Pushing steric bias in the Scholl reaction to access liquid crystalline crown ethers

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Supporting Information

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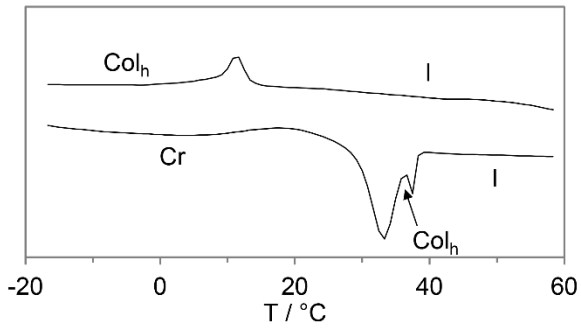
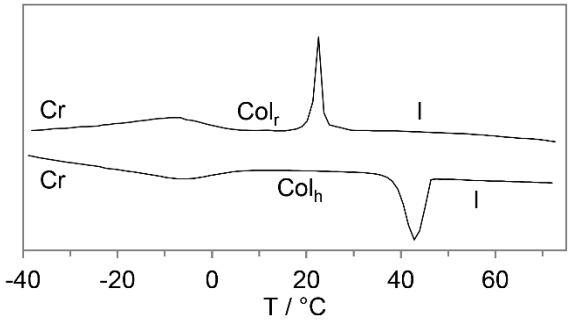
DSC traces:

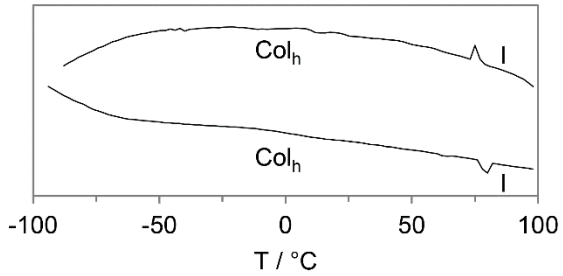
3a



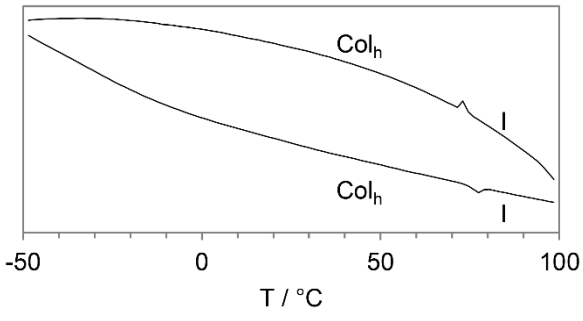
3c



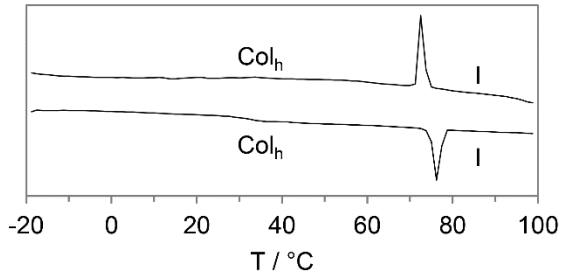
5a



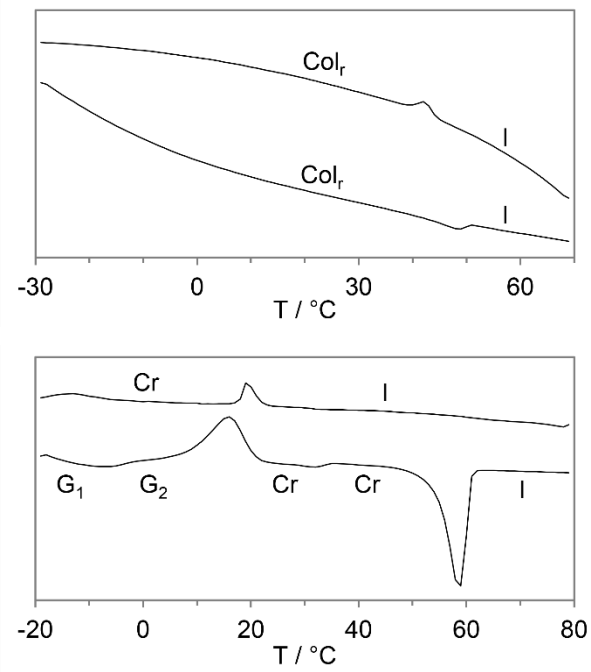
5b



5c



6a

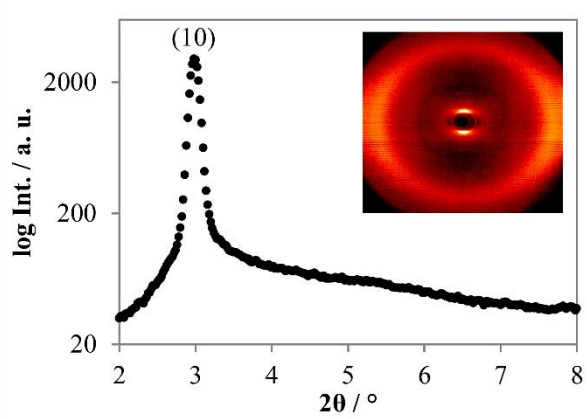


6c

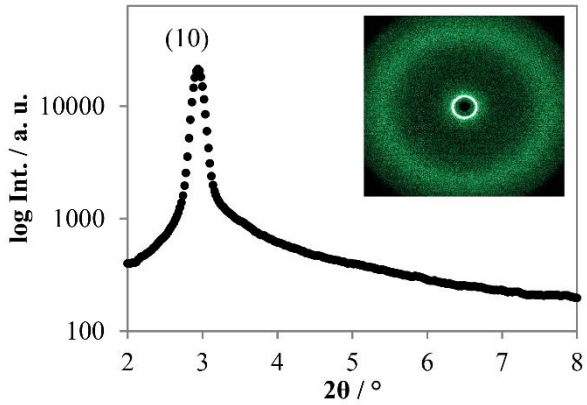
Figure S1. DSC traces of *o*-terphenyls **3a,b**, of triphenylenes **5a-c** and **6a,c** (second heating / cooling; heating/cooling rate: 5 K min^{-1}).

XRD investigations:

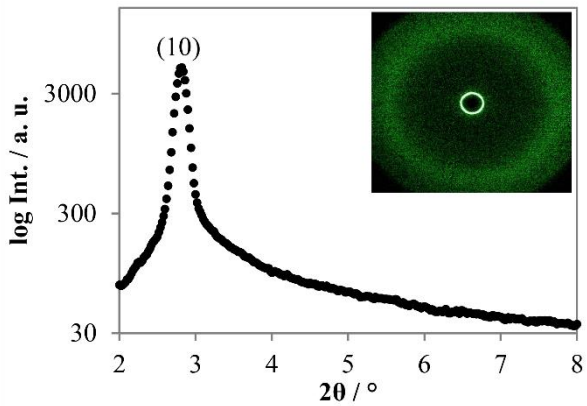
5a



5b



5c



6a

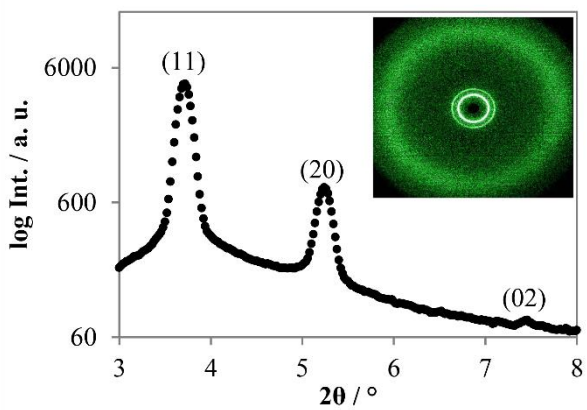
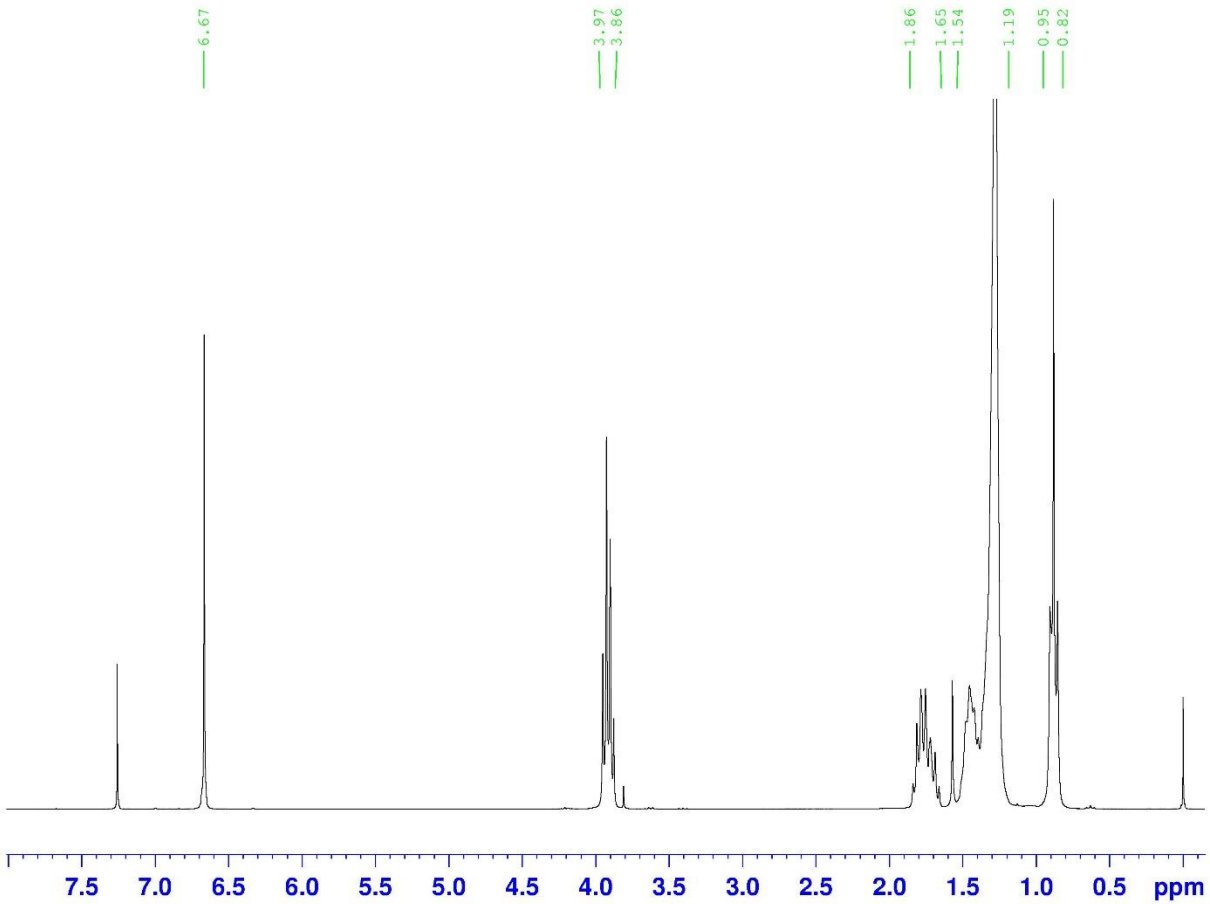


Figure S2. SAXS profile and WAXS diffraction pattern (inlay) of **5a** at 15 °C, **5b** at 85 °C **5c** at 25 °C (exemplary for series **5**) and **6a** at 37 °C.

Table S1. XRD results for *o*-terphenyl **3c** and triphenylene crown ethers **5a**, **6a**.

Compound	Mesophase	Lattice Spacing / Å	*d*-spacing / Å observed	Miller Indices
3a	Col_h at 25 °C	*a* = 35.3	30.5	(10)
	p6mm		17.6	(11)
			15.3	(20)
			4.4	halo
3c	Col_r at 25°C	*a* = 19.1	33.2	(02)
	c2mm	*b* = 66.4	22.5	(03)
			19.1	(10)
			16.6	(12)
			14.6	(13)
			13.4	(05)
			12.5	(14)
			11.0	(06)
			4.4	halo
5a	Col_h at 15 °C	*a* = 34.7	29.6	(10)
	p6mm		4.3	halo
5b	Col_h at 84 °C	*a* = 34.7	30.0	(10)
	p6mm		4.5	halo
5c	Col_h at 25 °C	*a* = 36.2	31.4	(10)
	p6mm		4.3	halo
6a	Colr at 37 °C	*a* = 47.9	28.1	(11)
	c2mm	*b* = 34.8	23.9	(20)
			16.9	(02)
			4.4	halo

9a ^{1}H



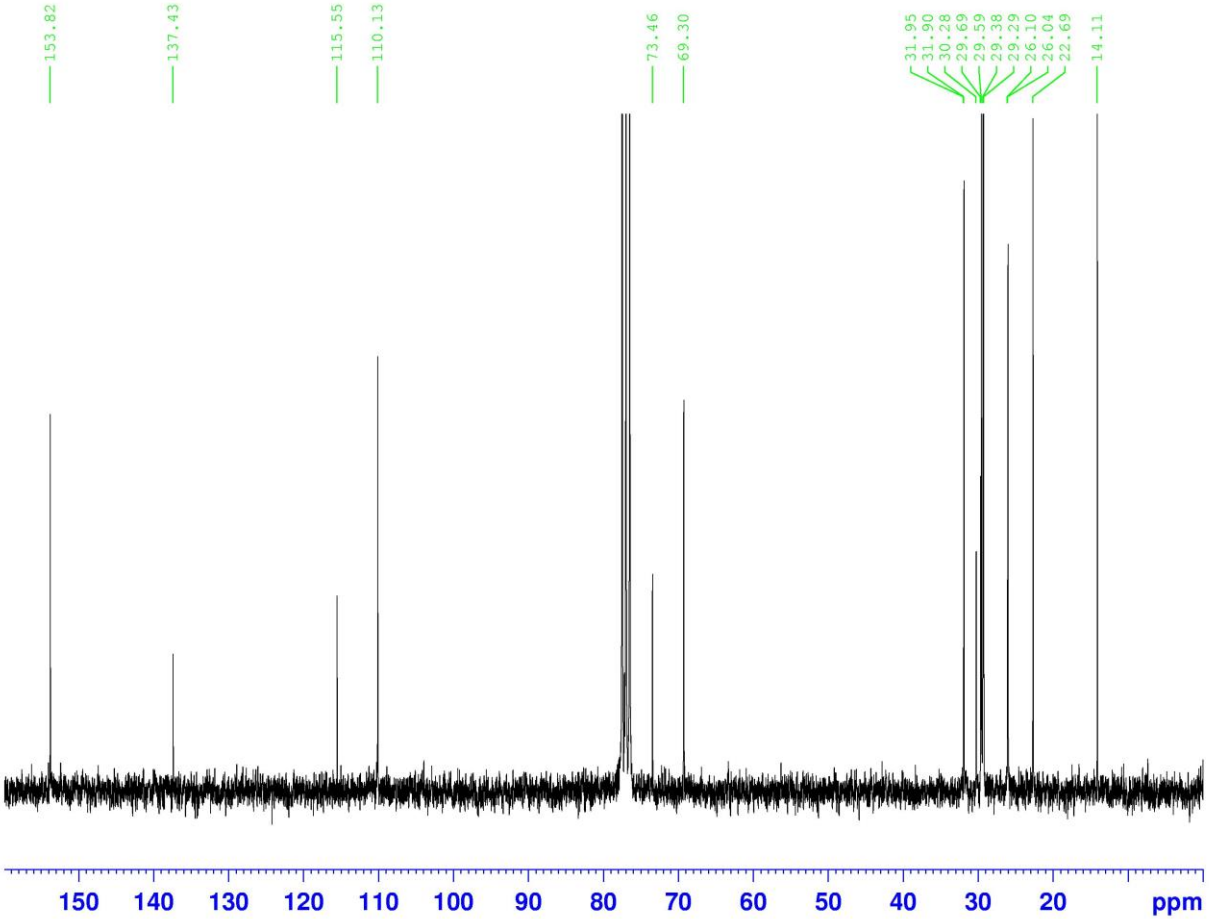

```
Current Data Parameters
NAME          Jun27-2011
EXPNO                 30
PROCNO                 1

F2 - Acquisition Parameters
Date_            20110627
Time               10.01
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     2
SWH             5175.983 Hz
FIDRES          0.078979 Hz
AQ             6.3308277 sec
RG                 143.7
DW                96.600 usec
DE                 8.00 usec
TE                300.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.40 usec
PL1               -6.00 dB
SFO1        250.1315447 MHz

F2 - Processing parameters
SI                 65536
SF          250.1300076 MHz
WDW                   EM
SSB      0
LB                 0.30 Hz
GB       0
PC                 1.00
```

9a ^{13}C

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NAME          Jun28-2011
EXPNO                 90
PROCNO                 1

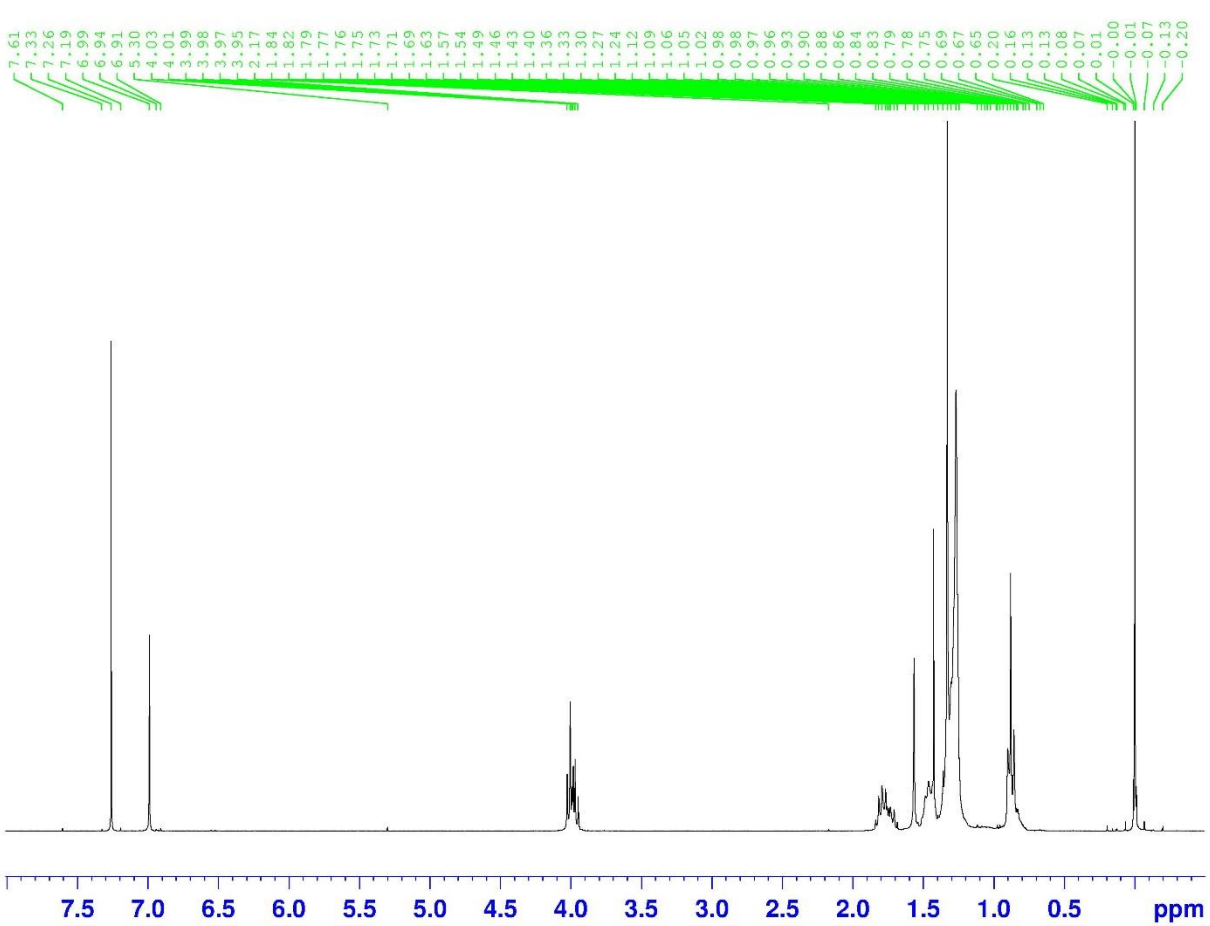
F2 - Acquisition Parameters
Date_            20110628
Time                18.22
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            15060.241 Hz
FIDRES          0.229801 Hz
AQ             2.1758451 sec
RG                2896.3
DW                33.200 usec
DE                  8.00 usec
TE                 300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                  11.70 usec
PL1       0 dB
SFO1          62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2             100.00 usec
PL2                -6.00 dB
PL12               18.50 dB
PL13               15.00 dB
SFO2         250.1310005 MHz

F2 - Processing parameters
SI                 32768
SF            62.8952390 MHz
WDW                   EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

9b ^{1}H

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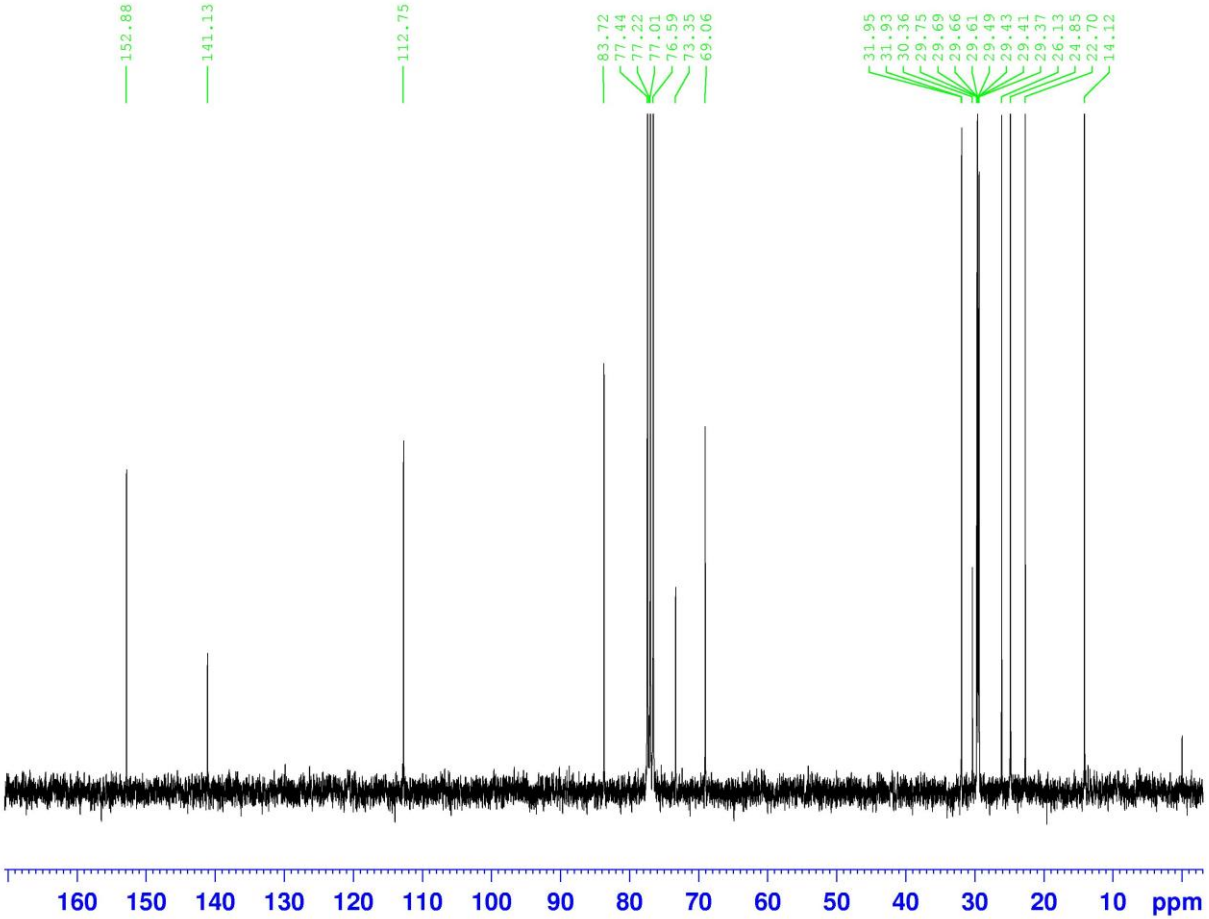
EXPNO                310
PROCNO                 1

F2 - Acquisition Parameters
Date_            20131022
Time               16.03
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    48
DS                     2
SWH             6188.119 Hz
FIDRES          0.188846 Hz
AQ             2.6477044 sec
RG                   322
DW                80.800 usec
DE                  8.00 usec
TE                 296.0 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 11.05 usec
PL1                -2.00 dB
PL1W        37.02396774 W
SFO1        300.1318534 MHz

F2 - Processing parameters
SI                16384
SF          300.1300062 MHz
WDW                  EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

9b ^{13}C

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EXPNO                381
PROCNO                 1

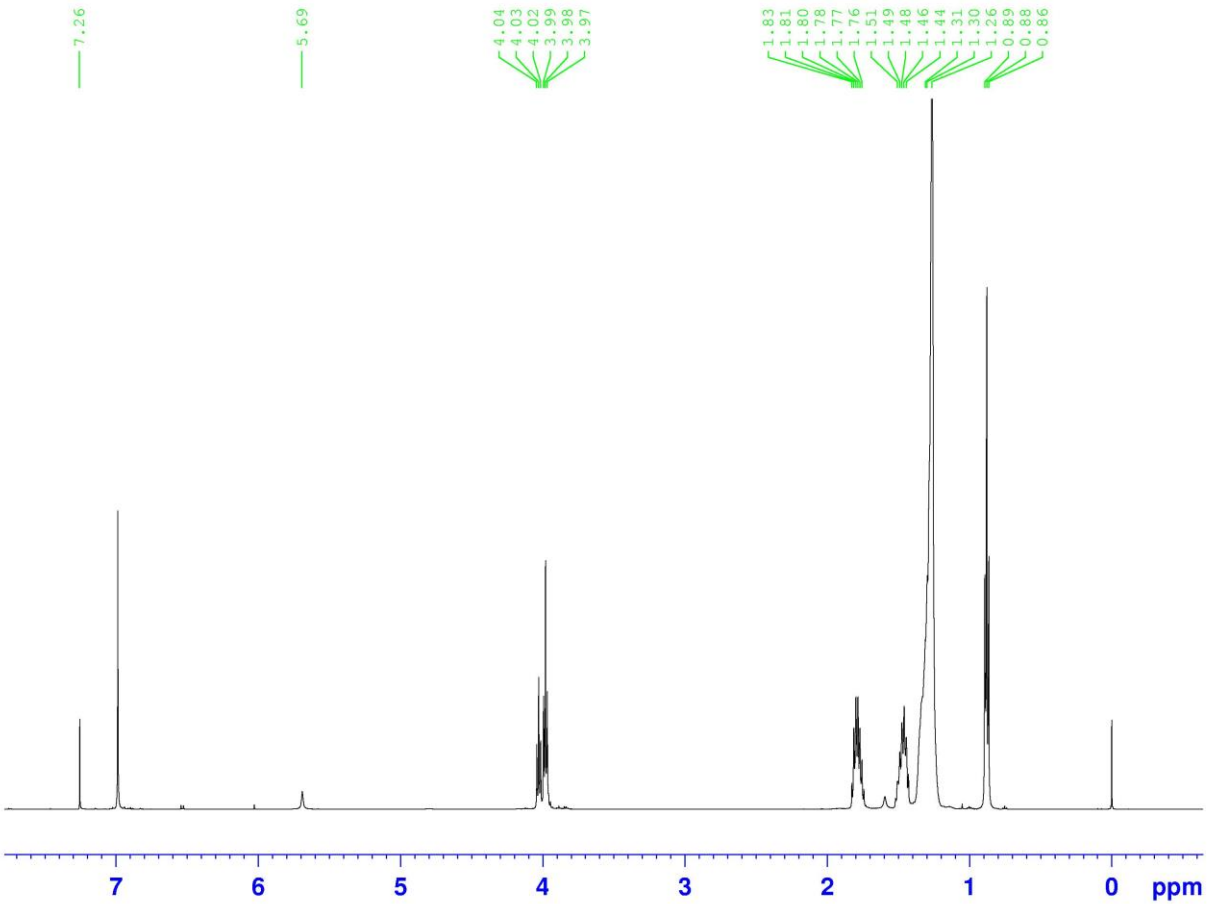
F2 - Acquisition Parameters
Date_           20140731
Time               22.52
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           18028.846 Hz
FIDRES         0.275098 Hz
AQ            1.8175818 sec
RG                 2580
DW               27.733 usec
DE                8.00 usec
TE                297.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                11.75 usec
PL1      0 dB
PL1W        31.14739227 W
SFO1         75.4752953 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2               -2.00 dB
PL12              17.05 dB
PL13              19.00 dB
PL2W        37.02396774 W
PL12W        0.46076876 W
PL13W        0.29409182 W
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                32768
SF           75.4677490 MHz
WDW                  EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
```

9c ^{1}H

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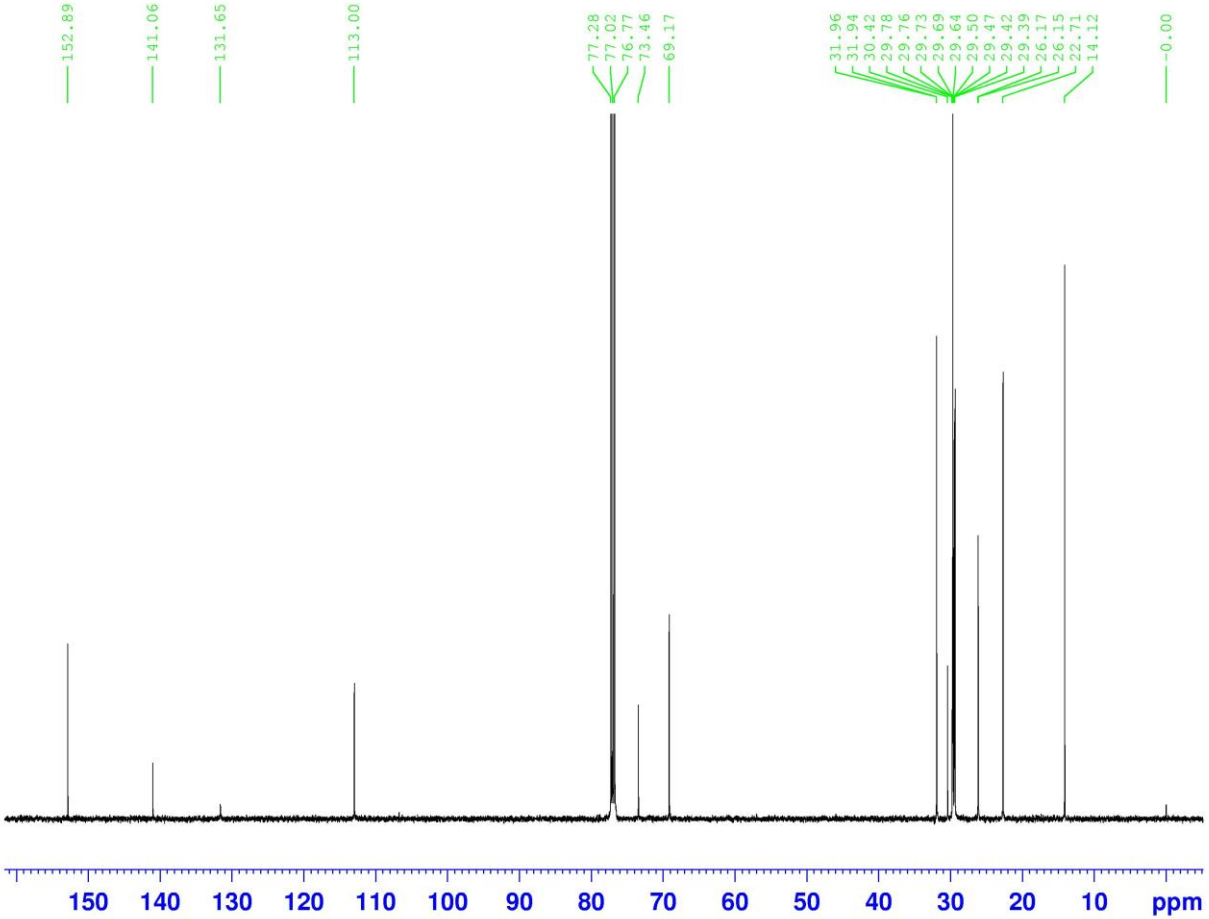
EXPNO                 80
PROCNO                 1

F2 - Acquisition Parameters
Date_            20130610
Time                20.57
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     32
DS                      0
SWH            10330.578 Hz
FIDRES          0.315264 Hz
AQ             1.5860212 sec
RG                     57
DW                48.400 usec
DE                 10.00 usec
TE                 296.8 K
D1            2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 11.23 usec
PL1                 1.00 dB
PL1W         19.75309753 W
SFO1         500.1560886 MHz

F2 - Processing parameters
SI                 16384
SF           500.1530180 MHz
WDW                   EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

9c ^{13}C




```
Current Data Parameters
NAME          Jun10-2013
EXPNO                 81
PROCNO                 1

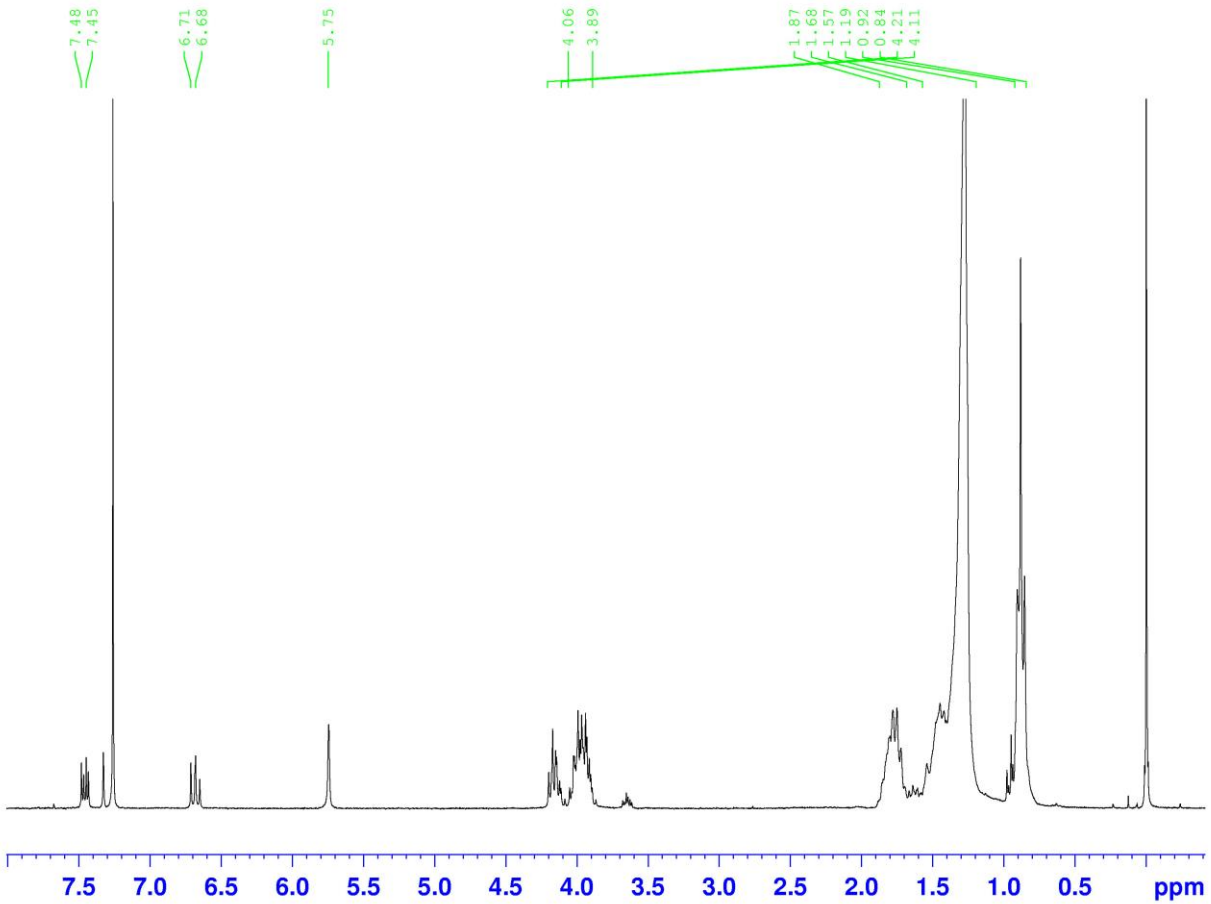
F2 - Acquisition Parameters
Date_           20130610
Time               21.50
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           32894.738 Hz
FIDRES         0.501934 Hz
AQ            0.9961972 sec
RG                 2890
DW               15.200 usec
DE                10.00 usec
TE                296.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.20 usec
PL1                1.50 dB
PL1W        51.74793243 W
SFO1        125.7761482 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2                1.00 dB
PL12              19.99 dB
PL13              21.00 dB
PL2W        19.75309753 W
PL12W        0.24925002 W
PL13W        0.19753097 W
SFO2        500.1550006 MHz

F2 - Processing parameters
SI                32768
SF          125.7635739 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

12a ^{1}H




```
Current Data Parameters
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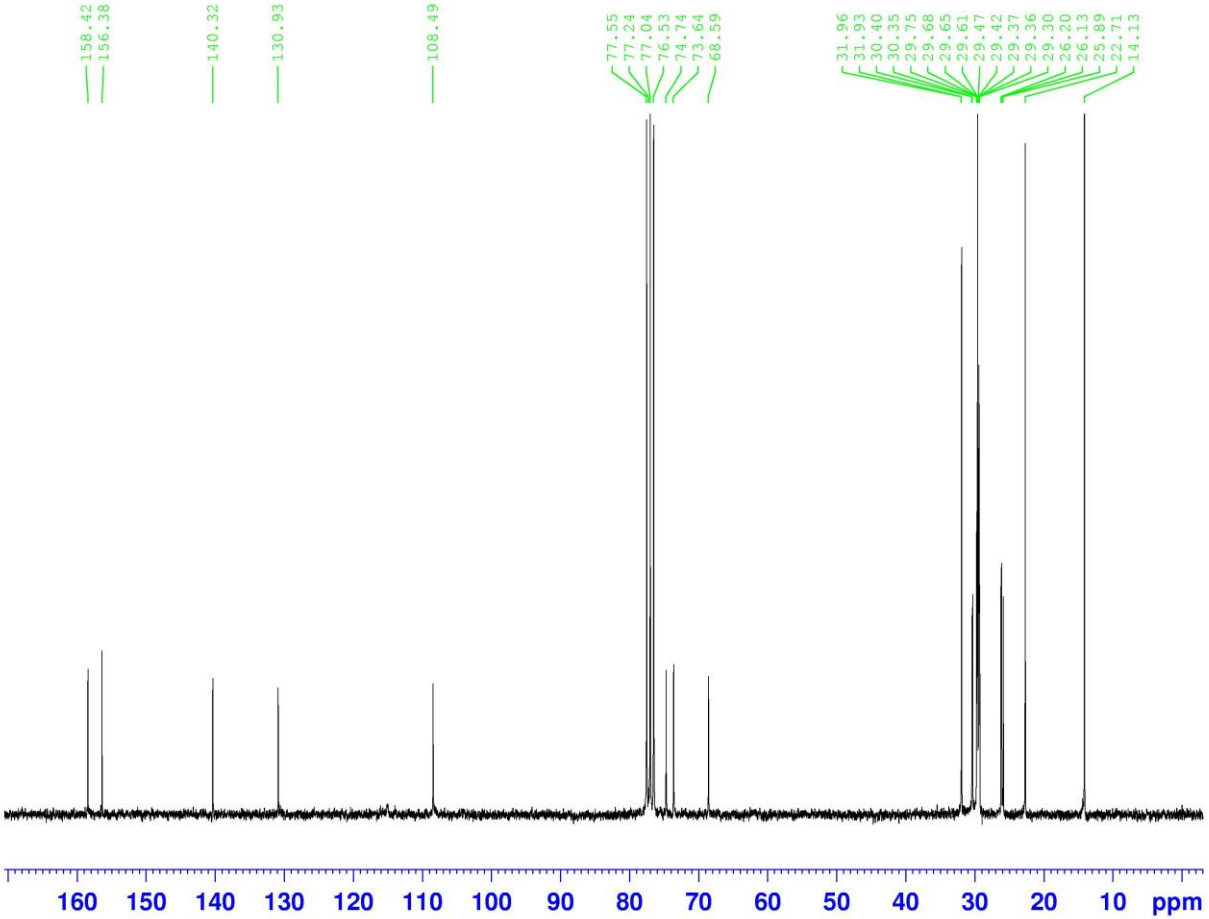
EXPNO                 50
PROCNO                 1

F2 - Acquisition Parameters
Date_             20110706
Time                  9.02
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     32
DS                      2
SWH             5175.983 Hz
FIDRES          0.078979 Hz
AQ             6.3308277 sec
RG                    512
DW                 96.600 usec
DE                  8.00 usec
TE                 300.0 K
D1            1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.40 usec
PL1                -6.00 dB
SFO1         250.1315447 MHz

F2 - Processing parameters
SI                  65536
SF           250.1300077 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

12a ^{13}C

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NAME          Aug01-2014
EXPNO                 20
PROCNO                 1

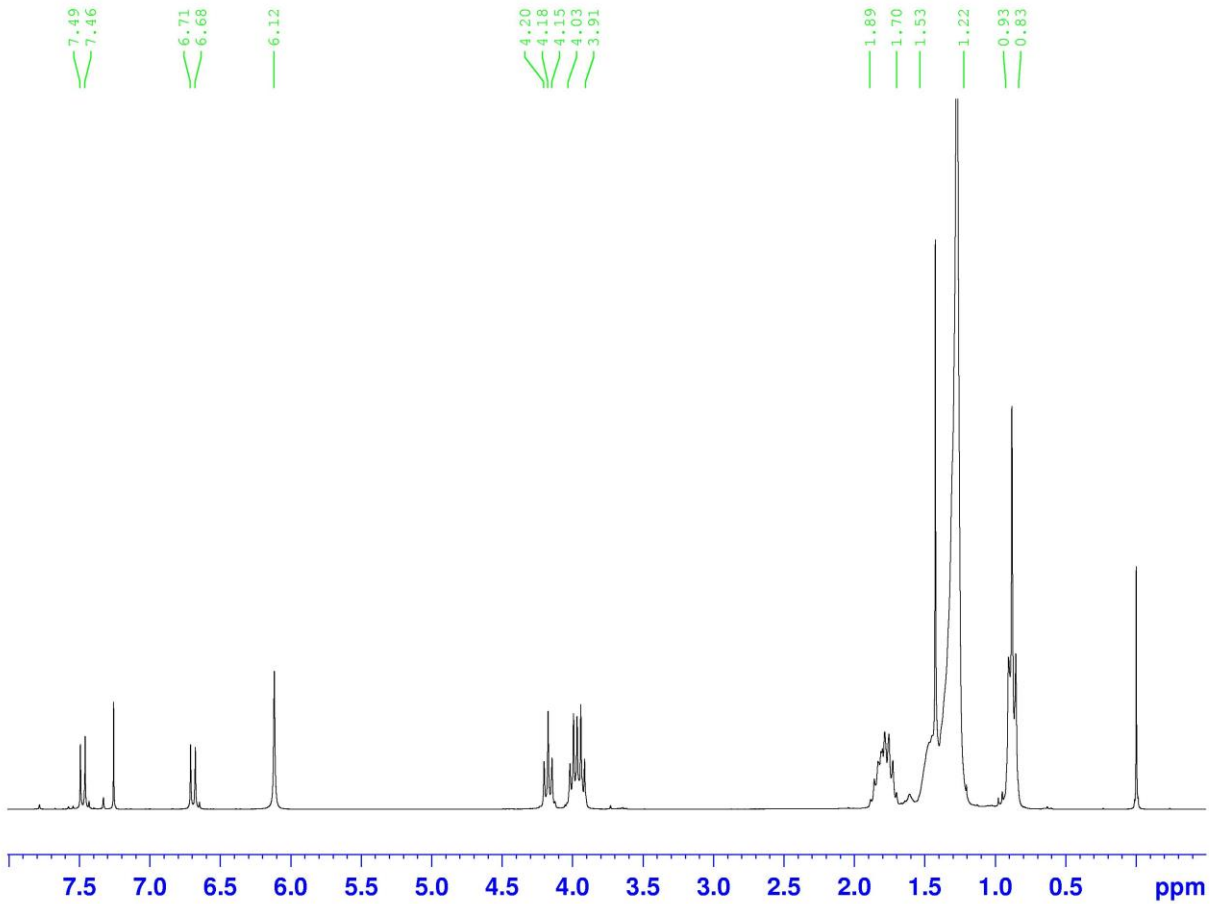
F2 - Acquisition Parameters
Date_            20140801
Time                10.02
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            15060.241 Hz
FIDRES          0.229801 Hz
AQ             2.1758451 sec
RG                2896.3
DW                33.200 usec
DE                  8.00 usec
TE                 300.0 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                  11.70 usec
PL1       0 dB
SFO1          62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2             100.00 usec
PL2                -6.00 dB
PL12               18.50 dB
PL13               15.00 dB
SFO2         250.1310005 MHz

F2 - Processing parameters
SI                 32768
SF            62.8952390 MHz
WDW                   EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

12b ^{1}H



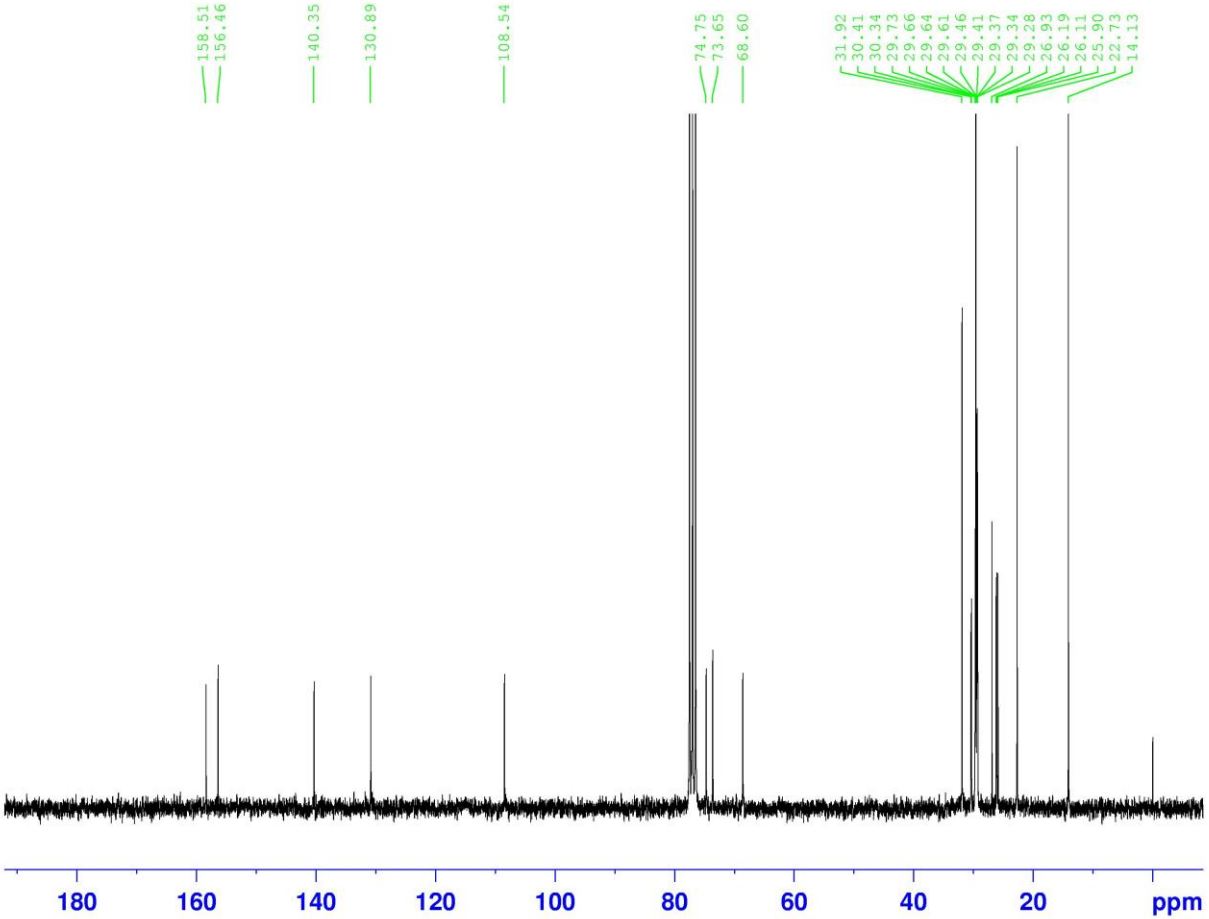

```
Current Data Parameters
NAME          Jul05-2011
EXPNO                 60
PROCNO                 1

F2 - Acquisition Parameters
Date_            20110705
Time                 9.03
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     32
DS                      2
SWH             5175.983 Hz
FIDRES          0.078979 Hz
AQ             6.3308277 sec
RG                    128
DW                 96.600 usec
DE                  8.00 usec
TE                 300.0 K
D1            1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 10.40 usec
PL1                -6.00 dB
SFO1         250.1315447 MHz

F2 - Processing parameters
SI                  65536
SF           250.1300077 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

12b ^{13}C




```
Current Data Parameters
NAME          Jul05-2011
EXPNO                 61
PROCNO                 1

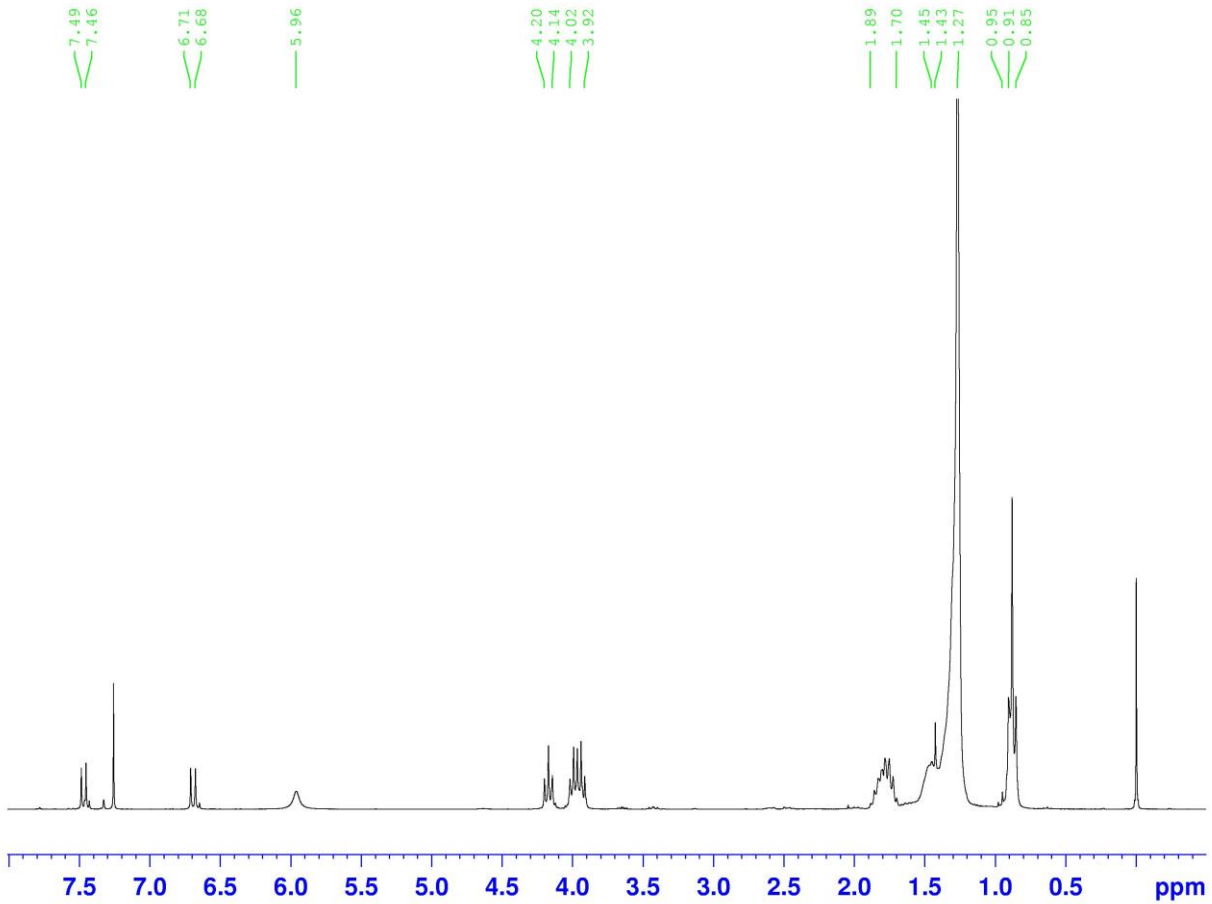
F2 - Acquisition Parameters
Date_            20110705
Time               10.03
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           15060.241 Hz
FIDRES         0.229801 Hz
AQ            2.1758451 sec
RG               2896.3
DW               33.200 usec
DE                 8.00 usec
TE                300.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                11.70 usec
PL1      0 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2            100.00 usec
PL2               -6.00 dB
PL12              18.50 dB
PL13              15.00 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                32768
SF           62.8952388 MHz
WDW                  EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
```

12c ^{1}H



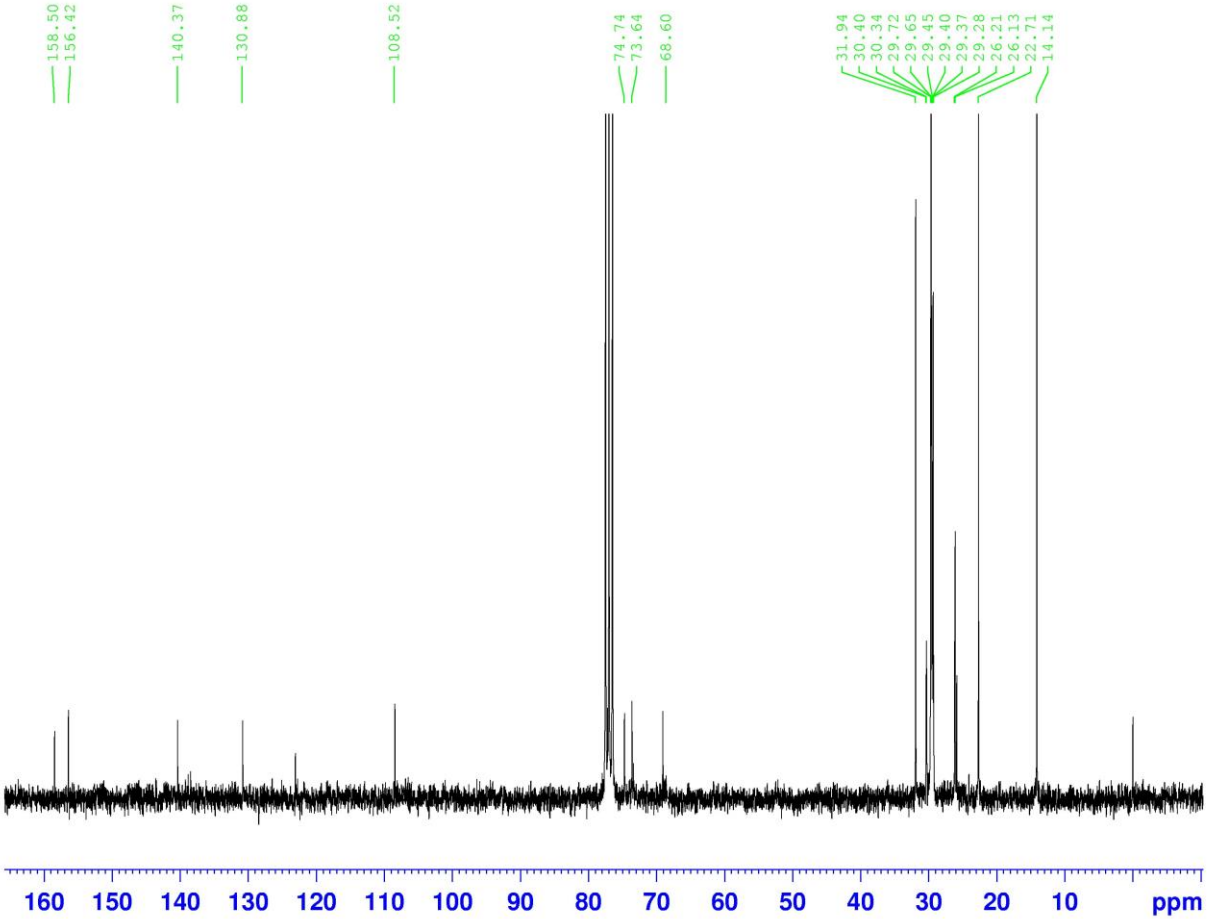

```
Current Data Parameters
NAME          Jun07-2011
EXPNO                 90
PROCNO                 1

F2 - Acquisition Parameters
Date_            20110607
Time               12.56
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    32
DS                     2
SWH             5175.983 Hz
FIDRES          0.078979 Hz
AQ             6.3308277 sec
RG                 228.1
DW                96.600 usec
DE                 8.00 usec
TE                300.0 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.40 usec
PL1               -6.00 dB
SFO1        250.1315447 MHz

F2 - Processing parameters
SI                 65536
SF          250.1300075 MHz
WDW                   EM
SSB      0
LB                 0.30 Hz
GB       0
PC                 1.00
```

12c ^{13}C




```
Current Data Parameters
NAME          Jul11-2011
EXPNO                 41
PROCNO                 1

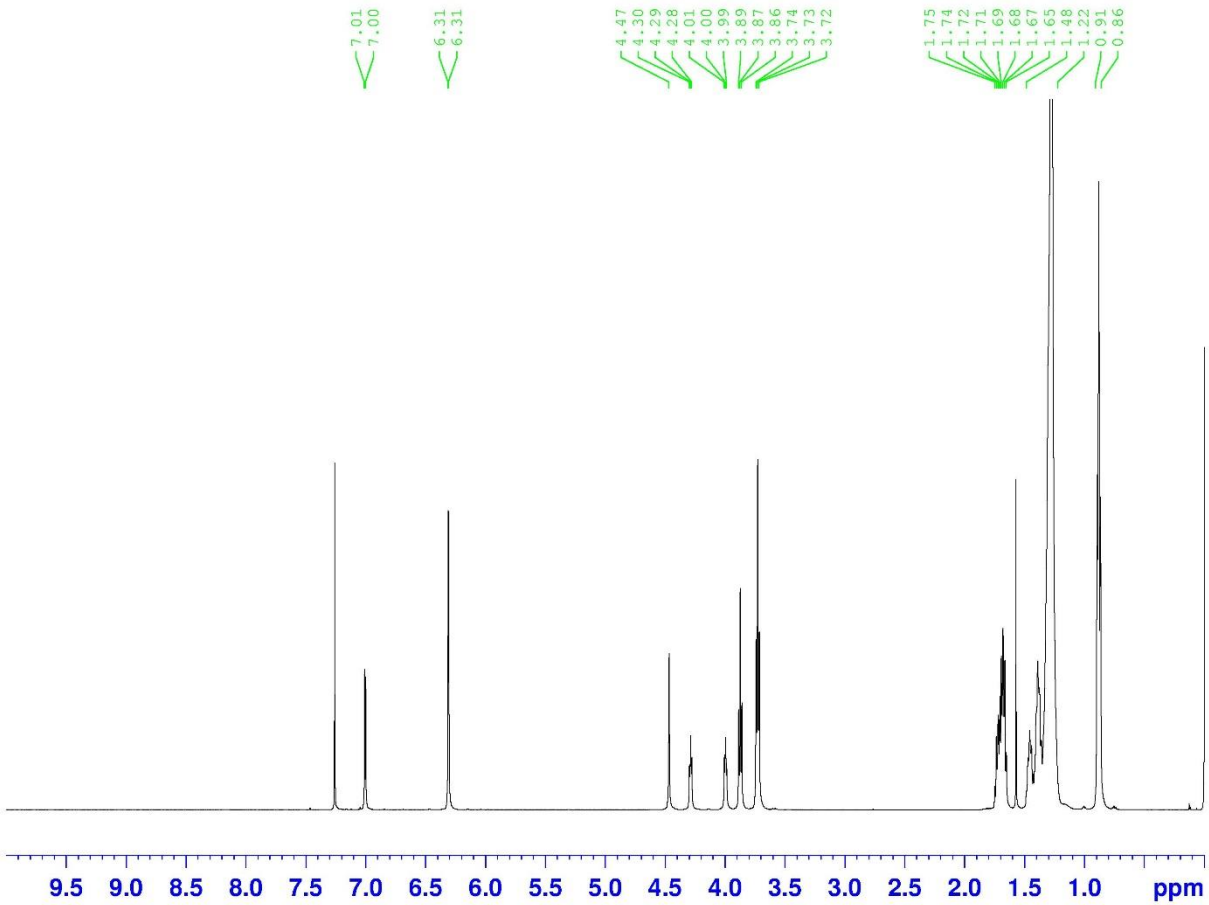
F2 - Acquisition Parameters
Date_            20110711
Time                13.11
INSTRUM             spect
PROBHD   5 mm QNP 1H/13
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            15060.241 Hz
FIDRES          0.229801 Hz
AQ             2.1758451 sec
RG                2298.8
DW                33.200 usec
DE                  8.00 usec
TE                 300.0 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                  11.70 usec
PL1      0 dB
SFO1         62.9015280 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                   1H
PCPD2             100.00 usec
PL2                -6.00 dB
PL12               18.50 dB
PL13               15.00 dB
SFO2        250.1310005 MHz

F2 - Processing parameters
SI                 32768
SF           62.8952390 MHz
WDW                   EM
SSB      0
LB                  1.00 Hz
GB       0
PC                  1.40
```

3a ^{1}H



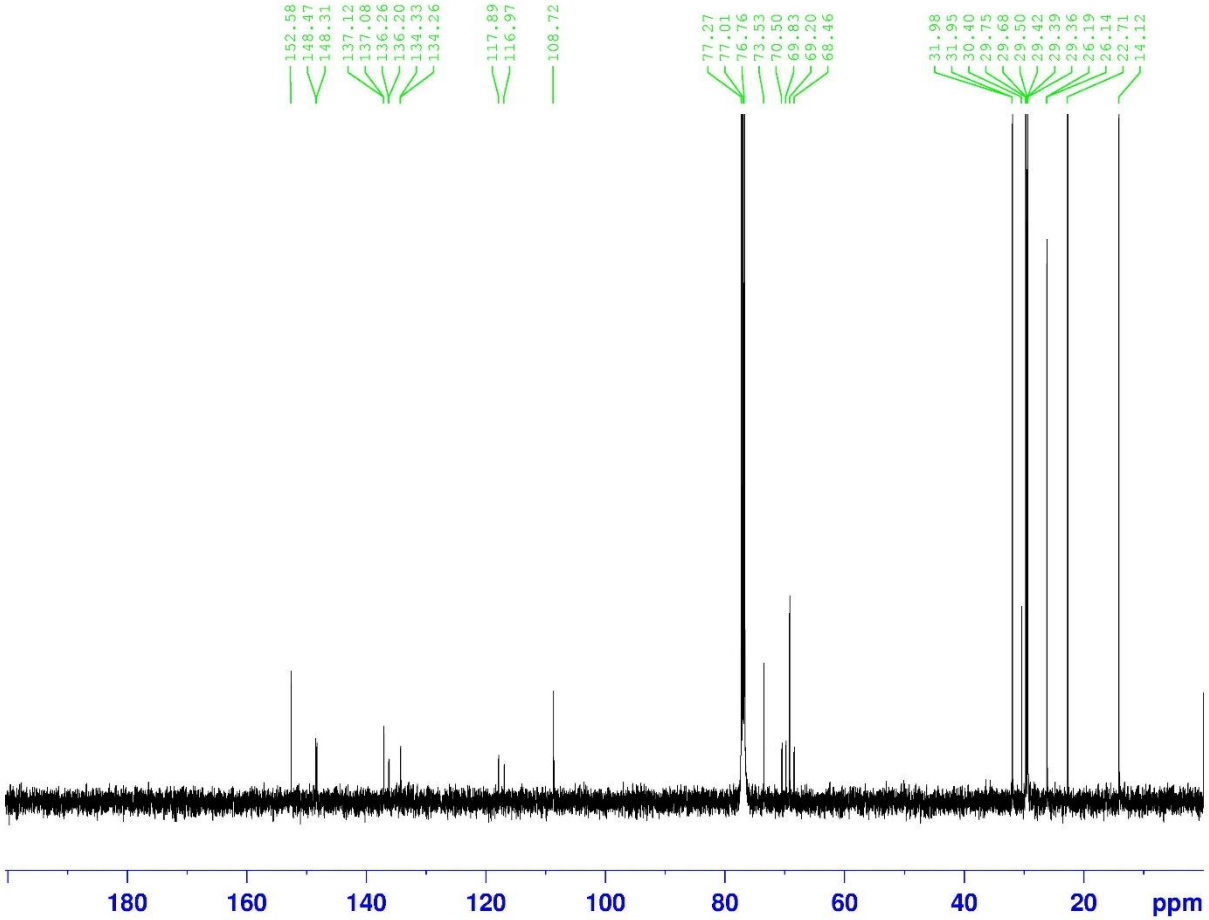

```
Current Data Parameters
NAME          May19-2011
EXPNO                100
PROCNO                 1

F2 - Acquisition Parameters
Date_            20110520
Time                 3.30
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     64
DS                      0
SWH            10330.578 Hz
FIDRES          0.315264 Hz
AQ             1.5860212 sec
RG                    228
DW                48.400 usec
DE                 10.00 usec
TE                 296.8 K
D1            2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  11.05 usec
PL1                  1.00 dB
PL1W         19.75309753 W
SFO1         500.1560886 MHz

F2 - Processing parameters
SI                 16384
SF           500.1530157 MHz
WDW                   EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

3a ^{13}C




```
Current Data Parameters
NAME          May20-2011
EXPNO                 30
PROCNO                 1

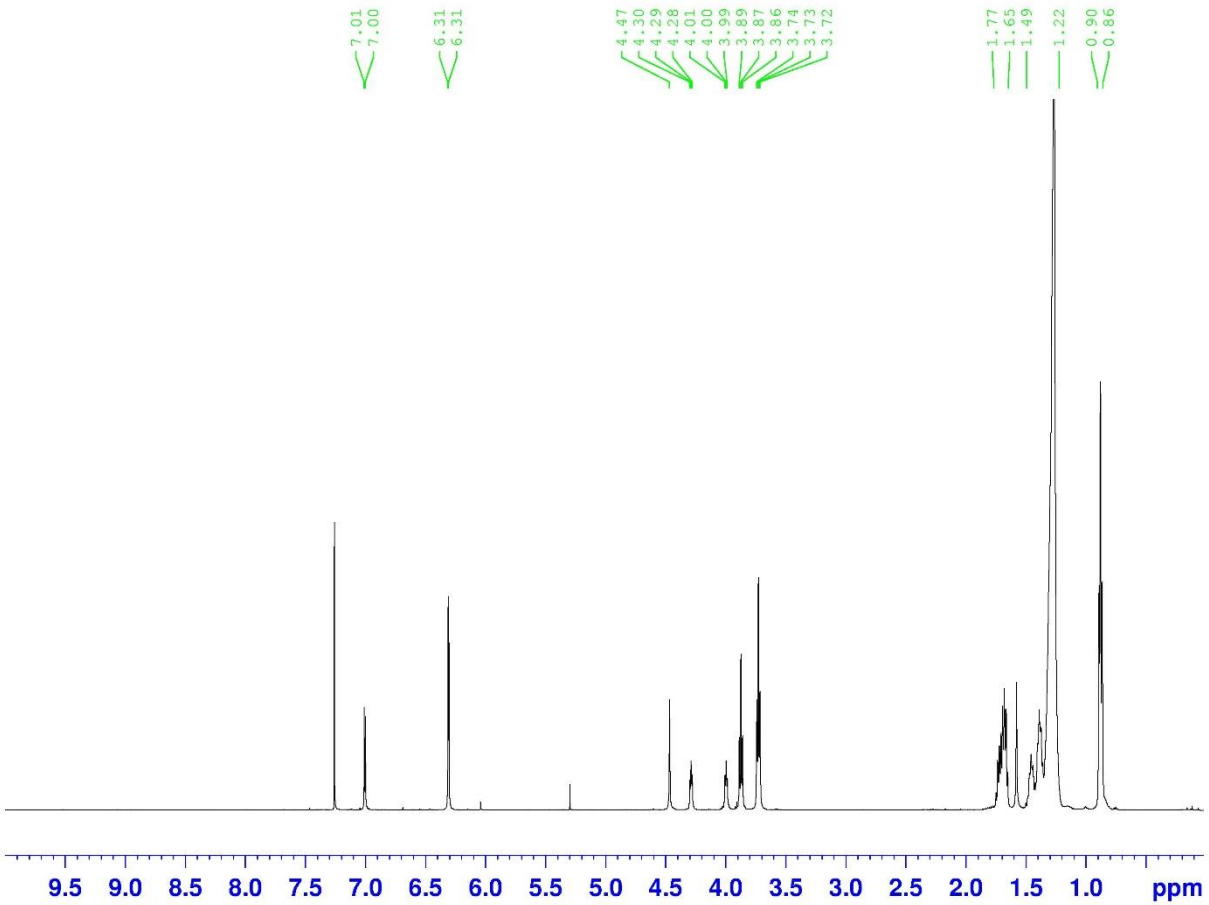
F2 - Acquisition Parameters
Date_           20110520
Time               16.45
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           32894.738 Hz
FIDRES         0.501934 Hz
AQ            0.9961972 sec
RG                 3250
DW               15.200 usec
DE                10.00 usec
TE                297.6 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.40 usec
PL1                1.50 dB
PL1W        51.74793243 W
SFO1        125.7761482 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2                1.00 dB
PL12              18.79 dB
PL13              21.00 dB
PL2W        19.75309753 W
PL12W        0.32857543 W
PL13W        0.19753097 W
SFO2        500.1550006 MHz

F2 - Processing parameters
SI                32768
SF          125.7635736 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

3b ^{1}H



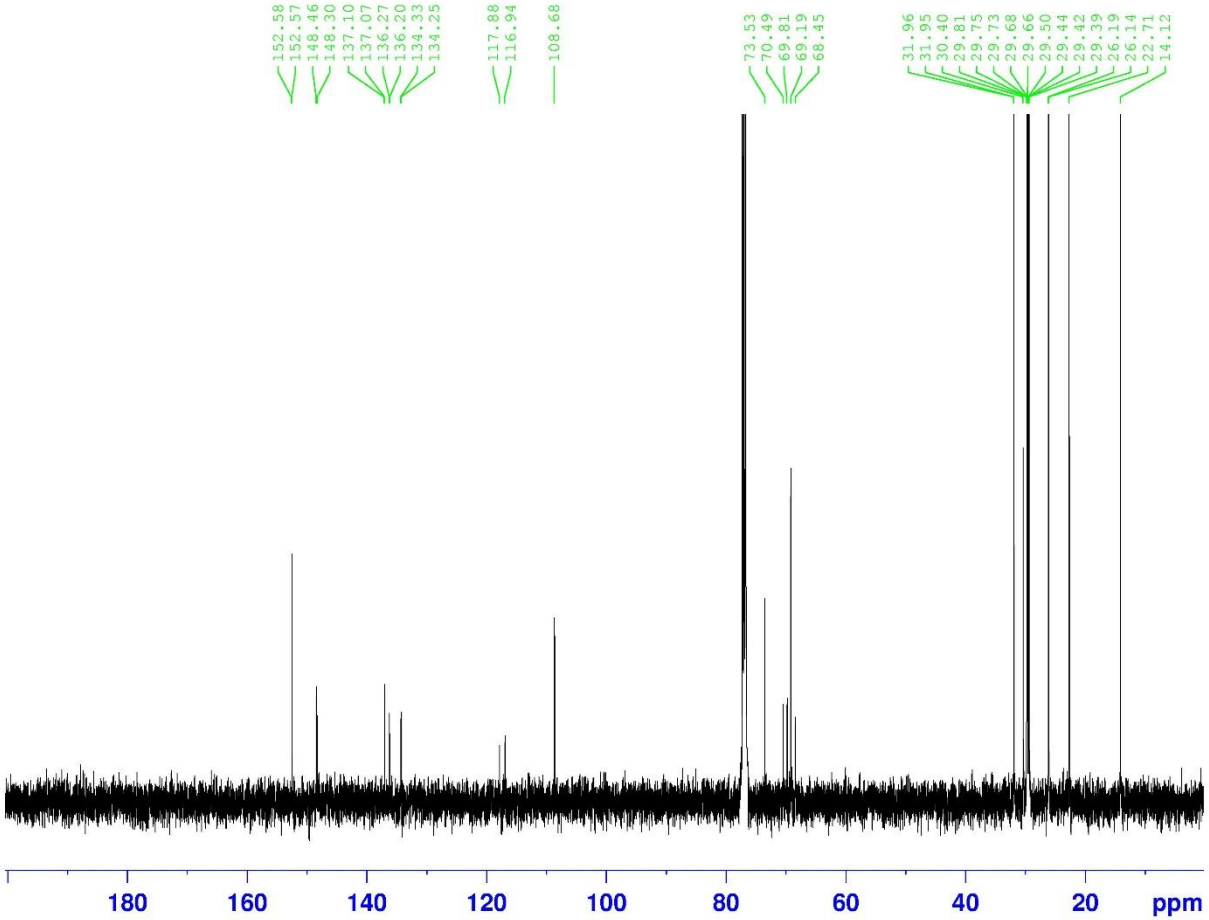

```
Current Data Parameters
NAME          Oct25-2013
EXPNO                 40
PROCNO                 1

F2 - Acquisition Parameters
Date_            20131025
Time                12.06
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     32
DS                      0
SWH            10330.578 Hz
FIDRES          0.315264 Hz
AQ             1.5860212 sec
RG                    203
DW                48.400 usec
DE                 10.00 usec
TE                 296.8 K
D1            2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  11.23 usec
PL1                  1.00 dB
PL1W         19.75309753 W
SFO1         500.1560886 MHz

F2 - Processing parameters
SI                  16384
SF           500.1530161 MHz
WDW                    EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```

3b ^{13}C




```
Current Data Parameters
NAME          Oct25-2013
EXPNO                 41
PROCNO                 1

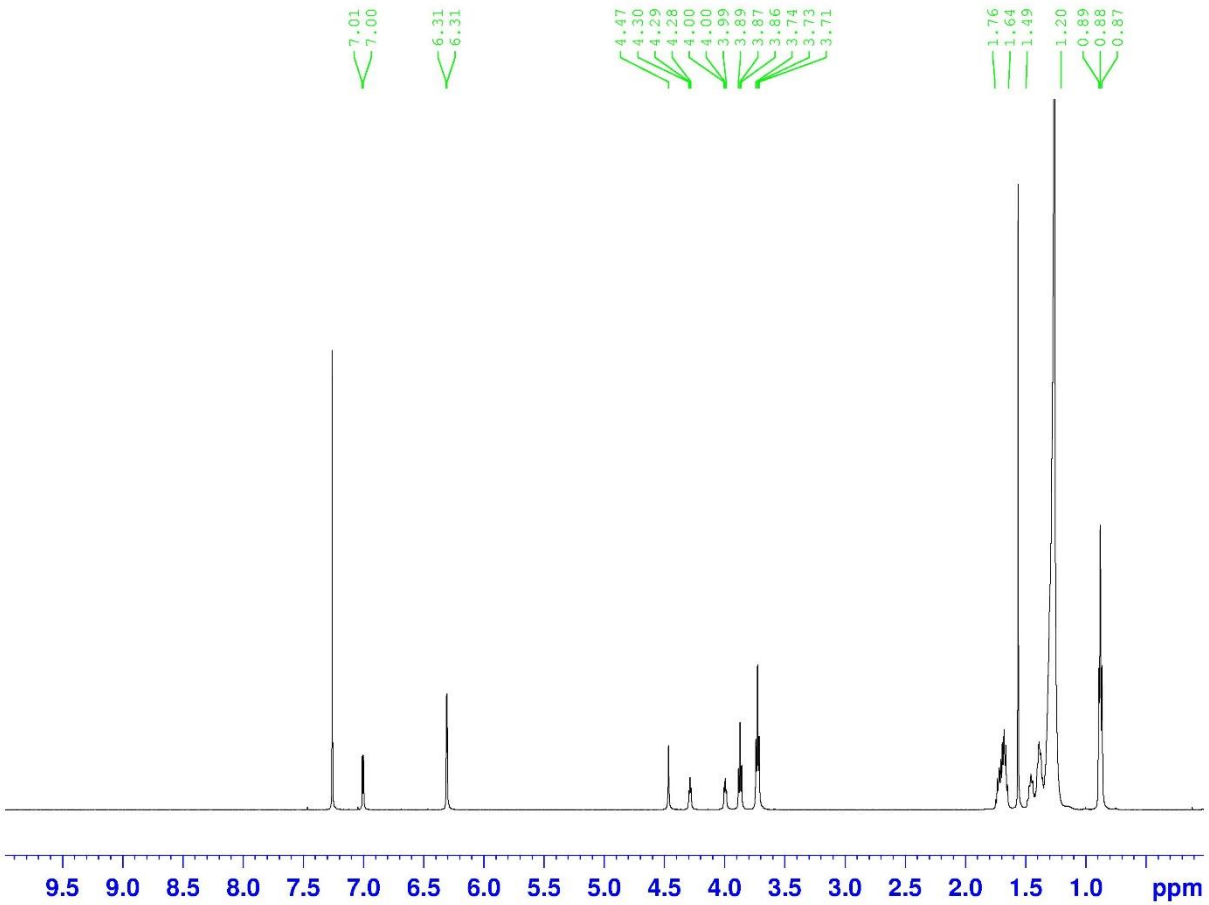
F2 - Acquisition Parameters
Date_           20131025
Time               12.59
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           32894.738 Hz
FIDRES         0.501934 Hz
AQ            0.9961972 sec
RG                 3250
DW               15.200 usec
DE                10.00 usec
TE                296.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.20 usec
PL1                1.50 dB
PL1W        51.74793243 W
SFO1        125.7761482 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2                1.00 dB
PL12              19.99 dB
PL13              21.00 dB
PL2W        19.75309753 W
PL12W        0.24925002 W
PL13W        0.19753097 W
SFO2        500.1550006 MHz

F2 - Processing parameters
SI                32768
SF          125.7635738 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

3c ^{1}H



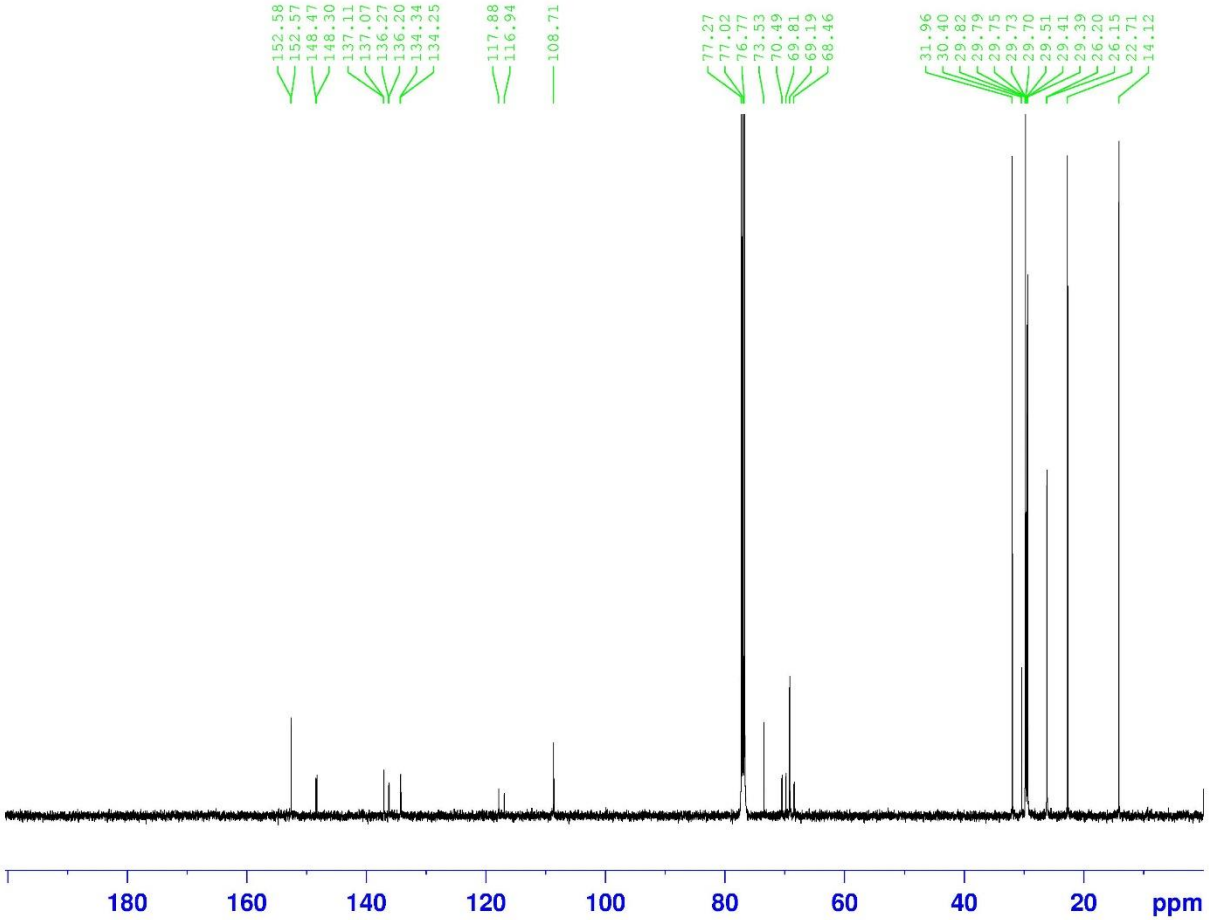

```
Current Data Parameters
NAME          Jul01-2011
EXPNO                 20
PROCNO                 1

F2 - Acquisition Parameters
Date_            20110701
Time                 8.50
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     32
DS                      0
SWH            10330.578 Hz
FIDRES          0.315264 Hz
AQ             1.5860212 sec
RG                    406
DW                 48.400 usec
DE                 10.00 usec
TE                 296.8 K
D1            2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  11.05 usec
PL1                  1.00 dB
PL1W         19.75309753 W
SFO1         500.1560886 MHz

F2 - Processing parameters
SI                  16384
SF           500.1530154 MHz
WDW                    EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```

3c ^{13}C




```
Current Data Parameters
NAME          Jul26-2011
EXPNO                 70
PROCNO                 1

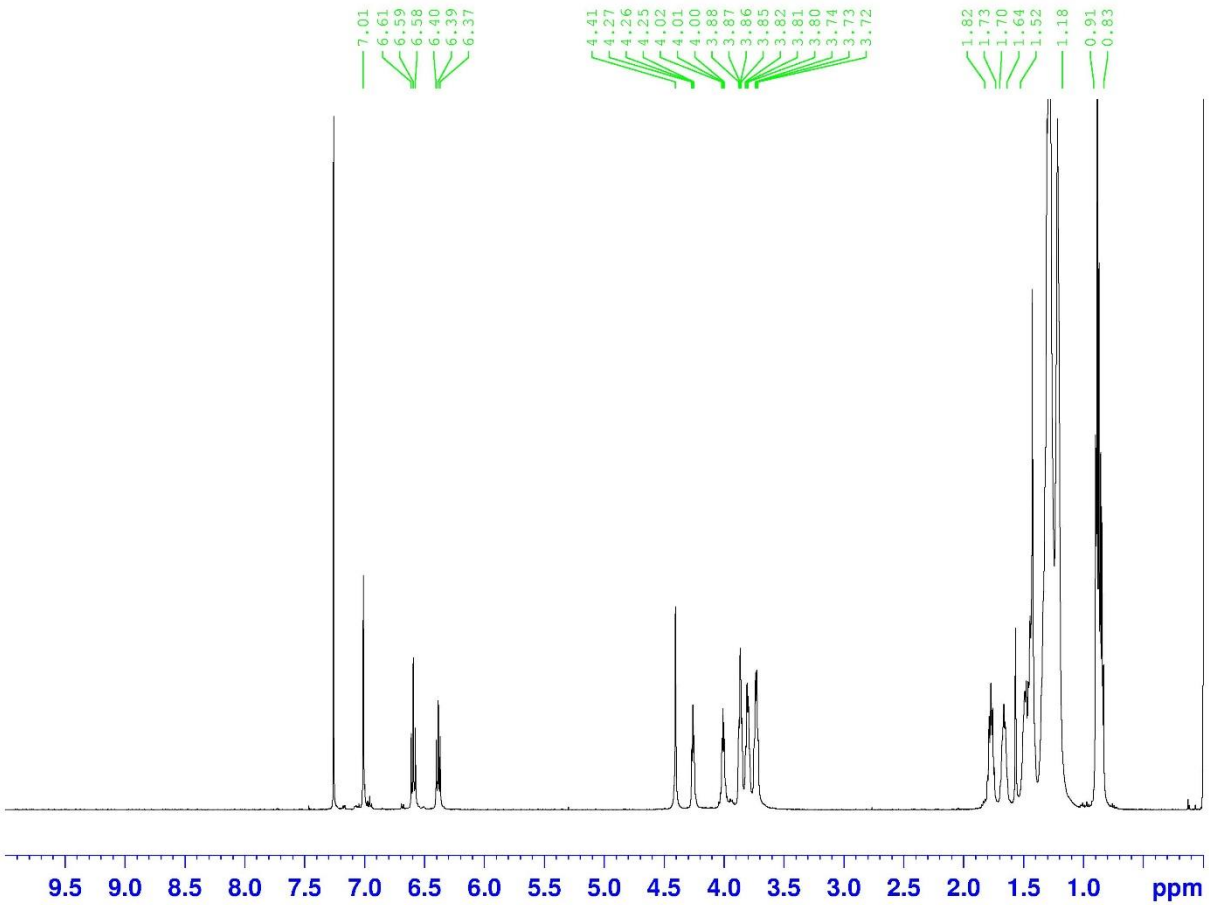
F2 - Acquisition Parameters
Date_           20110726
Time               22.20
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2048
DS                    4
SWH           32894.738 Hz
FIDRES         0.501934 Hz
AQ            0.9961972 sec
RG                 2890
DW               15.200 usec
DE                10.00 usec
TE                297.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.40 usec
PL1                1.50 dB
PL1W        51.74793243 W
SFO1        125.7761482 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2                 1.00 dB
PL12               18.79 dB
PL13               21.00 dB
PL2W        19.75309753 W
PL12W        0.32857543 W
PL13W        0.19753097 W
SFO2        500.1550006 MHz

F2 - Processing parameters
SI                 32768
SF          125.7635736 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

4a ^{1}H



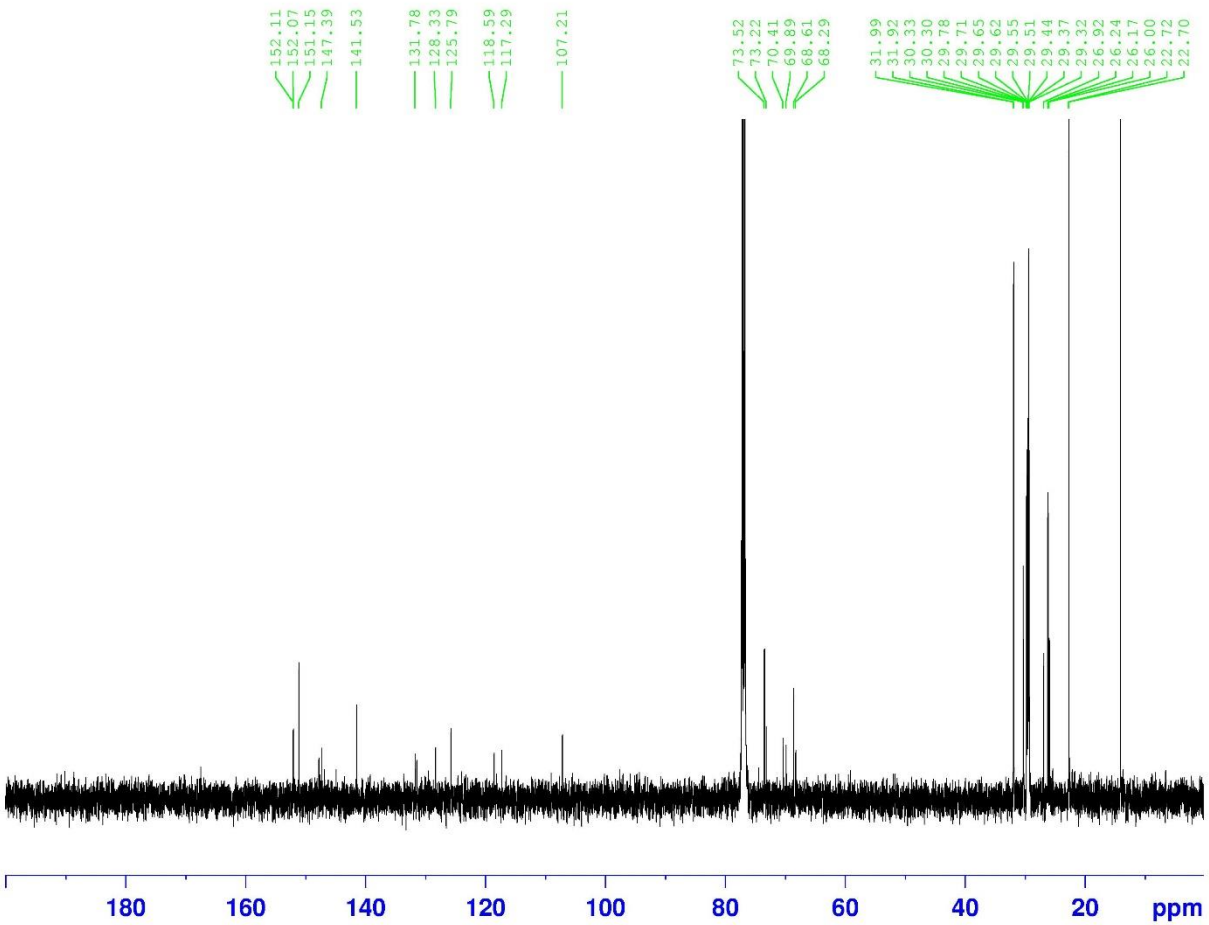

```
Current Data Parameters
NAME      May31-2011-guest
EXPNO                   40
PROCNO                   1

F2 - Acquisition Parameters
Date_             20110531
Time                 12.56
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG               zg30
TD                   32768
SOLVENT              CDCl3
NS                      32
DS                       0
SWH             10330.578 Hz
FIDRES           0.315264 Hz
AQ              1.5860212 sec
RG                     228
DW                 48.400 usec
DE                 10.00 usec
TE                 295.8 K
D1             2.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   11.05 usec
PL1                   1.00 dB
PL1W          19.75309753 W
SFO1          500.1560886 MHz

F2 - Processing parameters
SI                   16384
SF            500.1530155 MHz
WDW                     EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

4a ^{13}C




```
Current Data Parameters
NAME      May31-2011-guest
EXPNO                   41
PROCNO                   1

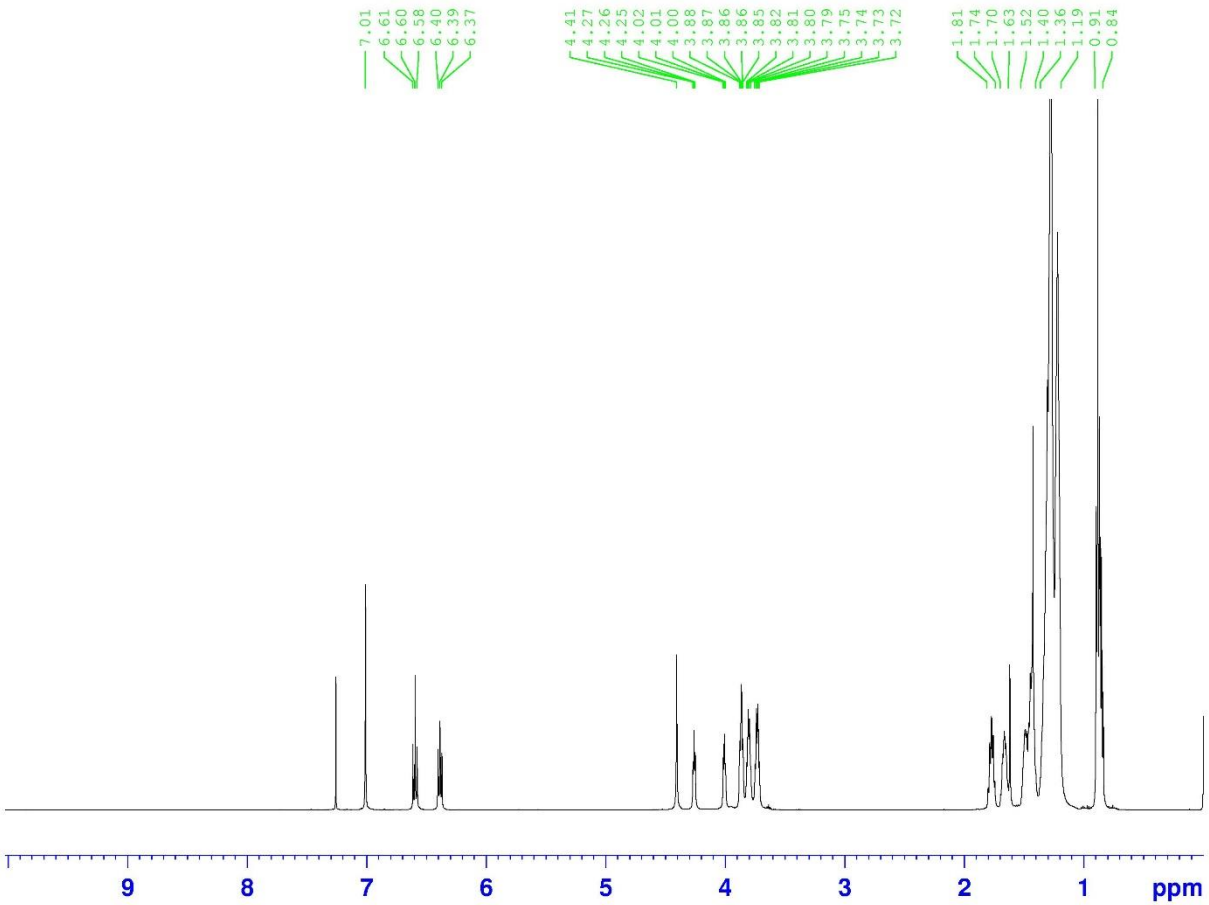
F2 - Acquisition Parameters
Date_            20110531
Time               13.49
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           32894.738 Hz
FIDRES         0.501934 Hz
AQ            0.9961972 sec
RG                 3250
DW               15.200 usec
DE                10.00 usec
TE                296.9 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.40 usec
PL1                1.50 dB
PL1W        51.74793243 W
SFO1        125.7761482 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2                1.00 dB
PL12              18.79 dB
PL13              21.00 dB
PL2W        19.75309753 W
PL12W        0.32857543 W
PL13W        0.19753097 W
SFO2        500.1550006 MHz

F2 - Processing parameters
SI                32768
SF          125.7635738 MHz
WDW                  EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
```

4b ^{1}H



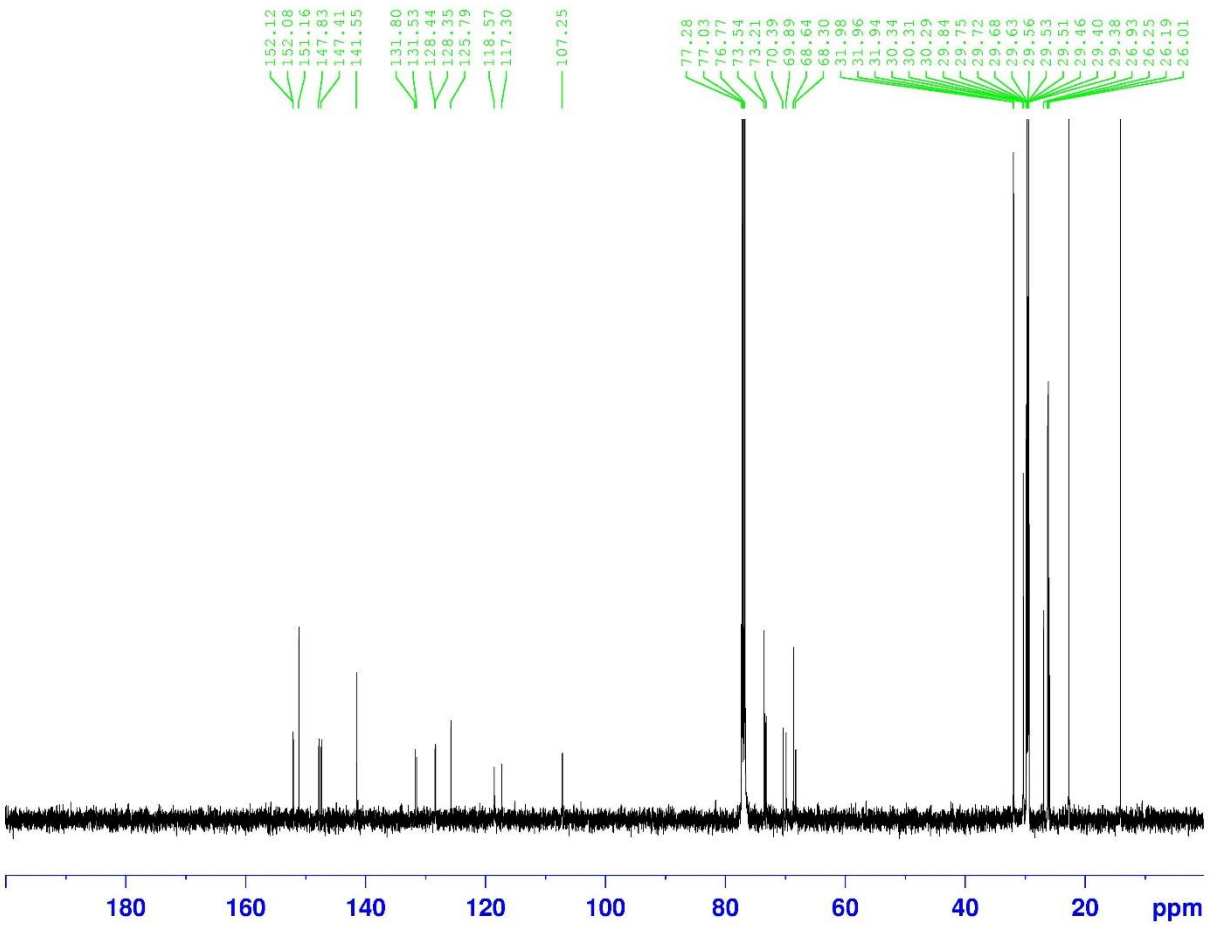

```
Current Data Parameters
NAME          Jul13-2011
EXPNO                 60
PROCNO                 1

F2 - Acquisition Parameters
Date_            20110713
Time                11.21
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     32
DS                      0
SWH            10330.578 Hz
FIDRES          0.315264 Hz
AQ             1.5860212 sec
RG                  50.8
DW                48.400 usec
DE                 10.00 usec
TE                 297.8 K
D1            2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  11.05 usec
PL1                  1.00 dB
PL1W         19.75309753 W
SFO1         500.1560886 MHz

F2 - Processing parameters
SI                  16384
SF           500.1530160 MHz
WDW                    EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```

4b ^{13}C




```
Current Data Parameters
NAME          Jul13-2011
EXPNO                 61
PROCNO                 1

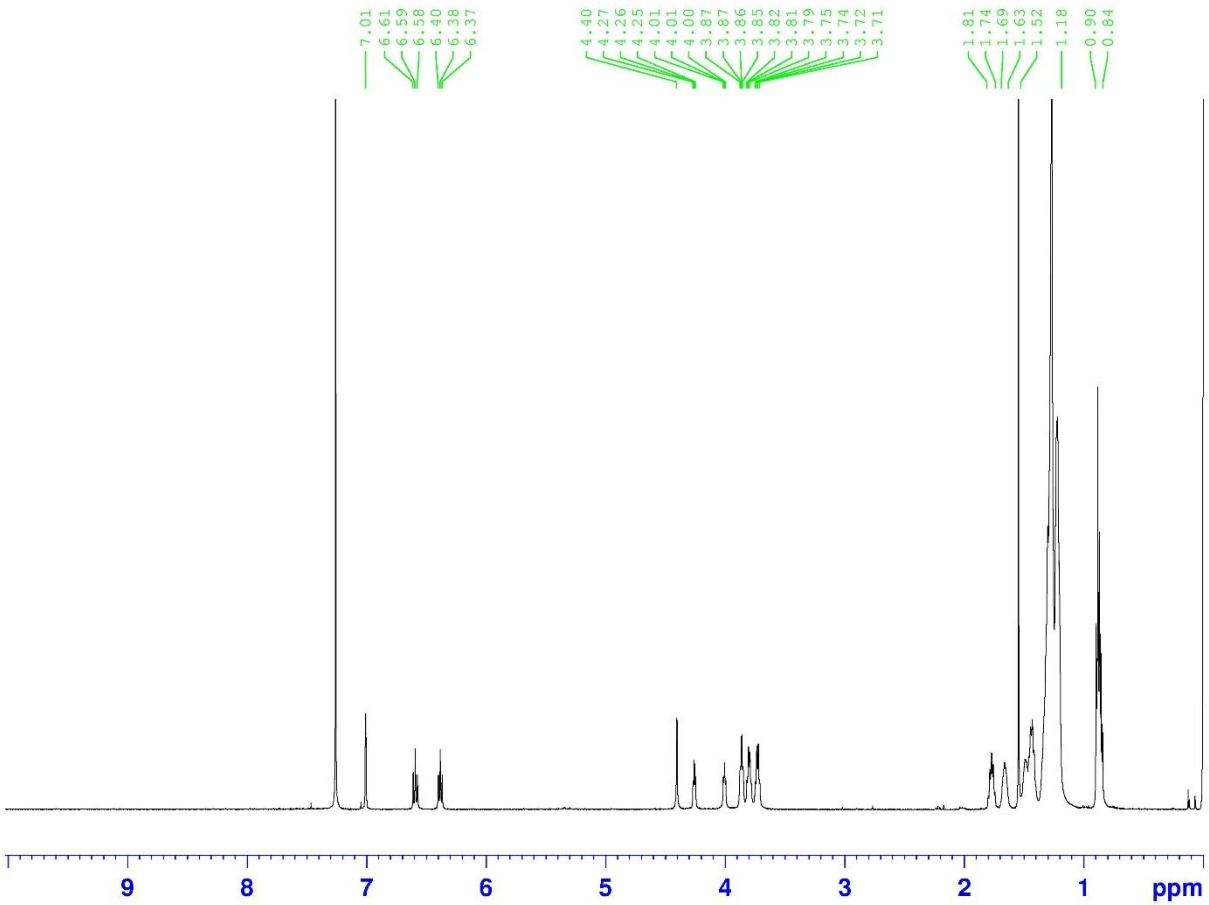
F2 - Acquisition Parameters
Date_           20110713
Time               12.14
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           32894.738 Hz
FIDRES         0.501934 Hz
AQ            0.9961972 sec
RG                 2890
DW               15.200 usec
DE                10.00 usec
TE                298.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.40 usec
PL1                1.50 dB
PL1W        51.74793243 W
SFO1        125.7761482 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2                1.00 dB
PL12              18.79 dB
PL13              21.00 dB
PL2W        19.75309753 W
PL12W        0.32857543 W
PL13W        0.19753097 W
SFO2        500.1550006 MHz

F2 - Processing parameters
SI                32768
SF          125.7635725 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

4c ^{1}H



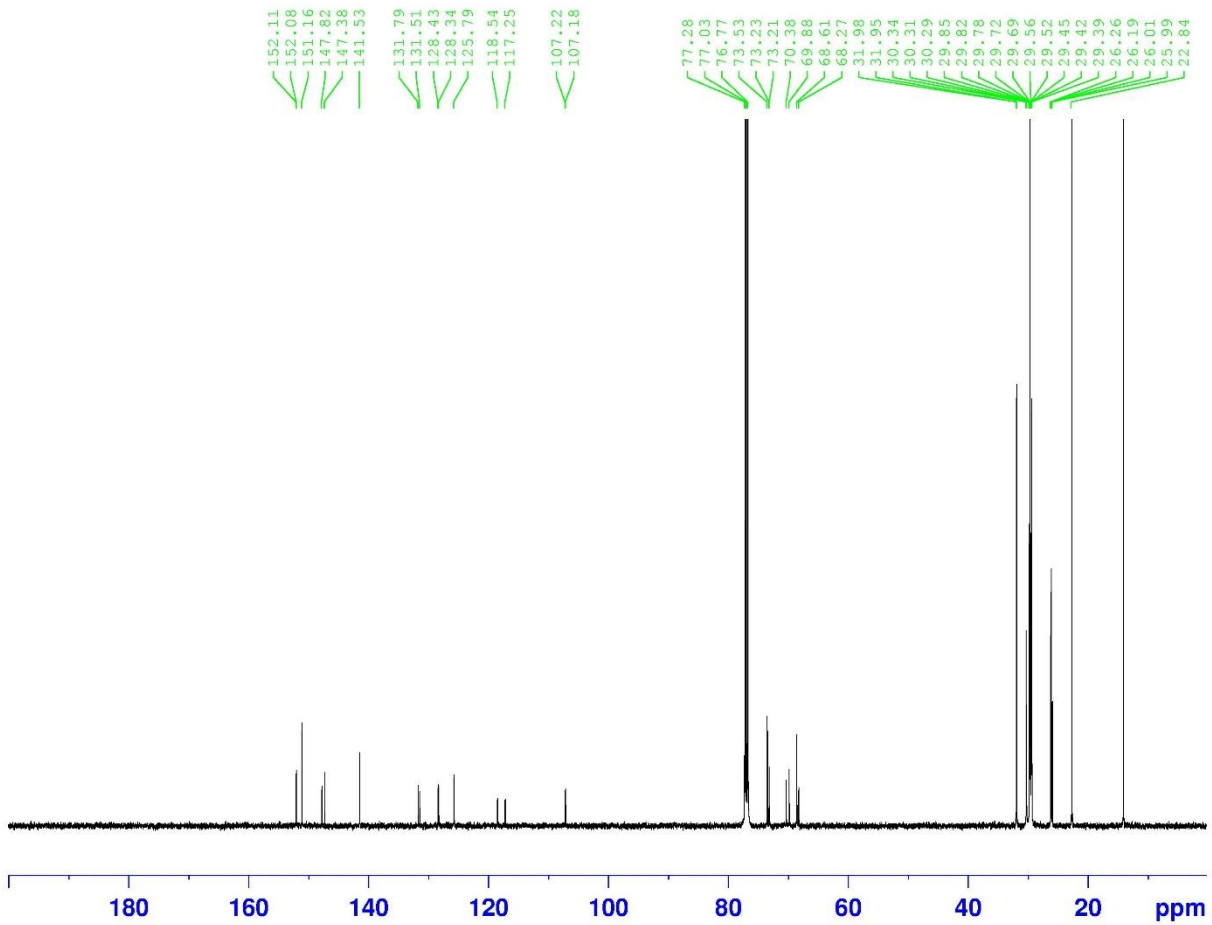

```
Current Data Parameters
NAME          May24-2011
EXPNO                 50
PROCNO                 1

F2 - Acquisition Parameters
Date_            20110524
Time                17.45
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     32
DS                      0
SWH            10330.578 Hz
FIDRES          0.315264 Hz
AQ             1.5860212 sec
RG                    575
DW                48.400 usec
DE                 10.00 usec
TE                 300.0 K
D1            2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  11.05 usec
PL1                  1.00 dB
PL1W         19.75309753 W
SFO1         500.1560886 MHz

F2 - Processing parameters
SI                  16384
SF           500.1530156 MHz
WDW                    EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```

4c ^{13}C




```
Current Data Parameters
NAME          Jul26-2011
EXPNO                120
PROCNO                 1

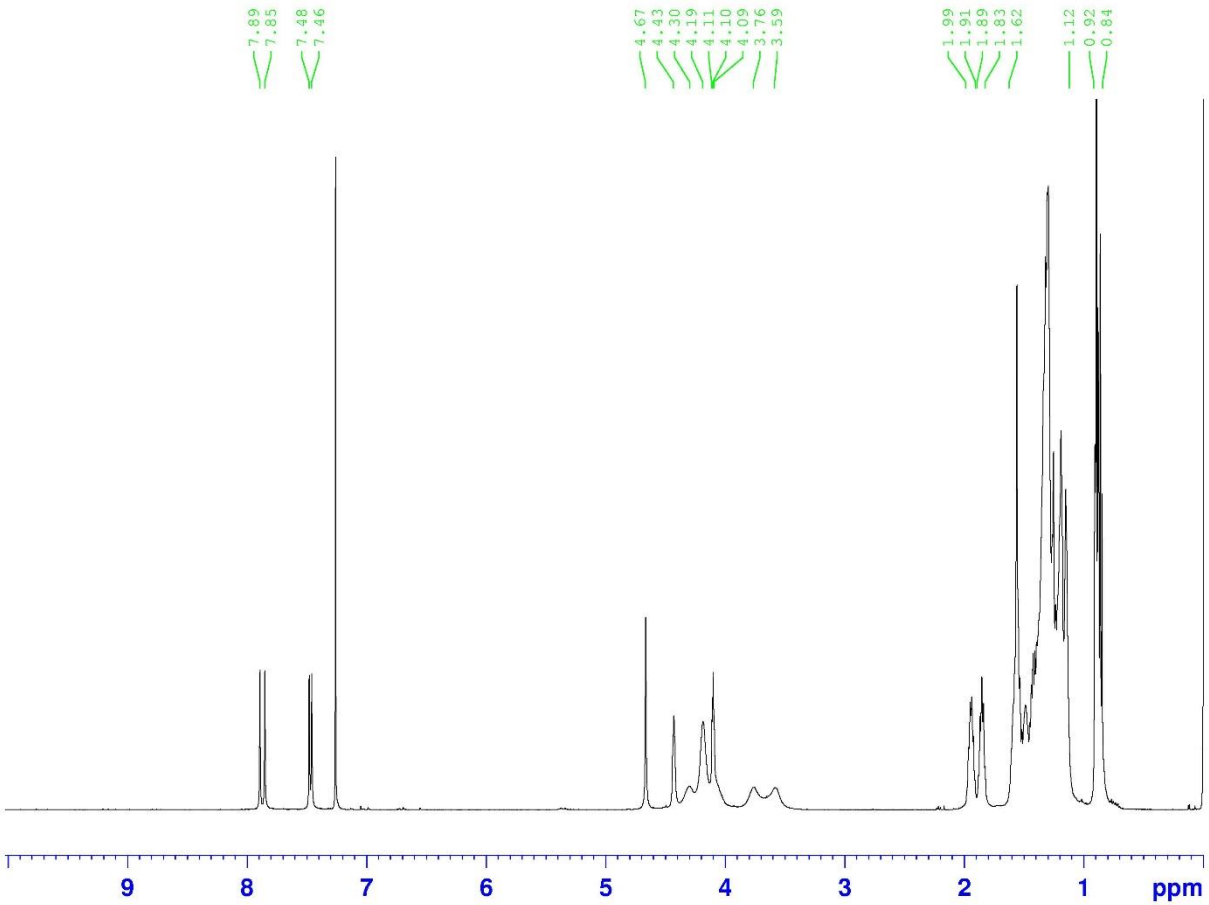
F2 - Acquisition Parameters
Date_           20110727
Time                5.16
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2048
DS                    4
SWH           32894.738 Hz
FIDRES         0.501934 Hz
AQ            0.9961972 sec
RG                 2890
DW               15.200 usec
DE                10.00 usec
TE                296.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.40 usec
PL1                1.50 dB
PL1W        51.74793243 W
SFO1        125.7761482 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2                1.00 dB
PL12              18.79 dB
PL13              21.00 dB
PL2W        19.75309753 W
PL12W        0.32857543 W
PL13W        0.19753097 W
SFO2        500.1550006 MHz

F2 - Processing parameters
SI                32768
SF          125.7635732 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

5a ^{1}H



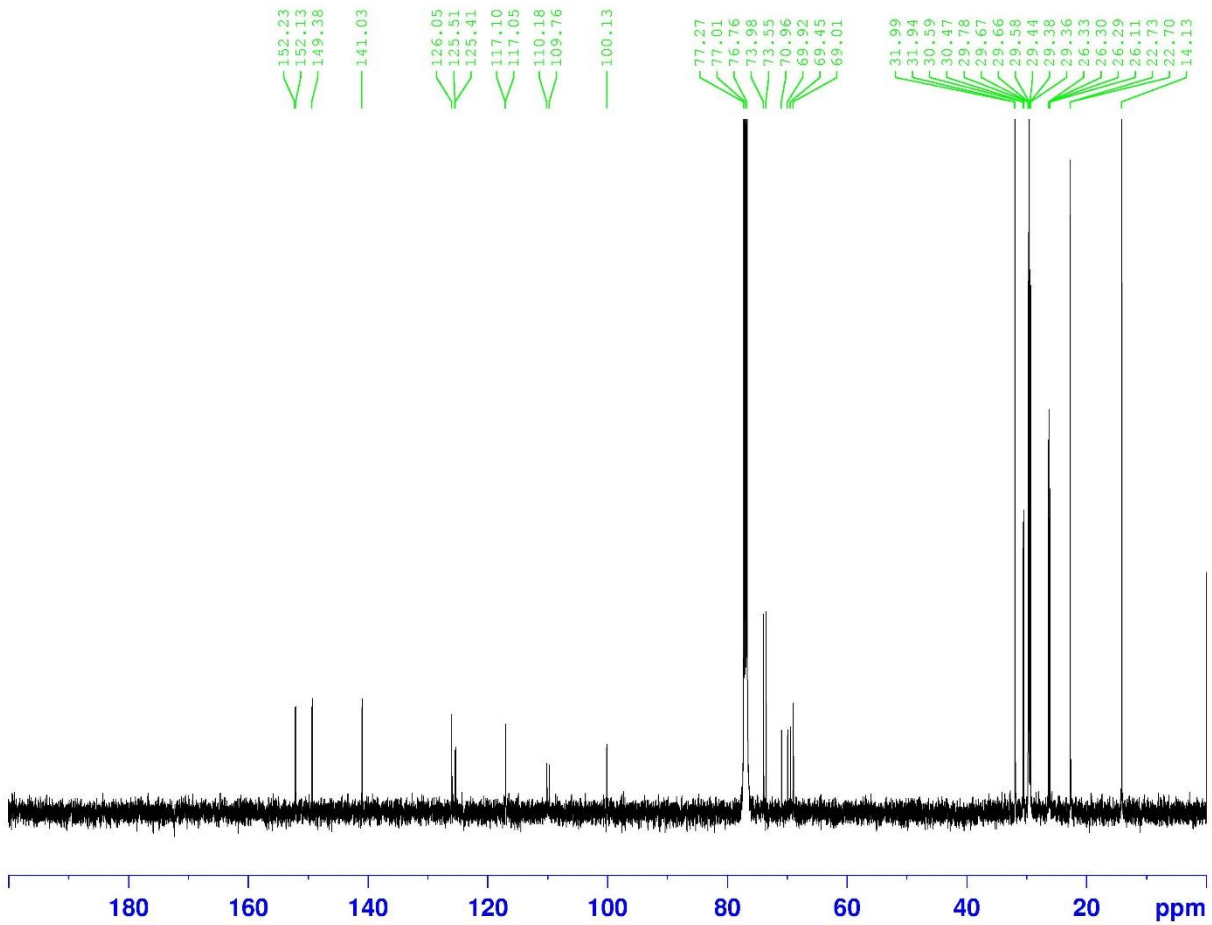

```
Current Data Parameters
NAME          Jun07-2011
EXPNO                100
PROCNO                 1

F2 - Acquisition Parameters
Date_            20110607
Time               11.09
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                   128
DS                     0
SWH           10330.578 Hz
FIDRES         0.315264 Hz
AQ            1.5860212 sec
RG                   256
DW               48.400 usec
DE                10.00 usec
TE                298.1 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.05 usec
PL1                1.00 dB
PL1W        19.75309753 W
SFO1        500.1560886 MHz

F2 - Processing parameters
SI                16384
SF          500.1530161 MHz
WDW                  EM
SSB      0
LB                0.30 Hz
GB       0
PC                1.00
```

5a ^{13}C




```
Current Data Parameters
NAME          Jun09-2011
EXPNO                160
PROCNO                 1

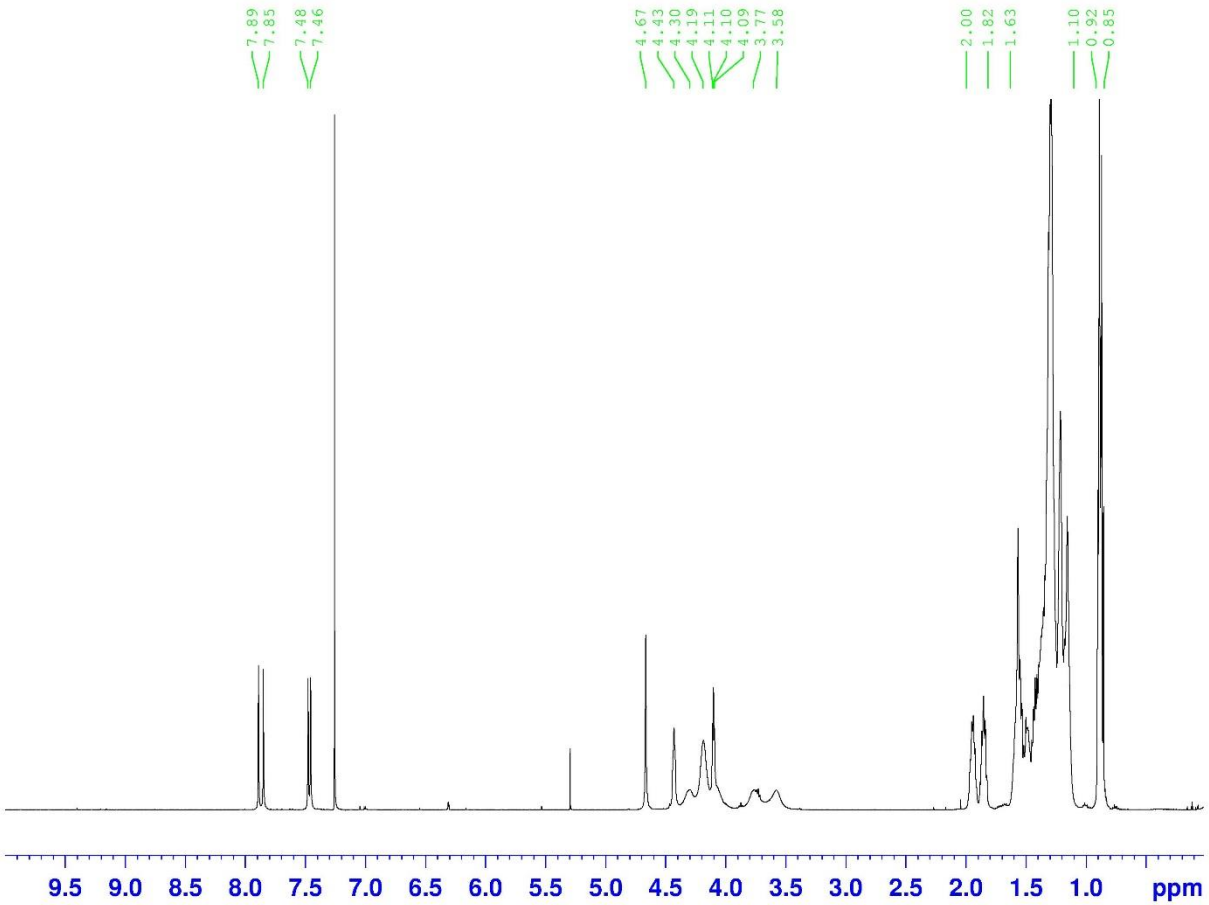
F2 - Acquisition Parameters
Date_           20110610
Time                5.22
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3072
DS                    4
SWH           32894.738 Hz
FIDRES         0.501934 Hz
AQ            0.9961972 sec
RG                 2890
DW               15.200 usec
DE                10.00 usec
TE                296.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.40 usec
PL1                1.50 dB
PL1W        51.74793243 W
SFO1        125.7761482 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2                 1.00 dB
PL12               18.79 dB
PL13               21.00 dB
PL2W        19.75309753 W
PL12W        0.32857543 W
PL13W        0.19753097 W
SFO2        500.1550006 MHz

F2 - Processing parameters
SI                 32768
SF          125.7635738 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

5b ^{1}H



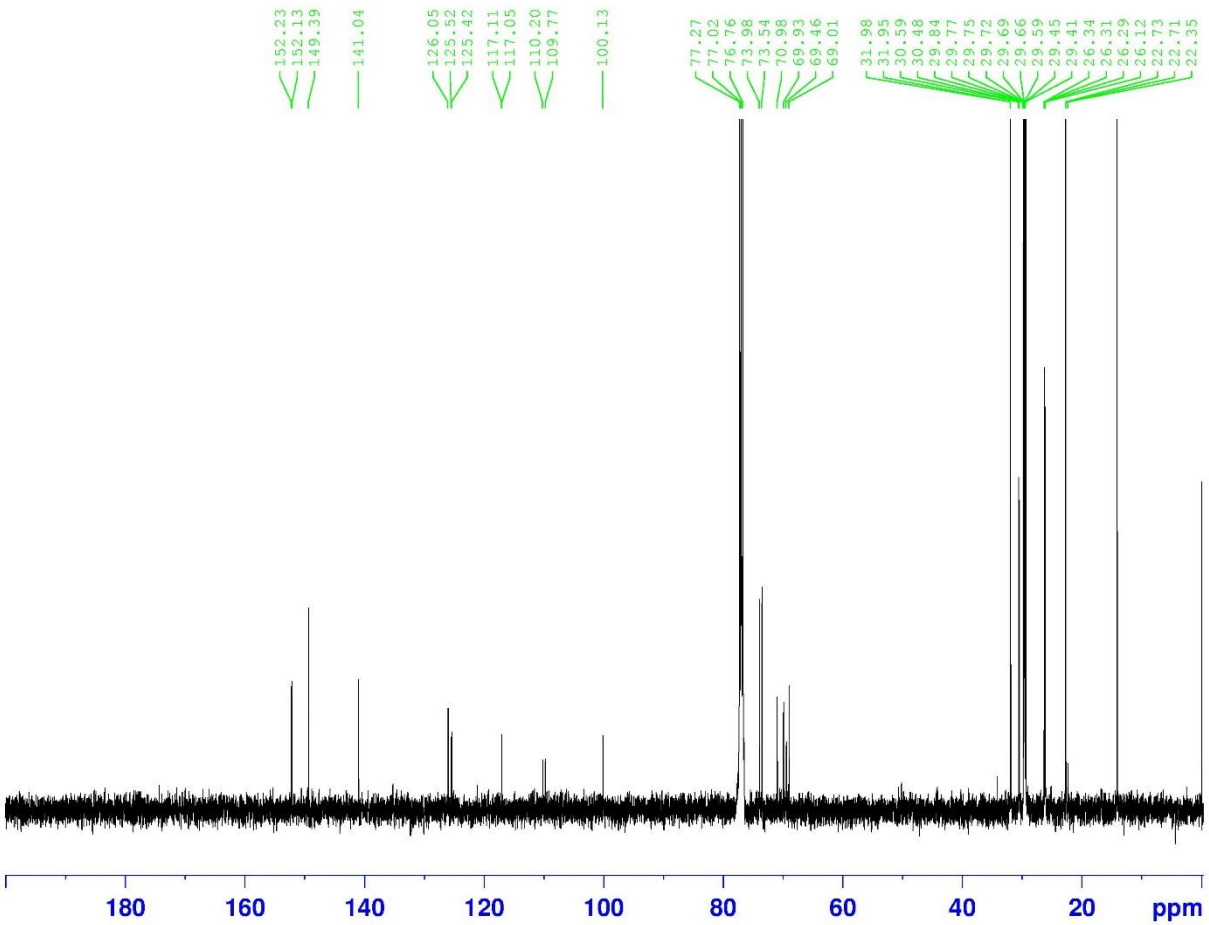

```
Current Data Parameters
NAME          Oct31-2013
EXPNO                 90
PROCNO                 1

F2 - Acquisition Parameters
Date_            20131031
Time                18.51
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                     64
DS                      0
SWH            10330.578 Hz
FIDRES          0.315264 Hz
AQ             1.5860212 sec
RG                    203
DW                48.400 usec
DE                 10.00 usec
TE                 296.8 K
D1            2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  11.23 usec
PL1                  1.00 dB
PL1W         19.75309753 W
SFO1         500.1560886 MHz

F2 - Processing parameters
SI                  16384
SF           500.1530167 MHz
WDW                    EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```

5b ^{13}C




```
Current Data Parameters
NAME          Oct31-2013
EXPNO                 91
PROCNO                 1

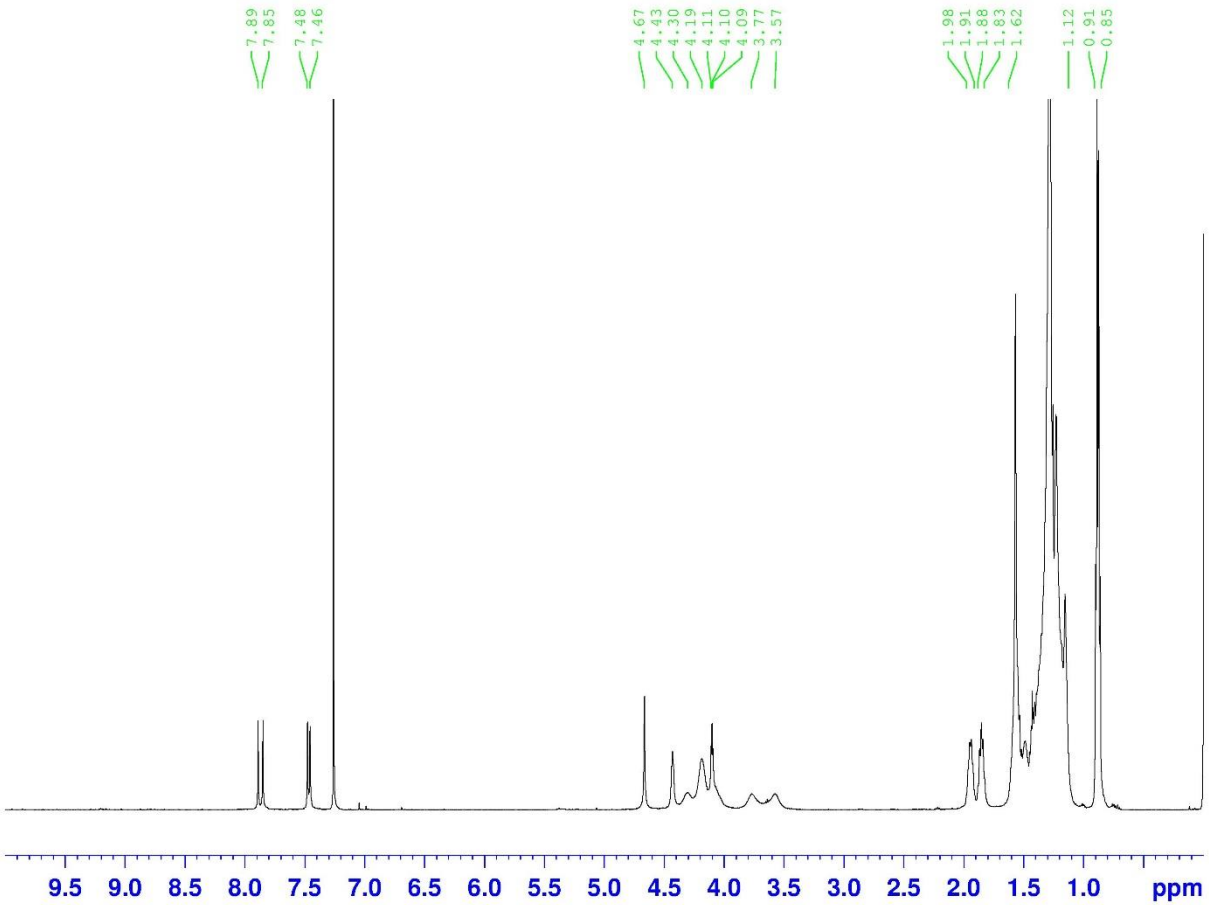
F2 - Acquisition Parameters
Date_           20131031
Time               20.36
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2048
DS                    4
SWH           32894.738 Hz
FIDRES         0.501934 Hz
AQ            0.9961972 sec
RG                 3250
DW               15.200 usec
DE                10.00 usec
TE                296.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.20 usec
PL1                1.50 dB
PL1W        51.74793243 W
SFO1        125.7761482 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2                 1.00 dB
PL12               19.99 dB
PL13               21.00 dB
PL2W        19.75309753 W
PL12W        0.24925002 W
PL13W        0.19753097 W
SFO2        500.1550006 MHz

F2 - Processing parameters
SI                 32768
SF          125.7635738 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

5c ^{1}H



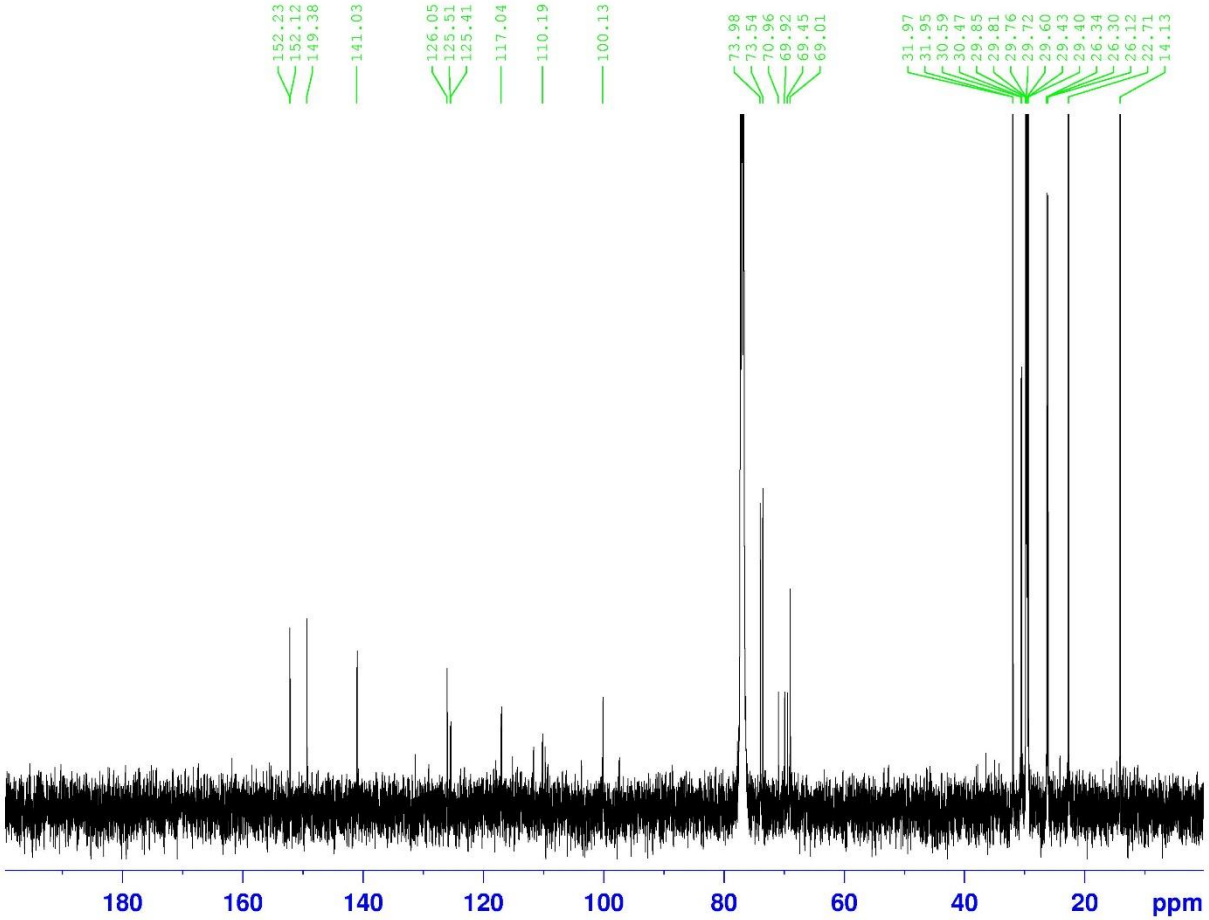

```
Current Data Parameters
NAME          Jul27-2011
EXPNO                 30
PROCNO                 1

F2 - Acquisition Parameters
Date_            20110727
Time               10.37
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    64
DS                     0
SWH           10330.578 Hz
FIDRES         0.315264 Hz
AQ            1.5860212 sec
RG                   362
DW               48.400 usec
DE                10.00 usec
TE                296.8 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.05 usec
PL1                1.00 dB
PL1W        19.75309753 W
SFO1        500.1560886 MHz

F2 - Processing parameters
SI                16384
SF          500.1530152 MHz
WDW                  EM
SSB      0
LB                0.30 Hz
GB       0
PC                1.00
```

5c ^{13}C




```
Current Data Parameters
NAME          Jul29-2011
EXPNO                120
PROCNO                 1

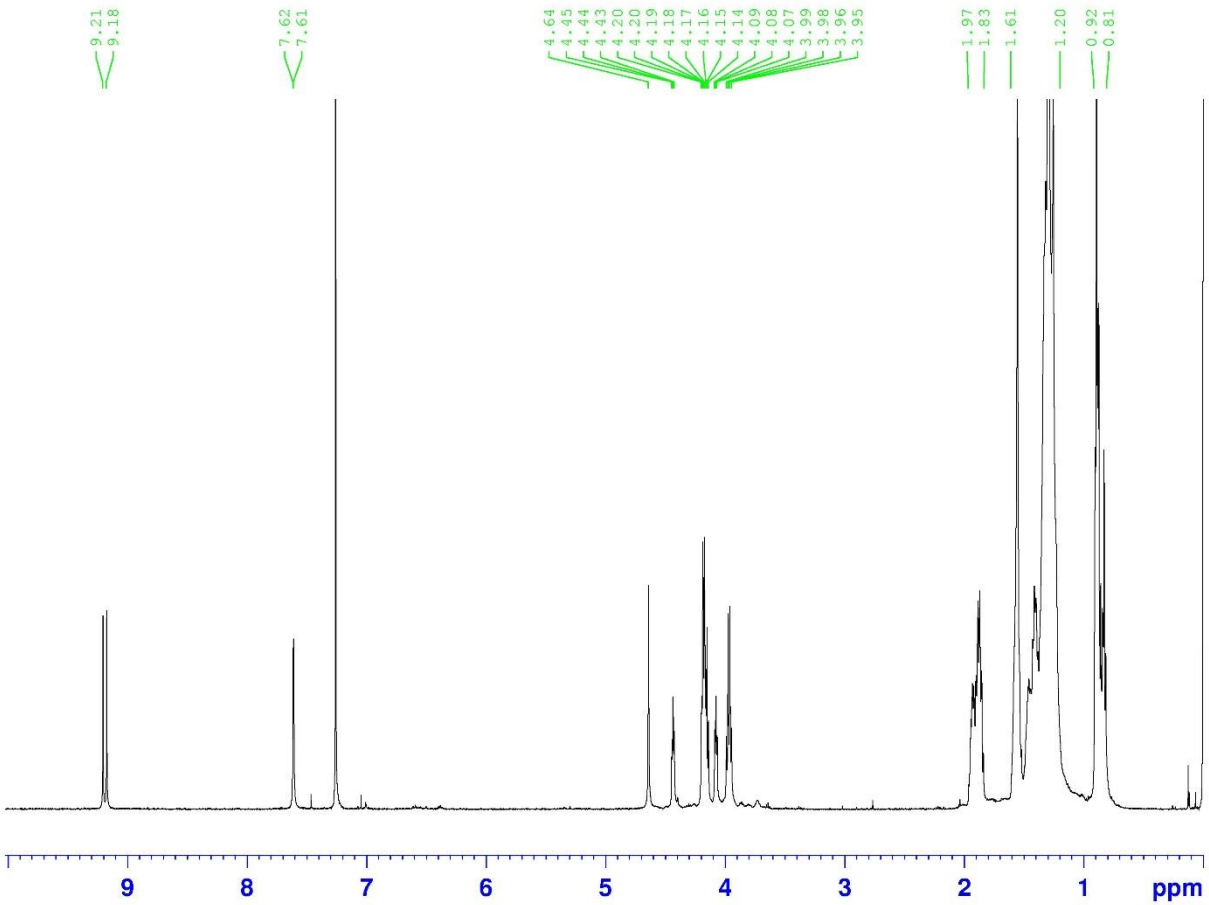
F2 - Acquisition Parameters
Date_           20110731
Time                8.29
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 4096
DS                    4
SWH           32894.738 Hz
FIDRES         0.501934 Hz
AQ            0.9961972 sec
RG                 2890
DW               15.200 usec
DE                10.00 usec
TE                296.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.40 usec
PL1                1.50 dB
PL1W        51.74793243 W
SFO1        125.7761482 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2                1.00 dB
PL12              18.79 dB
PL13              21.00 dB
PL2W        19.75309753 W
PL12W        0.32857543 W
PL13W        0.19753097 W
SFO2        500.1550006 MHz

F2 - Processing parameters
SI                32768
SF          125.7635738 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

6a ^{1}H



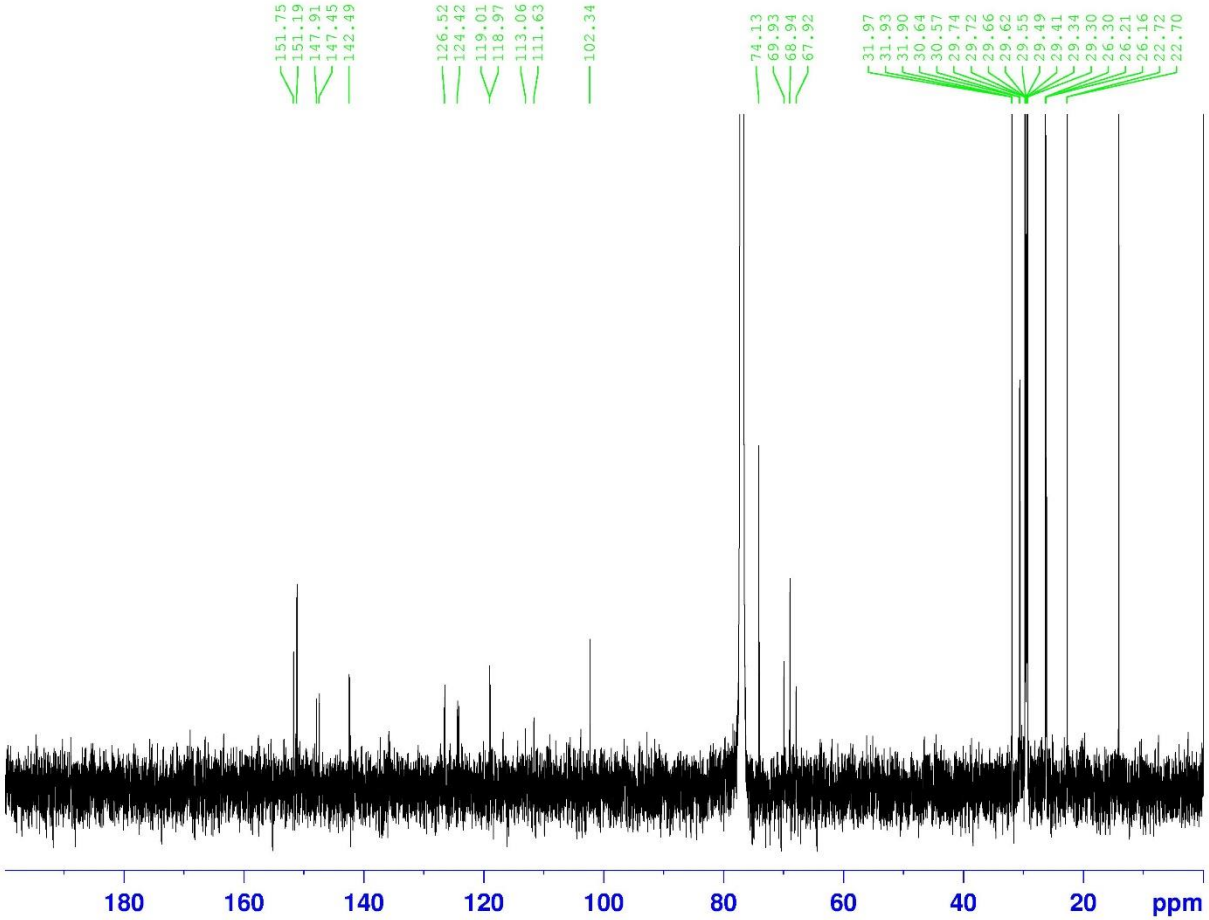

```
Current Data Parameters
NAME          Jun09-2011
EXPNO                171
PROCNO                 1

F2 - Acquisition Parameters
Date_            20110610
Time                 9.04
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     64
DS                      2
SWH            10330.578 Hz
FIDRES          0.157632 Hz
AQ             3.1719923 sec
RG                    456
DW                 48.400 usec
DE                  8.50 usec
TE                 296.8 K
D1            1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  11.05 usec
PL1                  1.00 dB
PL1W         19.75309753 W
SFO1         500.1560886 MHz

F2 - Processing parameters
SI                  32768
SF           500.1530156 MHz
WDW                    EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```

6a ^{13}C




```
Current Data Parameters
NAME          Jun10-2011
EXPNO                190
PROCNO                 1

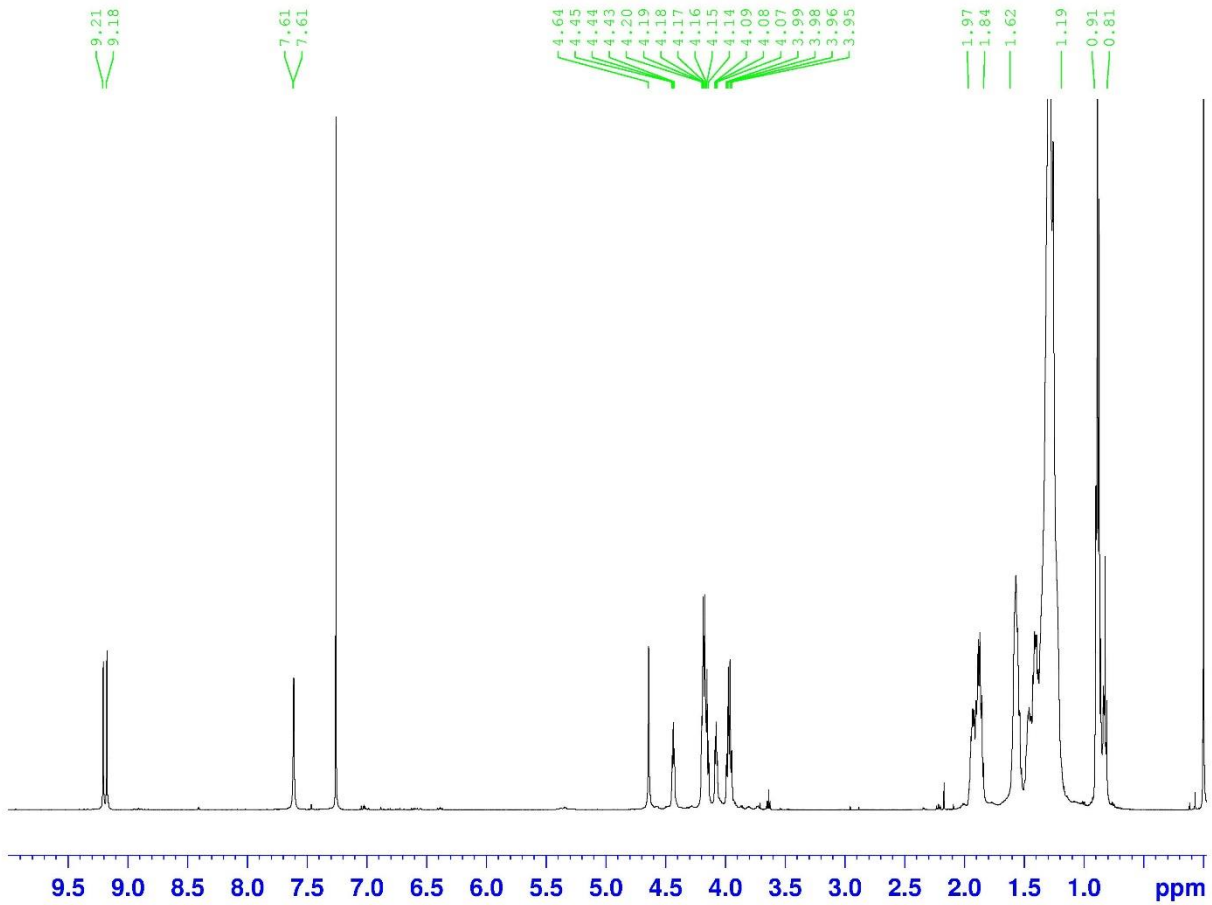
F2 - Acquisition Parameters
Date_           20110612
Time                1.56
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 8192
DS                    4
SWH           32894.738 Hz
FIDRES         0.501934 Hz
AQ            0.9961972 sec
RG                 2890
DW               15.200 usec
DE                10.00 usec
TE                296.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.40 usec
PL1                1.50 dB
PL1W        51.74793243 W
SFO1        125.7761482 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2                1.00 dB
PL12              18.79 dB
PL13              21.00 dB
PL2W        19.75309753 W
PL12W        0.32857543 W
PL13W        0.19753097 W
SFO2        500.1550006 MHz

F2 - Processing parameters
SI                 32768
SF          125.7635738 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

6b ^{1}H



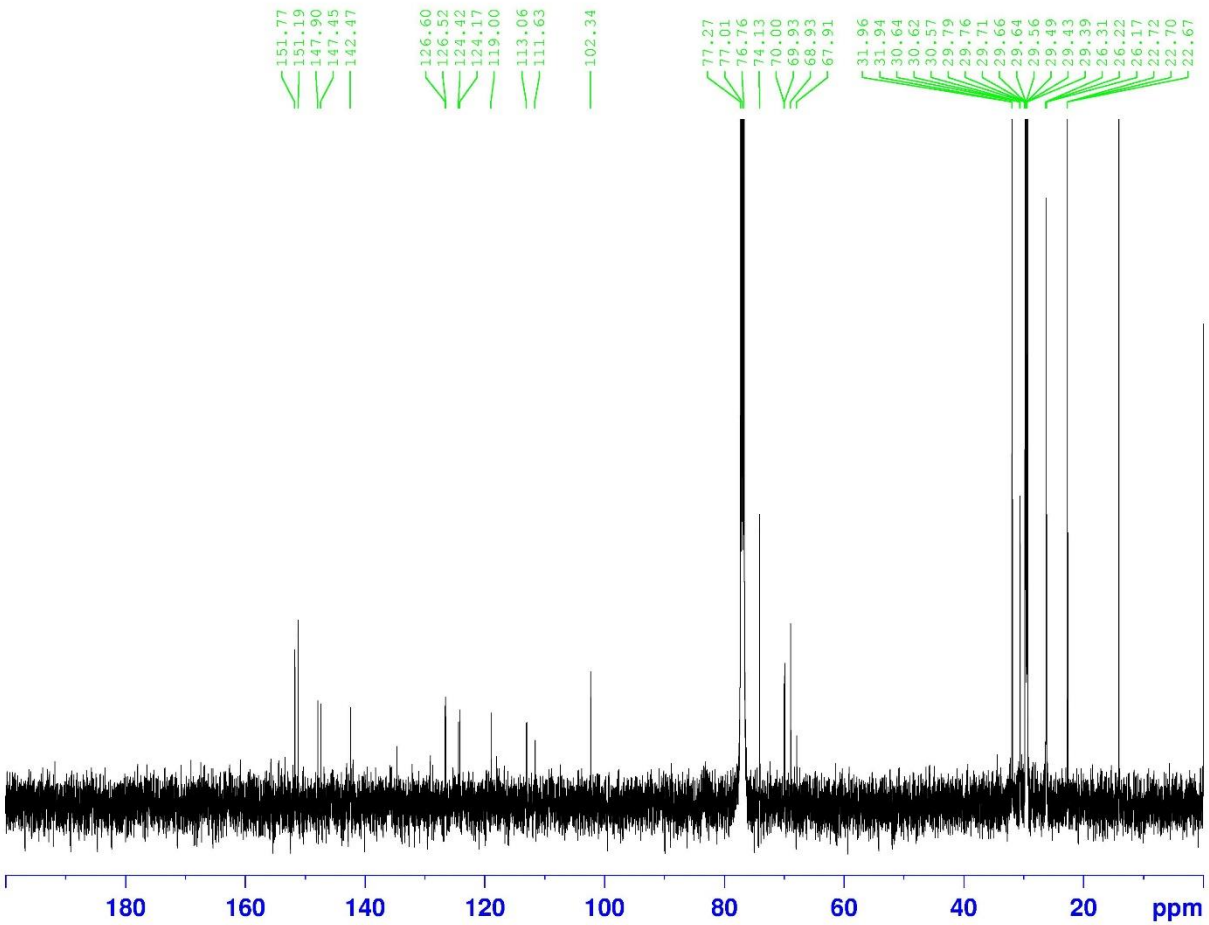

```
Current Data Parameters
NAME          Jul19-2011
EXPNO                130
PROCNO                 1

F2 - Acquisition Parameters
Date_            20110719
Time               22.17
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                   128
DS                     0
SWH           10330.578 Hz
FIDRES         0.315264 Hz
AQ            1.5860212 sec
RG                   256
DW               48.400 usec
DE               10.00 usec
TE               300.0 K
D1           2.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                11.05 usec
PL1                1.00 dB
PL1W        19.75309753 W
SFO1        500.1560886 MHz

F2 - Processing parameters
SI                16384
SF          500.1530159 MHz
WDW                  EM
SSB      0
LB                0.30 Hz
GB       0
PC                1.00
```

6b ^{13}C




```
Current Data Parameters
NAME          Jul19-2011
EXPNO                131
PROCNO                 1

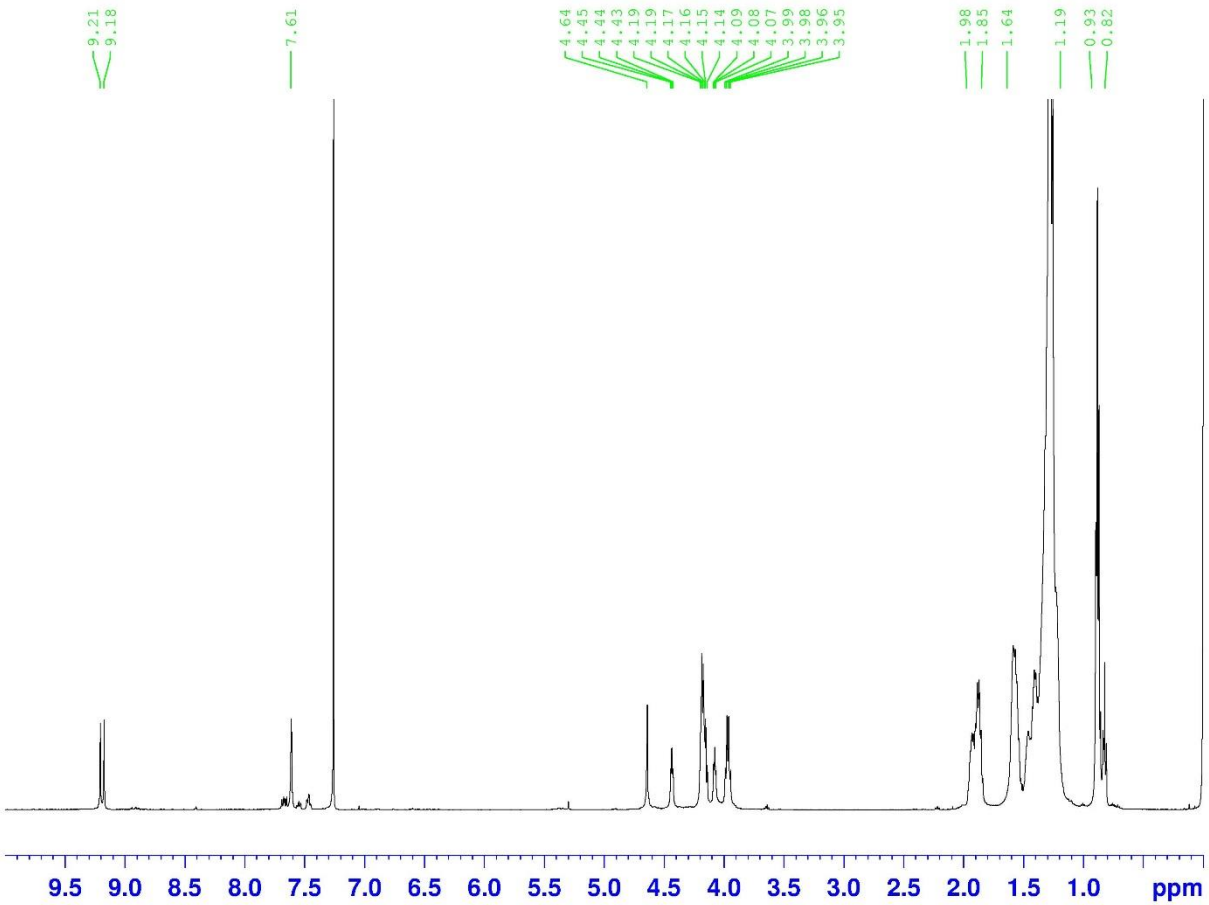
F2 - Acquisition Parameters
Date_           20110720
Time                0.02
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2048
DS                    4
SWH           32894.738 Hz
FIDRES         0.501934 Hz
AQ            0.9961972 sec
RG                 2580
DW               15.200 usec
DE                10.00 usec
TE                296.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.40 usec
PL1                1.50 dB
PL1W        51.74793243 W
SFO1        125.7761482 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2                 1.00 dB
PL12               18.79 dB
PL13               21.00 dB
PL2W        19.75309753 W
PL12W        0.32857543 W
PL13W        0.19753097 W
SFO2        500.1550006 MHz

F2 - Processing parameters
SI                 32768
SF          125.7635738 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

6c ^{1}H



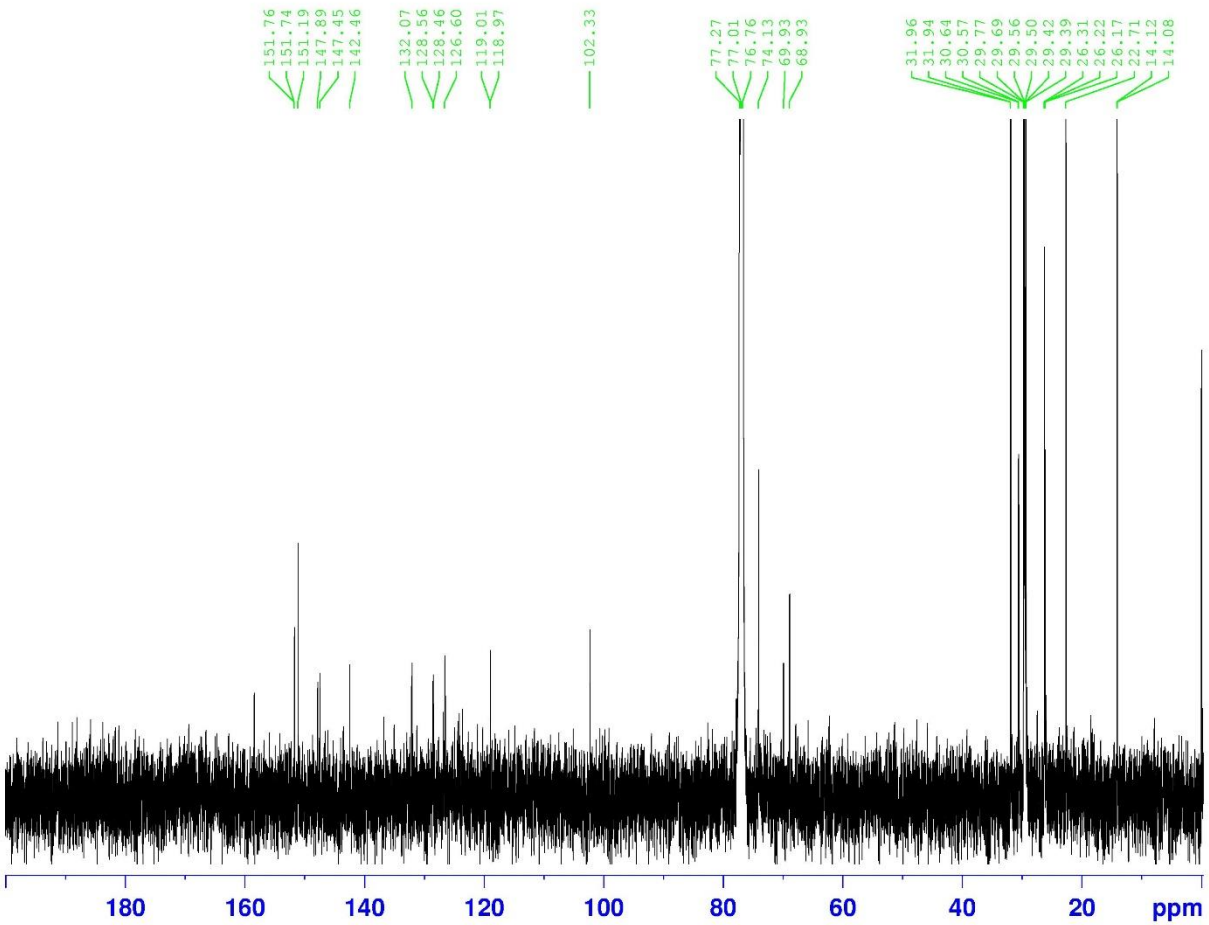

```
Current Data Parameters
NAME          Jul19-2011
EXPNO                140
PROCNO                 1

F2 - Acquisition Parameters
Date_            20110720
Time                 0.16
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                    128
DS                      0
SWH            10330.578 Hz
FIDRES          0.315264 Hz
AQ             1.5860212 sec
RG                    322
DW                48.400 usec
DE                 10.00 usec
TE                 296.8 K
D1            2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  11.05 usec
PL1                  1.00 dB
PL1W         19.75309753 W
SFO1         500.1560886 MHz

F2 - Processing parameters
SI                  16384
SF           500.1530155 MHz
WDW                    EM
SSB       0
LB                   0.30 Hz
GB        0
PC                   1.00
```

6c ^{13}C




```
Current Data Parameters
NAME          Jul29-2011
EXPNO                110
PROCNO                 1

F2 - Acquisition Parameters
Date_           20110731
Time                4.54
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 4096
DS                    4
SWH           32894.738 Hz
FIDRES         0.501934 Hz
AQ            0.9961972 sec
RG                 2890
DW               15.200 usec
DE                10.00 usec
TE                296.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                10.40 usec
PL1                1.50 dB
PL1W        51.74793243 W
SFO1        125.7761482 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2            100.00 usec
PL2                 1.00 dB
PL12               18.79 dB
PL13               21.00 dB
PL2W        19.75309753 W
PL12W        0.32857543 W
PL13W        0.19753097 W
SFO2        500.1550006 MHz

F2 - Processing parameters
SI                 32768
SF          125.7635738 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```