Supporting Information for

# Arenium Acid-Catalyzed Deuteration of Aromatic Hydrocarbons

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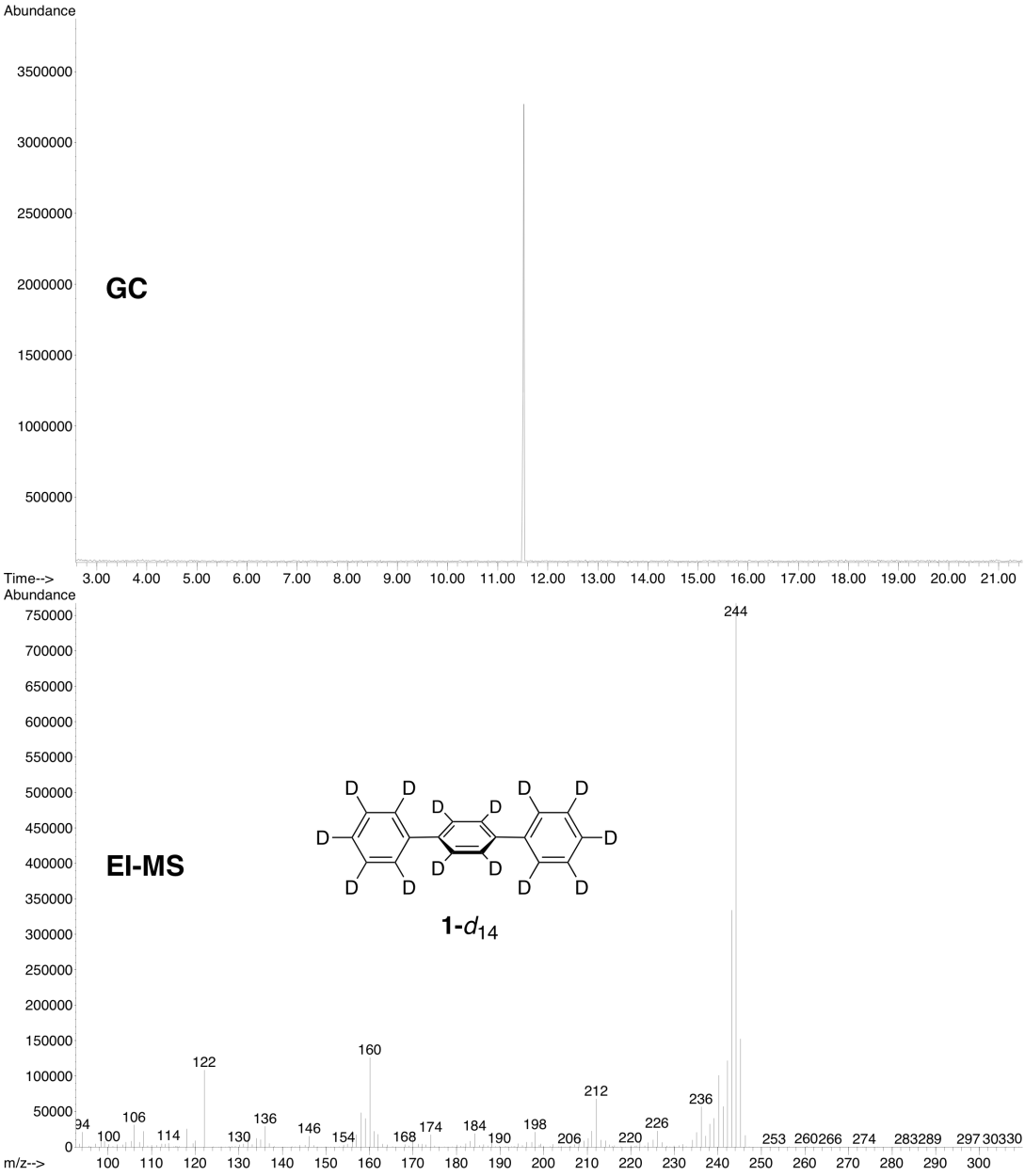
## GC-MS Data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Abundance
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300000
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200000
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50000
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244
160
122
212
236
226
106
136
146
198
184
174
168
154
130
114
100
94
253 260266 274 283289 297 30330
m/z-->
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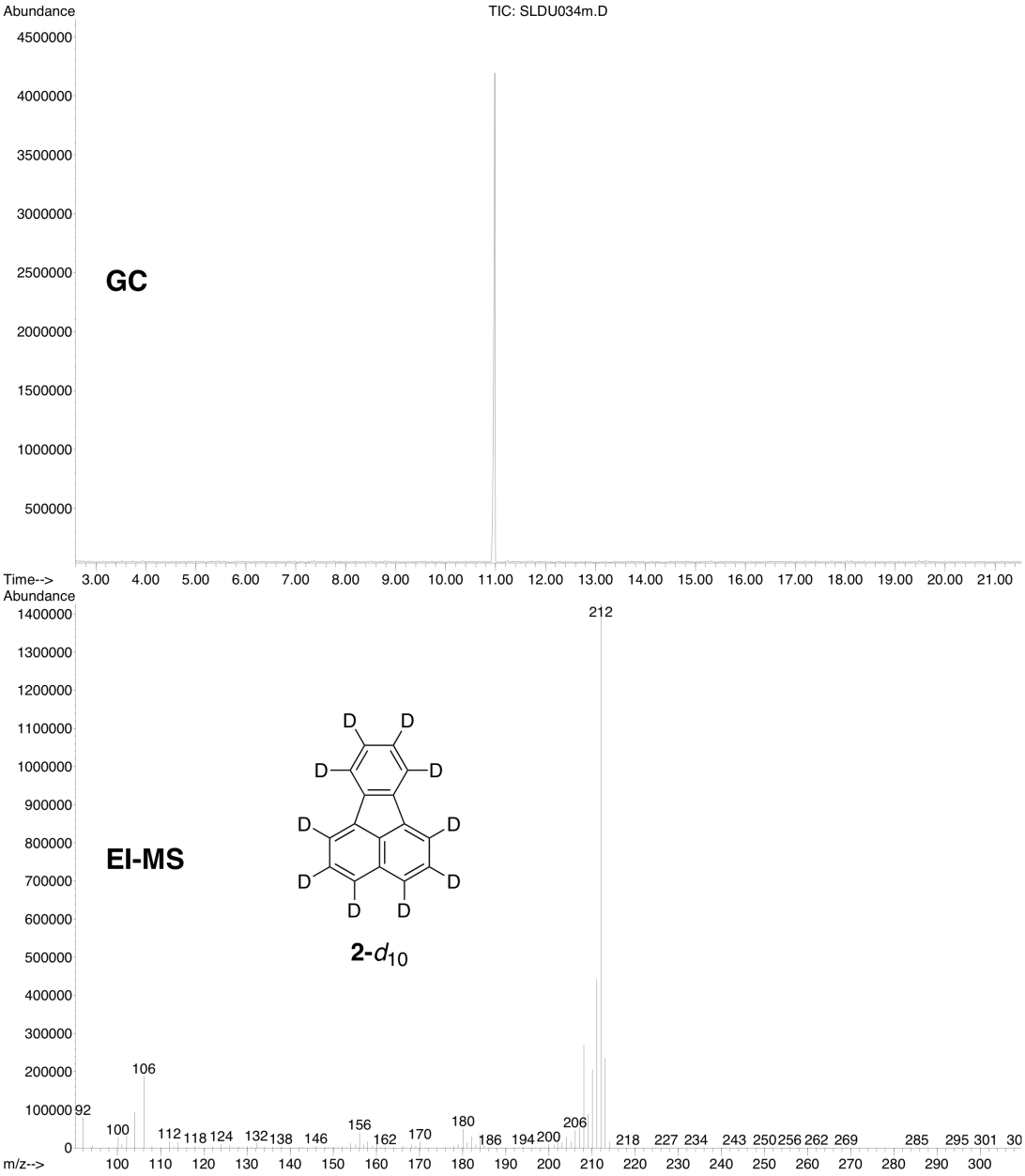
D
1-$d_{14}$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Abundance
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1100000
1000000
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800000
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600000
500000
400000
300000
200000
100000
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EI-MS
212
106
92
100
112
118
124
132
138
146
156
162
170
180
186
194
200
206
218
227
234
243
250
256
262
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m/z-->
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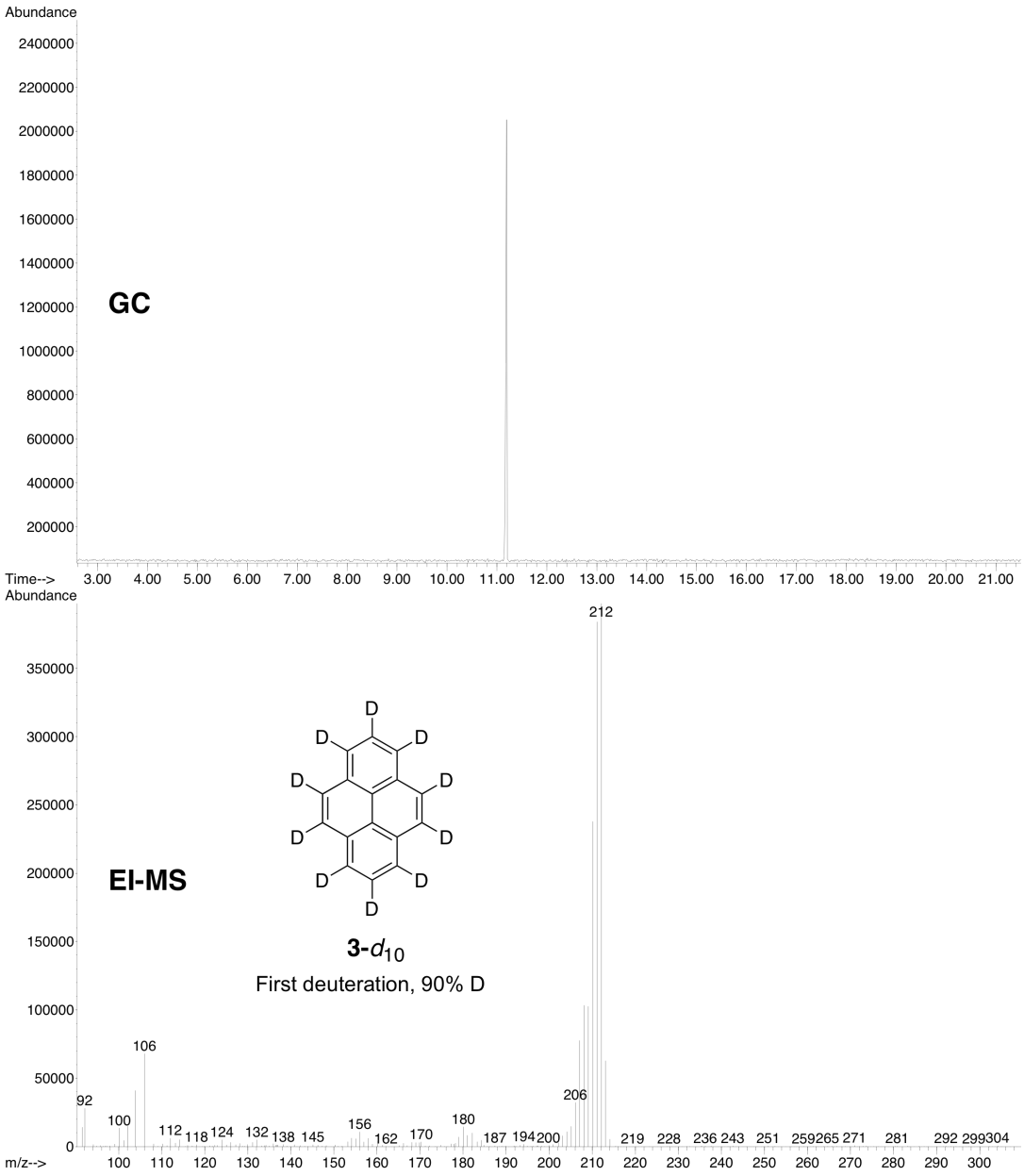
D
2-$d_{10}$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200000
GC
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Abundance
350000
300000
250000
200000
150000
100000
50000
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EI-MS
212
206
106
92
100
112
118
124
132
138
145
156
162
170
180
187
194
200
219
228
236
243
251
259
265
271
281
292
299
304
m/z-->
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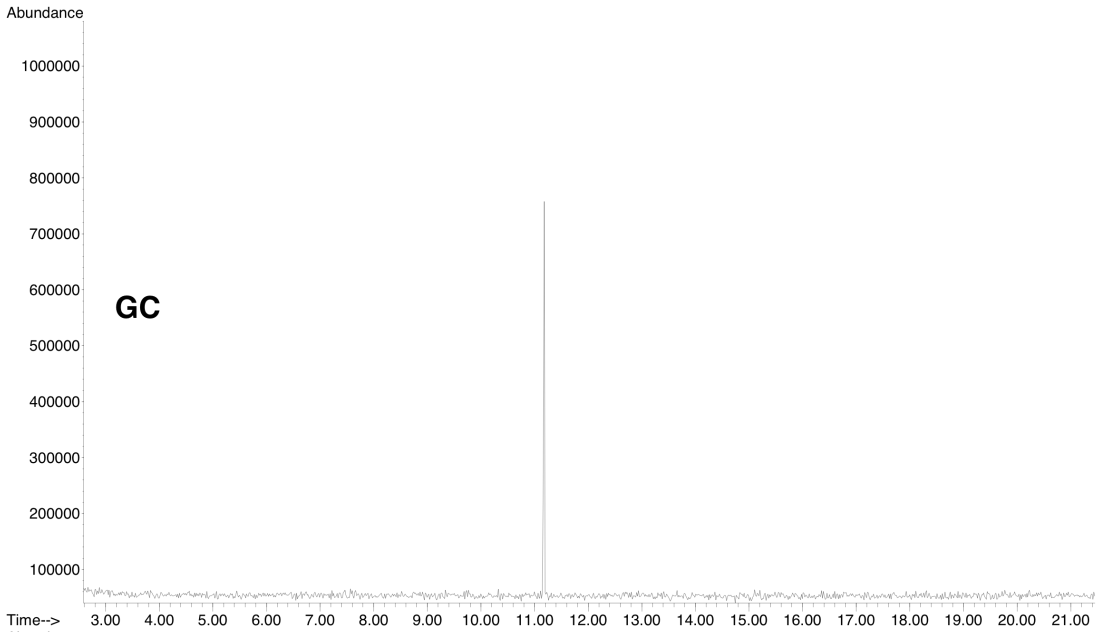
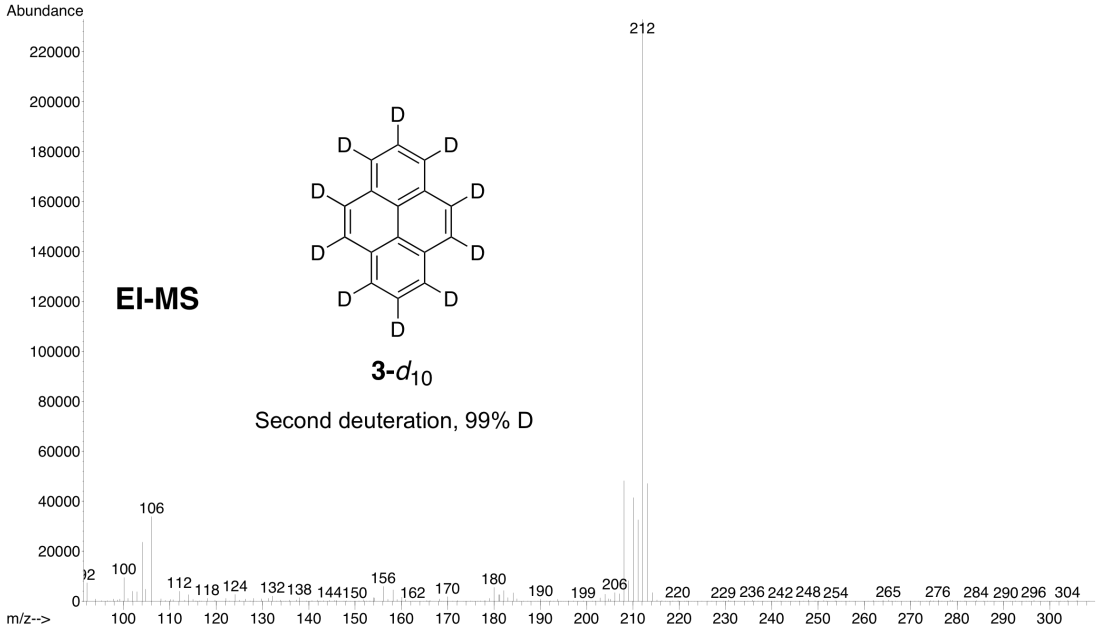
D
3-$d_{10}$
First deuteration, 90% D



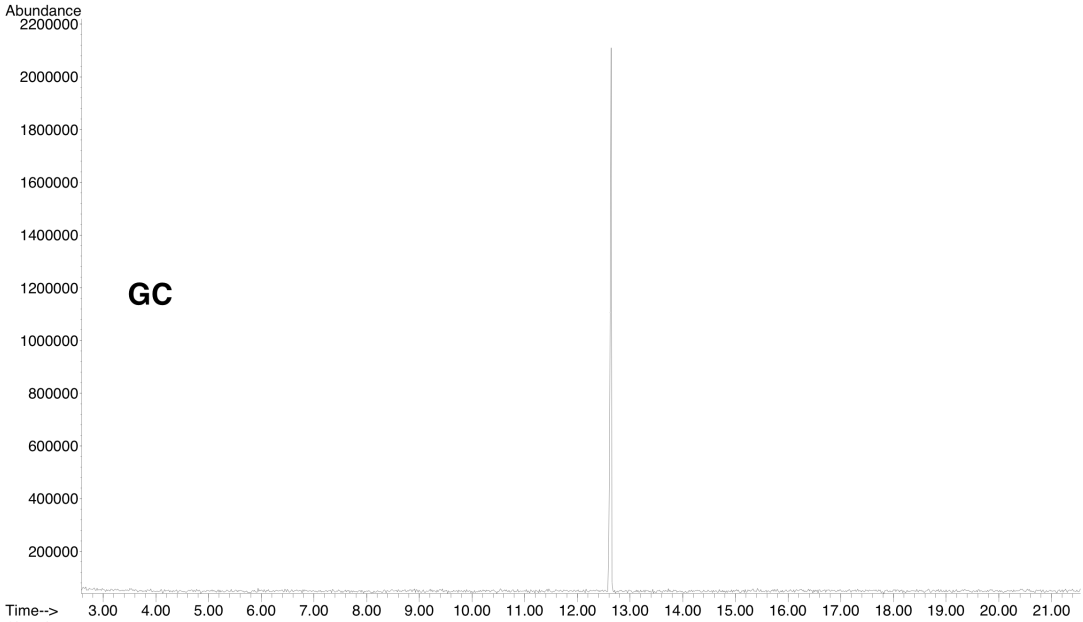







**3-$d_{10}$**

Second deuteration, 99% D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1000000
800000
600000
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200000
GC
Time-->
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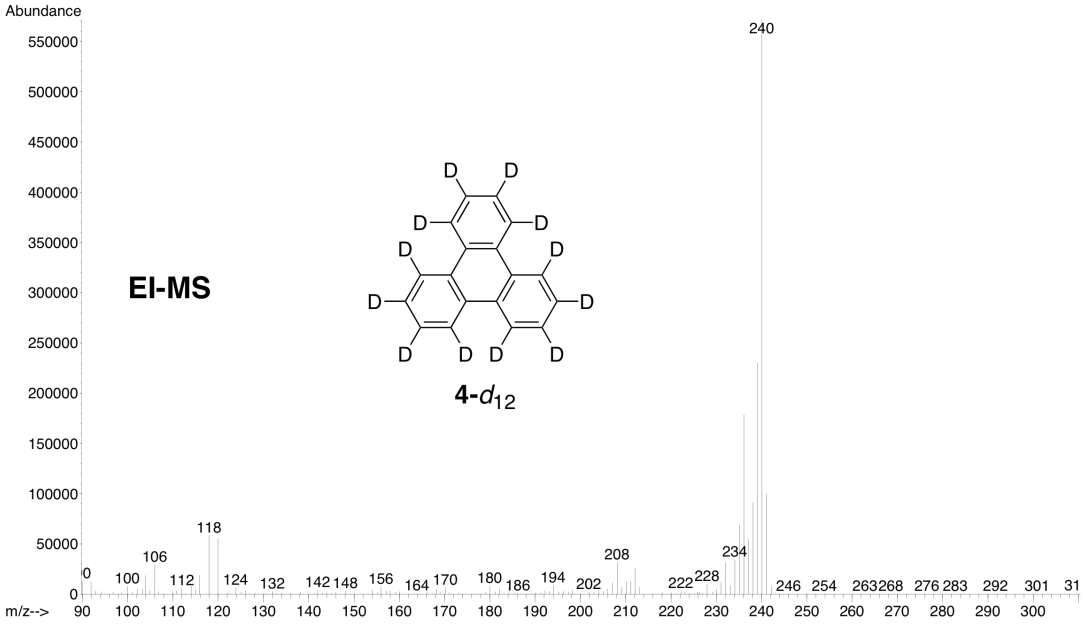
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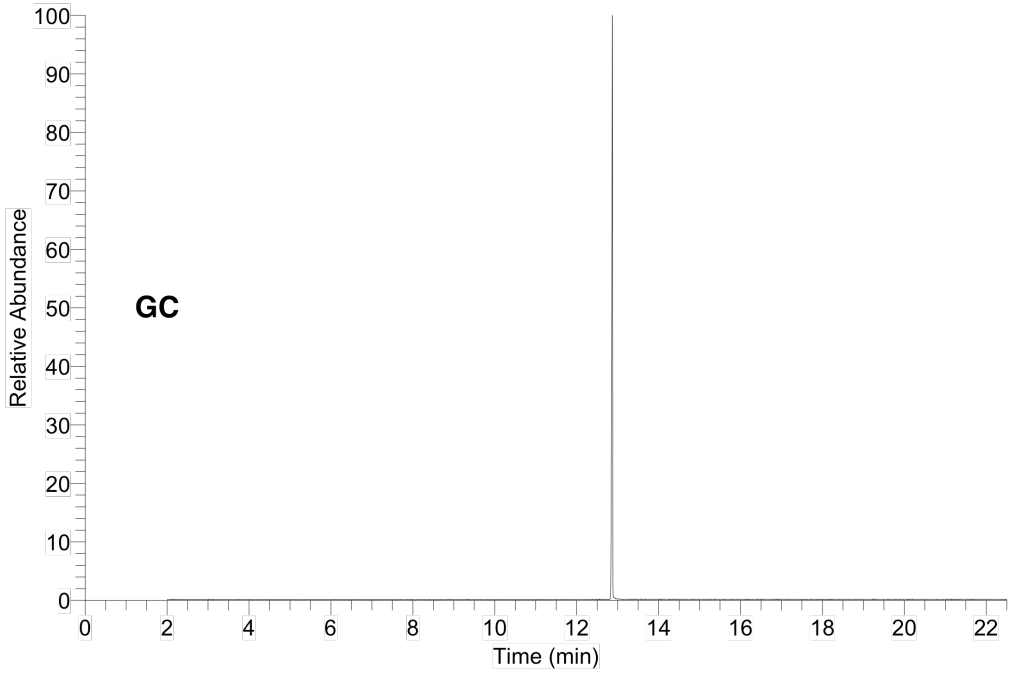
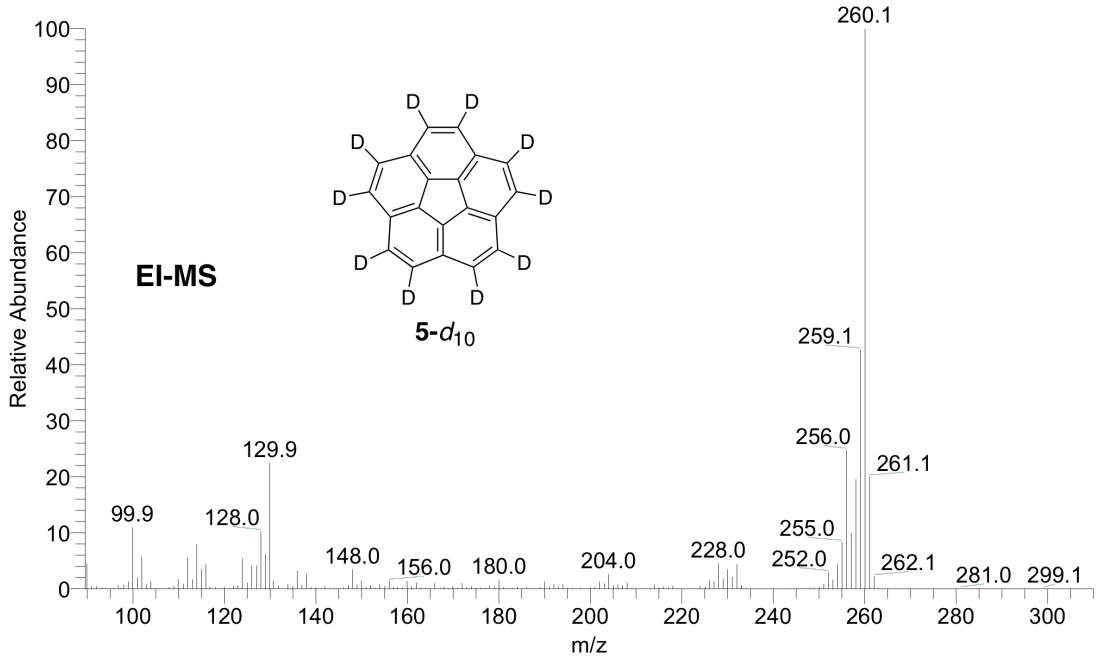
450000
400000
350000
300000
250000
200000
150000
100000
50000
0
EI-MS
240
118
106
208
234
m/z-->
90 100 110 120 130 140 150 160 170 180 190 200 210 220 230 240 250 260 270 280 290 300


D
D
D
D
D
D
D
D
D
D
D
D

**4-$d_{12}$**


GC
Relative Abundance
Time (min)


EI-MS
Relative Abundance
m/z
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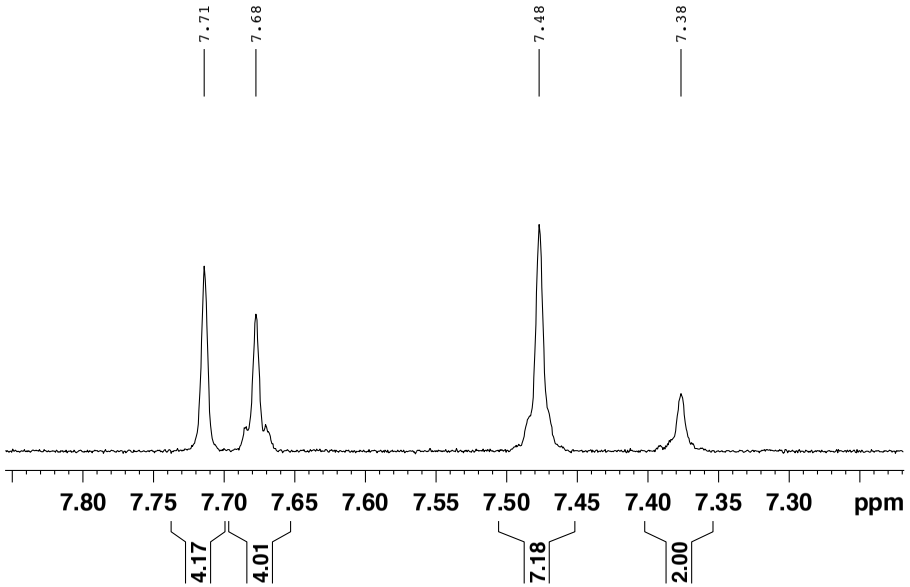
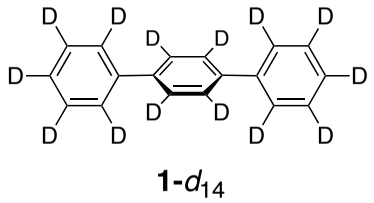
256.0
261.1
255.0
252.0
262.1
129.9
99.9
128.0
148.0
156.0
180.0
204.0
228.0
281.0
299.1
D

**5-$d_{10}$**

# 1H NMR, 19.4 mg in 0.9 mL CD2Cl2, CHDCl2 = 5.32 ppm




**1-$d_{14}$**

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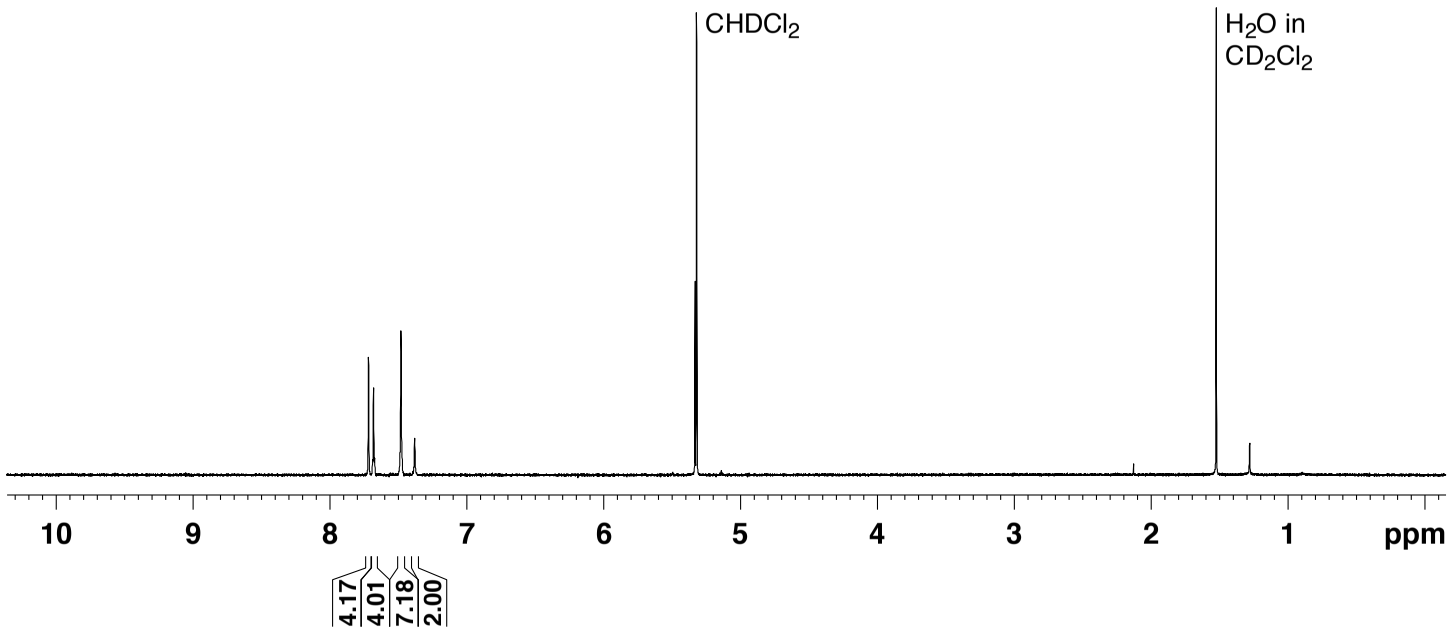
Current Data Parameters
NAME       sld_uzh_0032a
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG             zg30
TD                 61980
SOLVENT           CD2Cl2
NS                    16
DS                     0
SWH           10330.578 Hz
FIDRES         0.166676 Hz
AQ            2.9998820 sec
RG                574.7
DW                48.400 usec
DE                 7.50 usec
TE                298.2 K
D1           3.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.28 usec
PL1               -1.00 dB
SFO1        499.9530874 MHz

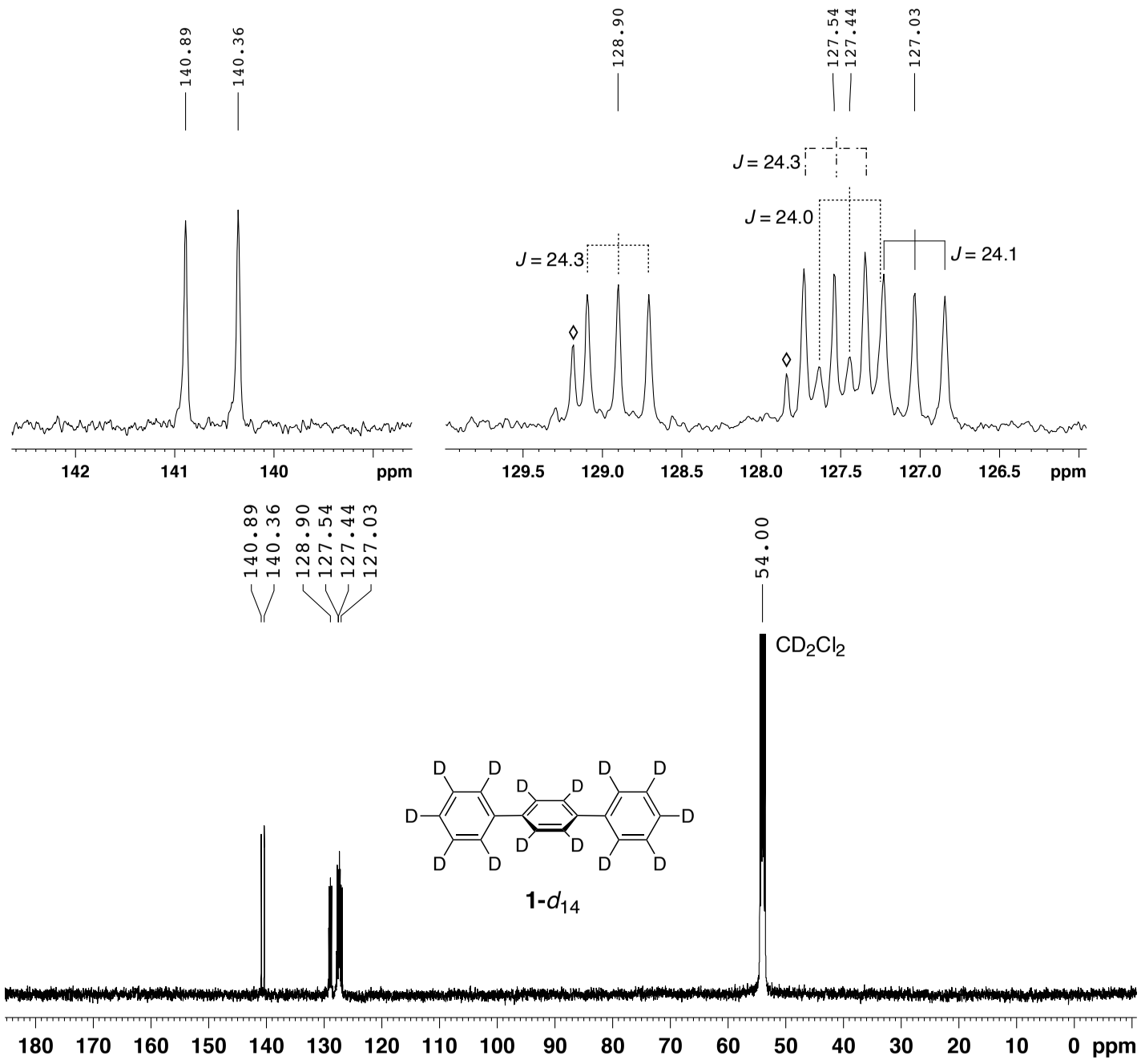
F2 - Processing parameters
SI                 32768
SF          499.9499952 MHz
WDW                   EM
SSB       0
LB               -0.10 Hz
GB        0
PC                 1.00
```

S8



## 13C{1H} NMR, 19.4 mg in 0.9 mL CD2Cl2, CD2Cl2 = 54.0 ppm

◊ = resonances from partially deuterated product




6S

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Current Data Parameters
NAME      sld_uzh_0032a
EXPNO                 3
PROCNO                1

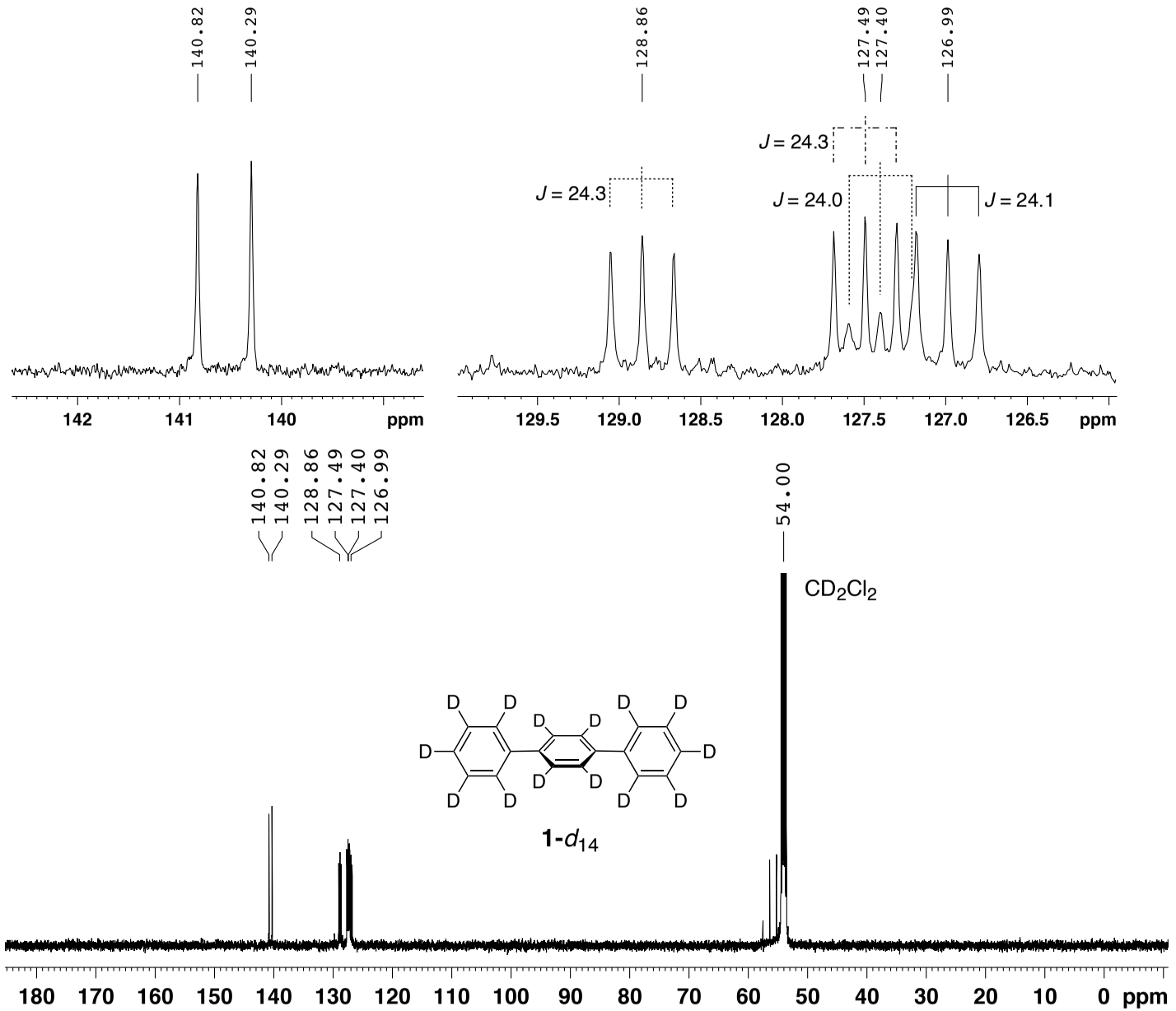
F2 - Acquisition Parameters
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG         zgpg30
TD              600596
SOLVENT          CD2Cl2
NS                  951
DS                    0
SWH           30030.029 Hz
FIDRES            0.050000 Hz
AQ             9.9999733 sec
RG                13004
DW               16.650 usec
DE                7.50 usec
TE                298.2 K
D1            30.00000000 sec
d11            0.03000000 sec
DELTA         29.89999962 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                 7.25 usec
PL1               -2.00 dB
SFO1         125.7250987 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               -1.00 dB
PL12              16.82 dB
PL13              17.00 dB
SFO2         499.9519998 MHz

F2 - Processing parameters
SI                32768
SF           125.7124482 MHz
WDW                  EM
SSB       0
LB                2.00 Hz
GB        0
PC                1.40
```

**13C NMR without 1H decoupling, 19.4 mg in 0.9 mL CD2Cl2, + 1.5 mg $Cr(acac)_3$ as a relaxation agent, CD2Cl2 = 54.0 ppm**



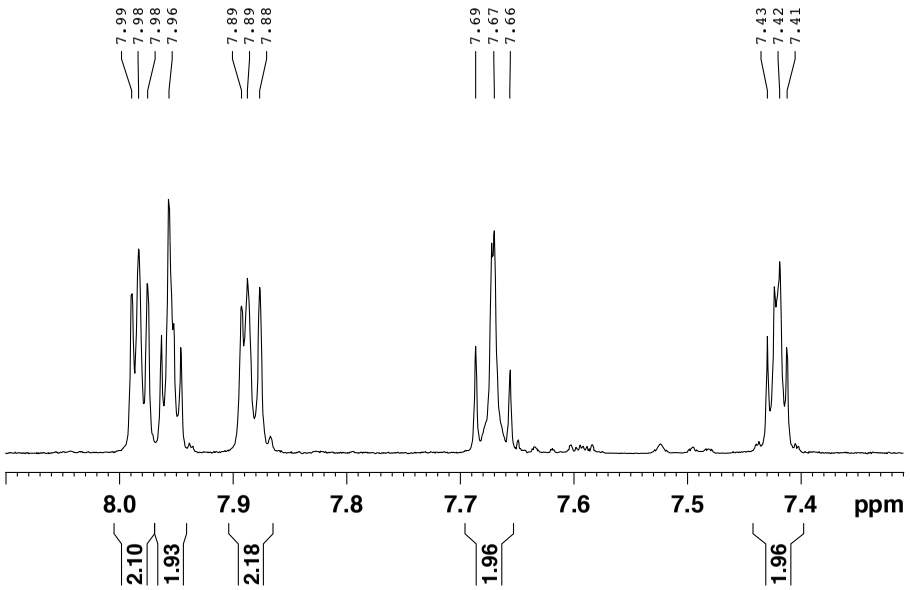

```
Current Data Parameters
NAME       sld_uzh_0032a
EXPNO                 50
PROCNO                 1

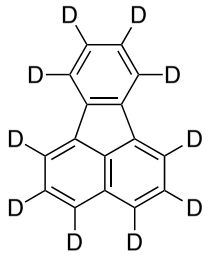
F2 - Acquisition Parameters
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 54050
SOLVENT           CD2Cl2
NS                  3584
DS                     0
SWH            30030.029 Hz
FIDRES          0.555597 Hz
AQ              0.8999825 sec
RG                10321.3
DW                16.650 usec
DE                 7.50 usec
TE                297.1 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  7.25 usec
PL1                -2.00 dB
SFO1         125.7250987 MHz

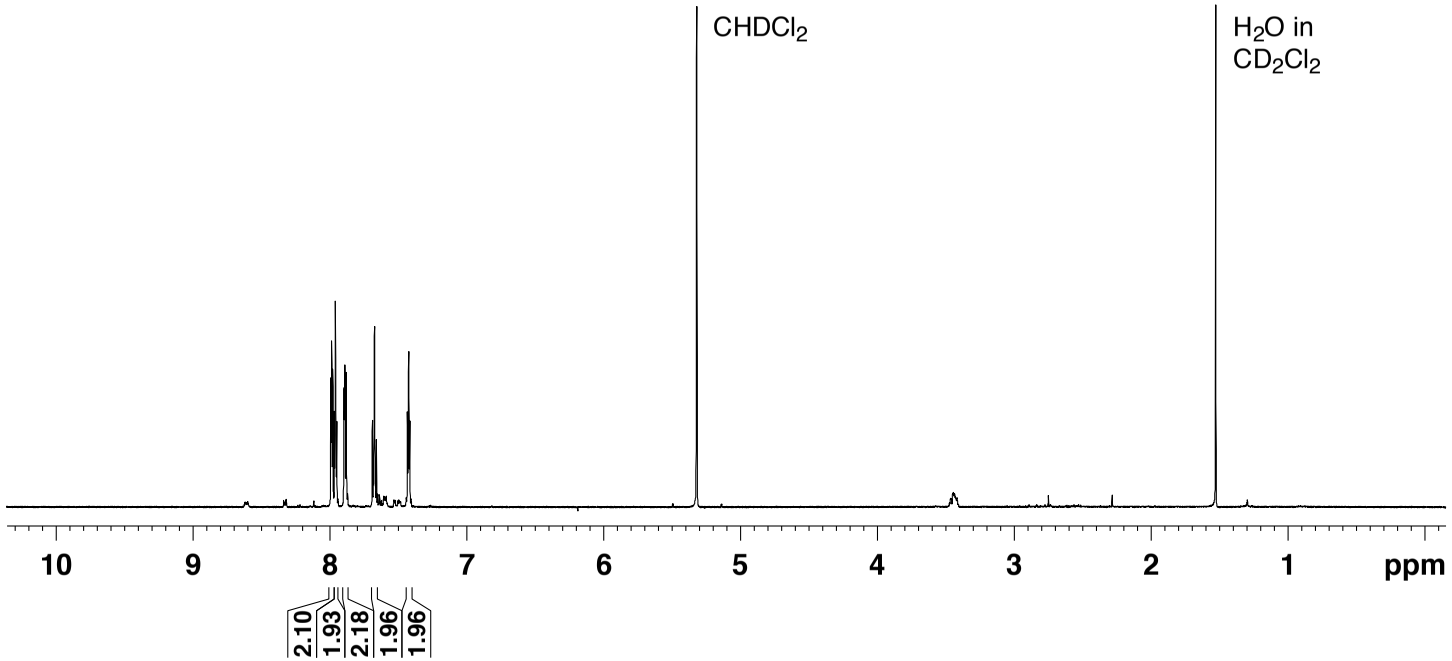
F2 - Processing parameters
SI                 32768
SF           125.7124551 MHz
WDW                   EM
SSB       0
LB                 0.80 Hz
GB        0
PC                 1.40
```

# 1H NMR, 29.7 mg in 0.6 mL CD2Cl2, CHDCl2 = 5.32 ppm




**2-$d_{10}$**




```
Current Data Parameters
NAME       sld_uzh_0034a
EXPNO                  1
PROCNO                 1

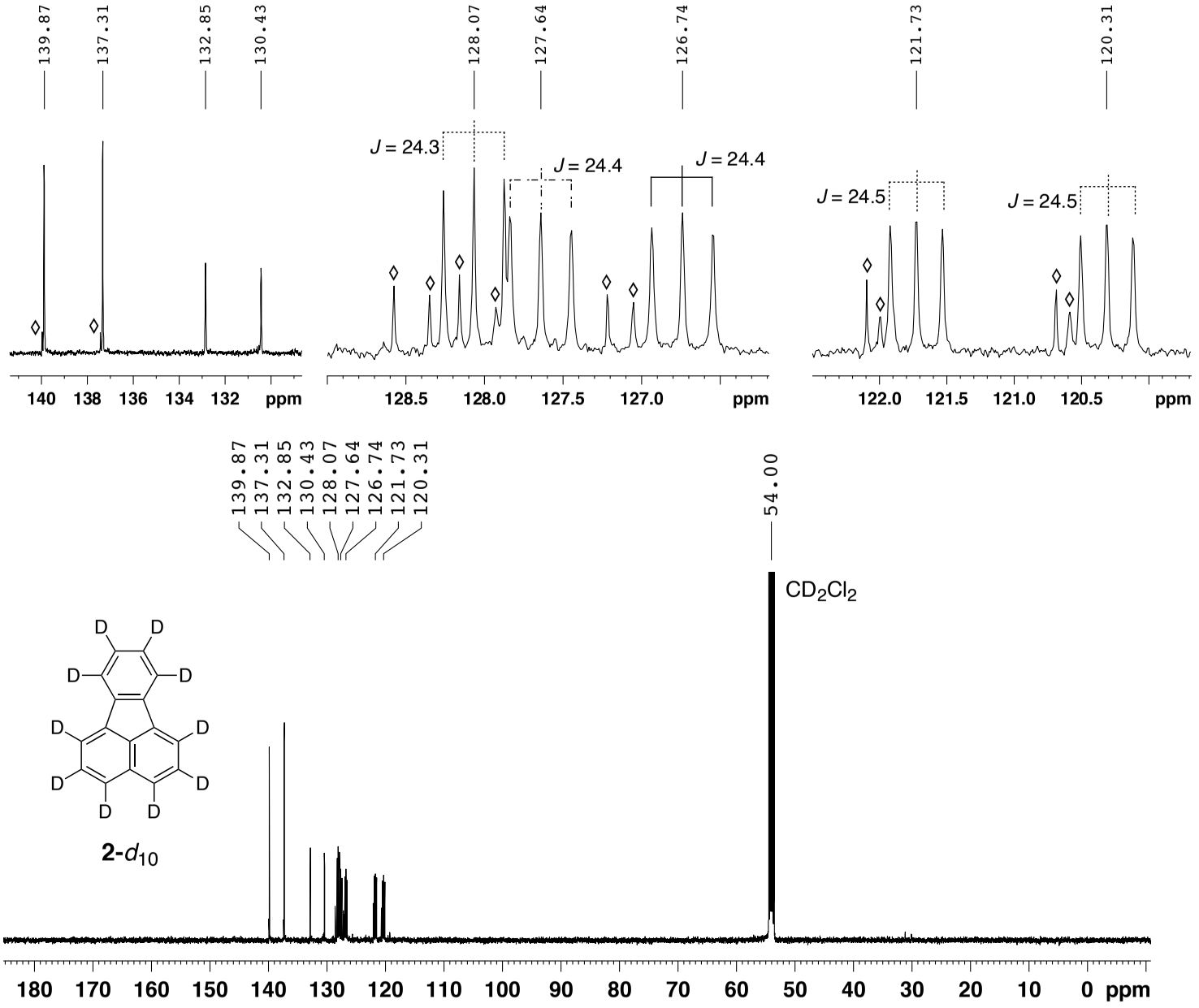
F2 - Acquisition Parameters
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                103302
SOLVENT           CD2Cl2
NS                    16
DS                     0
SWH           10330.578 Hz
FIDRES         0.100004 Hz
AQ            4.9998670 sec
RG                456.1
DW                48.400 usec
DE                 7.50 usec
TE                297.2 K
D1           30.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.28 usec
PL1               -1.00 dB
SFO1        499.9530874 MHz

F2 - Processing parameters
SI                 32768
SF          499.9499952 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```

## 13C{1H} NMR, 29.7 mg in 0.6 mL CD2Cl2, CD2Cl2 = 54.0 ppm

◊ = resonances from partially deuterated product




**2-$d_{10}$**

```
Current Data Parameters
NAME      sld_uzh_0034a
EXPNO                 2
PROCNO                1

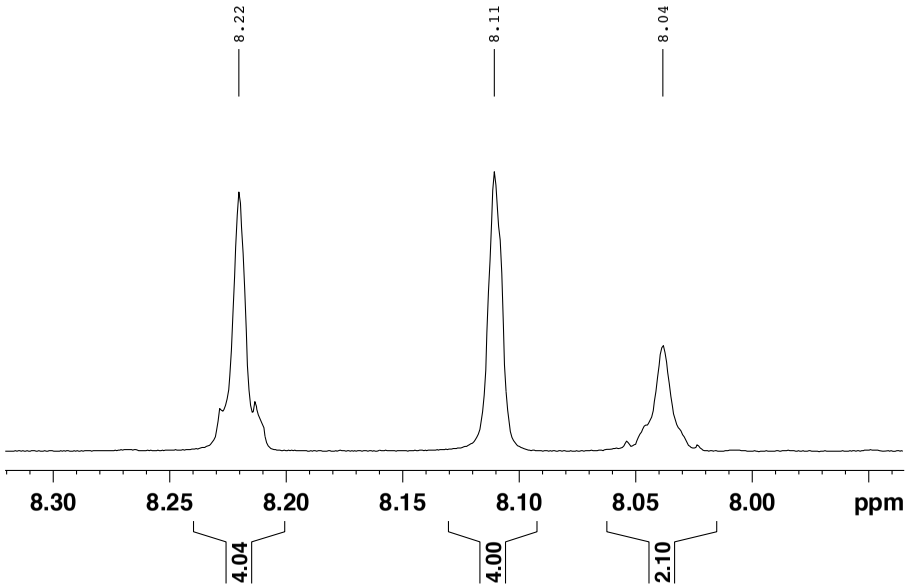
F2 - Acquisition Parameters
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD               600596
SOLVENT          CD2Cl2
NS                 1017
DS                    0
SWH           30030.029 Hz
FIDRES            0.050000 Hz
AQ            9.9999733 sec
RG                13004
DW               16.650 usec
DE                7.50 usec
TE                297.5 K
D1           30.00000000 sec
d11           0.03000000 sec
DELTA        29.89999962 sec
TD0                   1

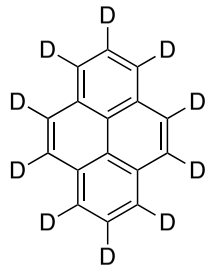
======== CHANNEL f1 ========
NUC1                 13C
P1                 7.25 usec
PL1               -2.00 dB
SFO1        125.7250987 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2               -1.00 dB
PL12              16.82 dB
PL13              17.00 dB
SFO2        499.9519998 MHz

F2 - Processing parameters
SI                32768
SF          125.7124522 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

## 1H NMR, 24.9 mg in 0.6 mL CD2Cl2, CHDCl2 = 5.32 ppm



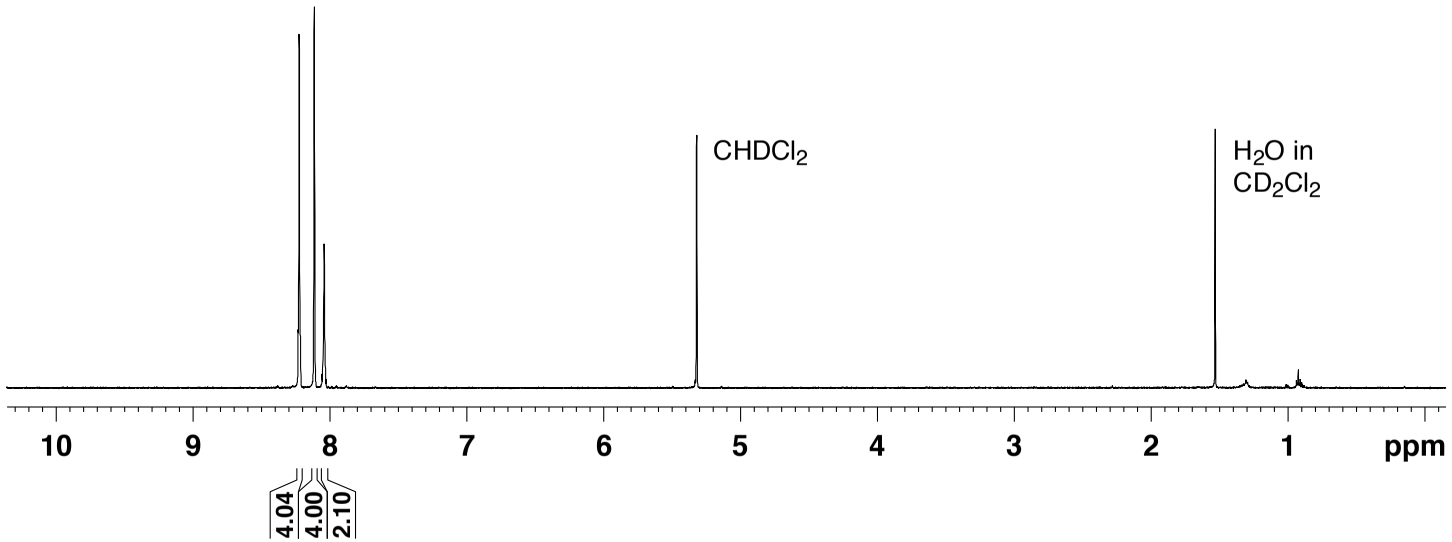

**3-$d_{10}$**

```
Current Data Parameters
NAME       sld_uzh_0035a
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 61980
SOLVENT           CD2Cl2
NS                    16
DS                     0
SWH           10330.578 Hz
FIDRES         0.166676 Hz
AQ            2.9998820 sec
RG                456.1
DW                48.400 usec
DE                 7.50 usec
TE                297.2 K
D1            3.00000000 sec
TD0                    1

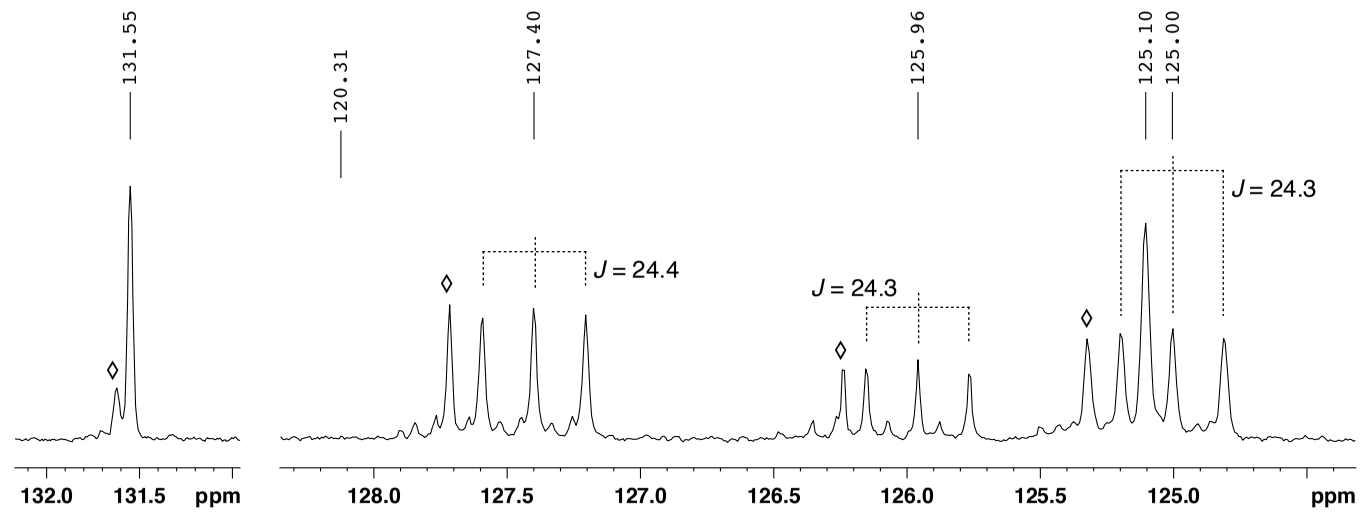
======== CHANNEL f1 ========
NUC1                  1H
P1                10.28 usec
PL1               -1.00 dB
SFO1        499.9530874 MHz

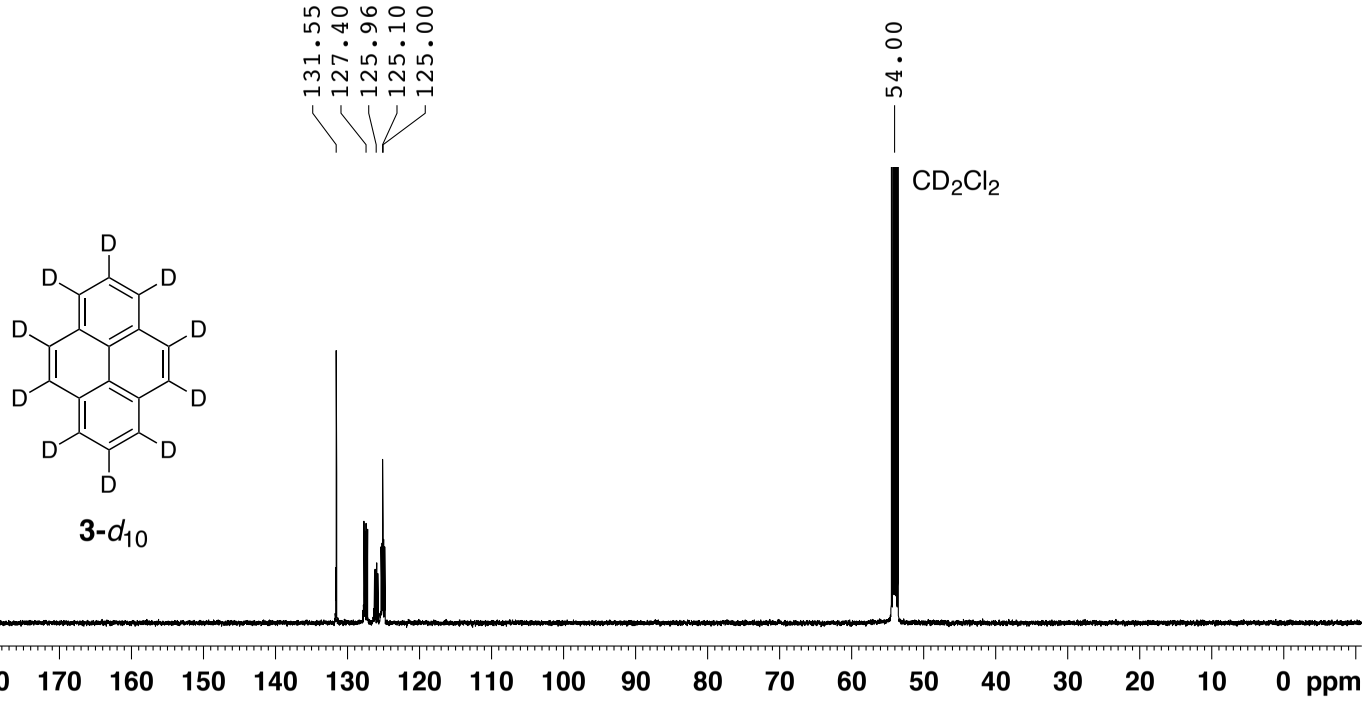
F2 - Processing parameters
SI                 32768
SF          499.9499952 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```



## 13C{1H} NMR, 24.9 mg in 0.6 mL CD2Cl2, CD2Cl2 = 54.0 ppm

◊ = resonances from partially deuterated product

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Current Data Parameters
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EXPNO                 2
PROCNO                1

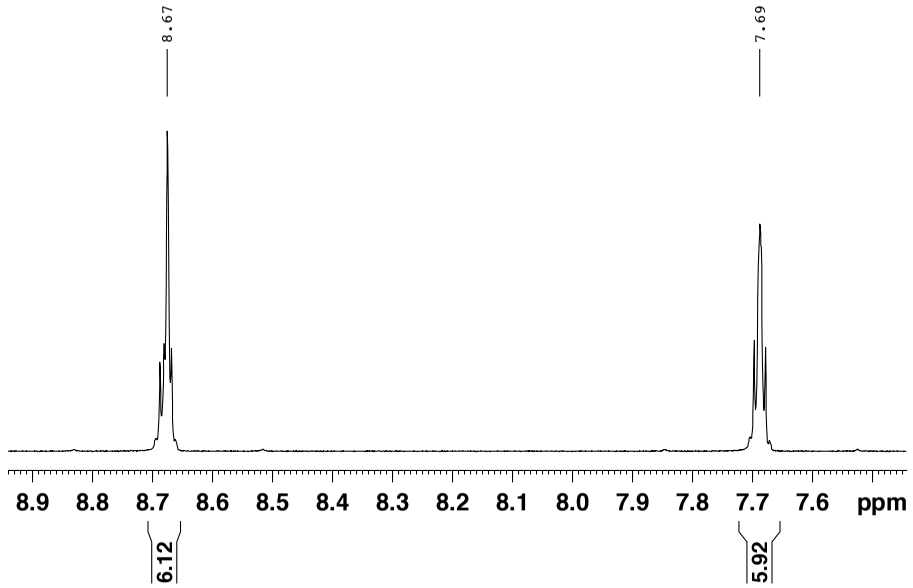
F2 - Acquisition Parameters
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG          zgpg30
TD                600596
SOLVENT           CD2Cl2
NS                   912
DS                     0
SWH            30030.029 Hz
FIDRES             0.050000 Hz
AQ             9.9999733 sec
RG                 10321.3
DW                  16.650 usec
DE                   7.50 usec
TE                  297.4 K
D1            30.00000000 sec
d11            0.03000000 sec
DELTA         29.89999962 sec
TD0                    1

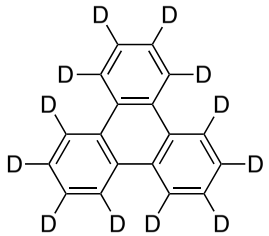
======== CHANNEL f1 ========
NUC1                  13C
P1                   7.25 usec
PL1                 -2.00 dB
SFO1         125.7250987 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2               80.00 usec
PL2                 -1.00 dB
PL12                16.82 dB
PL13                17.00 dB
SFO2         499.9519998 MHz

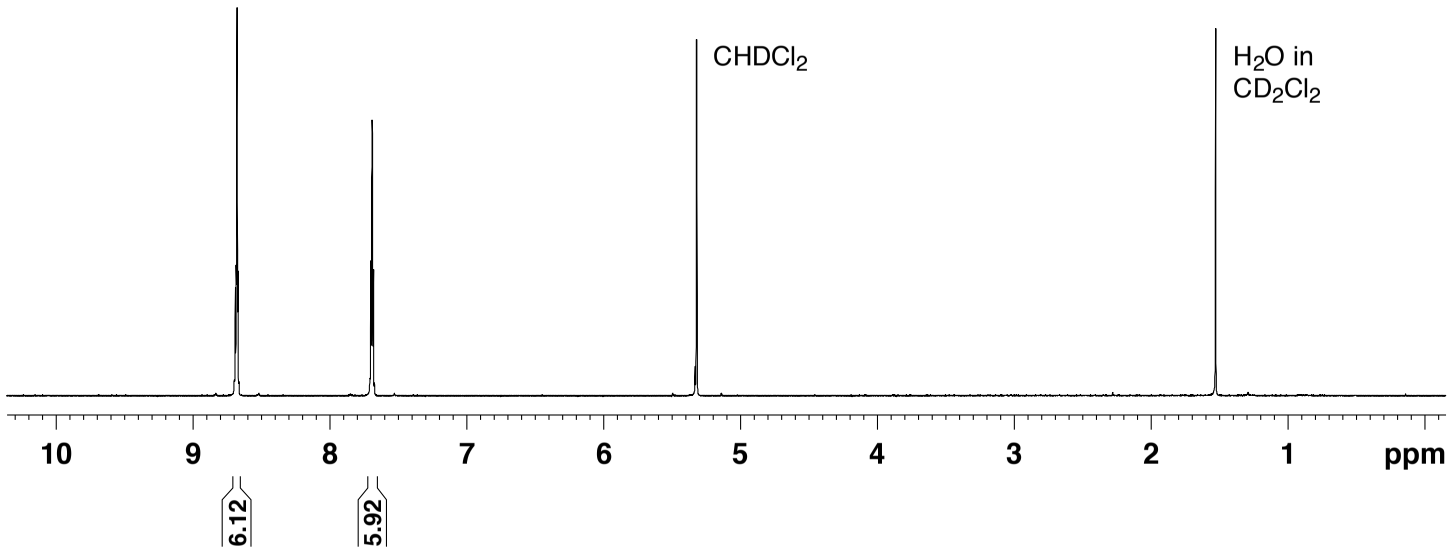
F2 - Processing parameters
SI                 32768
SF           125.7124522 MHz
WDW                   EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

## 1H NMR, 27.1 mg in 0.6 mL CD2Cl2, CHDCl2 = 5.32 ppm




**4-$d_{12}$**




```
Current Data Parameters
NAME       sld_uzh_0036a
EXPNO                  1
PROCNO                 1

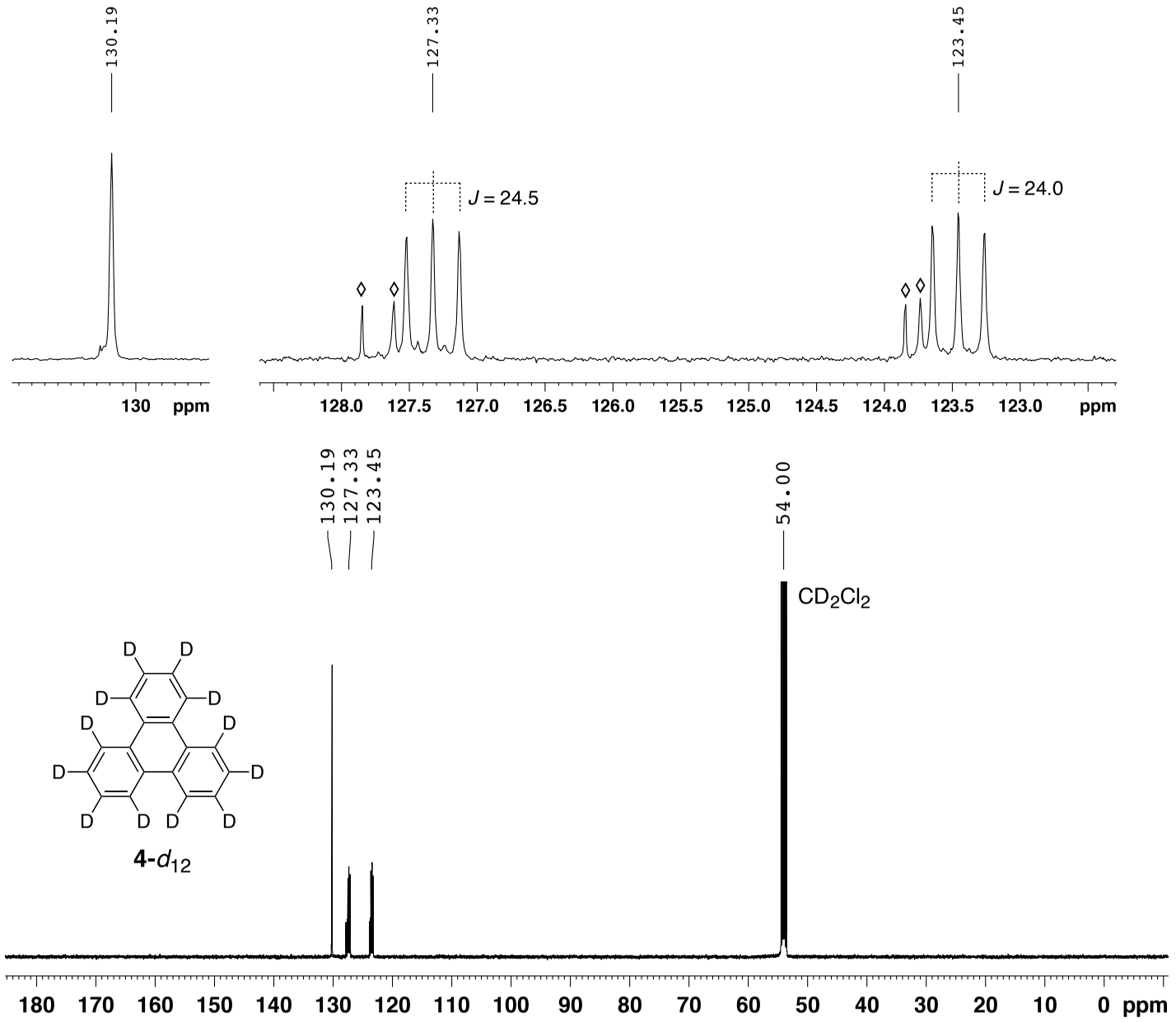
F2 - Acquisition Parameters
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 61980
SOLVENT           CD2Cl2
NS                    16
DS                     0
SWH            10330.578 Hz
FIDRES          0.166676 Hz
AQ             2.9998820 sec
RG                 456.1
DW                48.400 usec
DE                 7.50 usec
TE                297.5 K
D1            3.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                10.28 usec
PL1               -1.00 dB
SFO1         499.9530874 MHz

F2 - Processing parameters
SI                 32768
SF           499.9499952 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                 1.00
```

## 13C{1H} NMR, 27.1 mg in 0.6 mL CD2Cl2, CD2Cl2 = 54.0 ppm

◊ = resonances from partially deuterated product




```
Current Data Parameters
NAME      sld_uzh_0036a
EXPNO                 2
PROCNO                1

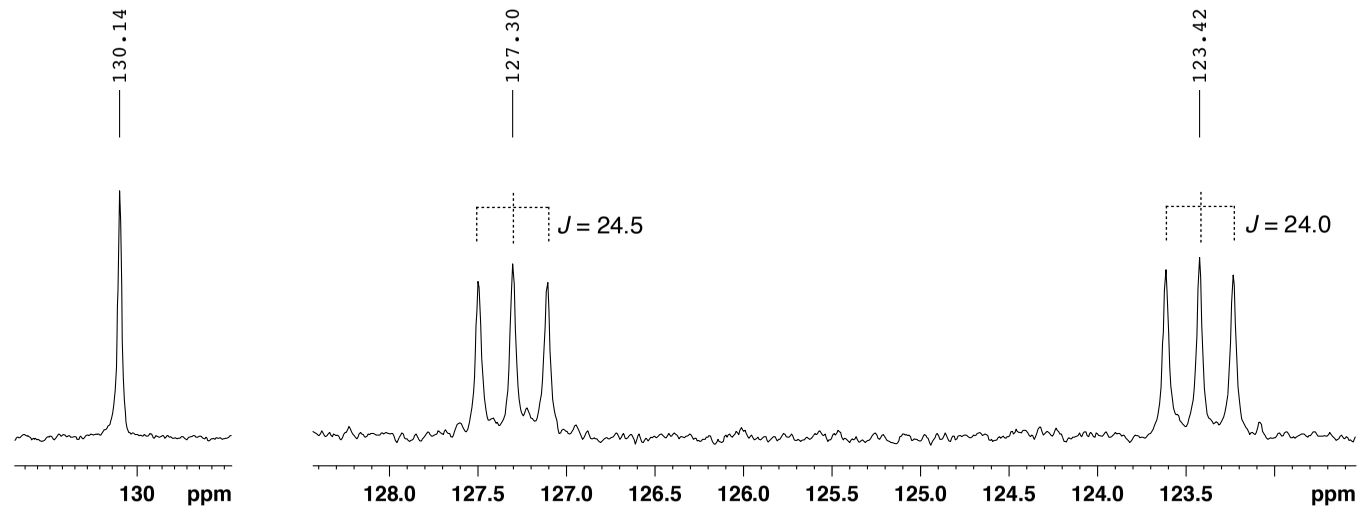
F2 - Acquisition Parameters
INSTRUM            spect
PROBHD    5 mm PABBO BB-
PULPROG          zgpg30
TD                600596
SOLVENT           CD2Cl2
NS                  1024
DS                     0
SWH           30030.029 Hz
FIDRES            0.050000 Hz
AQ             9.9999733 sec
RG               10321.3
DW                16.650 usec
DE                 7.50 usec
TE                297.9 K
D1            30.00000000 sec
d11            0.03000000 sec
DELTA         29.89999962 sec
TD0                   1

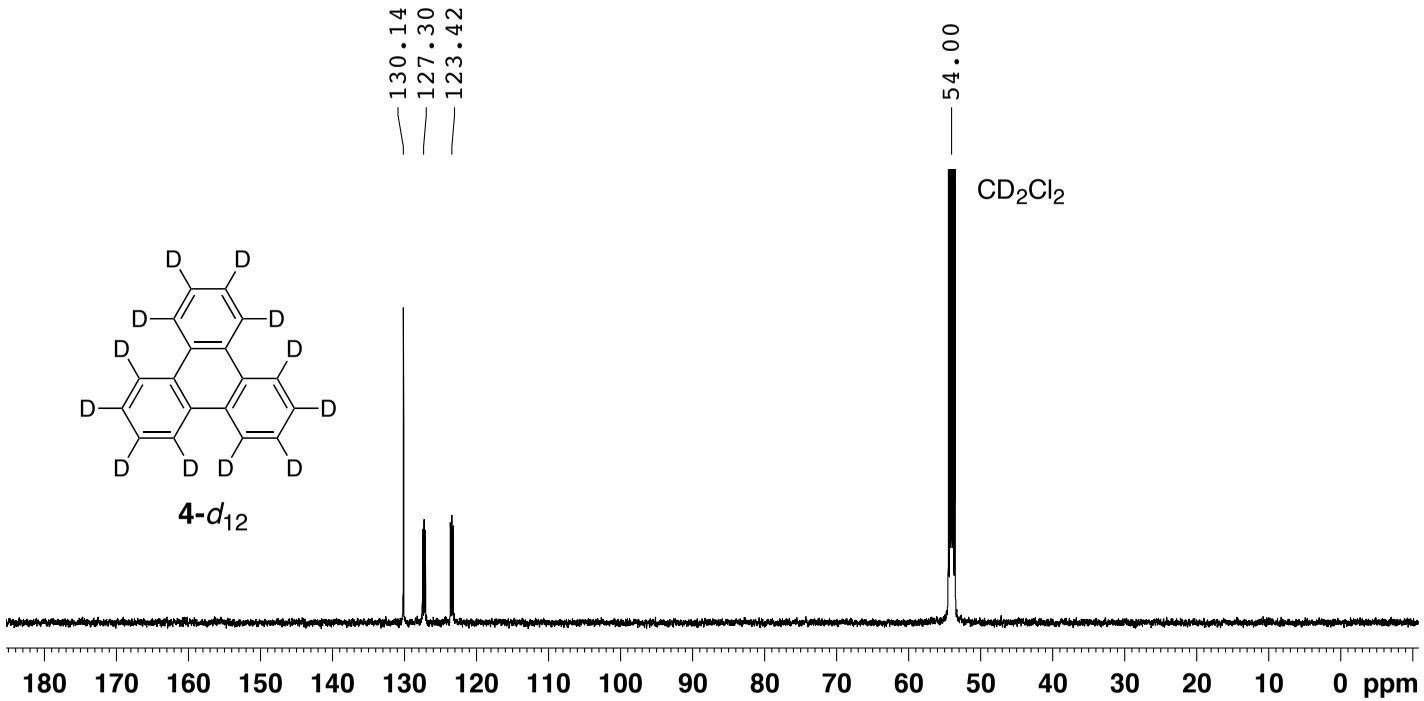
======== CHANNEL f1 ========
NUC1                 13C
P1                  7.25 usec
PL1                -2.00 dB
SFO1         125.7250987 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                -1.00 dB
PL12               16.82 dB
PL13               17.00 dB
SFO2         499.9519998 MHz

F2 - Processing parameters
SI                 32768
SF           125.7124522 MHz
WDW                  EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

**13C NMR without 1H decoupling, 15 mg in 0.7 mL CD2Cl2, + 1.0 mg $Cr(acac)_3$ as a relaxation agent, CD2Cl2 = 54.0 ppm**







**4-$d_{12}$**

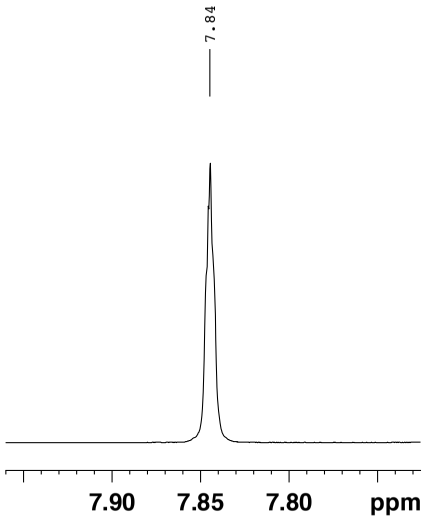
```
Current Data Parameters
NAME       sld_uzh_0036a
EXPNO                 60
PROCNO                 1

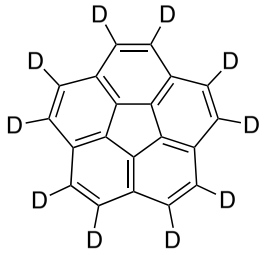
F2 - Acquisition Parameters
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG             zg30
TD                 54050
SOLVENT           CD2Cl2
NS                  1024
DS                     0
SWH          30030.029 Hz
FIDRES        0.555597 Hz
AQ            0.8999825 sec
RG              10321.3
DW               16.650 usec
DE                7.50 usec
TE               297.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  7.25 usec
PL1                -2.00 dB
SFO1        125.7250987 MHz

F2 - Processing parameters
SI                 32768
SF          125.7124563 MHz
WDW                   EM
SSB       0
LB                  2.00 Hz
GB        0
PC                  1.40
```

## 1H NMR, 20.5 mg in 0.6 mL CD2Cl2, CHDCl2 = 5.32 ppm



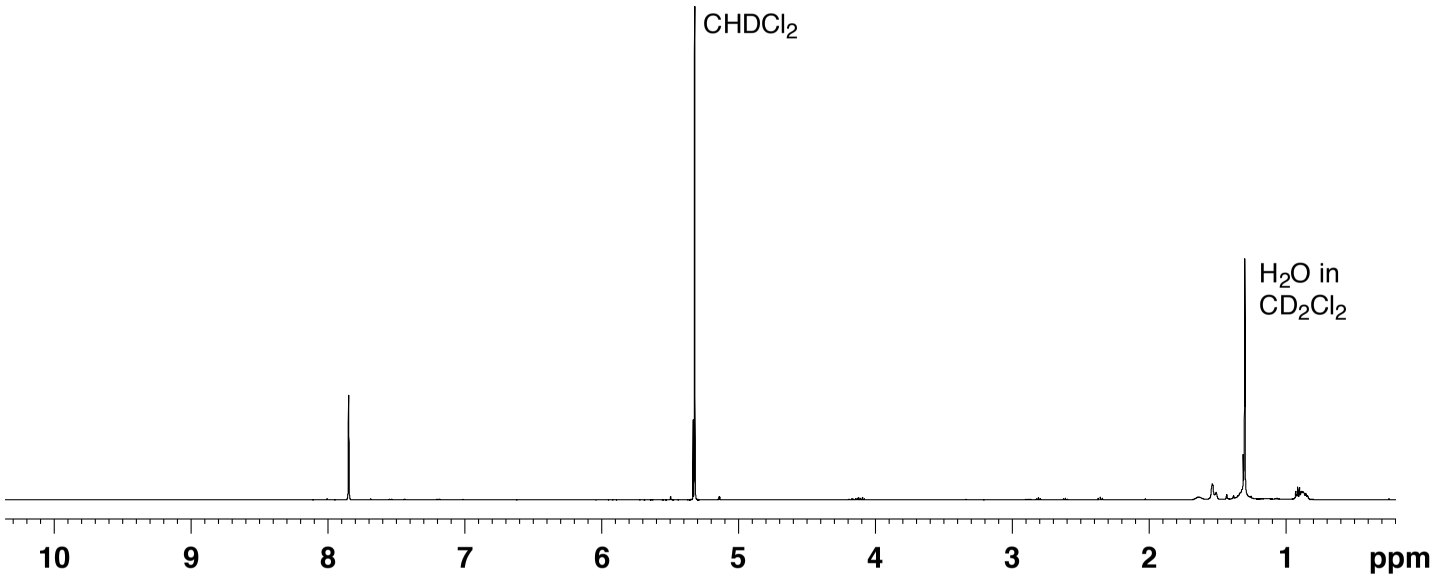

**5-$d_{10}$**

```
Current Data Parameters
NAME            Anna_Cor
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
INSTRUM             spect
PROBHD   5 mm PATXI 1H/
PULPROG                zg
TD                  61982
SOLVENT            CD2Cl2
NS                     32
DS                      0
SWH             10330.578 Hz
FIDRES          0.166671 Hz
AQ              2.9999788 sec
RG                    406
DW                48.400 usec
DE                20.00 usec
TE                300.0 K
D1             3.00000000 sec
TD0                    1

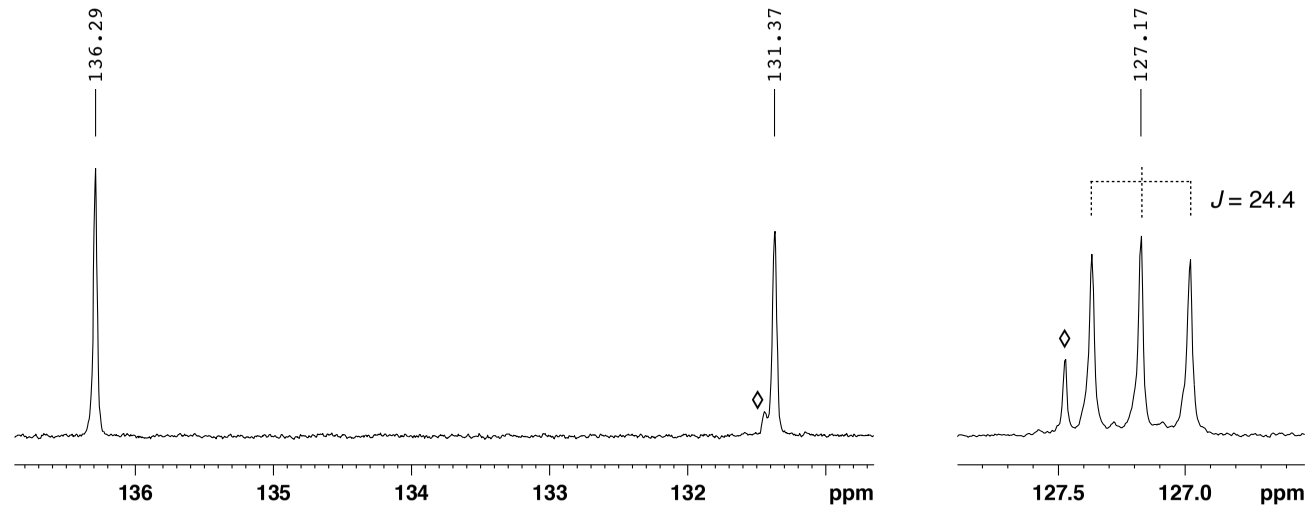
======== CHANNEL f1 ========
NUC1                  1H
P1                 7.70 usec
PL1                1.50 dB
PL1W         15.41768265 W
SFO1         500.1330885 MHz

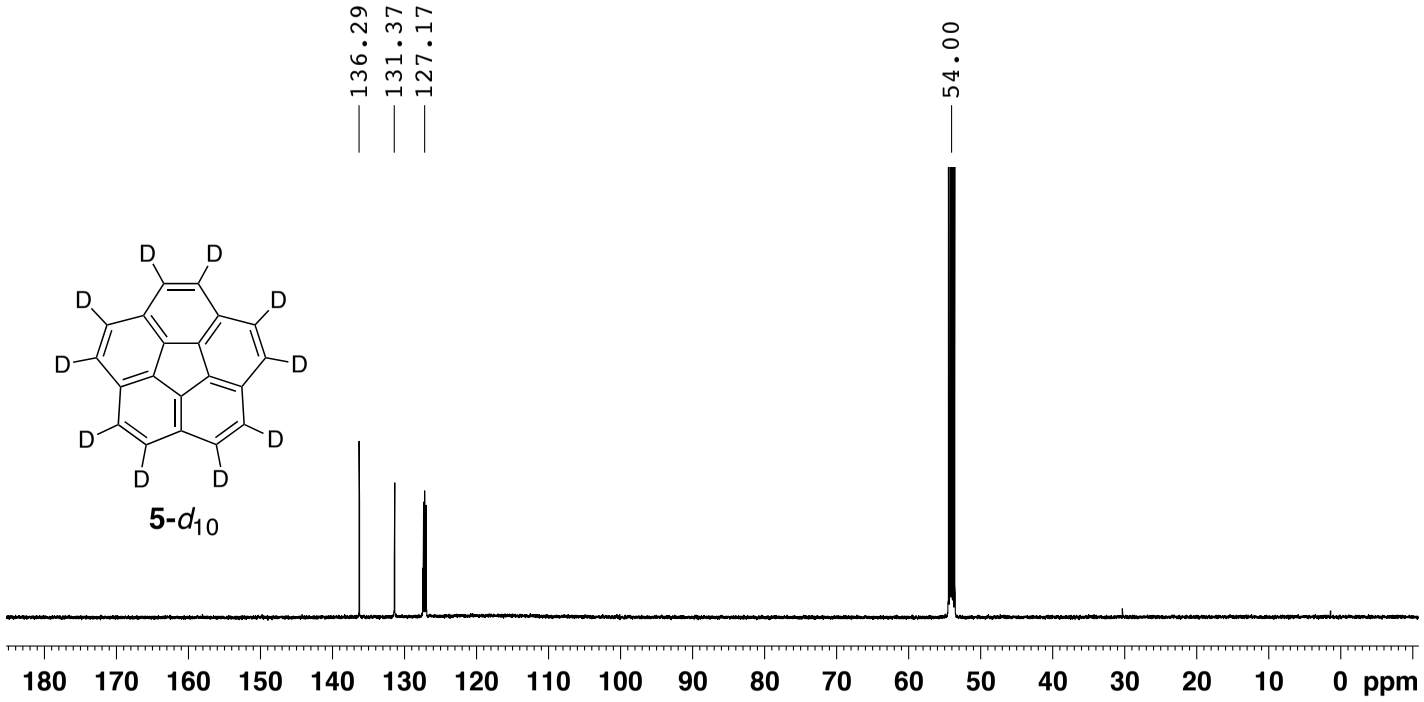
F2 - Processing parameters
SI                 65536
SF           500.1300204 MHz
WDW                   no
SSB       0
LB        0 Hz
GB        0
PC                 1.40
```



## 13C{1H} NMR, 20.5 mg in 0.6 mL CD2Cl2, CD2Cl2 = 54.0 ppm

◊ = resonances from partially deuterated product







**5-$d_{10}$**

```
Current Data Parameters
NAME            Anna_Cor
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
INSTRUM              spect
PROBHD    5 mm PATXI 1H/
PULPROG           zgpg30
TD                781246
SOLVENT           CD2Cl2
NS                  1464
DS                     4
SWH            39062.500 Hz
FIDRES          0.050000 Hz
AQ              9.9999990 sec
RG                  2050
DW                12.800 usec
DE                20.00 usec
TE                300.0 K
D1           30.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 11.55 usec
PL1                -4.00 dB
PL1W        167.83465576 W
SFO1         125.7703052 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                 1.50 dB
PL12               21.83 dB
PL13               25.00 dB
PL2W         15.41768265 W
PL12W         0.14289568 W
PL13W         0.06886826 W
SFO2         500.1320005 MHz

F2 - Processing parameters
SI                 65536
SF           125.7577160 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```