Supplementary Material

β-Pinene and camphor based, pyrazole-tethered triarylphosphines as chiral P,N ligands for palladium

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Crystallographic information

X-ray crystal structure of ligand (C3) (Figure 1).

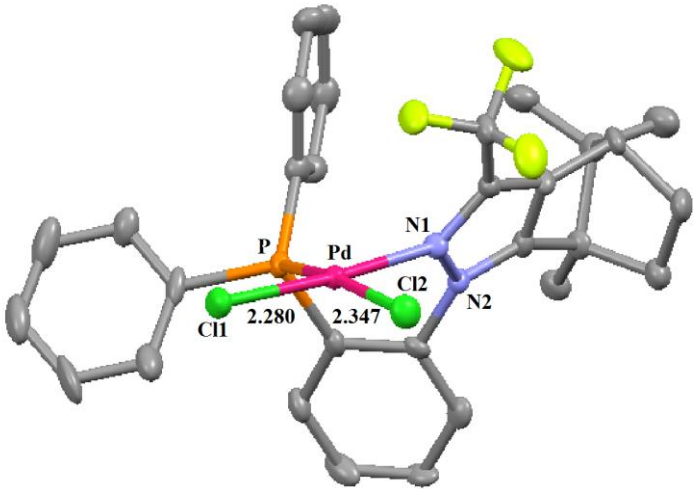
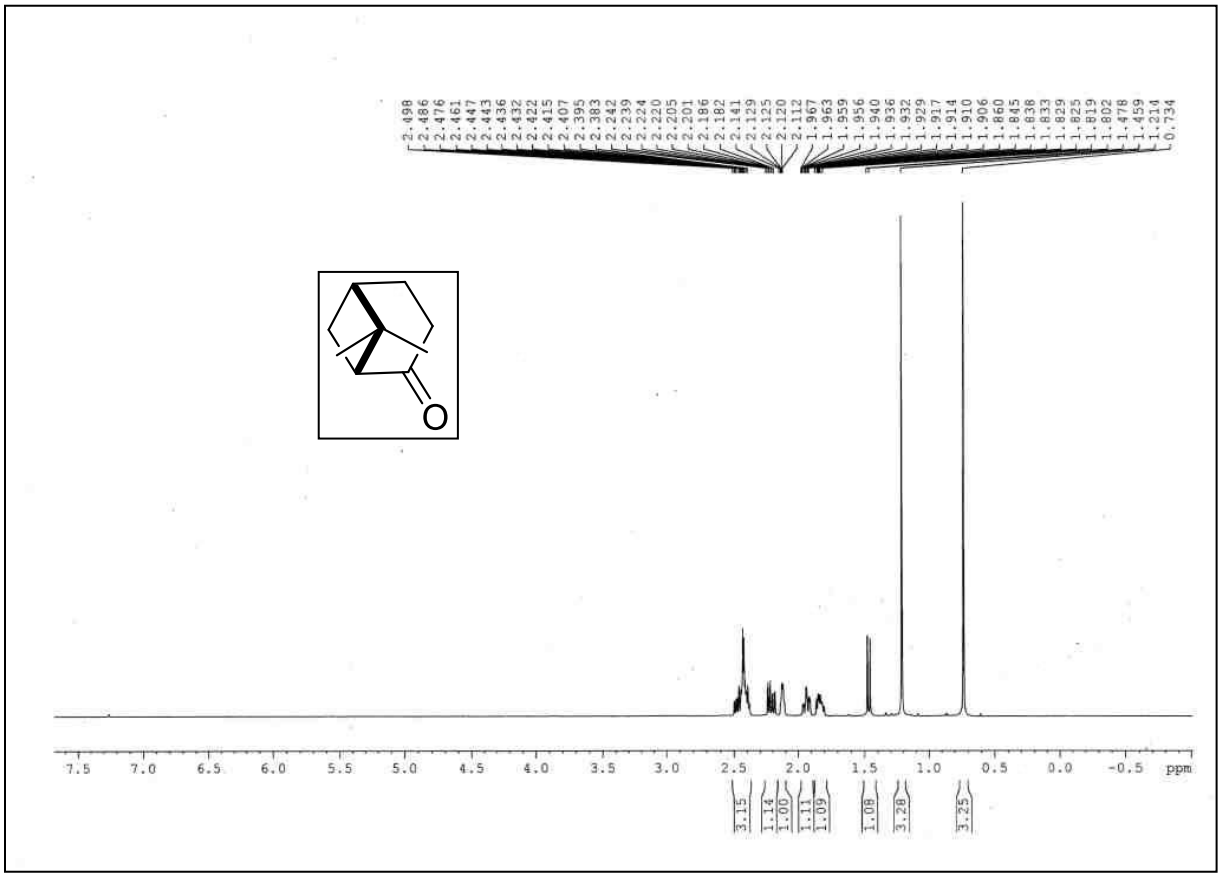
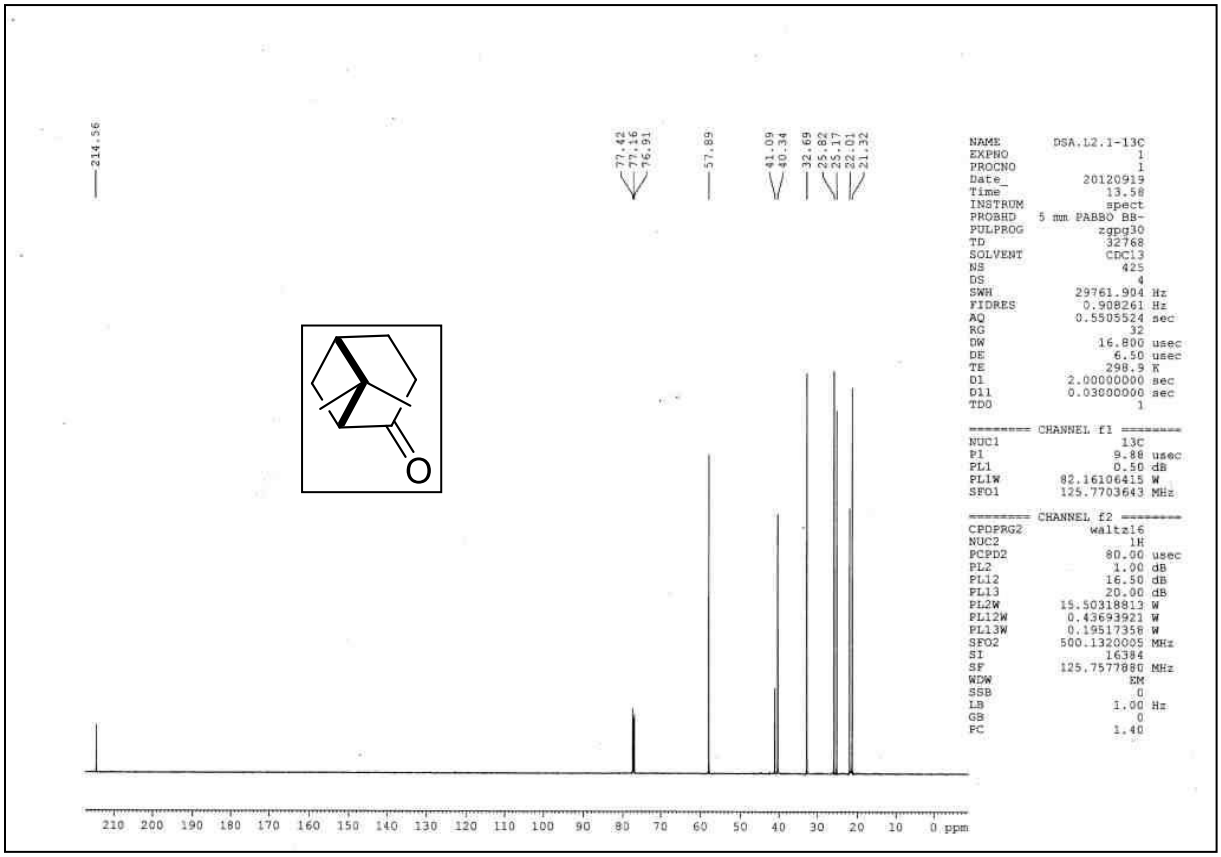


Figure 1: Thermal ellipsoid plot of Pd-L3 (C3) complex drawn at 50 % probability level.

Crystal data of Pd-L1 complex (C3):A colorless block shaped crystal (0.28 X 0.19 X 0.08 mm) was analyzed. Empirical formula$C_{30}H_{28}Cl_2F_3N_2PPd$, *FW*= 681.81, monoclinic space group $P2_1$, a = 8.8797(7)Å, b = 15.9122(12)Å, c = 11.4502(9)Å, β = 102.348(2)°, V = 1580.4(2) Å^3, T = 150 K, Z = 2. ρ_{calcd} = 1.433 g cm^{-3}. F (000) = 688, λ (Mo–Kα) = 0.71073 Å, μMoKα /mm^{-1} = 0.846, $2\theta_{max}$ = 50.0°, 15013 total reflections, 5237 unique reflections, 5001 observed (I>2σ (I)) 355 parameters; R_{int}= 0.0327, R_1 = 0.0322; wR_2 = 0.0762 (I>2σ (I)), R_1 = 0.0338; wR_2 = 0.0771 (all data) with GOF = 1.016.

Spectrum of all compounds

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40.34
32.69
25.82
25.17
22.01
21.32
O
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PROCNO 1
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DE 6.50 usec
TE 298.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
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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
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SSB 0
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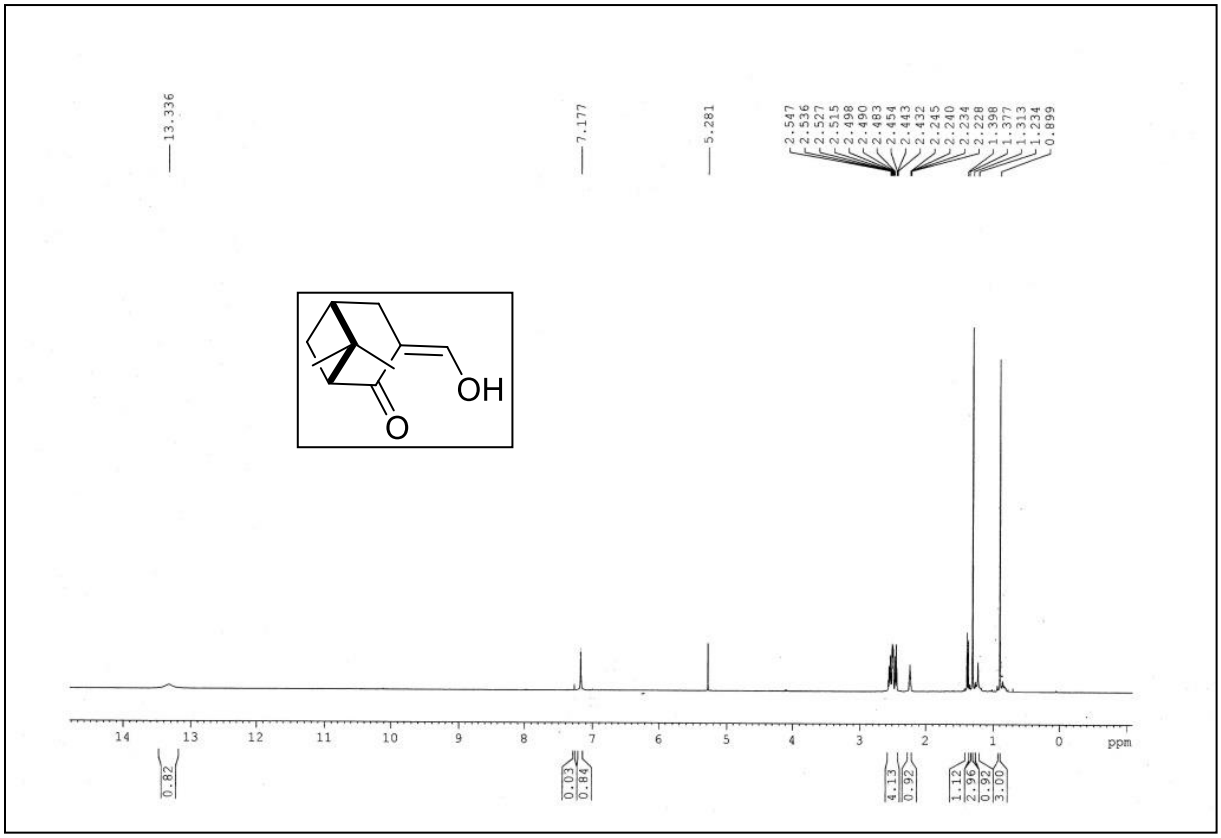
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2.515
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2.490
2.483
2.454
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2.432
2.245
2.240
2.234
2.228
1.398
1.377
1.313
1.234
0.899
OH
O
14 13 12 11 10 9 8 7 6 5 4 3 2 1 0 ppm
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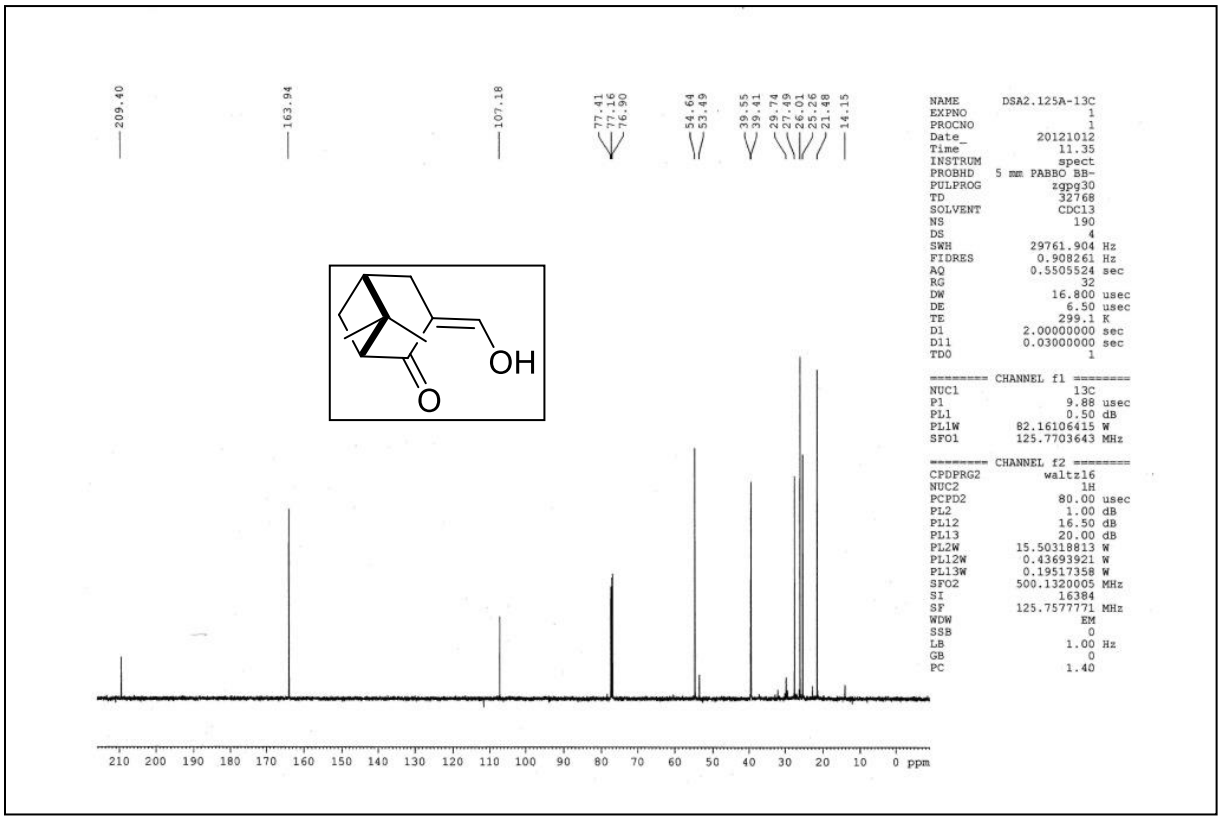
0.92
1.12
2.96
0.92
3.00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76.90
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26.01
25.26
21.48
14.15
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O
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TE 299.1 K
D1 2.00000000 sec
D11 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
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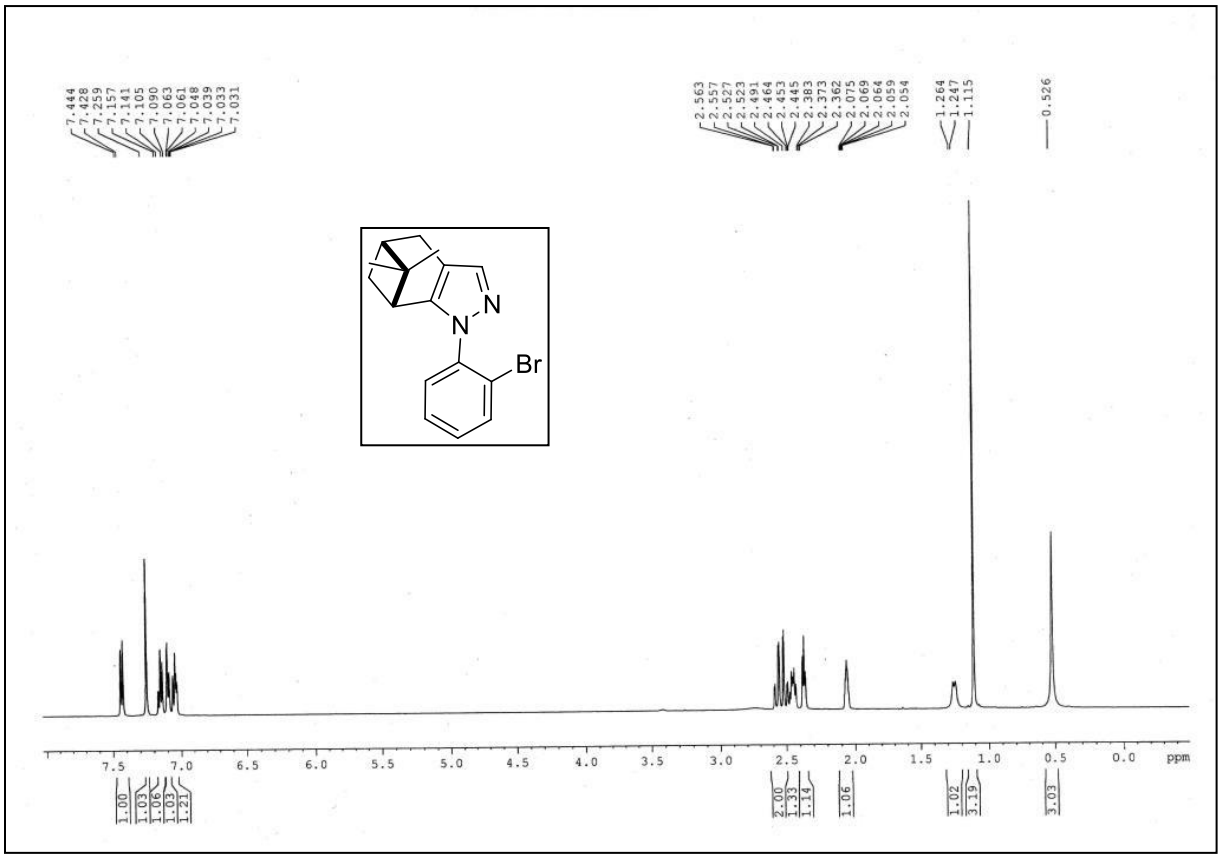
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7.105
7.090
7.063
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7.048
7.039
7.033
7.031
2.563
2.557
2.527
2.523
2.491
2.464
2.453
2.445
2.383
2.373
2.362
2.075
2.069
2.064
2.059
2.054
1.264
1.247
1.115
0.526
N
N
Br
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1.06
1.03
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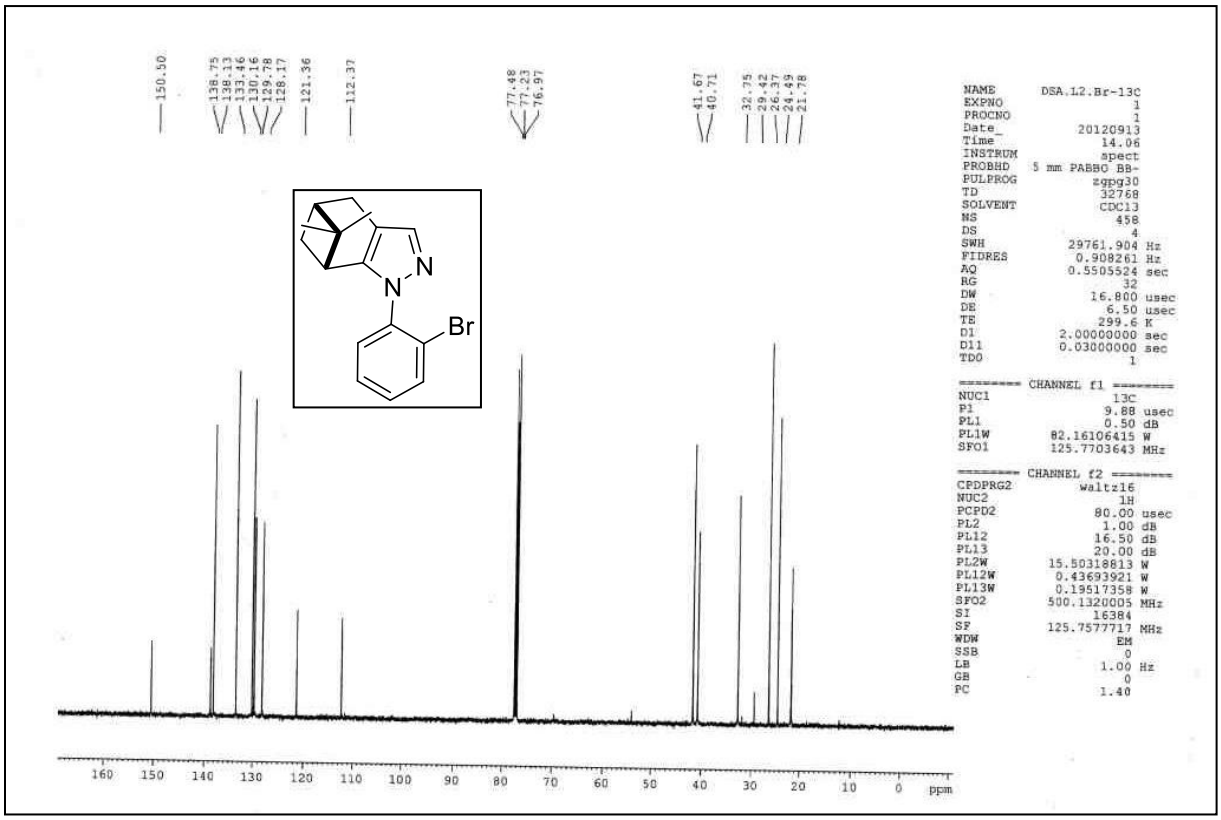
1.06
1.02
3.19
3.03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129.78
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40.71
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21.78
Br
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EXPNO 1
PROCNO 1
Date_ 20120913
Time 14.06
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PULPROG zgpg30
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SOLVENT CDCl3
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DE 6.50 usec
TE 299.6 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
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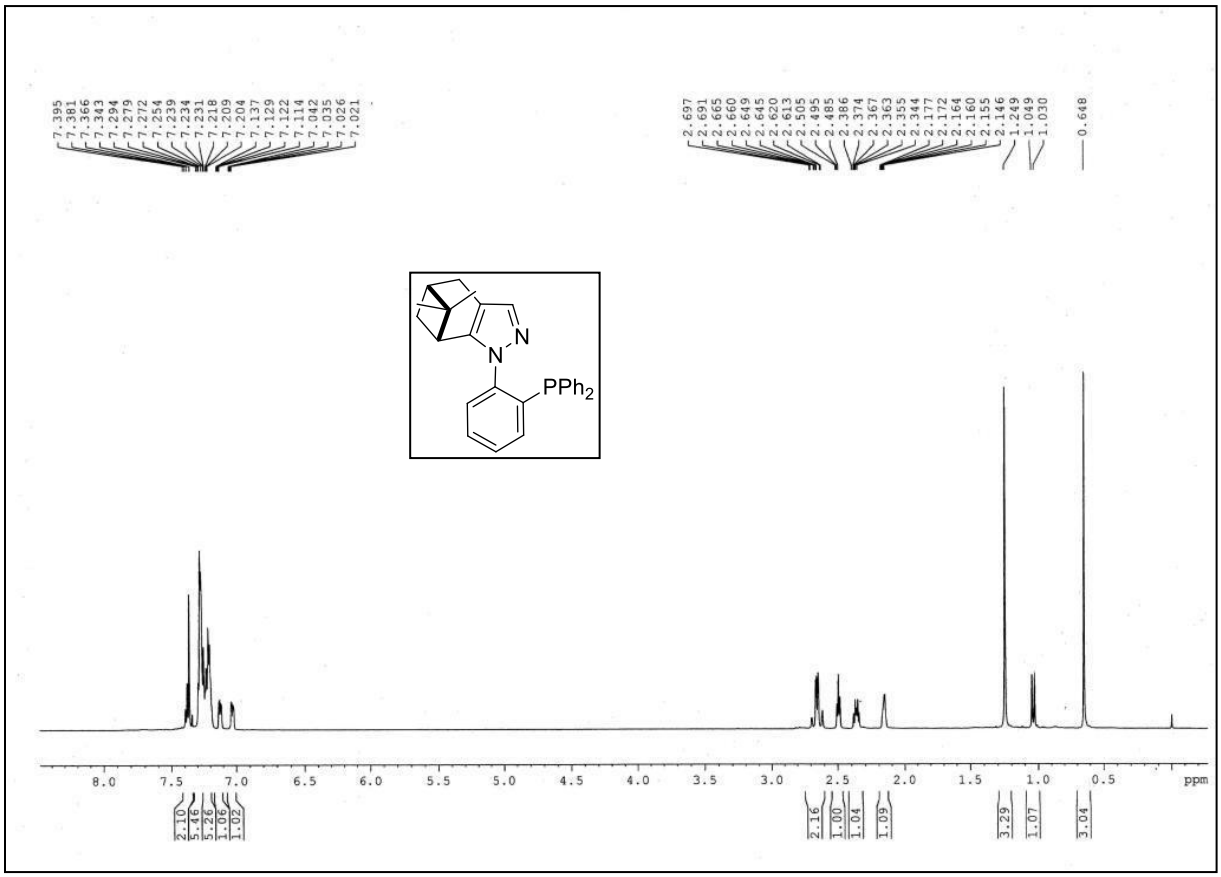
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7.234
7.231
7.218
7.209
7.204
7.137
7.129
7.122
7.114
7.042
7.035
7.026
7.021
2.697
2.691
2.665
2.660
2.649
2.645
2.620
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2.363
2.355
2.344
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2.172
2.164
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2.146
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PPh2
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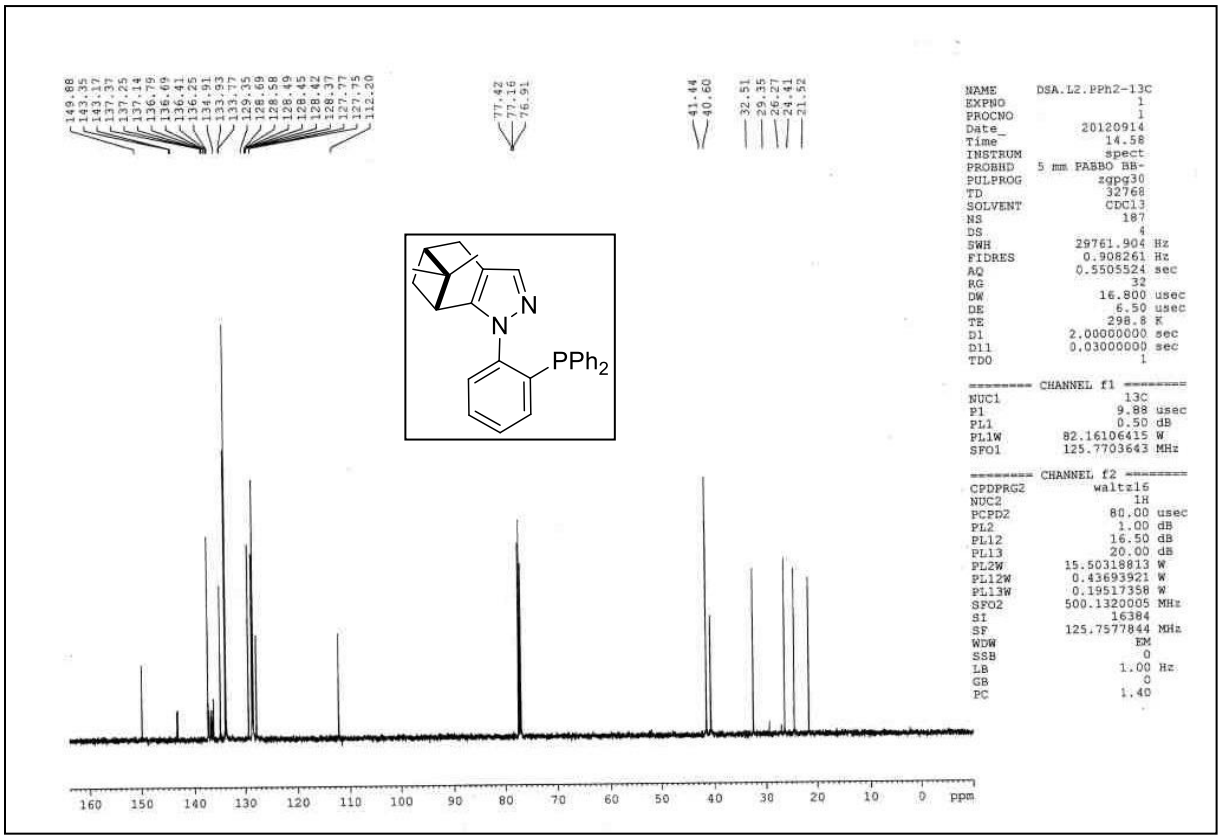

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RG 32
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DE 6.50 usec
TE 298.8 K
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D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
NUC1 13C
P1 9.88 usec
PL1 0.50 dB
PL1W 82.16106415 W
SFO1 125.7703643 MHz

======== CHANNEL f2 ========
CPDPRGZ 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
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SI 16384
SF 125.7577844 MHz
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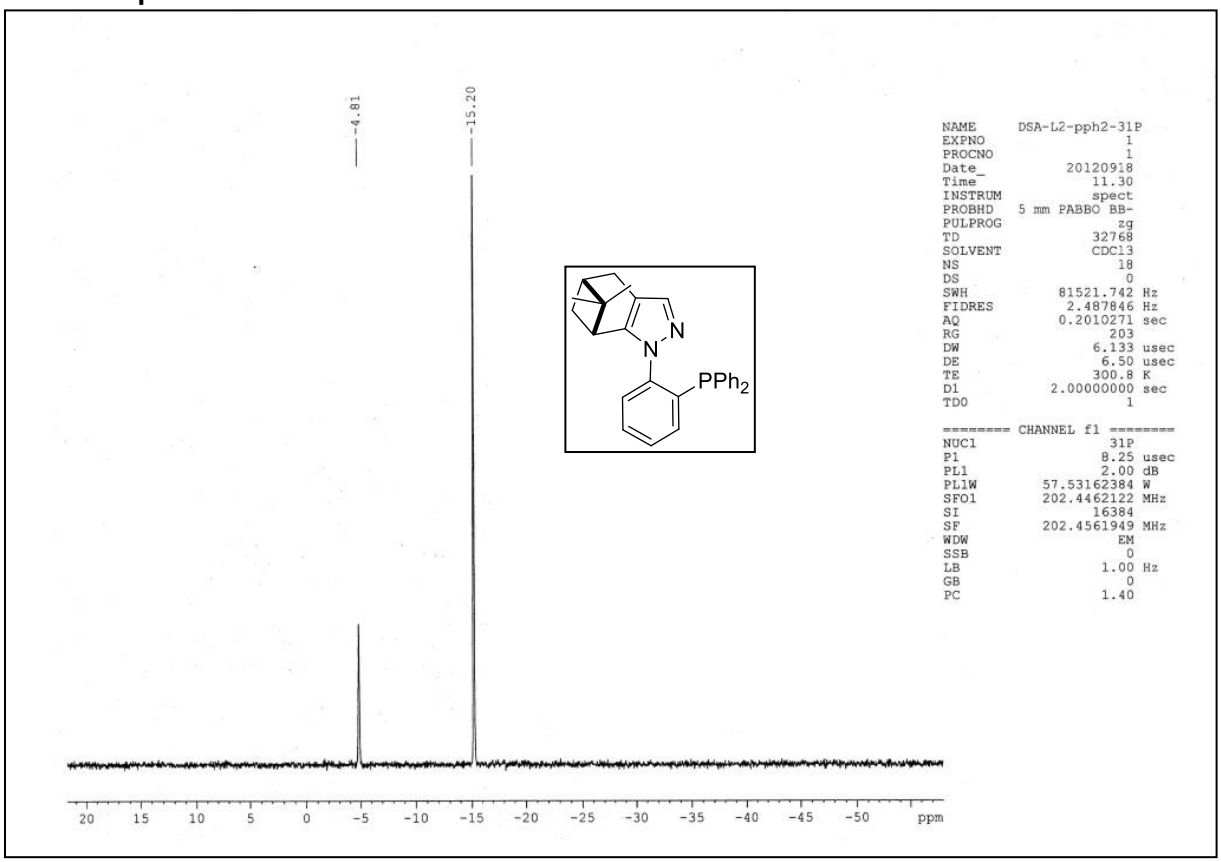
LB 1.00 Hz
GB 0
PC 1.40

^{31}P NMR Spectrum



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PULPROG zg
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FIDRES 2.487846 Hz
AQ 0.2010271 sec
RG 203
DW 6.133 usec
DE 6.50 usec
TE 300.8 K
D1 2.00000000 sec
TD0 1

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P1 8.25 usec
PL1 2.00 dB
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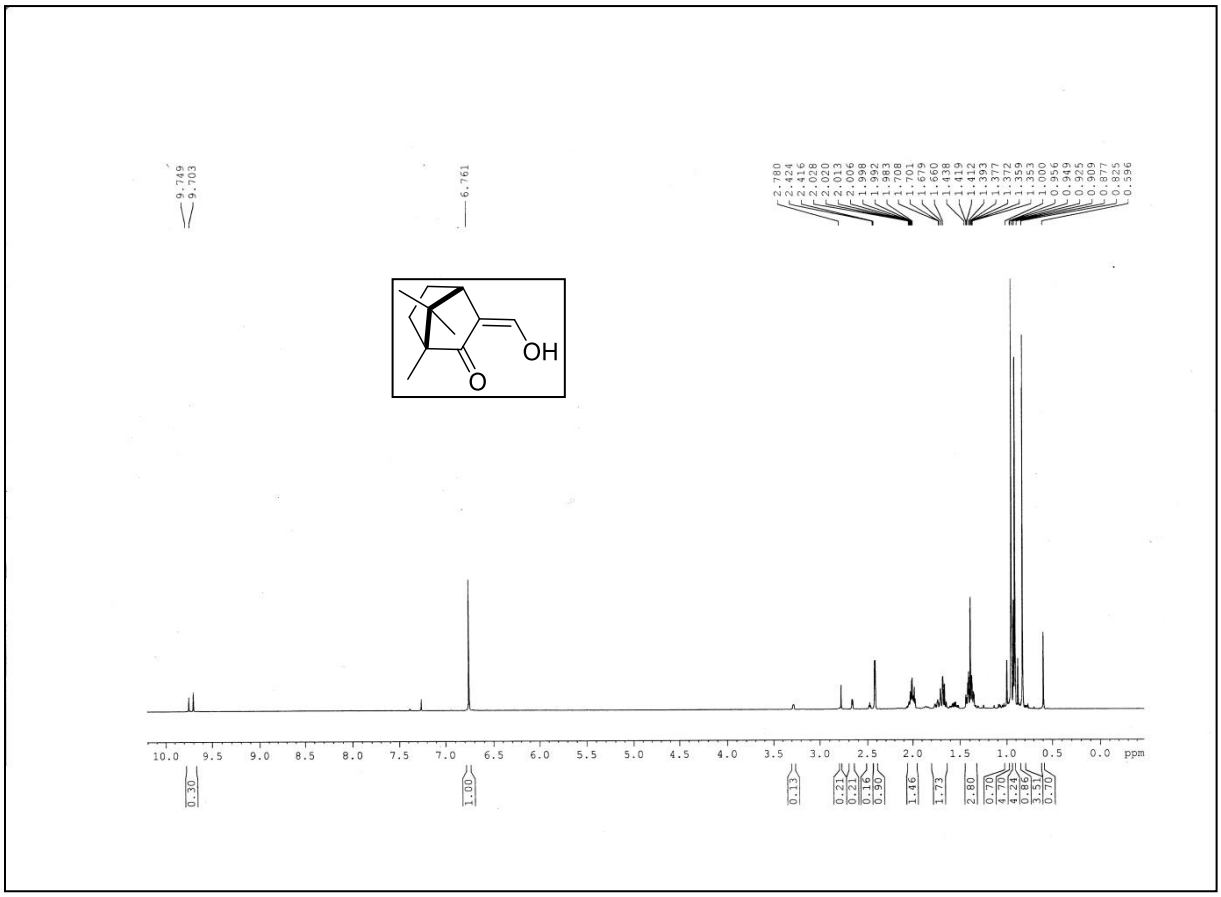
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1.708
1.701
1.679
1.660
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1.419
1.412
1.383
1.377
1.372
1.359
1.353
1.000
0.956
0.944
0.925
0.909
0.877
0.825
0.596
OH
O
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
0.30
1.00
0.13
0.21
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4.70
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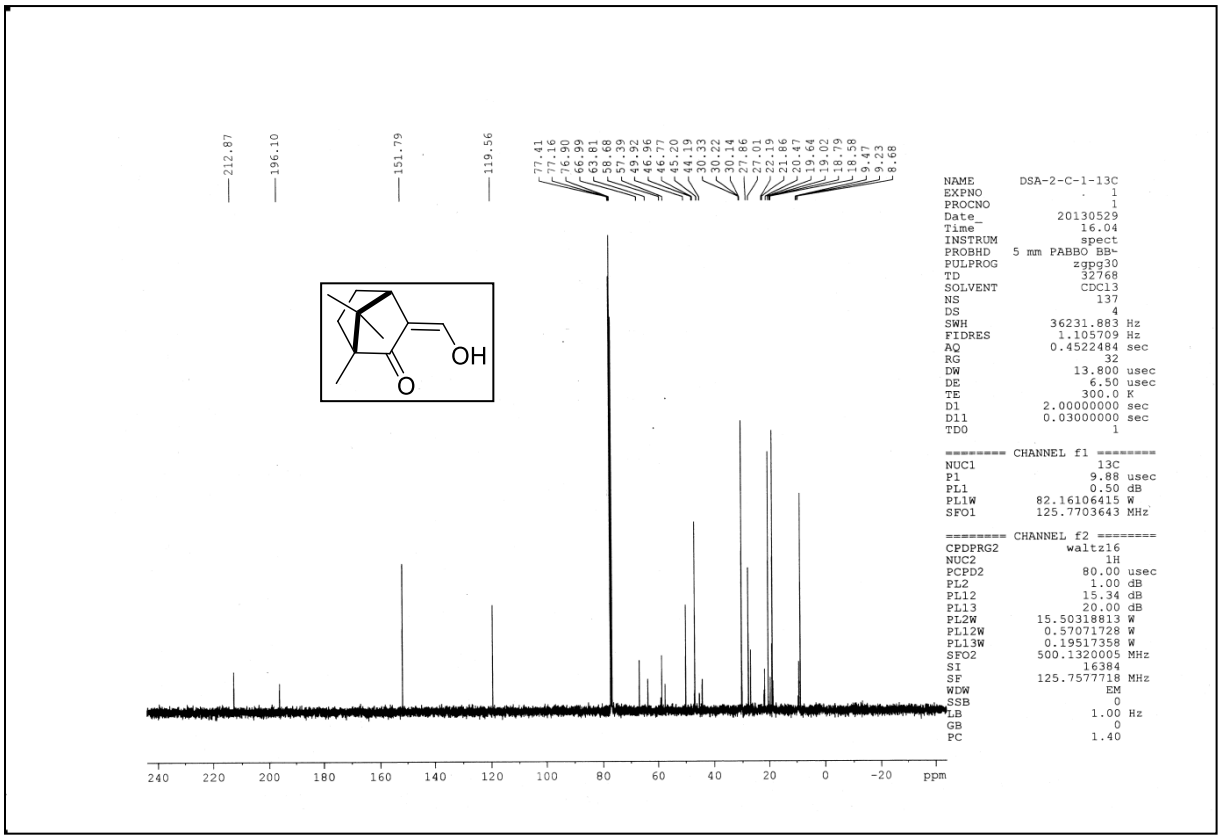
0.70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30.33
30.22
30.14
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27.01
22.19
21.86
20.47
19.64
19.02
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O
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D11 0.03000000 sec
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NUC1 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 15.34 dB
PL13 20.00 dB
PL2W 15.50318813 W
PL12W 0.57071728 W
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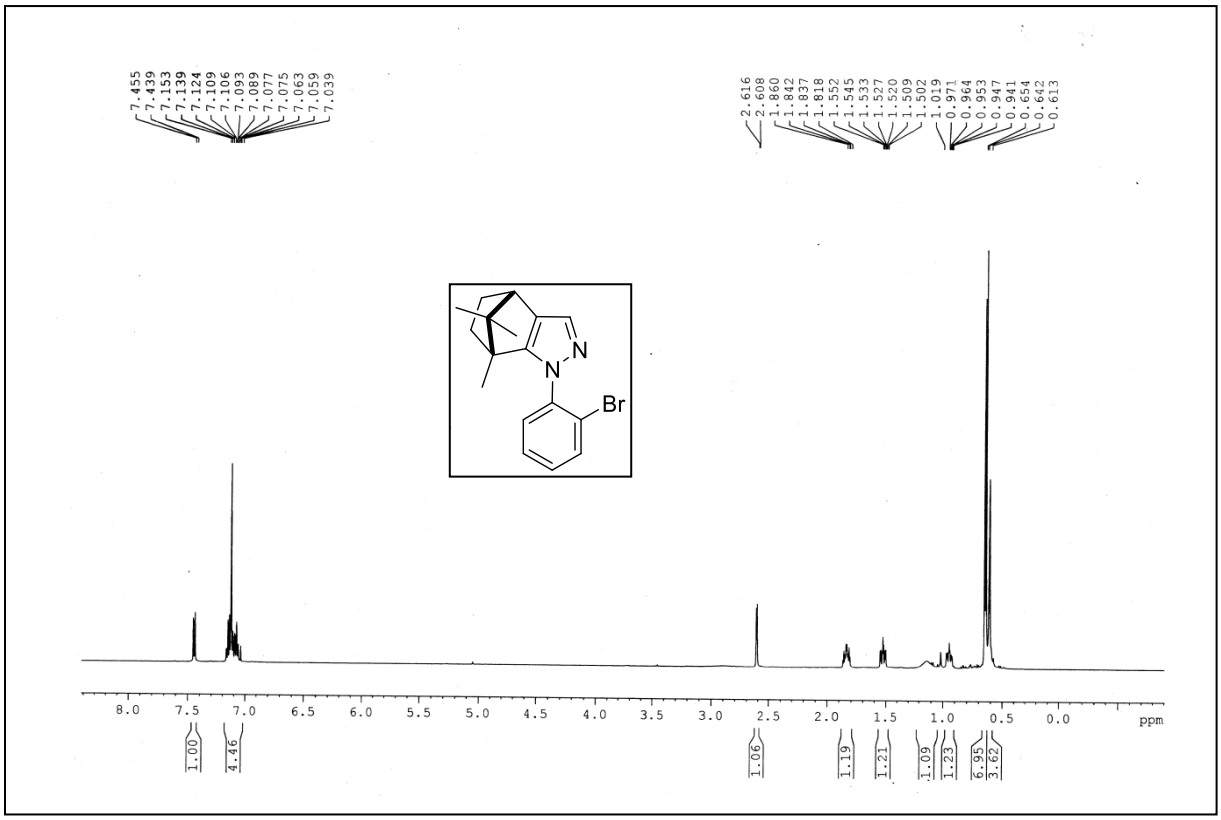
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7.059
7.039
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2.608
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1.837
1.818
1.552
1.545
1.533
1.527
1.520
1.509
1.502
1.019
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6.0
5.5
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3.0
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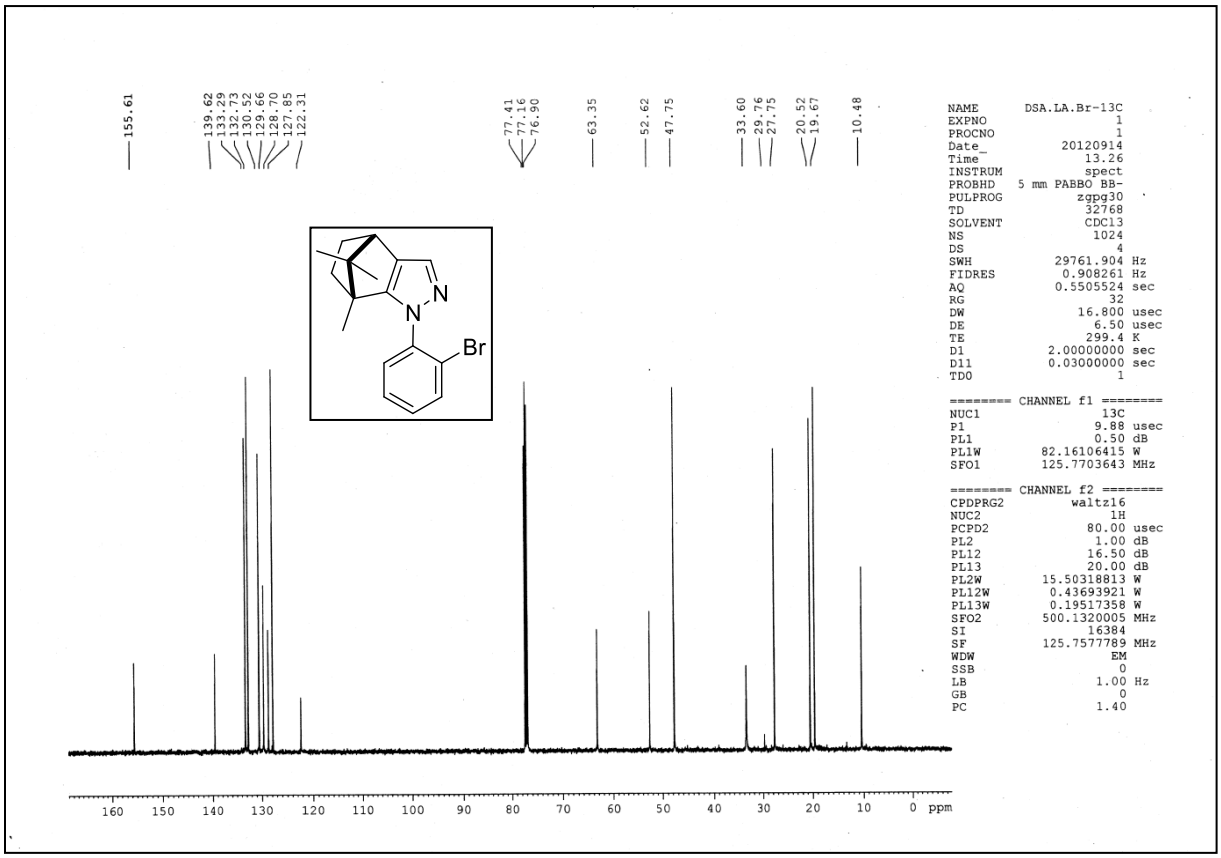
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10.48
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Br
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150
140
130
120
110
100
90
80
70
60
50
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20
10
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PROCNO 1
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PULPROG zgpg30
TD 32768
SOLVENT CDCl3
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FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 32
DW 16.800 usec
DE 6.50 usec
TE 299.4 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
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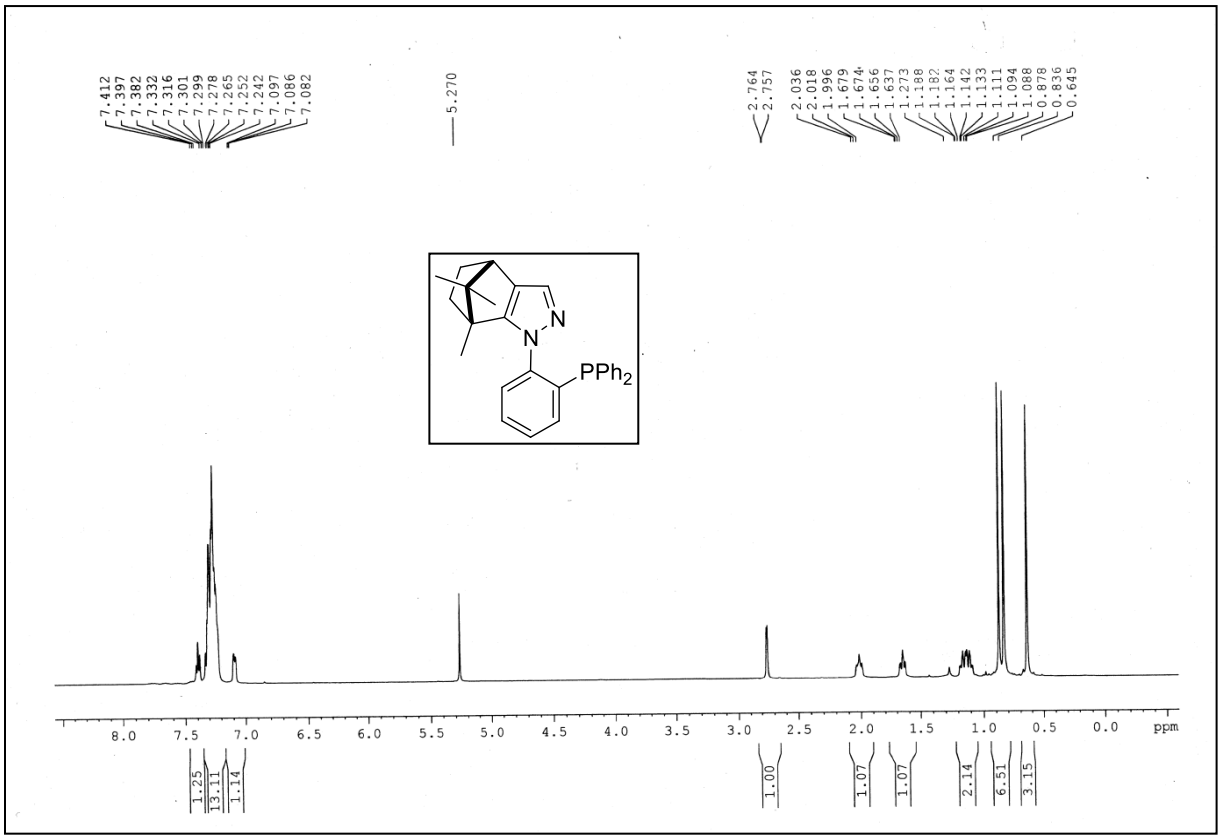
SSB 0
LB 1.00 Hz
GB 0
PC 1.40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7.316
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7.252
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7.082
5.270
2.764
2.757
2.036
2.018
1.996
1.679
1.674
1.656
1.637
1.273
1.188
1.182
1.164
1.142
1.133
1.111
1.094
1.088
0.878
0.836
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1.07
1.07
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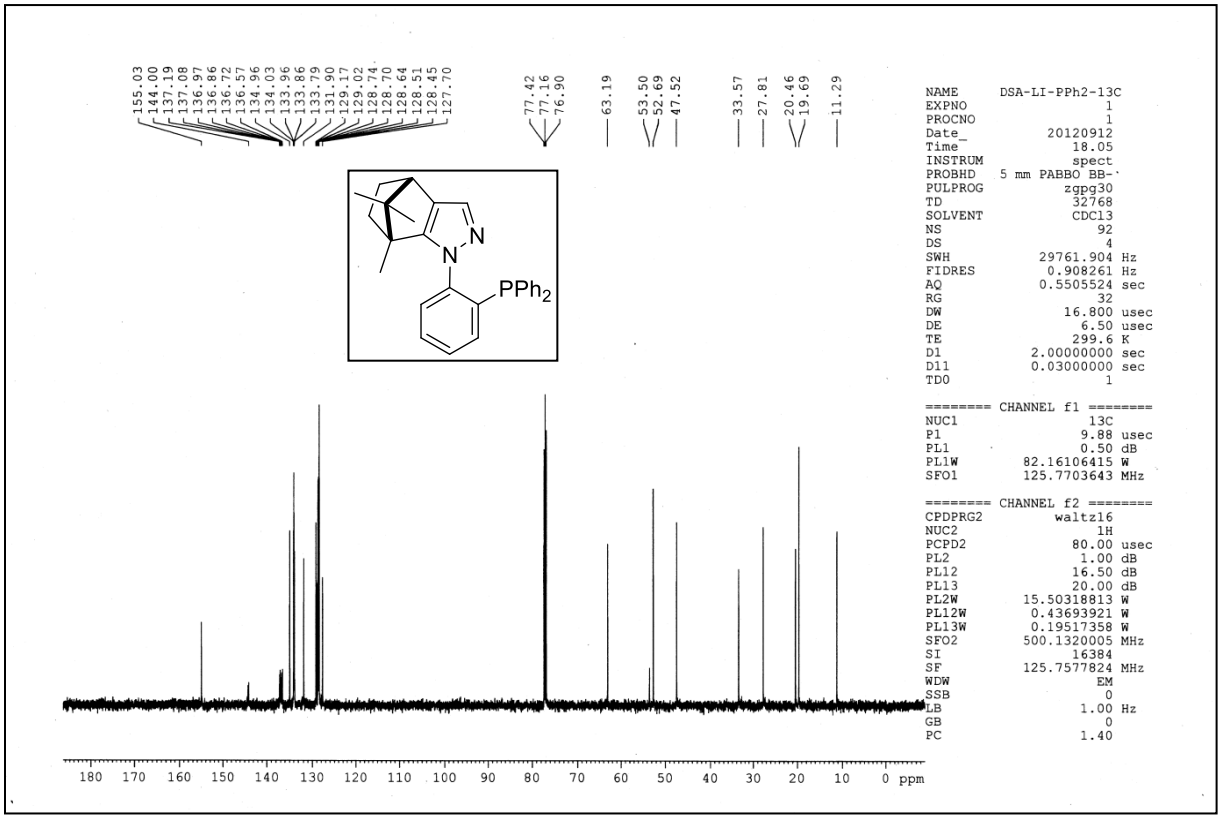
3.15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134.96
134.03
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133.86
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129.17
129.02
128.74
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52.69
47.52
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27.81
20.46
19.69
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PPh2
ppm
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PROCNO 1
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TD 32768
SOLVENT CDCl3
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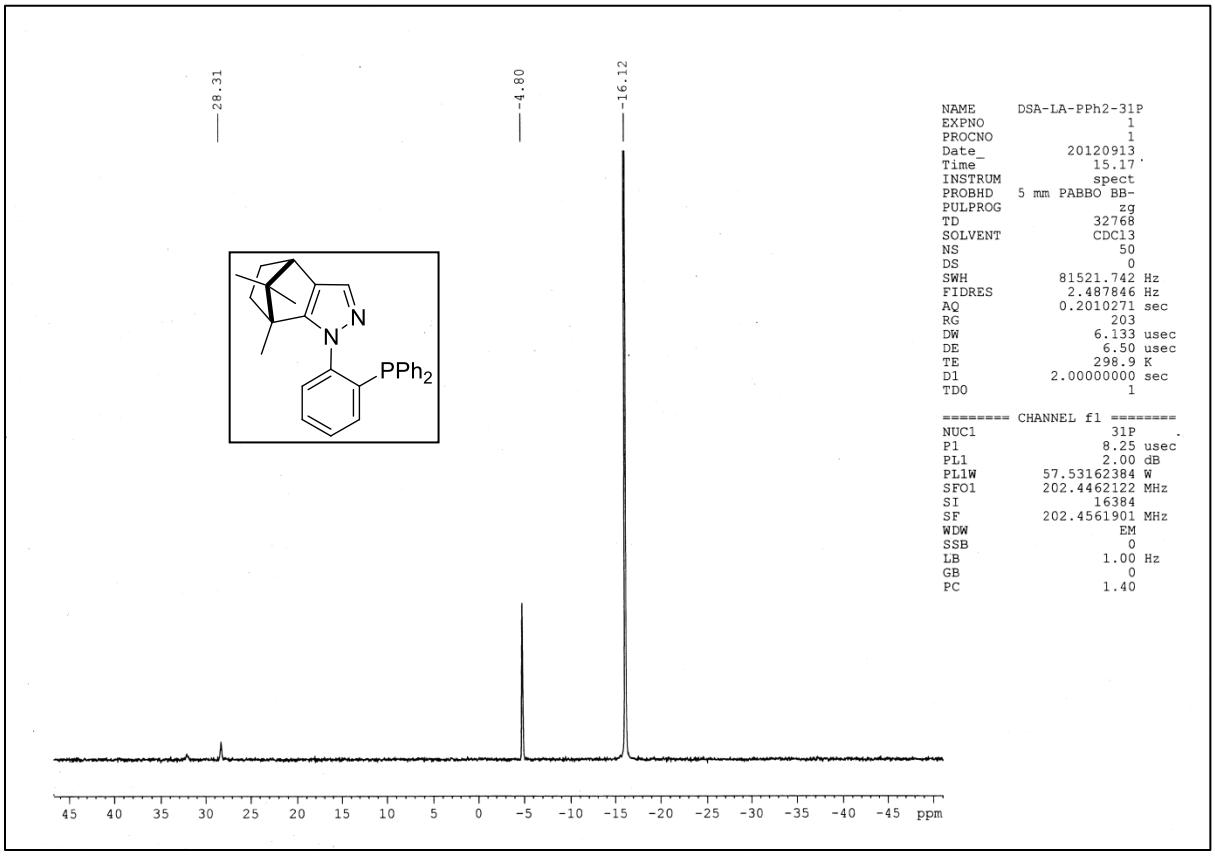
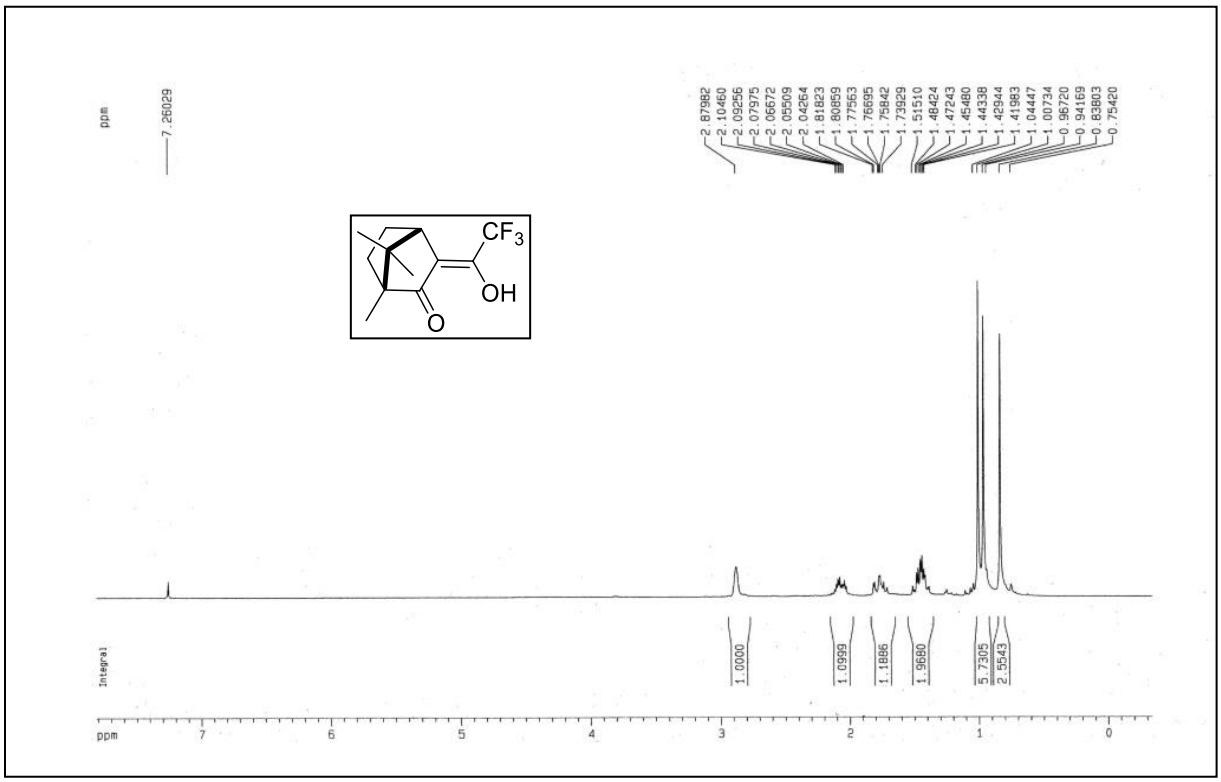
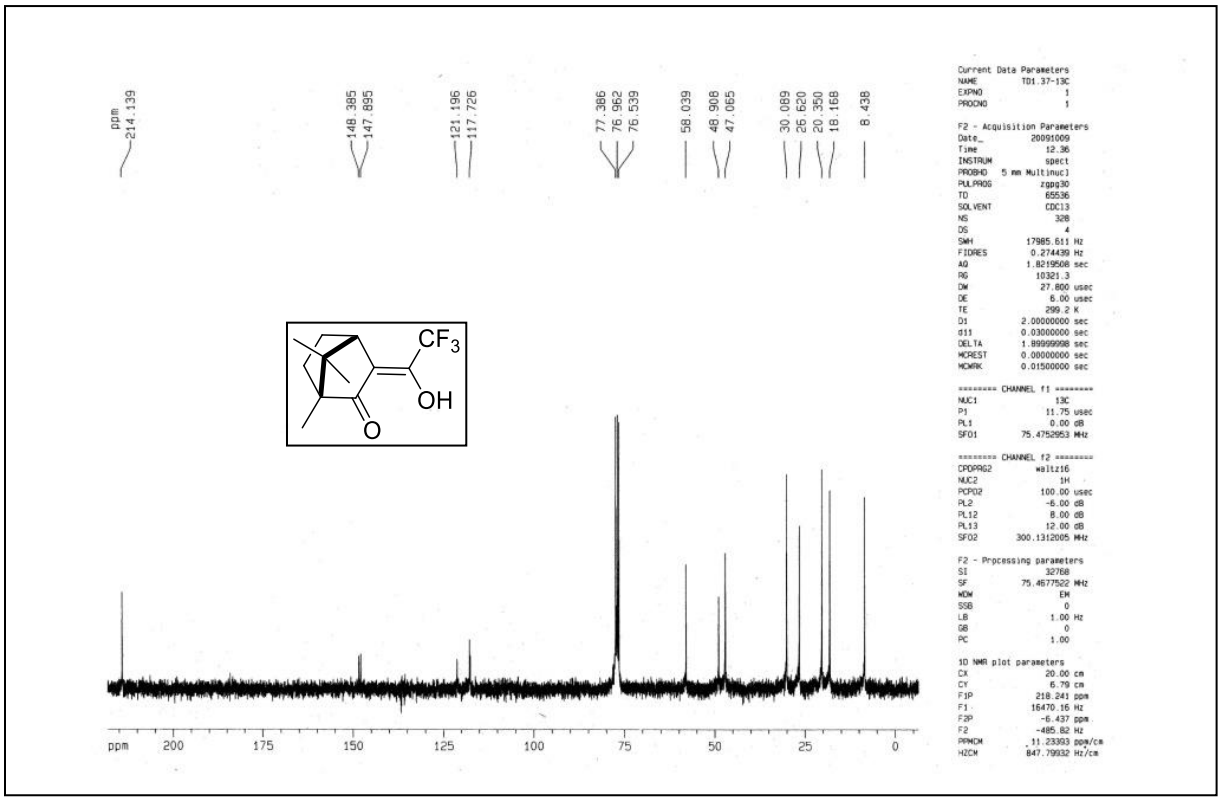
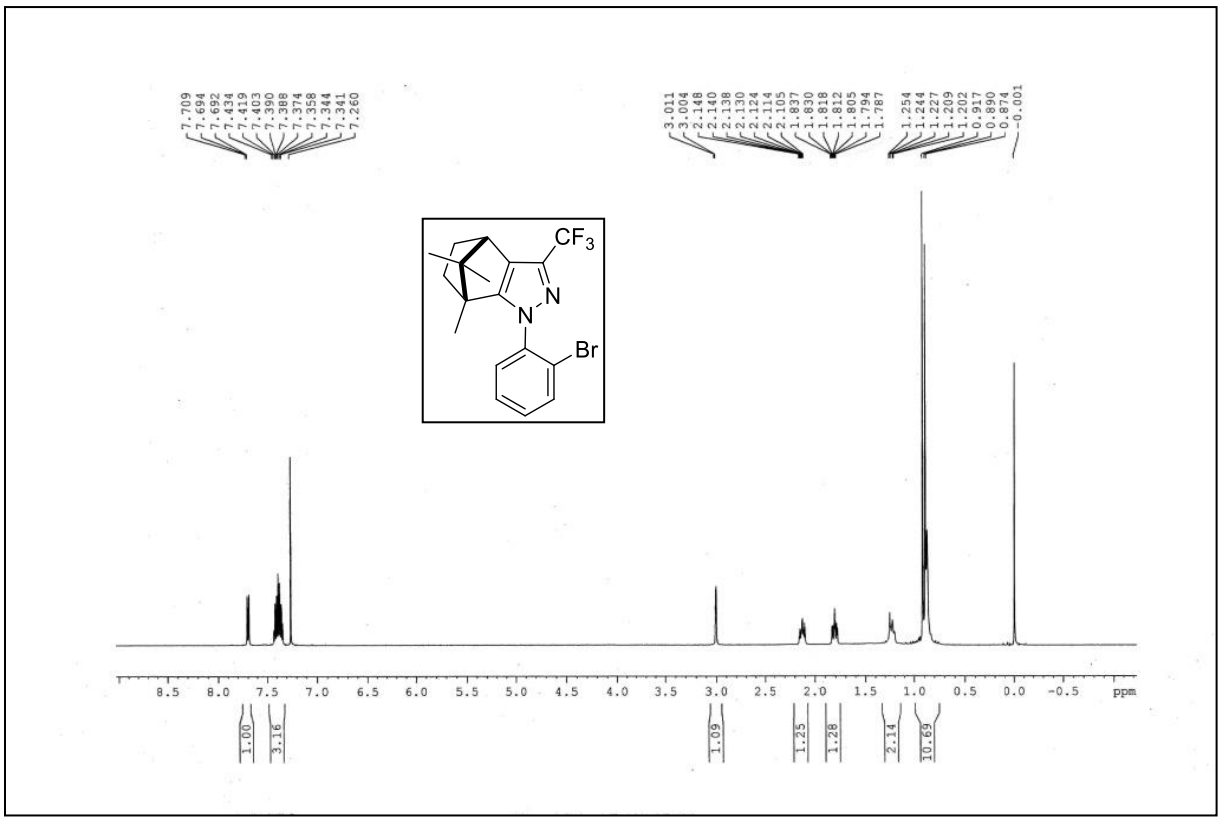
FIDRES 0.908261 Hz
AQ 0.5505524 sec
RG 32
DW 16.800 usec
DE 6.50 usec
TE 299.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.88 usec
PL1 0.50 dB
PL1W 82.16106415 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 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 125.7577824 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

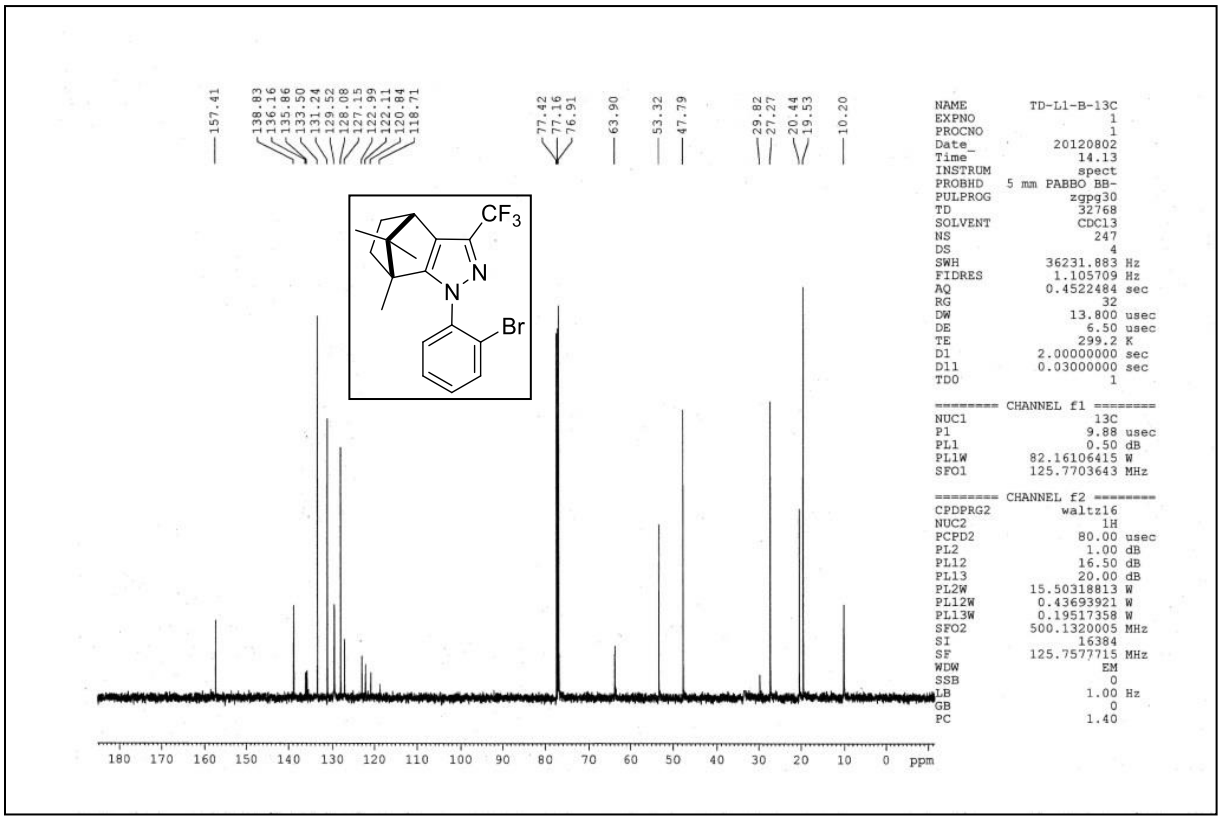
^{31}P NMR Spectrum



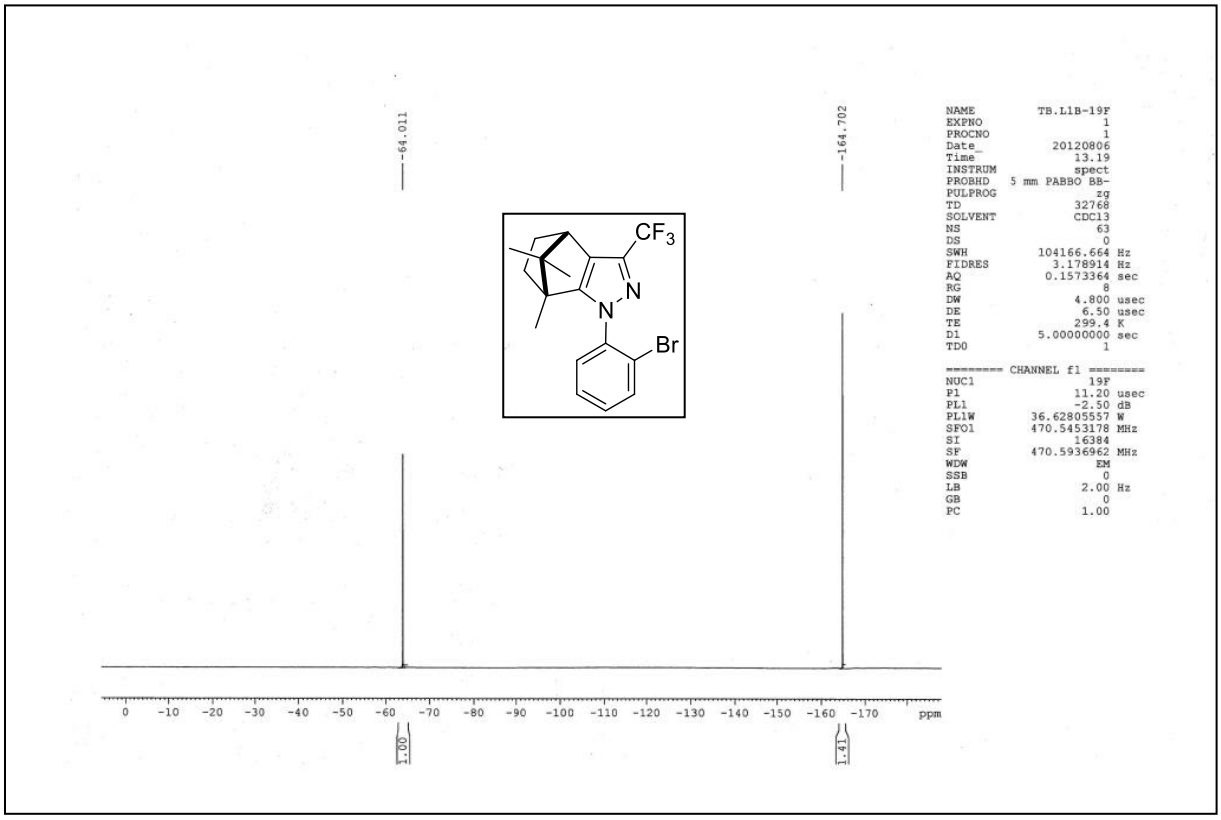


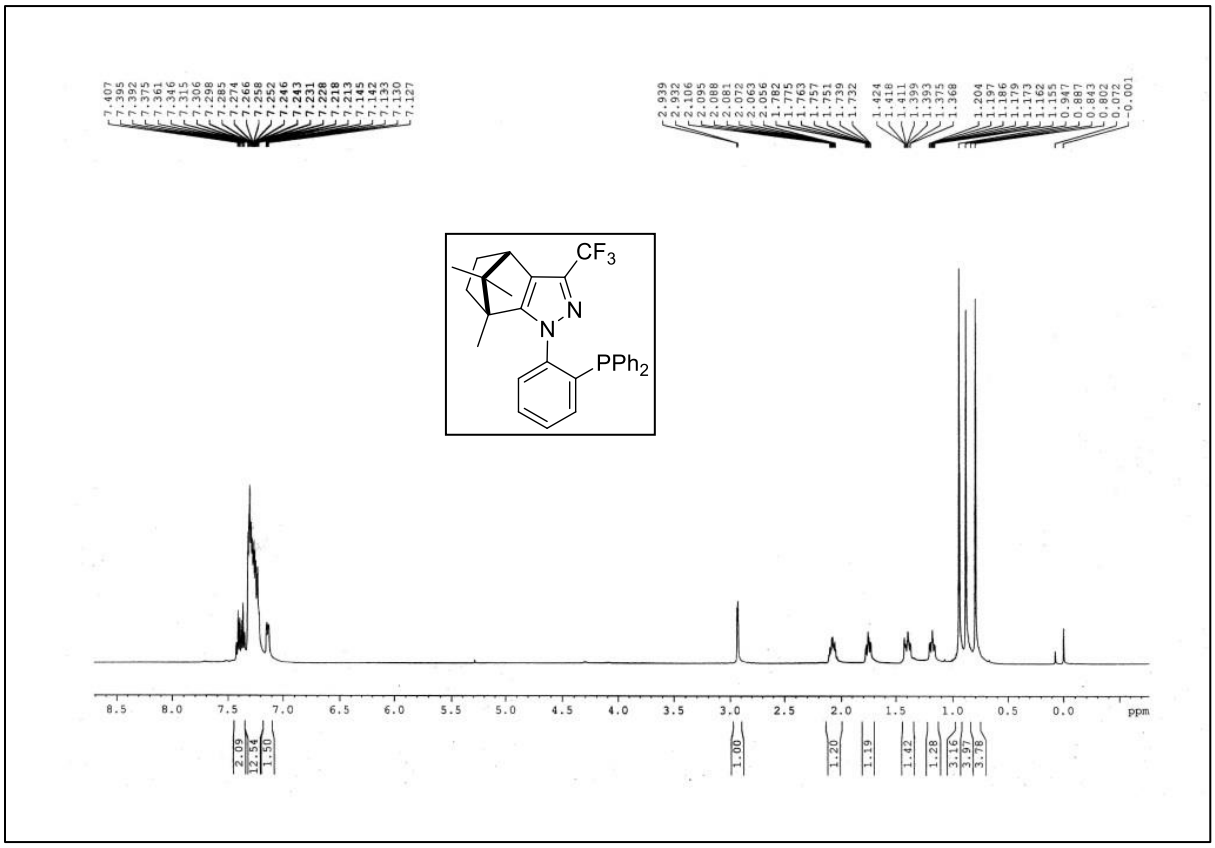

ppm
214.139
148.385
147.895
121.196
117.726
77.386
76.962
76.539
58.039
48.908
47.065
30.089
26.620
20.350
18.168
8.438
CF3
OH
O
ppm
200
175
150
125
100
75
50
25
0
Current Data Parameters
NAME TD1.37-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20091009
Time 12.36
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 328
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 10321.3
DW 27.800 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 75.4752953 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 75.4677522 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.00
1D NMR plot parameters
CX 20.00 cm
CY 6.79 cm
F1P 218.241 ppm
F1 16470.16 Hz
F2P -6.437 ppm
F2 -485.82 Hz
PPMCM 11.23393 ppm/cm
HZCM 847.79932 Hz/cm

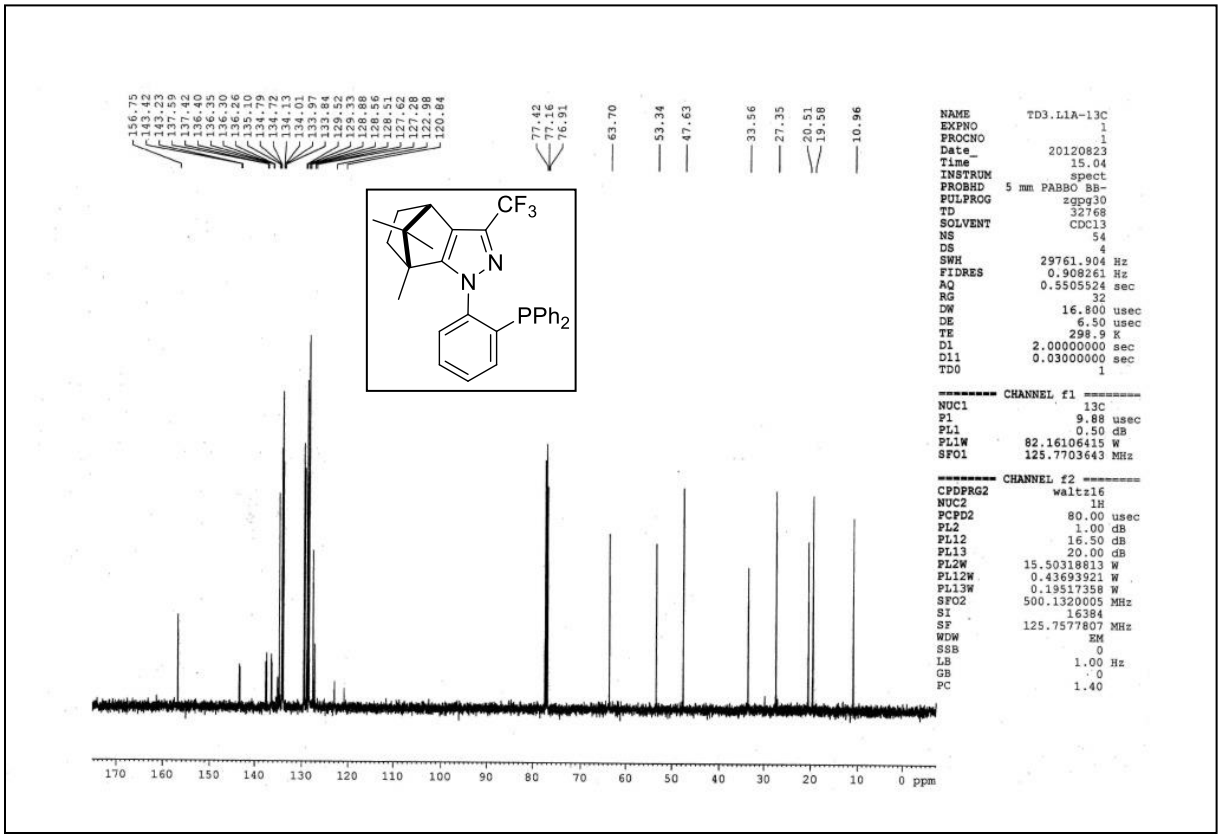

7.709
7.694
7.692
7.434
7.419
7.403
7.390
7.388
7.374
7.358
7.344
7.341
7.260
3.011
3.004
2.148
2.140
2.138
2.130
2.124
2.114
2.105
1.837
1.830
1.818
1.812
1.805
1.794
1.787
1.254
1.244
1.227
1.209
1.202
0.917
0.890
0.874
-0.001
CF3
N
N
Br
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
ppm
1.00
3.16
1.09
1.25
1.28
2.14
10.69



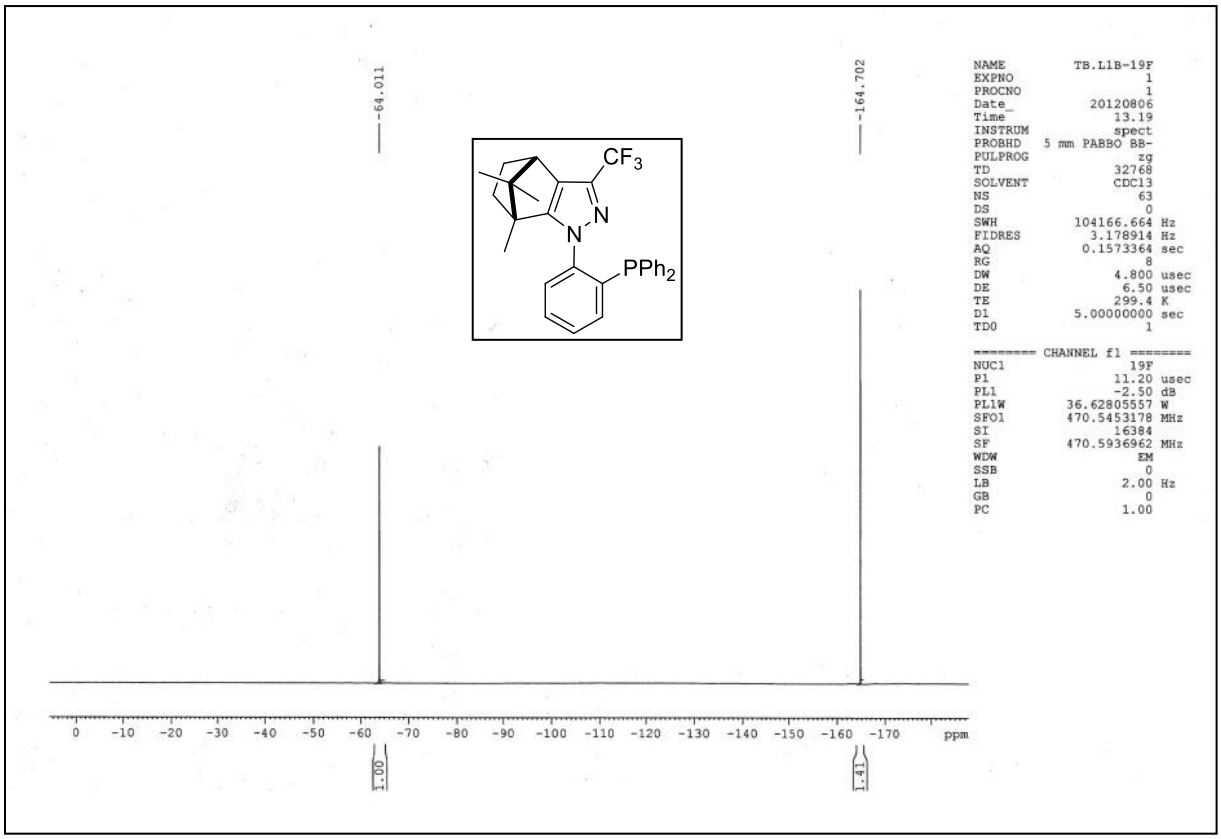
^{19}F NMR Spectrum



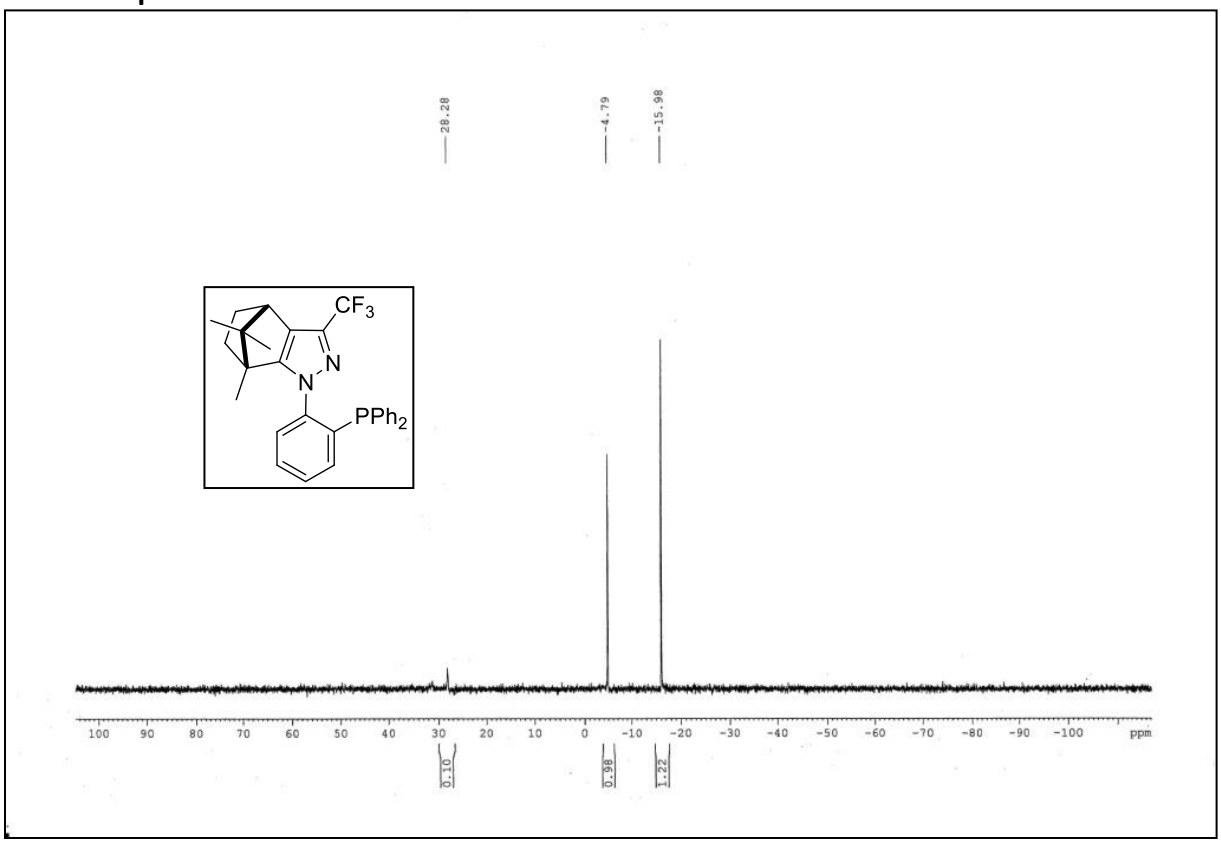


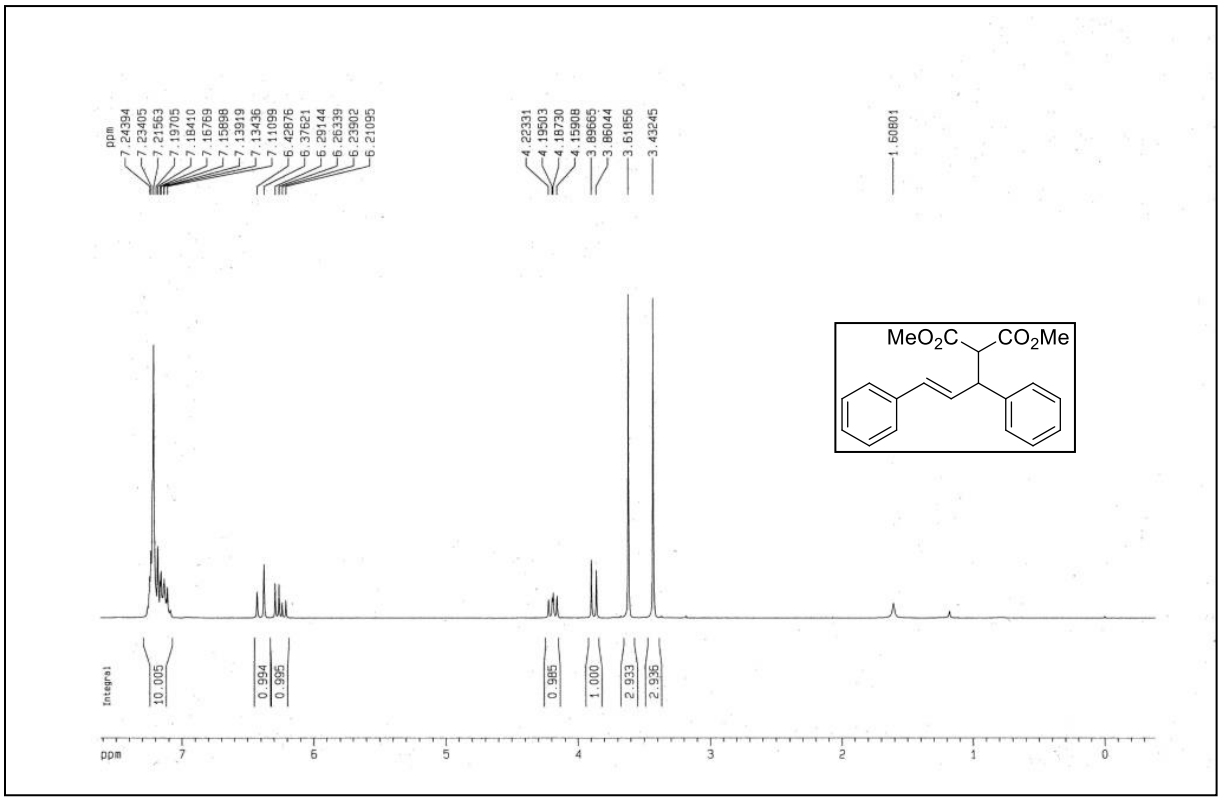


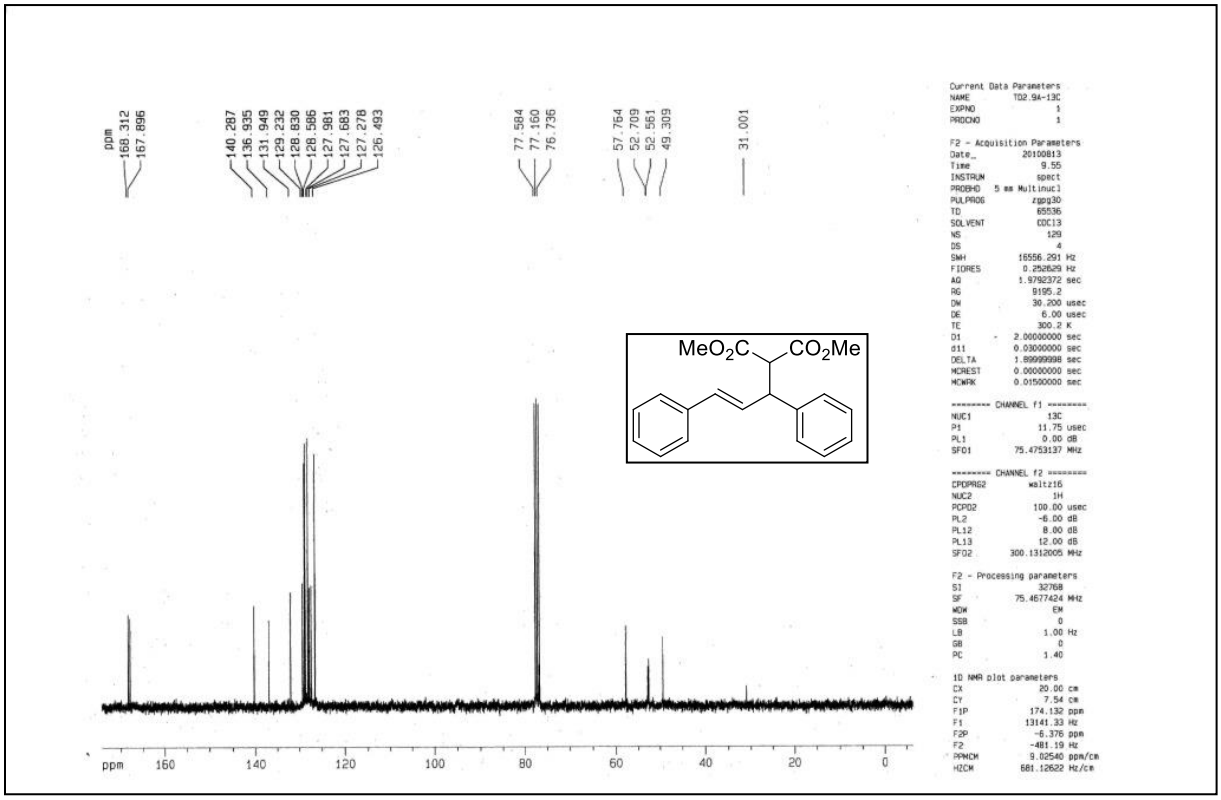
^{19}F NMR Spectrum :

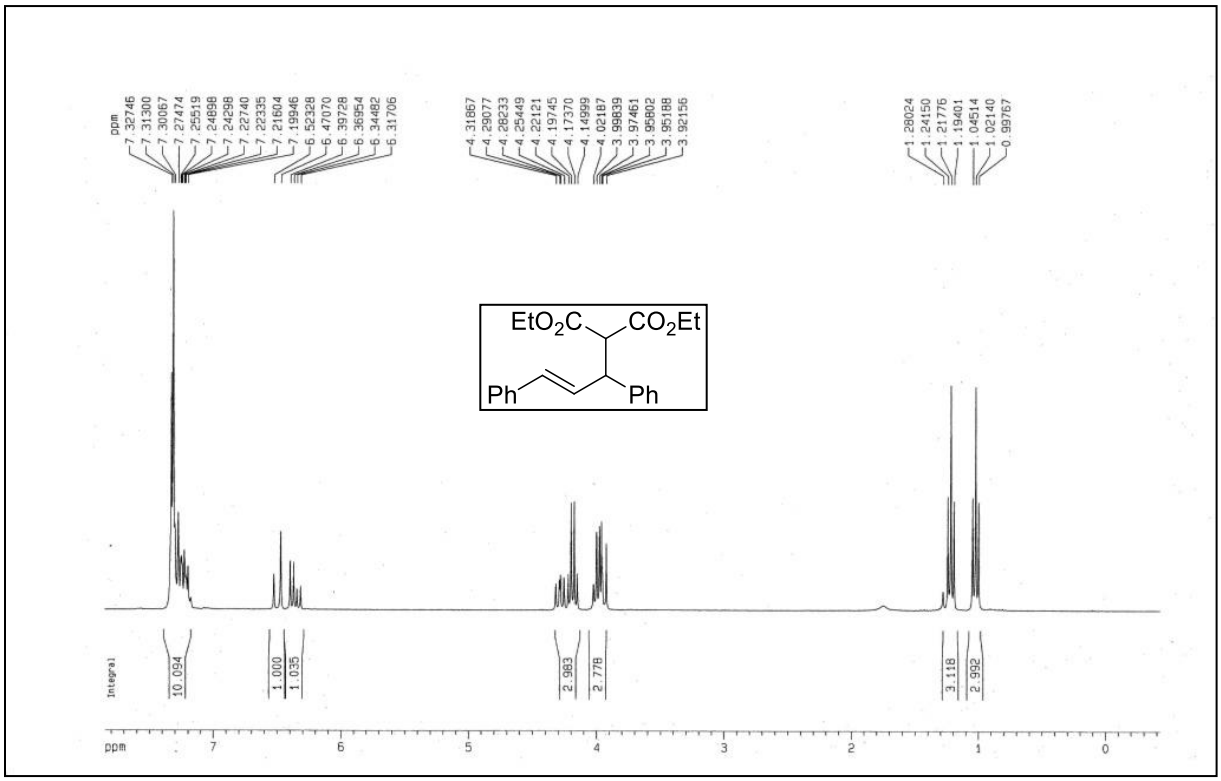


^{31}P NMR Spectrum




ppm
7.24394
7.23405
7.21563
7.19705
7.18410
7.16769
7.15898
7.13919
7.13436
7.11099
6.42676
6.37621
6.29144
6.26339
6.23902
6.21095
4.22331
4.19503
4.18730
4.15908
3.89665
3.86044
3.61856
3.43245
1.60801
MeO2C
CO2Me
Integral
10.005
0.994
0.995
0.985
1.000
2.933
2.936
ppm


ppm
168.312
167.896
140.287
136.935
131.949
129.232
128.830
128.586
127.981
127.683
127.278
126.493
77.584
77.160
76.736
57.764
52.709
52.561
49.309
31.001
MeO2C
CO2Me
Current Data Parameters
NAME TD2.9A-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100813
Time 9.55
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 128
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 75.4677424 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 7.54 cm
F1P 174.132 ppm
F1 13141.33 Hz
F2P -6.376 ppm
F2 -481.19 Hz
PPMCM 9.02540 ppm/cm
HZCM 681.12622 Hz/cm
ppm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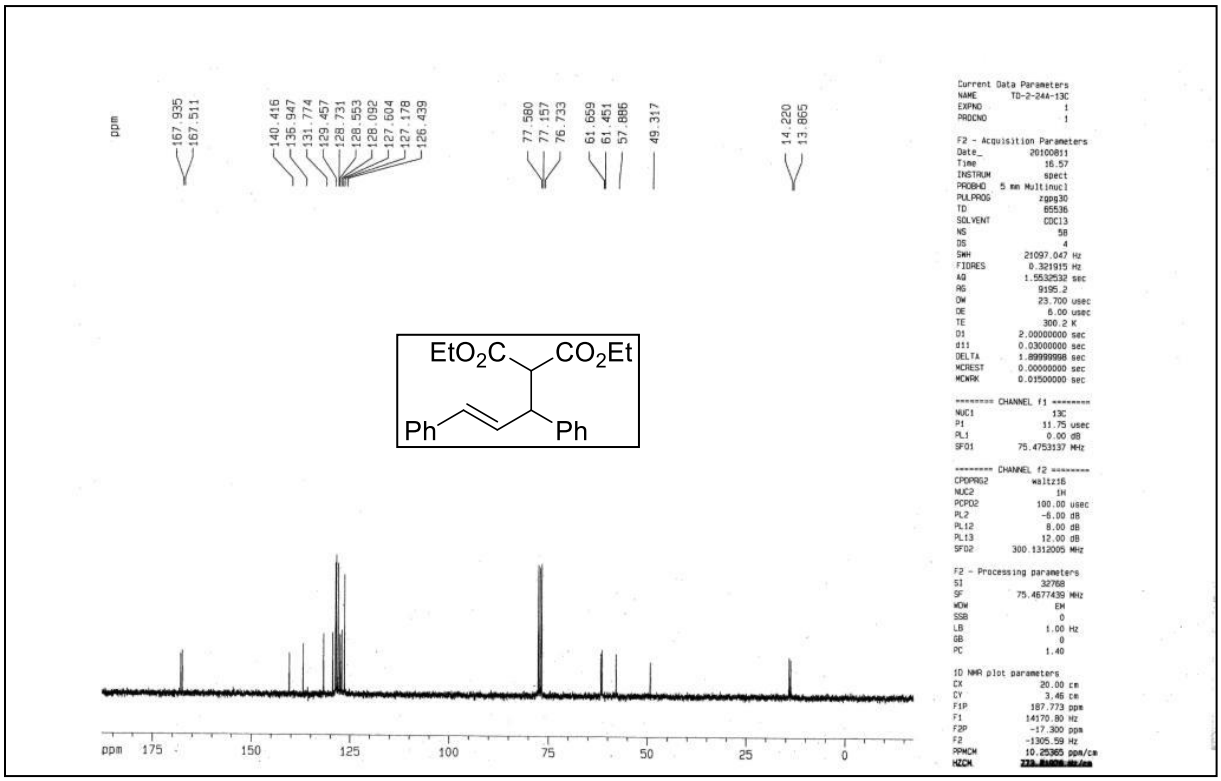
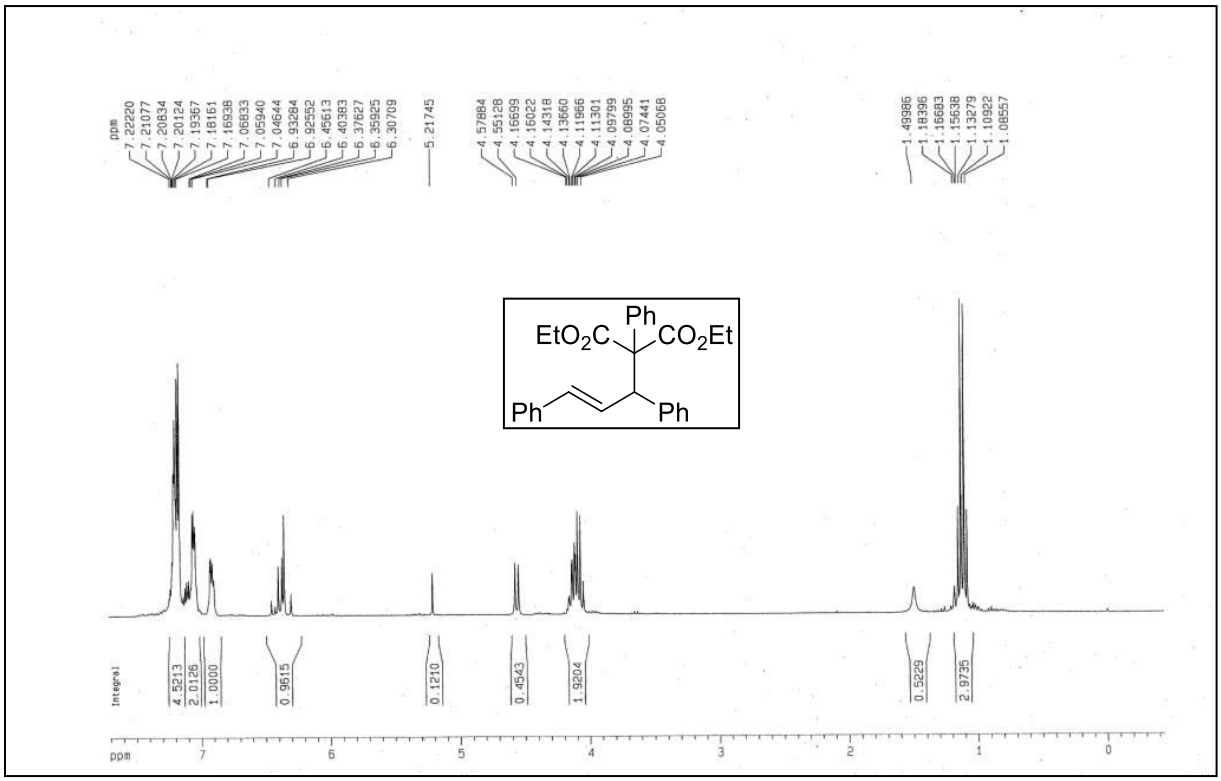
7.31300
7.30067
7.27474
7.25519
7.24898
7.24298
7.22740
7.22335
7.21604
7.19946
6.52328
6.47070
6.39728
6.36954
6.34482
6.31706
4.31867
4.29077
4.28233
4.25449
4.22121
4.19745
4.17370
4.14999
4.02187
3.99839
3.97461
3.95802
3.95188
3.92156
1.28024
1.24150
1.21776
1.19401
1.04514
1.02140
0.99767
EtO2C
CO2Et
Ph
Ph
Integral
10.094
1.000
1.035
2.983
2.778
3.118
2.992
ppm


ppm
167.935
167.511
140.416
136.947
131.774
129.457
128.731
128.553
128.092
127.604
127.178
126.439
77.580
77.157
76.733
61.659
61.451
57.886
49.317
14.220
13.865
EtO2C
CO2Et
Ph
Ph
Current Data Parameters
NAME TD-2-24A-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100811
Time 16.57
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 58
DS 4
SWH 21097.047 Hz
FIDRES 0.321915 Hz
AQ 1.5532532 sec
RG 9195.2
DW 23.700 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 75.4677439 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 3.46 cm
F1P 187.773 ppm
F1 14170.80 Hz
F2P -17.300 ppm
F2 -1305.59 Hz
PPMCM 10.25365 ppm/cm
HZCM 773.81806 Hz/cm
ppm


ppm
7.22220
7.21077
7.20834
7.20124
7.19367
7.18161
7.16938
7.06833
7.05940
7.04644
6.93284
6.92552
6.45613
6.40383
6.37627
6.35925
6.30709
5.21745
4.57884
4.55128
4.16699
4.16022
4.14318
4.13660
4.11966
4.11301
4.09799
4.08995
4.07441
4.05068
1.49986
1.18396
1.16683
1.15638
1.13279
1.10922
1.08557
Ph
EtO2C
CO2Et
Ph
Ph
Integral
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1.0000
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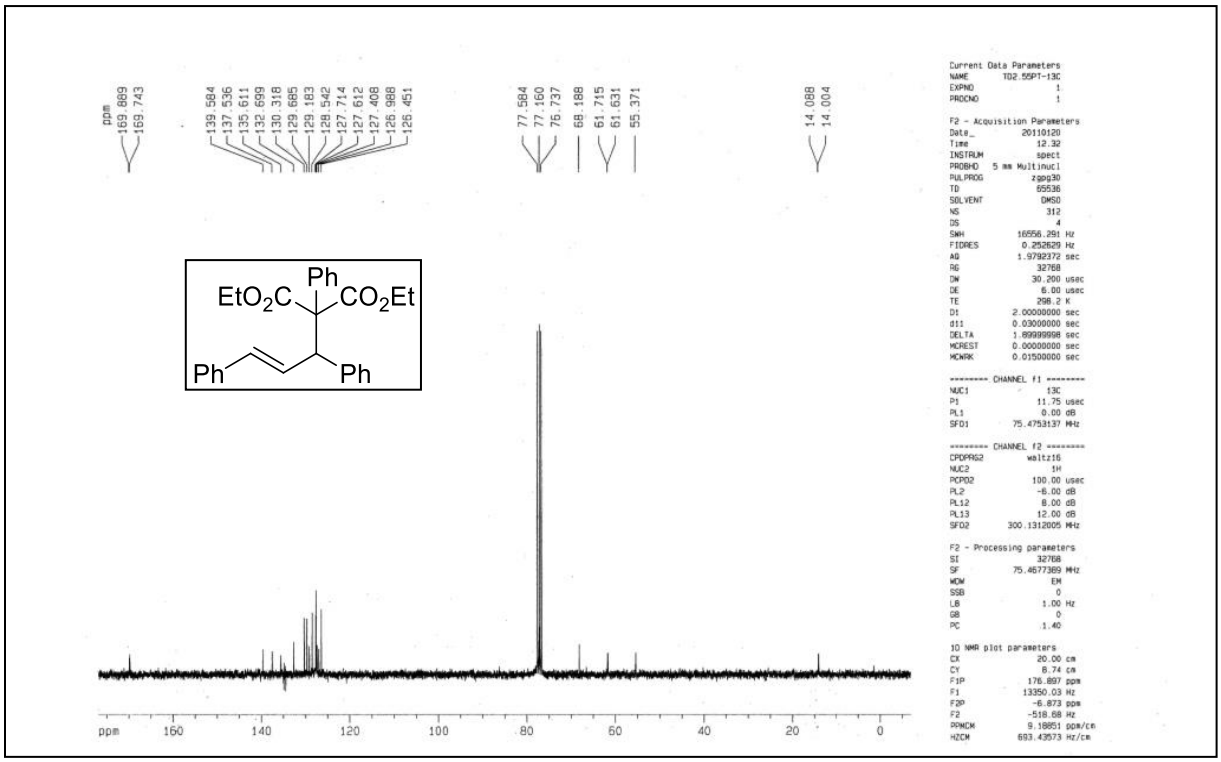
0.1210
0.4543
1.9204
0.5229
2.9735
ppm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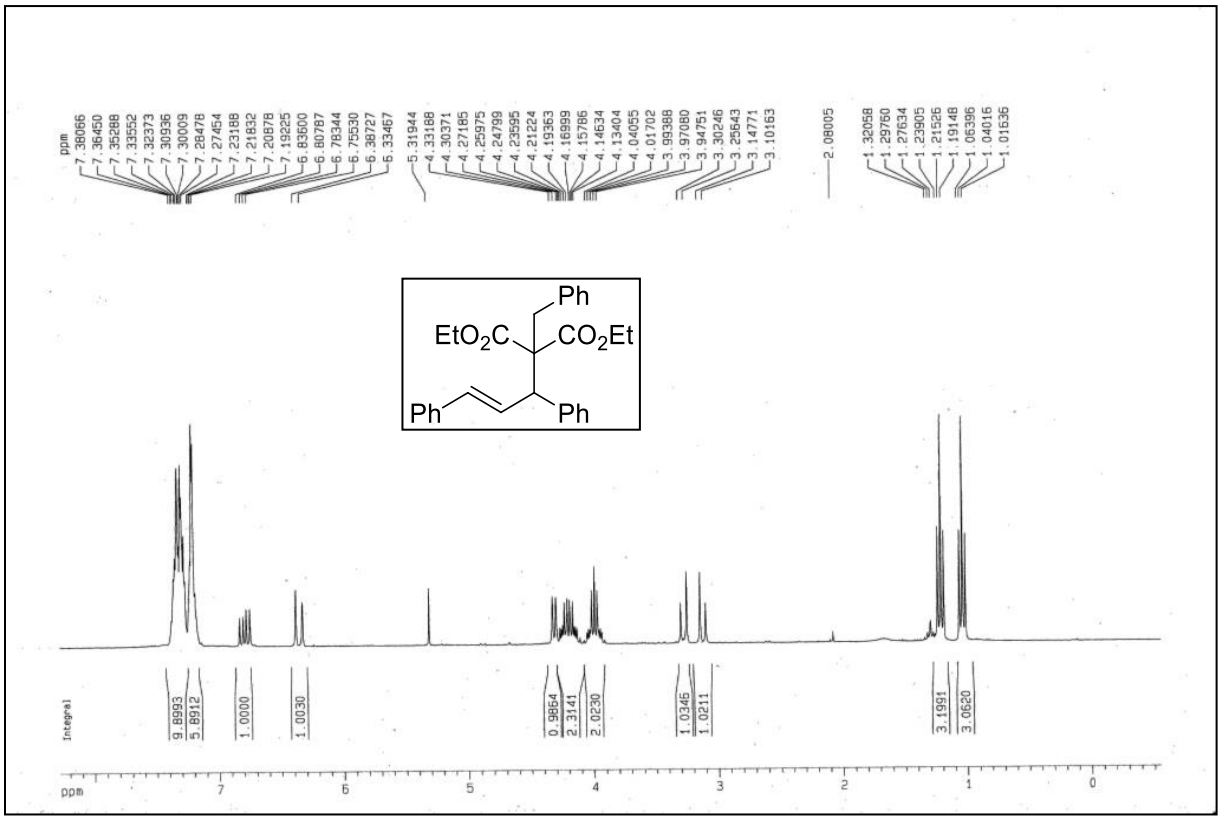
169.743
139.584
137.536
135.611
132.699
130.318
129.685
129.183
128.542
127.714
127.612
127.408
126.988
126.451
77.584
77.160
76.737
68.188
61.715
61.631
55.371
14.088
14.004
Ph
EtO2C
CO2Et
Ph
Ph
ppm
Current Data Parameters
NAME T02.55PT-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110120
Time 12.32
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 312
DS 4
SWH 16556.291 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 32768
DW 30.200 usec
DE 6.00 usec
TE 298.2 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 75.4677389 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 8.74 cm
F1P 176.897 ppm
F1 13350.03 Hz
F2P -6.873 ppm
F2 -518.68 Hz
PPMCM 9.18851 ppm/cm
HZCM 693.43573 Hz/cm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7.36450
7.35288
7.33552
7.32373
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7.28478
7.27454
7.23188
7.21832
7.20878
7.19225
6.83600
6.80787
6.78344
6.75530
6.38727
6.33467
5.31944
4.33188
4.30371
4.27185
4.25975
4.24799
4.23595
4.21224
4.19363
4.16999
4.15786
4.14634
4.13404
4.04055
4.01702
3.99388
3.97080
3.94751
3.30246
3.25643
3.14771
3.10163
2.08005
1.32058
1.29760
1.27634
1.23905
1.21526
1.19148
1.06396
1.04016
1.01636
Ph
EtO2C
CO2Et
Ph
Ph
Integral
9.8993
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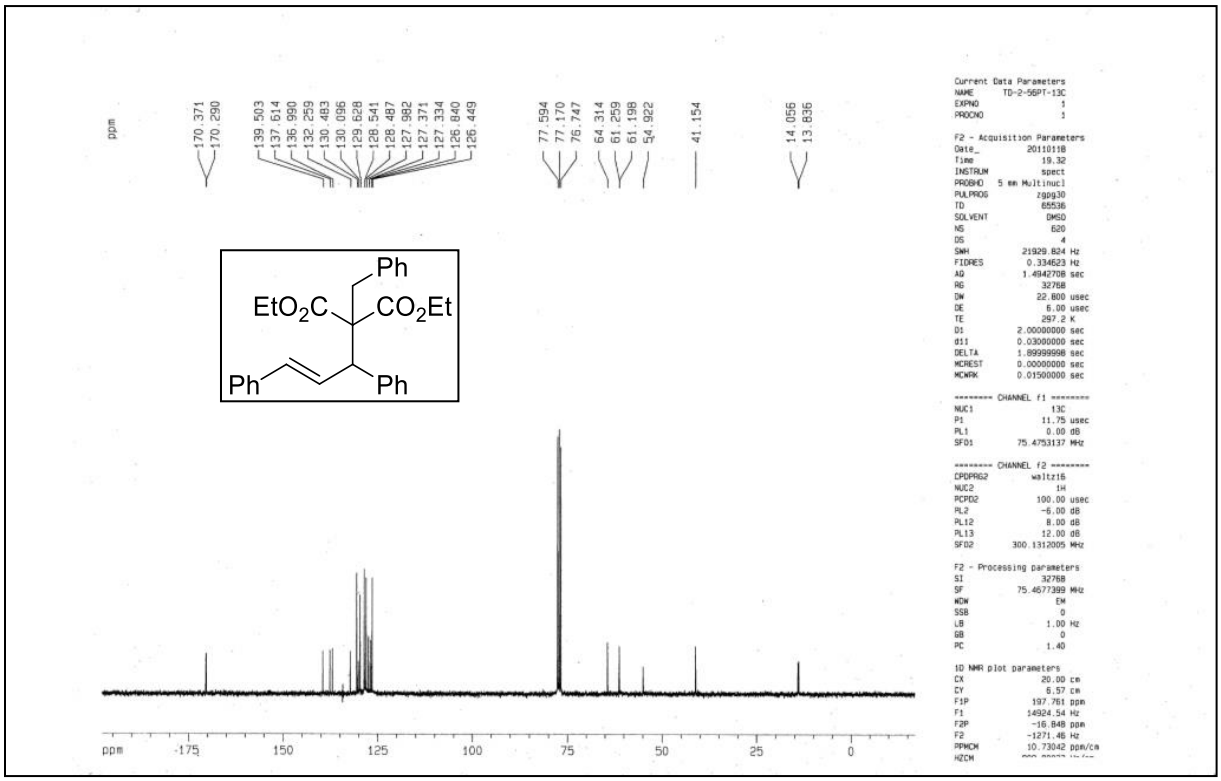
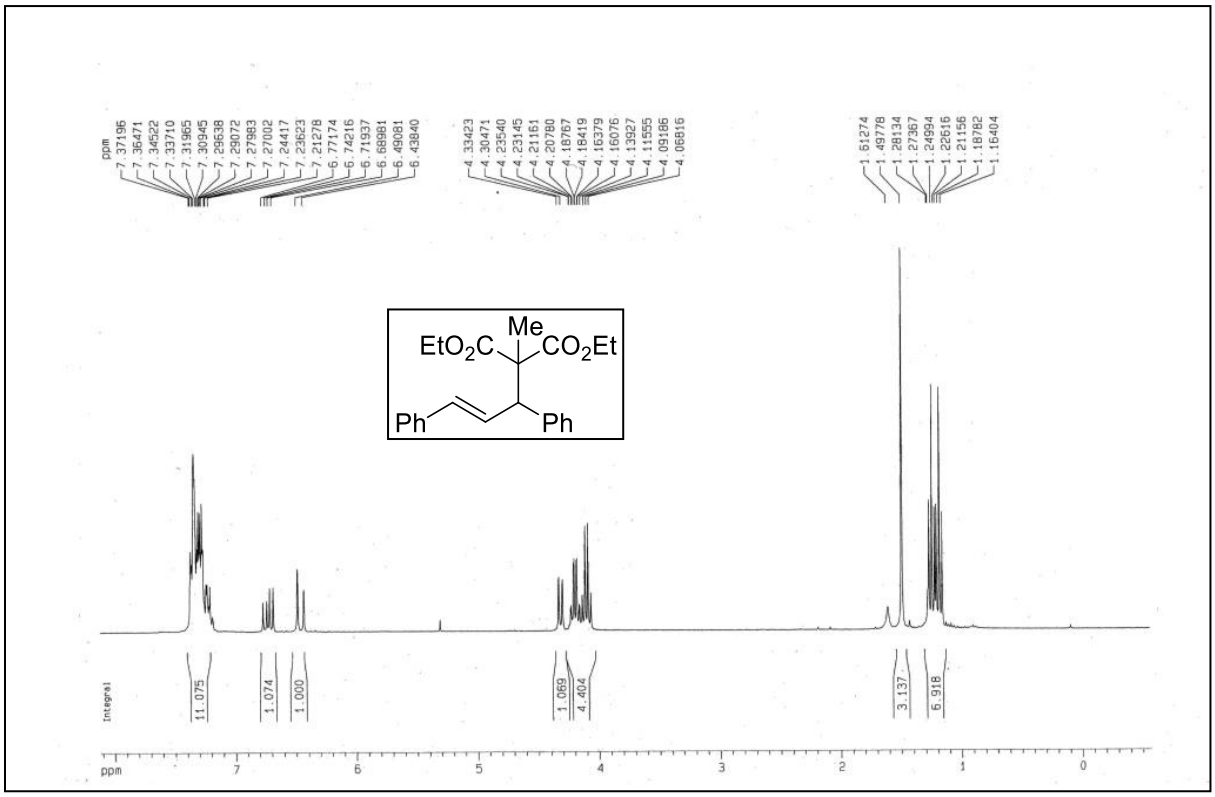
2.0230
1.0346
1.0211
3.1991
3.0620
ppm


ppm
170.371
170.290
139.503
137.614
136.990
132.259
130.483
130.096
129.628
128.541
128.487
127.982
127.371
127.334
126.840
126.449
77.594
77.170
76.747
64.314
61.259
61.198
54.922
41.154
14.056
13.836
Ph
EtO2C
CO2Et
Ph
Ph
Current Data Parameters
NAME TD-2-56PT-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110118
Time 19.32
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 820
DS 4
SWH 21929.824 Hz
FIDRES 0.334623 Hz
AQ 1.4942708 sec
RG 32768
DW 22.800 usec
DE 6.00 usec
TE 297.2 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
SF01 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
SF02 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677399 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 6.57 cm
F1P 197.761 ppm
F1 14924.54 Hz
F2P -16.848 ppm
F2 -1271.46 Hz
PPMCM 10.73042 ppm/cm
HZCM
ppm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7.33710
7.31965
7.30945
7.29638
7.29072
7.27983
7.27002
7.24417
7.23623
7.21278
6.77174
6.74216
6.71937
6.68981
6.49081
6.43840
4.33423
4.30471
4.23540
4.23145
4.21161
4.20780
4.18767
4.18419
4.16379
4.16076
4.13927
4.11555
4.09186
4.06816
1.61274
1.49778
1.28134
1.27367
1.24994
1.22616
1.21156
1.18782
1.16404
Me
EtO2C
CO2Et
Ph
Ph
Integral
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1.074
1.000
1.069
4.404
3.137
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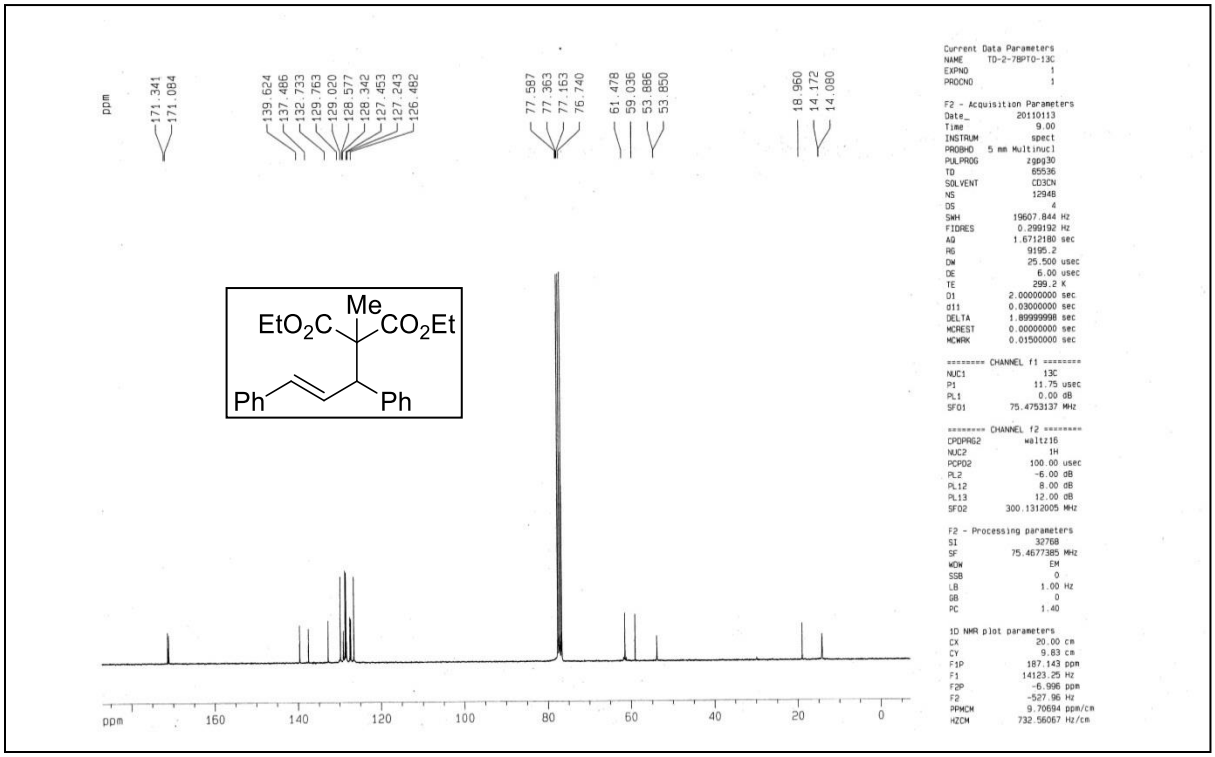
ppm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137.486
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129.763
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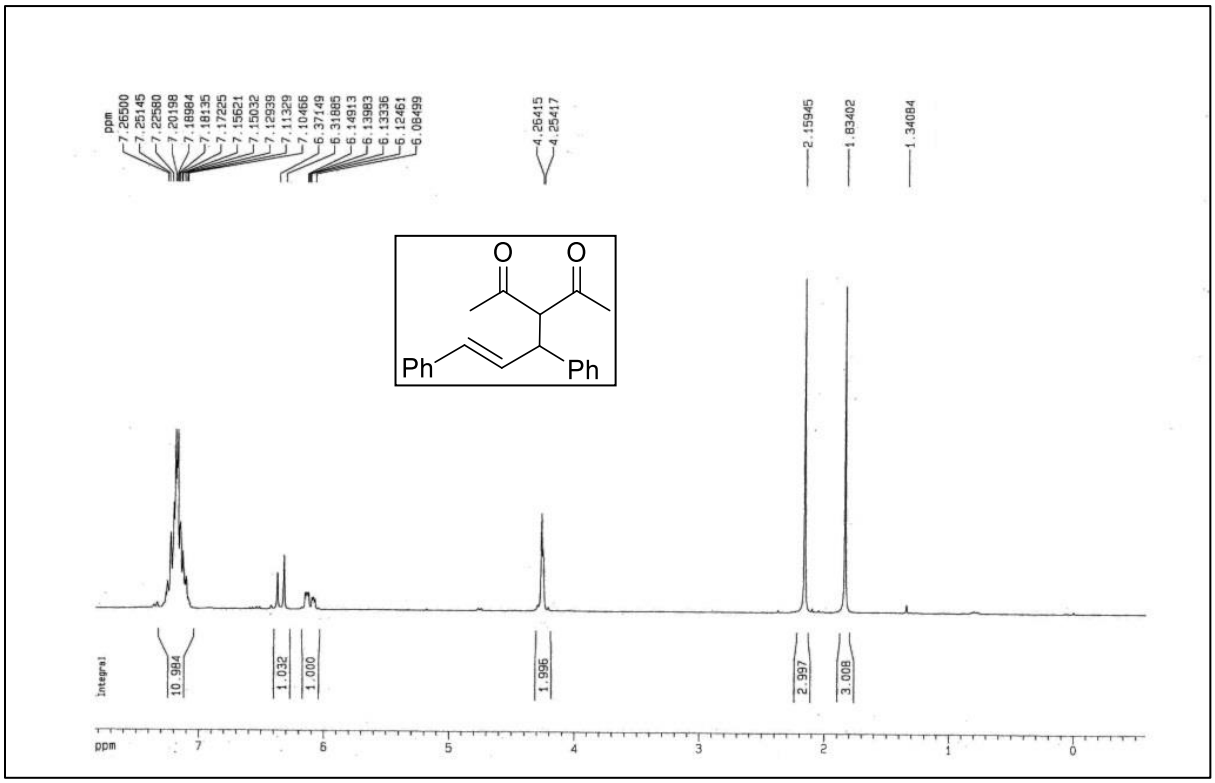
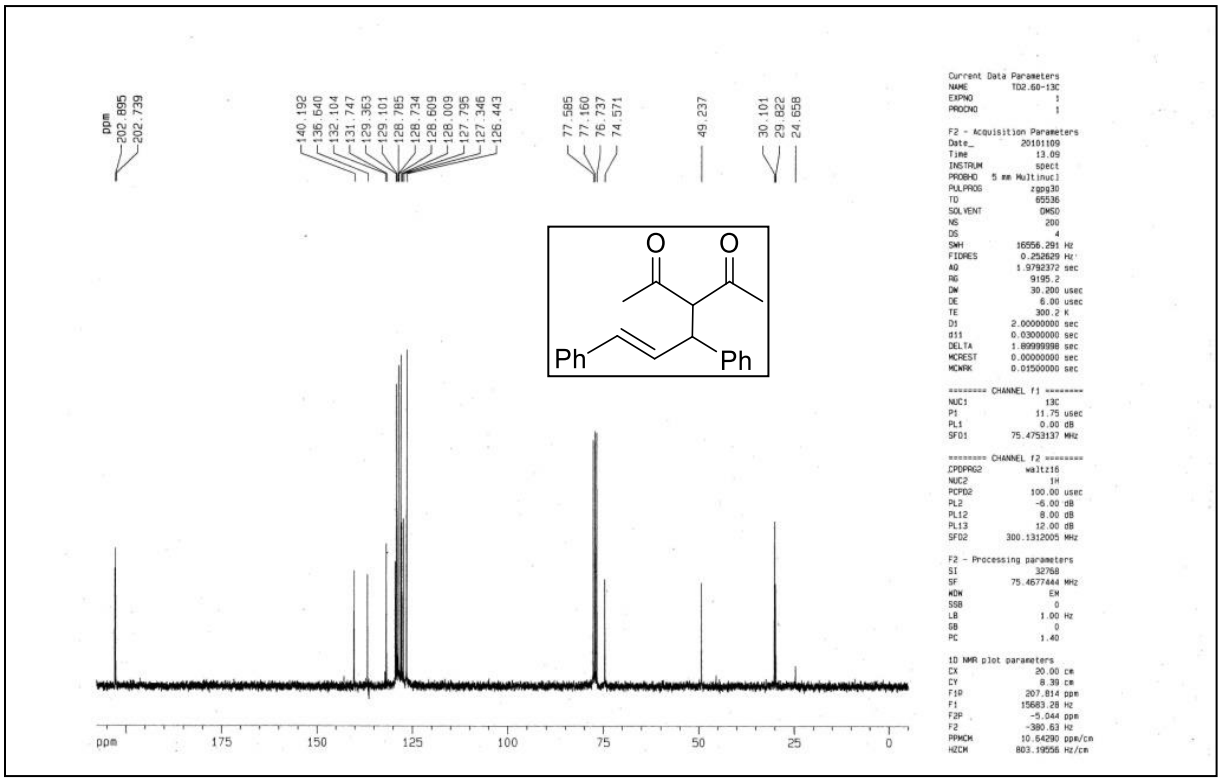
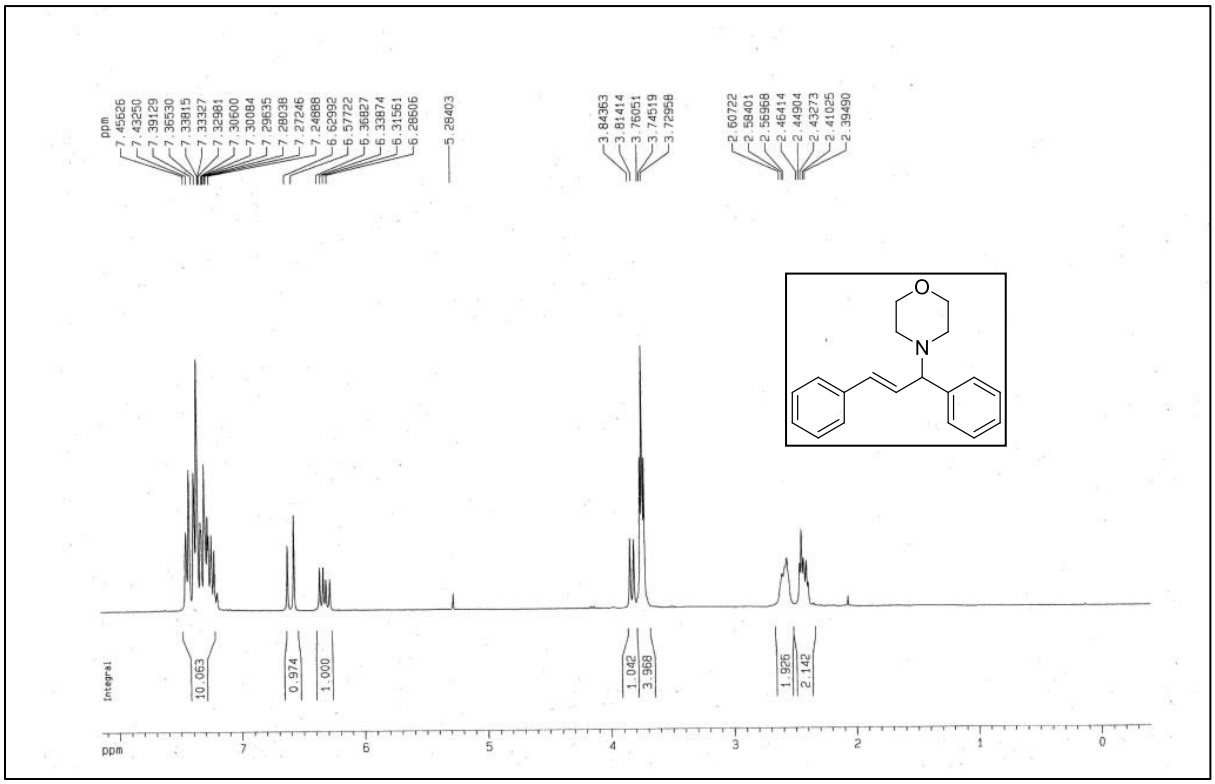
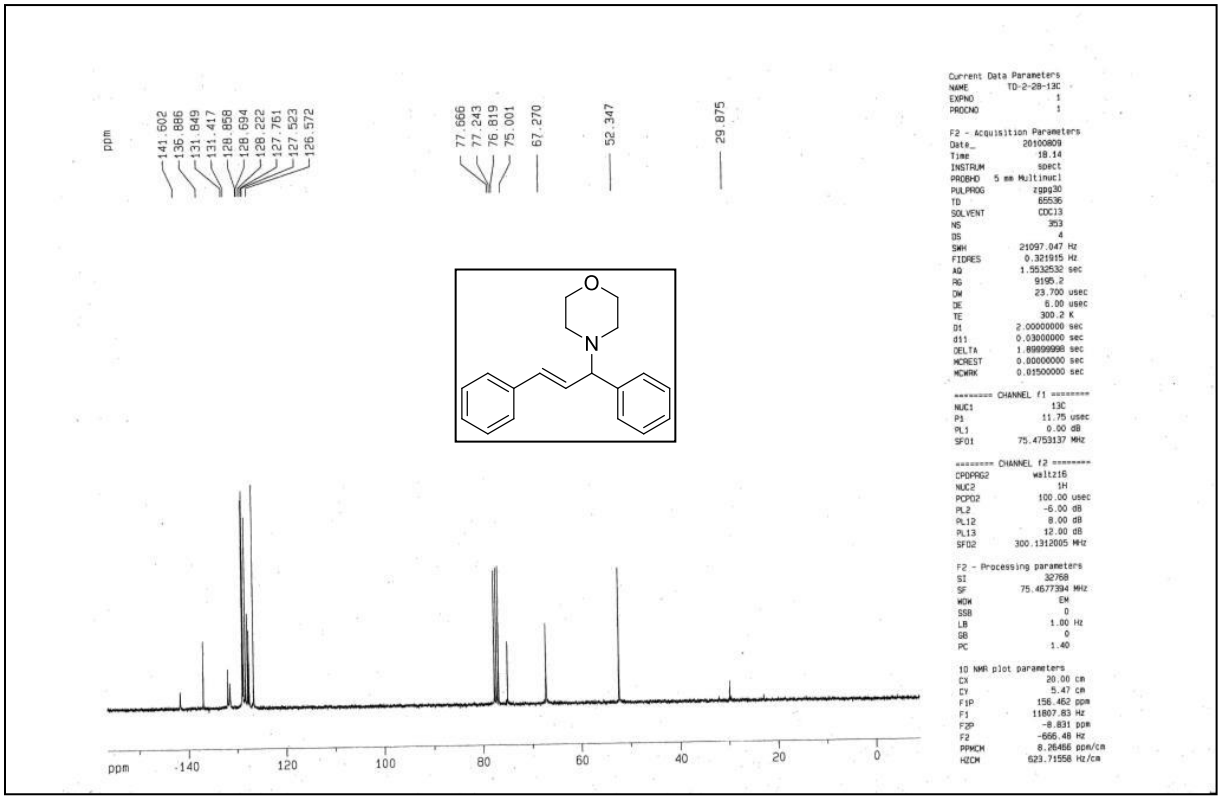
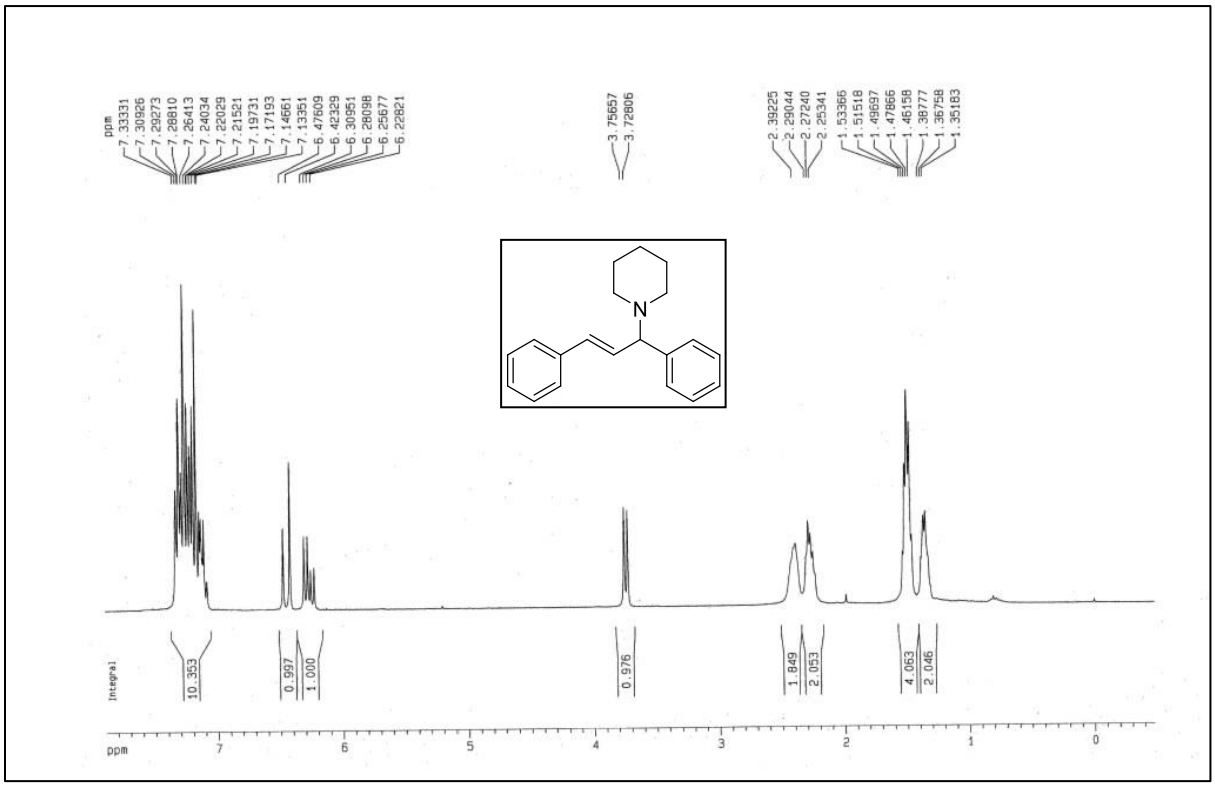
128.577
128.342
127.453
127.243
126.482
77.587
77.363
77.163
76.740
61.478
59.036
53.886
53.850
18.960
14.172
14.080
Me
EtO2C
CO2Et
Ph
Ph
ppm
Current Data Parameters
NAME TD-2-7BPTO-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110113
Time 9.00
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CD3CN
NS 1294
DS 4
SWH 19607.844 Hz
FIDRES 0.299192 Hz
AQ 1.6712180 sec
RG 9195.2
DW 25.500 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 75.4753137 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 75.4677385 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 9.83 cm
F1P 187.143 ppm
F1 14123.25 Hz
F2P -6.996 ppm
F2 -527.96 Hz
PPMCM 9.70694 ppm/cm
HZCM 732.56067 Hz/cm

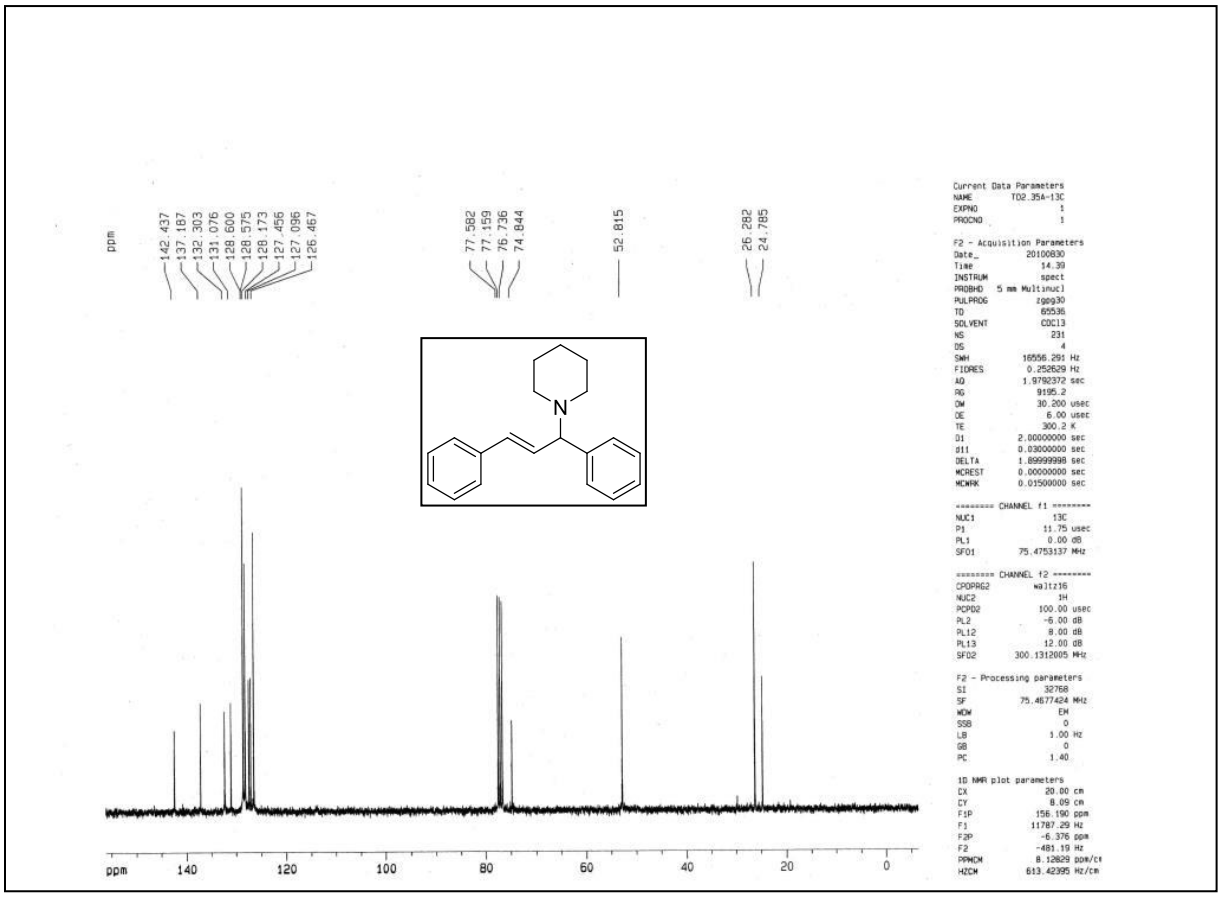

ppm
7.26500
7.25145
7.22580
7.20198
7.18984
7.18135
7.17225
7.15621
7.15032
7.12939
7.11329
7.10466
6.37149
6.31885
6.14913
6.13983
6.13336
6.12461
6.08499
4.26415
4.25417
2.15945
1.83402
1.34084
O
O
Ph
Ph
Integral
10.984
1.032
1.000
1.996
2.997
3.008
ppm

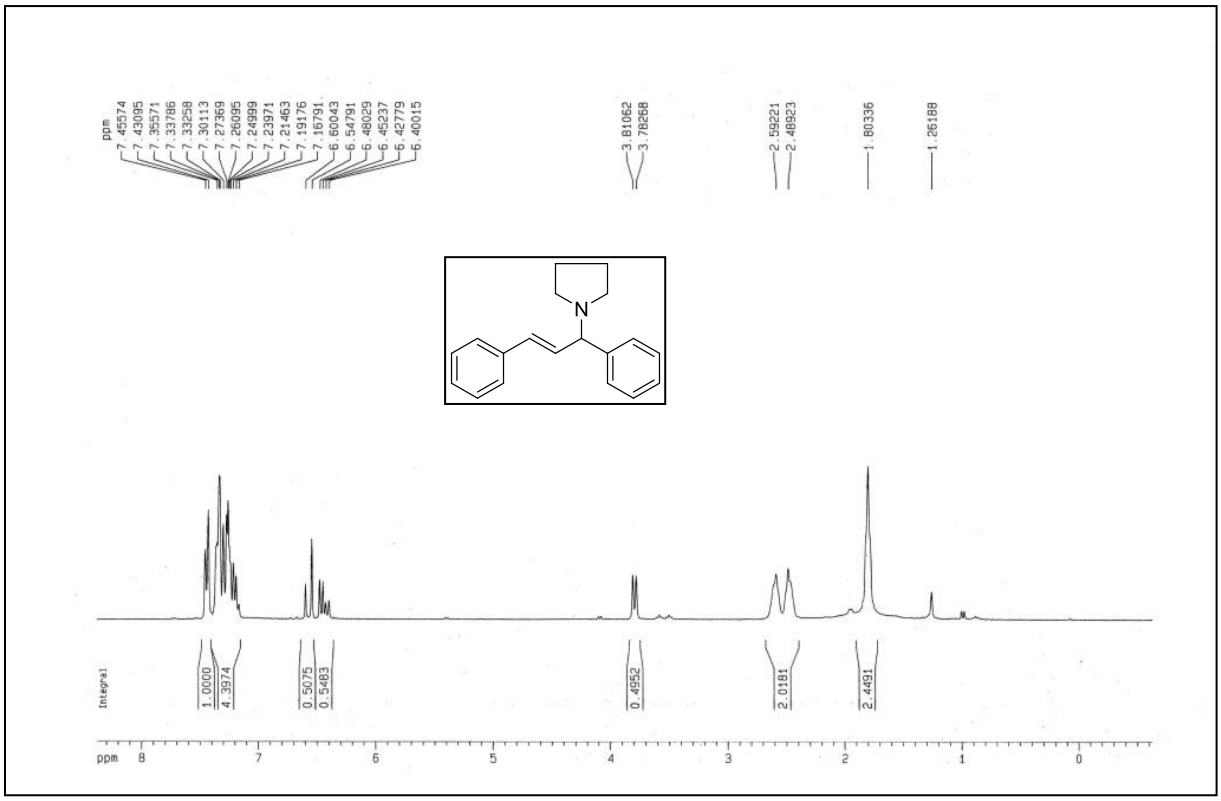

ppm
202.895
202.739
140.192
136.640
132.104
131.747
129.363
129.101
128.785
128.734
128.609
128.009
127.795
127.346
126.443
77.585
77.160
76.737
74.571
49.237
30.101
29.822
24.658
O
O
Ph
Ph
Current Data Parameters
NAME TD2.60-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20191109
Time 13.09
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 200
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 75.4677444 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 8.39 cm
F1P 207.814 ppm
F1 15683.28 Hz
F2P -5.044 ppm
F2 -380.63 Hz
PPMCM 10.64290 ppm/cm
HZCM 803.19556 Hz/cm

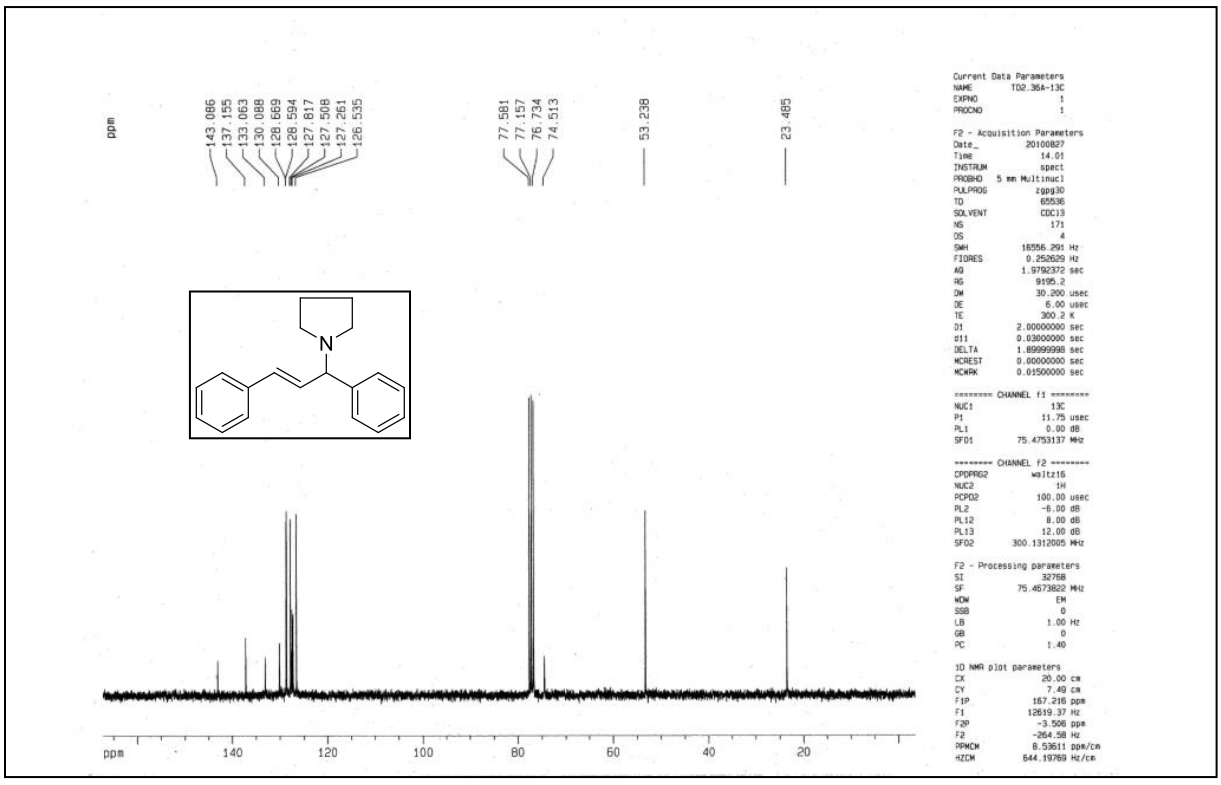

ppm
7.45626
7.43250
7.39129
7.36530
7.33815
7.33327
7.32981
7.30600
7.30084
7.29635
7.28038
7.27246
7.24888
6.62992
6.57722
6.36827
6.33874
6.31561
6.28606
5.28403
3.84363
3.81414
3.76051
3.74519
3.72958
2.60722
2.59401
2.56968
2.46414
2.44904
2.43273
2.41025
2.39490
Integral
10.063
0.974
1.000
1.042
3.968
1.926
2.142
ppm
7
6
5
4
3
2
1
0

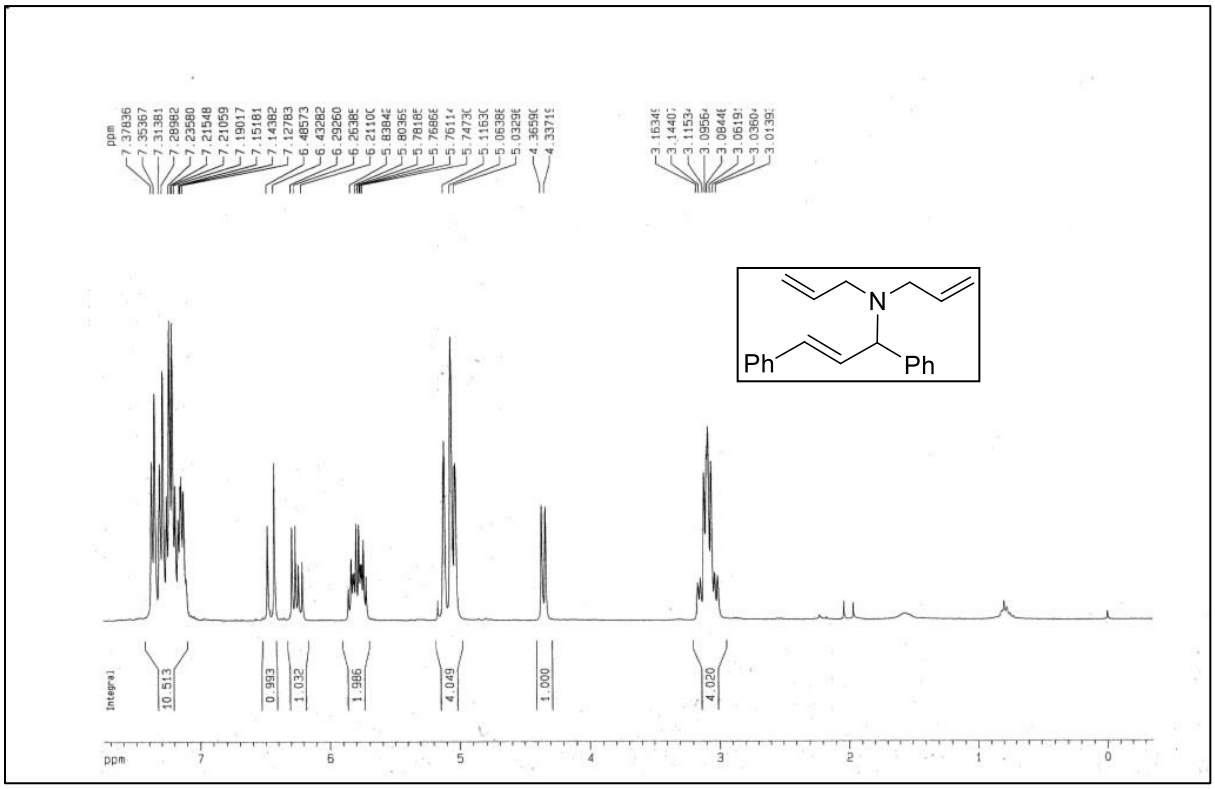

ppm
141.602
136.886
131.849
131.417
128.858
128.694
128.222
127.761
127.523
126.572
77.666
77.243
76.819
75.001
67.270
52.347
29.875
Current Data Parameters
NAME TD-2-28-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100809
Time 18.14
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 353
DS 4
SWH 21097.047 Hz
FIDRES 0.321915 Hz
AQ 1.5532532 sec
RG 9195.2
DW 23.700 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 75.4677394 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 5.47 cm
F1P 156.462 ppm
F1 11807.83 Hz
F2P -8.831 ppm
F2 -666.48 Hz
PPMCM 8.26466 ppm/cm
HZCM 623.71558 Hz/cm
ppm
140
120
100
80
60
40
20
0

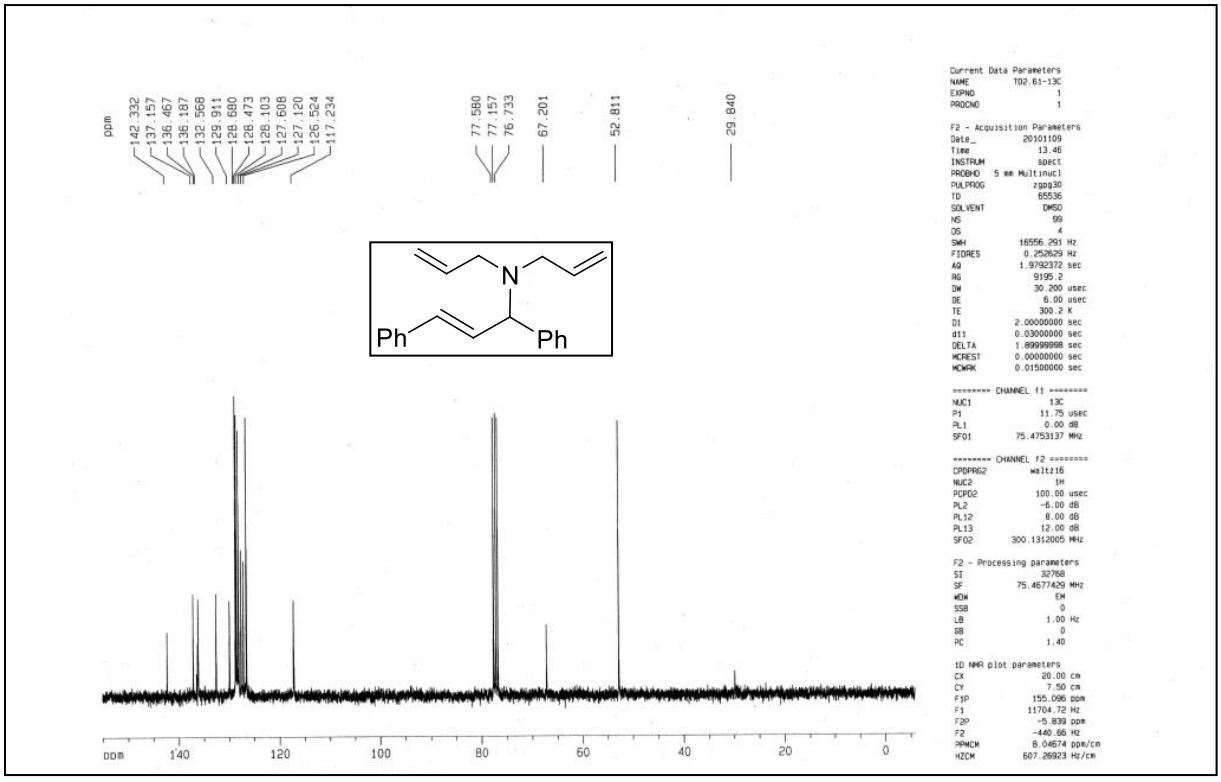

ppm
7.33331
7.30926
7.29273
7.28810
7.26413
7.24034
7.22029
7.21521
7.19731
7.17193
7.14661
7.13351
6.47609
6.42329
6.30951
6.28098
6.25677
6.22821
3.75657
3.72806
2.39225
2.29044
2.27240
2.25341
1.53366
1.51518
1.49697
1.47866
1.46158
1.38777
1.36758
1.35183
Integral
10.353
0.997
1.000
0.976
1.849
2.053
4.063
2.046
ppm

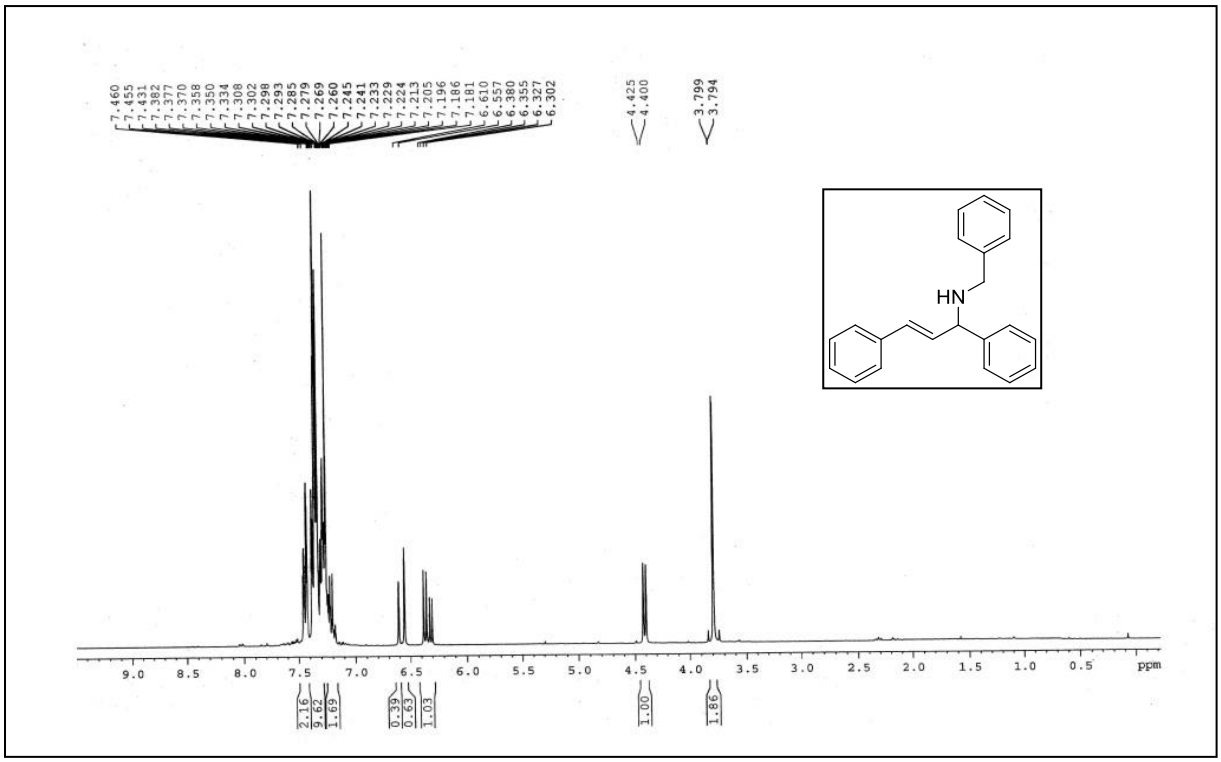

ppm
142.437
137.187
132.303
131.076
128.600
128.575
128.173
127.456
127.096
126.467
77.582
77.159
76.736
74.844
52.815
26.282
24.785
Current Data Parameters
NAME T02.35A-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100830
Time 14.39
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 231
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 75.4677424 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 8.09 cm
F1P 156.190 ppm
F1 11787.29 Hz
F2P -6.376 ppm
F2 -481.19 Hz
PPMCM 8.12829 ppm/cm
HZCM 613.42395 Hz/cm

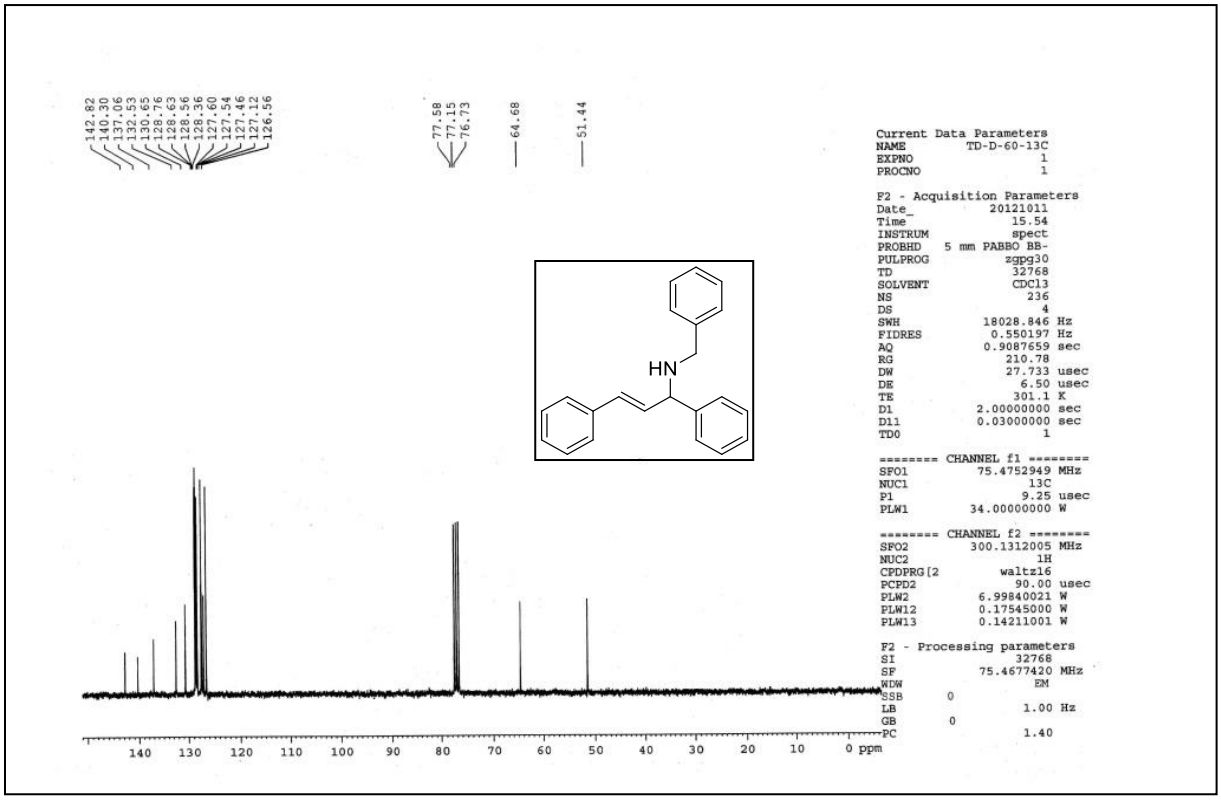

ppm
7.45574
7.43095
7.35571
7.33786
7.33258
7.30113
7.27369
7.26095
7.24999
7.23971
7.21463
7.19176
7.16791
6.60043
6.54791
6.48029
6.45237
6.42779
6.40015
3.81062
3.78268
2.59221
2.48923
1.80336
1.26188
N
Integral
1.0000
4.3974
0.5075
0.5483
0.4952
2.0181
2.4491
ppm 8 7 6 5 4 3 2 1 0

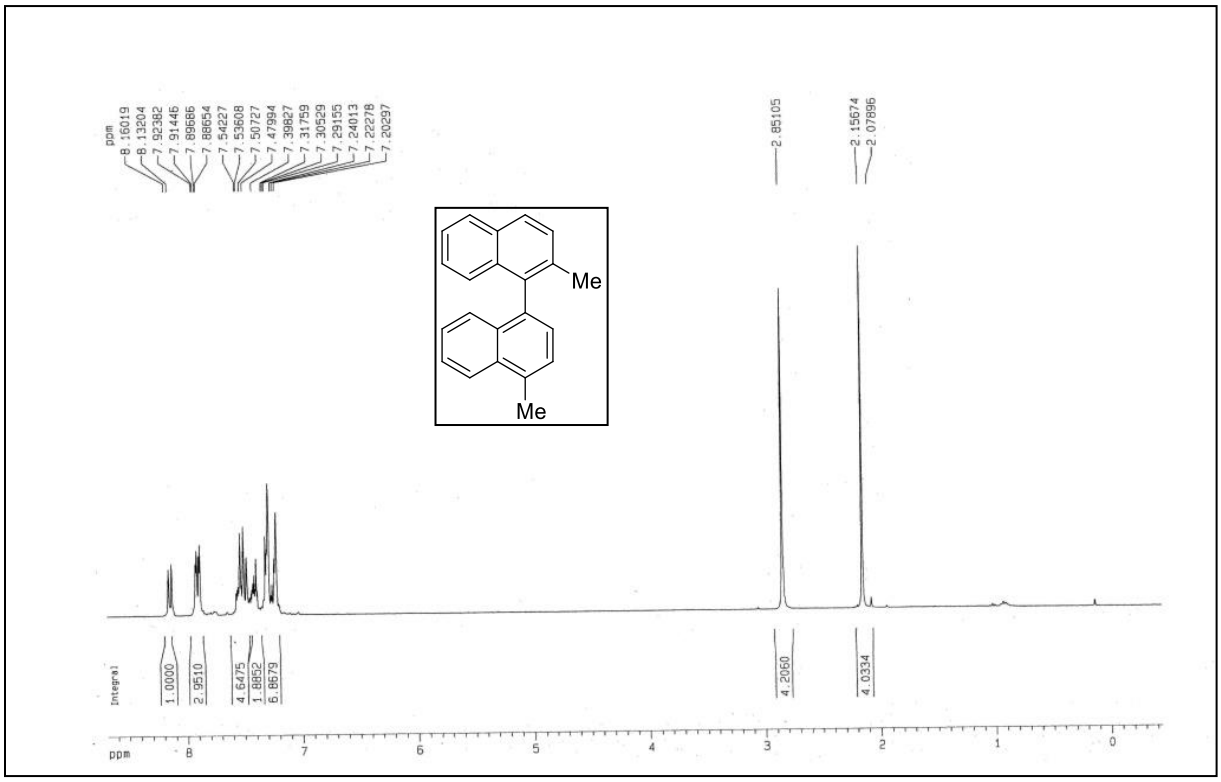

ppm
143.086
137.155
133.063
130.088
128.669
128.594
127.817
127.508
127.261
126.535
77.581
77.157
76.734
74.513
53.238
23.485
N
ppm 140 120 100 80 60 40 20
Current Data Parameters
NAME TD2.36A-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100827
Time 14.01
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 171
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
SF01 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
SF02 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4673822 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 7.49 cm
F1P 167.216 ppm
F1 12619.37 Hz
F2P -3.506 ppm
F2 -264.58 Hz
PPMCM 8.53611 ppm/cm
HZCM 644.19769 Hz/cm

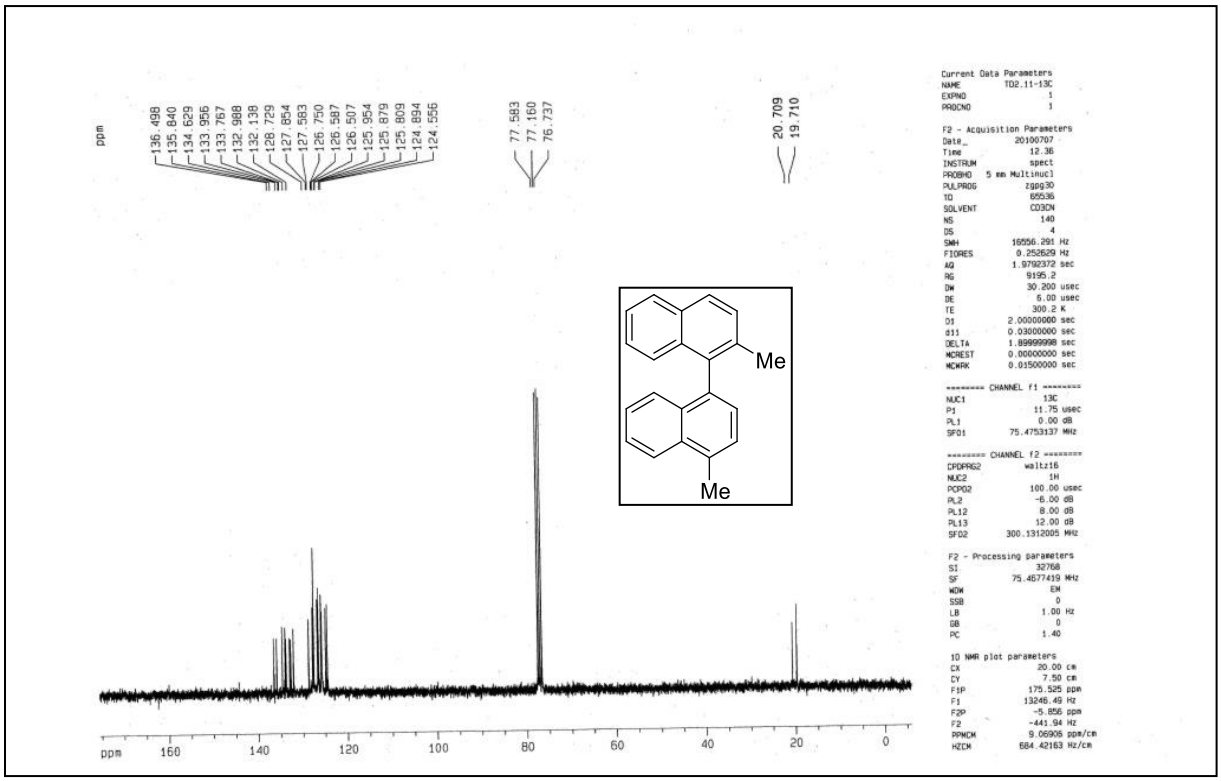

ppm
7.37836
7.35367
7.31381
7.28982
7.23580
7.21548
7.21059
7.19017
7.15181
7.14382
7.12783
6.48573
6.43282
6.29260
6.26385
6.21100
5.83842
5.80365
5.78185
5.76865
5.76114
5.74736
5.11630
5.06388
5.03298
4.36590
4.33715
3.16345
3.14407
3.11534
3.09564
3.08448
3.06195
3.03604
3.01395
N
Ph
Ph
Integral
10.513
0.993
1.032
1.986
4.049
1.000
4.020
ppm
7
6
5
4
3
2
1
0

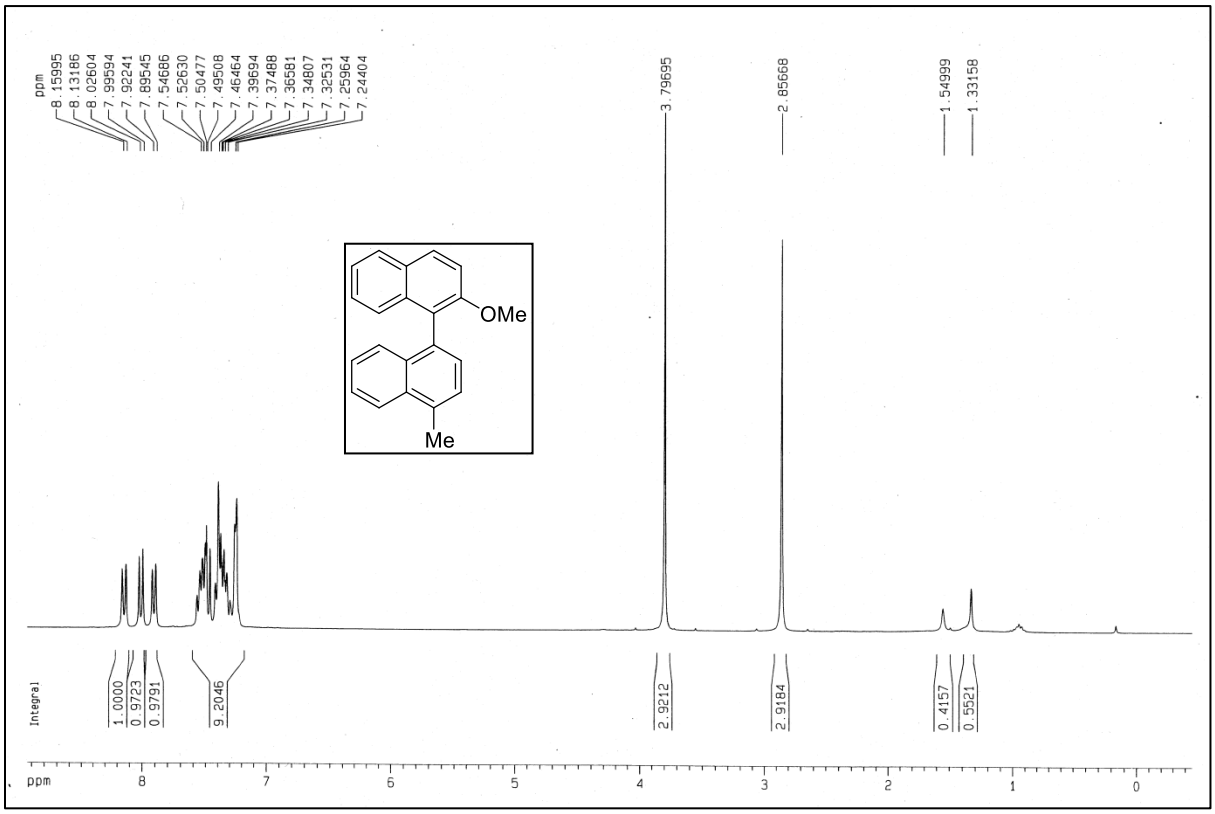

ppm
142.332
137.157
136.467
136.187
132.568
129.911
128.680
128.473
128.103
127.608
127.120
126.524
117.234
77.580
77.157
76.733
67.201
52.811
29.840
N
Ph
Ph
ppm
140
120
100
80
60
40
20
0
Current Data Parameters
NAME TD2.61-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20101109
Time 13.46
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 99
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
SF01 75.4753137 MHz
======== CHANNEL f2 ========
DPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 8.00 dB
PL13 12.00 dB
SF02 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677429 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 7.50 cm
F1P 155.096 ppm
F1 11704.72 Hz
F2P -5.839 ppm
F2 -440.66 Hz
PPMCM 8.04674 ppm/cm
HZCM 607.26923 Hz/cm

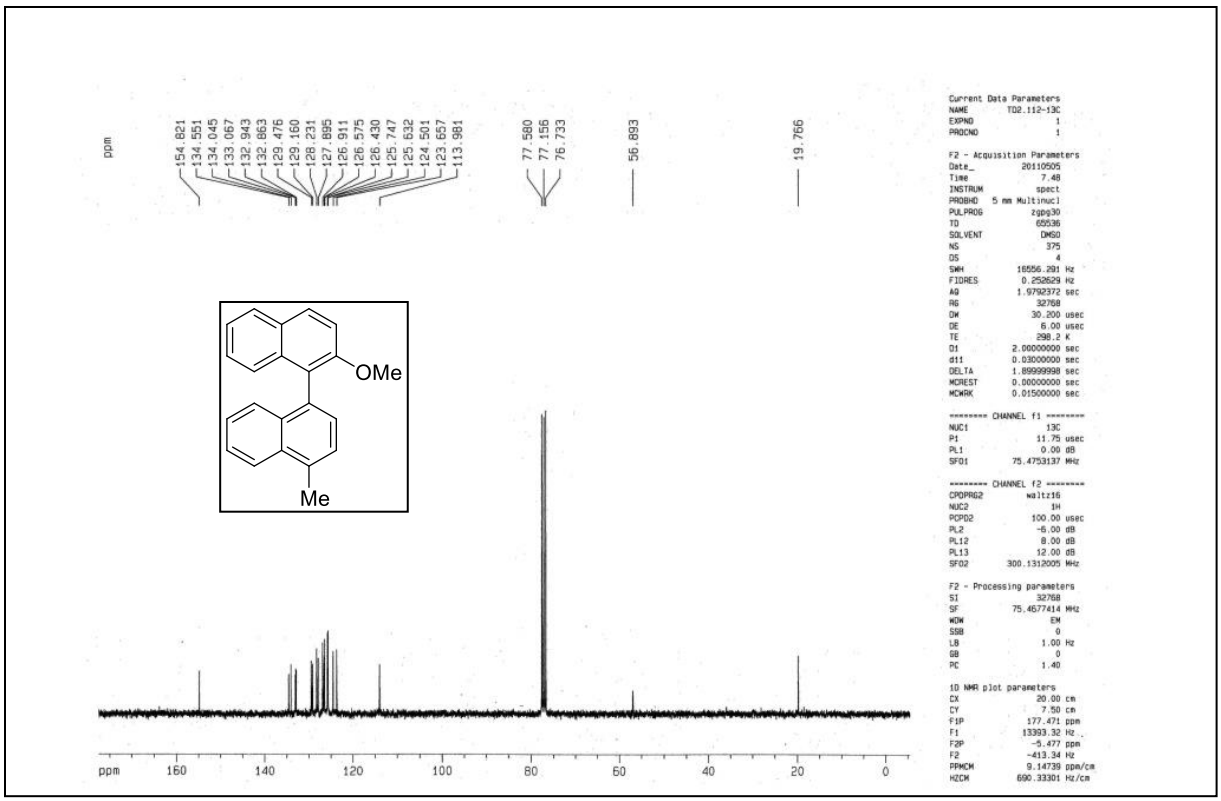

7.460
7.455
7.431
7.382
7.377
7.370
7.358
7.350
7.334
7.308
7.302
7.298
7.293
7.285
7.279
7.269
7.260
7.245
7.241
7.233
7.229
7.224
7.213
7.205
7.196
7.186
7.181
6.610
6.557
6.380
6.355
6.327
6.302
4.425
4.400
3.799
3.794
HN
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
2.16
9.62
1.69
0.39
0.63
1.03
1.00
1.86

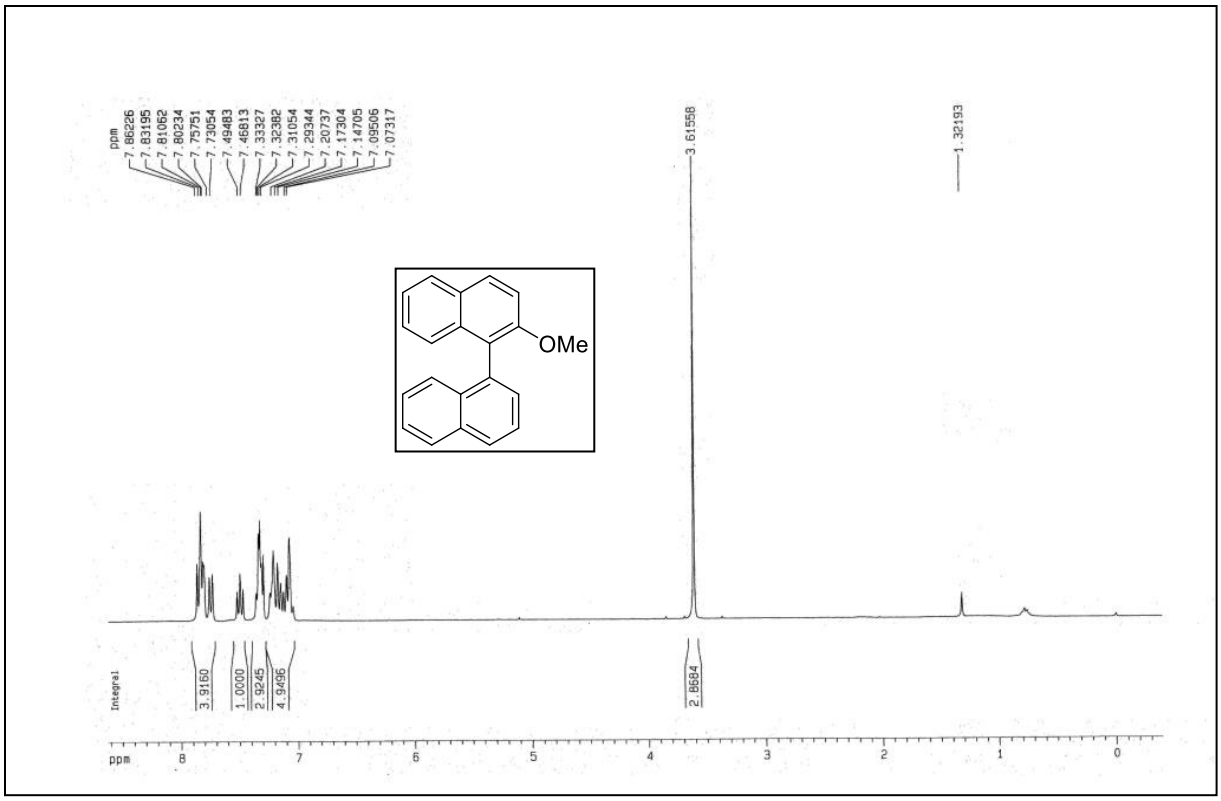

142.82
140.30
137.06
132.53
130.65
128.76
128.63
128.56
128.36
127.60
127.54
127.46
127.12
126.56
77.58
77.15
76.73
64.68
51.44
HN
140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm
Current Data Parameters
NAME TD-D-60-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20121011
Time 15.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 236
DS 4
SWH 18028.846 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 210.78
DW 27.733 usec
DE 6.50 usec
TE 301.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 75.4752949 MHz
NUC1 13C
P1 9.25 usec
PLW1 34.00000000 W
======== CHANNEL f2 ========
SFO2 300.1312005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 6.99840021 W
PLW12 0.17545000 W
PLW13 0.14211001 W
F2 - Processing parameters
SI 32768
SF 75.4677420 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

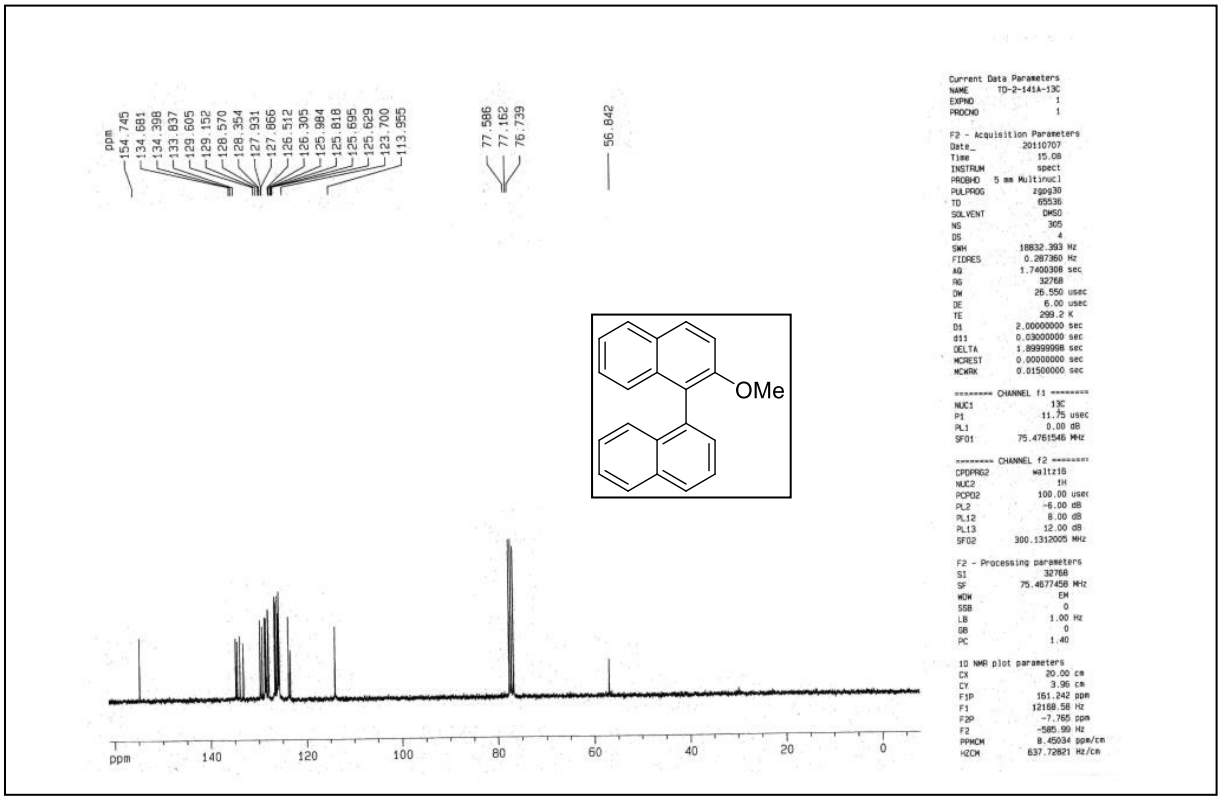

ppm
8.16019
8.13204
7.92382
7.91446
7.89666
7.88654
7.54227
7.53608
7.50727
7.47994
7.39827
7.31759
7.30529
7.29155
7.24013
7.22278
7.20297
2.85105
2.15674
2.07896
Me
Me
Integral
1.0000
2.9510
4.6475
1.8852
6.8679
4.2060
4.0334
ppm
8
7
6
5
4
3
2
1
0

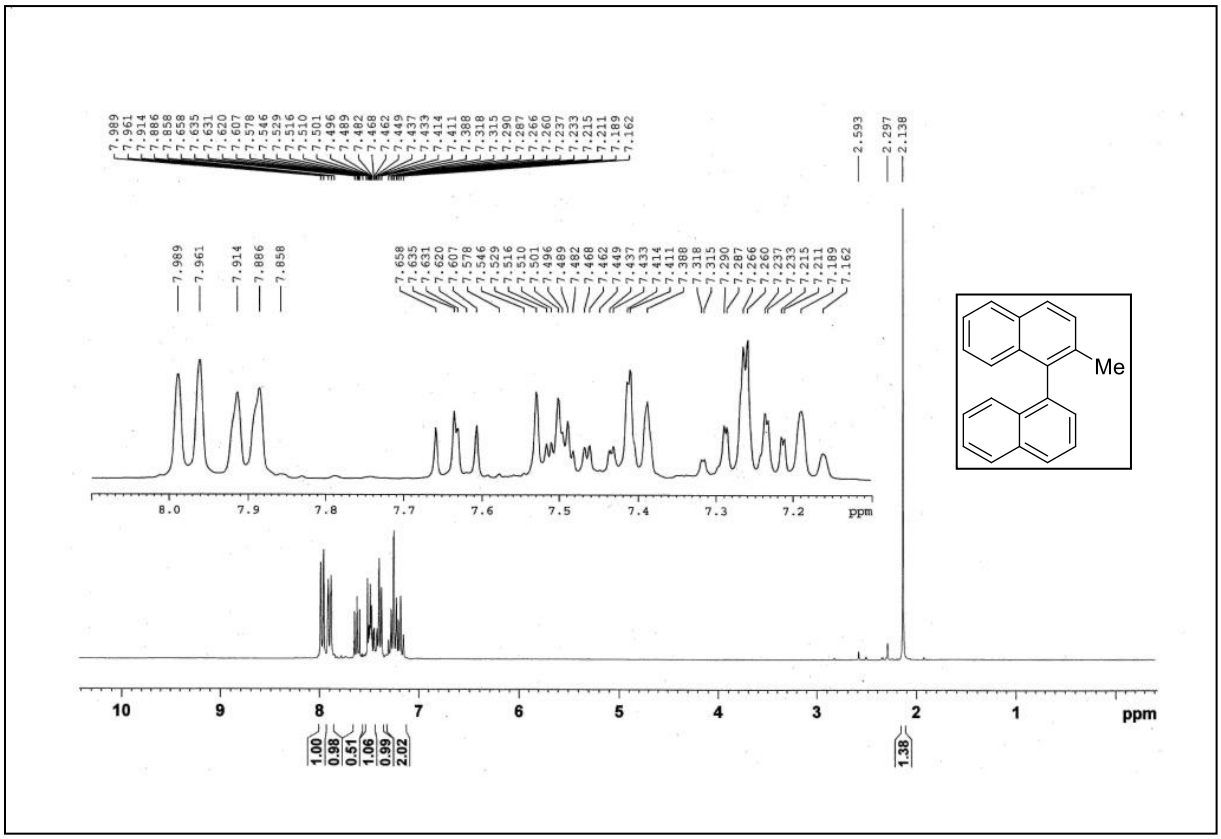

ppm
136.498
135.840
134.629
133.956
133.767
132.988
132.138
128.729
127.854
127.583
126.750
126.587
126.507
125.954
125.879
125.809
124.894
124.556
77.583
77.160
76.737
20.709
19.710
Me
Me
ppm
160
140
120
100
80
60
40
20
0
Current Data Parameters
NAME TD2.11-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100707
Time 12.36
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CD3CN
NS 140
DS 4
SWH 18556.291 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 75.4677419 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 7.50 cm
F1P 175.525 ppm
F1 13248.49 Hz
F2P -5.856 ppm
F2 -441.94 Hz
PPMCM 9.06905 ppm/cm
HZCM 684.42163 Hz/cm

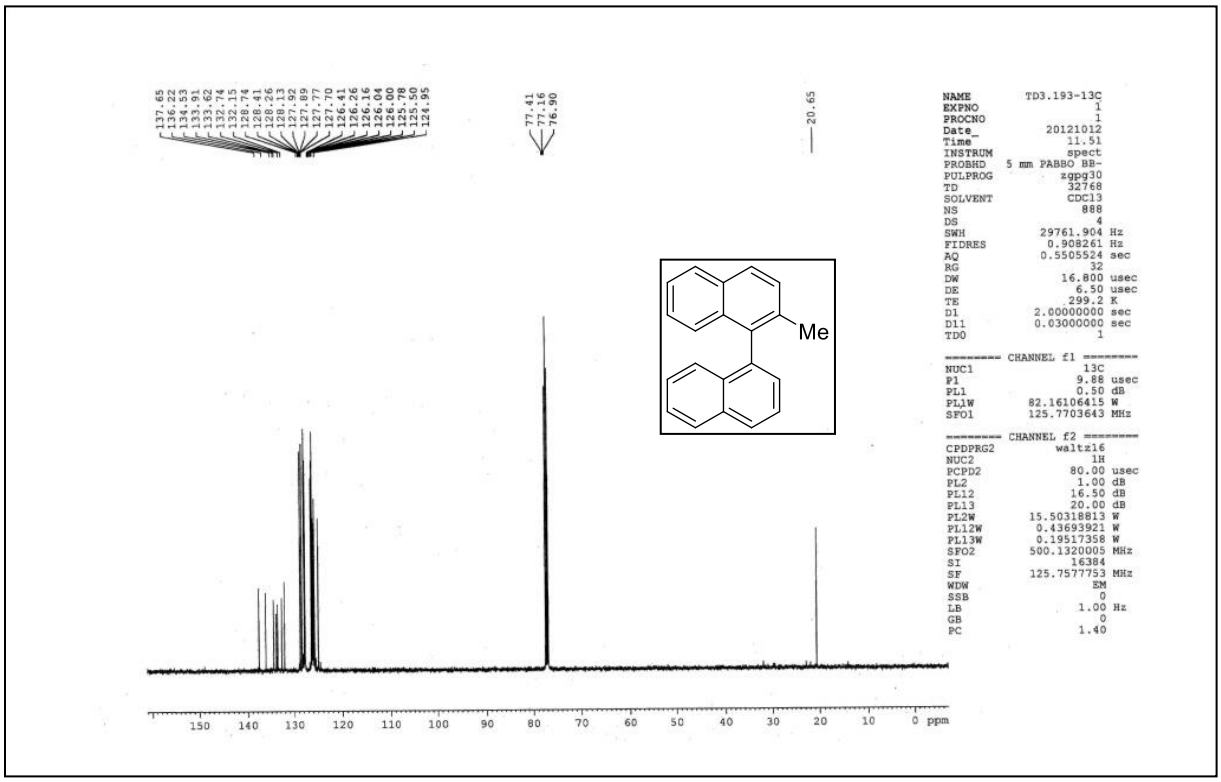

ppm
8.15995
8.13186
8.02604
7.99594
7.92241
7.89545
7.54686
7.52630
7.50477
7.49508
7.46464
7.39694
7.37488
7.36581
7.34807
7.32531
7.25964
7.24404
3.79695
2.85668
1.54999
1.33158
OMe
Me
Integral
1.0000
0.9723
0.9791
9.2046
2.9212
2.9184
0.4157
0.5521
ppm

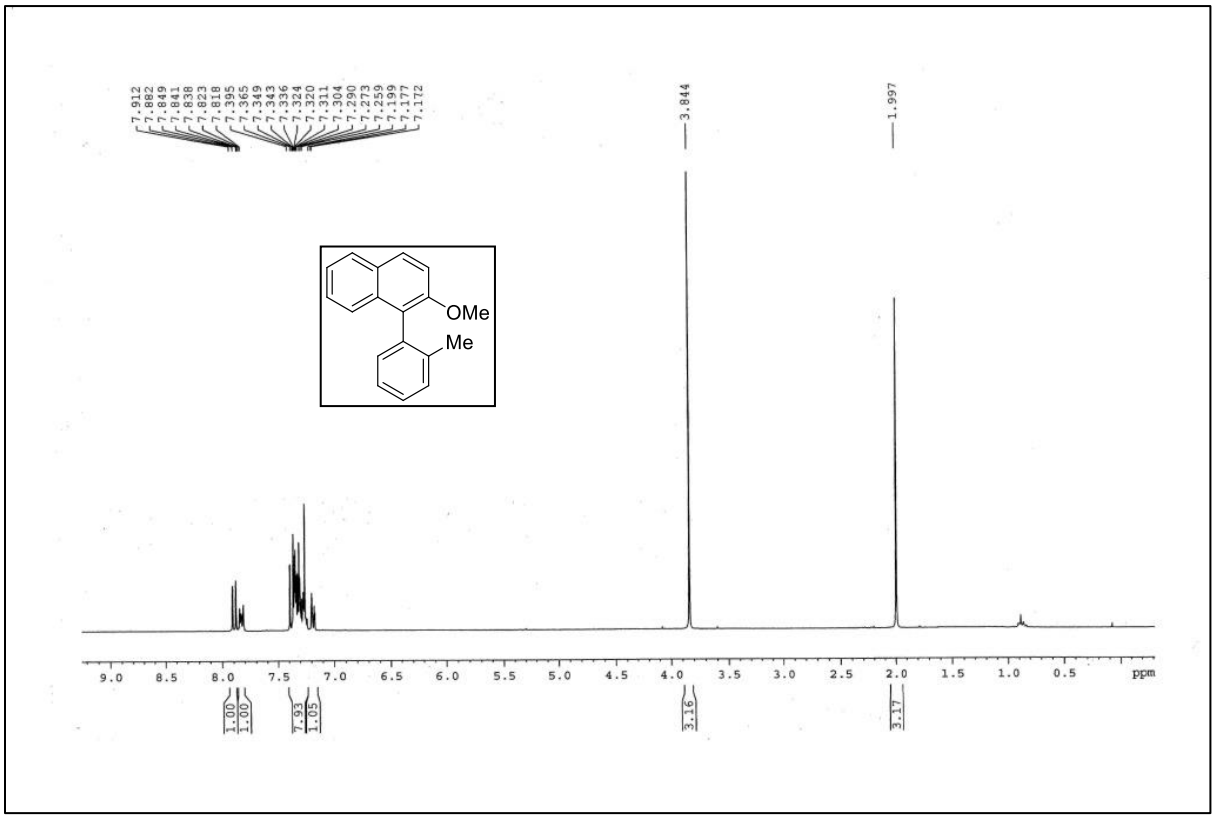

ppm
154.821
134.551
134.045
133.067
132.943
132.863
129.476
129.160
128.231
127.885
126.911
126.575
126.430
125.747
125.632
124.501
123.657
113.981
77.580
77.156
76.733
56.893
19.766
OMe
Me
ppm
Current Data Parameters
NAME TD2.112-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110505
Time 7.48
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 375
DS 4
SWH 16556.291 Hz
FIDRES 0.252629 Hz
AQ 1.9792372 sec
RG 32768
DW 30.200 usec
DE 6.00 usec
TE 298.2 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 75.4677414 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 7.50 cm
F1P 177.471 ppm
F1 13393.32 Hz
F2P -5.477 ppm
F2 -413.34 Hz
PPMCM 9.14739 ppm/cm
HZCM 690.33301 Hz/cm

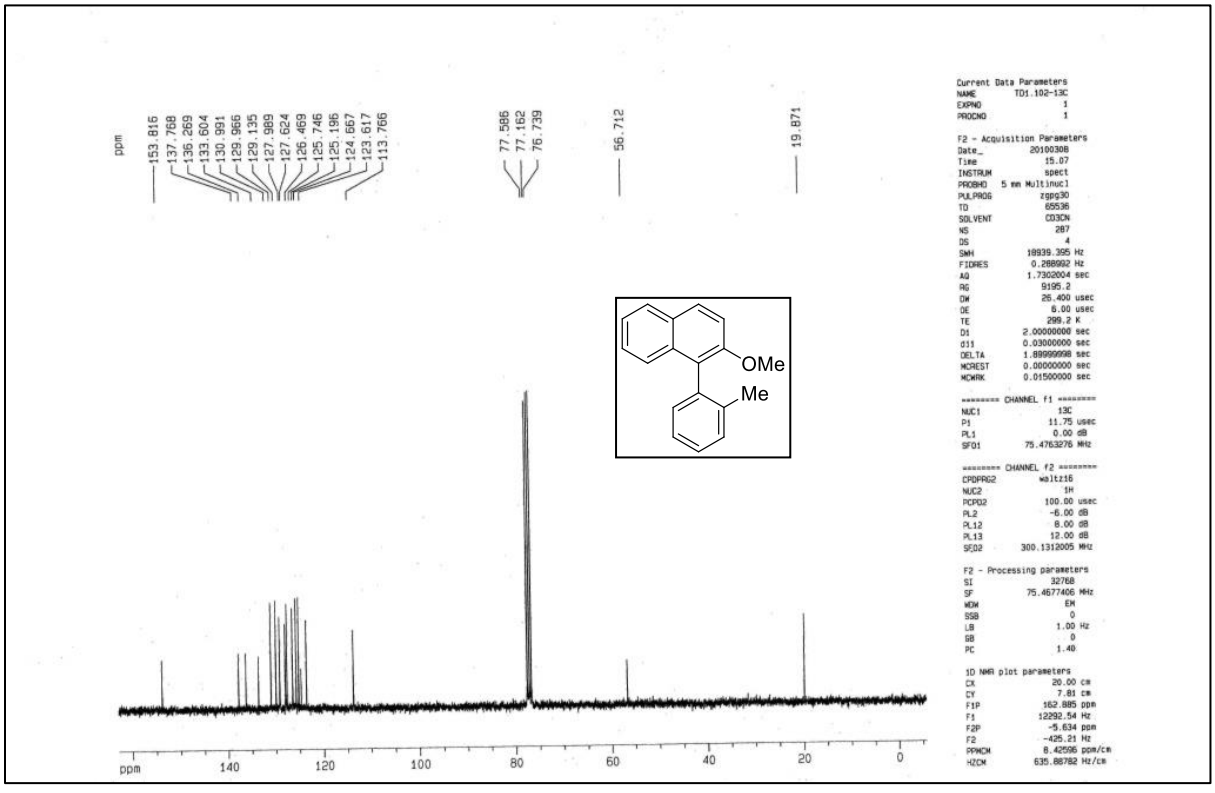

ppm
7.86226
7.83195
7.81062
7.80234
7.75751
7.73054
7.49483
7.46813
7.33327
7.32382
7.31054
7.29344
7.20737
7.17304
7.14705
7.09506
7.07317
3.61558
1.32193
OMe
Integral
3.9160
1.0000
2.9245
4.9496
2.8684
ppm
8
7
6
5
4
3
2
1
0


ppm
154.745
134.681
134.398
133.837
129.605
129.152
128.570
128.354
127.931
127.866
126.512
126.305
125.984
125.818
125.695
125.629
123.700
113.955
77.586
77.162
76.739
56.842
OMe
ppm
140
120
100
80
60
40
20
0
Current Data Parameters
NAME TD-2-141A-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20110707
Time 15.08
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 305
DS 4
SWH 18832.393 Hz
FIDRES 0.287360 Hz
AQ 1.7400308 sec
RG 32768
DW 26.550 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
SF01 75.4761546 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 100.00 usec
PL2 -6.00 dB
PL12 8.00 dB
PL13 12.00 dB
SF02 300.1312005 MHz
F2 - Processing parameters
SI 32768
SF 75.4677458 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 3.96 cm
F1P 161.242 ppm
F1 12168.58 Hz
F2P -7.765 ppm
F2 -585.99 Hz
PPMCM 8.45034 ppm/cm
HZCM 637.72821 Hz/cm


7.989
7.961
7.914
7.886
7.858
7.658
7.635
7.631
7.620
7.607
7.578
7.546
7.529
7.516
7.510
7.501
7.496
7.489
7.482
7.468
7.462
7.449
7.437
7.433
7.414
7.411
7.388
7.318
7.315
7.290
7.287
7.266
7.260
7.237
7.233
7.215
7.211
7.189
7.162
2.593
2.297
2.138
Me
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
ppm
10
9
8
7
6
5
4
3
2
1
ppm
1.00
0.98
0.51
1.06
0.99
2.02
1.38


137.65
137.22
136.53
134.53
133.91
133.62
132.74
132.15
128.74
128.41
128.26
128.13
127.92
127.89
127.77
127.70
126.41
126.16
126.04
126.00
125.78
125.50
124.95
77.41
77.16
76.90
20.65
Me
NAME TD3.193-13C
EXPNO 1
PROCNO 1
Date_ 20121012
Time 11.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 32768
SOLVENT CDCl3
NS 888
DS 4
SWH 29761.904 Hz
FIDRES 0.90826l Hz
AQ 0.5505524 sec
RG 32
DW 16.800 usec
DE 6.50 usec
TE 299.2 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 125.7577753 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm


7.912
7.882
7.849
7.841
7.838
7.823
7.818
7.395
7.365
7.349
7.343
7.336
7.324
7.320
7.311
7.304
7.290
7.273
7.259
7.199
7.177
7.172
3.844
1.997
OMe
Me
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
ppm
1.00
1.00
7.03
1.05
3.16
3.17


ppm
153.816
137.768
136.269
133.604
130.991
129.966
129.135
127.989
127.624
126.469
125.746
125.196
124.667
123.617
113.766
77.586
77.162
76.739
56.712
19.871
OMe
Me
ppm
140
120
100
80
60
40
20
0
Current Data Parameters
NAME TD1.102-13C
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20100308
Time 15.07
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zgpg30
TD 65536
SOLVENT CD3CN
NS 287
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 298.2 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 7.81 cm
F1P 162.885 ppm
F1 12292.54 Hz
F2P -5.634 ppm
F2 -425.21 Hz
PPMCM 8.42595 ppm/cm
HZCM 635.88782 Hz/cm