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Supporting Information
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Thieme

A Simple and Convenient Method for the Synthesis of *N*,*N*-Diaryl Tertiary Amines

Supporting Information

Francis S. Wekesa, Neha Phadke, Claire Jahier, David B. Cordes and Michael Findlater*

Department of Chemistry and Biochemistry, Texas Tech University,
Lubbock, TX, 79409, USA

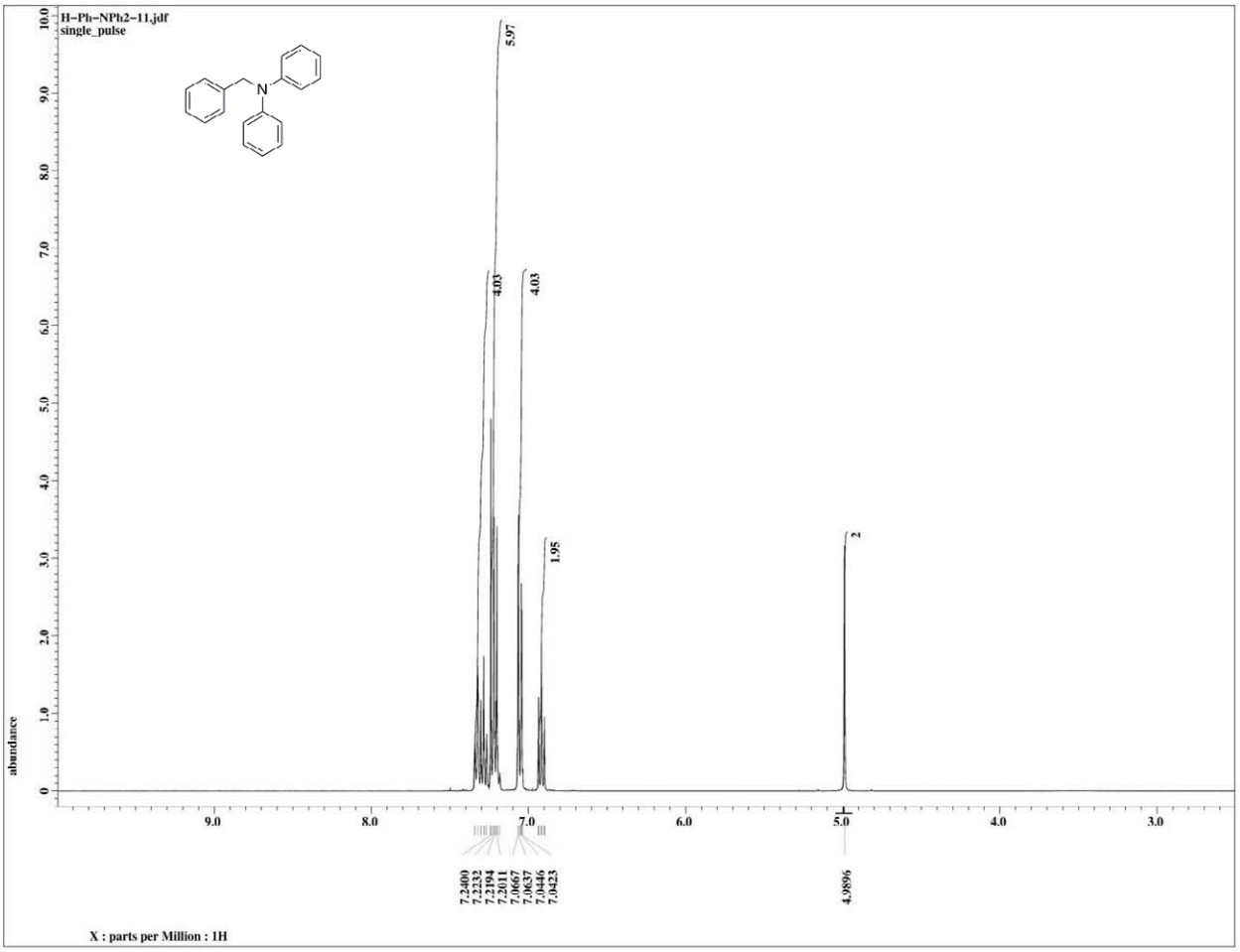
Contents

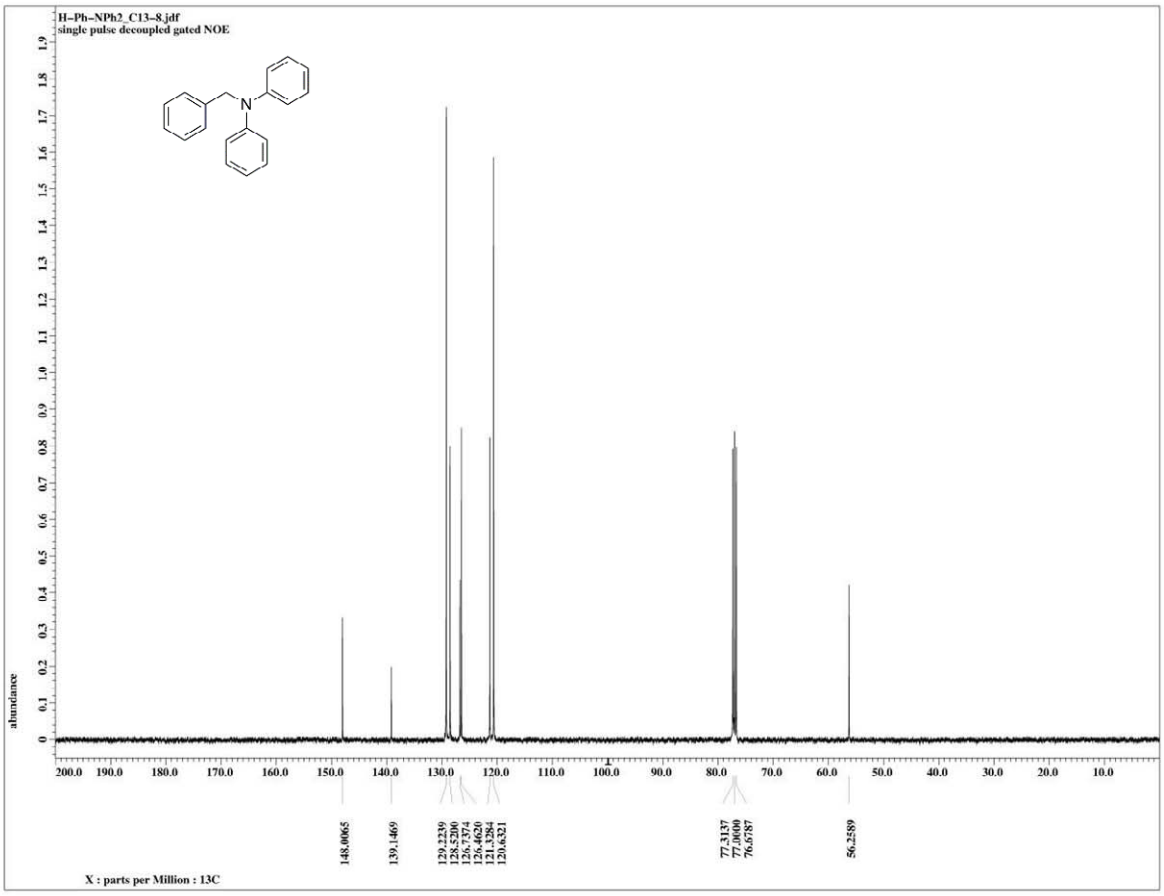
Details of X-ray Experiments

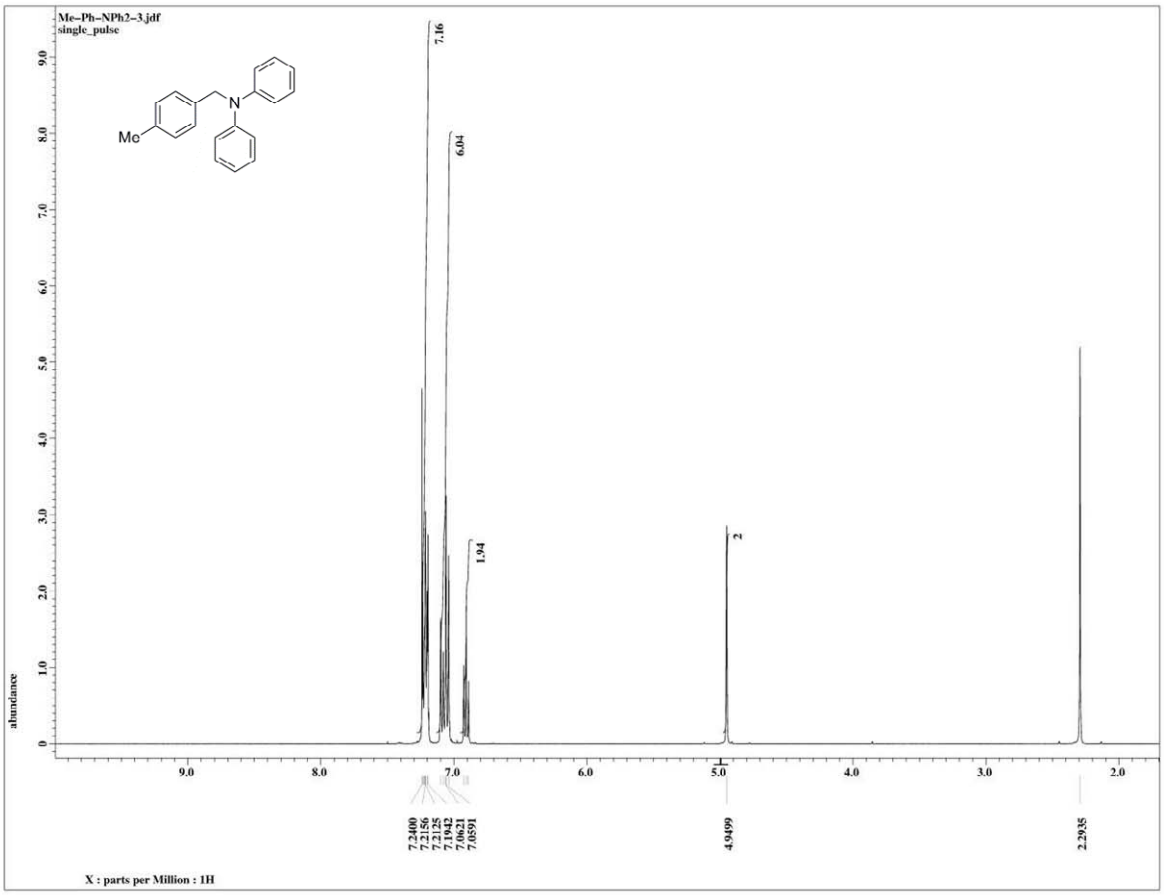
X-ray diffraction data for compounds **2a**, **2c**, and **4g** were obtained on a Bruker Smart Apex II CCD diffractometer, and data for compounds **2b** and **6** were obtained on a Rigaku SCXMini CCD diffractometer. All data were collected at room temperature using graphite-monochromated Mo-K□ radiation (λ = 0.71073 Å). Intensity data were collected using □-steps accumulating area detector images spanning at least a hemisphere of reciprocal space. All the data were corrected for Lorentz polarization effects. A multi-scan absorption correction was applied using SADABS15[S1] (compounds **2a**, **2c**, and **4g**), or CrystalClear[S2] (compounds **2b** and **6**). Structures were solved by direct methods and refined by full-matrix least squares against F^2 (SHELXTL[S3]). All hydrogen atoms were assigned riding isotropic displacement parameters and constrained to idealized geometries. The $-CF_3$ group in the structure of **2d** was disordered by rotation over two sites, with occupancies of 0.7 and 0.3. Restraints to bond distances and angles, and to thermal parameters was required for the minor component of the disorder. The structure of compound **4g** shows two independent molecules in the asymmetric unit.

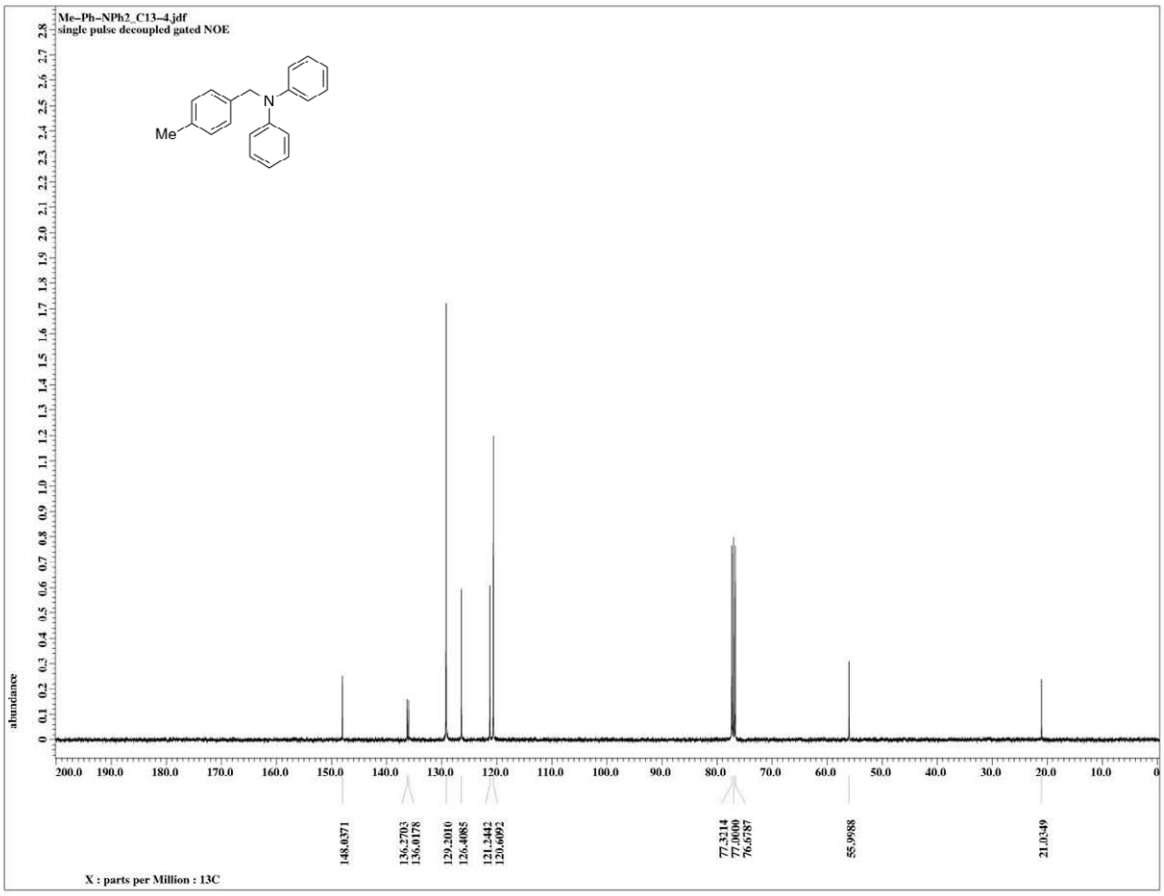
S1. Sheldrick, G. M., *SADABS* v**2008**/1, **2008**.
S2. CrystalClear-SM Expert v2.0. Rigaku Americas, The Woodlands, Texas, USA, and Rigaku Corporation, Tokyo, Japan, **2010**.
S3. Sheldrick, G. M., *Acta Crystallogr*., **2008**, *A64*, 112-122.

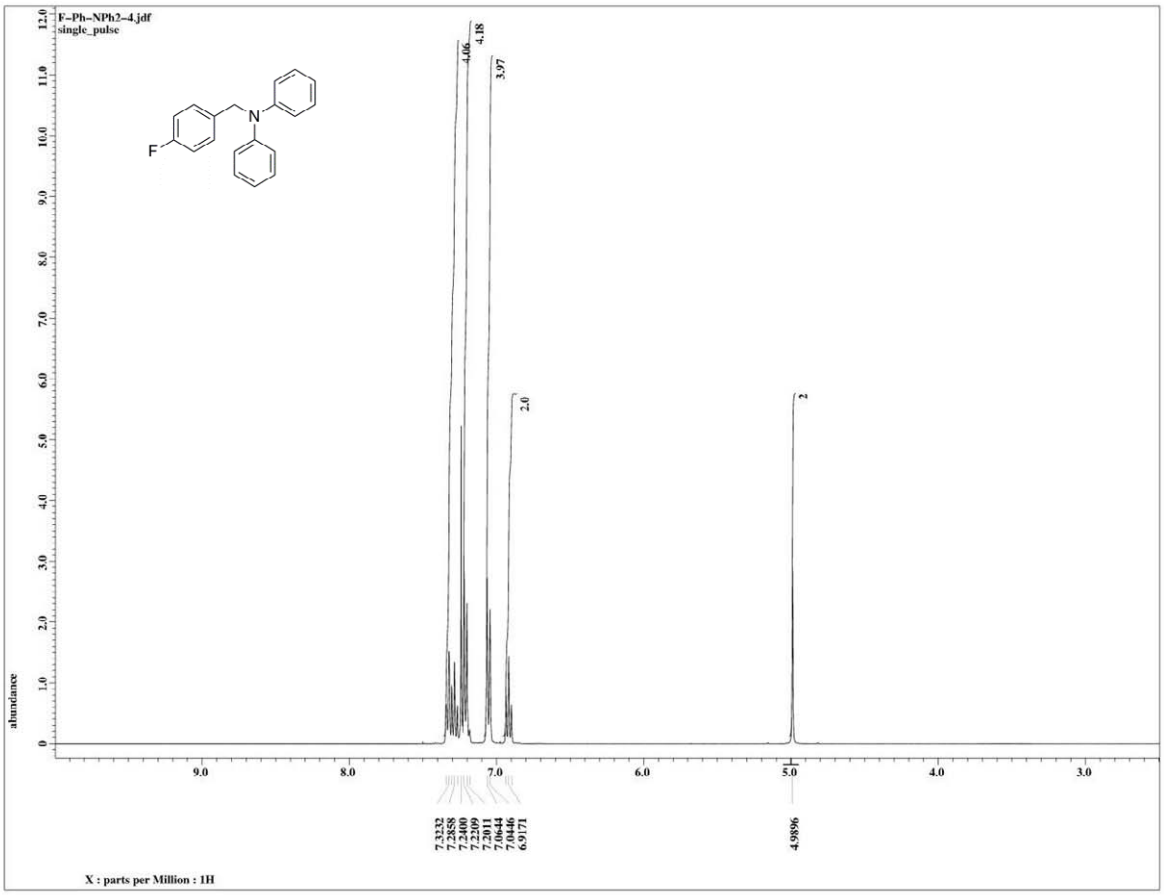
^{1}H and ^{13}C Spectra for all compounds:

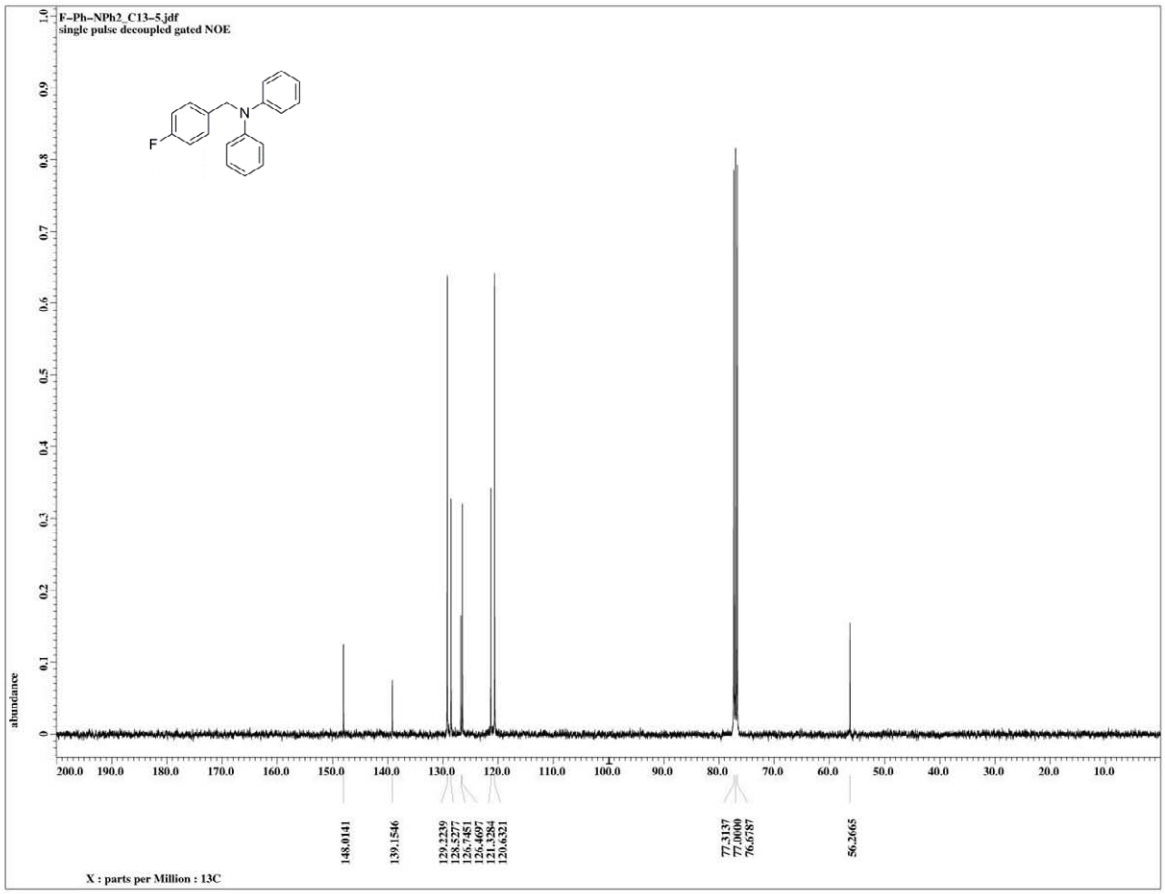


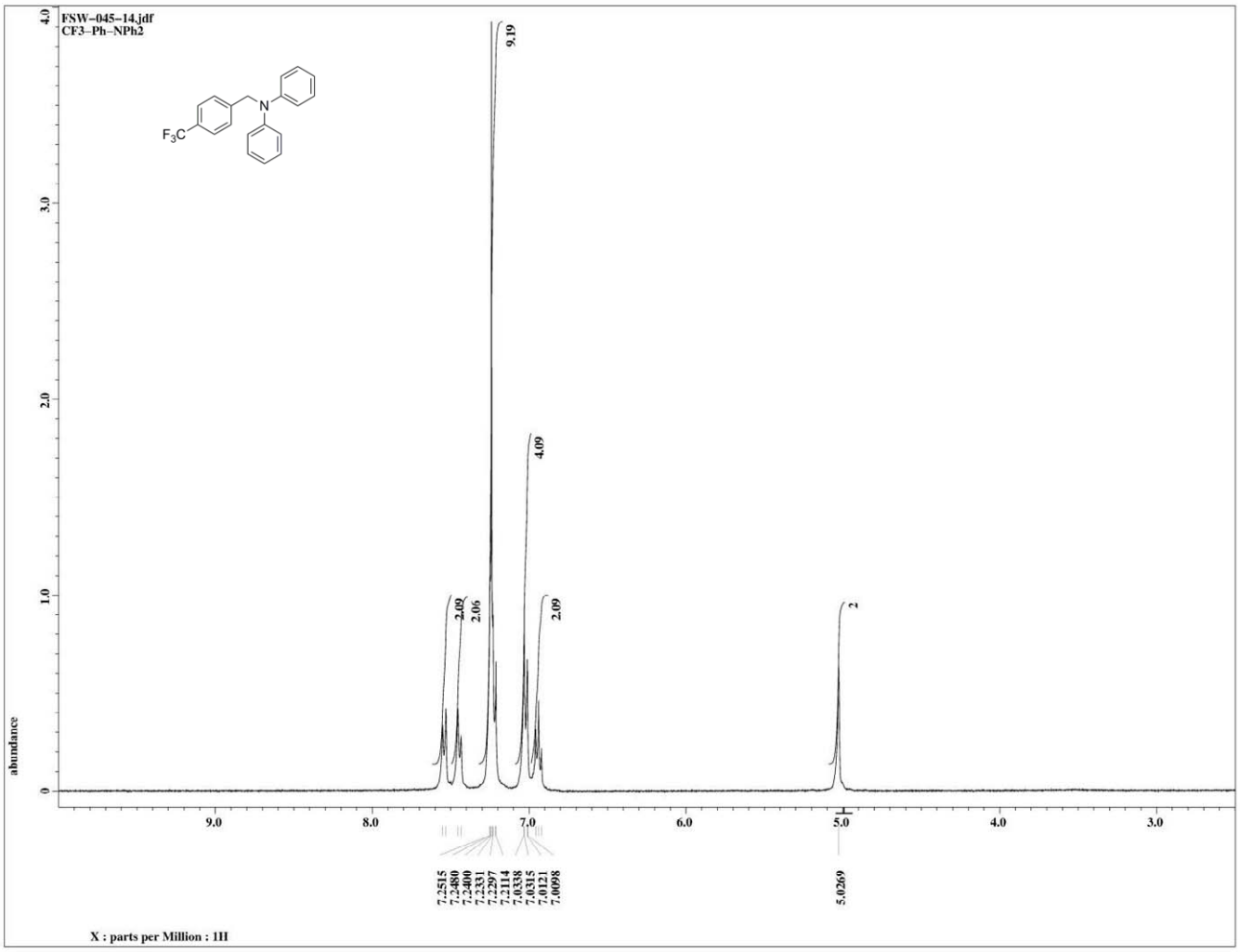

H-Ph-NPh2_C13-8.jdf
single pulse decoupled gated NOE
abundance
X : parts per Million : 13C
148.0065
139.1469
129.2239
128.5290
126.7374
126.4620
121.3284
120.6321
77.3137
77.0800
76.6787
56.2589

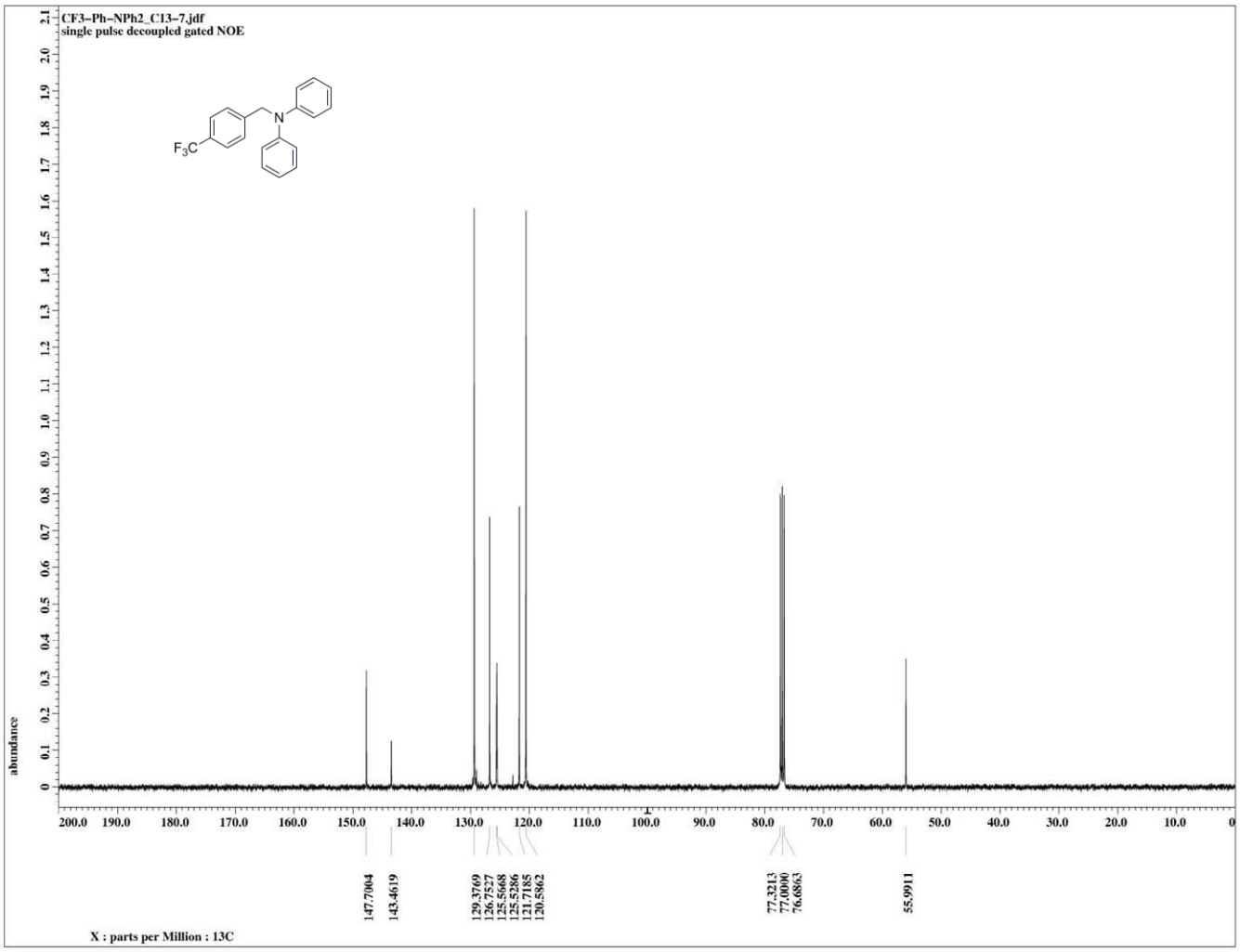

Me-Ph-NPh2-3.jdf
single_pulse
Me
N
7.16
6.04
1.94
2
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
7.2400
7.2156
7.2125
7.1942
7.0621
7.0591
4.9499
2.2935
X : parts per Million : 1H

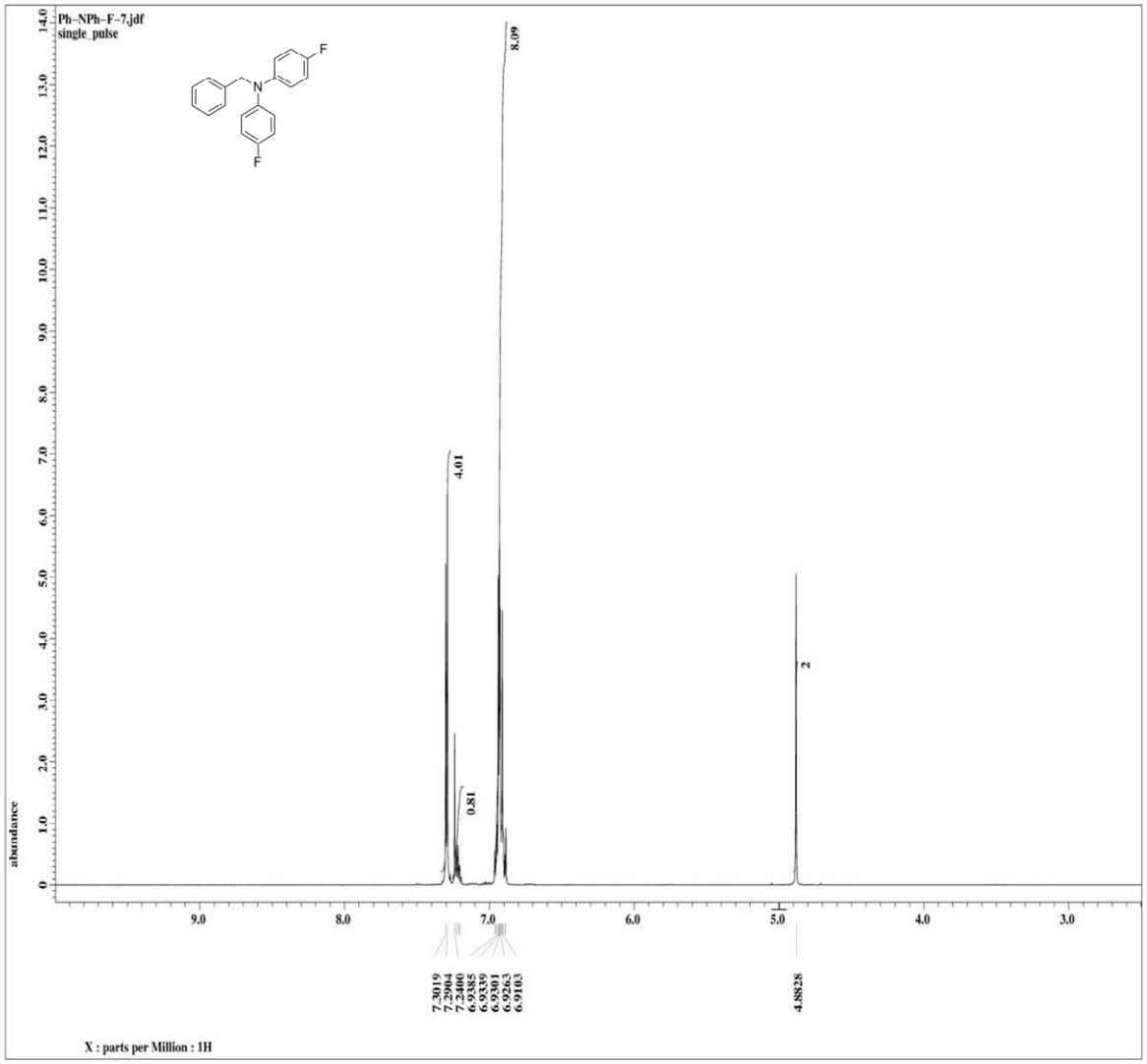

Me-Ph-NPh2_C13-4.jdf
single pulse decoupled gated NOE
Me
N
abundance
X : parts per Million : 13C
148.0371
136.2703
136.0178
129.2010
126.4085
121.3442
120.6092
77.3214
77.0000
76.6787
55.9988
21.0349

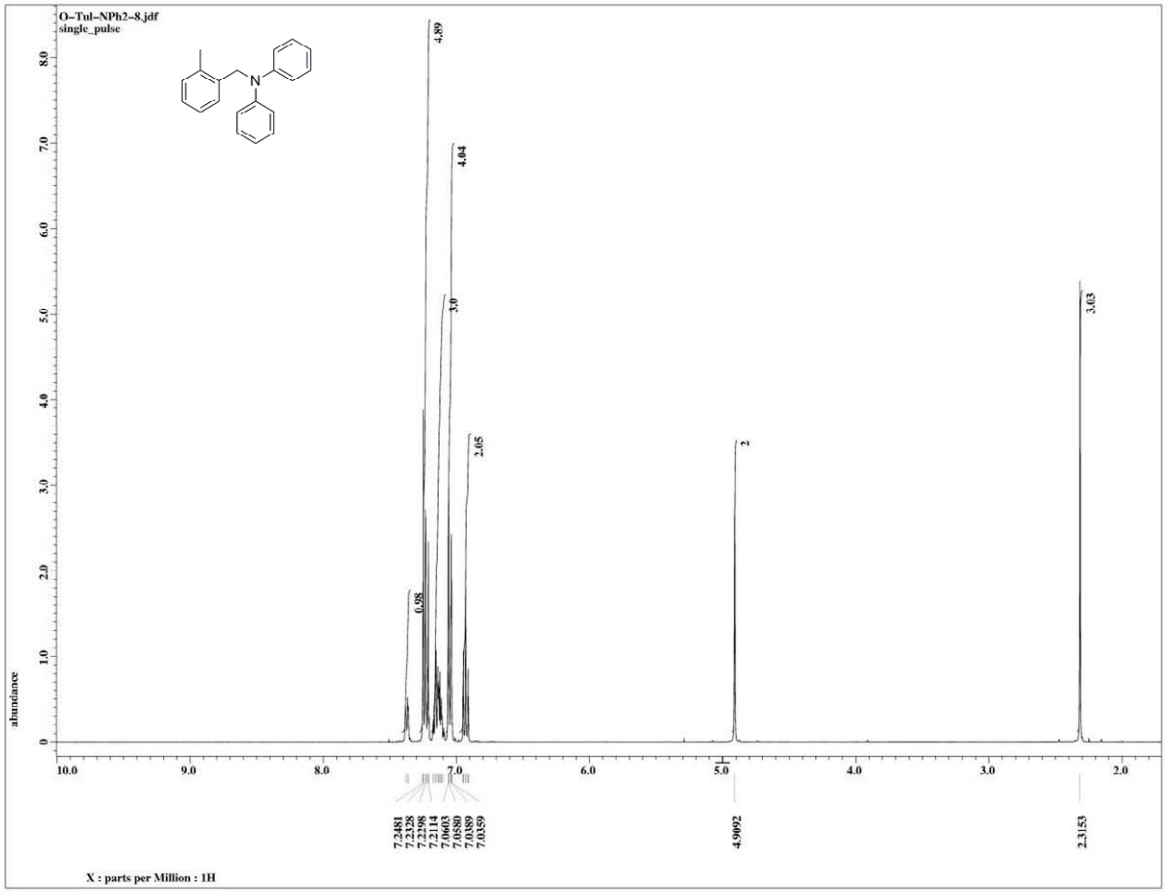

F-Ph-NPh2-4.jdf
single_pulse
F
N
4.06
4.18
3.97
2.0
2
abundance
9.0
8.0
7.0
6.0
5.0
4.0
3.0
7.3332
7.2858
7.2400
7.2209
7.2011
7.0644
7.0446
6.9171
4.9896
X : parts per Million : 1H

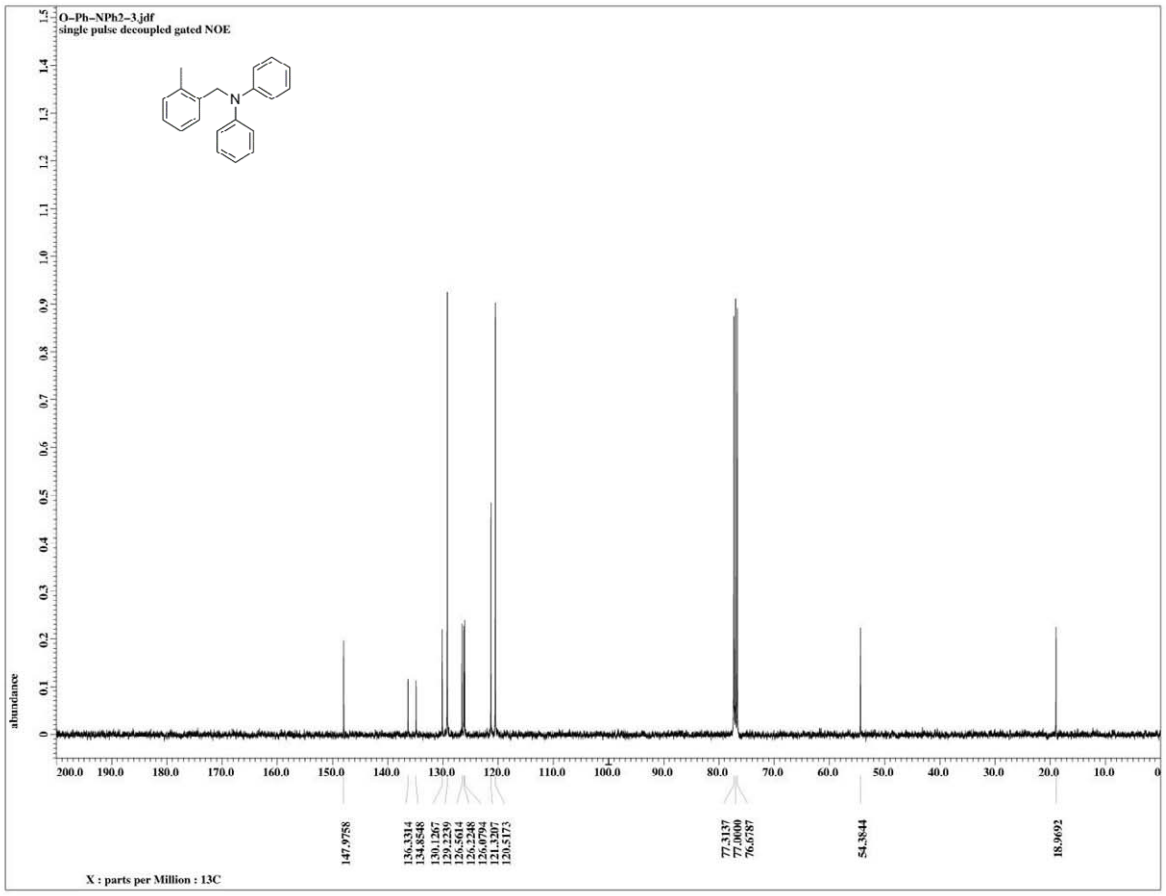

F-Ph-NPh2_C13-5.jdf
single pulse decoupled gated NOE
N
F
abundance
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0
148.0141
139.1546
129.2239
128.5277
126.7451
126.4697
121.3284
120.6321
77.3137
77.0000
76.6787
56.2665
X : parts per Million : 13C

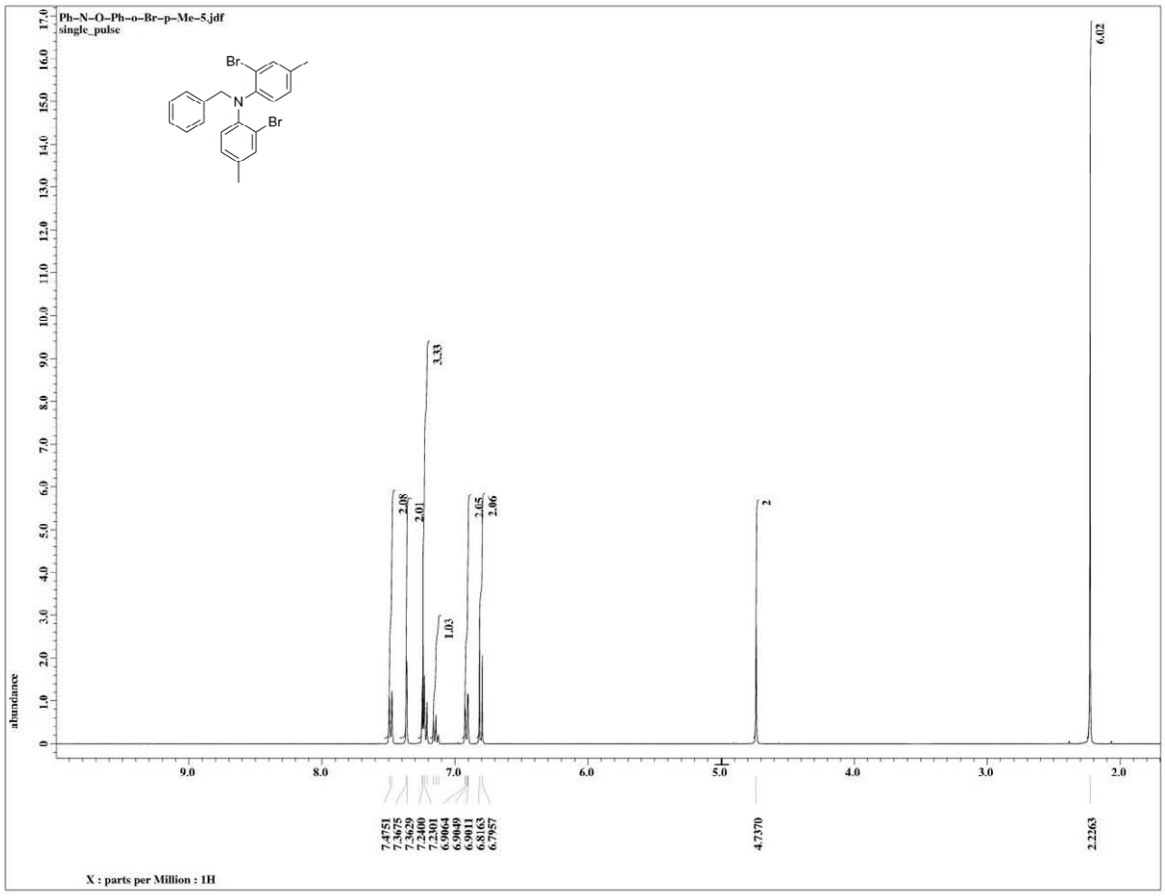

FSW-045-14.jdf
CF3-Ph-NPh2
F3C
N
9.19
4.09
2.09
2.06
2.02
2
abundance
4.0
3.0
2.0
1.0
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
7.2515
7.2480
7.2400
7.2331
7.2297
7.2114
7.0338
7.0315
7.0121
7.0098
5.0269
X : parts per Million : 1H

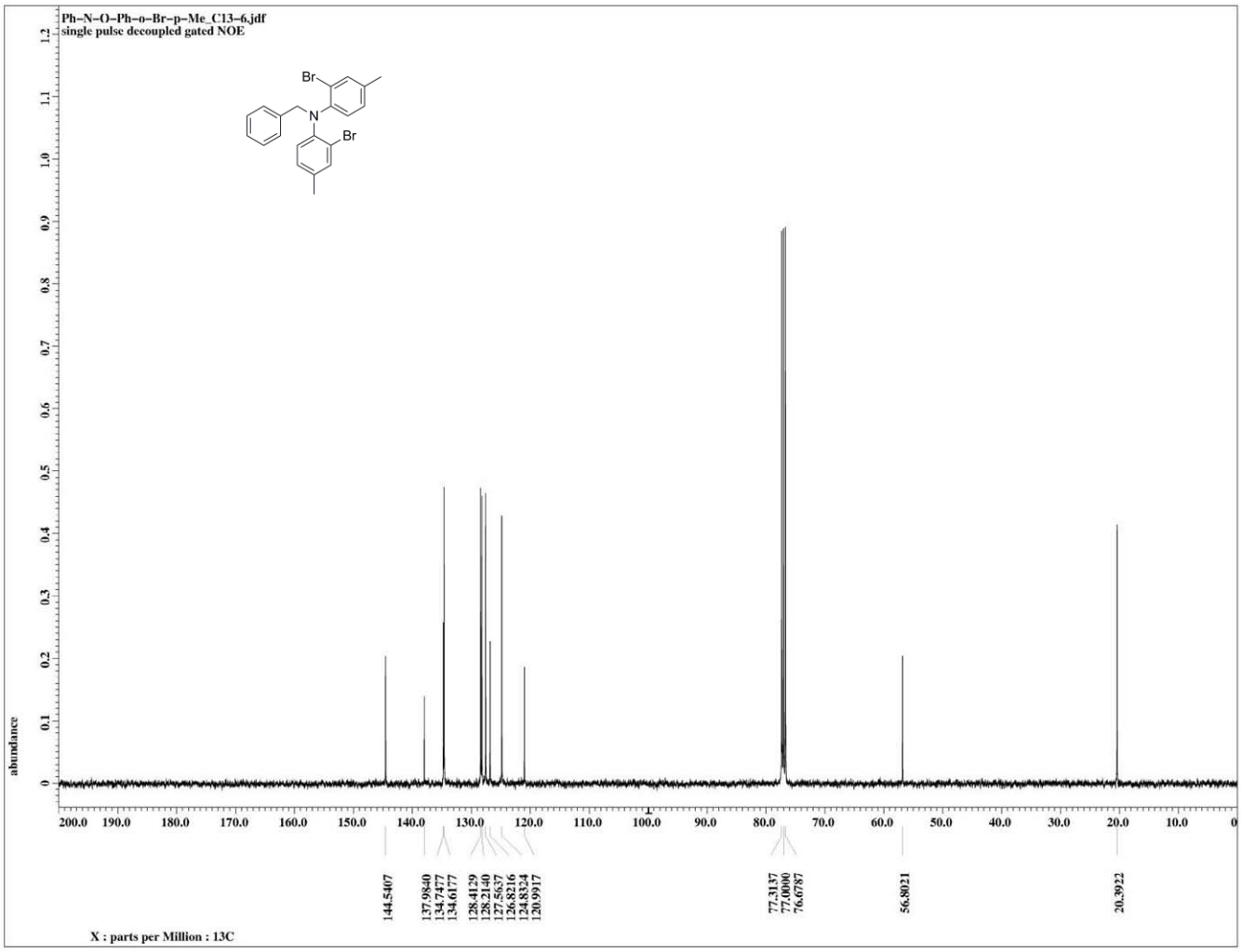

CF3–Ph–NPh2_C13–7.jdf
single pulse decoupled gated NOE
abundance
147.7004
143.4619
129.3769
126.7527
125.5668
125.5286
121.7185
120.5862
77.3213
77.0000
76.6863
55.9911
X : parts per Million : 13C

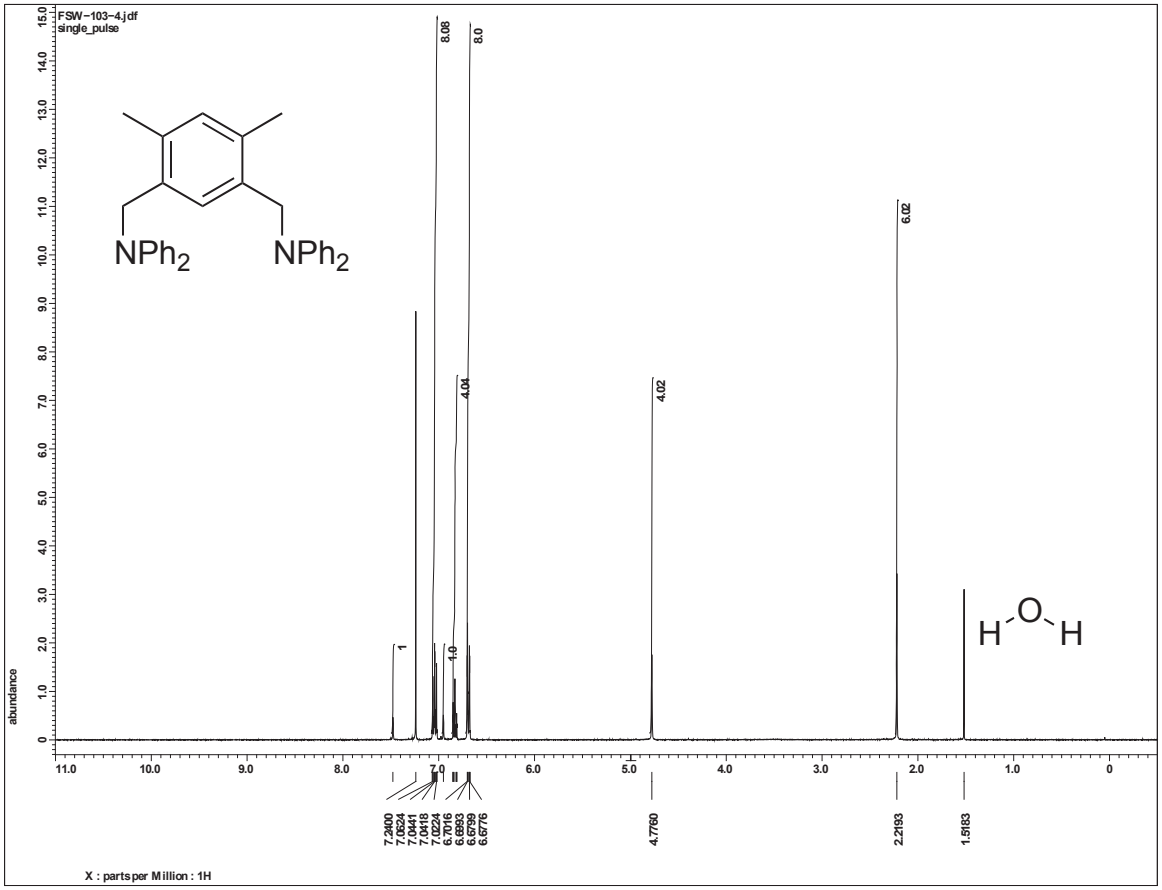

Ph-NPh-F-7.jdf
single_pulse
F
N
F
8.09
4.01
0.81
2
abundance
14.0
13.0
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
7.3019
7.2904
7.2400
6.9385
6.9339
6.9301
6.9263
6.9103
4.8828
X : parts per Million : 1H


O-Tul-NPh2-8.jdf
single_pulse
4.89
4.04
3.0
2.05
2
3.03
0.98
abundance
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
7.2481
7.2328
7.2298
7.2114
7.0603
7.0589
7.0389
7.0359
4.9092
2.3153
X : parts per Million : 1H


O-Ph-NPh2-3.jdf
single pulse decoupled gated NOE
N
abundance
147.9758
136.3314
134.8548
130.1267
129.3239
126.5814
126.2168
126.0794
121.3207
120.5173
77.3137
77.0600
76.6787
54.3844
18.0692
X : parts per Million : 13C


Ph-N-O-Ph-o-Br-p-Me-5.jdf
single_pulse
Br
N
Br
abundance
6.02
3.33
2.08
2.01
2.05
2.06
2
1.03
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
7.4751
7.3675
7.3629
7.2400
7.2301
6.9064
6.9040
6.9011
6.8163
6.7957
4.7370
2.2263
X : parts per Million : 1H


Ph-N-O-Ph-o-Br-p-Me_C13-6.jdf
single pulse decoupled gated NOE
Br
N
Br
abundance
144.5407
137.9840
134.7477
134.6177
128.4129
128.2140
127.5637
126.8216
124.8334
120.9917
77.3137
77.0000
76.6787
56.8021
20.3922
X : parts per Million : 13C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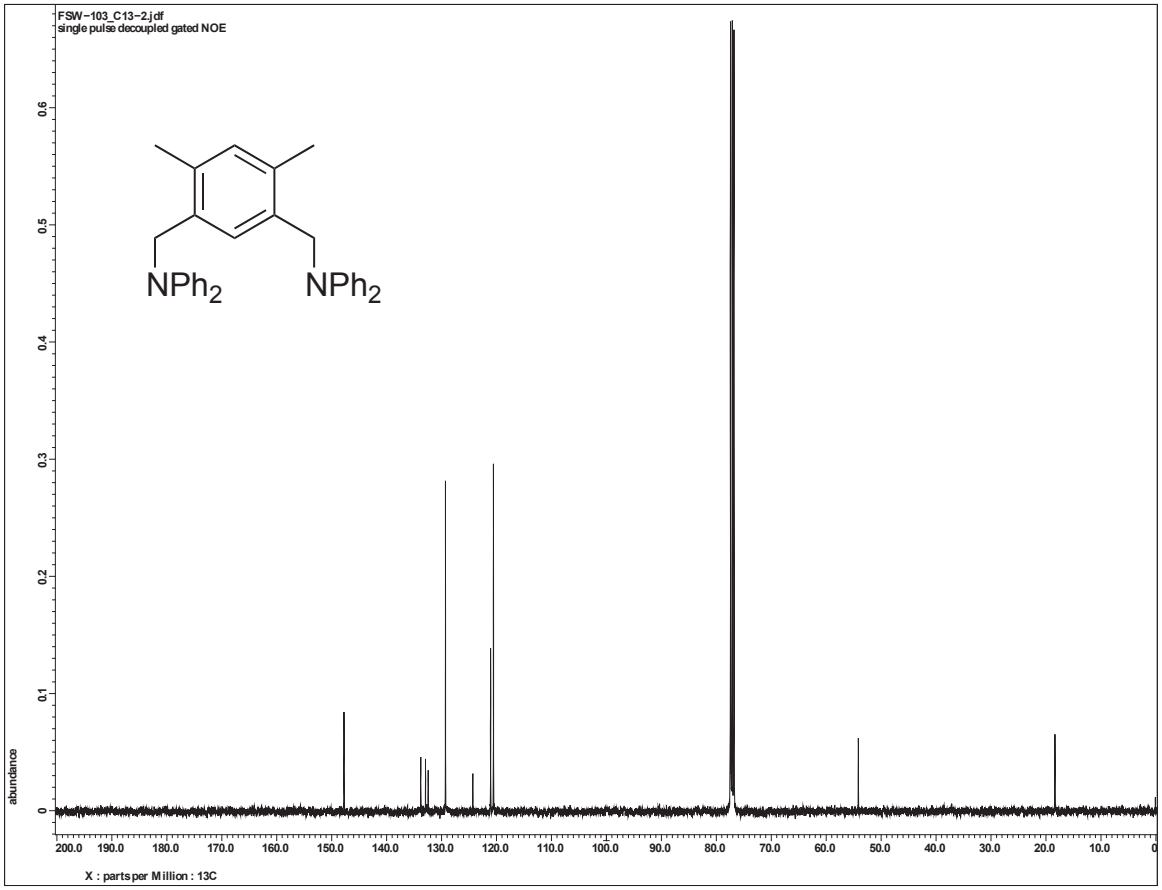
single_pulse
NPh2
NPh2
H
O
H
abundance
X : parts per Million : 1H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single pulse decoupled gated NOE
NPh2
NPh2
abundance
0
0.1
0.2
0.3
0.4
0.5
0.6
200.0 190.0 180.0 170.0 160.0 150.0 140.0 130.0 120.0 110.0 100.0 90.0 80.0 70.0 60.0 50.0 40.0 30.0 20.0 10.0 0
X : parts per Million : 13C