000	-0.879386000
C	1.798710000	2.715953000	-1.827053000
H	1.839449000	3.632427000	-2.410685000
C	3.910916000	2.654821000	-0.327262000
C	6.341479000	3.578314000	0.727357000
C	4.633542000	1.871975000	0.582406000
C	4.420122000	3.904926000	-0.700556000
C	5.626825000	4.363242000	-0.177508000
C	5.839740000	2.332654000	1.105109000
H	4.235810000	0.896240000	0.873764000
H	3.867276000	4.533178000	-1.405133000
H	6.011204000	5.341837000	-0.478086000
H	6.394333000	1.711696000	1.814145000
H	7.288079000	3.938556000	1.139418000
H	-1.879982000	-0.444778000	-3.065331000
Ru	-0.463942000	-0.805864000	-0.959248000
H	-1.679394000	0.230027000	-0.663702000
N	1.101870000	-2.275598000	-1.643876000
C	3.016839000	-4.160822000	-2.405837000
C	2.310185000	-2.313531000	-1.064589000
C	0.839508000	-3.143393000	-2.640342000
C	1.778597000	-4.101410000	-3.036166000
C	3.293765000	-3.235443000	-1.404886000
H	2.493647000	-1.559253000	-0.295681000
H	1.527214000	-4.796063000	-3.841493000
H	4.253769000	-3.219071000	-0.884336000
H	3.756376000	-4.910083000	-2.701427000
H	-1.298862000	-3.135540000	-2.640771000
P	-0.351513000	-0.919604000	1.260687000
H	-1.601419000	-1.982769000	-0.913865000
C	-1.789582000	-1.632144000	2.205249000
C	-4.070448000	-2.523746000	3.592330000
C	-1.673010000	-2.226362000	3.468356000
C	-3.066538000	-1.495131000	1.649749000
C	-4.199117000	-1.930670000	2.336362000
C	-2.803259000	-2.672832000	4.154598000
H	-0.688609000	-2.356337000	3.927547000
H	-3.141208000	-1.046216000	0.656047000
H	-5.189147000	-1.816373000	1.882993000
H	-2.690303000	-3.141606000	5.136478000
H	-4.955979000	-2.874215000	4.130440000
C	-0.223842000	0.688395000	2.203409000
C	-0.172253000	3.137081000	3.596359000
C	-0.536740000	1.889306000	1.557248000
C	0.103536000	0.735932000	3.566730000
C	0.134162000	1.946053000	4.256724000
C	-0.511431000	3.103776000	2.245775000
H	-0.819122000	1.857250000	0.501597000
H	0.342470000	-0.186071000	4.105148000
H	0.395062000	1.958558000	5.319001000
H	-0.765010000	4.028746000	1.718631000
H	-0.149403000	4.087652000	4.137258000
C	1.064956000	-1.887669000	1.963058000
C	3.315152000	-3.446410000	2.627448000
C	1.007992000	-3.288300000	1.924021000
C	2.273440000	-1.282499000	2.330597000
C	3.389057000	-2.054540000	2.660601000
C	2.118230000	-4.061537000	2.257812000
H	0.079787000	-3.783912000	1.619683000
H	2.352526000	-0.191580000	2.342506000
H	4.323200000	-1.561082000	2.945624000
H	2.049181000	-5.152690000	2.223538000
H	4.188372000	-4.051378000	2.888300000
C	-4.119177000	0.894898000	-2.057100000
O	-3.493260000	1.049316000	-3.091655000
C	-4.116868000	1.964701000	-1.005875000
C	-3.972163000	3.979600000	0.928662000
C	-4.560694000	1.723736000	0.299661000
C	-3.614498000	3.229230000	-1.336844000
C	-3.545850000	4.234102000	-0.376522000
C	-4.478908000	2.724799000	1.265358000
H	-4.950300000	0.741863000	0.580188000
H	-3.282686000	3.407455000	-2.363073000
H	-3.157134000	5.220743000	-0.643392000
H	-4.807879000	2.521550000	2.287663000
H	-3.910051000	4.764294000	1.687876000
C	-4.892973000	-0.372452000	-1.806291000
H	-4.354698000	-0.983586000	-1.064335000
H	-4.960691000	-0.940859000	-2.742272000
H	-5.899331000	-0.166832000	-1.414389000

Dihydride-is4-acetophenone-in-wB97X

C	-3.737019000	0.984940000	-2.646466000
H	-4.377881000	1.584267000	-3.313053000
C	-2.706151000	0.257260000	-3.494310000
H	-3.229751000	-0.452922000	-4.164702000
H	-2.191527000	0.992281000	-4.133672000
N	-1.690855000	-0.474098000	-2.713969000
C	-0.912854000	-1.375283000	-3.579106000
H	-0.877393000	-2.377331000	-3.121618000
H	-1.416097000	-1.495624000	-4.554126000
C	0.519833000	-0.926040000	-3.845334000
H	0.561505000	0.160266000	-4.012501000
H	0.929402000	-1.448738000	-4.720436000
N	1.385271000	-1.251819000	-2.724184000
N	1.115947000	-0.776324000	-1.515011000
N	1.950836000	-1.290084000	-0.671076000
C	2.801945000	-2.111458000	-1.337853000
C	2.437291000	-2.098898000	-2.670204000
H	2.836782000	-2.589250000	-3.554772000
C	3.912573000	-2.807482000	-0.662583000
C	6.049341000	-4.087407000	0.623655000
C	4.411709000	-2.309032000	0.547868000
C	4.492397000	-3.954112000	-1.219151000
C	5.556164000	-4.588739000	-0.580989000
C	5.472822000	-2.947557000	1.185359000
H	3.968160000	-1.404326000	0.972999000
H	4.100326000	-4.363153000	-2.155414000
H	5.999356000	-5.484307000	-1.025255000
H	5.858337000	-2.545900000	2.126762000
H	6.884241000	-4.585255000	1.124643000
H	-2.238472000	-1.062888000	-2.081418000
Ru	-0.427911000	0.716677000	-1.176779000
H	0.171990000	1.697800000	-2.306723000
N	-4.239663000	-1.133100000	-1.513341000
C	-6.568174000	-0.129350000	-0.379135000
C	-4.990445000	-1.889112000	-0.707181000
C	-4.617650000	0.121996000	-1.773388000
C	-5.791625000	0.656835000	-1.218786000
C	-6.161454000	-1.438130000	-0.110732000
H	-4.630779000	-2.908678000	-0.523306000
H	-6.079015000	1.686050000	-1.449779000
H	-6.739289000	-2.094731000	0.543579000
H	-7.484319000	0.271598000	0.063772000
H	-3.198397000	1.689513000	-1.990071000
P	0.749020000	1.894232000	0.290120000
H	-1.599245000	1.823472000	-0.952088000
C	0.644740000	3.750189000	0.321103000
C	0.448175000	6.555723000	0.367023000
C	1.532103000	4.520270000	1.088263000
C	-0.335332000	4.409202000	-0.426915000
C	-0.433607000	5.802367000	-0.404348000
C	1.434327000	5.909609000	1.115019000
H	2.314799000	4.029656000	1.674904000
H	-1.018809000	3.805170000	-1.029310000
H	-1.205583000	6.300908000	-0.997957000
H	2.134159000	6.492380000	1.720940000
H	0.371768000	7.646926000	0.384553000
C	2.600711000	1.708539000	0.246298000
C	5.390485000	1.419959000	0.001214000
C	3.215255000	1.709434000	-1.013544000
C	3.408195000	1.565215000	1.380284000
C	4.792633000	1.421490000	1.259540000
C	4.595787000	1.568589000	-1.136969000
H	2.588434000	1.803443000	-1.906387000
H	2.957206000	1.557902000	2.376869000
H	5.405299000	1.307306000	2.158825000
H	5.056022000	1.568864000	-2.129445000
H	6.473573000	1.301218000	-0.094629000
C	0.372427000	1.471691000	2.057696000
C	-0.409380000	0.592368000	4.614172000
C	-0.234410000	2.350737000	2.960474000
C	0.581039000	0.140172000	2.454732000
C	0.199012000	-0.294419000	3.721455000
C	-0.623726000	1.914158000	4.230229000
H	-0.414928000	3.390752000	2.674464000
H	1.032967000	-0.563185000	1.745258000
H	0.368435000	-1.335739000	4.011867000
H	-1.098018000	2.616678000	4.921910000
H	-0.713928000	0.250469000	5.607668000
O	-1.315785000	-0.842986000	0.219848000
C	-2.163169000	-0.877841000	1.100987000
C	-2.408206000	-2.176169000	1.808217000
C	-2.798393000	-4.634582000	3.084909000
C	-3.407449000	-2.317308000	2.779072000
C	-1.602551000	-3.276860000	1.487442000
C	-1.796019000	-4.499582000	2.121915000
C	-3.602301000	-3.543292000	3.413045000
H	-4.041762000	-1.468390000	3.046199000
H	-0.818799000	-3.148485000	0.736488000
H	-1.161274000	-5.352840000	1.868099000
H	-4.384709000	-3.646017000	4.169685000
H	-2.951191000	-5.595424000	3.584391000
C	-2.946494000	0.337629000	1.494122000
H	-2.715505000	0.602136000	2.539565000
H	-4.028375000	0.140277000	1.423250000
H	-2.664731000	1.164145000	0.828161000