SUPPORTING INFORMATION

Bidentate P, N-P Ligand for Nickel-Catalyzed Cross-Coupling of Aryl or Benzyl Chlorides with ArMgX

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General Information:

Unless otherwise noted all starting materials were obtained from commercial suppliers. Organic solvents were dried and distilled as described elsewhere.[1] All reactions were carried out in an oven-dried flask under argon atmosphere. Column chromatography was performed with silica gel 230 ~ 400 meshes. All ^{1}H NMR, ^{13}C NMR and ^{31}P NMR spectra were recorded on in $CDCl_3$ or CD_2Cl_2 solution and reported in ppm (δ). X-ray single crystal data were collected using MoKα (λ = 0.7107 Å) radiation. Data collection, data reduction, structure solution/refinement were carried out using the software package of BRUKER APEX II. The single crystal structures of the free ligand **(L2)** and Ni-L complex **(1d)** were solved by direct method respectively and refined in a routine manner.

Experimental Section:

(a) Preparation of 7-bromo-3-methyl-1H-indole (1c) from 1-bromo-2-nitrobenzene (1b).[2] To a stirred solution of 1-bromo-2-nitrobenzene (**1b**) (2.02 g, 10 mmol) in dry THF (100 mL) at - 45 °C under argon atmosphere 1-propenylmagnesium bromide (**1a**), 0.5(M) in THF, (60 mL, 30 mmol) was added rapidly and stirring continued for a further 30 min. Saturated ammonium chloride solution was added to the reaction mixture (at - 45 °C) before allowing the mixture warm to room temperature. The mixture was then extracted with diethyl ether (2 × 150 mL). The combined organic layer was washed subsequently with water and brine and dried over anhydrous Na_2SO_4. Evaporation of solvent under reduced pressure gave the crude product. Purification by flash column chromatography (silica gel, 2.7% ethyl acetate/ petroleum ether) afforded 7-bromo-3-methyl-1H-indole (**1c**) as yellowish white solid. (1.26 g, 60%). **^{1}H NMR** (300 MHz, $CDCl_3$, ppm): δ 8.07(brs, 1H), 7.54(d, *J*= 7.9 Hz, 1H), 7.36(d, *J*= 7.6 Hz, 1H), 7.04-6.99(m, 2H), 2.34(s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$, ppm): δ 135.0, 129.6, 124.3, 122.3, 120.4, 118.2, 113.1, 104.7, 9.9.

(b) Typical procedure for Synthesis of Ni-L2 complex

A solution of **L2** (100.0 mg, 0.2 mmol) and $Ni(CH_3CN)_2Cl_2$ (42.3 mg, 0.2 mmol) in dichloromethane (5 mL) was stirred for 30 min at RT under argon atmosphere. After that solvent was removed under reduced pressure. The residue was rinsed with hexane and dried in vacuo, affording complex (**1d)** as an orange powder (107.0 mg, 85%) which was crystallized from DCM/CH_3CN. **^{1}H NMR** (500 MHz, CD_2Cl_2, ppm): δ 7.76(d, *J*= 8.0 Hz, 1H), 7.59(q, *J*= 7.0 Hz, 7H), 7.49-7.43(m, 4H), 7.37-7.31(m,9H), 7.23(t, *J*= 7.5 Hz, 1H), 6.82(d, *J*= 7.5 Hz, 1H), 6.42(s, 1H), 2.2(s, 3H); **^{13}C NMR** (125 MHz, CD_2Cl_2, ppm): δ 142.6, 139.8, 134.2, 133.8, 133.7, 132.9, 132.4, 131.8, 131.2, 130.2, 129.0, 128.8, 128.6, 128.6, 128.5, 128.5, 123.6, 122.1, 118.0, 9.4; **^{31}P NMR** (202.44 MHz, CD_2Cl_2, ppm): δ 60.19, 14.83 (PPh_3 as a standard); Anal. Calcd for $C_{33}H_{27}Cl_2NNiP_2$: C, 63.00; H, 4.33; N, 2.23. Found: C, 62.98; H, 4.32; N, 2.21.

^{1}H and ^{13}C NMR Spectra data for all Compounds:

4-Methoxybiphenyl (3a);[3] ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.59-7.54 (m, 4H), 7.44(t, *J*= 7.3 Hz, 2H), 7.32 (t, *J*= 7.2 Hz, 1H), 7.00(d, *J*= 8.8 Hz, 2H), 3.87 (s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$, ppm): δ 159.2, 140.9, 133.9, 128.8, 128.2, 126.8, 126.7, 114.3, 55.4.

3-Methoxybiphenyl (3b);[3] ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.63 (d, *J*= 7.2 Hz, 2H), 7.46(t, *J*= 7.5 Hz, 2H), 7.42-7.37 (m, 2H), 7.24-7.17 (m, 2H), 6.93 (dd, *J*= 1.8 Hz, *J*= 8.0 Hz, 1H), 3.89 (s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$, ppm): δ 160.1, 142.9, 141.2, 129.9, 128.8, 127.5, 127.3, 119.8, 113.0, 112.8, 55.4.

3-Methylbiphenyl (3c);[3] ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.75(d, *J*= 7.2 Hz, 2H), 7.60-7.55 (m, 4H), 7.48 (t, *J*= 7.4 Hz, 2H), 7.31 (d, *J*= 7.3 Hz, 1H), 2.57 (s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$, ppm): δ 141.4, 141.3, 138.3, 128.9, 128.8, 128.7, 128.1, 128.0, 127.3, 124.3, 21.6.

4-methoxy-4'-methylbiphenyl (3d);[4] **^{1}H NMR** (300 MHz, $CDCl_3$, ppm): δ 7.56 (d, *J*= 8.8 Hz, 2H), 7.50 (d, *J*= 8.1 Hz, 2H), 7.27 (d, *J*= 8.0 Hz, 2H), 7.01 (d, *J*= 8.8 Hz, 2H), 3.88 (s, 3H), 2.45 (s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$, ppm): δ 159.0, 138.0, 136.4, 133.8, 129.5, 128.0, 126.6, 114.2, 55.4, 21.1.

3-methoxy-3'-methylbiphenyl (3e);[5] **^{1}H NMR** (300 MHz, $CDCl_3$, ppm): δ 7.44-7.36(m, 4H), 7.23-7.16(m, 3H), 6.94(m, 1H), 3.89(s, 3H), 2.46(s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$, ppm): δ160.0, 143.0, 141.2, 138.4, 129.8, 128.7, 128.2, 128.1, 124.4, 119.8, 113.0, 112.7, 55.4, 21.6.

2-(4'-Methylphenyl)pyridine (3f);[6] **^{1}H NMR** (500 MHz, $CDCl_3$, ppm): δ 8.58(d, *J*= 3.0 Hz, 1H), 7.81(d, *J*= 8.0 Hz, 2H), 7.64-7.59 (m, 2H), 7.17 (t, *J= 8.0* Hz, 2H), 7.11-7.08 (m, 1H), 2.31(s, 3H); **^{13}C NMR** (125 MHz, $CDCl_3$, ppm): δ 157.4, 149.4, 139.1, 136.9, 136.4, 129.5, 126.8, 121.8, 120.3, 21.3.

3-(4'-Methylphenyl)pyridine (3g);[7] **^{1}H NMR** (300 MHz, $CDCl_3$, ppm): δ 8.83(d, *J*= 1.6 Hz, 1H), 8.56 (d, *J*= 3.6 Hz, 1H), 7.86-7.82 (m, 1H), 7.47 (d, *J*= 8.1 Hz, 2H), 7.35-7.26 (m, 3H), 2.39(s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$, ppm): δ 148.1, 138.1, 136.6, 134.9, 134.2, 129.8, 127.0, 123.5, 21.1.

4-Methylbiphenyl (3h);[1] **^{1}H NMR** (300 MHz, $CDCl_3$, ppm): δ 7.62(d, *J*= 7.6 Hz, 2H), 7.55-7.43 (m, 4H), 7.37(d, *J*= 7.3 Hz, 1H), 7.28(d, *J*= 7.7 Hz, 2H), 2.43(s,3H); **^{13}C NMR** (75 MHz, $CDCl_3$, ppm): δ 141.3, 138.4, 137.1, 129.6, 128.8, 127.1, 127.1, 126.9, 21.2.

4-methoxy-3'-methylbiphenyl (3i);[4] **^{1}H NMR** (300 MHz, $CDCl_3$, ppm): δ 7.53(d, *J*= 8.5 Hz, 2H), 7.38-7.32 (m, 3H), 7.13(d, *J*= 7.0 Hz, 1H), 6.98(d, *J*= 8.6 Hz, 2H), 3.85(s, 3H), 2.42(s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$, ppm): δ 159.1, 140.9, 138.3, 134.0, 128.7, 128.2, 127.6, 127.5, 123.9, 114.2, 55.4, 21.6.

1-Benzyl-4-methoxybenzene (3j);[8] **^{1}H NMR** (300 MHz, $CDCl_3$, ppm): δ 7.35-7.30(m,2H), 7.24(m, 3H), 7.15(d, *J*= 8.6 Hz, 2H), 6.88(d, *J*= 8.6 Hz, 2H), 3.97(s, 2H), 3.82(s,3H); **^{13}C NMR** (75 MHz, $CDCl_3$, ppm): δ 158.1, 141.7, 133.4, 130.0, 128.9, 128.5, 126.1, 114.0, 55.3, 41.1.

1-Methoxy-4-(4-methylbenzyl)benzene (3k);[8] **^{1}H NMR** (300 MHz, $CDCl_3$, ppm): δ 7.26(m,6H), 7.00(d, *J*= 8.6 Hz, 2H), 4.06(s, 2H), 3.93(s,3H), 2.49(s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$, ppm): δ 158.0, 138.6, 135.4, 133.6, 129.9, 129.2, 128.7, 113.9, 55.2, 40.7, 21.0.

1-isopropyl-4-(4-methoxybenzyl)benzene (3l); ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 7.04(m, 6H), 6.77(d, *J*= 6.6 Hz, 2H), 3.83(s, 2H), 3.71(s, 3H), 2.81(m, 1H), 1.17(d, *J*= 6.9 Hz, 6H); **^{13}C NMR** (75 MHz, $CDCl_3$, ppm): δ 158.1, 146.6, 139.1, 133.6, 129.9, 128.8, 126.6, 113.9, 55.3, 40.8, 33.8, 24.2.

1-(4-methoxybenzyl)naphthalene (3m);[9] **^{1}H NMR** (300 MHz, $CDCl_3$, ppm): δ 8.03(m,1H), 7.90(m,1H), 7.79(d, *J*= 8.2 Hz, 1H), 7.49(m, 3H), 7.31(d, *J*= 6.9 Hz, 1H), 7.15(d, *J*= 8.2 Hz, 2H), 6.85(d, *J*= 8.6 Hz, 2H), 4.43(s, 2H), 3.81(s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$, ppm): δ 158.1, 137.2, 134.1, 132.8, 132.2, 129.8, 128.8, 127.3, 126.0, 125.7, 124.4, 113.9, 55.3, 38.3.

1-(4-methoxybenzyl)-4-methylnaphthalene (3n); ^{1}H NMR (300 MHz, $CDCl_3$, ppm): δ 8.10(d, *J*= 8.1 Hz, 2H), 7.55(m, 2H), 7.33(d, *J*= 7.1 Hz, 1H), 7.25(d, *J*= 7.1 Hz, 1H), 7.18(d, *J*= 8.5 Hz, 2H), 6.88(d, *J*= 8.6 Hz, 2H), 4.44(s, 2H), 3.83(s, 3H), 2.76(s, 3H); **^{13}C NMR** (75 MHz, $CDCl_3$, ppm): δ 158.0, 135.3, 133.2, 133.1, 132.3, 129.7, 127.0, 126.4, 125.7, 125.5, 125.0, 124.9, 113.9, 55.3, 38.3, 19.6.

Crystallographic information:

X-ray crystal structure of ligand (Fig.A):

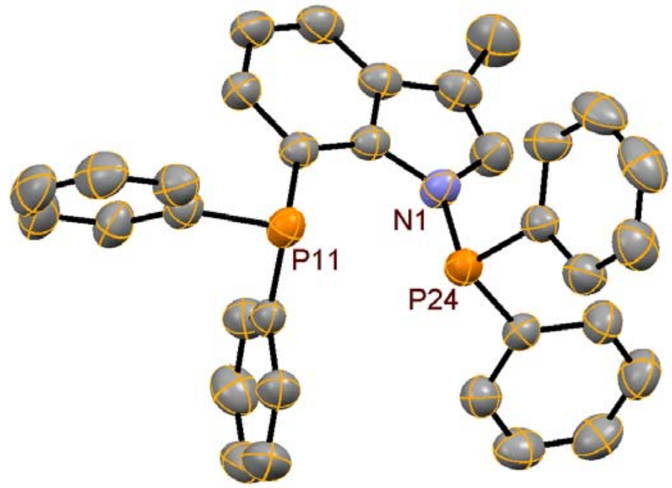

Figure A: Thermal ellipsoid plot of free ligand drawn at 50 % probability level

X-ray crystal structure of Ni-L2 complex (Fig.B):

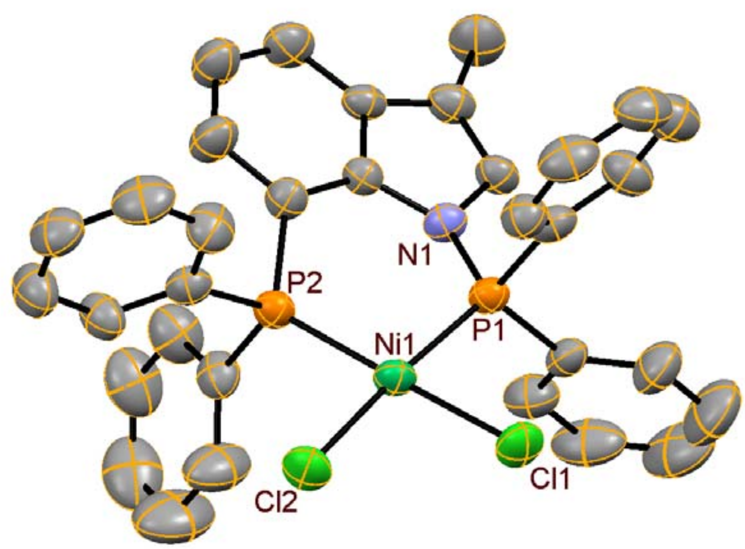

Figure B: Thermal ellipsoid plot of Ni-L2 complex drawn at 50 % probability level

Crystal data of **Ligand**: $C_{33}H_{27}NP_2$, M = 499.50, monoclinic, $P2_1/c$, a = 9.4292(10), b = 14.3380(15), c = 19.960(2)Å. ß = 91.711(3). V = 2697.3(5) Å3, T = 298 K, Z = 4. F (000) = 1048, λ (Mo–Kα) = 0.71073 Å, μ = 0.183 mm^{-1}, $2\theta_{max}$ = 46.16°, 3784 reflections measured, 2978 observed (I>2σ (I)) 326 parameters; R_{int} = 0.047, R_1 = 0.0359; wR_2 = 0.0844 [(I>2σ (I)], R_1 = 0.0508; wR_2 = 0.0910 (all data) with GOF = 1.033; **Ni complex**: $C_{33}H_{27}Cl_2NP_2Ni$, FW = 629.11, monoclinic, $P2_1$, a = 9.9428(16), b = 15.399(2), c = 9.9985(17) Å. ß = 109.144(4). V = 1446.3(4) Å3, T = 298 K, Z = 2. F (000) = 648, λ (Mo–Kα) = 0.71073 Å, μ = 0.990 mm-1, $2\theta_{max}$ = 50.0°, 5106 reflections measured, 4528 observed [(I>2σ (I)] 356 parameters; R_1 = 0.0379; wR_2 = 0.0843 (I>2σ (I)), R_1 = 0.0454; wR_2 = 0.0881 (all data) with GOF = 1.055

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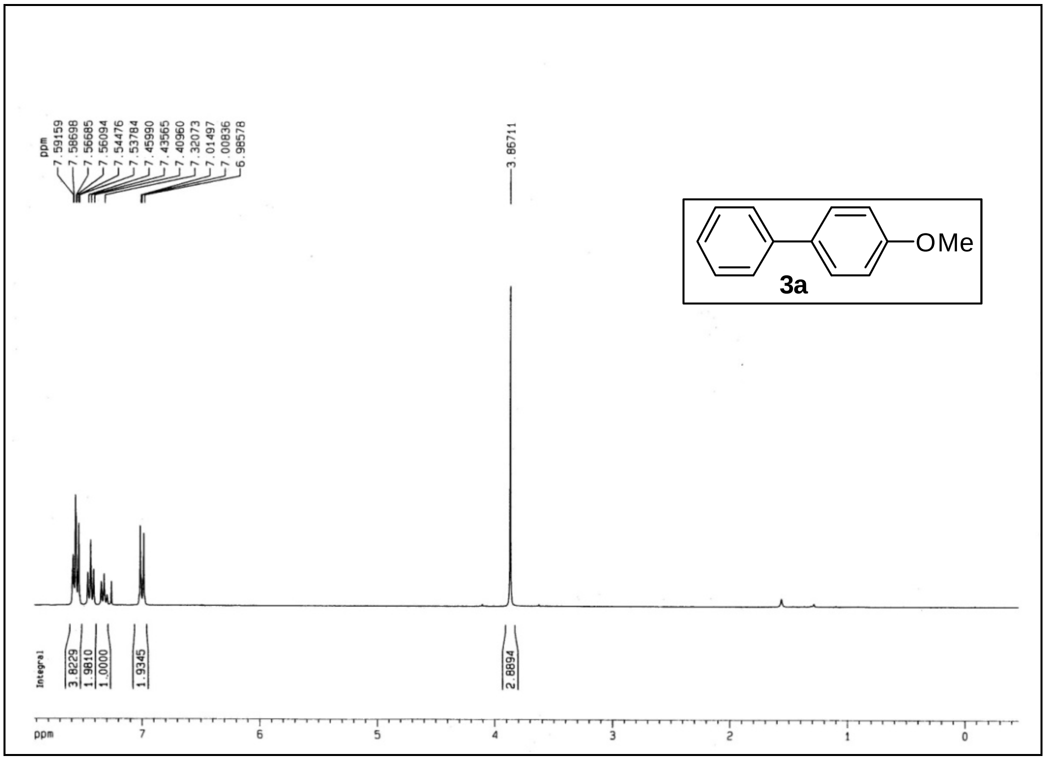

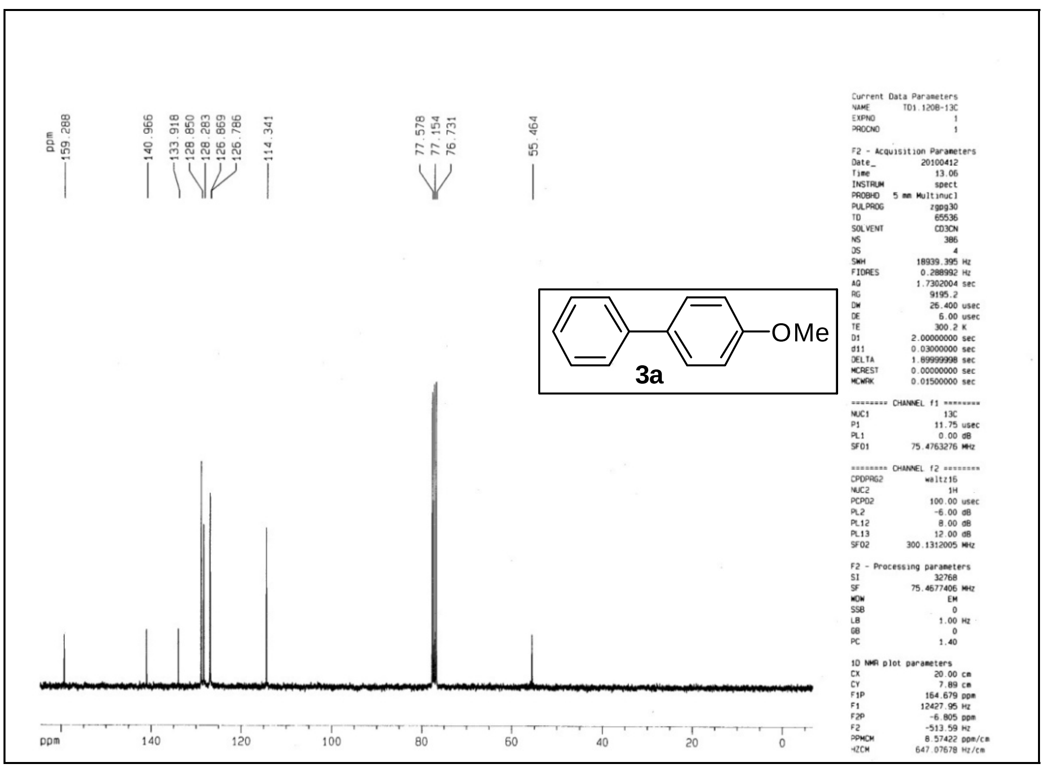

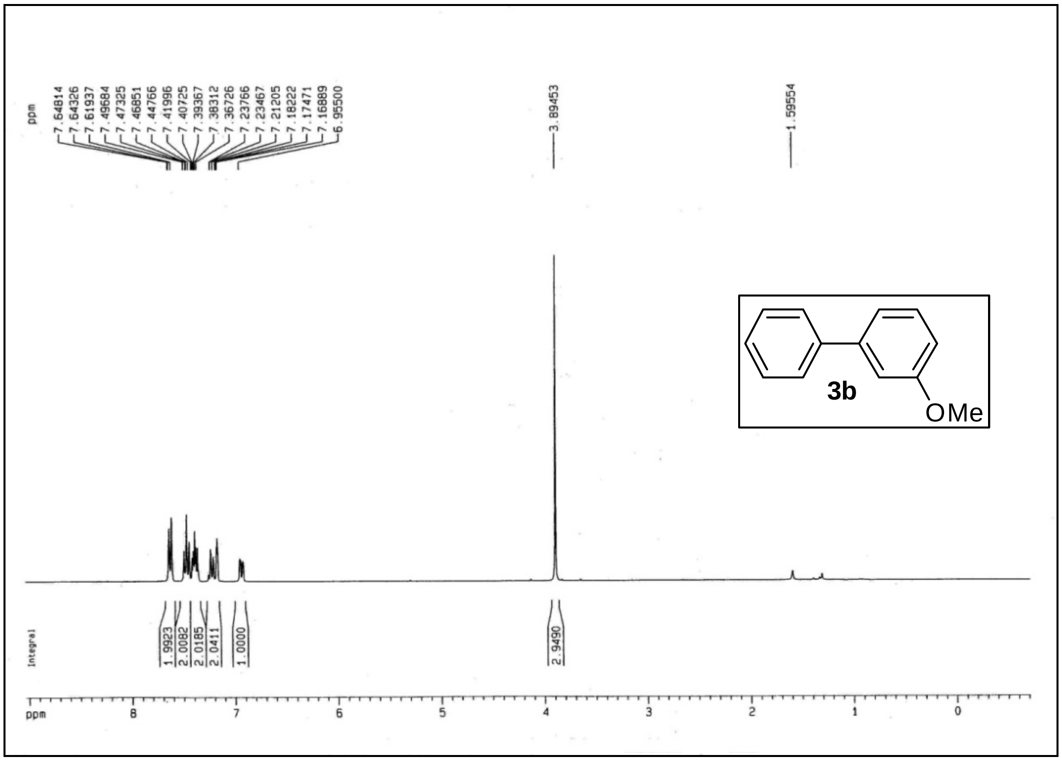

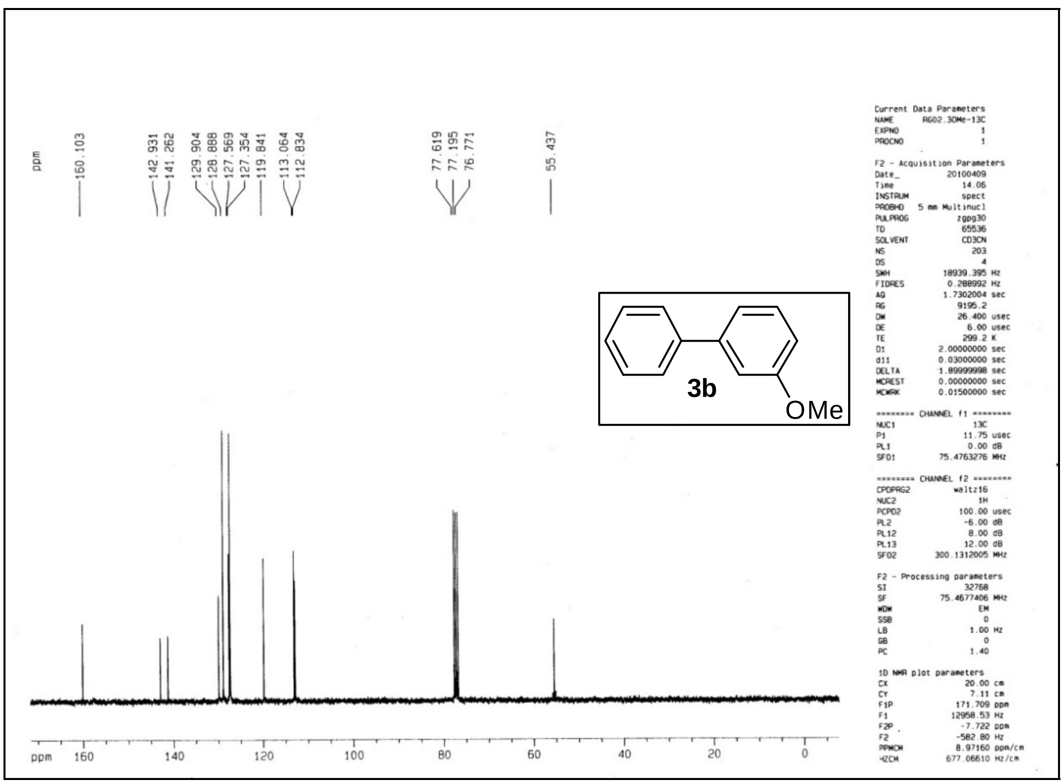

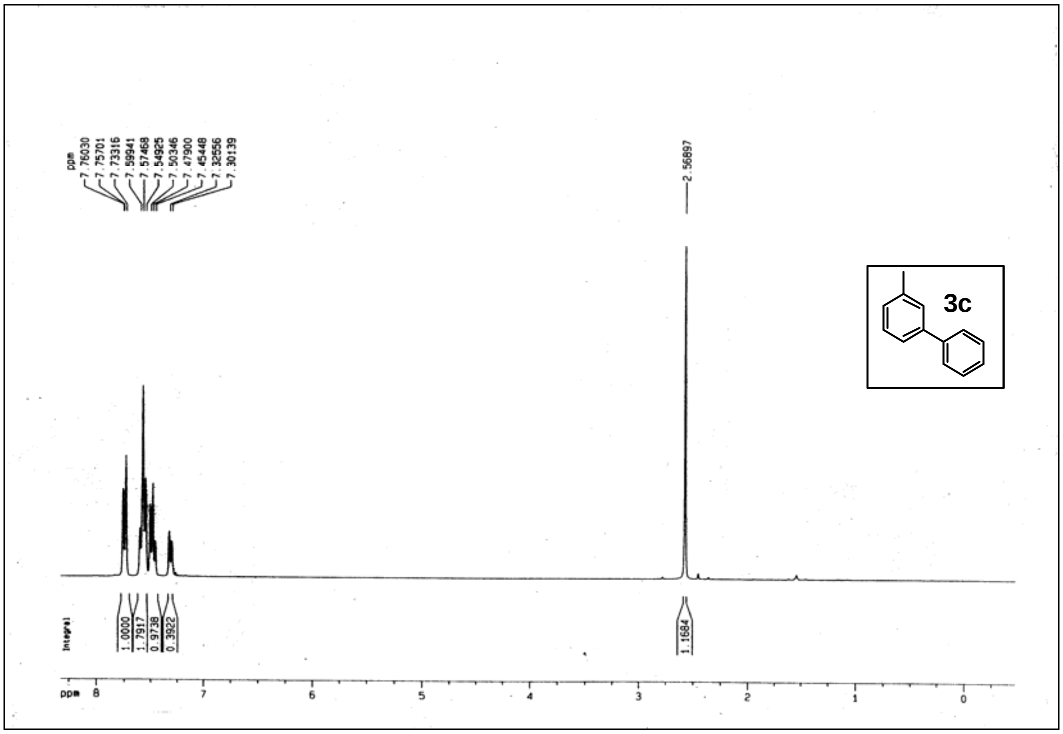
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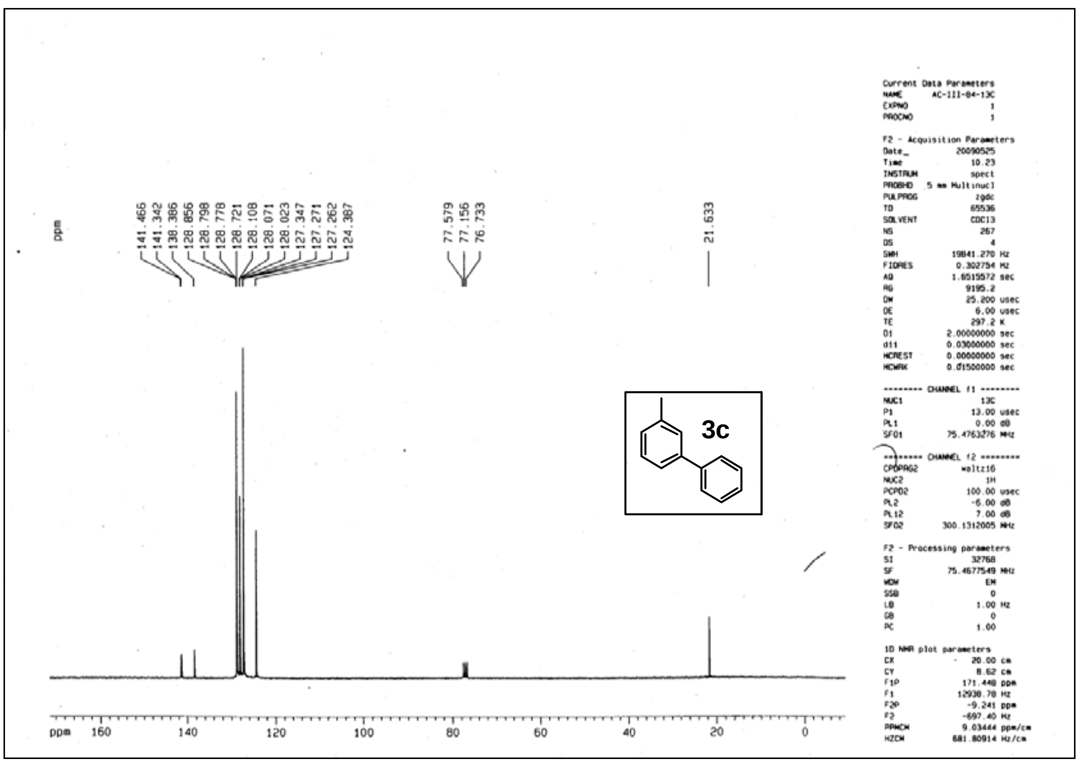
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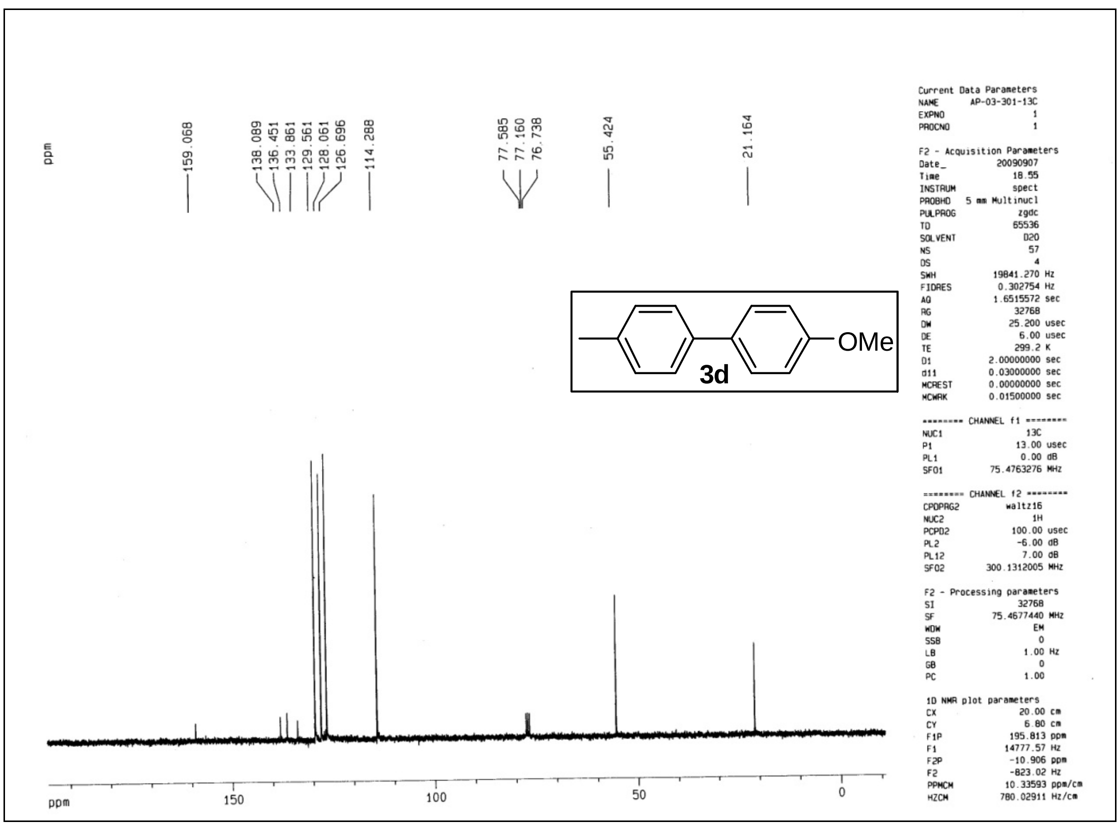
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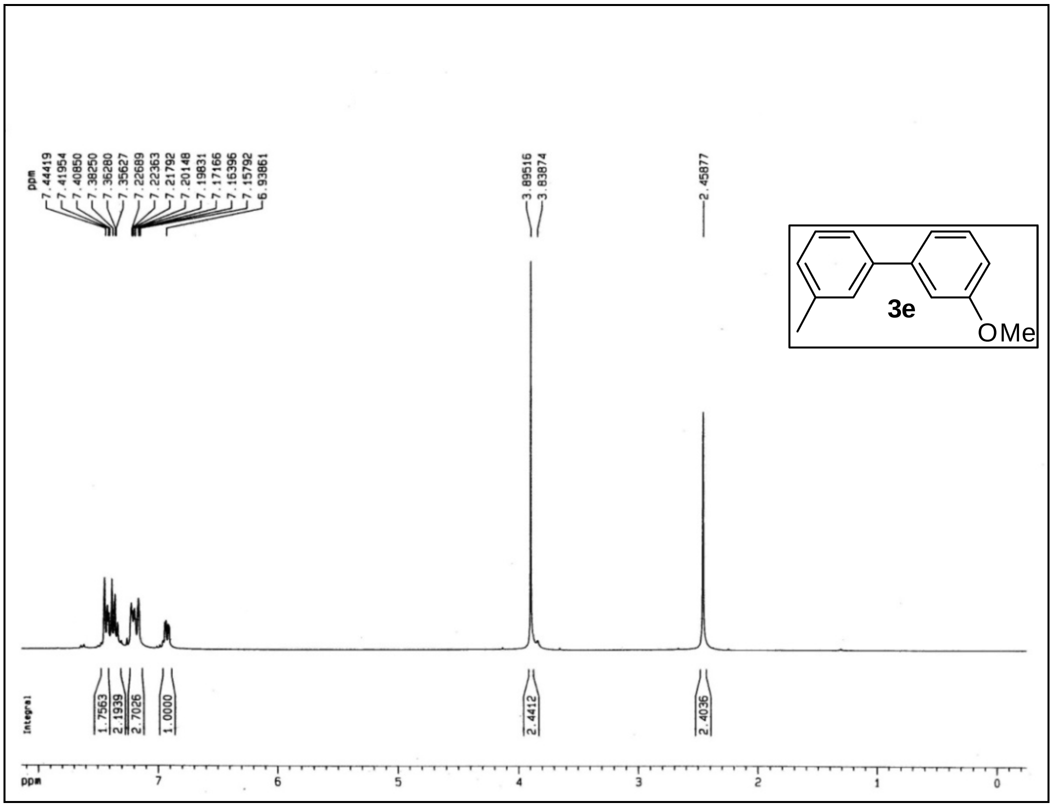
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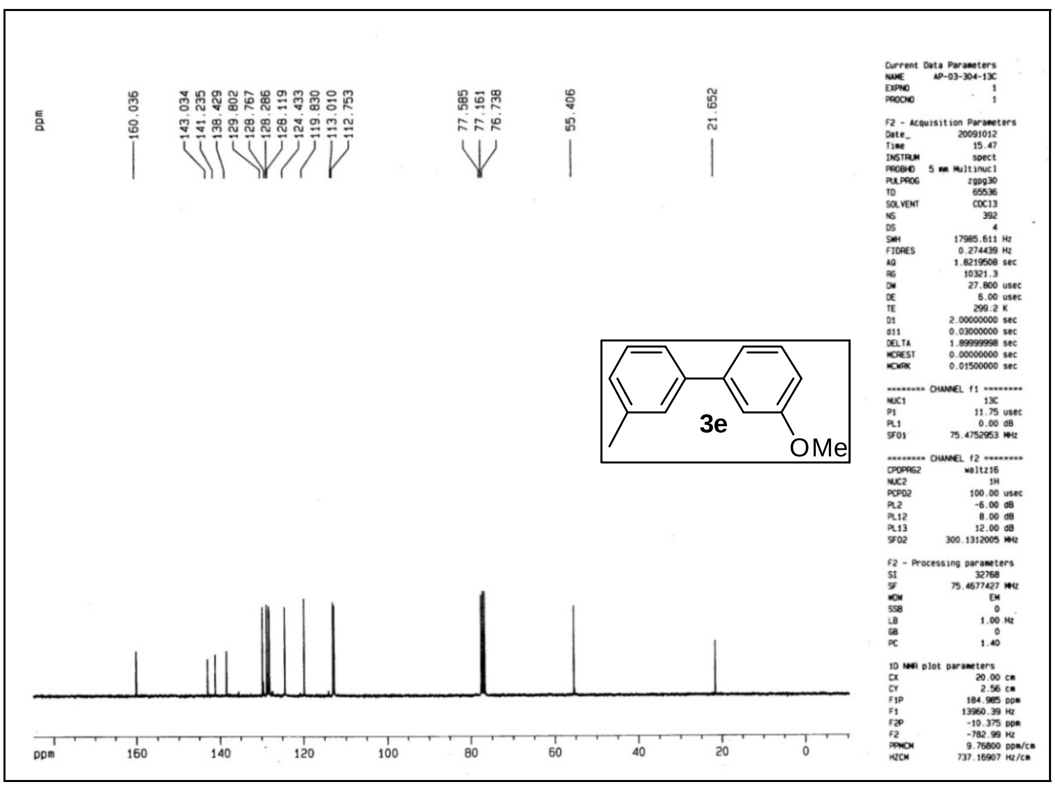
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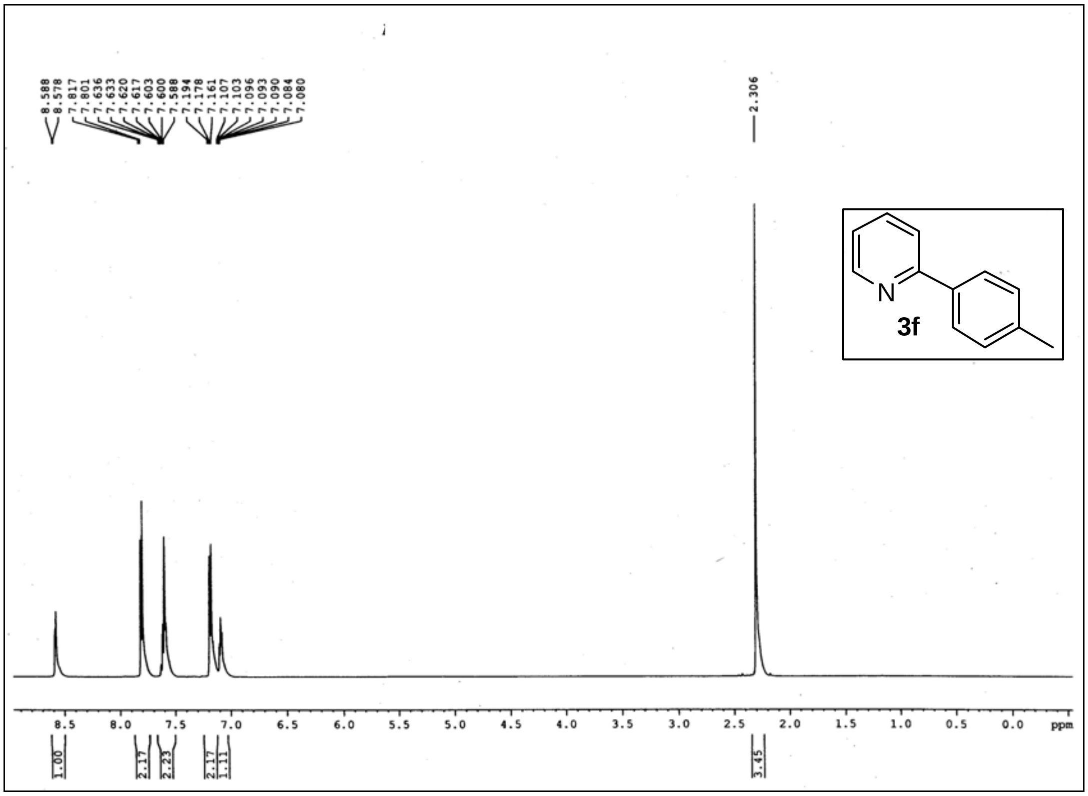
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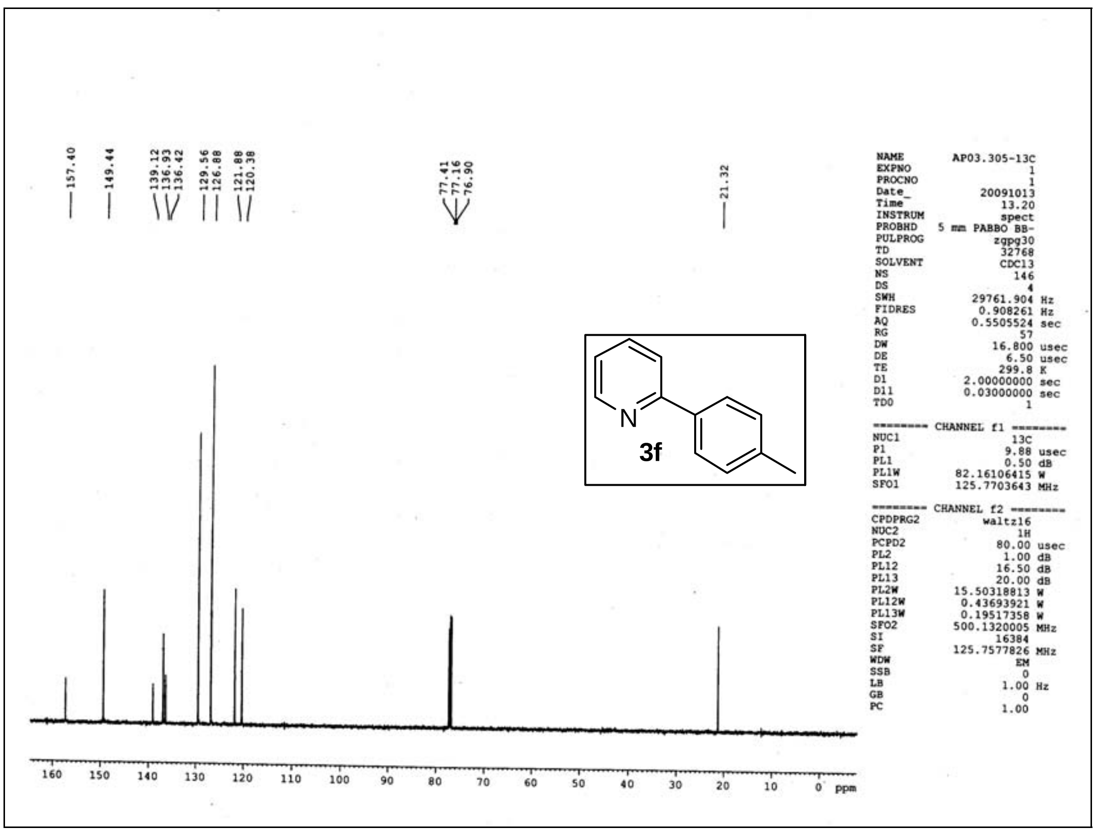
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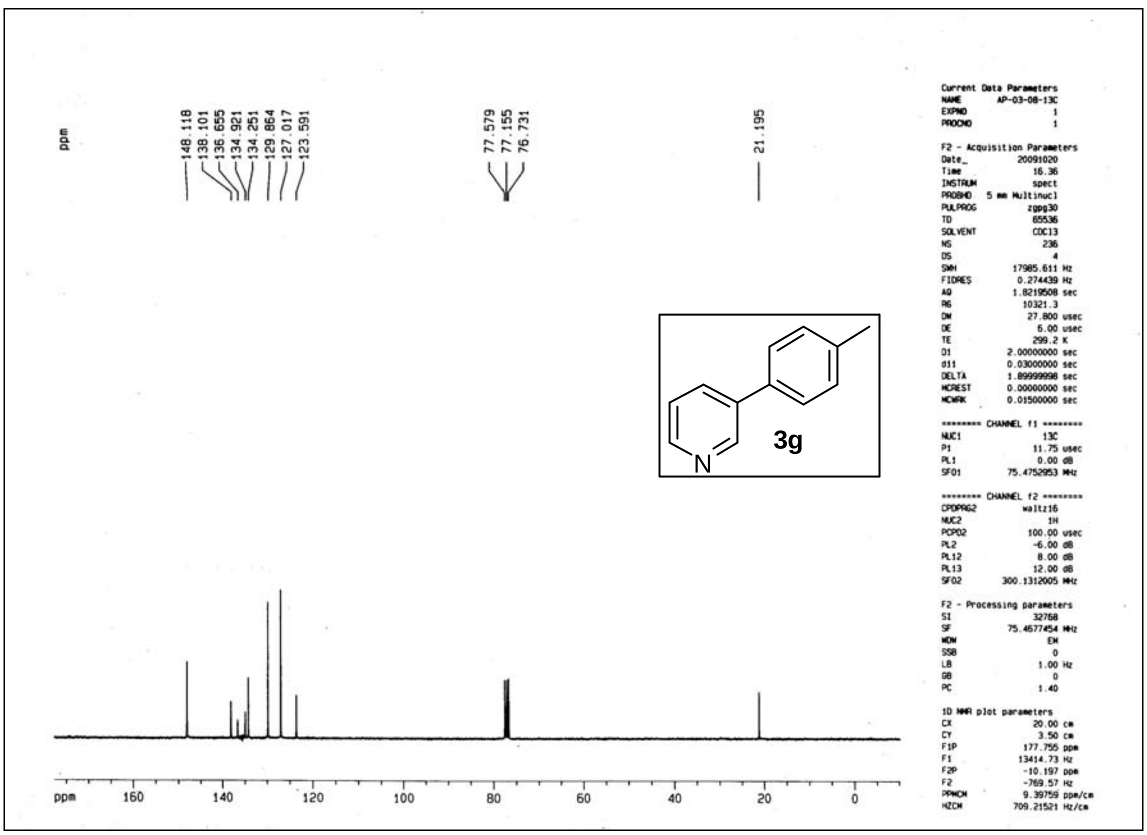

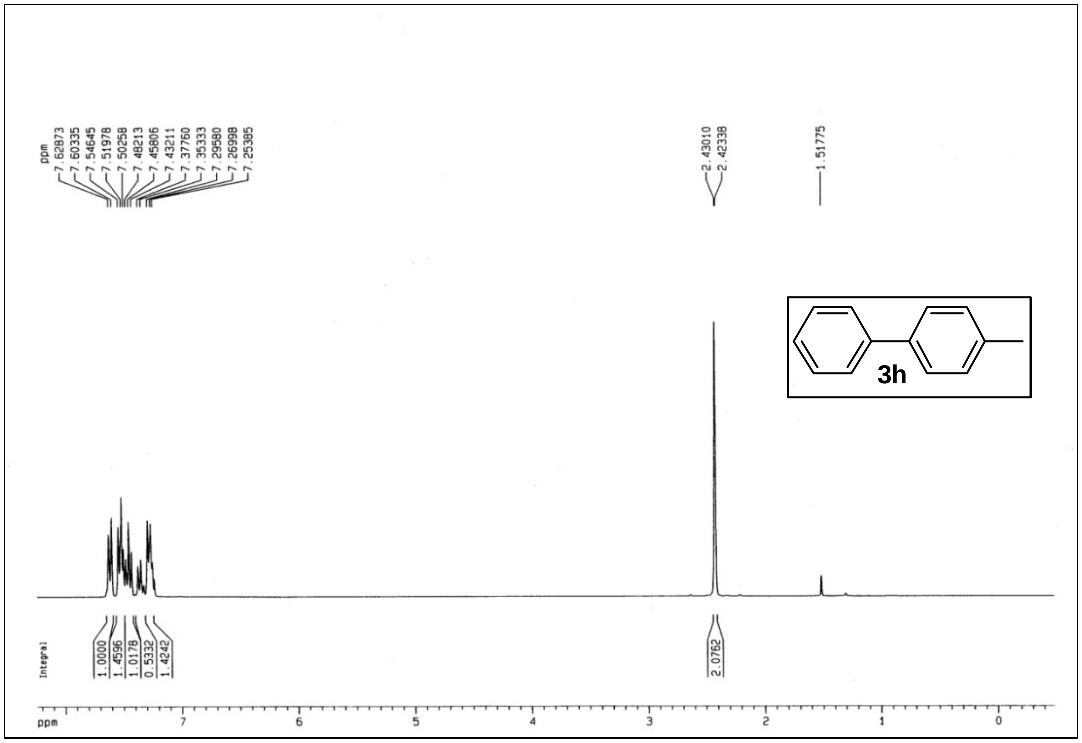

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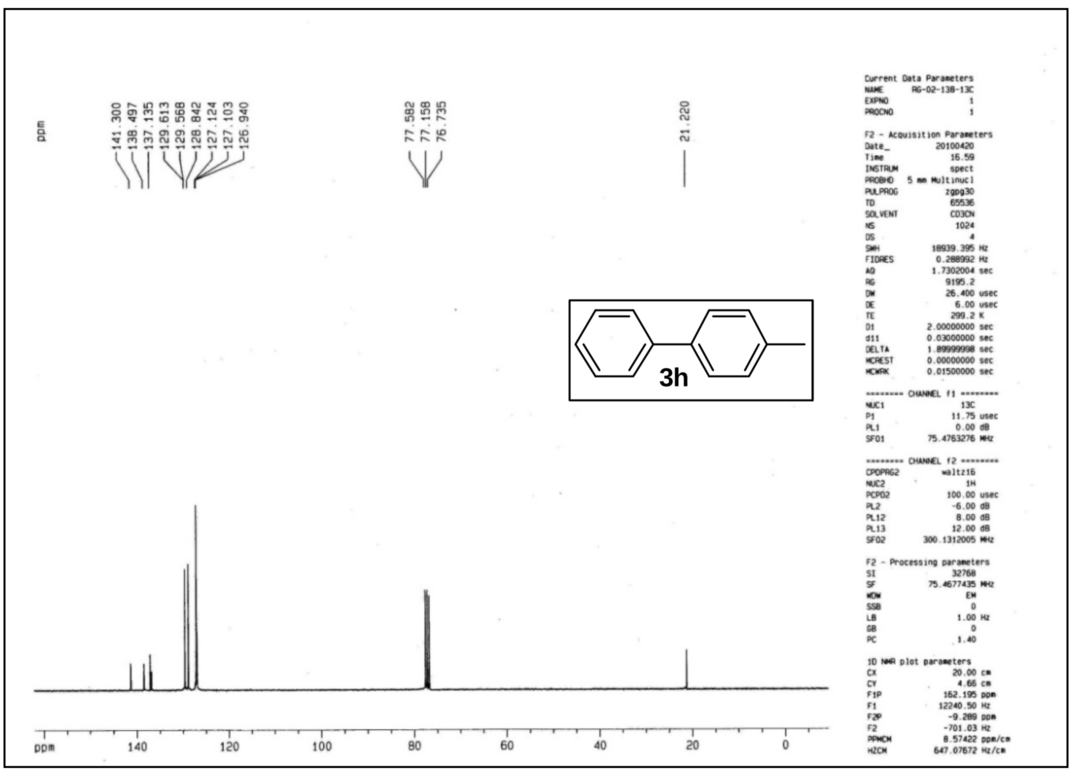
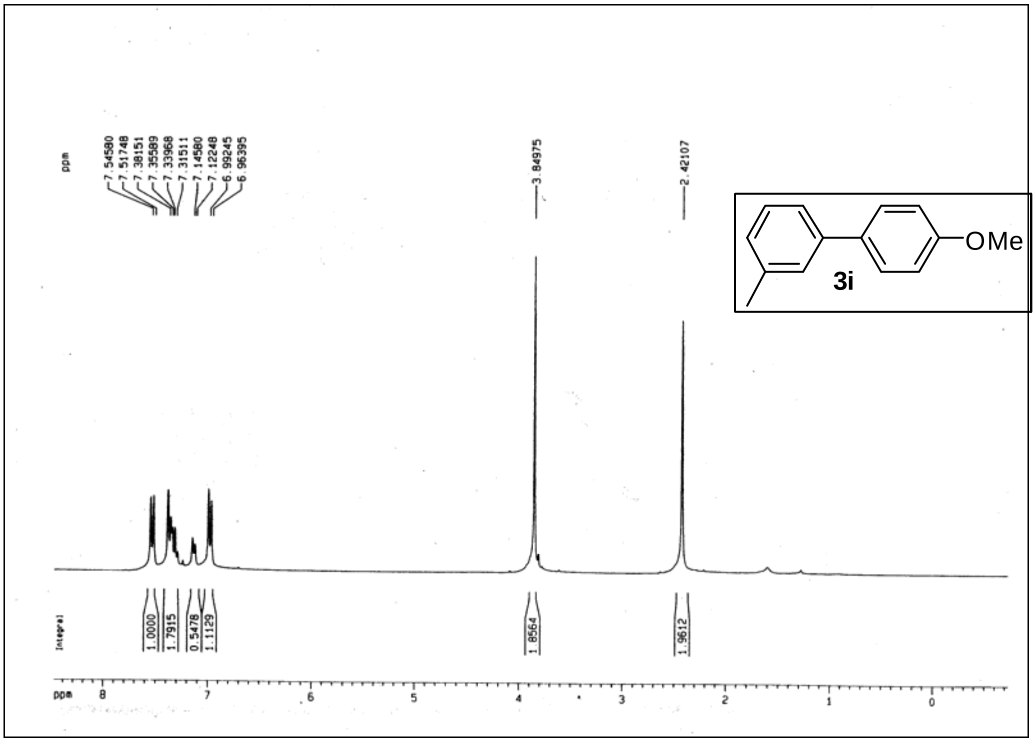
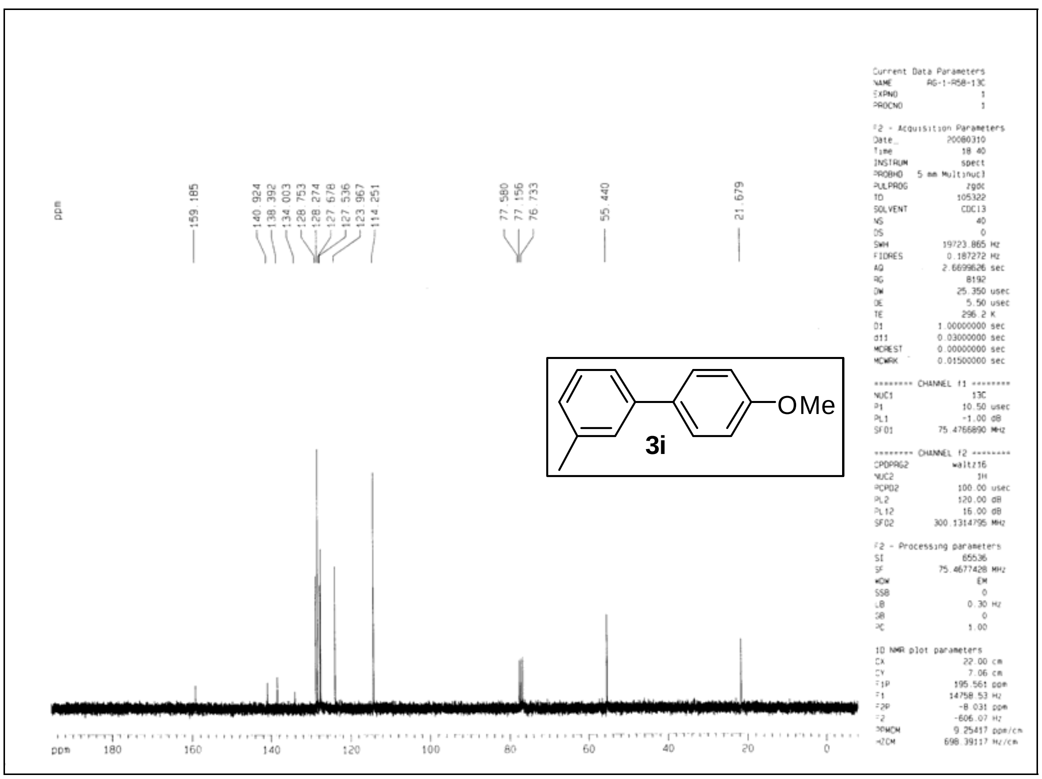


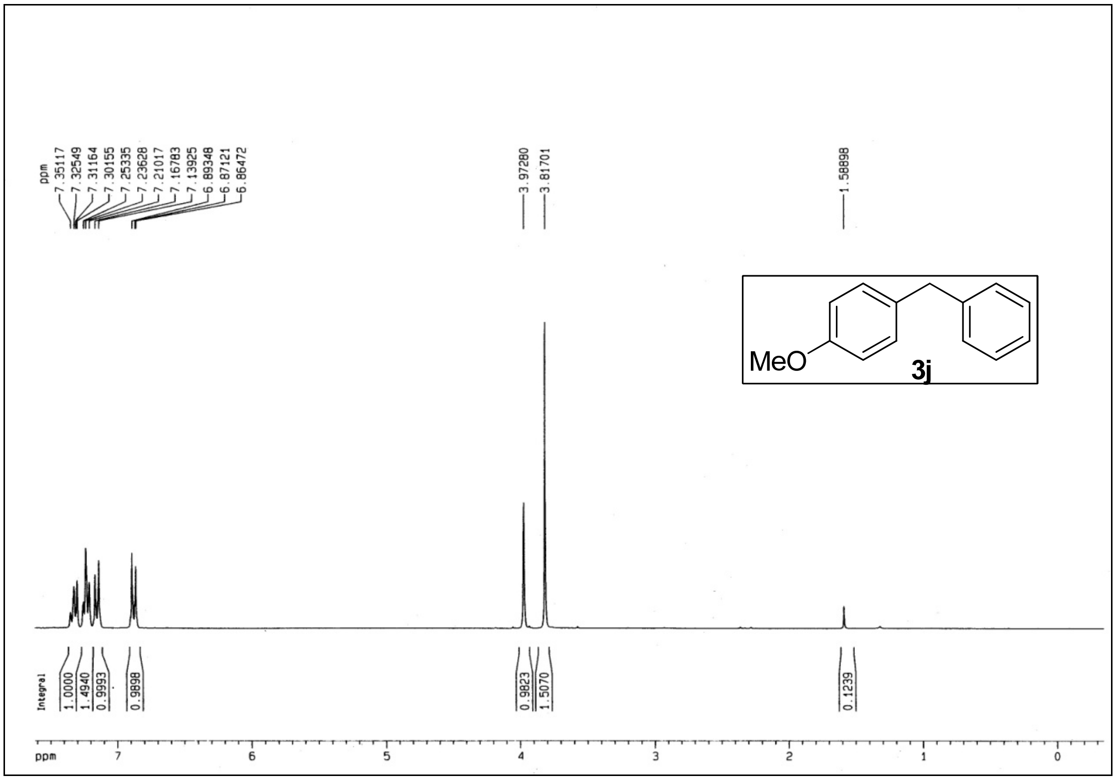
ppm
141.300
138.497
137.135
129.613
129.568
128.842
127.124
127.103
126.940
77.582
77.158
76.735
21.220
3h
Current Data Parameters
NAME RG-02-138-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100420
Time 16.59
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CD3CN
NS 1024
DS 4
SWH 18939.395 Hz
FIDRES 0.288992 Hz
AQ 1.7302004 sec
RG 9195.2
DW 26.400 usec
DE 6.00 usec
TE 299.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 11.75 usec
PL1 0.00 dB
SFO1 75.4763276 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 8.00 dB
PL13 12.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677435 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 4.66 cm
F1P 162.195 ppm
F1 12240.50 Hz
F2P -9.289 ppm
F2 -701.03 Hz
PPMCM 8.57422 ppm/cm
HZCM 647.07672 Hz/cm

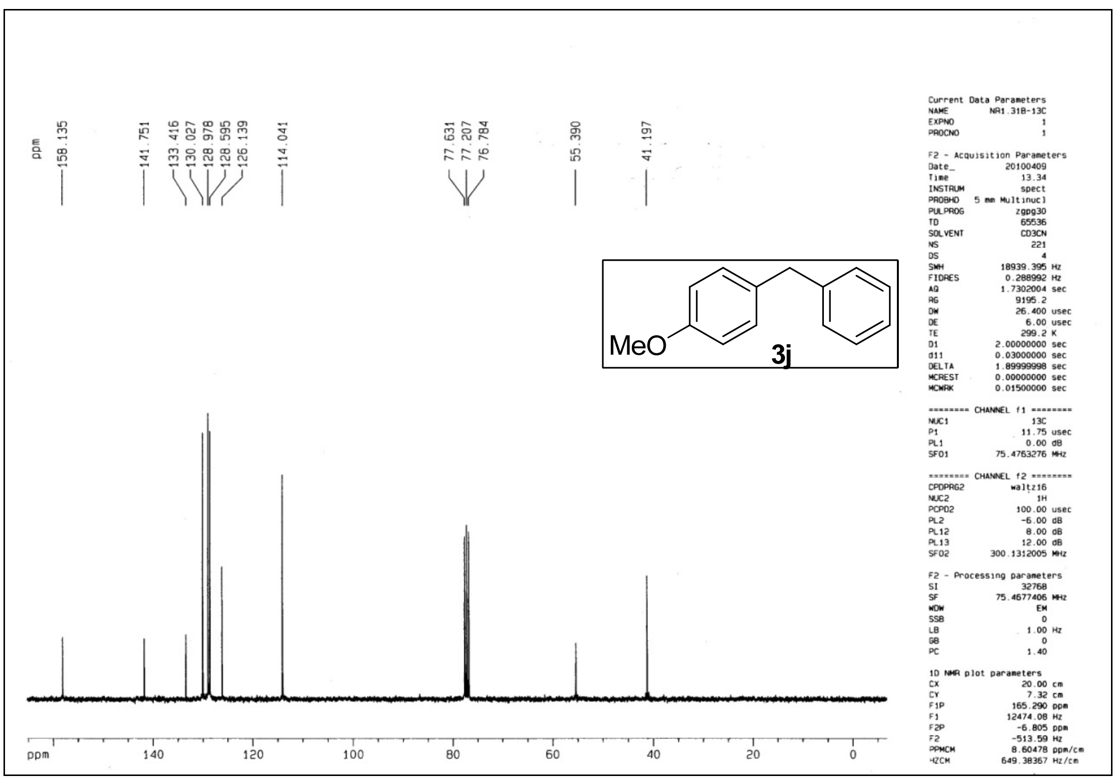


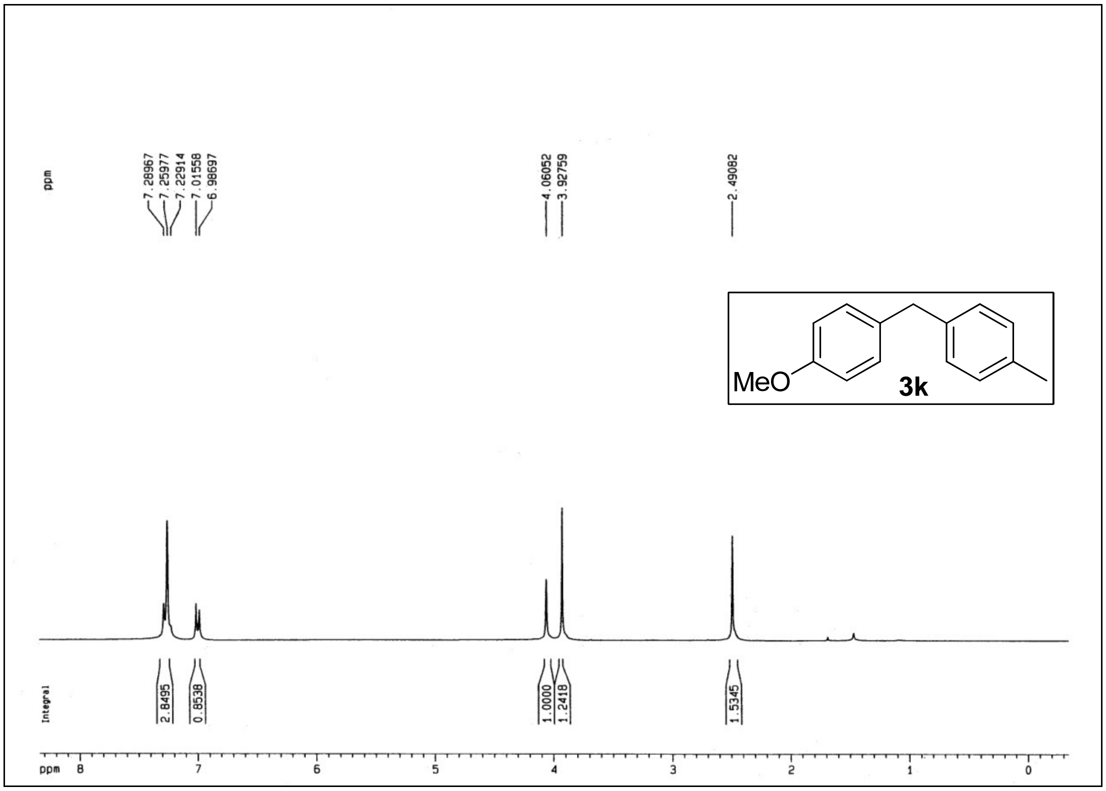
ppm
7.54580
7.51748
7.38151
7.35589
7.33968
7.31511
7.14580
7.12248
6.99245
6.96395
3.84975
2.42107
OMe
3i
Integral
1.0000
1.7915
0.5478
1.1129
1.8564
1.9612
ppm 8 7 6 5 4 3 2 1 0

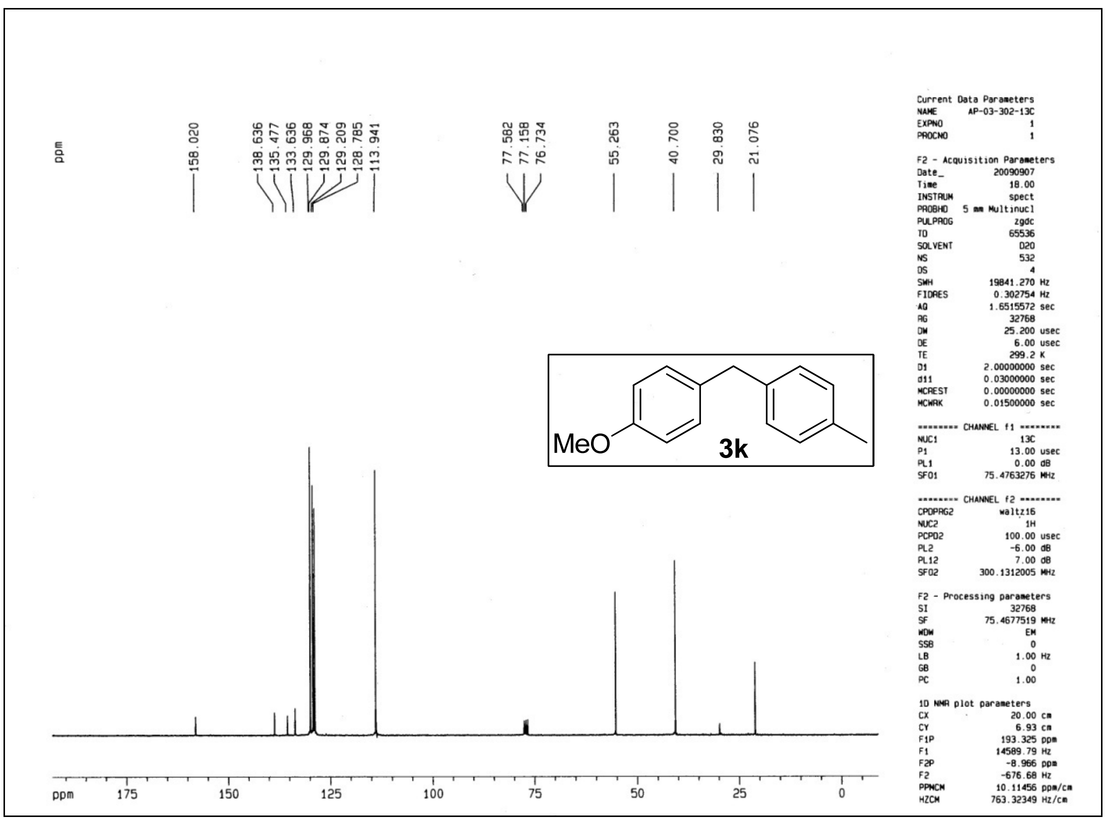


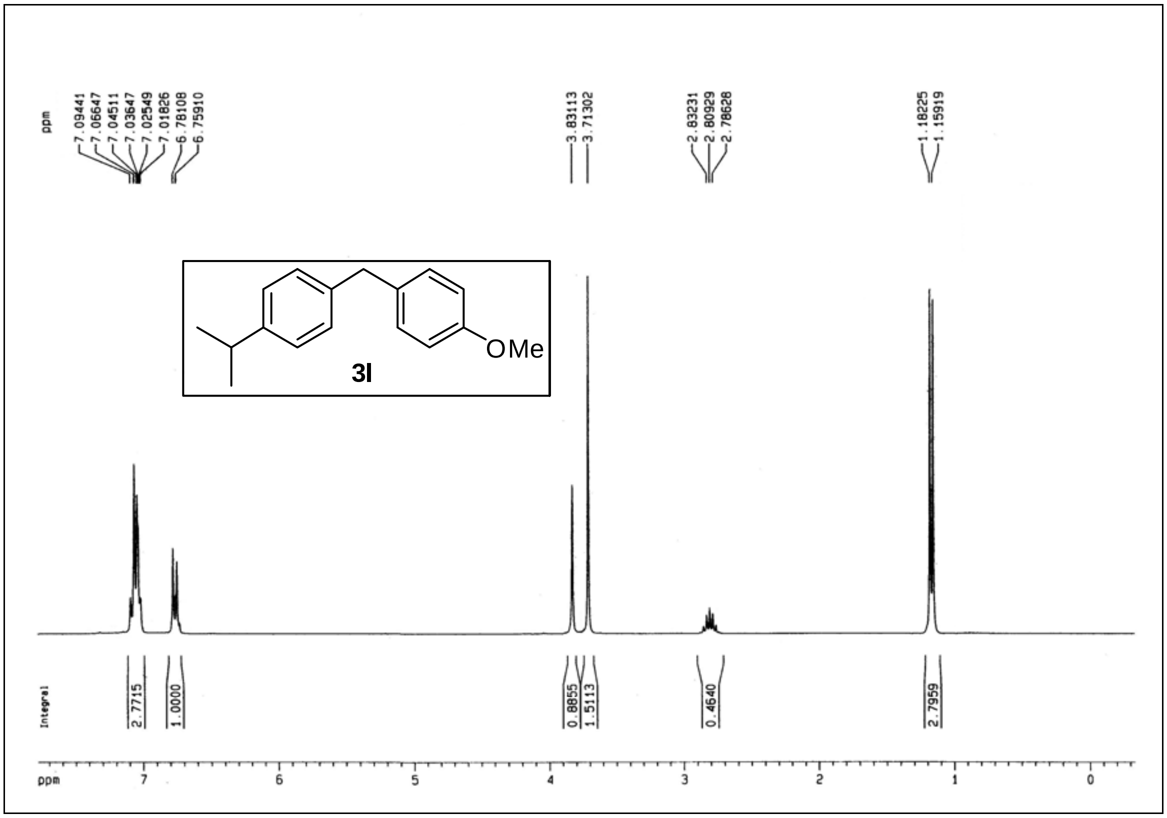
ppm
159.185
140.924
138.392
134.003
128.753
128.274
127.678
127.536
123.967
114.251
77.580
77.156
76.733
55.440
21.679
OMe
3i
ppm 180 160 140 120 100 80 60 40 20 0

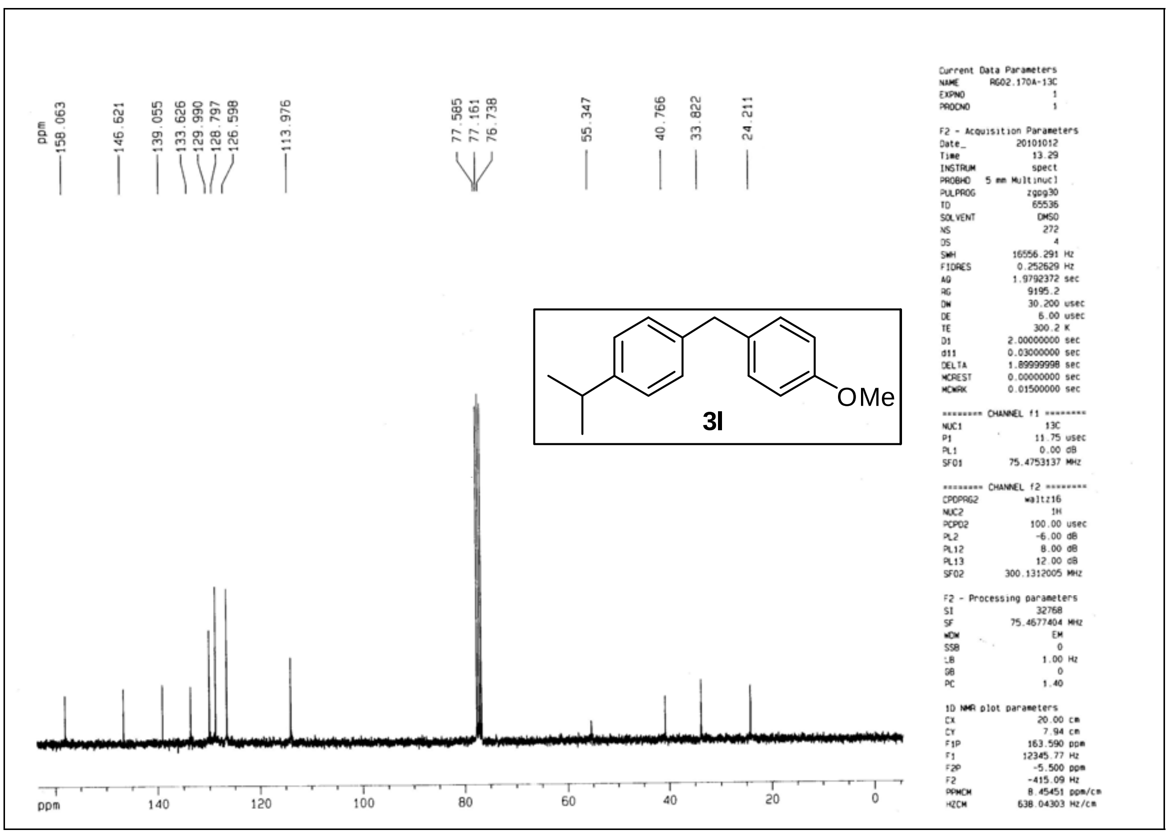

ppm
7.35117
7.32549
7.31164
7.30155
7.25335
7.23628
7.21017
7.16783
7.13925
6.89348
6.87121
6.86472
3.97280
3.81701
1.58898
MeO
3j
Integral
1.0000
1.4940
0.9993
0.9898
0.9823
1.5070
0.1239
ppm
7
6
5
4
3
2
1
0

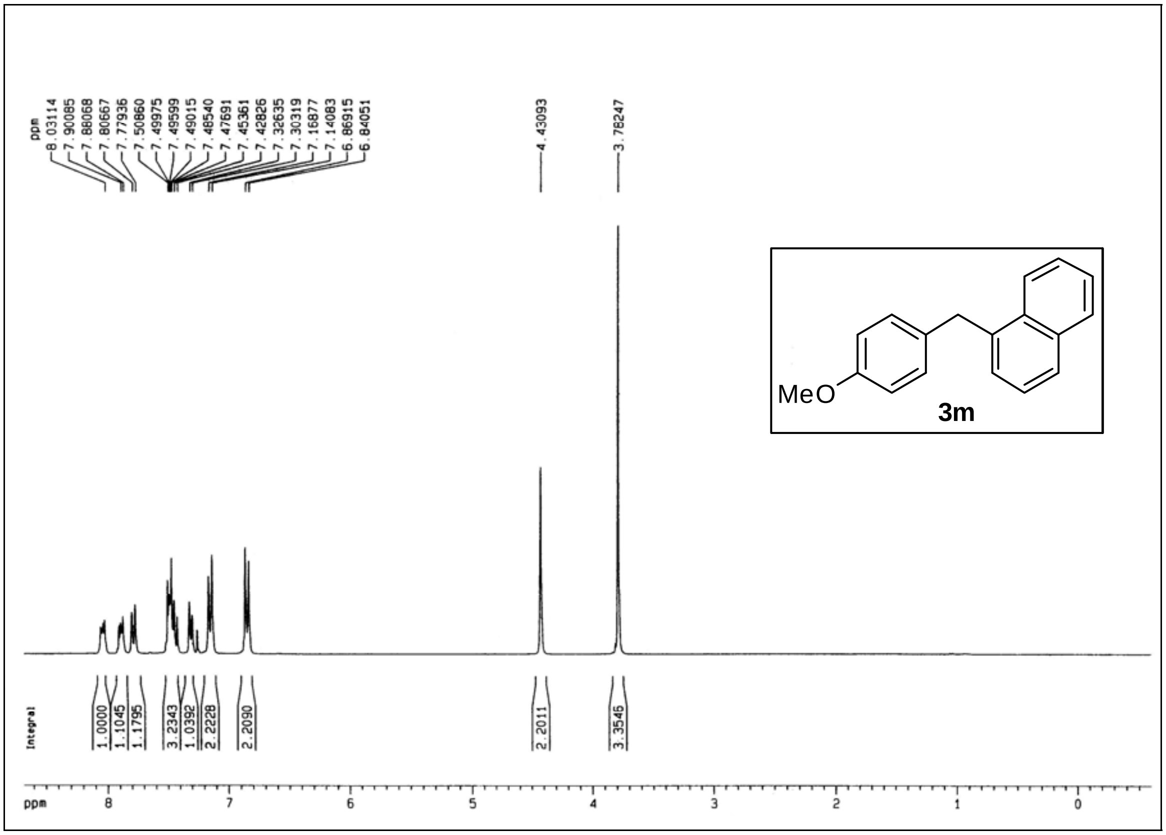

ppm
158.135
141.751
133.416
130.027
128.978
128.595
126.139
114.041
77.631
77.207
76.784
55.390
41.197
MeO
3j
Current Data Parameters
NAME NR1.31B-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100409
Time 13.34
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CD3CN
NS 221
DS 4
SWH 18939.395 Hz
FIDRES 0.288992 Hz
AQ 1.7302004 sec
RG 9195.2
DW 26.400 usec
DE 6.00 usec
TE 299.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 11.75 usec
PL1 0.00 dB
SFO1 75.4763276 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 8.00 dB
PL13 12.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677406 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 7.32 cm
F1P 165.290 ppm
F1 12474.08 Hz
F2P -6.805 ppm
F2 -513.59 Hz
PPMCM 8.60478 ppm/cm
HZCM 649.38367 Hz/cm
ppm
140
120
100
80
60
40
20
0


ppm
7.28967
7.25977
7.22914
7.01558
6.98697
4.06052
3.92759
2.49082
MeO
3k
Integral
2.8495
0.8538
1.0000
1.2418
1.5345
ppm 8 7 6 5 4 3 2 1 0

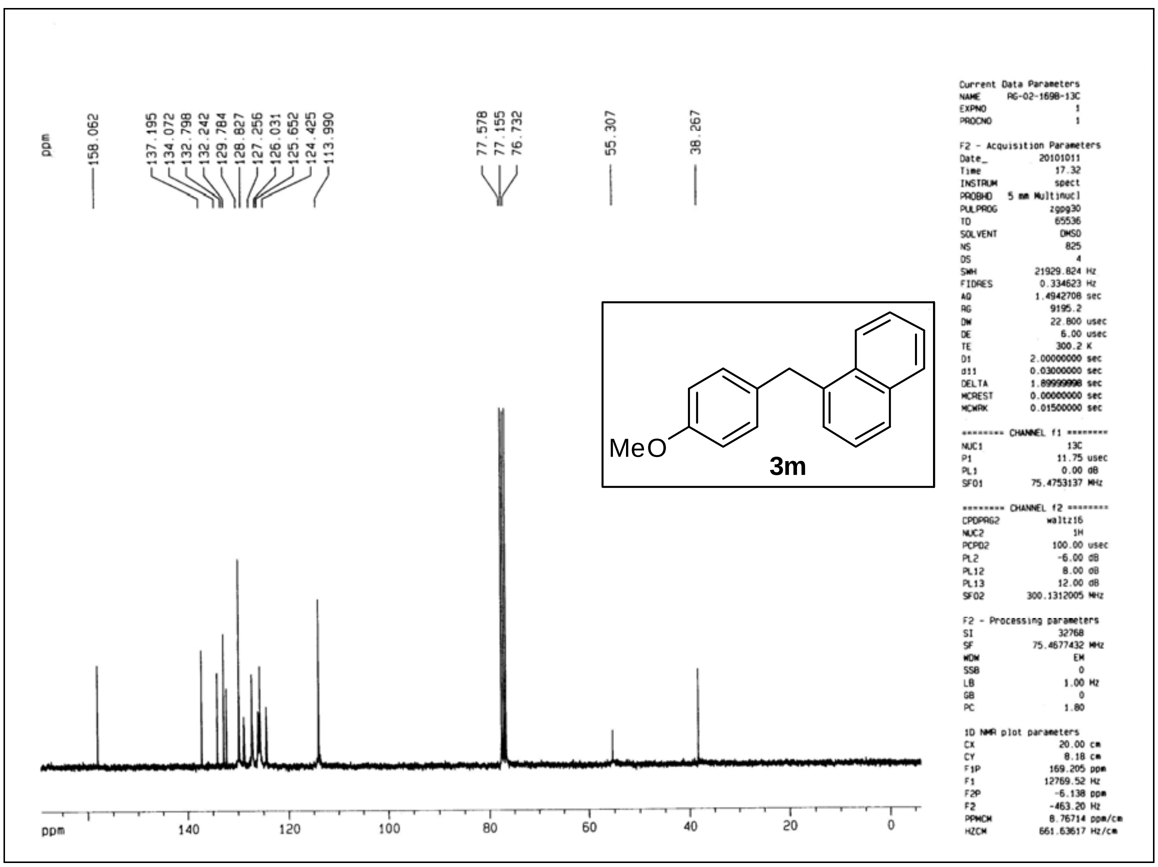

ppm
158.020
138.636
135.477
133.636
129.968
129.874
129.209
128.785
113.941
77.582
77.158
76.734
55.263
40.700
29.830
21.076
MeO
3k
ppm 175 150 125 100 75 50 25 0
Current Data Parameters
NAME AP-03-302-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090907
Time 18.00
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgdc
TD 65536
SOLVENT D20
NS 532
DS 4
SWH 19841.270 Hz
FIDRES 0.302754 Hz
AQ 1.6515572 sec
RG 32768
DW 25.200 usec
DE 6.00 usec
TE 299.2 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 13.00 usec
PL1 0.00 dB
SFO1 75.4763276 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 7.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677519 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 6.93 cm
F1P 193.325 ppm
F1 14589.79 Hz
F2P -8.966 ppm
F2 -676.68 Hz
PPMCM 10.11456 ppm/cm
HZCM 763.32349 Hz/cm


ppm
7.09441
7.06647
7.04511
7.03647
7.02549
7.01826
6.78108
6.75910
3.83113
3.71302
2.83231
2.80929
2.78628
1.18225
1.15919
OMe
3l
Integral
2.7715
1.0000
0.8855
1.5113
0.4640
2.7959
ppm
7
6
5
4
3
2
1
0

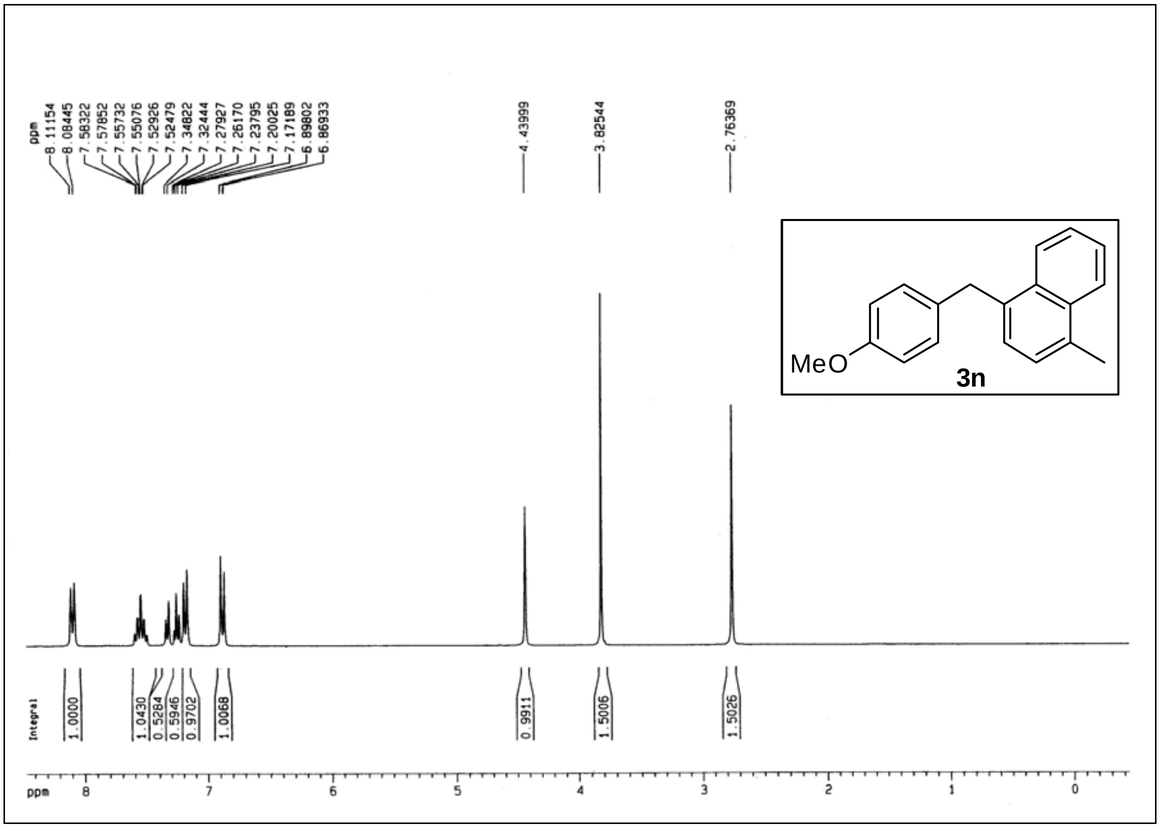

ppm
158.063
146.621
139.055
133.626
129.990
128.797
126.598
113.976
77.585
77.161
76.738
55.347
40.766
33.822
24.211
OMe
3l
ppm
140
120
100
80
60
40
20
0
Current Data Parameters
NAME RG02.170A-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101012
Time 13.29
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 272
DS 4
SWH 16556.291 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 9195.2
DW 30.200 usec
DE 6.00 usec
TE 300.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 11.75 usec
PL1 0.00 dB
SFO1 75.4753137 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 8.00 dB
PL13 12.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677404 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 7.94 cm
F1P 163.590 ppm
F1 12345.77 Hz
F2P -5.500 ppm
F2 -415.09 Hz
PPMCM 8.45451 ppm/cm
HZCM 638.04303 Hz/cm

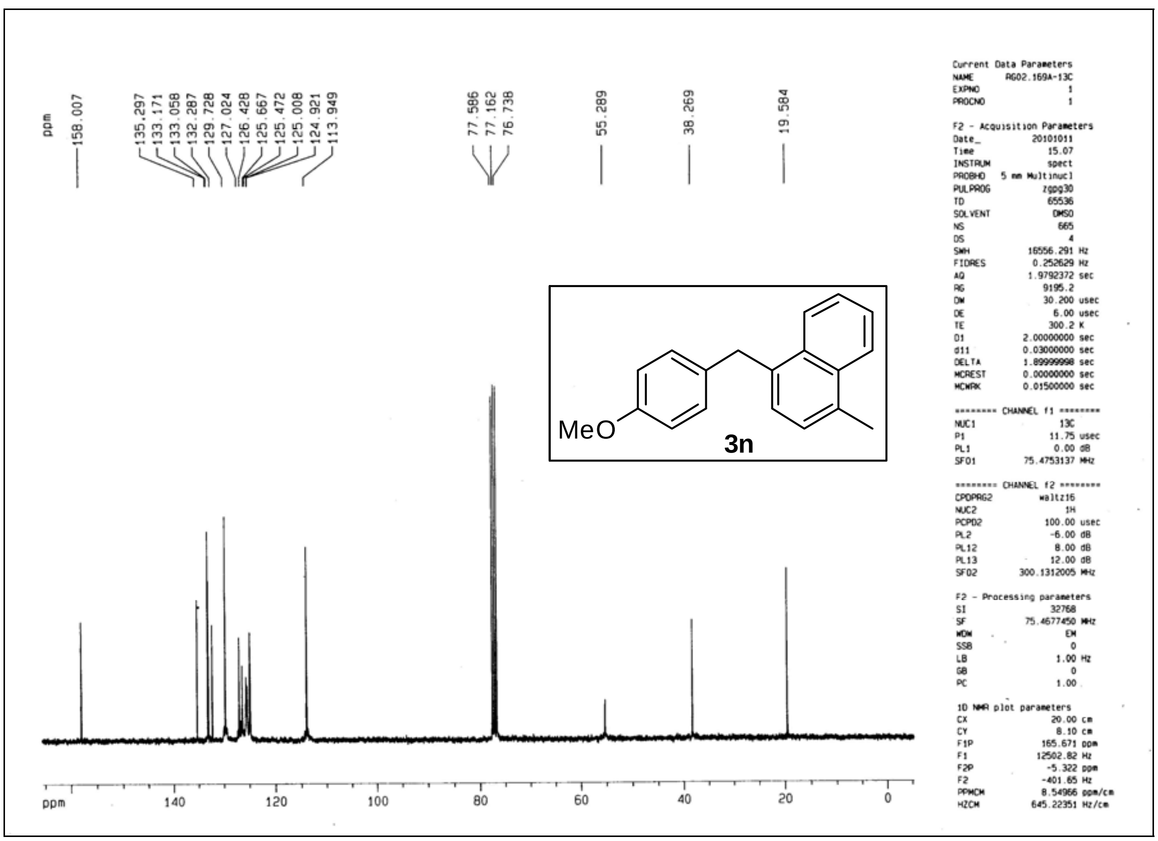


ppm
8.03114
7.90085
7.88068
7.80667
7.77936
7.50860
7.49975
7.49599
7.49015
7.48540
7.47691
7.45361
7.42826
7.32635
7.30319
7.16877
7.14083
6.86915
6.84051
4.43093
3.78247
MeO
3m
Integral
1.0000
1.1045
1.1795
3.2343
1.0392
2.2228
2.2090
2.2011
3.3545
ppm
8
7
6
5
4
3
2
1
0

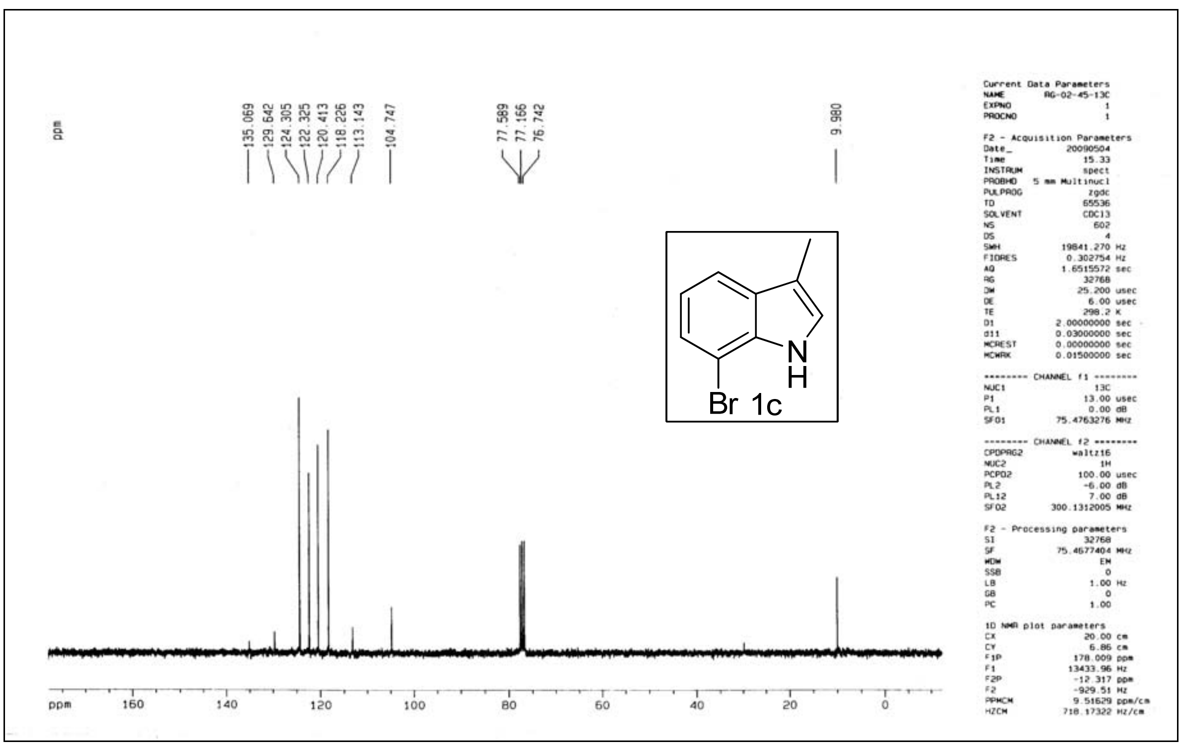


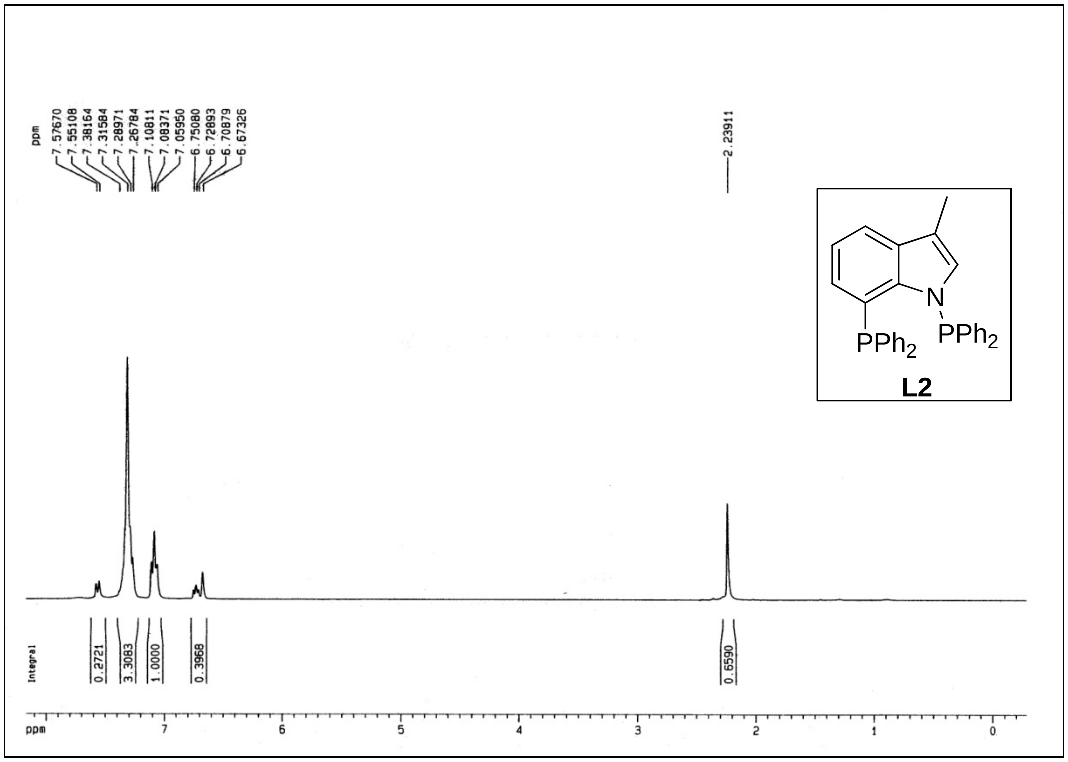
ppm
158.062
137.195
134.072
132.798
132.242
129.784
128.827
127.256
126.031
125.652
124.425
113.990
77.578
77.155
76.732
55.307
38.267
MeO
3m
Current Data Parameters
NAME RG-02-169B-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101011
Time 17.32
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 825
DS 4
SWH 21929.824 Hz
FIDRES 0.334623 Hz
AQ 1.4942708 sec
RG 9195.2
DW 22.800 usec
DE 6.00 usec
TE 300.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 11.75 usec
PL1 0.00 dB
SFO1 75.4753137 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 8.00 dB
PL13 12.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677432 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.80
1D NMR plot parameters
CX 20.00 cm
CY 8.18 cm
F1P 169.205 ppm
F1 12769.52 Hz
F2P -6.138 ppm
F2 -463.20 Hz
PPMCM 8.76714 ppm/cm
HZCM 661.63617 Hz/cm
ppm
140
120
100
80
60
40
20
0

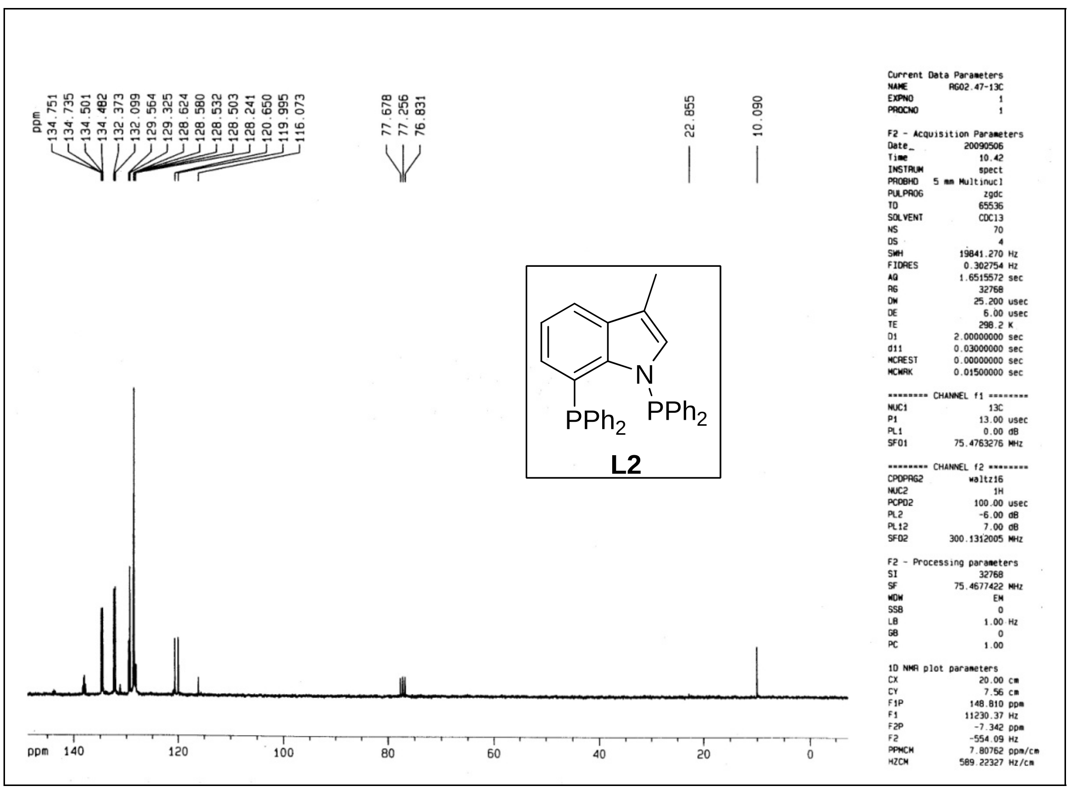

ppm
8.11154
8.08445
7.58322
7.57852
7.55732
7.55076
7.52926
7.52479
7.34822
7.32444
7.27927
7.26170
7.23795
7.20025
7.17189
6.89802
6.86933
4.43999
3.82544
2.76369
MeO
3n
Integral
1.0000
1.0430
0.5284
0.5946
0.9702
1.0068
0.9911
1.5006
1.5026
ppm
8
7
6
5
4
3
2
1
0

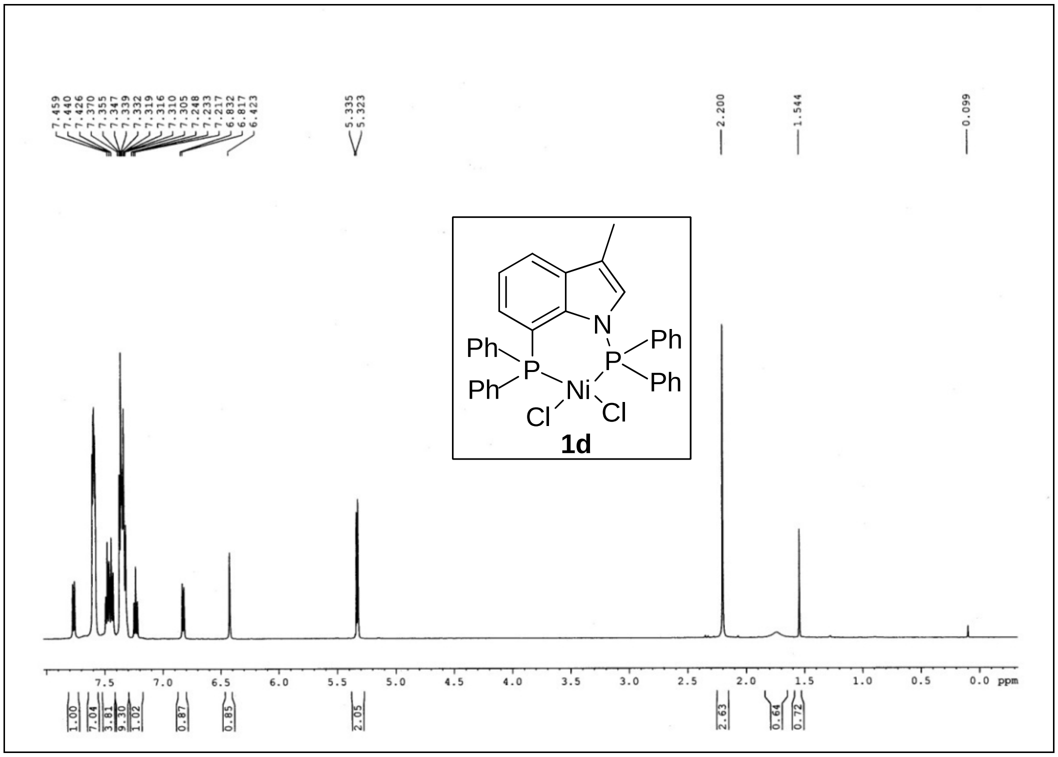

ppm
158.007
135.297
133.171
133.058
132.287
129.728
127.024
126.428
125.667
125.472
125.008
124.921
113.949
77.586
77.162
76.738
55.289
38.269
19.584
MeO
3n
ppm
140
120
100
80
60
40
20
0
Current Data Parameters
NAME RG02.169A-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101011
Time 15.07
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 665
DS 4
SWH 16556.291 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 9195.2
DW 30.200 usec
DE 6.00 usec
TE 300.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 11.75 usec
PL1 0.00 dB
SFO1 75.4753137 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 8.00 dB
PL13 12.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677450 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 8.10 cm
F1P 165.671 ppm
F1 12502.82 Hz
F2P -5.322 ppm
F2 -401.65 Hz
PPMCM 8.54966 ppm/cm
HZCM 645.22351 Hz/cm

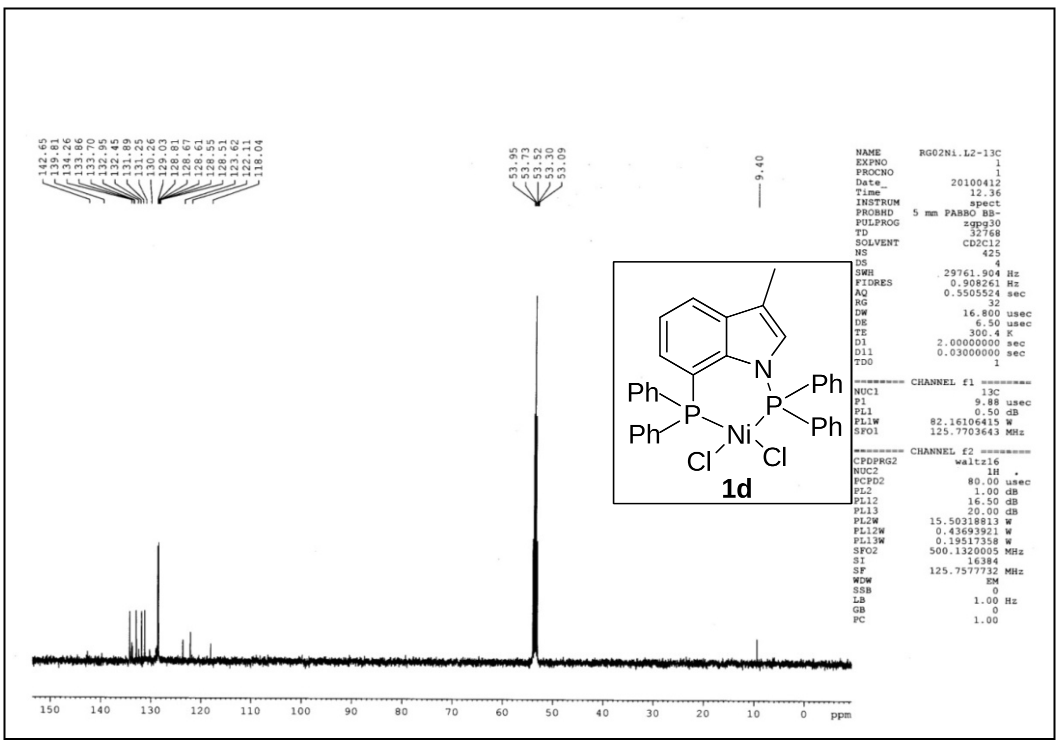

ppm
8.06823
7.54971
7.52348
7.36898
7.34380
7.25938
7.04301
7.02899
7.01876
6.99153
2.33974
2.33691
Br 1c
N
H
Integral
0.8357
1.0000
1.0562
2.1035
3.2691
ppm
8
7
6
5
4
3
2
1
0


ppm
135.069
129.642
124.305
122.325
120.413
118.226
113.143
104.747
77.589
77.166
76.742
9.980
Br 1c
N
H
ppm
160
140
120
100
80
60
40
20
0
Current Data Parameters

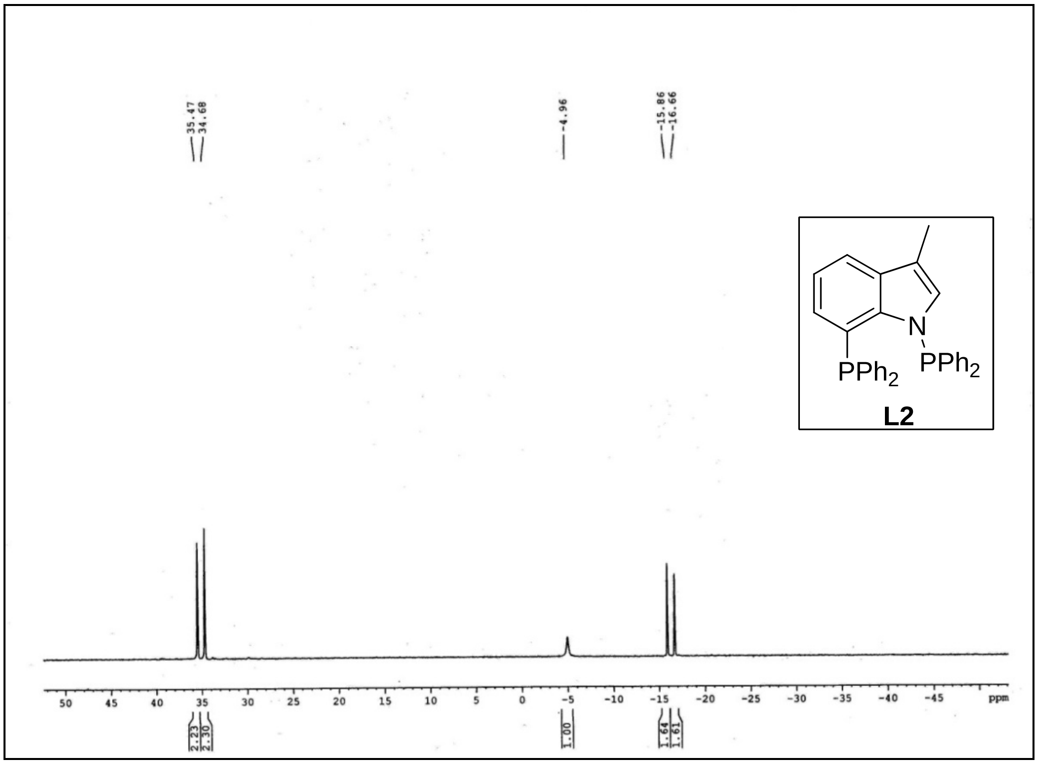

ppm
7.57670
7.55108
7.38164
7.31584
7.28971
7.26784
7.10811
7.08371
7.05950
6.75080
6.72893
6.70879
6.67326
2.23911
PPh2
N
PPh2
L2
Integral
0.2721
3.3083
1.0000
0.3968
0.6590
ppm
7
6
5
4
3
2
1
0

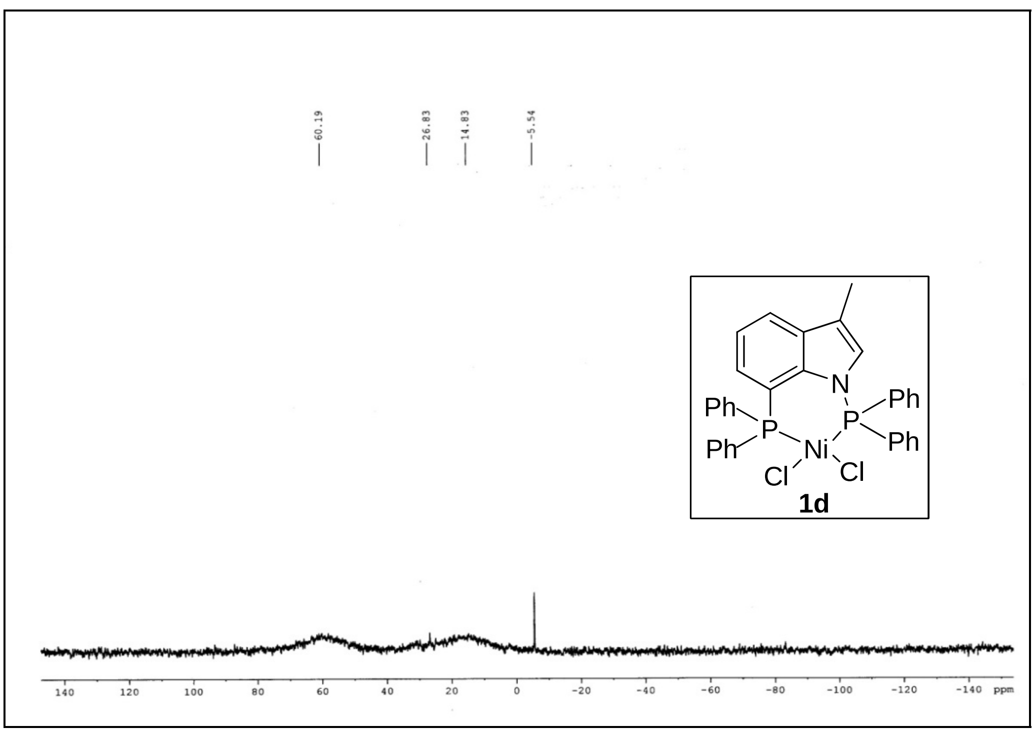

ppm
134.751
134.735
134.501
134.482
132.373
132.099
129.564
129.325
128.624
128.580
128.532
128.503
128.241
120.650
119.995
116.073
77.678
77.256
76.831
22.855
10.090
PPh2
N
PPh2
L2
ppm 140
120
100
80
60
40
20
0
Current Data Parameters
NAME RG02.47-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20090506
Time 10.42
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgdc
TD 65536
SOLVENT CDCl3
NS 70
DS 4
SWH 19841.270 Hz
FIDRES 0.302754 Hz
AQ 1.6515572 sec
RG 32768
DW 25.200 usec
DE 6.00 usec
TE 298.2 K
D1 2.00000000 sec
d11 0.03000000 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 13.00 usec
PL1 0.00 dB
SFO1 75.4763276 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 7.00 dB
SFO2 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677422 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 7.56 cm
F1P 148.810 ppm
F1 11230.37 Hz
F2P -7.342 ppm
F2 -554.09 Hz
PPMCM 7.80762 ppm/cm
HZCM 589.22327 Hz/cm


7.459
7.440
7.426
7.370
7.355
7.347
7.339
7.332
7.319
7.316
7.310
7.305
7.248
7.233
7.217
6.832
6.817
6.423
5.335
5.323
2.200
1.544
0.099
Ph
Ph
P
N
Ph
P
Ph
Ni
Cl
Cl
1d
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 ppm
1.00
7.04
3.81
9.30
1.02
0.87
0.85
2.05
2.63
0.64
0.72


142.65
139.81
134.26
133.86
133.70
132.95
132.45
131.89
131.25
130.26
129.03
128.81
128.67
128.61
128.55
128.51
123.62
122.11
118.04
53.95
53.73
53.52
53.30
53.09
9.40
NAME RG02Ni.L2-13C
EXPNO 1
PROCNO 1
Date_ 20100412
Time 12.36
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CD2Cl2
NS 425
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 32
DW 16.800 usec
DE 6.50 usec
TE 300.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.88 usec
PL1 0.50 dB
PL1W 82.16106415 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.50 dB
PL13 20.00 dB
PL2W 15.50318813 W
PL12W 0.43693921 W
PL13W 0.19517358 W
SFO2 500.1320005 MHz
SI 16384
SF 125.7577732 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
Ph
Ph
P
N
Ph
P
Ph
Ni
Cl
Cl
1d
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm

31P NMR Spectrum:





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