Supporting Information

Acceptorless Dehydrogenative Construction of C=N and C=C bond through Catalytic Aza-Wittig and Wittig Reaction in the Presence of Air-stable Ruthenium Pincer Complex

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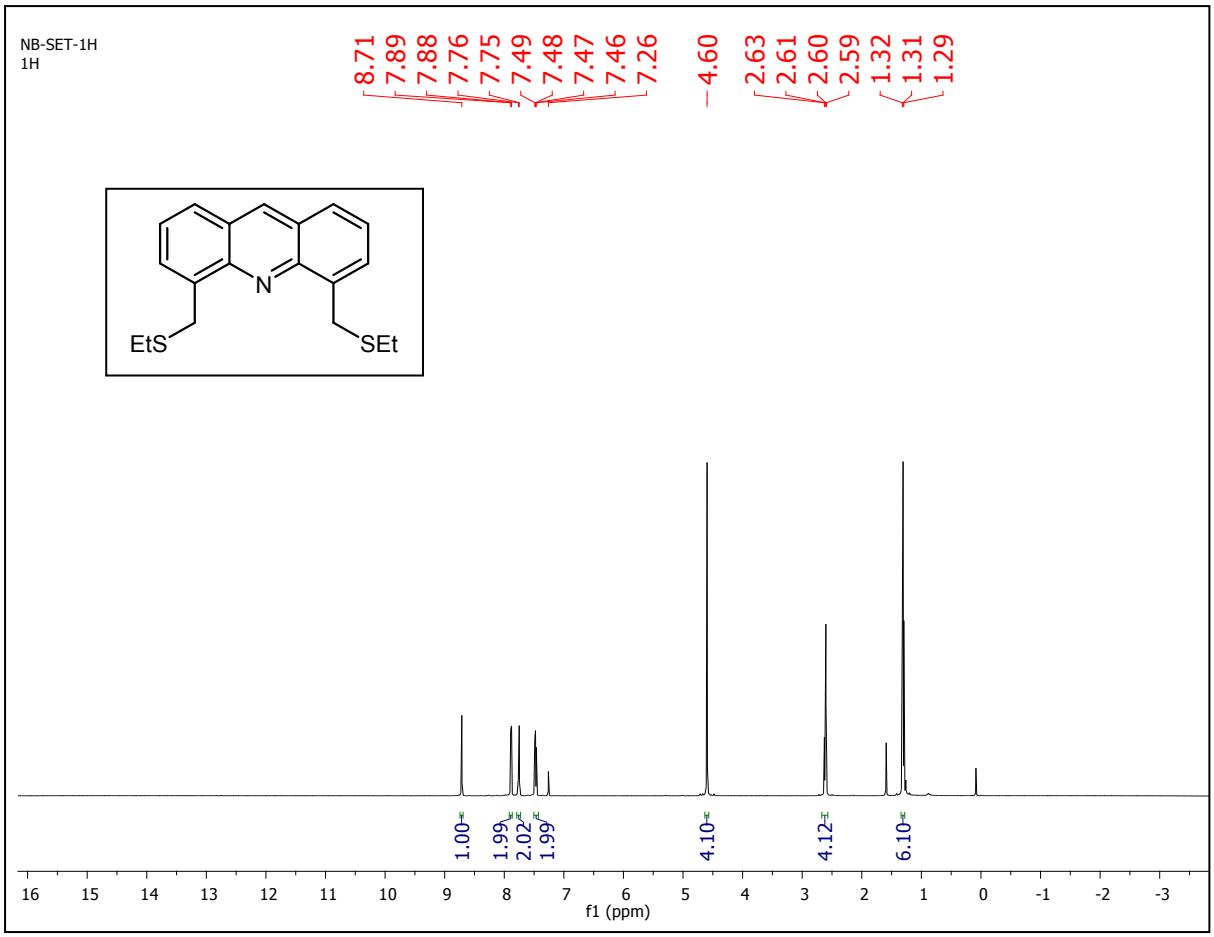
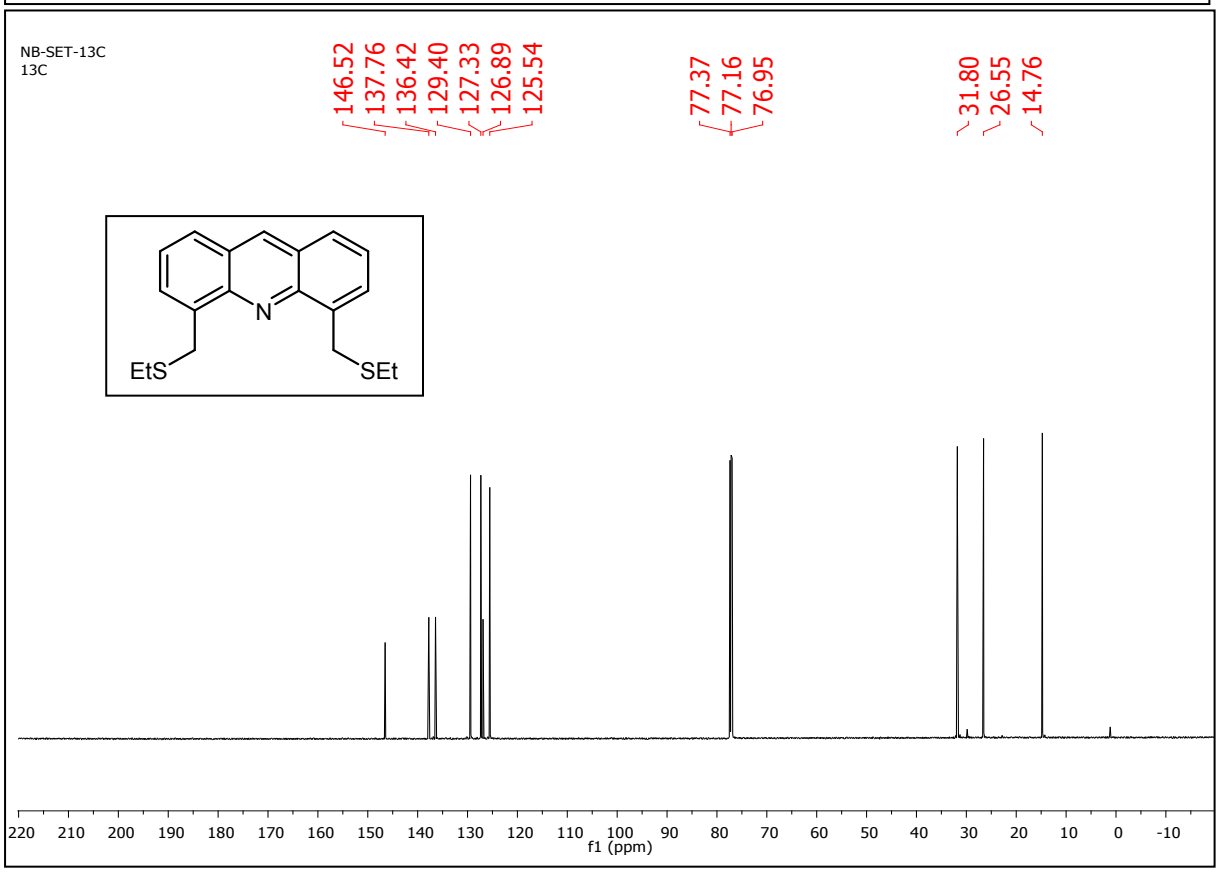
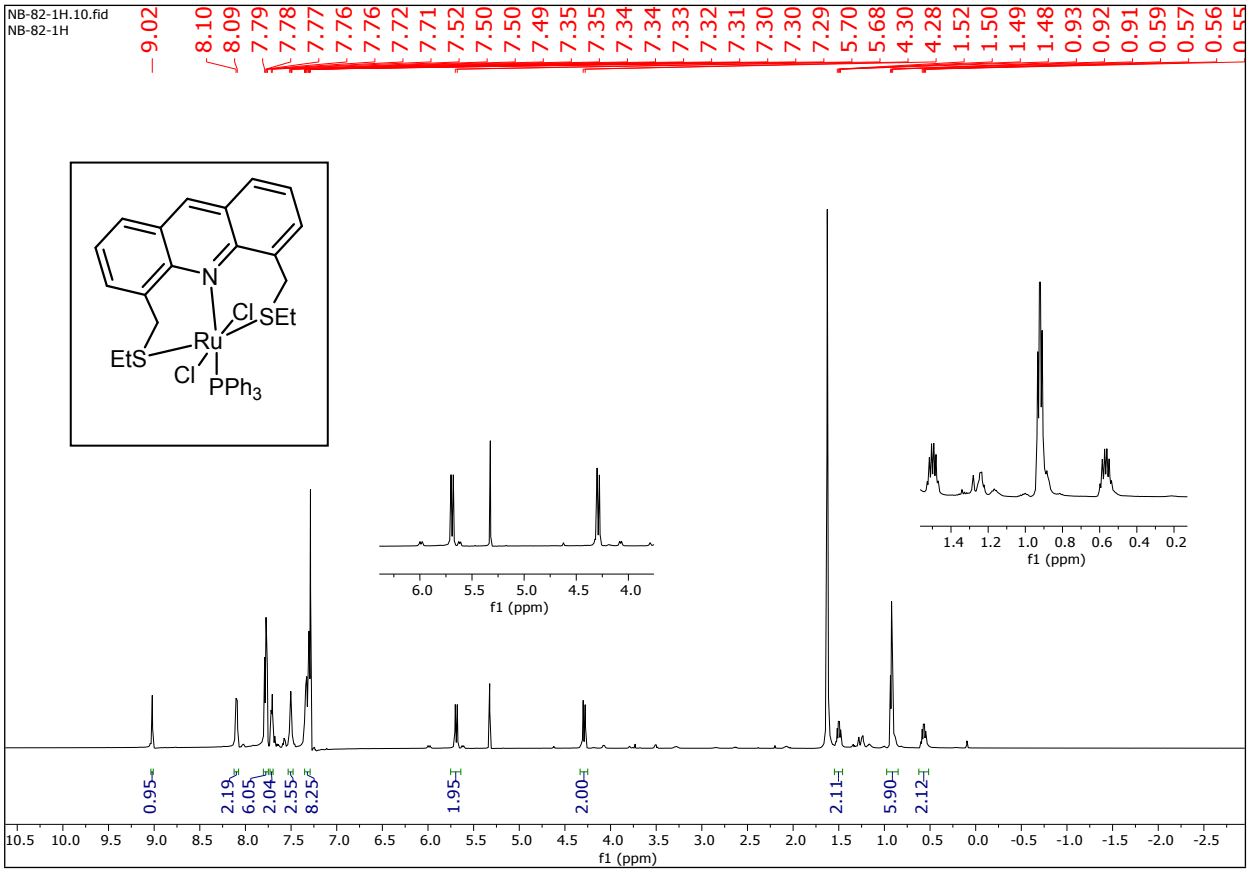
1. Characterization data of Ligands and the corresponding Ru-pincer complexes (1-3):



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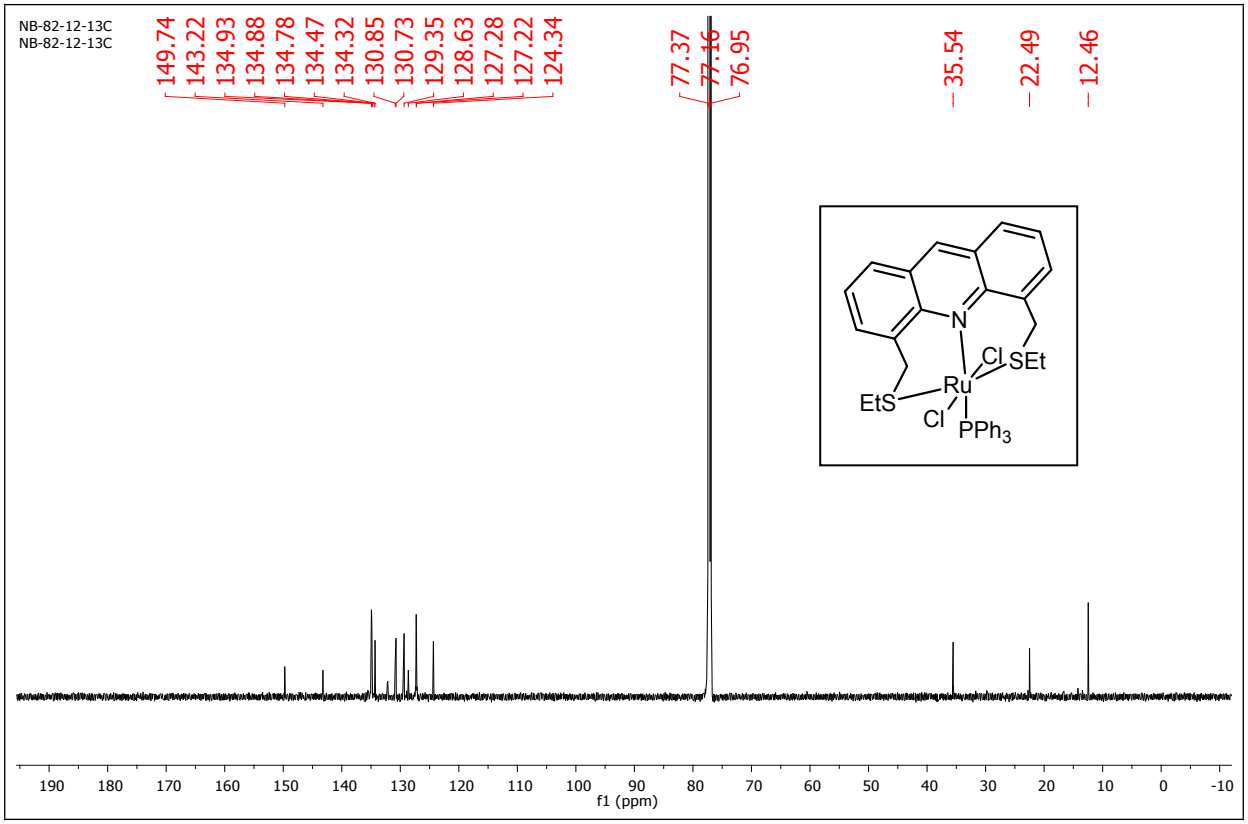
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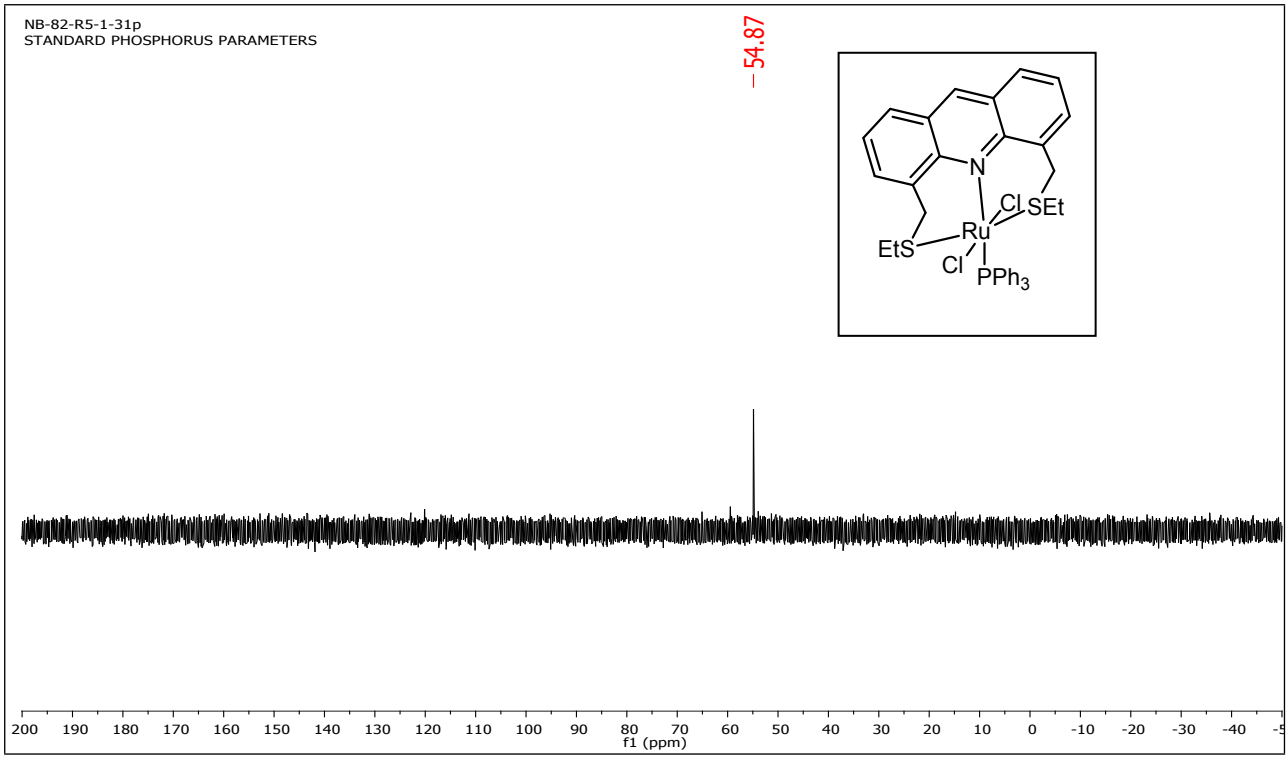


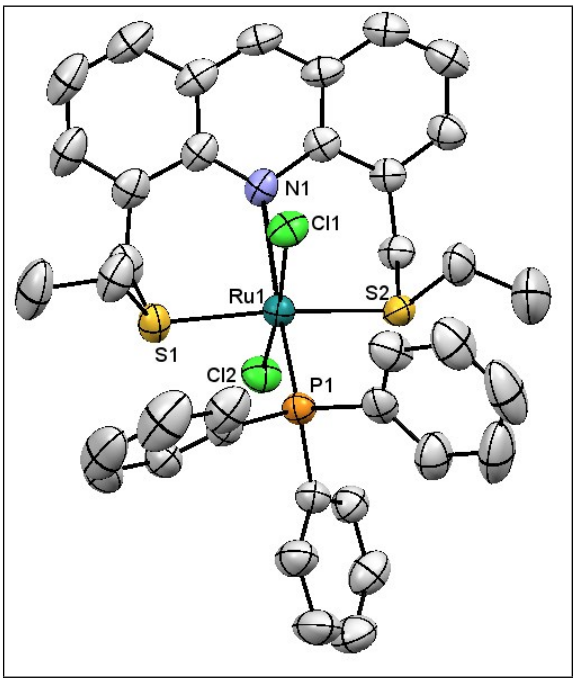


Figure 1. Molecular structure of **1** with thermal ellipsoids at 50% probability.

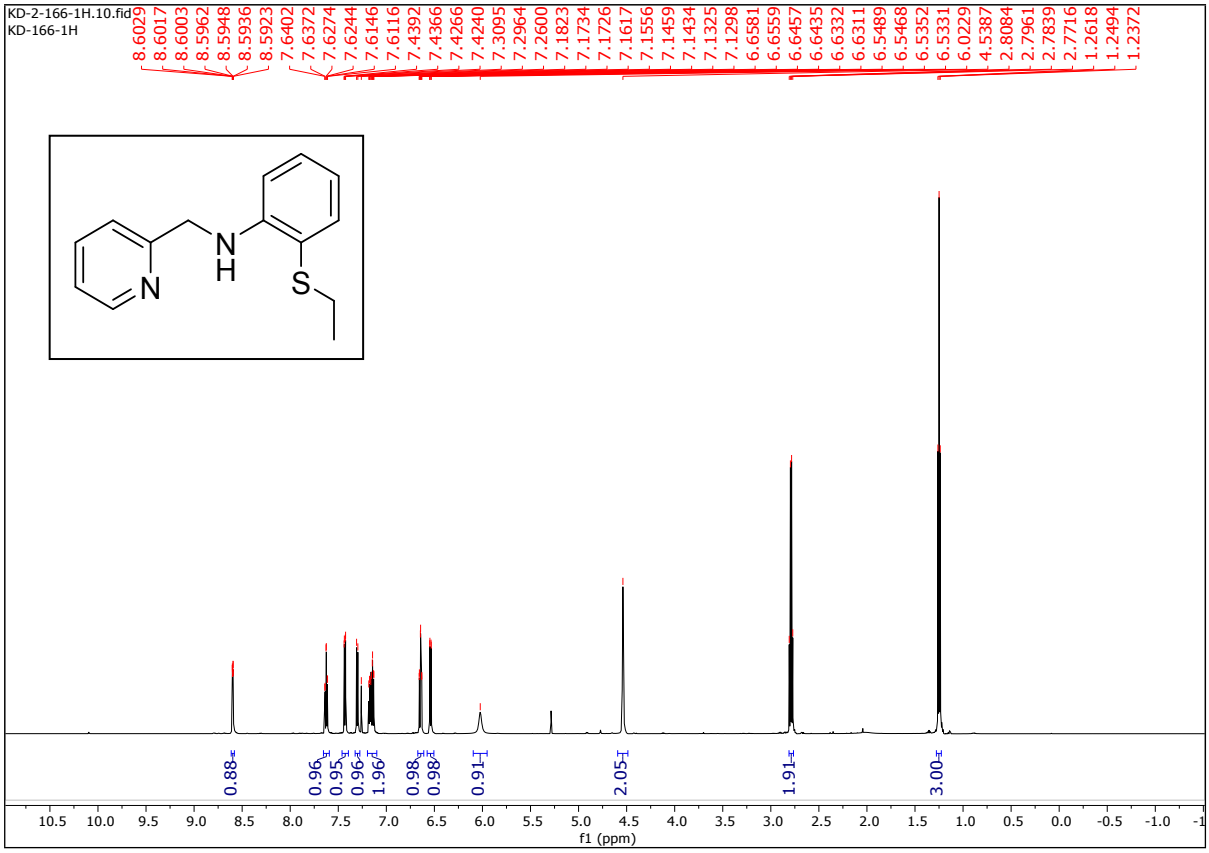
Crystallographic data for complex 1:

Formula	C_{39} H_{39} Cl_2 N_2 P Ru S_2
Mol. wt.	802.78
Crystal system	Triclinic
Space group	P -1

Temperature /K	296(2)
Wavelength /Å	0.71073
a /Å	9.7186(6)
b /Å	11.8743(7)
c /Å	18.0974(11)
α/°	71.496(4)
β/°	79.588(4)
γ/°	79.316(4)
V/ Å^3	1929.4(2)
Z	2
Density/Mgm^{-3}	1.382
Abs. Coeff. /mm^{-1}	0.724
Abs. correction	MULTI-SCAN
F(000)	824
Total no. of reflections	18723
Reflections, I > 2σ(I)	4342
Max. 2θ/°	25.00
Ranges (h, k, l)	-11≤ h ≤11 -14≤ k ≤13 -21≤ l ≤ 20
Complete to 2θ (%)	98.9
Refinement method	Full-matrix least-squares on F^2
Goof (F^2)	1.033
R indices [I > 2σ(I)]	0.0633
R indices (all data)	0.0900

Table 1. Selected bond lengths and angles:

Bond Distances [Å]		**Bond angles [°]**	
Ru1 N1	12.561(5)	P1 Ru1 N1	170.02(12)
Ru1 P1	2.2587(16)	S1 Ru1 N1	89.53(12)
Ru1 S1	2.3394(16)	S2 Ru1 N1	90.43(12)
Ru1 S2	2.3210 (16)	Cl1 Ru1 N1	76.51(12)
Ru1 Cl1	2.3989(16)	Cl2 Ru1 N1	93.22(12)
Ru1 Cl2	2.4317(16)	Cl1 Ru1 Cl2	169.47(6)
		P1 Ru1 S1	92.60(6)
		S2 Ru1 S1	167.27(6)
		P1 Ru1 S2	89.63(6)
		P1 Ru1 Cl1	93.59(6)
		S2 Ru1 Cl1	98.06(6)
		S1 Ru1 Cl1	94.32(6)
		P1 Ru1 Cl2	96.72(6)
		S2 Ru1 Cl2	84.13(6)
		S1 Ru1 Cl2	83.16(6)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7.4392
7.4366
7.4266
7.4240
7.3095
7.2964
7.2600
7.1823
7.1734
7.1726
7.1617
7.1556
7.1459
7.1434
7.1325
7.1298
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6.6559
6.6457
6.6435
6.6332
6.6311
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6.5331
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H
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S
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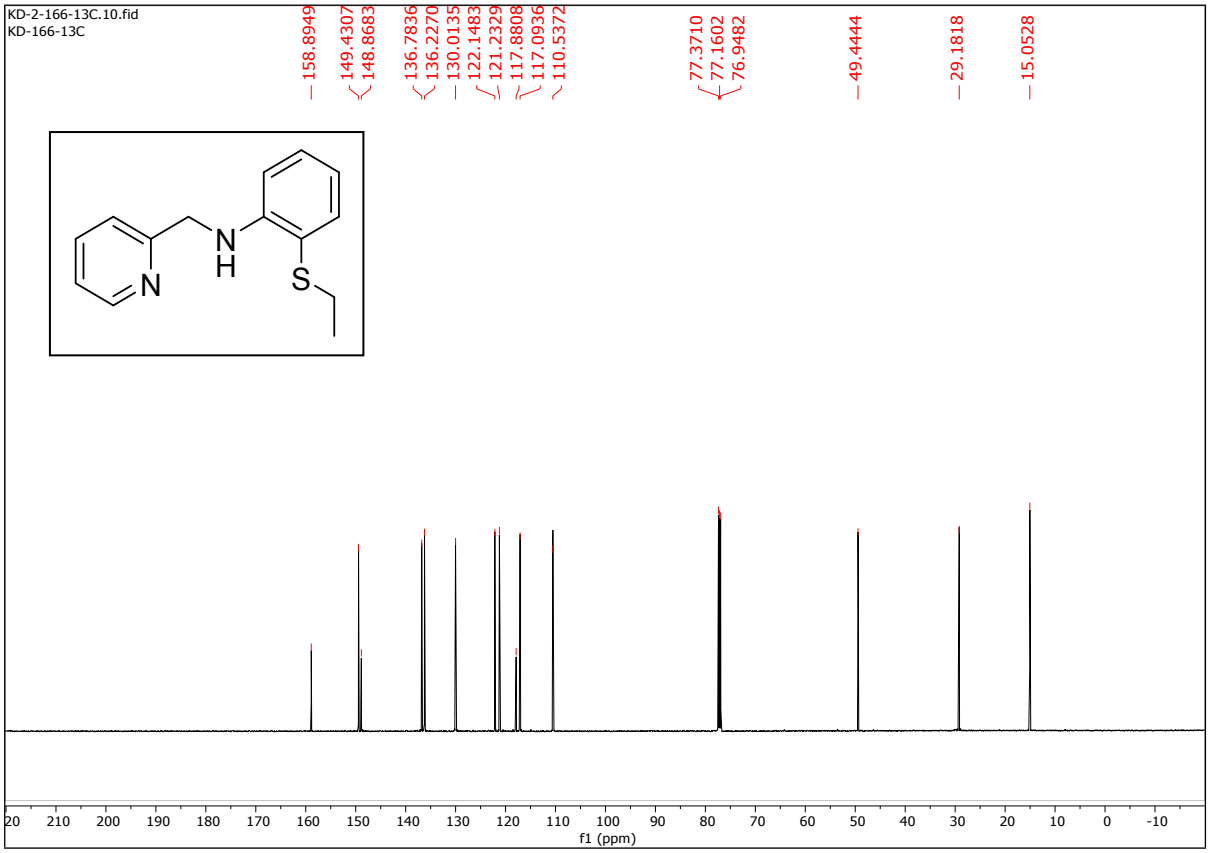
f1 (ppm)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S
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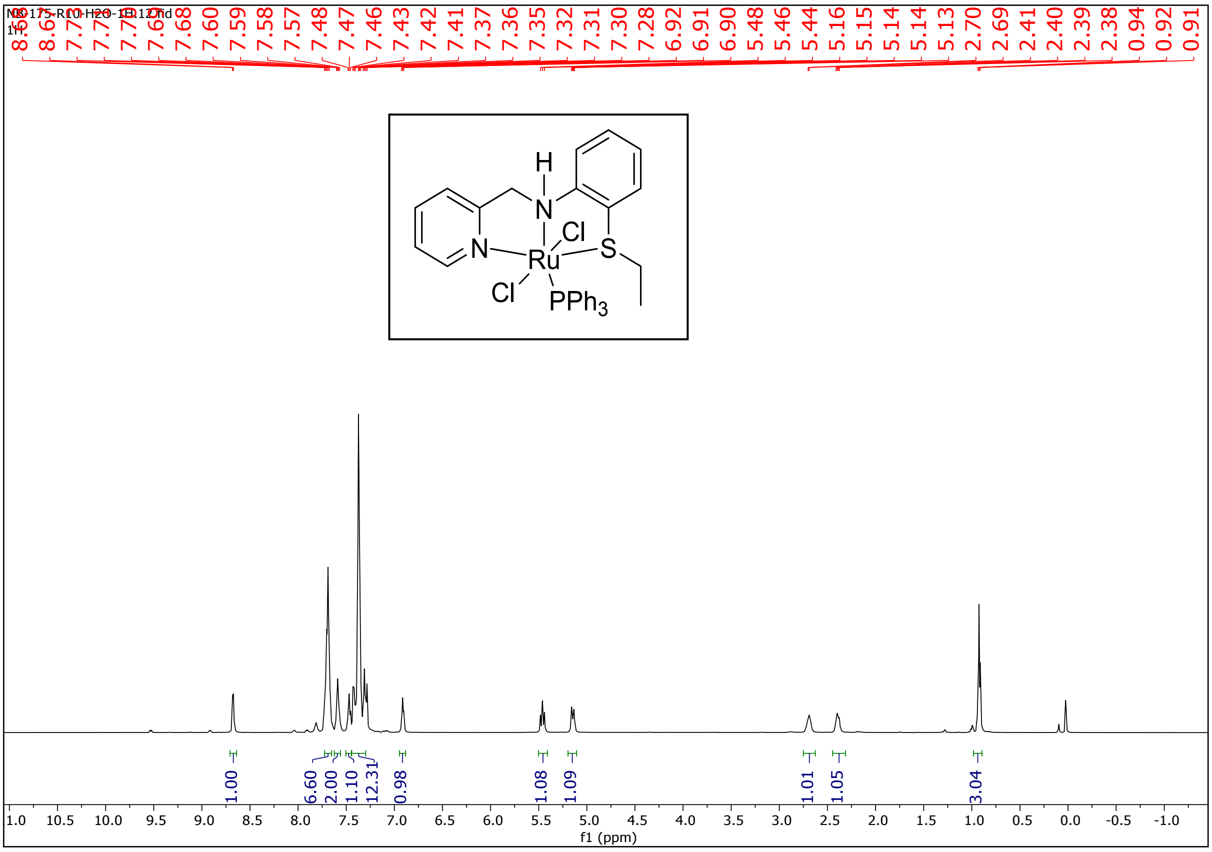
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5.15
5.14
5.14
5.13
2.70
2.69
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0.92
0.91
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N
N
Ru
Cl
Cl
S
PPh3
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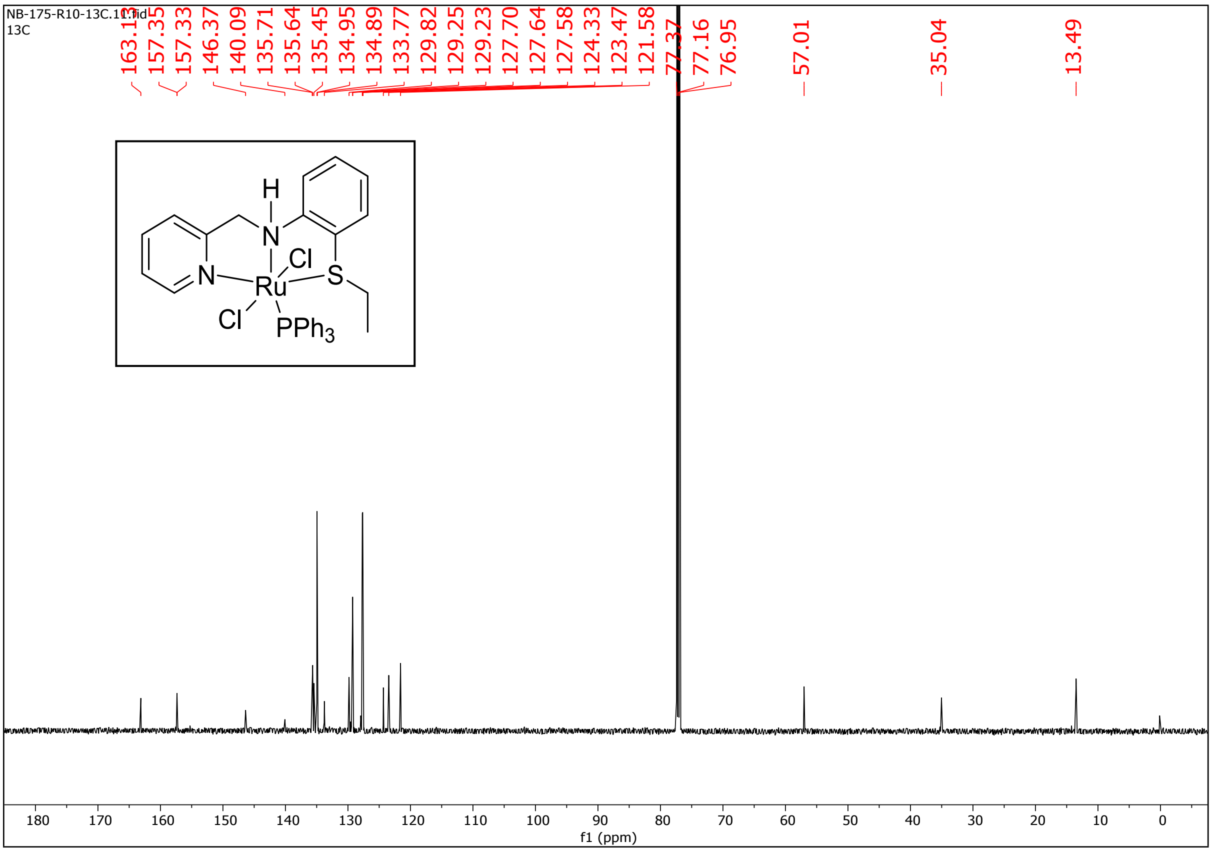
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127.64
127.58
124.33
123.47
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S
PPh3
f1 (ppm)

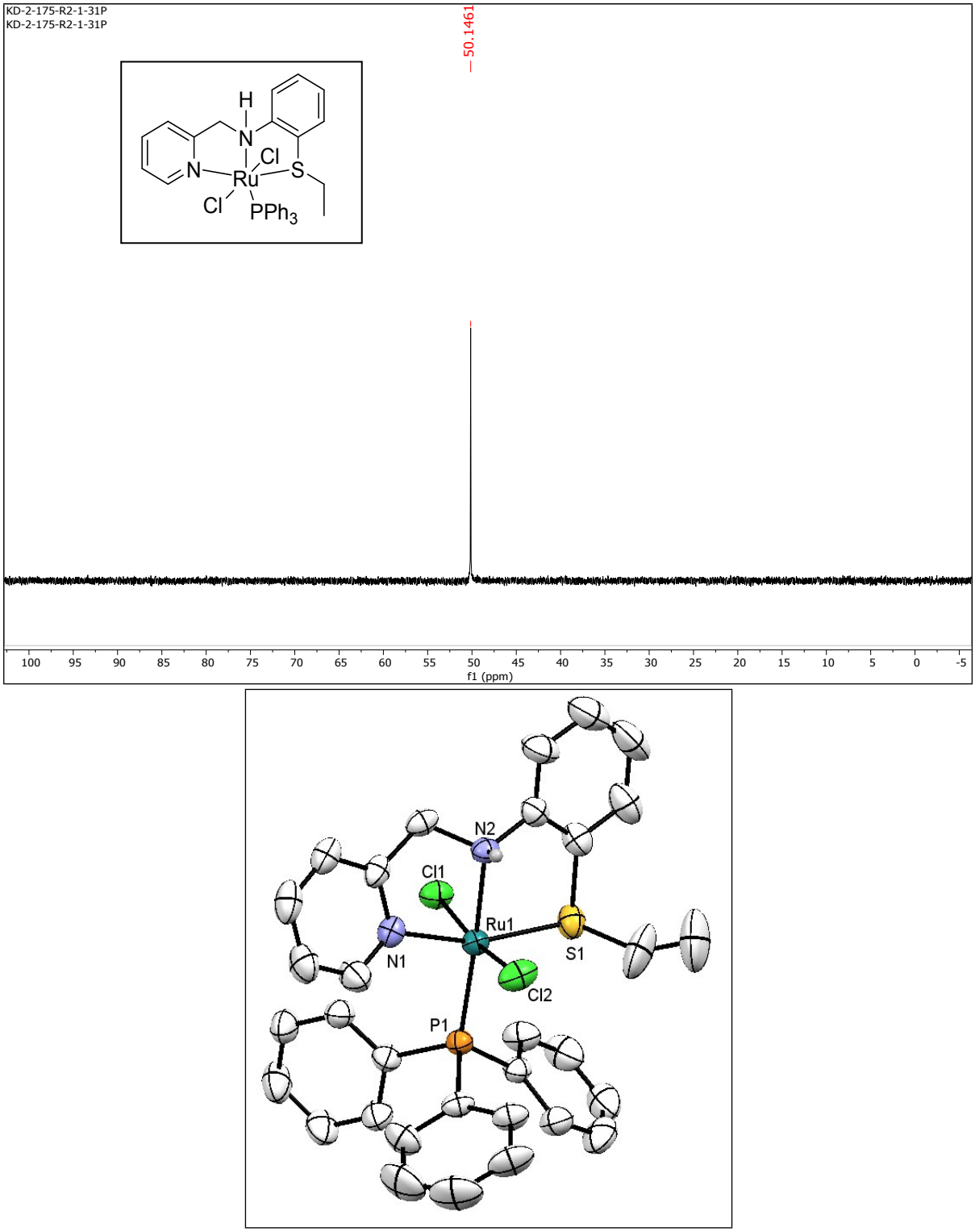


Figure 2. Molecular structure of **2** with thermal ellipsoids at 30% probability.

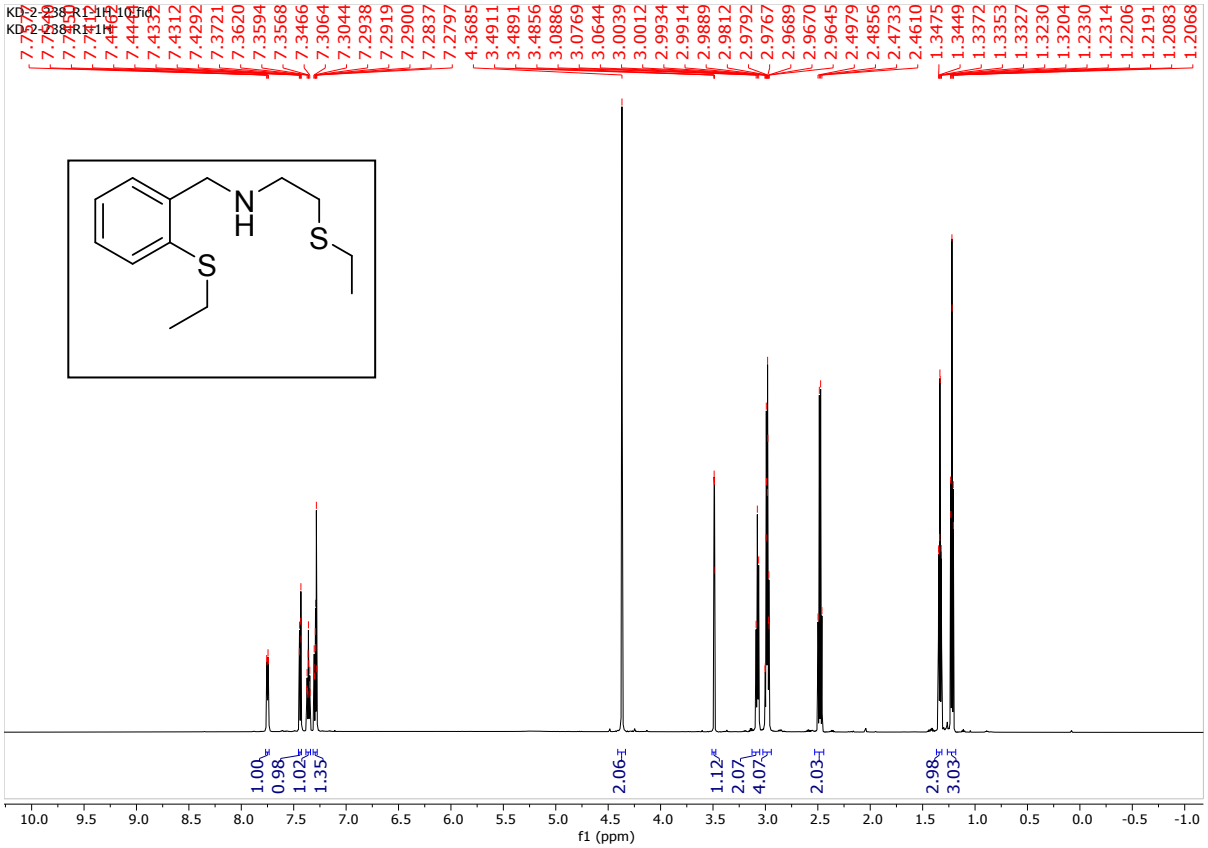
Crystallographic data for complex 2:

Empirical formula	C68 H72 Cl4 N4 O P2 Ru2 S2 C68
Formula weight	1431.30
Temperature, T	293 K
Crystal system	Triclinic

Space group	P-1
Unit cell dimensions	a= 10.1370(4) Å α= 73.196(2)° b= 11.4066(4) Å β= 80.920(2)° c= 16.0632(6) Å γ= 67.294(2)°
Volume, V (Å^3)	1638.01(11)
Z	1
Density (calculated), Mg·m^{-3}	1.451
Absorption coefficient, μ (mm^{-1})	0.782
F(000)	734.0
Crystal size, mm^3	0.32 × 0.28 × 0.19
Theta range for data collection	0.997 to 24.75
Index ranges	-11 ≤ h ≤ 11, -12 ≤ k ≤ 13, -18 ≤ l ≤ 18
Reflections collected	4204
Independent reflections	5581
Completeness to theta	0.997
Absorption correction	none
Max. and min. transmission	0.862 to 0.779
Refinement method	'SHELXL-97(Sheldrick, 1997)'
Data / restraints / parameters	5581 / 6/388
Goodness-of-fit on F^2	0.909
Final R indices [I>2sigma(I)]	R1 = 0.0473(3792), wR=0.1146(5581)
R indices (all data)	R1 = 0.0730, wR=0.0975
Extinction coefficient	0.782
Largest diff. peak and hole	1.089 and -0.549 e·Å^{-3}

Selected bond length and bond angle:

Bond lengths [Å]	**Bond angles [°]**
Ru1 N1 2.078(4)	N1 Ru1 N2 78.49(16)
Ru1 N2 2.124(4)	N1 Ru1 P1 98.45(13)
Ru1 P1 2.2967(14)	N2 Ru1 P1 176.93(12
Ru1 S1 2.3214(15)	N1 Ru1 S1 162.58(13)
Ru1 Cl2 2.3935(15)	N2 Ru1 S1 84.42(12)
Ru1 Cl1 2.4227(15)	P1 Ru1 S1 98.65(5)
	N1 Ru1 Cl2 85.61(12)
	N2 Ru1 Cl2 84.37(12
	P1 Ru1 Cl2 95.20(5)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7.3466
7.3064
7.3044
7.2938
7.2919
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7.2837
7.2797
4.3685
3.4911
3.4891
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3.0886
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3.0039
3.0012
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2.9812
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2.4979
2.4856
2.4733
2.4610
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1.3449
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1.3353
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1.3230
1.3204
1.2330
1.2314
1.2206
1.2191
1.2083
1.2068
N
H
S
S
1.00
0.98
1.02
1.35
2.06
1.12
2.07
4.07
2.03
2.98
3.03
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 -1.0
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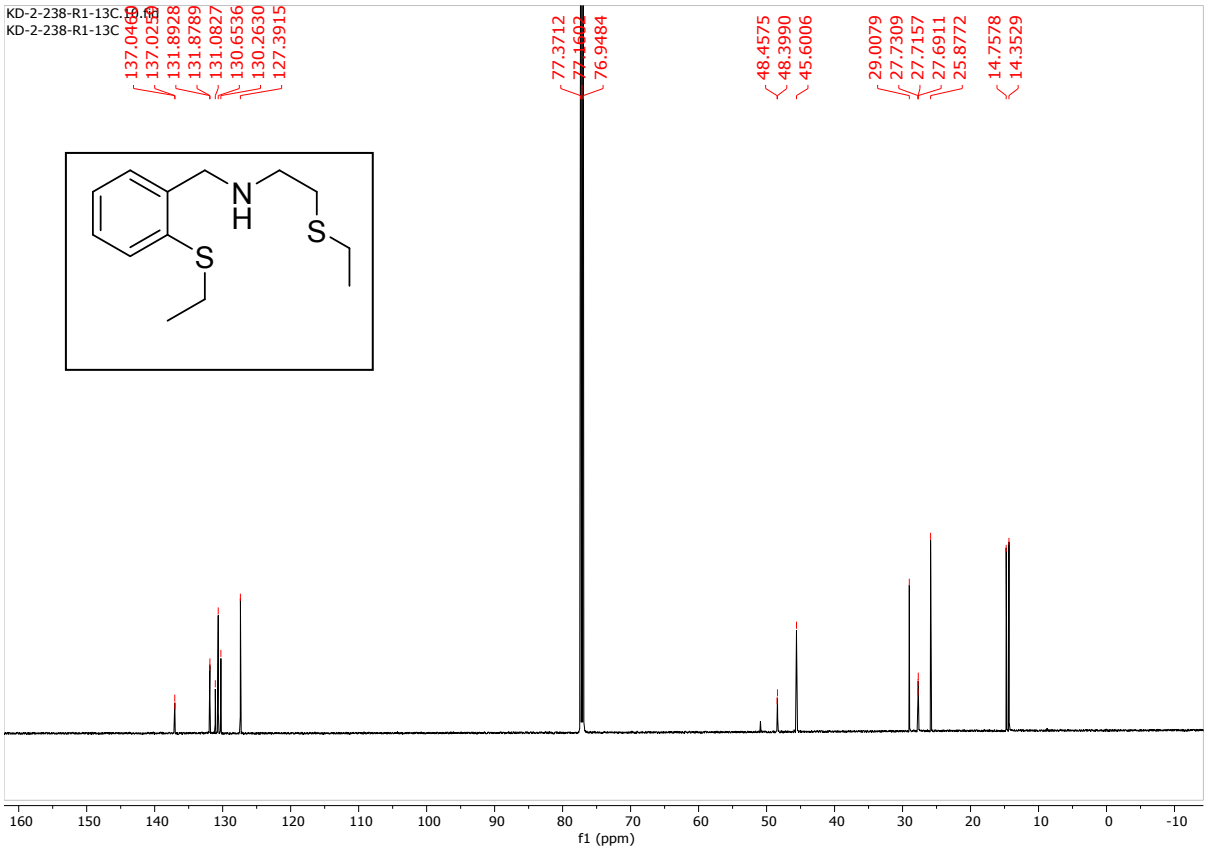
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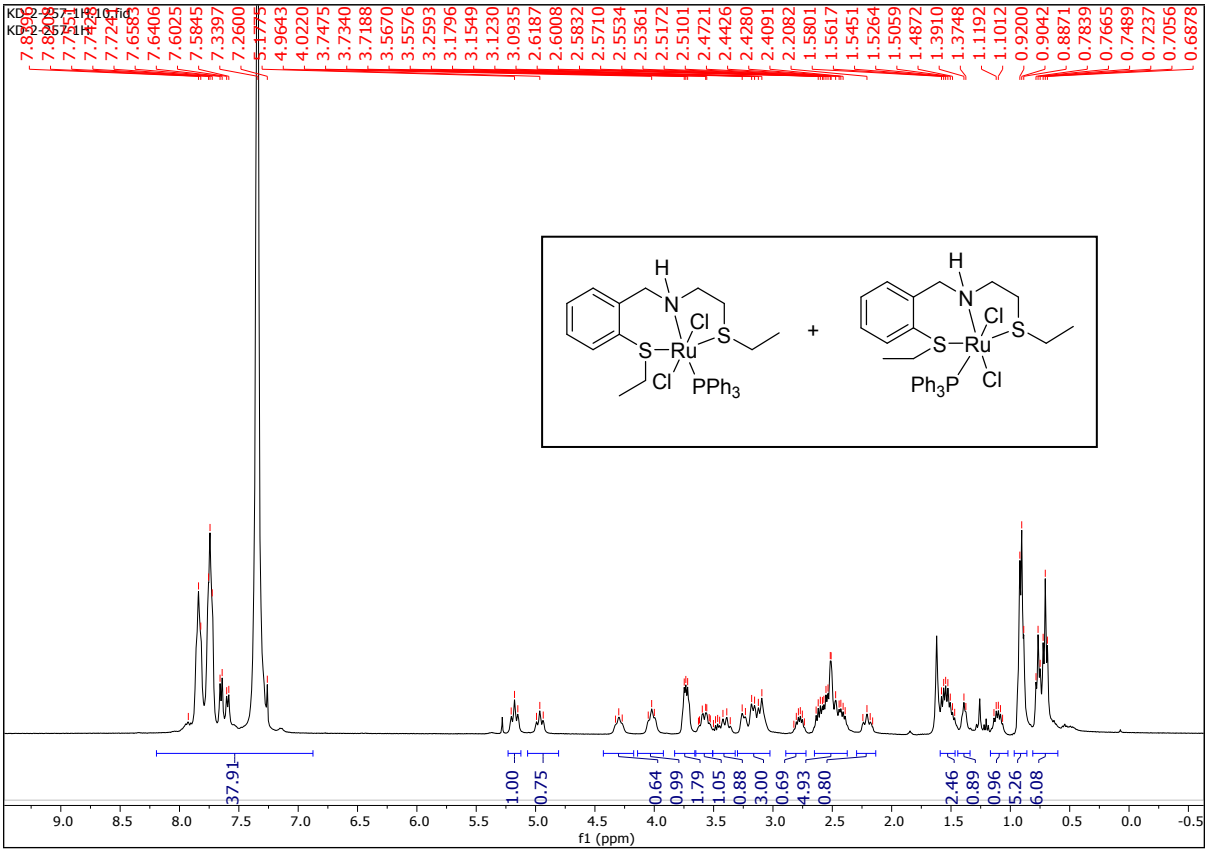
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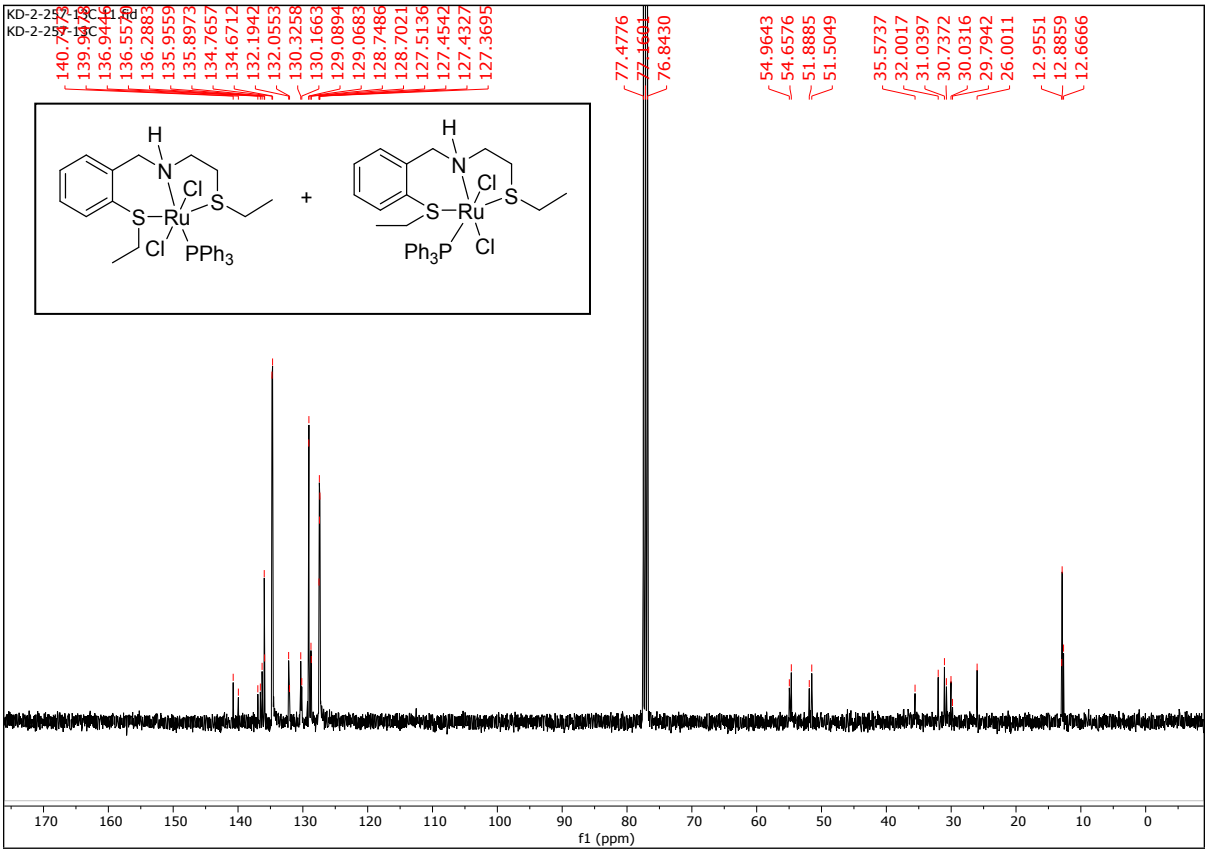
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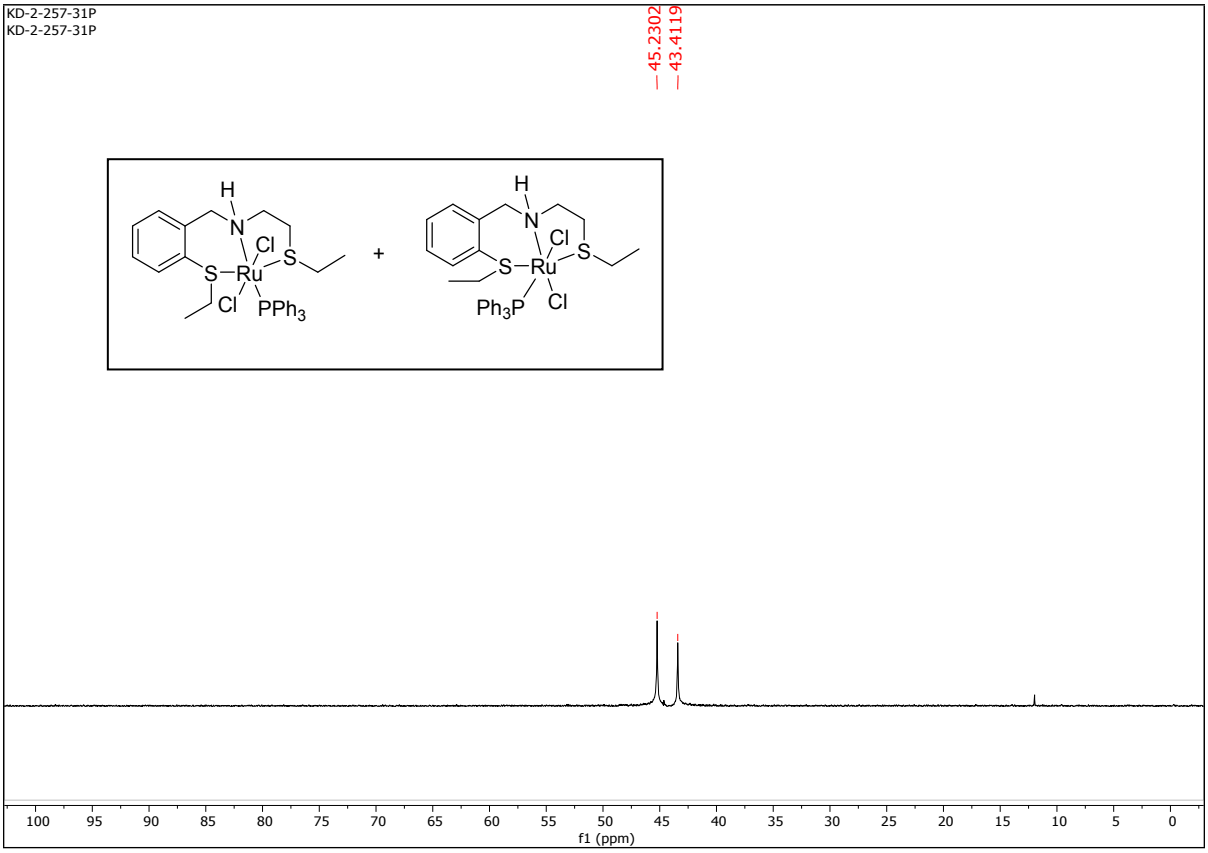


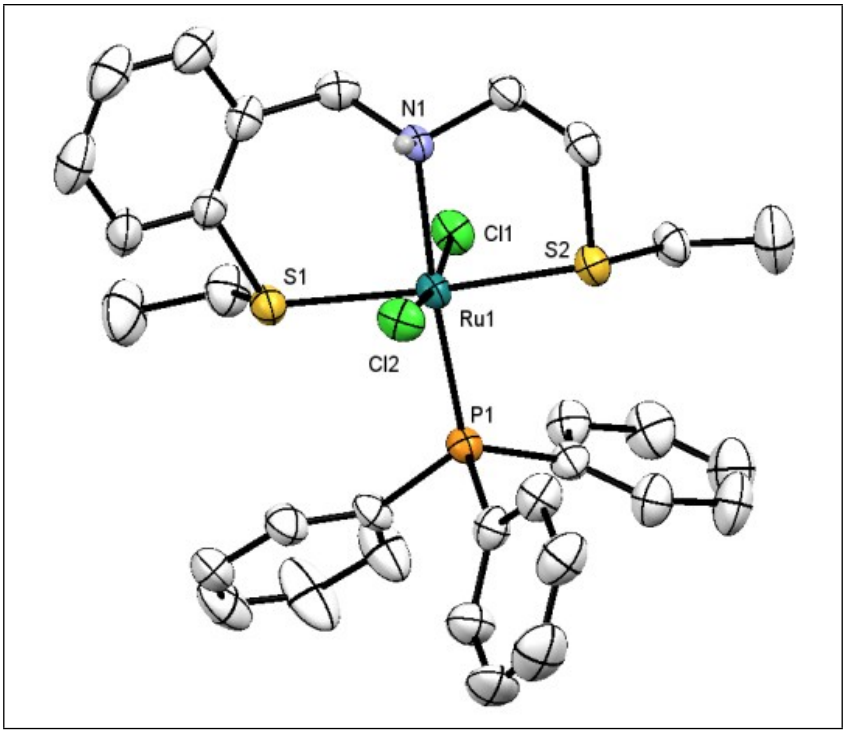


Figure 3. Molecular structure of **3** with thermal ellipsoids at 30% probability.

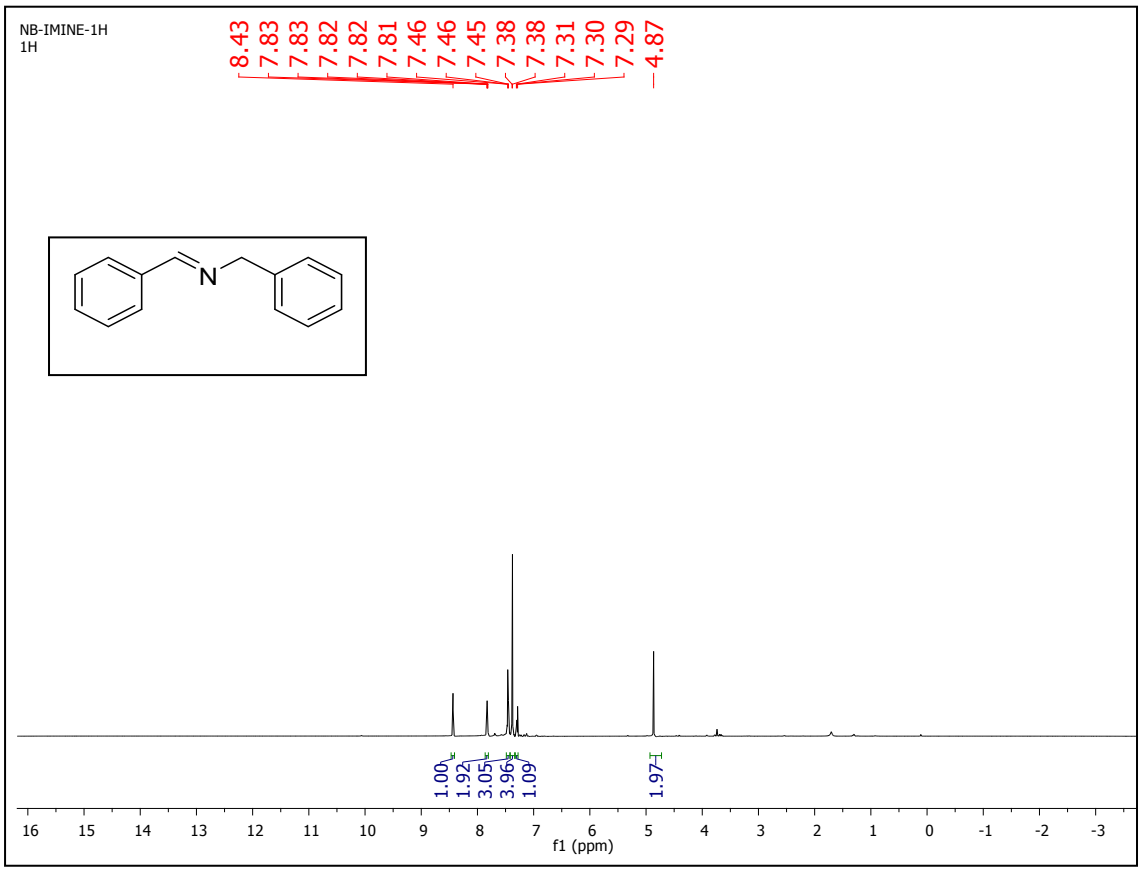
Crystallographic data for complex 3:

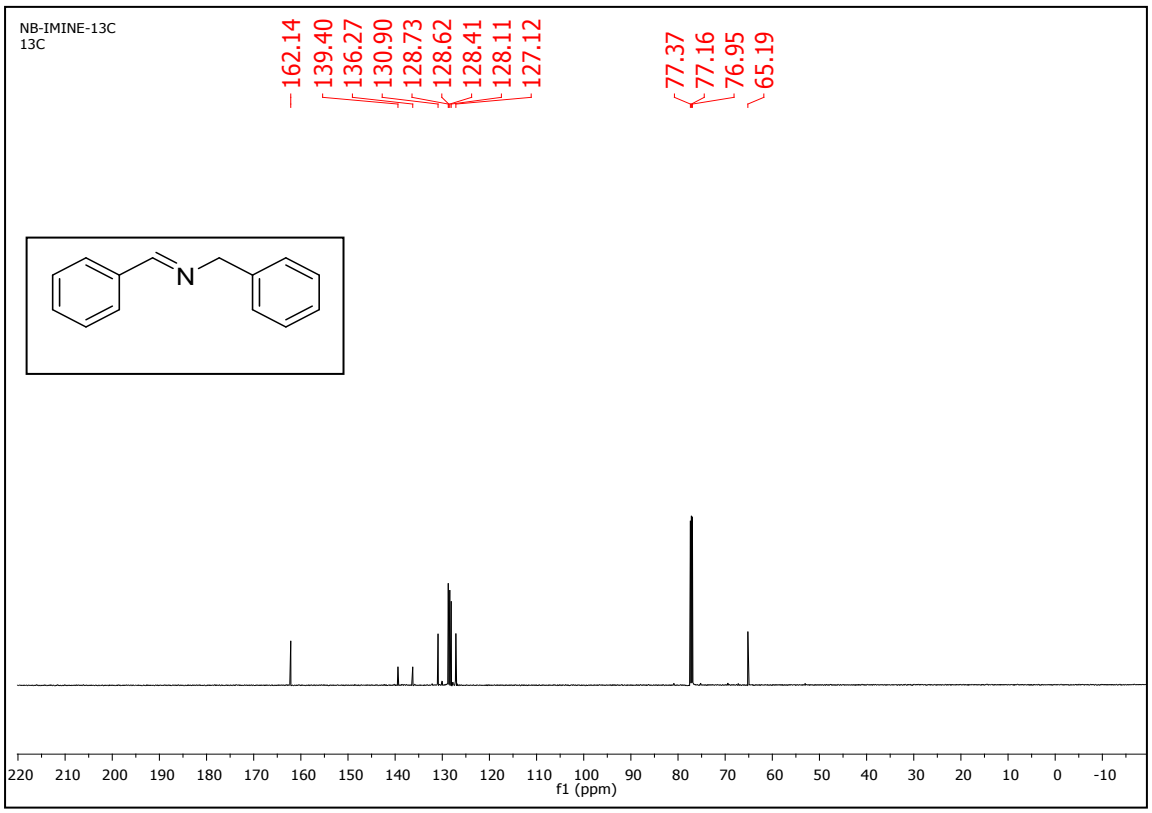
Empirical formula	C31 H36 Cl2 N P Ru S2
Formula weight	689.67
Temperature, T	293 K
Crystal system	triclinic
Space group	P -1
Unit cell dimensions	a= 10.7565(6) Å α= 90.215(5) ° b= 12.0194(7) Å β= 92.041(5) ° c= 12.7360(8) Å γ=107.252(5) °
Volume, V (Å^3)	1571.34(16)
Z	2
Density (calculated), Mg·m^{-3}	1.458
Absorption coefficient, μ (mm^{-1})	0.874
F(000)	708.0
Crystal size, mm^3	0.34 × 0.30 × 0.27
Theta range for data collection	0.998 to 25.00
Index ranges	-10 ≤ h ≤ 12, -14 ≤ k ≤ 14, -15 ≤ l ≤ 13
Reflections collected	3007
Independent reflections	5525
Completeness to theta	0.998
Absorption correction	multi-scan
Max. and min. transmission	0.792 to 1.000
Refinement method	'SHELXL-97(Sheldrick, 1997)'
Data / restraints / parameters	5525 / 0/345
Goodness-of-fit on F^2	0.977
Final R indices [I>2sigma(I)]	R1 = 0.0492(4271), wR=0.1385(5525)
R indices (all data)	R1 = 0.0705, wR=0.1196
Extinction coefficient	0.874
Largest diff. peak and hole	1.098and -0.566 e·Å^{-3}

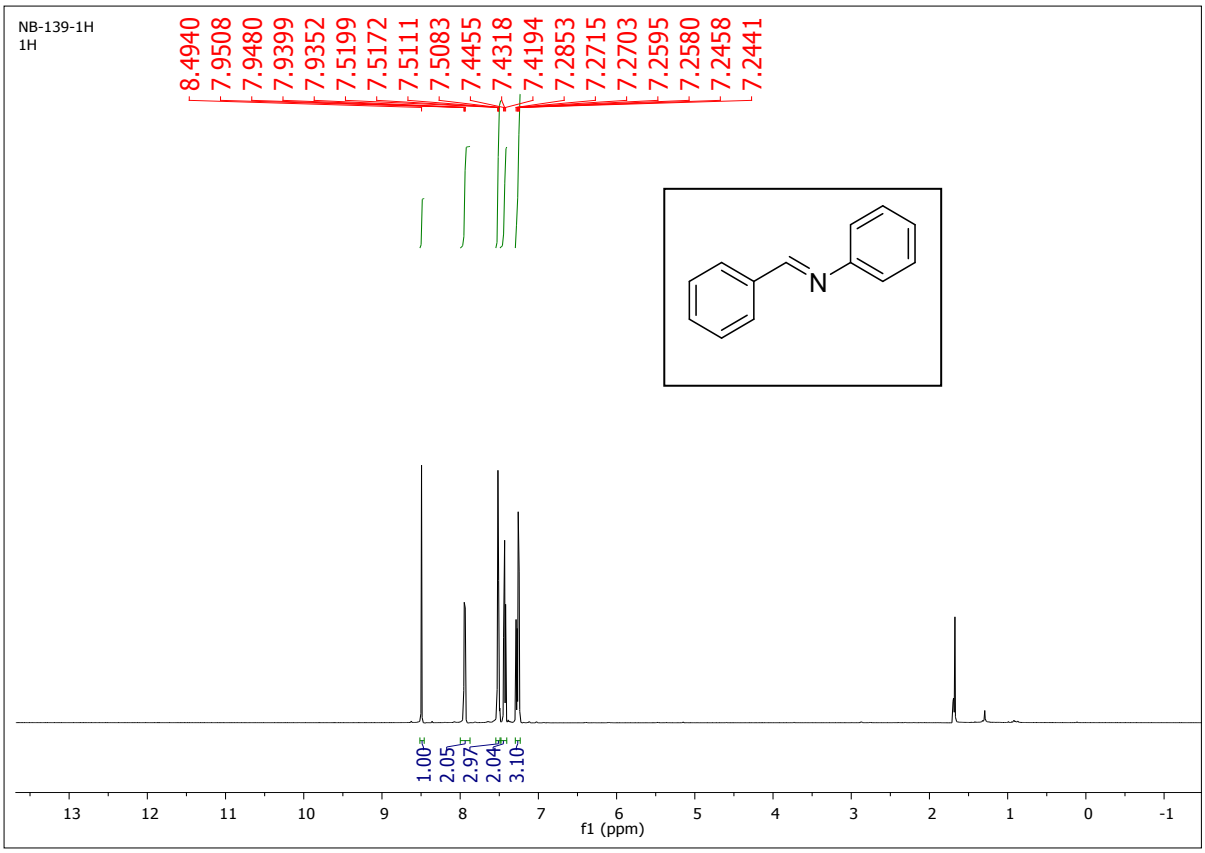
Selected bond length and bond angle:

Bond lengths [Å]	**Bond angles [°]**
Ru1 N1 2.179(4)	N1 Ru1 P1 175.43(10)
Ru1 P1 2.3110(14)	N1 Ru1 S2 84.13(10)
Ru1 S2 2.3506(13)	P1 Ru1 S2 91.32(5)
Ru1 S1 2.3646(13)	N1 Ru1 S1 90.08(10)
Ru1 Cl1 2.4107(13)	P1 Ru1 S1 94.41(5)
Ru1 Cl2 2.4299(13)	S2 Ru1 S1 171.28(5)
	N1 Ru1 Cl1 86.79(11)
	P1 Ru1 Cl1 93.86(5)
	S2 Ru1 Cl1 93.84(5)

2. ^{1}H and ^{13}C NMR spectra of Aza-Wittig and Wittig reaction products:



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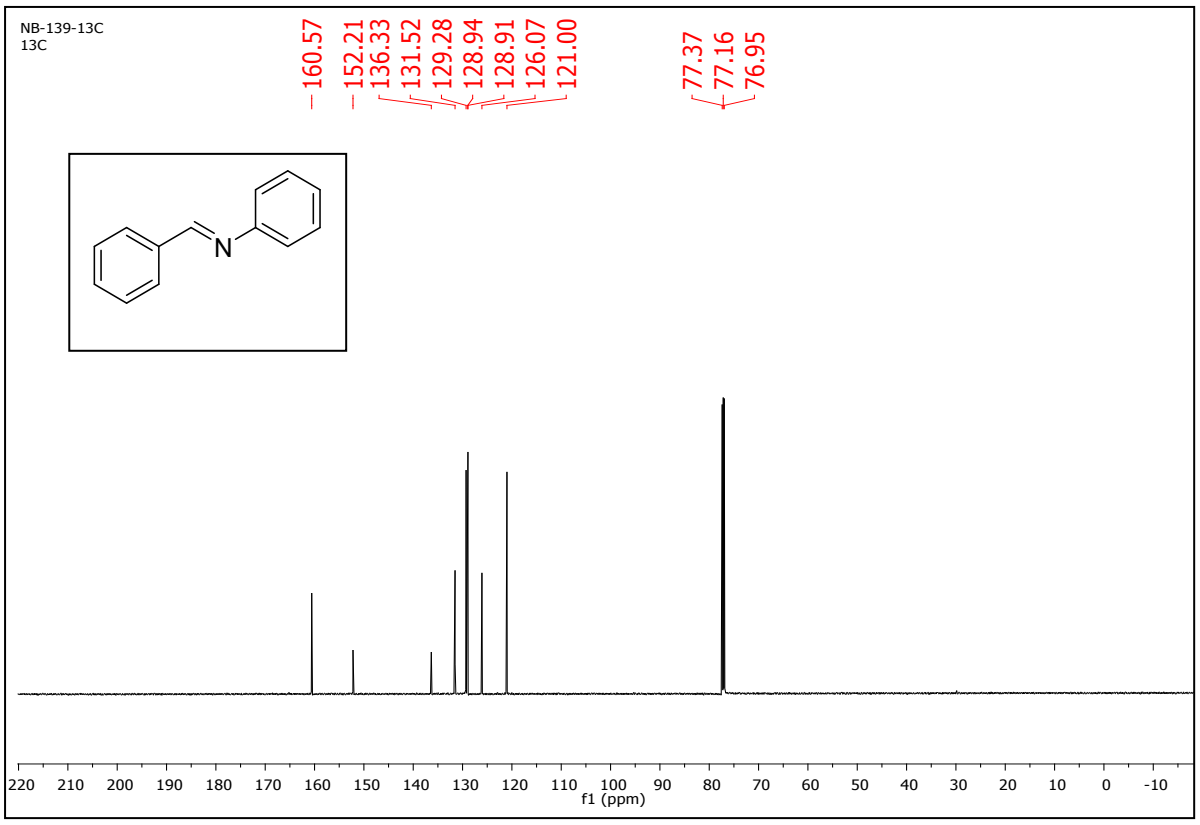
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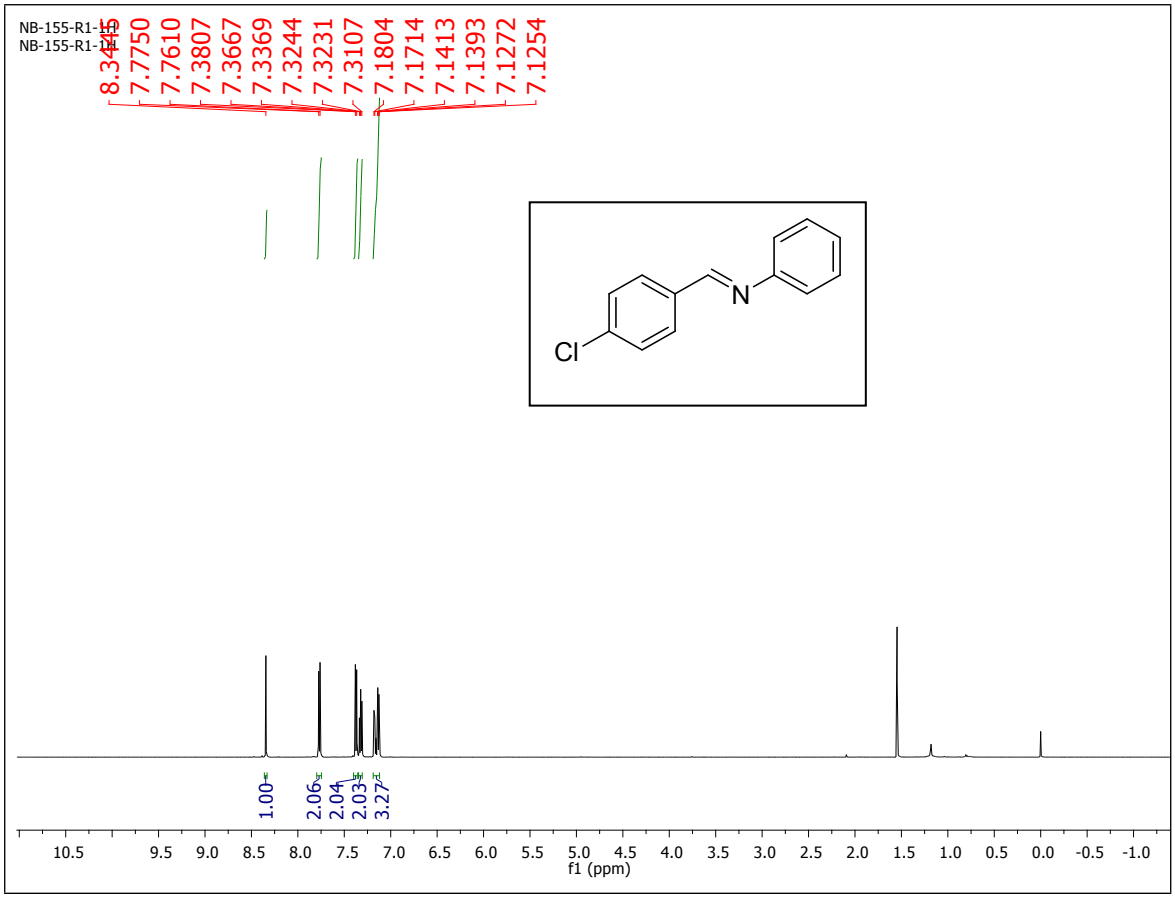
N
f1 (ppm)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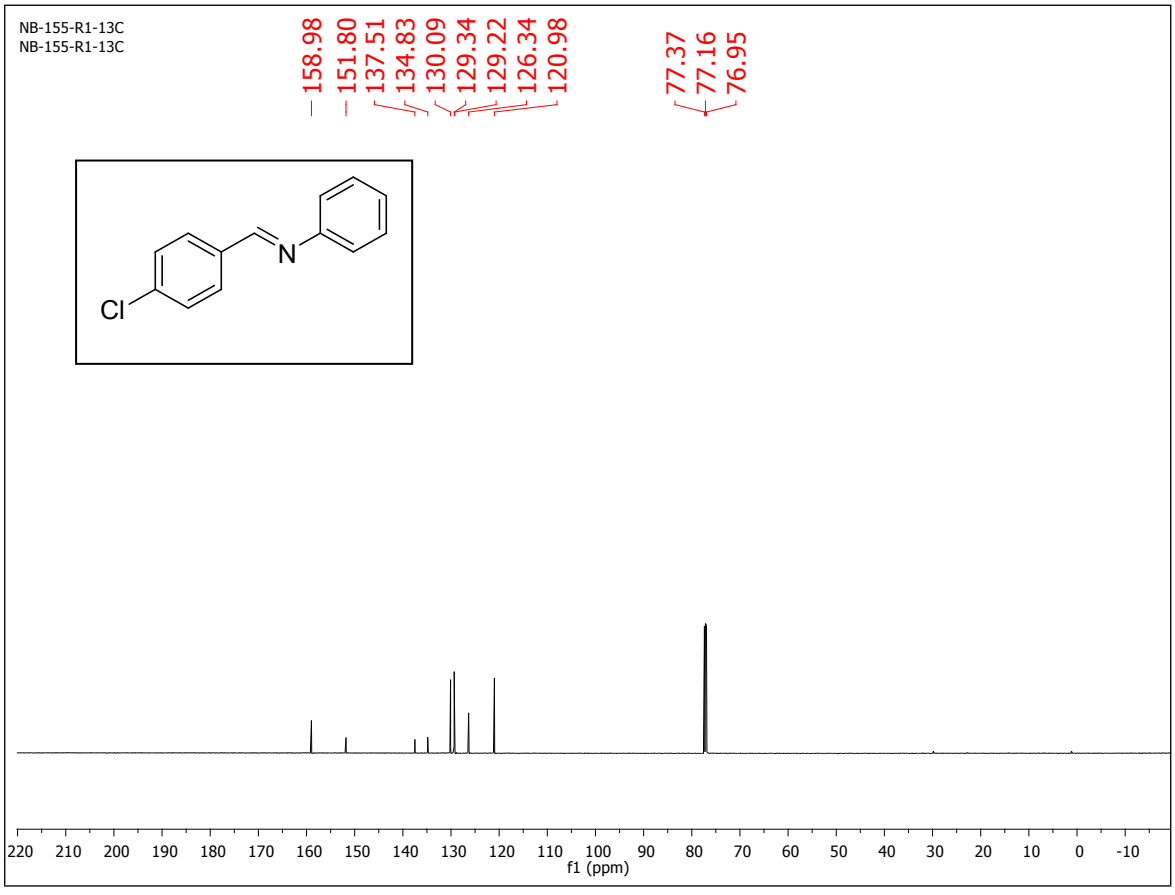
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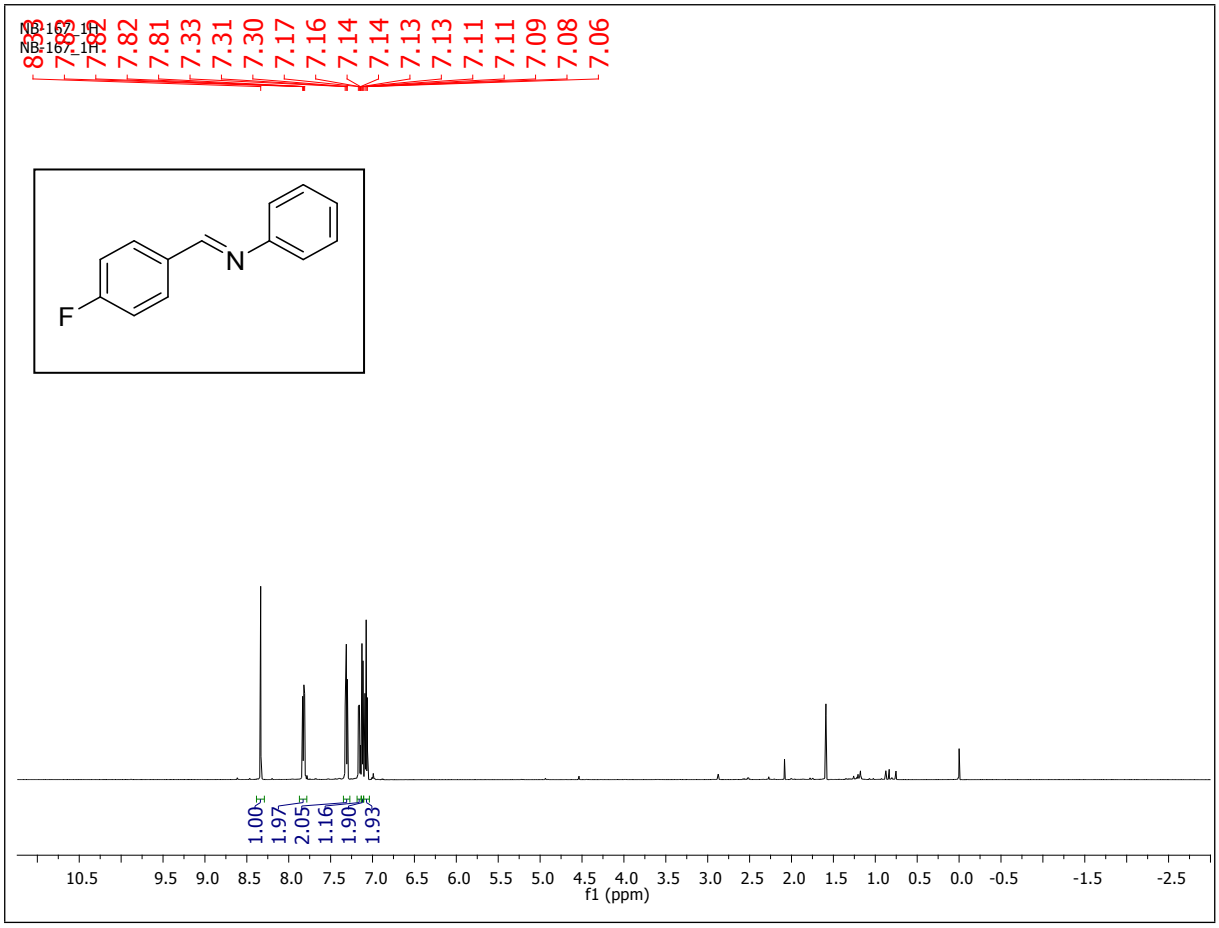
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N
F
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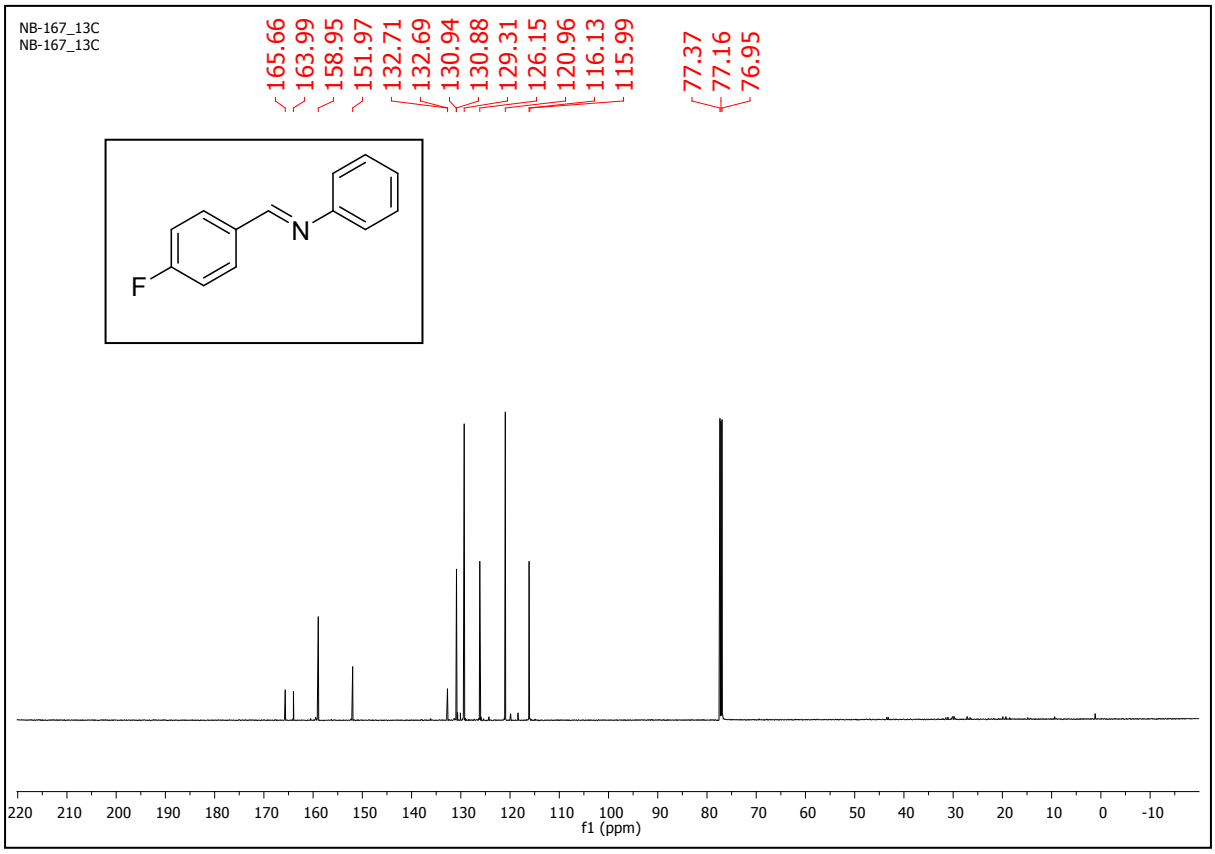
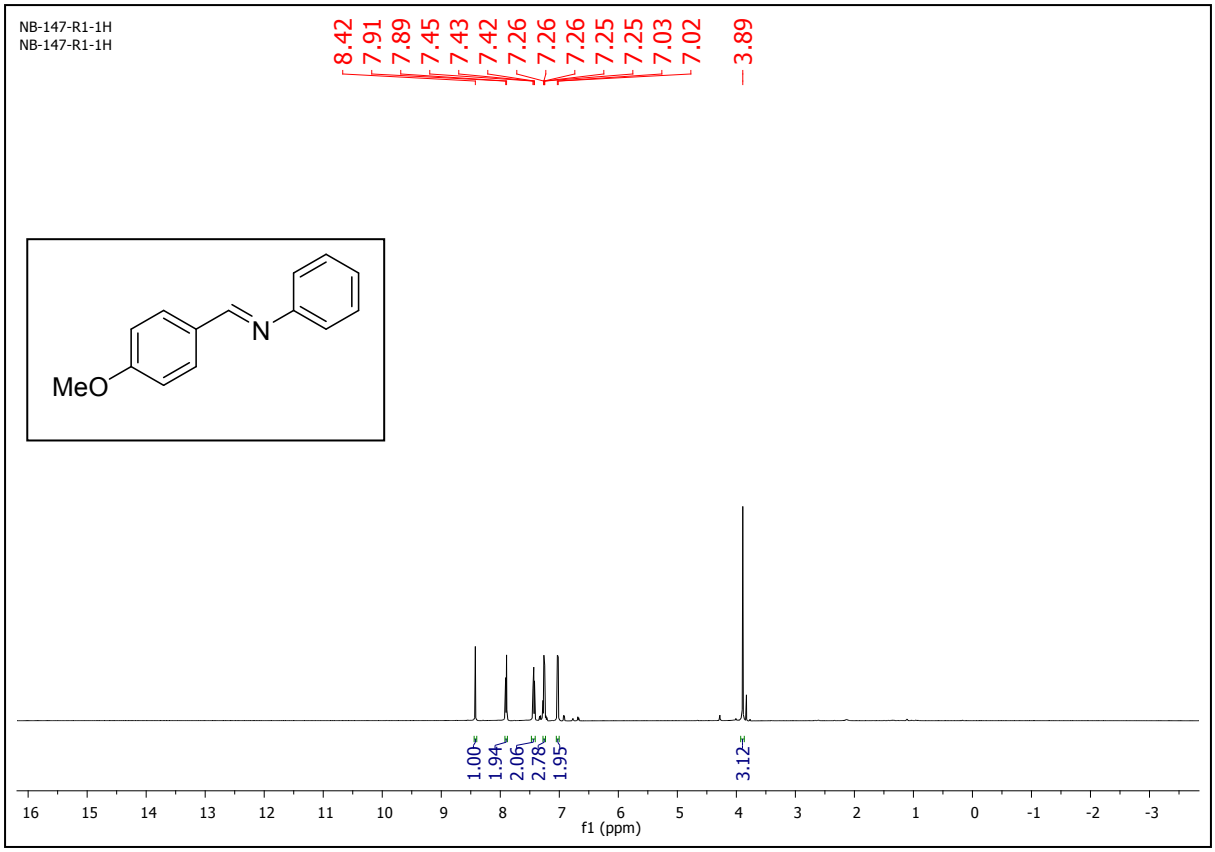
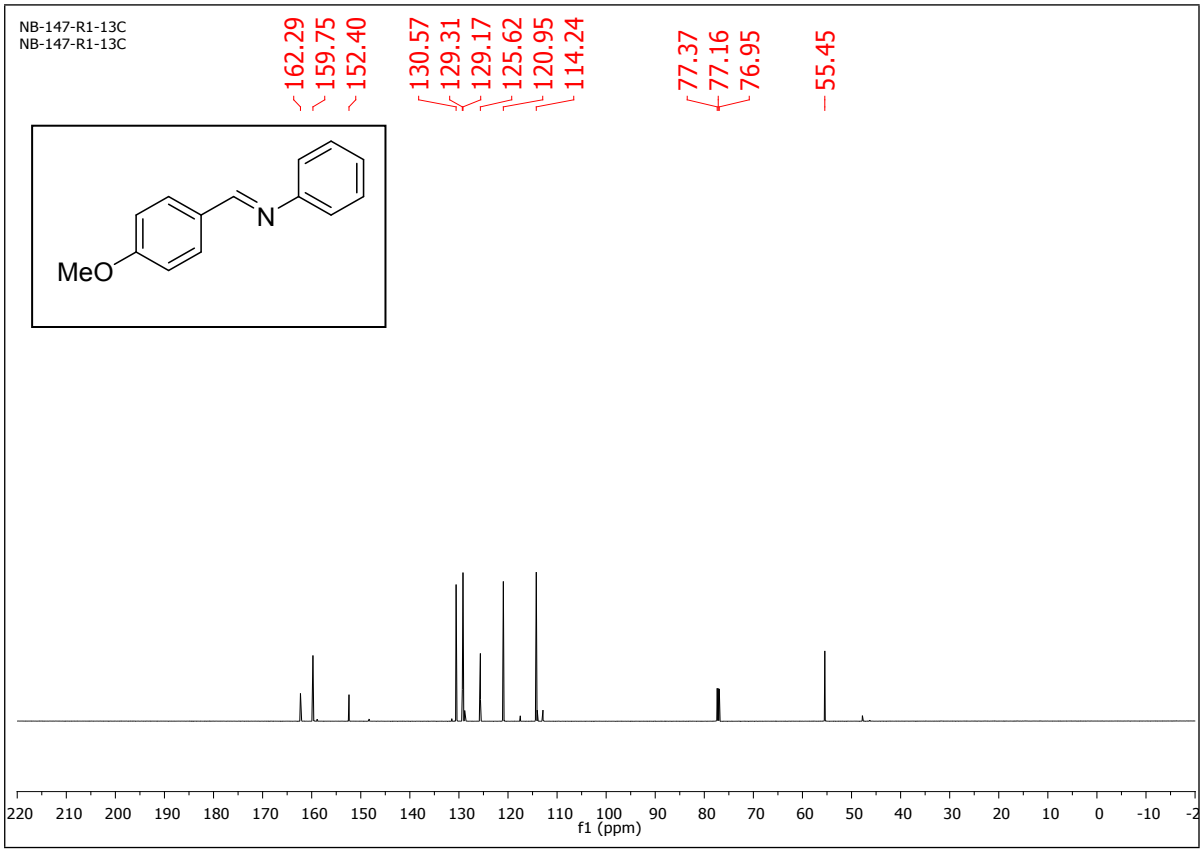
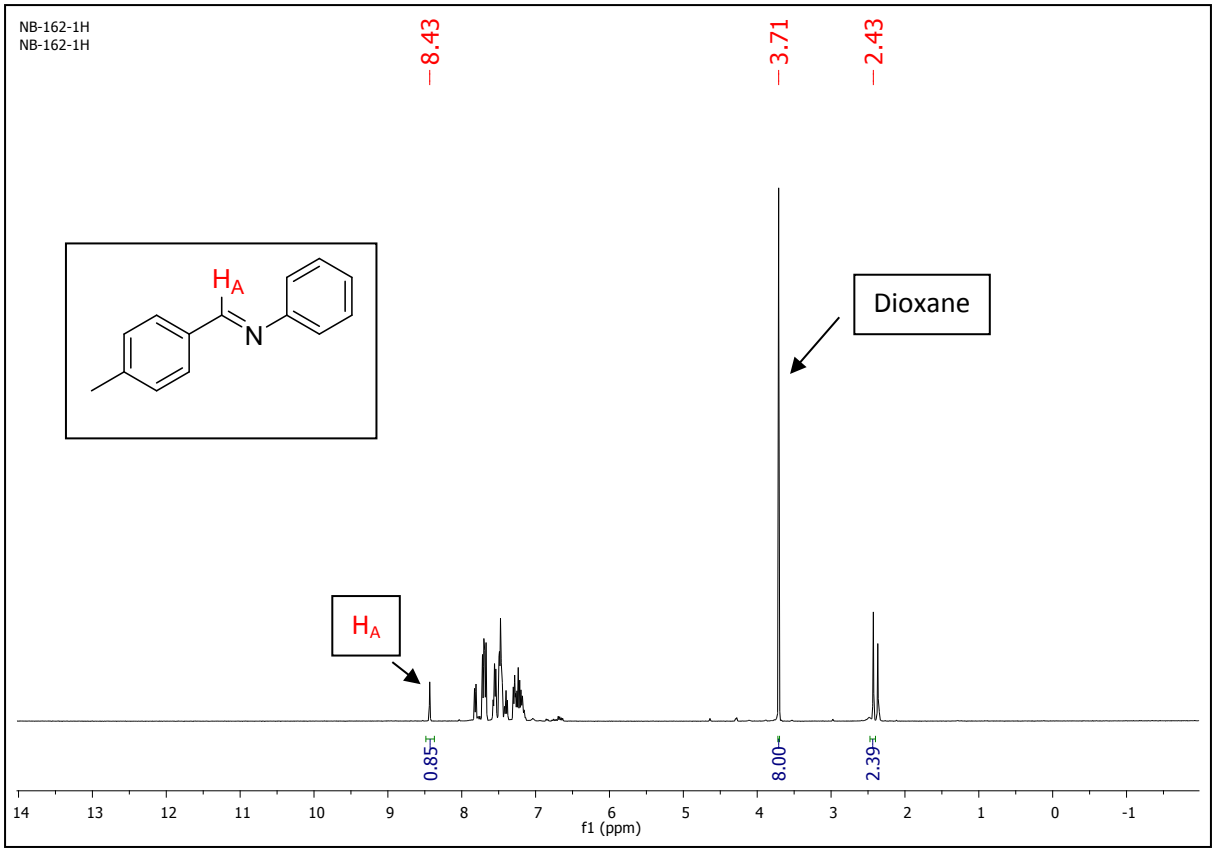
1.90
1.93
10.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.5
-2.5
f1 (ppm)

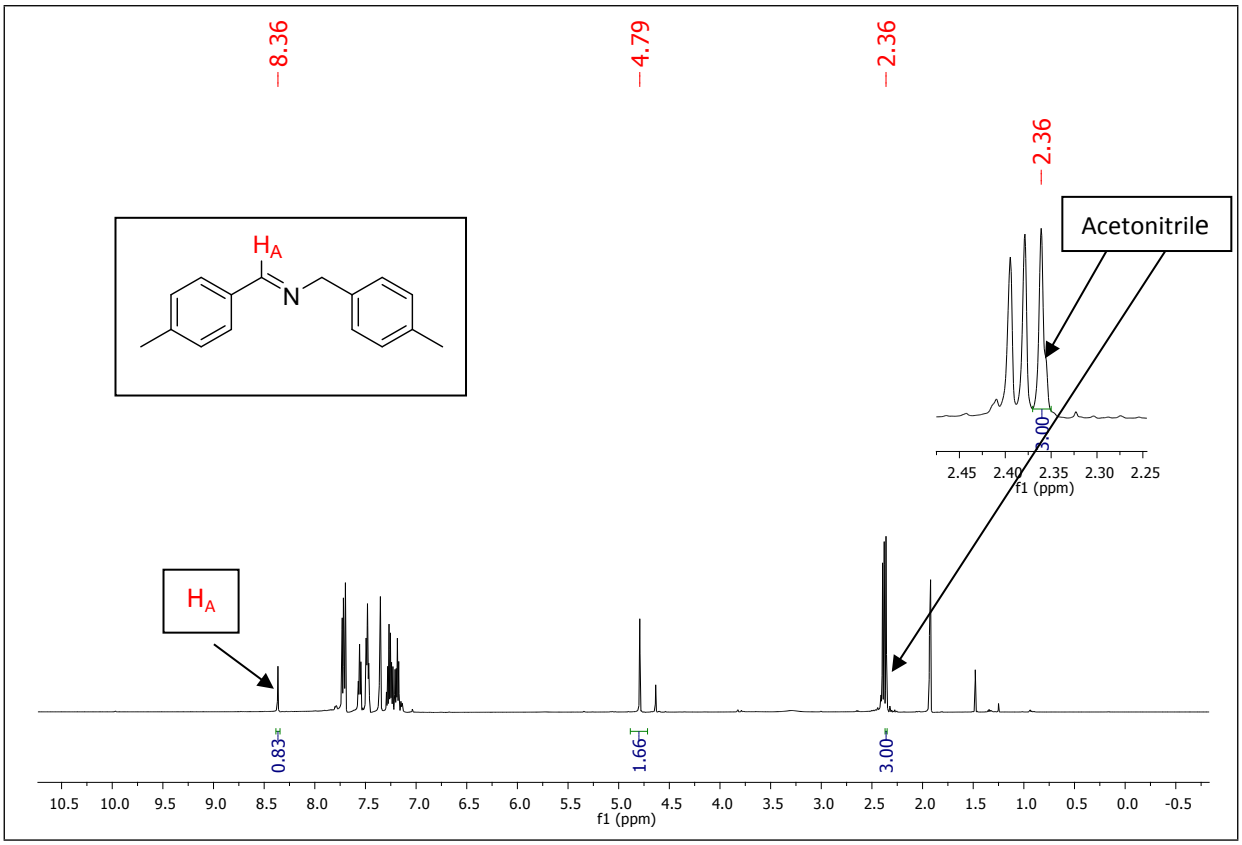

NB-167_13C
NB-167_13C
165.66
163.99
158.95
151.97
132.71
132.69
130.94
130.88
129.31
126.15
120.96
116.13
115.99
77.37
77.16
76.95
N
F
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


NB-147-R1-1H
NB-147-R1-1H
8.42
7.91
7.89
7.45
7.43
7.42
7.26
7.26
7.26
7.25
7.25
7.03
7.02
3.89
MeO
N
1.00
1.94
2.06
2.78
1.95
3.12
f1 (ppm)

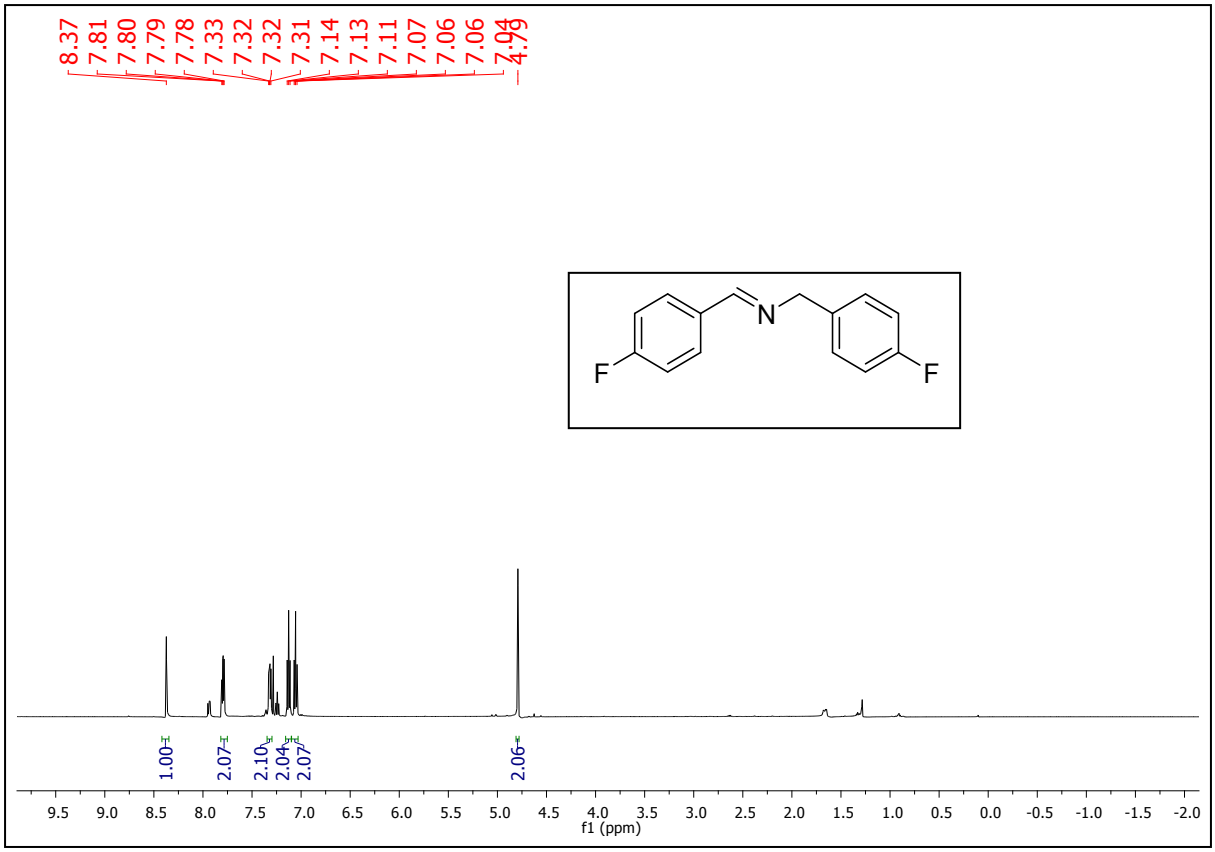

NB-147-R1-13C
NB-147-R1-13C
162.29
159.75
152.40
130.57
129.31
129.17
125.62
120.95
114.24
77.37
77.16
76.95
55.45
MeO
N
f1 (ppm)

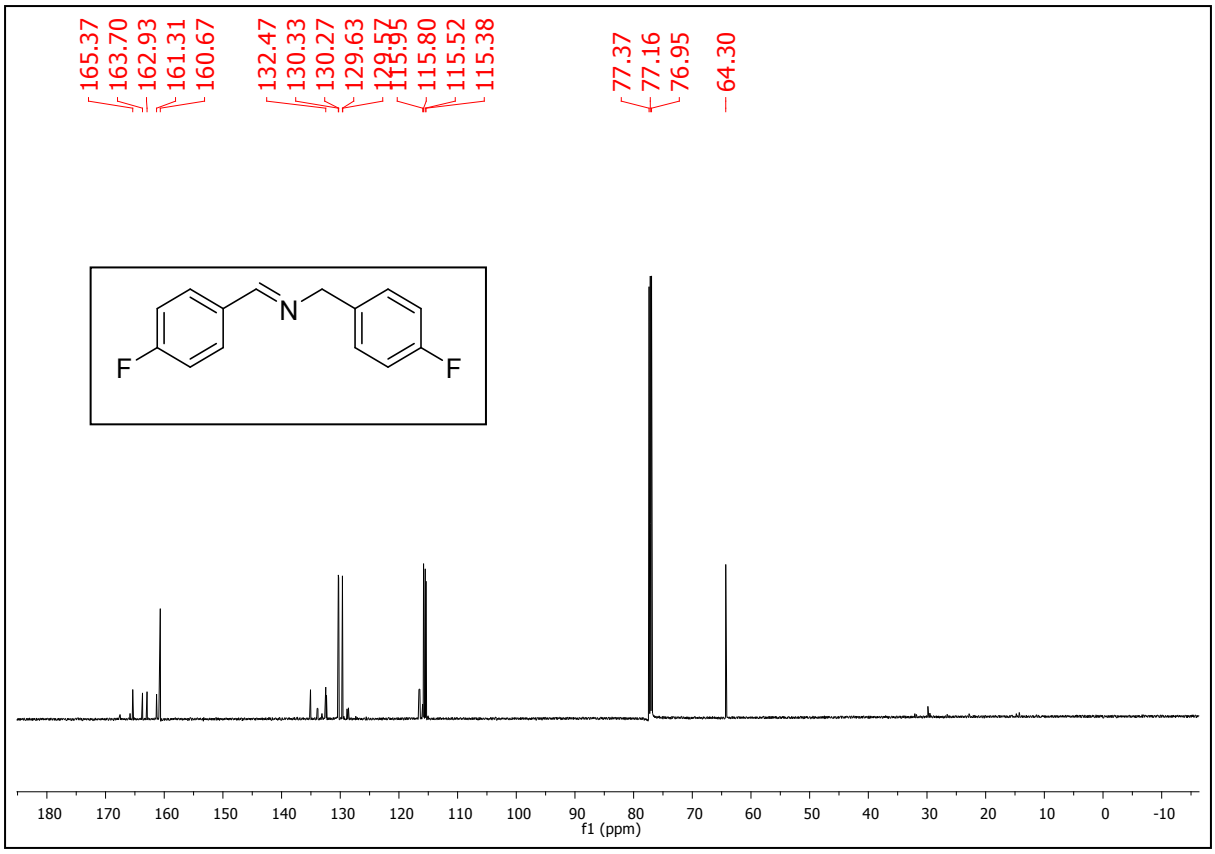


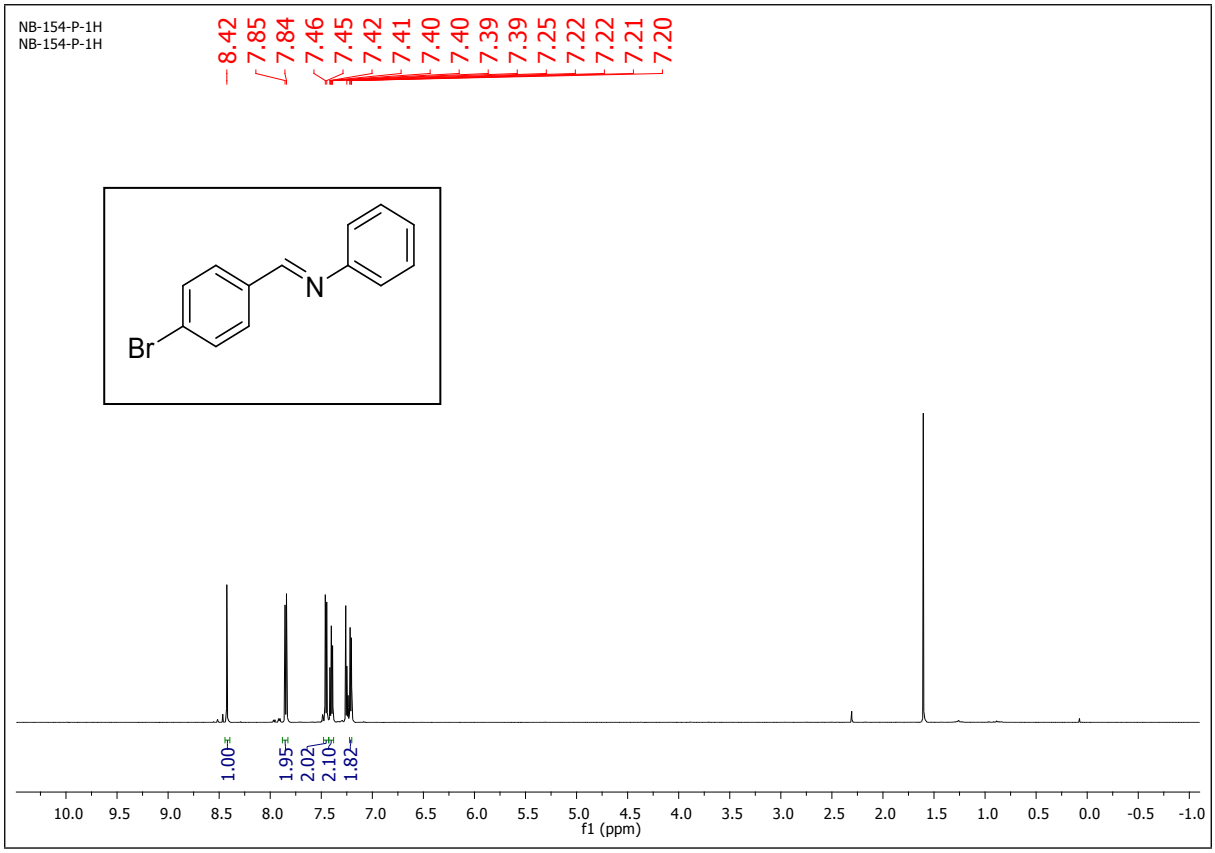
Reaction mixture of 4-methylbenzyl alcohol and phenyl azide using dioxane as internal standard

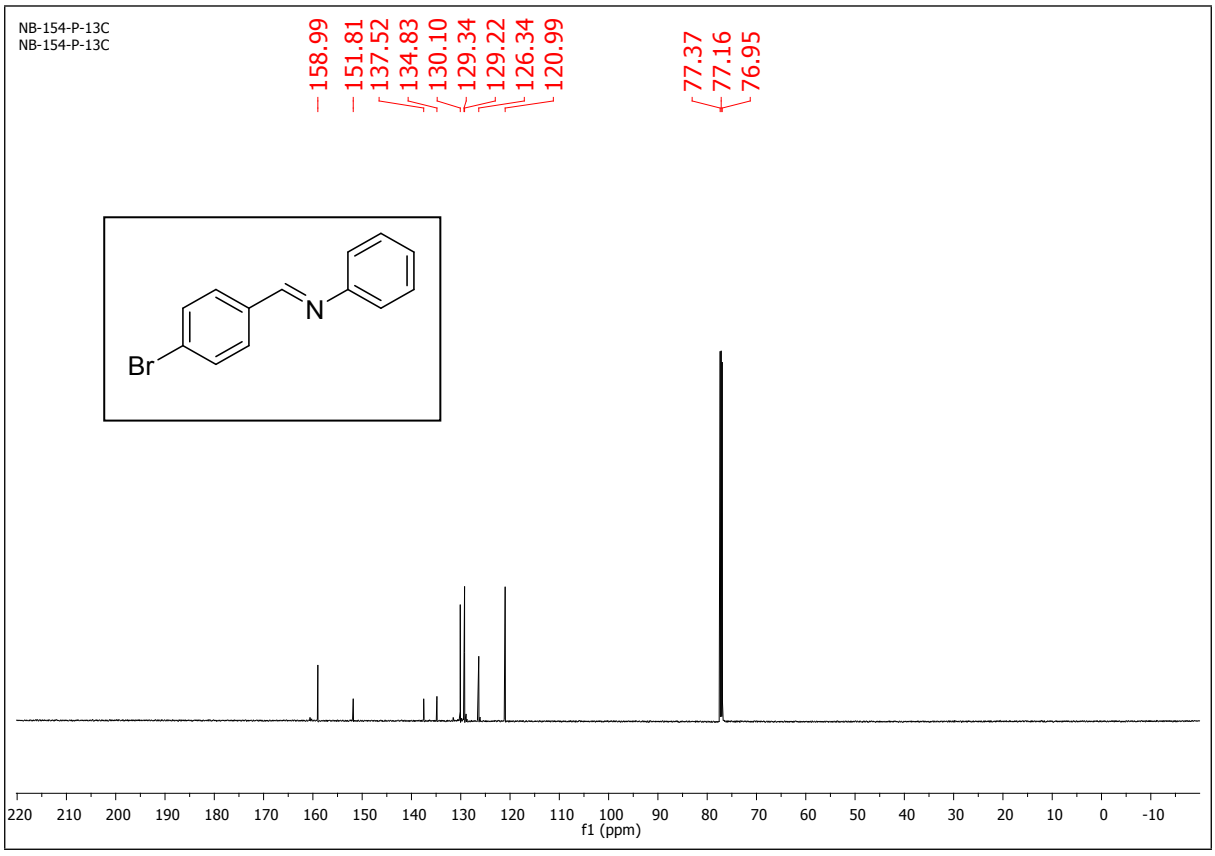


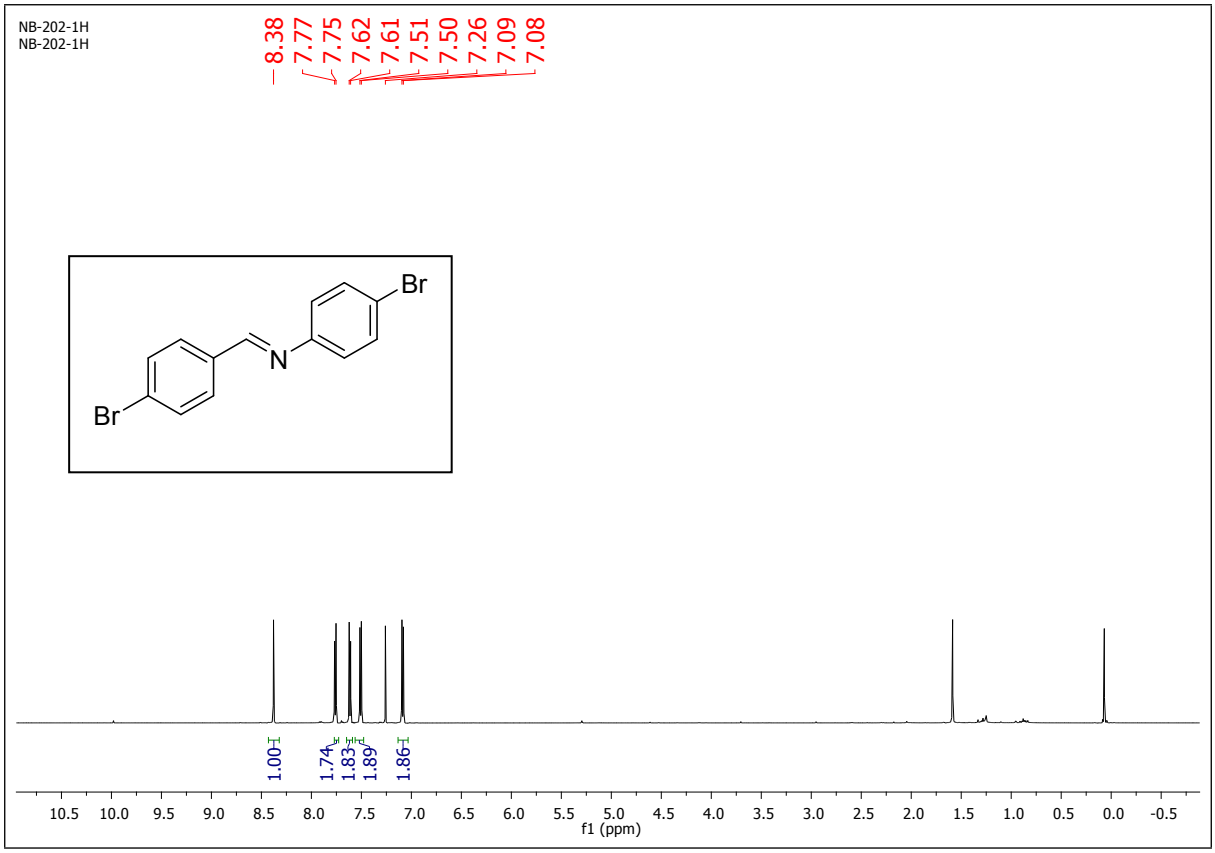
Reaction mixture of 4-methylbenzyl alcohol and 4-methylbenzyl azide using Acetonitrile as internal standard

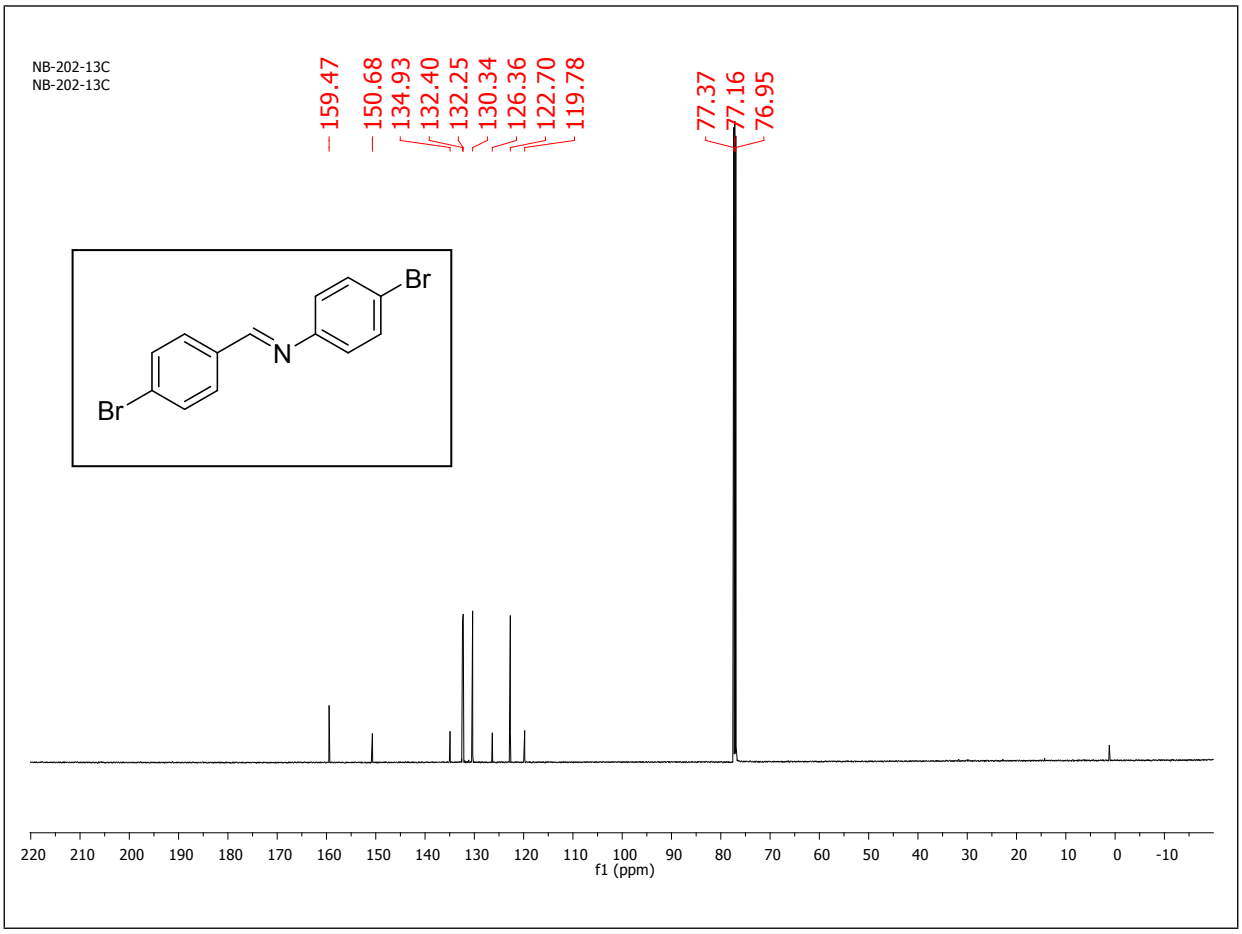

8.37
7.81
7.80
7.79
7.78
7.33
7.32
7.32
7.31
7.14
7.13
7.11
7.07
7.06
7.06
7.04
4.79
N
F
F
1.00
2.07
2.10
2.04
2.07
2.06
f1 (ppm)

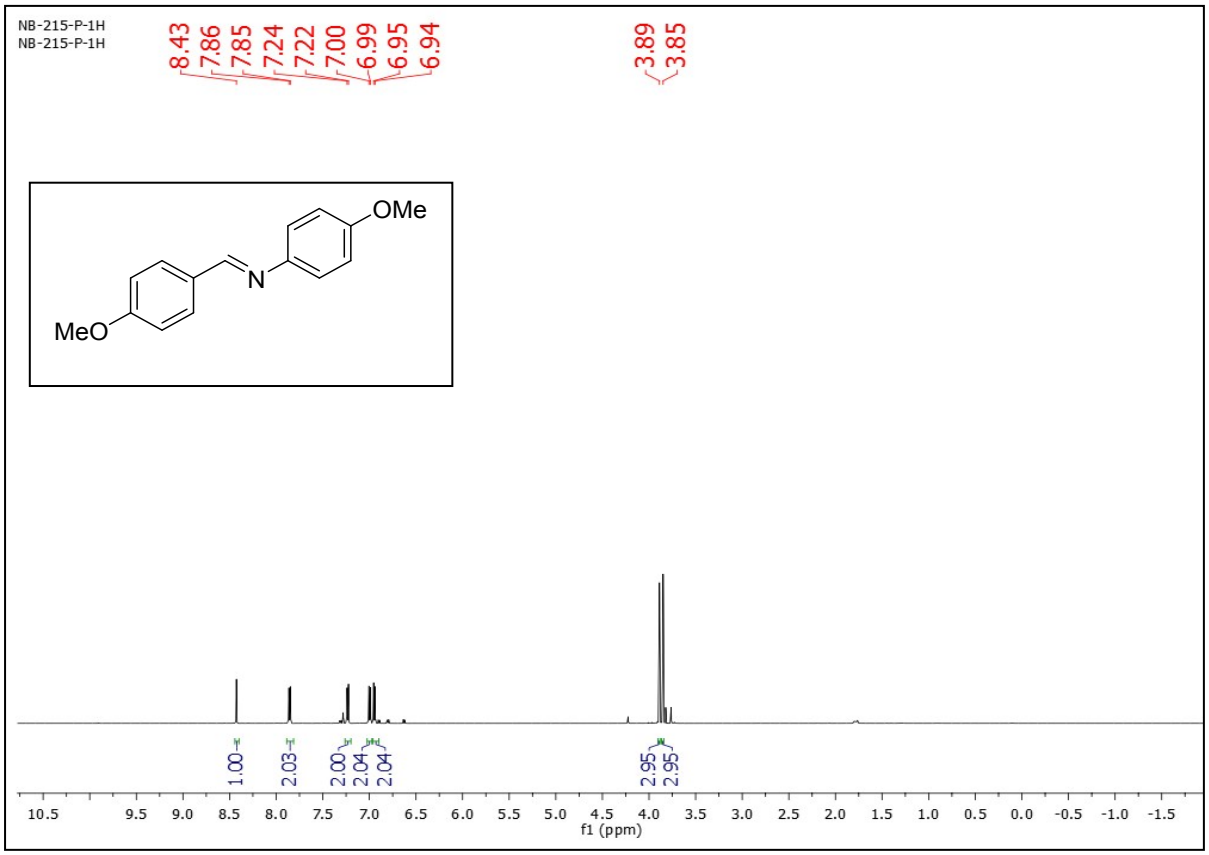

165.37
163.70
162.93
161.31
160.67
132.47
130.33
130.27
129.63
115.80
115.52
115.38
77.37
77.16
76.95
64.30
N
F
F
f1 (ppm)

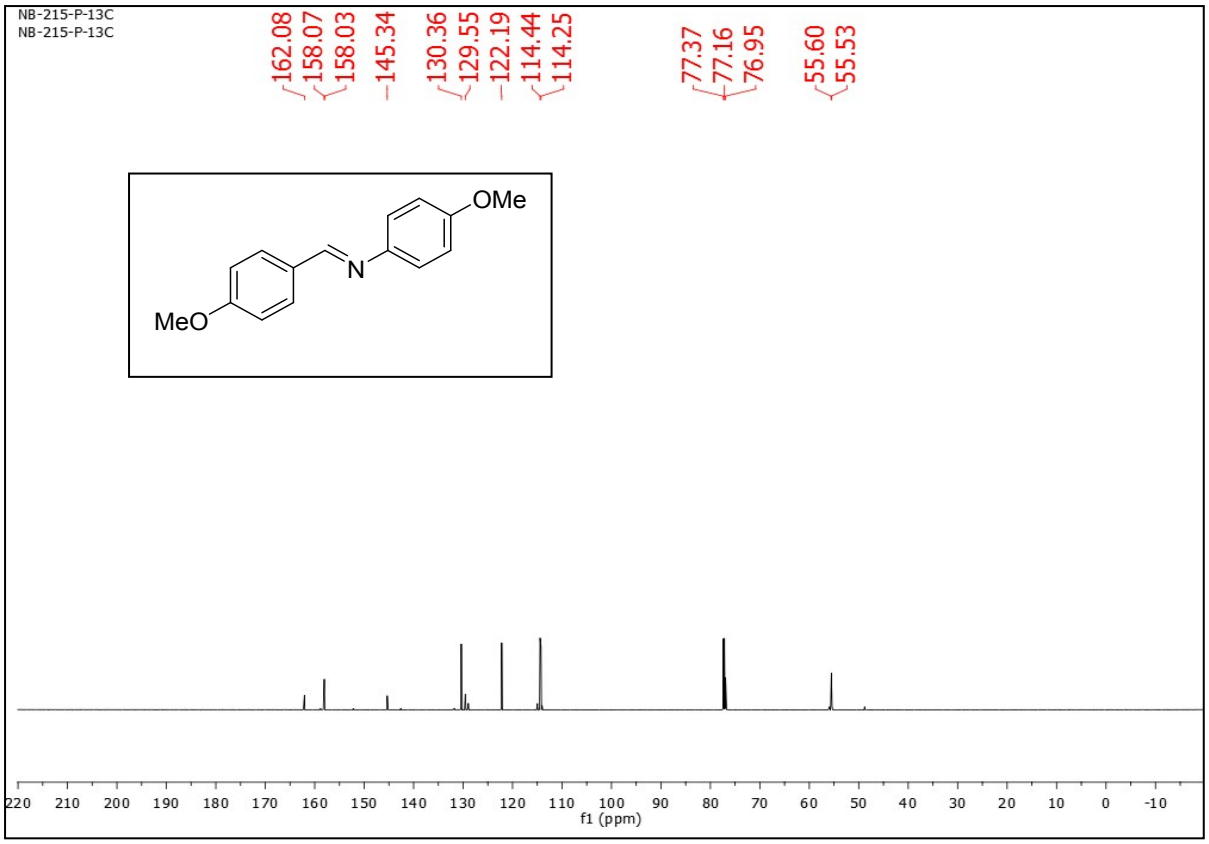

NB-154-P-1H
NB-154-P-1H
8.42
7.85
7.84
7.46
7.45
7.42
7.41
7.40
7.40
7.39
7.39
7.25
7.22
7.22
7.21
7.20
Br
N
1.00
1.95
2.02
2.10
1.82
f1 (ppm)

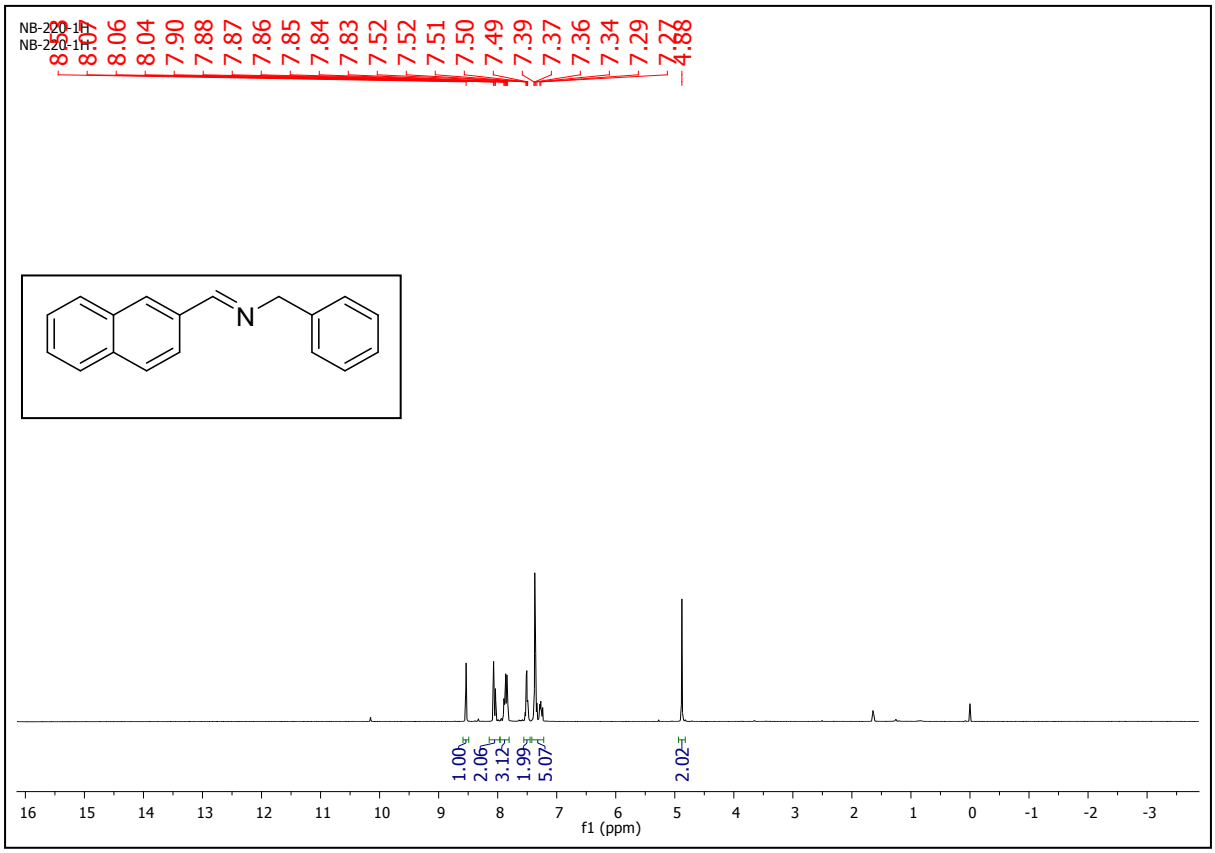

NB-154-P-13C
NB-154-P-13C
158.99
151.81
137.52
134.83
130.10
129.34
129.22
126.34
120.99
77.37
77.16
76.95
Br
N
f1 (ppm)

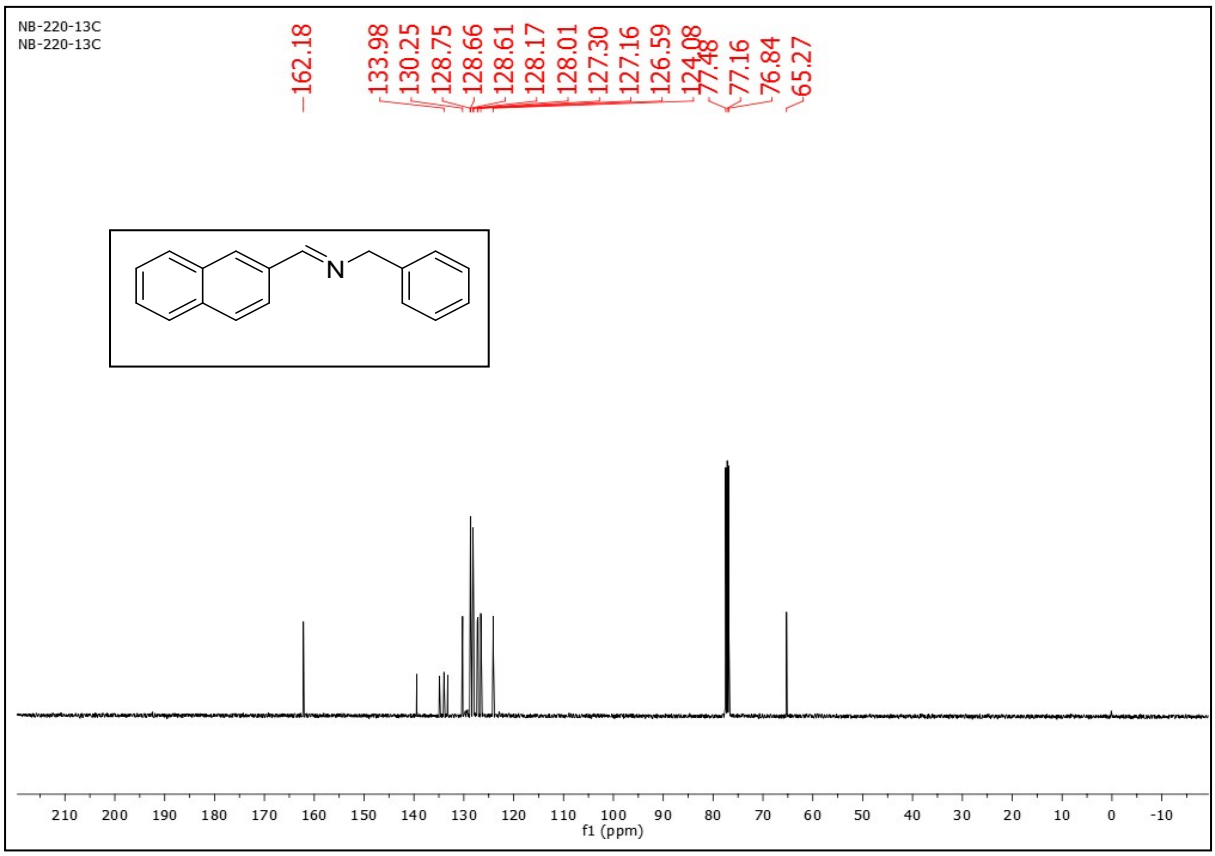

NB-202-1H
NB-202-1H
8.38
7.77
7.75
7.62
7.61
7.51
7.50
7.26
7.09
7.08
Br
N
Br
1.00
1.74
1.83
1.89
1.86
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

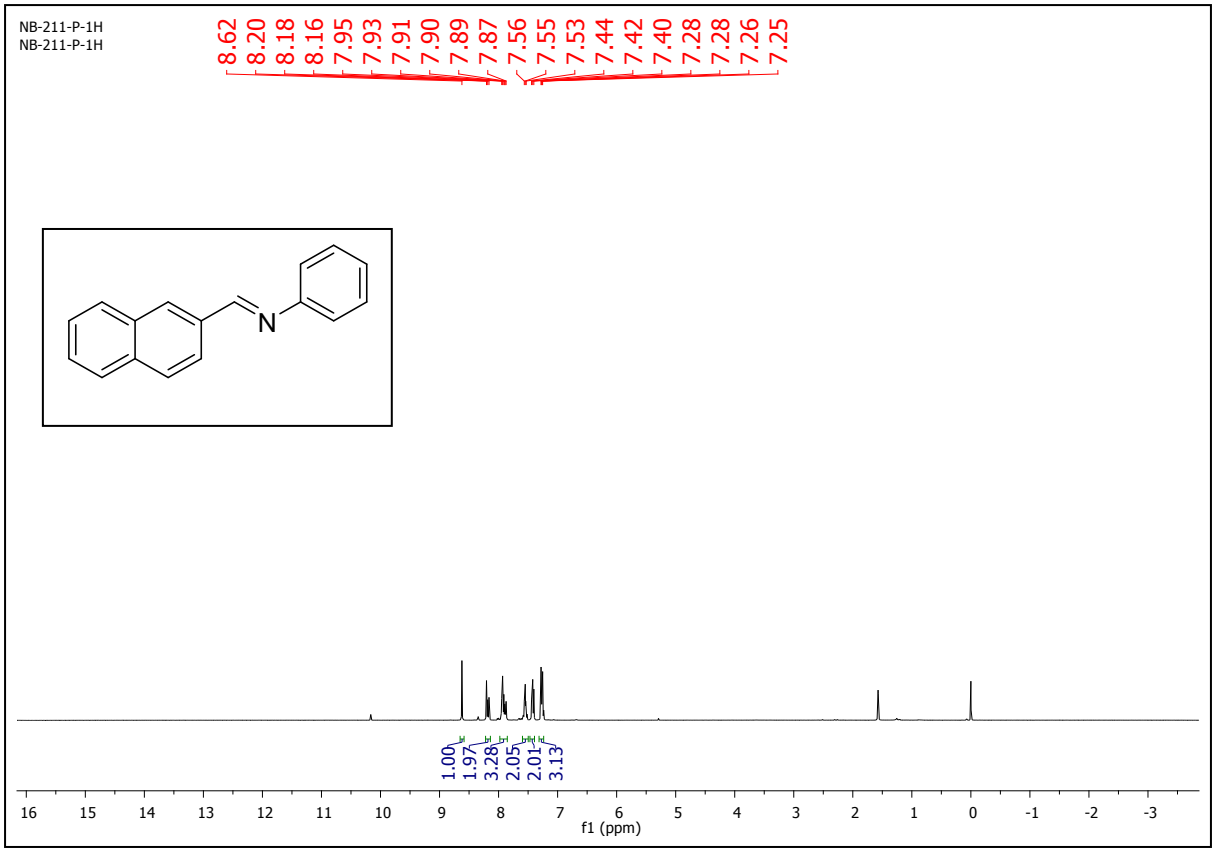

NB-202-13C
NB-202-13C
159.47
150.68
134.93
132.40
132.25
130.34
126.36
122.70
119.78
77.37
77.16
76.95
Br
N
Br
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

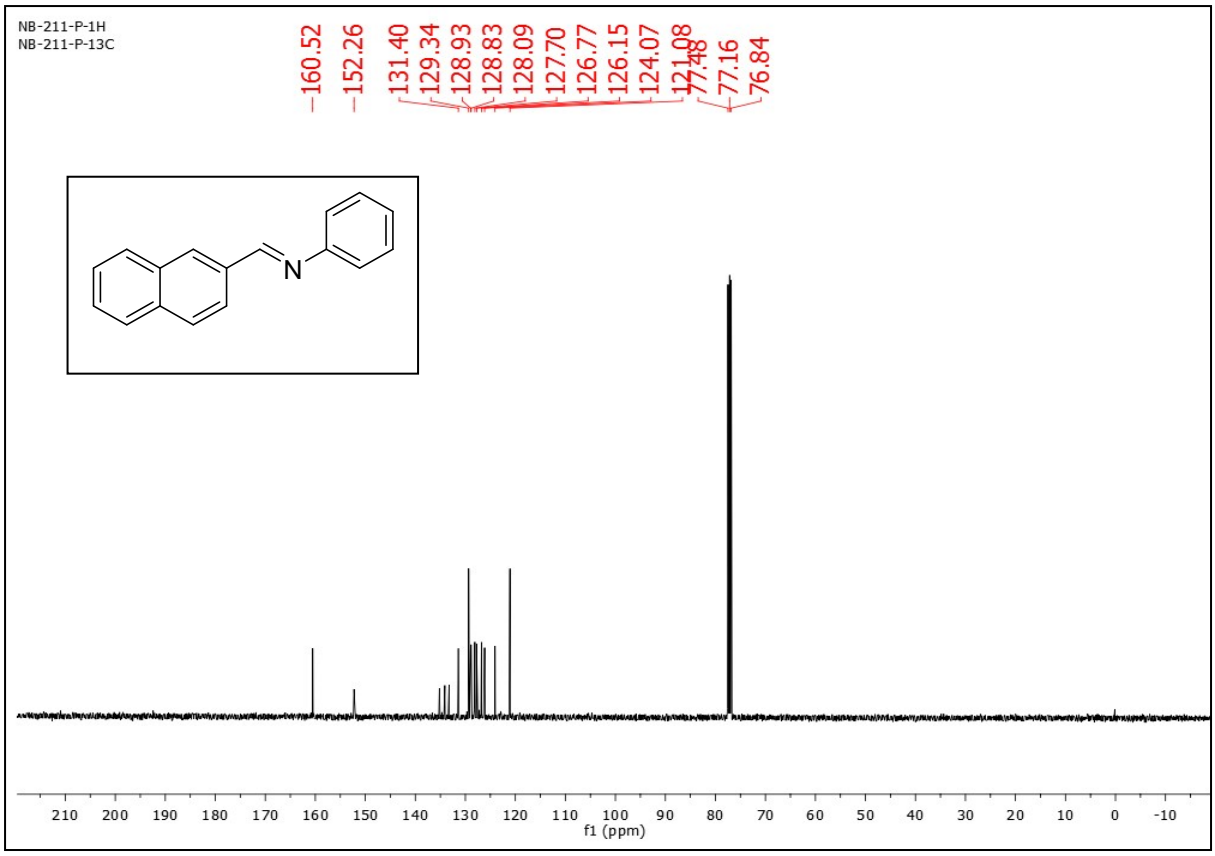

NB-215-P-1H
NB-215-P-1H
8.43
7.86
7.85
7.24
7.22
7.00
6.99
6.95
6.94
3.89
3.85
OMe
N
MeO
1.00
2.03
2.00
2.04
2.04
2.95
2.95
f1 (ppm)

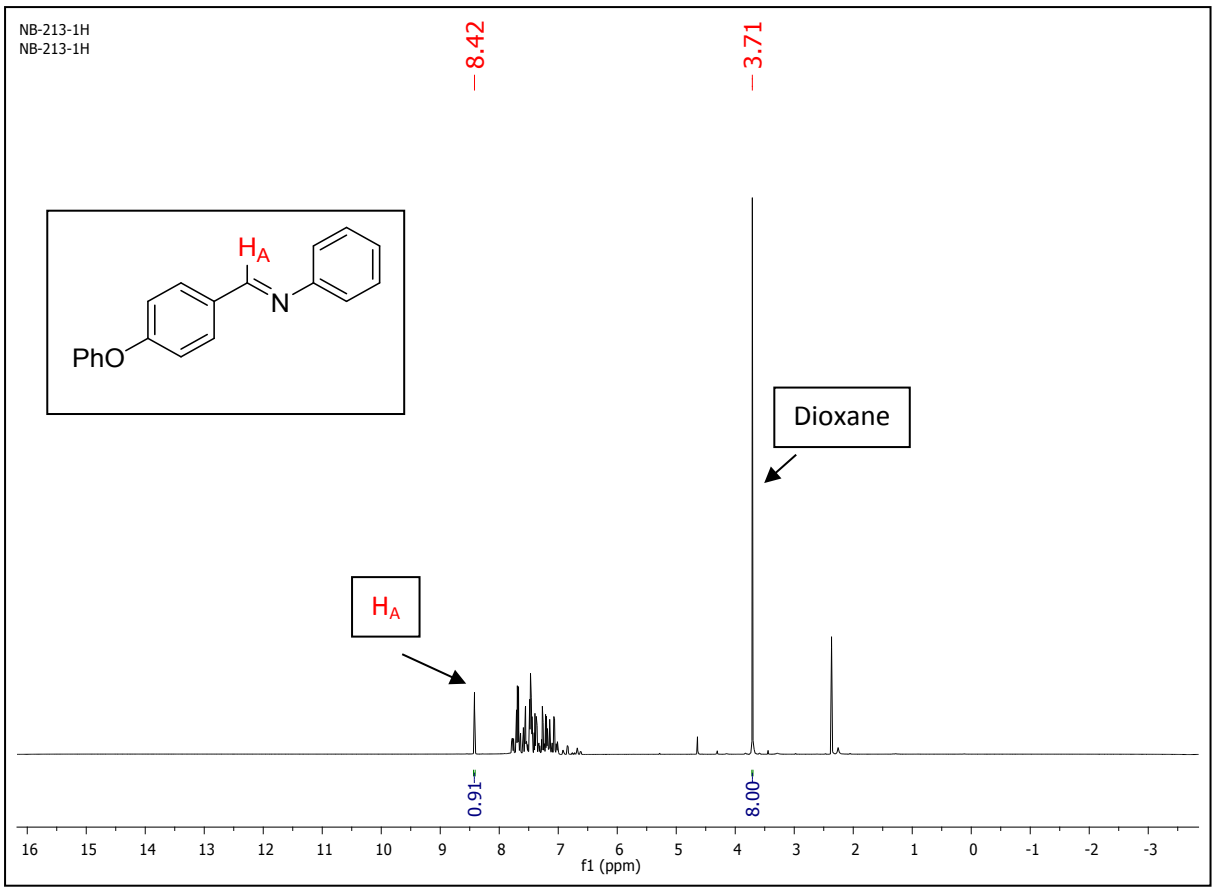

NB-215-P-13C
NB-215-P-13C
162.08
158.07
158.03
145.34
130.36
129.55
122.19
114.44
114.25
77.37
77.16
76.95
55.60
55.53
OMe
N
MeO
f1 (ppm)


NB-220-1H
NB-220-1H
8.09
8.07
8.06
8.04
7.90
7.88
7.87
7.86
7.85
7.84
7.83
7.52
7.52
7.51
7.50
7.49
7.39
7.37
7.36
7.34
7.29
7.27
4.88
N
1.00
2.06
3.12
1.99
5.07
2.02
f1 (ppm)

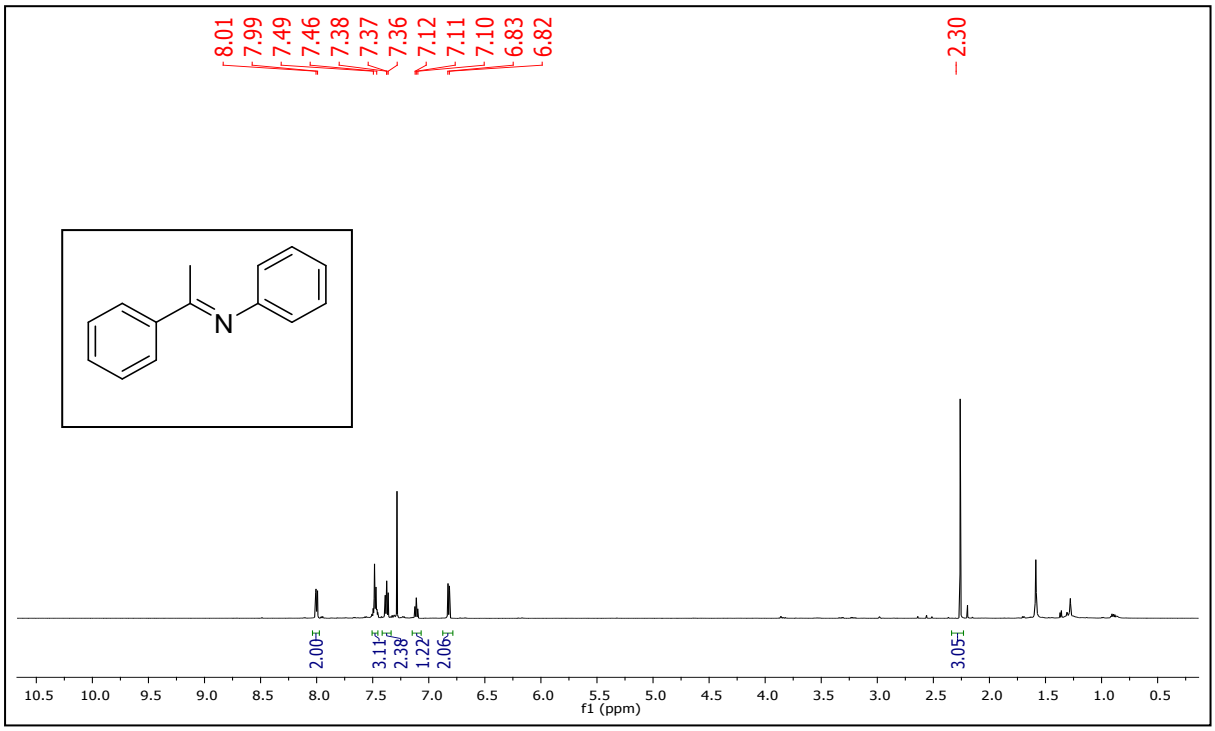

NB-220-13C
NB-220-13C
162.18
133.98
130.25
128.75
128.66
128.61
128.17
128.01
127.30
127.16
126.59
124.08
77.48
77.16
76.84
65.27
N
f1 (ppm)

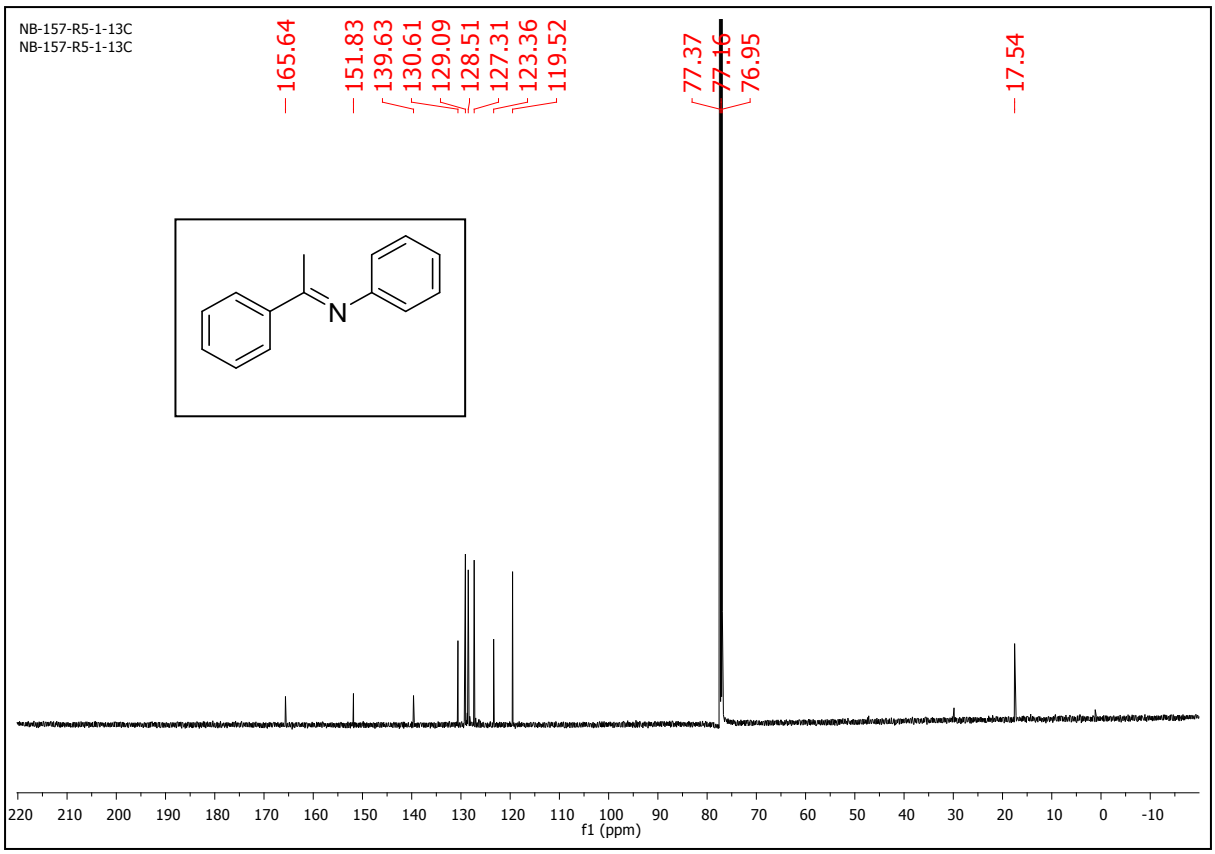

NB-211-P-1H
NB-211-P-1H
8.62
8.20
8.18
8.16
7.95
7.93
7.91
7.90
7.89
7.87
7.56
7.55
7.53
7.44
7.42
7.40
7.28
7.28
7.26
7.25
N
1.00
1.97
3.28
2.05
2.01
3.13
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

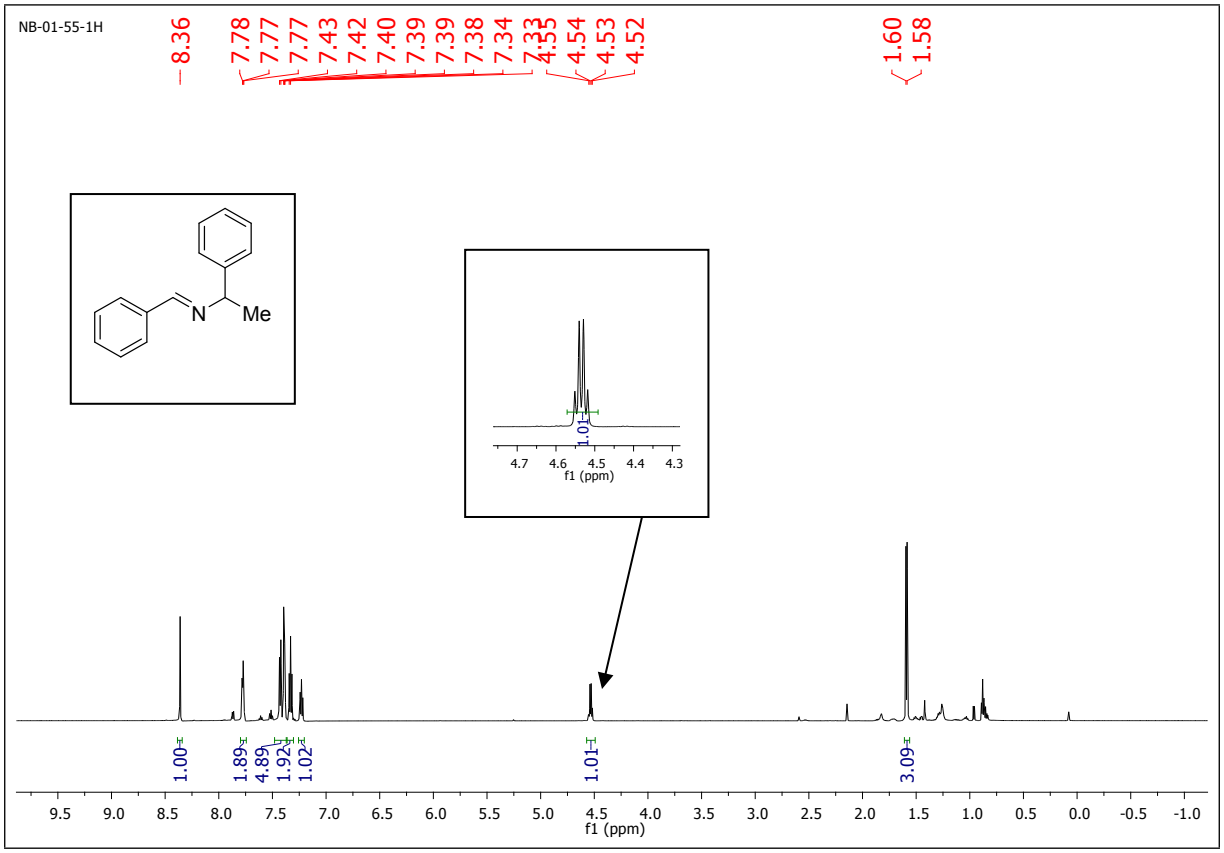

NB-211-P-1H
NB-211-P-13C
160.52
152.26
131.40
129.34
128.93
128.83
128.09
127.70
126.77
126.15
124.07
121.08
77.48
77.16
76.84
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

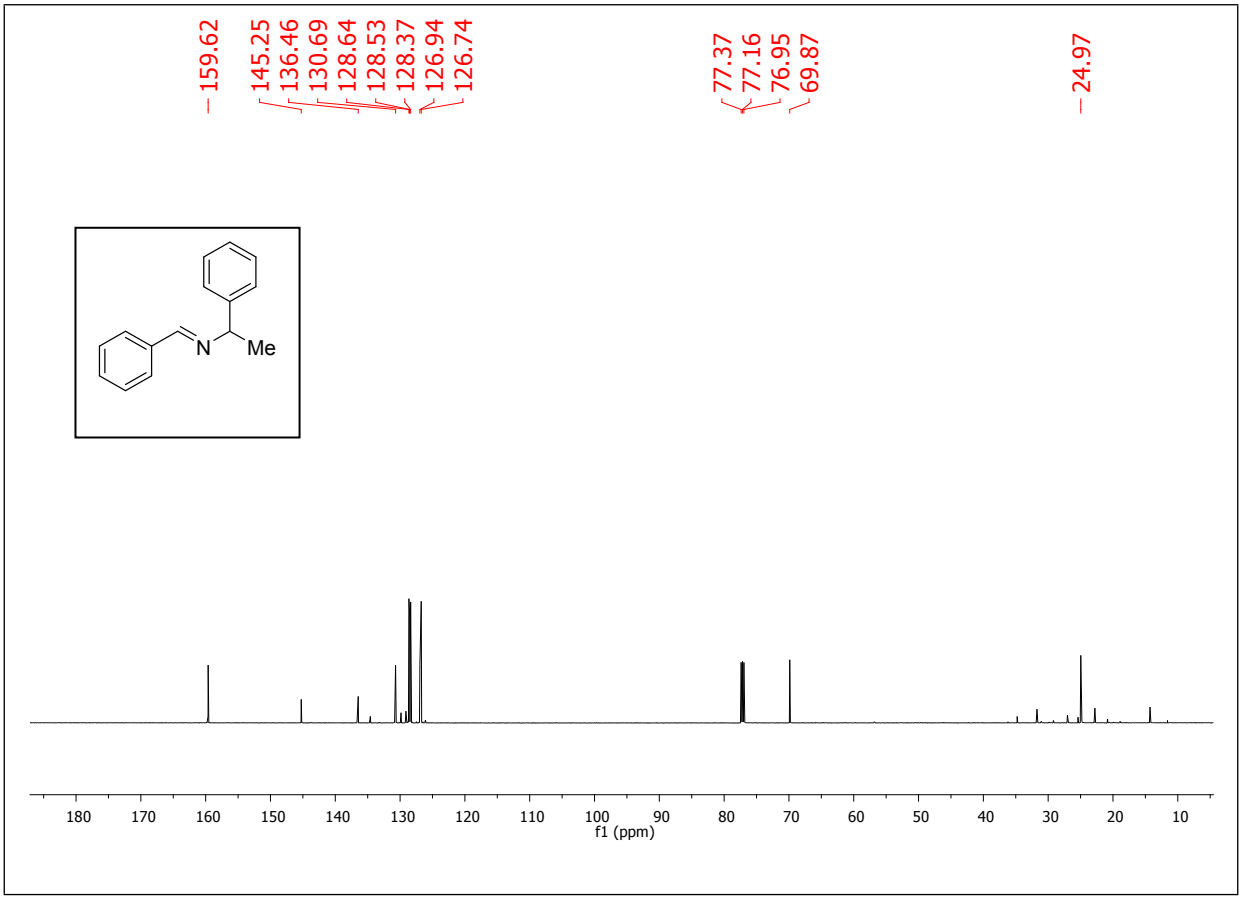


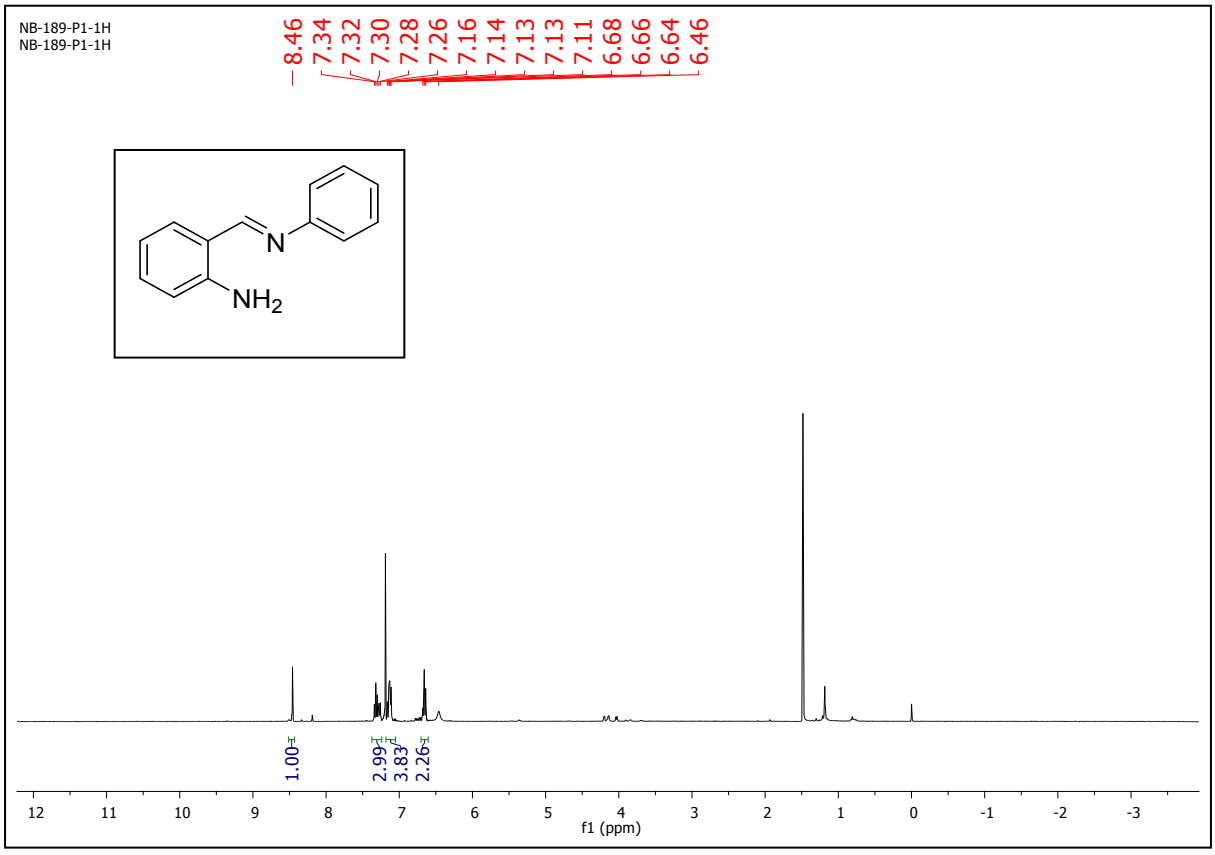
Reaction mixture of 4-phenoxybenzyl alcohol and phenyl azide using dioxane as internal standard

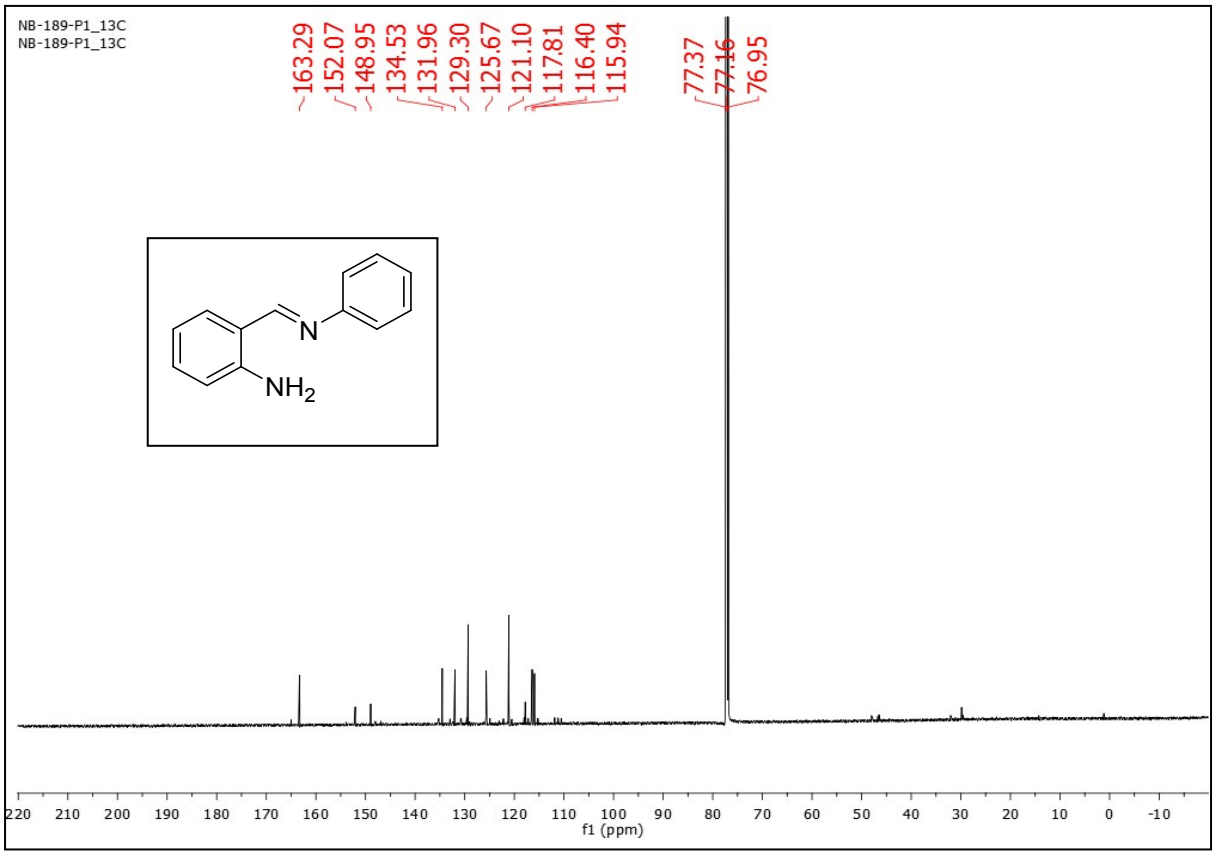


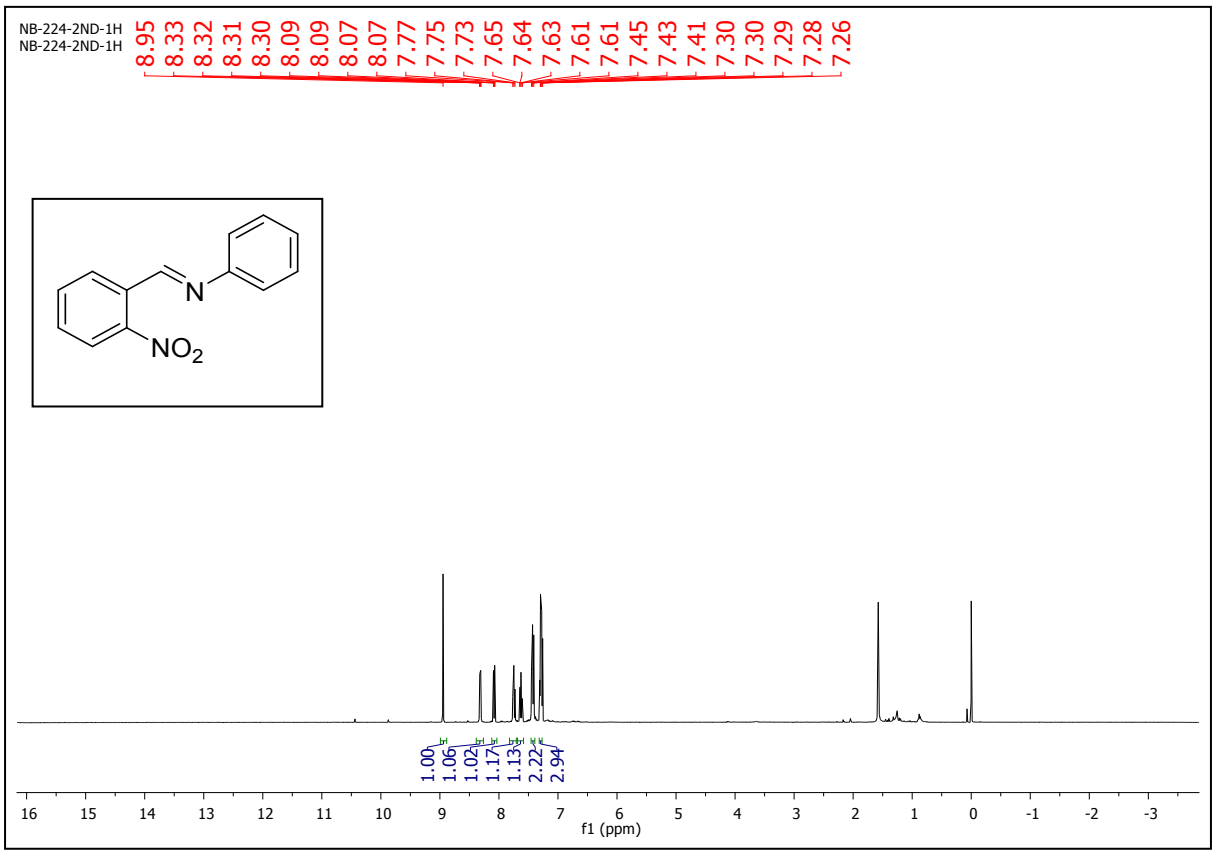

NB-157-R5-1-13C
NB-157-R5-1-13C
165.64
151.83
139.63
130.61
129.09
128.51
127.31
123.36
119.52
77.37
77.16
76.95
17.54
N
f1 (ppm)

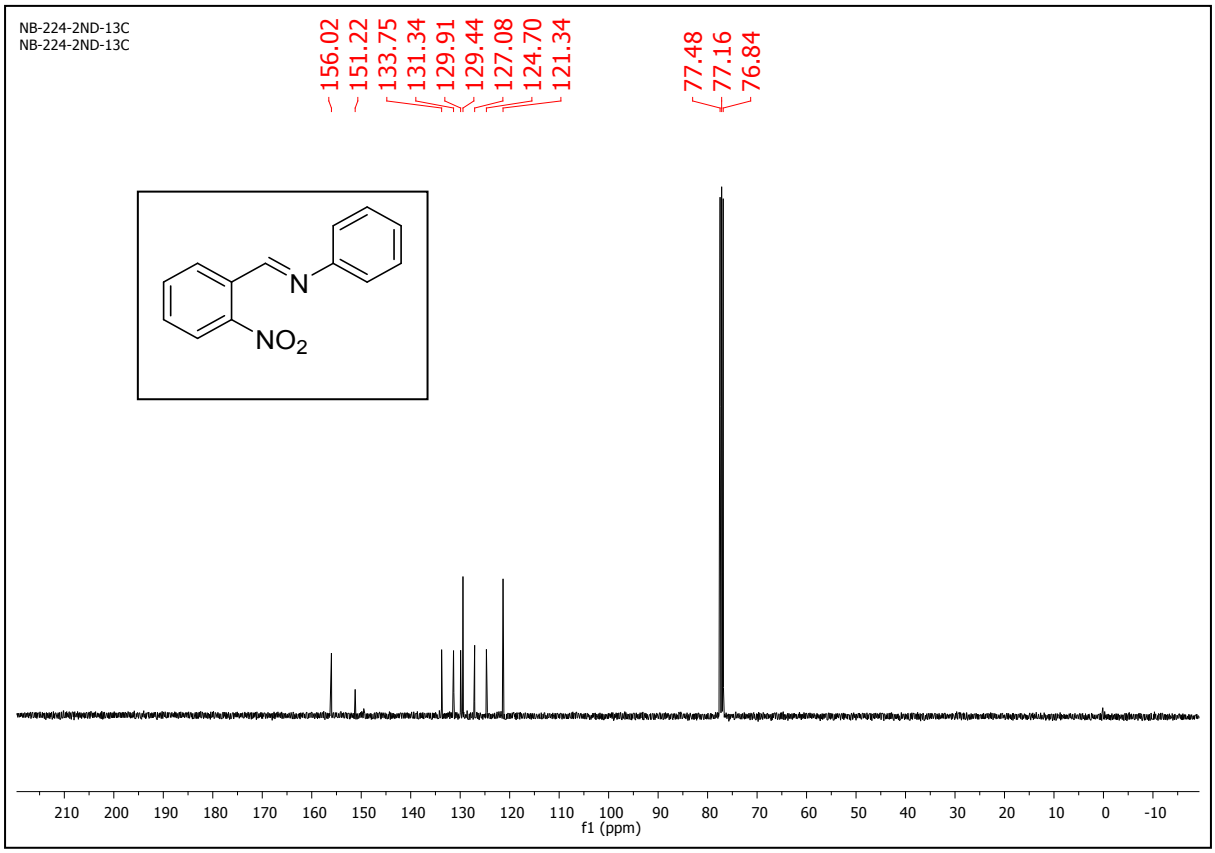

NB-01-55-1H
8.36
7.78
7.77
7.77
7.43
7.42
7.40
7.39
7.39
7.38
7.34
7.33
4.55
4.54
4.53
4.52
1.60
1.58
N
Me
1.01
f1 (ppm)
1.00
1.89
4.89
1.92
1.02
1.01
3.09
f1 (ppm)

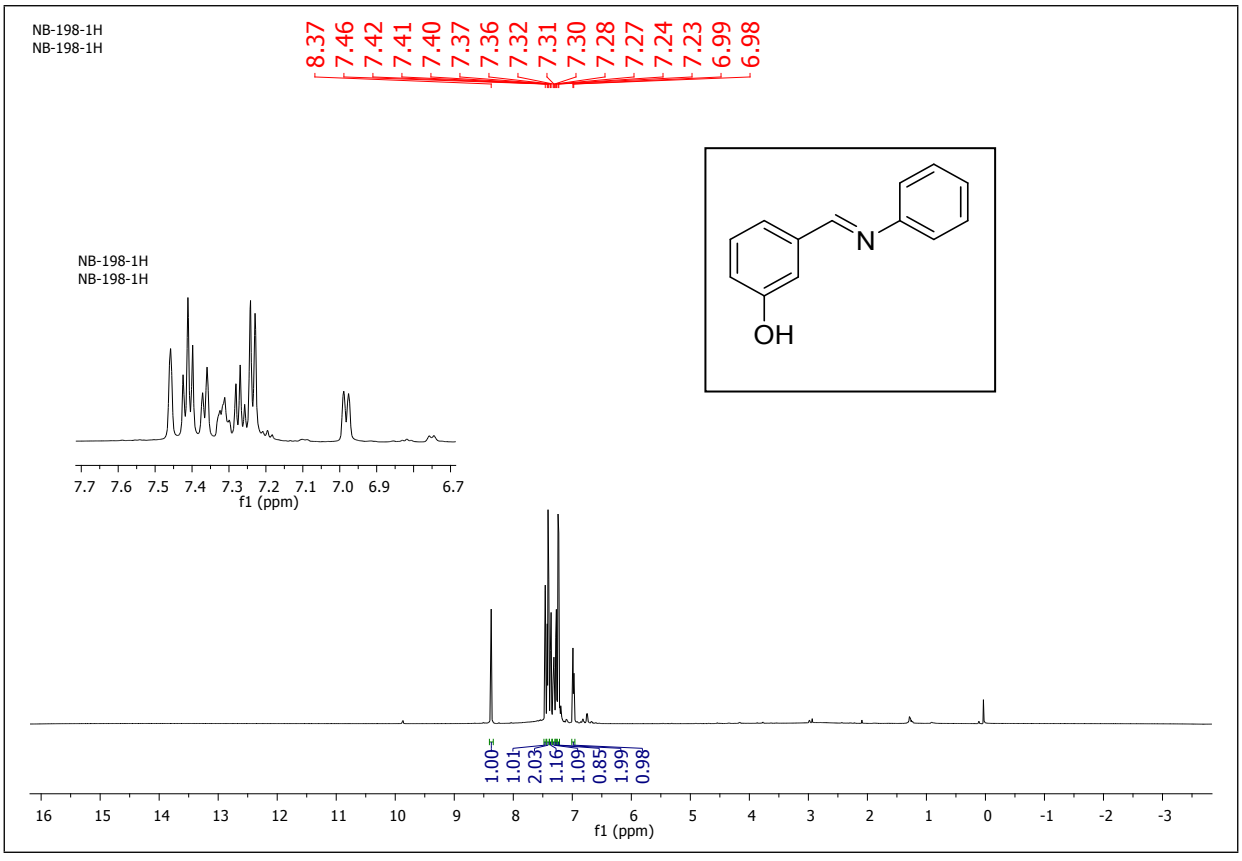

159.62
145.25
136.46
130.69
128.64
128.53
128.37
126.94
126.74
77.37
77.16
76.95
69.87
24.97
N
Me
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

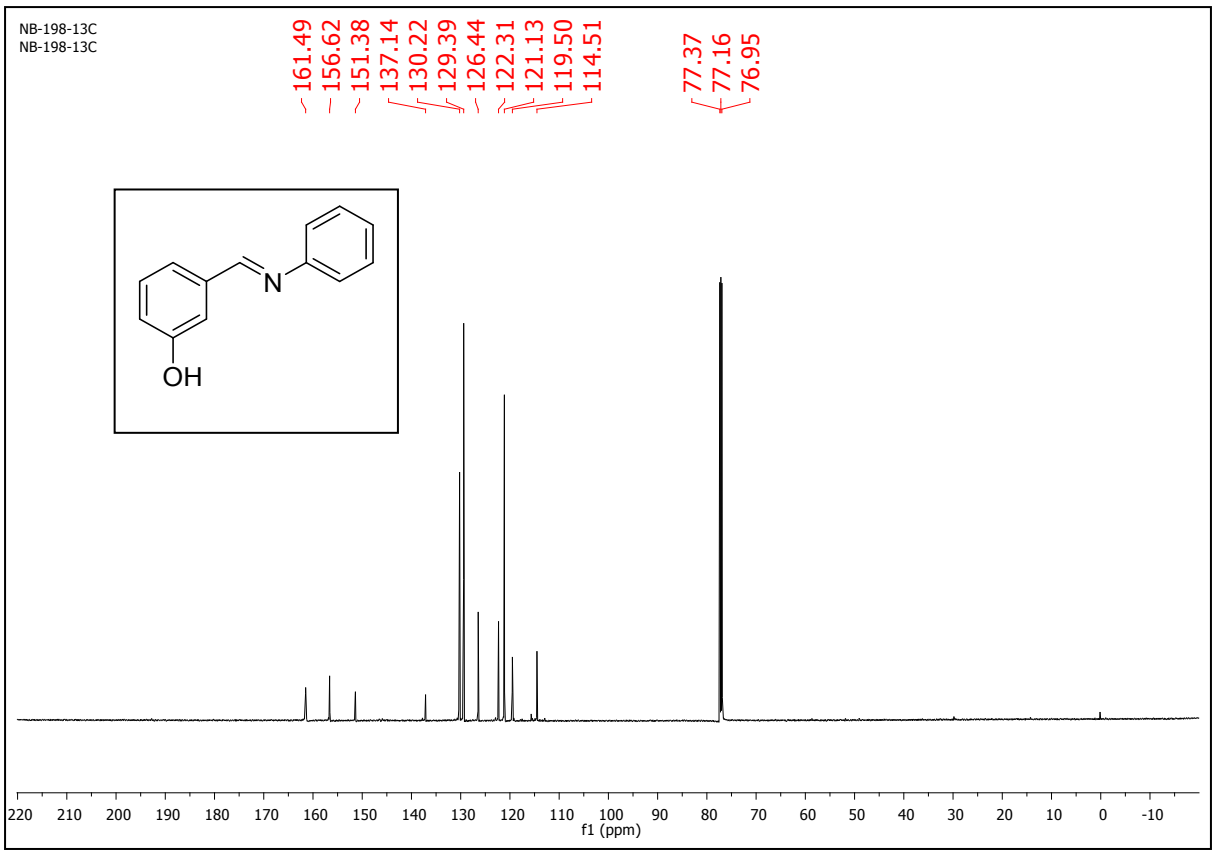

NB-189-P1-1H
NB-189-P1-1H
8.46
7.34
7.32
7.30
7.28
7.26
7.16
7.14
7.13
7.13
7.11
6.68
6.66
6.64
6.46
N
NH2
1.00
2.99
3.83
2.26
12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

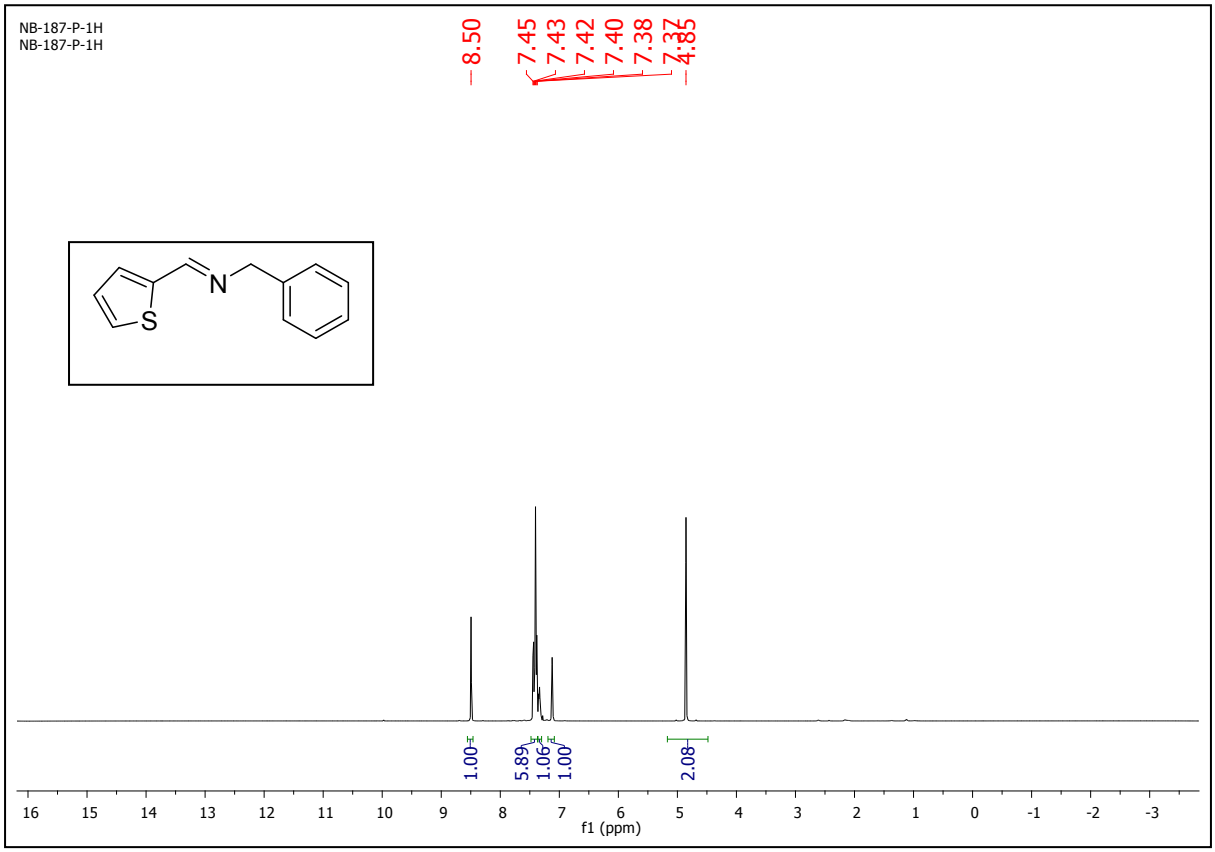

NB-189-P1_13C
NB-189-P1_13C
163.29
152.07
148.95
134.53
131.96
129.30
125.67
121.10
117.81
116.40
115.94
77.37
77.16
76.95
N
NH2
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

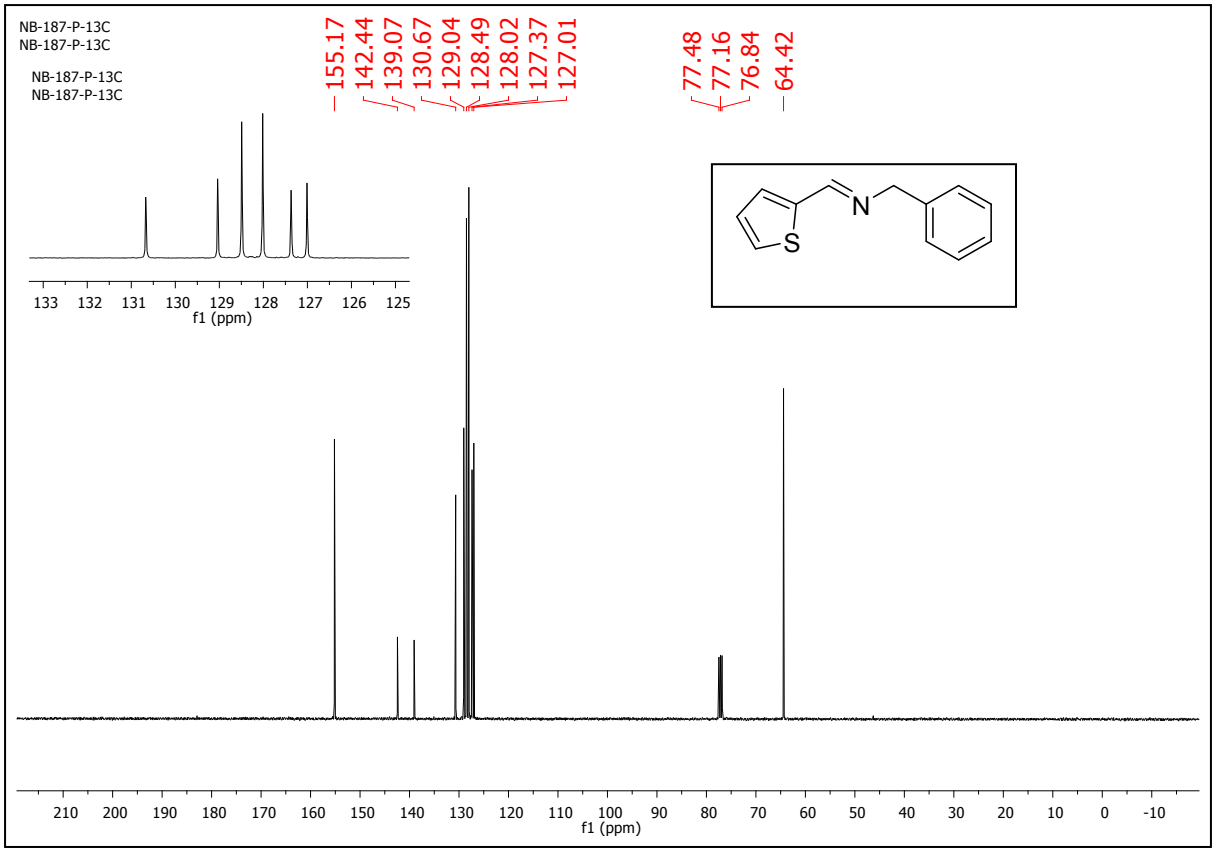

NB-224-2ND-1H
NB-224-2ND-1H
8.95
8.33
8.32
8.31
8.30
8.09
8.09
8.07
8.07
7.77
7.75
7.73
7.65
7.64
7.63
7.61
7.61
7.45
7.43
7.41
7.30
7.30
7.29
7.28
7.26
N
NO2
1.00
1.06
1.02
1.17
1.13
2.22
2.94
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

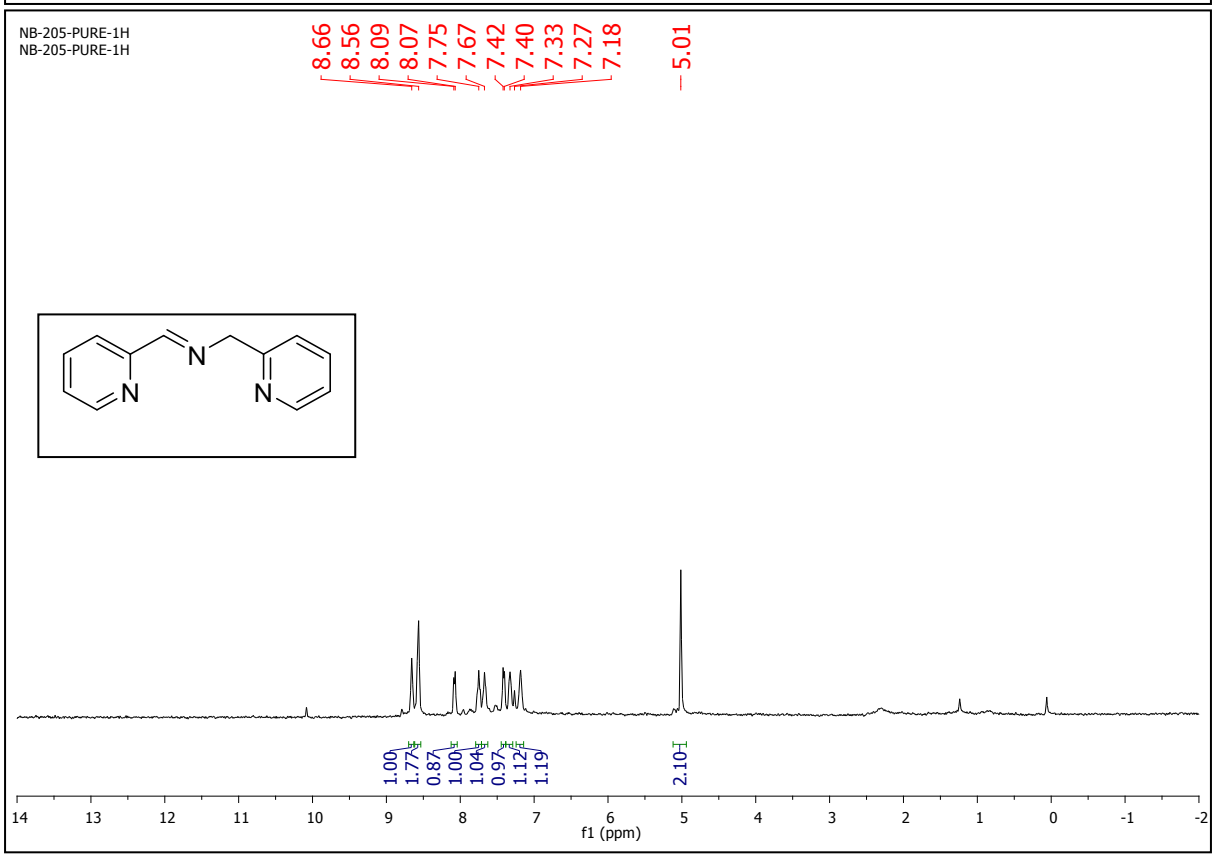

NB-224-2ND-13C
NB-224-2ND-13C
156.02
151.22
133.75
131.34
129.91
129.44
127.08
124.70
121.34
77.48
77.16
76.84
N
NO2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

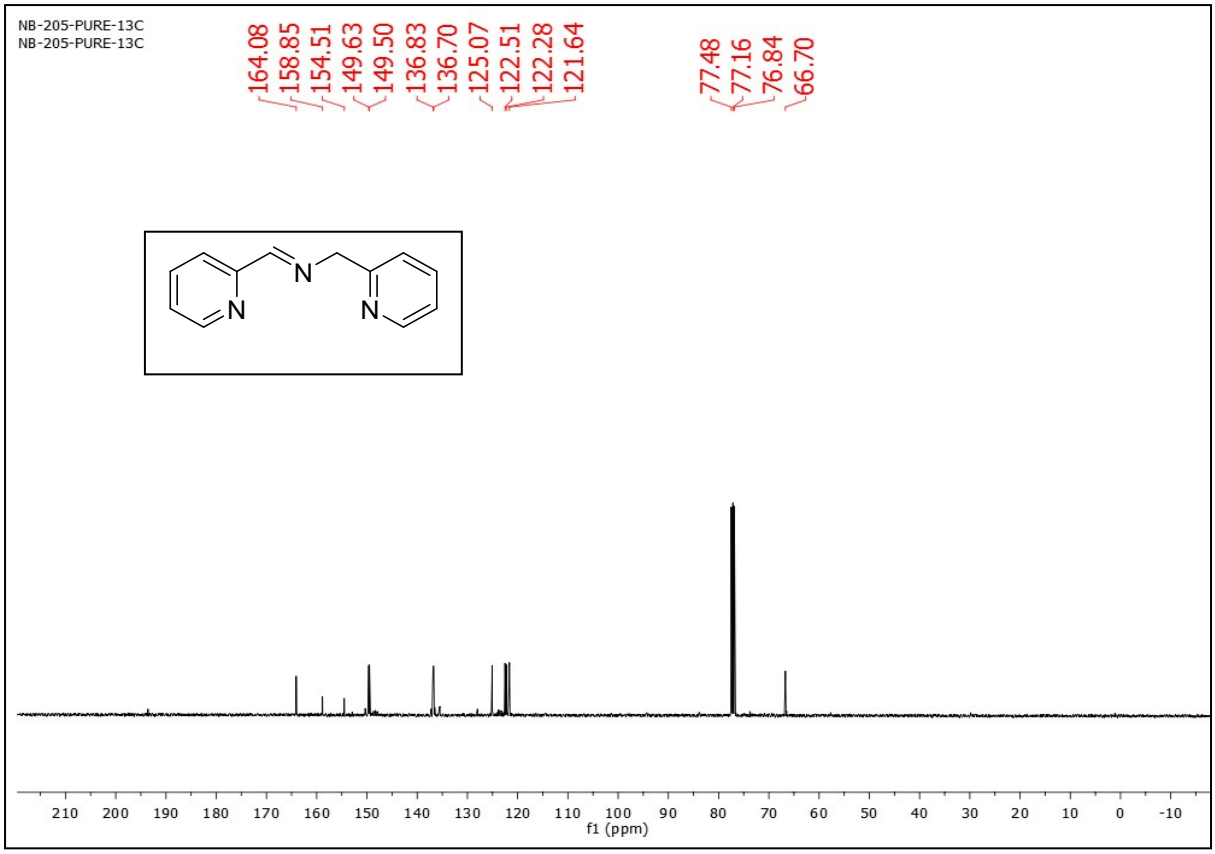

NB-198-1H
NB-198-1H
8.37
7.46
7.42
7.41
7.40
7.37
7.36
7.32
7.31
7.30
7.28
7.27
7.24
7.23
6.99
6.98
N
OH
NB-198-1H
NB-198-1H
7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.7
f1 (ppm)
1.00
1.01
2.03
1.16
1.09
0.85
1.99
0.98
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

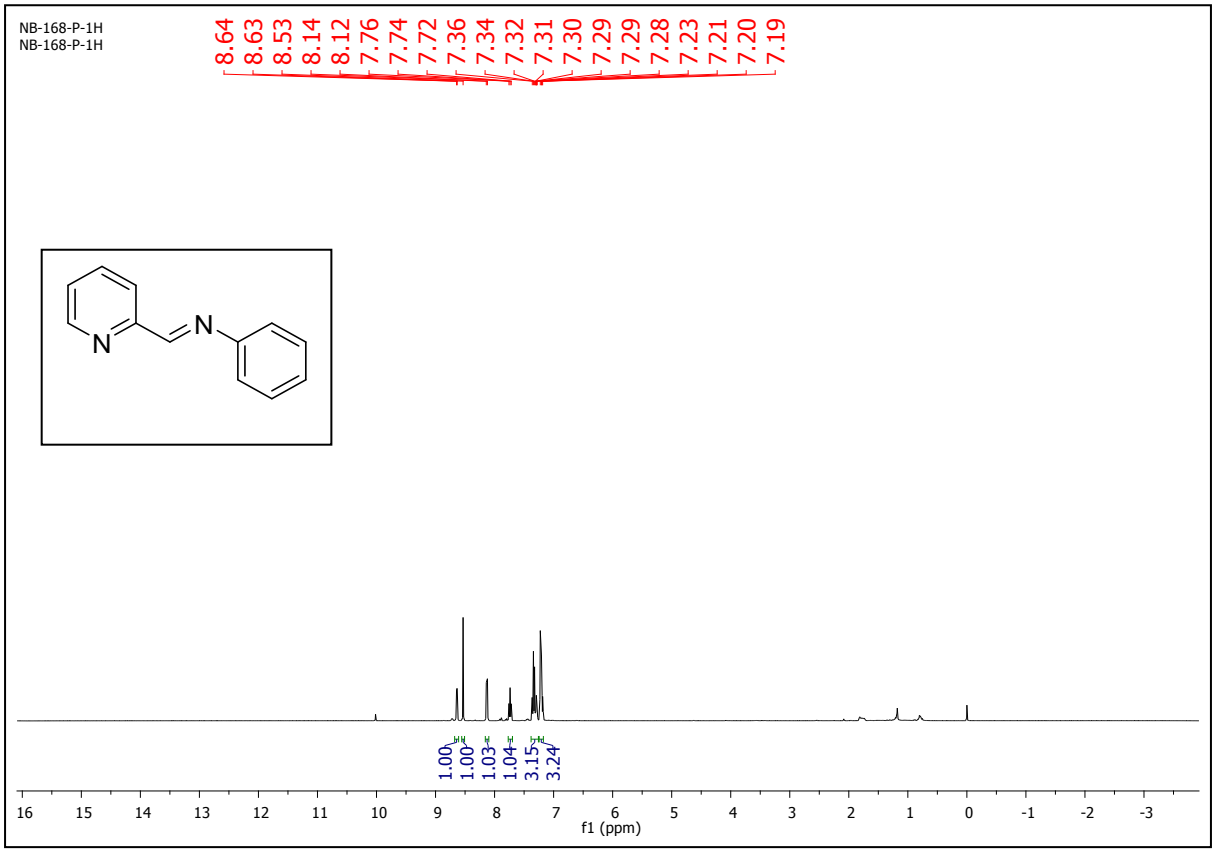

NB-198-13C
NB-198-13C
161.49
156.62
151.38
137.14
130.22
129.39
126.44
122.31
121.13
119.50
114.51
77.37
77.16
76.95
N
OH
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

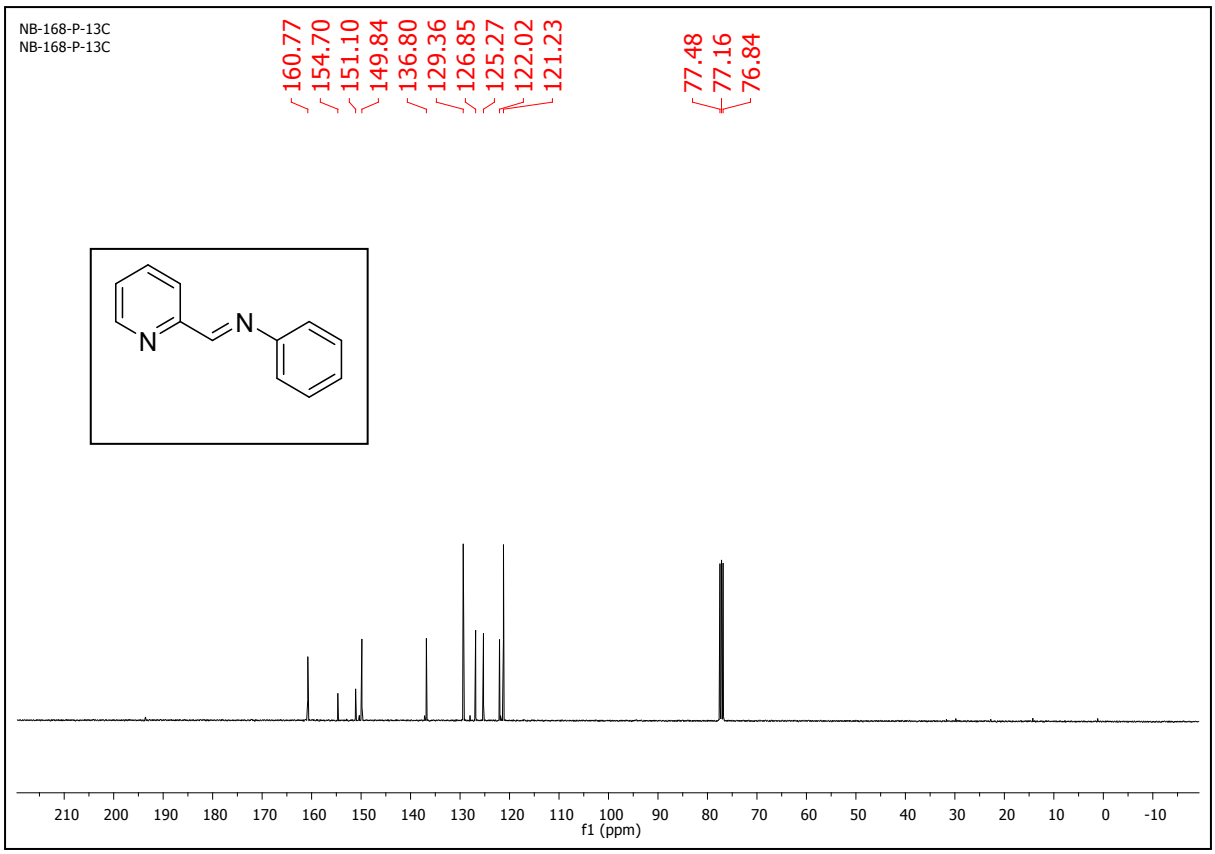

NB-187-P-1H
NB-187-P-1H
8.50
7.45
7.43
7.42
7.40
7.38
7.37
4.85
N
S
1.00
5.89
1.06
1.00
2.08
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

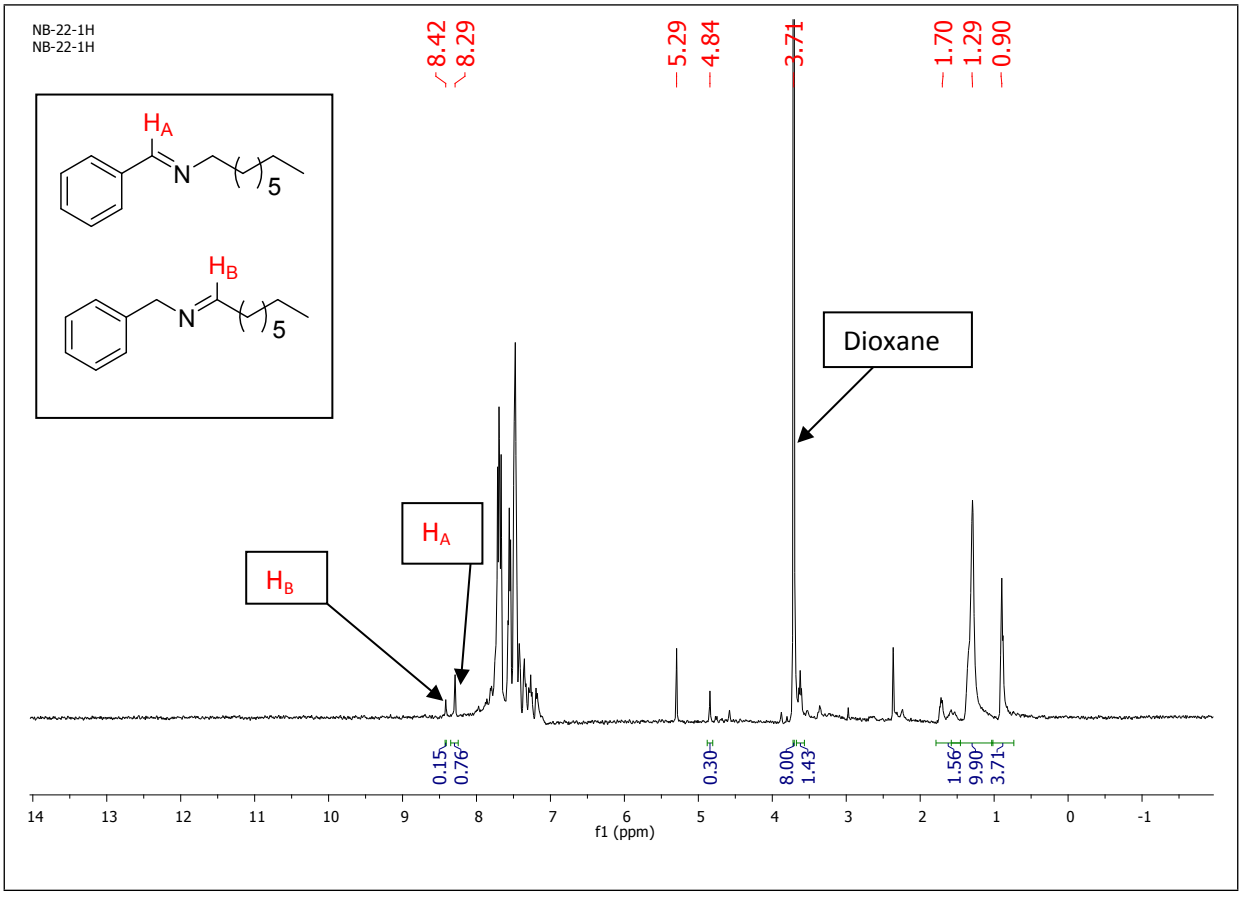

NB-187-P-13C
NB-187-P-13C
NB-187-P-13C
NB-187-P-13C
155.17
142.44
139.07
130.67
129.04
128.49
128.02
127.37
127.01
77.48
77.16
76.84
64.42
N
S
133 132 131 130 129 128 127 126 125
f1 (ppm)
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


NB-205-PURE-1H
NB-205-PURE-1H
8.66
8.56
8.09
8.07
7.75
7.67
7.42
7.40
7.33
7.27
7.18
5.01
N
N
N
1.00
1.77
0.87
1.00
1.04
0.97
1.12
1.19
2.10
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2
f1 (ppm)

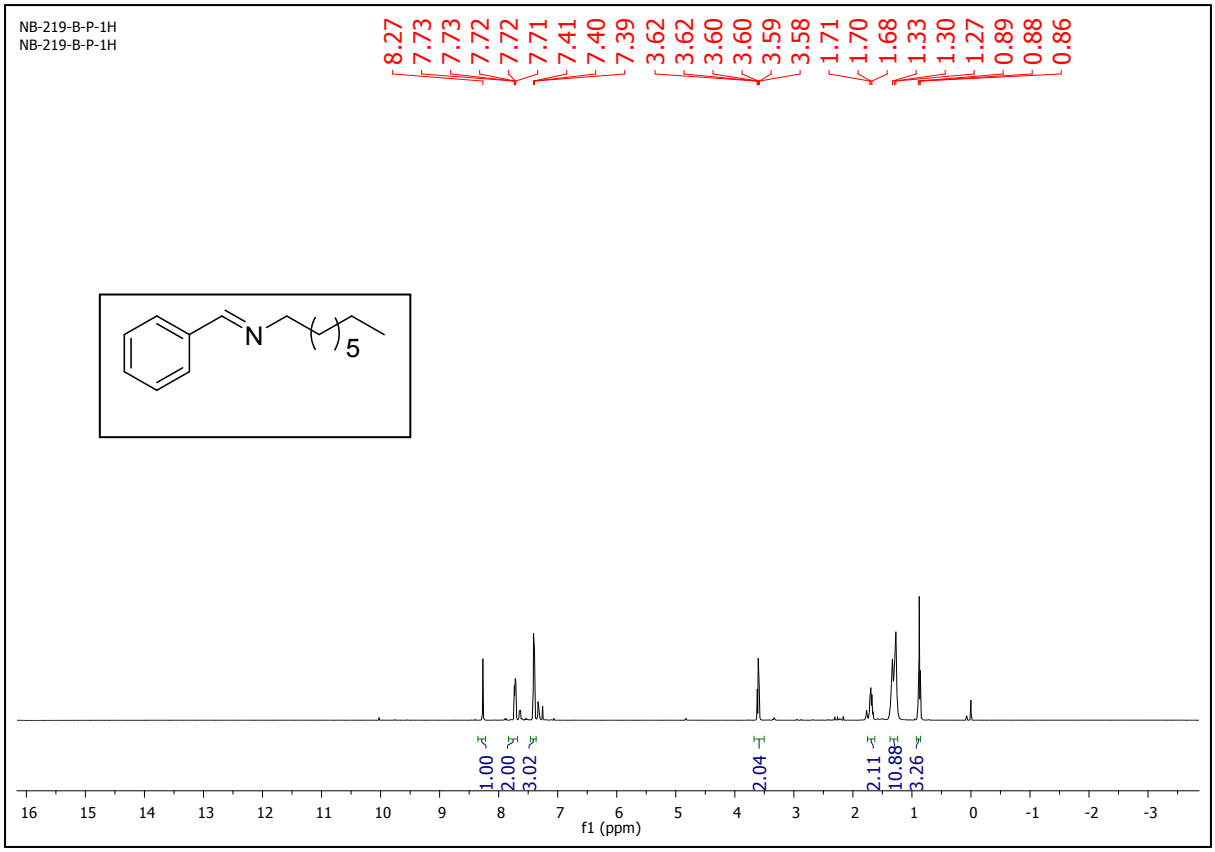

NB-205-PURE-13C
NB-205-PURE-13C
164.08
158.85
154.51
149.63
149.50
136.83
136.70
125.07
122.51
122.28
121.64
77.48
77.16
76.84
66.70
N
N
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

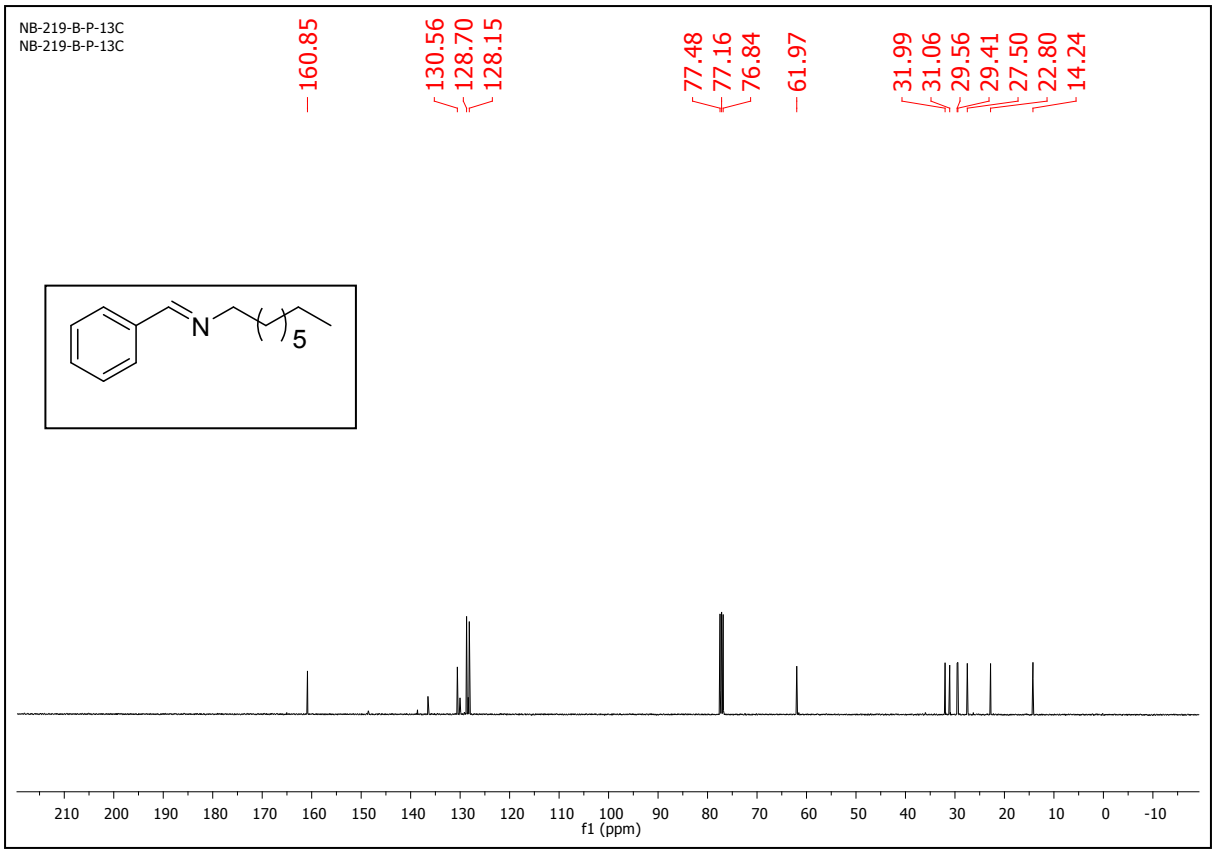

NB-168-P-1H
NB-168-P-1H
8.64
8.63
8.53
8.14
8.12
7.76
7.74
7.72
7.36
7.34
7.32
7.31
7.30
7.29
7.29
7.28
7.23
7.21
7.20
7.19
N
N
1.00
1.00
1.03
1.04
3.15
3.24
16 15 14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 -1 -2 -3
f1 (ppm)

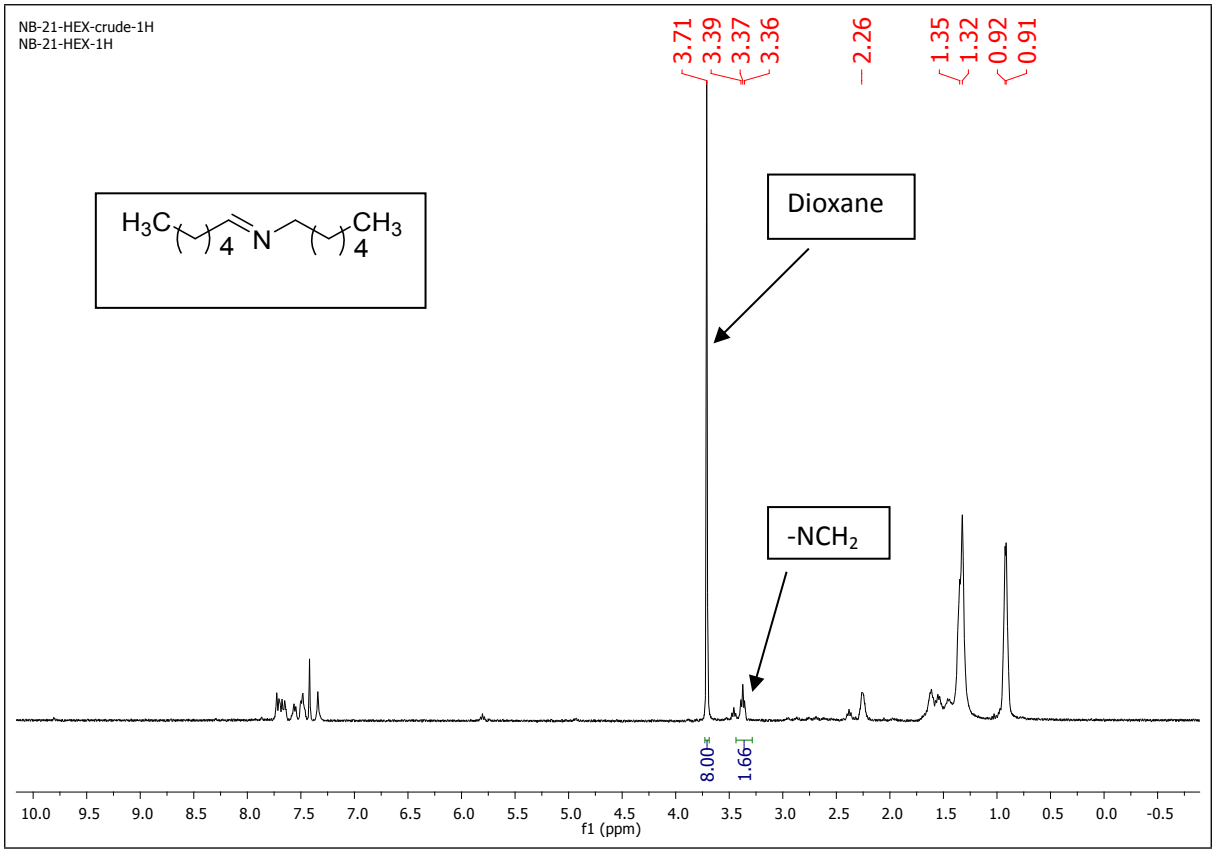




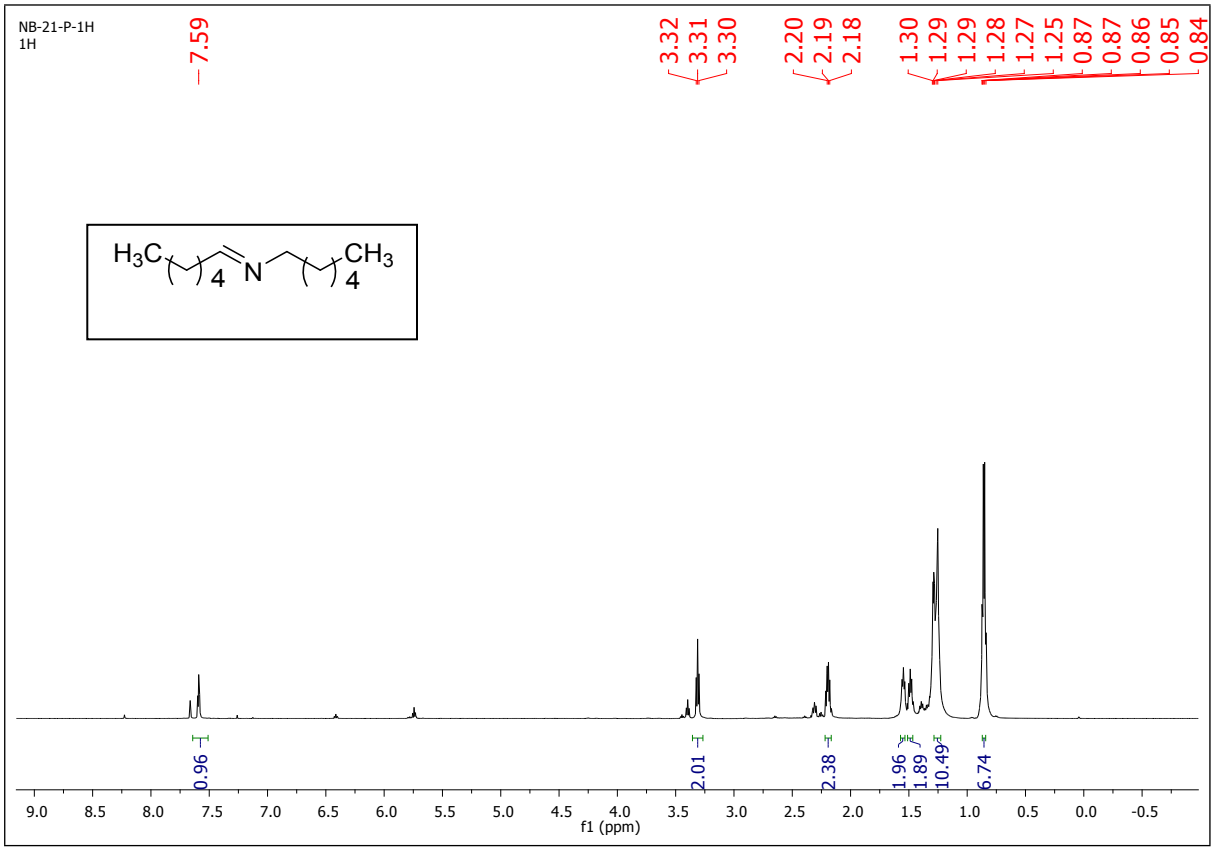
Reaction mixture of 1-Octanol and benzyl azide using dioxane as internal standard

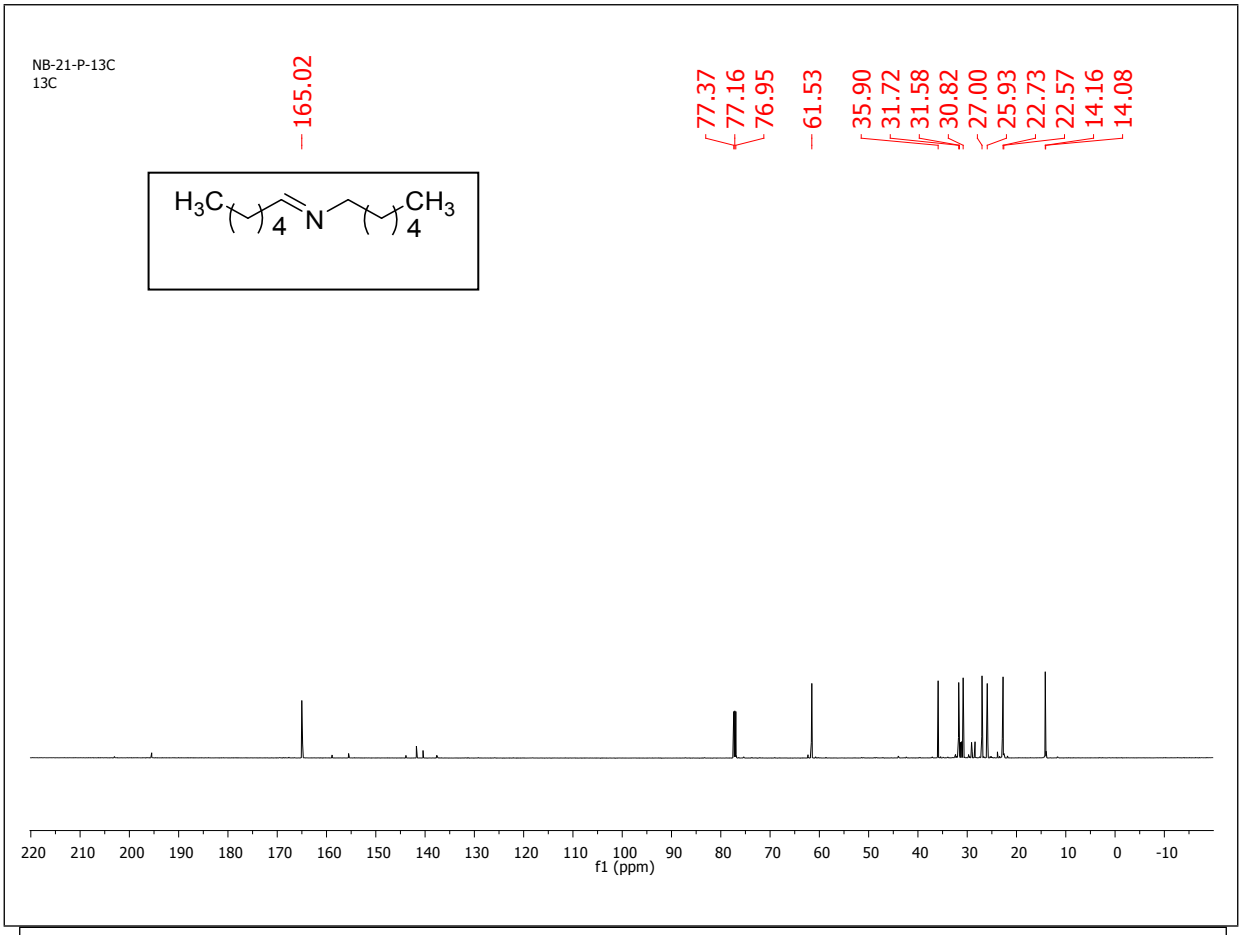

NB-219-B-P-1H
NB-219-B-P-1H
8.27
7.73
7.73
7.72
7.72
7.71
7.41
7.40
7.39
3.62
3.62
3.60
3.60
3.59
3.58
1.71
1.70
1.68
1.33
1.30
1.27
0.89
0.88
0.86
N
5
1.00
2.00
3.02
2.04
2.11
10.88
3.26
f1 (ppm)

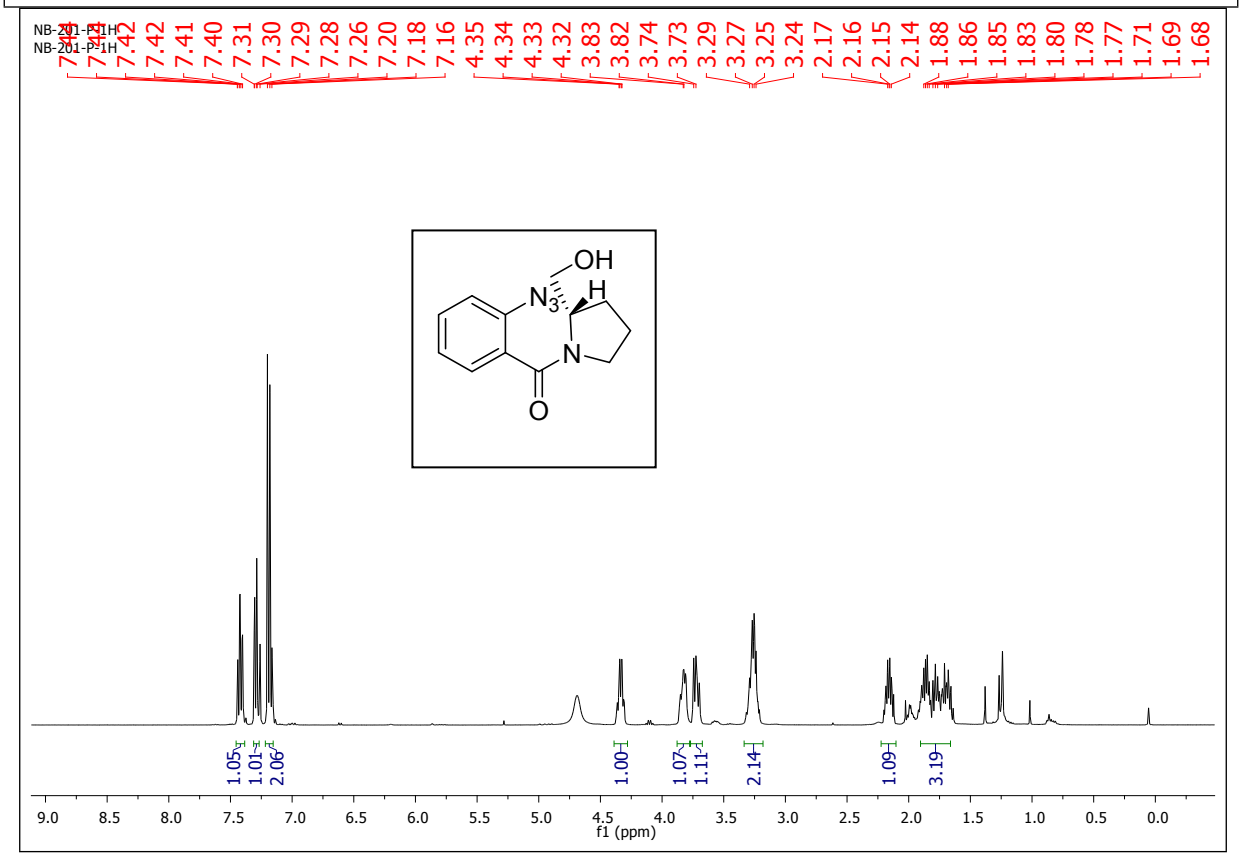

NB-219-B-P-13C
NB-219-B-P-13C
160.85
130.56
128.70
128.15
77.48
77.16
76.84
61.97
31.99
31.06
29.56
29.41
27.50
22.80
14.24
N
5
f1 (ppm)

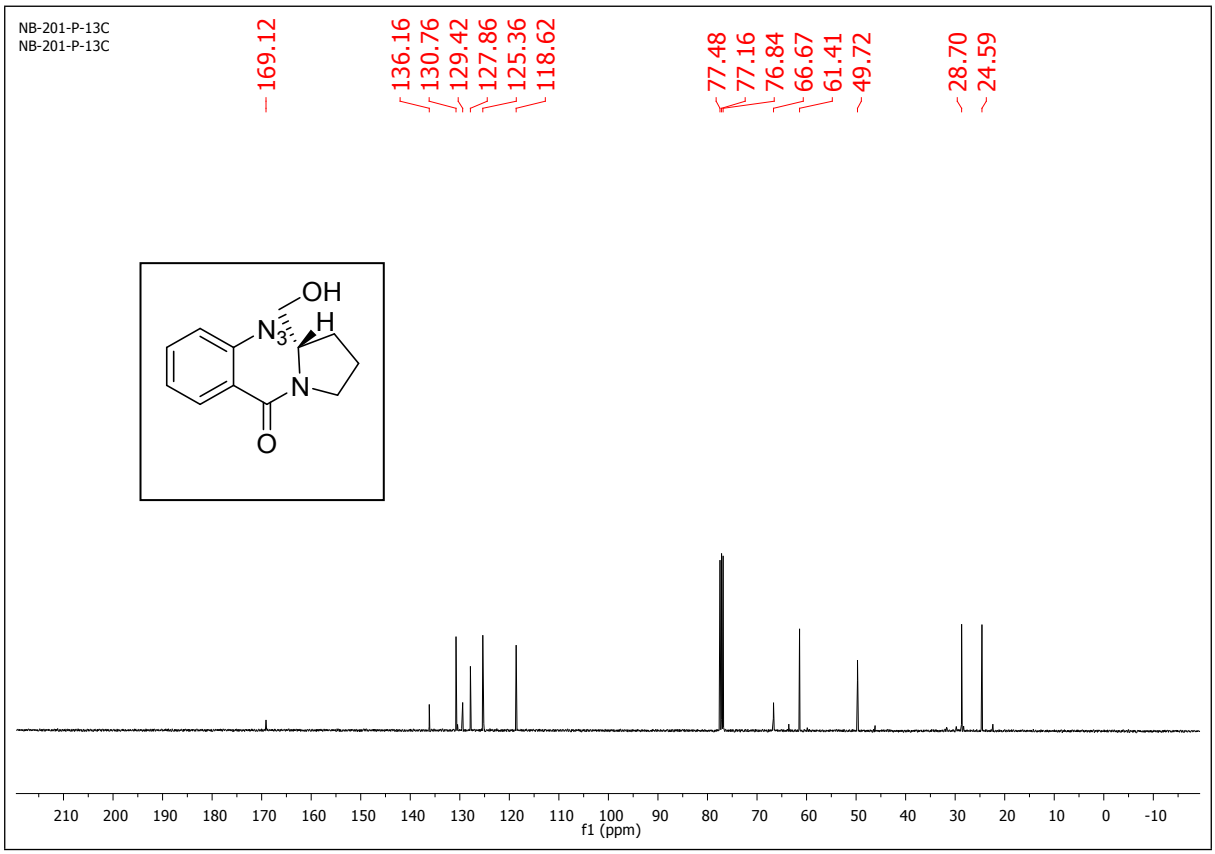


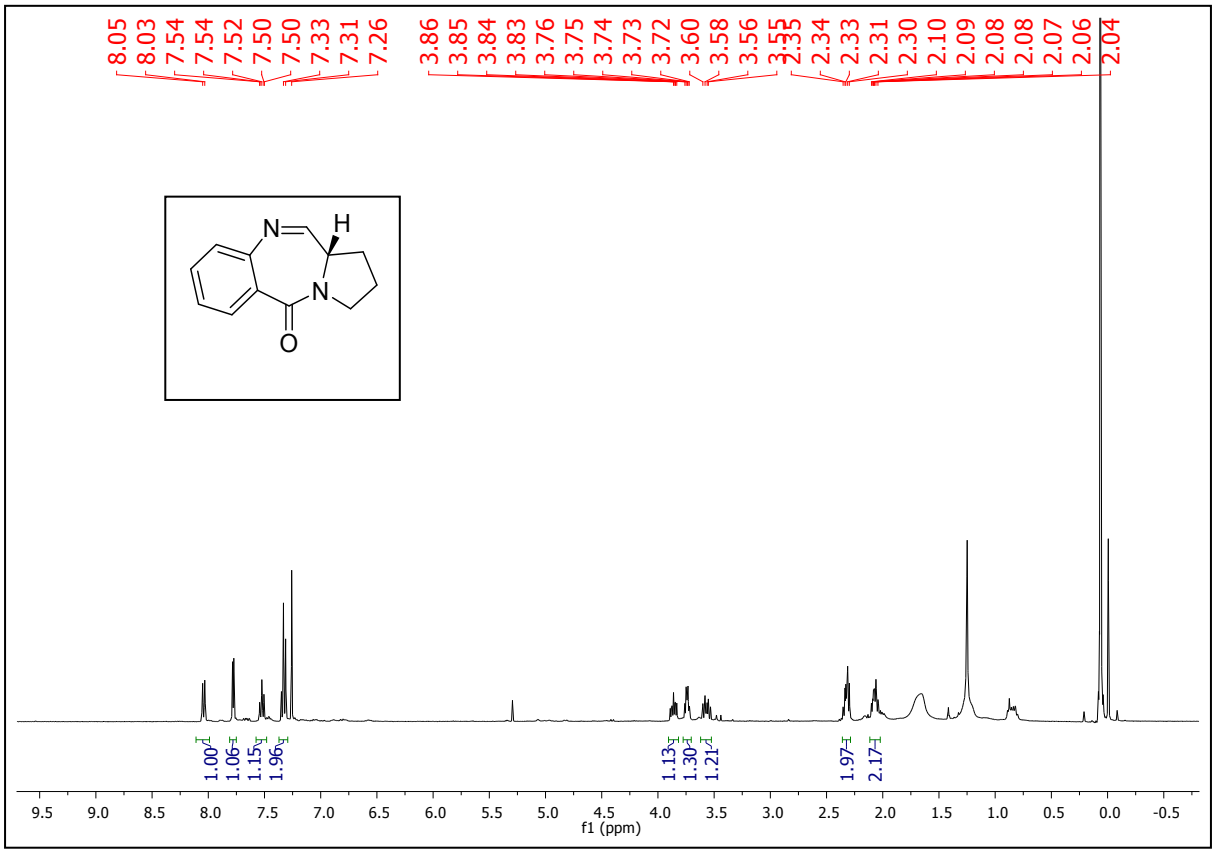
Reaction mixture of 1-hexanol and hexyl azide using dioxane as internal standard

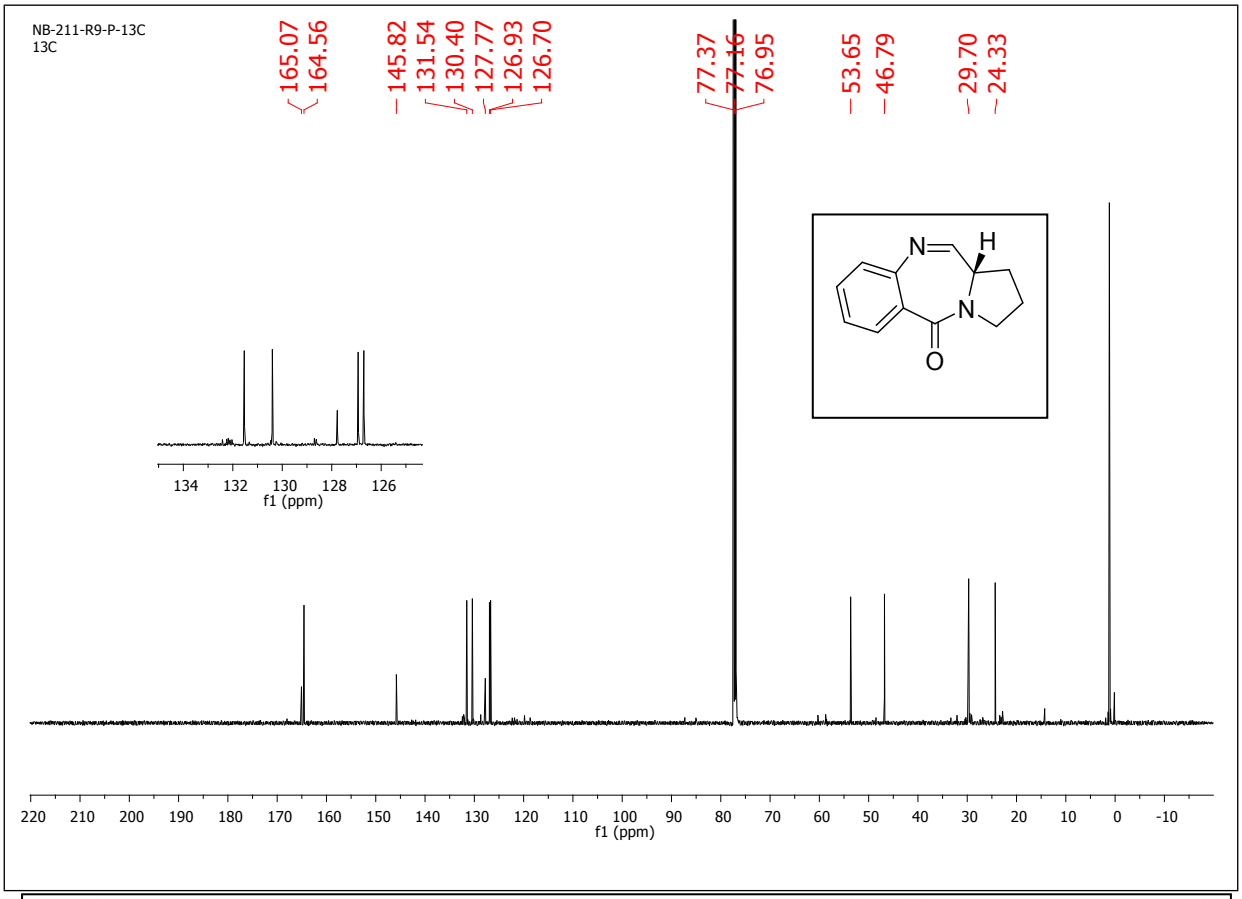


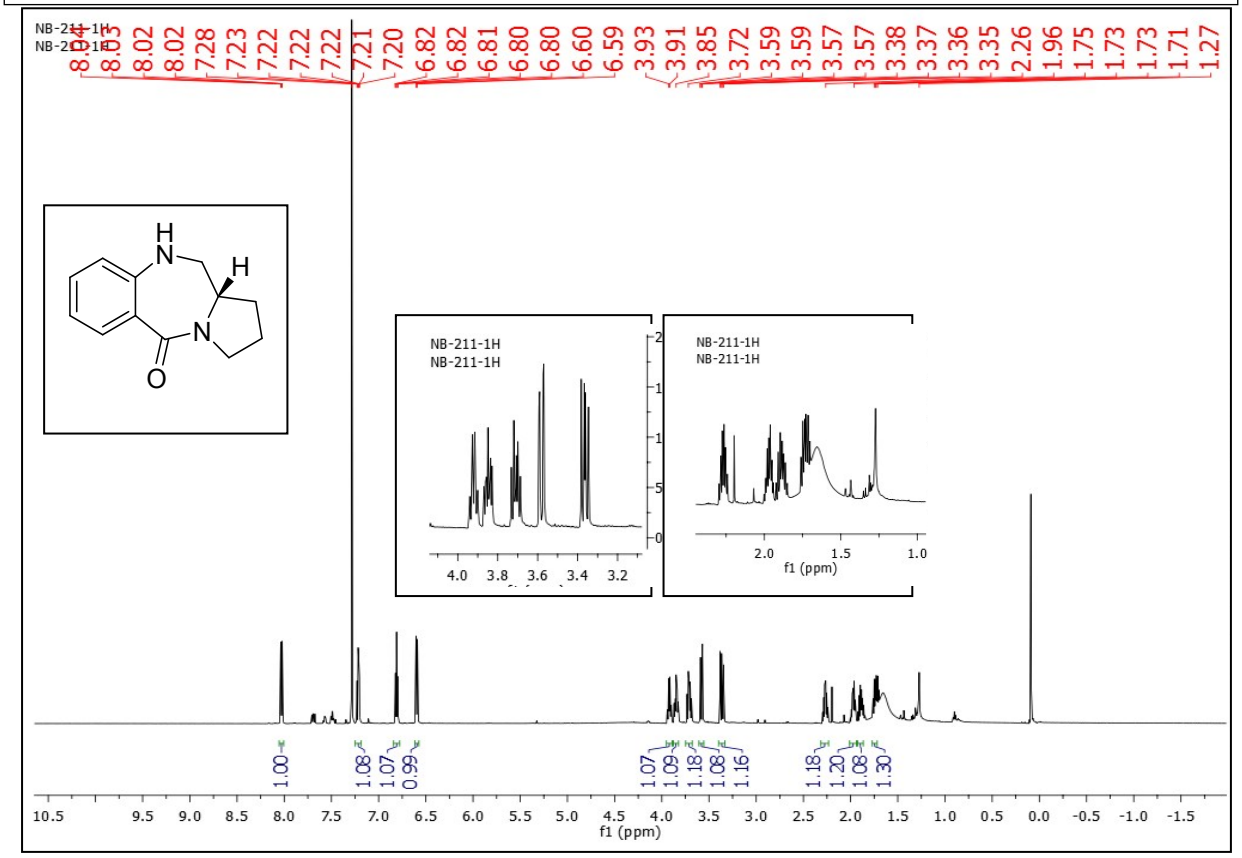

NB-21-P-13C
13C
165.02
77.37
77.16
76.95
61.53
35.90
31.72
31.58
30.82
27.00
25.93
22.73
22.57
14.16
14.08
H3C
4
N
CH3
4
f1 (ppm)

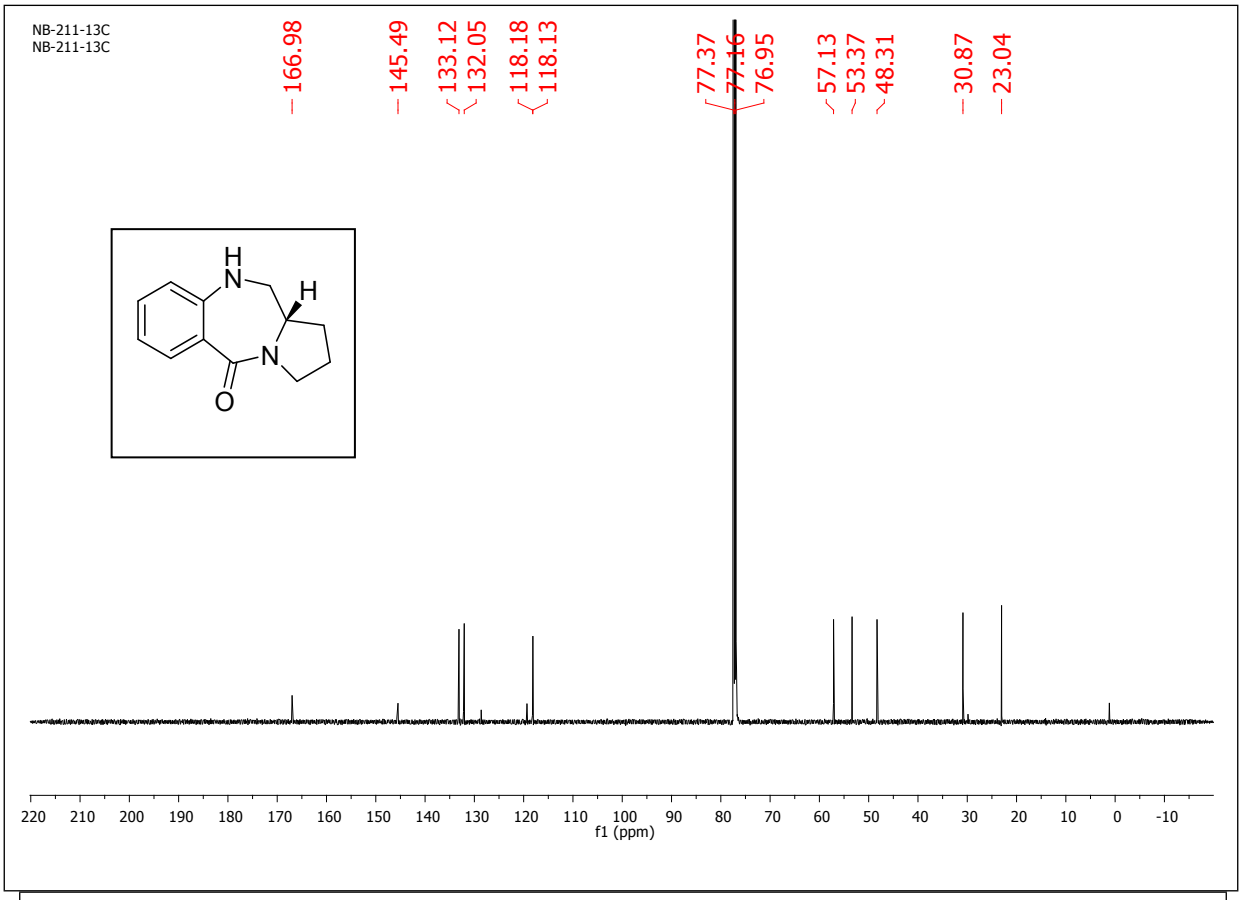

NB-201-P-1H
NB-201-P-1H
7.42
7.42
7.41
7.40
7.31
7.30
7.29
7.28
7.26
7.20
7.18
7.16
4.35
4.34
4.33
4.32
3.83
3.82
3.74
3.73
3.29
3.27
3.25
3.24
2.17
2.16
2.15
2.14
1.88
1.86
1.85
1.83
1.80
1.78
1.77
1.71
1.69
1.68
OH
H
N3
N
O
1.05
1.01
2.06
1.00
1.07
1.11
2.14
1.09
3.19
f1 (ppm)

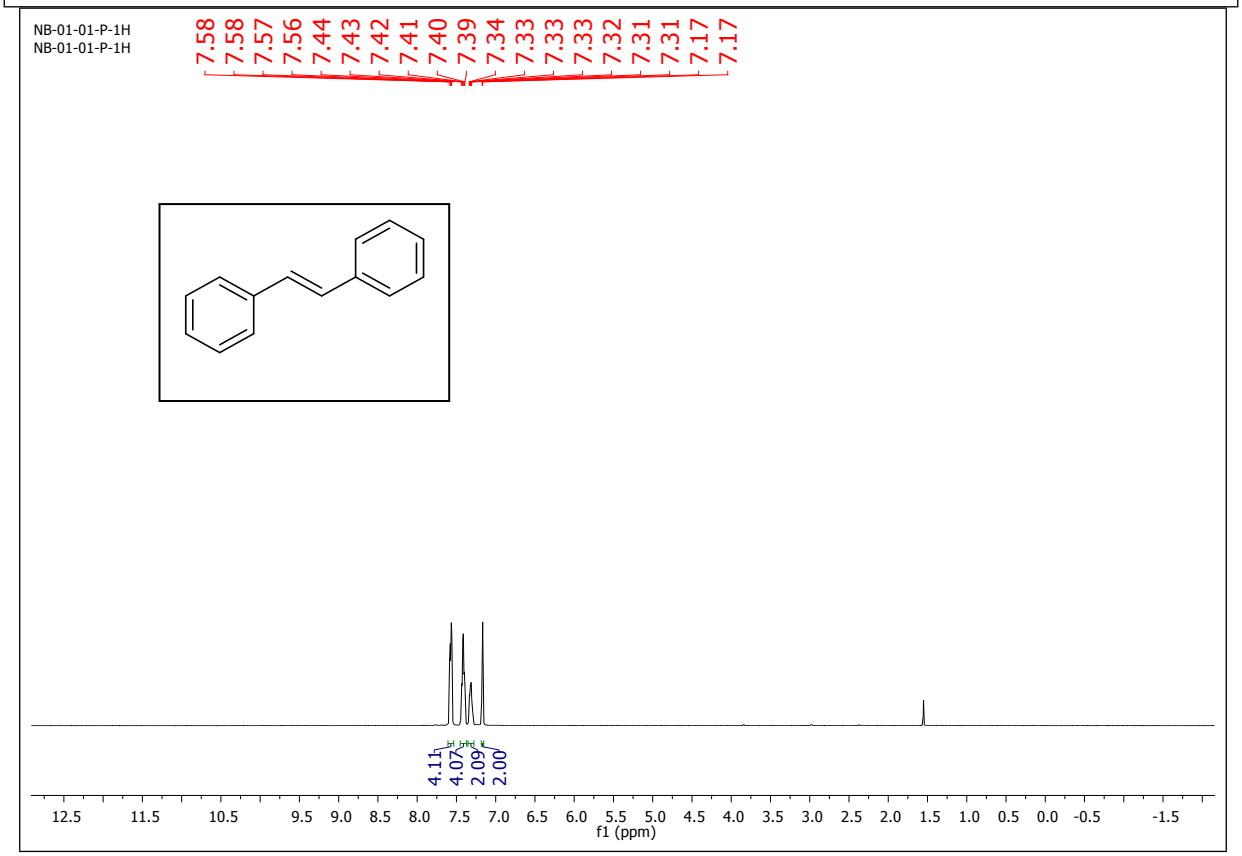

NB-201-P-13C
NB-201-P-13C
169.12
136.16
130.76
129.42
127.86
125.36
118.62
77.48
77.16
76.84
66.67
61.41
49.72
28.70
24.59
OH
N
3
H
N
O
f1 (ppm)

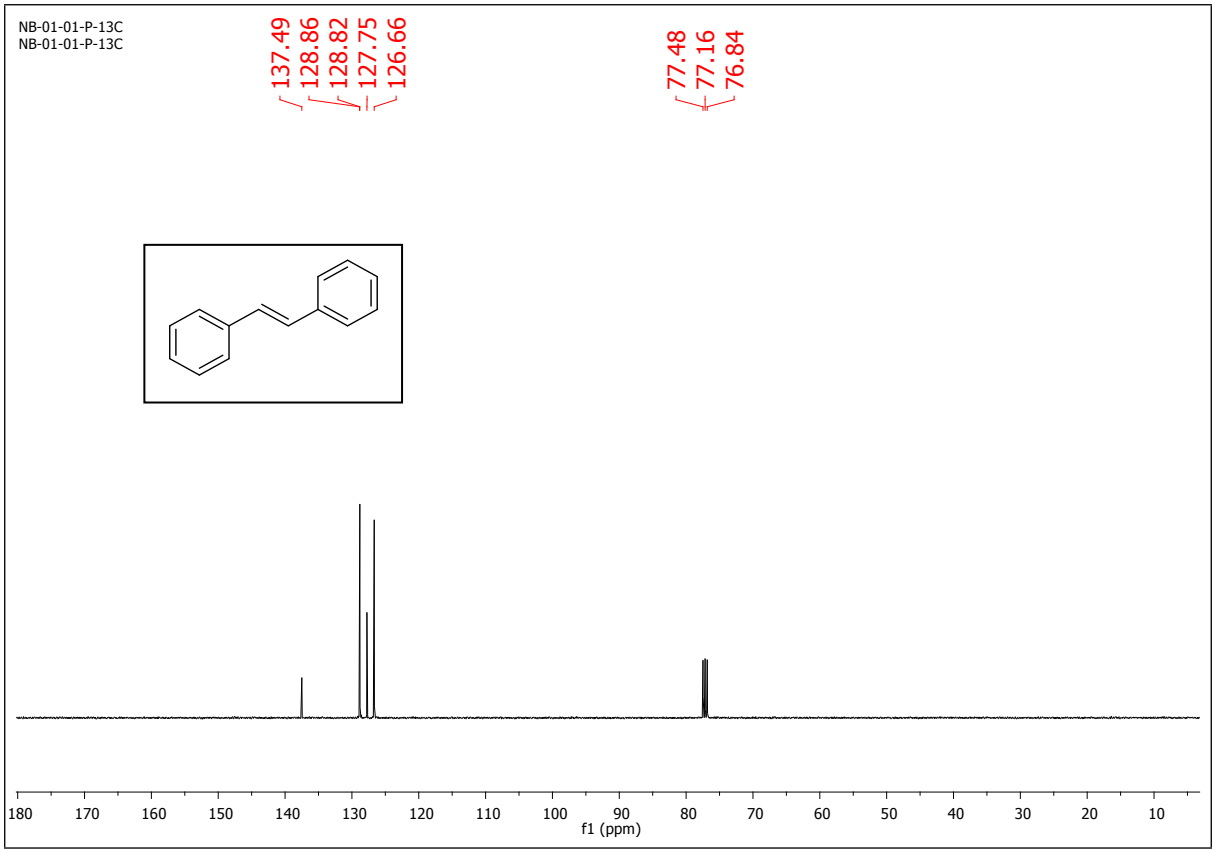

8.05
8.03
7.54
7.54
7.52
7.50
7.50
7.33
7.31
7.26
3.86
3.85
3.84
3.83
3.76
3.75
3.74
3.73
3.72
3.60
3.58
3.56
2.34
2.33
2.31
2.30
2.10
2.09
2.08
2.08
2.07
2.06
2.04
N
H
N
O
1.00
1.06
1.15
1.96
1.13
1.30
1.21
1.97
2.17
f1 (ppm)

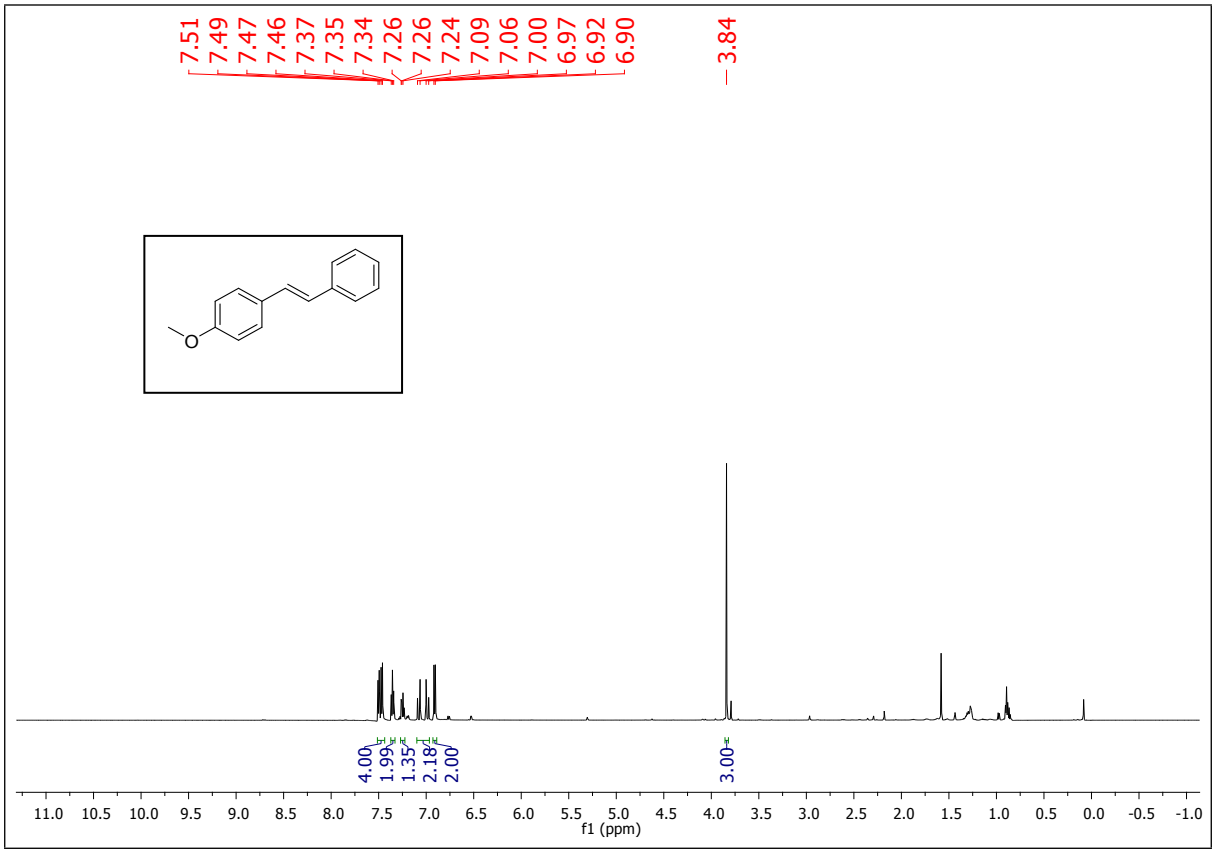

NB-211-R9-P-13C
13C
165.07
164.56
145.82
131.54
130.40
127.77
126.93
126.70
77.37
77.16
76.95
53.65
46.79
29.70
24.33
f1 (ppm)

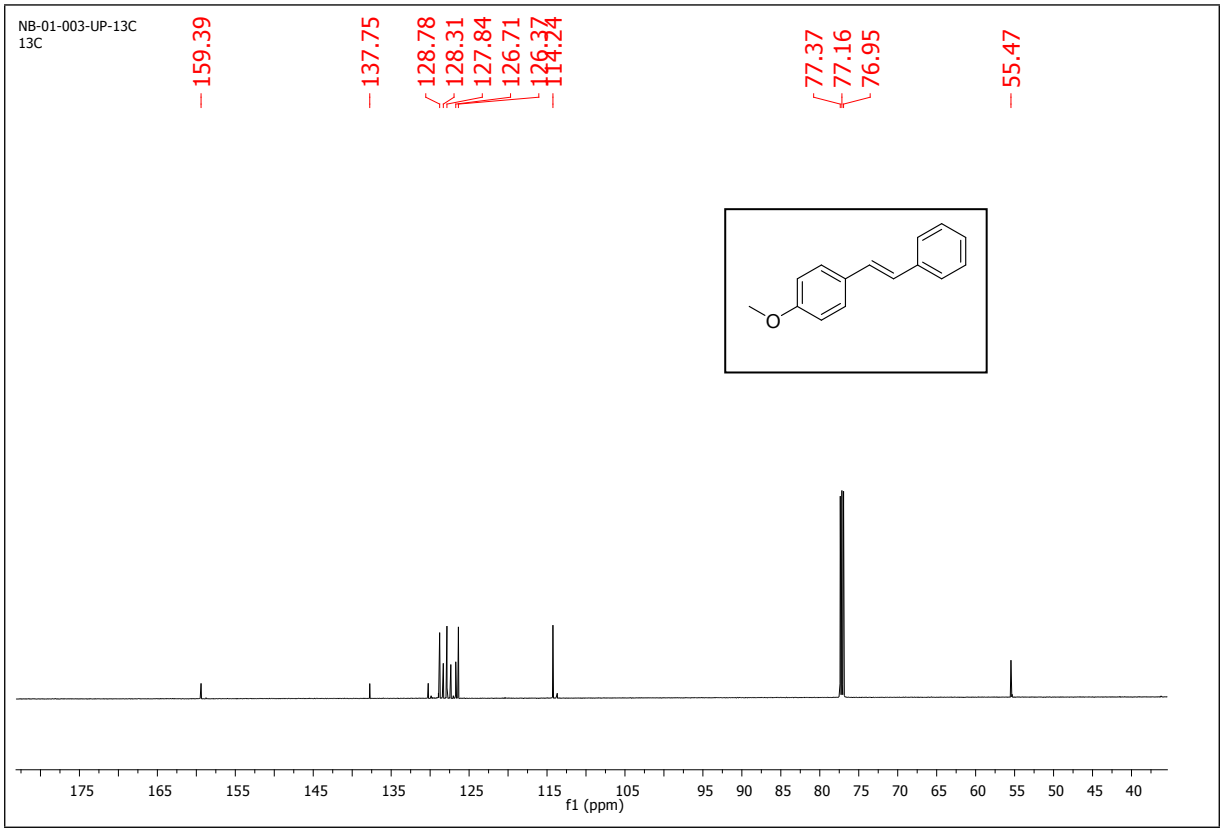

NB-211-1H
NB-211-1H
f1 (ppm)

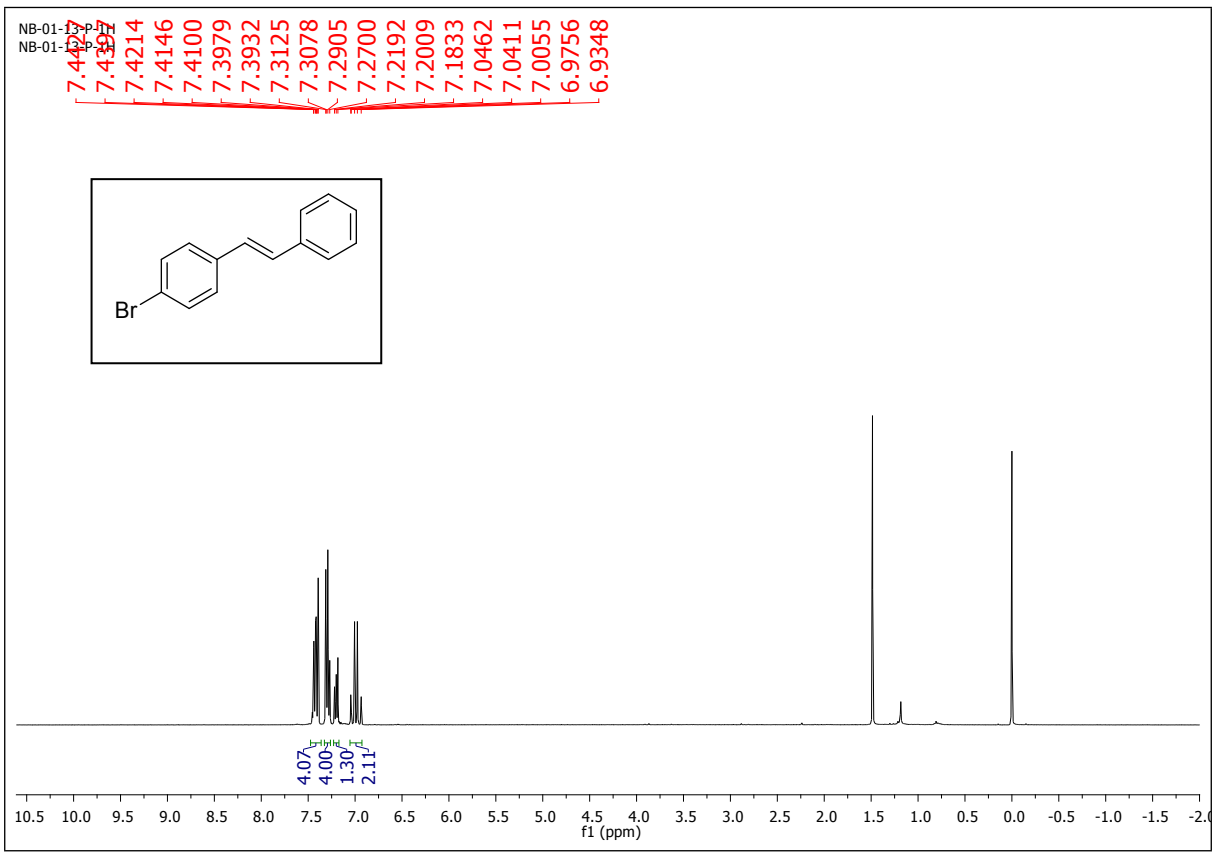

NB-211-13C
NB-211-13C
166.98
145.49
133.12
132.05
118.18
118.13
77.37
77.16
76.95
57.13
53.37
48.31
30.87
23.04
H
N
H
N
O
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

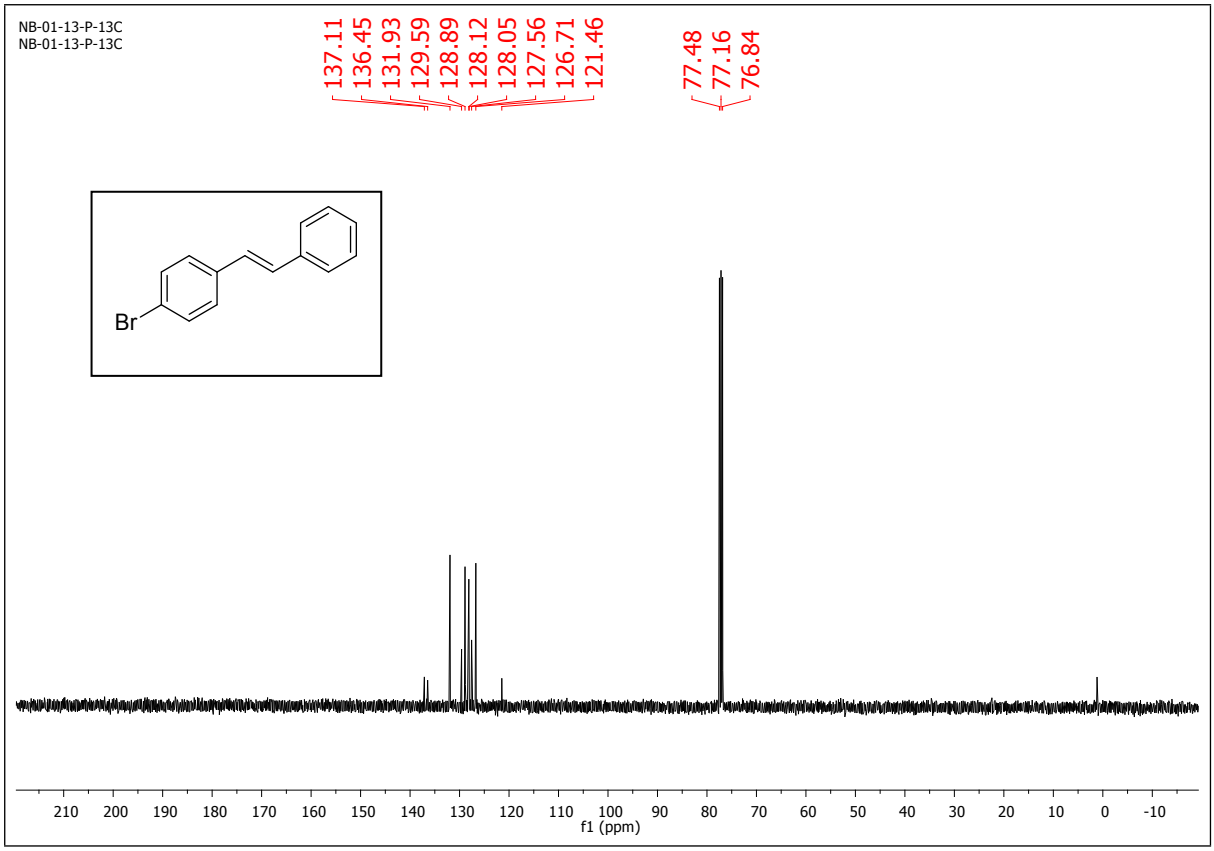

NB-01-P-1H
NB-01-P-1H
7.58
7.58
7.57
7.56
7.44
7.43
7.42
7.41
7.40
7.39
7.34
7.33
7.33
7.33
7.32
7.31
7.31
7.17
7.17
4.11
4.07
2.09
2.00
12.5 11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.5
f1 (ppm)

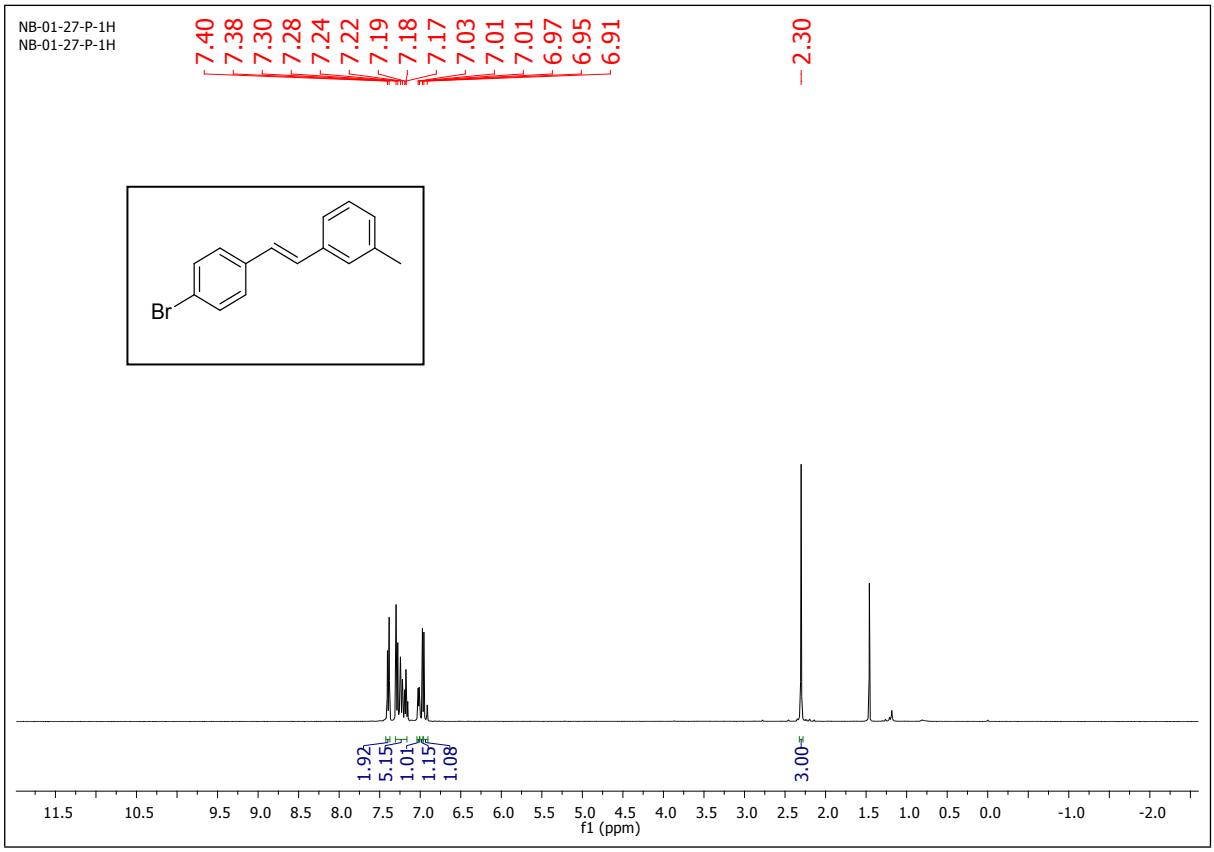

NB-01-01-P-13C
NB-01-01-P-13C
137.49
128.86
128.82
127.75
126.66
77.48
77.16
76.84
f1 (ppm)

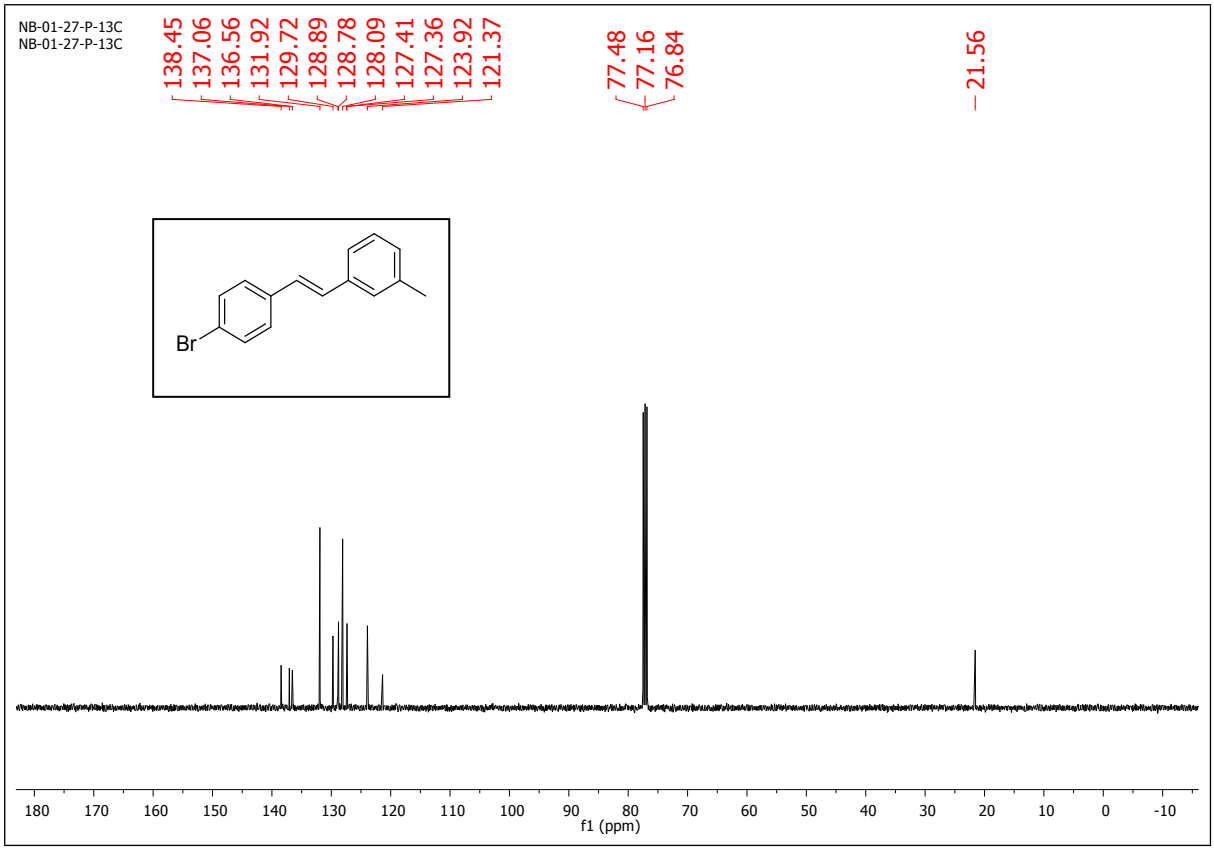

7.51
7.49
7.47
7.46
7.37
7.35
7.34
7.26
7.26
7.24
7.09
7.06
7.00
6.97
6.92
6.90
3.84
O
4.00
1.99
1.35
2.18
2.00
3.00
f1 (ppm)

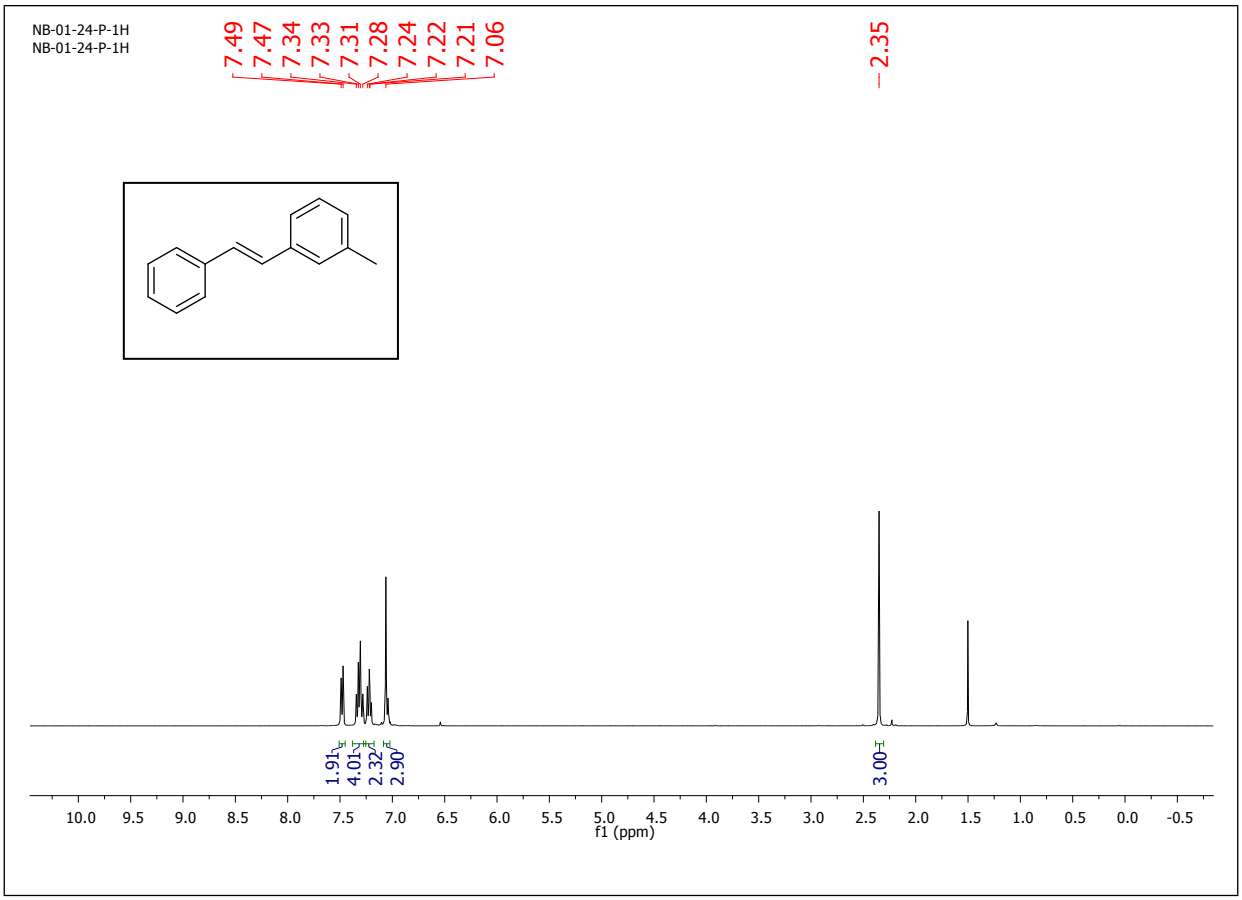

NB-01-003-UP-13C
13C
159.39
137.75
128.78
128.31
127.84
126.71
126.37
114.24
77.37
77.16
76.95
55.47
O
175 165 155 145 135 125 115 105 95 90 85 80 75 70 65 60 55 50 45 40
f1 (ppm)

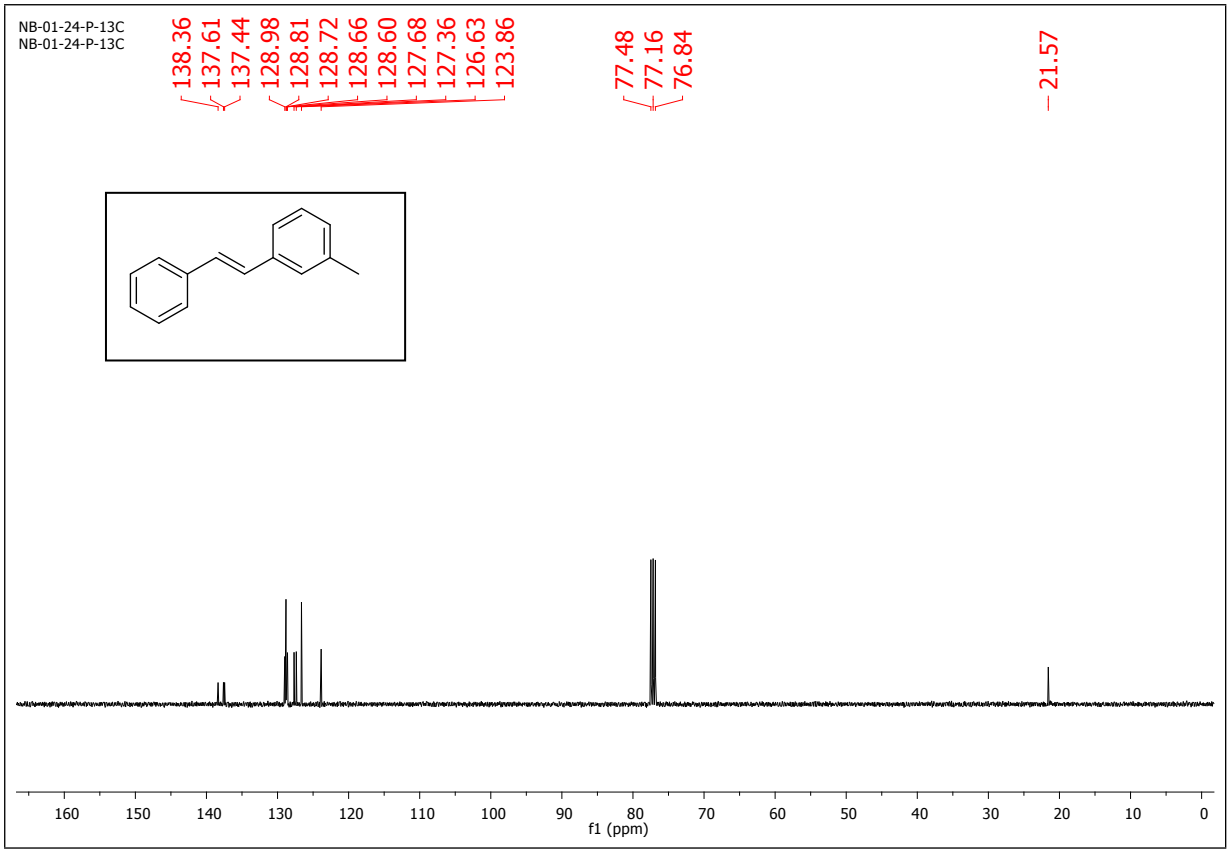

NB-01-13-P-1H
NB-01-13-P-1H
7.4427
7.4397
7.4214
7.4146
7.4100
7.3979
7.3932
7.3125
7.3078
7.2905
7.2700
7.2192
7.2009
7.1833
7.0462
7.0411
7.0055
6.9756
6.9348
Br
4.07
4.00
1.30
2.11
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0 -1.5
f1 (ppm)

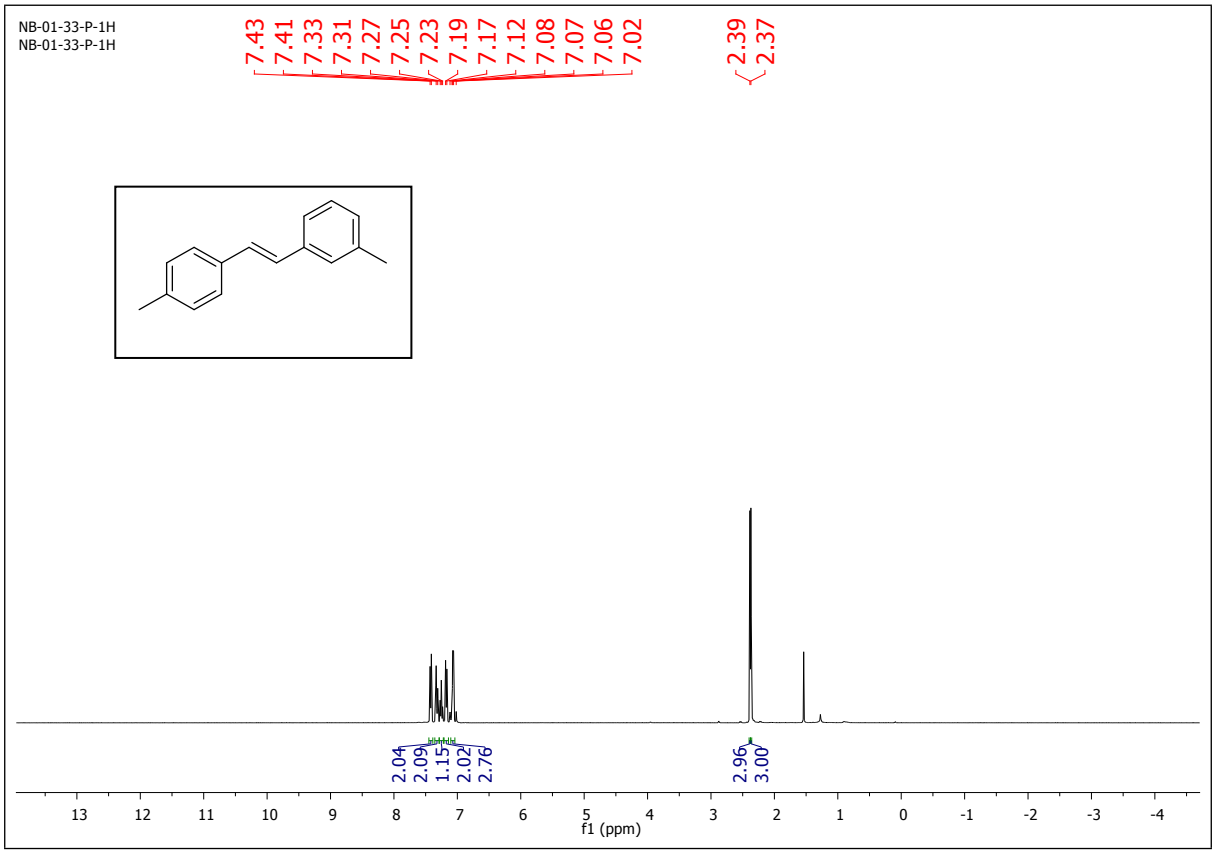

NB-01-13-P-13C
NB-01-13-P-13C
137.11
136.45
131.93
129.59
128.89
128.12
128.05
127.56
126.71
121.46
77.48
77.16
76.84
Br
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

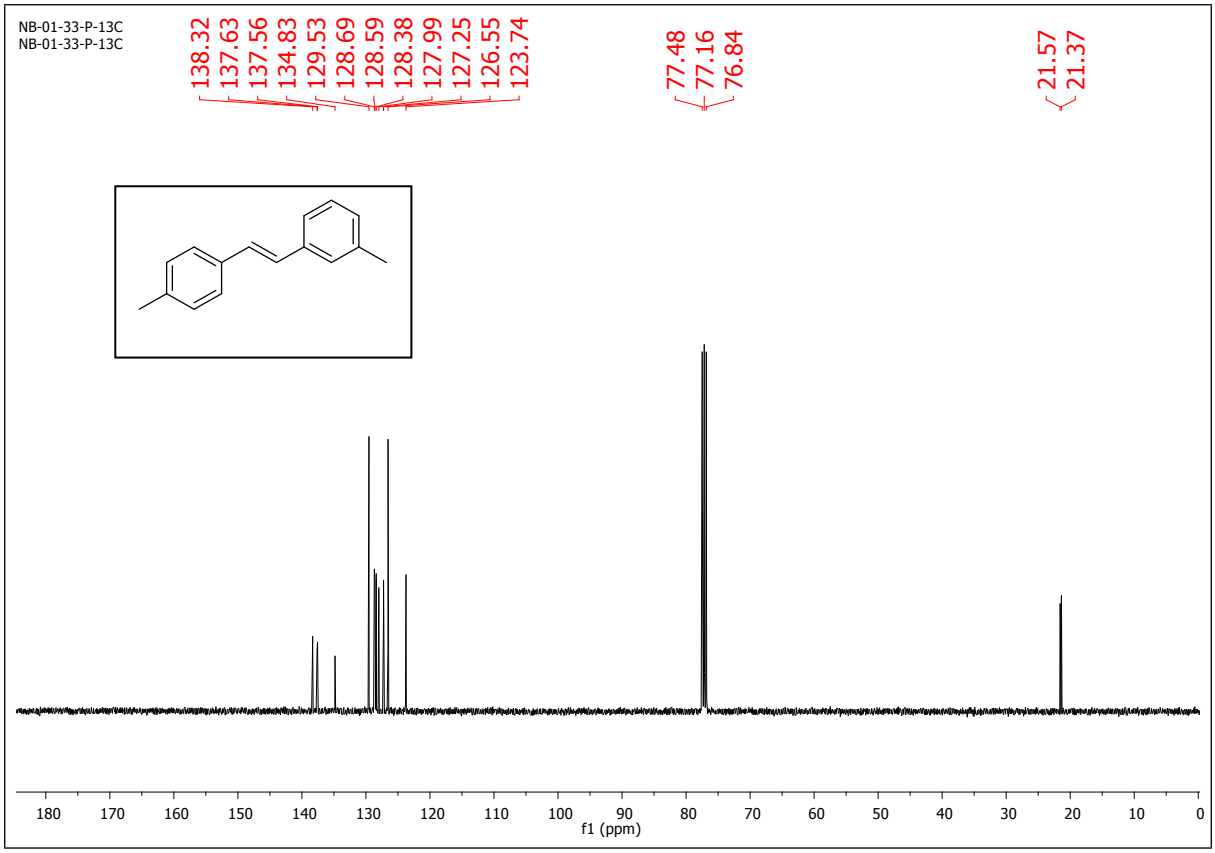

NB-01-27-P-1H
NB-01-27-P-1H
7.40
7.38
7.30
7.28
7.24
7.22
7.19
7.18
7.17
7.03
7.01
7.01
6.97
6.95
6.91
2.30
Br
1.92
5.15
1.01
1.15
1.08
3.00
11.5 10.5 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -1.0 -2.0
f1 (ppm)

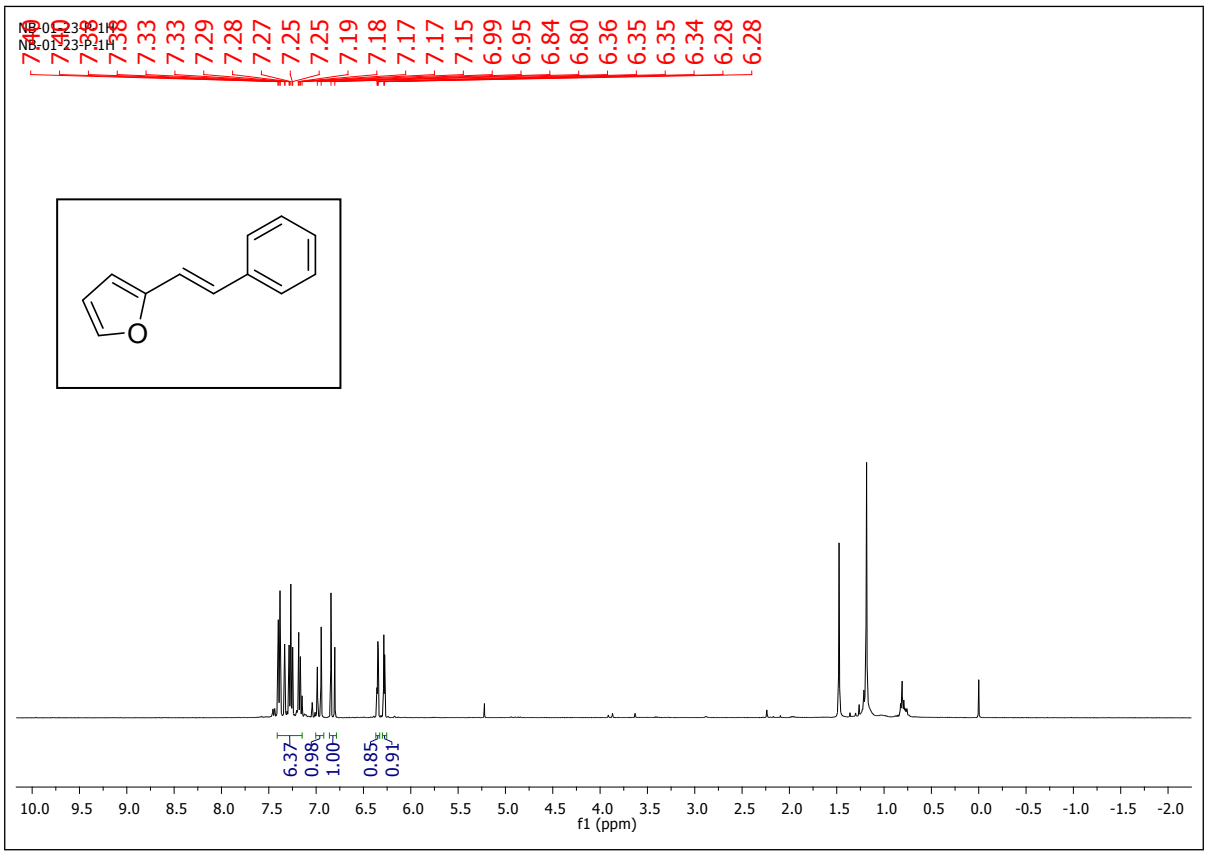

NB-01-27-P-13C
NB-01-27-P-13C
138.45
137.06
136.56
131.92
129.72
128.89
128.78
128.09
127.41
127.36
123.92
121.37
77.48
77.16
76.84
21.56
Br
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

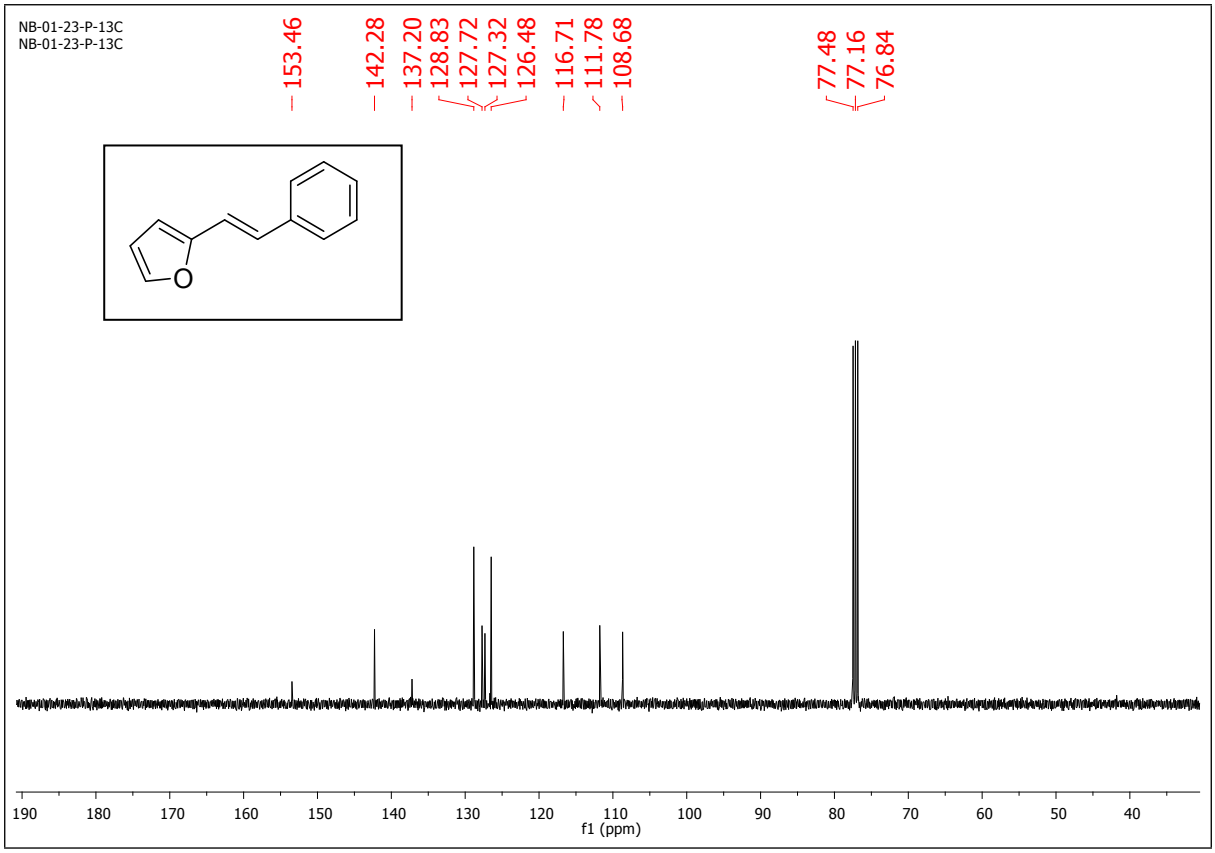

NB-01-24-P-1H
NB-01-24-P-1H
7.49
7.47
7.34
7.33
7.31
7.28
7.24
7.22
7.21
7.06
2.35
1.91
4.01
2.32
2.90
3.00
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)

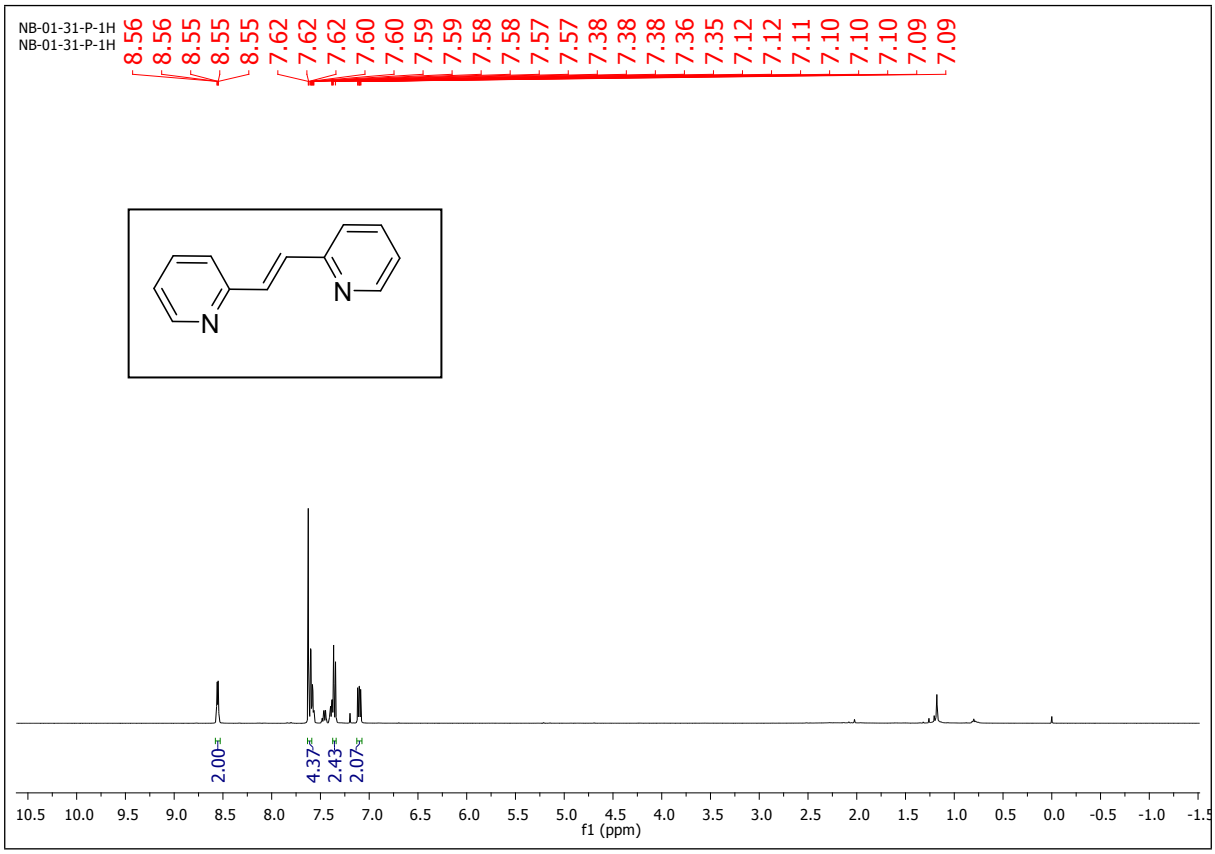

NB-01-24-P-13C
NB-01-24-P-13C
138.36
137.61
137.44
128.98
128.81
128.72
128.66
128.60
127.68
127.36
126.63
123.86
77.48
77.16
76.84
21.57
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

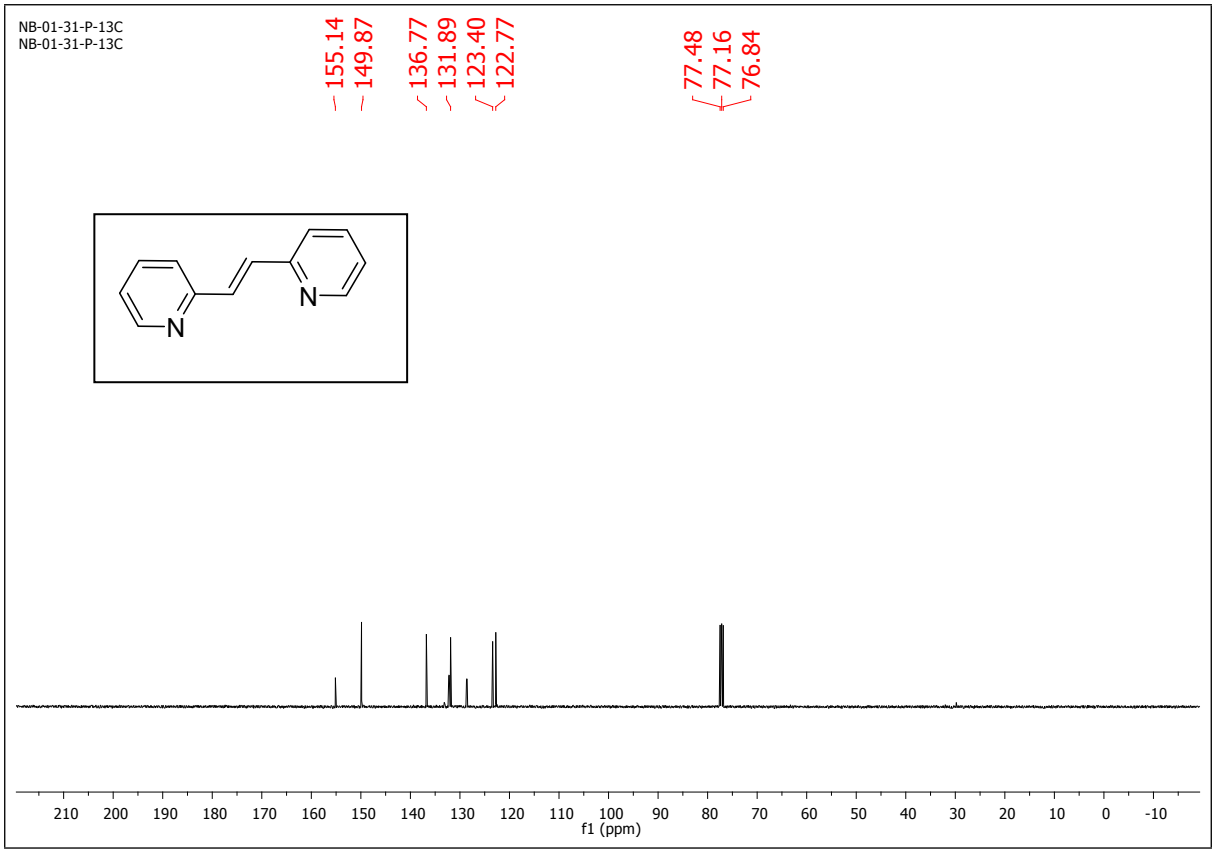

NB-01-33-P-1H
NB-01-33-P-1H
7.43
7.41
7.33
7.31
7.27
7.25
7.23
7.19
7.17
7.12
7.08
7.07
7.06
7.02
2.39
2.37
2.04
2.09
1.15
2.02
2.76
2.96
3.00
13
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
-4
f1 (ppm)

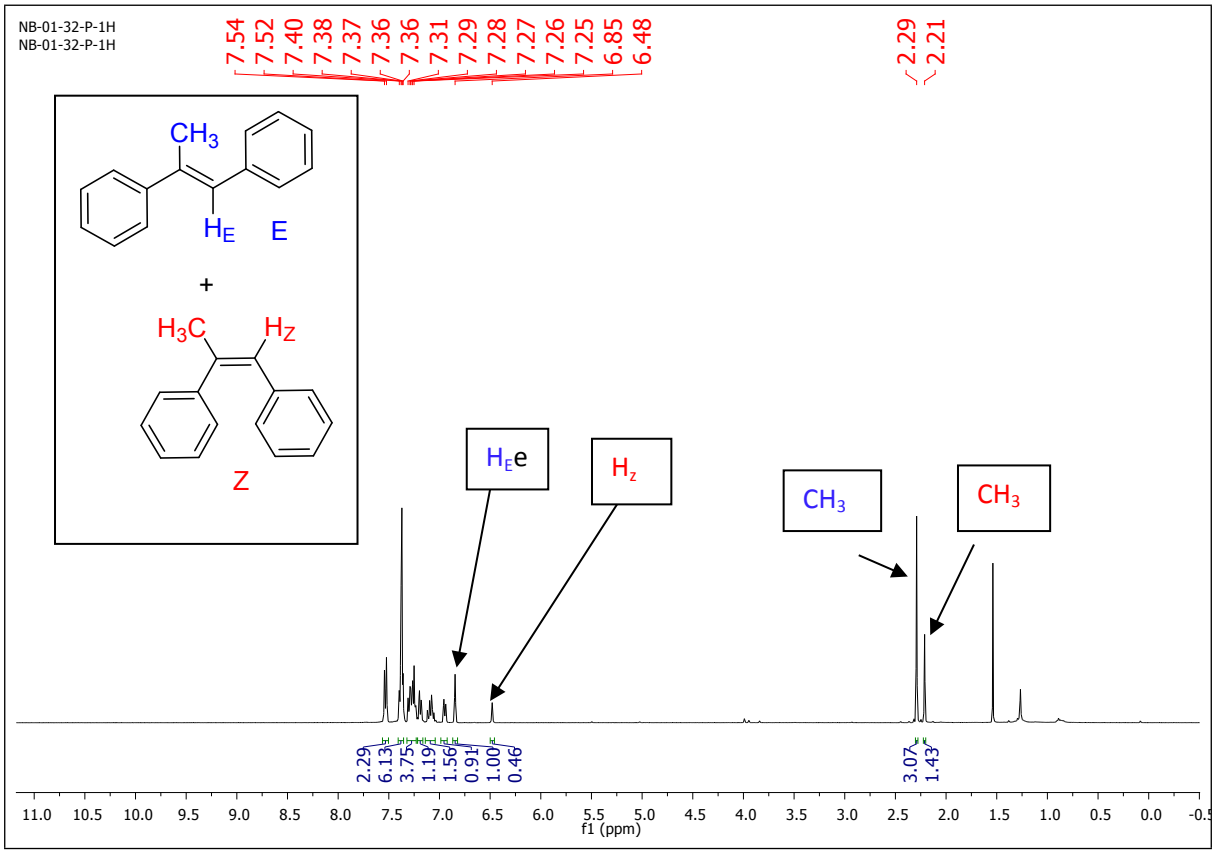

NB-01-33-P-13C
NB-01-33-P-13C
138.32
137.63
137.56
134.83
129.53
128.69
128.59
128.38
127.99
127.25
126.55
123.74
77.48
77.16
76.84
21.57
21.37
f1 (ppm)

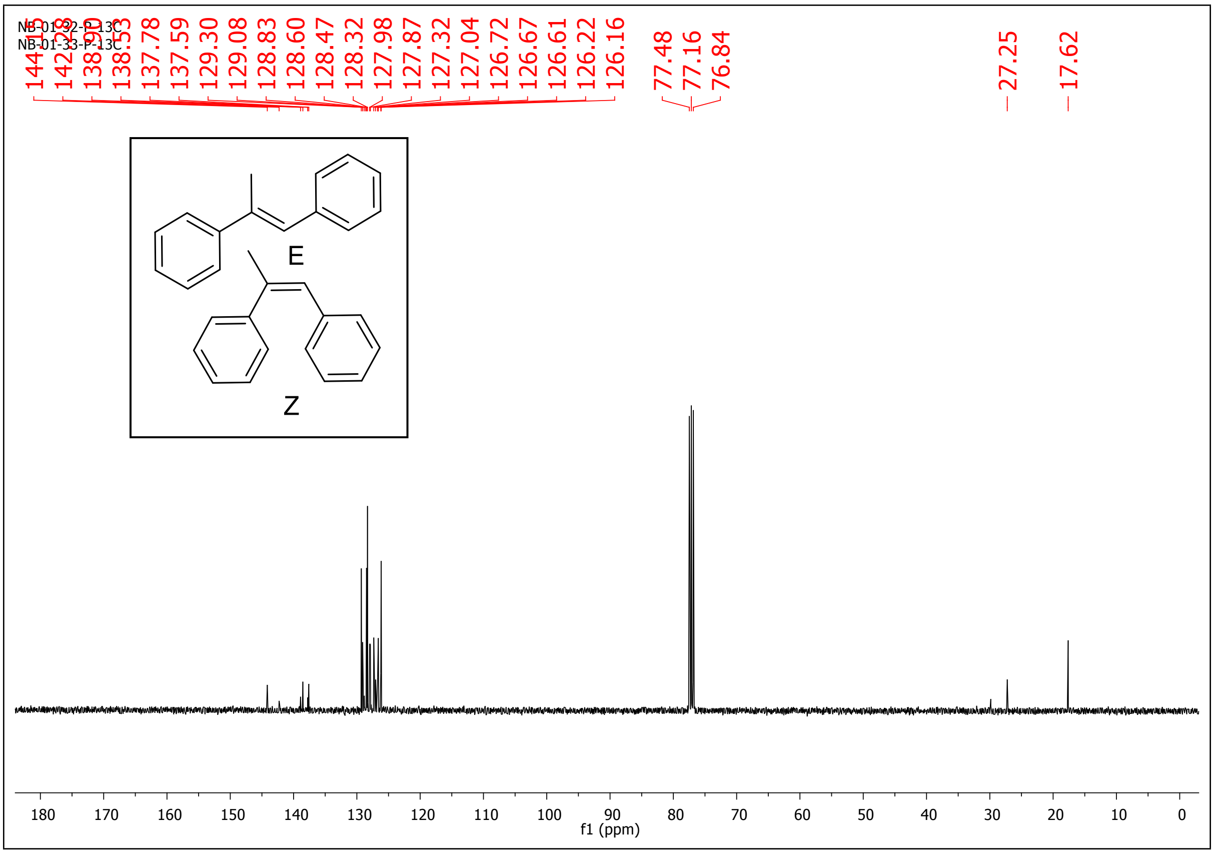

7.33
7.33
7.29
7.28
7.27
7.25
7.25
7.19
7.18
7.17
7.17
7.15
6.99
6.95
6.84
6.80
6.36
6.35
6.35
6.34
6.28
6.28
O
6.37
0.98
1.00
0.85
0.91
f1 (ppm)


NB-01-23-P-13C
NB-01-23-P-13C
153.46
142.28
137.20
128.83
127.72
127.32
126.48
116.71
111.78
108.68
77.48
77.16
76.84
O
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40
f1 (ppm)

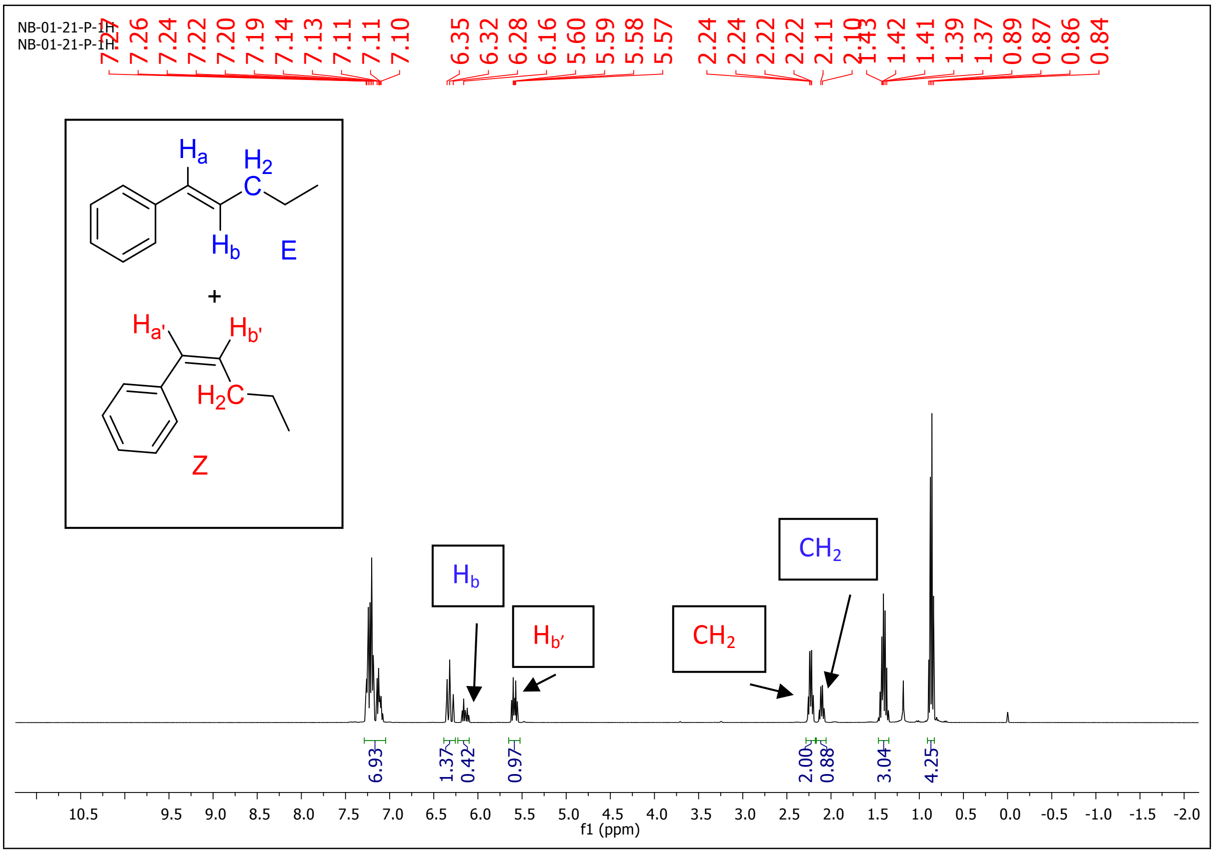

NB-01-31-P-1H
NB-01-31-P-1H
8.56 8.56 8.55 8.55 8.55 7.62 7.62 7.62 7.60 7.60 7.59 7.59 7.58 7.58 7.57 7.57 7.38 7.38 7.38 7.36 7.35 7.12 7.12 7.11 7.10 7.10 7.10 7.09 7.09
N
N
2.00
4.37
2.43
2.07
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1.0
f1 (ppm)


NB-01-31-P-13C
NB-01-31-P-13C
155.14
149.87
136.77
131.89
123.40
122.77
77.48
77.16
76.84
N
N
f1 (ppm)

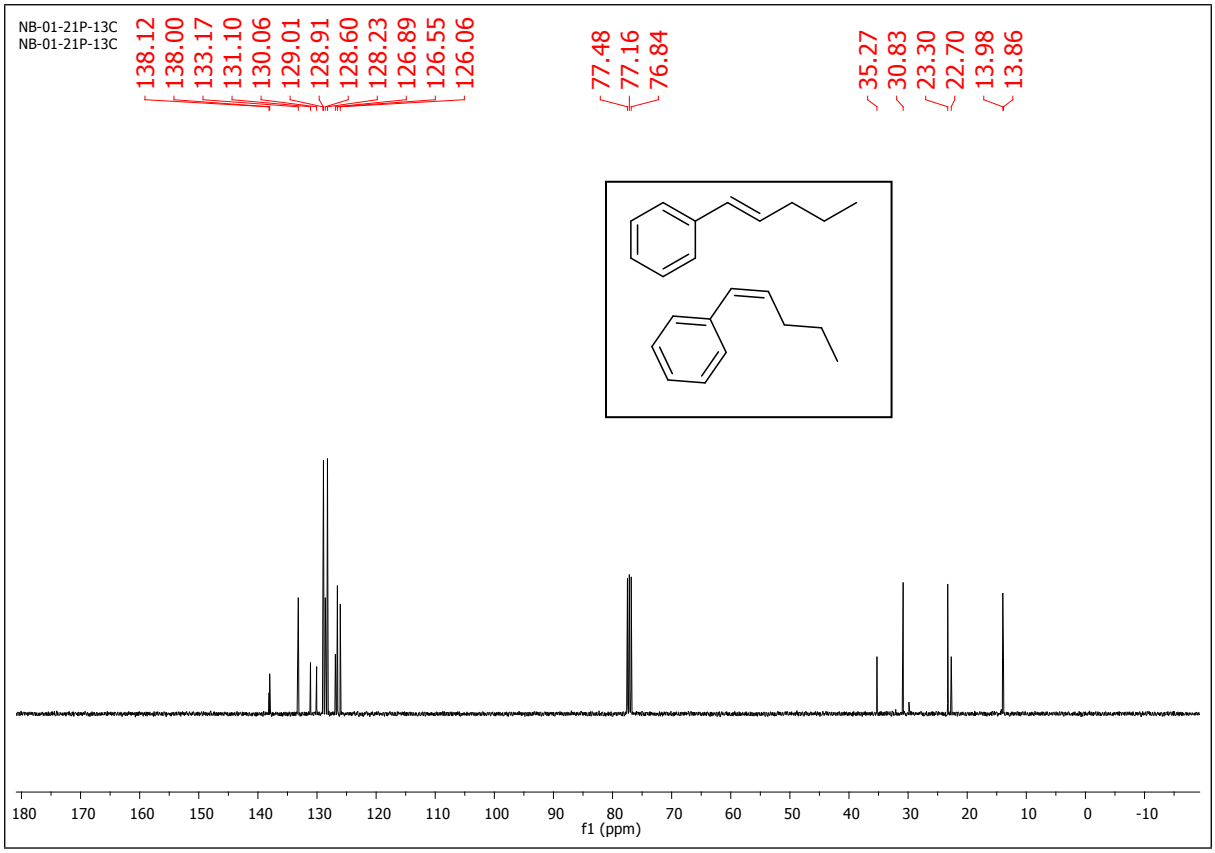

NB-01-32-P-1H
NB-01-32-P-1H
7.54
7.52
7.40
7.38
7.37
7.36
7.36
7.31
7.29
7.28
7.27
7.26
7.25
6.85
6.48
2.29
2.21
CH3
HE
E
+
H3C
HZ
Z
HEe
Hz
CH3
CH3
2.29
6.13
3.75
1.19
1.56
0.91
1.00
0.46
3.07
1.43
f1 (ppm)

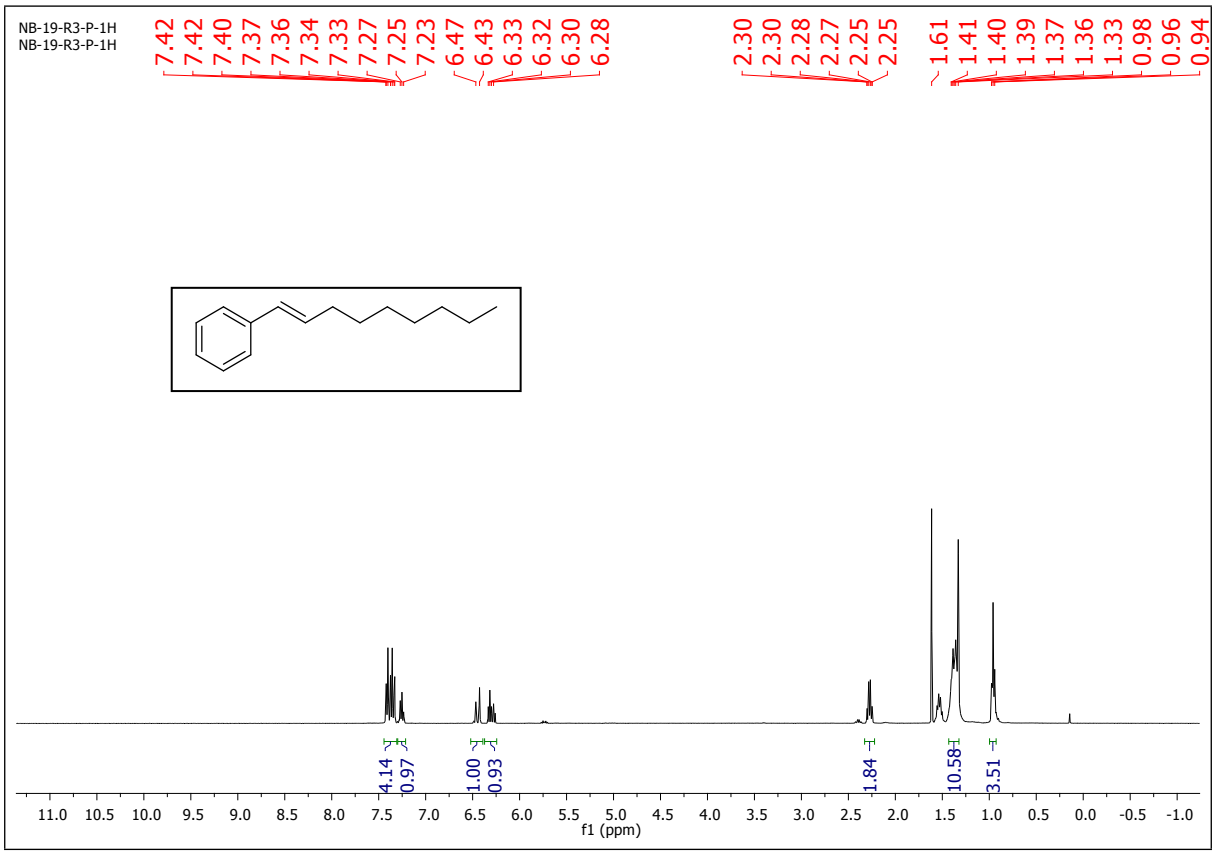


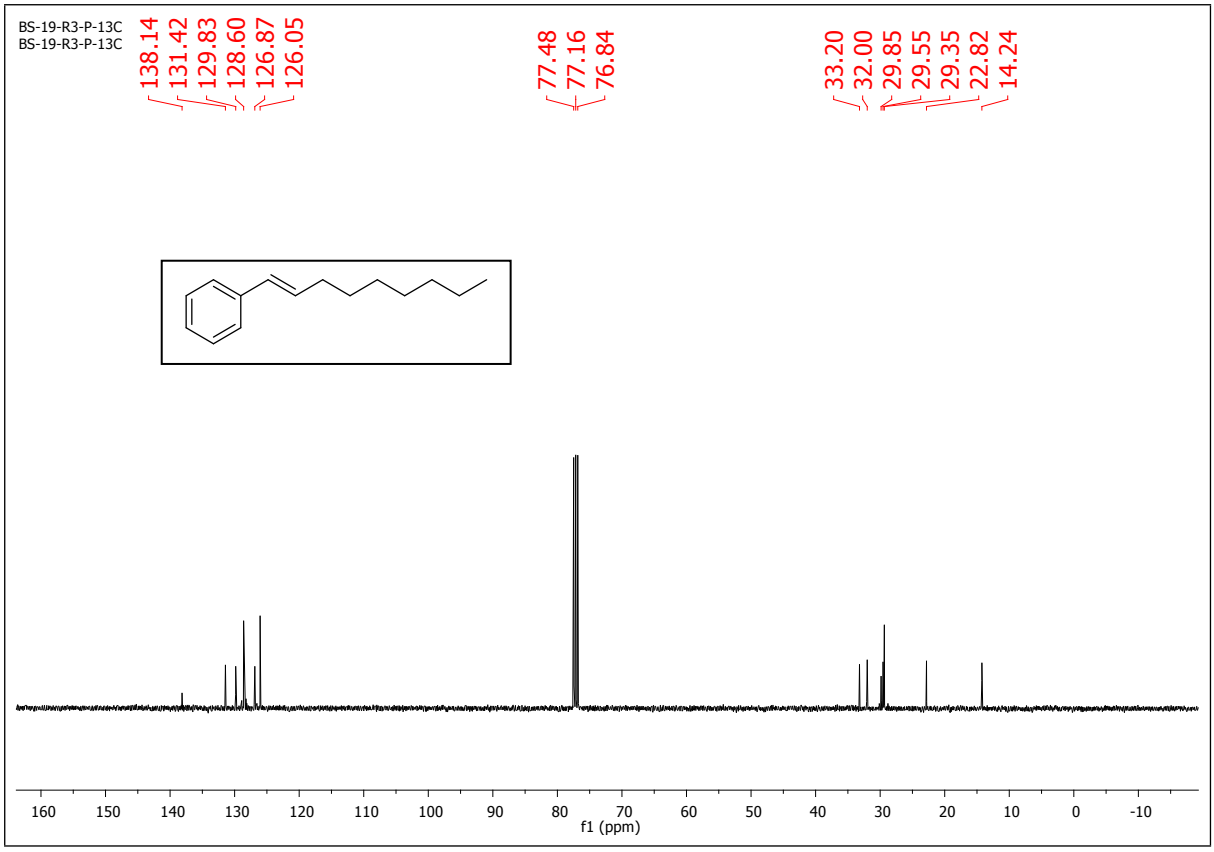
138.53
137.78
137.59
129.30
129.08
128.83
128.60
128.47
128.32
127.98
127.87
127.32
127.04
126.72
126.67
126.61
126.22
126.16
77.48
77.16
76.84
27.25
17.62
E
Z
f1 (ppm)

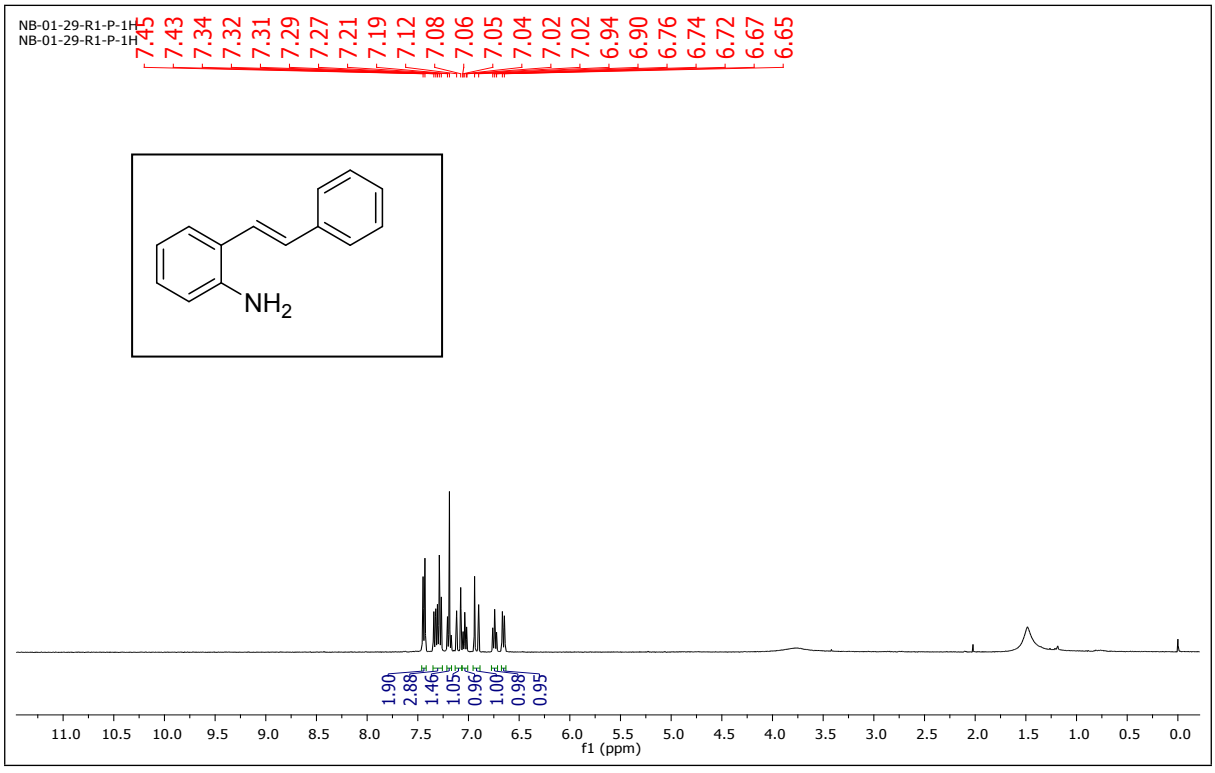


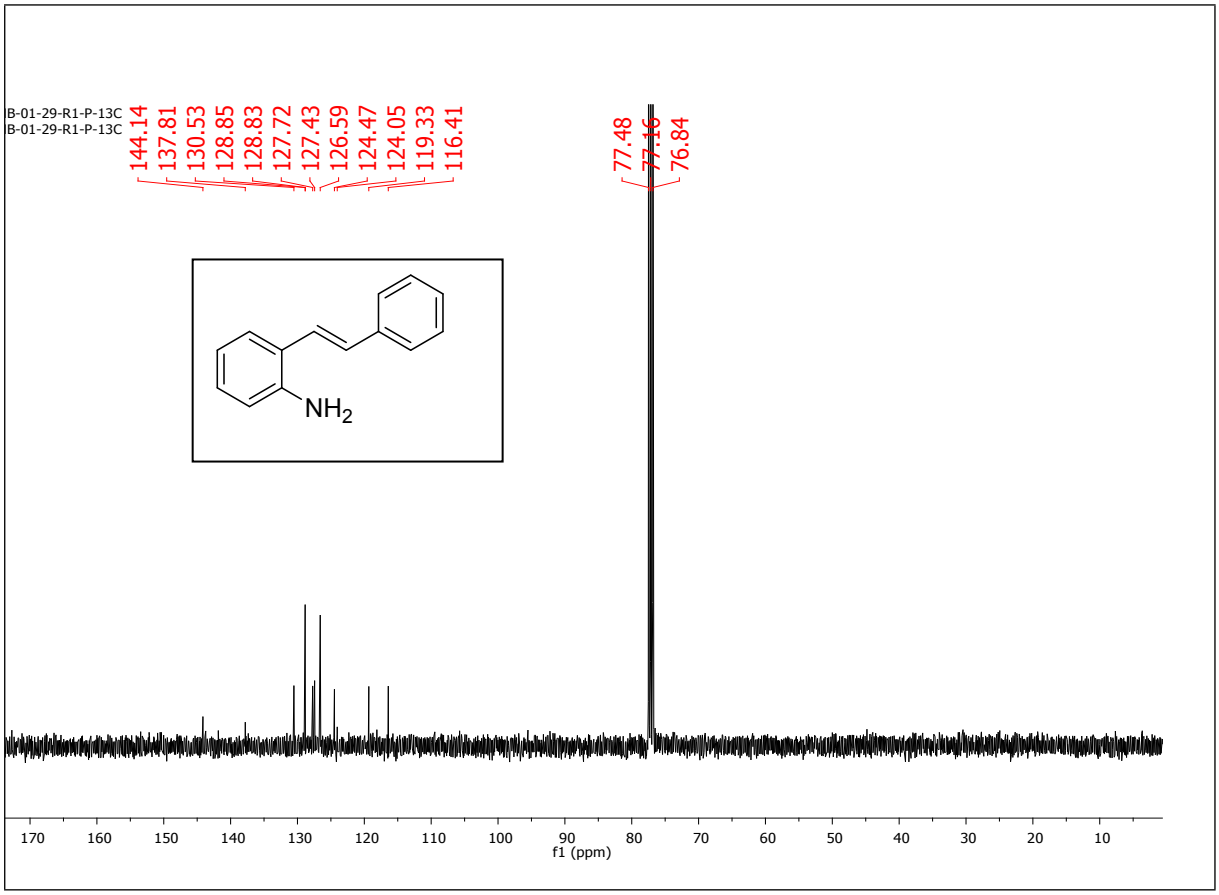
NB-01-21-P-1H
7.26
7.24
7.22
7.20
7.19
7.14
7.13
7.11
7.11
7.10
6.35
6.32
6.28
6.16
5.60
5.59
5.58
5.57
2.24
2.24
2.22
2.22
2.11
1.42
1.41
1.39
1.37
0.89
0.87
0.86
0.84
Ha
H2
C
Hb
E
+
Ha'
Hb'
H2C
Z
Hb
Hb'
CH2
CH2
6.93
1.37
0.42
0.97
2.00
0.88
3.04
4.25
f1 (ppm)


NB-01-21P-13C
NB-01-21P-13C
138.12
138.00
133.17
131.10
130.06
129.01
128.91
128.60
128.23
126.89
126.55
126.06
77.48
77.16
76.84
35.27
30.83
23.30
22.70
13.98
13.86
f1 (ppm)


NB-19-R3-P-1H
NB-19-R3-P-1H
7.42
7.42
7.40
7.37
7.36
7.34
7.33
7.27
7.25
7.23
6.47
6.43
6.33
6.32
6.30
6.28
2.30
2.30
2.28
2.27
2.25
2.25
1.61
1.41
1.40
1.39
1.37
1.36
1.33
0.98
0.96
0.94
4.14
0.97
1.00
0.93
1.84
10.58
3.51
f1 (ppm)


BS-19-R3-P-13C
BS-19-R3-P-13C
138.14
131.42
129.83
128.60
126.87
126.05
77.48
77.16
76.84
33.20
32.00
29.85
29.55
29.35
22.82
14.24
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


NB-01-29-R1-P-1H
NB-01-29-R1-P-1H
7.45
7.43
7.34
7.32
7.31
7.29
7.27
7.21
7.19
7.12
7.08
7.06
7.05
7.04
7.02
7.02
6.94
6.90
6.76
6.74
6.72
6.67
6.65
NH2
1.90
2.88
1.46
1.05
0.96
1.00
0.98
0.95
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


B-01-29-R1-P-13C
B-01-29-R1-P-13C
144.14
137.81
130.53
128.85
128.83
127.72
127.43
126.59
124.47
124.05
119.33
116.41
77.48
77.16
76.84
NH2
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)