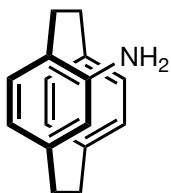
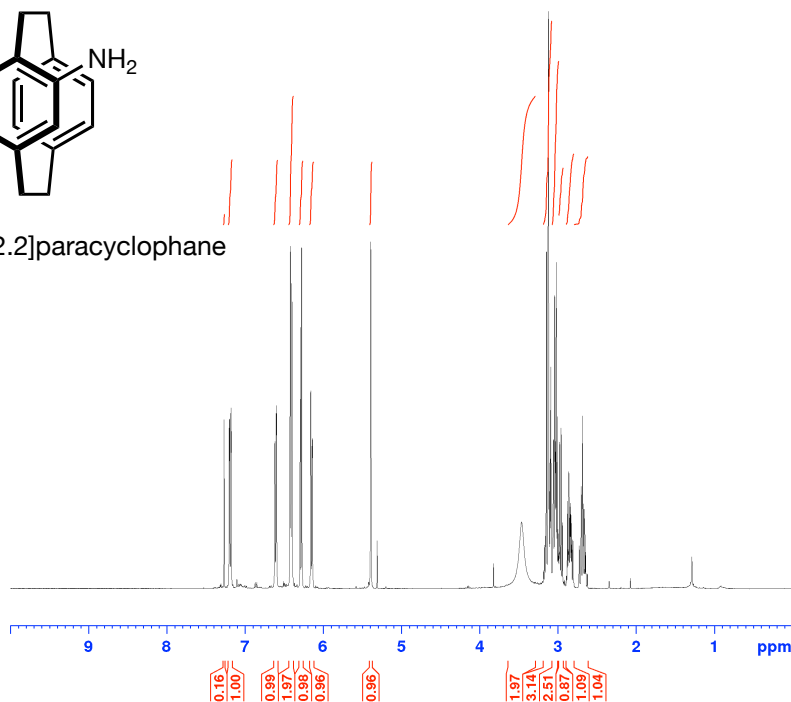


Supplementary information: The synthesis of substituted amino[2.2]paracyclophanes



4-amino[2.2]paracyclophane



Current Data Parameters
NAME XIV-GJR-77B
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111207
Time 10.16
INSTRUM spect
PROBHD 5 mm Multinucl
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9583745 sec
RG 90.5
DW 60.400 usec
DE 6.00 usec
TE 295.2 K
D1 1.00000000 sec
TD0 1

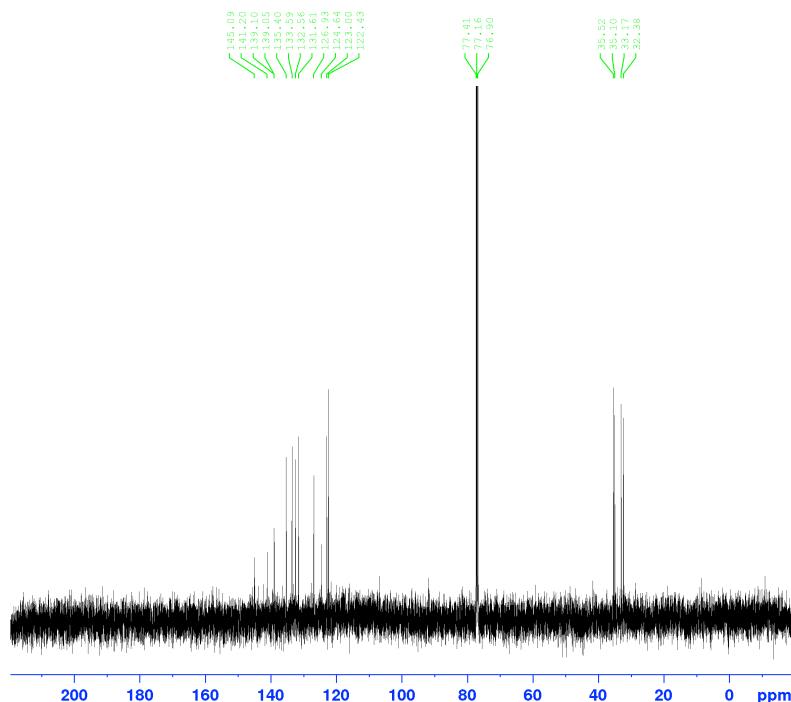
===== CHANNEL f1 =====
NUC1 1H
P1 10.00 usec
PL1 4.00 dB
SFO1 400.1324710 MHz

F1 - Acquisition parameters
TD 256
SFO1 100.6203 MHz
FIDRES 130.208328 Hz
SW 165.639 ppm
FnMODE Echo-Antiecho

F2 - Processing parameters
SI 32768
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

F1 - Processing parameters
SI 1024
MC2 echo-antiecho
SF 100.6127690 MHz
WDW QSINE
SSB 2
LB 0.30 Hz
GB 0.1

kj-13-016



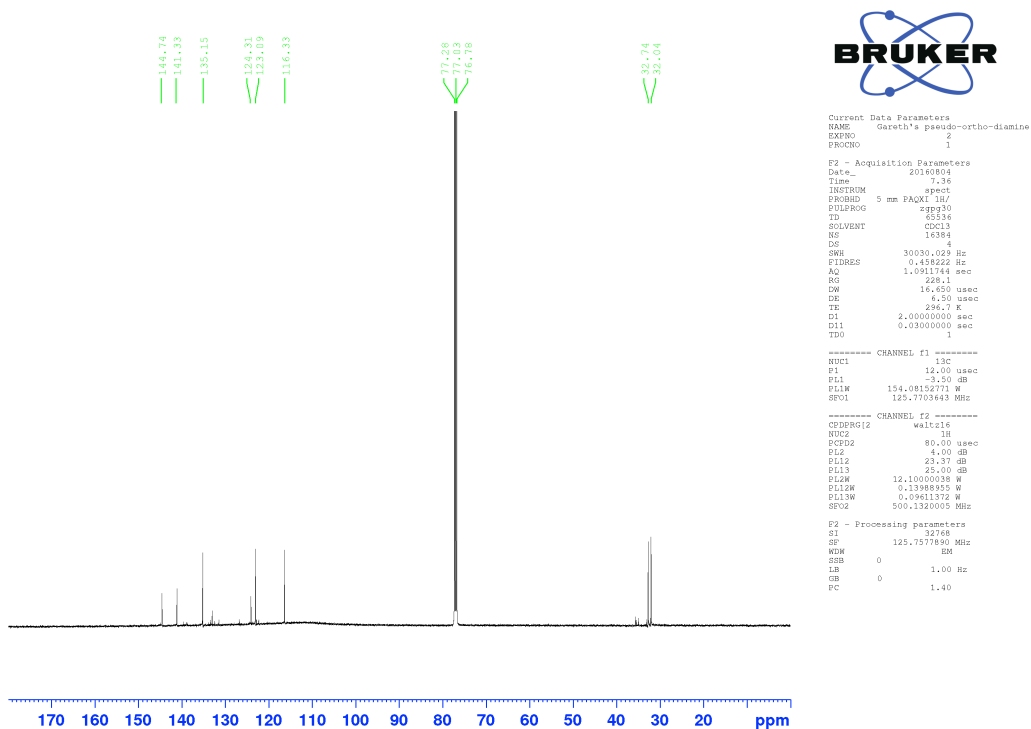
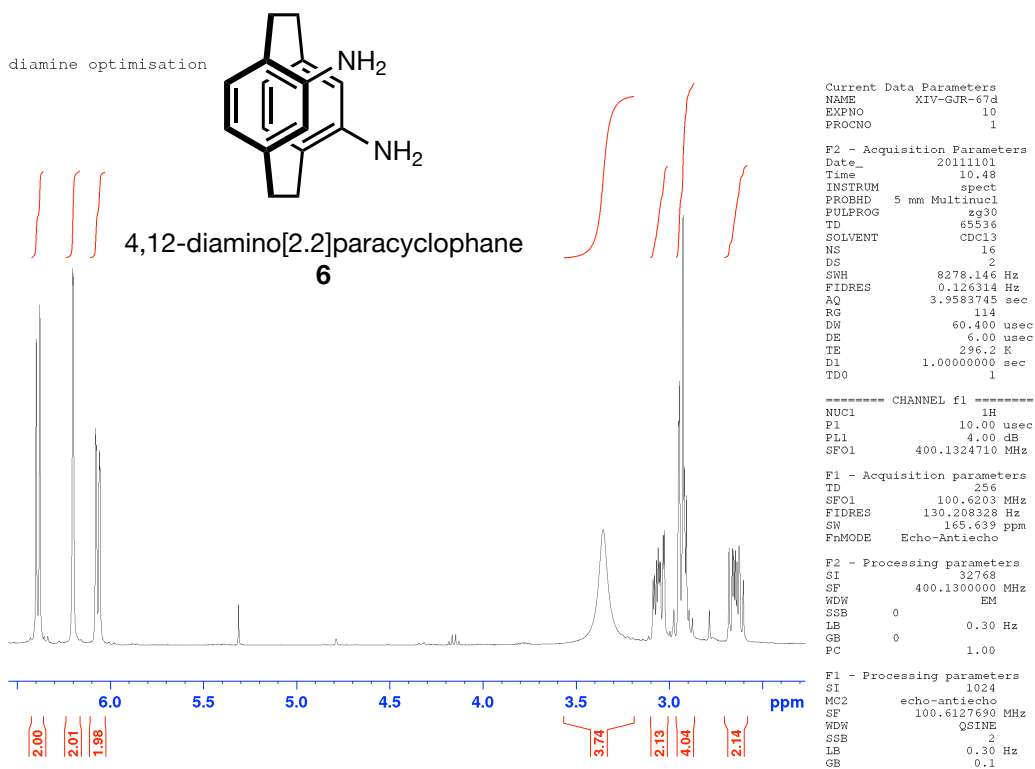
Current Data Parameters
NAME kj-13-016
EXPNO 2
PROCNO 1

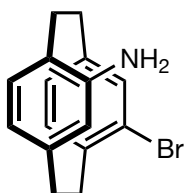
F2 - Acquisition Parameters
Date_ 20160203
Time 13.57
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 127
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 32768
DW 16.650 usec
DE 6.50 usec
TE 301.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -3.50 dB
PL1W 154.08152771 W
SFO1 125.7703643 MHz

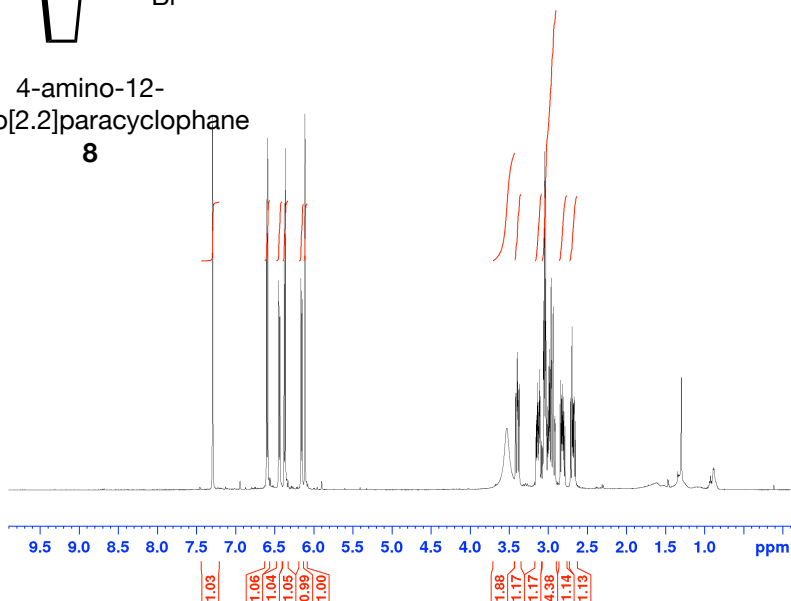
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 23.37 dB
PL13 25.00 dB
PL12W 12.10000038 W
PL12W 0.13988955 W
PL13W 0.09611372 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577720 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40





4-amino-12-bromo[2.2]paracyclophane
8



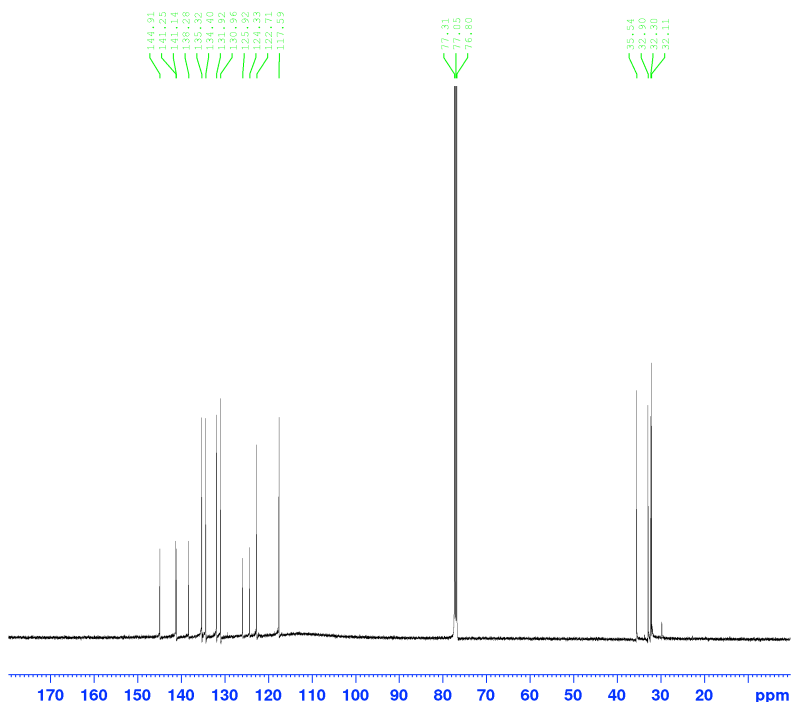
Current Data Parameters
NAME XIVGJR67B
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160721
Time 11.34
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 71.8
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 4.00 dB
PL1W 12.10000038 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Carbon NMR for XIV-GJR-67B for Gareth



Current Data Parameters
NAME XIV-GJR-67B
EXPNO 1
PROCNO 1

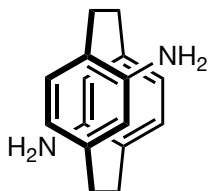
F2 - Acquisition Parameters
Date_ 20160721
Time 18.18
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 14336
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 32768
DW 16.650 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 14

===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -3.50 dB
PL1W 154.08152771 W
SFO1 125.7703643 MHz

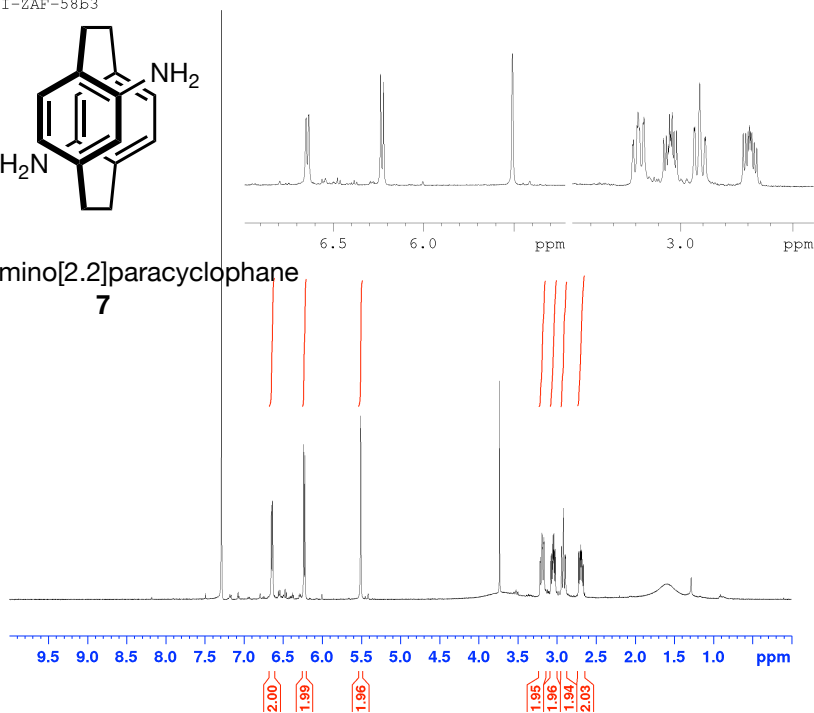
===== CHANNEL f2 =====
CPDPRG2 waitz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 23.37 dB
PL13 25.00 dB
PL2W 12.10000038 W
PL12W 0.13988955 W
PL13W 0.09611372 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

I-ZAF-58b3



4,16-diamino[2.2]paracyclophane
7



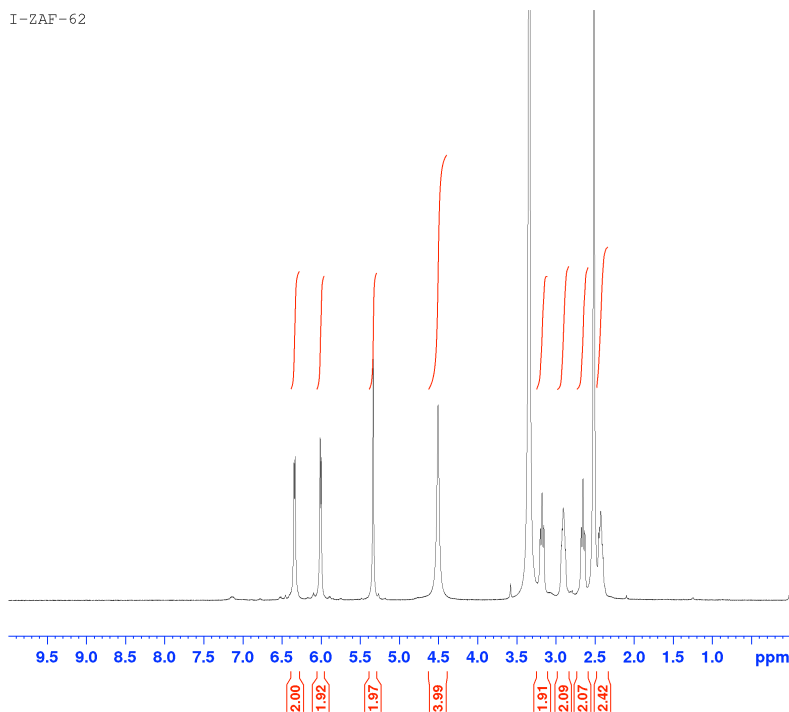
Current Data Parameters
NAME I-ZAF-58b3
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160930
Time 14.32
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 512
DW 48.400 usec
DE 6.50 usec
TE 298.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 4.00 dB
PL1W 12.10000038 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

I-ZAF-62



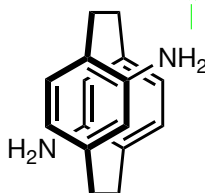
Current Data Parameters
NAME I-ZAF-62
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161003
Time 14.35
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 18
DS 0
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 228.1
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
TD0 1

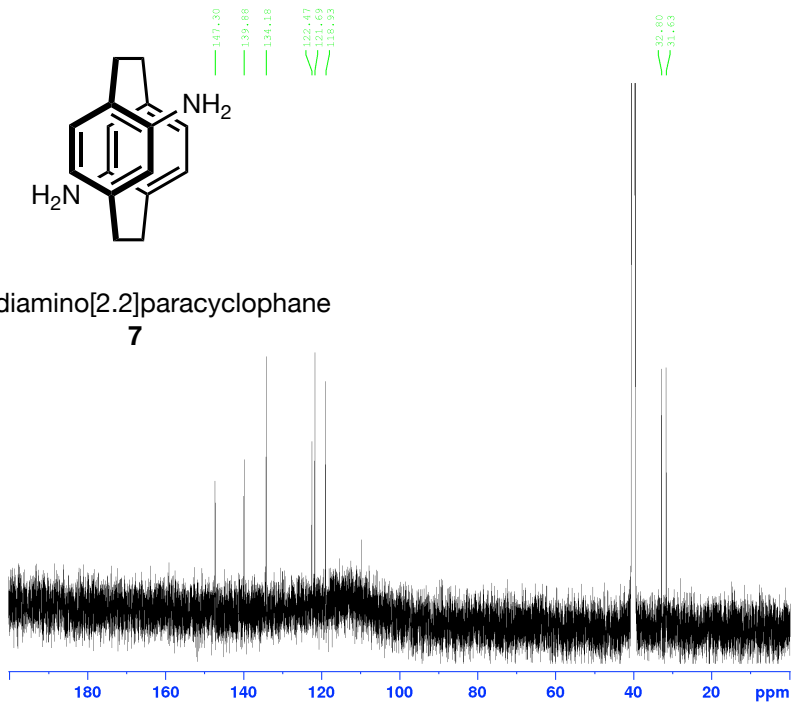
===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 4.00 dB
PL1W 12.10000038 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

I-ZAF-62 13C NMR



4,16-diamino[2.2]paracyclophane
7



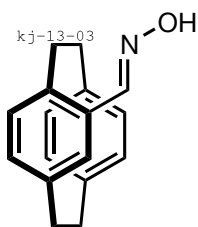
Current Data Parameters
NAME I-ZAF-62
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161003
Time 15.32
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 32768
DW 16.650 usec
DE 6.50 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

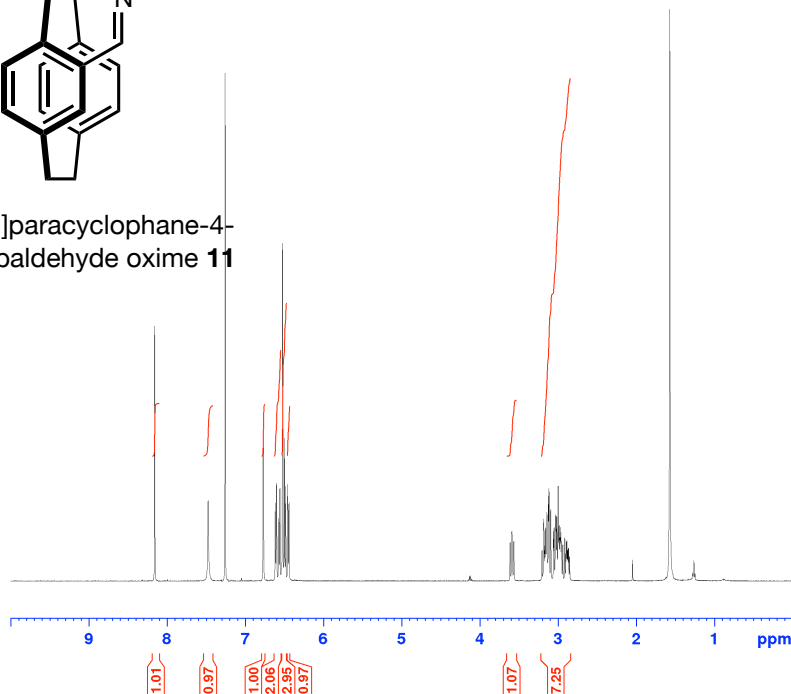
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -3.50 dB
PL1W 154.08152771 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 23.37 dB
PL13 25.00 dB
PL2W 12.10000038 W
PL12W 0.13988955 W
PL13W 0.09611372 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



[2.2]paracyclophane-4-carbaldehyde oxime **11**



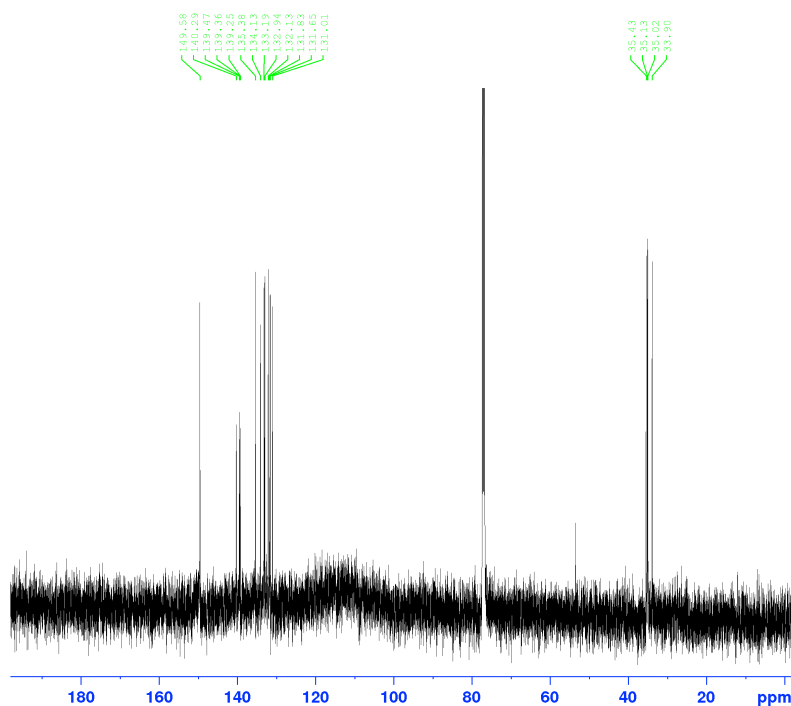
Current Data Parameters
NAME kj-13-03
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160203
Time 13.21
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 362
DW 48.400 usec
DE 6.50 usec
TE 301.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 4.00 dB
PL1W 12.10000038 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300134 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Oxime NMR data for Gareth



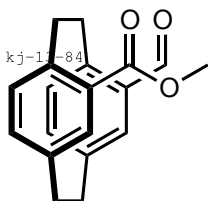
Current Data Parameters
NAME oxamine
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160830
Time 14.01
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 30030.029 Hz
FIDRES 0.456222 Hz
AQ 1.0911744 sec
RG 256
DW 16.650 usec
DE 6.50 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 3

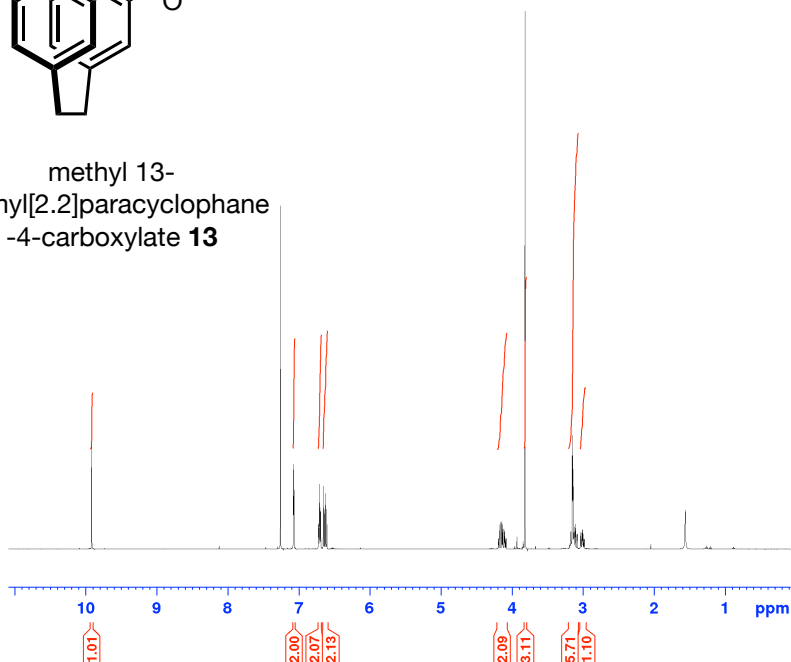
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -3.50 dB
PL1W 154.08152771 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 23.37 dB
PL13 25.00 dB
PL2W 12.10000038 W
PL12W 0.13988955 W
PL13W 0.09611372 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



methyl 13-
formyl[2.2]paracyclophane
-4-carboxylate **13**



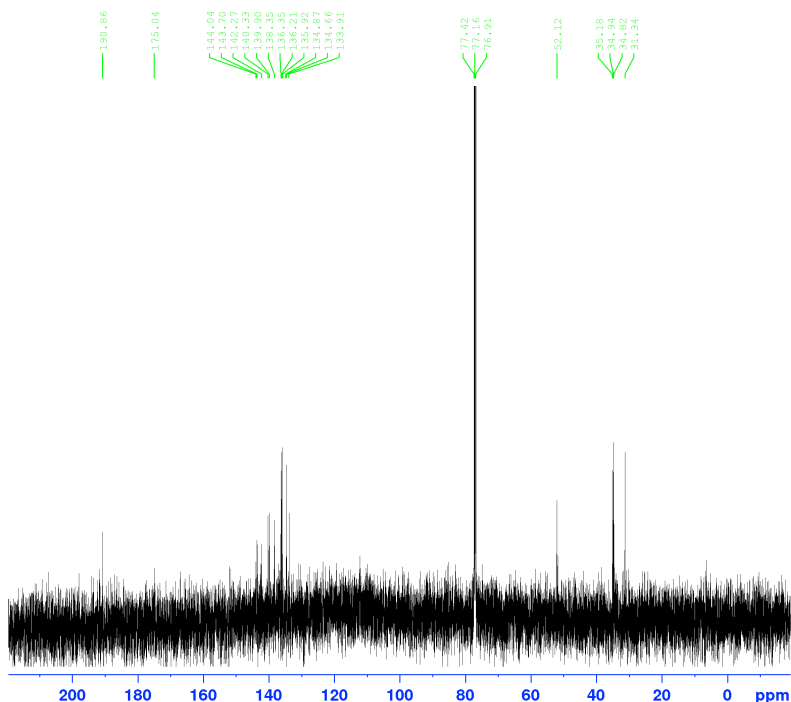
```
Current Data Parameters
NAME      kj-13-84
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20160210
Time      12.47
INSTRUM   spect
PROBHD    5 mm PAQXI 1H/
PULPROG   zg30
TD         65536
SOLVENT   CDCl3
NS         16
DS         2
SWH        10330.578 Hz
FIDRES     0.157632 Hz
AQ         3.1719425 sec
RG         362
DW         48.400 usec
DE         6.50 usec
TE         298.2 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         8.60 usec
PL1        4.00 dB
PL1W       12.10000038 W
SFO1       500.130885 MHz

F2 - Processing parameters
SI         32768
SF         500.1300135 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
```

kj-13-84



```
Current Data Parameters
NAME      kj-13-84
EXPNO     2
PROCNO    1

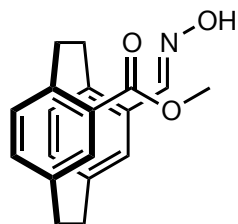
F2 - Acquisition Parameters
Date_     20160210
Time      12.54
INSTRUM   spect
PROBHD    5 mm PAQXI 1H/
PULPROG   zgpg30
TD         65536
SOLVENT   CDCl3
NS         231
DS         4
SWH        30030.029 Hz
FIDRES     0.458222 Hz
AQ         1.0911744 sec
RG         32768
DW         16.650 usec
DE         6.50 usec
TE         298.2 K
D1         2.00000000 sec
D11        0.03000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       13C
P1         12.00 usec
PL1        -3.50 dB
PL1W       154.08152771 W
SFO1       125.7703643 MHz

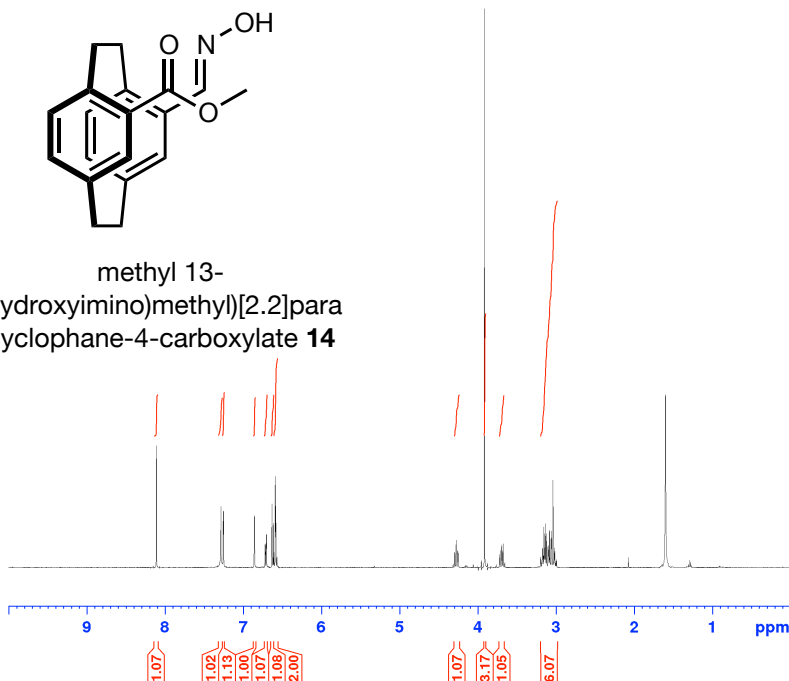
===== CHANNEL f2 =====
CPDPRG2    waltz16
NUC2       1H
PCPD2      80.00 usec
PL2        4.00 dB
PL12       23.37 dB
PL13       25.00 dB
PL2W       12.10000038 W
PL12W      0.13988955 W
PL13W      0.09611372 W
SFO2       500.1320005 MHz

F2 - Processing parameters
SI         32768
SF         125.7577710 MHz
WDW        EM
SSB        0
LB         1.00 Hz
GB         0
PC         1.40
```

31e6b oxime-coome-22pc column 4:1 H:EA



methyl 13-(hydroxyimino)methyl[2.2]paracyclophane-4-carboxylate **14**



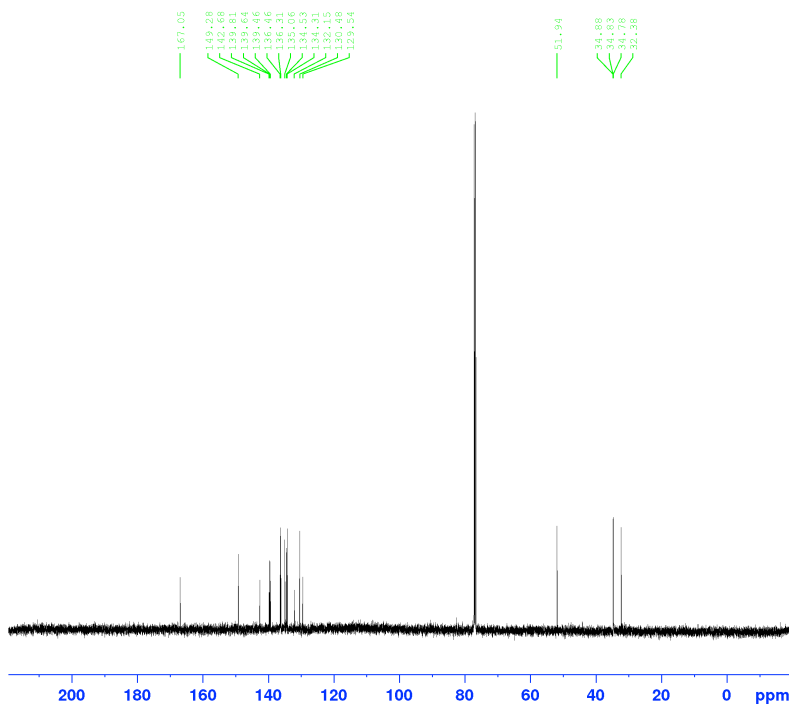
Current Data Parameters
NAME 31e6b
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160719
Time 13.41
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 512
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 4.00 dB
PL1W 12.10000038 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

31e6b



Current Data Parameters
NAME 31e6b
EXPNO 5
PROCNO 1

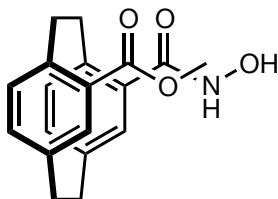
F2 - Acquisition Parameters
Date_ 20160804
Time 16.38
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 346
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 32768
DW 16.650 usec
DE 6.50 usec
TE 296.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -3.50 dB
PL1W 154.08152771 W
SFO1 125.7703643 MHz

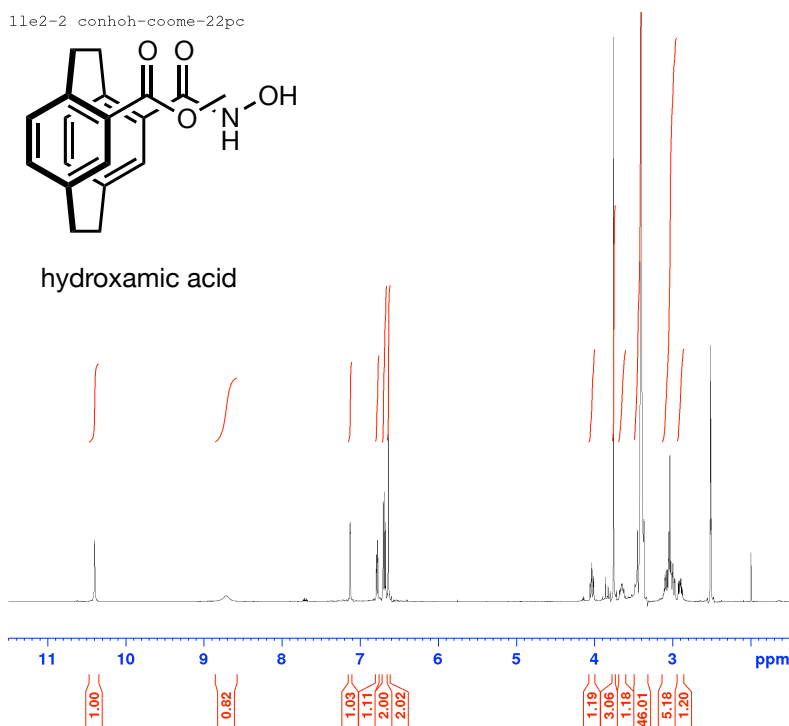
===== CHANNEL f2 =====
CPDPRG12 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 23.37 dB
PL13 25.00 dB
EL2W 12.10000038 W
PL12W 0.13988955 W
PL13W 0.09611372 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

11e2-2 conhoh-coome-22pc



hydroxamic acid



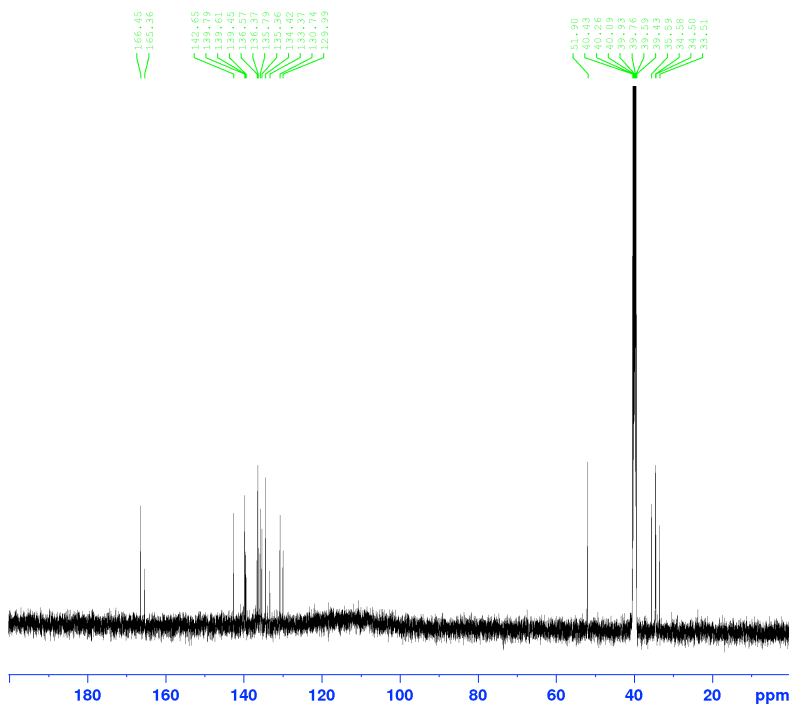
Current Data Parameters
NAME 11e2-2
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160817
Time 16.07
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 57
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 4.00 dB
PL1W 12.10000038 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

11e2-2 conhoh-coome-22pc



Current Data Parameters
NAME 11e2-2
EXPNO 6
PROCNO 1

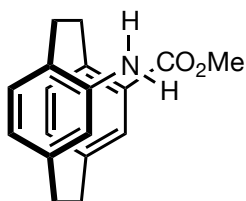
F2 - Acquisition Parameters
Date_ 20160817
Time 16.45
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 32768
DW 16.650 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -3.50 dB
PL1W 154.08152771 W
SFO1 125.7703643 MHz

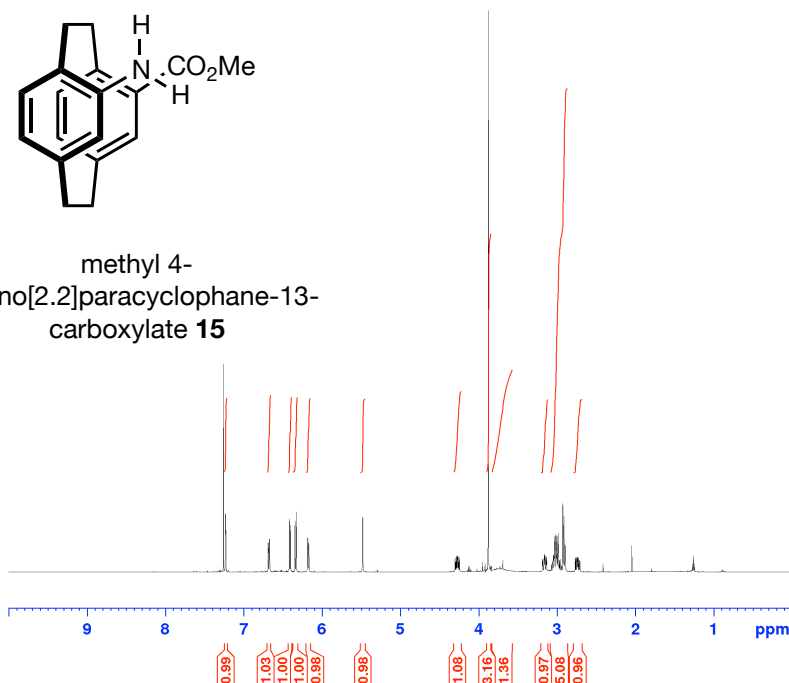
===== CHANNEL f2 =====
CPDPRG12 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 23.37 dB
PL13 25.00 dB
PL2W 12.10000038 W
PL12W 0.13988935 W
PL13W 0.09611372 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

kj-13-87



methyl 4-amino[2.2]paracyclophane-13-carboxylate **15**



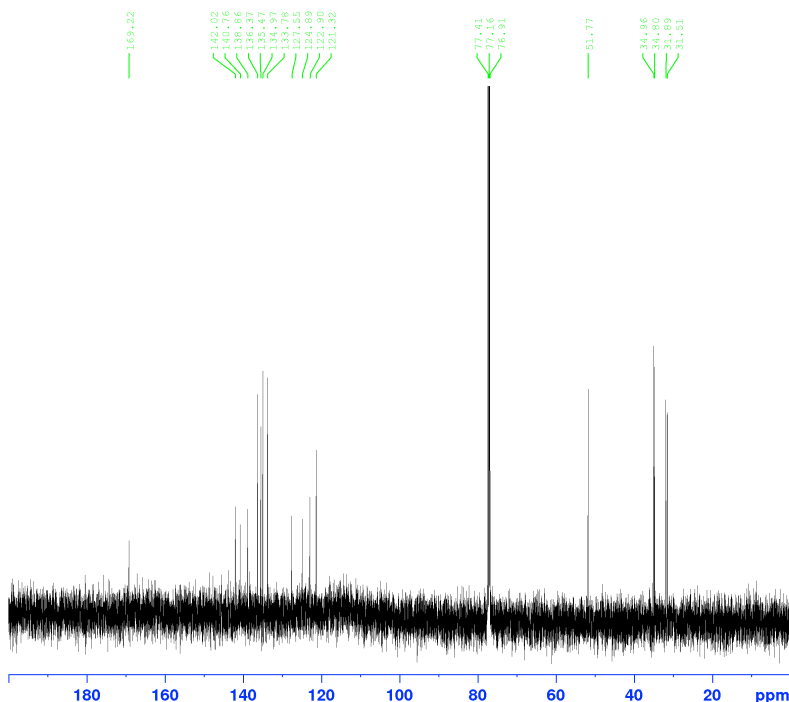
Current Data Parameters
NAME kj-13-87
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150430
Time 11.40
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 128
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 4.00 dB
PL1W 12.10000038 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300137 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

kj-13-87



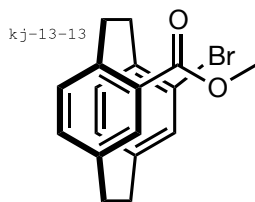
Current Data Parameters
NAME kj-13-87
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150430
Time 11.52
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 270
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 32768
DW 16.650 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

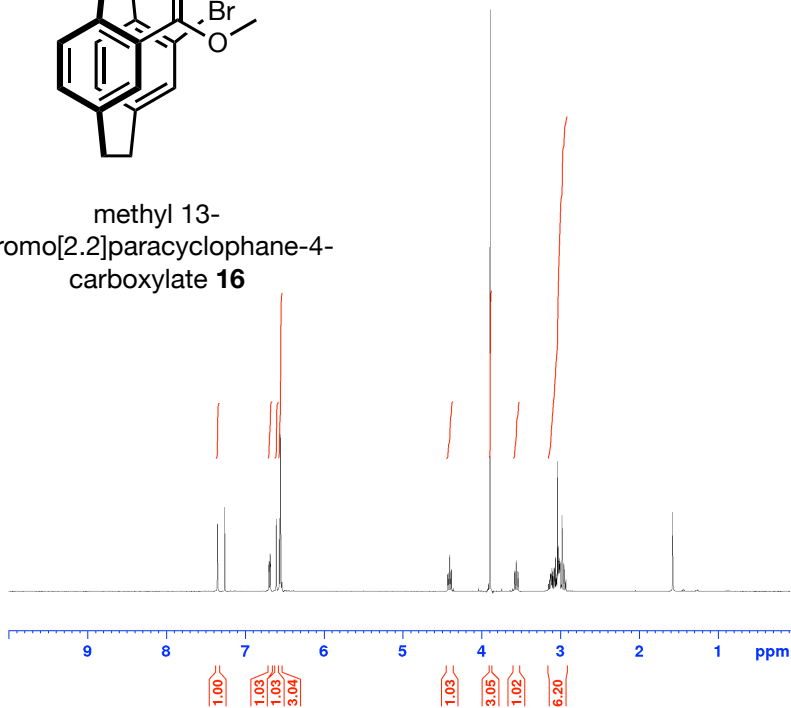
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -3.50 dB
PL1W 154.08152771 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG12 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 23.37 dB
PL13 25.00 dB
PL2W 12.10000038 W
PL12W 0.13988935 W
PL13W 0.09611372 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577721 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



methyl 13-bromo[2.2]paracyclophane-4-carboxylate **16**



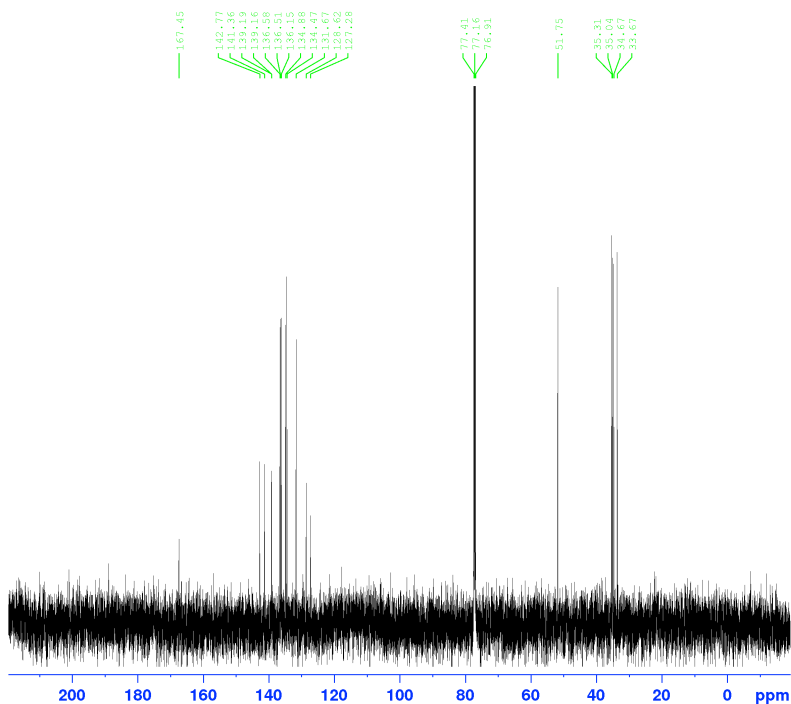
Current Data Parameters
NAME kj-13-13
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140703
Time 9.34
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT cdcl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 114
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 4.00 dB
PL1W 12.10000038 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300132 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

kj-13-13



Current Data Parameters
NAME kj-13-13
EXPNO 2
PROCNO 1

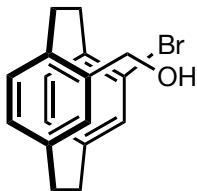
F2 - Acquisition Parameters
Date_ 20140703
Time 9.41
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 123
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 32768
DW 16.650 usec
DE 6.50 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -3.50 dB
PL1W 154.08152771 W
SFO1 125.7703643 MHz

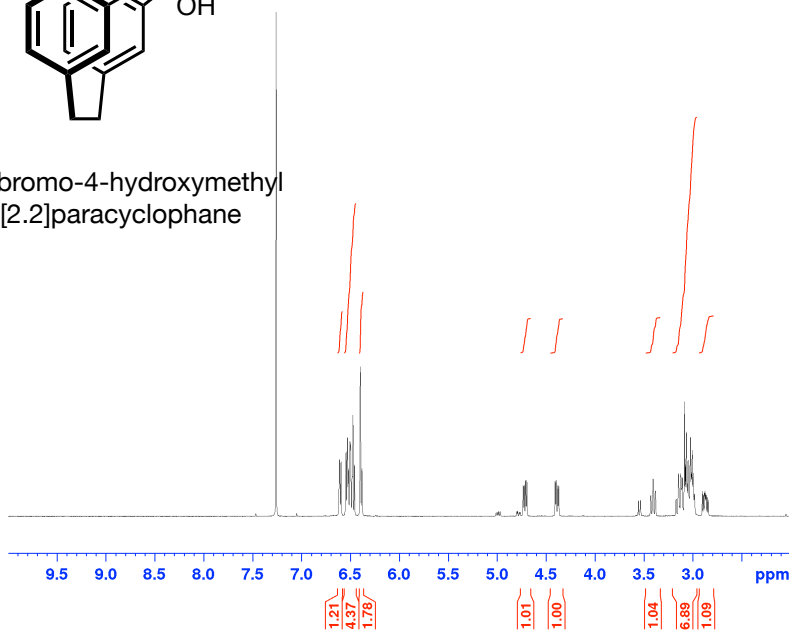
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPDZ 80.00 usec
PL2 4.00 dB
PL12 23.37 dB
PL13 25.00 dB
PL1W 12.10000038 W
PL12W 0.13988955 W
PL13W 0.09611372 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577726 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

kj-13-81 SM for C



13-bromo-4-hydroxymethyl
[2.2]paracyclophane



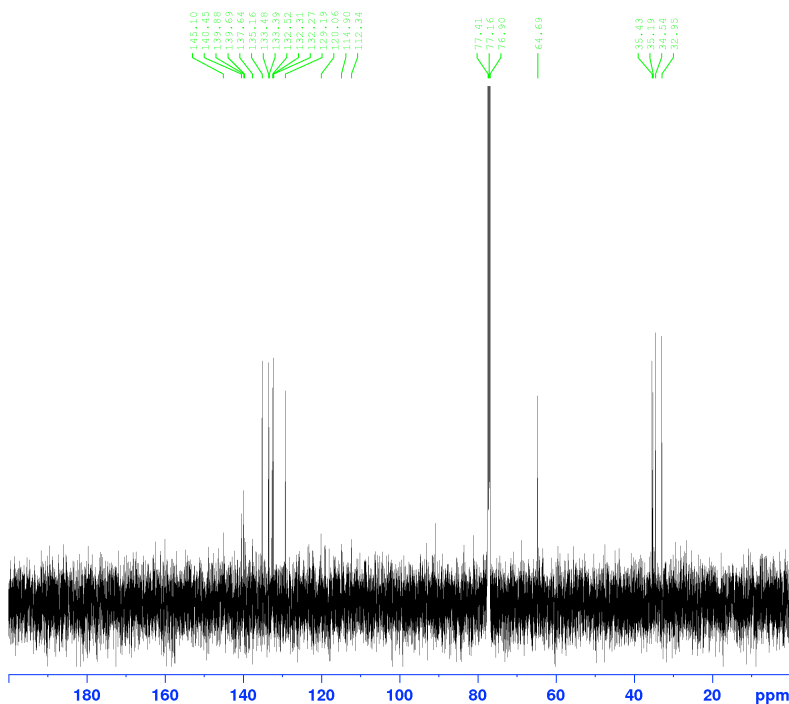
Current Data Parameters
NAME kj-13-81 for C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160317
Time 12.26
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719423 sec
RG 256
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 4.00 dB
PL1W 12.10000038 W
SFO1 500.1330889 MHz

F2 - Processing parameters
SI 32768
SF 500.1300139 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

kj-13-81 for C



Current Data Parameters
NAME kj-13-81 for C
EXPNO 2
PROCNO 1

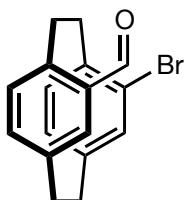
F2 - Acquisition Parameters
Date_ 20160317
Time 13.21
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 32768
DW 16.650 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -3.50 dB
PL1W 154.08152771 W
SFO1 125.7703643 MHz

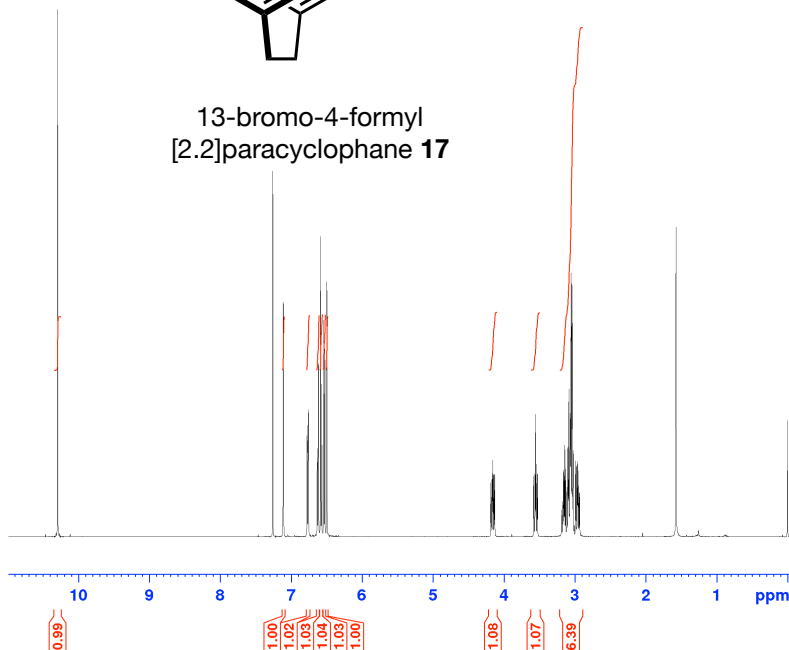
===== CHANNEL f2 =====
CPDPRG12 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 23.37 dB
PL13 25.00 dB
EL2W 12.10000038 W
EL12W 0.13988925 W
PL13W 0.09611372 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577717 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

13-25 CHO, Br



13-bromo-4-formyl
[2.2]paracyclophane 17



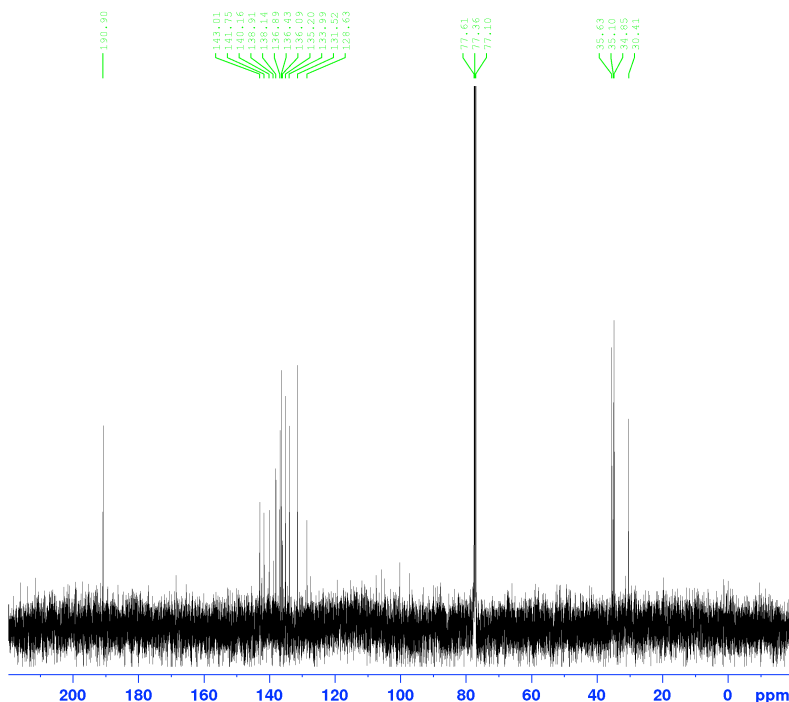
Current Data Parameters
NAME kj-13-25
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140709
Time 9.50
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 181
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 4.00 dB
PL1W 12.10000038 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.130133 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

13-25 CHO, Br



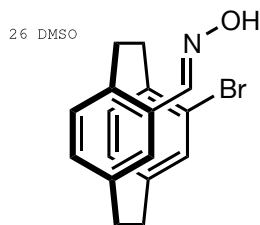
Current Data Parameters
NAME kj-13-25
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140709
Time 9.55
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 157
DS 4
SWH 30030.029 Hz
FIDRES 0.456222 Hz
AQ 1.0911744 sec
RG 114
DW 16.650 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

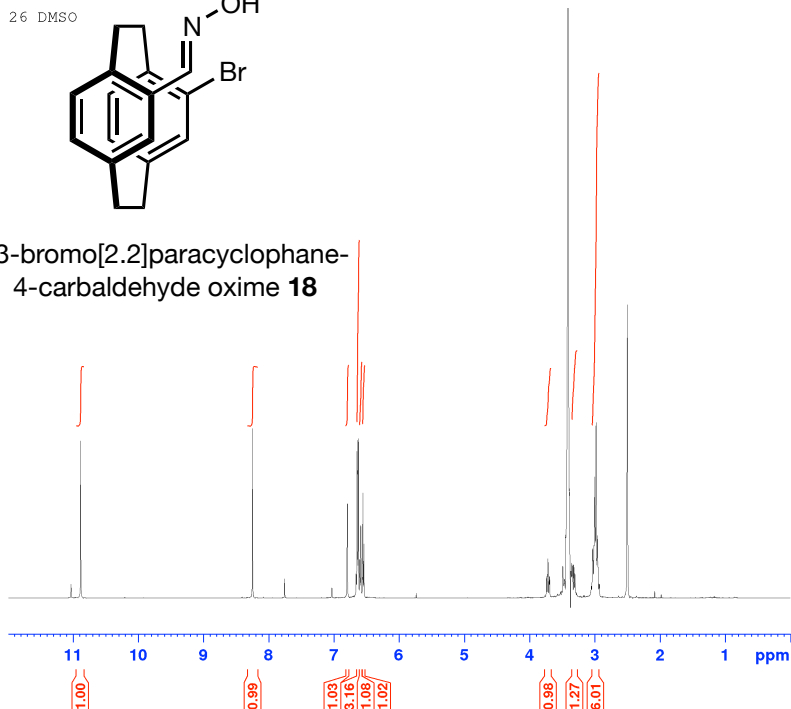
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -3.50 dB
PL1W 154.08152771 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG12 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 23.37 dB
PL13 25.00 dB
PL2W 12.10000038 W
PL12W 0.13988955 W
PL13W 0.09611372 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577475 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



13-bromo[2.2]paracyclophane-4-carbaldehyde oxime **18**



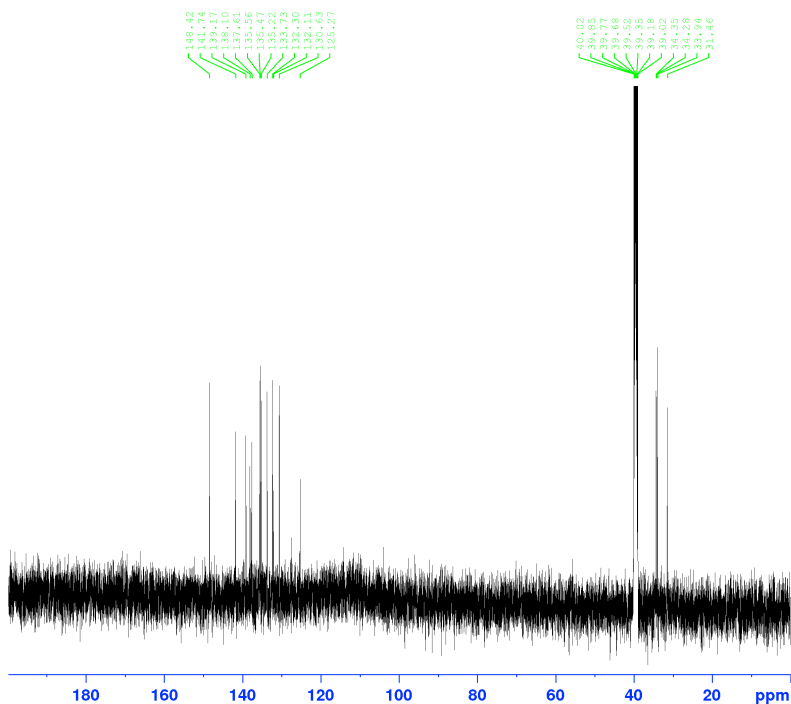
Current Data Parameters
NAME kj-13-26 DMSO
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140723
Time 10.58
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SNR 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 40.3
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 4.00 dB
PL1W 12.10000038 W
SF01 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300048 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

26 DMSO



Current Data Parameters
NAME kj-13-26 DMSO
EXPNO 2
PROCNO 1

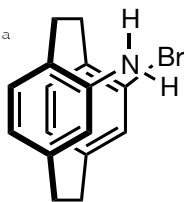
F2 - Acquisition Parameters
Date_ 20140723
Time 11.04
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 204
DS 4
SNR 30030.029 Hz
FIDRES 0.456222 Hz
AQ 1.0911744 sec
RG 32768
DW 16.650 usec
DE 6.50 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -3.50 dB
PL1W 154.08152771 W
SF01 125.7703643 MHz

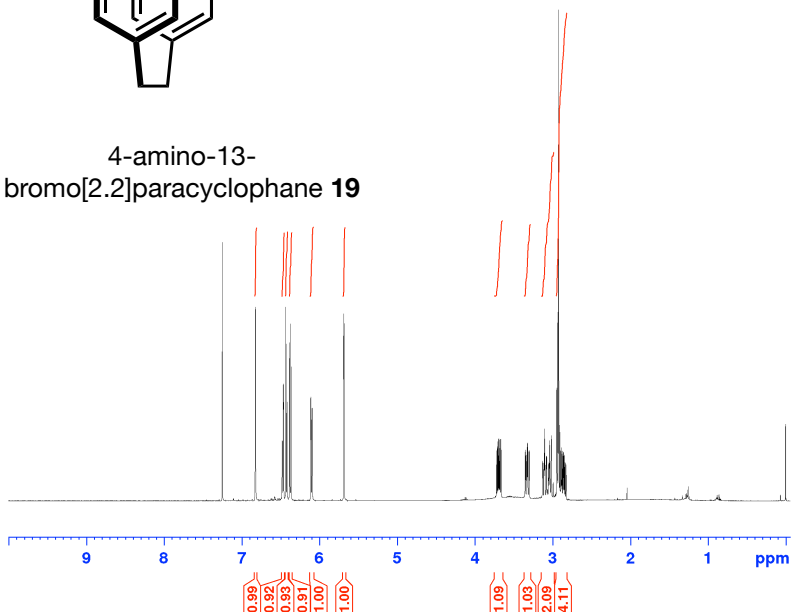
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 23.37 dB
PL13 25.00 dB
PL2W 12.10000038 W
PL12W 0.13989855 W
PL13W 0.09611372 W
SF02 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7578389 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

kj-13-28a



4-amino-13-bromo[2.2]paracyclophane **19**



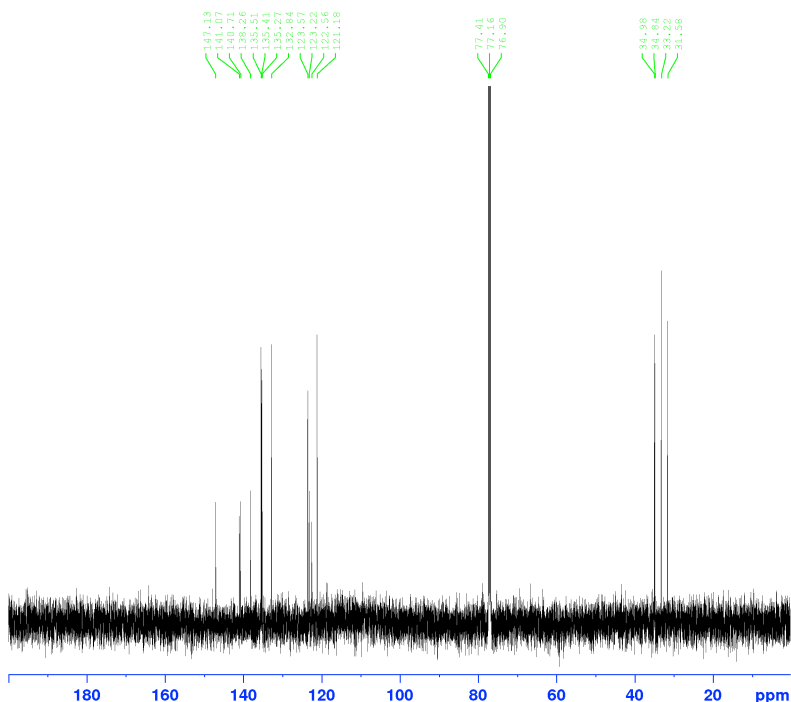
Current Data Parameters
NAME kj-13-28a
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140717
Time 14.24
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 128
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec

===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PLW1 12.10000038 W
SFO1 500.1330865 MHz

F2 - Processing parameters
SI 65536
SF 500.1300162 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

kj-13-28a



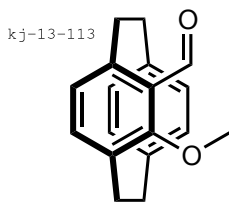
Current Data Parameters
NAME kj-13-28a
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140717
Time 14.39
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 148
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 181
DW 16.650 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec

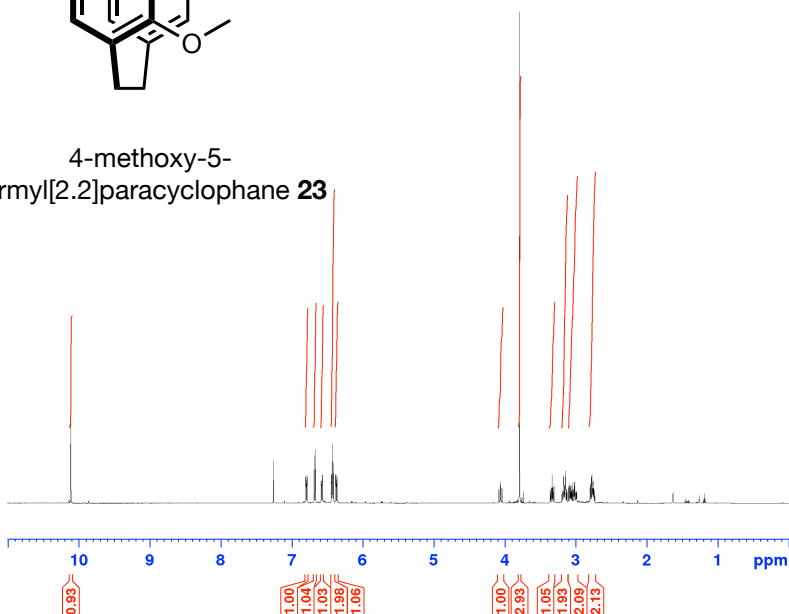
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PLW1 154.08000183 W
SFO1 125.7703637 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PLW2 12.10000038 W
PLW12 0.13982999 W
PLW13 0.08949200 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577740 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



4-methoxy-5-formyl[2.2]paracyclophane **23**



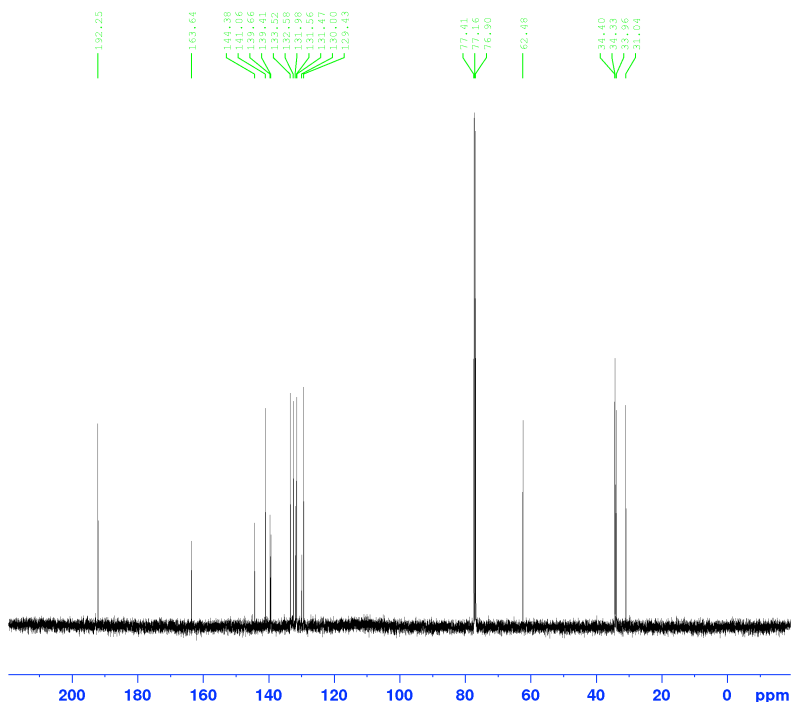
Current Data Parameters
NAME kj-13-113
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150617
Time 12.15
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 45.3
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 4.00 dB
PL1W 12.10000038 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300129 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

kj-13-113



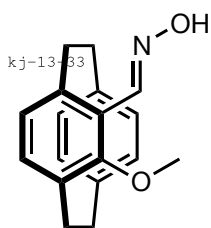
Current Data Parameters
NAME kj-13-113
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150617
Time 12.27
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 191
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 32768
DW 16.650 usec
DE 6.50 usec
TE 298.2 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

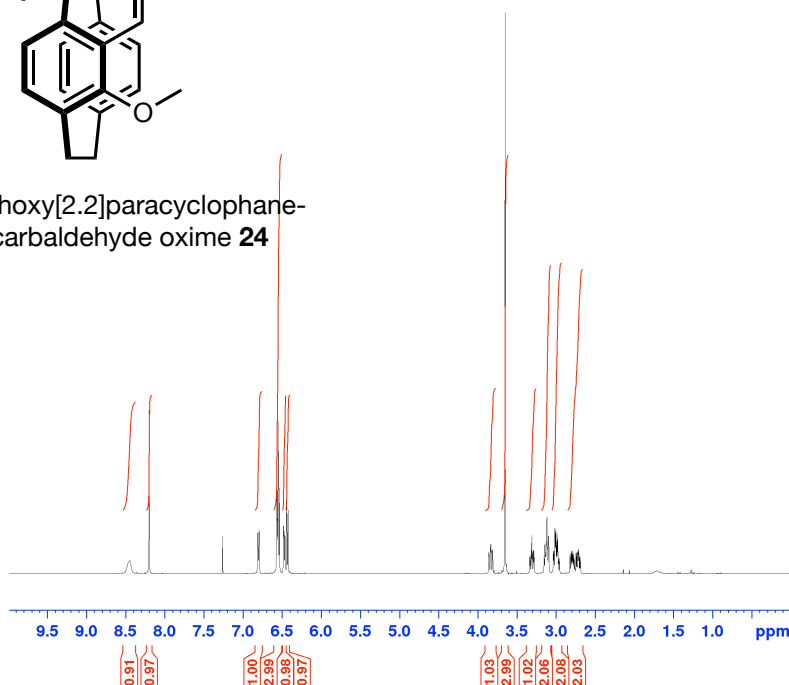
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -3.50 dB
PL1W 154.08152771 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 23.37 dB
PL13 25.00 dB
PL2W 12.10000038 W
PL12W 0.13988855 W
PL13W 0.09611372 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577768 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



4-methoxy[2.2]paracyclophane-
5-carbaldehyde oxime **24**



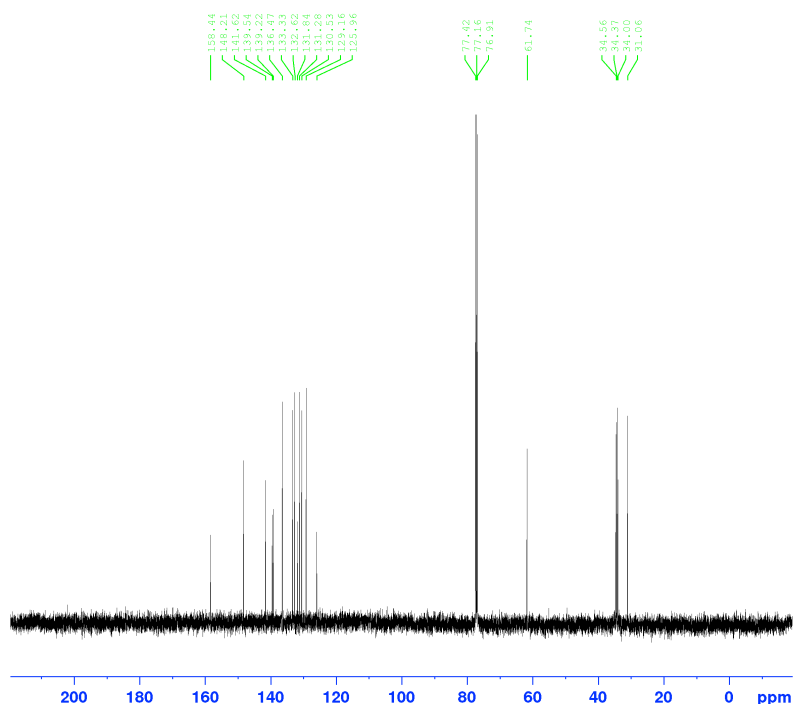
Current Data Parameters
NAME kj-13-33
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140730
Time 9.51
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 40.3
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 4.00 dB
PL1W 12.10000038 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.130129 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

kj-13-33



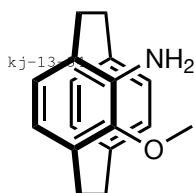
Current Data Parameters
NAME kj-13-33
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140730
Time 9.57
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 109
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 32768
DW 16.650 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

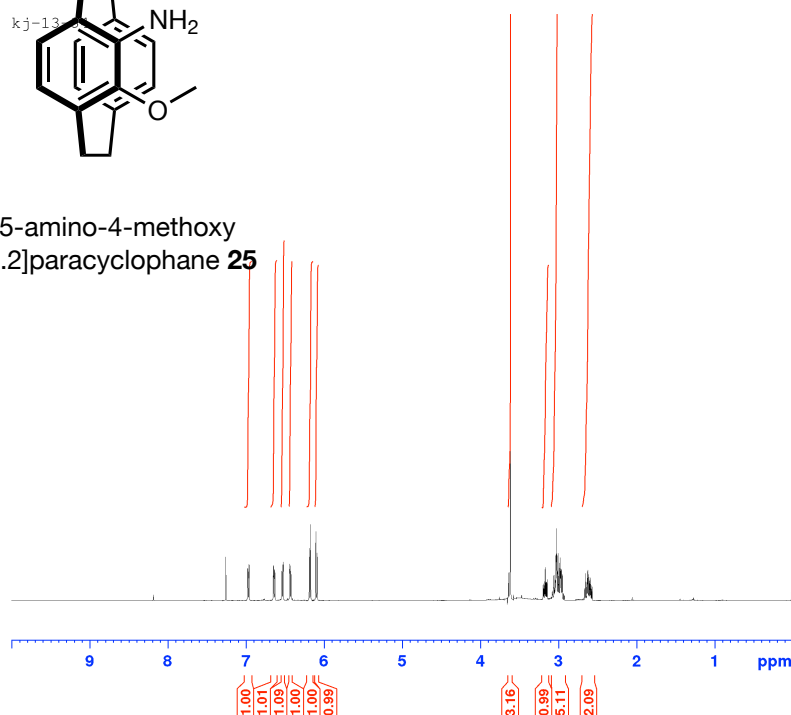
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -3.50 dB
PL1W 154.08152771 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 23.37 dB
PL13 25.00 dB
PL2W 12.10000038 W
PL12W 0.13988953 W
PL13W 0.09611372 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577763 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



5-amino-4-methoxy
[2.2]paracyclophane **25**



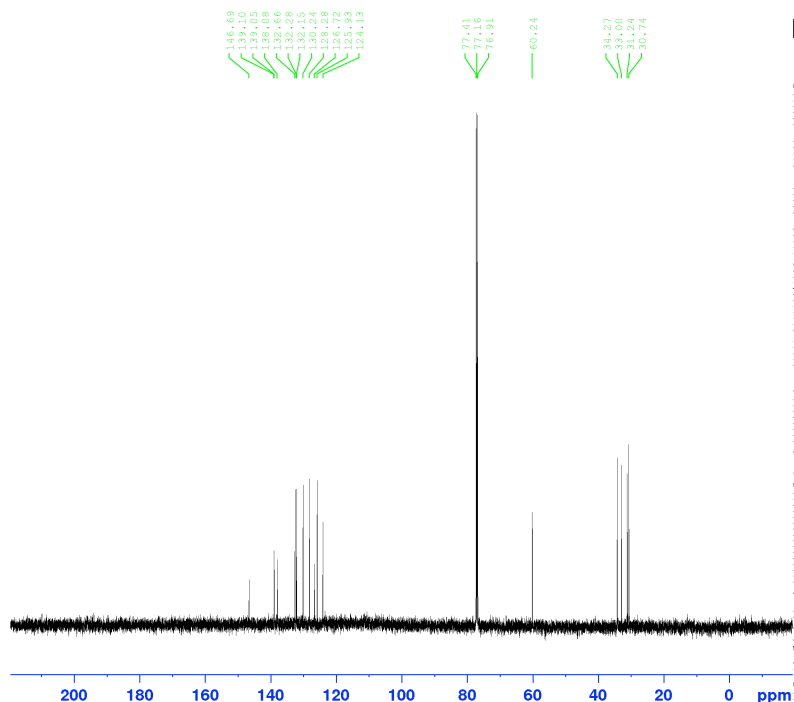
Current Data Parameters
NAME kj-13-34
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140731
Time 9.39
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.137632 Hz
AQ 3.1719425 sec
RG 64
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 4.00 dB
PL1W 12.10000038 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300132 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

kj-13-34



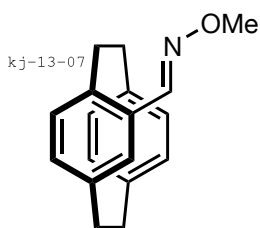
Current Data Parameters
NAME kj-13-34
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140731
Time 9.47
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 157
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 32768
DW 16.650 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

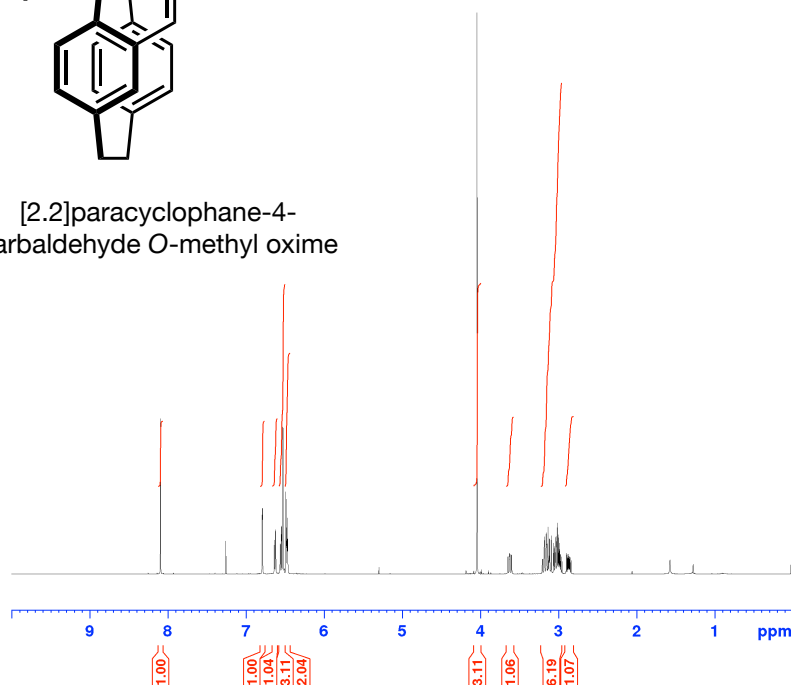
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -3.50 dB
PL1W 154.08152771 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG12 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 23.37 dB
PL13 25.00 dB
EL2W 12.10000038 W
PL12W 0.13988955 W
PL13W 0.09611372 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577753 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



[2.2]paracyclophane-4-carbaldehyde O-methyl oxime



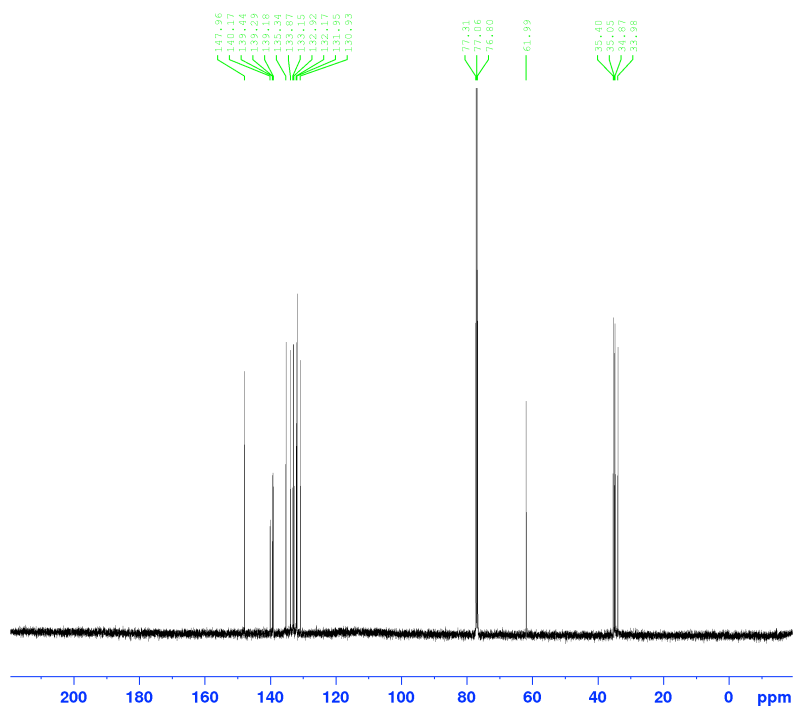
Current Data Parameters
NAME kj-13-07
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140617
Time 16.20
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 45.3
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 4.00 dB
PL1W 12.10000038 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300131 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

kj-13-07



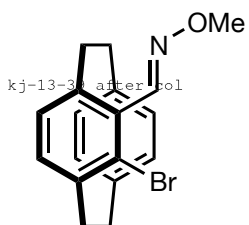
Current Data Parameters
NAME kj-13-07
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140617
Time 16.53
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 590
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 32768
DW 16.650 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

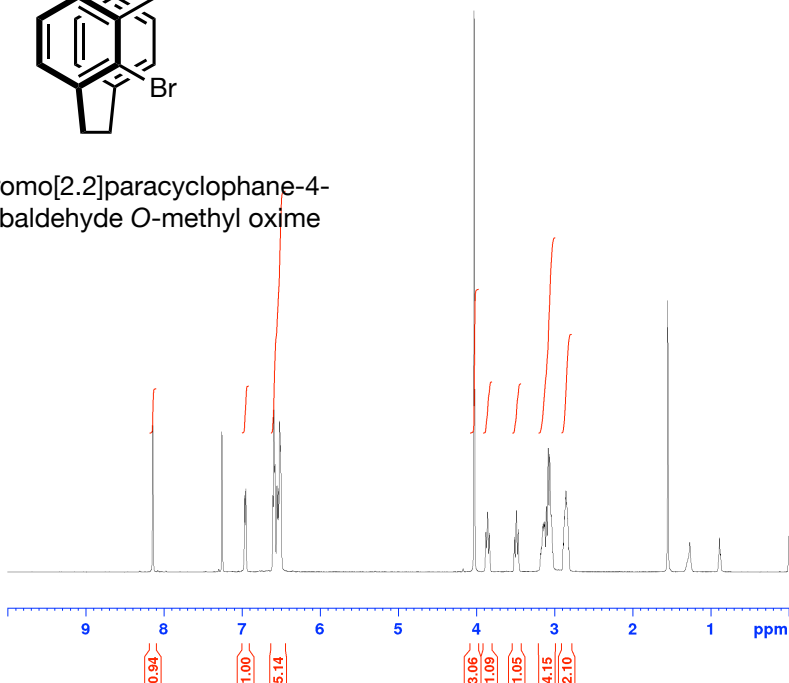
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -3.50 dB
PL1W 154.08152771 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 23.37 dB
PL13 25.00 dB
PL2W 12.10000038 W
PL12W 0.13988955 W
PL13W 0.09611372 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



5-bromo[2.2]paracyclophane-4-carbaldehyde O-methyl oxime



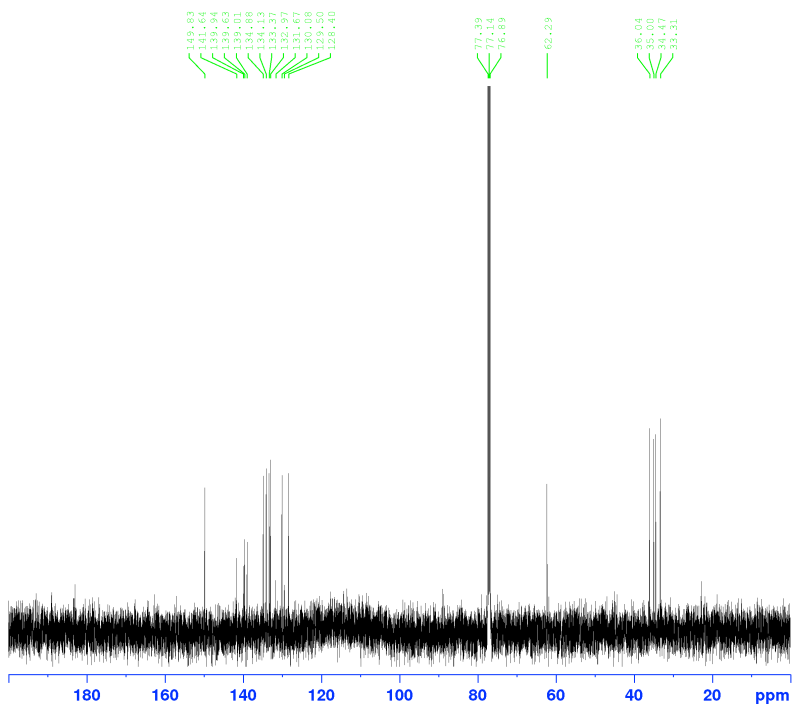
Current Data Parameters
NAME kj-13-39 after col
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140910
Time 9.27
INSIRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 161.3
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 8.60 usec
PL1 4.00 dB
PL1W 12.10000038 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.130142 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

kj-13-39 after col



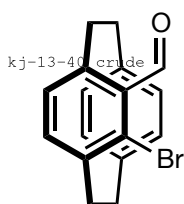
Current Data Parameters
NAME kj-13-39 after col
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140910
Time 9.34
INSIRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 406
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 32768
DW 16.650 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

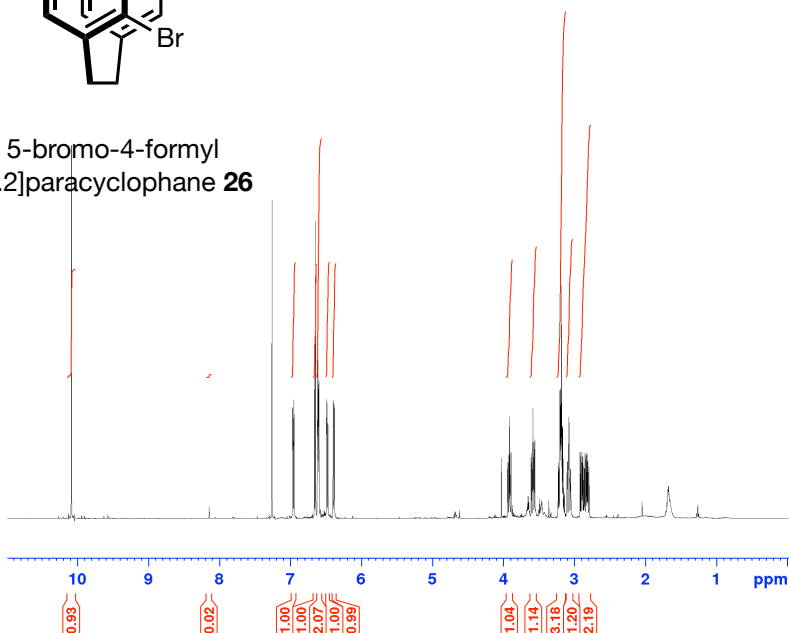
----- CHANNEL f1 -----
NUC1 13C
P1 12.00 usec
PL1 -3.50 dB
PL1W 154.08152771 W
SFO1 125.7703643 MHz

----- CHANNEL f2 -----
CPDPRG2 waitz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 23.37 dB
PL13 25.00 dB
PL2W 12.10000038 W
PL12W 0.13988955 W
PL13W 0.09611372 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577743 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



5-bromo-4-formyl
[2.2]paracyclophane **26**



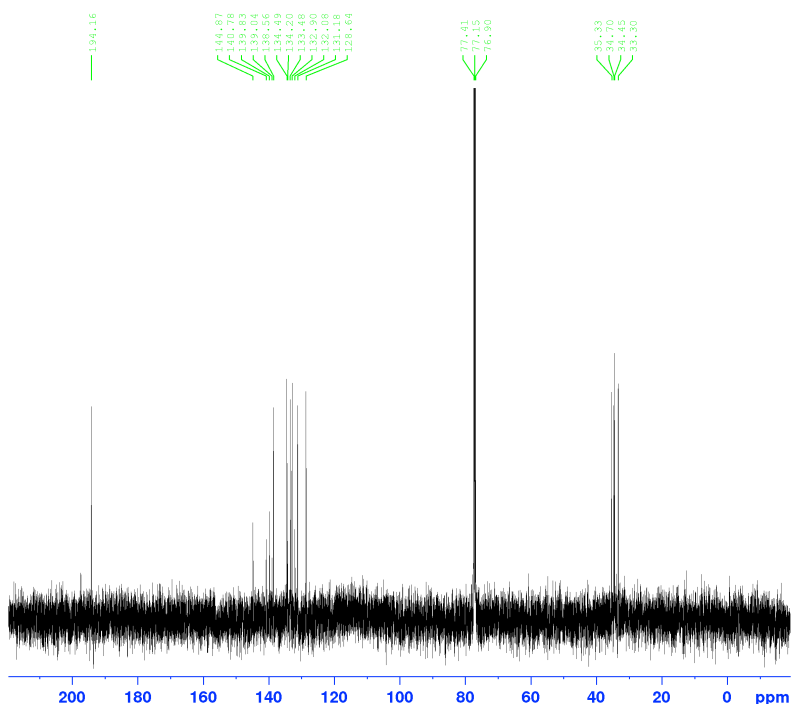
Current Data Parameters
NAME kj-13-40 crude
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140911
Time 11.57
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 90.5
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 4.00 dB
PL1W 12.1000038 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1330133 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

kj-13-40 crude



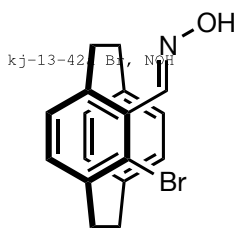
Current Data Parameters
NAME kj-13-40 crude
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140911
Time 12.05
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 228
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 32768
DW 16.650 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

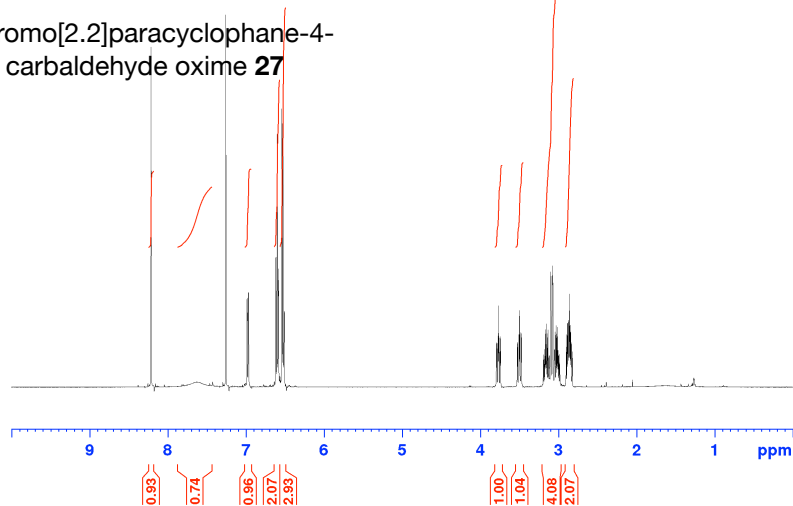
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -3.50 dB
PL1W 154.08152771 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 23.37 dB
PL13 25.00 dB
PL1W 12.1000038 W
PL12W 0.13988955 W
PL13W 0.09611372 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577735 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



5-bromo[2.2]paracyclophane-4-carbaldehyde oxime **27**



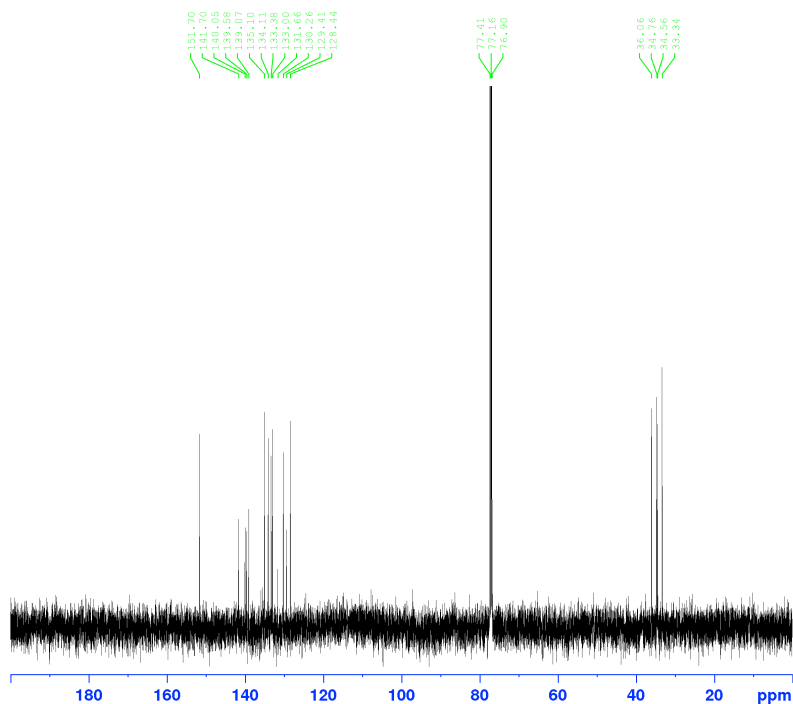
Current Data Parameters
NAME kj-13-42a Br, NOH
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140915
Time 11.22
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 128
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 4.00 dB
PL1W 12.10000038 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300132 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

kj-13-42a Br, NOH



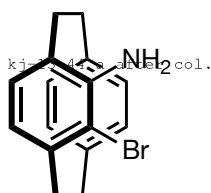
Current Data Parameters
NAME kj-13-42a Br, NOH
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140915
Time 11.28
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 199
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 32768
DW 16.650 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

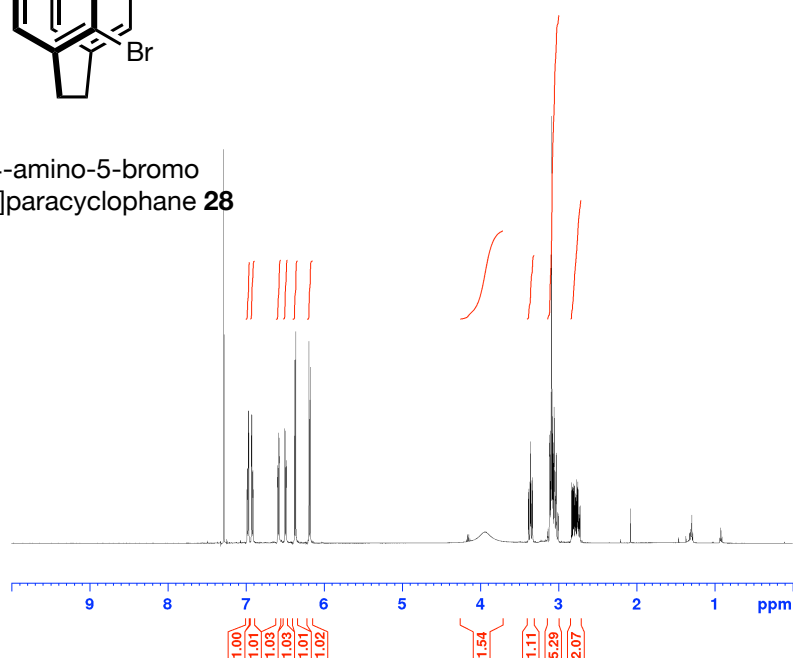
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -3.50 dB
PL1W 154.08152771 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG12 waltz16
NUC2 1H
PCPDZ 80.00 usec
PL2 4.00 dB
PL12 23.37 dB
PL13 25.00 dB
PL12W 12.10000038 W
PL12W 0.13988955 W
PL13W 0.09611372 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577726 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



4-amino-5-bromo
[2.2]paracyclophane **28**



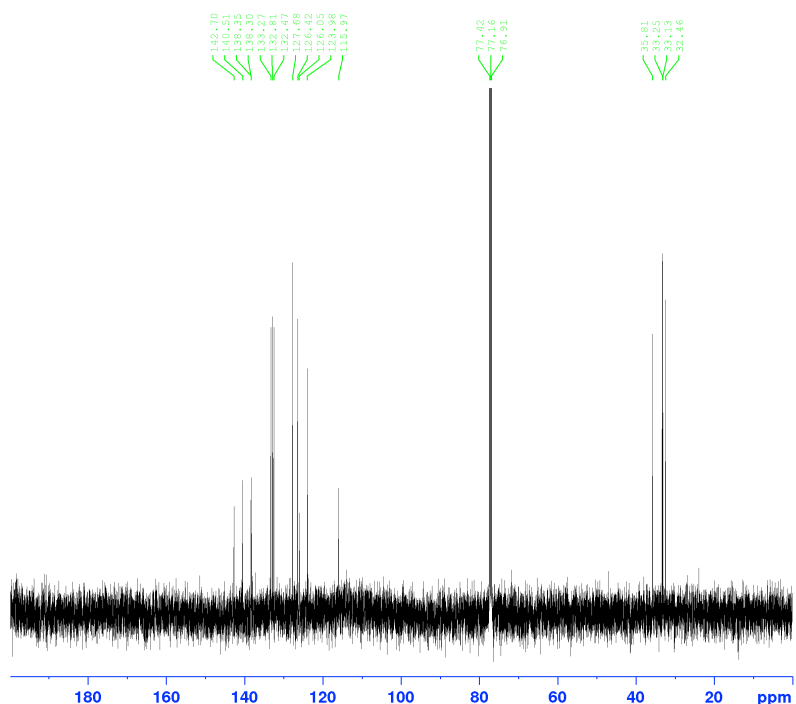
Current Data Parameters
NAME kj-13-44a
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140917
Time 14.46
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 161.3
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 4.00 dB
PL1W 12.10000038 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.130000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

kj-13-44 a after col.



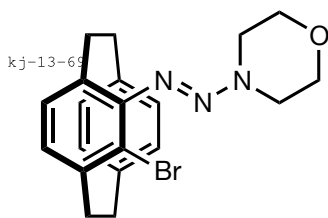
Current Data Parameters
NAME kj-13-44a
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140917
Time 14.58
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 203
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 32768
DW 16.650 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

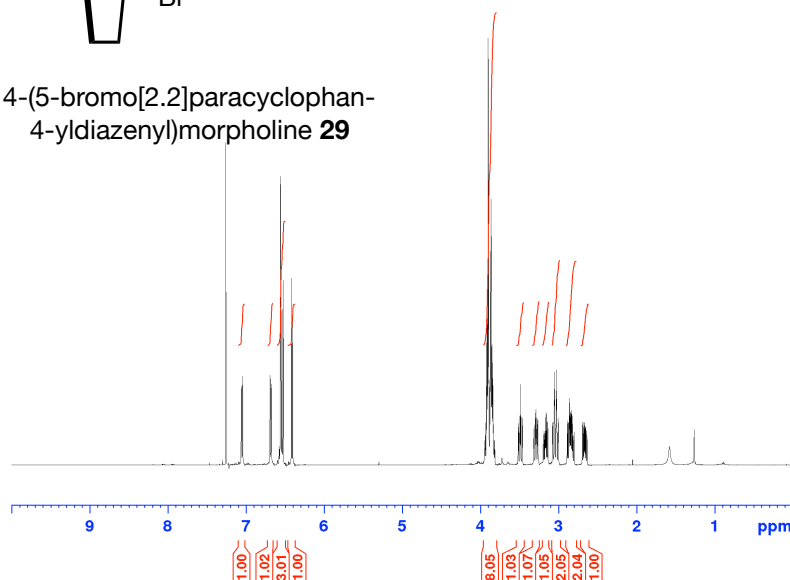
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 3.50 dB
PL1W 154.08152771 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 23.37 dB
PL13 25.00 dB
PL12W 12.10000038 W
PL12W 0.13988925 W
PL13W 0.09611372 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577726 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



4-(5-bromo[2.2]paracyclophan-4-yl-diazenyl)morpholine **29**



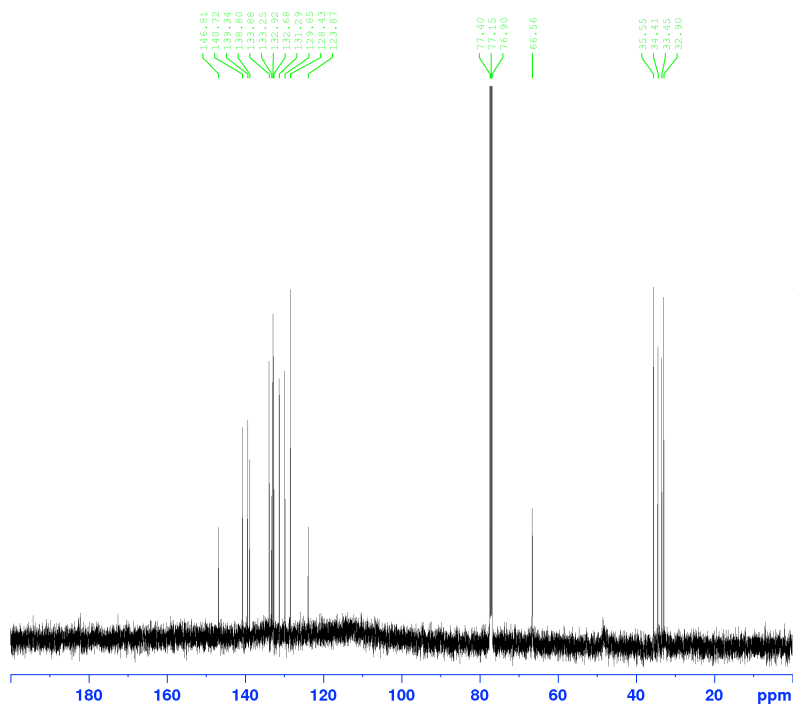
Current Data Parameters
NAME kj-13-69
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150312
Time 10.05
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 128
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 4.00 dB
PL1W 12.10000038 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300141 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

kj-13-69



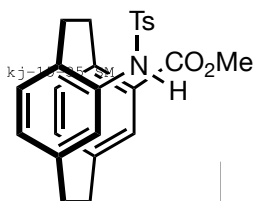
Current Data Parameters
NAME kj-13-69
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150312
Time 10.46
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 783
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 32768
DW 16.650 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

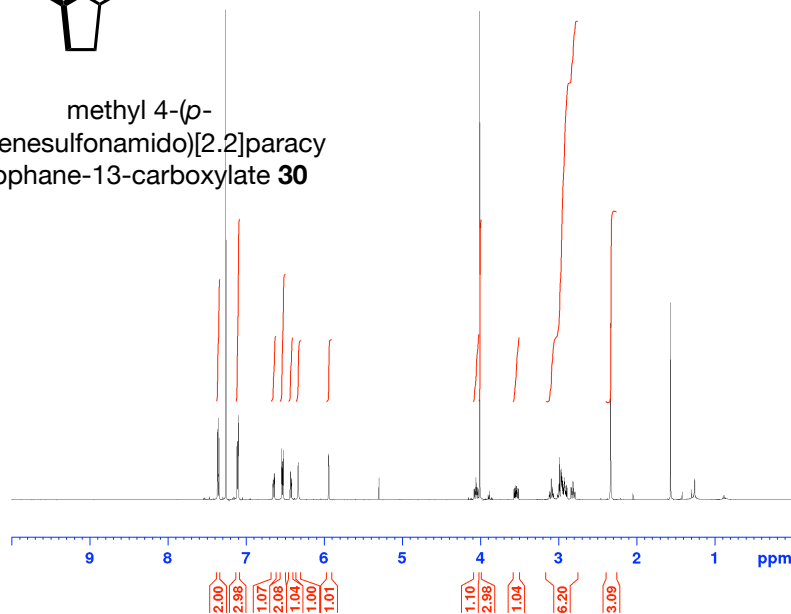
===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -3.50 dB
PL1W 154.08152771 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG12 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 23.37 dB
PL13 25.00 dB
PL2W 12.10000038 W
PL12W 0.13988955 W
PL13W 0.09611372 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577747 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



methyl 4-(*p*-toluenesulfonamido)[2.2]paracyclophane-13-carboxylate **30**



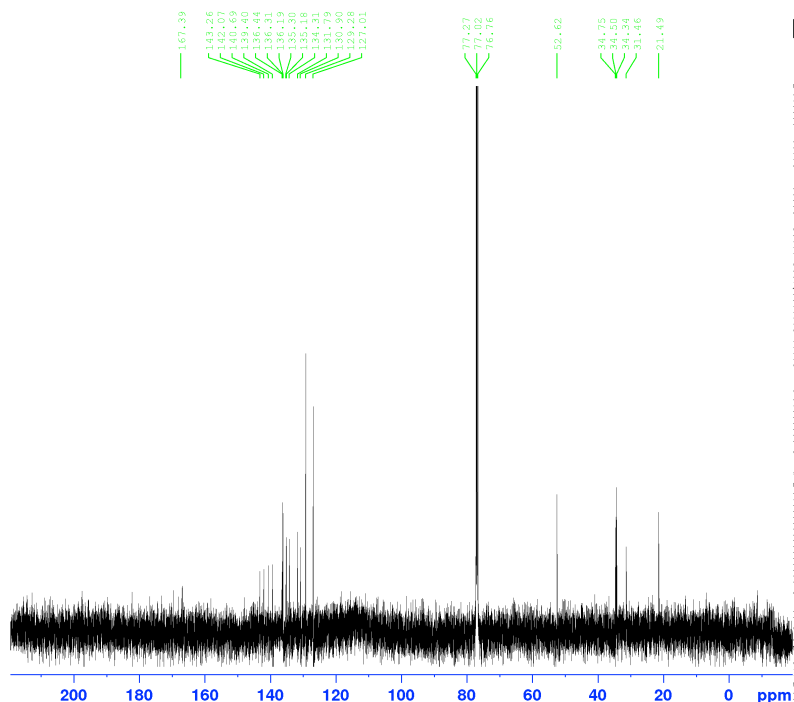
Current Data Parameters
NAME kj-15-35 SM
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160212
Time 13.18
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 322.5
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 4.00 dB
PL1W 12.10000038 W
SF01 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300136 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
FC 1.00

kj-15-35 SM



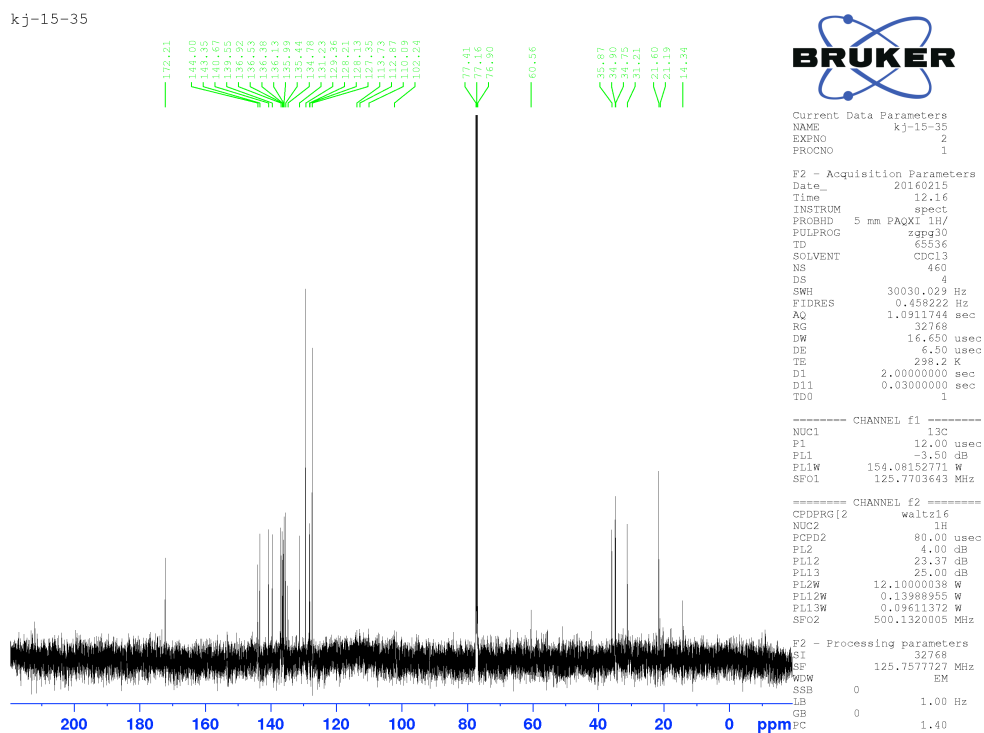
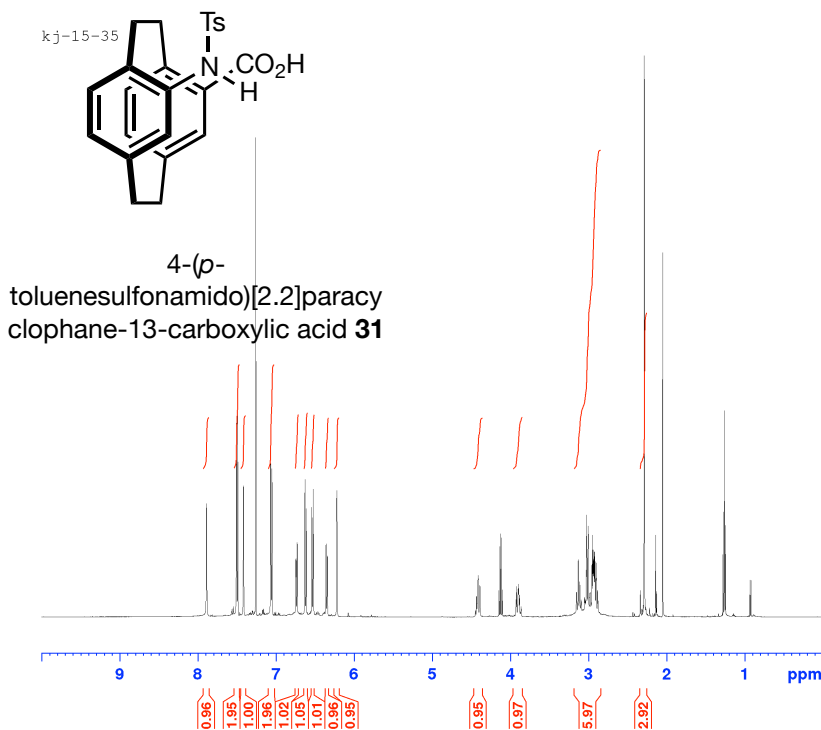
Current Data Parameters
NAME kj-15-35 SM
EXPNO 2
PROCNO 1

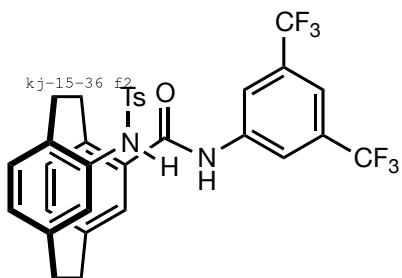
F2 - Acquisition Parameters
Date_ 20160212
Time 13.27
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 736
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 32768
DW 16.650 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -3.50 dB
PL1W 154.08152771 W
SF01 125.7703643 MHz

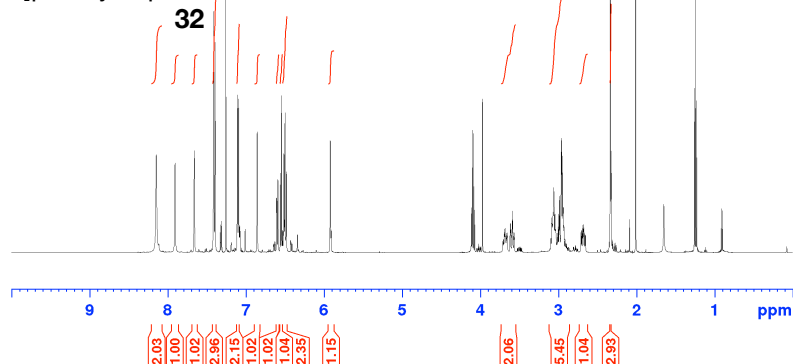
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 23.37 dB
PL13 25.00 dB
EL2W 12.10000038 W
PL12W 0.13988935 W
PL13W 0.09611372 W
SF02 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
FC 1.40





**N-(3,5-bis(trifluoromethyl)phenyl)-4-(*p*-toluenesulfonamido)
[2.2]paracyclophane-13-carbamide**



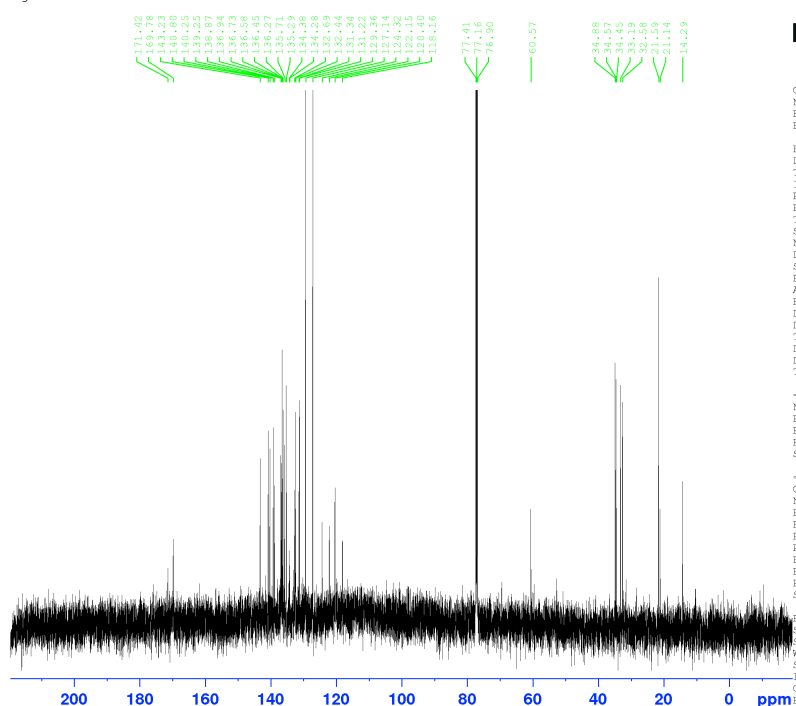
Current Data Parameters
NAME kj-15-36 f2
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160218
Time 15.45
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 71.8
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 1H
P1 8.60 usec
PL1 4.00 dB
PL1W 12.10000038 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1300135 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

kj-15-36 f2



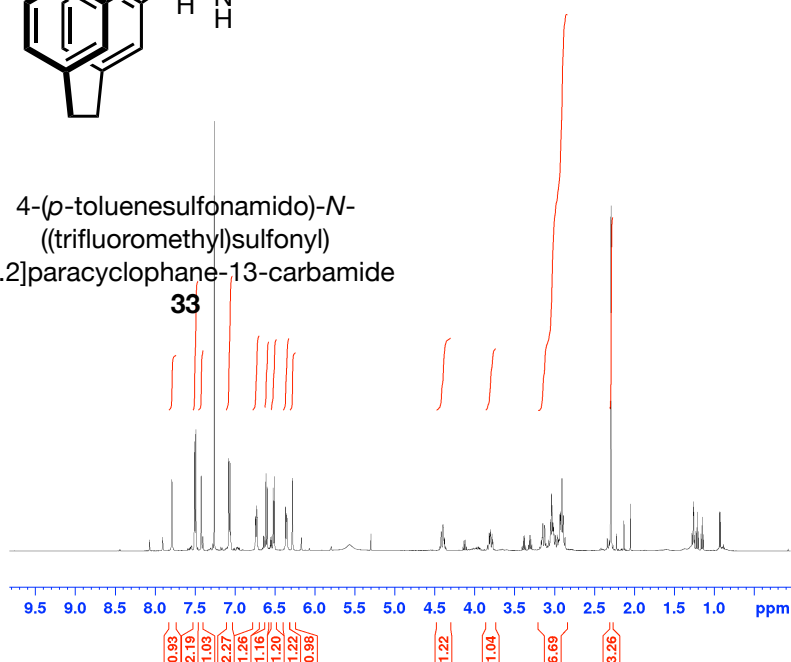
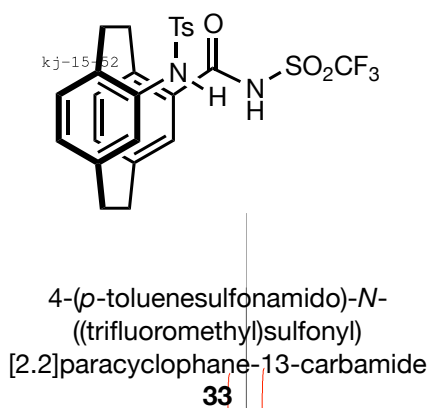
Current Data Parameters
NAME kj-15-36 f2
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160218
Time 15.52
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 260
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 32768
DW 16.650 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

----- CHANNEL f1 -----
NUC1 13C
P1 12.00 usec
PL1 -3.50 dB
PL1W 154.08152771 W
SFO1 125.7703643 MHz

----- CHANNEL f2 -----
CPDPRG12 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 23.37 dB
PL13 25.00 dB
PL2W 12.10000038 W
PL12W 0.13988955 W
PL13W 0.09611372 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577735 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40



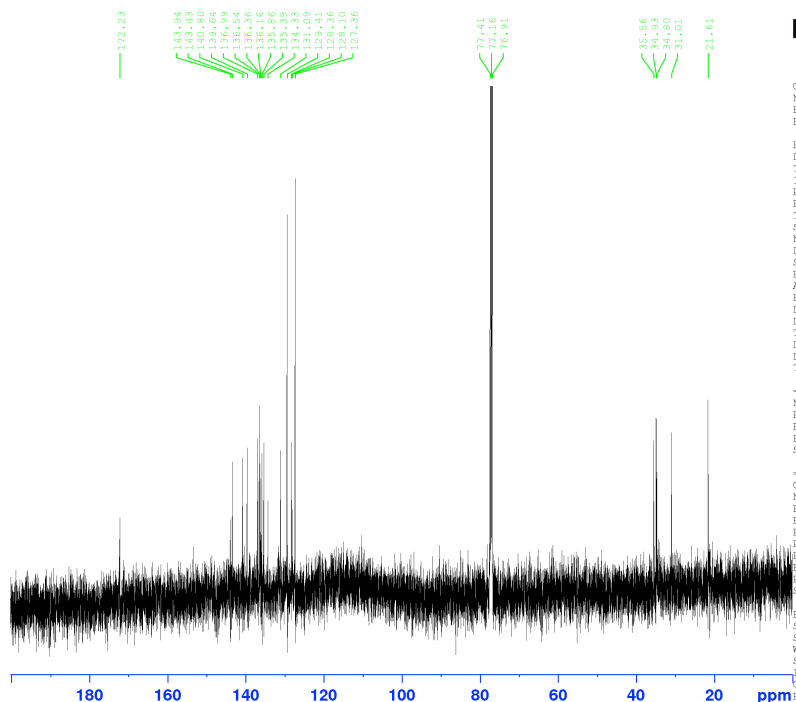
Current Data Parameters
NAME kj-15-52
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160311
Time 12.07
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719425 sec
RG 128
DW 48.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.60 usec
PL1 4.00 dB
PL1W 12.10000038 W
SFO1 500.1330885 MHz

F2 - Processing parameters
SI 32768
SF 500.1330135 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

kj-15-52



Current Data Parameters
NAME kj-15-52
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160311
Time 12.17
INSTRUM spect
PROBHD 5 mm PAQXI 1H/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 738
DS 4
SWH 30030.029 Hz
FIDRES 0.458222 Hz
AQ 1.0911744 sec
RG 32768
DW 16.650 usec
DE 6.50 usec
TE 298.2 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PL1 -3.50 dB
PL1W 154.08152771 W
SFO1 125.7703643 MHz

===== CHANNEL f2 =====
CPDPRG12 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 4.00 dB
PL12 23.37 dB
PL13 25.00 dB
EL2W 12.10000038 W
EL12W 0.13988925 W
PL13W 0.09611372 W
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577717 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

HPLC traces for acid 31

Racemic (±)-31

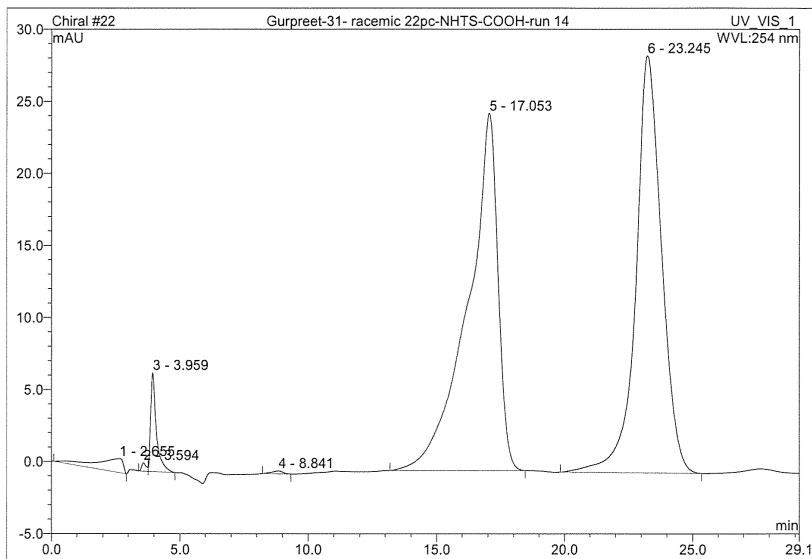
Operator:vfiliche Timebase:ANALYTICAL_500loop Sequence:Chiral

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22 Gurpreet-31- racemic 22pc-NHTS-COOH-run 14

AD-H column, 20:80 iPr-OH/Hex @ 1.0mL/min

Sample Name:	Gurpreet-31- racemic 22pc-NHTS-COOH-ru	Injection Volume:	30.0
Vial Number:	GA5	Channel:	UV_VIS_1
Sample Type:	unknown	Wavelength:	254.0
Control Program:	Gurpreet Chiral AD-10march	Bandwidth:	2
Quantif. Method:	Caffeine test	Dilution Factor:	1.0000
Recording Time:	10/3/2015 17:35	Sample Weight:	1.0000
Run Time (min):	29.15	Sample Amount:	1.0000



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	2.65	n.a.	0.967	1.175	1.67	n.a.	BMB
2	3.59	n.a.	0.588	0.121	0.17	n.a.	BM
3	3.96	n.a.	6.881	1.763	2.50	n.a.	MB
4	8.84	n.a.	0.207	0.100	0.14	n.a.	BMB
5	17.05	n.a.	24.792	33.739	47.85	n.a.	BMB
6	23.25	n.a.	28.945	33.617	47.67	n.a.	BMB
Total:			62.380	70.515	100.00	0.000	

Enantiomer 1 31

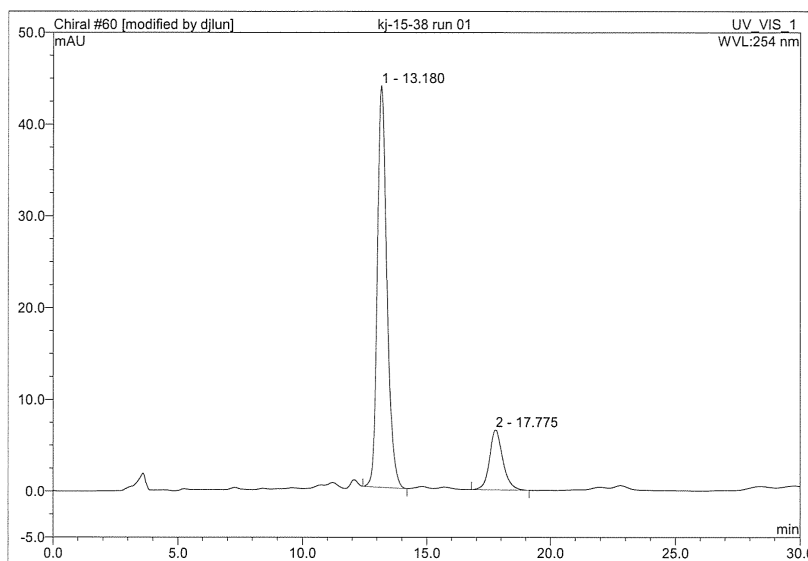
Operator:vfiliche Timebase:ANALYTICAL_500loop Sequence:Chiral

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60 kj-15-38 run 01

AD-H column, 20:80 iPr-OH/Hex @ 1.0mL/min

Sample Name:	kj-15-38 run 01	Injection Volume:	25.0
Vial Number:	BB5	Channel:	UV_VIS_1
Sample Type:	unknown	Wavelength:	254.0
Control Program:	Gurpreet Chiral AD-11march v2	Bandwidth:	2
Quantif. Method:	Caffeine test	Dilution Factor:	1.0000
Recording Time:	26/2/2016 11:02	Sample Weight:	1.0000
Run Time (min):	30.00	Sample Amount:	1.0000



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	13.18	n.a.	43.756	19.892	82.82	n.a.	BMB*
2	17.78	n.a.	6.554	4.126	17.18	n.a.	BMB
Total:			50.310	24.018	100.00	0.000	

Enantiomer 2 31

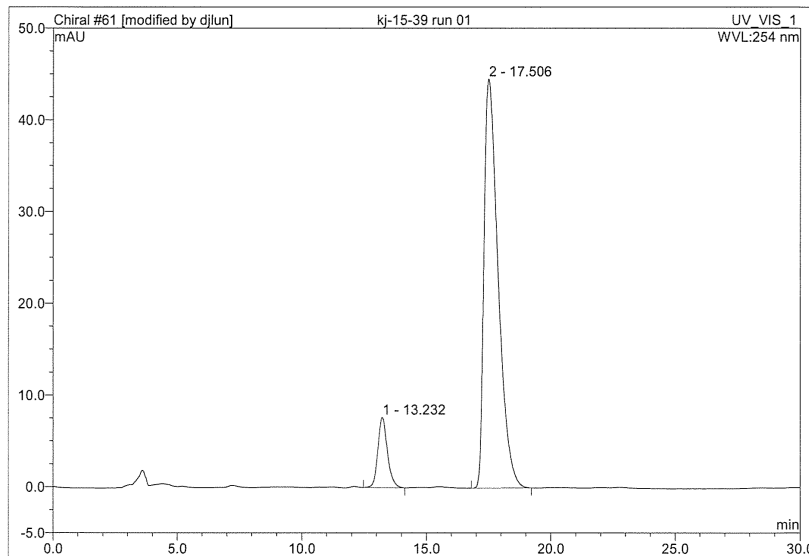
Operator:vfllche Timebase:ANALYTICAL_500loop Sequence:Chiral

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61 kj-15-39 run 01

AD-H column, 20:80 iPr-OH/Hex @ 1.0mL/min

Sample Name:	kj-15-39 run 01	Injection Volume:	25.0
Vial Number:	BB6	Channel:	UV_VIS_1
Sample Type:	unknown	Wavelength:	254.0
Control Program:	Gurpreet Chiral AD-11march v2	Bandwidth:	2
Quantif. Method:	Caffeine test	Dilution Factor:	1.0000
Recording Time:	26/2/2016 11:33	Sample Weight:	1.0000
Run Time (min):	30.00	Sample Amount:	1.0000



No.	Ret.Time min	Peak Name	Height mAU	Area mAU*min	Rel.Area %	Amount	Type
1	13.23	n.a.	7.670	3.409	10.33	n.a.	BMB
2	17.51	n.a.	44.601	29.610	89.67	n.a.	BMB
Total:			52.271	33.019	100.00	0.000	