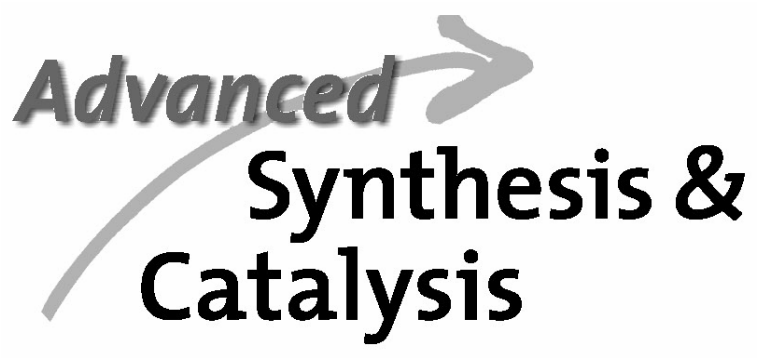

Supporting Information

Supporting Information

Cadmium Catalyzed *C-N* Cross-Coupling of Amines with Aryl Iodides

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Materials and Methods

Amines, bromobenzene (99%), chlorobenzene (99%), iodobenzene (98%) and $Cd(OAc)_2.2H_2O$ (99%), $CdCl_2 \cdot 2H_2O$ (99%), $CdCl_2$ (99%) and CdI_2 (99%) were purchased from Aldrich. NMR spectra (400 MHz for ^1H and 100 MHz for ^{13}C) were recorded using DRX-400 Varian spectrometer using $CDCl_3$ as solvent and Me_4Si as internal standard. Flash column chromatography was performed on silica gel (230-400 mesh) using ethyl acetate and hexane as eluent. Melting points determined using Buchi B-540 melting point apparatus and uncorrected.

***N*-(Phenyl)aniline.**[1] Colorless solid; yield 92%; m.p. 52 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.27-7.22 (m, 4H), 7.07-7.04 (d, J = 7.2 Hz, 4H), 6.93-6.89 (m, 2H), 5.69 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.33, 129.55, 121.21, 118.01.

***N*-(4-Bromophenyl)aniline**.[2] Colorless solid; yield 88%; m.p. 88 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.35-7.25 (m, 5H), 7.08-6.92 (m, 4H), 5.69 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.23, 145.34, 129.76, 129.48, 128.01, 126.57, 117.57, 114.30.

***N*-(4-Chlorophenyl)aniline.**[2] Colorless solid; yield 90%; m.p. 73 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.27-7.16 (m, 5H), 7.03-6.91 (m, 4H), 5.66 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.3, 146.3, 132.4, 129.7, 121.4, 119.2, 115.4.

***N*-(2-Methylphenyl)aniline**.[2] Light brown solid; yield 98%; m.p. 38 ^oC; ^1H NMR (400 MHz, $CDCl_3$) δ 7.25-7.17 (m, 5H), 7.13 (t, J = 6.8 Hz, 1H), 6.95-6.88 (m, 3H) 5.48 (s, 1H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.4, 142.9, 130.4, 129.7, 127.6, 125.8, 121.9, 119.2, 118.5, 17.6.

***N*-(2-Methoxyphenyl)aniline**.[3] Yellow oil; yield 94%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.32-7.26 (m, 3H), 7.16-7.12 (m, 2H), 7.03 (t, *J* = 7.2 Hz, 1H), 6.94-6.55 (m, 3H) 6.19 (s, 1H), 3.91 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.4, 143.4, 132.4, 129.7, 121.9, 119.2, 118.5, 115.9, 110.6, 58.6.

***N*-(4-Methoxyphenyl)aniline**.[1] Colorless solid; yield 91%; m.p. 105 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.42 (d, *J* = 8.4 Hz, 2H), 7.24-7.12 (m, 5H) 6.90 (d, *J* = 8.4 Hz, 2H), 5.51 (s,1H), 3.81 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.5, 145.8, 135.6, 129.1, 123.4, 120.1, 115.2, 55.3.

***N*-(4-Nitrophenyl)aniline**.[3] Yellow powder; yield 70%; m.p. 134 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (d, *J* = 9.2 Hz, 2H), 7.38 (t, *J* = 8.0 Hz, 2H) 7.20-7.12 (m, 3H), 6.93 (d, *J* = 7.6 Hz, 2H), 6.34 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.5, 138.2, 137.6, 129.7, 127.6, 125.7, 123.4, 114.0.

***N*-(2,4-Dimethyl phenyl)phenylamine**.[4] Colorless liquid; yield 92%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19-7.13 (m, 2H), 7.07 (d, *J* = 8.0 Hz, 1H) 6.96 (s, 1H), 6.90 (d, *J* = 8.0 Hz, 1H), 6.88-6.75 (m, 3H), 5.25 (s, 1H), 2.23 (s, 3H), 2.15 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.3, 139.5, 129.4, 124.5, 121.3, 117.6, 116.8, 21.2, 20.8.

***N*-Phenylbenzylamine**.[5] Yellow solid; yield 98%; m.p. 34 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34-7.22 (m, 5H), 7.15 (t, *J* = 7.2 Hz, 2H), 6.71 (t, *J* = 7.6 Hz, 1H), 6.61 (d, *J* = 7.63 Hz, 2H), 4.31 (s, 2H), 4.09 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.6, 139.5, 130.1, 129.1, 128.7, 127.4, 118.3, 113.3, 48.6.

***N*-(Phenyl)furfurylamine**.[6] Colorless oil; yield 82%; ^{1}H NMR (400 MHz, $CDCl_3$,) δ 7.33 (s, 1H), 7.16 (t, *J* = 8.0 Hz, 2H), 6.73-6.64 (m, 3H), 6.29 (br s, 1H), 6.21 (br s, 1H), 4.29 (s, 2H), 4.01 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.3, 148.6, 142.1, 129.4, 118.2, 113.4, 110.5, 107.2, 41.6.

***N*-Phenyl butylamine**.[7] Colorless liquid; yield 92%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16–7.12 (m, 2H), 6.66 (t, *J* = 7.2 Hz, 1H), 6.59 (d, *J* = 8.4 Hz, 2H), 3.51(s, 1H), 3.10-3.06

(m, 2H), 1.61-1.54 (m, 2H), 1.45-1.36 (m, 2H), 0.95-0.91 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 129.4, 117.3, 112.9, 43.9, 31.9, 20.5, 14.1.

***N*-Cyclohexylaniline**.[3] Colorless oil; yield 90%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13-7.03 (m, 2H), 6.66-6.56 (m, 3H), 3.24-3.21 (m, 1H), 2.05-2.03 (m, 2H), 1.77-1.72 (m, 2H), 1.66-1.61 (m, 1H), 1.40-1.10 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.3, 129.6, 116.8, 113.3, 53.1, 33.0, 26.6, 25.2.

***N*-Phenylpyrrolidine**.[7] Colorless liquid; yield 94%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18–7.13 (m, 2H), 6.58 (t, *J* = 7.2 Hz, 1H), 6.50 (d, *J* = 8.4 Hz, 2H), 3.20 (t, *J* = 6.8 Hz, 4H), 1.94-1.90 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.3, 129.0, 115.2, 111.5, 47.4, 25.3.

***N*-Phenylpiperidine**.[1] Colorless liquid; yield 98%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24-7.20 (m, 2H), 6.93-6.91 (m, 2H), 6.80 (t, *J* = 7.2 Hz, 1H), 3.19 (t, *J* = 5.6 Hz, 4H), 1.71-1.66 (m, 4H), 1.58-1.53 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.8, 129.5, 119.1, 117.6, 51.5, 29.6, 26.3.

***N*-Phenylmorpholine**.[1] Colorless solid; yield 97%; m.p. 55 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 (t, *J* = 8.0 Hz, 2H), 6.90-6.84 (m, 3H), 3.85 (t, *J* = 4.8 Hz, 4H), 3.14 (t, *J* = 4.8 Hz, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.5, 129.4, 120.3, 115.9, 67.1, 49.6.

***N*-Phenylpyrrole.**[8] Colorless solid; yield 96%; m.p. 62 ^{o}C, ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 7.6 Hz, 2H), 7.46-7.26 (m, 3H), 7.14-7.11 (m, 2H) 6.38-6.37 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.7, 130.4, 129.7, 127.6, 125.7, 120.7, 119.5, 110.6.

***N*-Phenylindole**.[1] Colorless oil; yield 97%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 7.6 Hz, 1H), 7.66 (d, *J* = 8.0 Hz, 1H), 7.57-7.56 (m, 3H), 7.41-7.40 (m, 2H), 7.30-7.25 (m, 3H), 6.58 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.0, 136.0, 129.8, 129.5, 128.1, 126.6, 124.5, 122.5, 121.3, 120.5, 110.7, 103.7.

***N*-(Phenyl)imidazole.**[9] Colorless liquid; yield 98%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87 (s, 1H), 7.50-7.47 (m, 2H), 7.40-7.37 (m, 3H), 7.29 (s, 1H), 7.21 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.5 135.8 130.5 130.1 127.7, 121.7 118.5, 107.4

***N*-(Phenyl)-5-methyl-imidazole.** Colorless oil; yield 96%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43-7.35 (m, 5H), 7.22-7.20 (m, 3H), 6.96 (s, 1H), 6.93 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 129.7 128.4,127.7, 125.7,120.8, 13.9

***N*-(Phenyl)benzimidazole**.[10] Colorless solid, yield 98%; m.p. 96 ^{o}C; ^{1}H NMR (400 MHz, $CDCl_3$,) δ 8.16 (s, 1H), 7.90-7.87 (m, 1H), 7.57-7.43 (m, 6H), 7.34-7.30 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.6, 130.3 128.4, 124.3, 124.1 123.2, 120.6, 110.8

***N*-(3,5-Dimethylphenyl)pyrrolidine**. Colorless liquid; yield 55%; ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.30 (s, 1H), 6.18 (s, 2H), 3.22 (t, J = 6.4 Hz, 4H), 2.35 (s, 6H), 1.93 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.0, 138.9, 128.4, 109.9 108.5, 47.8, 25.6, 21.9.

***N*-(2,4-Dimethylphenyl)pyrrolidine**.[11] Colorless liquid; yield 37%; ^{1}H NMR (400 MHz, $CDCl_3$,) δ 6.91 (s, 1H), 6.88 (d, J = 8.0 Hz, 1H), 6.78 (d, J = 8.0 Hz, 1H), 3.09 (m, 4H), 2.26 (s, 3H), 2.21 (s, 3H), 1.89 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.3, 131.3, 127.6, 126.0, 115.8, 54.6, 24.9, 21.3, 14.4.

***N*-(4-Methoxyphenyl)pyrrolidine**.[12] White solid; m.p. 44-45 ^{o}C; yield 26%; ^{1}H NMR (400 MHz, $CDCl_3$,) δ 6.79 (d, J = 9 Hz, 2H), 6.48 (d, J = 11 Hz, 2H), 3.69 (s, 3H), 3.18-3.15 (m, 4H), 1.93-1.90 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.2, 144.2, 115.3, 114.9, 56.2, 48.2, 25.6.

***N*-(3-Methoxyphenyl)pyrrolidine**.[13] Yellow oil; yield 42%; ^{1}H NMR (400 MHz, $CDCl_3$,) δ 7.11(t, J = 9.5 Hz, 1H), 6.22-6.18 (dd, J = 1.2, 8 Hz, 2H), 6.08 (s, 1H), 3.77 (s, 3H), 3.26-3.23 (m, 4H), 1.97-1.94 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.6, 149.1, 130.0, 105.1, 100.6, 98.1, 55.3, 47.8, 25.7.

***N*-(2-Methoxyphenyl)pyrrolidine**.[12] Yellow liquid; yield 22%; ^{1}H NMR (400 MHz, $CDCl_3$,) δ 6.82–6.71 (m , 4H), 3.77 (s, 3H), 3.22-3.19 (m, 4H), 1.88-1.84 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.7, 139.9, 121.3, 119.9, 115.7, 111.9, 55.8, 50.7, 24.9.

***N*-(4-Nitrophenyl)pyrrolidine**.[14] Yellow solid; m.p. 177-178 °C; yield 77%; ^{1}H NMR (400 MHz, $CDCl_3$,) δ 8.14 (d, *J* = 9.2 Hz, 2H), 6.48 (d, *J* = 8.8 Hz, 2H), 3.42-3.39 (m, 4H), 2.09-2.06 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.0, 136.7, 126.3, 110.6, 48.1, 25.7.

***N*-(3-Nitrophenyl)pyrrolidine**.[14] Orange solid; m.p. 97-99 °C; yield 18%; ^{1}H NMR (400 MHz, $CDCl_3$,) δ 7.45 (d, *J* = 6.4 Hz, 1H), 7.33-7.28 (m, 2H), 6.81-6.78 (d, *J* = 6.4 Hz, 1H), 3.35-3.32 (m, 4H), 2.07-2.04 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 149.6, 148.4, 129.7, 117.4, 110.0, 105.8, 94.7, 48.0, 25.7.

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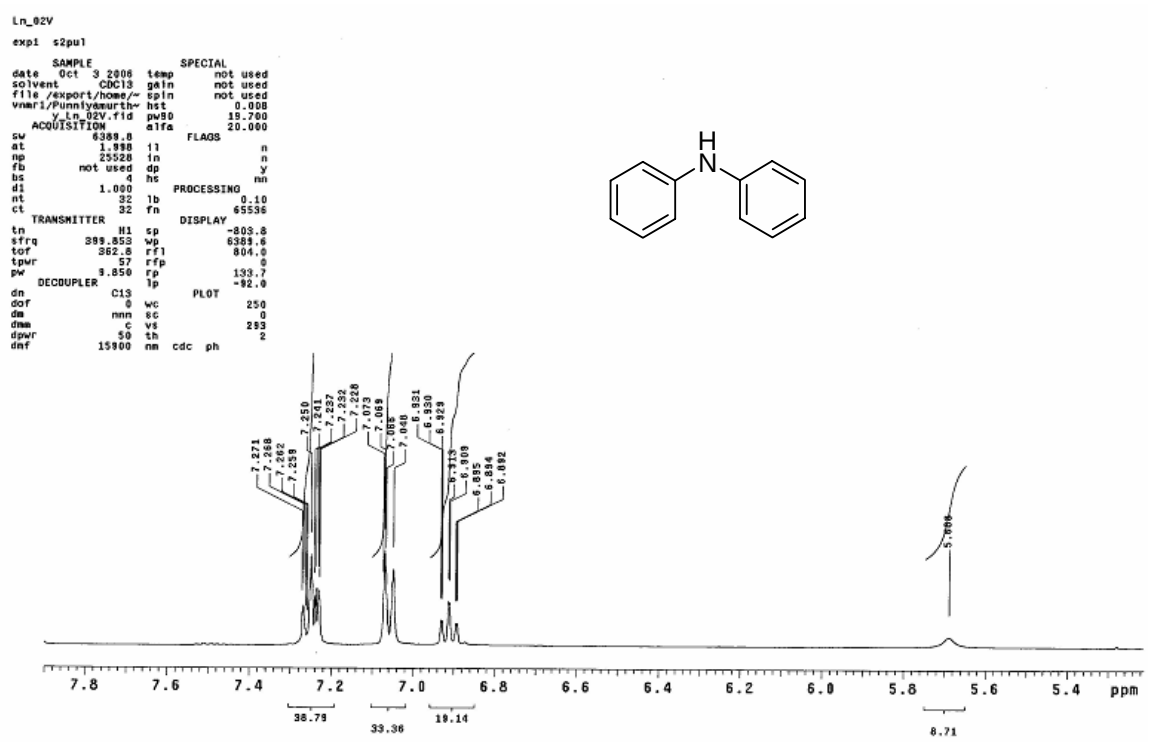
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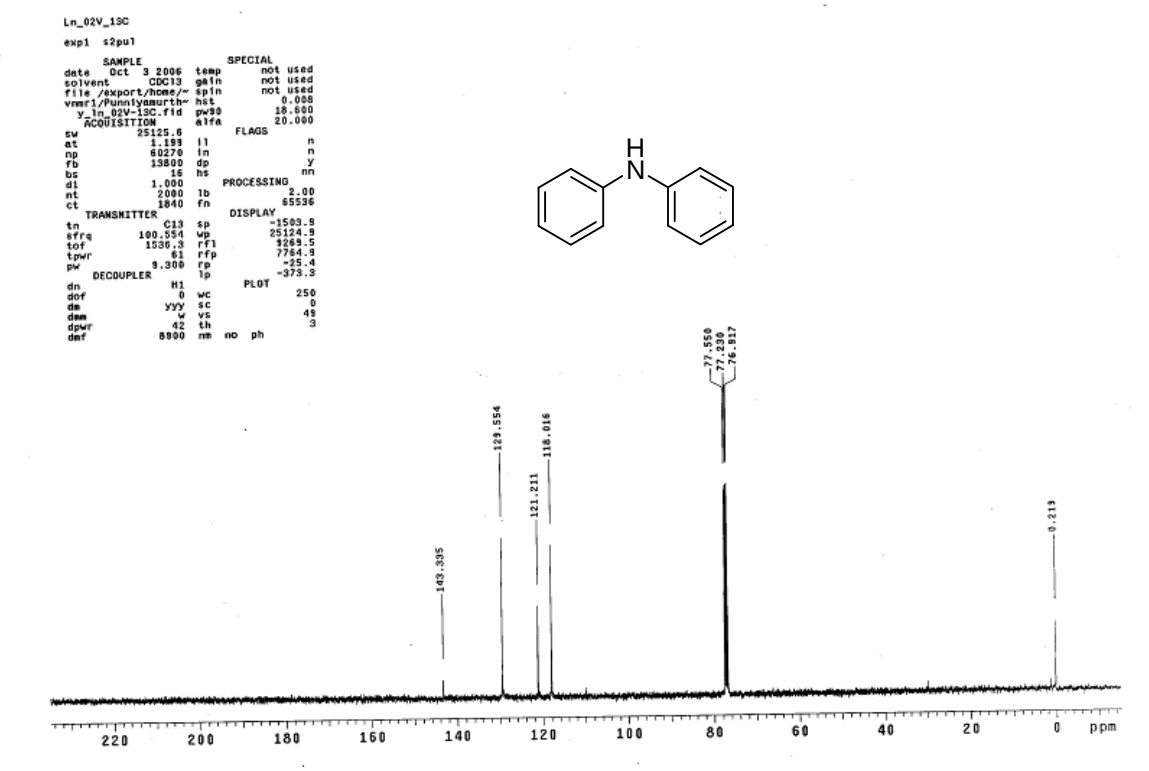
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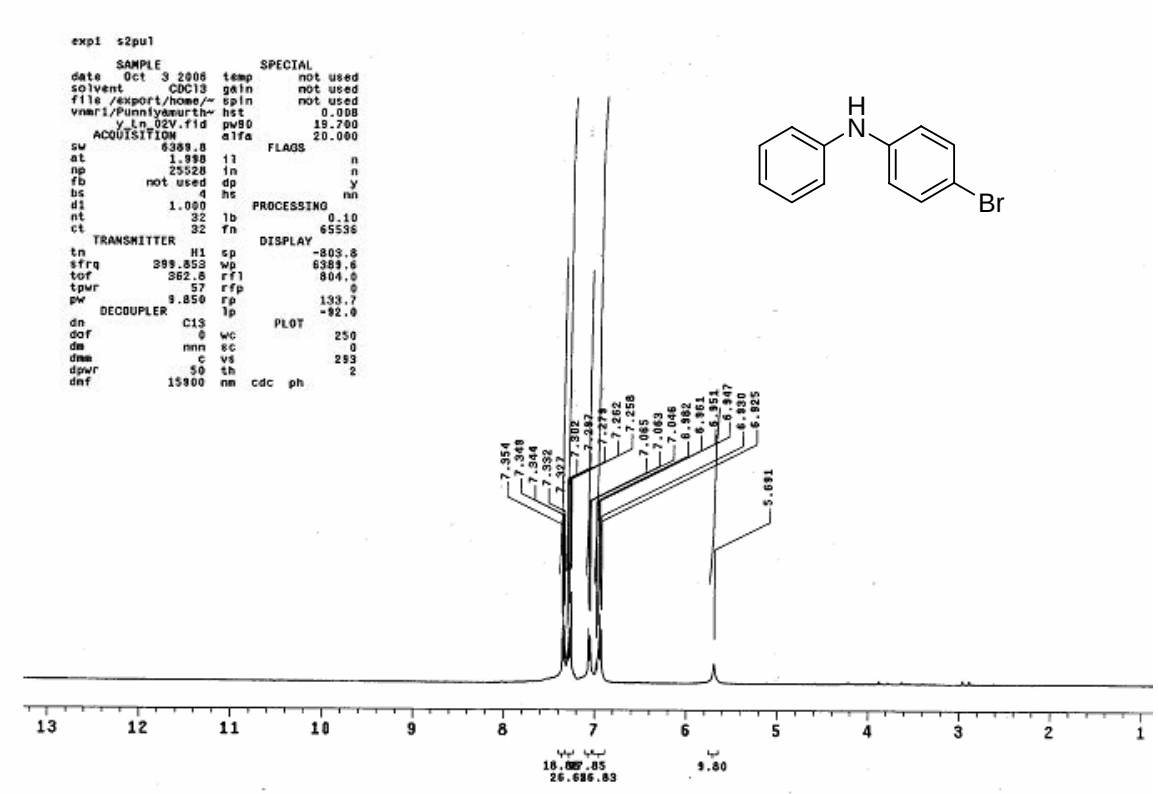
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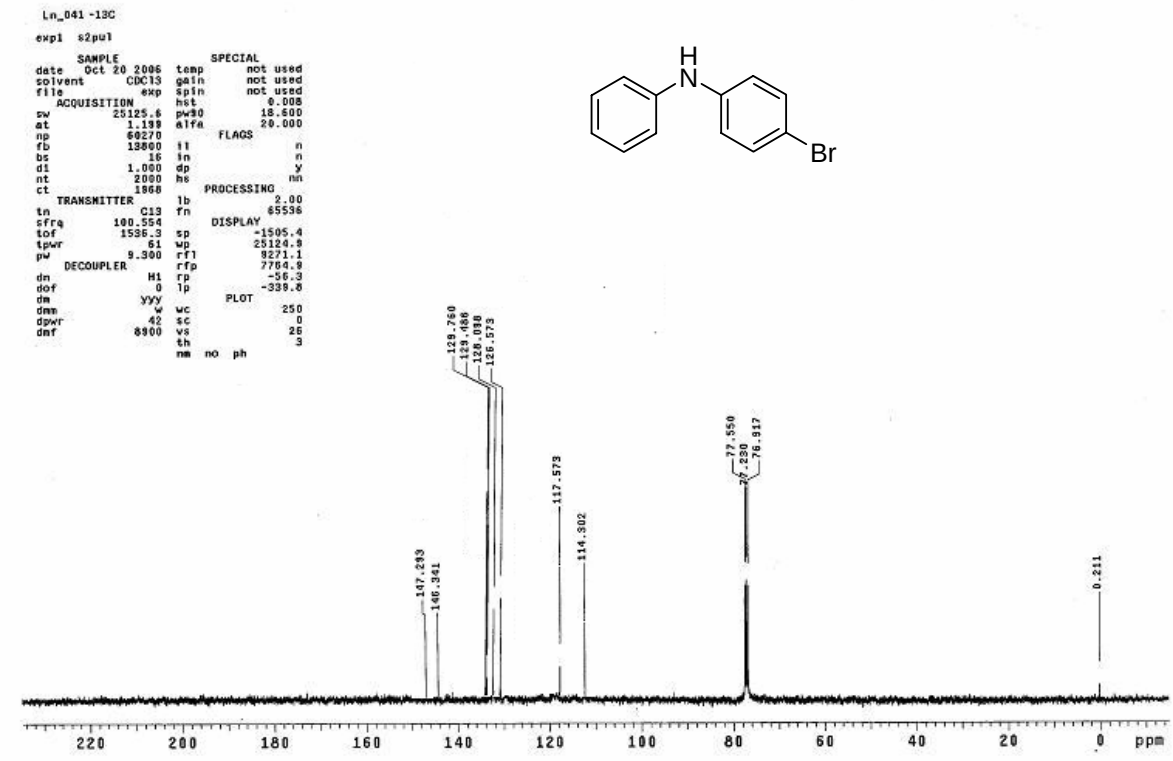
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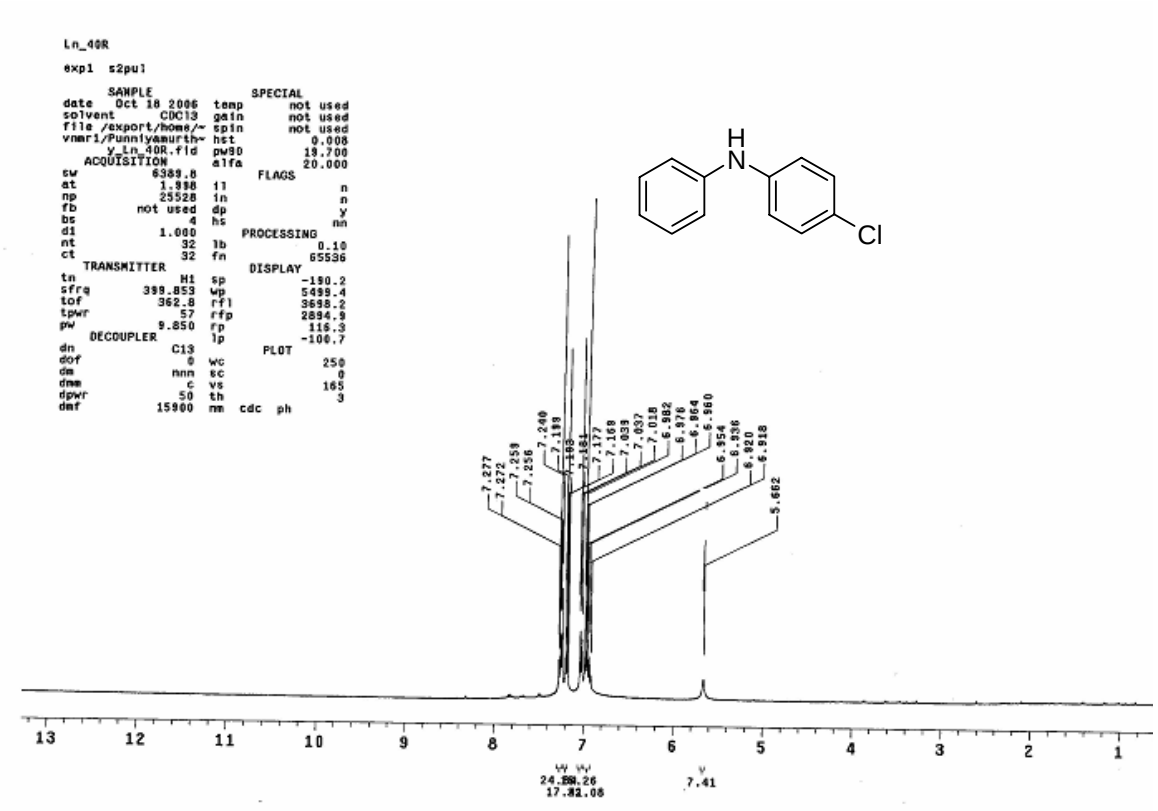
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th 3
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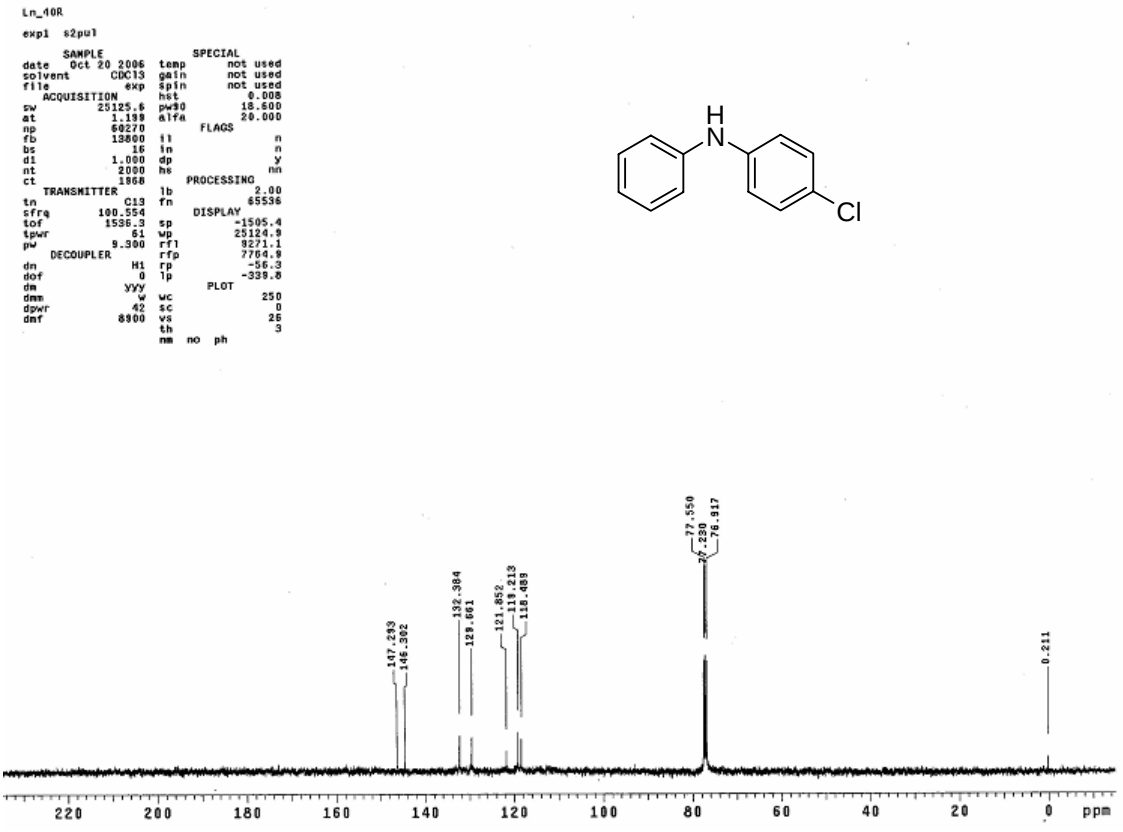
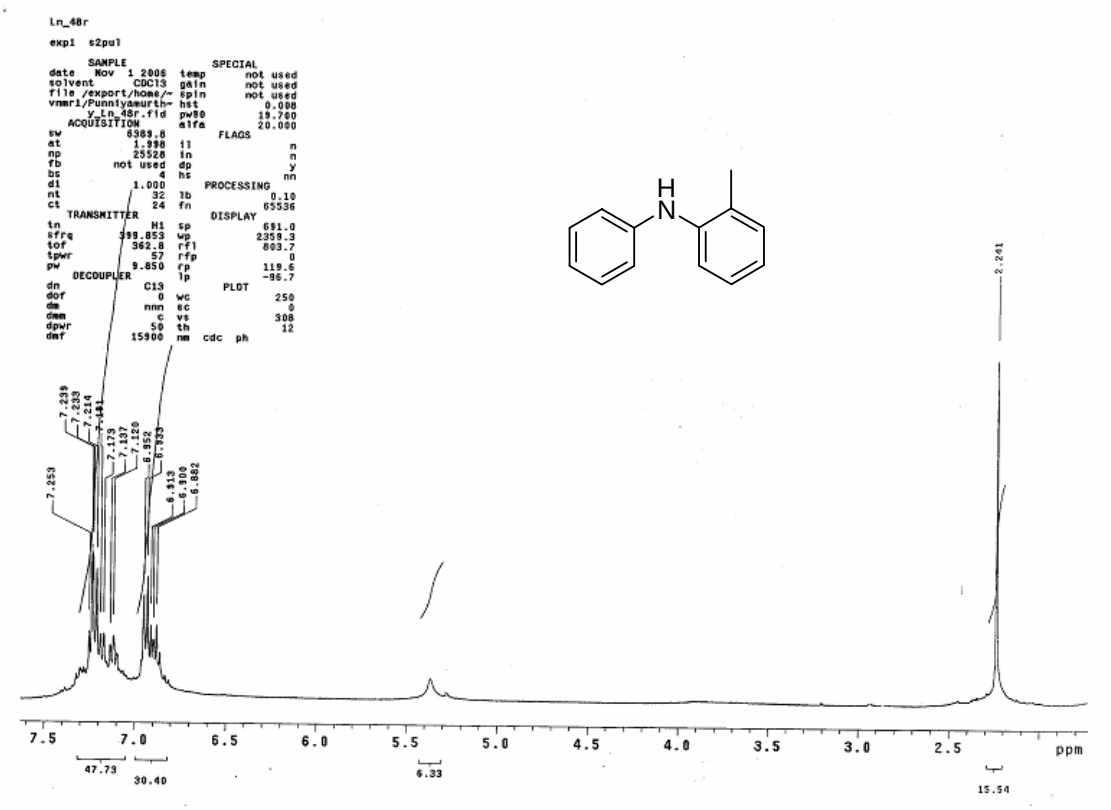
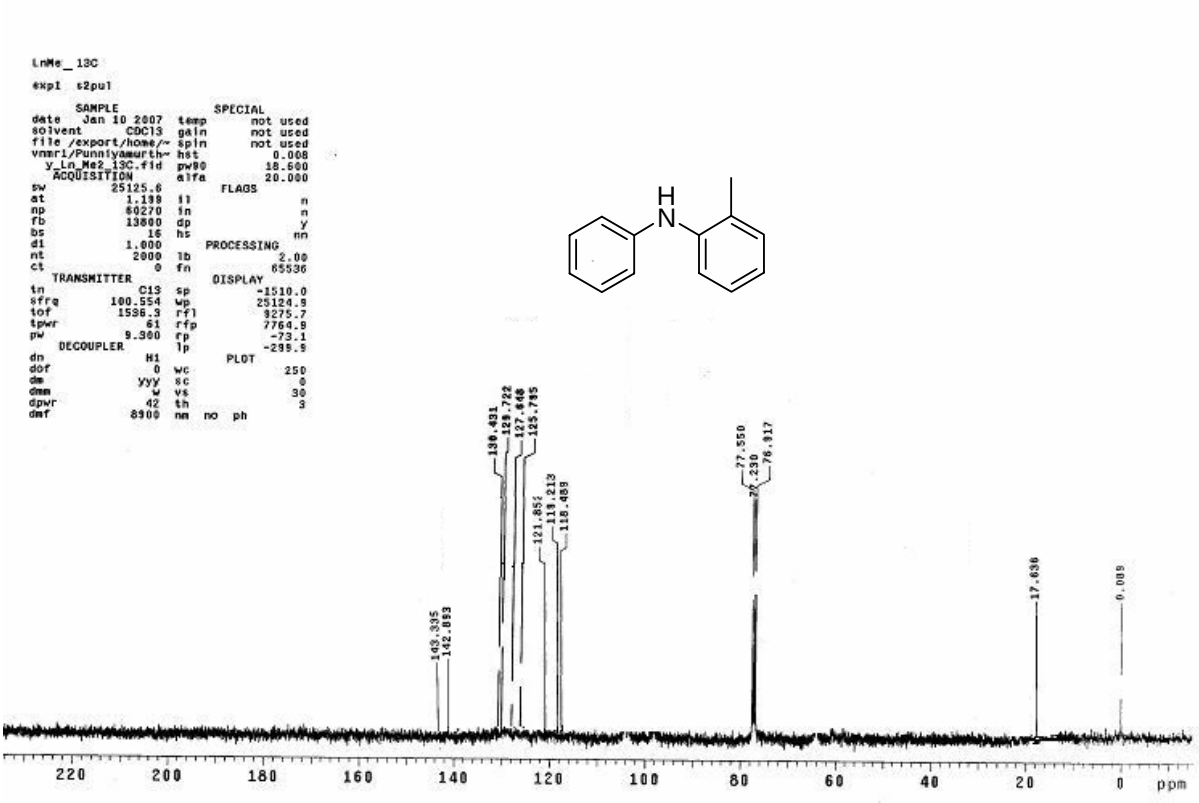
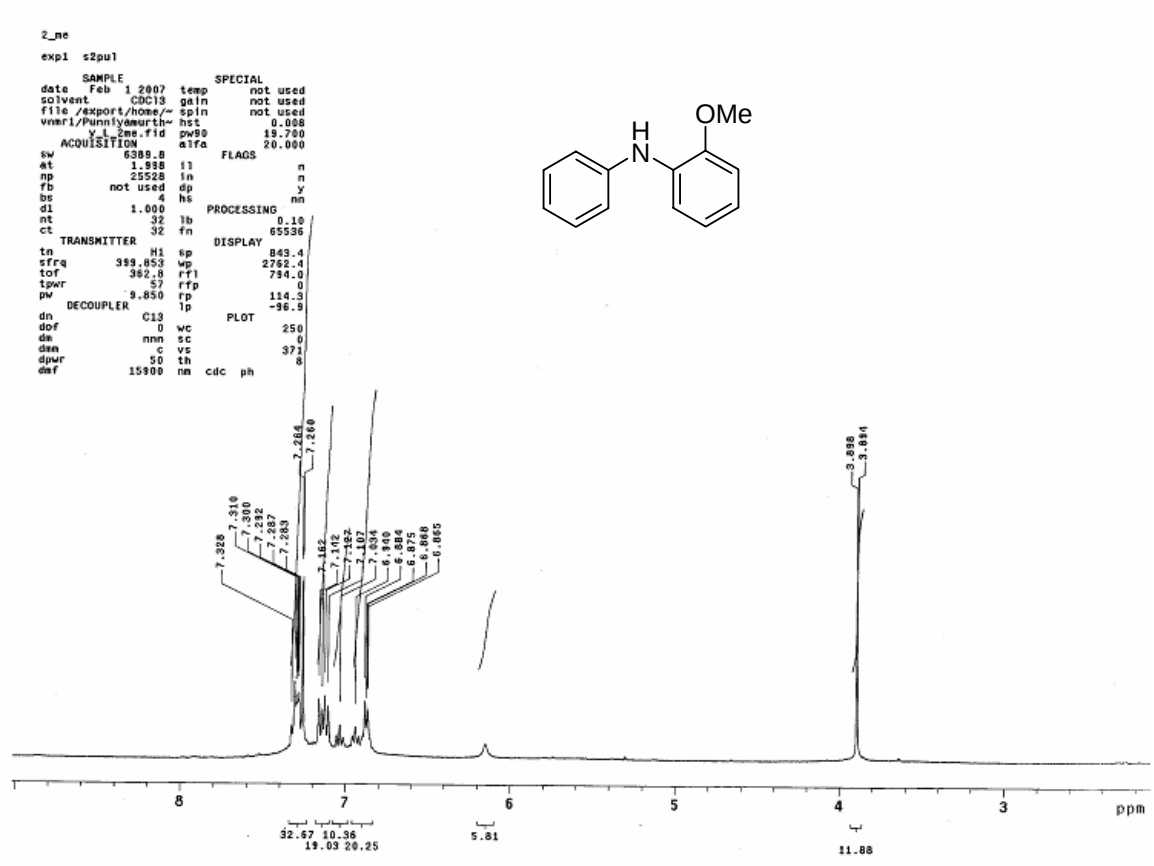
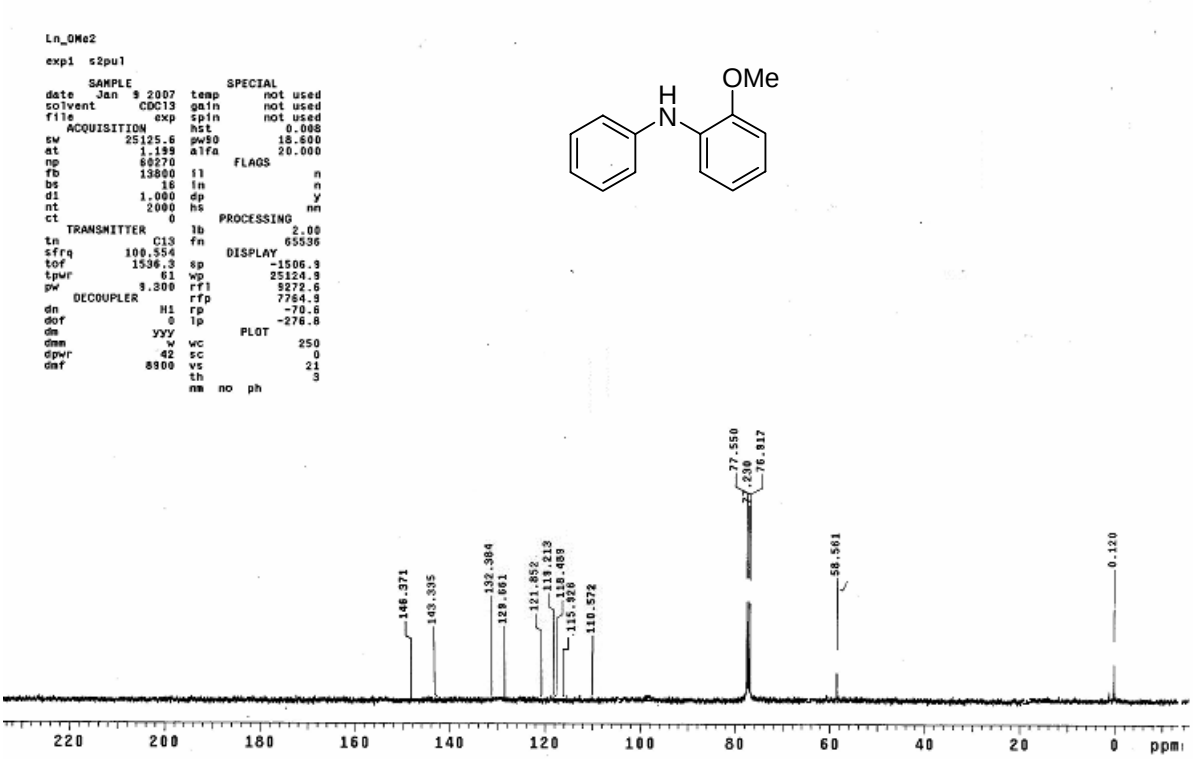
H
N
Cl
7.277
7.272
7.259
7.256
7.240
7.199
7.195
7.187
7.178
7.038
7.037
7.018
6.982
6.978
6.964
6.960
6.554
6.536
6.920
6.918
5.662
24.88
17.82
21.08
7.41

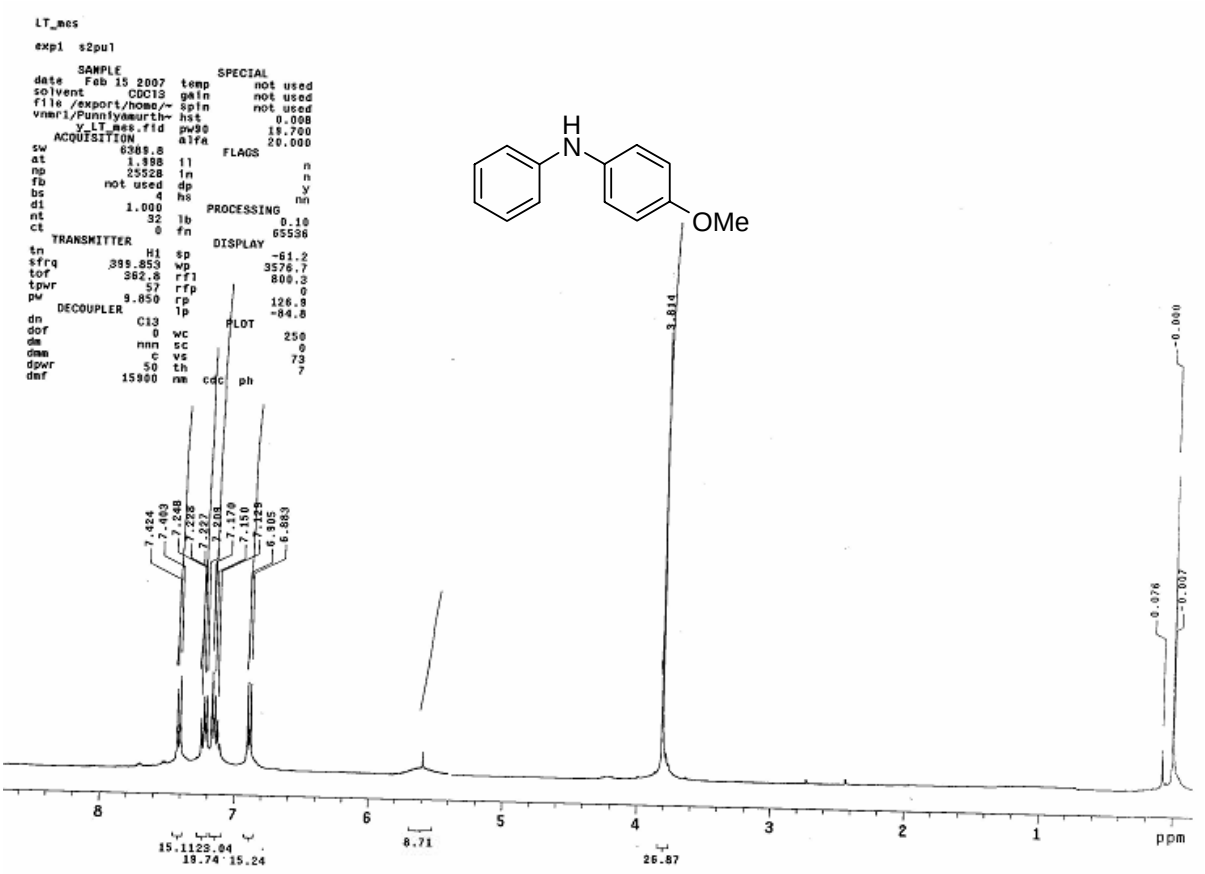

Ln_40R
exp1 s2pul
SAMPLE
date Oct 20 2006
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.199
np 60270
fb 13800
bs 16
di 1.000
nt 2000
ct 1868
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1505.4
wp 25124.9
rfl 9271.1
rfp 7764.9
rp -56.3
lp -338.8
PLOT
wc 250
sc 0
vs 26
th 3
nm no ph
H
N
Cl
147.243
146.392
132.384
129.661
121.852
119.213
118.489
77.550
77.230
76.917
0.211
ppm

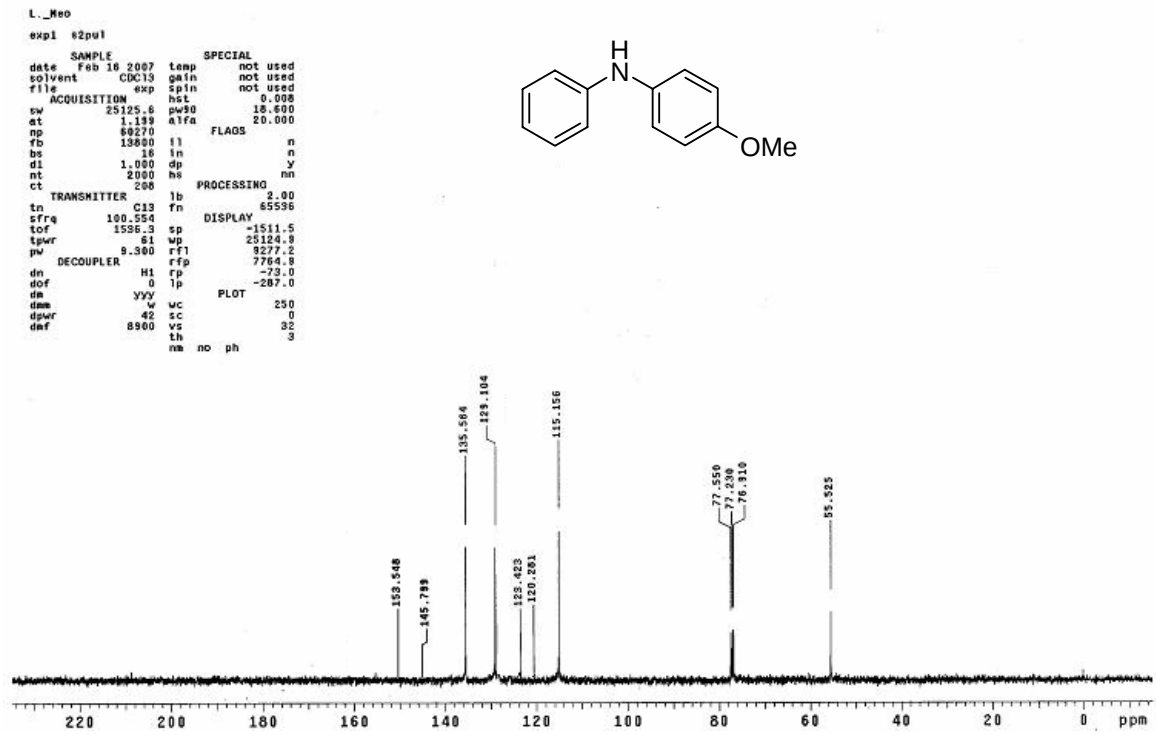

Ln_48r
expl s2pul
SAMPLE
date Nov 1 2006
solvent CDCl3
file /export/home/~
vnmrj/Punniyamurth~
y_Ln_48r.fid
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 24
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 19.700
alfa 20.000
FLAGS
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp 681.0
wp 2359.3
rfl 803.7
rfp 0
rp 119.6
lp -96.7
PLOT
wc 250
sc 0
vs 308
th 12
nm cdc ph
7.239
7.233
7.214
7.141
7.173
7.157
7.120
6.952
6.933
7.253
6.913
6.908
6.882
2.261
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
47.73
30.40
6.33
15.54

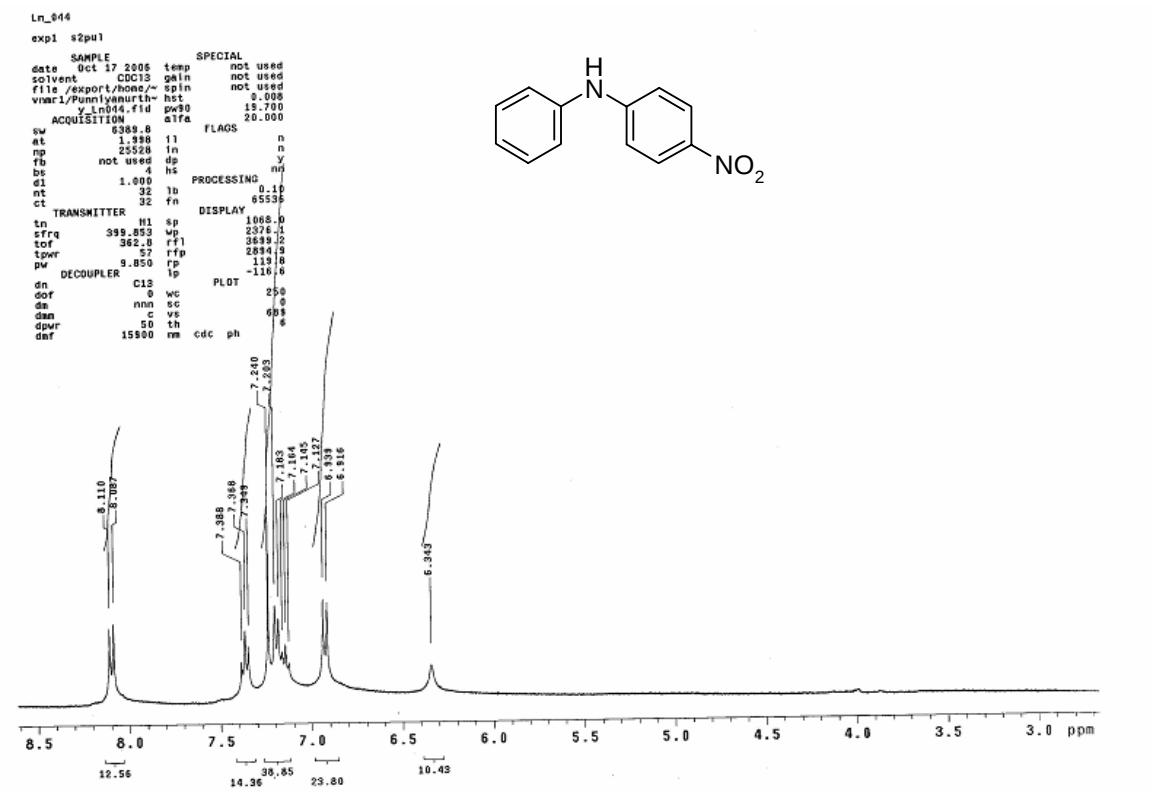

LnMe_13C
expl s2pul
SAMPLE
date Jan 10 2007
solvent CDCl3
file /export/home/~
vnmrj/Punniyamurth~
y_Ln_Me2_13C.fid
ACQUISITION
sw 25125.6
at 1.199
np 60270
fb 13800
bs 16
d1 1.000
nt 2000
ct 0
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.5
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1510.0
wp 25124.9
rfl 9275.7
rfp 7764.8
rp -73.1
lp -299.9
PLOT
wc 250
sc 0
vs 30
th 3
nm no ph
143.305
142.893
130.431
129.722
127.648
125.795
121.852
119.213
118.489
77.550
77.230
76.917
17.636
0.008
220
200
180
160
140
120
100
80
60
40
20
0
ppm

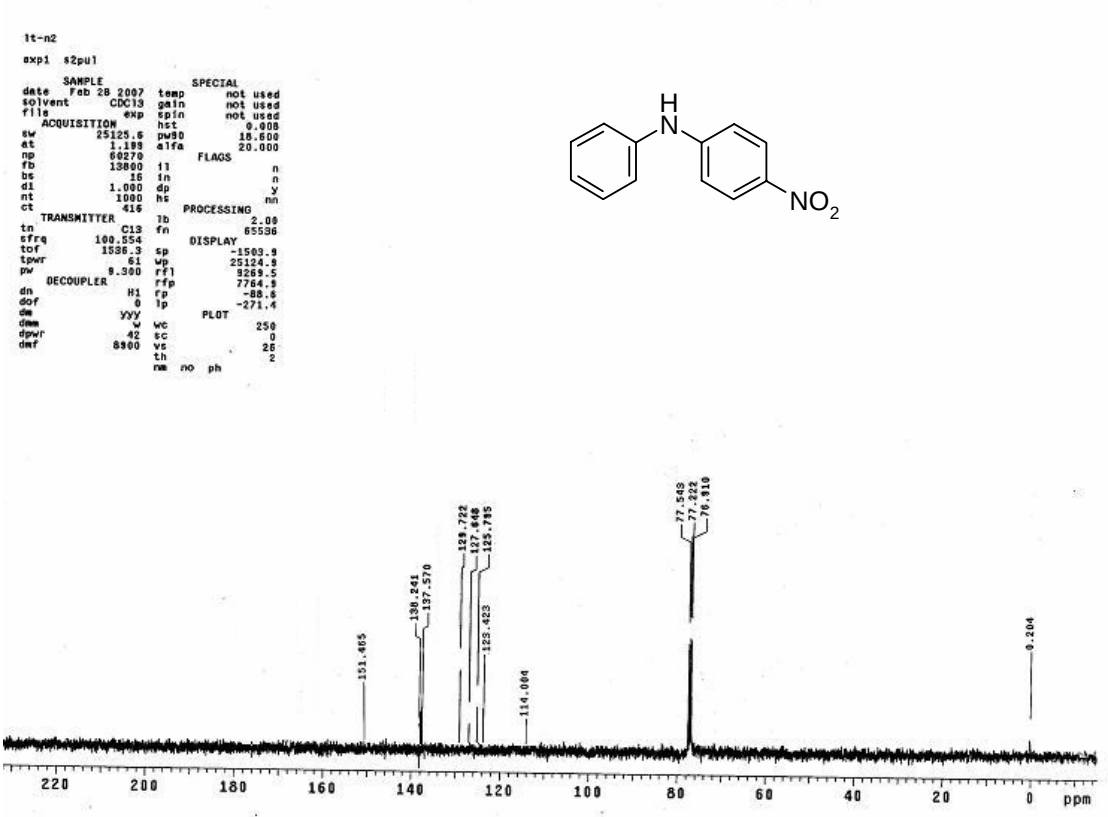

2_me
exp1 s2pul
SAMPLE
date Feb 1 2007
solvent CDCl3
file /export/home/~
vnmr1/Punniyamurth~
y_1_2me.fid
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 19.700
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp 843.4
wp 2762.4
rfl 794.0
rfp 0
rp 114.9
lp -96.9
PLOT
wc 250
sc 0
vs 371
th 8
nm cdc ph
OMe
H
N
7.328
7.316
7.300
7.292
7.287
7.283
7.284
7.260
7.162
7.142
7.102
7.107
7.084
7.064
6.884
6.875
6.868
6.865
3.898
3.884
8
7
6
5
4
3
ppm
32.67
10.36
19.03
20.25
5.81
11.88

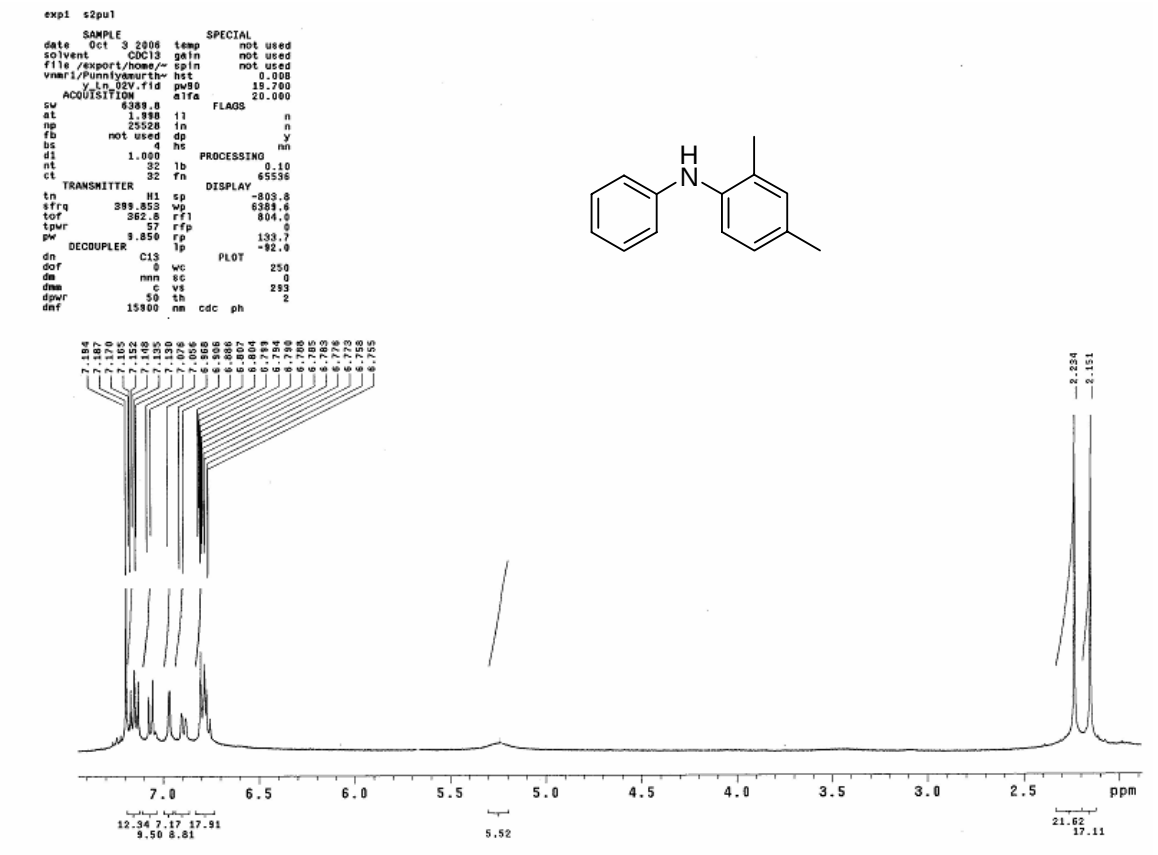

Ln_OMe2
exp1 s2pul
SAMPLE
date Jan 9 2007
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.199
np 60270
fb 13800
bs 16
d1 1.000
nt 2000
ct 0
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1506.9
wp 25124.8
rfl 9272.6
rfp 7764.9
rp -70.6
lp -276.8
PLOT
wc 250
sc 0
vs 21
th 3
nm no ph
OMe
H
N
146.371
143.335
132.384
129.061
121.852
119.213
118.489
115.920
110.572
77.550
77.230
76.817
58.561
0.120
220
200
180
160
140
120
100
80
60
40
20
0
ppm

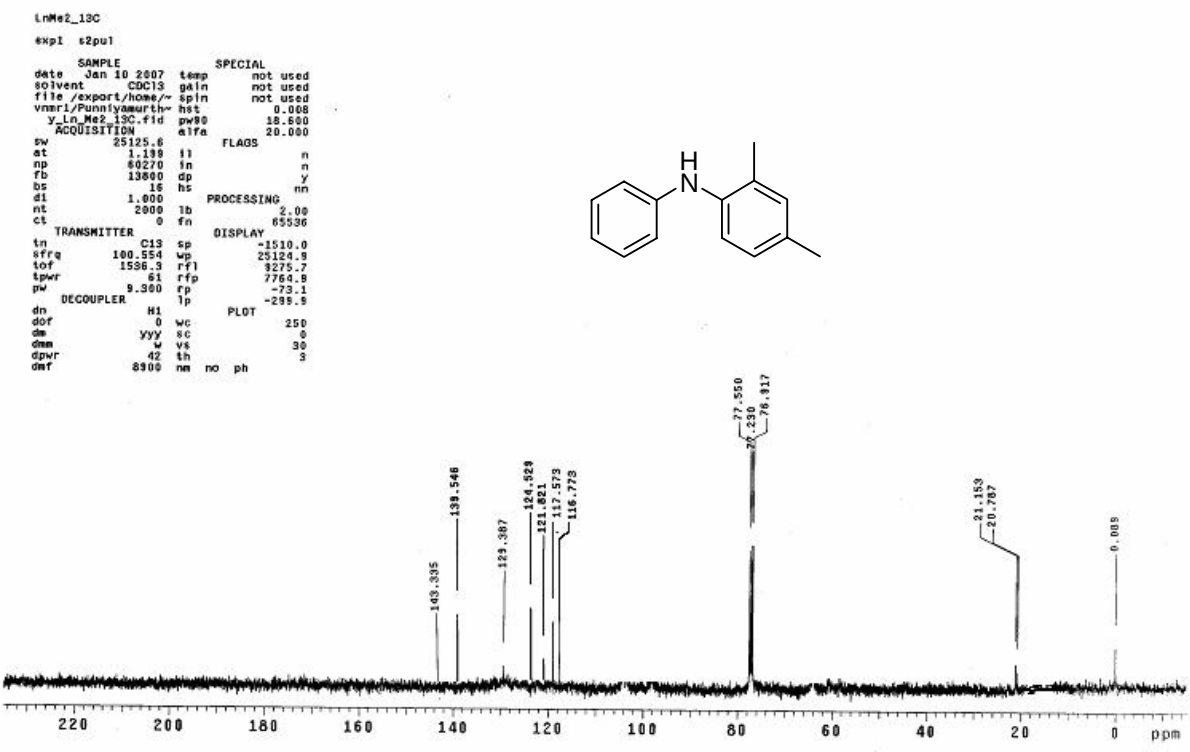

LT_mes
exp1 s2pul
SAMPLE
date Feb 15 2007
solvent CDCl3
file /export/home/v
vmarj/Punnyamurth
y_LT_mes.fid
ACQUISITION
sw 6389.8
at 1.988
np 25528
fb not used
bs 4
di 1.000
nt 32
ct 0
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.700
alfa 20.000
FLAGS
ll n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp -61.2
wp 3576.7
rf1 800.3
rfp 0
rp 126.8
lp -84.8
PLOT
wc 250
sc 0
vs 73
th 7
nm cdc ph
7.424
7.403
7.248
7.226
7.227
7.209
7.170
7.150
7.129
6.905
6.883
3.814
0.076
0.000
15.11
23.04
18.74
15.24
8.71
26.87
OMe
8
7
6
5
4
3
2
1
ppm

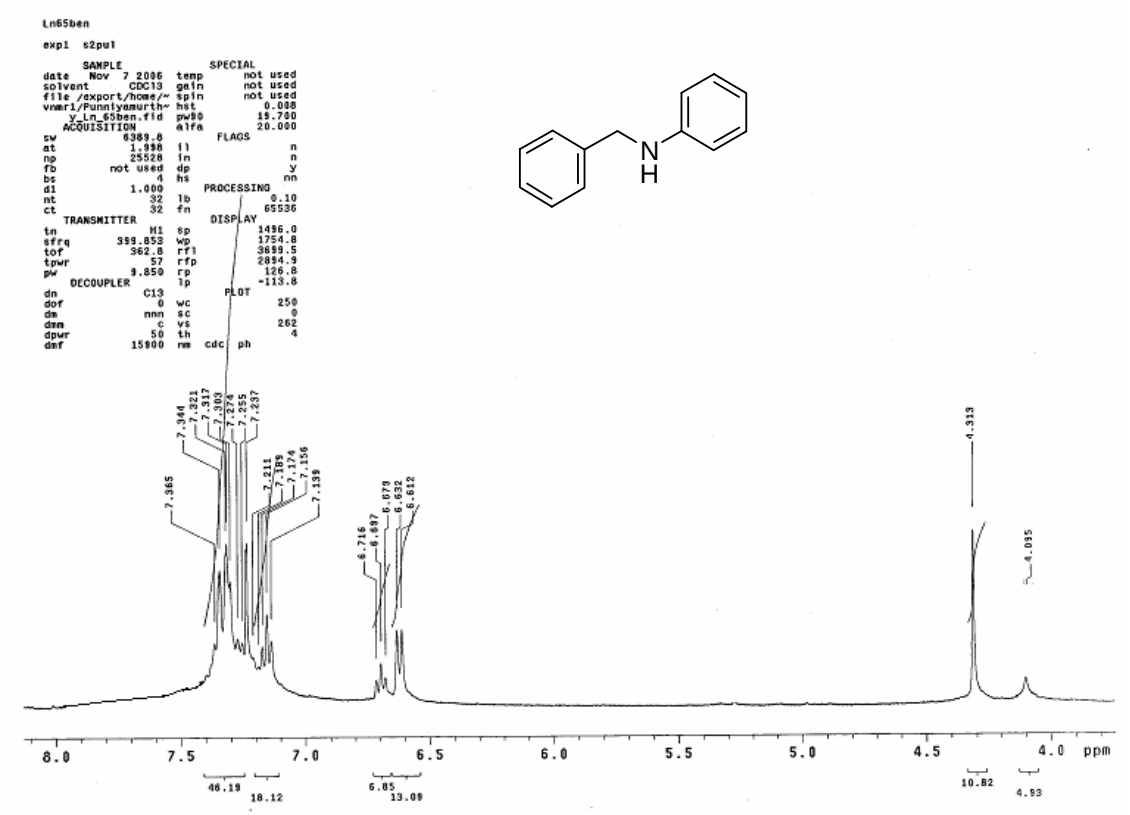

L._Meo
exp1 s2pul
SAMPLE
date Feb 16 2007
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.199
np 60270
fb 13800
bs 16
di 1.000
nt 2000
ct 208
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
ll n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1511.5
wp 25124.9
rf1 9277.2
rfp 7764.8
rp -73.0
lp -287.0
PLOT
wc 250
sc 0
vs 32
th 3
nm no ph
158.548
145.799
135.564
129.104
123.423
120.281
115.156
77.550
77.230
76.910
55.525
OMe
220
200
180
160
140
120
100
80
60
40
20
0
ppm

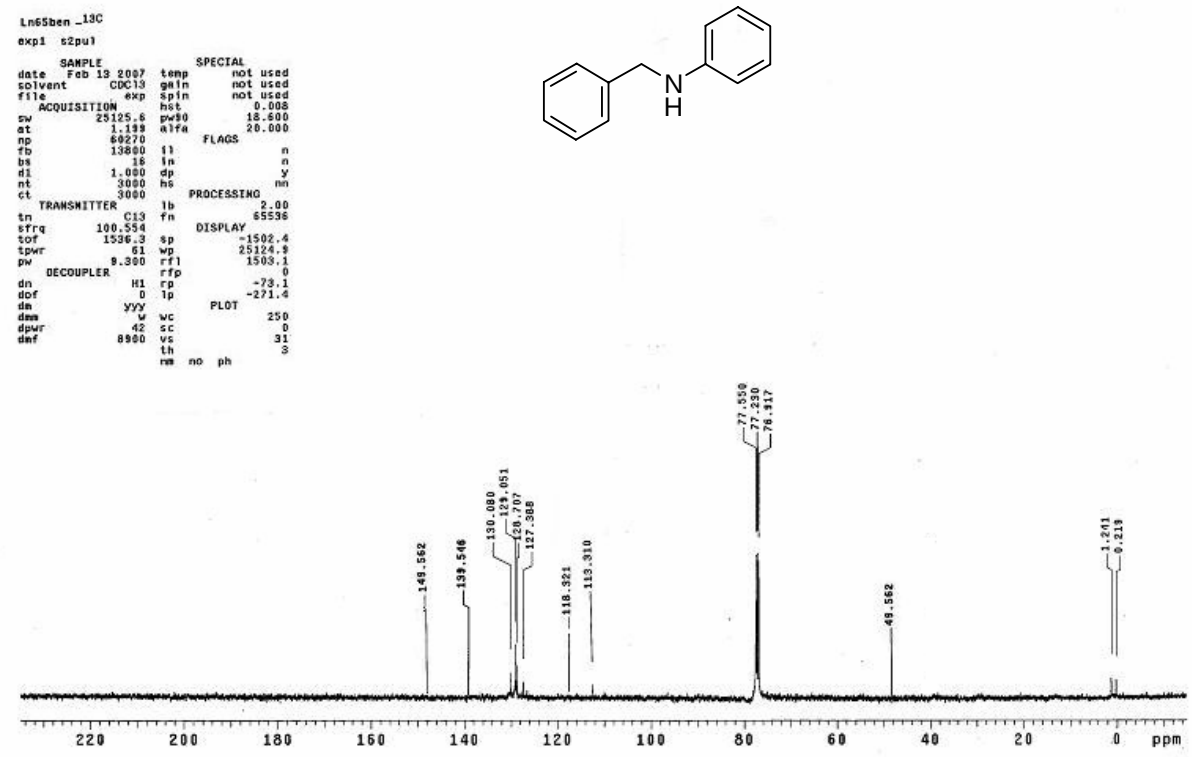

Ln_044
exp1 s2pul
SAMPLE
date Oct 17 2008
solvent CDCl3
file /export/home/~
vnmr1/Punniyamurth~
y_ln044.fid
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15500
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 19.700
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp 1068.0
wp 2376.1
rfl 3699.2
rfp 2894.9
rp 119.8
lp -116.6
PLOT
wc 250
sc 0
vs 688
th 6
cdc ph
8.110
8.087
7.388
7.368
7.349
7.240
7.203
7.183
7.164
7.145
7.127
6.939
6.816
6.343
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0 ppm
12.56
14.36
38.85
23.80
10.43
H
N
NO2

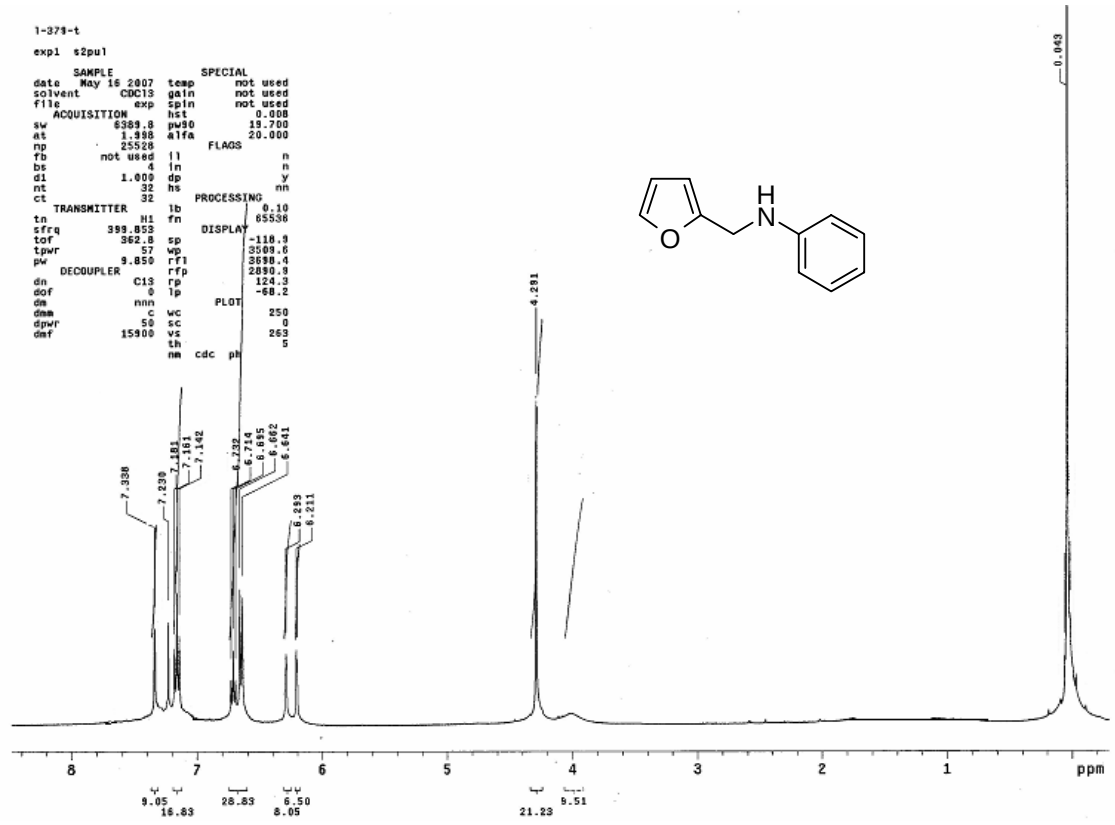

lt-n2
exp1 s2pul
SAMPLE
date Feb 28 2007
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.199
np 60270
fb 13800
bs 16
d1 1.000
nt 1000
ct 416
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 8.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1503.9
wp 25124.8
rfl 9269.5
rfp 7764.8
rp -88.6
lp -271.4
PLOT
wc 250
sc 0
vs 26
th 2
nm no ph
151.465
130.241
127.570
129.722
127.448
125.785
125.423
114.064
77.548
77.222
76.910
0.204
220
200
180
160
140
120
100
80
60
40
20
0 ppm
H
N
NO2

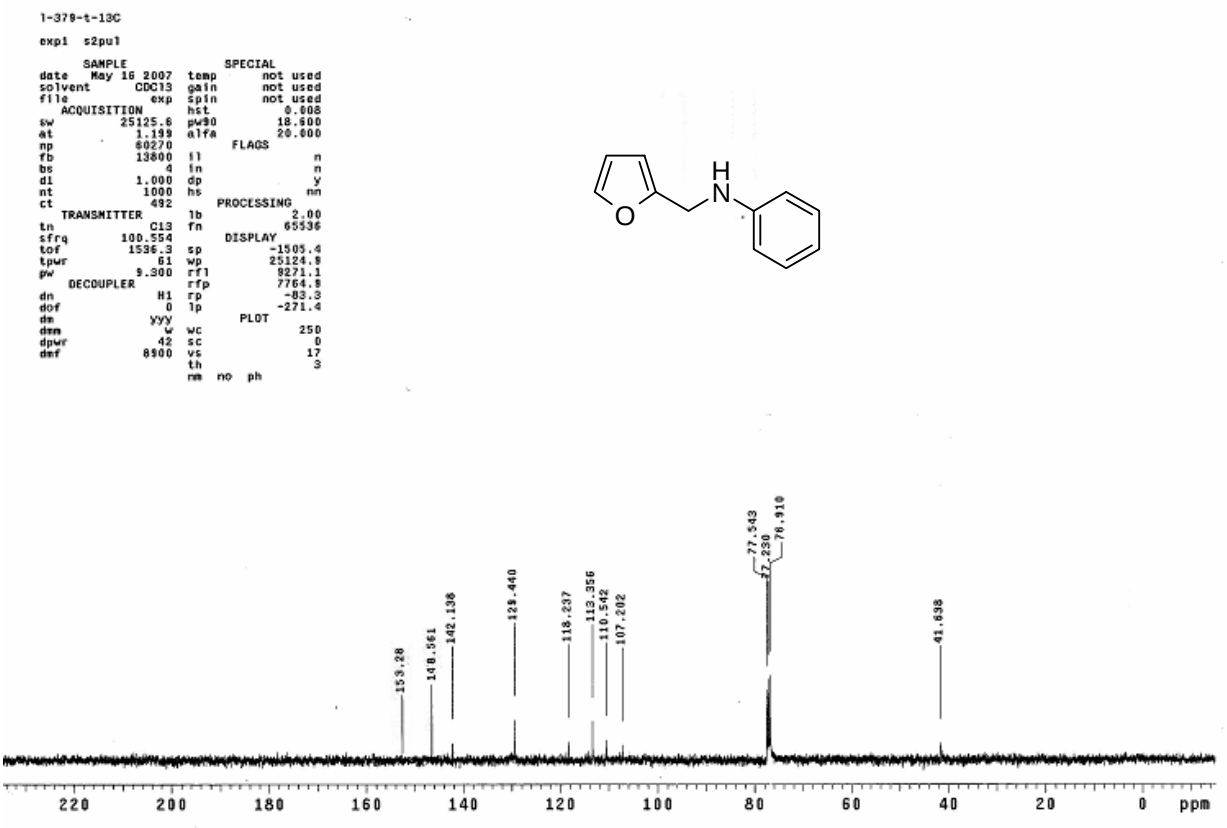

expl s2pul
SAMPLE
date Oct 3 2006
solvent CDCl3
file /export/home/~
vnmr1/Punniyamurth~
y_Ln_02V.fid
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.700
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp -803.8
wp 6389.6
rfl 804.0
rfp 0
rp 133.7
lp -92.0
PLOT
wc 250
sc 0
vs 293
th 2
nm cdc ph
7.194
7.187
7.170
7.155
7.152
7.148
7.135
7.130
7.076
7.066
6.895
6.886
6.807
6.804
6.799
6.794
6.788
6.785
6.783
6.776
6.773
6.758
6.755
2.234
2.151
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
ppm
12.34
9.50
7.17
8.81
17.91
5.52
21.62
17.11
H
N

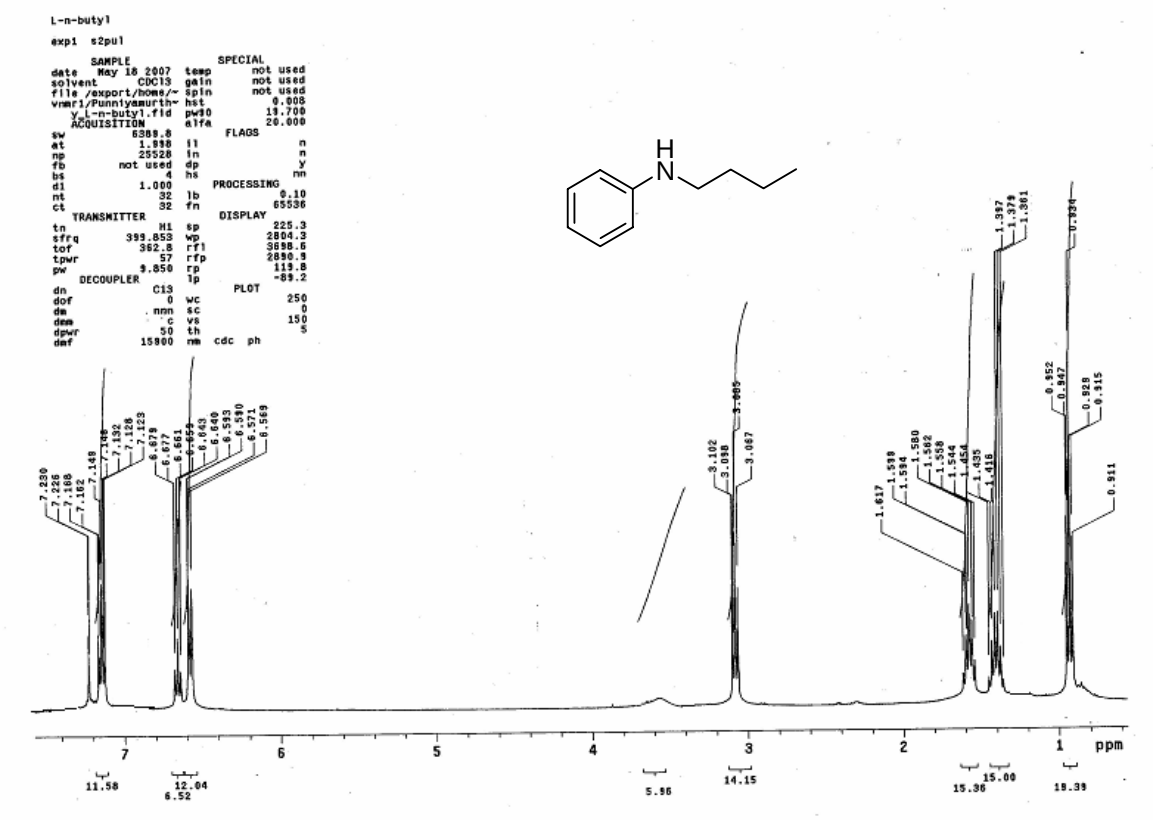

LnMe2_13C
expl s2pul
SAMPLE
date Jan 10 2007
solvent CDCl3
file /export/home/~
vnmr1/Punniyamurth~
y_Ln_Me2_13C.fid
ACQUISITION
sw 25125.6
at 1.138
np 60270
fb 13800
bs 16
d1 1.000
nt 2000
ct 0
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1510.0
wp 25124.9
rfl 9275.7
rfp 7764.9
rp -73.1
lp -295.9
PLOT
wc 250
sc 0
vs 30
th 3
nm no ph
143.335
139.546
129.387
124.529
121.821
117.573
116.773
77.550
77.230
76.917
21.153
20.767
0.089
220
200
180
160
140
120
100
80
60
40
20
0
ppm
H
N

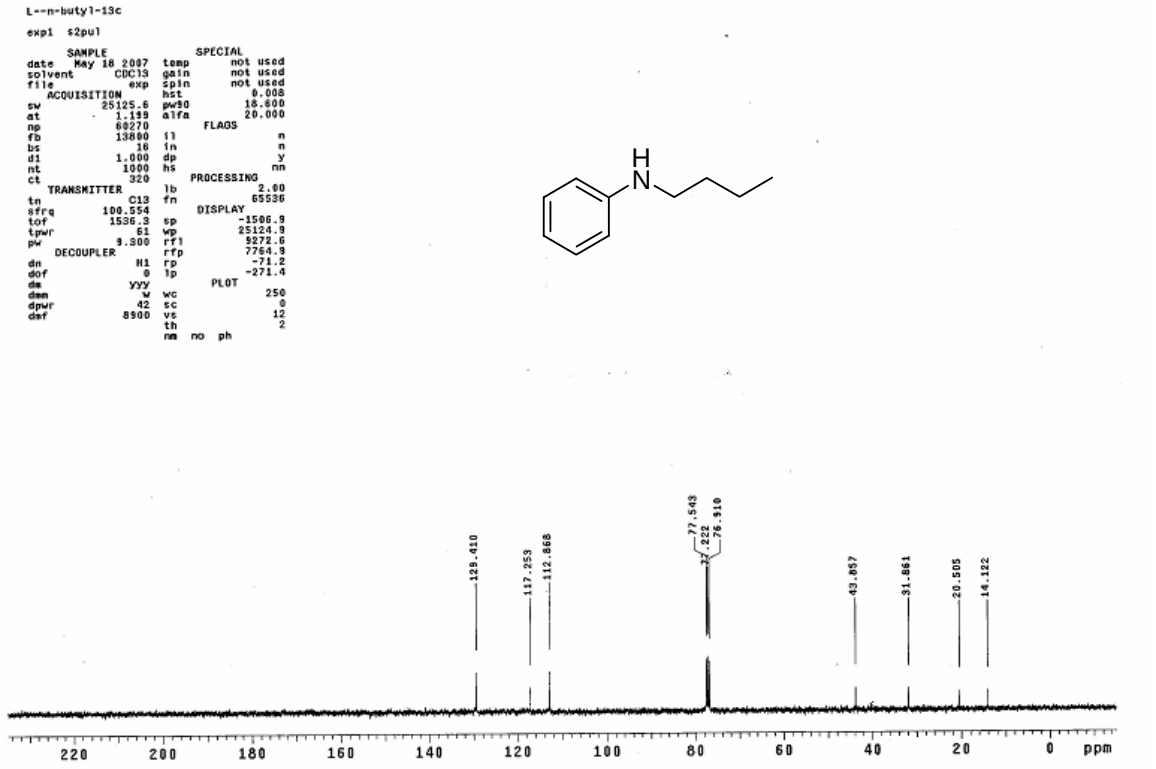

Ln65ben
exp1 s2pul
SAMPLE
date Nov 7 2006
solvent CDCl3
file /export/home/~
vnmr1/Punniyamurth~
y_Ln_65ben.fid
ACQUISITION
sw 6389.8
at 1.898
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.700
alfa 20.000
FLAGS
li n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp 1496.0
wp 1754.8
rfl 3699.5
rfp 2894.9
rp 126.8
lp -113.8
PLOT
wc 250
sc 0
vs 262
th 4
nm cdc ph
7.365
7.344
7.321
7.317
7.303
7.274
7.255
7.237
7.211
7.189
7.174
7.156
7.139
6.716
6.697
6.679
6.632
6.612
4.313
4.035
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
ppm
46.19
18.12
6.85
13.09
10.82
4.93

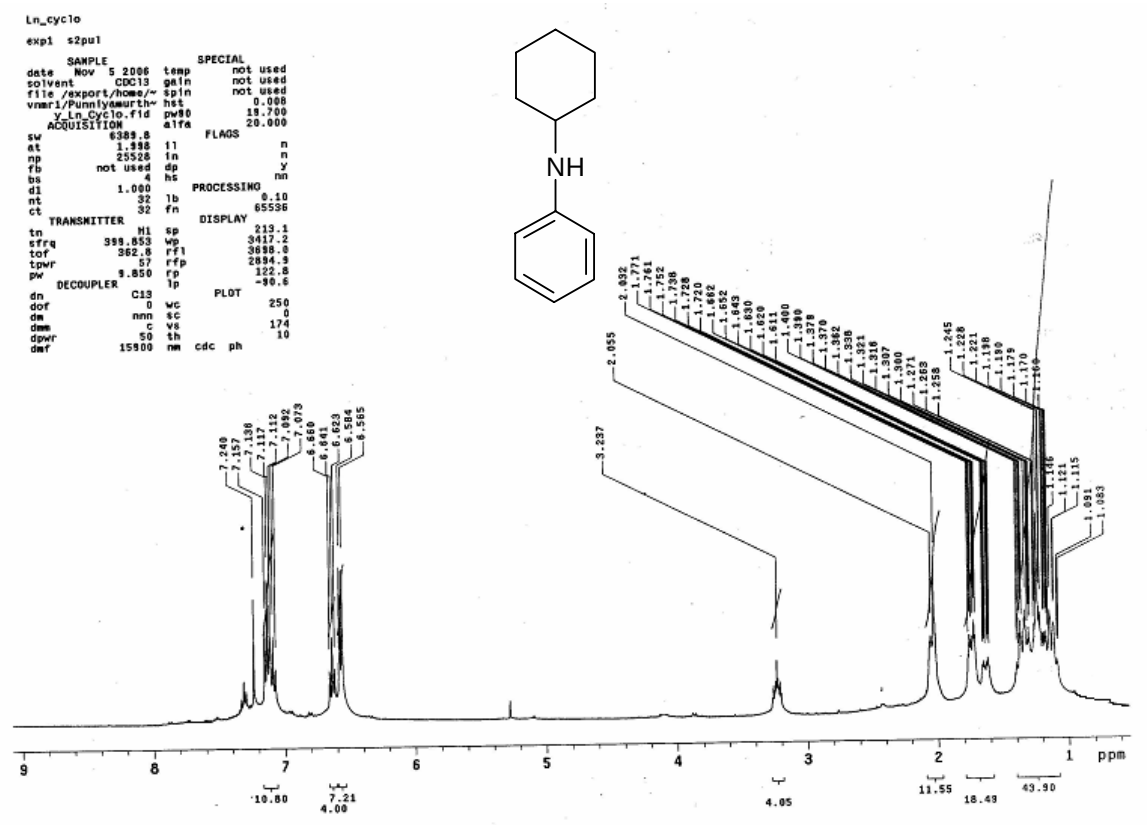

Ln65ben _13C
exp1 s2pul
SAMPLE
date Feb 13 2007
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.199
np 60270
fb 13880
bs 16
d1 1.000
nt 3000
ct 3000
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
li n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1502.4
wp 25124.9
rfl 1503.1
rfp 0
rp -73.1
lp -271.4
PLOT
wc 250
sc 0
vs 31
th 3
nm no ph
149.562
139.546
130.080
129.051
128.707
127.388
118.321
113.310
77.550
77.230
76.917
48.562
1.201
0.213
220
200
180
160
140
120
100
80
60
40
20
0
ppm

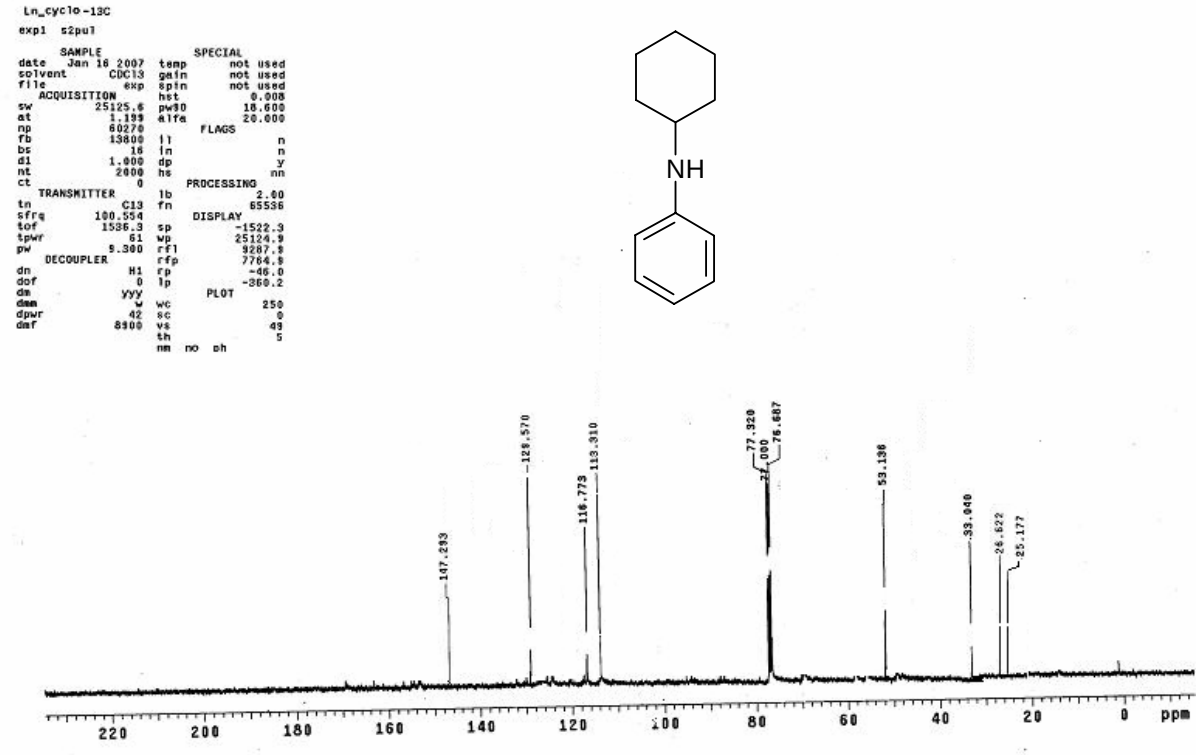

1-379-t
exp1 s2pul
SAMPLE
date May 16 2007
solvent CDCl3
file exp
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
dl 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 19.700
alfa 20.000
FLAGS
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp -118.9
wp 3508.6
rf1 3698.4
rfp 2890.9
rp 124.3
lp -68.2
PLOT
wc 250
sc 0
vs 263
th 5
nm cdc ph
7.338
7.230
7.181
7.161
7.142
6.738
6.715
6.662
6.641
6.293
6.211
4.291
0.043
8
7
6
5
4
3
2
1
ppm
9.05
16.83
28.83
6.50
8.05
21.23
9.51

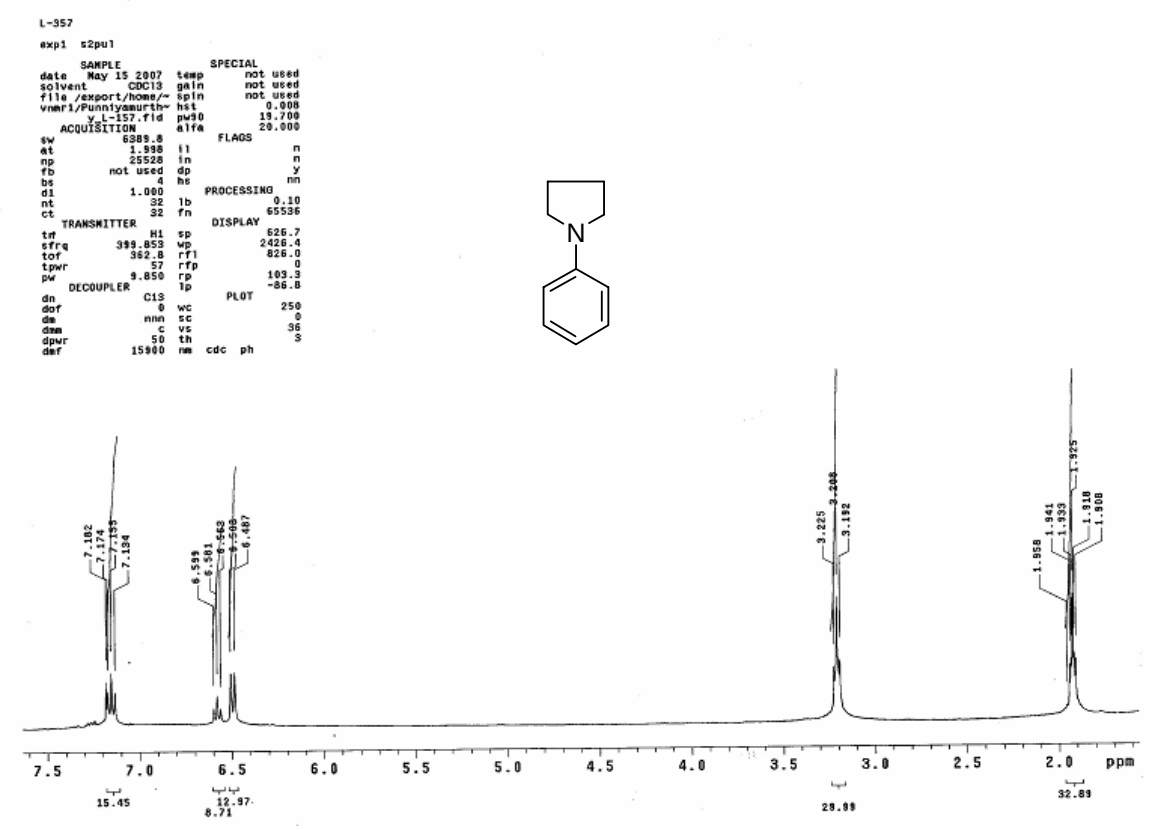

1-379-t-13C
exp1 s2pul
SAMPLE
date May 16 2007
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.199
np 60270
fb 13800
bs 4
dl 1.000
nt 1000
ct 492
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1505.4
wp 25124.9
rf1 9271.1
rfp 7764.8
rp -83.3
lp -271.4
PLOT
wc 250
sc 0
vs 17
th 3
nm no ph
153.28
148.561
142.136
129.440
118.237
113.356
110.542
107.202
77.543
77.230
76.918
41.638
220
200
180
160
140
120
100
80
60
40
20
0
ppm

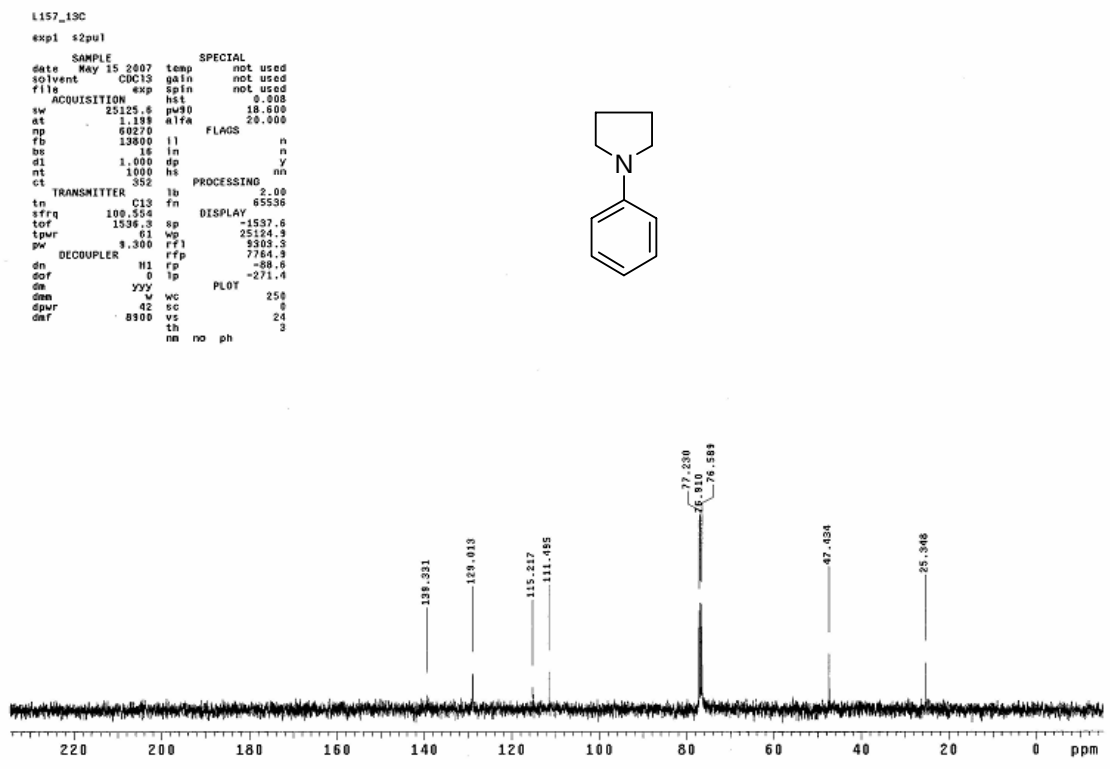

L-n-butyl
exp1 s2pul
SAMPLE
date May 18 2007
solvent CDCl3
file /export/home/~
vnmr1/Punniyamurth~
y_L-n-butyl.fid
ACQUISITION
sw 6388.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.005
pw90 13.700
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp 225.3
wp 2804.3
rfl 3898.6
rfp 2890.9
rp 119.8
lp -89.2
PLOT
wc 250
sc 0
vs 150
th 5
nm cdc ph
7.230
7.226
7.188
7.182
7.149
7.134
7.132
7.128
7.123
6.679
6.677
6.661
6.659
6.643
6.640
6.593
6.590
6.571
6.569
3.102
3.088
3.085
3.067
1.617
1.598
1.594
1.582
1.558
1.544
1.454
1.435
1.416
0.952
0.947
0.928
0.915
0.911
ppm
11.58
12.04
6.52
5.96
14.15
15.36
15.00
18.39

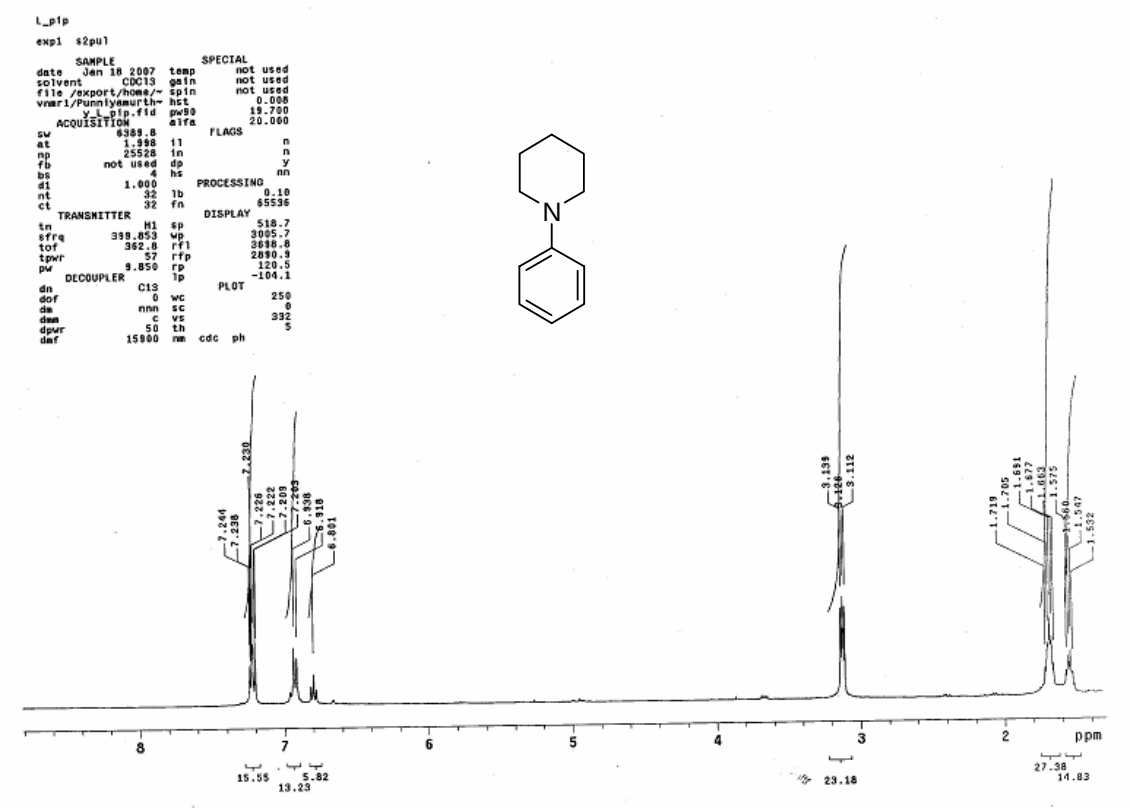

L--n-butyl-13c
exp1 s2pul
SAMPLE
date May 18 2007
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.199
np 60270
fb 13800
bs 16
d1 1.000
nt 1000
ct 320
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.500
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1506.9
wp 25124.9
rfl 9272.6
rfp 7764.9
rp -71.2
lp -271.4
PLOT
wc 250
sc 0
vs 12
th 2
nm no ph
129.410
117.259
112.868
77.543
77.222
76.910
43.857
31.861
20.505
14.122
ppm

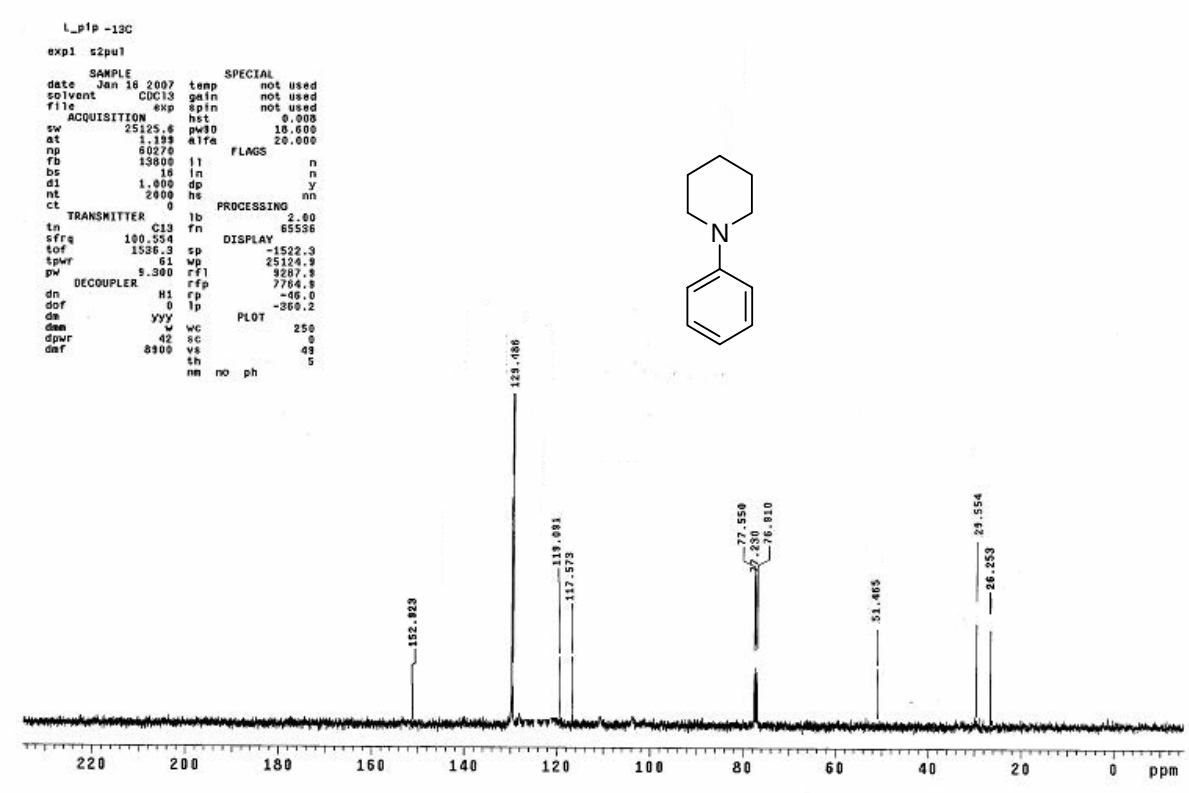

Ln_cyclo
exp1 s2pul
SAMPLE
date Nov 5 2006
solvent CDCl3
file /export/home/v
vnmr1/Punnyamurth
y_Ln_Cyclo.fid
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.700
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp 213.1
wp 3417.2
rfl 3698.8
rfp 2894.9
rp 122.8
lp -90.6
PLOT
wc 250
sc 0
vs 174
th 10
nm cdc ph
NH
ppm
10.80
7.21
4.00
4.05
11.55
18.49
43.90

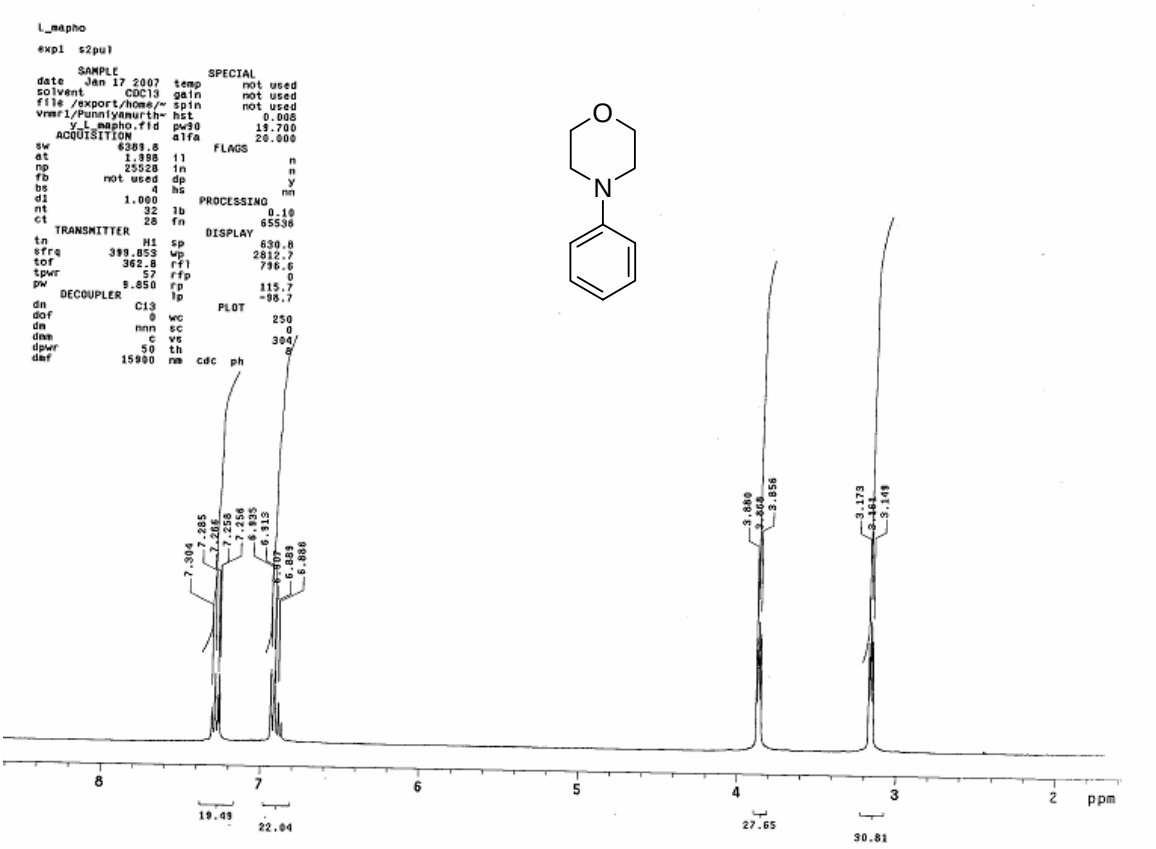

Ln_cyclo-13C
exp1 s2pul
SAMPLE
date Jan 18 2007
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.139
np 60270
fb 13800
bs 16
d1 1.000
nt 2000
ct 0
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8100
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1522.3
wp 25124.9
rfl 9287.8
rfp 7764.8
rp -46.0
lp -360.2
PLOT
wc 250
sc 0
vs 48
th 5
nm no ph
NH
147.293
128.570
116.773
113.310
77.320
77.000
76.687
53.138
33.040
26.622
25.177
ppm

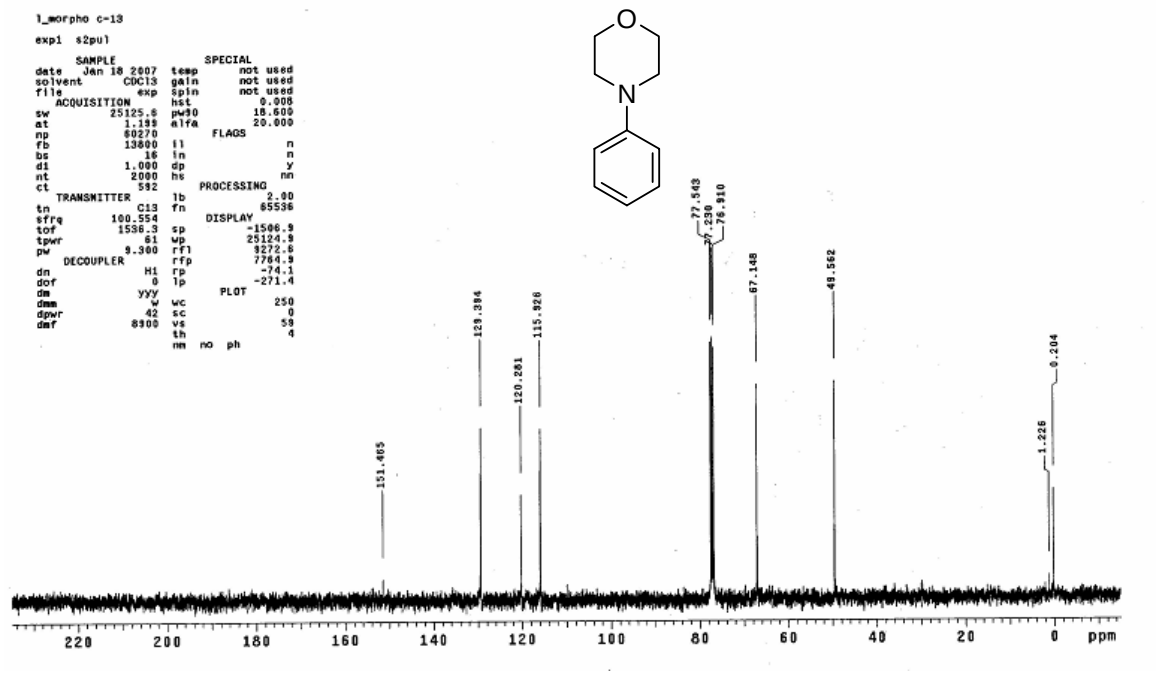

L-157
exp1 s2pul
SAMPLE
date May 15 2007
solvent CDCl3
file /export/home/~
vnmr1/Punniyamurth~
y_L-157.fid
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 19.700
alfa 20.000
FLAGS
ll n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp 626.7
wp 2426.4
rfl 826.0
rfp 0
rp 103.3
lp -86.8
PLOT
wc 250
sc 0
vs 36
th 3
nm cdc ph
N
7.182
7.174
7.155
7.134
6.599
6.581
6.563
6.548
6.487
3.225
3.208
3.192
1.958
1.941
1.933
1.918
1.908
1.925
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm
15.45
12.97
8.71
28.89
32.89

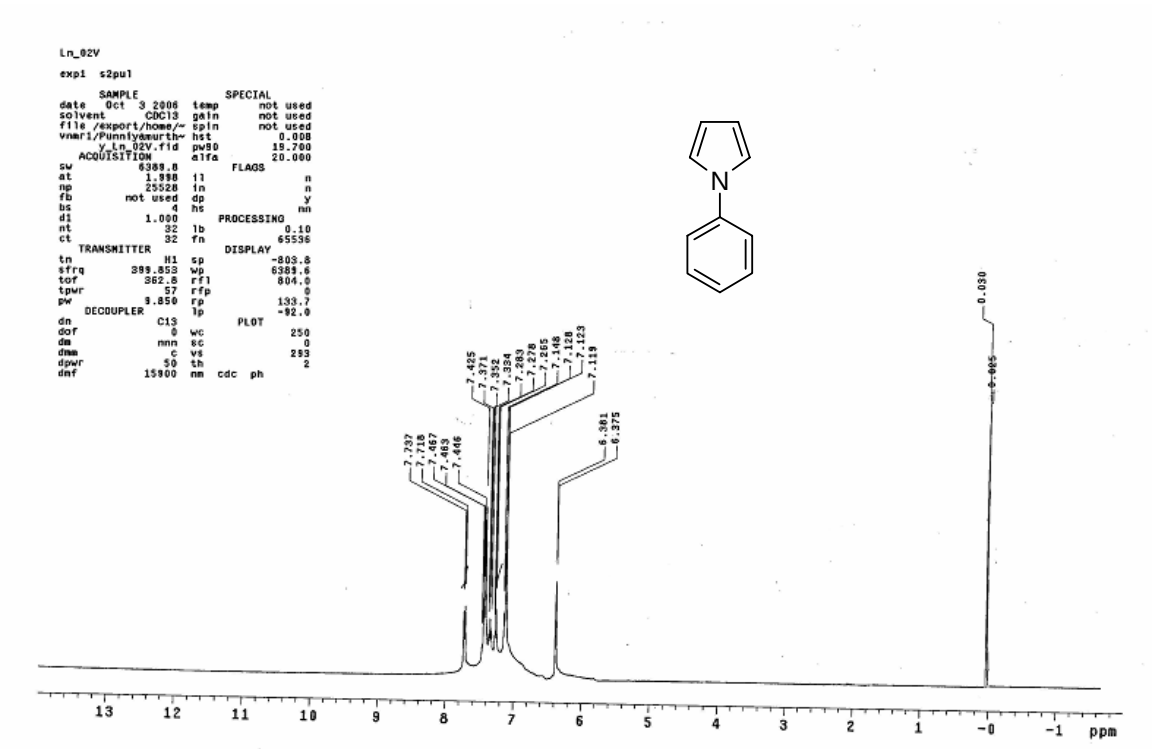

L157_13C
exp1 s2pul
SAMPLE
date May 15 2007
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.199
np 60270
fb 13800
bs 16
d1 1.000
nt 1000
ct 352
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
ll n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1537.6
wp 25124.9
rfl 9303.3
rfp 7764.9
rp -88.6
lp -271.4
PLOT
wc 250
sc 0
vs 24
th 3
nm no ph
N
139.331
129.013
115.217
111.455
77.230
76.910
76.589
47.434
25.348
220
200
180
160
140
120
100
80
60
40
20
0
ppm

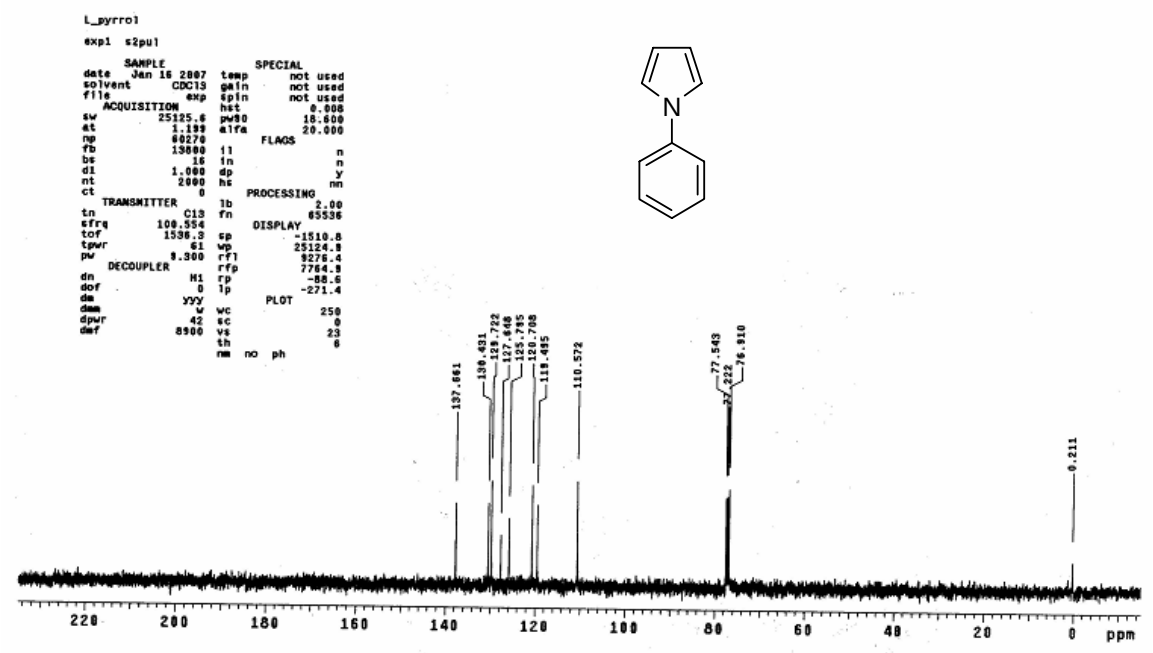

L_p1p
exp1 s2pul
SAMPLE
date Jan 18 2007
solvent CDCl3
file /export/home/~
vnmr1/Punnlyamurth~
y_L_p1p.fid
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.000
pw90 19.700
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp 518.7
wp 3005.7
rfl 3698.8
rfp 2890.8
rp 120.5
lp -104.1
PLOT
wc 250
sc 0
vs 332
th 5
nm cdc ph
7.264
7.238
7.230
7.226
7.222
7.209
7.203
6.938
6.918
6.901
3.139
3.126
3.112
1.719
1.705
1.681
1.677
1.663
1.575
1.560
1.547
1.532
8
7
6
5
4
3
2
ppm
15.55
13.23
5.82
23.18
27.38
14.83

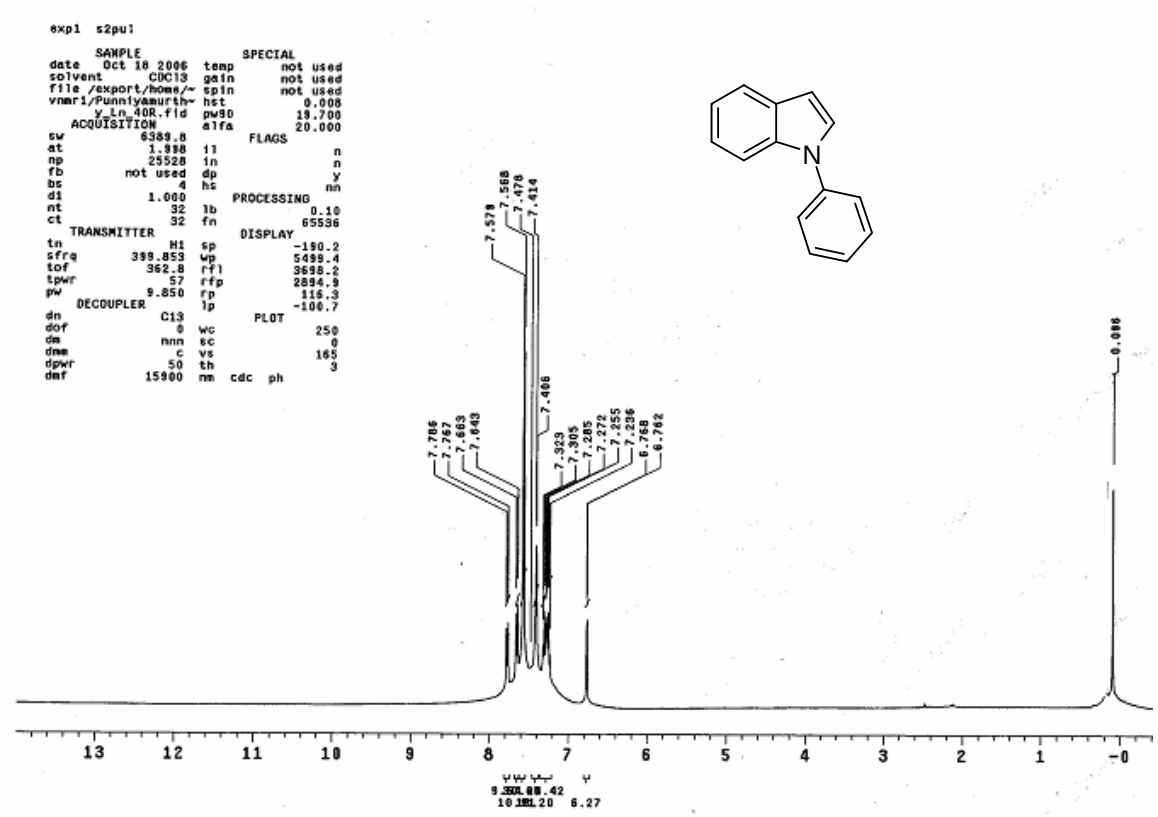

L_p1p -13C
exp1 s2pul
SAMPLE
date Jan 16 2007
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.193
np 60270
fb 13800
bs 16
d1 1.000
nt 2000
ct 0
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8900
SPECIAL
temp not used
gain not used
spin not used
hst 0.000
pw90 18.600
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1522.3
wp 25124.9
rfl 9287.8
rfp 7764.8
rp -46.0
lp -360.2
PLOT
wc 250
sc 0
vs 48
th 5
nm no ph
152.823
129.486
119.091
117.573
77.550
77.230
76.810
51.465
25.554
25.253
220
200
180
160
140
120
100
80
60
40
20
0
ppm

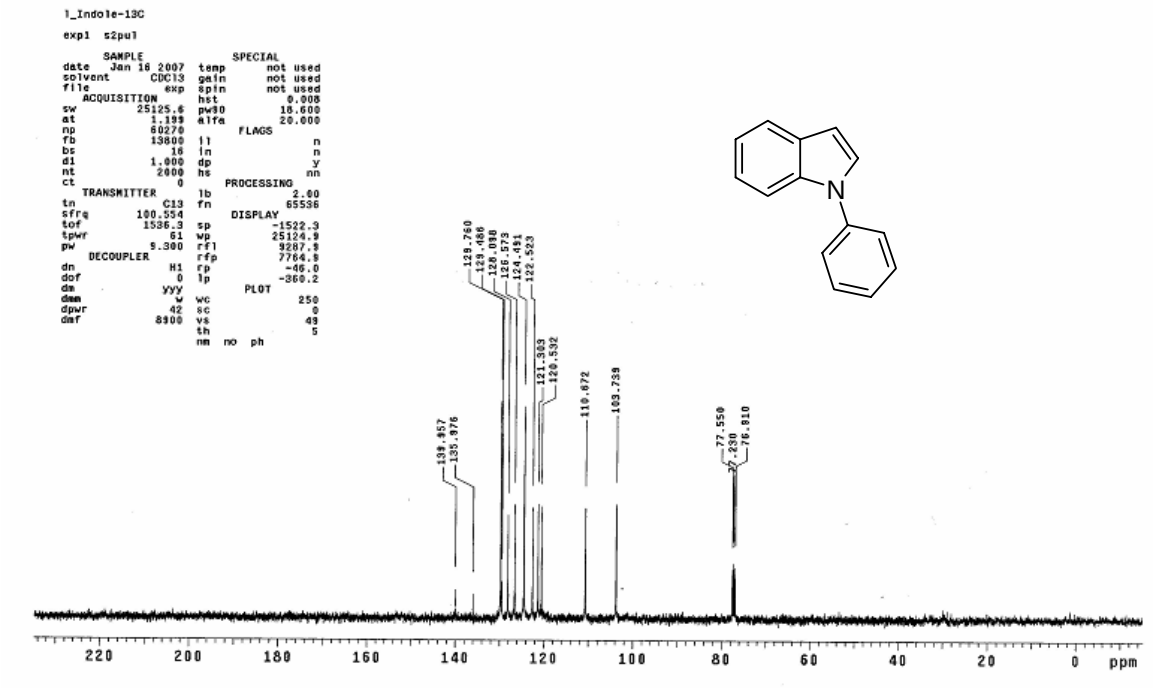

l_mapho
expl s2pul
SAMPLE
date Jan 17 2007
solvent CDCl3
file /export/home/v
vnmr1/Punniyamurth
y_l_mapho.fid
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 28
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.700
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp 630.8
wp 2812.7
rfl 796.6
rfp 0
rp 115.7
lp -98.7
PLOT
wc 250
sc 0
vs 304
th 8
nm cdc ph
7.304
7.285
7.266
7.258
7.256
6.935
6.913
6.907
6.889
6.886
3.880
3.868
3.856
3.173
3.161
3.149
8
7
6
5
4
3
2
ppm
19.49
22.04
27.65
30.81

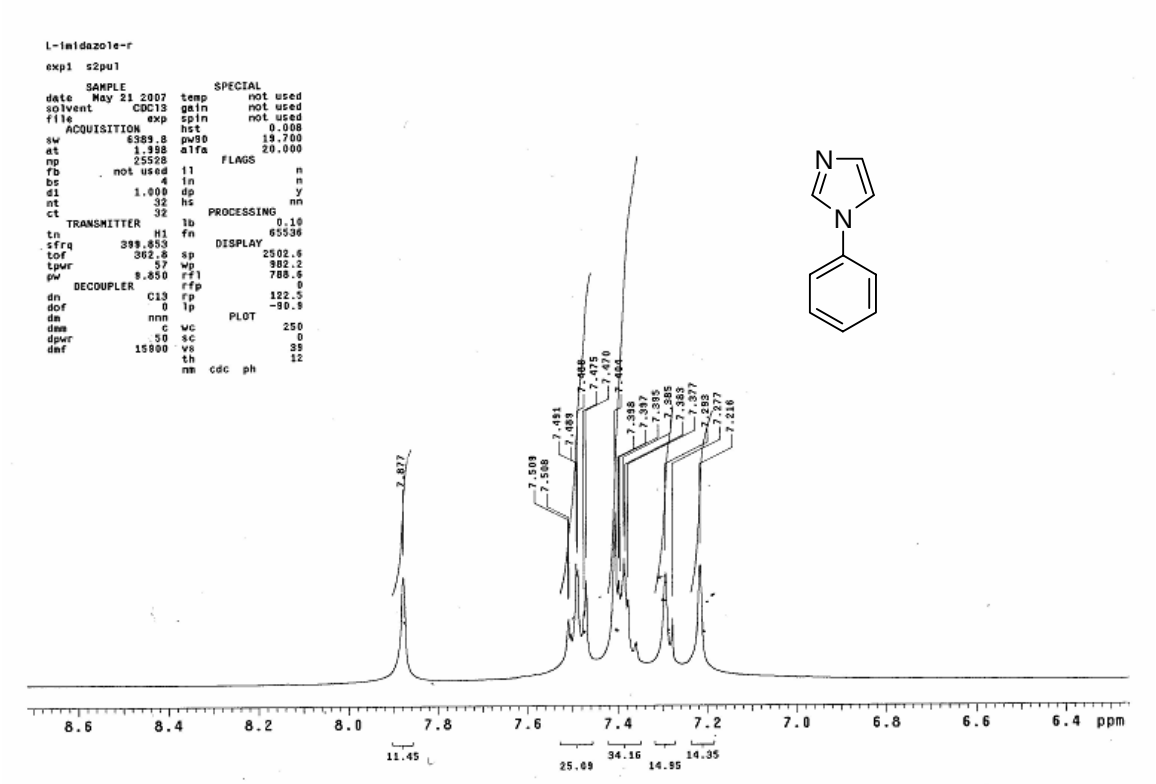

l_morpho c-13
expl s2pul
SAMPLE
date Jan 18 2007
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.193
np 60270
fb 13800
bs 16
d1 1.000
nt 2000
ct 582
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8300
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1506.9
wp 25124.8
rfl 9272.6
rfp 7764.9
rp -74.1
lp -271.4
PLOT
wc 250
sc 0
vs 59
th 4
nm no ph
151.465
129.384
120.281
115.926
77.543
77.230
76.910
67.148
48.562
1.226
0.204
220
200
180
160
140
120
100
80
60
40
20
0
ppm

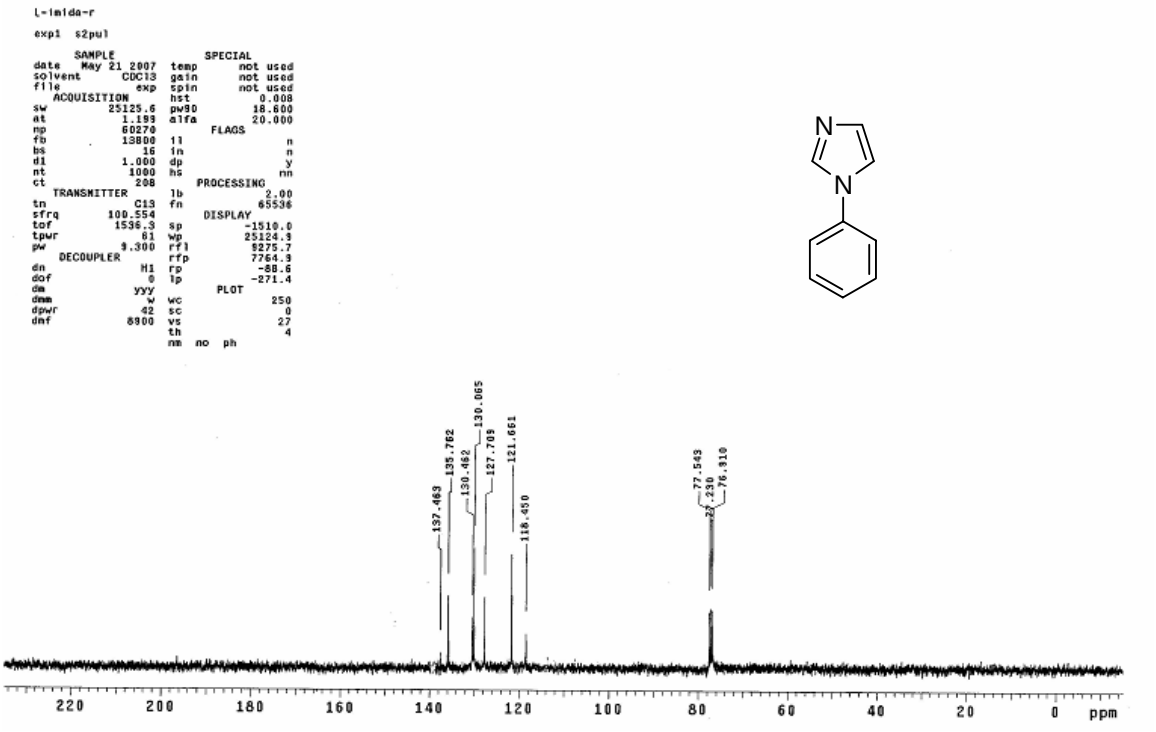

Ln_02V
exp1 s2pul
SAMPLE
date Oct 3 2006
solvent CDCl3
file /export/home/~
vnmr1/Punniya&urth~
y_Ln_02V.fid
ACQUISITION
sw 6389.8
at 1.598
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 15.700
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp -803.8
wp 6389.6
rfl 804.0
rfp 0
rp 133.7
lp -92.0
PLOT
wc 250
vs 293
th 2
nm cdc ph
7.737
7.718
7.467
7.463
7.446
7.425
7.371
7.352
7.284
7.283
7.278
7.265
7.146
7.118
7.123
7.119
6.381
6.375
0.030
0.000
13 12 11 10 9 8 7 6 5 4 3 2 1 -0 -1 ppm

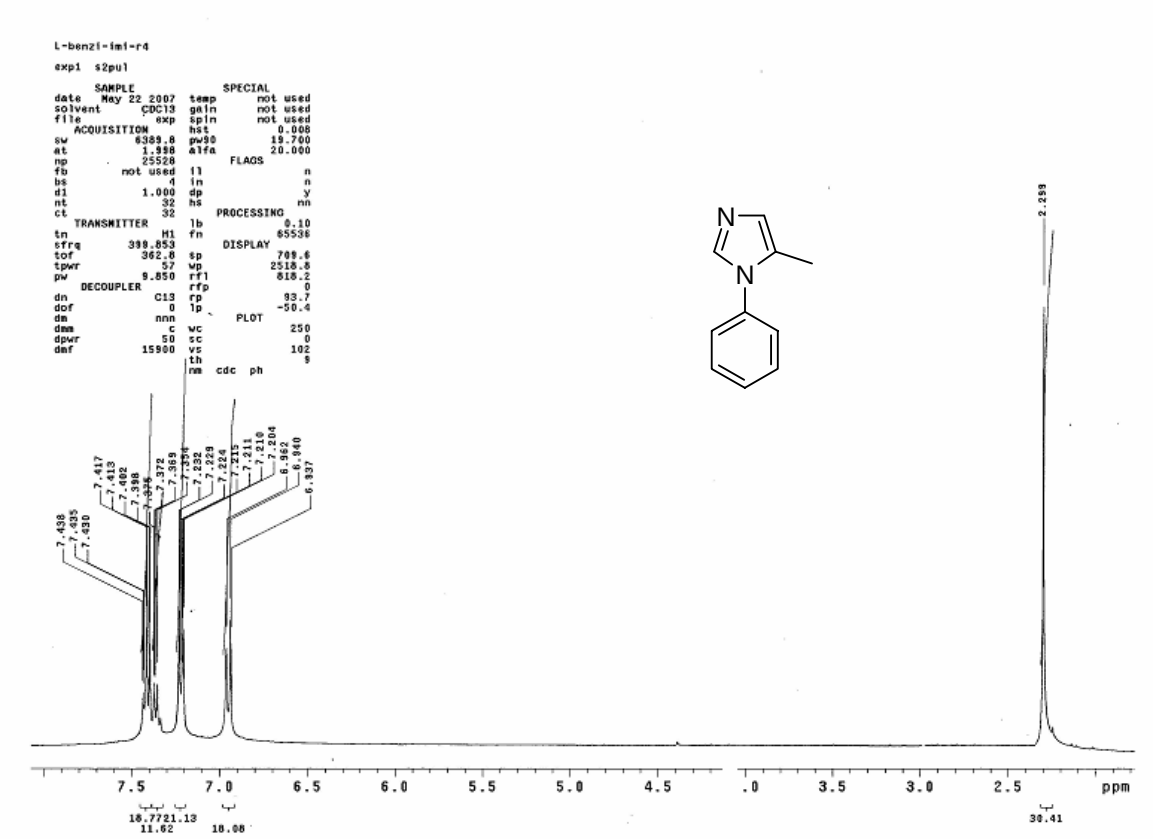

L_pyrrol
exp1 s2pul
SAMPLE
date Jan 16 2007
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.193
np 60270
fb 13800
bs 16
d1 1.000
nt 2000
ct 0
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 8.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8500
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1510.8
wp 25124.8
rfl 9276.4
rfp 7764.8
rp -88.6
lp -271.4
PLOT
wc 250
sc 0
vs 23
th 6
nm no ph
137.661
130.431
129.722
127.648
125.795
120.708
118.495
110.572
77.543
77.222
76.810
0.211
220 200 180 160 140 120 100 80 60 40 20 0 ppm

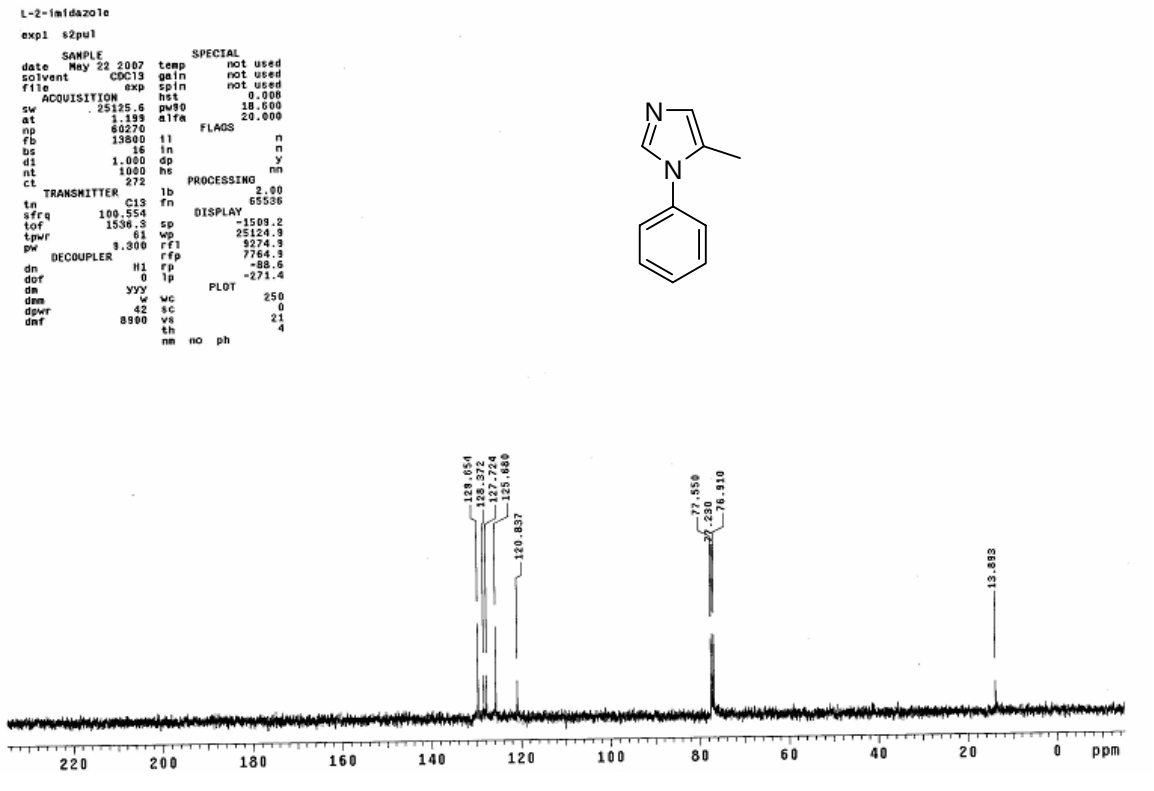

exp1 s2pul
SAMPLE
date Oct 16 2006
solvent CDCl3
file /export/home/~
vnmr1/Punniyamurth~
y_Ln_40R.fid
ACQUISITION
sw 6389.8
at 1.988
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.700
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp -180.2
wp 5499.4
rfl 3698.2
rfp 2894.9
rp 116.3
lp -100.7
PLOT
wc 250
sc 0
vs 165
th 3
nm cdc ph
7.579
7.568
7.478
7.414
7.406
7.786
7.767
7.663
7.643
7.323
7.305
7.285
7.272
7.255
7.236
6.768
6.762
0.000
13
12
11
10
9
8
7
6
5
4
3
2
1
-0
10.18
1.20
6.27

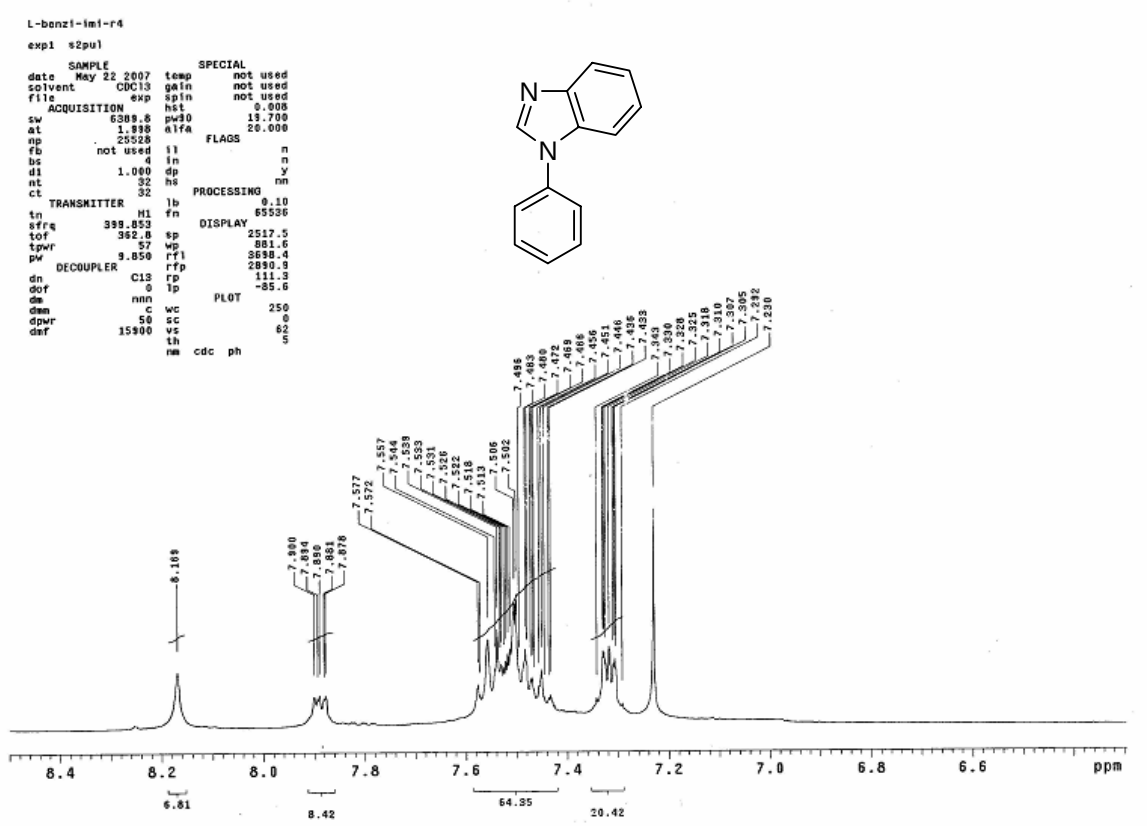

1_Indole-13C
exp1 s2pul
SAMPLE
date Jan 16 2007
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.199
np 60270
fb 13800
bs 16
d1 1.000
nt 2000
ct 0
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm c
dpwr 42
dmf 8900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1522.3
wp 25124.9
rfl 9287.8
rfp 7764.9
rp -46.0
lp -360.2
PLOT
wc 250
sc 0
vs 49
th 5
nm no ph
139.457
135.976
129.760
129.486
128.030
126.573
124.491
122.523
121.369
120.592
110.672
103.739
77.550
77.230
76.910
220
200
180
160
140
120
100
80
60
40
20
0
ppm

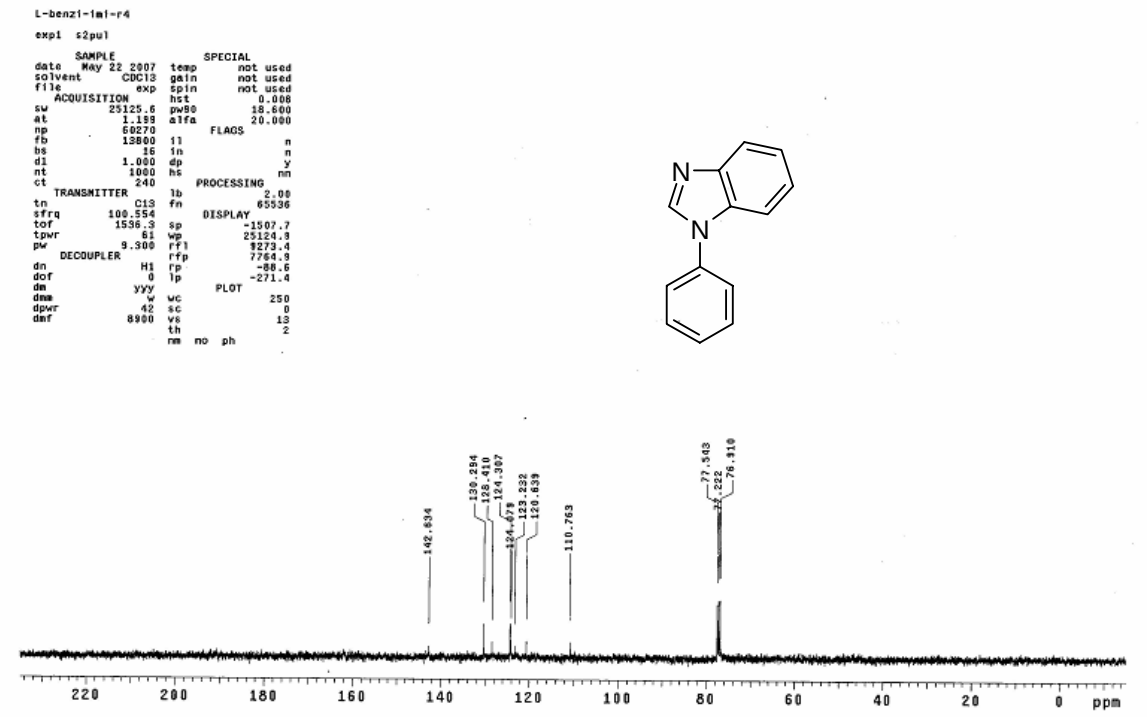

L-imidazole-r
exp1 s2pul
SAMPLE
date May 21 2007
solvent CDCl3
file exp
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 302.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15800
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 19.700
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp 2502.6
wp 982.2
rfl 788.6
rfp 0
rp 122.5
lp -90.9
PLOT
wc 250
sc 0
vs 38
th 12
nm cdc ph
7.877
7.508
7.503
7.491
7.489
7.488
7.475
7.470
7.464
7.398
7.397
7.385
7.383
7.377
7.288
7.277
7.216
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
6.4 ppm
11.45
25.69
34.16
14.95
14.35

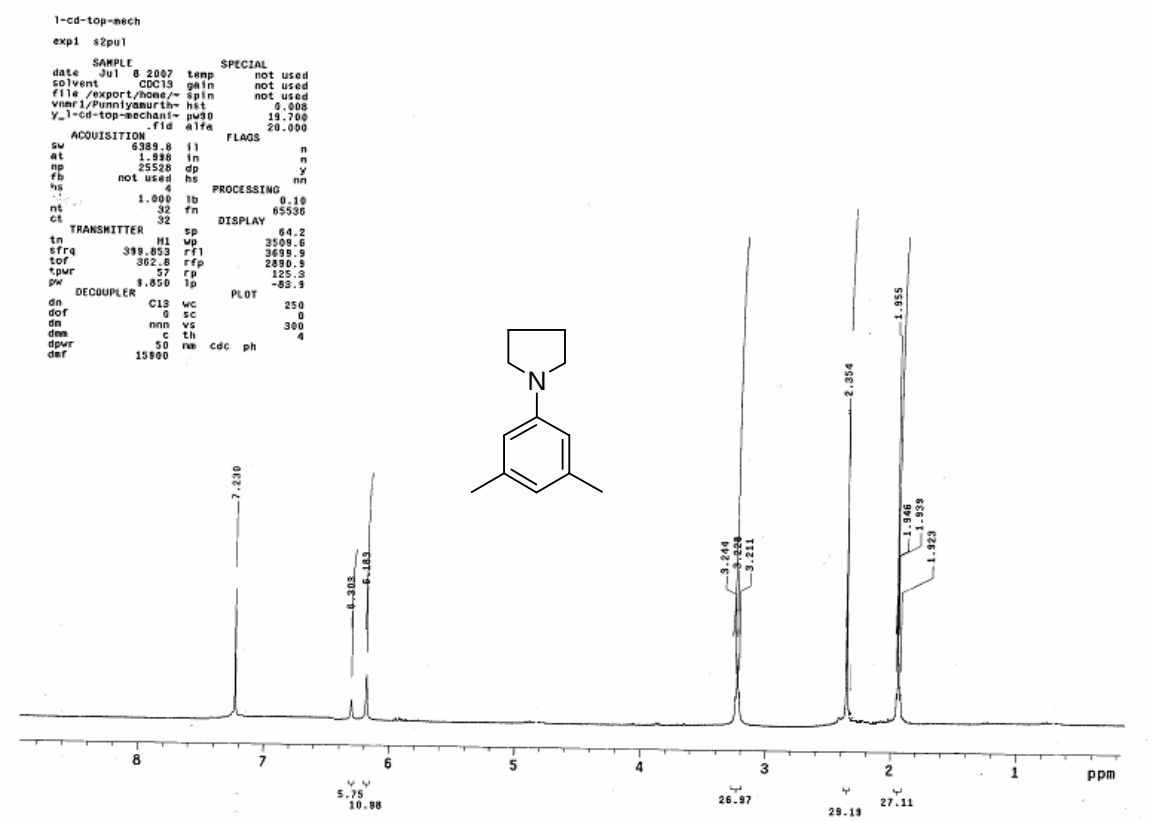

L-imida-r
exp1 s2pul
SAMPLE
date May 21 2007
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.193
np 60270
fb 13800
bs 16
d1 1.000
nt 1000
ct 208
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1510.0
wp 25124.8
rfl 9275.7
rfp 7764.9
rp -88.6
lp -271.4
PLOT
wc 250
sc 0
vs 27
th 4
nm no ph
137.463
135.762
130.462
130.065
127.709
121.661
118.450
77.543
77.230
76.810
220
200
180
160
140
120
100
80
60
40
20
0 ppm

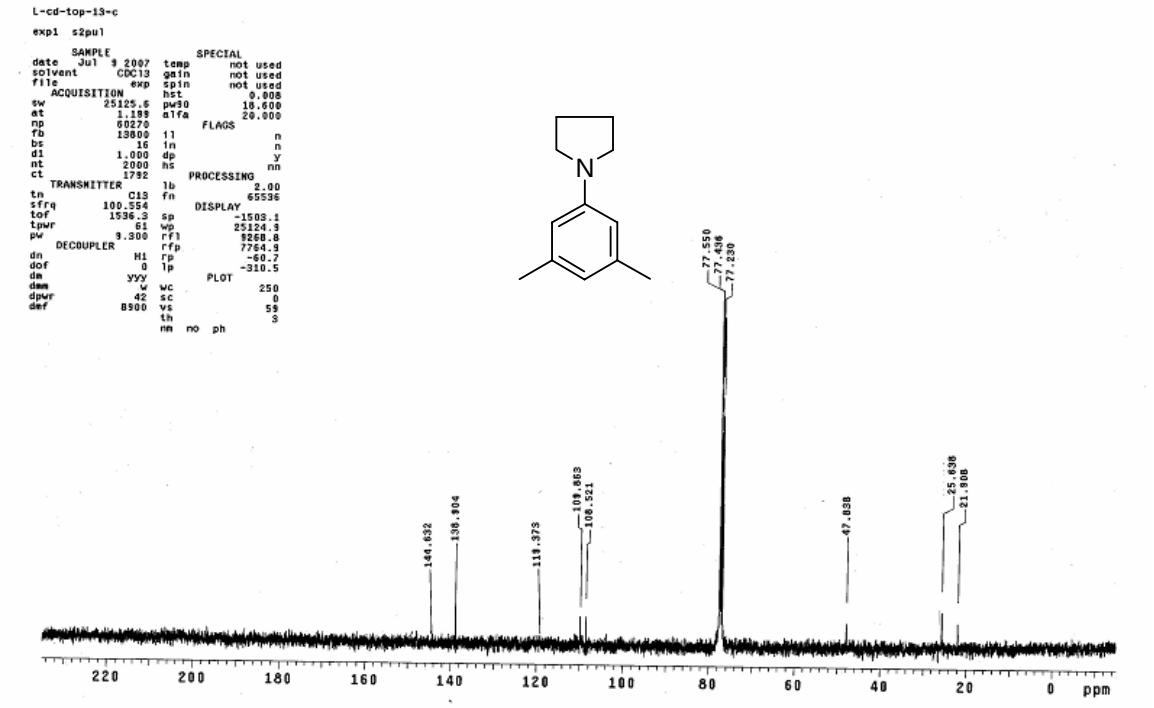

L-benzi-imi-r4
exp1 s2pul
SAMPLE
date May 22 2007
solvent CDCl3
file exp
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 19.700
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp 709.6
wp 2518.8
rfl 818.2
rfp 0
rp 93.7
lp -50.4
PLOT
wc 250
sc 0
vs 102
th 9
nm cdc ph
7.438
7.435
7.430
7.417
7.413
7.402
7.398
7.388
7.372
7.369
7.354
7.232
7.229
7.224
7.215
7.211
7.210
7.204
6.962
6.940
6.937
2.299
7.5
7.0
6.5
6.0
5.5
5.0
4.5
.0
3.5
3.0
2.5
ppm
18.77
21.13
11.62
18.08
30.41

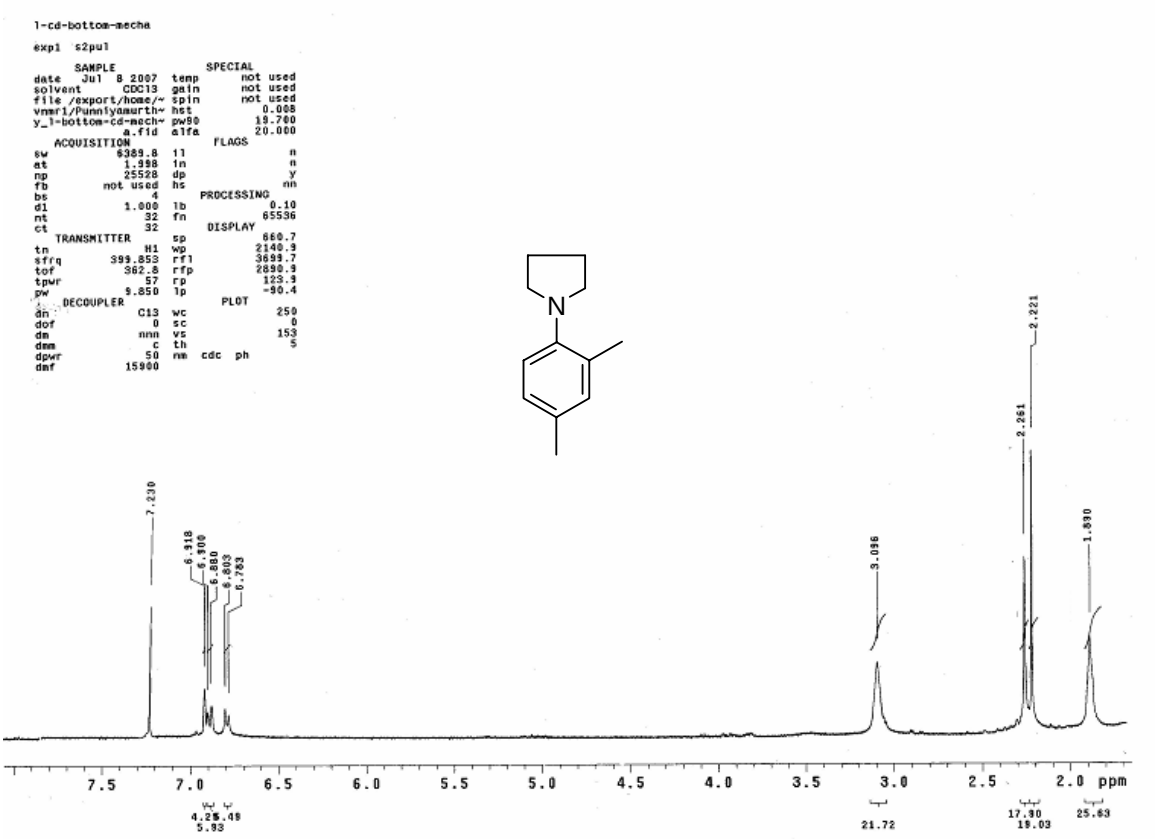

L-2-imidazole
exp1 s2pul
SAMPLE
date May 22 2007
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.189
np 60270
fb 13800
bs 16
d1 1.000
nt 1000
ct 272
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1509.2
wp 25124.9
rfl 9274.9
rfp 7764.9
rp -88.6
lp -271.4
PLOT
wc 250
sc 0
vs 21
th 4
nm no ph
128.654
128.372
127.724
125.680
120.837
77.550
77.230
76.910
13.893
220
200
180
160
140
120
100
80
60
40
20
0
ppm

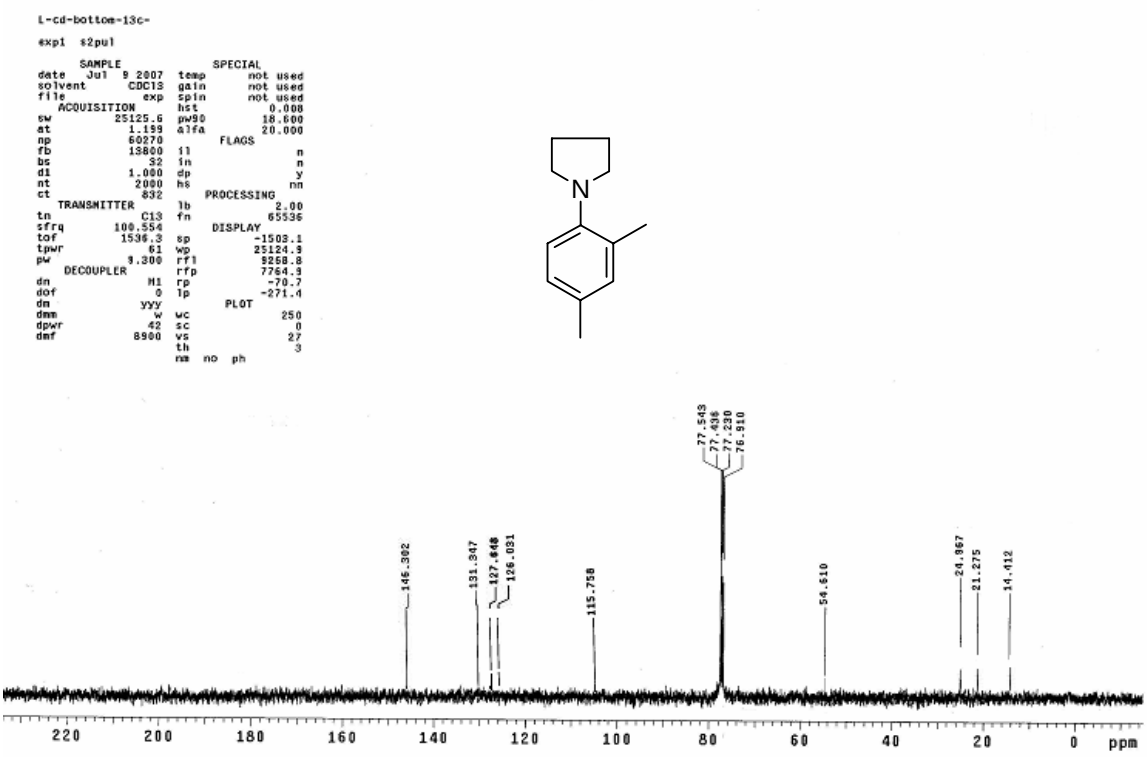

L-benzi-imi-r4
exp1 s2pul
SAMPLE
date May 22 2007
solvent CDCl3
file exp
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 19.700
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp 2517.5
wp 881.6
rfl 3698.4
rfp 2890.9
rp 111.3
lp -85.6
PLOT
wc 250
sc 0
vs 62
th 5
nm cdc ph
8.169
7.980
7.834
7.850
7.881
7.878
7.577
7.572
7.557
7.544
7.539
7.533
7.531
7.526
7.522
7.518
7.513
7.506
7.502
7.496
7.483
7.480
7.472
7.469
7.466
7.455
7.451
7.446
7.436
7.433
7.363
7.330
7.325
7.320
7.310
7.307
7.305
7.292
7.230
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
ppm
6.81
8.42
64.95
20.42

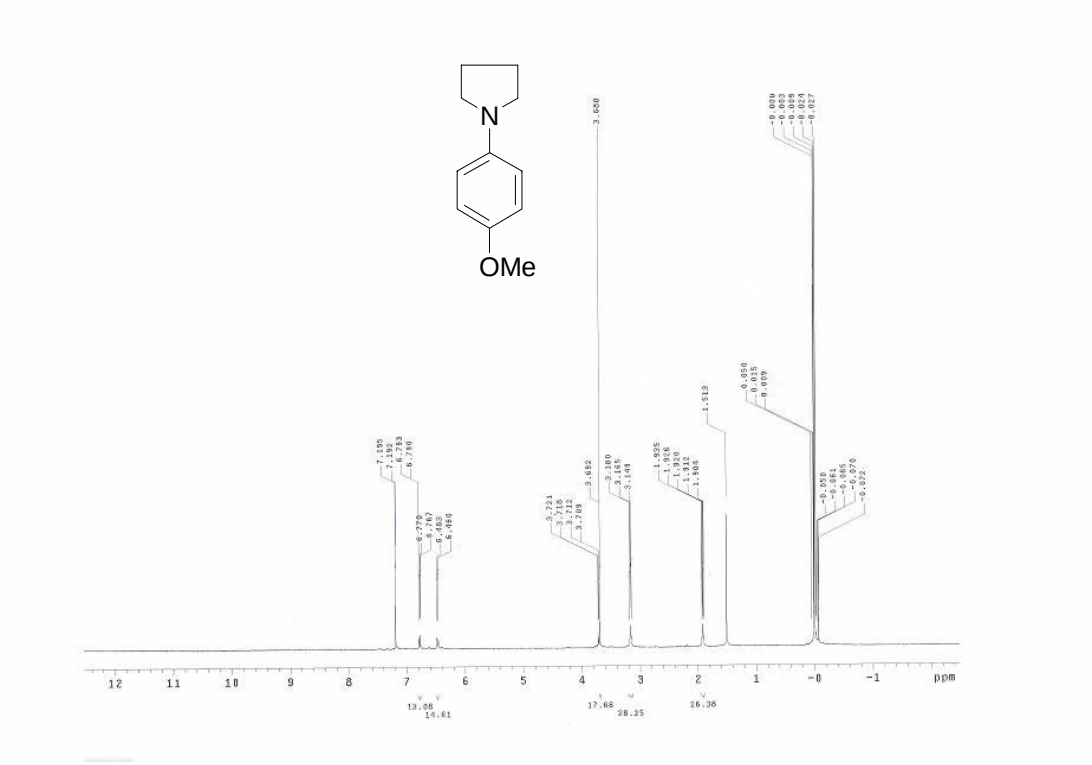

L-benzi-imi-r4
exp1 s2pul
SAMPLE
date May 22 2007
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.199
np 60270
fb 13800
bs 16
d1 1.000
nt 1000
ct 240
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1507.7
wp 25124.3
rfl 9273.4
rfp 7764.9
rp -88.6
lp -271.4
PLOT
wc 250
sc 0
vs 13
th 2
nm no ph
142.634
130.284
128.410
124.307
124.079
123.232
120.639
110.763
77.543
77.222
76.910
220
200
180
160
140
120
100
80
60
40
20
0
ppm

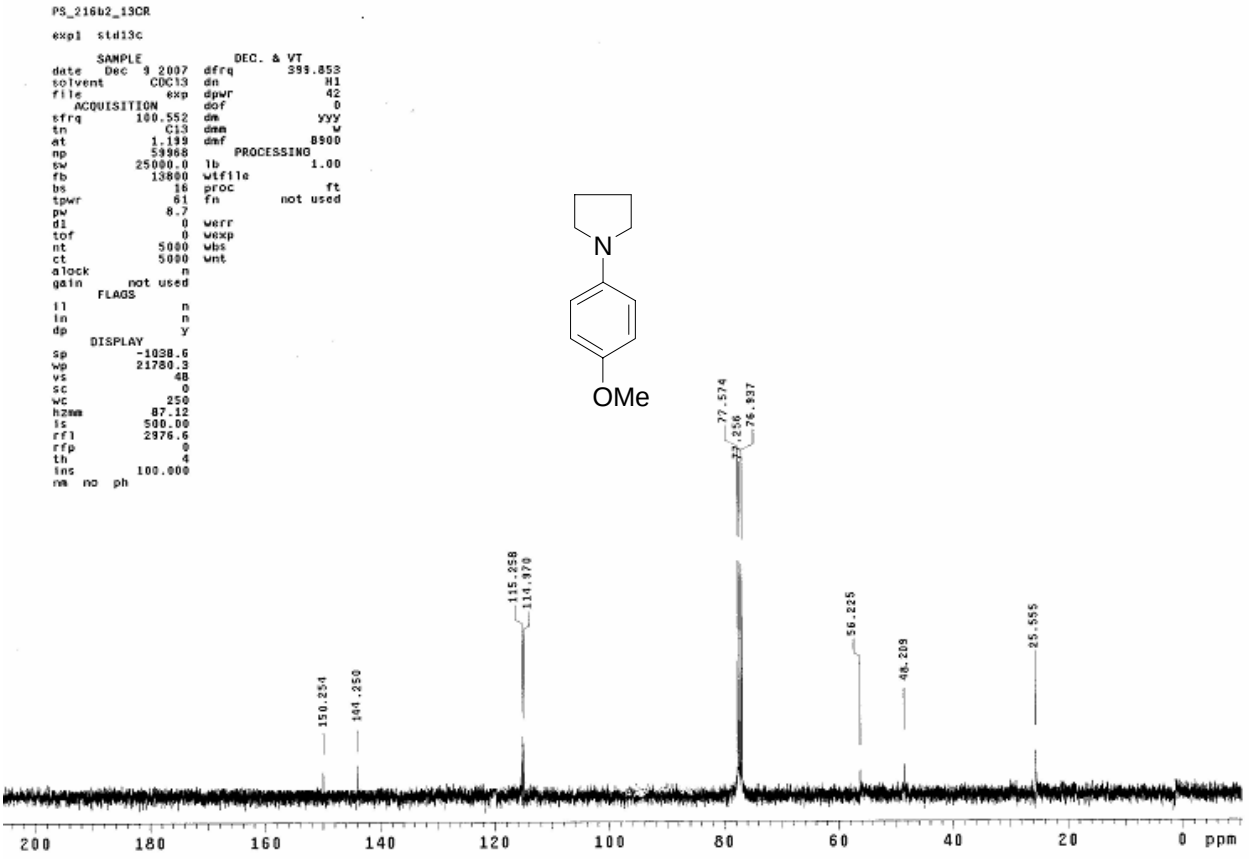

1-cd-top-mech
exp1 s2pul
SAMPLE
date Jul 8 2007
solvent CDCl3
file /export/home/~
vnmr1/Punnlyamurth~
y_1-cd-top-mechani~
.fid
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
def 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 19.700
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp 64.2
wp 3509.6
rf1 3699.9
rfp 2890.9
rp 125.2
lp -83.9
PLOT
wc 250
sc 0
vs 300
th 4
nm cdc ph
7.230
6.303
6.183
3.244
3.228
3.211
2.354
1.955
1.946
1.939
1.928
8
7
6
5
4
3
2
1
ppm
5.75
10.98
26.97
29.19
27.11

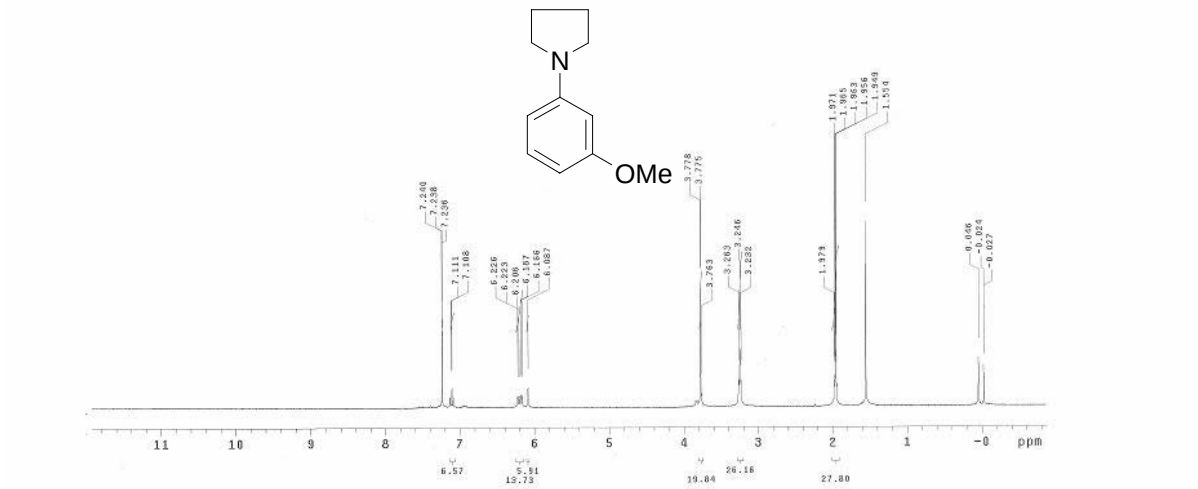

L-cd-top-13-c
exp1 s2pul
SAMPLE
date Jul 9 2007
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.199
np 60270
fb 13800
bs 16
d1 1.000
nt 2000
ct 1792
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
def 8900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1503.1
wp 25124.8
rf1 9268.8
rfp 7764.8
rp -60.7
lp -310.5
PLOT
wc 250
sc 0
vs 59
th 3
nm no ph
77.550
77.438
77.230
144.632
138.804
119.373
109.863
108.521
47.838
25.638
21.908
220
200
180
160
140
120
100
80
60
40
20
0
ppm

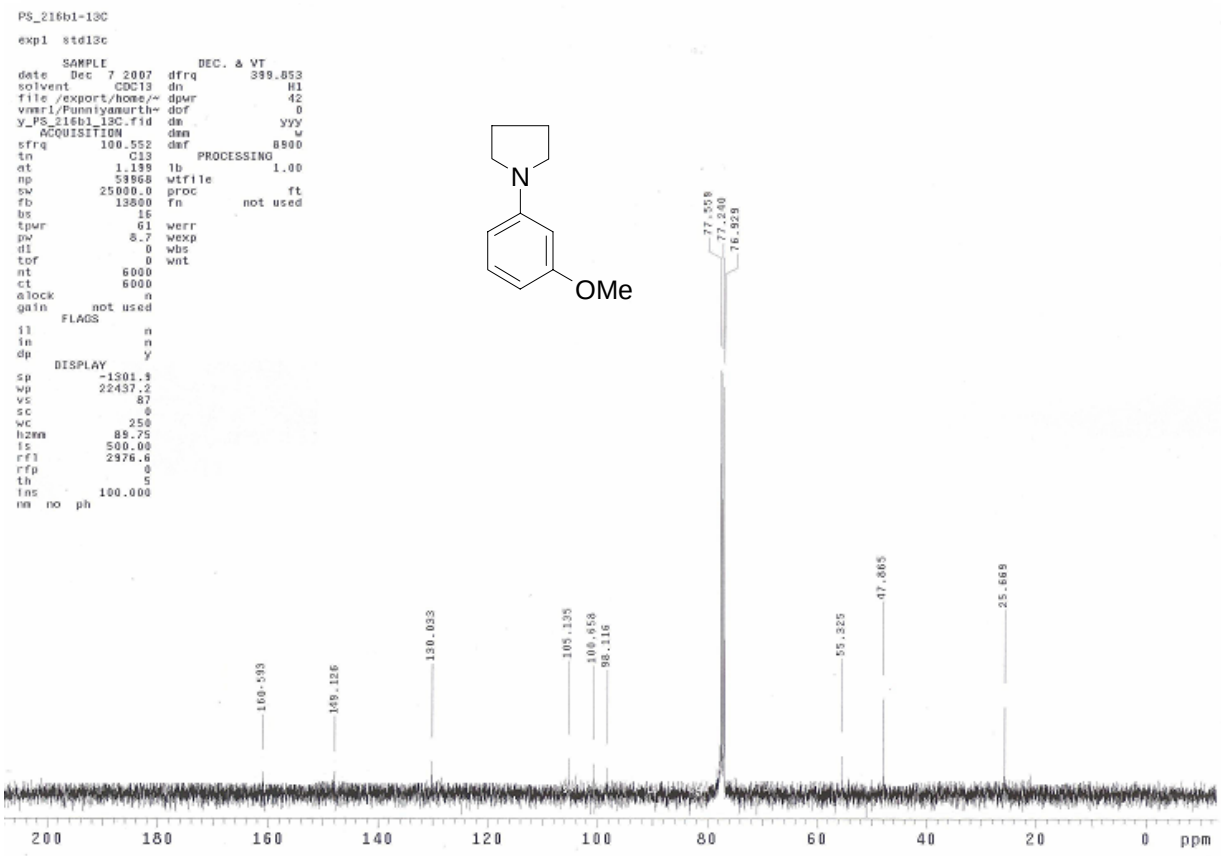

1-cd-bottom-mecha
exp1 s2pul
SAMPLE
date Jul 8 2007
solvent CDCl3
file /export/home/v
vmr1/Punniyamurth~
y_1-bottom-cd-mech~
a.fid
ACQUISITION
sw 6389.8
at 1.998
np 25528
fb not used
bs 4
d1 1.000
nt 32
ct 32
TRANSMITTER
tn H1
sfrq 399.853
tof 362.8
tpwr 57
pw 9.850
DECOUPLER
dn C13
dof 0
dm nnn
dmm c
dpwr 50
dmf 15900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 19.700
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 0.10
fn 65536
DISPLAY
sp 660.7
wp 2140.9
rf1 3699.7
rfp 2890.9
rp 123.9
lp -90.4
PLOT
wc 250
sc 0
vs 153
th 5
nm cdc ph
7.230
6.918
6.900
6.880
6.803
6.783
3.096
2.261
2.221
1.830
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0 ppm
4.25
5.49
5.93
21.72
17.90
19.03
25.83

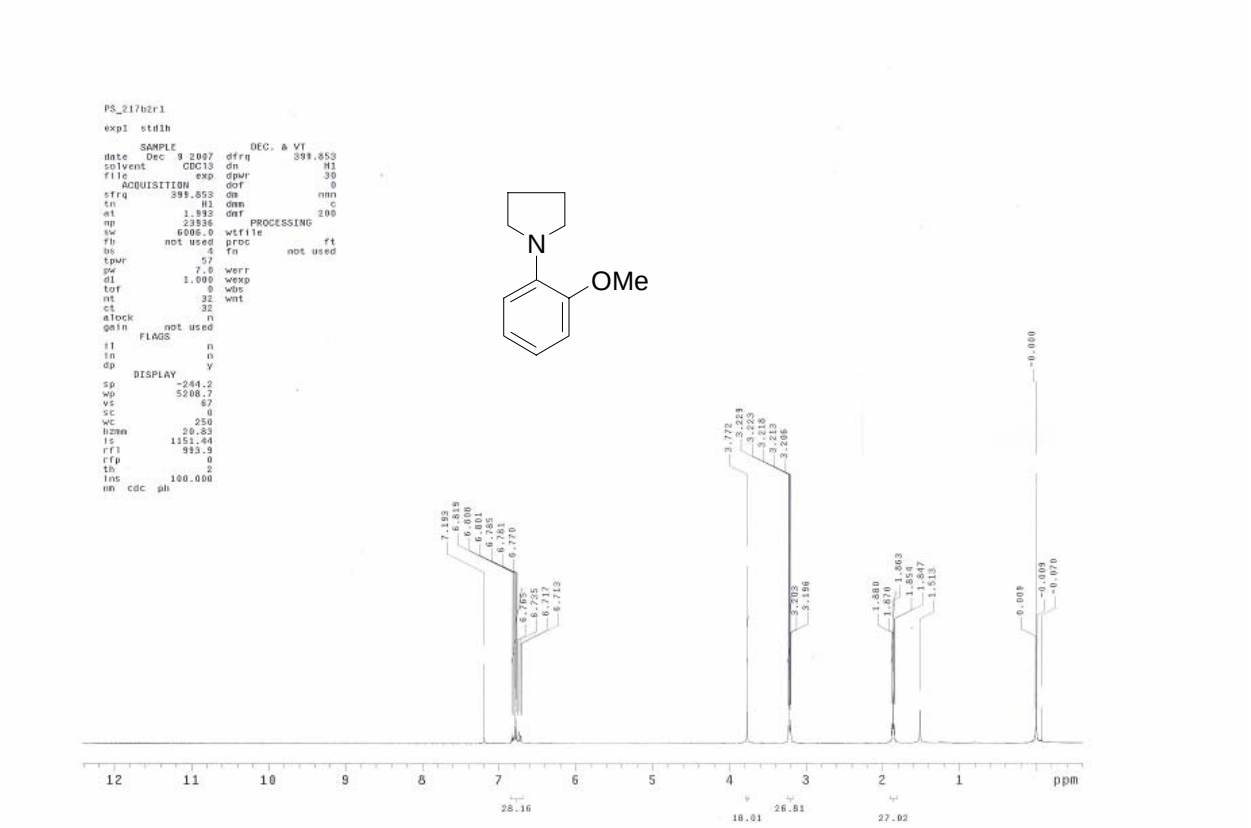

L-cd-bottom-13c-
exp1 s2pul
SAMPLE
date Jul 9 2007
solvent CDCl3
file exp
ACQUISITION
sw 25125.6
at 1.199
np 60270
fb 13800
bs 32
d1 1.000
nt 2000
ct 832
TRANSMITTER
tn C13
sfrq 100.554
tof 1536.3
tpwr 61
pw 9.300
DECOUPLER
dn H1
dof 0
dm yyy
dmm w
dpwr 42
dmf 8900
SPECIAL
temp not used
gain not used
spin not used
hst 0.008
pw90 18.600
alfa 20.000
FLAGS
il n
in n
dp y
hs nn
PROCESSING
lb 2.00
fn 65536
DISPLAY
sp -1503.1
wp 25124.9
rf1 8258.8
rfp 7764.9
rp -70.7
lp -271.4
PLOT
wc 250
sc 0
vs 27
th 3
nm no ph
146.302
131.347
127.648
126.031
115.758
77.543
77.438
77.230
76.910
54.610
24.967
21.275
14.412
220
200
180
160
140
120
100
80
60
40
20
0 ppm

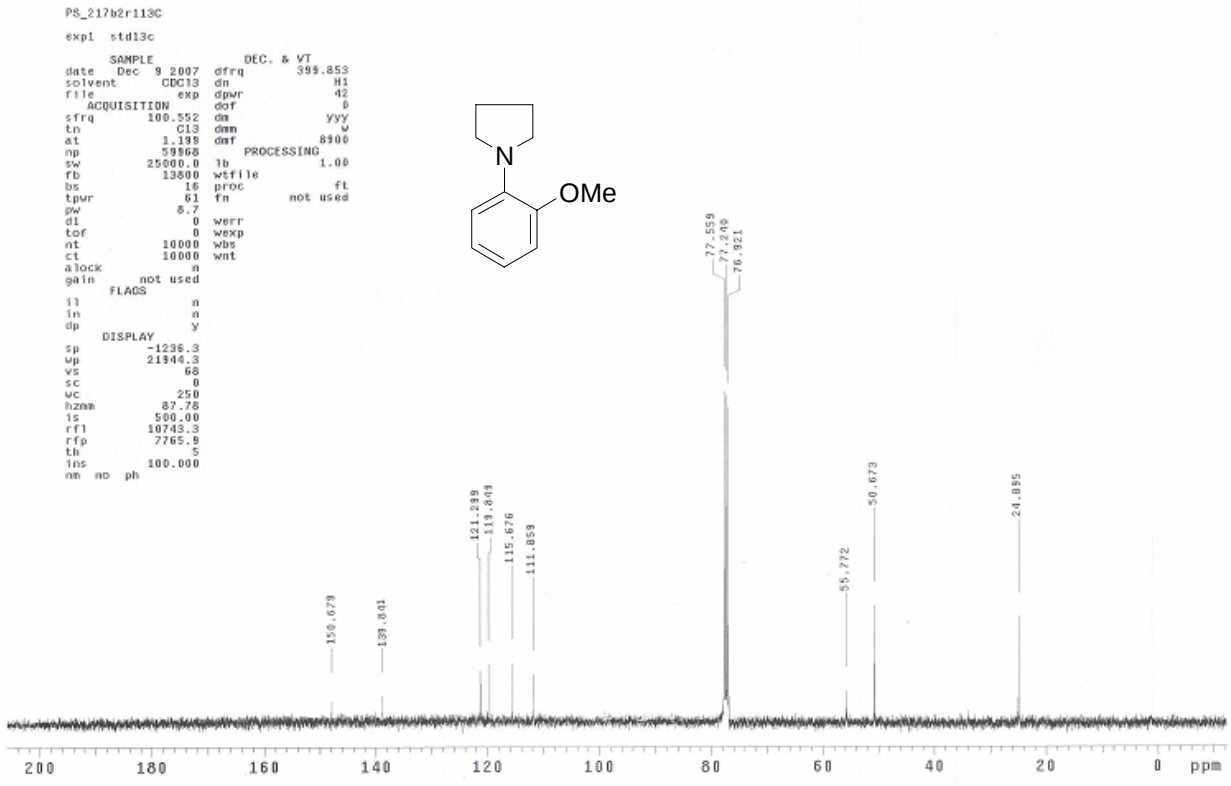

N
OMe
12
11
10
9
8
7
6
5
4
3
2
1
0
−1
ppm


PS_216b2_13CR
expl std13c
SAMPLE
date Dec 9 2007
solvent CDCl3
file exp
ACQUISITION
sfrq 100.552
tn C13
at 1.199
np 59968
sw 25000.0
fb 13800
bs 16
tpwr 61
pw 8.7
d1 0
tof 0
nt 5000
ct 5000
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -1038.6
wp 21780.3
vs 48
sc 0
wc 250
hzmm 87.12
is 500.00
rfl 2976.6
rfp 0
th 4
ins 100.000
nm no ph
DEC. & VT
dfrq 399.853
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 8900
PROCESSING
lb 1.00
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
N
OMe
77.574
77.256
76.937
150.254
144.250
115.258
114.970
56.225
48.209
25.555
200
180
160
140
120
100
80
60
40
20
0
ppm


N
OMe
7.240
7.238
7.236
7.111
7.108
6.226
6.223
6.208
6.205
6.187
6.166
6.087
3.778
3.775
3.763
3.249
3.246
3.232
1.971
1.965
1.963
1.955
1.949
1.504
1.473
0.046
0.024
0.027
11
10
9
8
7
6
5
4
3
2
1
-0
ppm
6.57
5.91
13.73
19.84
26.16
27.80


PS_216b1-13C
exp1 stdl3c
SAMPLE
date Dec 7 2007
solvent CDCl3
file /export/home/~
vmrl/Punniyamurth~
y_PS_216b1_13C.fid
ACQUISITION
sfrq 100.552
tn C13
at 1.199
np 53968
sw 25000.0
fb 13800
bs 16
tpwr 61
pw 8.7
dl 0
tof 0
nt 6000
ct 6000
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -1301.9
wp 22437.2
vs 87
sc 0
wc 250
hzmm 89.75
is 500.00
rfl 2976.6
rfp 0
th 5
ins 100.000
nm no ph
DEC. & VT
dfrq 399.853
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 8900
PROCESSING
lb 1.00
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
N
OMe
77.558
77.240
76.929
160.593
149.126
130.033
105.135
100.658
98.116
55.325
47.865
25.669
200
180
160
140
120
100
80
60
40
20
0
ppm


PS_217b2r1
expl stdlh
SAMPLE
date Dec 9 2007
solvent CDCl3
file exp
ACQUISITION
sfrq 399.853
tn H1
at 1.993
np 23936
sw 6006.0
fb not used
bs 4
tpwr 57
pw 7.0
d1 1.000
tof 0
nt 32
ct 32
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -264.2
wp 5208.7
vs 67
sc 0
wc 250
hzmm 20.83
is 1151.44
rfl 933.9
rfp 0
th 2
ins 100.000
nm cdc ph
DEC. & VT
dfrq 399.853
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
N
OMe
7.183
6.819
6.808
6.801
6.785
6.761
6.770
6.765
6.735
6.717
6.713
3.772
3.229
3.223
3.218
3.213
3.206
3.208
3.198
1.880
1.870
1.863
1.854
1.847
1.515
0.000
0.009
-0.070
12
11
10
9
8
7
6
5
4
3
2
1
ppm
28.16
18.01
26.81
27.02


PS_217b2r113C
expl stdl3c
SAMPLE
date Dec 9 2007
solvent CDCl3
file exp
ACQUISITION
sfrq 100.552
tn C13
at 1.195
np 59868
sw 25000.0
fb 13800
bs 16
tpwr 61
pw 8.7
d1 0
tof 0
nt 10000
ct 10000
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -1236.3
wp 21944.3
vs 68
sc 0
wc 250
hzmm 87.78
is 500.00
rfl 10743.3
rfp 7765.9
th 5
ins 100.000
nm no ph
DEC. & VT
dfrq 399.853
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 8900
PROCESSING
lb 1.00
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
N
OMe
77.559
77.240
76.921
150.679
139.801
121.299
119.848
115.676
111.859
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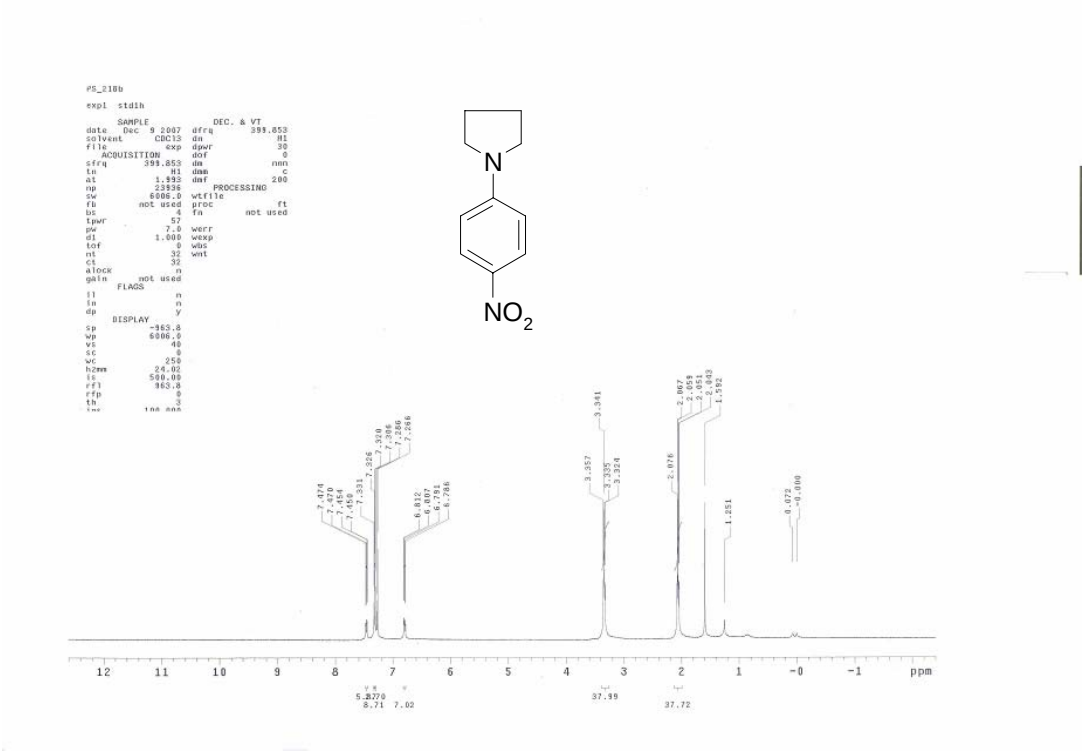
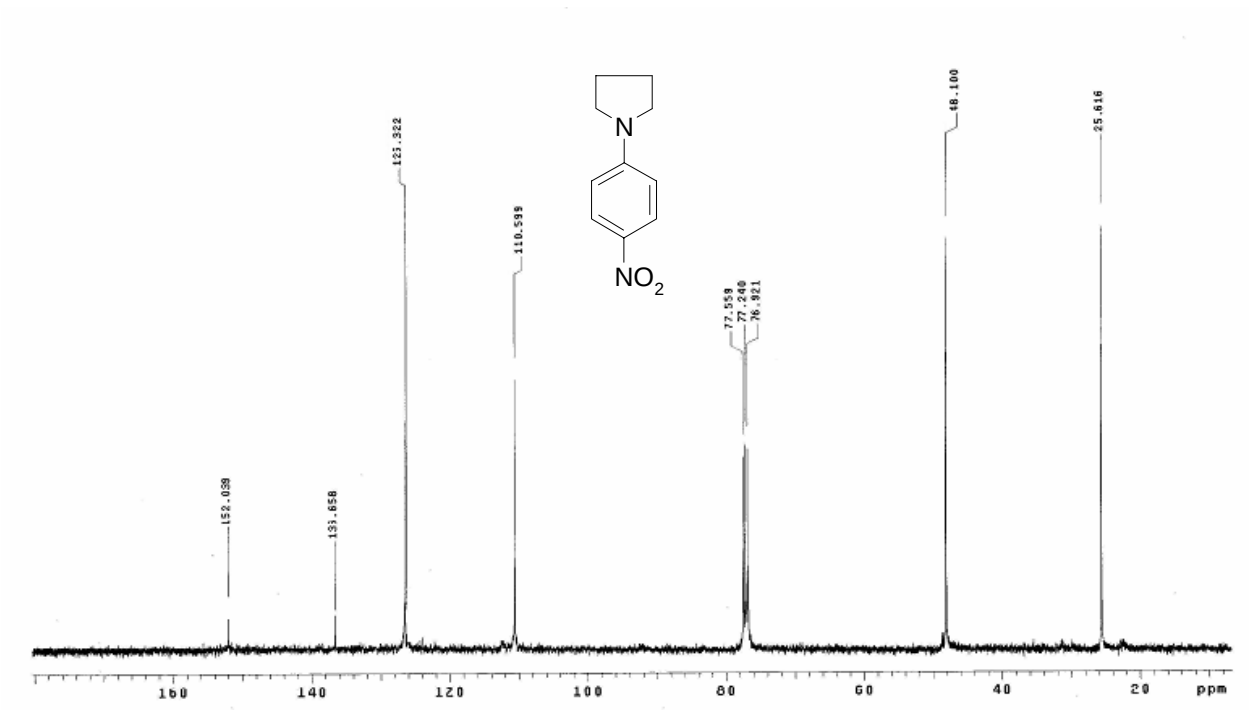
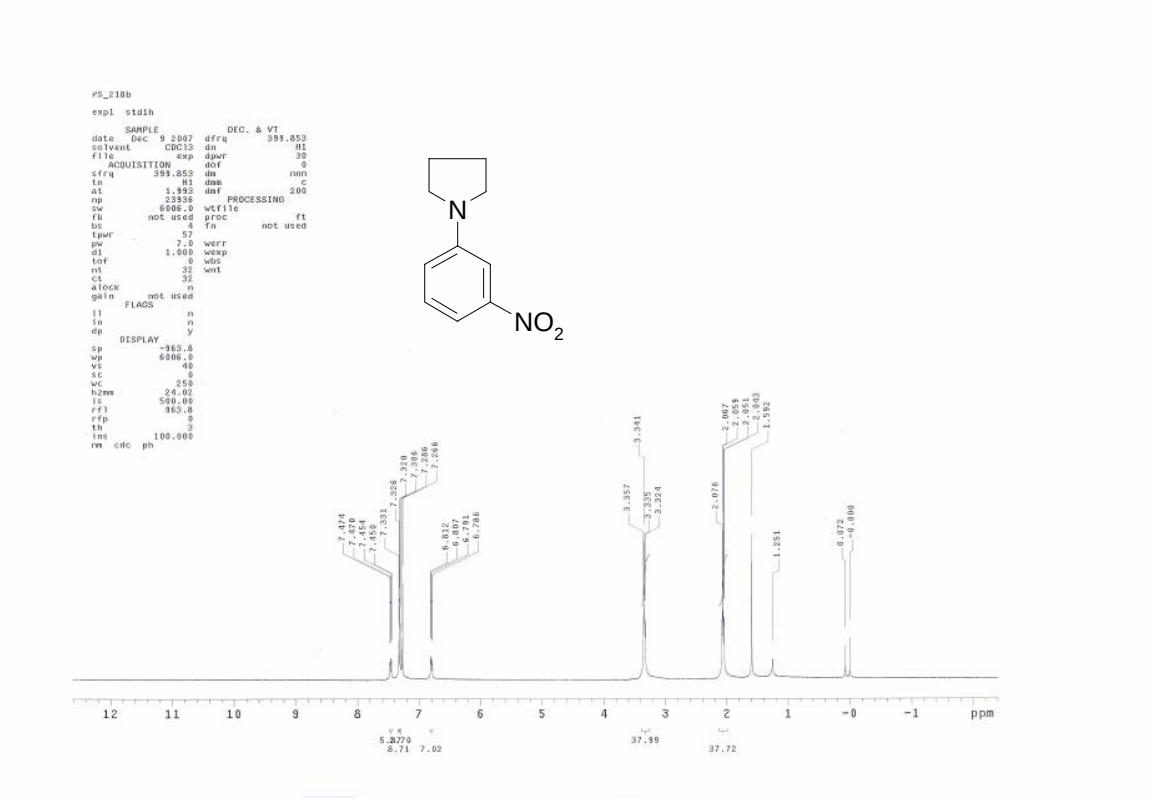
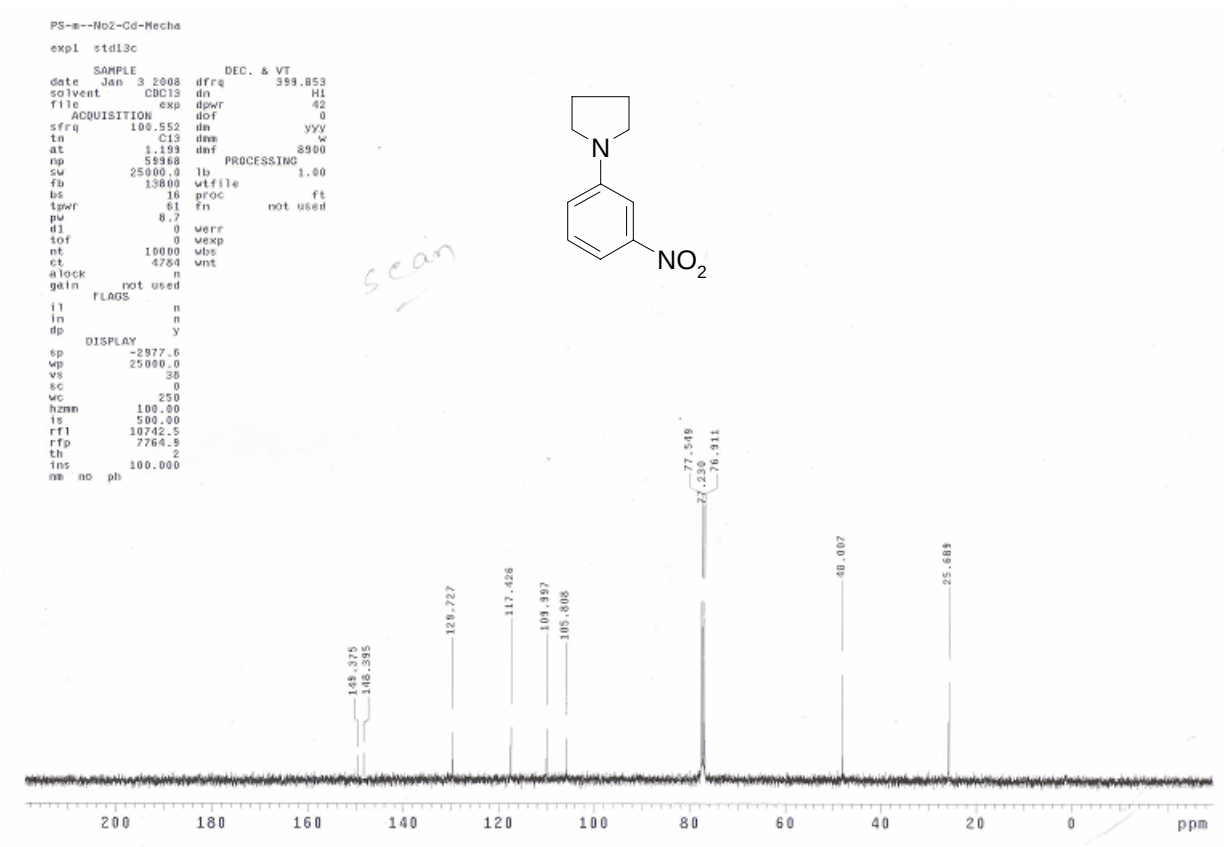
50.673
24.855
200
180
160
140
120
100
80
60
40
20
0
ppm


PS_218b
expl stdih
SAMPLE
date Dec 9 2007
solvent CDCl3
file exp
ACQUISITION
sfrq 399.853
tn H1
at 1.993
np 23936
sw 6006.0
fb not used
bs 4
tpwr 57
pw 7.0
dl 1.000
tof 0
nt 32
ct 32
alock n
gain not used
FLAGS
DISPLAY
sp -165.8
wp 6006.0
vs 40
sc 0
wc 250
hzmm 24.02
is 500.00
rfl 363.8
rfp 0
th 3
DEC. & VT
dfrq 399.853
dn H1
dpwr 30
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
N
NO2
7.474
7.470
7.454
7.451
7.326
7.310
7.306
7.286
7.266
6.812
6.807
6.791
6.786
3.357
3.341
3.335
3.324
2.867
2.059
2.051
2.048
1.592
1.261
0.072
0.000
12
11
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm
5.8270
8.71
7.02
37.99
37.72


152.039
131.658
123.322
110.599
77.559
77.240
76.921
48.100
25.616
N
NO2
160
140
120
100
80
60
40
20
ppm


PS_218b
expl stdlh
SAMPLE
date Dec 9 2007
solvent CDCl3
file exp
ACQUISITION
sfrq 399.853
tn H1
at 1.893
np 23936
sw 6008.0
fb not used
bs 4
tpwr 57
pw 7.0
dl 1.000
tof 0
nt 32
ct 32
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -963.8
wp 6006.0
vs 40
sc 0
wc 250
hzmm 24.02
is 500.00
rfl 963.8
rfp 0
th 3
ins 100.000
nm cdc ph
DEC. & VT
dfrq 399.853
dn H1
dpwr 20
dof 0
dm nnn
dmm c
dmf 200
PROCESSING
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
N
NO2
7.474
7.470
7.454
7.450
7.331
7.326
7.320
7.306
7.288
7.286
6.812
6.807
6.791
6.786
3.341
3.357
3.335
3.324
2.076
2.067
2.059
2.051
2.043
1.592
1.251
0.072
+0.000
12
11
10
9
8
7
6
5
4
3
2
1
-0
-1
ppm
5.2770
8.71
7.02
37.99
37.72


PS-m--No2-Cd-Mecha
expl stdl3c
SAMPLE
date Jan 3 2008
solvent CDCl3
file exp
ACQUISITION
sfrq 100.552
tn C13
at 1.193
np 59968
sw 25000.0
fb 13800
bs 16
tpwr 61
pw 8.7
dl 0
tof 0
nt 10000
ct 4784
alock n
gain not used
FLAGS
il n
in n
dp y
DISPLAY
sp -2977.6
wp 25000.0
vs 38
sc 0
wc 250
hzmm 100.00
is 500.00
rfl 10742.5
rfp 7764.9
th 2
ins 100.000
nm no ph
DEC. & VT
dfrq 399.853
dn H1
dpwr 42
dof 0
dm yyy
dmm w
dmf 8900
PROCESSING
lb 1.00
wtfile
proc ft
fn not used
werr
wexp
wbs
wnt
scan
N
NO2
77.549
77.230
76.911
148.375
148.395
129.727
117.426
109.397
105.808
40.007
25.689
200
180
160
140
120
100
80
60
40
20
0
ppm