

Supplementary data

Environmental friendly domino multicomponent strategy for the synthesis of pyrroloquinolinone hybrid heterocycles

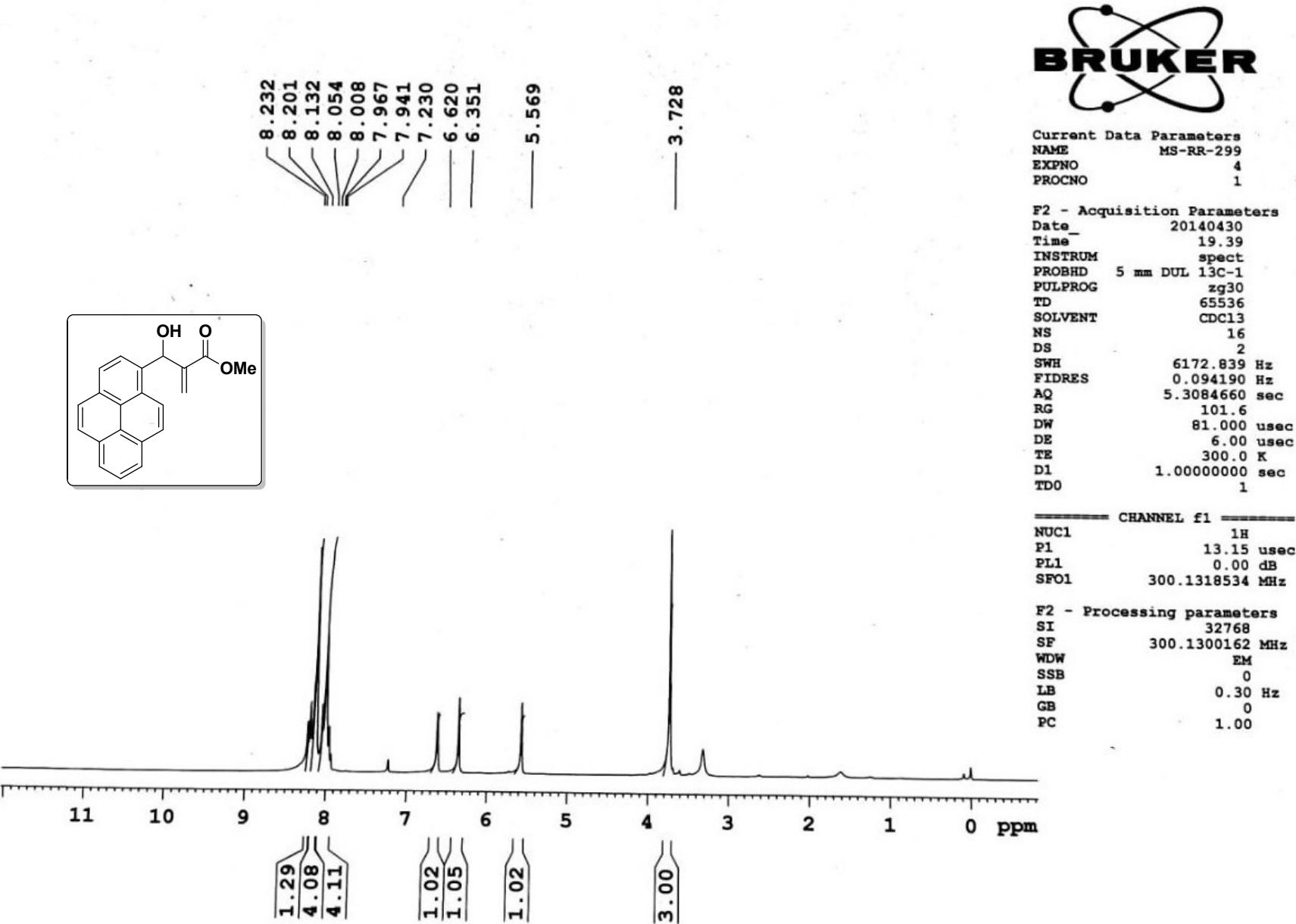
Suresh Mani,^a Rajesh Raju,^{a*} Raghavachary Raghunathan,^{a*} Natarajan Arumugam,^b Abdulrahman I. Almansour,^b Raju Suresh Kumar,^b Karthikeyan Perumal^c

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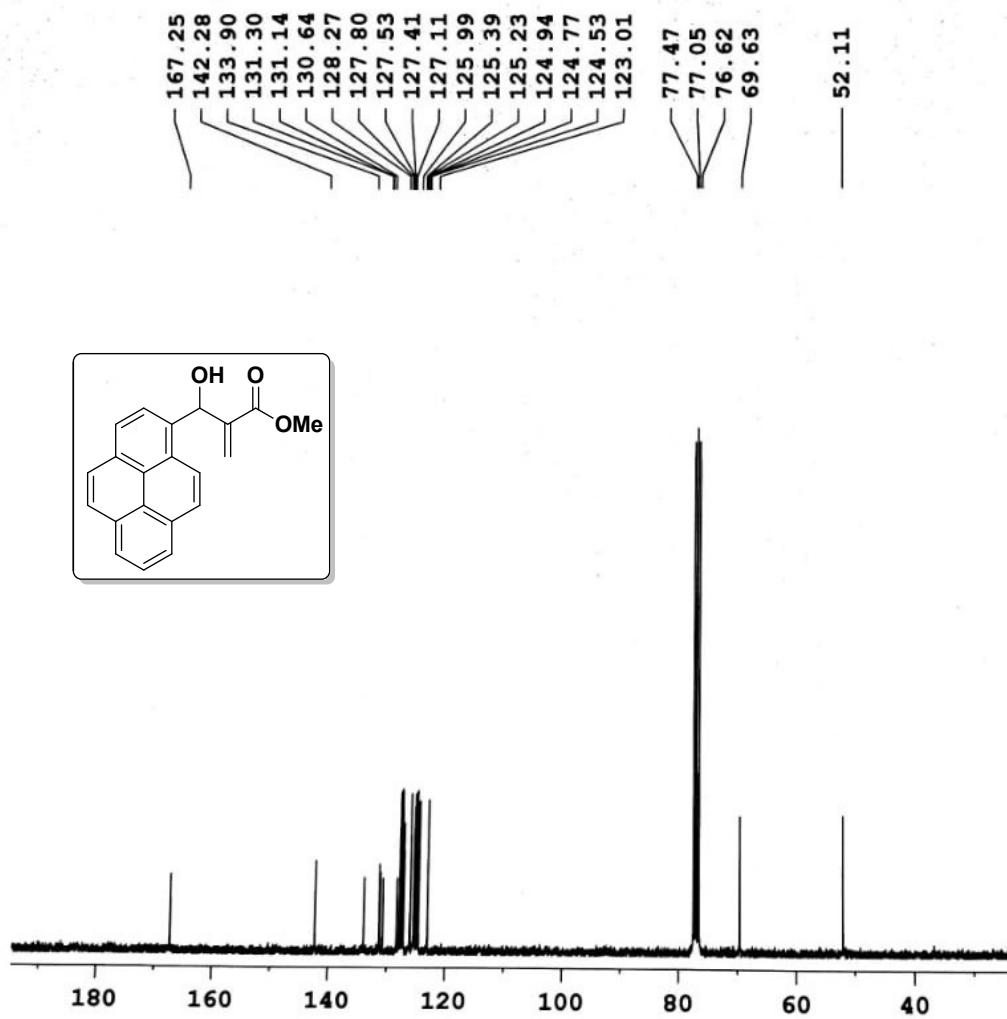
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^cDepartment of Chemistry and Biochemistry, The Ohio State University, 151 W. Woodruff Ave, Columbus, OH 43210, USA

Selected ^1H and ^{13}C NMR spectra



¹H-NMR spectrum of compound 3



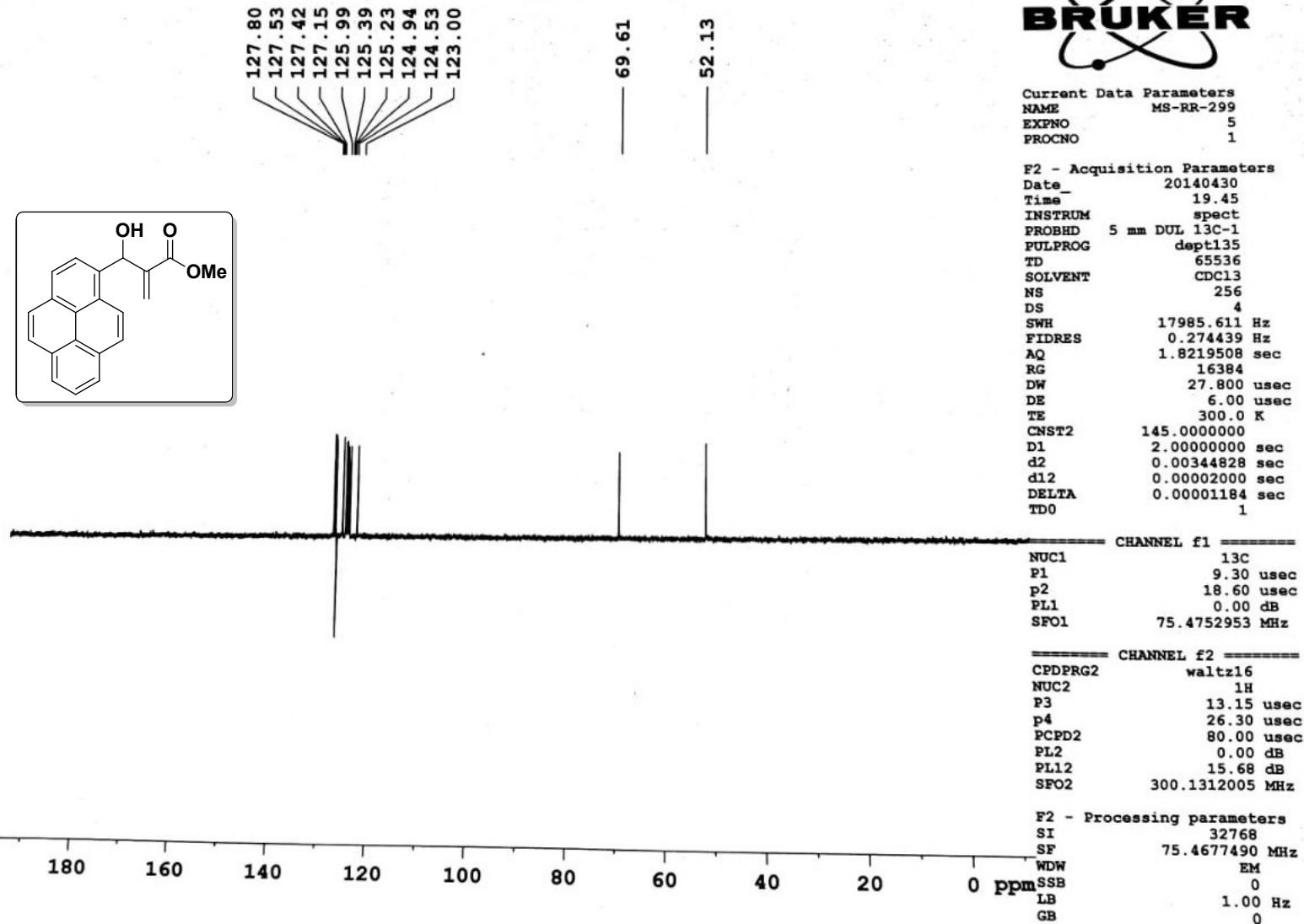
Current Data Parameters
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 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
 Date 20140430
 Time 20.21
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PROBPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 445
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 2298.8
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.03000000 sec
 DELTA 1.8999998 sec
 TDO 1

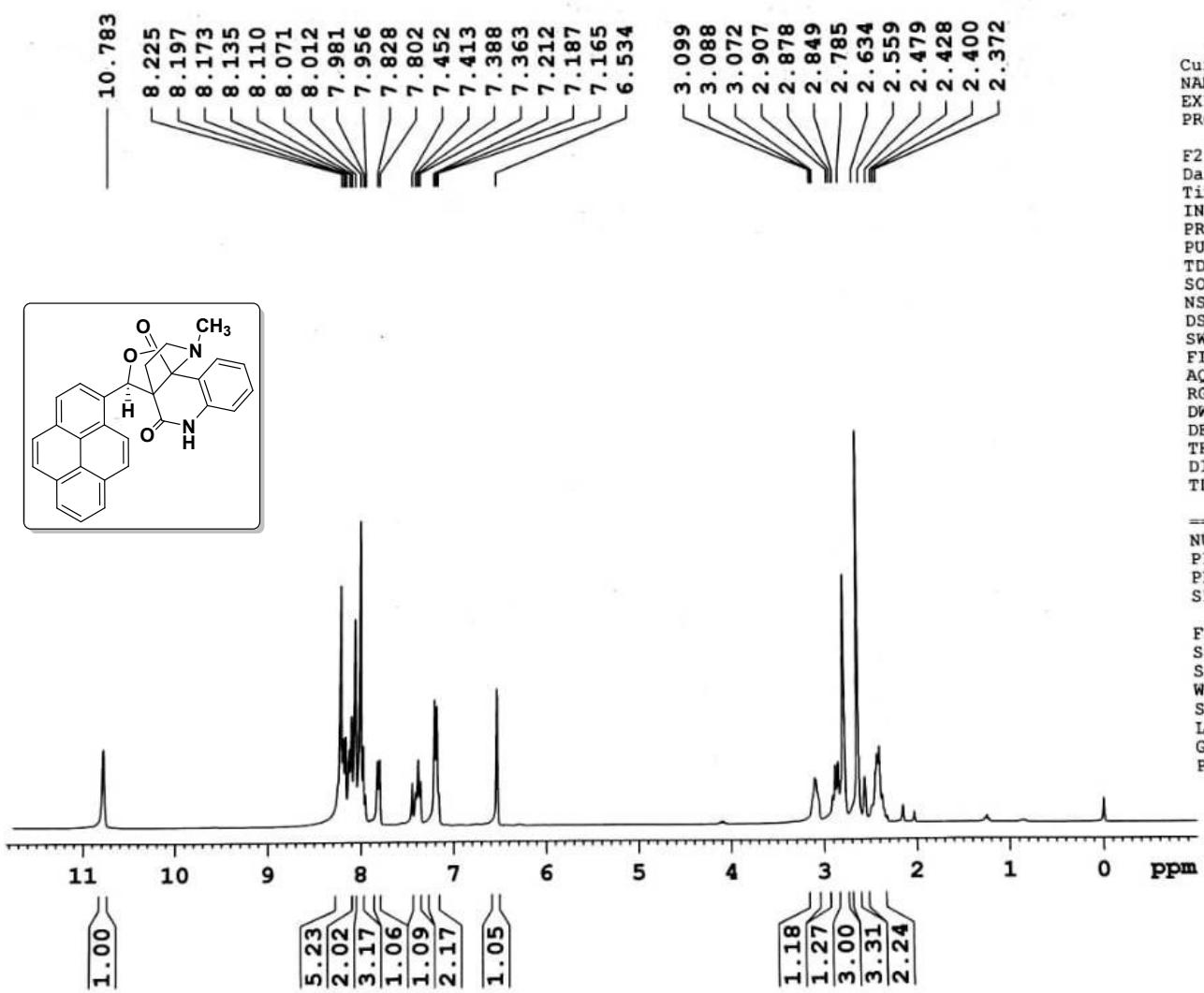
===== CHANNEL f1 =====
 NUC1 13C
 P1 9.30 usec
 PLL 0.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 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



DEPT-NMR spectrum of compound 3

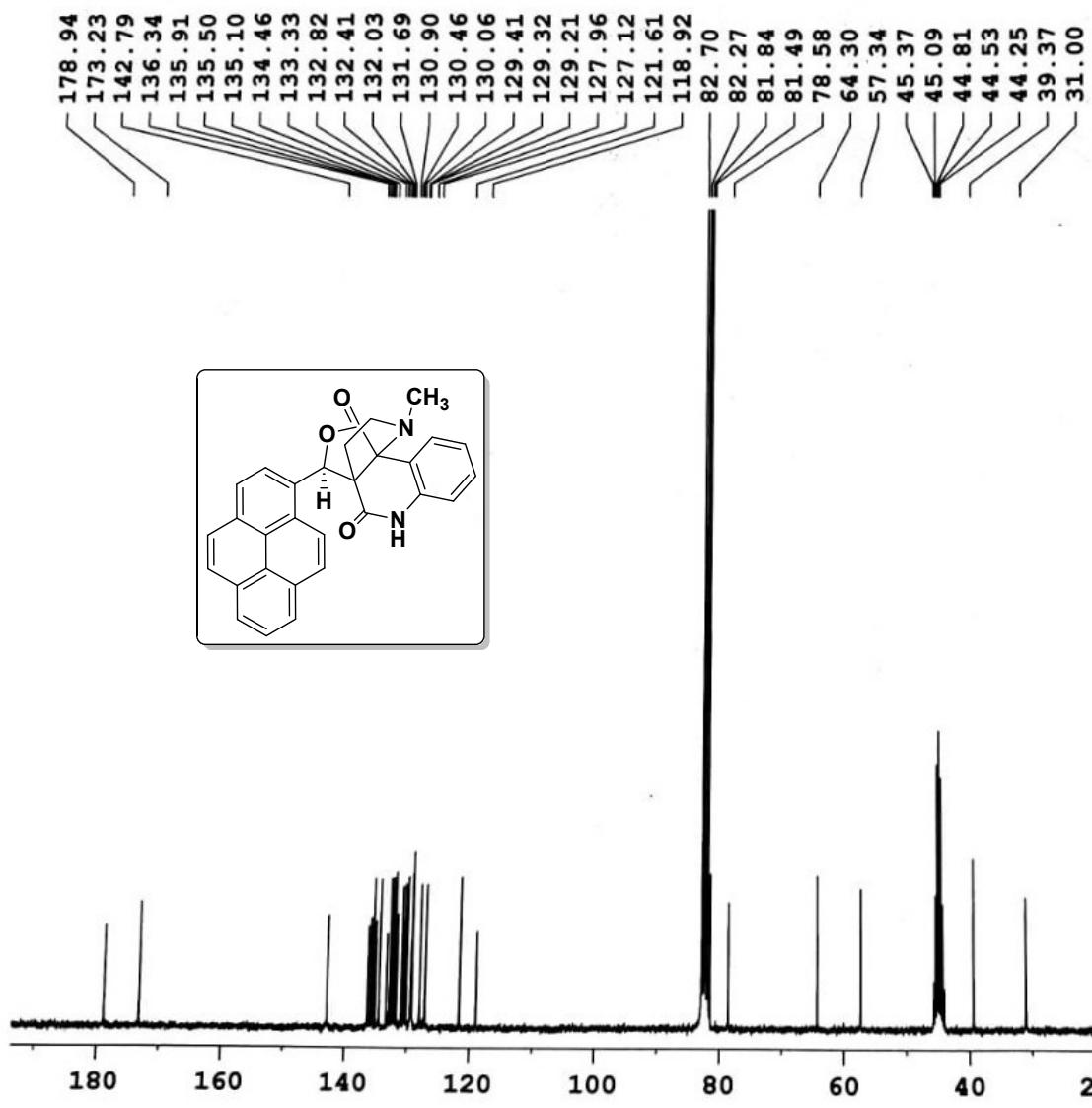


Current Data Parameters
 NAME MS-RR-300
 EXPNO 4
 PROCNO 1

F2 - Acquisition Parameters
 Date 20140418
 Time 8.33
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl₃
 NS 18
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 128
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.0000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.15 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1314113 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
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 PC 1.00



Current Data Parameters
NAME MS-RR-300
EXPNO 3
PROCNO 1

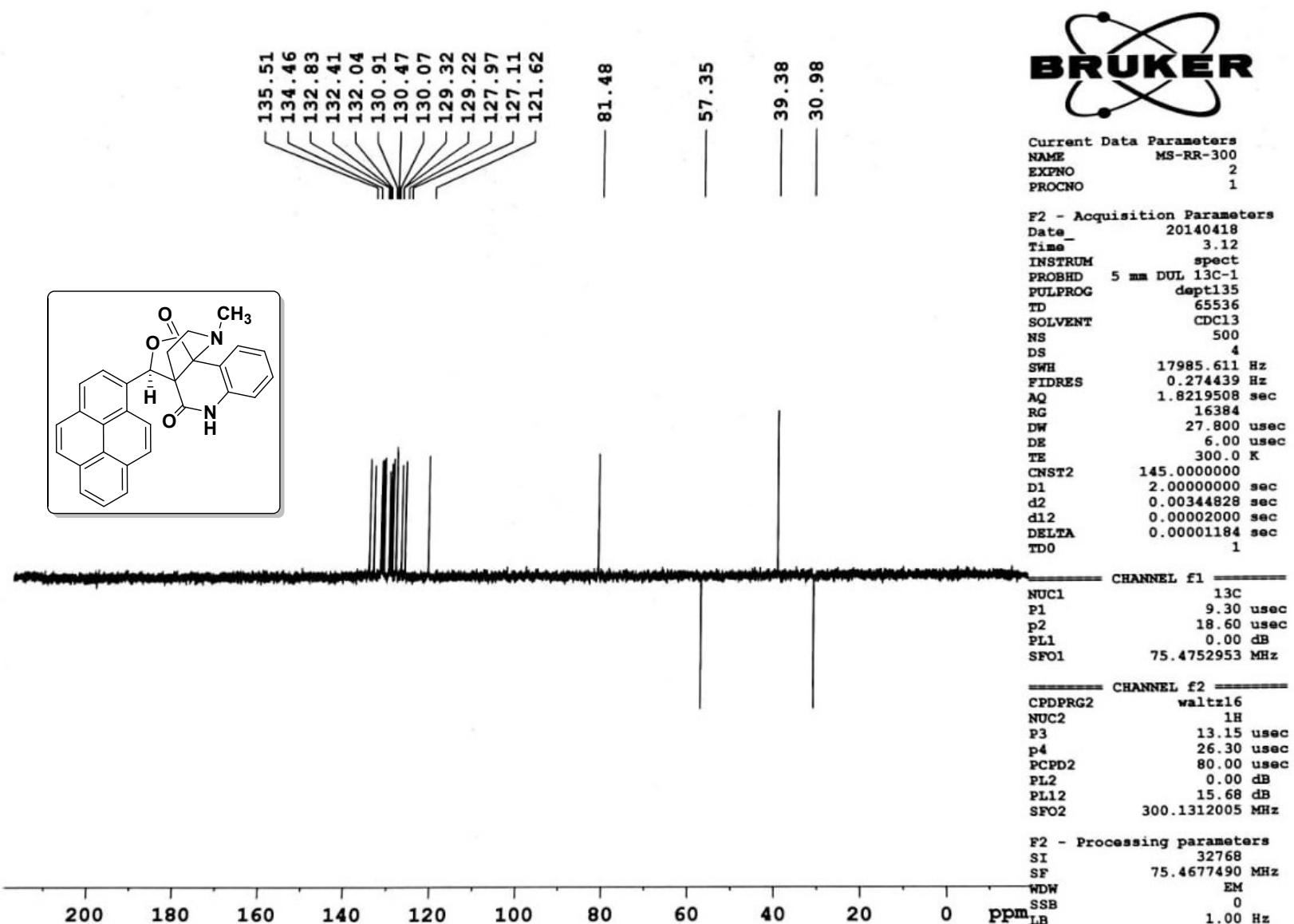
F2 - Acquisition Parameters
Date 20140418
Time 8.31
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PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 4926
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 2896.3
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999999 sec
TDO 1

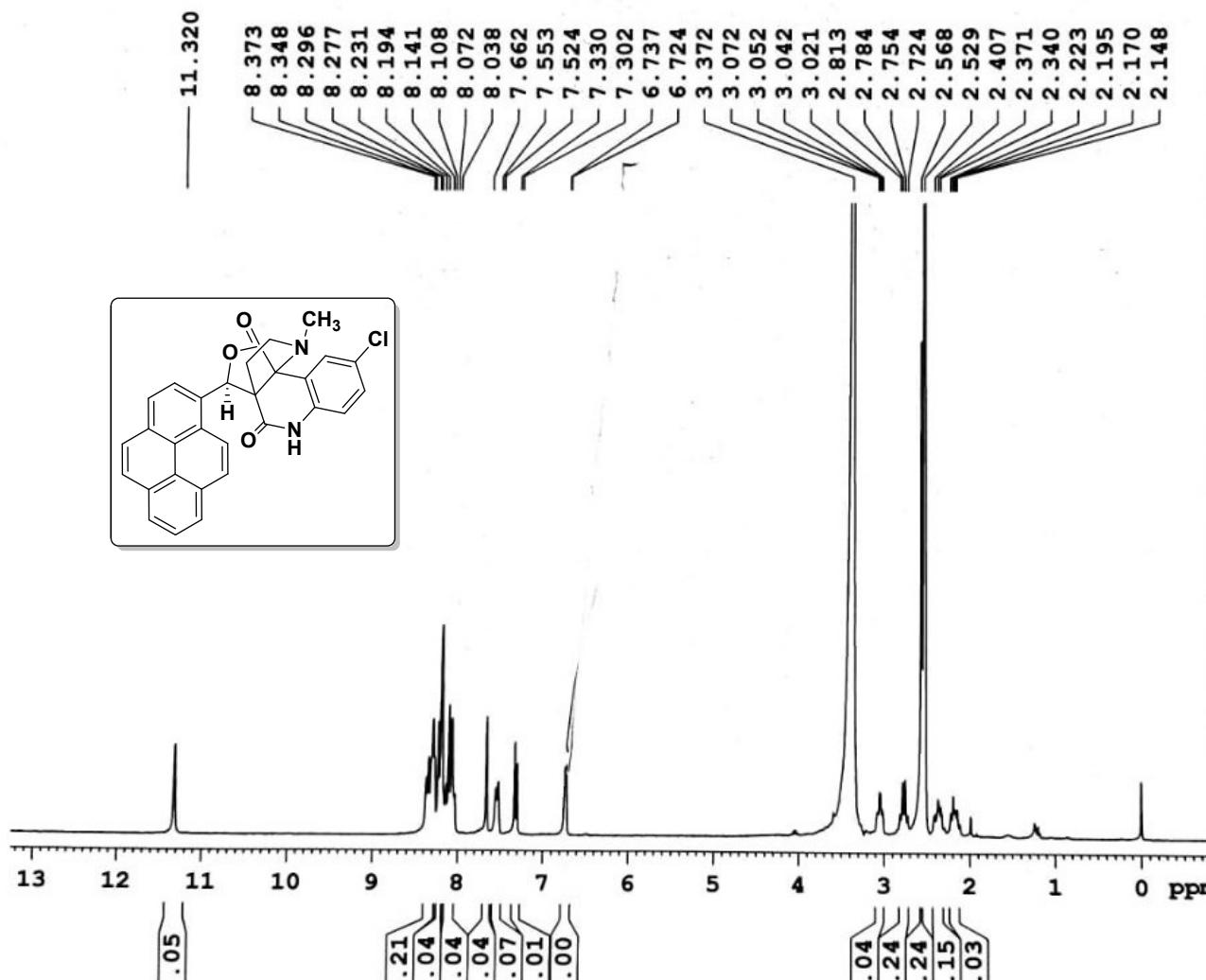
===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPDP2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
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

¹³C NMR spectrum of compound 9a



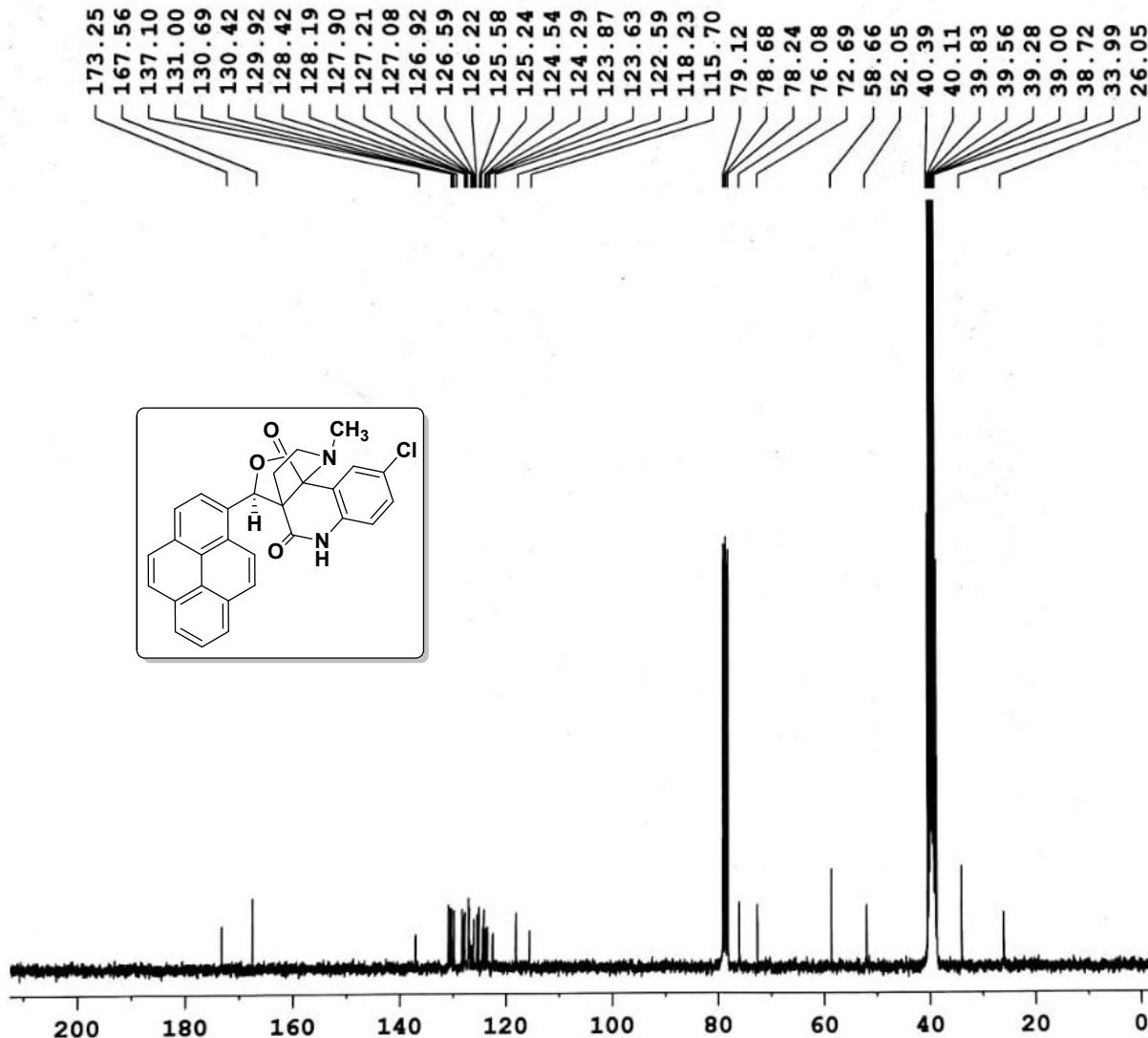


Current Data Parameters
 NAME MS-RR-308
 EXPNO 3
 PROCNO 1

F2 - Acquisition Parameters
 Date 20140411
 Time 9.45
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 128
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.0000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.15 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1299940 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



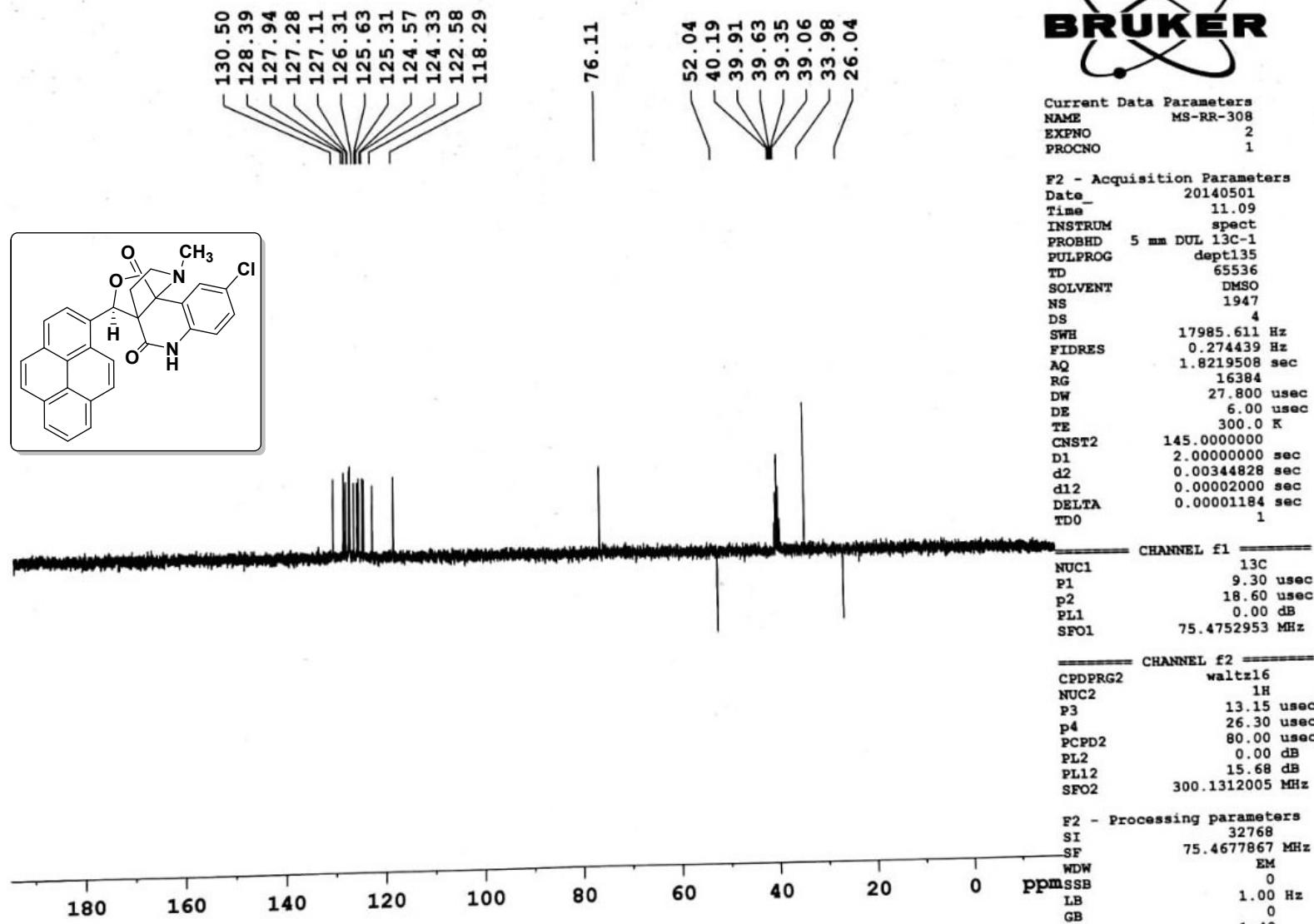
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 NAME MS-RR-308
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date 20140411
 Time 4.46
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgppg30
 TD 65536
 SOLVENT DMSO
 NS 5915
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 9195.2
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.8999998 sec
 TDO 1

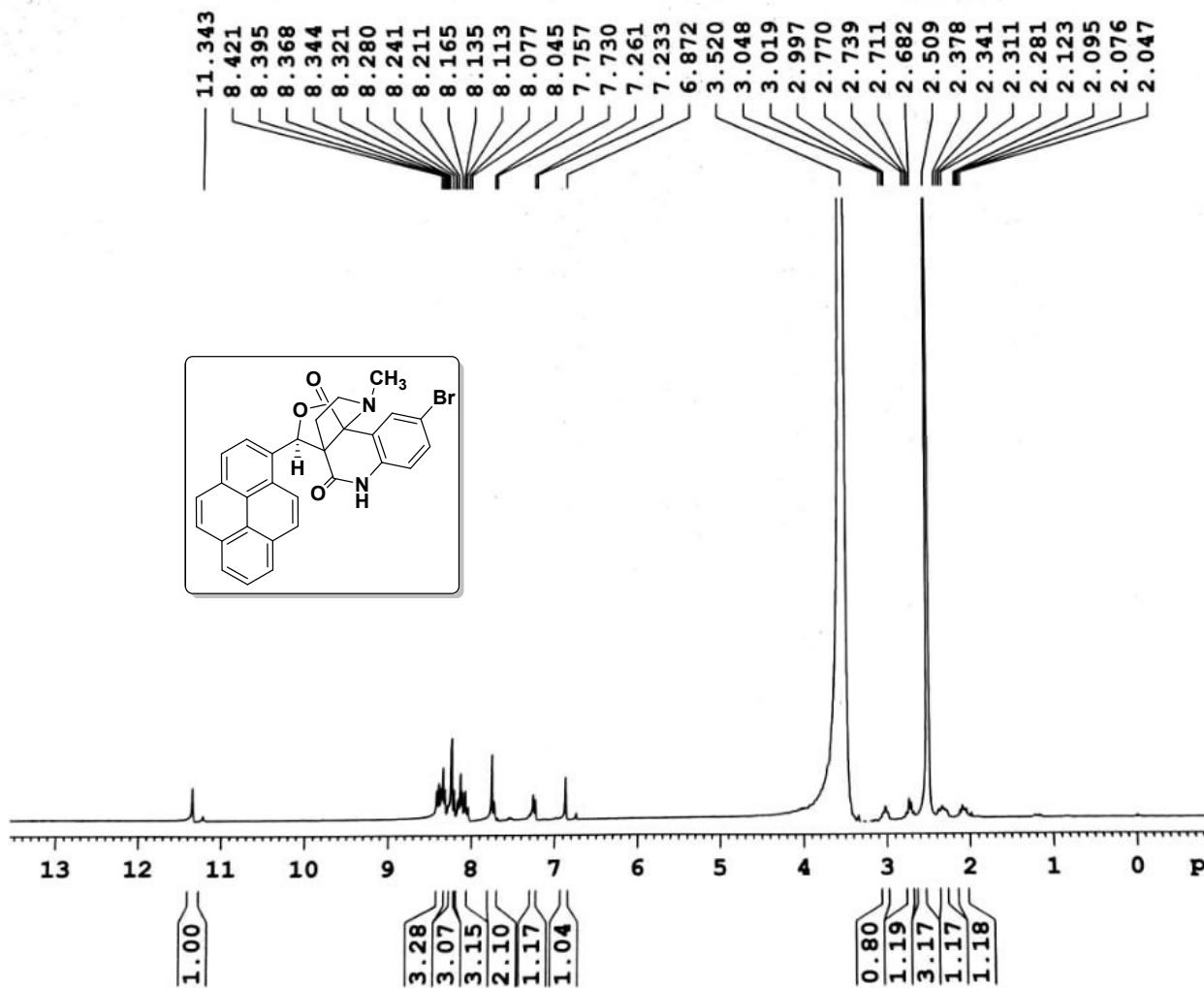
===== CHANNEL f1 =====
 NUC1 13C
 P1 9.30 usec
 PLL 0.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

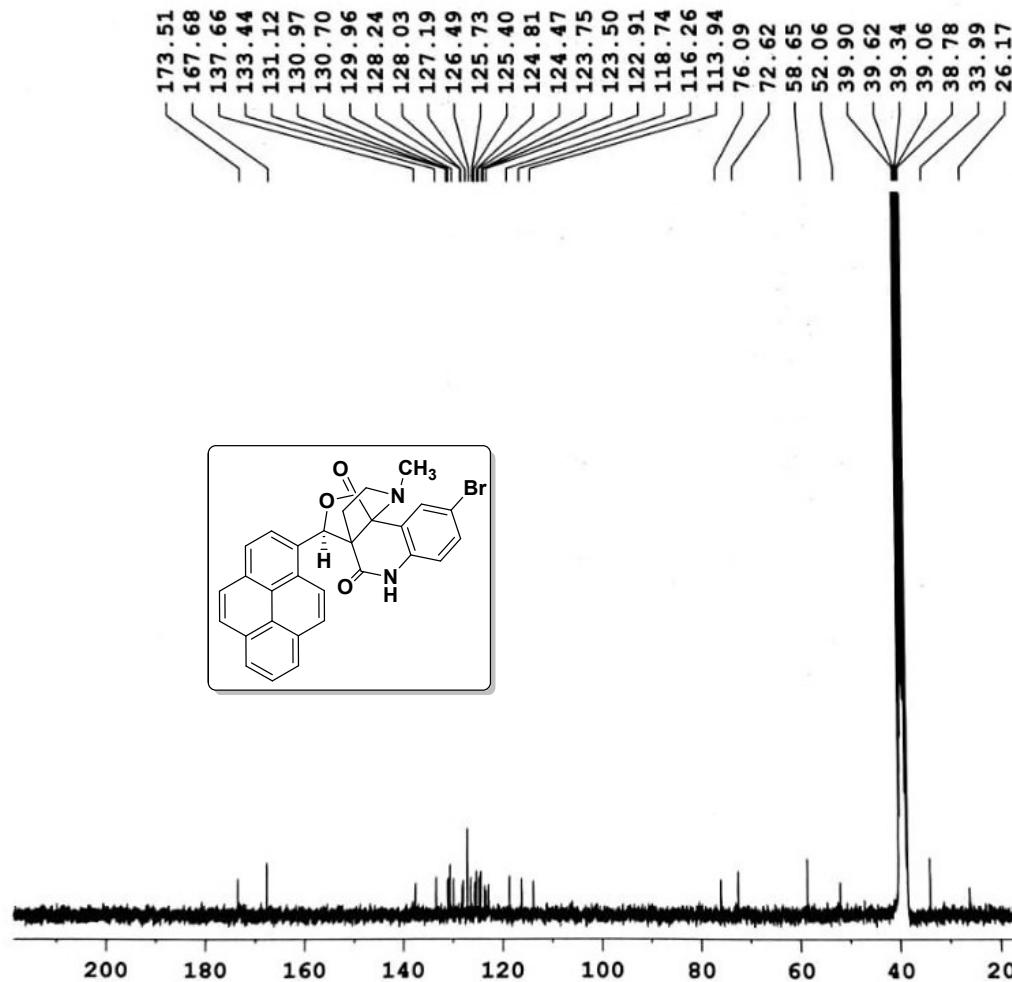
F2 - Processing parameters
 SI 32768
 SF 75.4677867 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



DEPT 135 NMR spectrum of compound **9b**



¹H NMR spectrum of compound 9c



Current Data Parameters
 NAME MS-RR-315
 EXPNO 3
 PROCNO 1

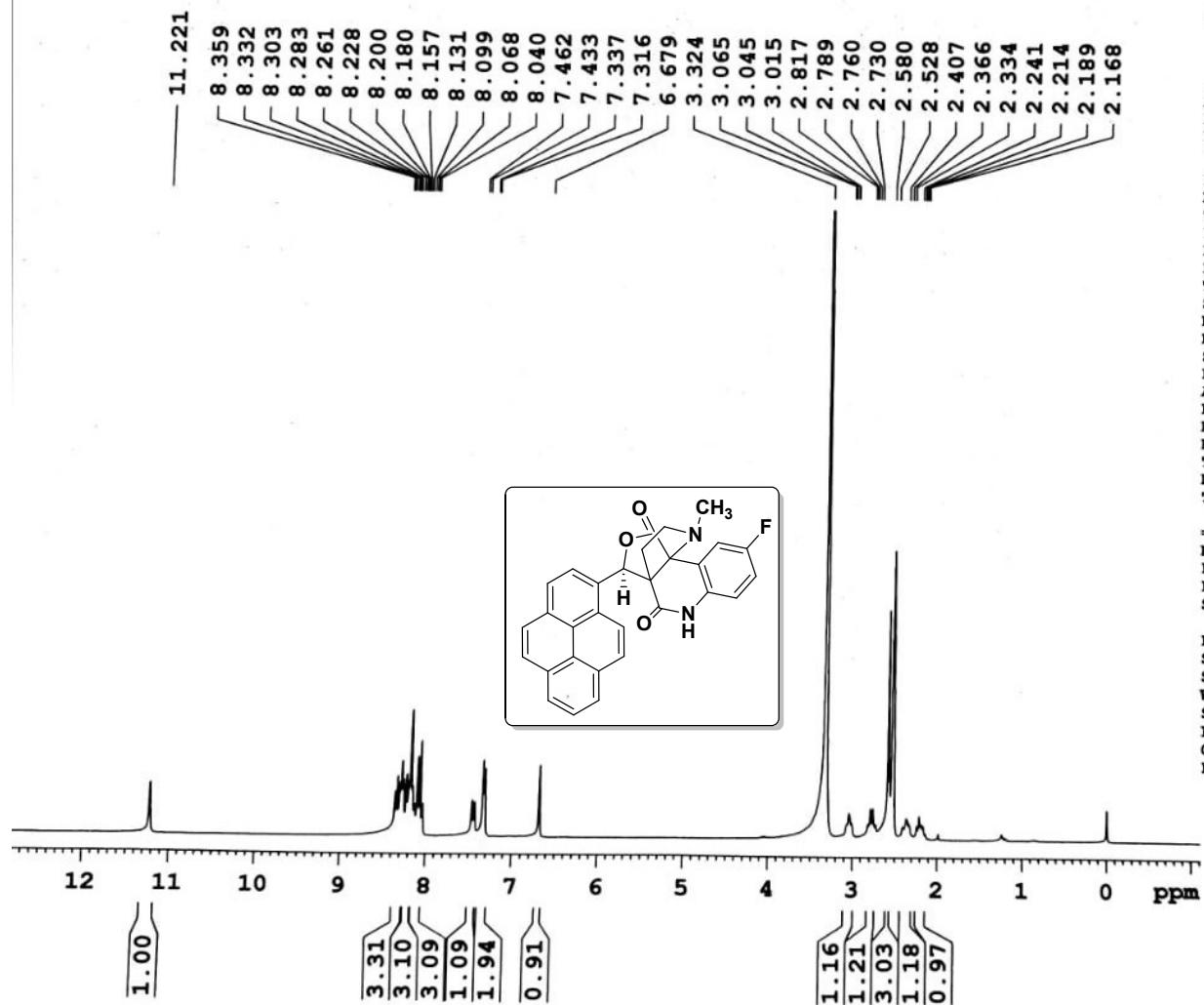
F2 - Acquisition Parameters
 Date 20140410
 Time 23.58
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 4965
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 8192
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.8999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.30 usec
 PL1 0.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPDP2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters
 SI 32768
 SF 75.4677867 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

¹³C NMR spectrum of compound 9c



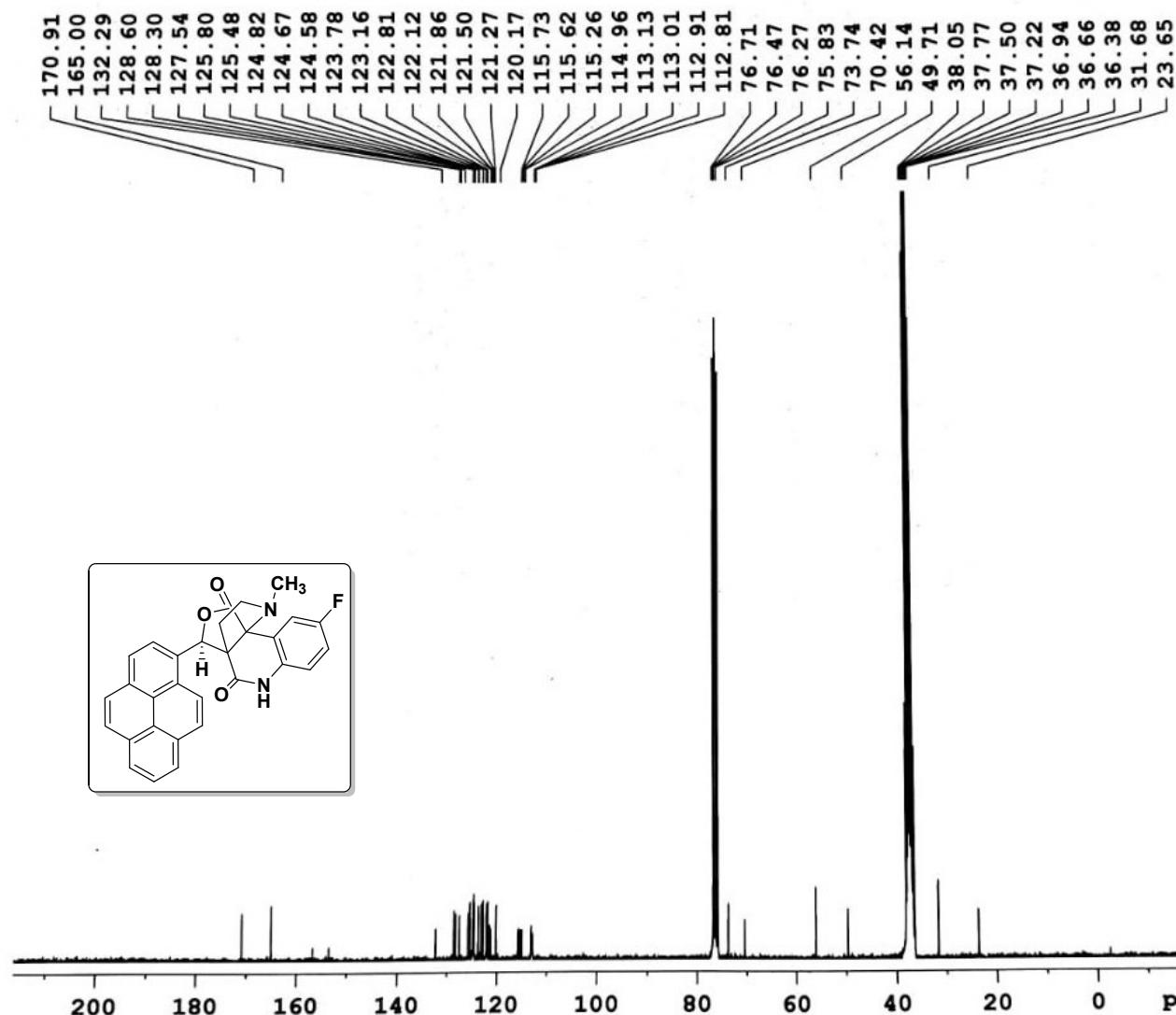
Current Data Parameters
NAME MS-RR-321
EXPNO 7
PROCNO 1

F2 - Acquisition Parameters
Date 20140502
Time 8.25
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 181
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SF01 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1299947 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H NMR spectrum of compound 9d



Current Data Parameters
NAME MS-RR-321
EXPNO 6
PROCNO 1

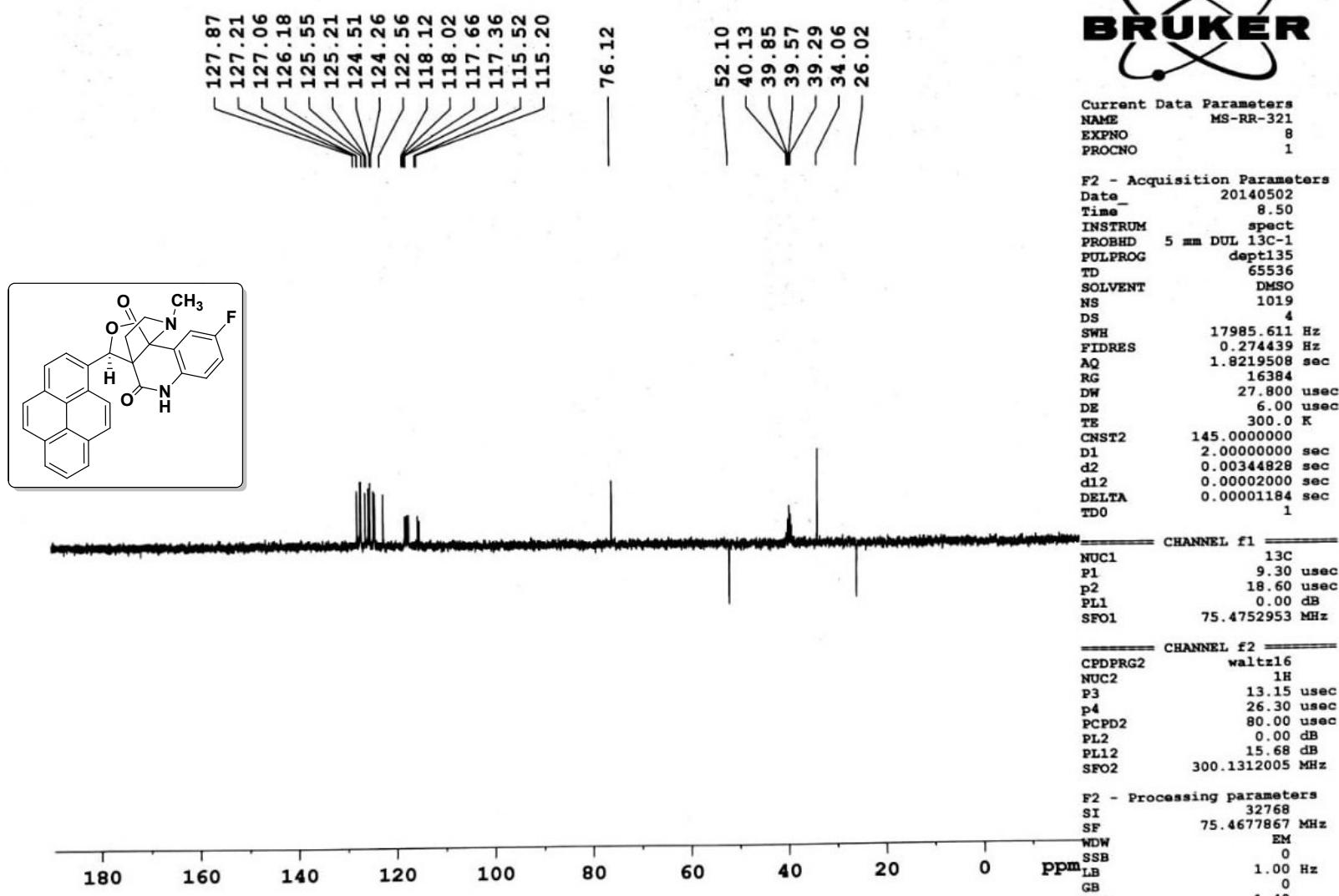
F2 - Acquisition Parameters
Date_ 20140502
Time 5.42
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 6568
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 1625.5
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.03000000 sec
DELTA 1.8999998 sec
TD0 1

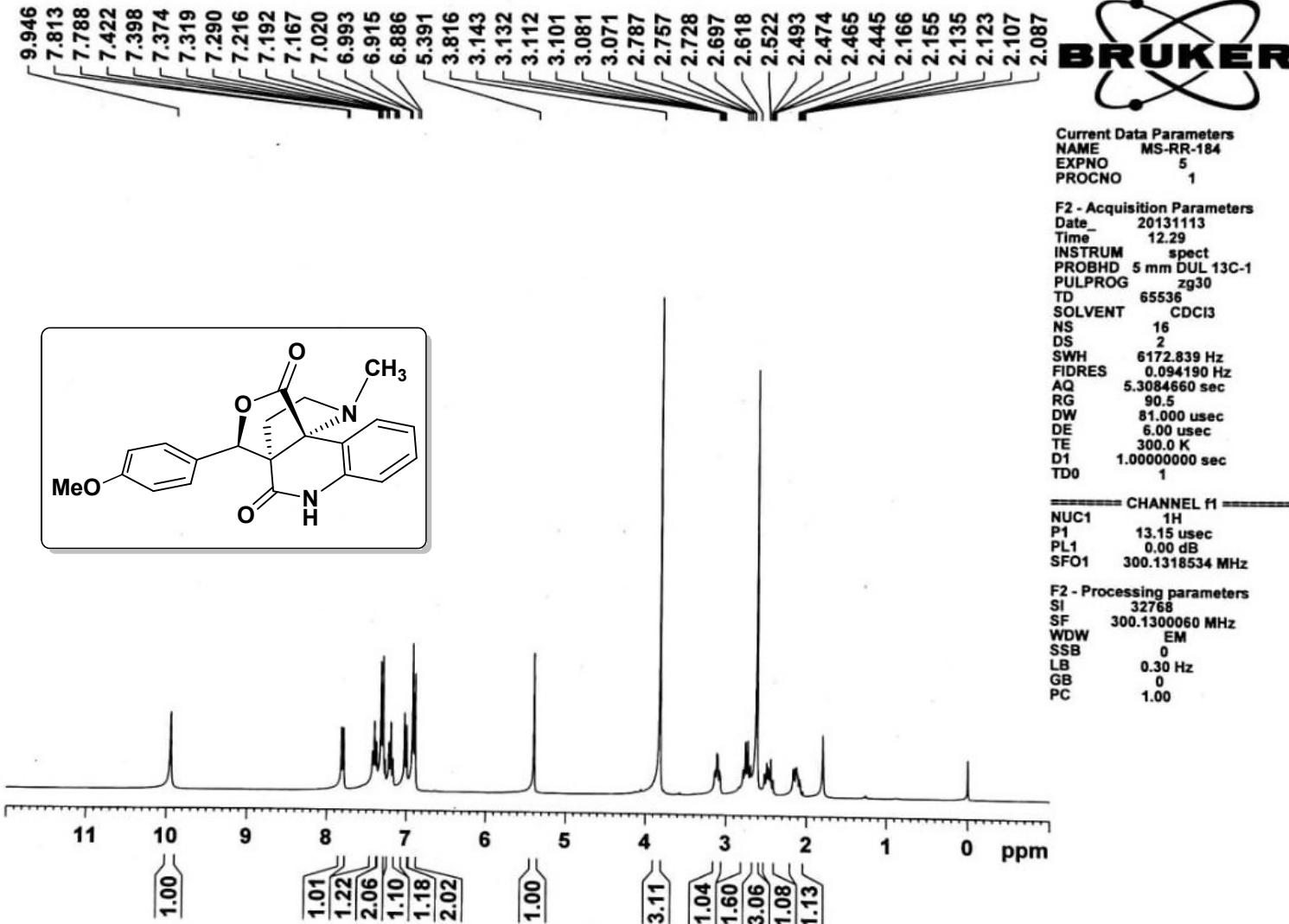
===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

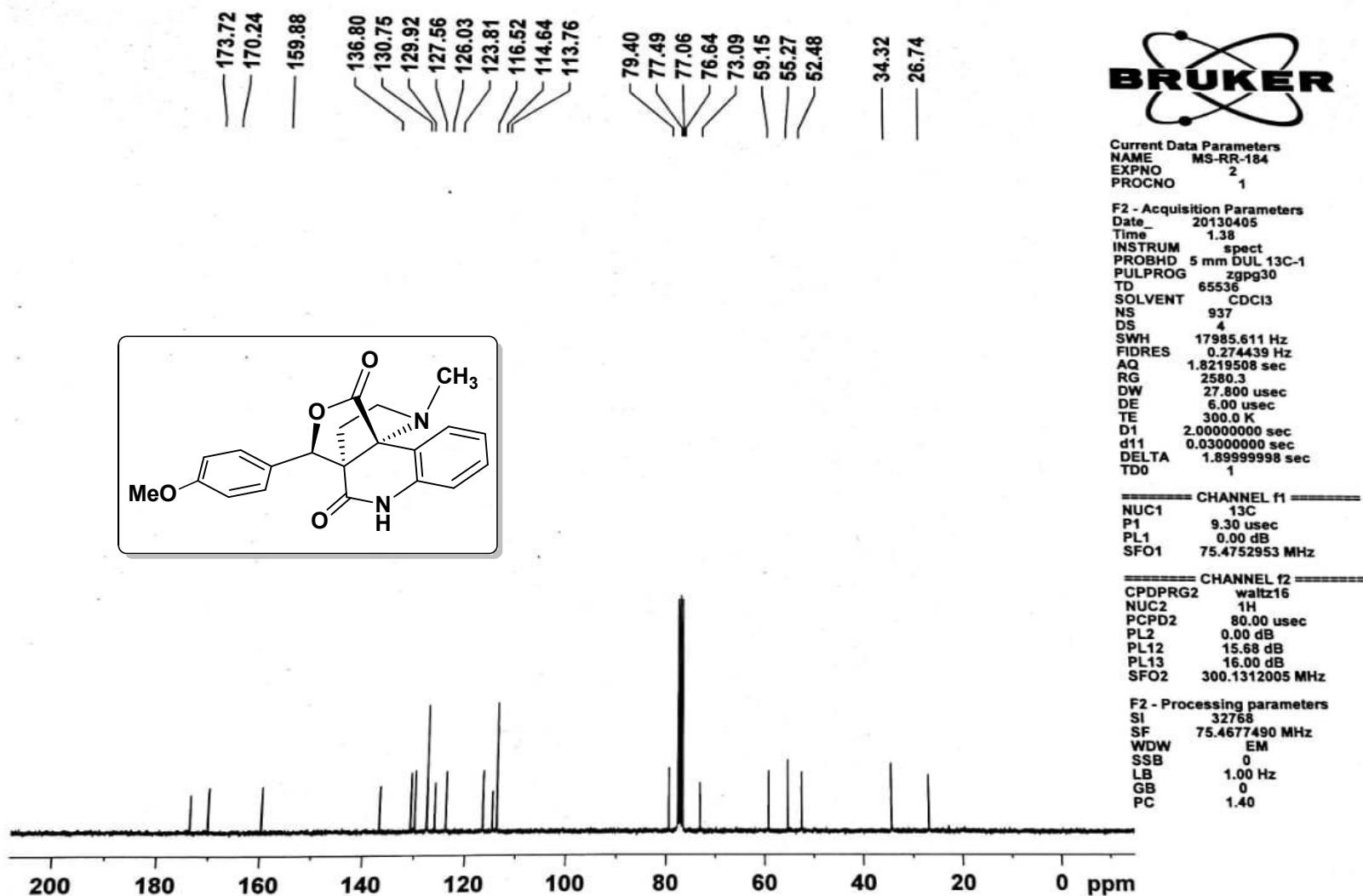
F2 - Processing parameters
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SF 75.4679671 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

¹³C NMR spectrum of compound 9d

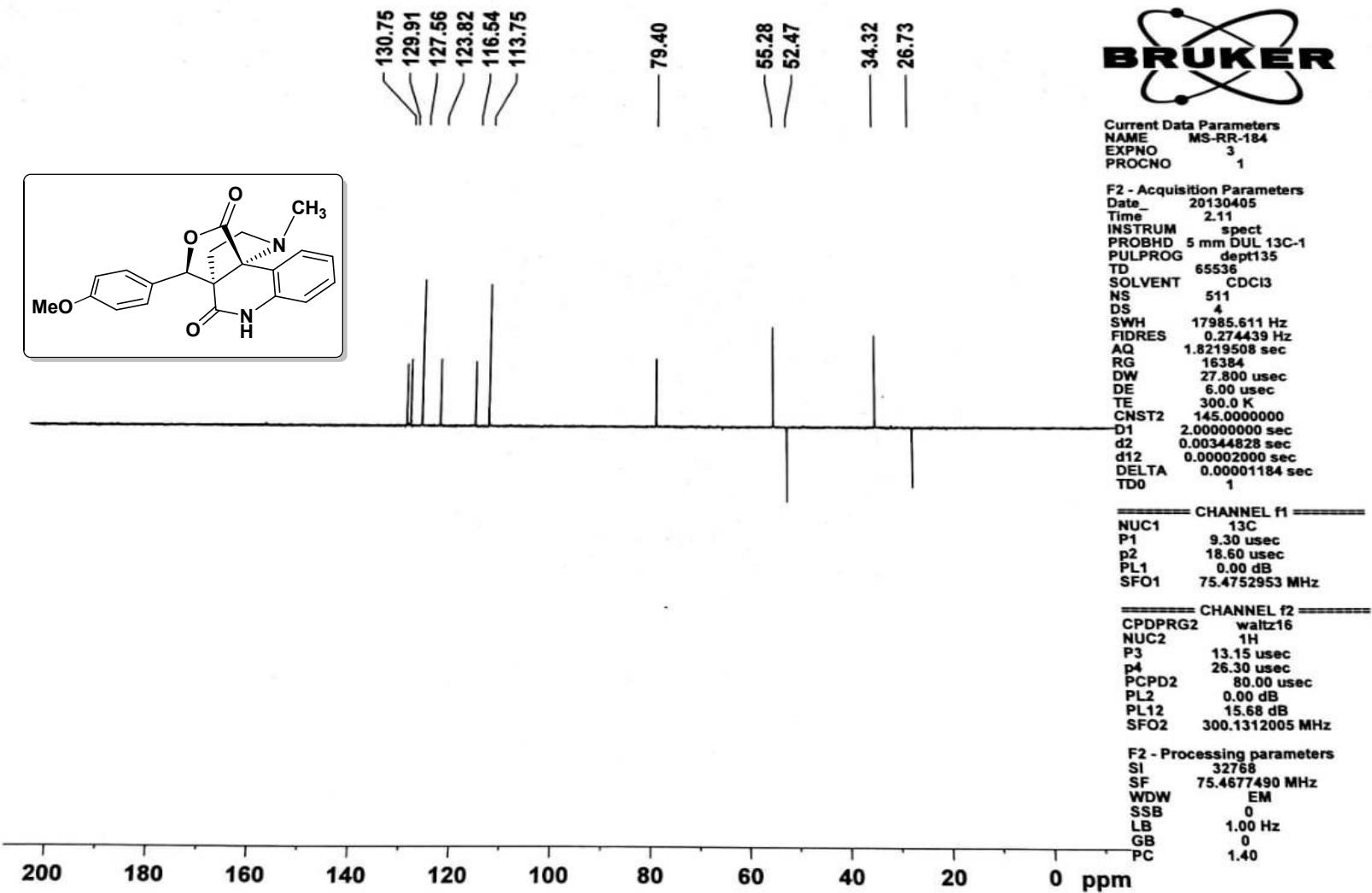




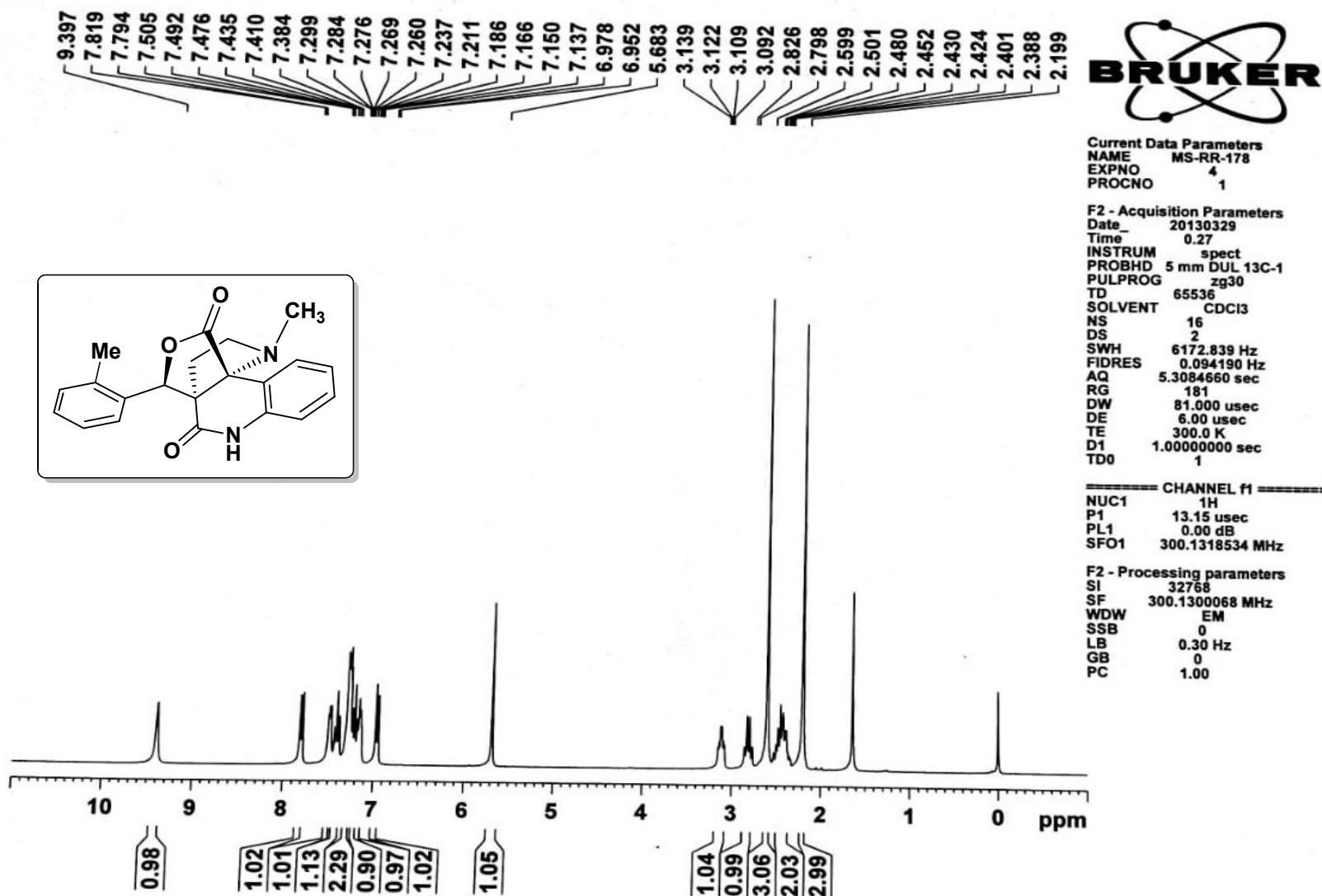
¹H-NMR spectrum of compound 10a



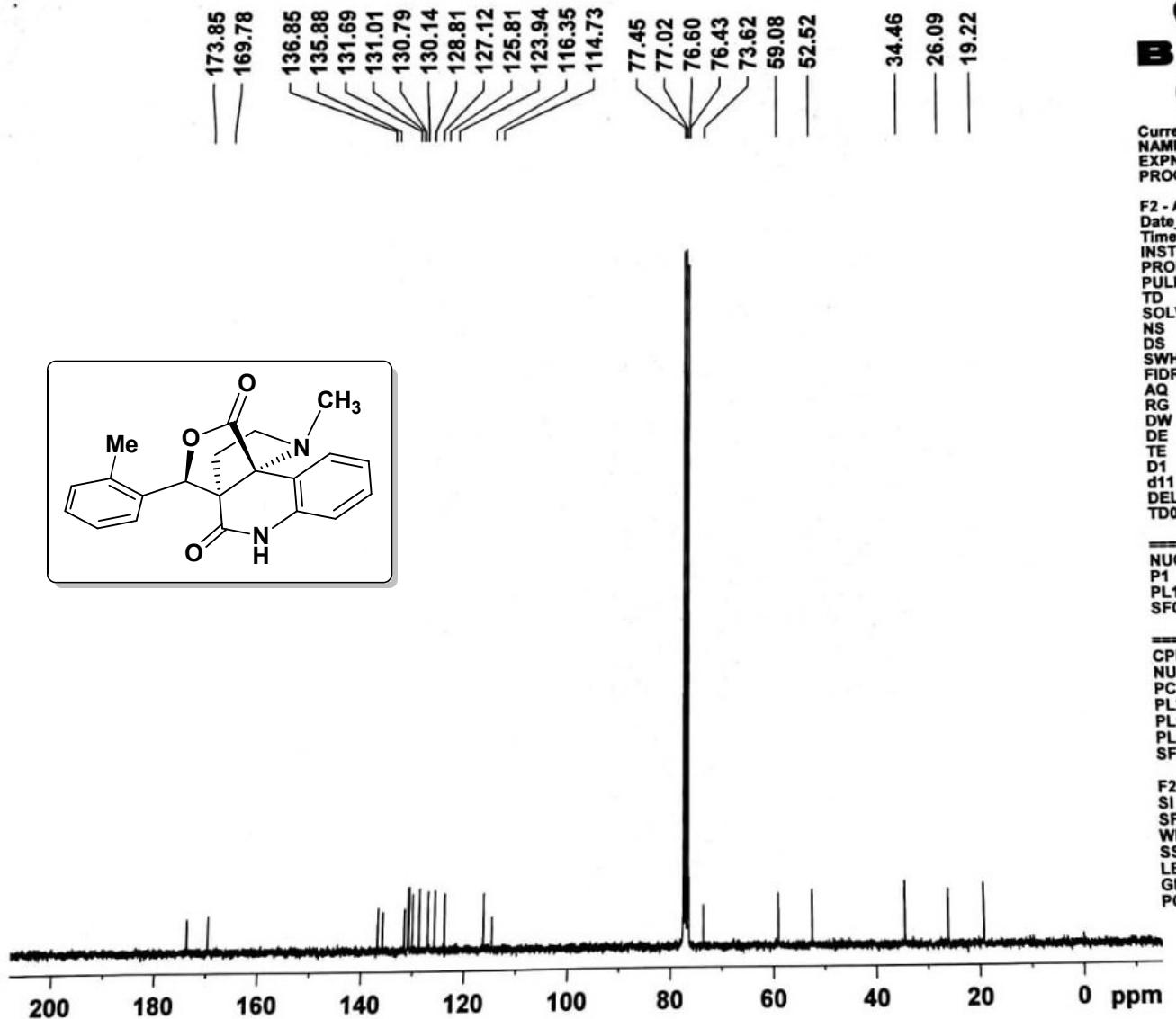
¹³C-NMR spectrum of compound 10a



DEPT 135-NMR spectrum of compound 10a



¹H NMR spectrum of compound 10b



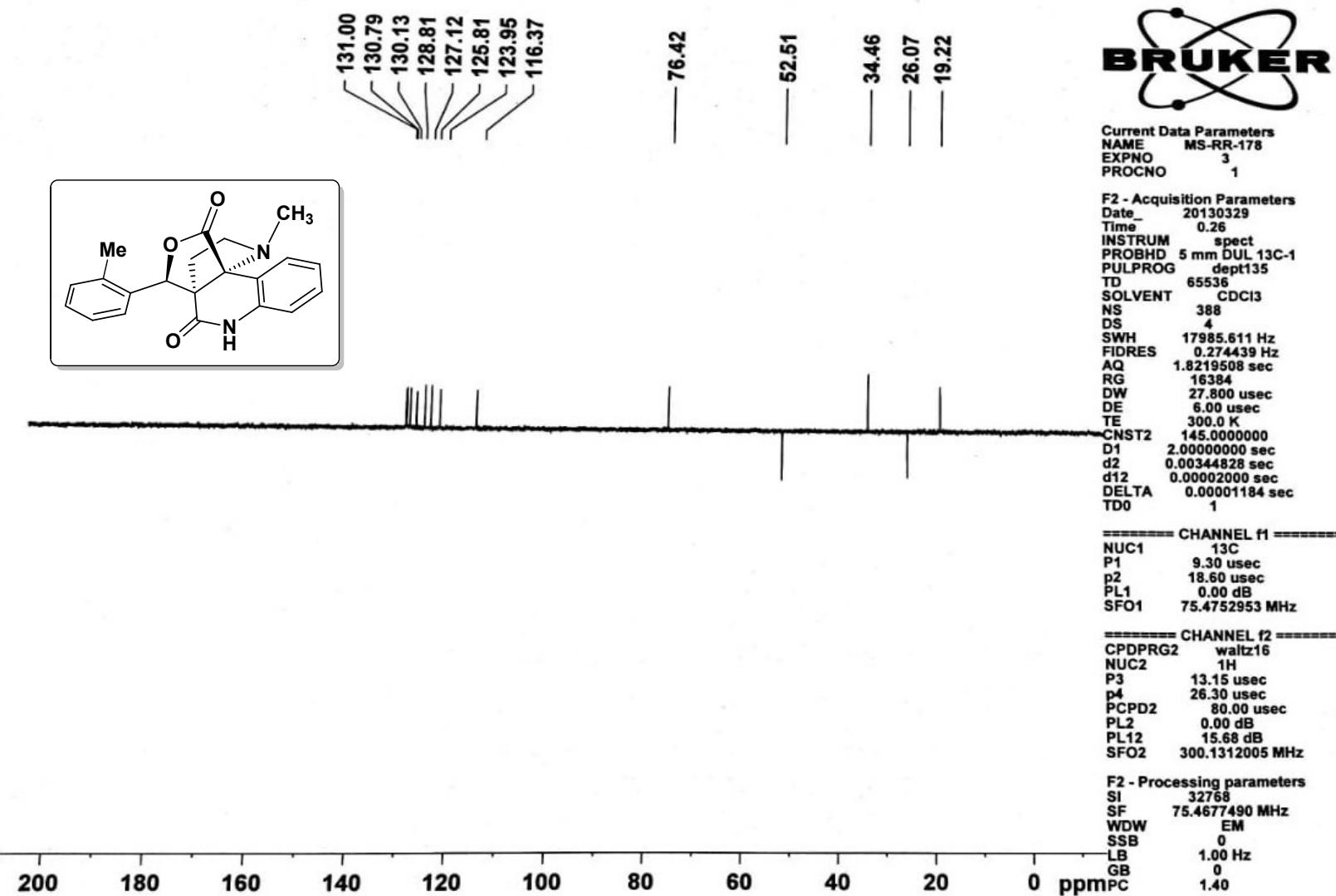
Current Data Parameters
 NAME MS-RR-178
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date 20130328
 Time 23.46
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 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 1024
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 1290.2
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.03000000 sec
 DELTA 1.8999998 sec
 TDO 1

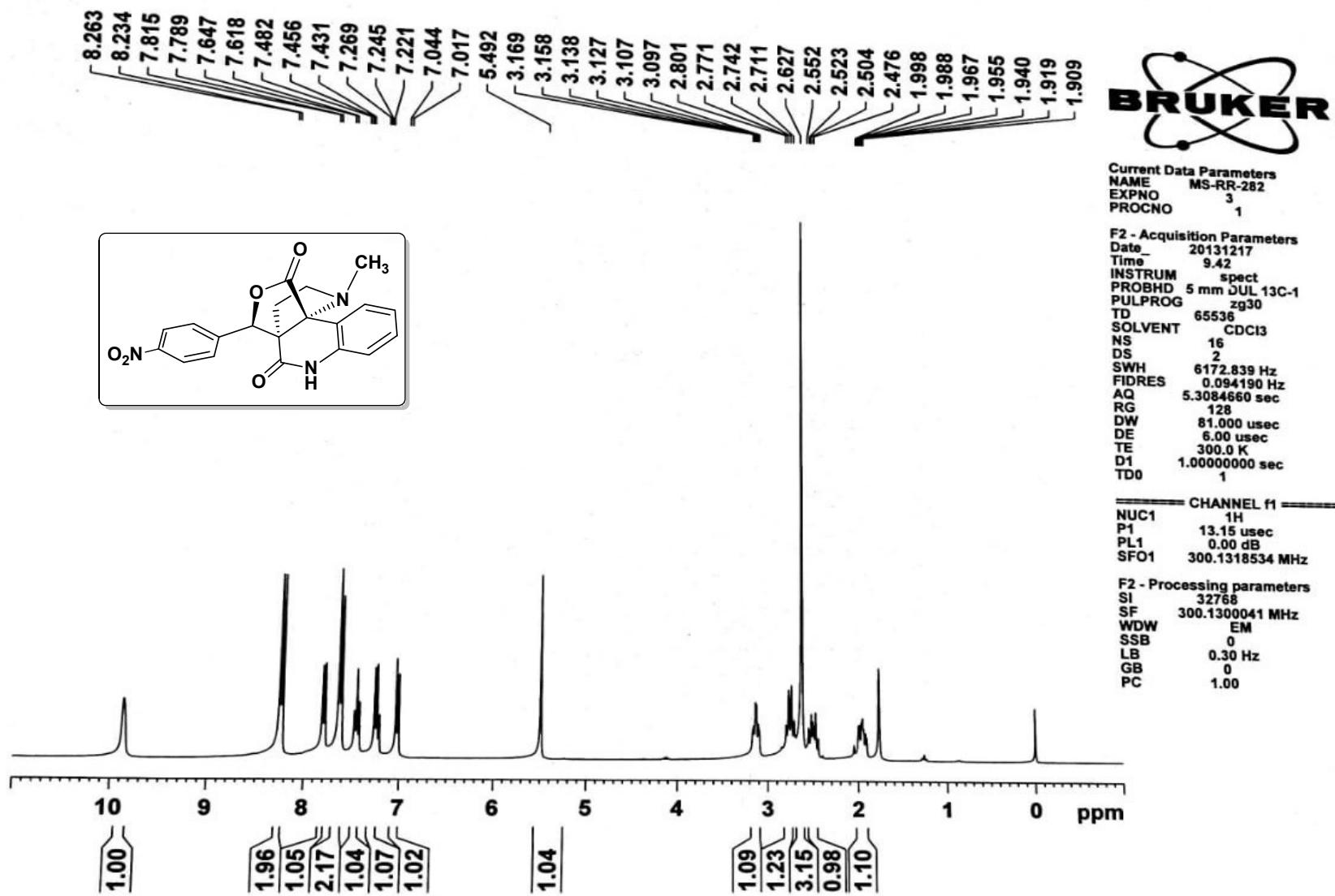
===== CHANNEL f1 =====
 NUC1 13C
 P1 9.30 usec
 PL1 0.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

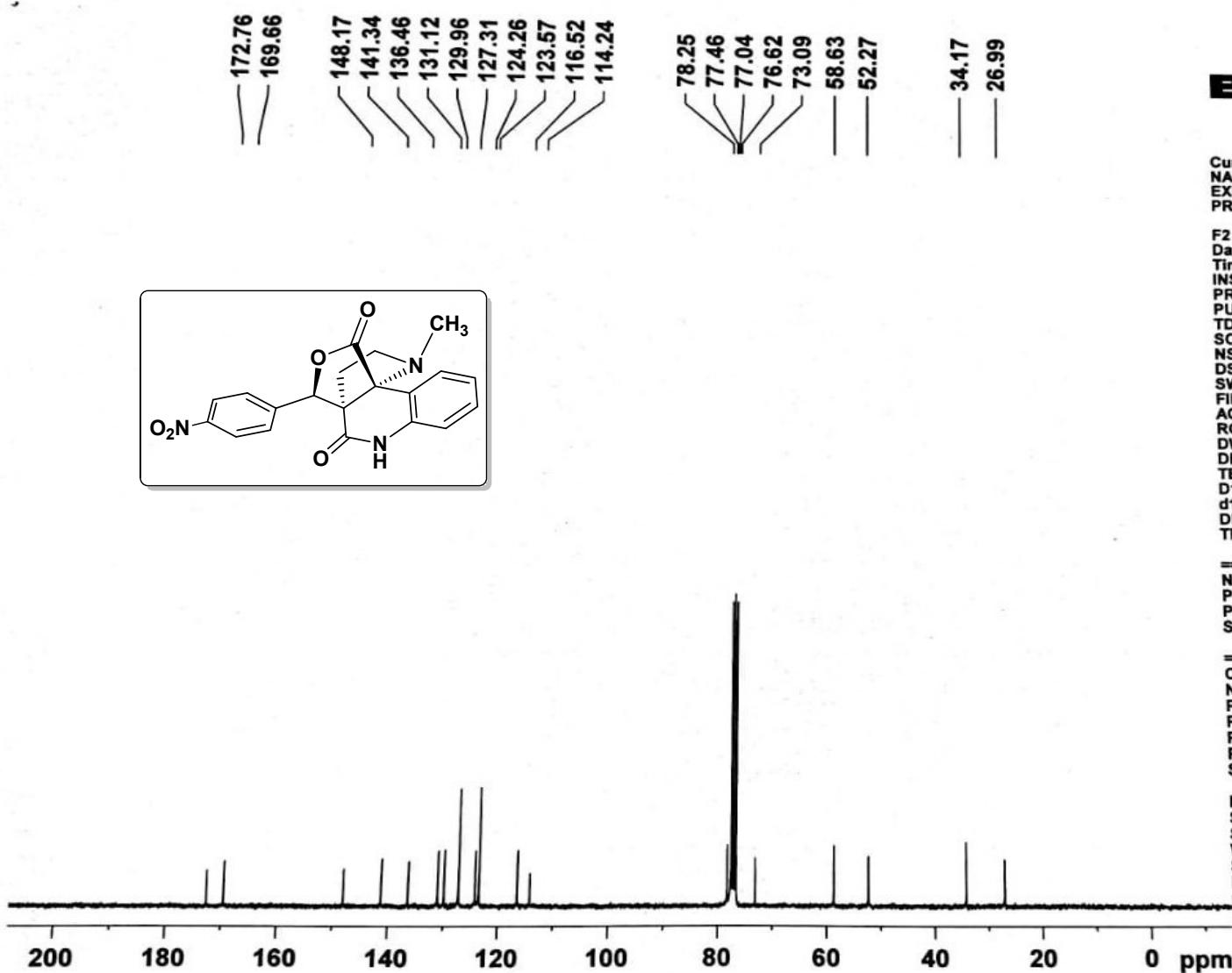
F2 - Processing parameters
 SI 32768
 SF 75.4677483 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40



DEPT 135-NMR spectrum of compound **10b**



¹H NMR spectrum of compound 10c



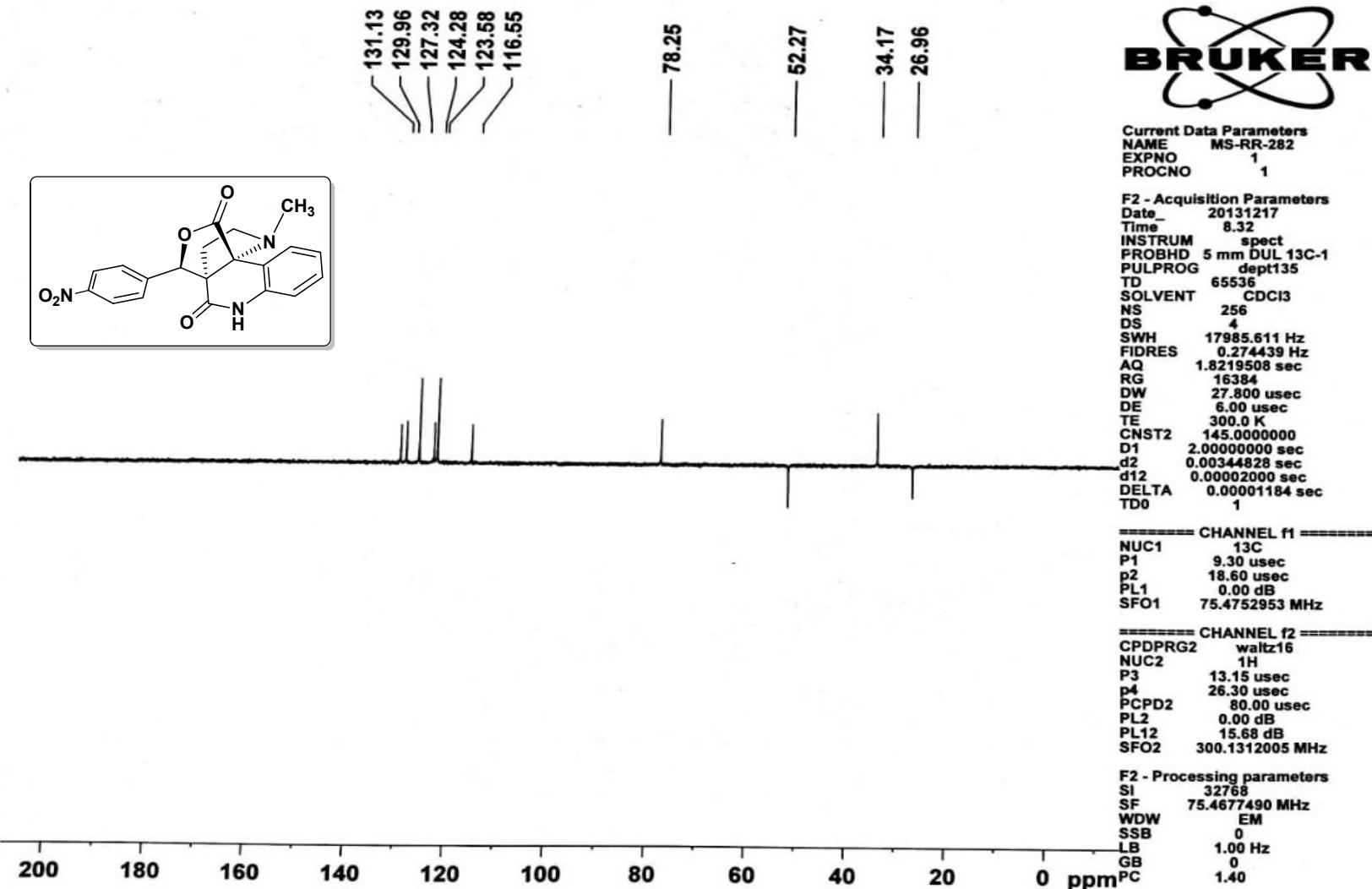
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 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date 20131217
 Time 9.40
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 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl₃
 NS 1024
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 574.7
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.03000000 sec
 DELTA 1.8999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 9.30 usec
 PL1 0.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ¹H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 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



DEPT 135-NMR Spectrum of compound **10c**

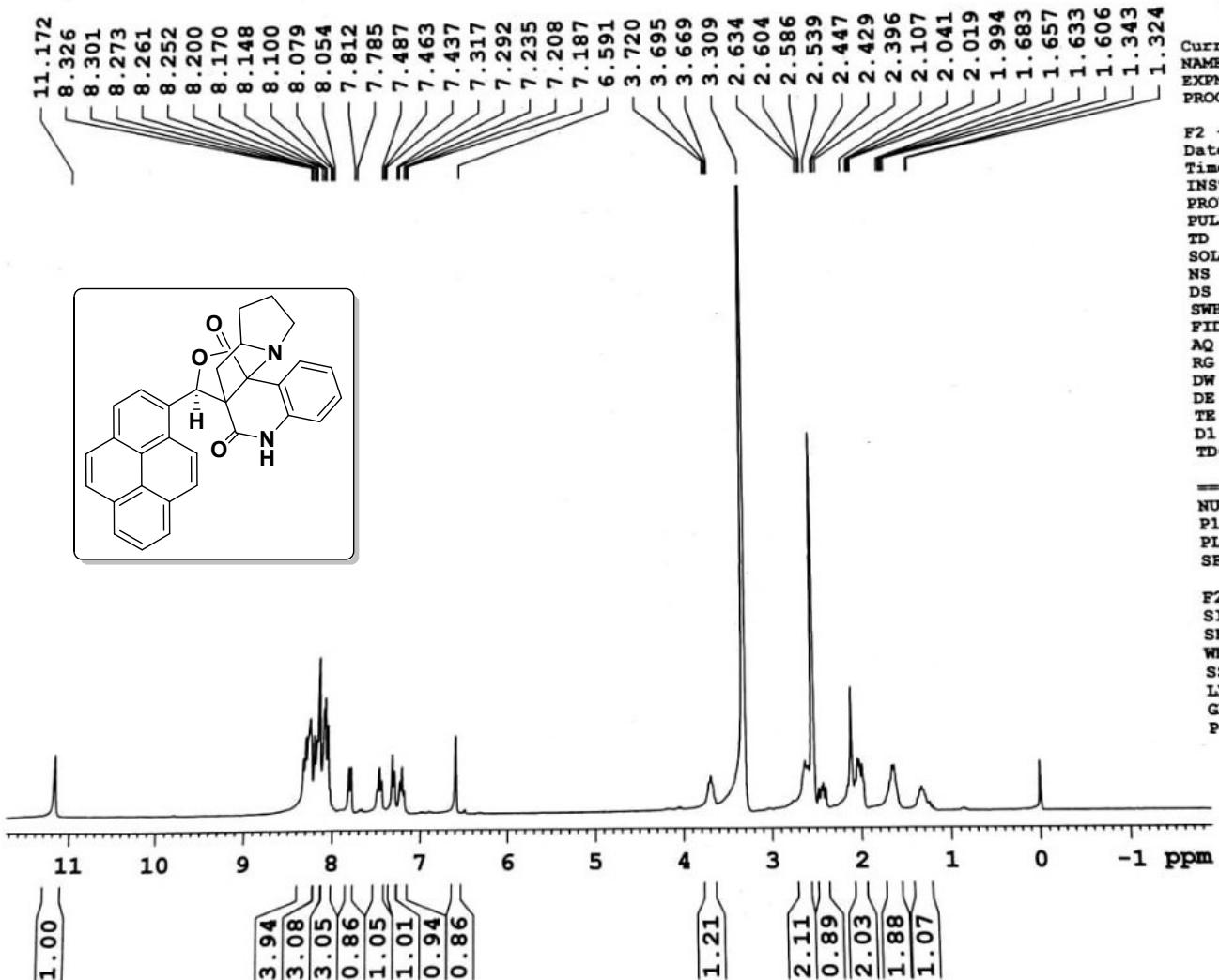


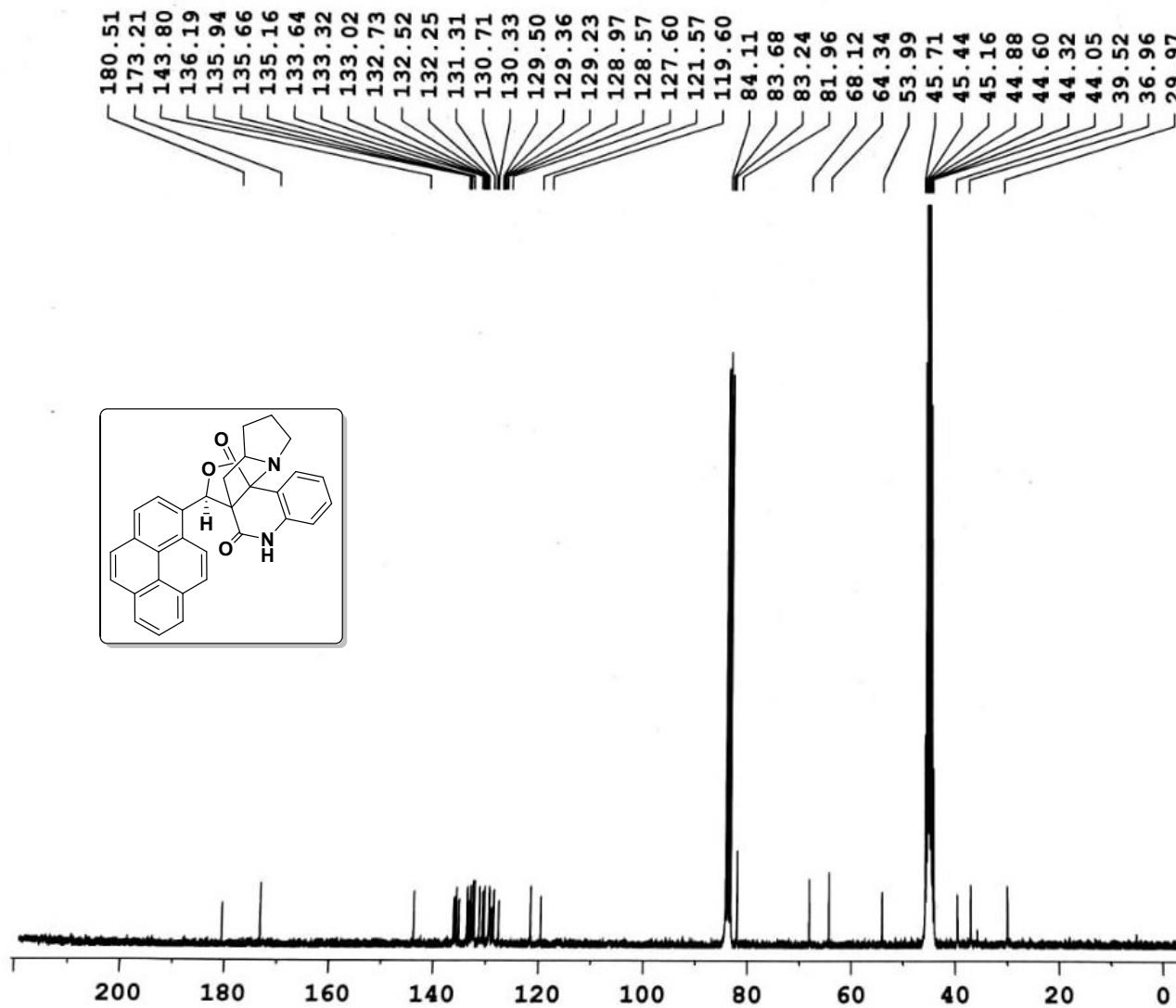
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 EXPNO 6
 PROCNO 1

F2 - Acquisition Parameters
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 Time 6.28
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 PROBHD 5 mm DUL 13C-1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 6172.839 Hz
 FIDRES 0.094190 Hz
 AQ 5.3084660 sec
 RG 203.2
 DW 81.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 1.0000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 13.15 usec
 PL1 0.00 dB
 SFO1 300.1318534 MHz

F2 - Processing parameters
 SI 32768
 SF 300.1314174 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00





Current Data Parameters

NAME MS-RR-324
 EXPNO 5
 PROCNO 1

F2 - Acquisition Parameters

Date 20140425
 Time 0.18
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgppg30
 TD 65536
 SOLVENT CDC13
 NS 5704
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 574.7
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.03000000 sec
 DELTA 1.8999998 sec
 TDO 1

===== CHANNEL f1 =====

NUC1 13C
 P1 9.30 usec
 PL1 0.00 dB
 SFO1 75.4752953 MHz

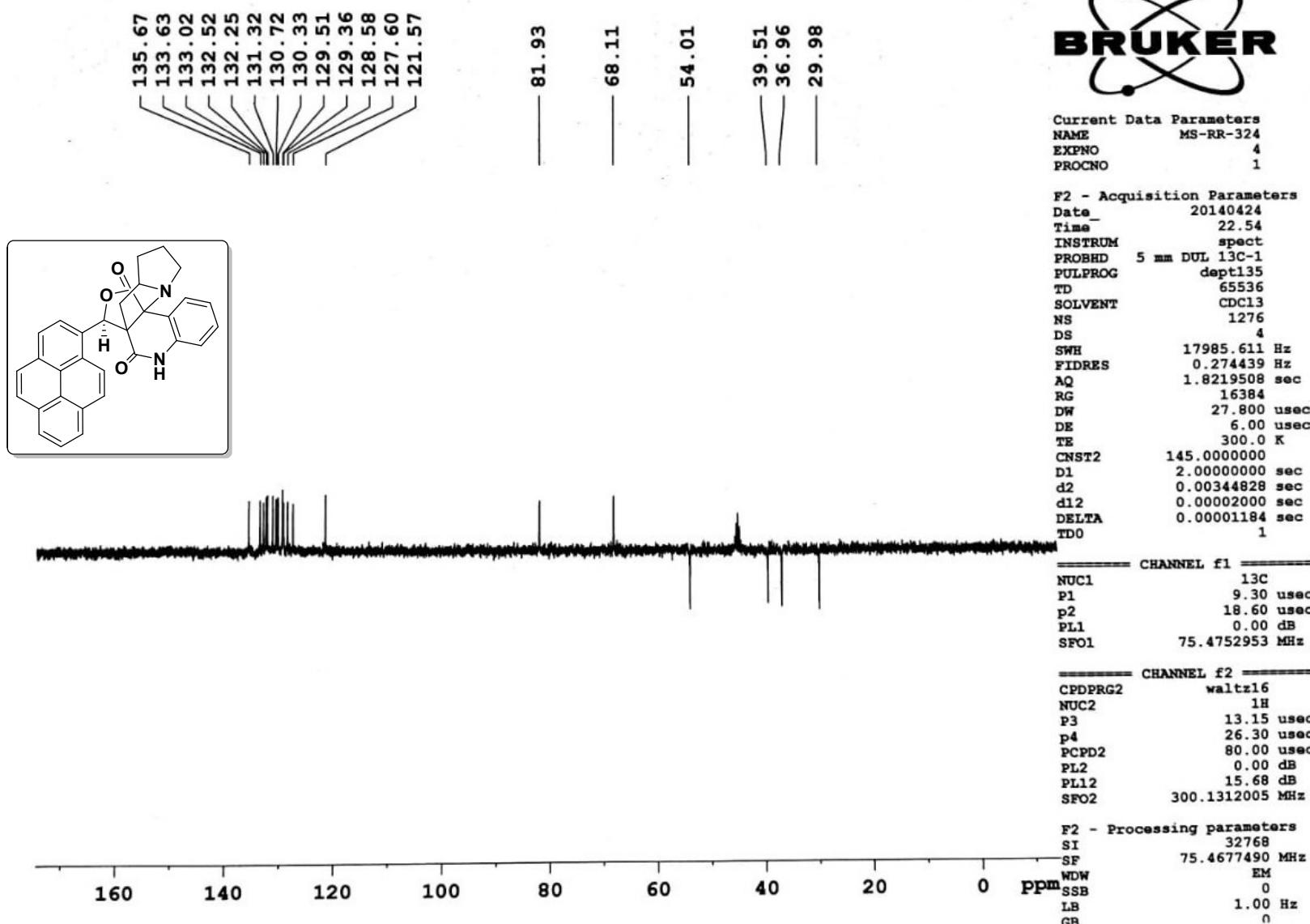
===== CHANNEL f2 =====

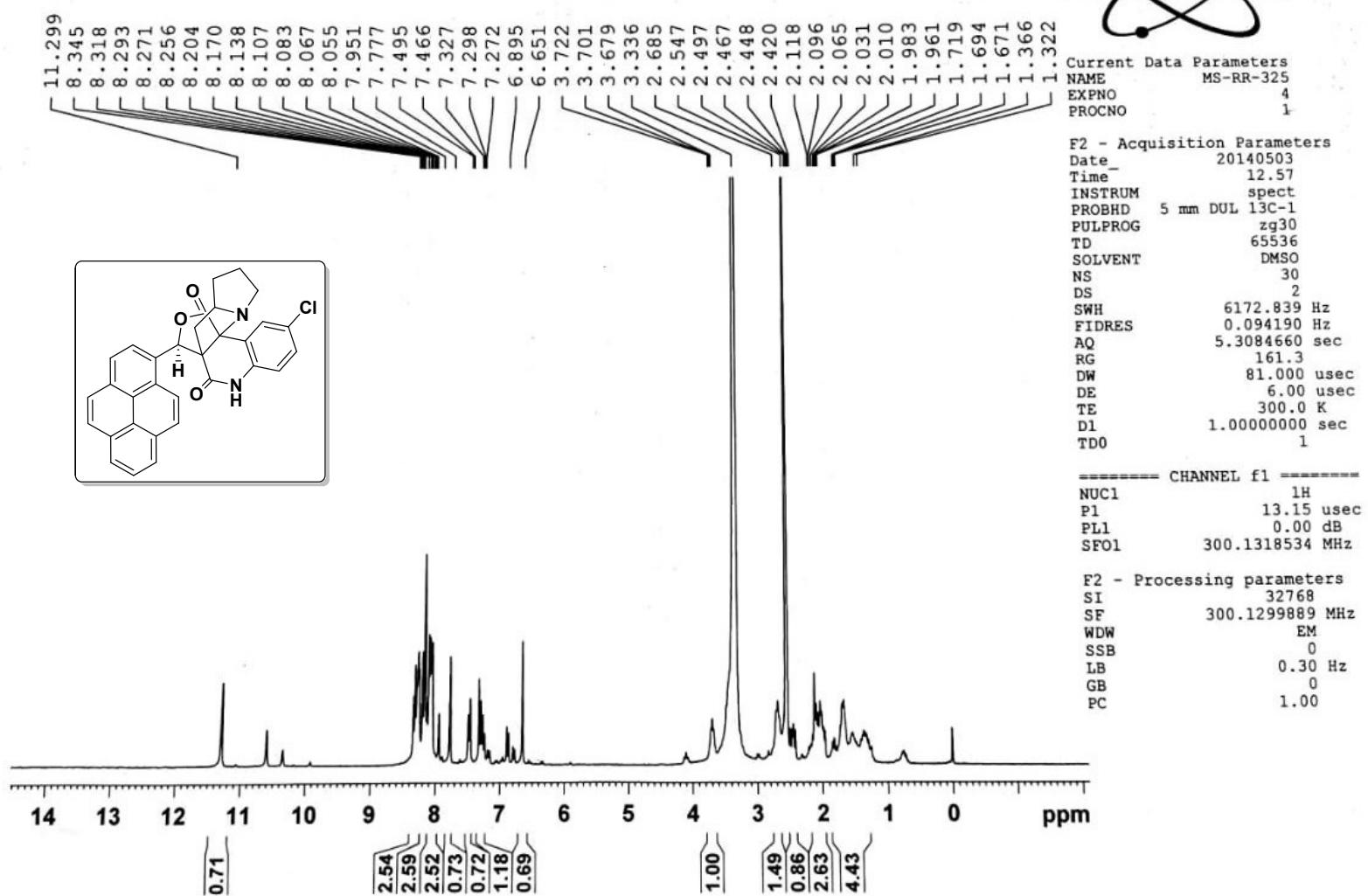
CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 SFO2 300.1312005 MHz

F2 - Processing parameters

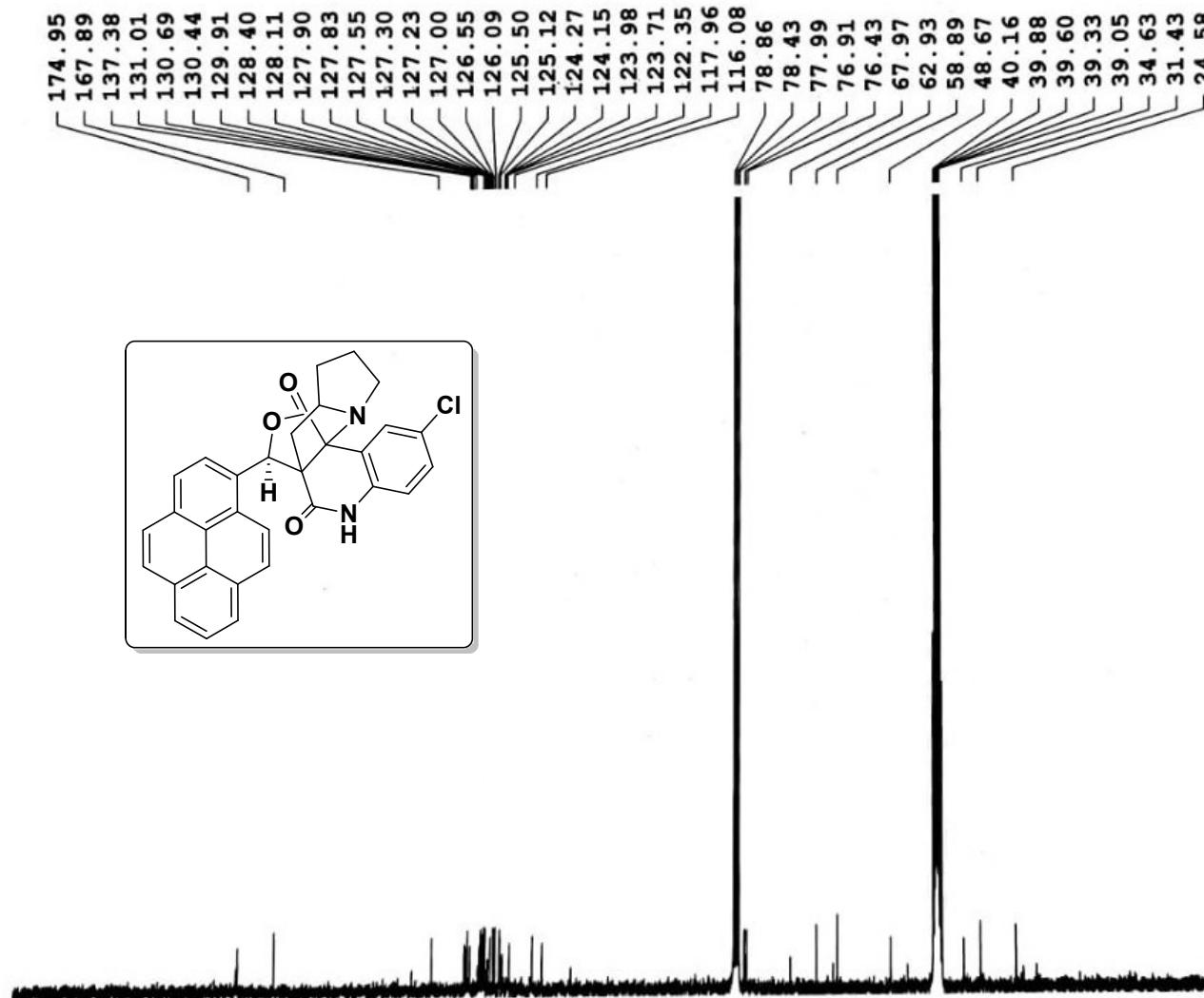
SI 32768
 SF 75.4677490 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

¹³C NMR spectrum of compound 12a





¹H NMR spectrum of compound 12b



Current Data Parameters
NAME MS-RR-325
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140503
Time_ 10.22
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zpg30
TD 65536
SOLVENT DMSO
NS 3603
DS 4
SWH 17985.611 Hz
FIDRES 0.274439 Hz
AQ 1.8219508 sec
RG 812.7
DW 27.800 usec
DE 6.00 usec
TE 300.0 K
D1 2.0000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

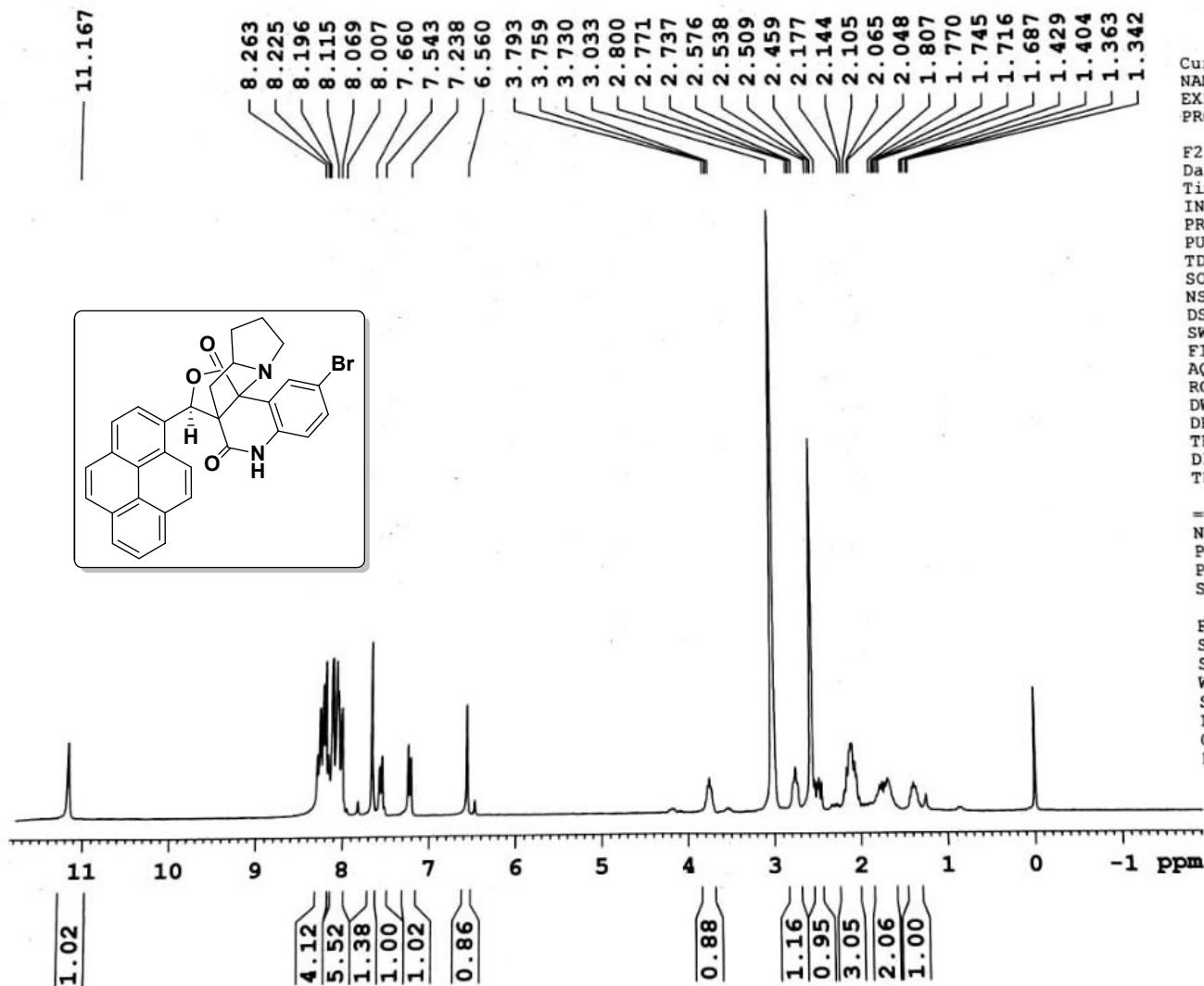
===== CHANNEL f1 =====
NUC1 13C
P1 9.30 usec
PL1 0.00 dB
SFO1 75.4752953 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 15.68 dB
PL13 16.00 dB
SFO2 300.1312005 MHz

F2 - Processing parameters
SI 32768
SF 75.4677867 MHz
WDW EM
SSB 0
LB 1.00 Hz

¹³C NMR spectrum of compound 12b

— 11.167 —



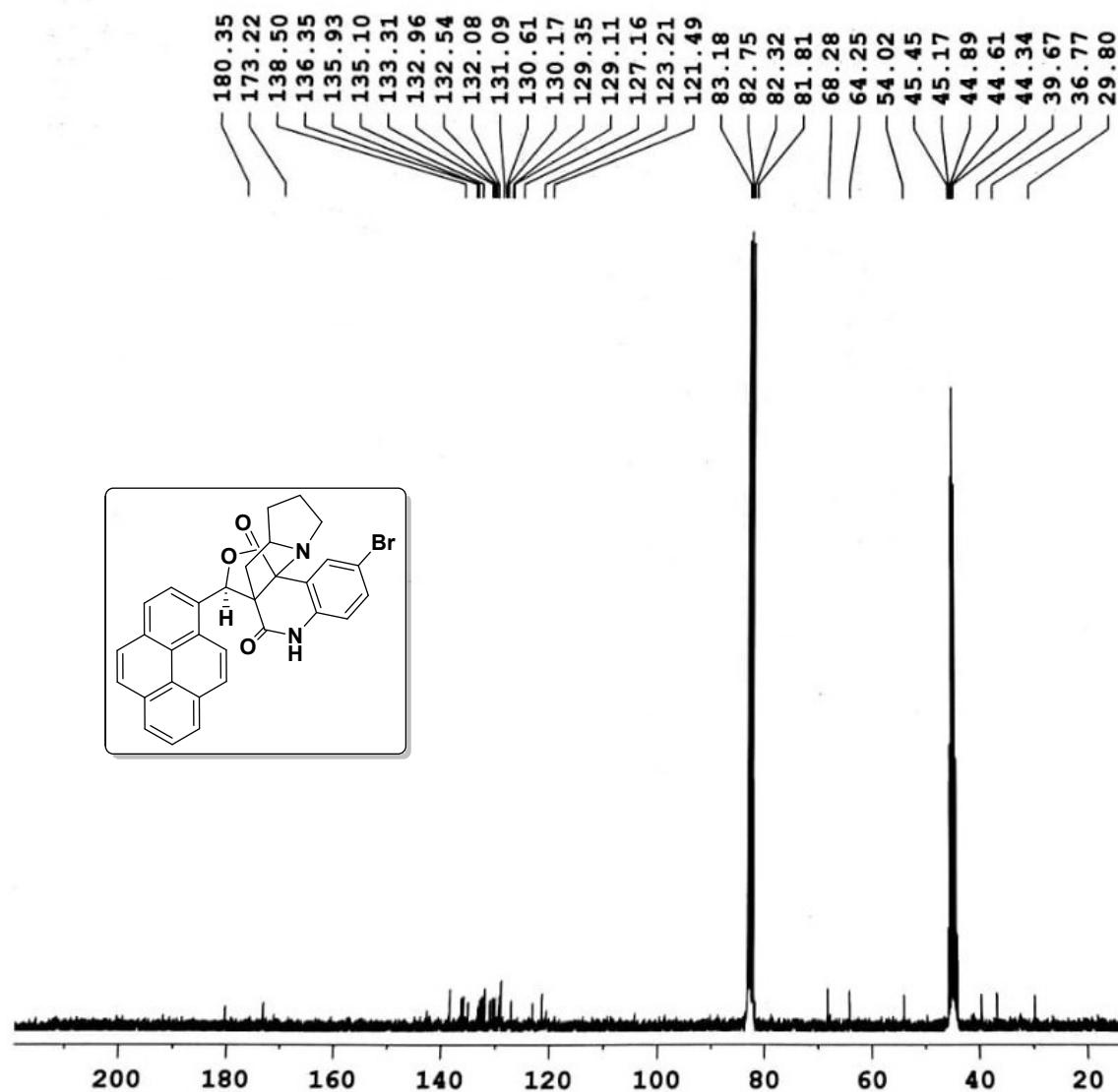
Current Data Parameters
NAME MS-RR-326
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20140504
Time 17.03
INSTRUM spect
PROBHD 5 mm DUL 13C-1
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 30
DS 2
SWH 6172.839 Hz
FIDRES 0.094190 Hz
AQ 5.3084660 sec
RG 456.1
DW 81.000 usec
DE 6.00 usec
TE 300.0 K
D1 1.0000000 sec
TDO 1

===== CHANNEL f1 =====
NUC1 1H
P1 13.15 usec
PL1 0.00 dB
SFO1 300.1318534 MHz

F2 - Processing parameters
SI 32768
SF 300.1314065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹H NMR spectrum of compound 12c



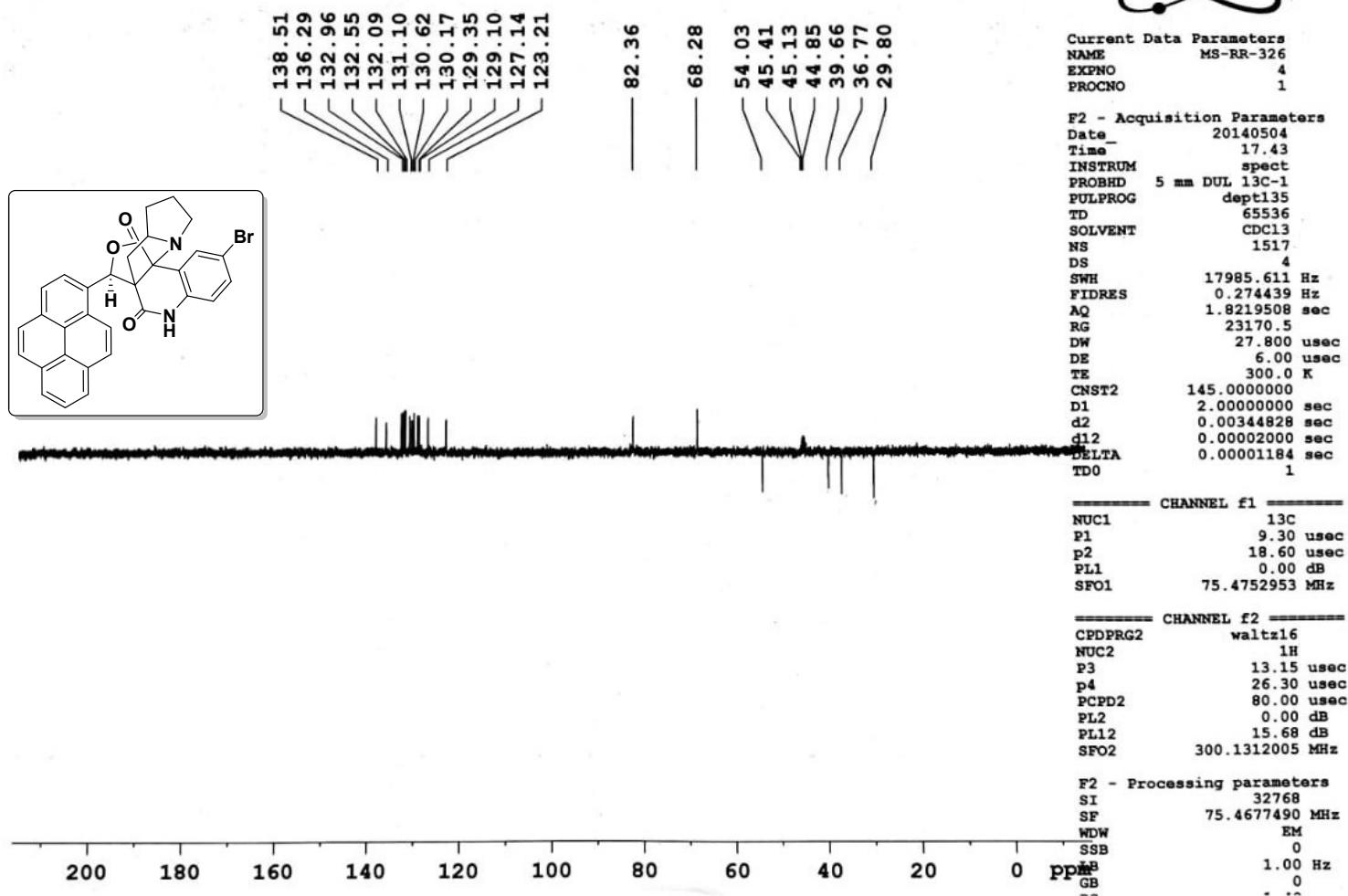
Current Data Parameters
 NAME MS-RR-326
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date 20140504
 Time 15.04
 INSTRUM spect
 PROBHD 5 mm DUL 13C-1
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 2000
 DS 4
 SWH 17985.611 Hz
 FIDRES 0.274439 Hz
 AQ 1.8219508 sec
 RG 2298.8
 DW 27.800 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.0000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 ¹³C
 P1 9.30 usec
 PL1 0.00 dB
 SFO1 75.4752953 MHz

===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 ¹H
 PCPD2 80.00 usec
 PL2 0.00 dB
 PL12 15.68 dB
 PL13 16.00 dB
 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



DEPT 135 NMR spectrum of compound 12c