

NaHSO₄/SiO₂ catalyzed generation of *o*-quinone/*o*-thioquinone methides: Synthesis of arylxanthenes/arylthioxanthenes via oxa-6π-electrocyclization

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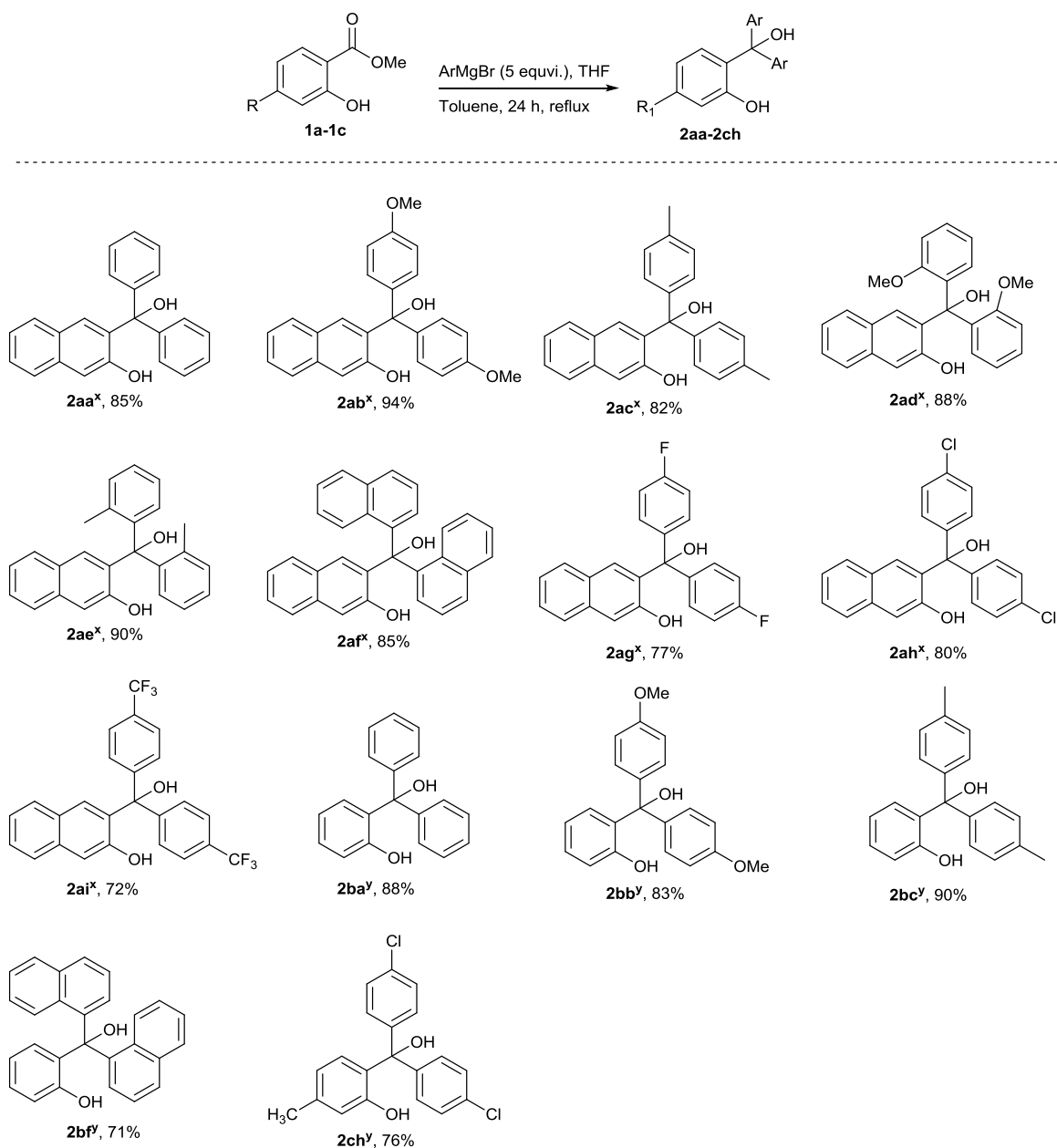
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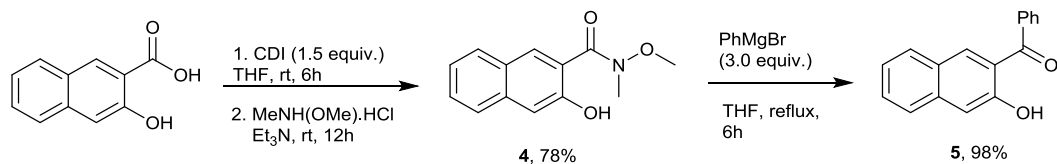
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Scheme 1: Synthesis of symmetrical *ortho*-(hydroxydiarylmethyl)arene-2-ol derivatives, 2aa-2ch¹⁸

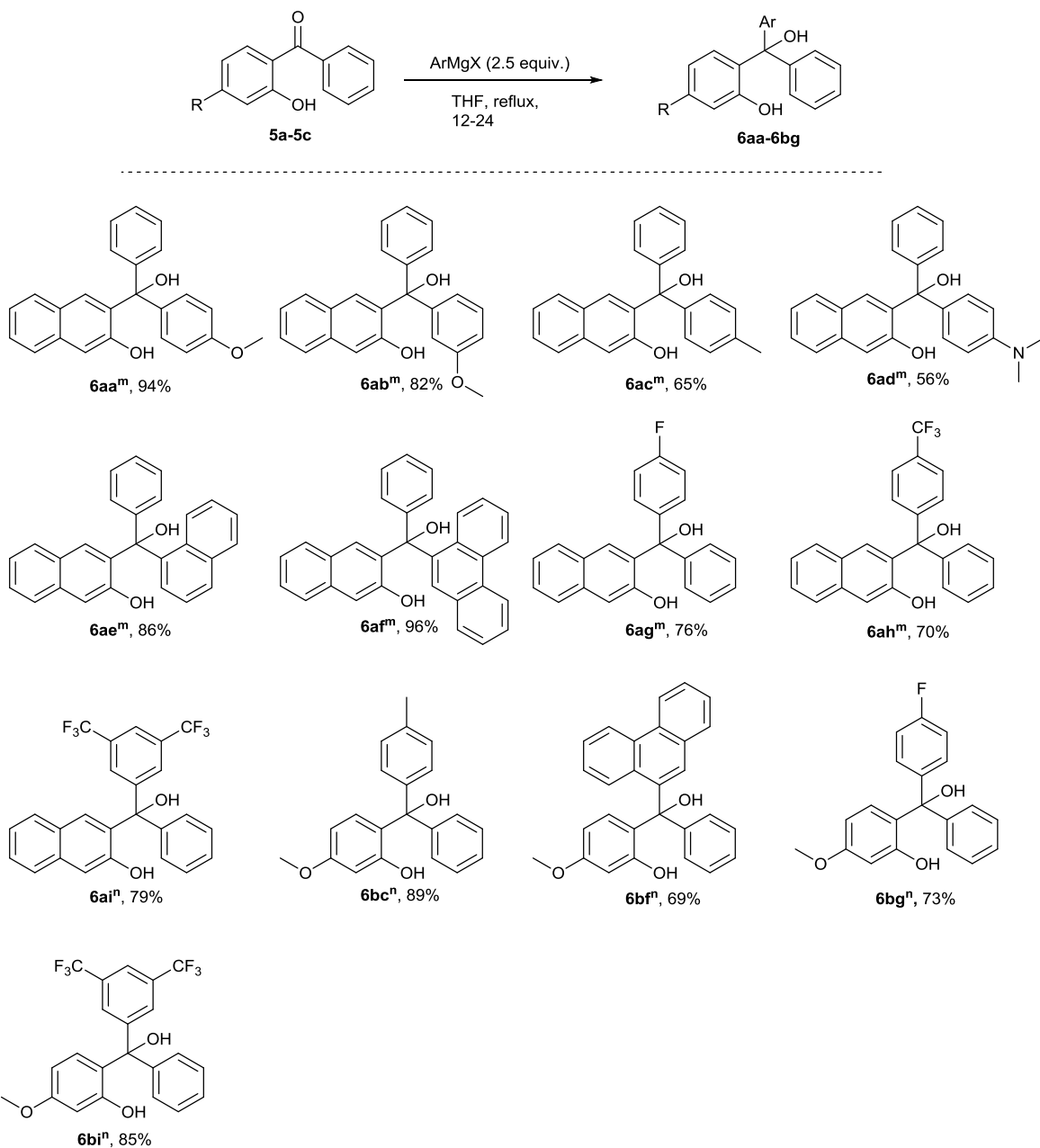


x = 5.0 mmol of ArMgBr for 1 mmol of substrate, y = 3.0 mmol of ArMgBr for 1 mmol of substrate

Scheme 2: Synthesis of compound 4 & 5

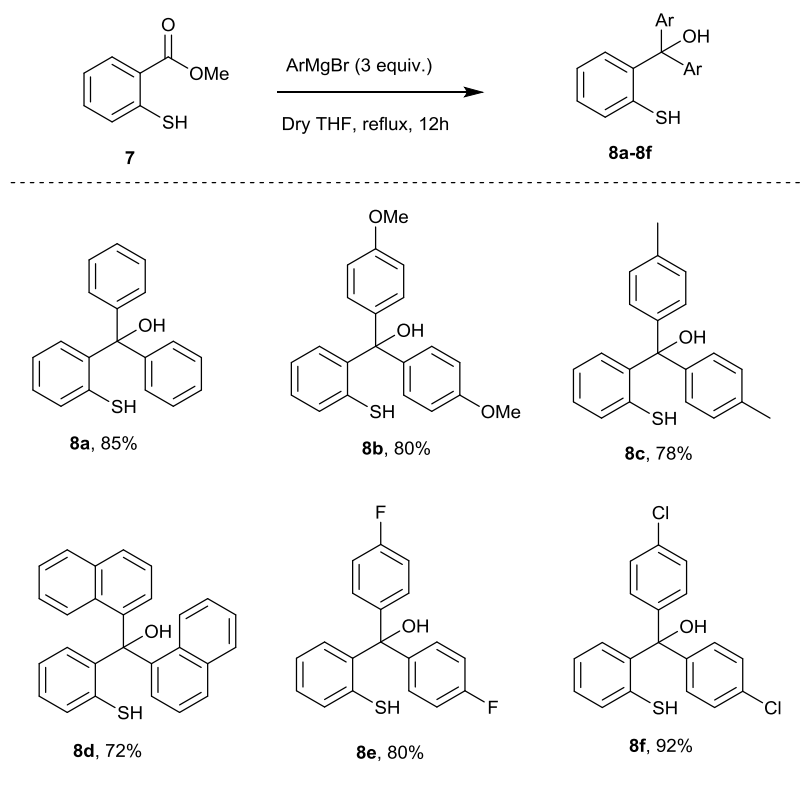


Scheme 3: Synthesis of unsymmetrical *ortho*-(hydroxydiarylmethyl)arene-2-ol derivatives, 6aa-6bi



m = 2.5 mmol of ArMgBr for 1 mmol of substrate, n = 2.5 mmol of ArMgBr for 1 mmol of substrate

Scheme 4: Synthesis of (2-mercaptophenyl)diarylmethanol derivatives, 8a-8f



PROTON CDCL3-M.KARTHICK



Current Data Parameters
NAME MK-ED-28
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190306
Time 10.58
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 406
DW 60.800 usec
DE 6.00 usec
TE 293.8 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
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SF 400.1300609 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

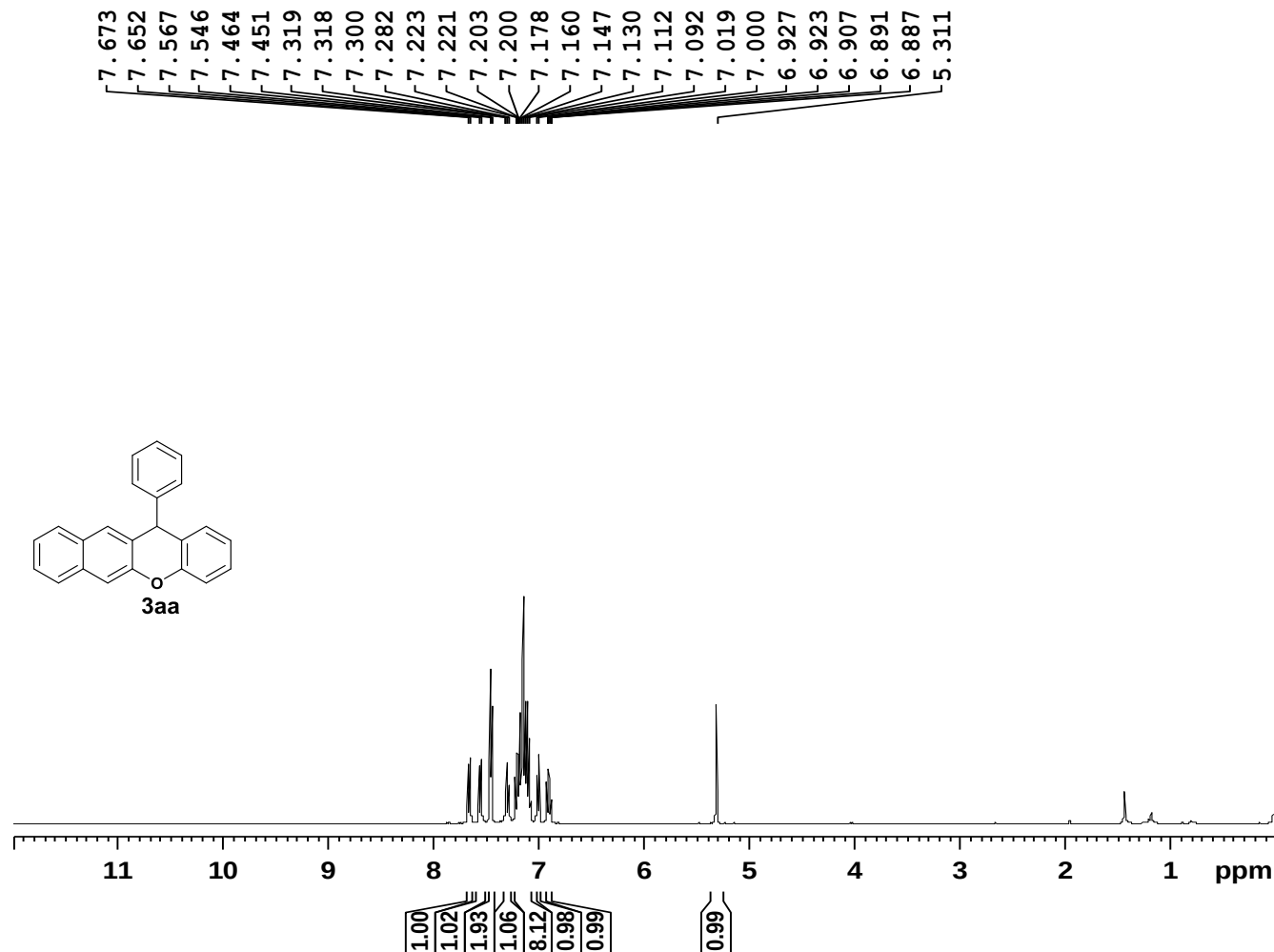


Figure 1: ¹H-NMR spectra for compound 3aa

PROTON CDCL₃-M.KARTHICK

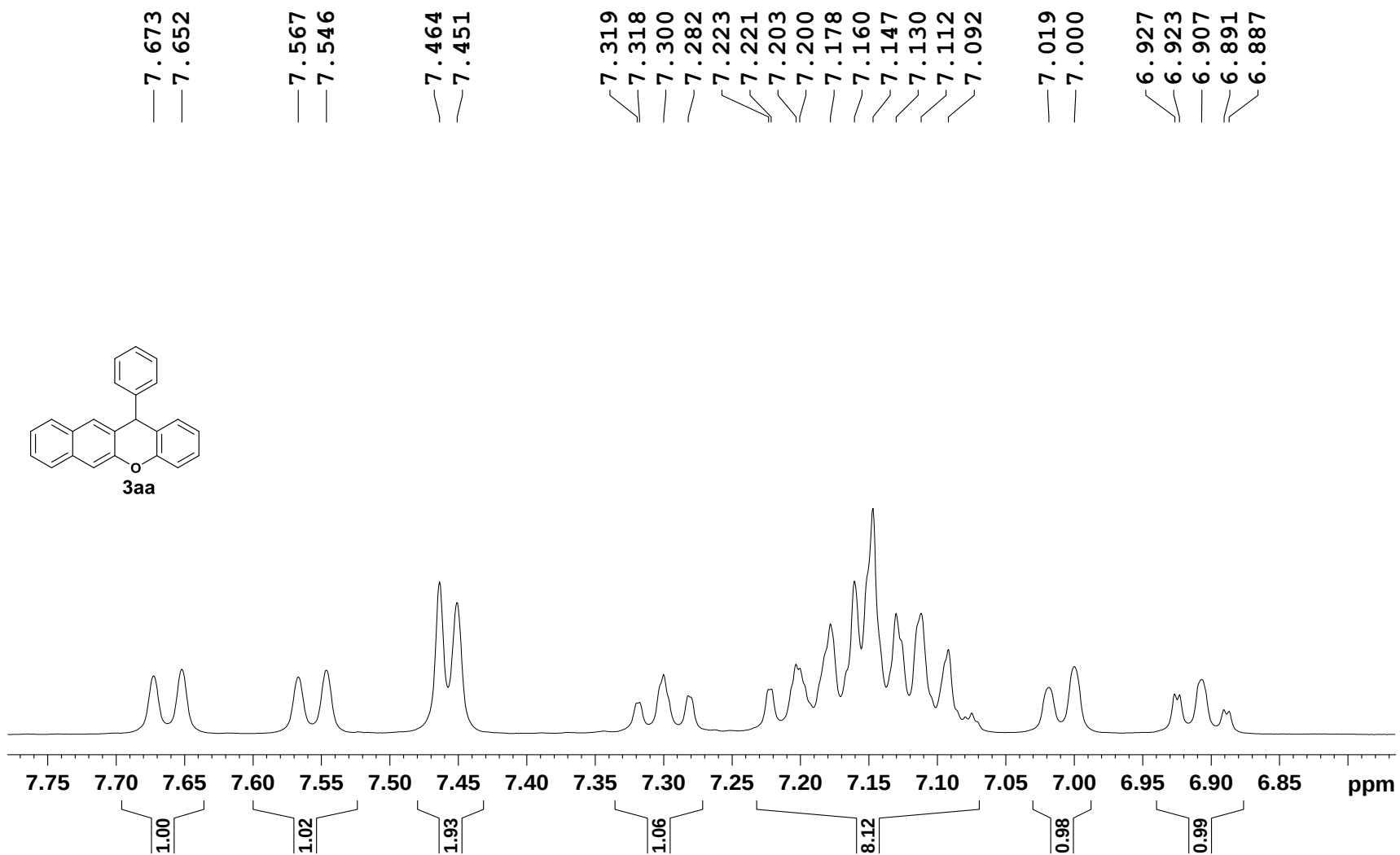
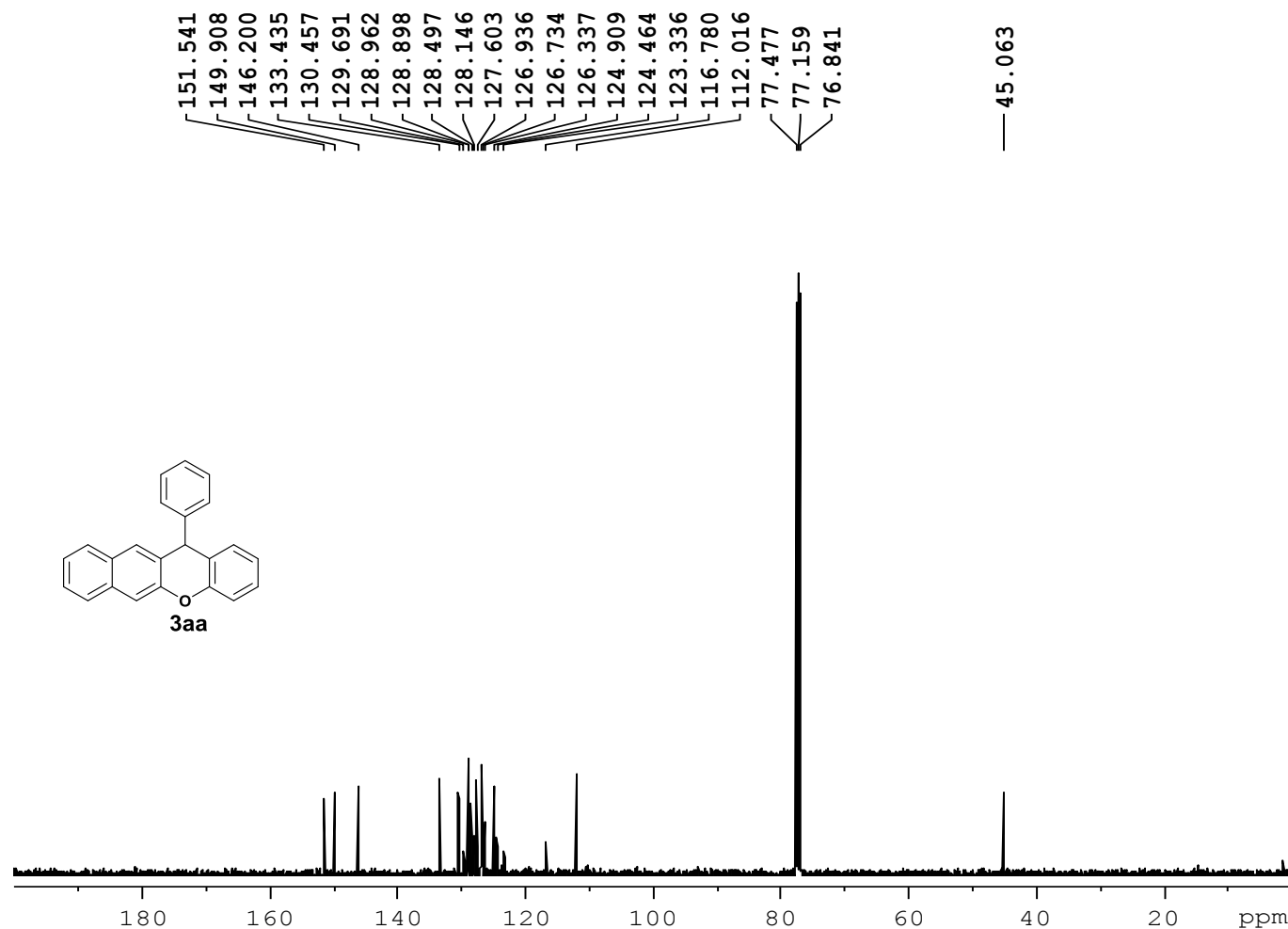


Figure 1a: ¹H-NMR spectra expansion for compound **3aa**

C13CPD CDCL3-M.KARTHICK



Current Data Parameters
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 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
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 Time 11.12
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCL3
 NS 256
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 362
 DW 20.800 usec
 DE 6.00 usec
 TE 294.3 K
 D1 2.0000000 sec
 d11 0.0300000 sec
 DELTA 1.89999998 sec
 TDO 1

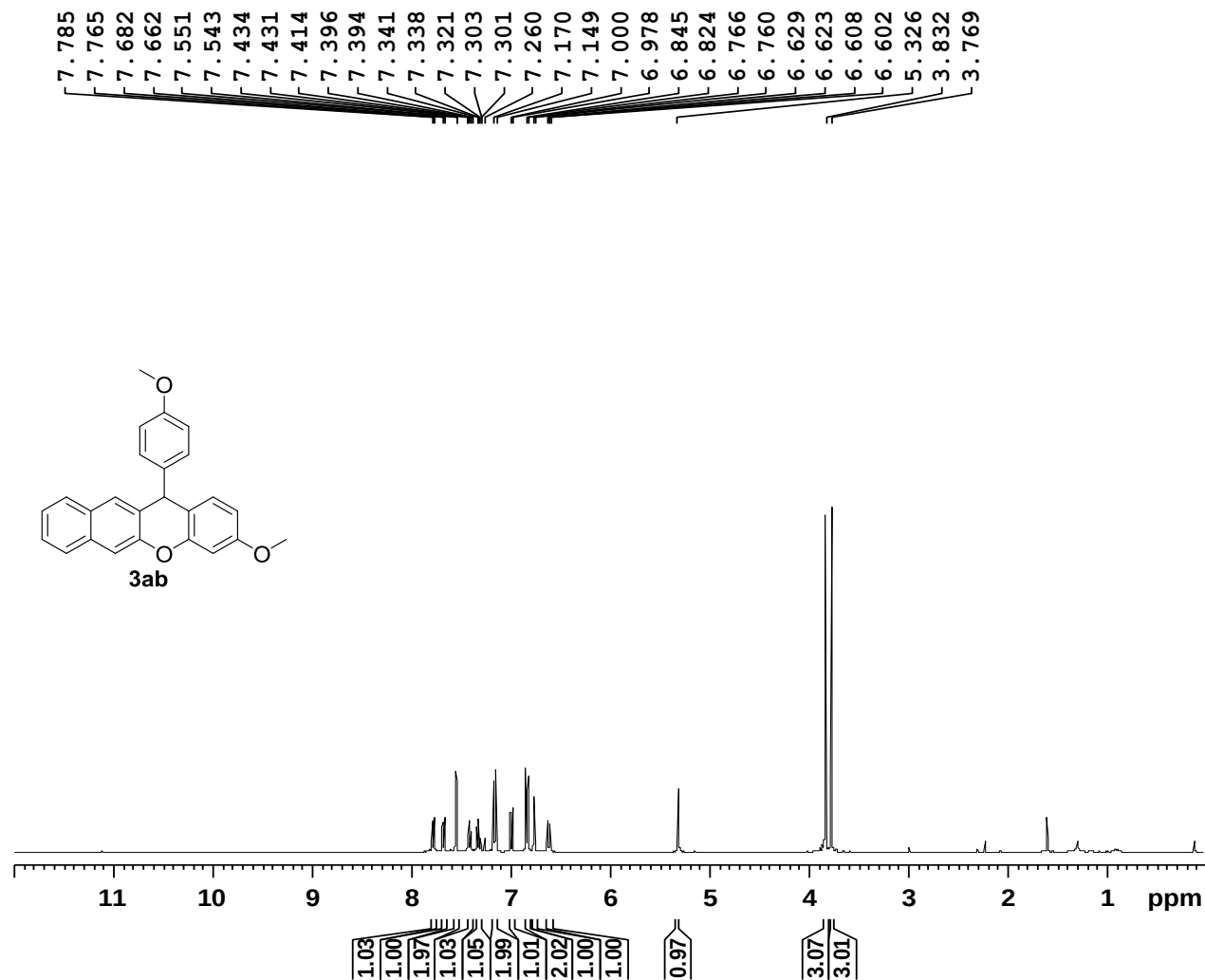
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 NUC1 13C
 P1 9.15 usec
 PL1 0 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 FCPD2 90.00 usec
 PL12 14.90 dB
 PL13 14.90 dB
 PL2 -3.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127604 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure 2: ¹³C-NMR spectra for compound **3aa**

PROTON CDC13 {D:\CRR} KOPAL 1



Current Data Parameters
NAME MK-ED-5
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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Time 10.29
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 144
DW 60.800 usec
DE 6.00 usec
TE 292.8 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300046 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 3: ¹H-NMR spectra for compound **3ab**

PROTON CDC13 {D:\CRR} KOPAL 1

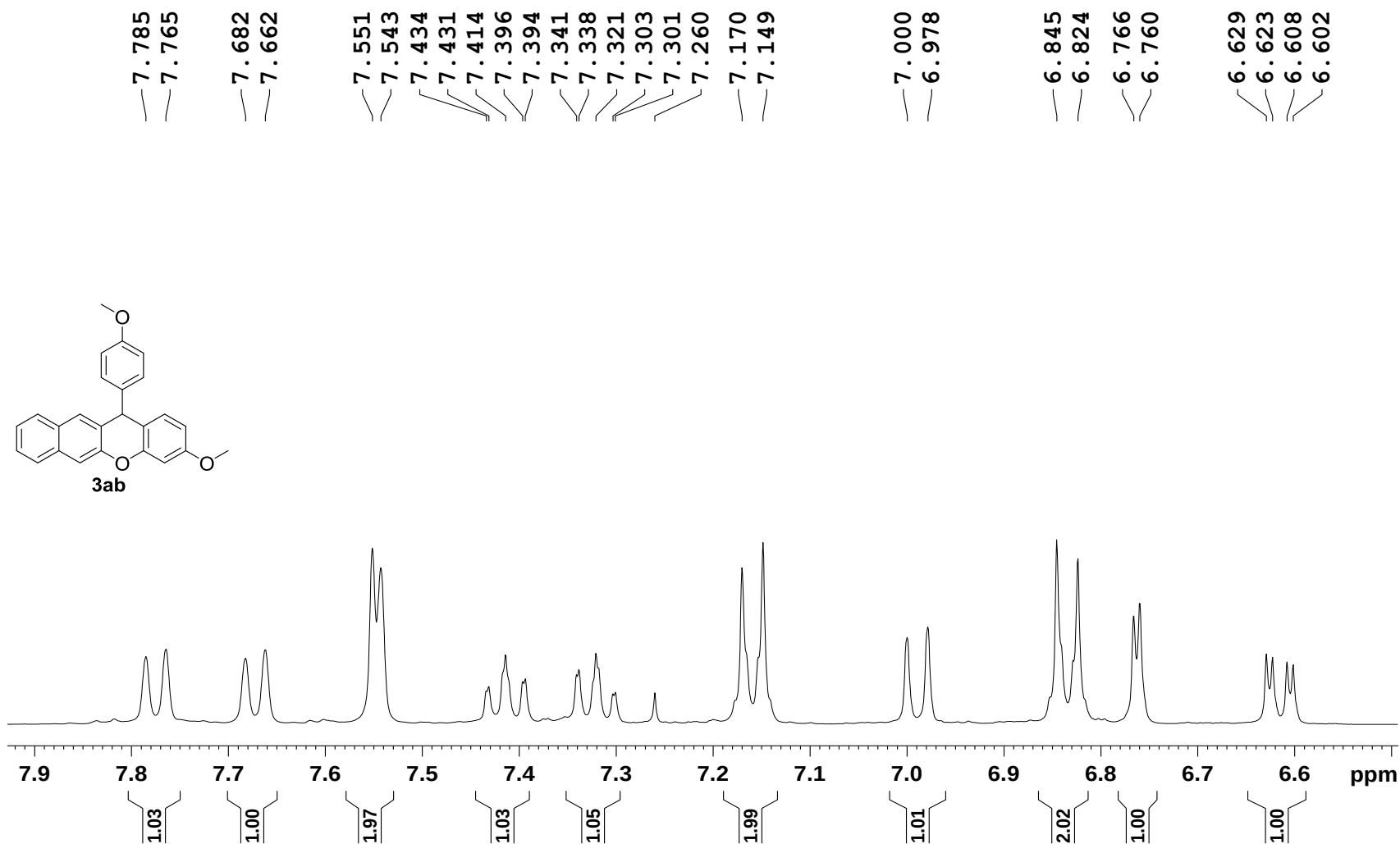


Figure 3: ^1H -NMR spectra for compound **3ab**

C13CPD CDC13 {D:\CRR} KOPAL 1

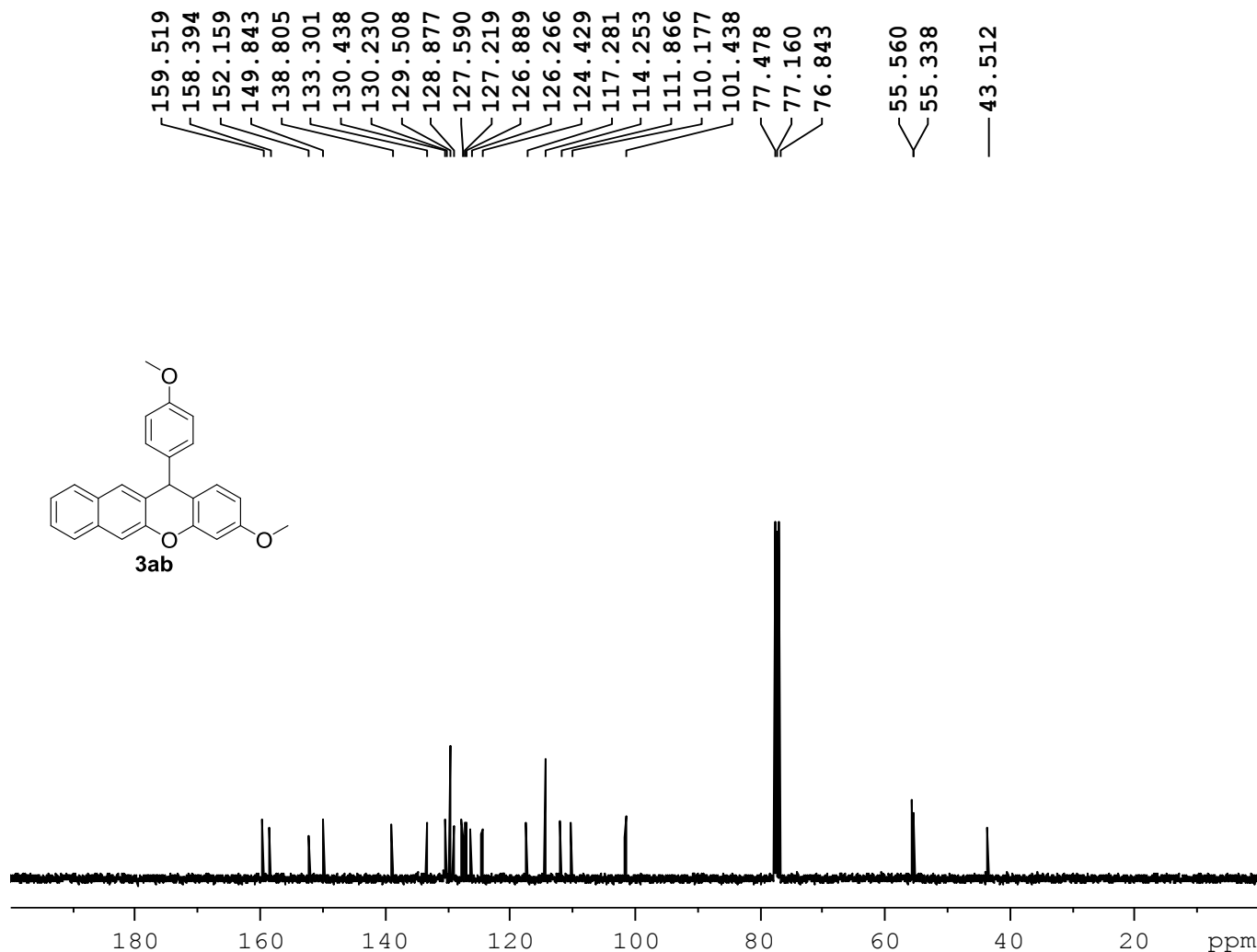
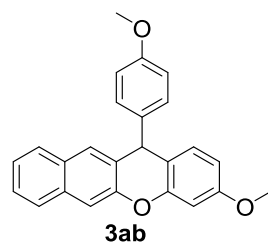


Figure 4: ^{13}C -NMR spectra for compound **3ab**

Current Data Parameters
 NAME MK-ED-5
 EXPNO 2
 PROCNO 1

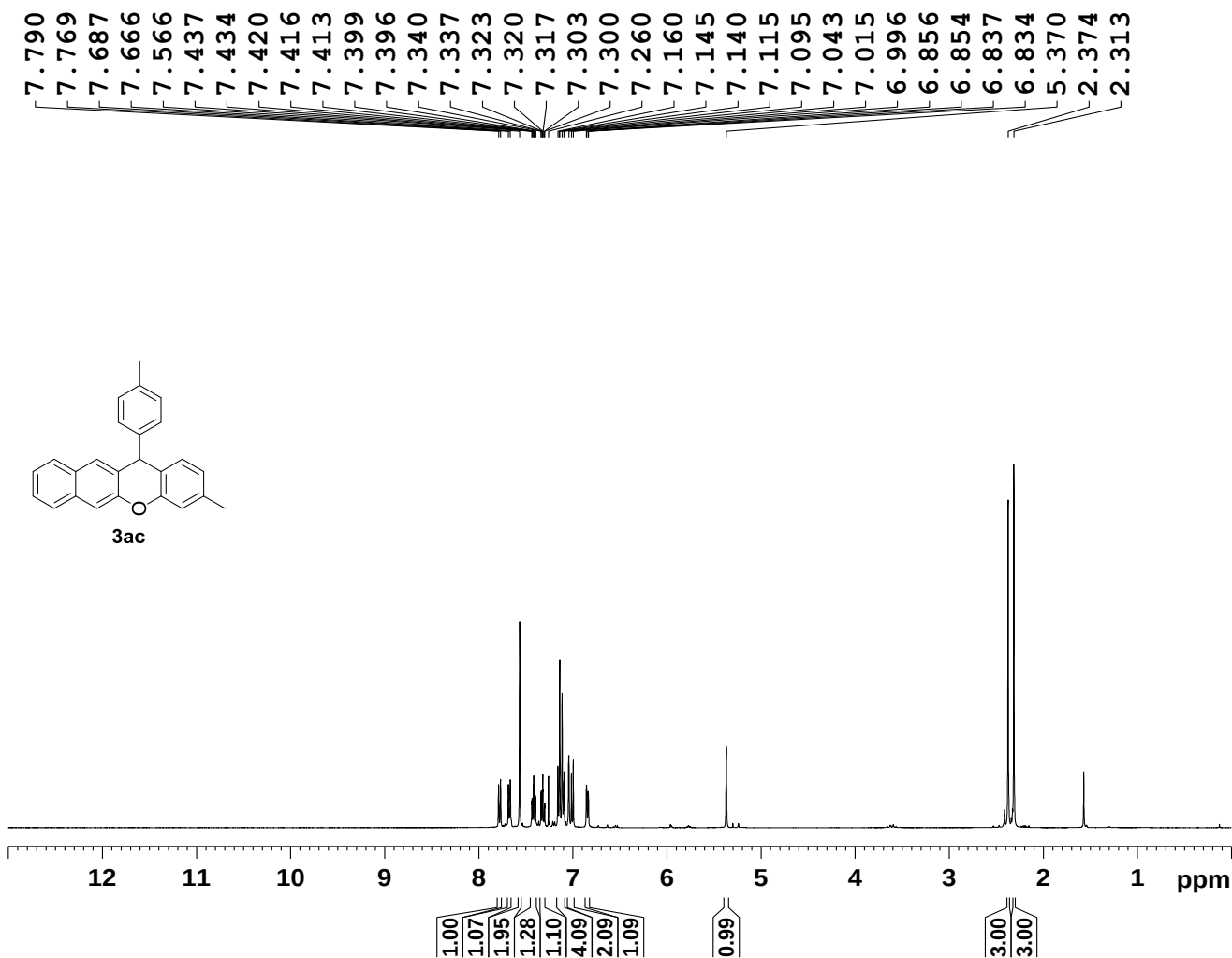
F2 - Acquisition Parameters
 Date_ 20180803
 Time 10.33
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 256
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 40.3
 DW 20.800 usec
 DE 6.00 usec
 TE 293.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 ^{13}C
 P1 9.95 usec
 PL1 -1.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 ^1H
 PCPD2 90.00 usec
 PL12 14.95 dB
 PL13 120.00 dB
 PL2 -1.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127593 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

PROTON CDC13 {D:\CRR} nmr 1



Current Data Parameters
 NAME MK-XN-N4
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190105
 Time 10.19
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 161
 DW 60.800 usec
 DE 6.00 usec
 TE 293.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.35 usec
 PL1 -1.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300048 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure 5: ¹H-NMR spectra for compound **3ac**

PROTON CDCl3 {D:\CRR} nmr 1

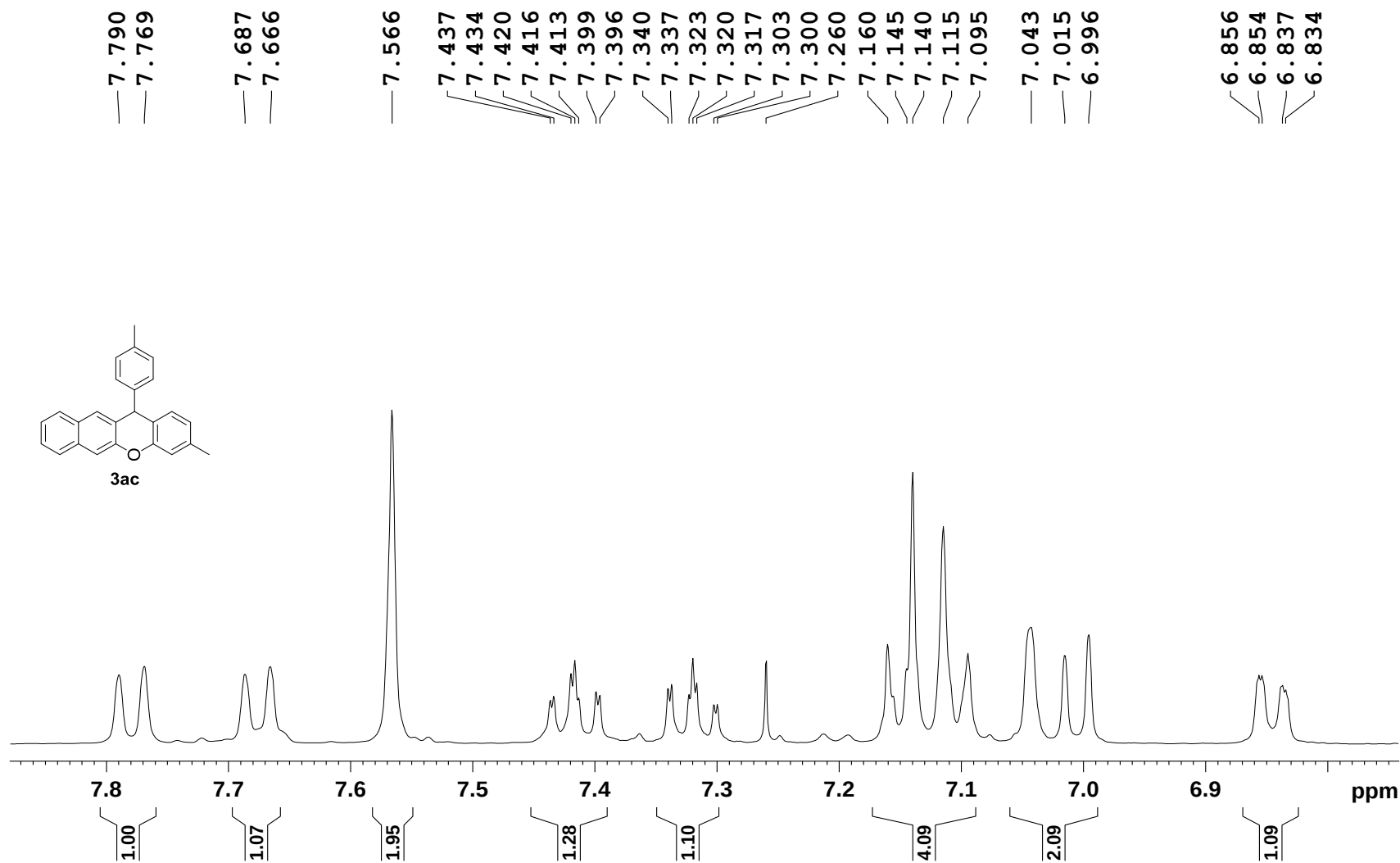
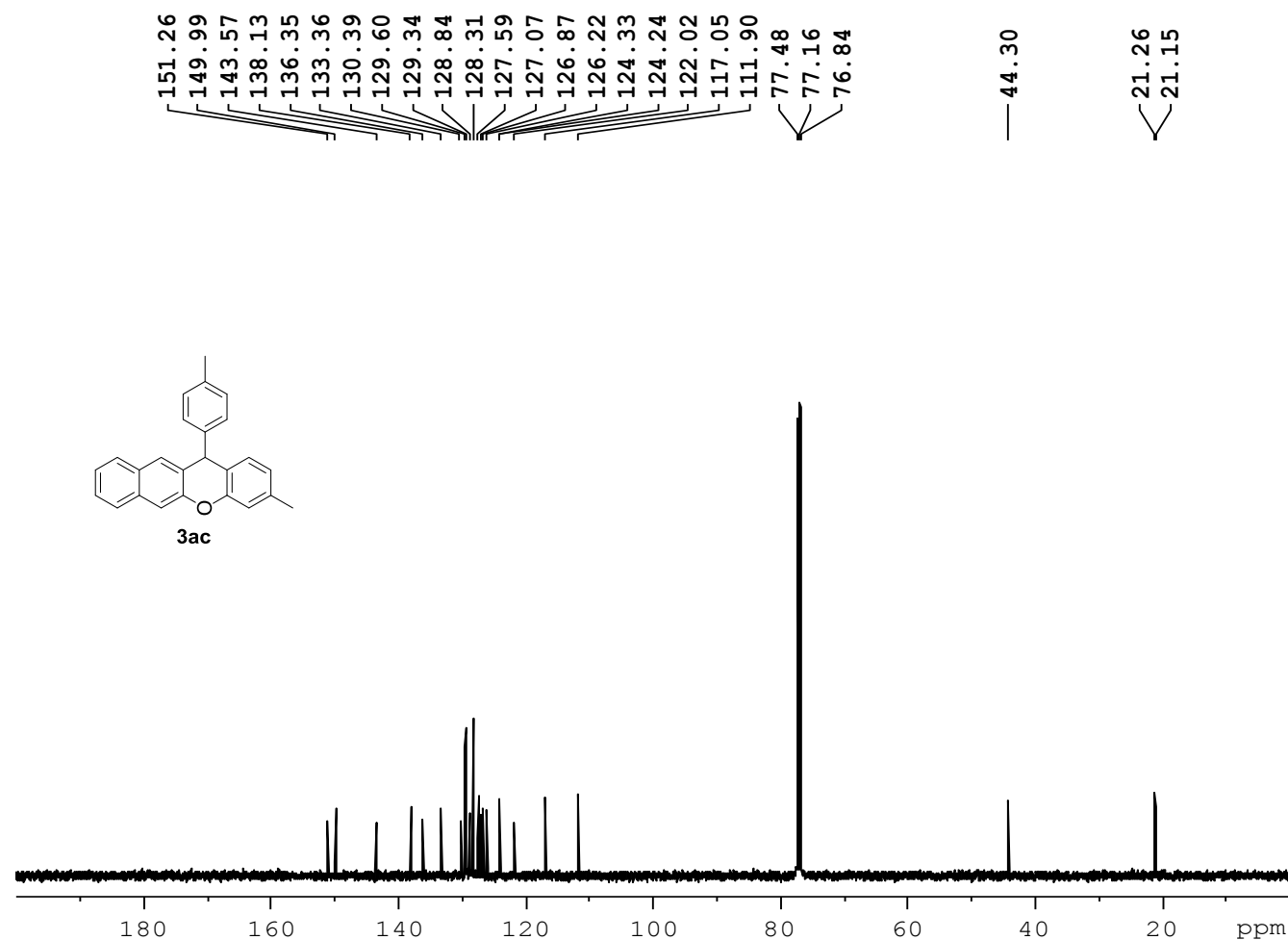


Figure 5a: ¹H-NMR spectra expansion for compound **3ac**

C13CPD CDC13 {D:\CRR} nmr 1



Current Data Parameters
NAME MK-XN-N4
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190106
Time 13.40
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 362
DW 20.800 usec
DE 6.00 usec
TE 290.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

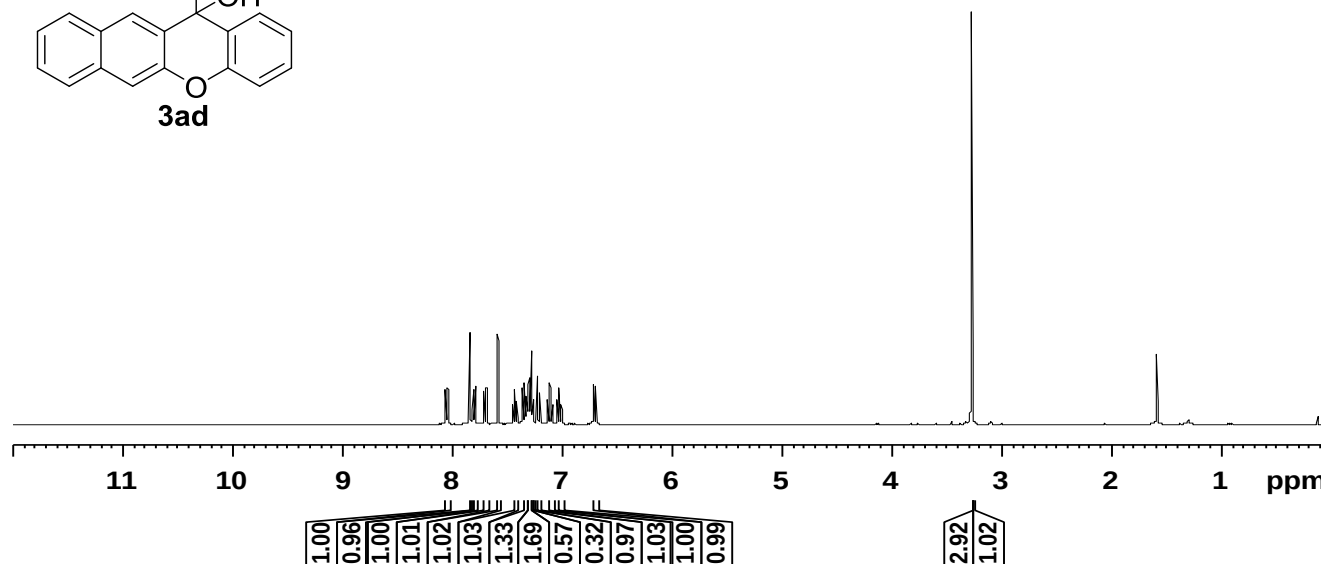
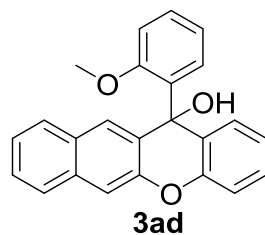
F2 - Processing parameters
SI 32768
SF 100.6127612 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 6: ^{13}C -NMR spectra for compound **3ac**

PROTON CDC13 {D:\CRR} CIF_NMR 1



8.053
8.048
8.033
8.029
7.827
7.797
7.777
7.699
7.679
7.573
7.423
7.420
7.352
7.348
7.332
7.328
7.319
7.316
7.299
7.293
7.290
7.286
7.282
7.273
7.268
7.260
7.213
7.210
7.192
7.190
7.117
7.101
7.098
7.014
6.703
6.702
6.683
6.681
3.258
3.249



Current Data Parameters
NAME MK-II-429
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190612
Time_ 13.01
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 203
DW 60.800 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 7: ^1H -NMR spectra for compound **3ad**

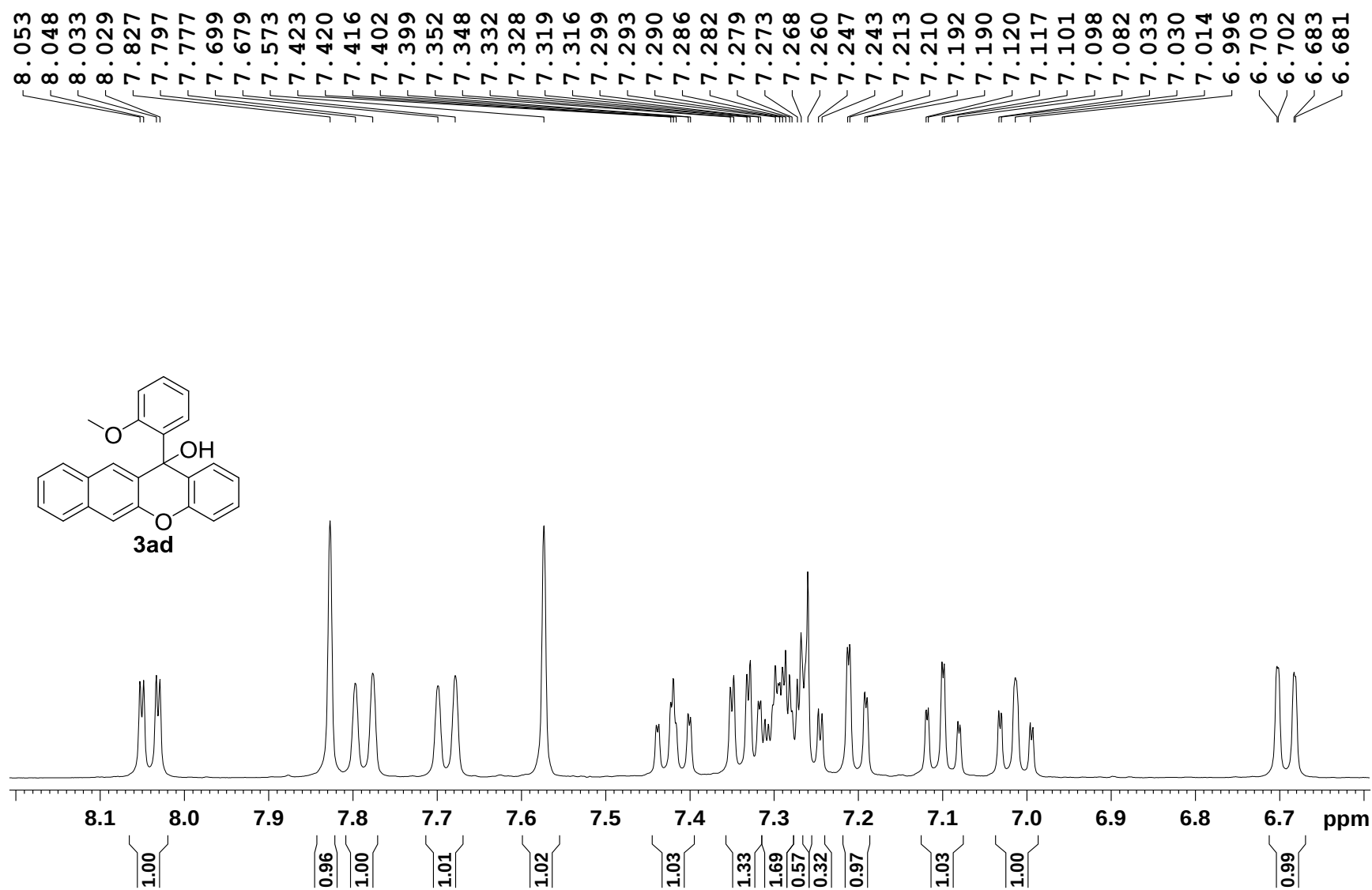
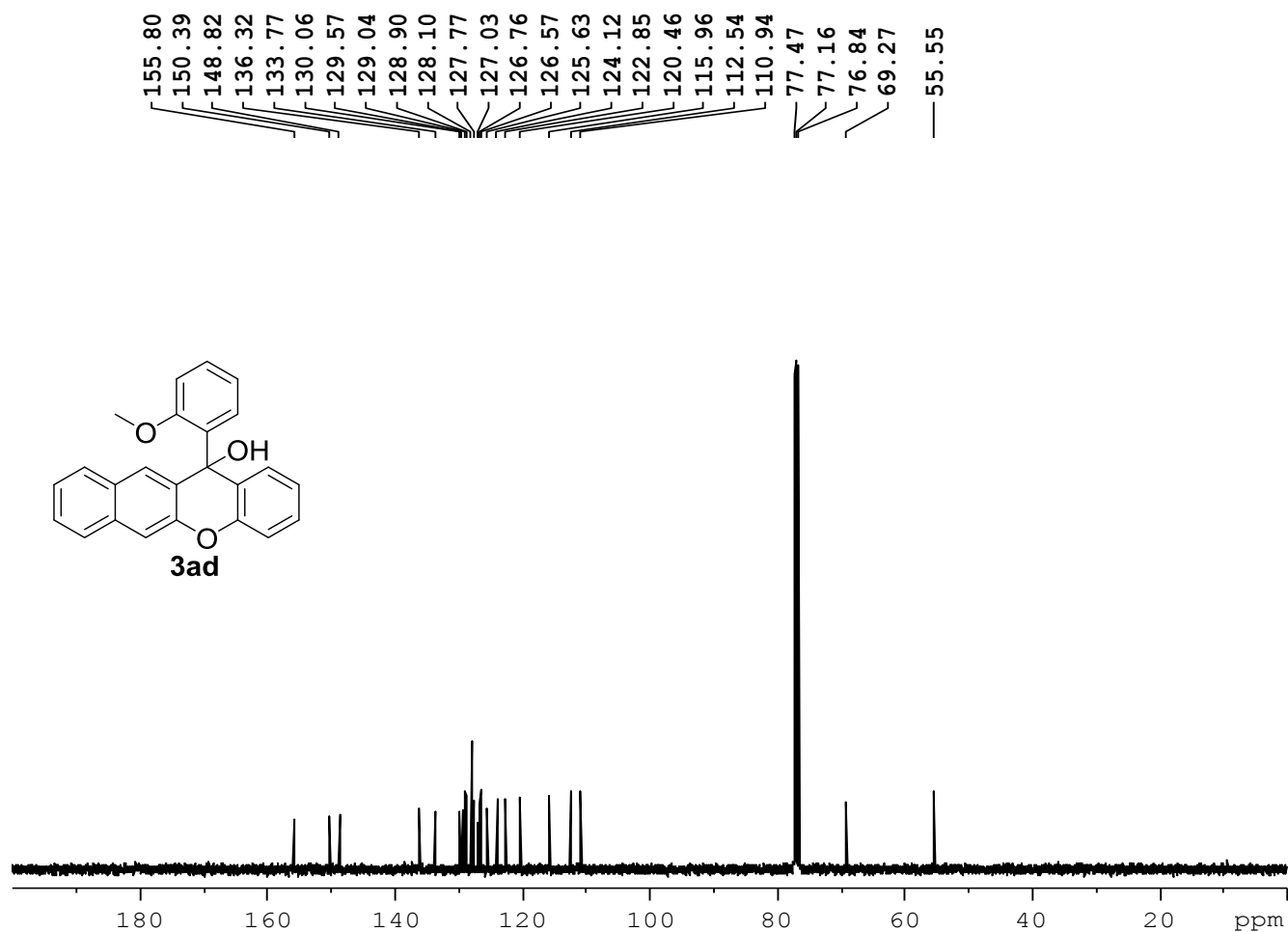


Figure 7a: ^1H -NMR spectra expansion for compound **3ad**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-429
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190620
Time 13.07
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 40.3
DW 20.800 usec
DE 6.00 usec
TE 293.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

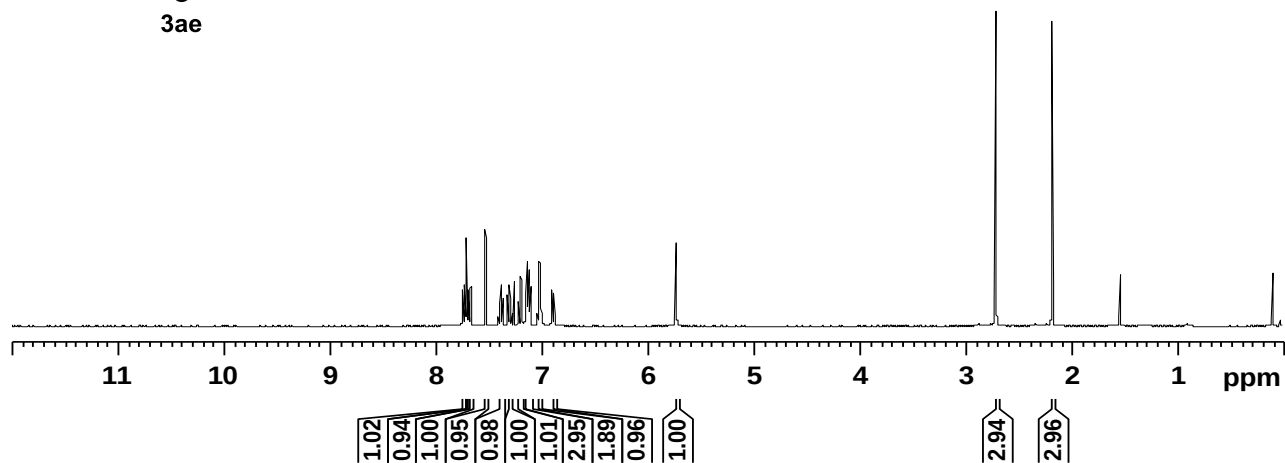
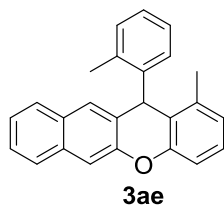
F2 - Processing parameters
SI 32768
SF 100.6127599 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 8: ^{13}C -NMR spectra for compound 3ad

PROTON CDCl3 {D:\CRR} CIF_NMR 1



7.742
7.721
7.707
7.687
7.666
7.527
7.385
7.382
7.379
7.365
7.362
7.321
7.318
7.304
7.301
7.298
7.260
7.221
7.201
7.182
7.153
7.145
7.142
7.136
7.134
7.129
7.121
7.116
7.113
7.105
7.027
7.025
7.020
7.014
7.003
6.900
6.882
5.729
2.712
2.180



Current Data Parameters
NAME MK-II-407
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190424
Time 18.50
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 203
DW 60.800 usec
DE 6.00 usec
TE 293.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 9: ^1H -NMR spectra for compound **3ae**

PROTON CDCl3 {D:\CRR} CIF_NMR 1

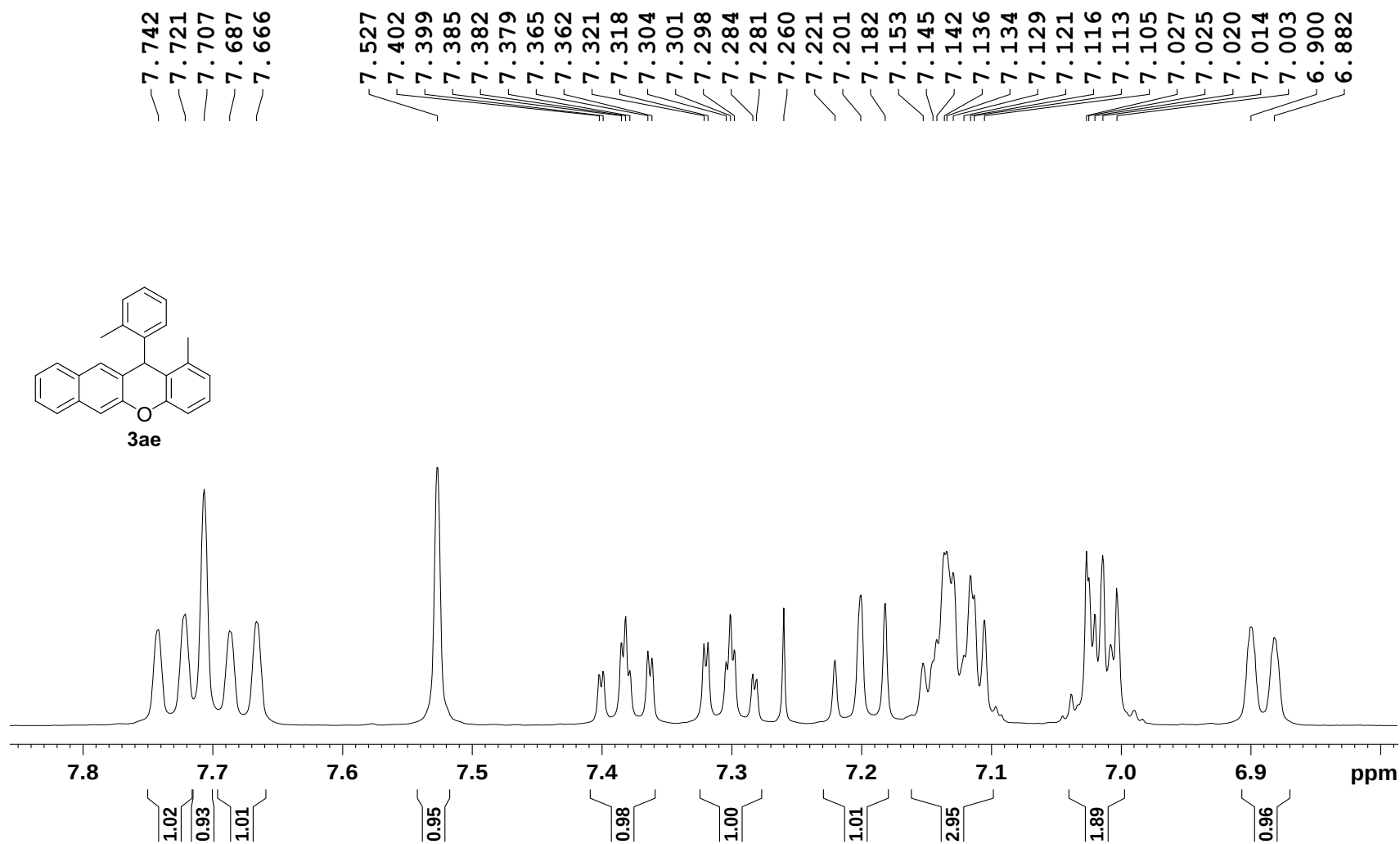
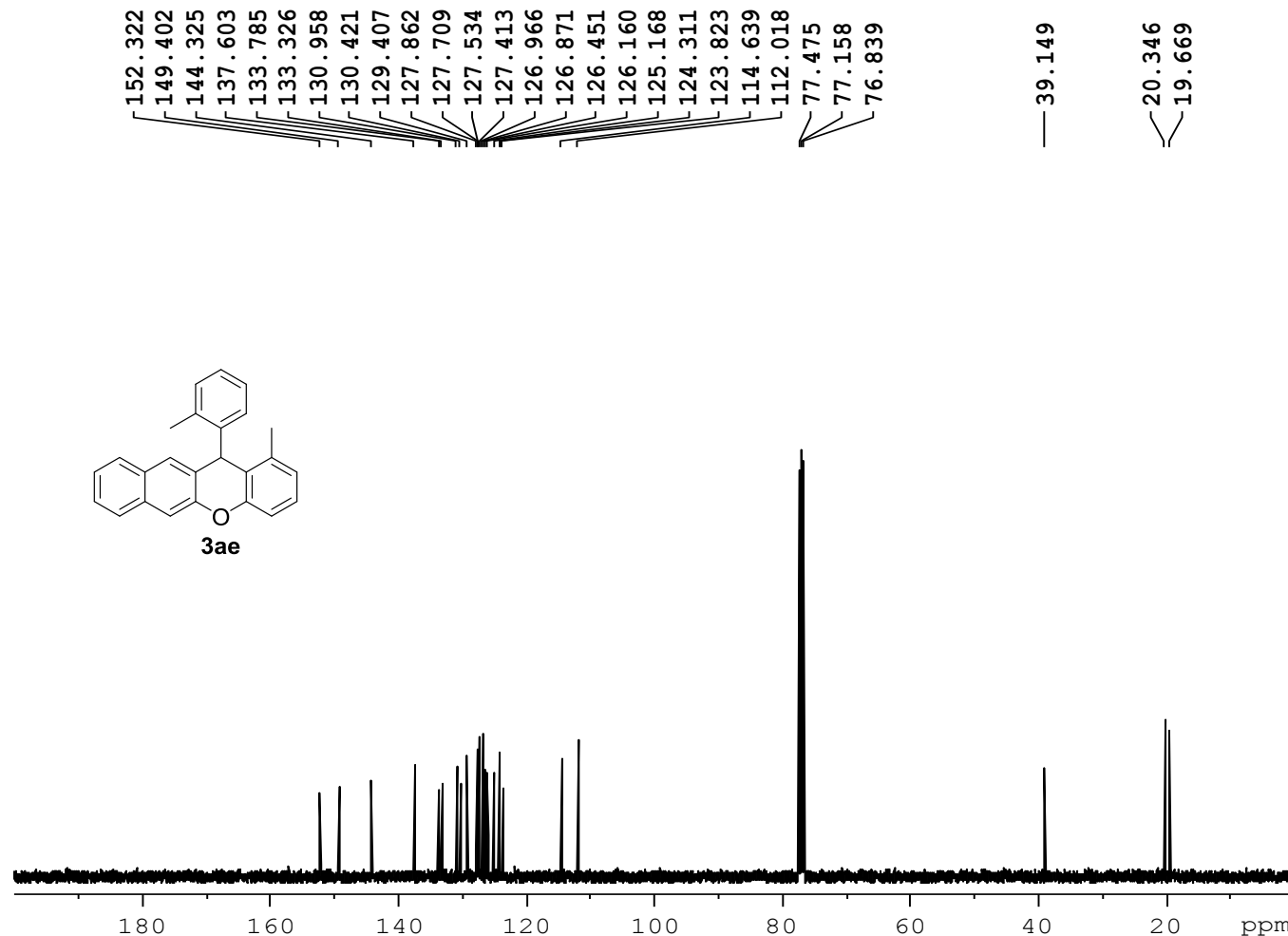


Figure 9a: ^1H -NMR spectra expansion for compound **3ae**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-407
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190424
Time 22.37
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 147
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 40.3
DW 20.800 usec
DE 6.00 usec
TE 293.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

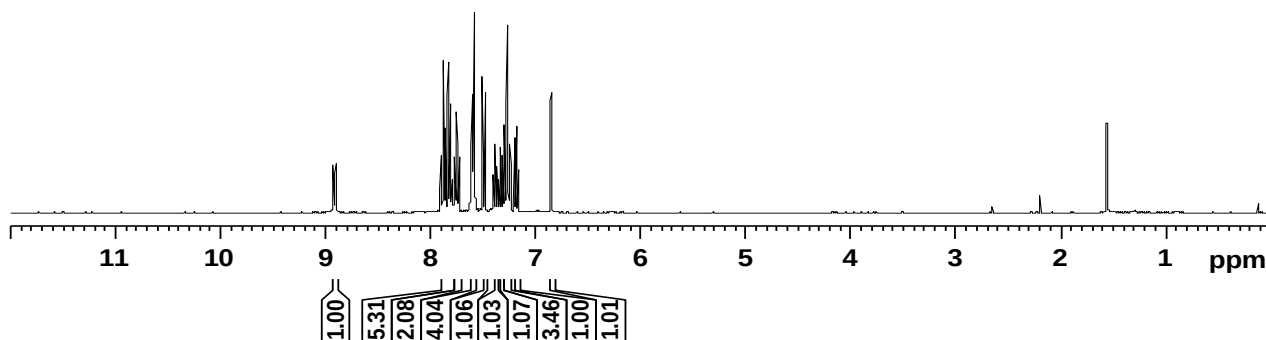
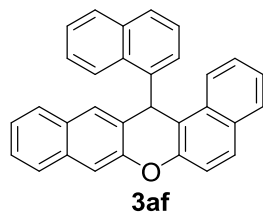
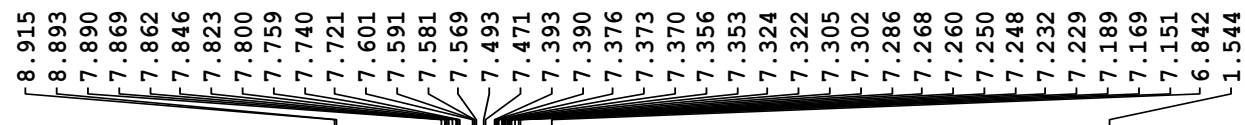
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127628 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 10: ^{13}C -NMR spectra for compound **3ae**

PROTON CDCl3 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-XN-N4-F
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190802
Time 14.19
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 362
DW 60.800 usec
DE 6.00 usec
TE 294.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 11: ¹H-NMR spectra for compound 3af

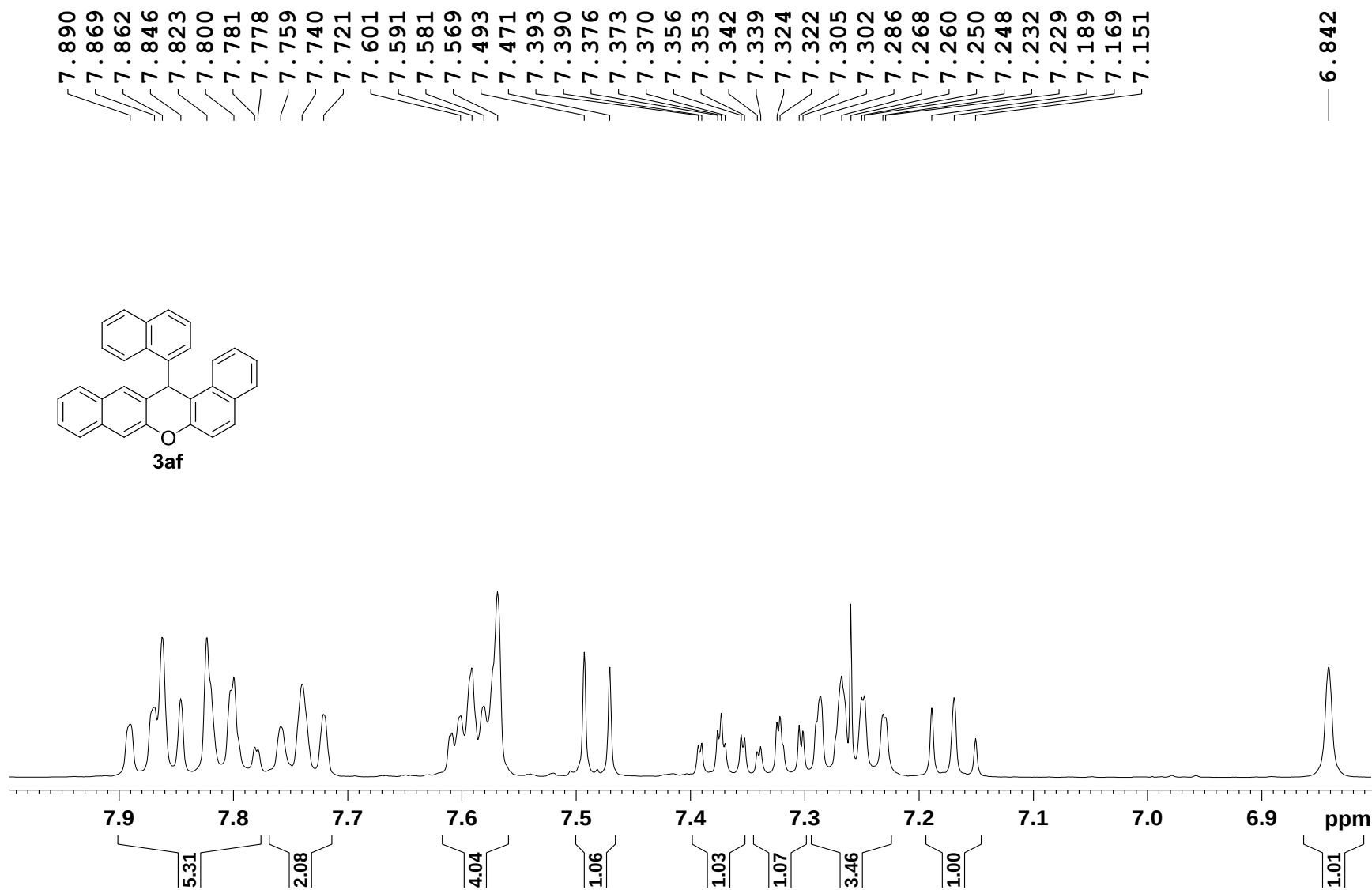
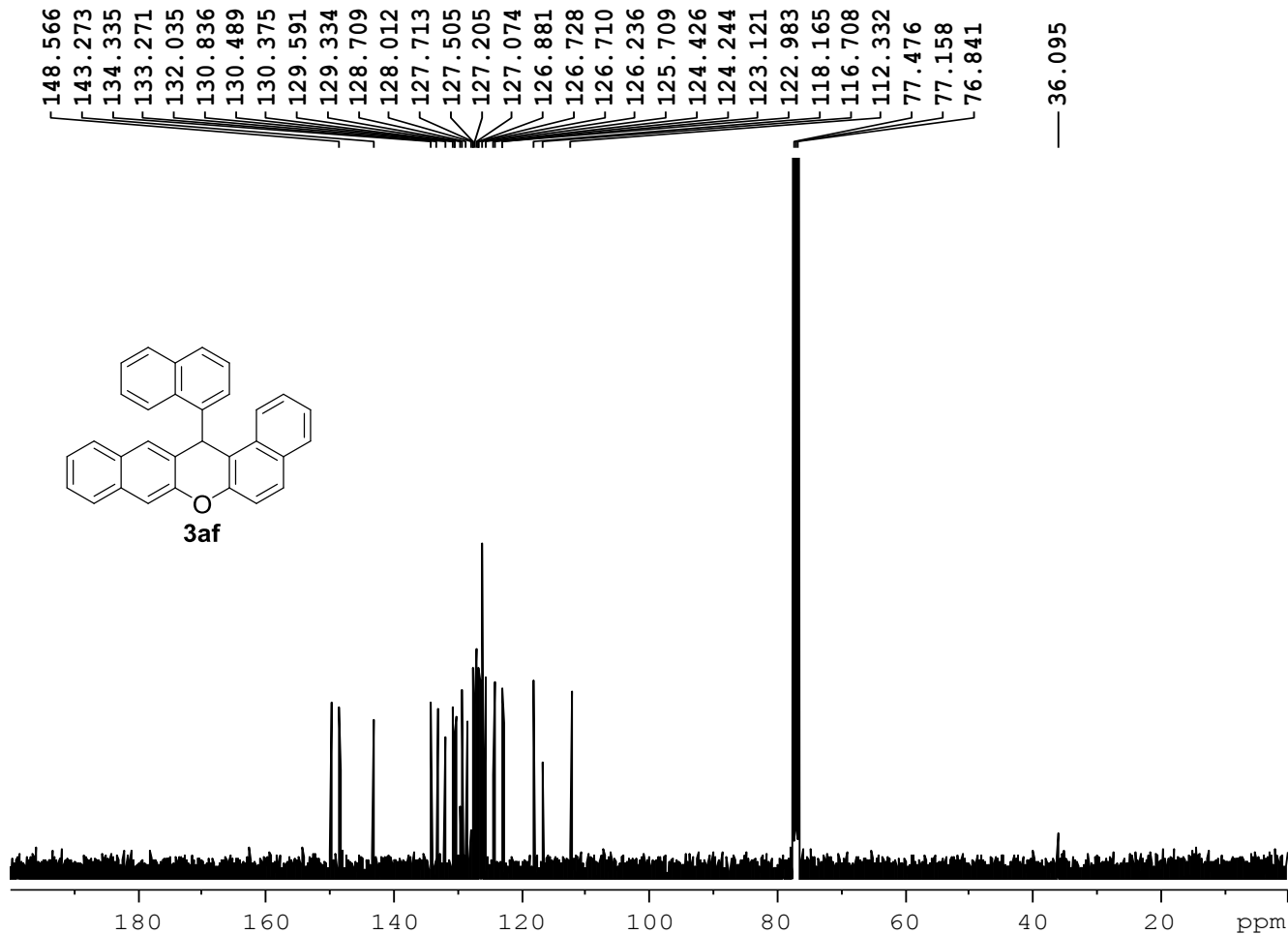


Figure 11a: ^1H -NMR spectra expansion for compound **3af**



Current Data Parameters
NAME MK-XN-N4-F
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190805
Time 10.11
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 40.3
DW 20.800 usec
DE 6.00 usec
TE 294.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

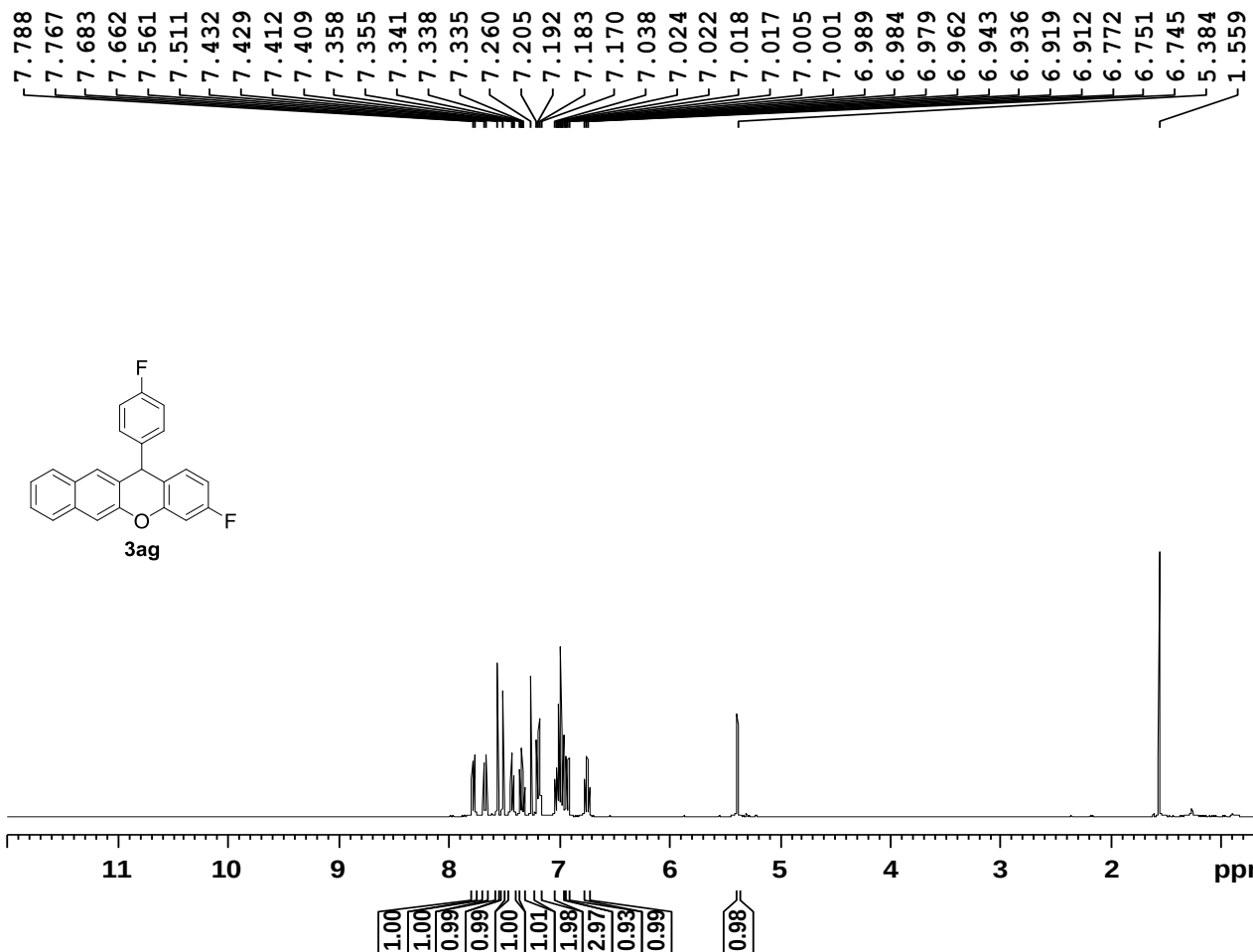
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127579 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 12: ^{13}C -NMR spectra for compound **3af**

PROTON CDCl3 {D:\CRR} CIF_NMR 1



Current Data Parameters
 NAME MK-II-400
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190422
 Time 12.38
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 456
 DW 60.800 usec
 DE 6.00 usec
 TE 292.6 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.35 usec
 PL1 -1.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300093 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure 13: ¹H-NMR spectra for compound **3ag**

PROTON CDCl3 {D:\CRR} ClF_NMR 1

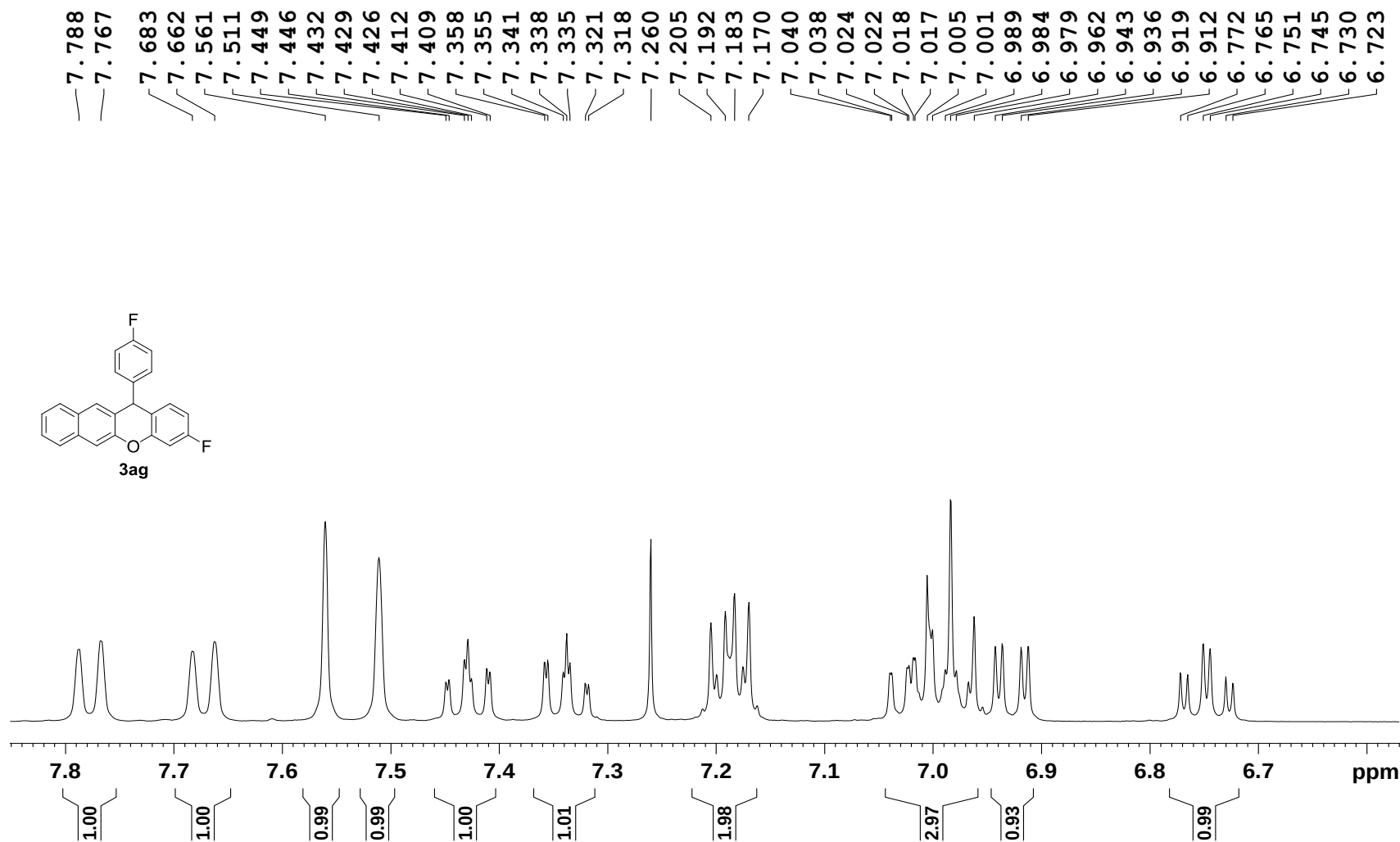
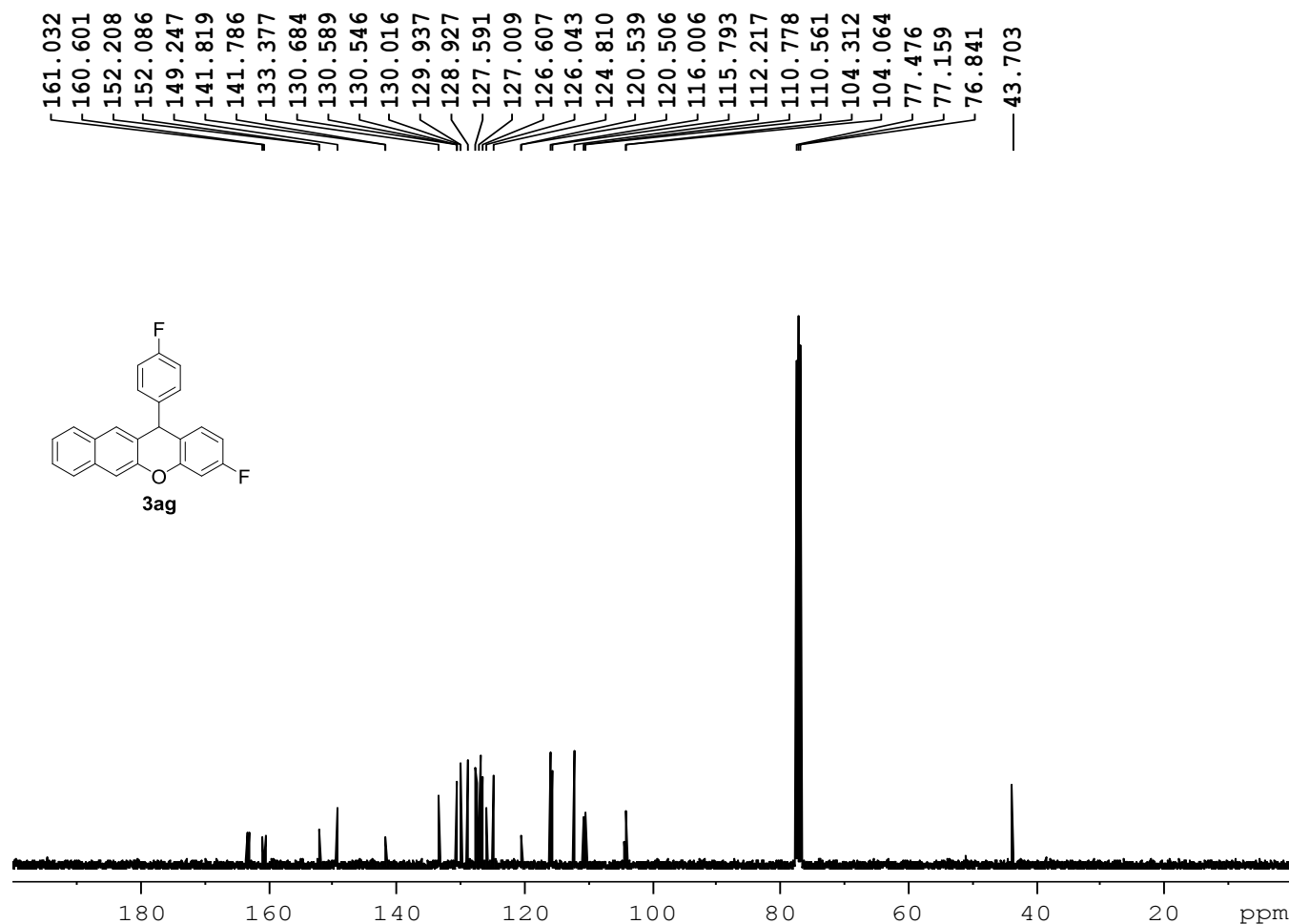


Figure 13a: ^1H -NMR spectra expansion for compound **3ag**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-400
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190423
Time 10.22
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 256
DW 20.800 usec
DE 6.00 usec
TE 291.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127591 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 14: ¹³C-NMR spectra for compound **3ag**

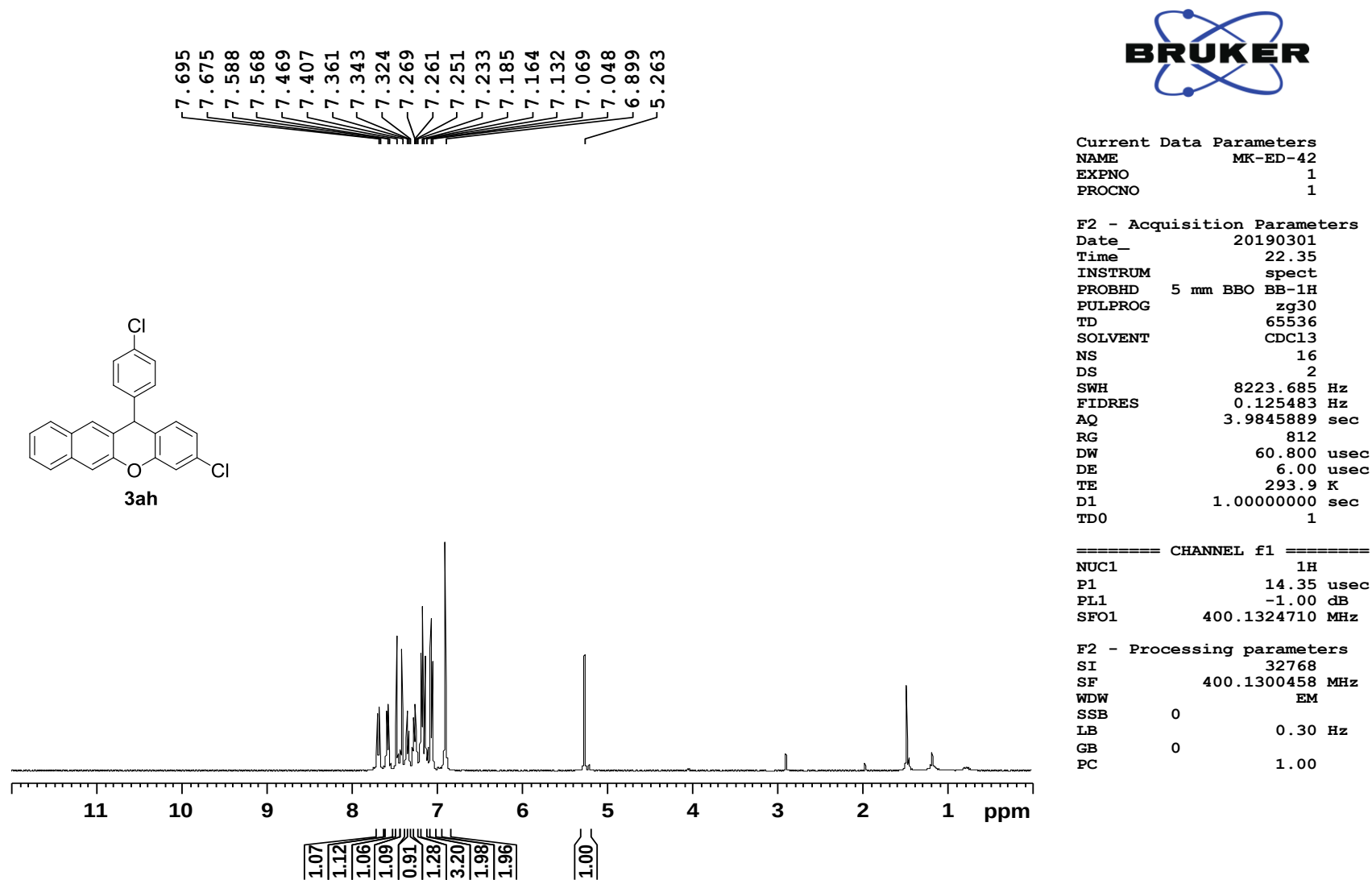


Figure 15: ¹H-NMR spectra for compound **3ah**

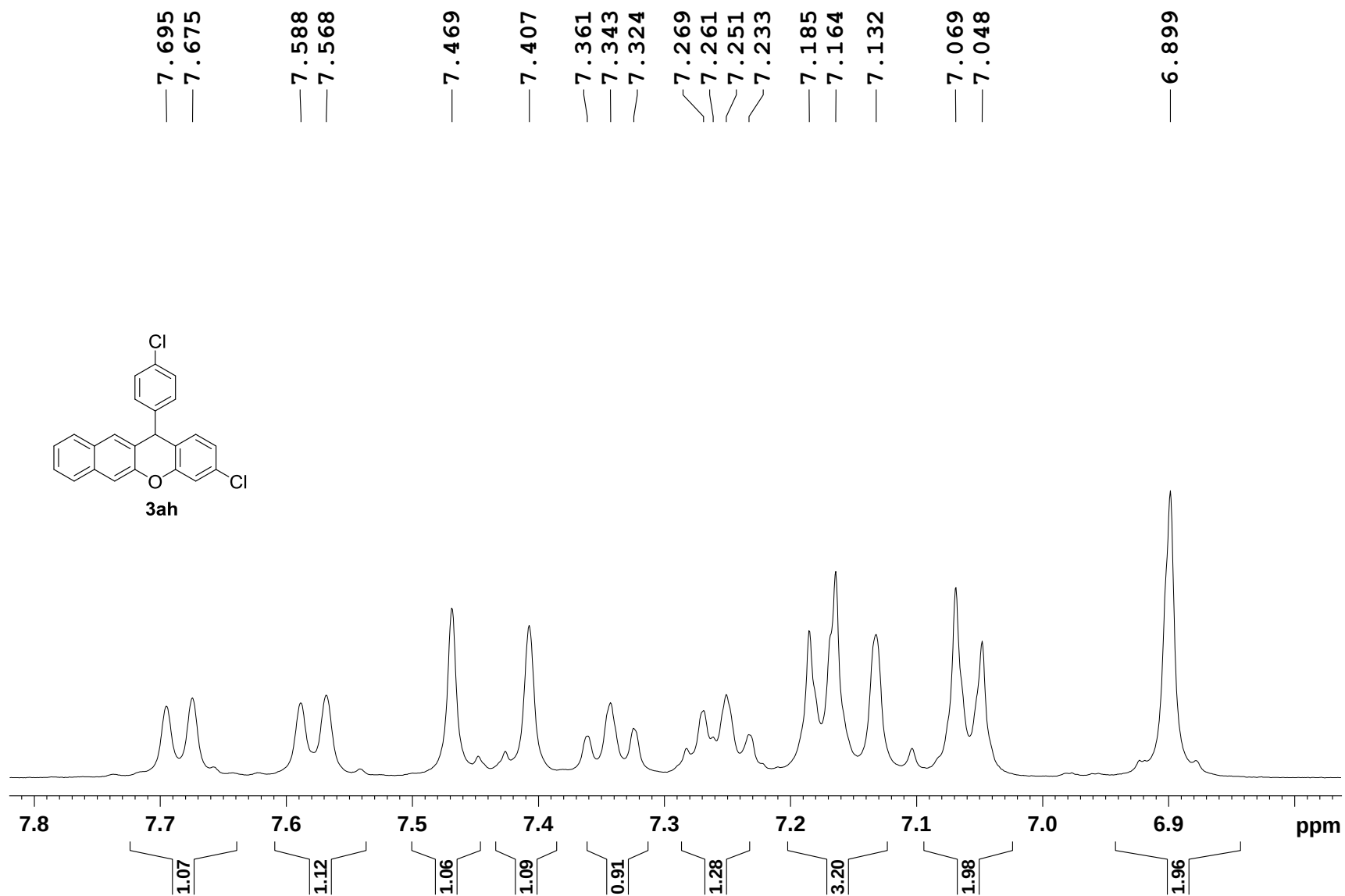
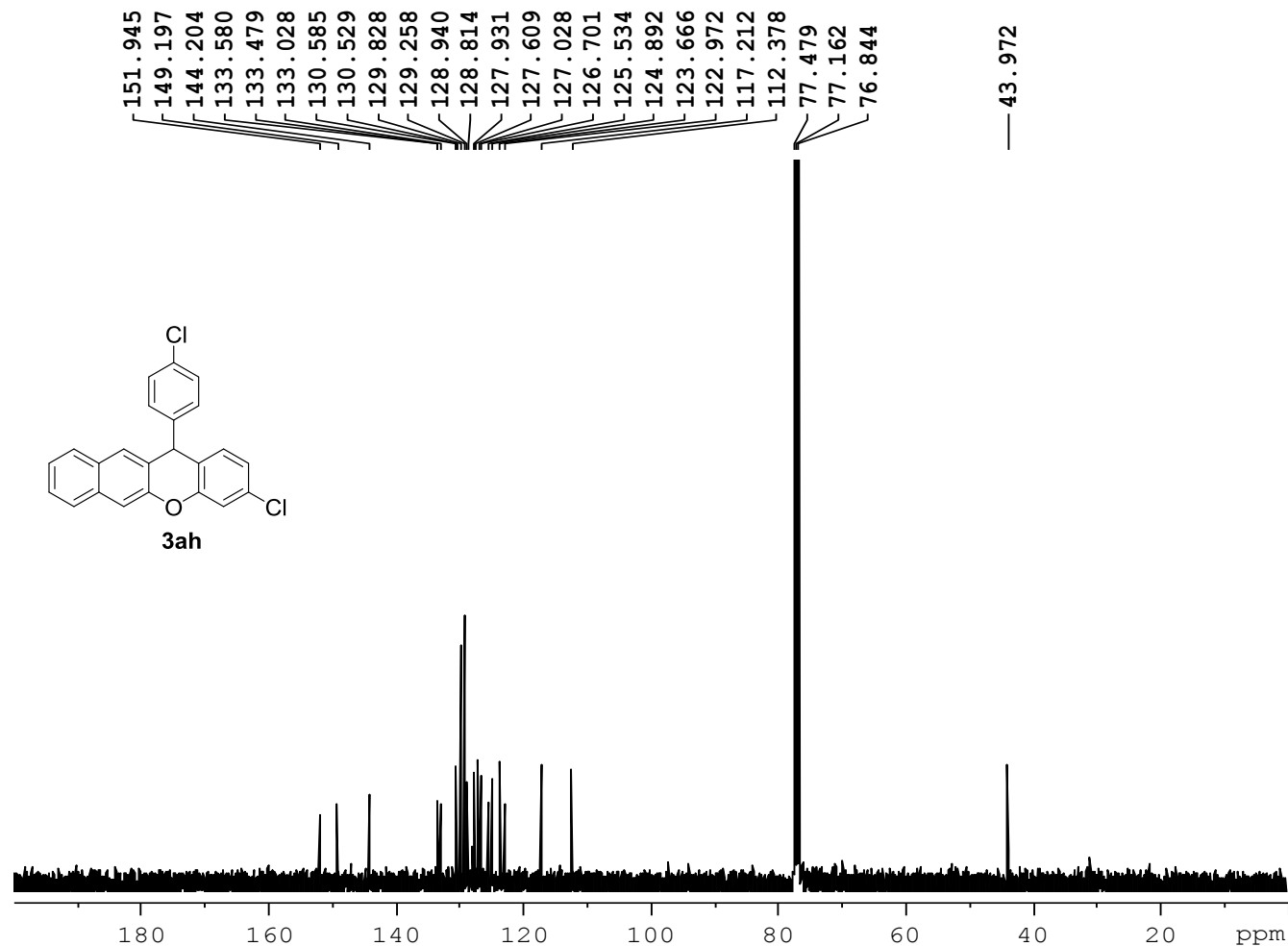


Figure 15a: $^1\text{H-NMR}$ spectra expansion for compound **3ah**

C13CPD CDCl3 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-ED-42-A
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190320
Time_ 19.30
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 40.3
DW 20.800 usec
DE 6.00 usec
TE 297.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

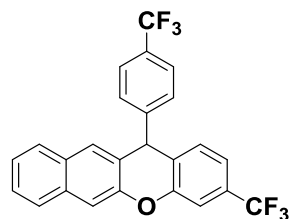
F2 - Processing parameters
SI 32768
SF 100.6127558 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 16: ¹³C-NMR spectra for compound **3ah**

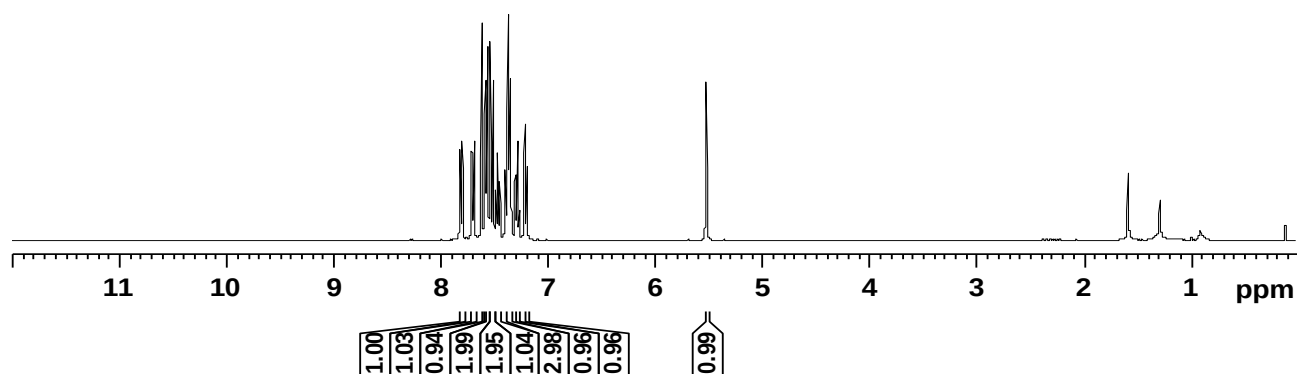
PROTON CDCl3



7.813
7.793
7.702
7.682
7.610
7.577
7.557
7.530
7.503
7.479
7.461
7.442
7.386
7.363
7.342
7.296
7.276
7.260
7.209
7.189
5.514



3ai



Current Data Parameters
NAME MK-ED-39
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190212
Time_ 10.50
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 181
DW 60.800 usec
DE 6.00 usec
TE 292.6 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 17: ¹H-NMR spectra for compound 3ai

PROTON CDCL₃

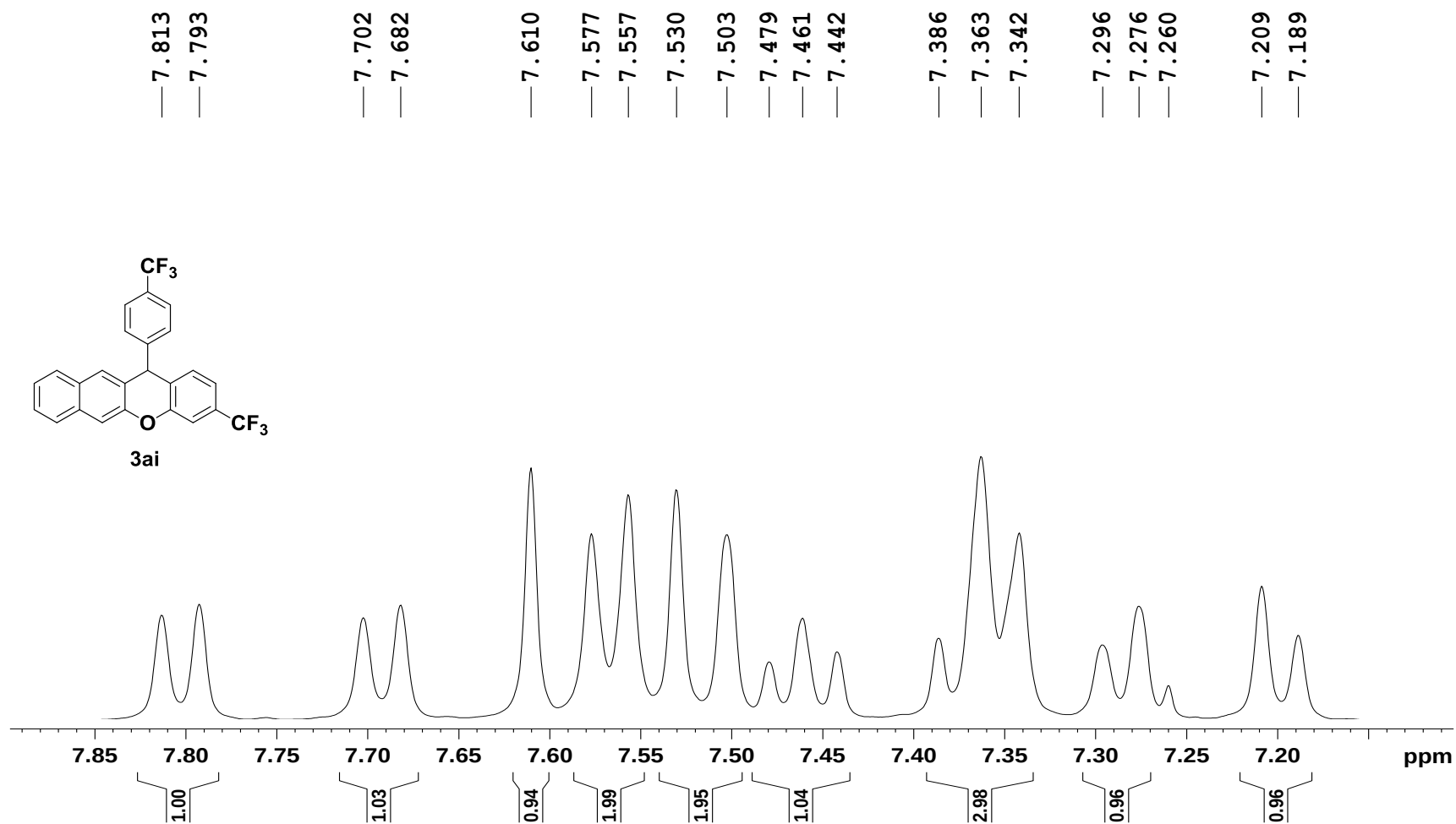
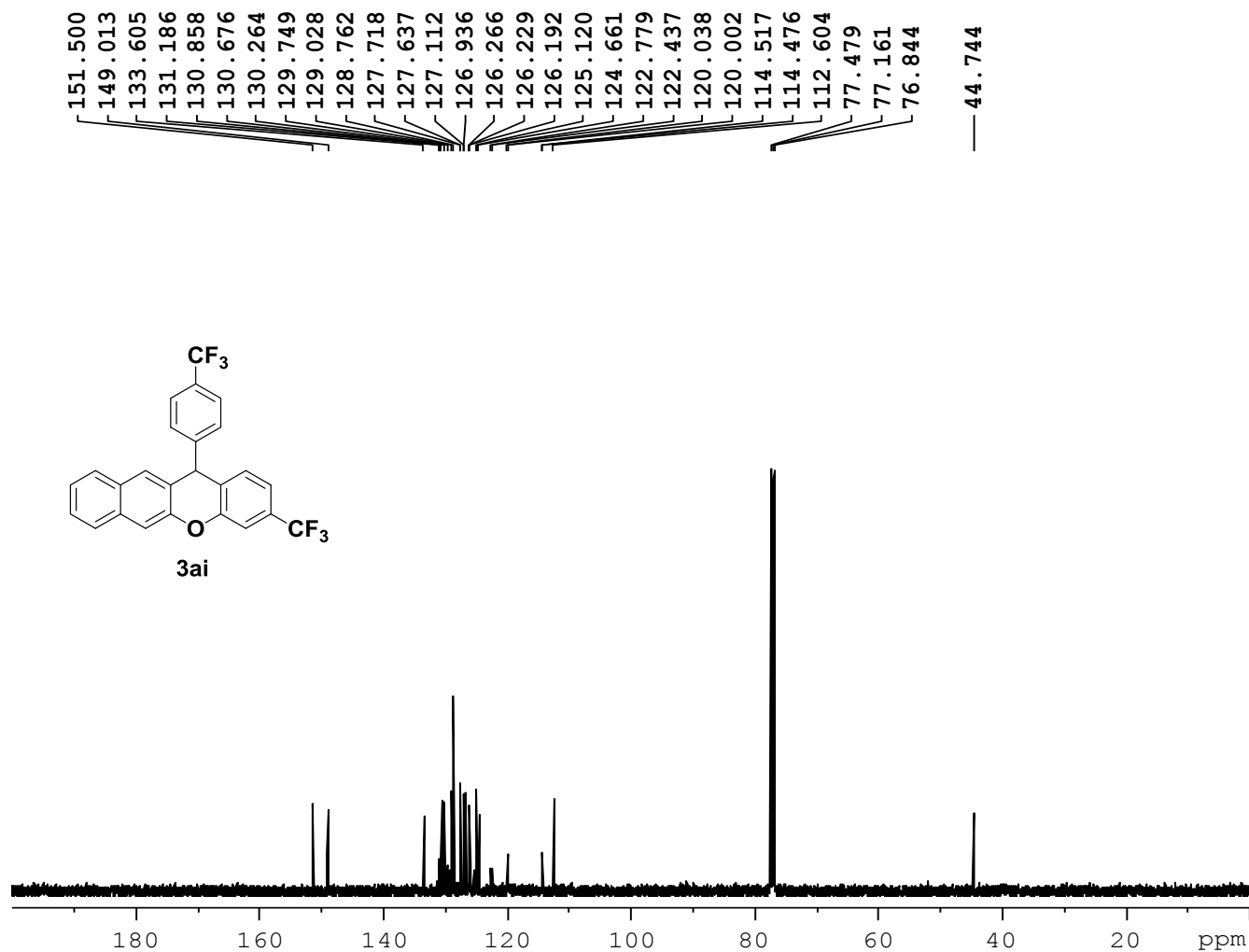


Figure 17a: ¹H-NMR spectra expansion for compound **3ai**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-ED-39A
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190322
Time 7.38
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 167
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 912
DW 20.800 usec
DE 6.00 usec
TE 295.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

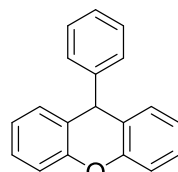
F2 - Processing parameters
SI 32768
SF 100.6127570 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 18: ¹³C-NMR spectra for compound **3ai**

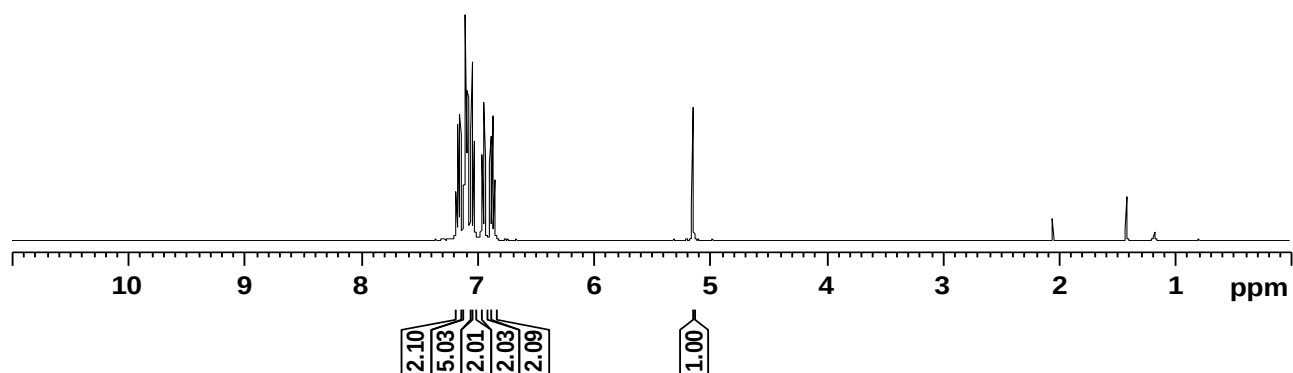
PROTON CDCl3 {D:\CRR} nmr 1



7.180
7.178
7.160
7.147
7.142
7.117
7.113
7.101
7.096
7.093
7.088
7.084
7.080
7.075
7.043
7.040
7.022
7.019
6.954
6.937
6.883
6.880
6.865
6.864
6.862
6.846
6.843
5.141



3ba



Current Data Parameters
NAME MK-XN-M1
EXPNO 1
PROCNO 1

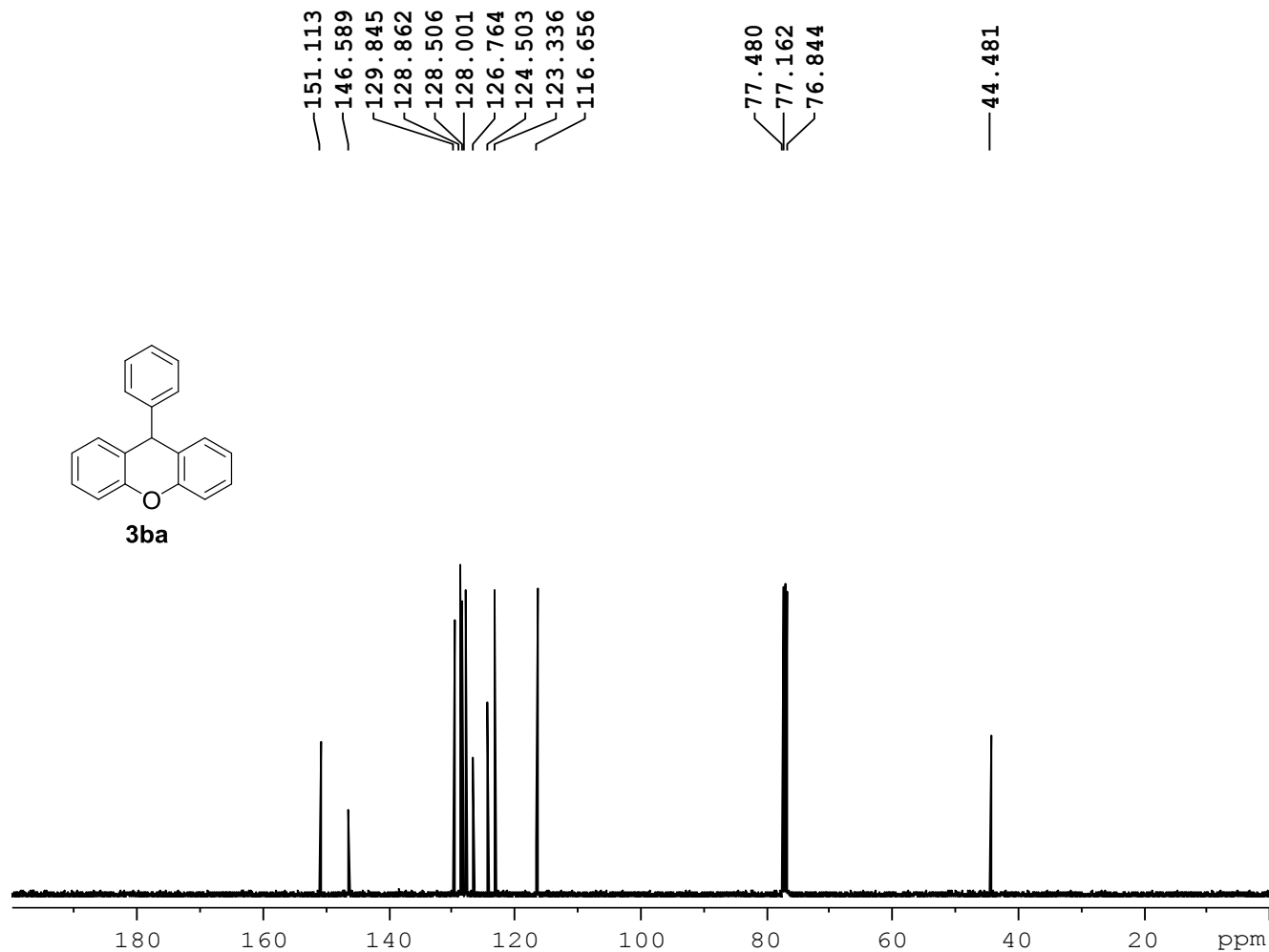
F2 - Acquisition Parameters
Date 20190102
Time 10.31
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 114
DW 60.800 usec
DE 6.00 usec
TE 289.8 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300673 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 19: ¹H-NMR spectra for compound **3ba**

C13CPD CDC13 {D:\CRR} nmr 1



Current Data Parameters
 NAME MK-XN-M1
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190102
 Time_ 10.48
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 256
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 406
 DW 20.800 usec
 DE 6.00 usec
 TE 290.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.95 usec
 PL1 -1.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL12 14.95 dB
 PL13 120.00 dB
 PL2 -1.00 dB
 SFO2 400.1316005 MHz

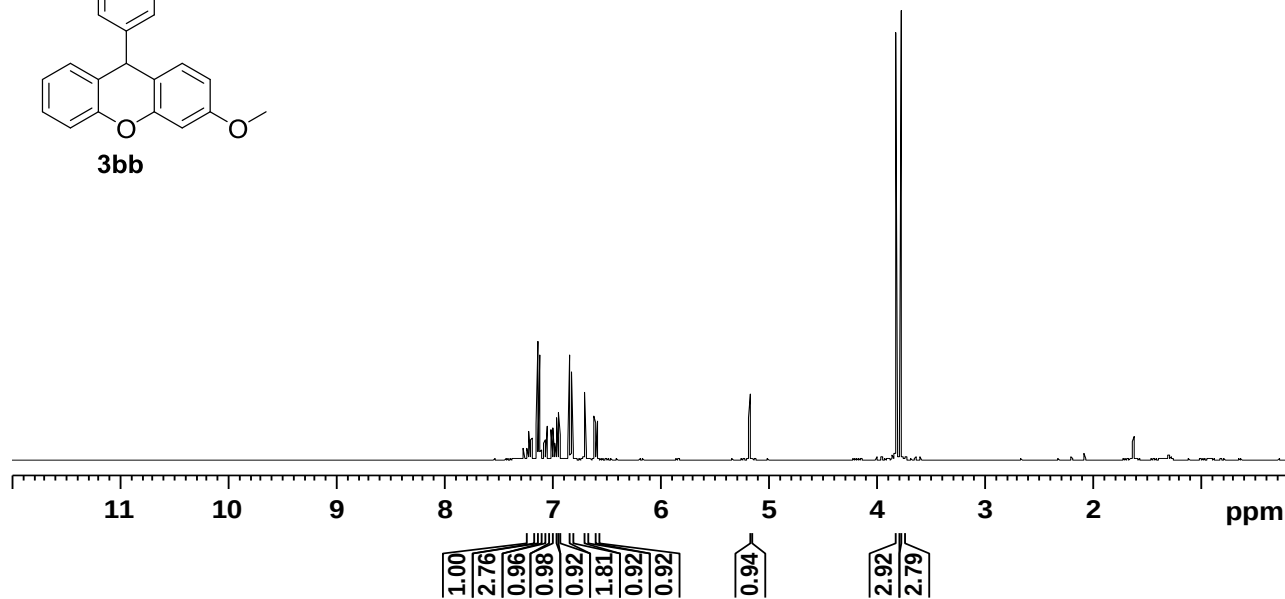
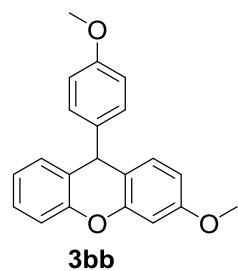
F2 - Processing parameters
 SI 32768
 SF 100.6127642 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure 20: ¹³C-NMR spectra for compound **3ba**

PROTON CDCl3 {D:\CRR} CIF_NMR 1



7.228
7.224
7.223
7.207
7.204
7.190
7.186
7.134
7.130
7.125
7.114
7.108
7.101
7.065
7.061
7.045
7.043
7.042
7.004
7.000
6.986
6.983
6.952
6.950
6.930
6.929
6.843
6.836
6.831
6.819
6.814
6.696
6.689
6.601
6.595
6.580
6.573
5.166
3.811
3.767



Current Data Parameters
NAME MK-ED-45
EXPNO 1
PROCNO 1

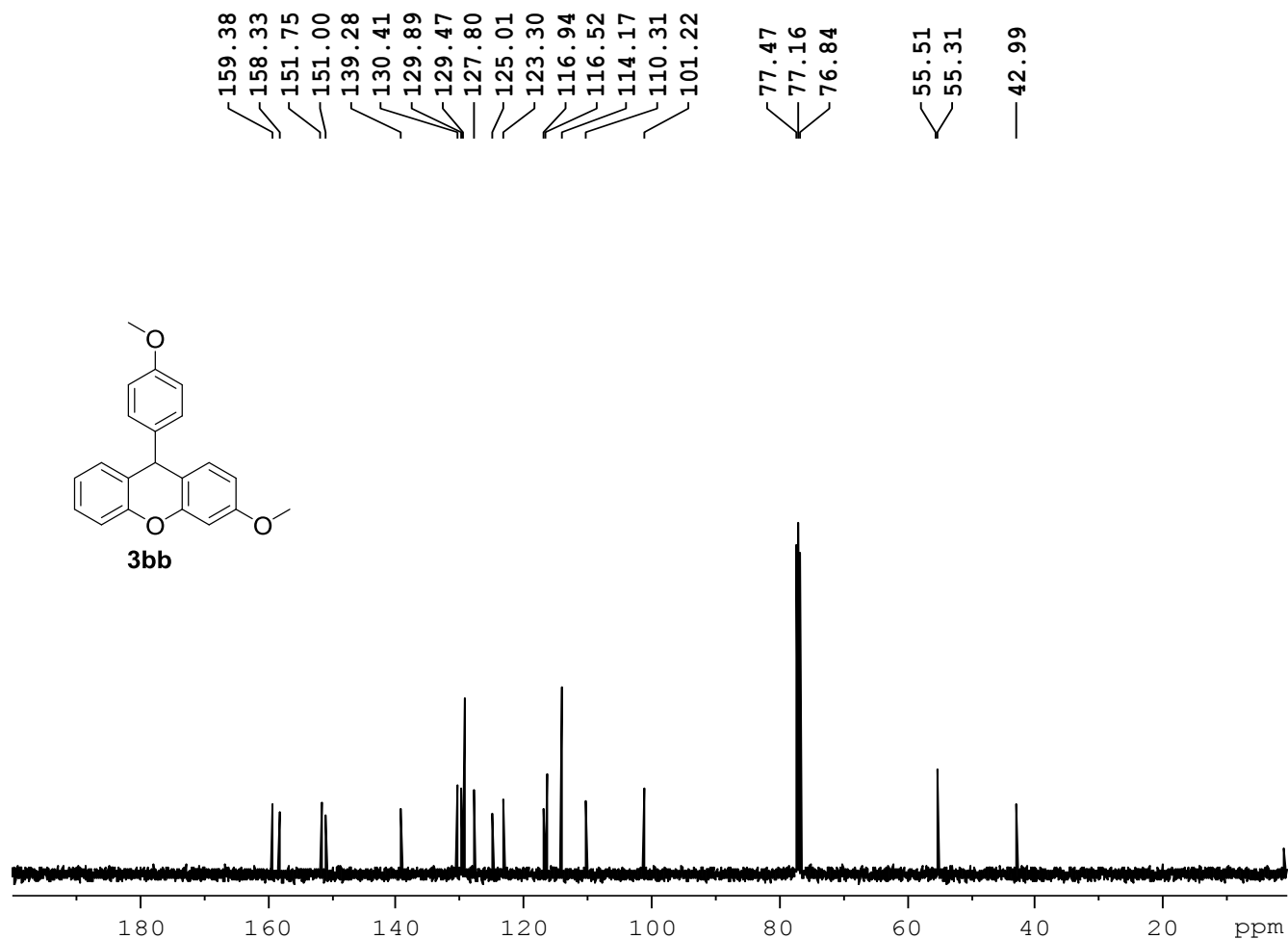
F2 - Acquisition Parameters
Date_ 20190318
Time 14.54
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 128
DW 60.800 usec
DE 6.00 usec
TE 294.7 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 21: ¹H-NMR spectra for compound **3bb**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-ED-45
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190318
Time 15.01
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 101
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 645
DW 20.800 usec
DE 6.00 usec
TE 294.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

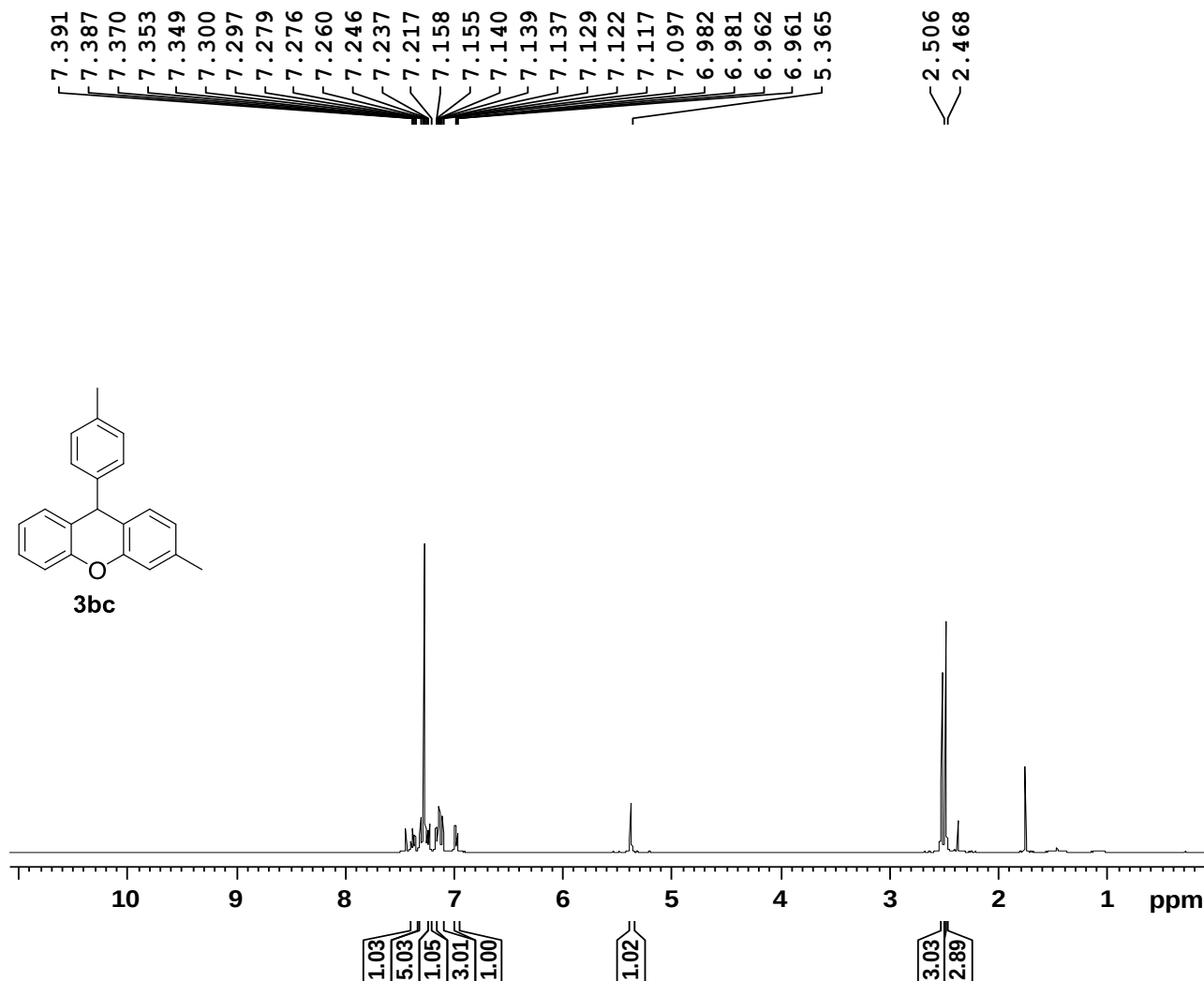
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127608 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 22: ^{13}C -NMR spectra for compound 3bb

PROTON CDCl3 {D:\CRR} nmr 1



Current Data Parameters
NAME MK-XN-M4
EXPNO 1
PROCNO 1

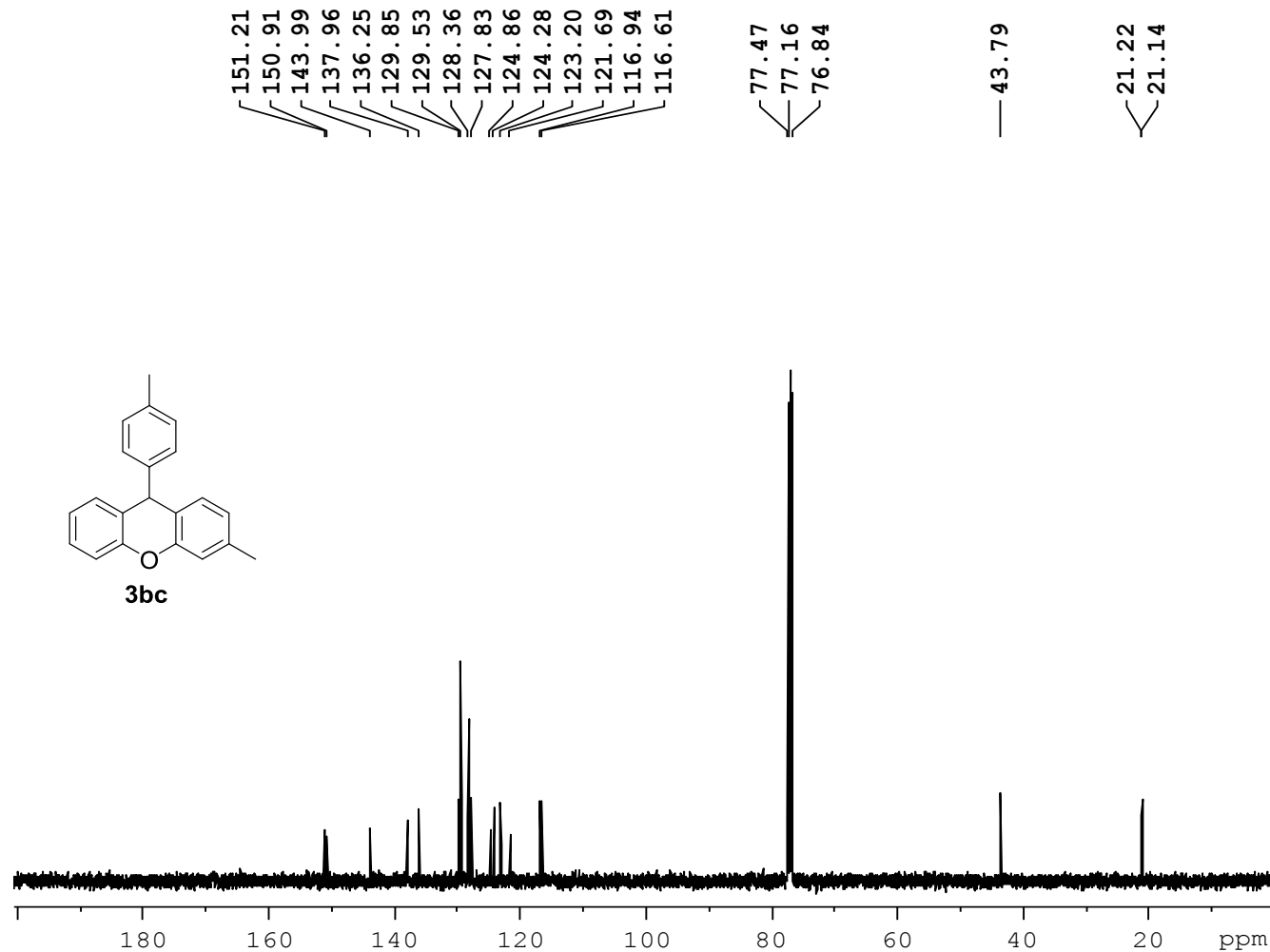
F2 - Acquisition Parameters
Date_ 20190104
Time 12.26
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 228
DW 60.800 usec
DE 6.00 usec
TE 293.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1299353 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 23: ¹H-NMR spectra for compound **3bc**

C13CPD CDC13 {D:\CRR} nmr 1



Current Data Parameters
 NAME MK-XN-M4
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190104
 Time_ 12.42
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 220
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 45.2
 DW 20.800 usec
 DE 6.00 usec
 TE 294.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

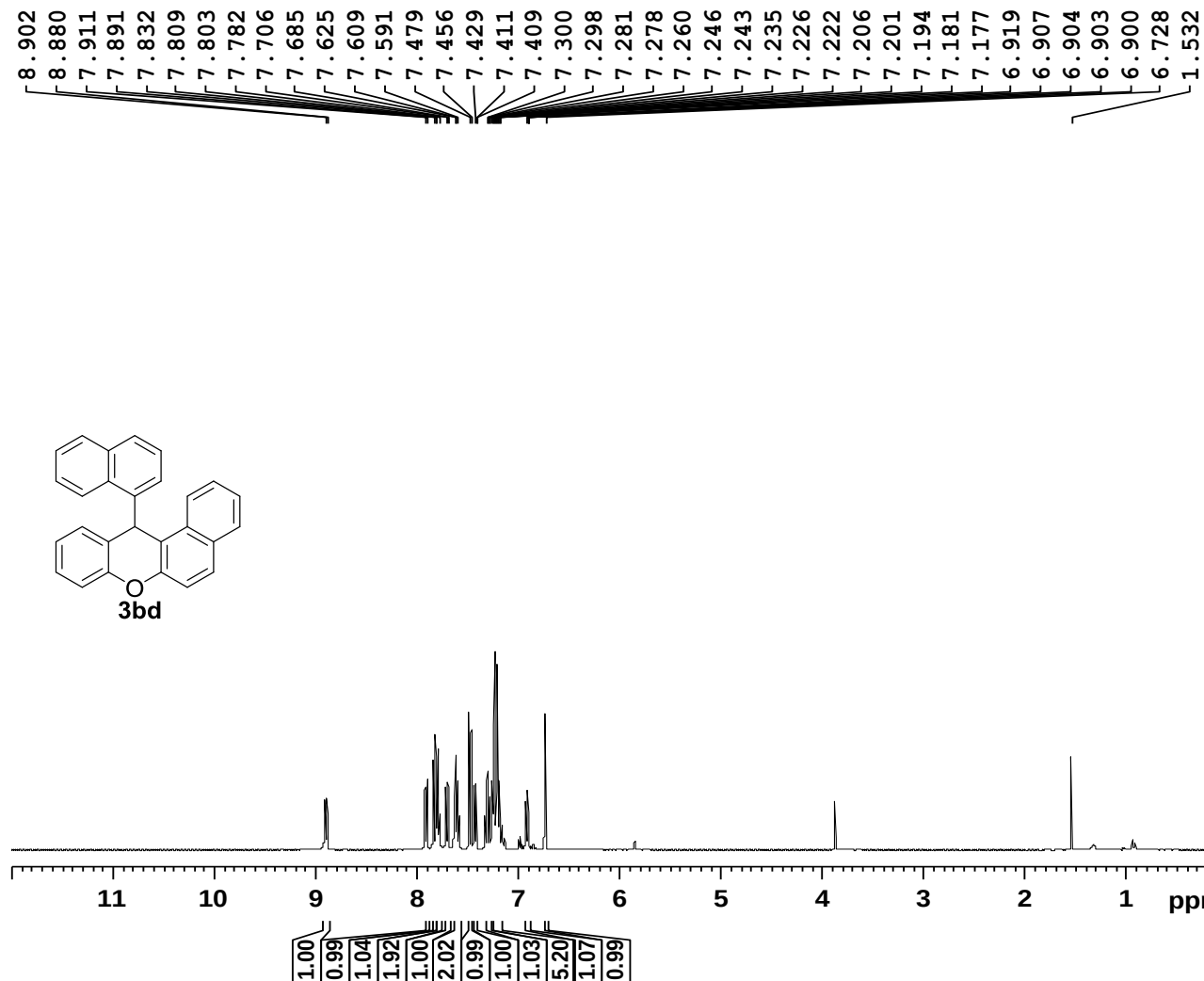
===== CHANNEL f1 =====
 NUC1 13C
 P1 9.95 usec
 PL1 -1.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL12 14.95 dB
 PL13 120.00 dB
 PL2 -1.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127570 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure 24: ¹³C-NMR spectra for compound **3bc**

PROTON CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
 NAME MK-XN-M5-F
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190622
 Time 18.40
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 161
 DW 60.800 usec
 DE 6.00 usec
 TE 293.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.35 usec
 PL1 -1.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300095 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure 25: ^1H -NMR spectra for compound **3bd**

PROTON CDCl3 {D:\CRR} CIF_NMR 1

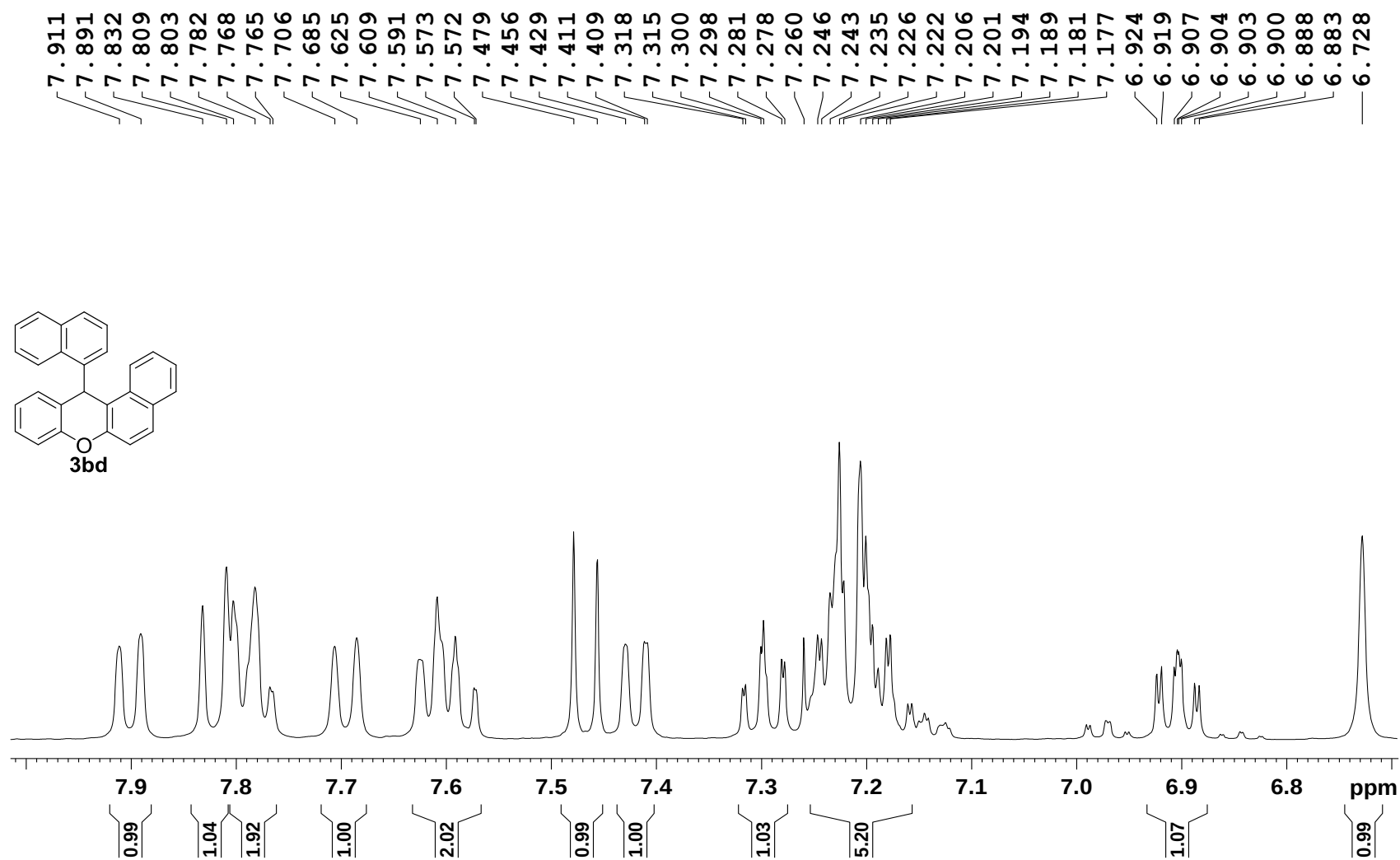
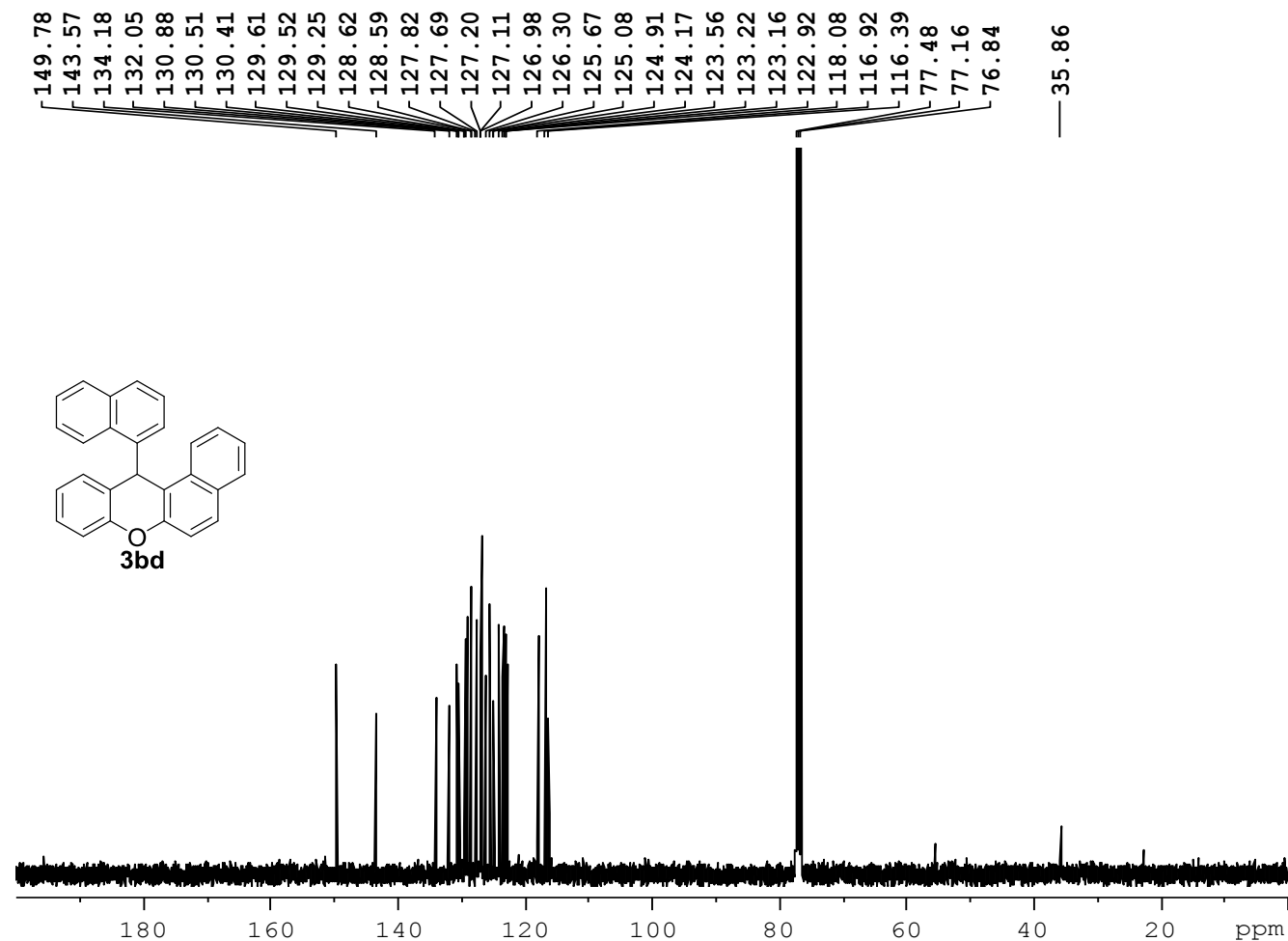


Figure 25a: ¹H-NMR spectra expansion for compound **3bd**



Current Data Parameters
NAME MK-XN-M5-F
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190622
Time 19.11
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 36
DW 20.800 usec
DE 6.00 usec
TE 293.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

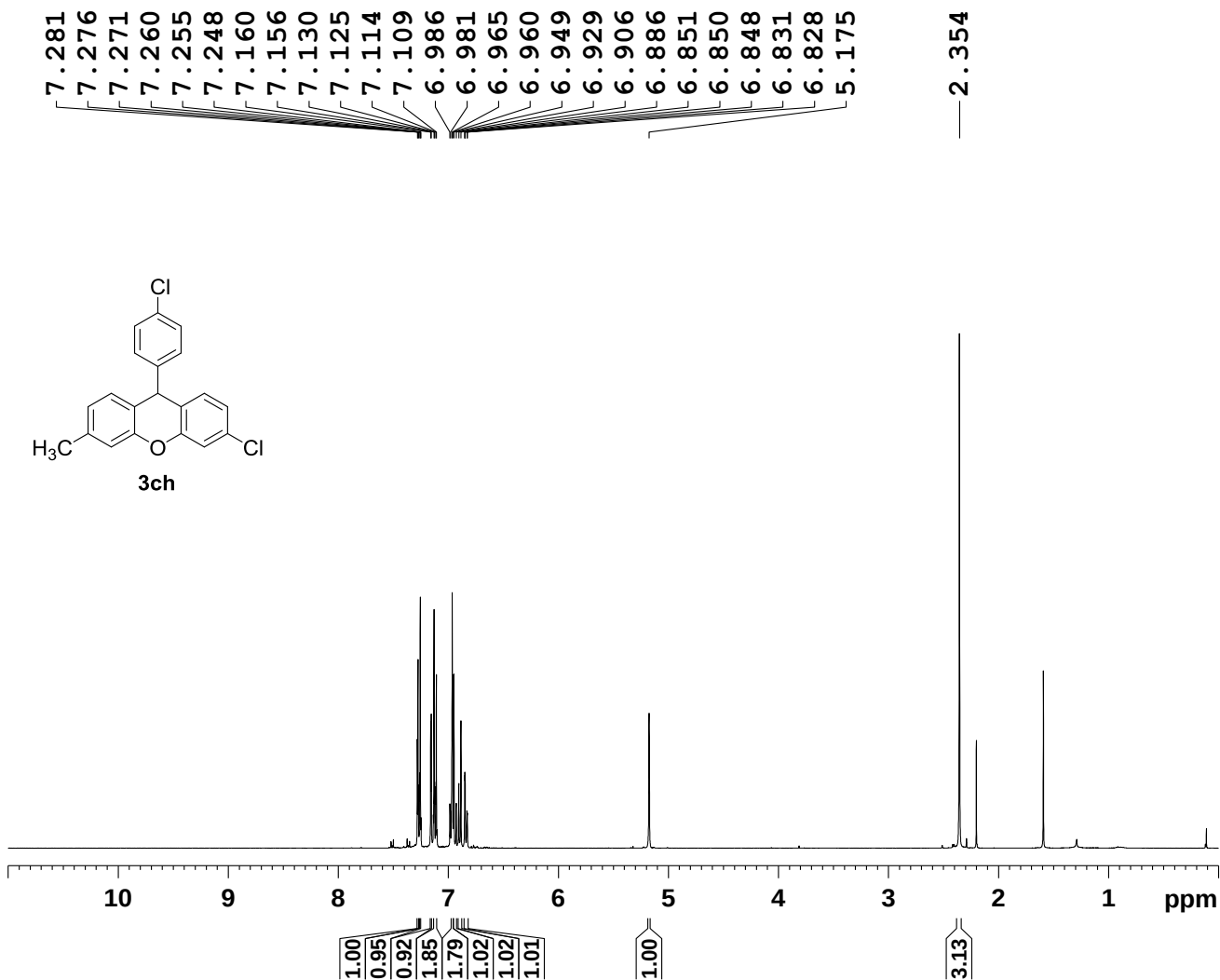
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127608 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 26: ^{13}C -NMR spectra for compound **3bd**

PROTON CDCl3 {D:\CRR} CIF_NMR 1



Current Data Parameters
 NAME MK-II-387
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190403
 Time 11.32
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 228
 DW 60.800 usec
 DE 6.00 usec
 TE 294.5 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.35 usec
 PL1 -1.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300009 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure 27: ¹H-NMR spectra for compound **3ch**

PROTON CDCl3 {D:\CRR} ClF_NMR 1

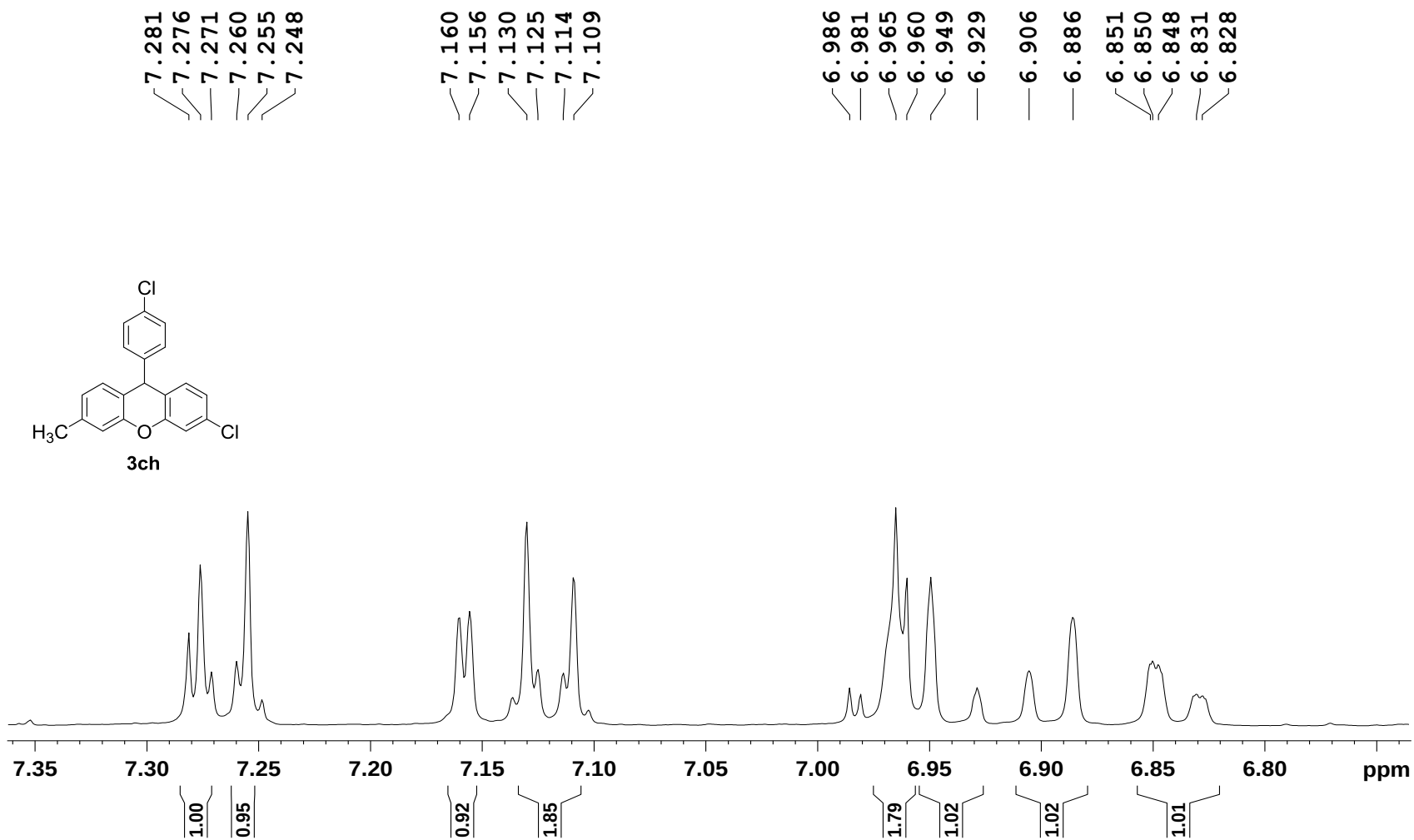
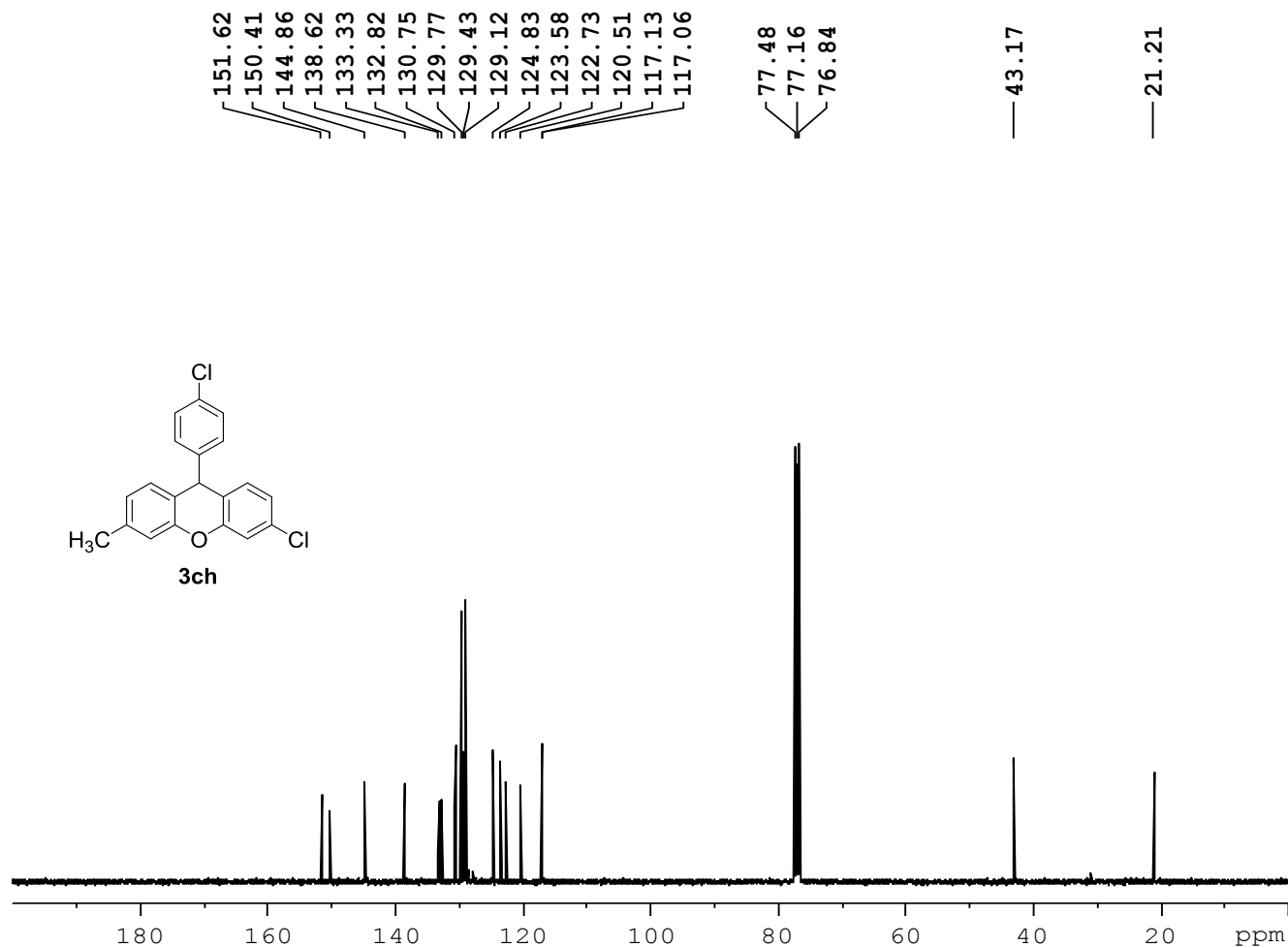


Figure 27a: ^1H -NMR spectra expansion for compound **3ch**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-387
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190403
Time_ 18.39
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 45.2
DW 20.800 usec
DE 6.00 usec
TE 297.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

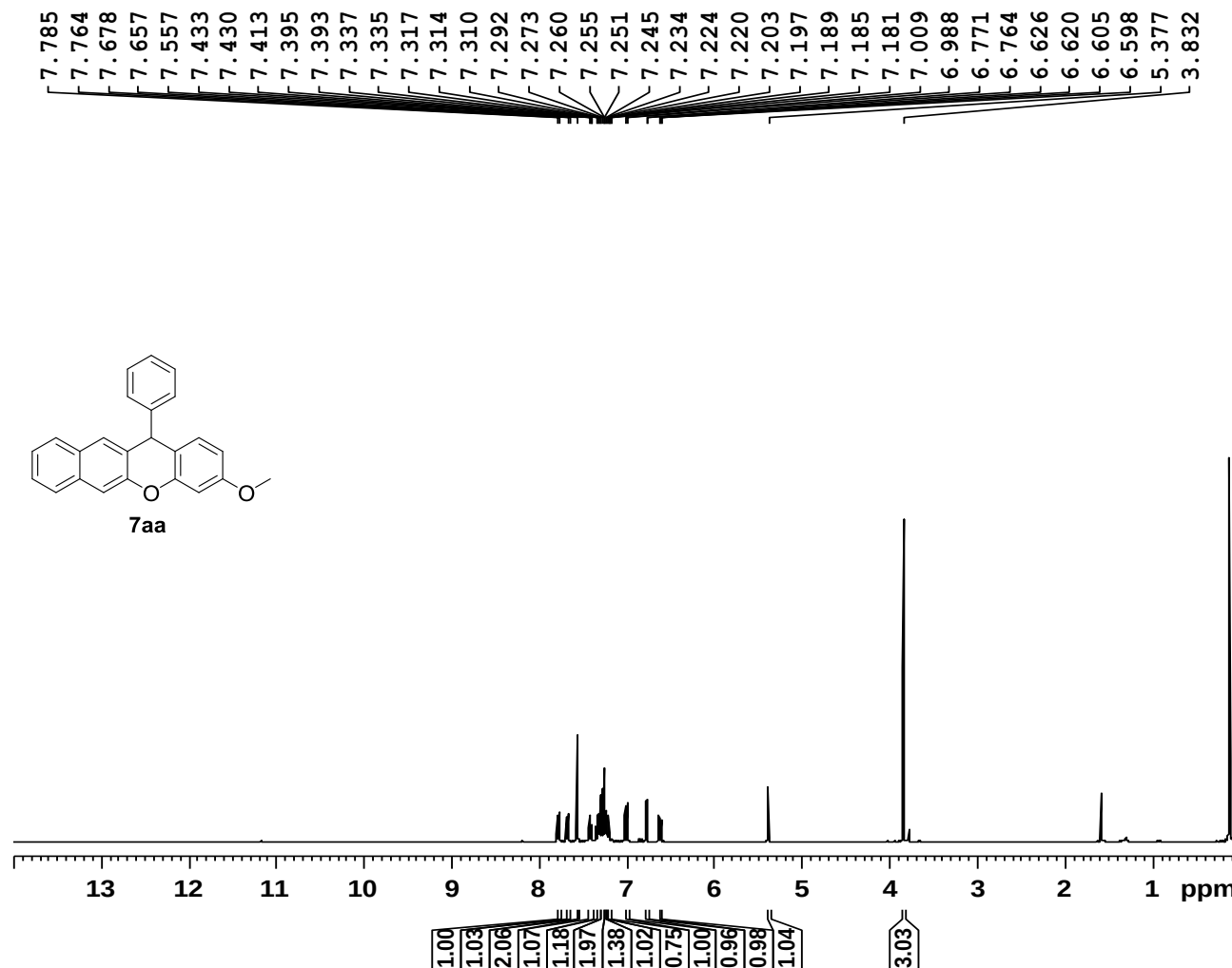
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127572 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 28: ¹³C-NMR spectra for compound **3ch**

PROTON CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-ED-47
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190320
Time 12.53
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 161
DW 60.800 usec
DE 6.00 usec
TE 295.7 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 29: ¹H-NMR spectra for compound **7aa**

PROTON CDCl3 {D:\CRR} CIF_NMR 1

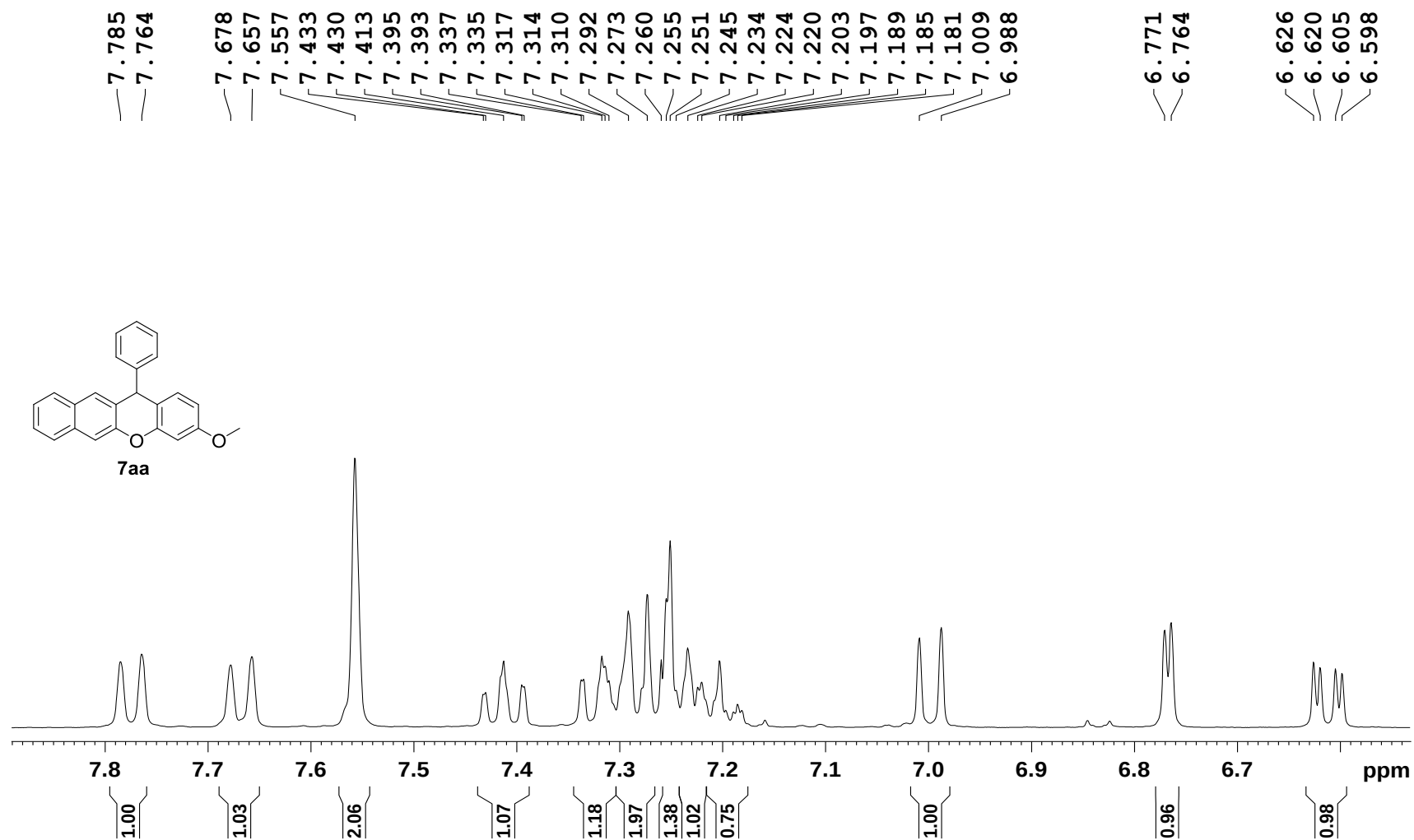
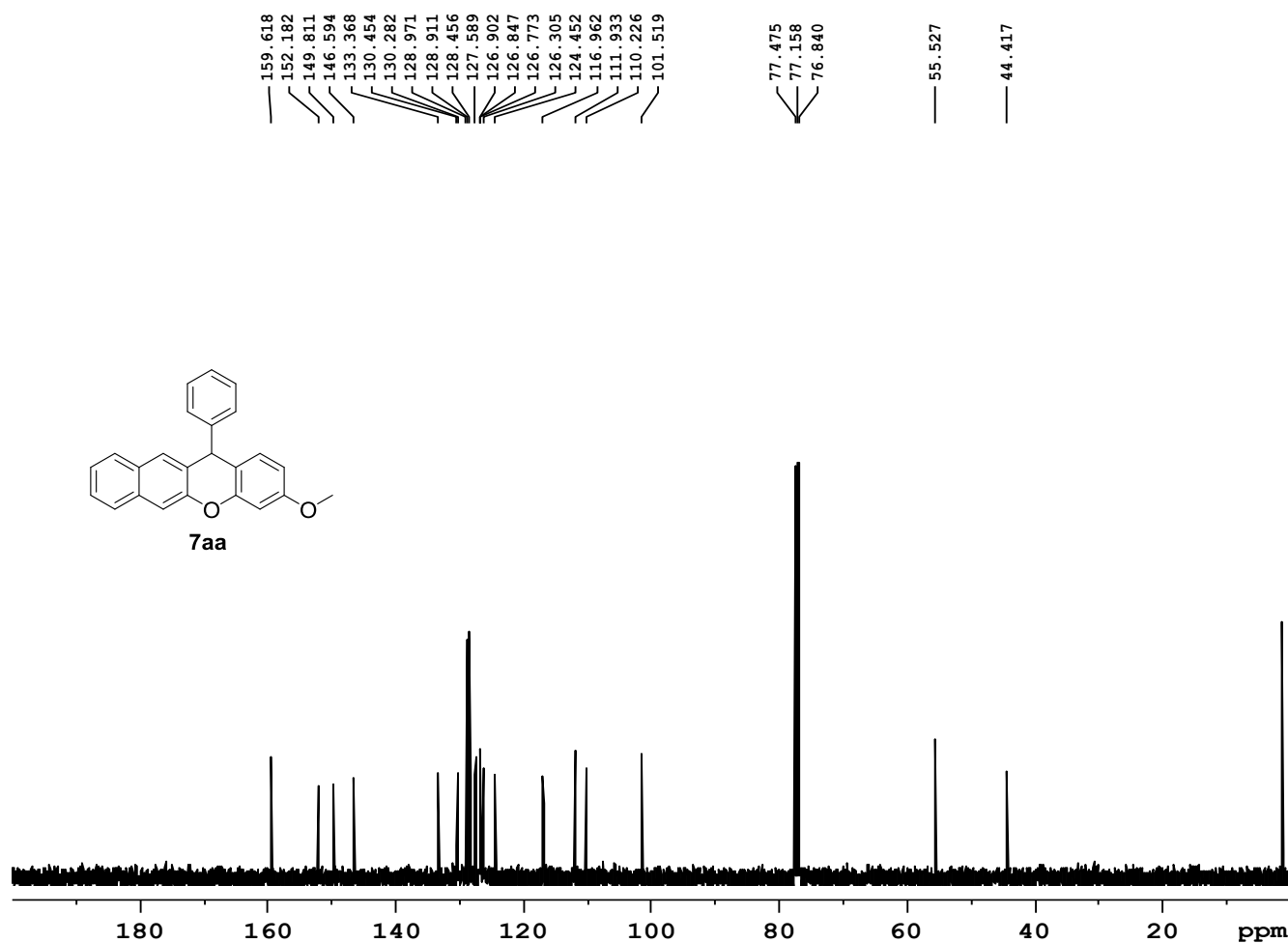


Figure 29: ¹H-NMR spectra for compound **7aa**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-ED-47A
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190320
Time 23.56
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 101
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 724
DW 20.800 usec
DE 6.00 usec
TE 298.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

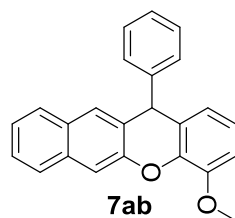
F2 - Processing parameters
SI 32768
SF 100.6127634 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 30: ^{13}C -NMR spectra for compound **7aa**

PROTON CDC13 {D:\CRR} CIF_NMR 1



8.695
8.690
8.672
8.294
8.272
7.815
7.808
7.797
7.792
7.520
7.516
7.509
7.503
7.496
7.490
7.486
7.313
7.304
7.299
7.294
7.289
7.280
7.260
7.190
7.185
7.171
7.167
7.114
7.027
7.021
7.006
7.000
6.897
6.891
5.084
3.810



Current Data Parameters
NAME MK-II-403
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190424
Time_ 10.50
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 256
DW 60.800 usec
DE 6.00 usec
TE 297.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

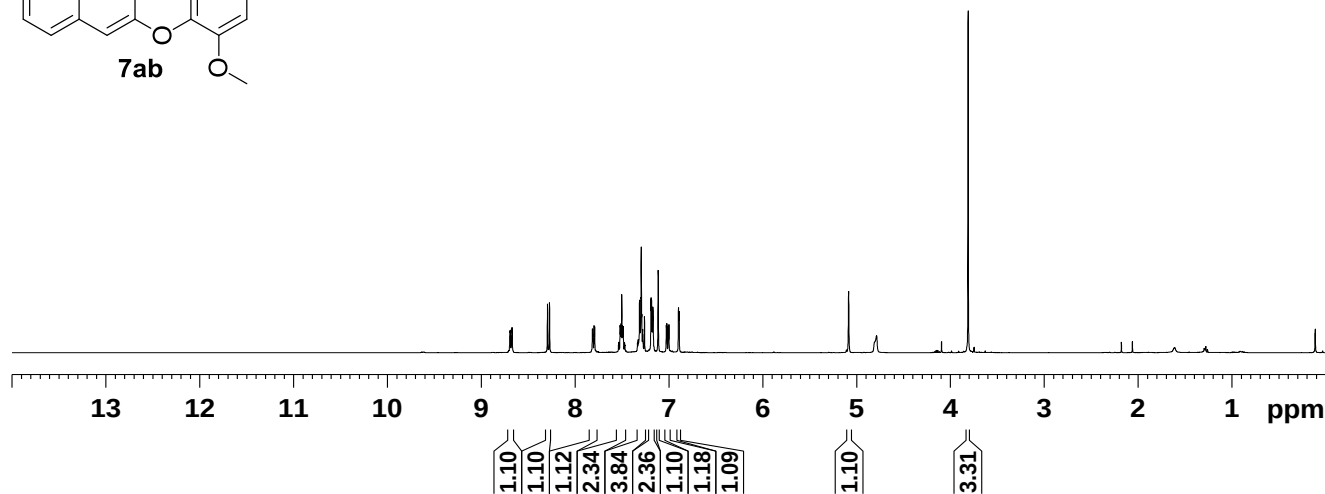


Figure 31: ¹H-NMR spectra for compound **7ab**

PROTON CDC13 {D:\CRR} CIF_NMR 1

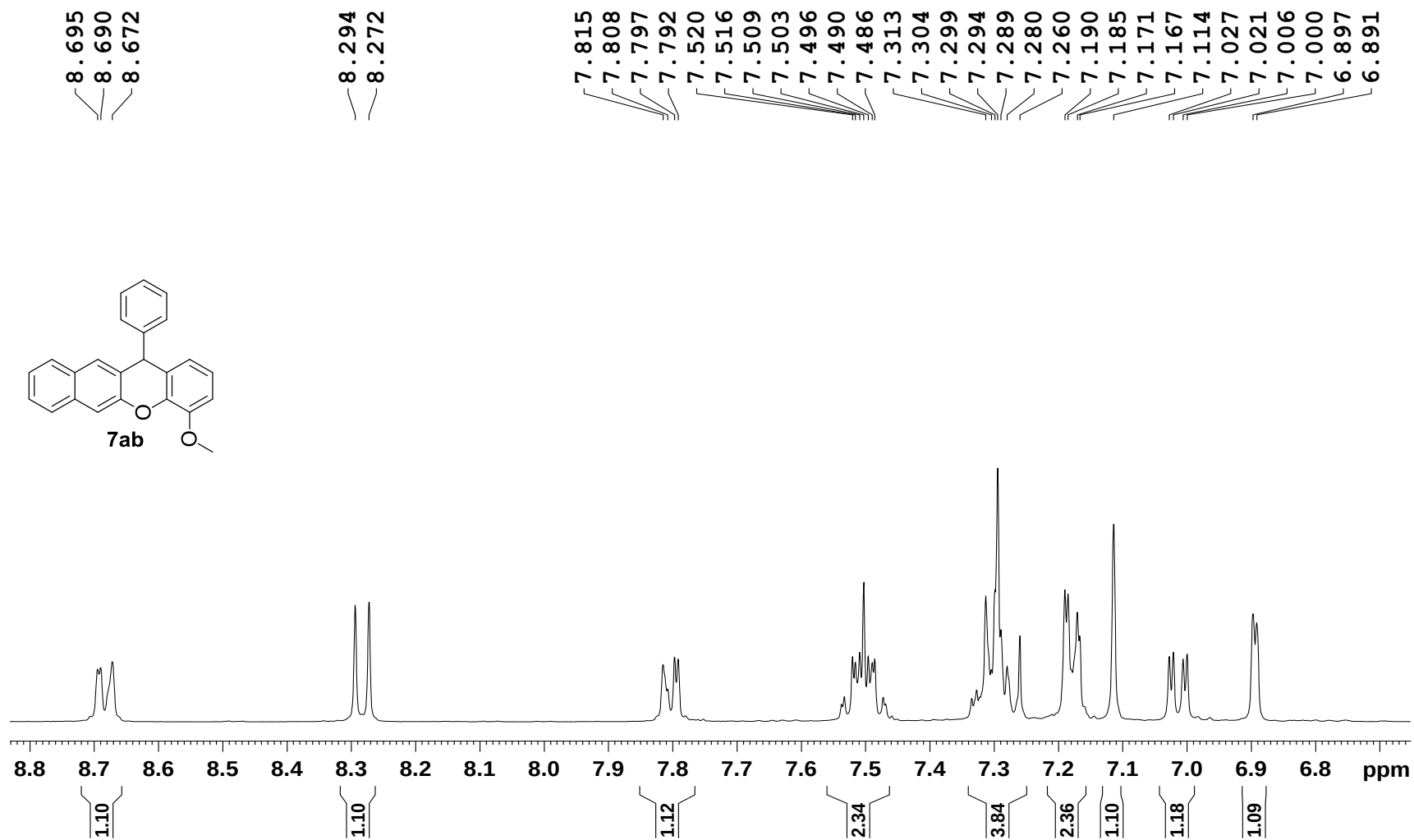
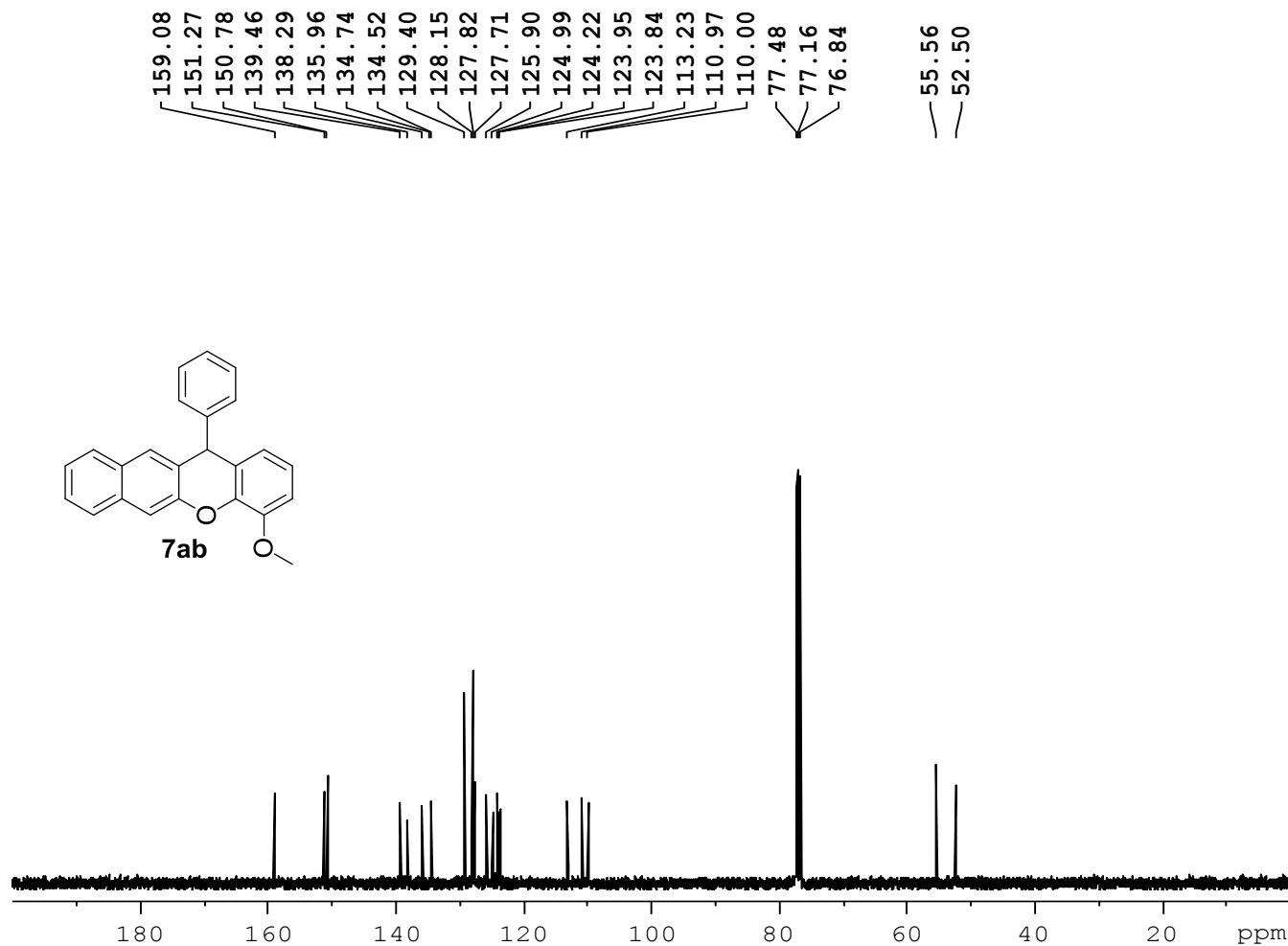


Figure 31a: ^1H -NMR spectra expansion for compound **7ab**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
 NAME MK-I-403
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190424
 Time_ 19.23
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 129
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 228
 DW 20.800 usec
 DE 6.00 usec
 TE 294.3 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.95 usec
 PL1 -1.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL12 14.95 dB
 PL13 120.00 dB
 PL2 -1.00 dB
 SFO2 400.1316005 MHz

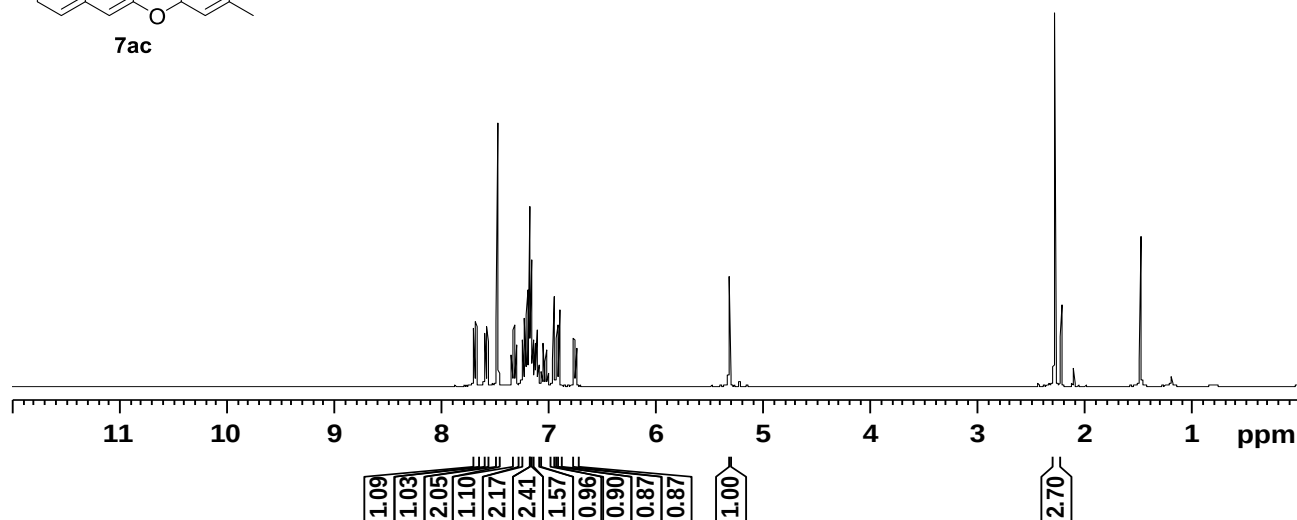
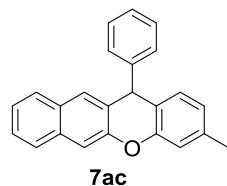
F2 - Processing parameters
 SI 32768
 SF 100.6127631 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure 32: ¹³C-NMR spectra for compound **7ab**

PROTON CDC13 {D:\CRR} CIF_NMR 1



7.668
7.585
7.564
7.473
7.464
7.335
7.332
7.318
7.315
7.297
7.295
7.238
7.236
7.218
7.215
7.200
7.192
7.174
7.171
7.163
7.159
7.142
7.121
7.104
7.041
7.015
6.941
6.911
6.891
6.754
6.752
6.735
6.733
5.306
2.270



Current Data Parameters
NAME MK-II-396
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190408
Time 12.38
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 406
DW 60.800 usec
DE 6.00 usec
TE 294.8 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300450 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 33: ¹H-NMR spectra for compound **7ac**

PROTON CDCl3 {D:\CRR} CIF_NMR 1

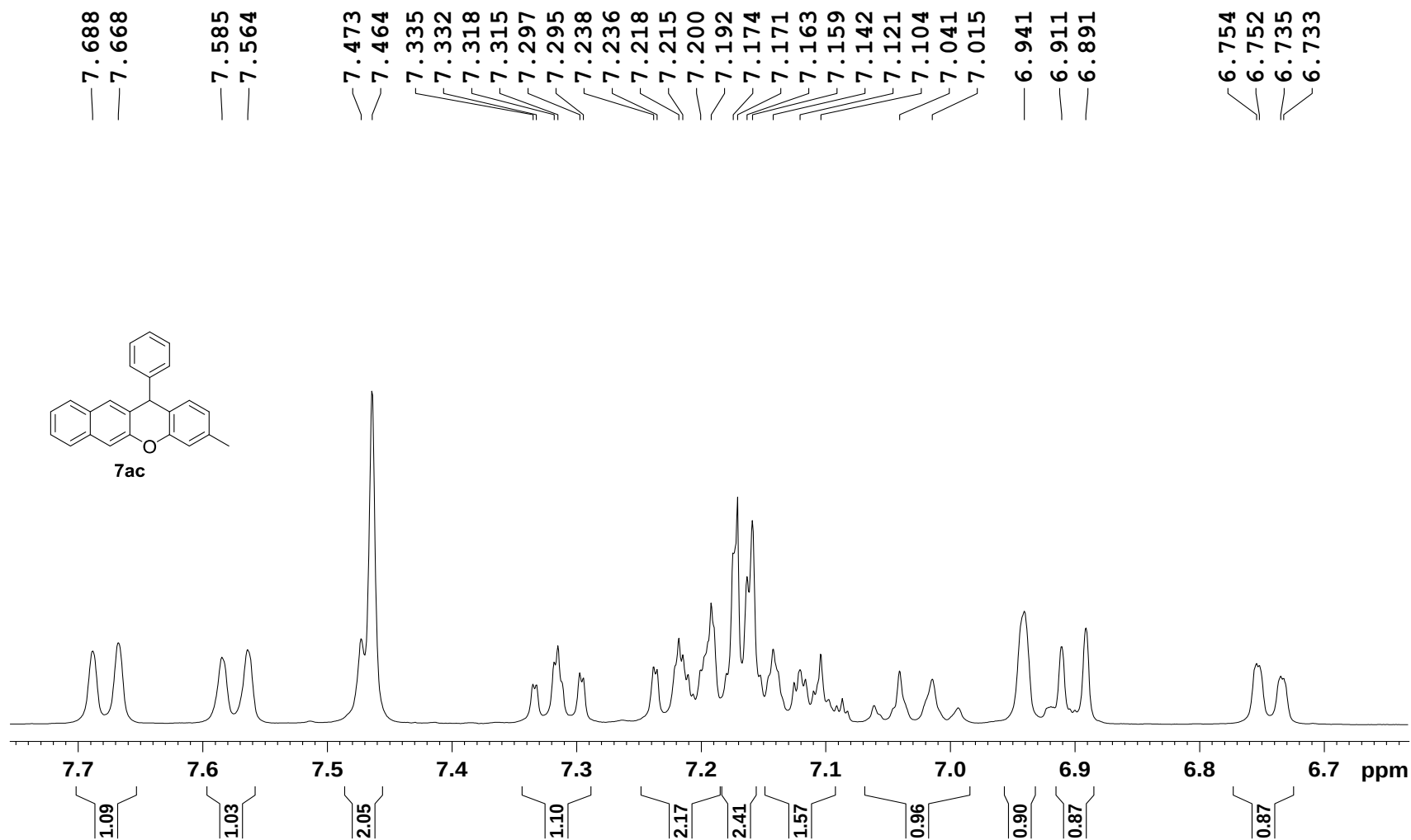
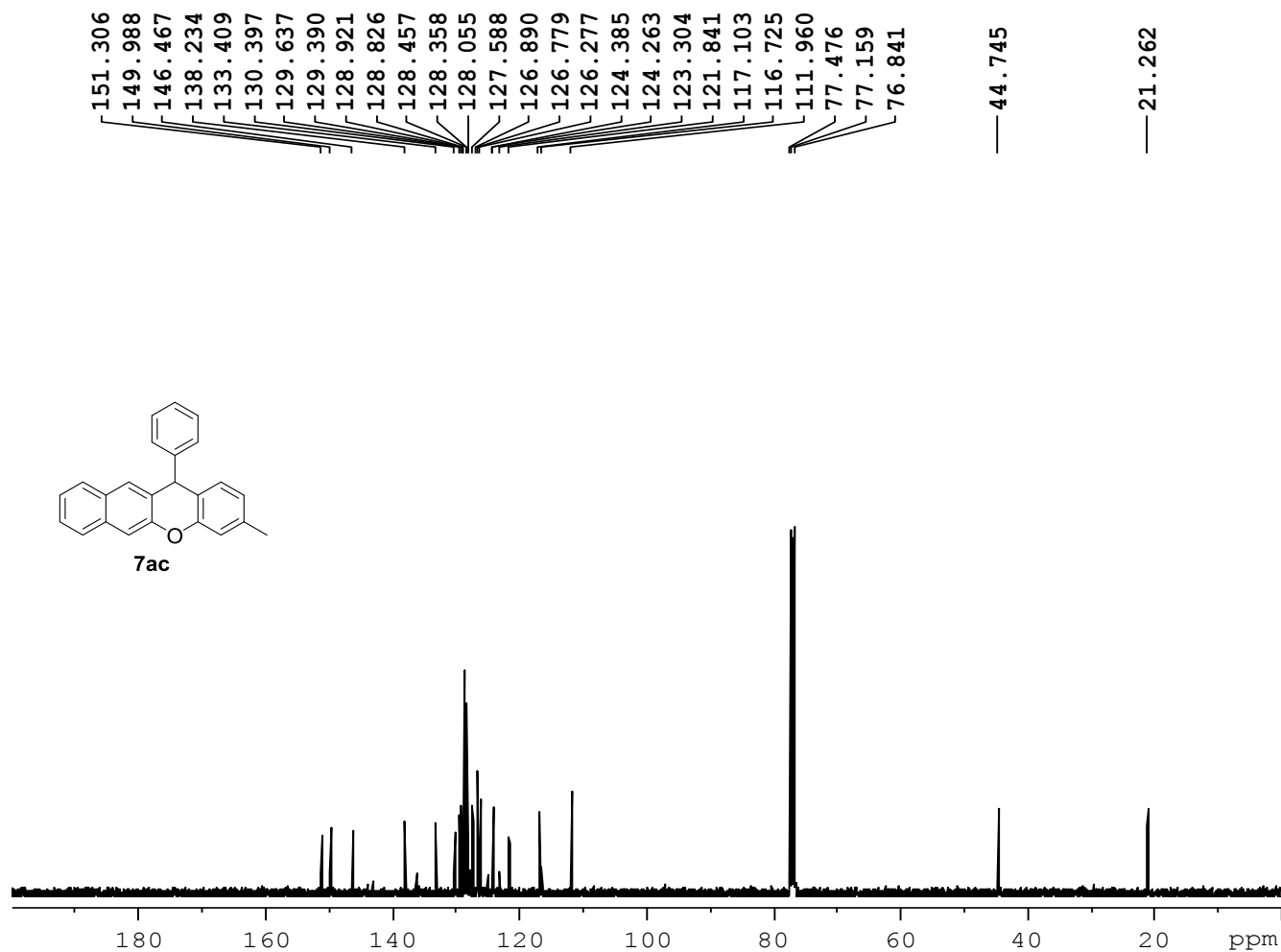


Figure 33a: ^1H -NMR spectra expansion for compound **7ac**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-396
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190408
Time 16.15
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 45.2
DW 20.800 usec
DE 6.00 usec
TE 294.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

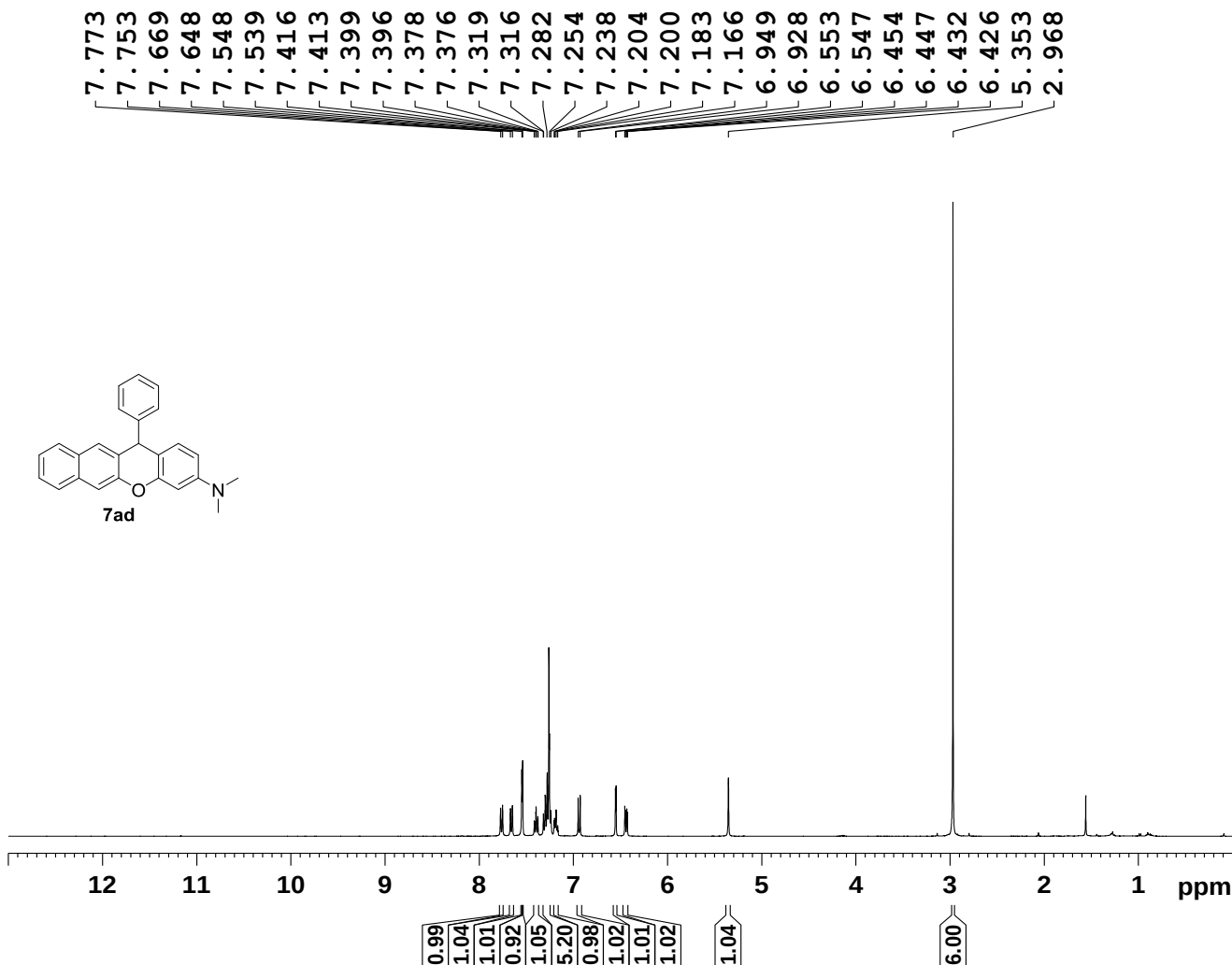
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127624 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 34: ^{13}C -NMR spectra for compound 7ac

PROTON CDC13 {D:\CRR} CIF_NMR 1



```

Current Data Parameters
NAME      MK-II-425 solved
EXPNO     1
PROCNO    1

F2 - Acquisition Parameters
Date_     20190531
Time      21.42
INSTRUM   spect
PROBHD    5 mm BBO BB-1H
PULPROG   zg30
TD        65536
SOLVENT   CDC13
NS         16
DS         2
SWH        8223.685 Hz
FIDRES     0.125483 Hz
AQ         3.9845889 sec
RG         228
DW         60.800 usec
DE         6.00 usec
TE         291.9 K
D1         1.00000000 sec
TD0        1

===== CHANNEL f1 =====
NUC1       1H
P1         14.35 usec
PL1        -1.00 dB
SFO1       400.1324710 MHz

F2 - Processing parameters
SI         32768
SF         400.1300095 MHz
WDW        EM
SSB        0
LB         0.30 Hz
GB         0
PC         1.00
  
```

Figure 35: ^1H -NMR spectra for compound **7ad**

PROTON CDC13 {D:\CRR} CIF_NMR 1

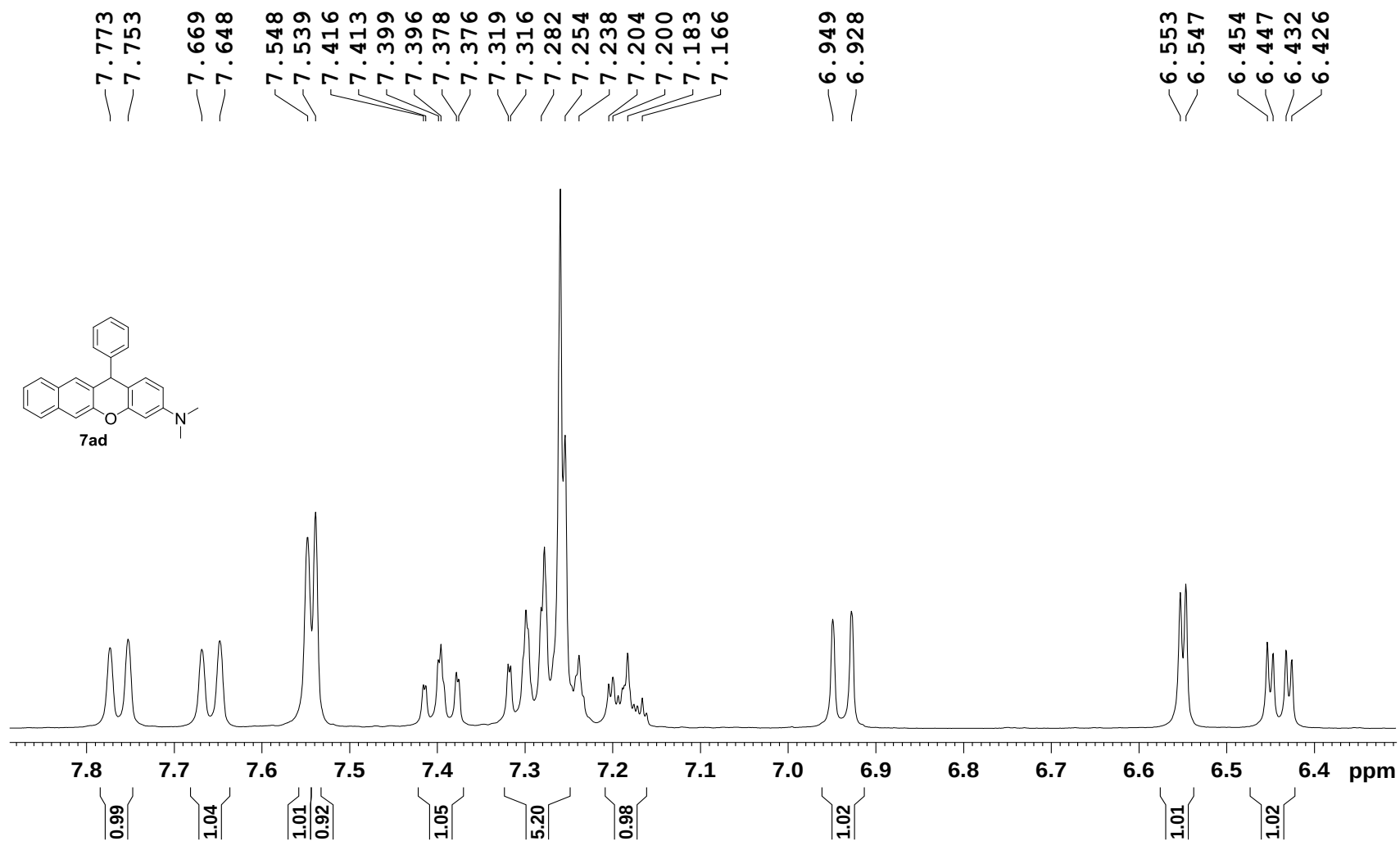
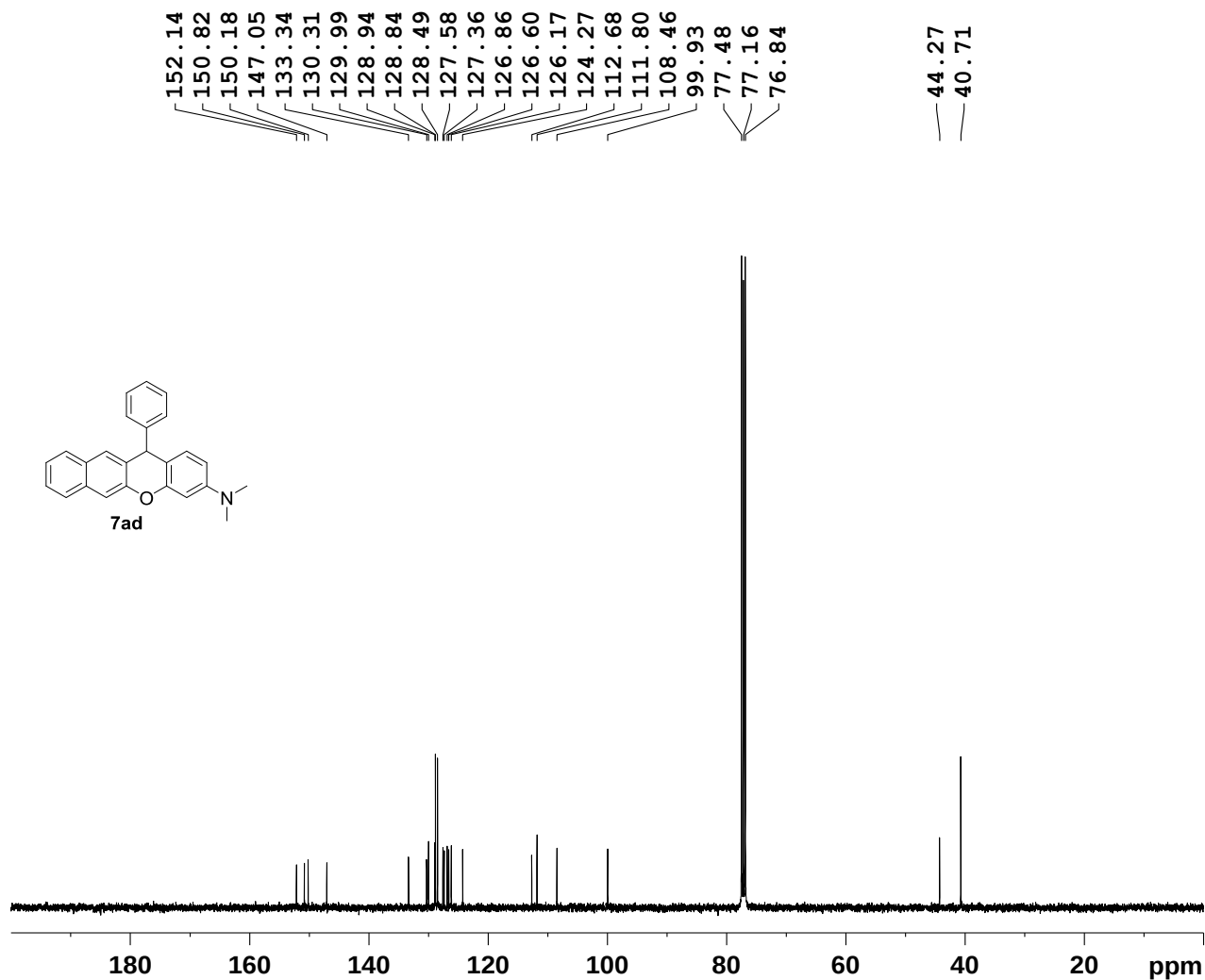


Figure 35a: ^1H -NMR spectra expansion for compound **7ad**



Current Data Parameters

NAME MK-II-425-A
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20190531
Time_ 22.26
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 406
DW 20.800 usec
DE 6.00 usec
TE 292.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters

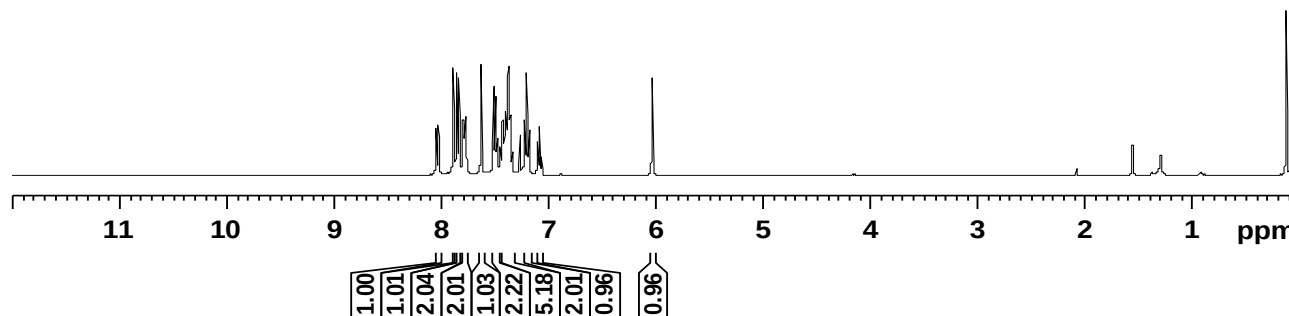
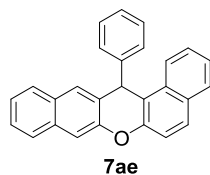
SI 32768
SF 100.6127588 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 36: ¹³C-NMR spectra for compound **7ad**

PROTON CDC13 {D:\CRR} CIF_NMR 1



8.041
8.020
7.880
7.849
7.827
7.790
7.781
7.770
7.761
7.620
7.502
7.488
7.480
7.470
7.421
7.393
7.378
7.367
7.360
7.354
7.351
7.260
7.215
7.196
7.177
7.094
7.076
7.057
6.025



Current Data Parameters
NAME MK-II-406
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190425
Time 22.37
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 203
DW 60.800 usec
DE 6.00 usec
TE 292.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 37: ¹H-NMR spectra for compound **7ae**

PROTON CDCl3 {D:\CRR} CIF_NMR 1

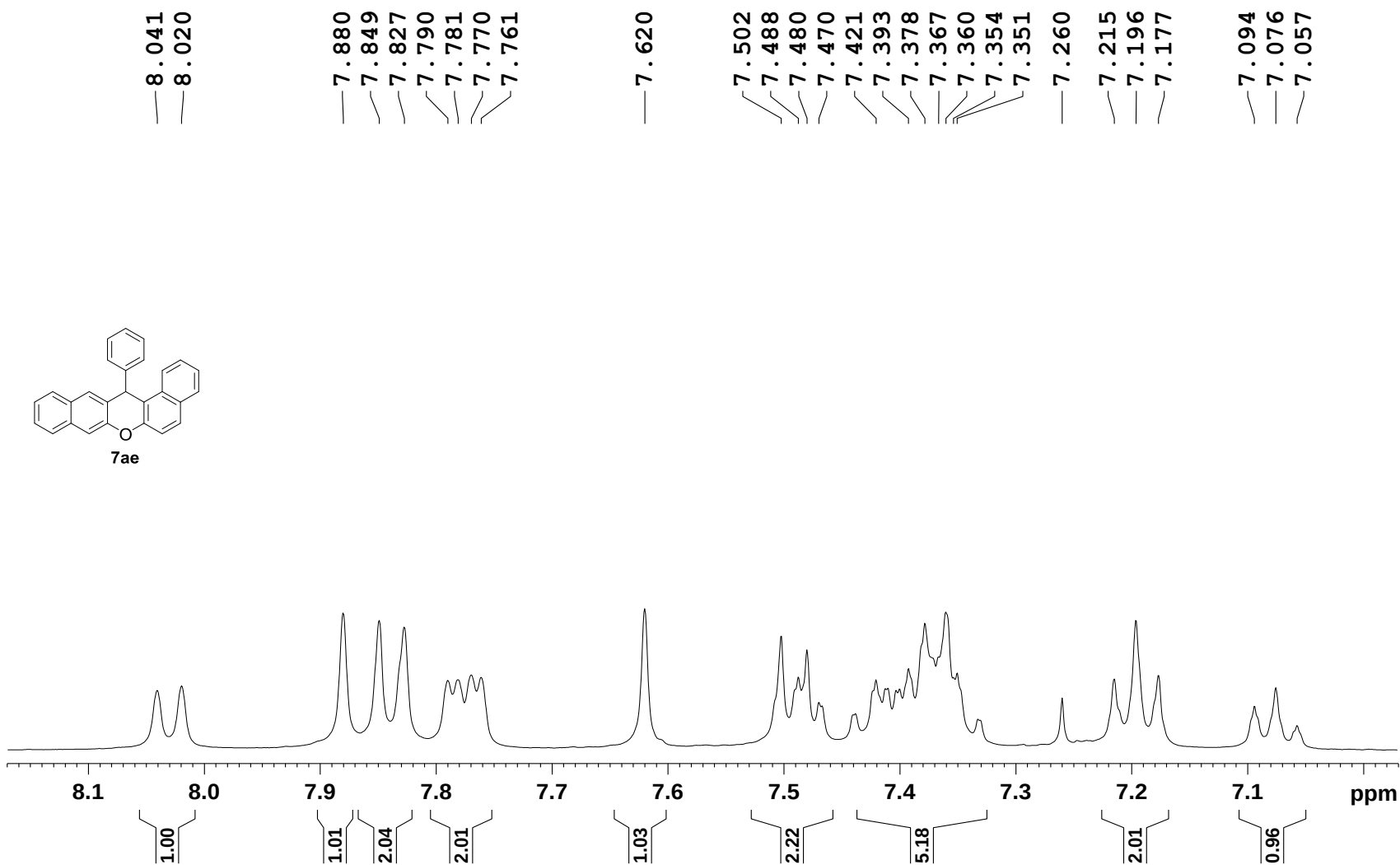
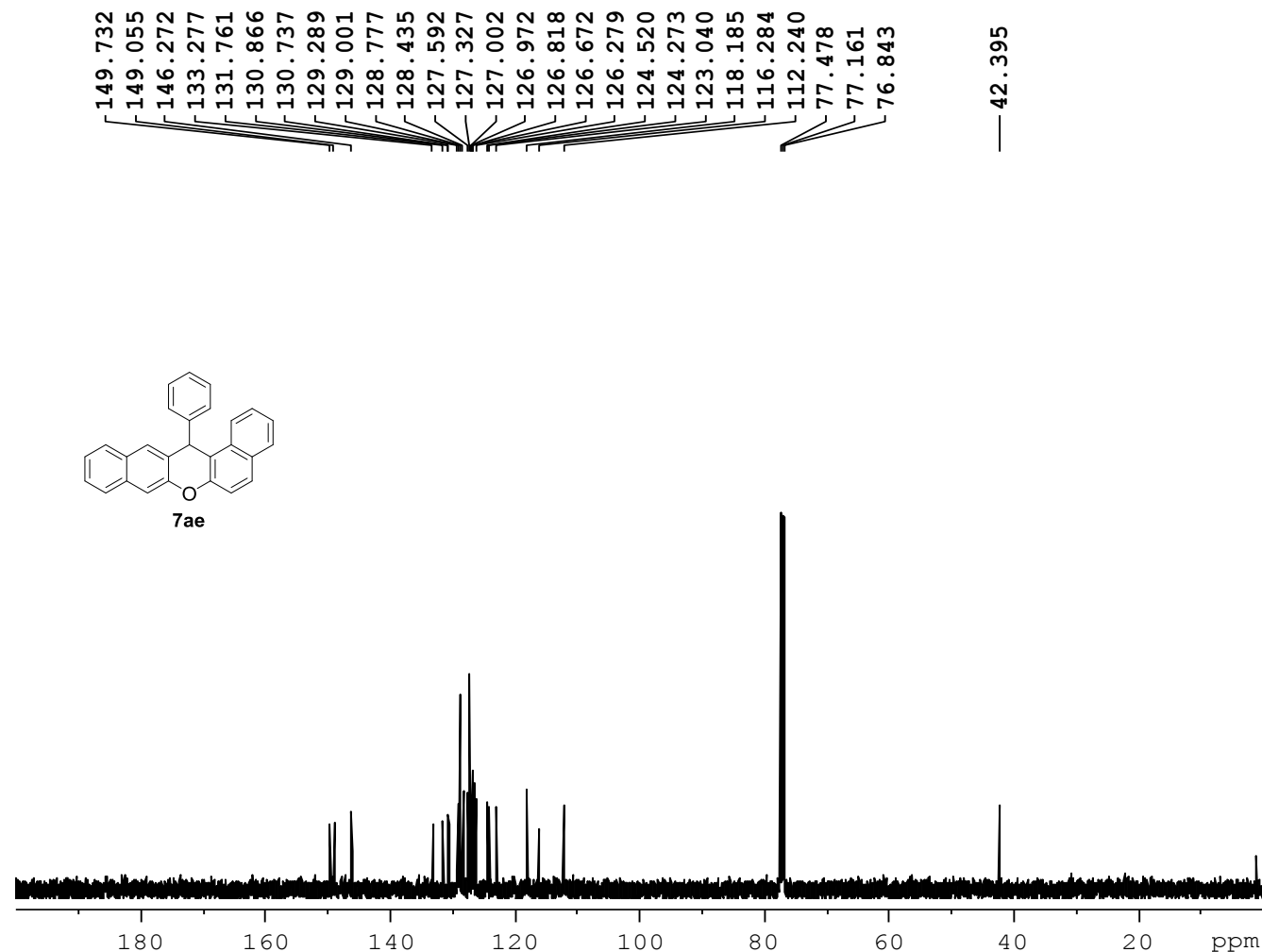


Figure 37a: ¹H-NMR spectra expansion for compound **7ae**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-406
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190426
Time_ 7.39
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 74
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 256
DW 20.800 usec
DE 6.00 usec
TE 295.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

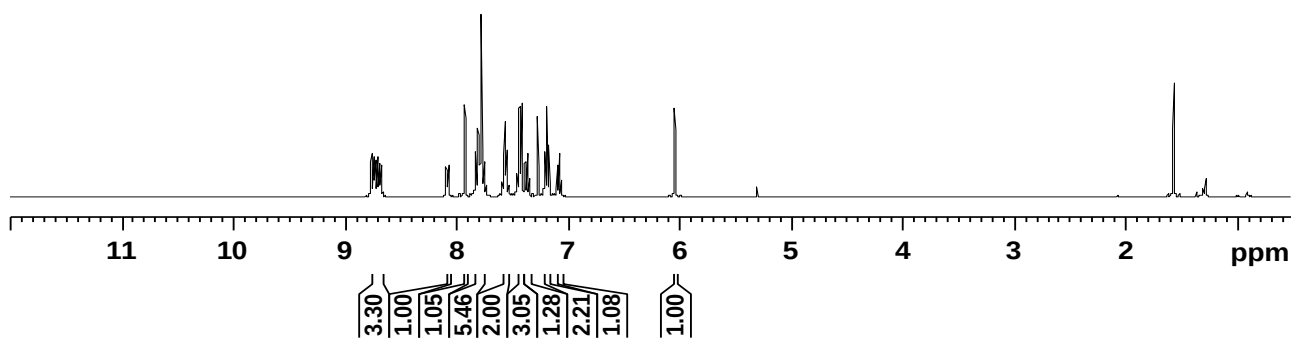
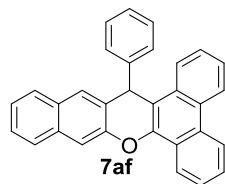
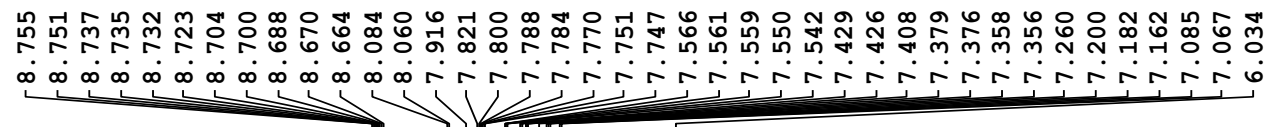
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127637 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 38: ^{13}C -NMR spectra for compound **7ae**

PROTON CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-417-A
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190514
Time_ 10.14
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 362
DW 60.800 usec
DE 6.00 usec
TE 292.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 39: ¹H-NMR spectra for compound **7af**

PROTON CDC13 {D:\CRR} CIF_NMR 1

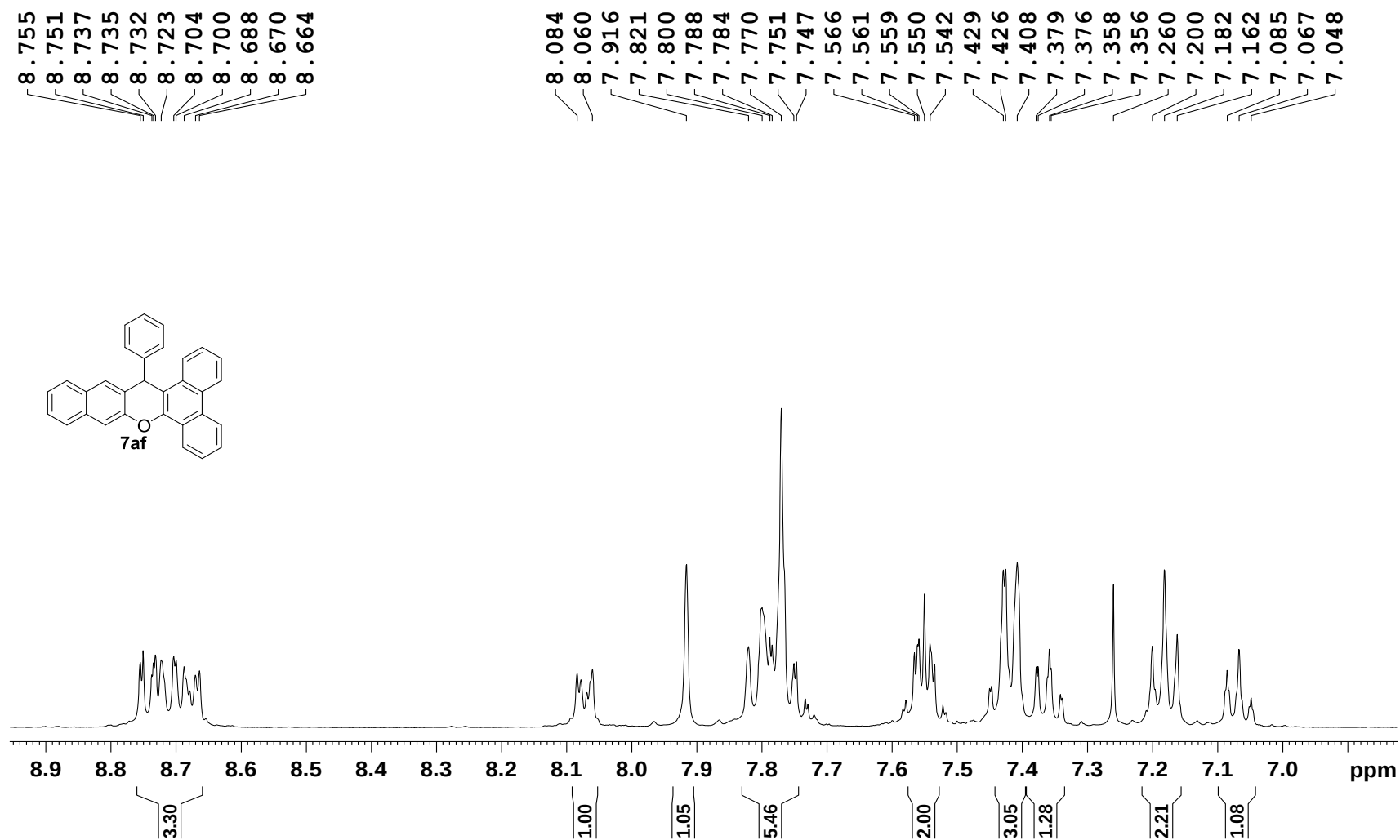
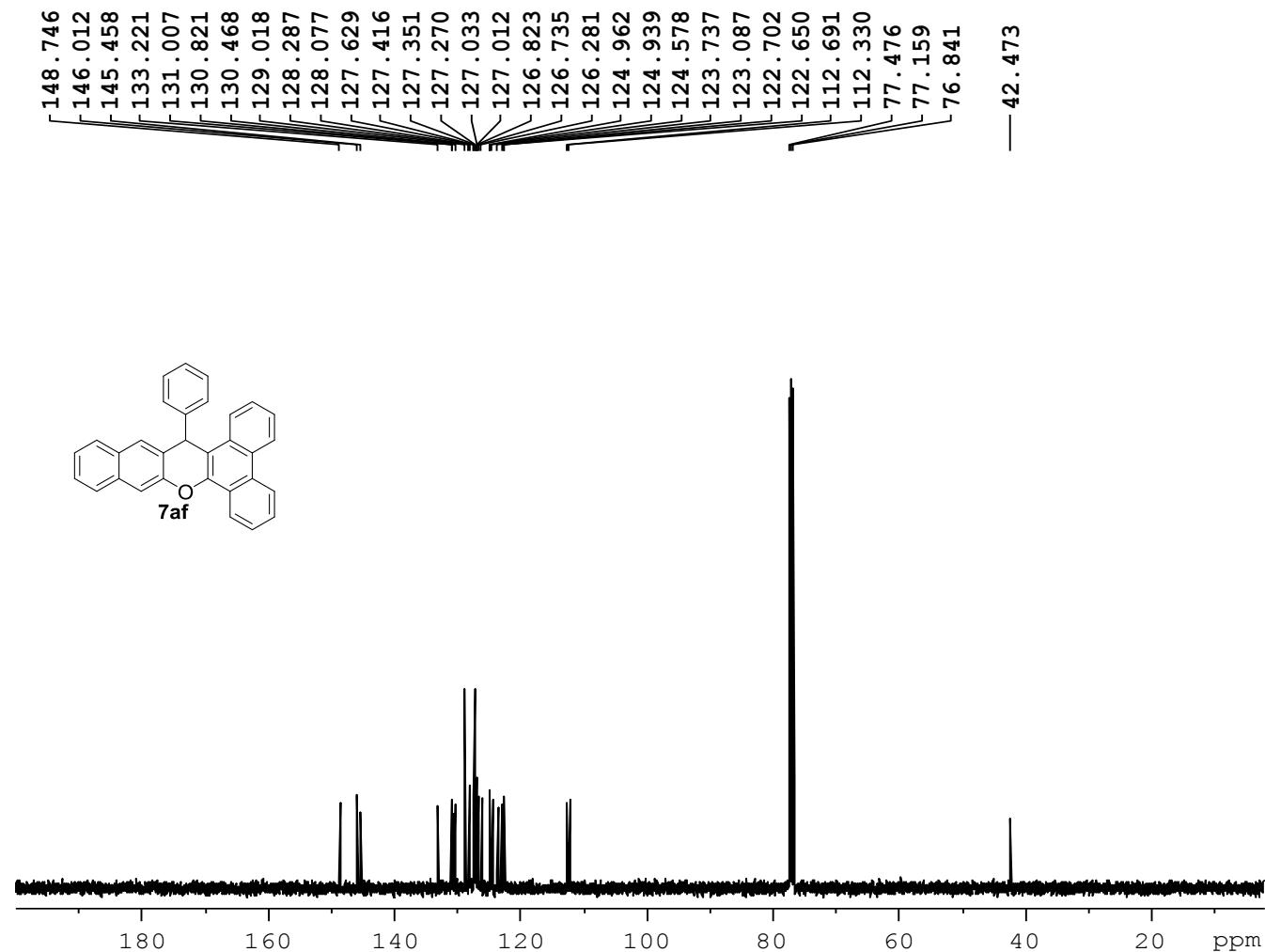


Figure 39a: ^1H -NMR spectra expansion for compound **7af**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-417-A
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190514
Time 11.59
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 220
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 40.3
DW 20.800 usec
DE 6.00 usec
TE 292.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

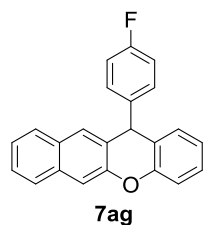
F2 - Processing parameters
SI 32768
SF 100.6127634 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 40: ^{13}C -NMR spectra for compound **7af**

PROTON CDC13 {D:\CRR} CIF_NMR 1



7.685
7.664
7.587
7.566
7.471
7.428
7.340
7.337
7.320
7.302
7.300
7.247
7.245
7.227
7.210
7.207
7.181
7.165
7.161
7.151
7.148
7.144
7.133
7.120
7.107
7.098
7.090
7.085
6.997
6.981
6.946
6.943
6.926
6.894
6.872
6.850
5.311
1.467



Current Data Parameters
NAME MK-II-394
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190408
Time 12.33
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 181
DW 60.800 usec
DE 6.00 usec
TE 294.9 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300529 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

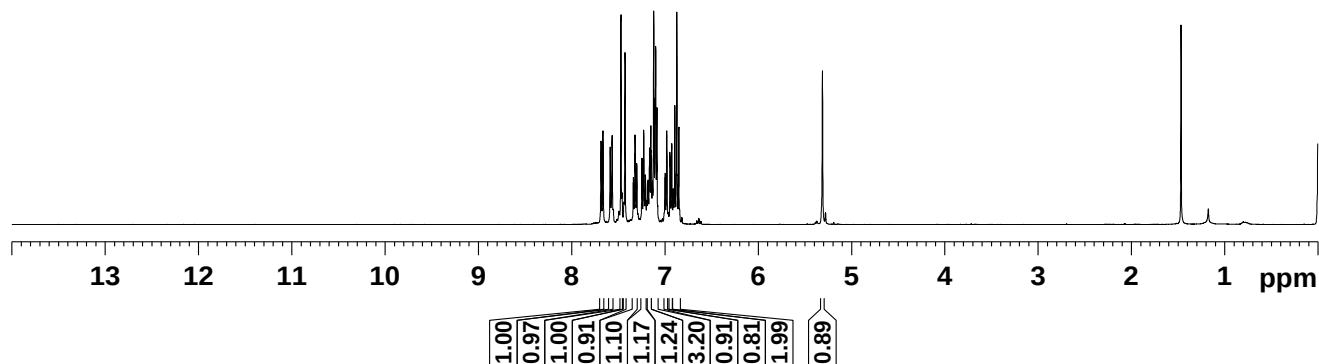


Figure 41: ^1H -NMR spectra for compound **7ag**

PROTON CDC13 {D:\CRR} CIF_NMR 1

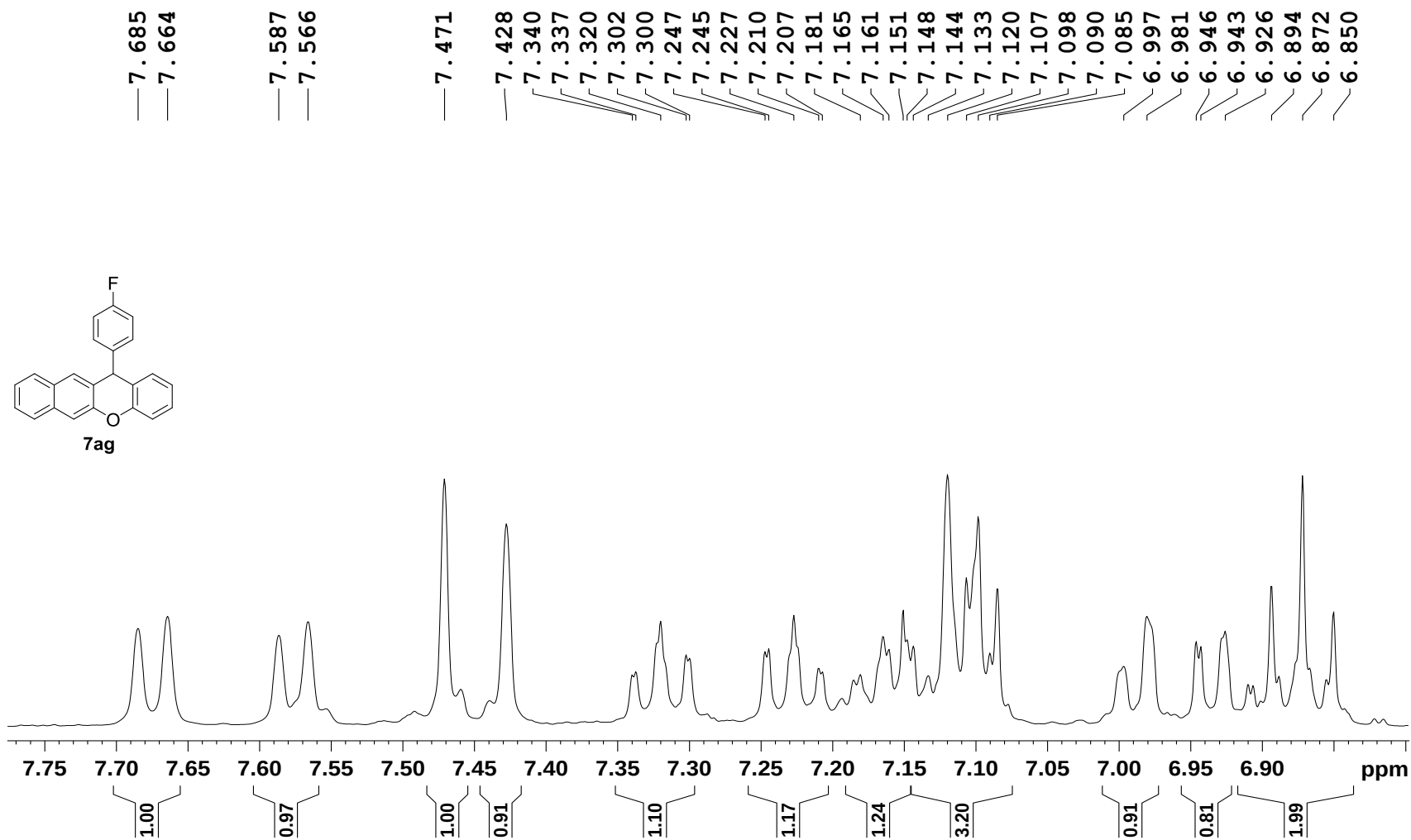
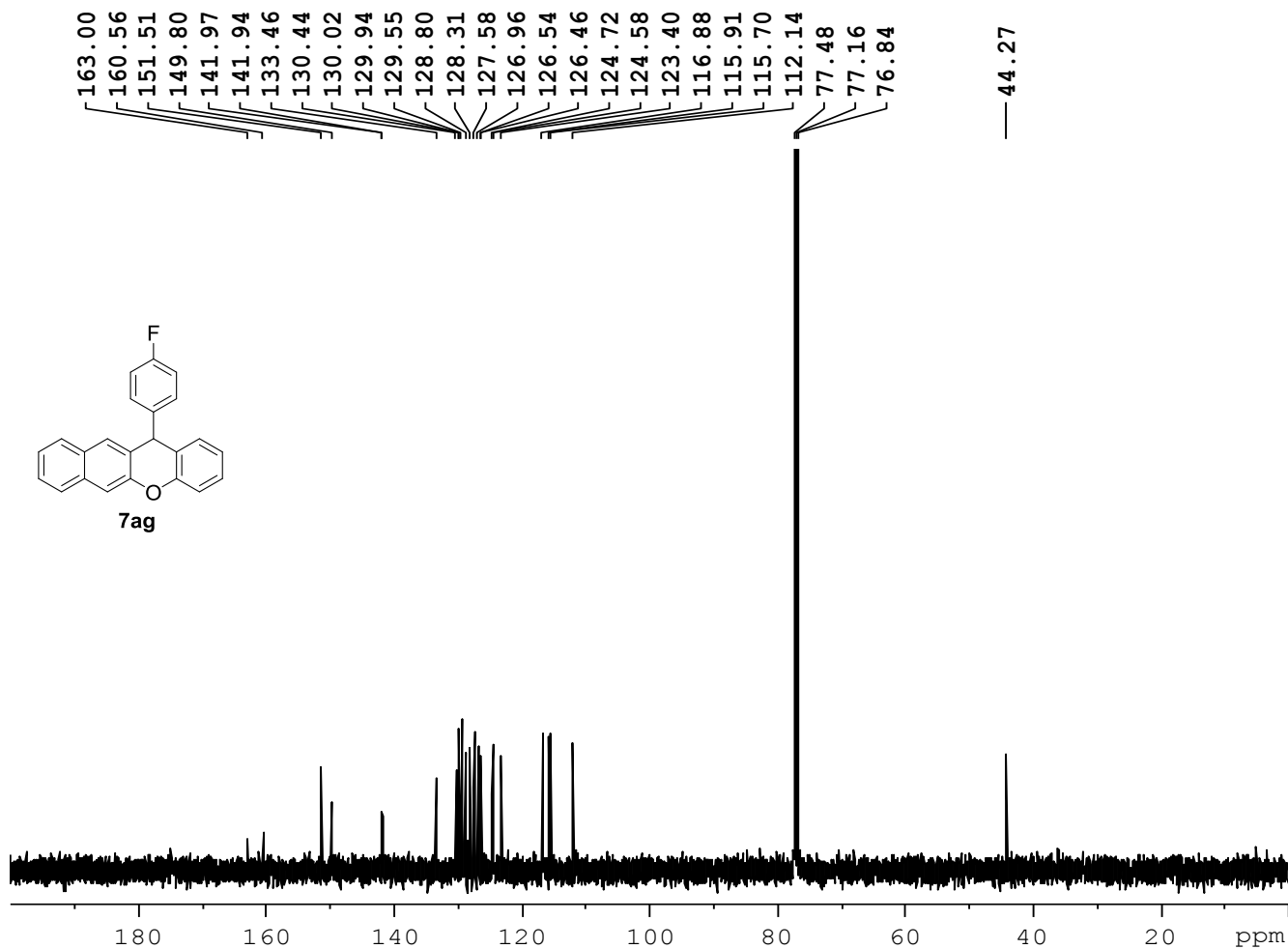


Figure 41a: ^1H -NMR spectra expansion for compound **7ag**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-394
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190408
Time 15.43
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 40.3
DW 20.800 usec
DE 6.00 usec
TE 294.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

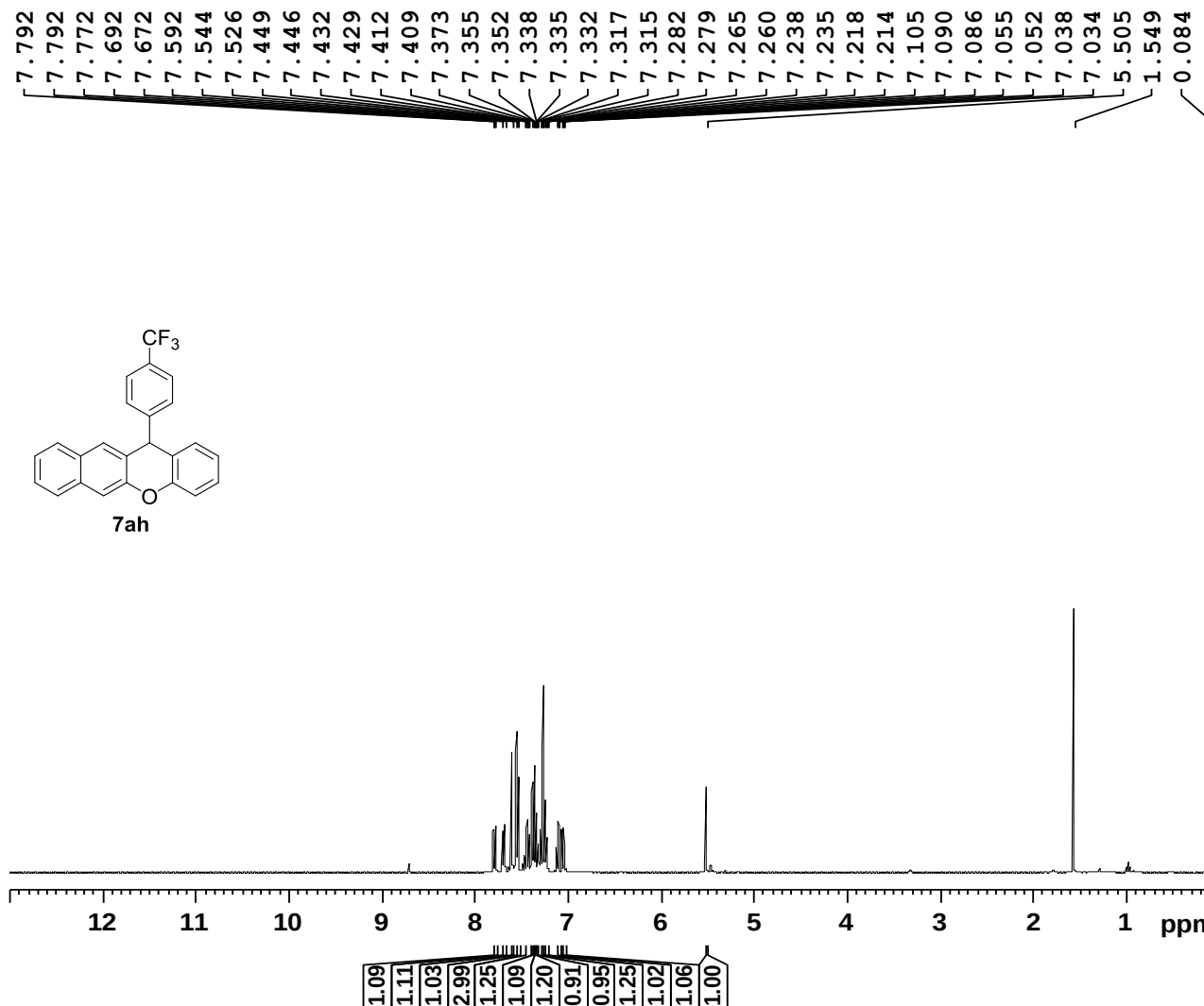
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127588 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 42: ¹³C-NMR spectra for compound **7ag**

PROTON CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
 NAME MK-II-385
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190329
 Time 15.35
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 322
 DW 60.800 usec
 DE 6.00 usec
 TE 297.5 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.35 usec
 PL1 -1.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.130094 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure 43: ¹H-NMR spectra for compound **7ah**

PROTON CDCl3 {D:\CRR} CIF_NMR 1

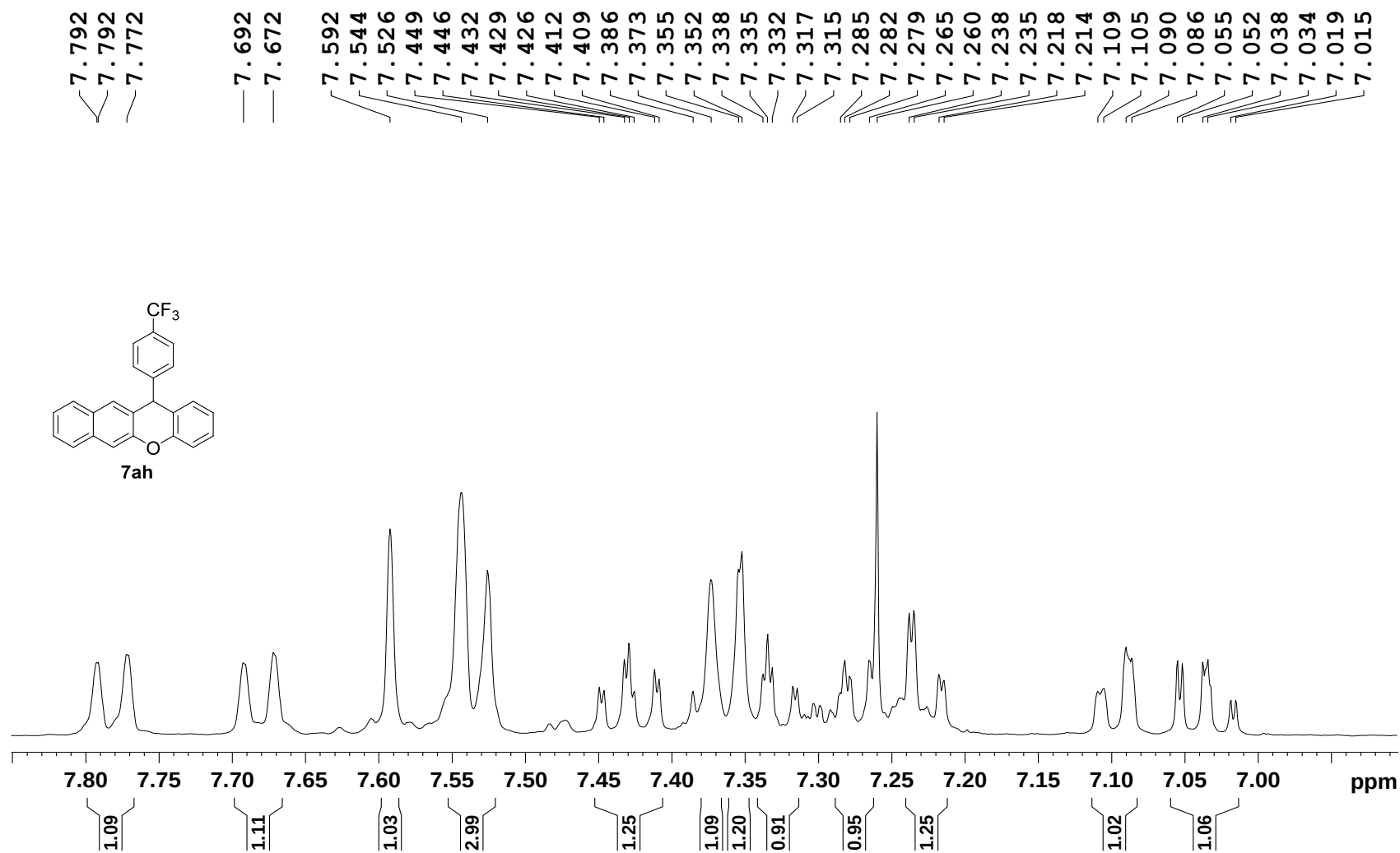
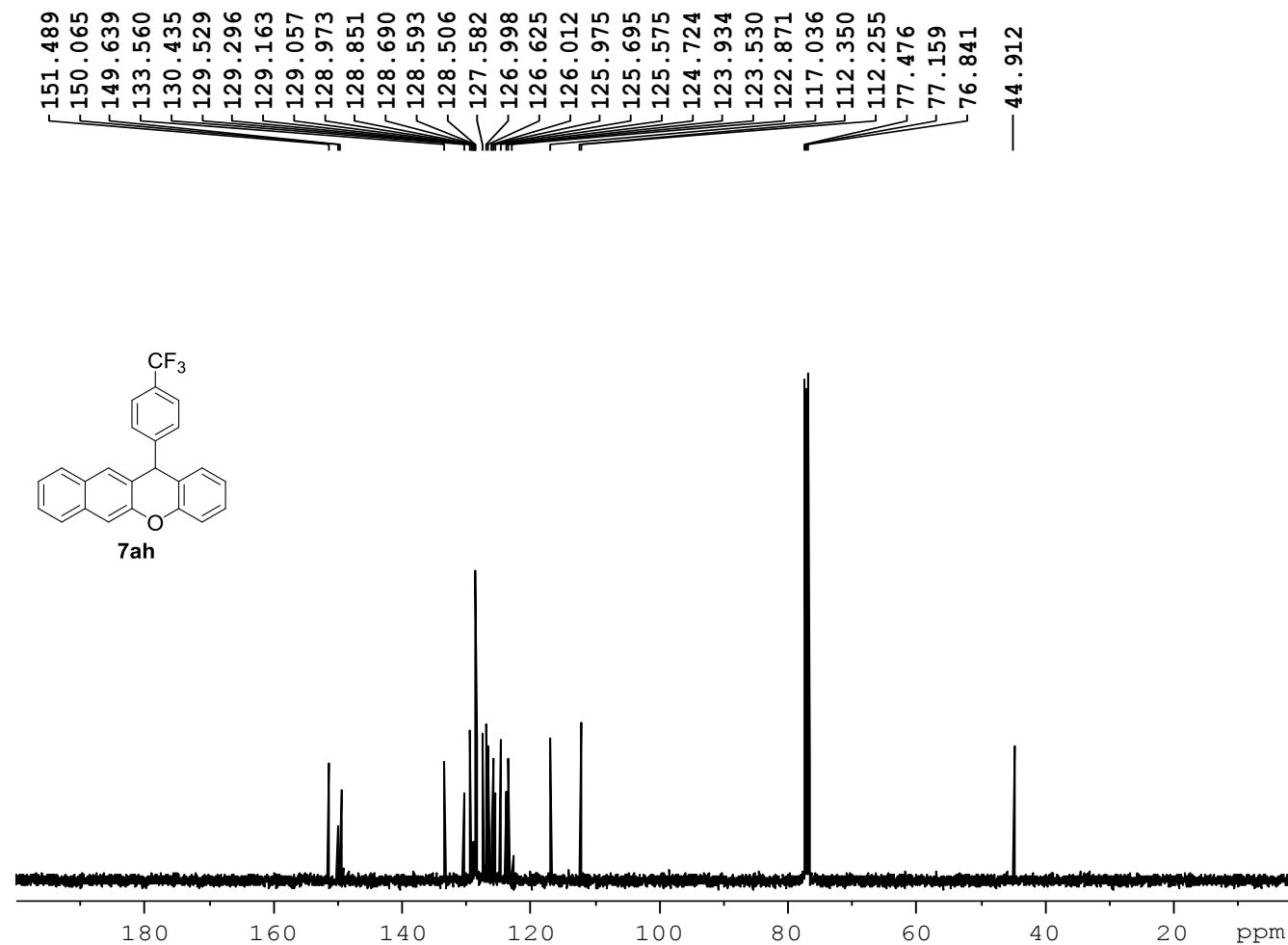


Figure 43a: ¹H-NMR spectra expansion for compound **7ah**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-385
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190331
Time 10.21
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 40.3
DW 20.800 usec
DE 6.00 usec
TE 292.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

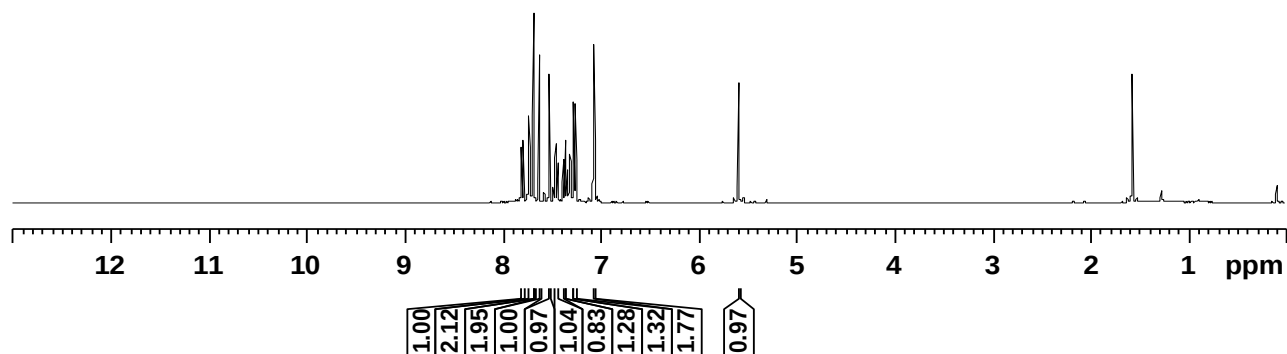
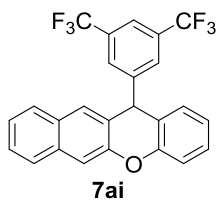
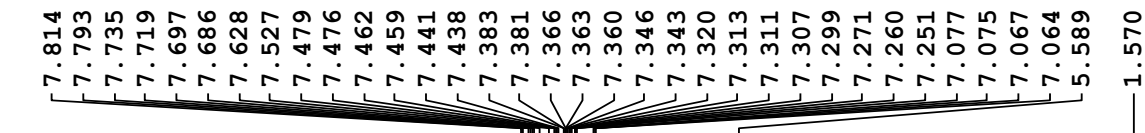
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127603 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 44: ¹³C-NMR spectra for compound 7ah

PROTON CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-398
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190411
Time_ 10.24
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 406
DW 60.800 usec
DE 6.00 usec
TE 292.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 45: ¹H-NMR spectra for compound 7ai

PROTON CDC13 {D:\CRR} CIF_NMR 1

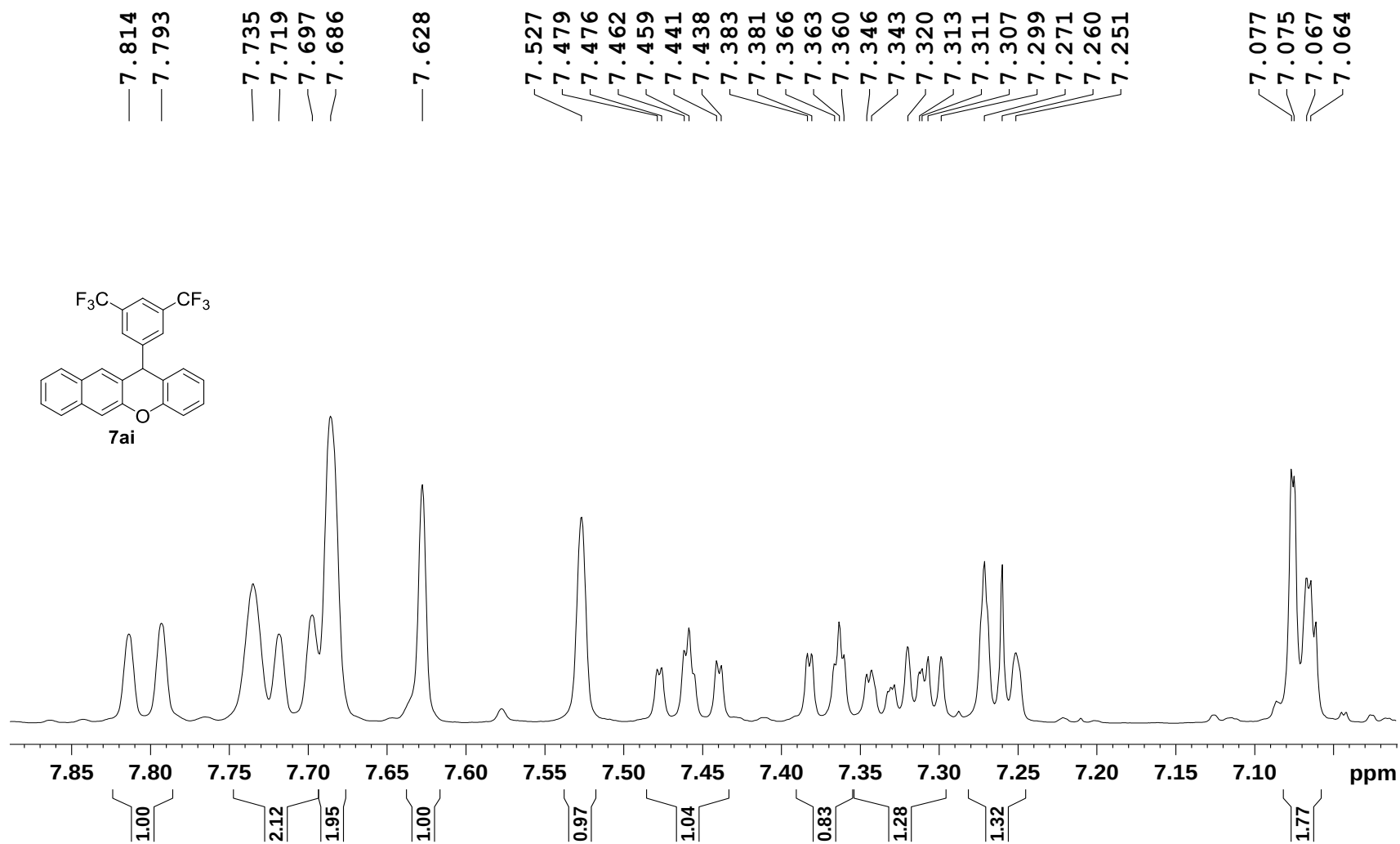
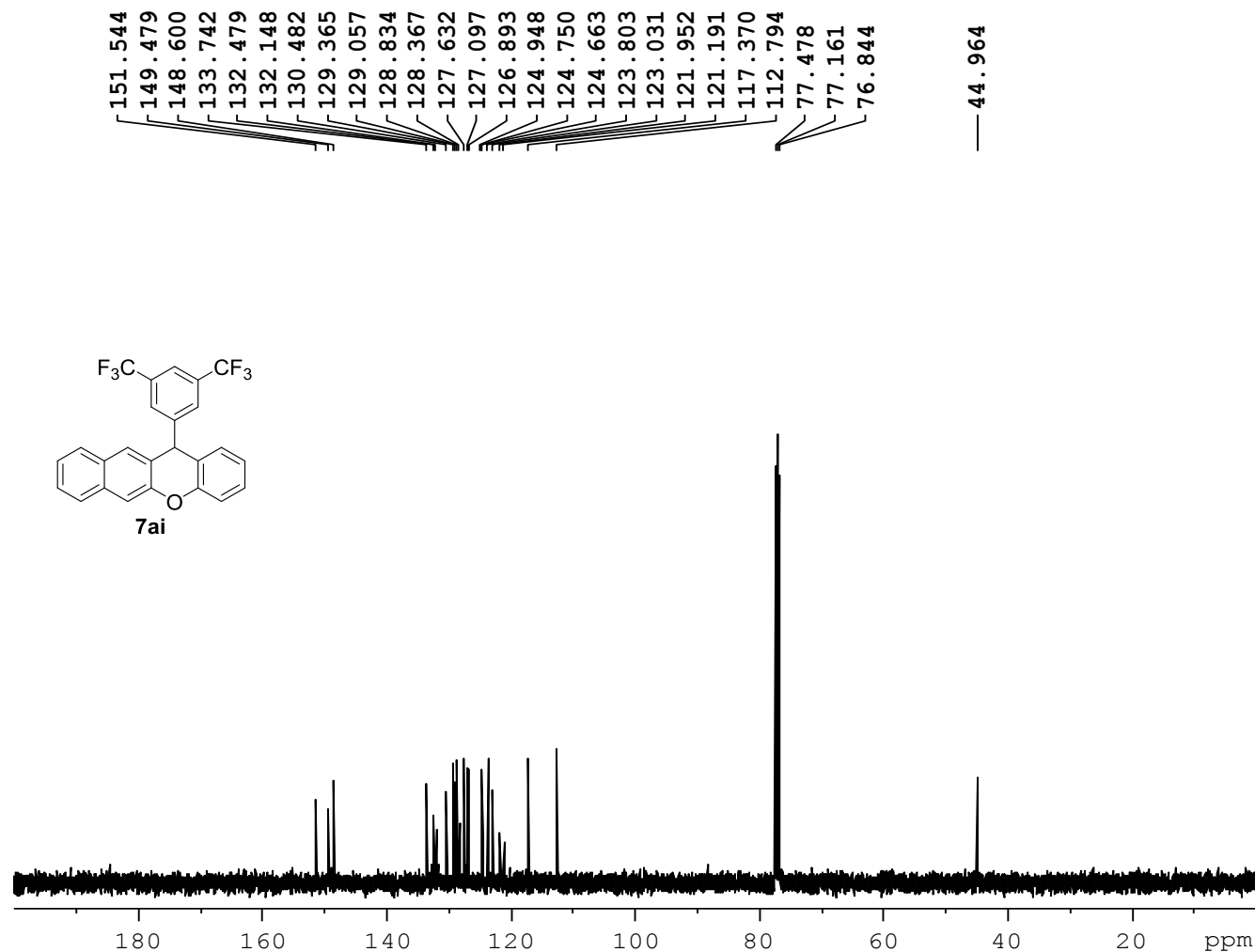


Figure 45a: ^1H -NMR spectra expansion for compound **7ai**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-398
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190411
Time 12.24
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 74
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 575
DW 20.800 usec
DE 6.00 usec
TE 295.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

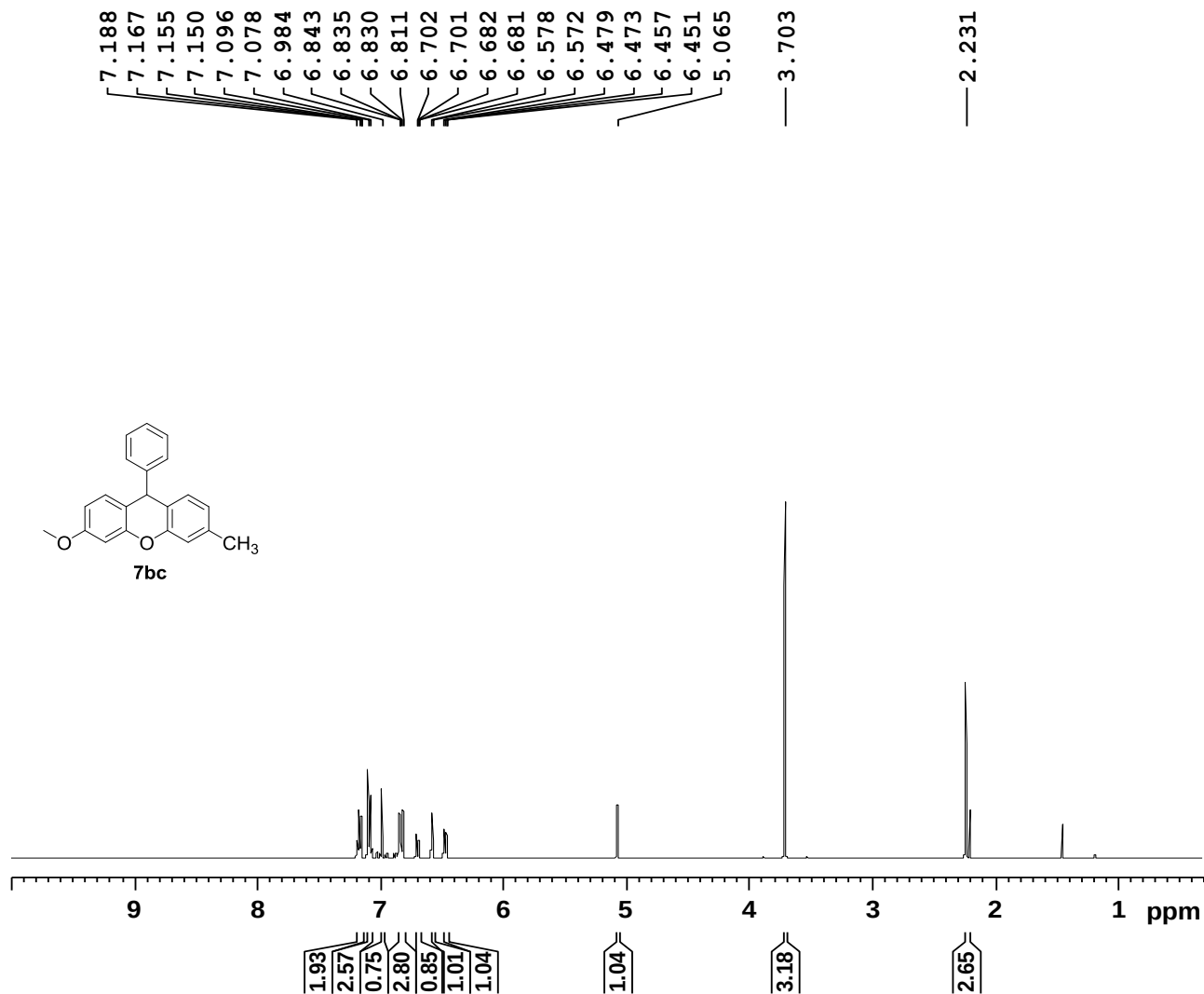
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127567 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 46: ¹³C-NMR spectra for compound 7ai

PROTON CDCl3 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-392
EXPNO 1
PROCNO 1

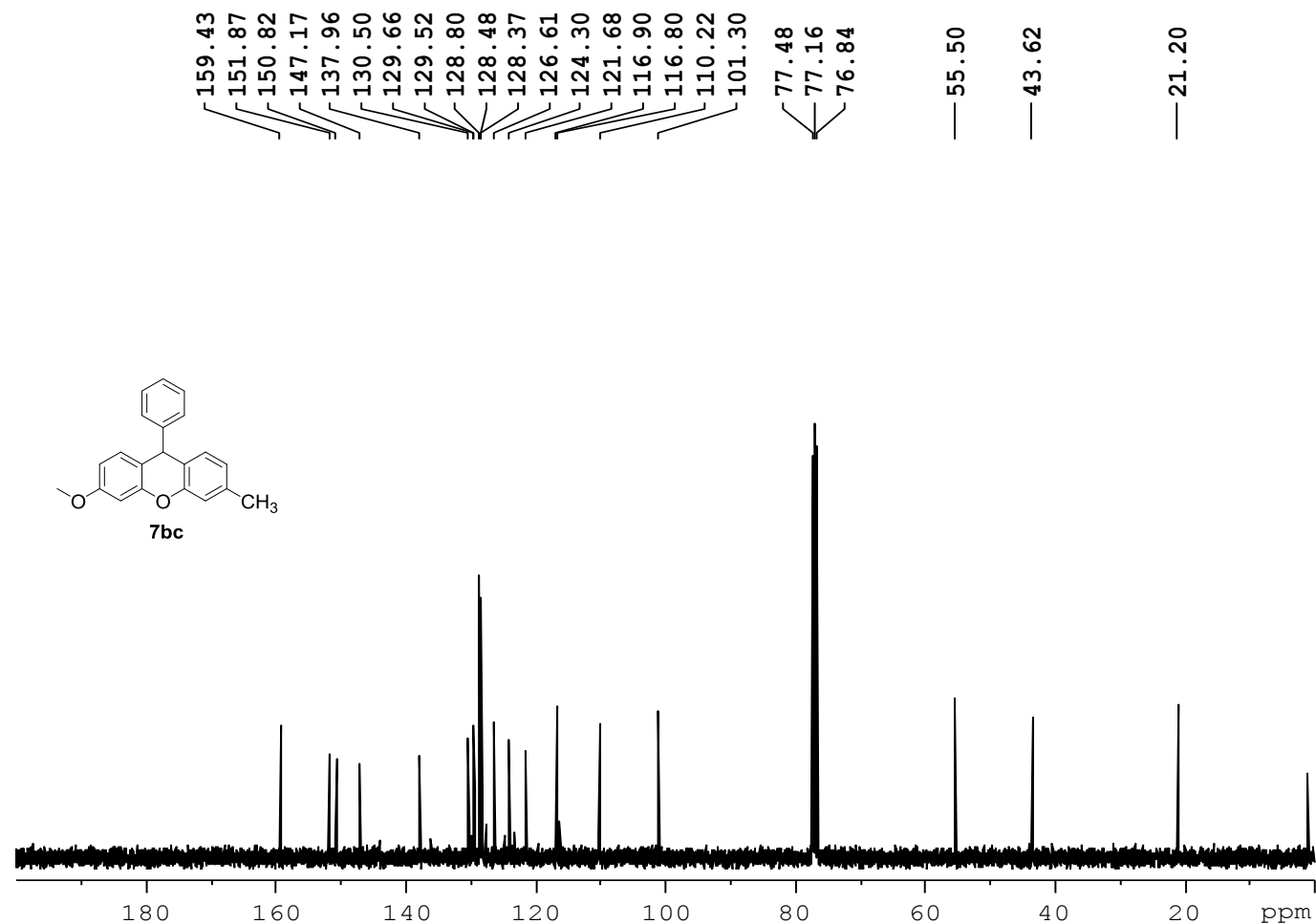
F2 - Acquisition Parameters
Date_ 20190403
Time 18.53
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 181
DW 60.800 usec
DE 6.00 usec
TE 297.6 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300514 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 47: ¹H-NMR spectra for compound **7bc**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-392
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190403
Time_ 20.37
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 72
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 45.2
DW 20.800 usec
DE 6.00 usec
TE 297.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

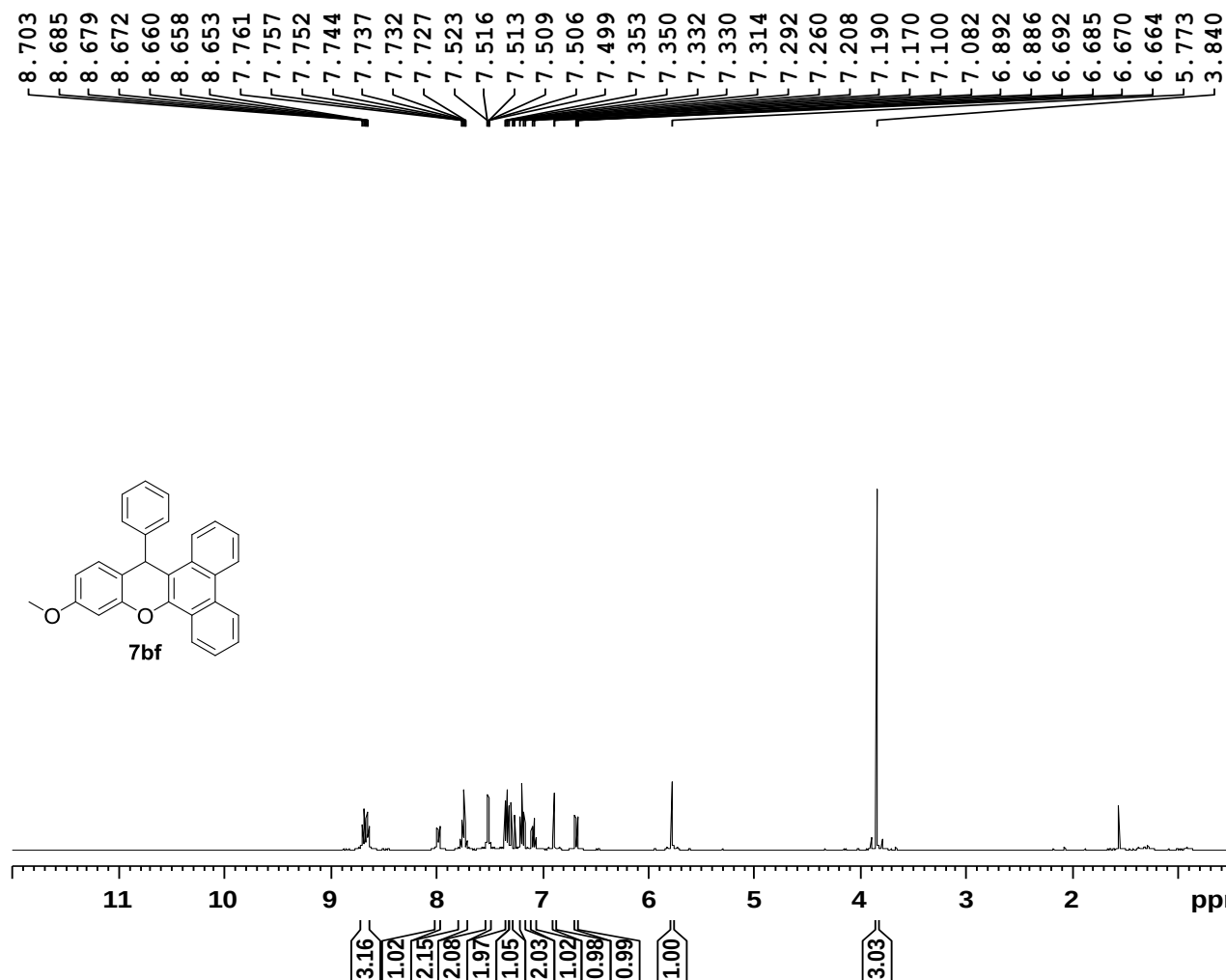
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127598 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 48: ¹³C-NMR spectra for compound **7bc**

PROTON CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-416
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190509
Time 10.52
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 181
DW 60.800 usec
DE 6.00 usec
TE 291.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 49: ^1H -NMR spectra for compound **7bf**

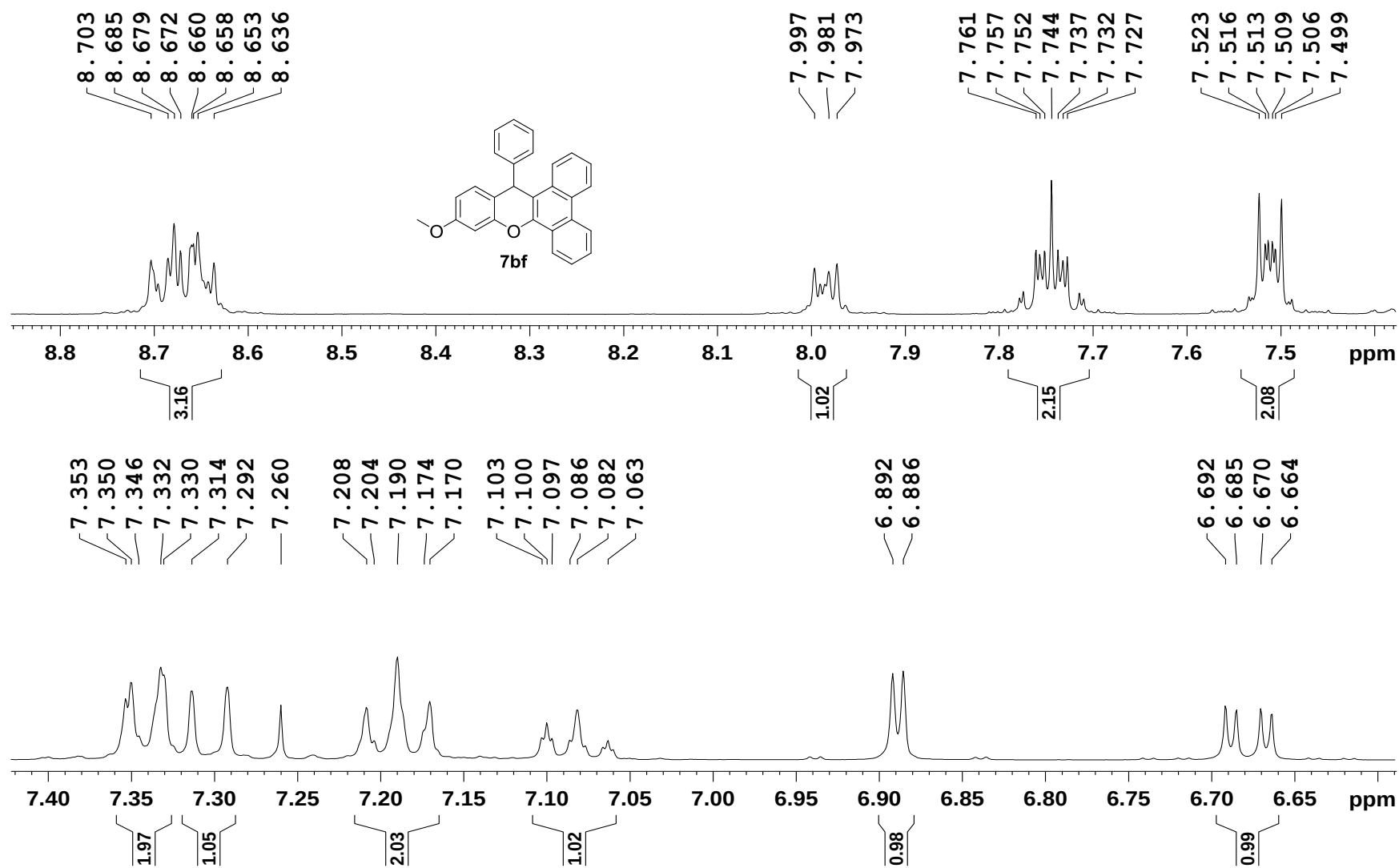
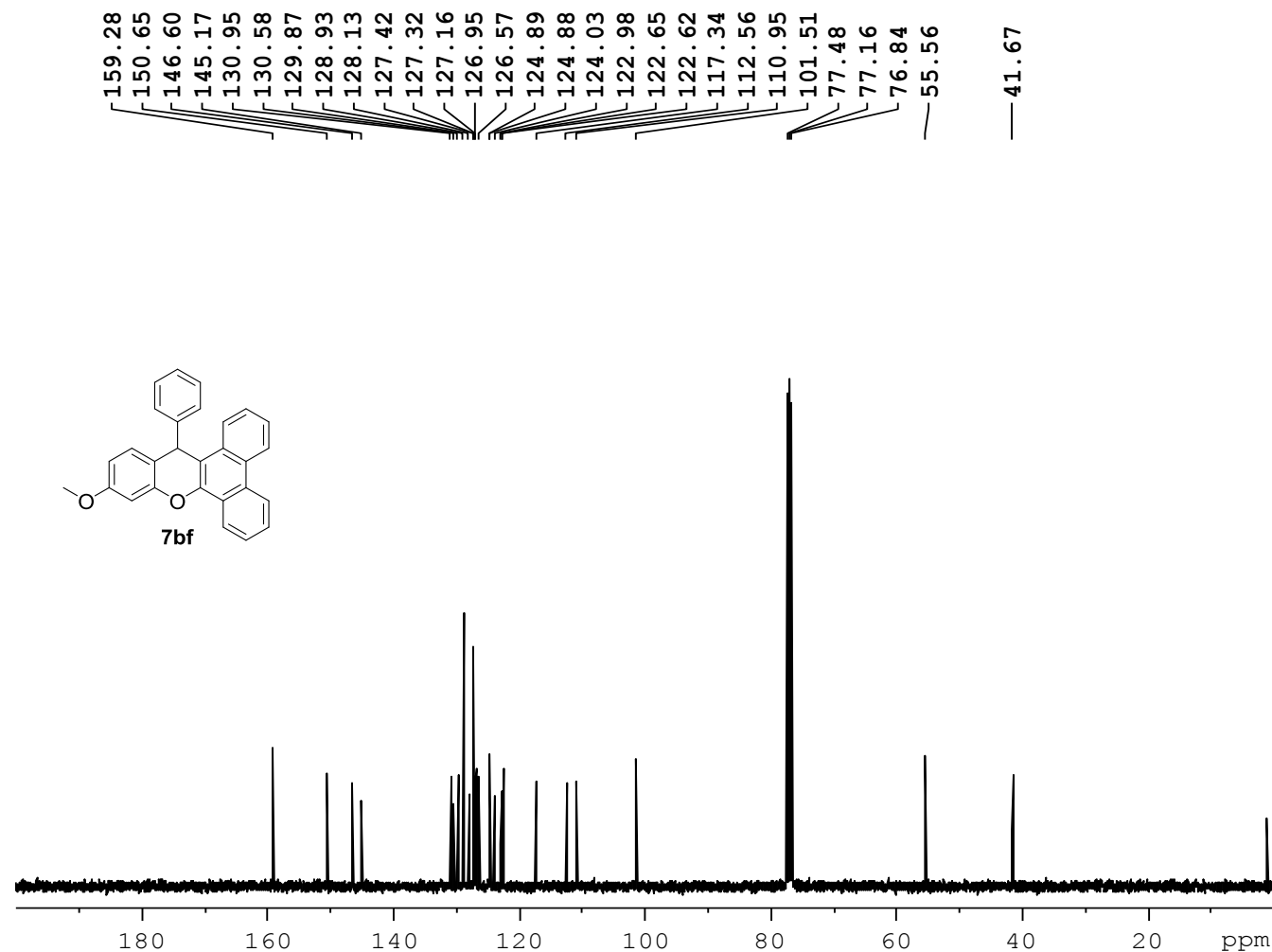


Figure 49a: ^1H -NMR spectra expansion for compound **7bf**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-416
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190509
Time 12.14
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 287
DW 20.800 usec
DE 6.00 usec
TE 293.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

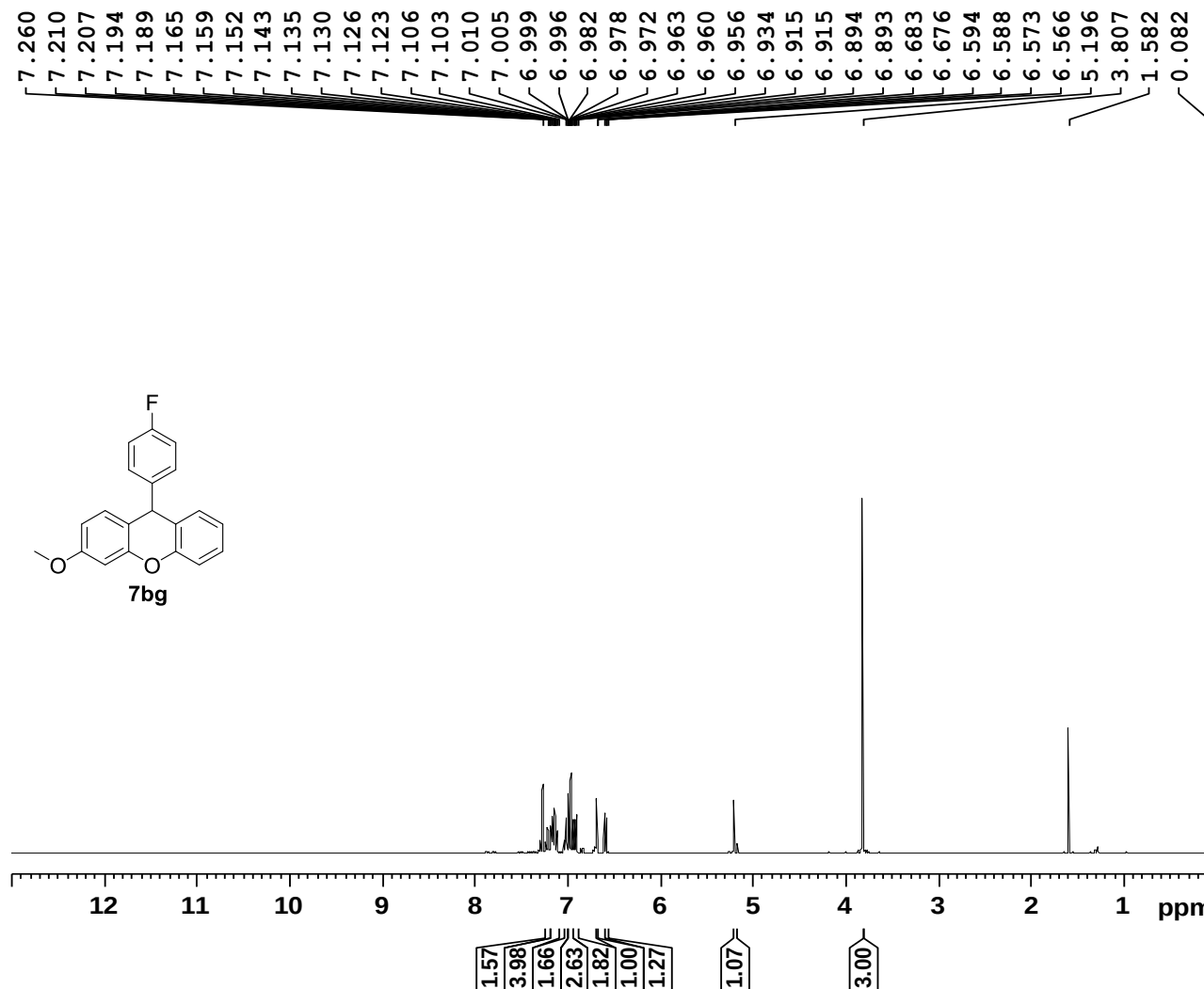
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127627 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 50: ¹³C-NMR spectra for compound **7bf**

PROTON CDCl3 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-414
EXPNO 1
PROCNO 1

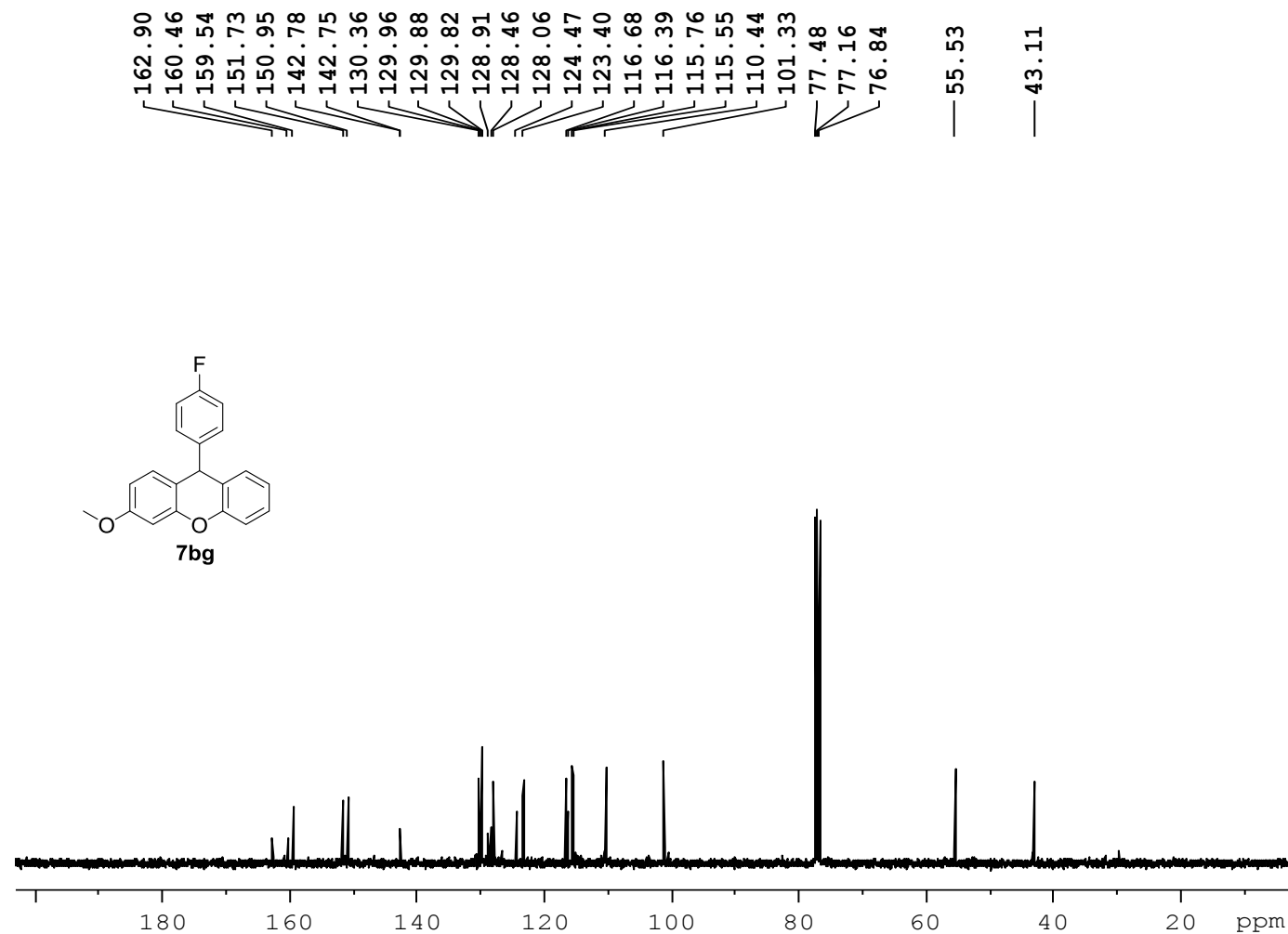
F2 - Acquisition Parameters
Date_ 20190506
Time 11.28
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 228
DW 60.800 usec
DE 6.00 usec
TE 291.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 51: ¹H-NMR spectra for compound **7bg**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



```

Current Data Parameters
NAME          MK-II-414-A
EXPNO         2
PROCNO        1

F2 - Acquisition Parameters
Date_         20190507
Time          15.32
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       zgpg30
TD            65536
SOLVENT       CDC13
NS            187
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG            322
DW            20.800 usec
DE            6.00 usec
TE            293.5 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999999 sec
TD0           1

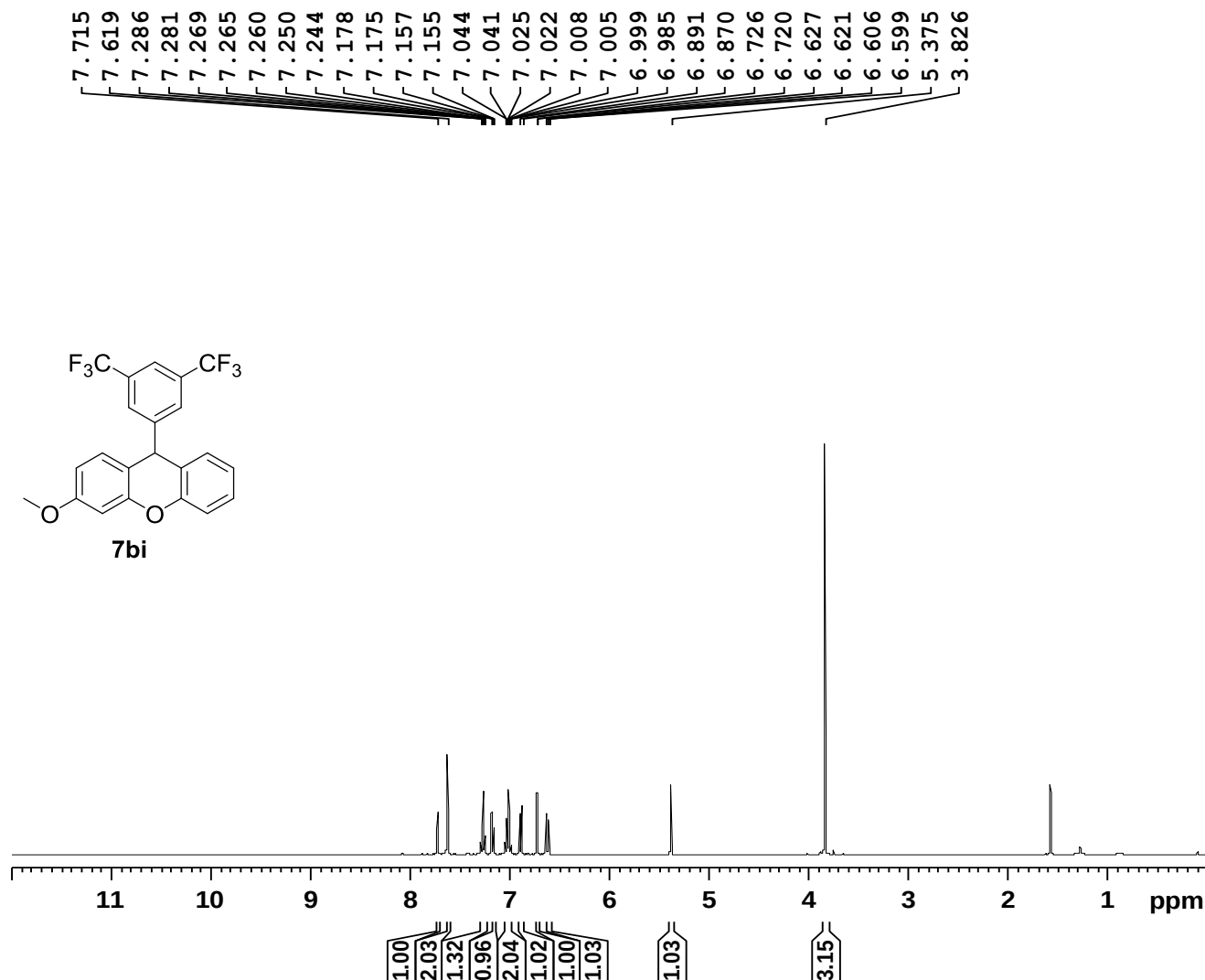
===== CHANNEL f1 =====
NUC1           13C
P1             9.95 usec
PL1            -1.00 dB
SFO1          100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2]     waltz16
NUC2           1H
PCPD2          90.00 usec
PL12           14.95 dB
PL13           120.00 dB
PL2            -1.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI            32768
SF           100.6127597 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

Figure 52: ^{13}C -NMR spectra for compound **7bg**

PROTON CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
 NAME MK-II-397-A
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190527
 Time_ 14.30
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 406
 DW 60.800 usec
 DE 6.00 usec
 TE 294.6 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.35 usec
 PL1 -1.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300094 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure 53: ¹H-NMR spectra for compound **7bi**

PROTON CDC13 {D:\CRR} CIF_NMR 1

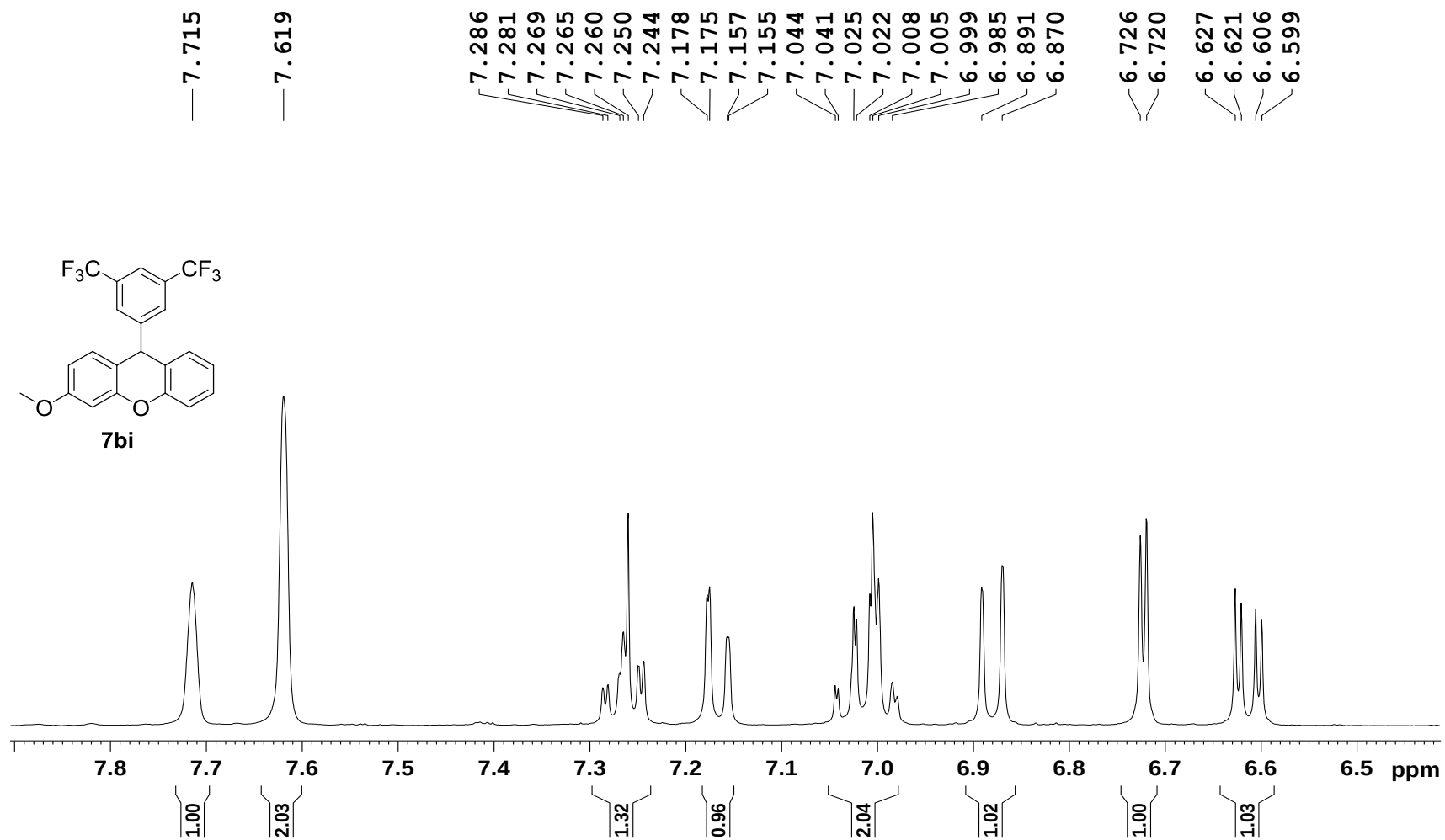
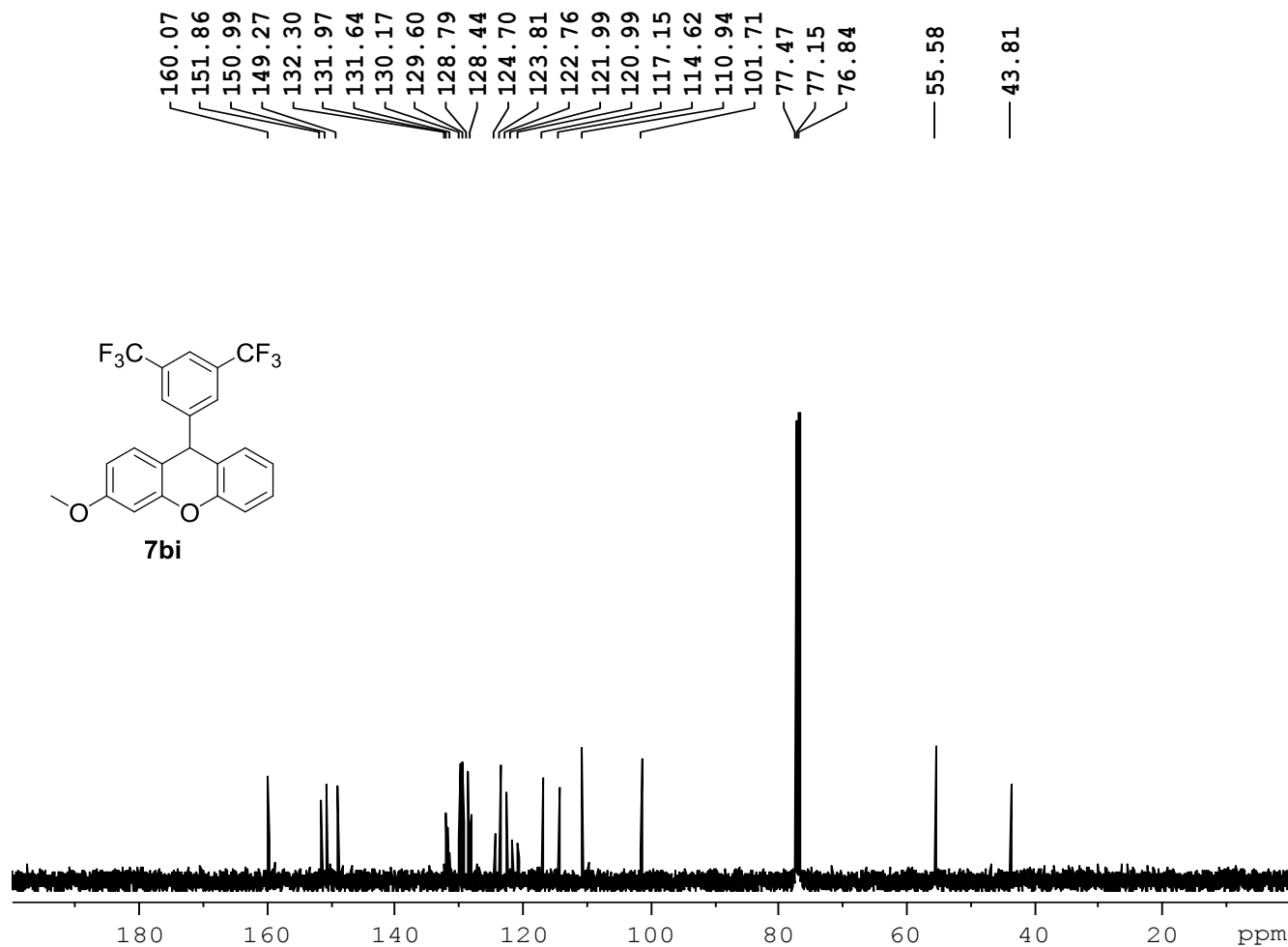


Figure 53a: ¹H-NMR spectra expansion for compound **7bi**

C13CPD CDC13 {D:\MB} CIF_NMR 1



Current Data Parameters
NAME MK-II-397-A
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190530
Time 11.29
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 40.3
DW 20.800 usec
DE 6.00 usec
TE 294.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

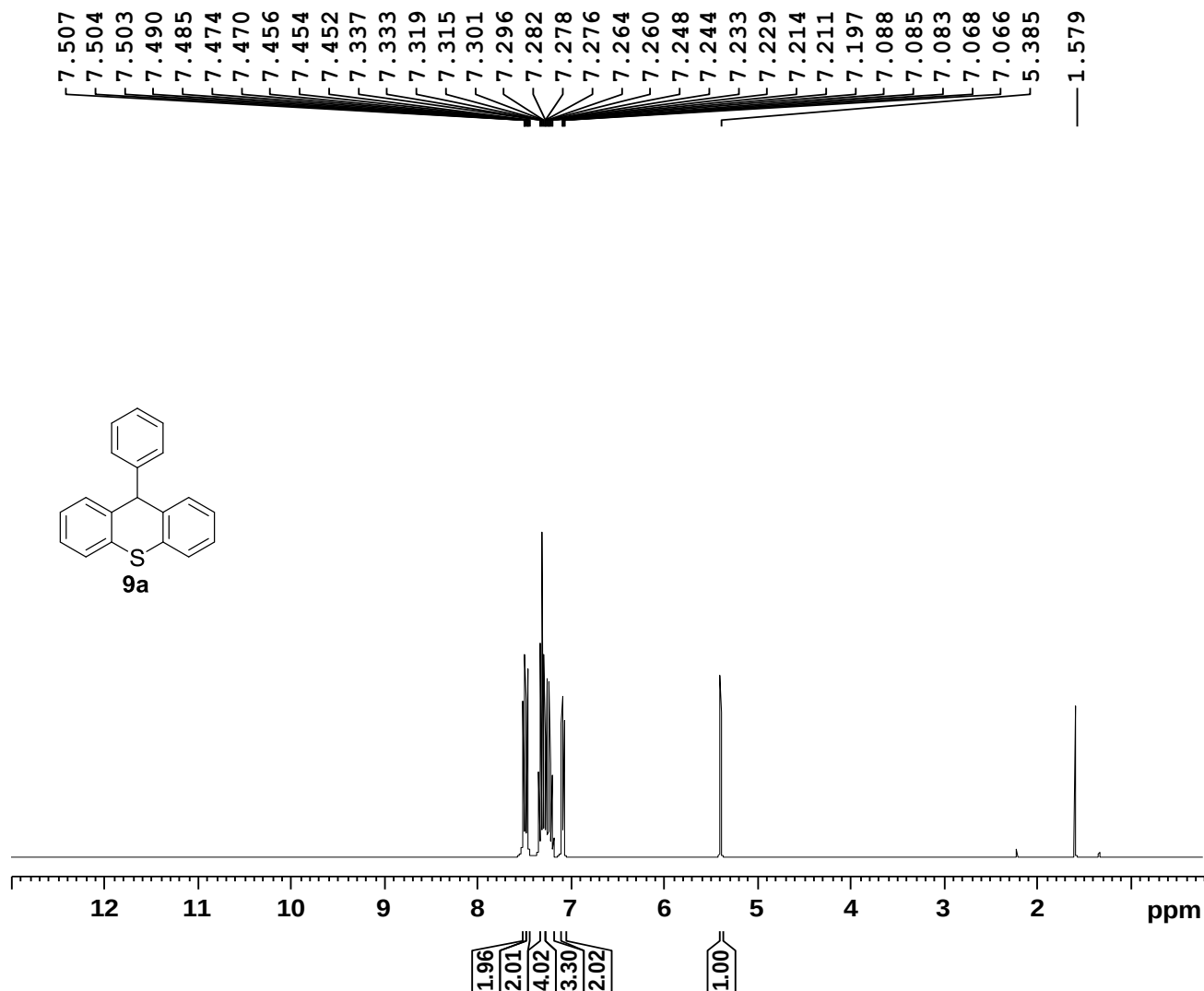
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127564 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 54: ^{13}C -NMR spectra for compound **7bi**

PROTON CDCl3 {D:\CRR} CIF_NMR 1



Current Data Parameters
 NAME MK-III-440
 EXPNO 1
 PROCNO 1

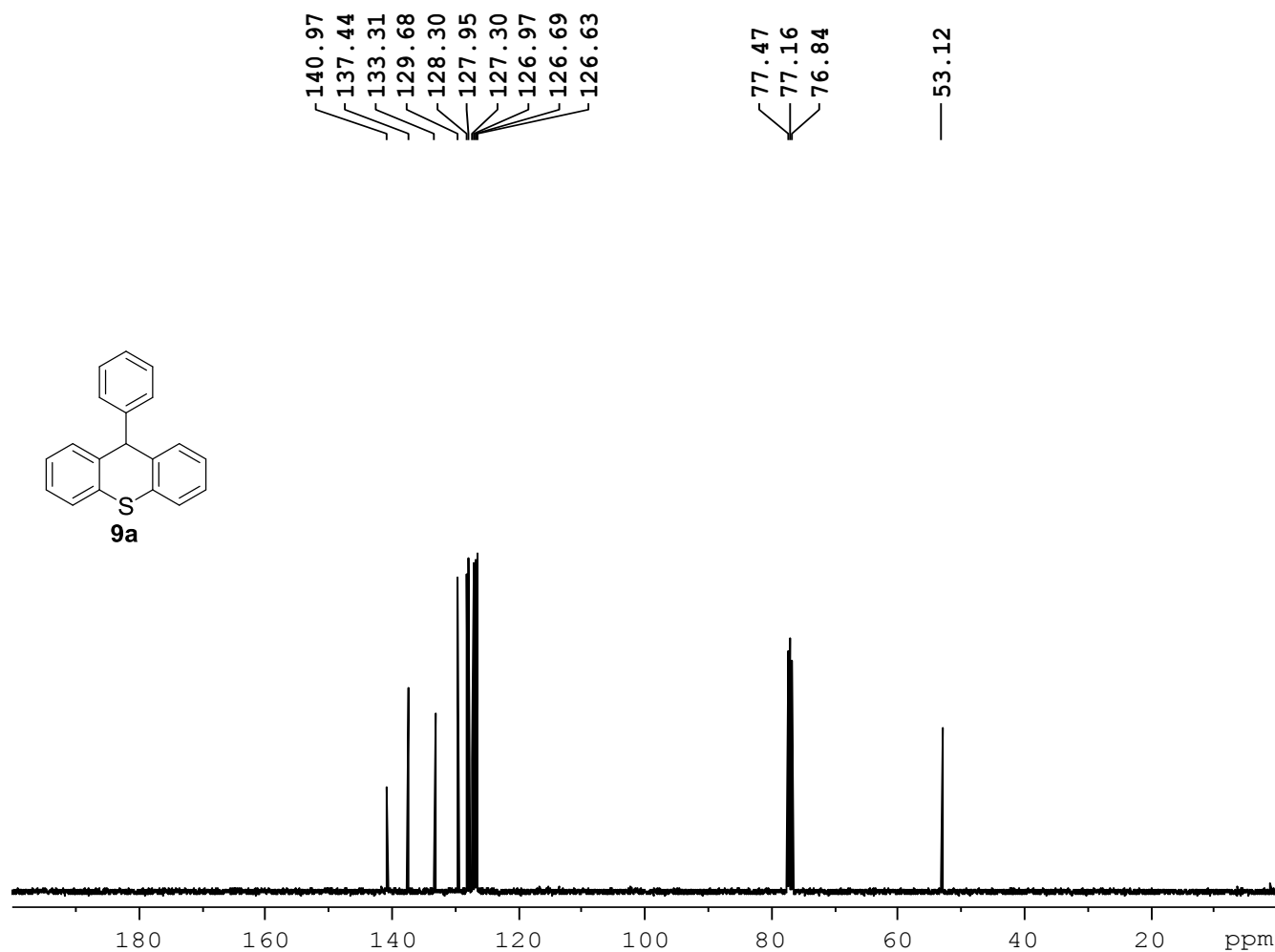
F2 - Acquisition Parameters
 Date_ 20190821
 Time 15.41
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 144
 DW 60.800 usec
 DE 6.00 usec
 TE 292.3 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.35 usec
 PL1 -1.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300030 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure 55: ¹H-NMR spectra for compound 9a

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-III-440
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190821
Time 17.23
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 36
DW 20.800 usec
DE 6.00 usec
TE 292.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

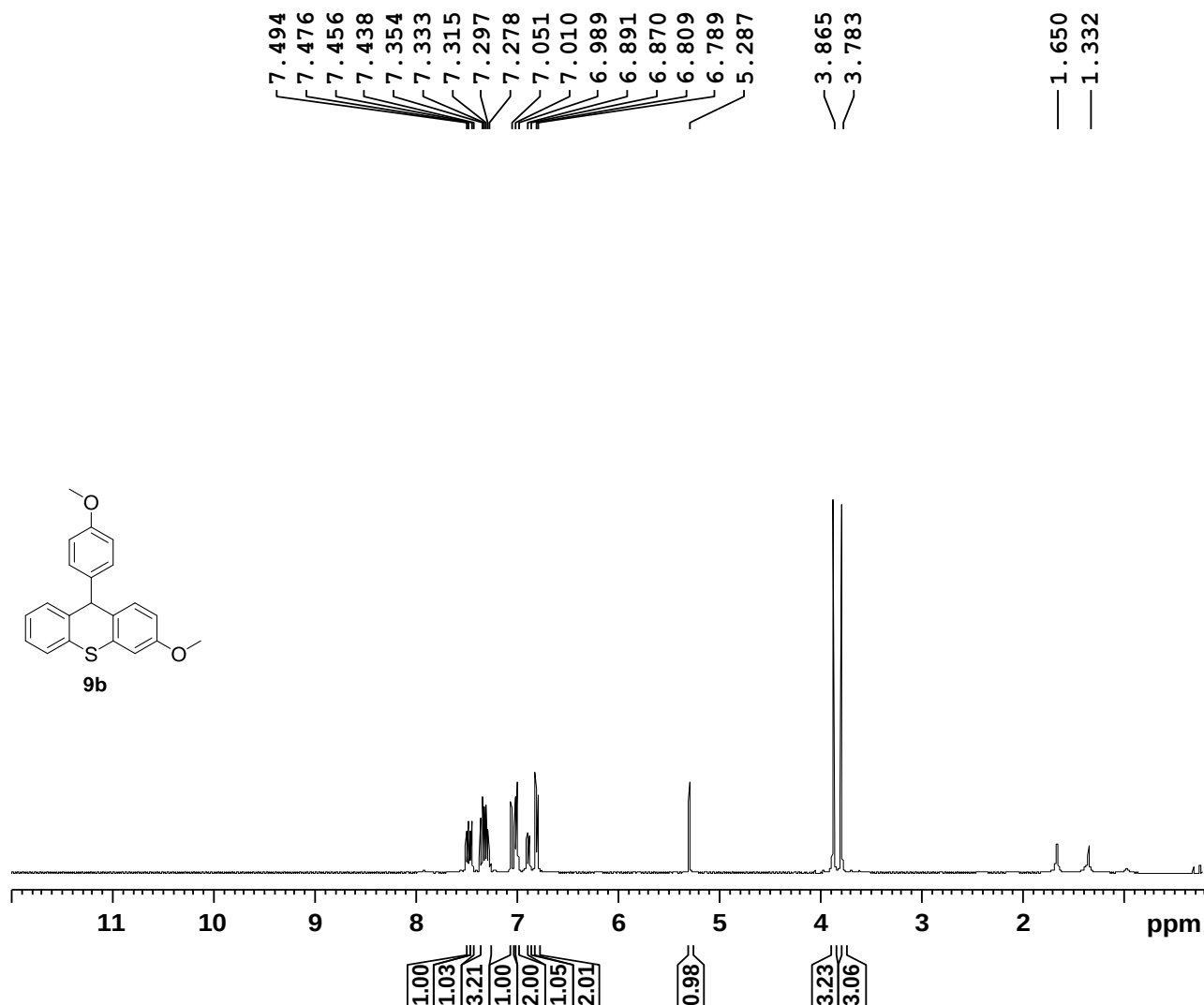
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127682 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 56: ^{13}C -NMR spectra for compound 9a

PROTON CDCL3



Current Data Parameters
NAME MK-ED-43
EXPNO 1
PROCNO 1

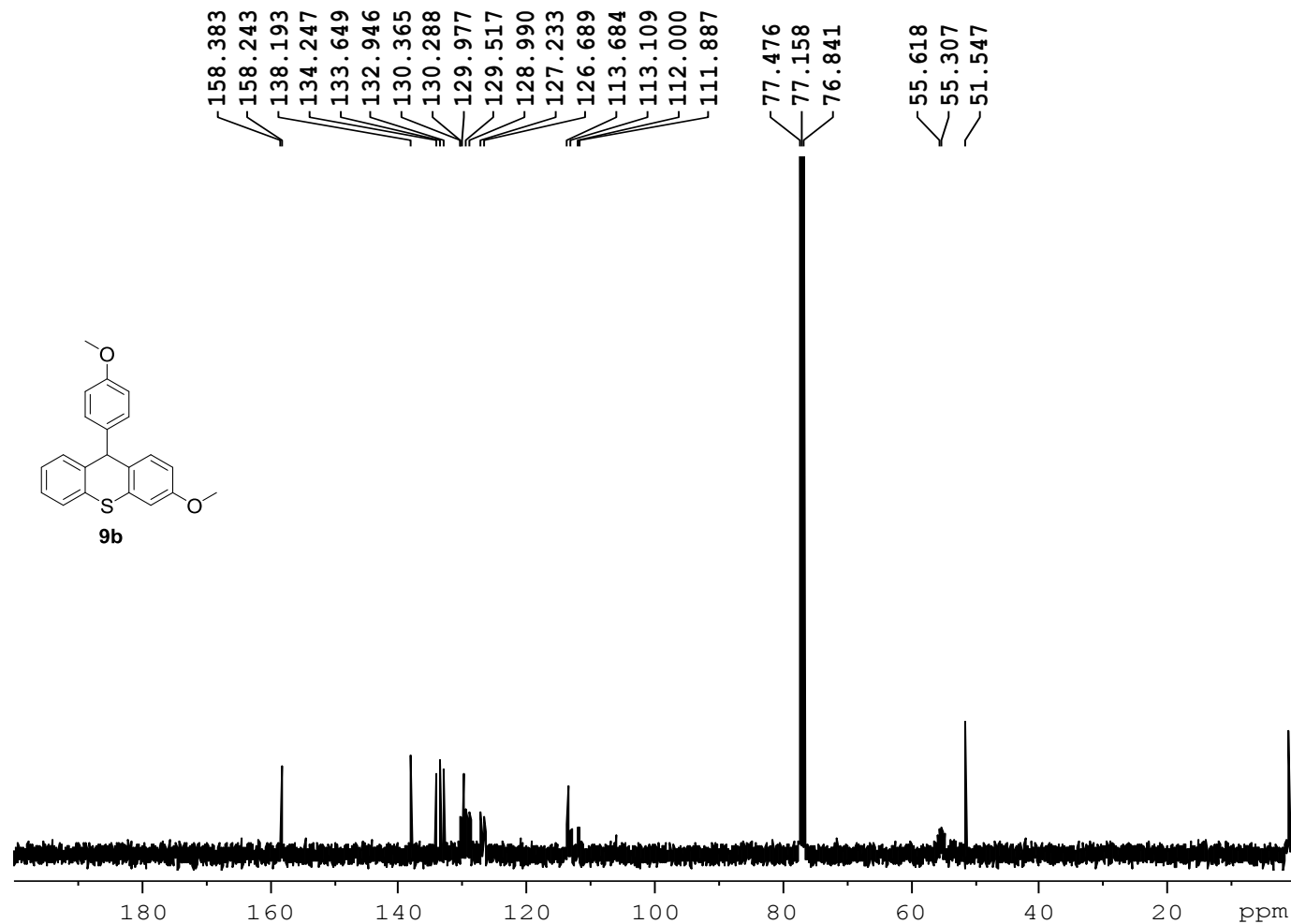
F2 - Acquisition Parameters
Date_ 20190311
Time_ 12.56
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCL3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 406
DW 60.800 usec
DE 6.00 usec
TE 295.8 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1299874 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 57: ¹H-NMR spectra for compound 9a

C13CPD



Current Data Parameters
NAME MK-ED-43
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190311
Time_ 13.01
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 362
DW 20.800 usec
DE 6.00 usec
TE 295.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

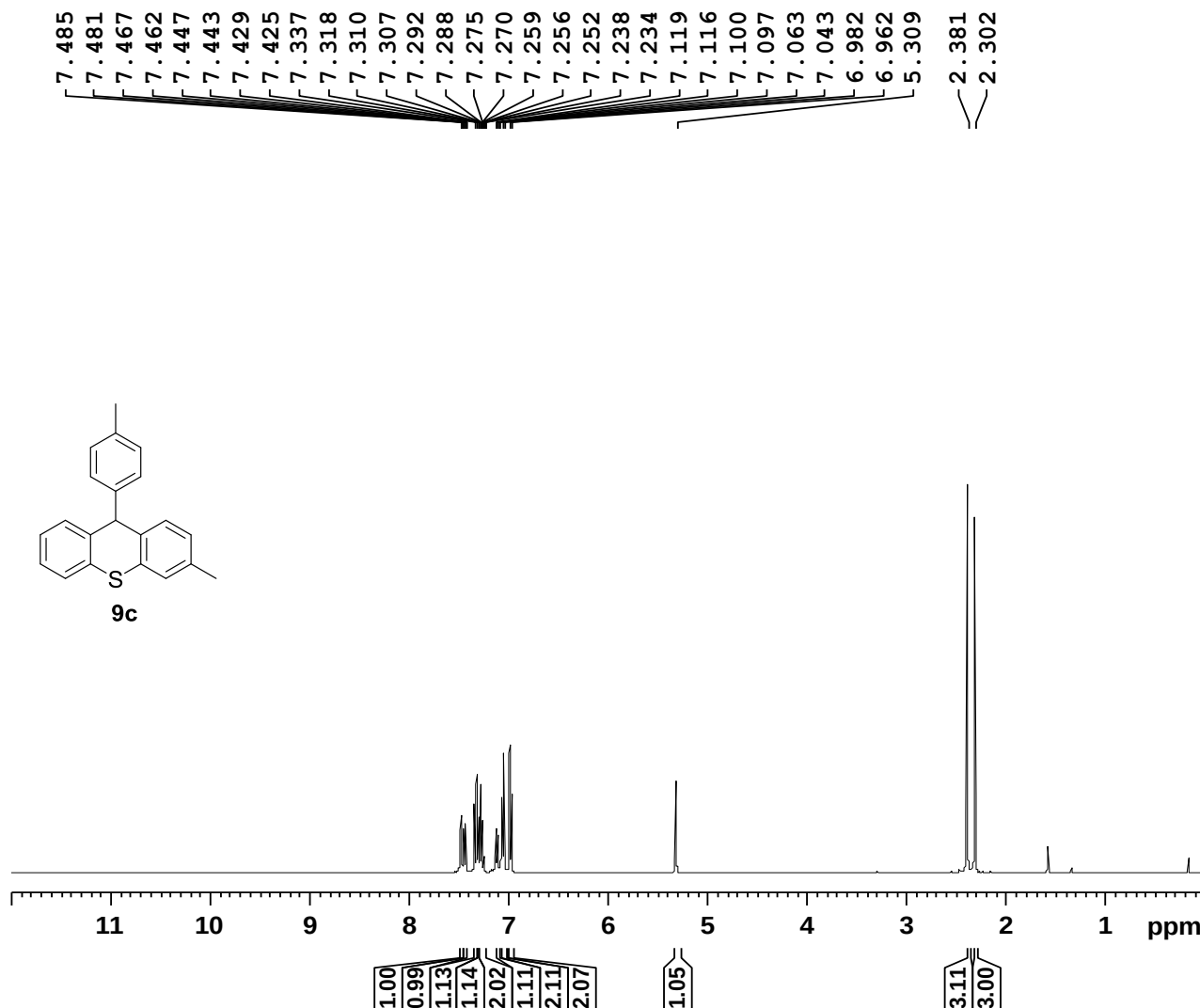
===== CHANNEL f1 =====
NUC1 13C
P1 9.15 usec
PL1 0 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.90 dB
PL13 14.90 dB
PL2 -3.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127578 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 58: ^{13}C -NMR spectra for compound **9b**

PROTON CDCl3 {D:\CRR} CIF_NMR 1



Current Data Parameters
 NAME MK-III-444
 EXPNO 1
 PROCNO 1

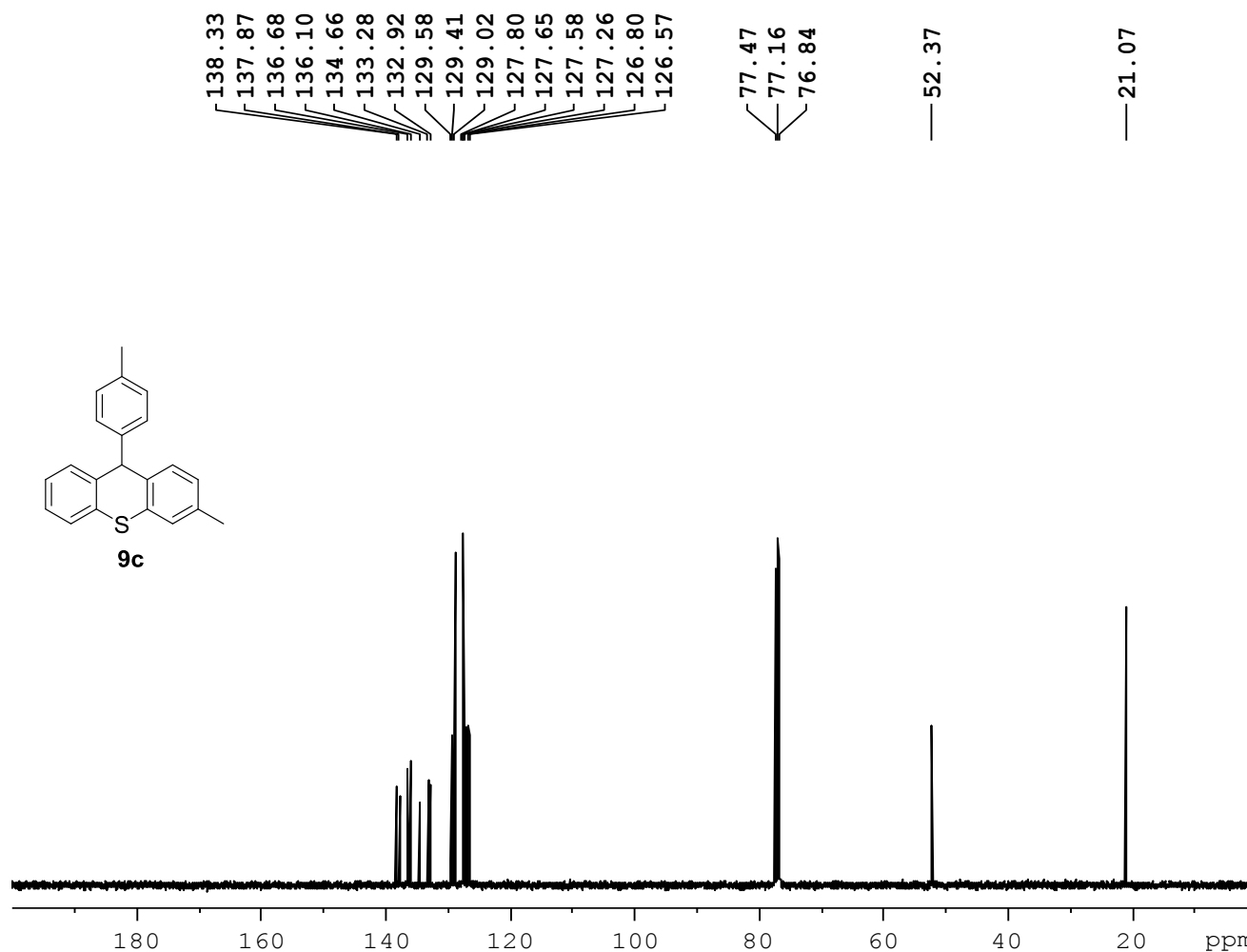
F2 - Acquisition Parameters
 Date_ 20190828
 Time_ 12.08
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 114
 DW 60.800 usec
 DE 6.00 usec
 TE 292.2 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.35 usec
 PL1 -1.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300093 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure 59: ¹H-NMR spectra for compound 9c

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-III-444
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190828
Time 12.23
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 362
DW 20.800 usec
DE 6.00 usec
TE 292.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

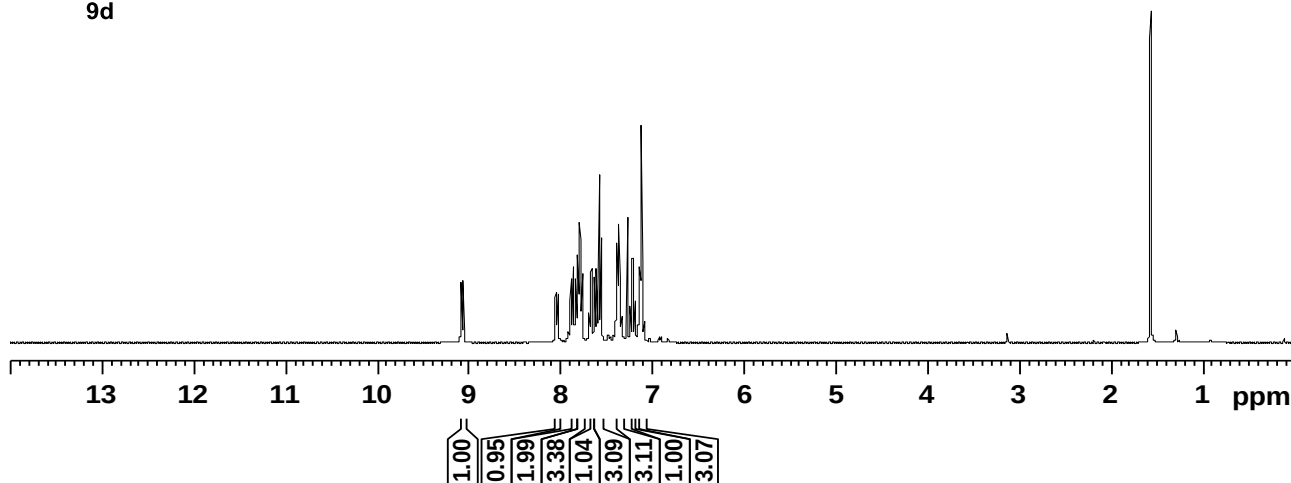
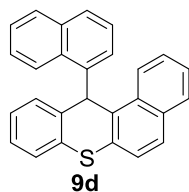
F2 - Processing parameters
SI 32768
SF 100.6127659 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 60: ¹³C-NMR spectra for compound **9c**

PROTON CDC13 {D:\CRR} CIF_NMR 1



9.075
9.053
7.876
7.856
7.832
7.828
7.809
7.803
7.794
7.786
7.780
7.772
7.759
7.673
7.671
7.654
7.652
7.623
7.602
7.586
7.566
7.544
7.383
7.378
7.368
7.364
7.361
7.351
7.345
7.338
7.333
7.260
7.224
7.204
7.124
7.119
7.108
7.101
7.096
7.091



Current Data Parameters
NAME MK-III-446
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190830
Time_ 12.39
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 406
DW 60.800 usec
DE 6.00 usec
TE 295.6 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 61: ¹H-NMR spectra for compound **9d**

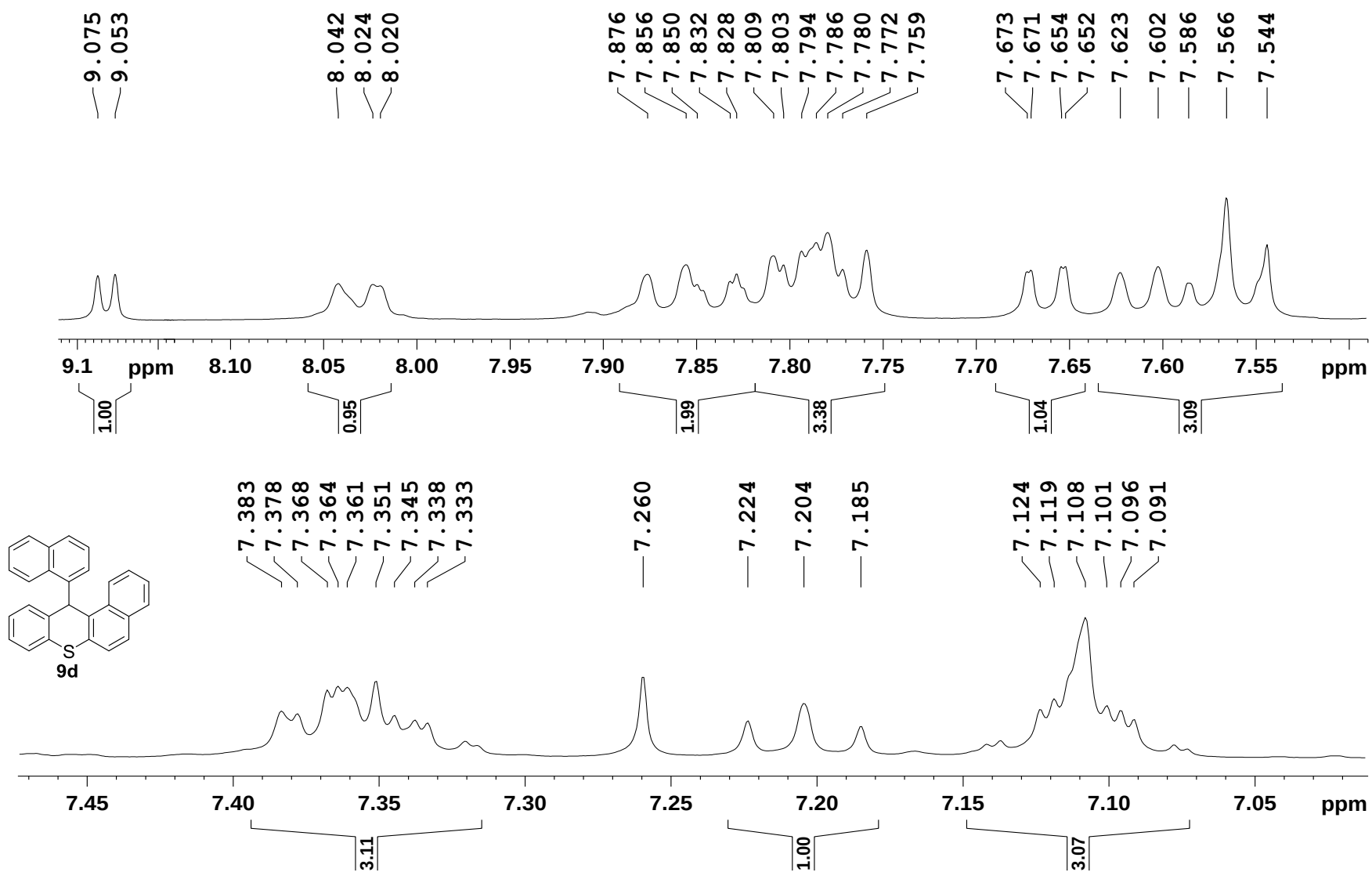
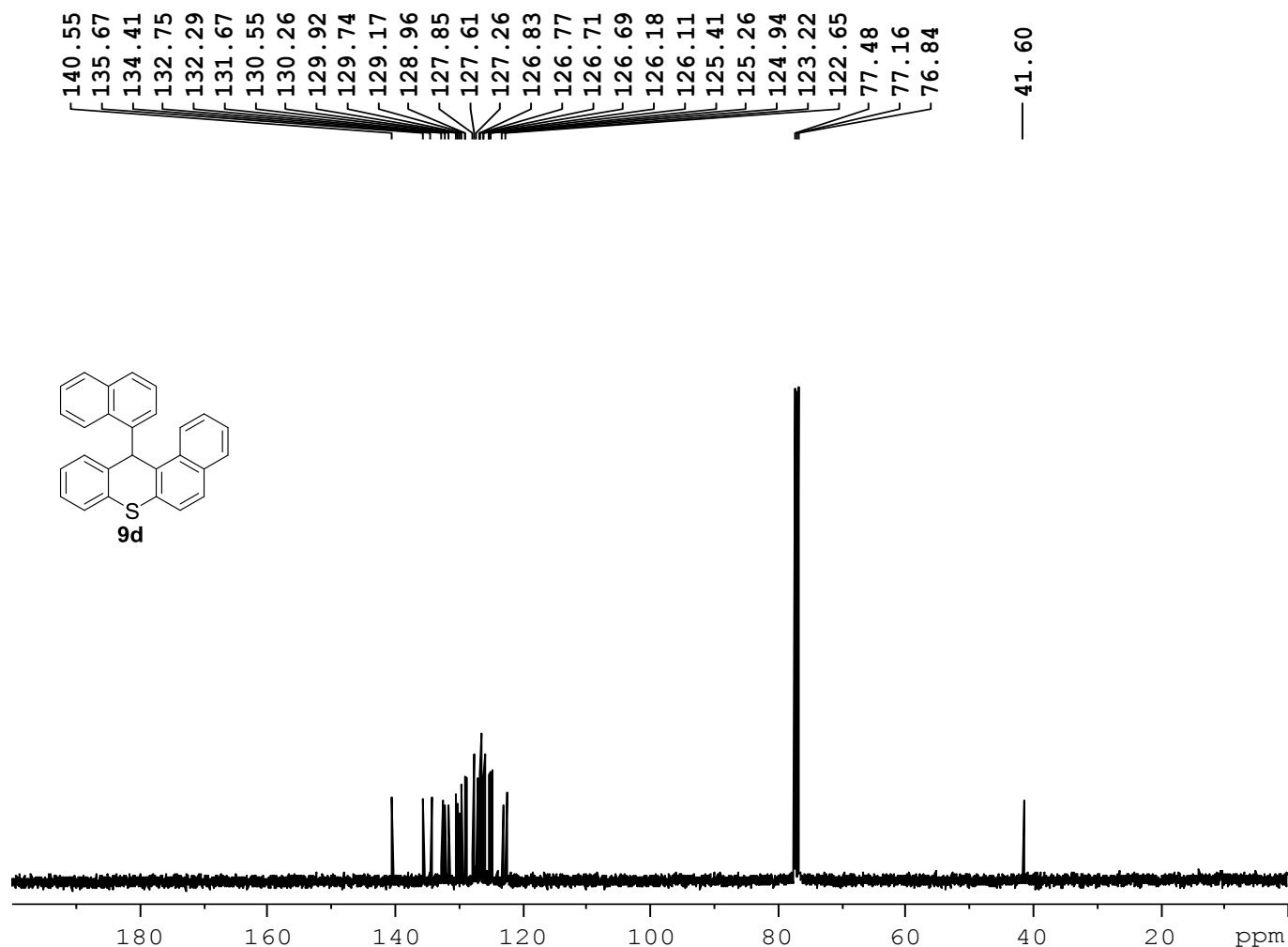


Figure 61a: ^1H -NMR spectra expansion for compound **9d**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-III-446
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190830
Time 16.16
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 322
DW 20.800 usec
DE 6.00 usec
TE 293.9 K
D1 2.0000000 sec
d11 0.0300000 sec
DELTA 1.8999999 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

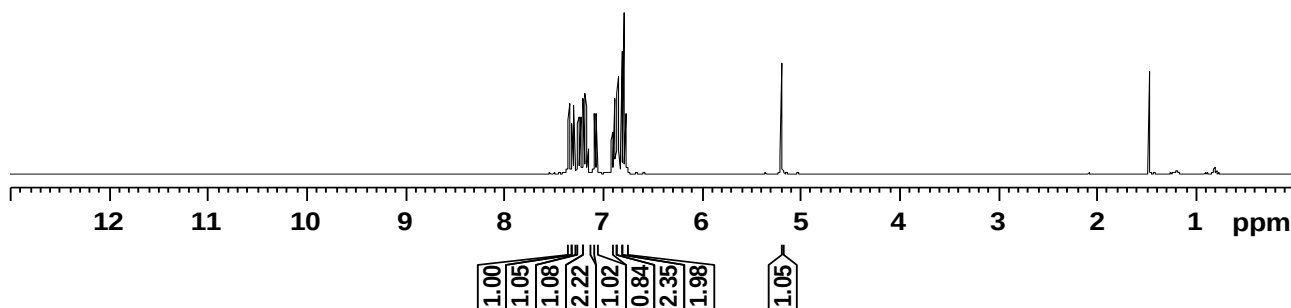
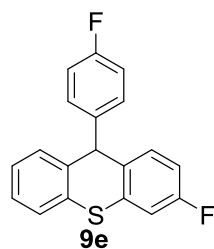
F2 - Processing parameters
SI 32768
SF 100.6127632 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 62: ^{13}C -NMR spectra for compound **9d**

PROTON CDC13 {D:\CRR} CIF_NMR 1



7.348
7.345
7.330
7.326
7.306
7.302
7.288
7.284
7.254
7.240
7.232
7.218
7.195
7.191
7.177
7.174
7.173
7.170
7.156
7.152
7.083
7.077
7.062
7.055
6.899
6.878
6.871
6.862
6.857
6.850
6.849
6.845
6.841
6.832
6.827
6.798
6.776
6.754
5.182
1.456



Current Data Parameters
NAME MK-III-449
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190910
Time_ 23.05
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 144
DW 60.800 usec
DE 6.00 usec
TE 295.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300567 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 63: ¹H-NMR spectra for compound 9e

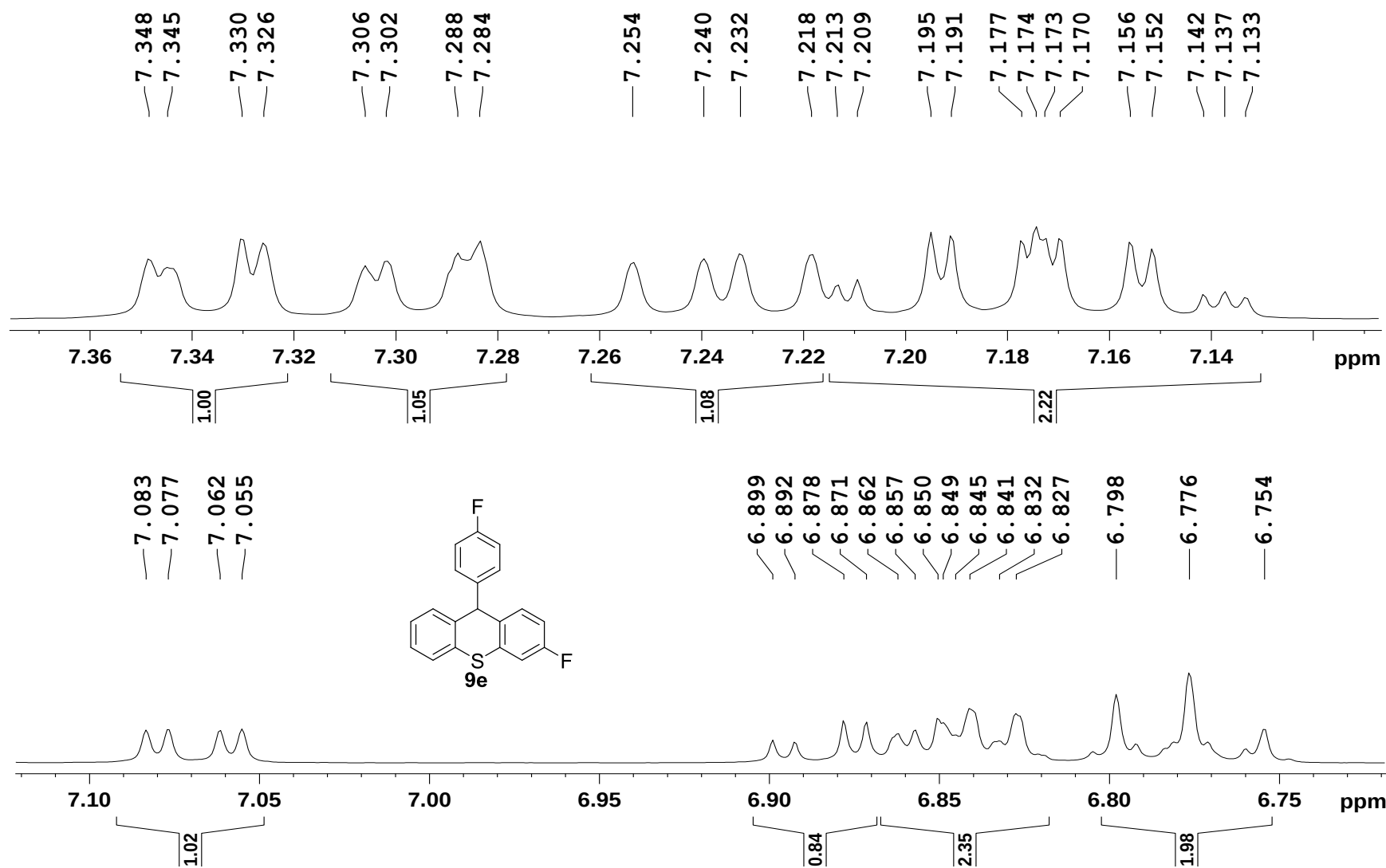
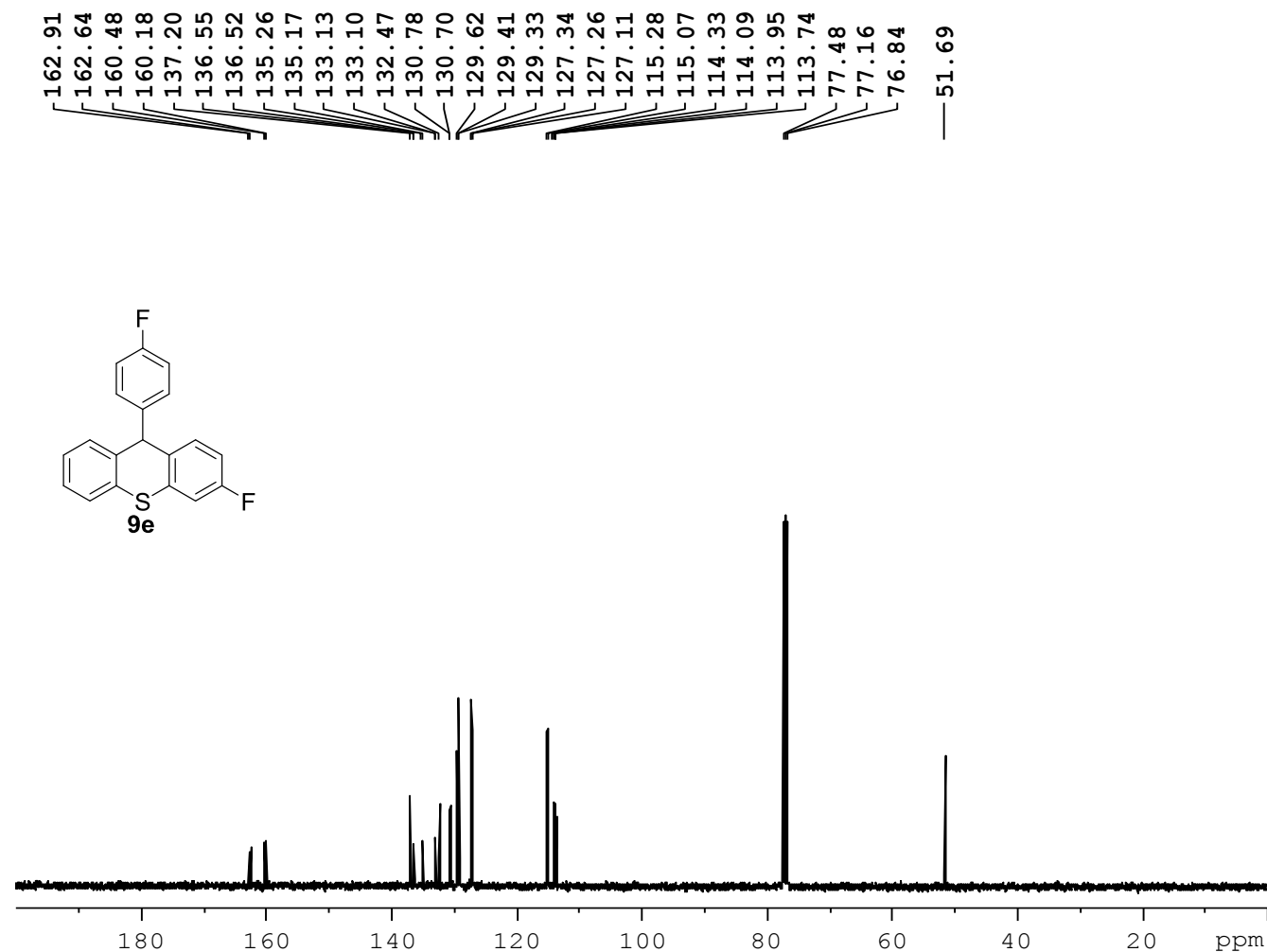


Figure 63a: ^1H -NMR spectra expansion for compound **9e**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
 NAME MK-III-449
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190911
 Time 9.23
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 300
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 36
 DW 20.800 usec
 DE 6.00 usec
 TE 294.5 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

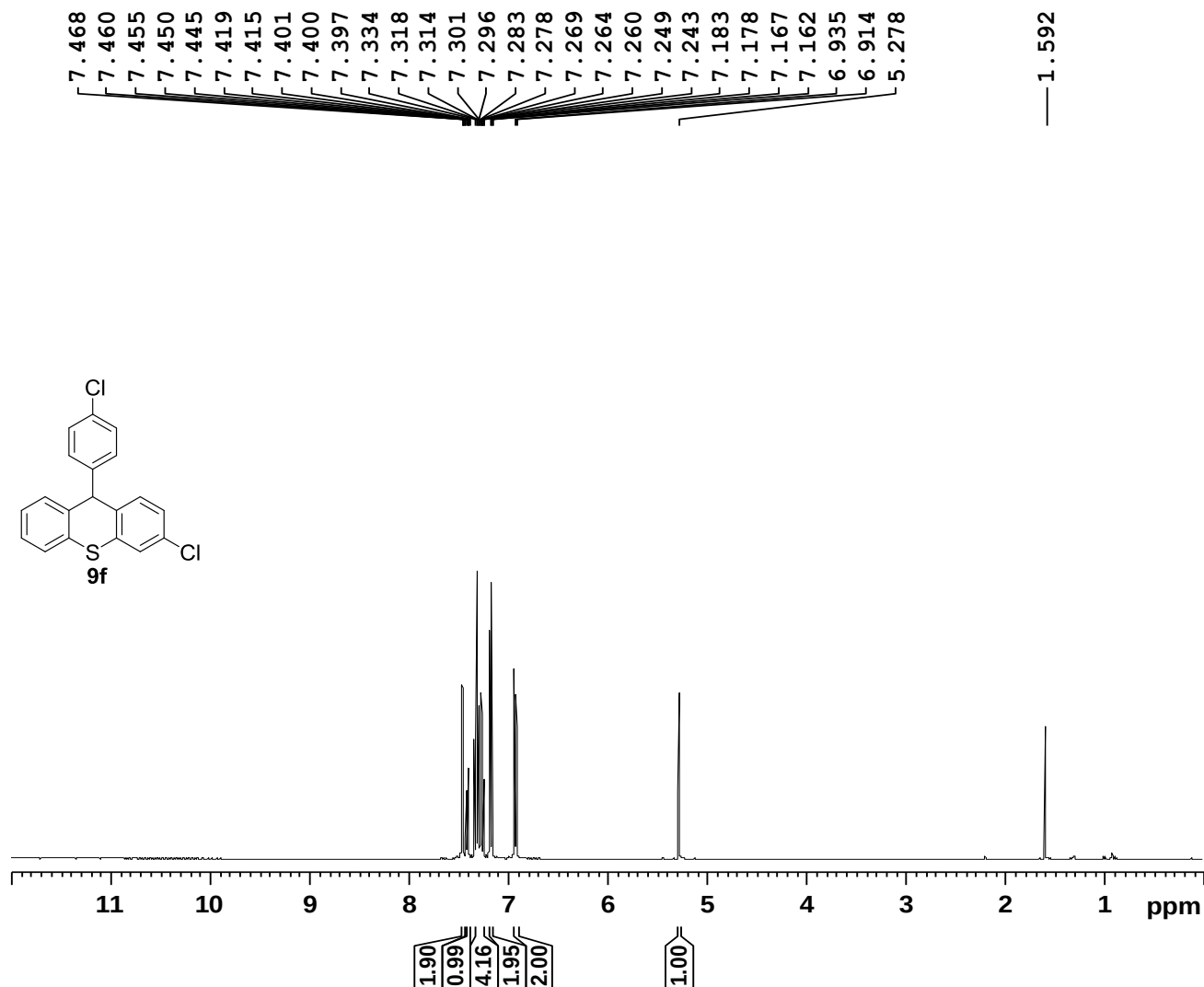
===== CHANNEL f1 =====
 NUC1 13C
 P1 9.95 usec
 PL1 -1.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL12 14.95 dB
 PL13 120.00 dB
 PL2 -1.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127599 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure 64: ¹³C-NMR spectra for compound **9e**

PROTON CDCl3 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-424-A
EXPNO 1
PROCNO 1

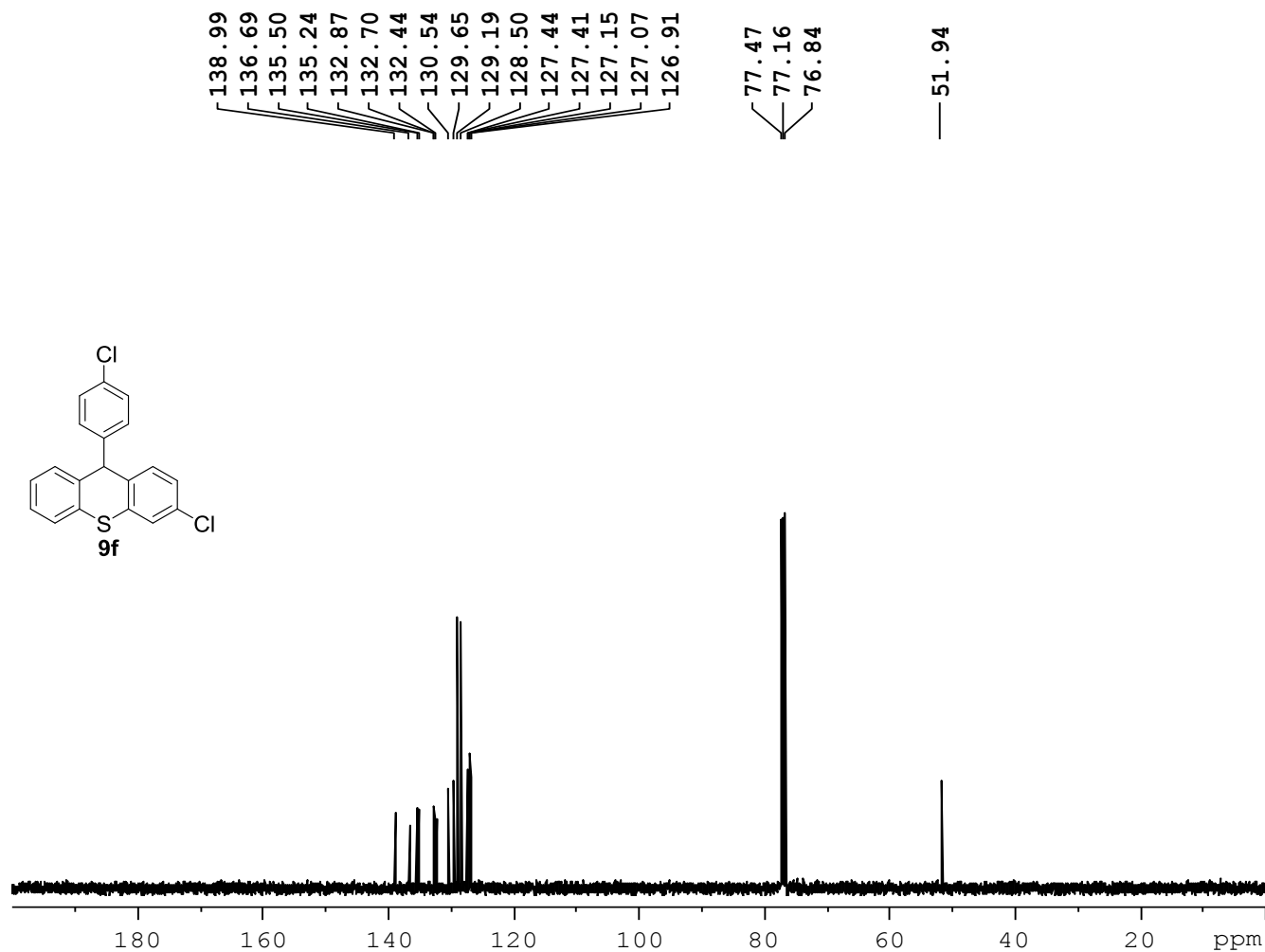
F2 - Acquisition Parameters
Date_ 20190926
Time 15.10
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 161
DW 60.800 usec
DE 6.00 usec
TE 293.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300065 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 65: ¹H-NMR spectra for compound 9f

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-424-A
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190926
Time 15.17
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 456
DW 20.800 usec
DE 6.00 usec
TE 293.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

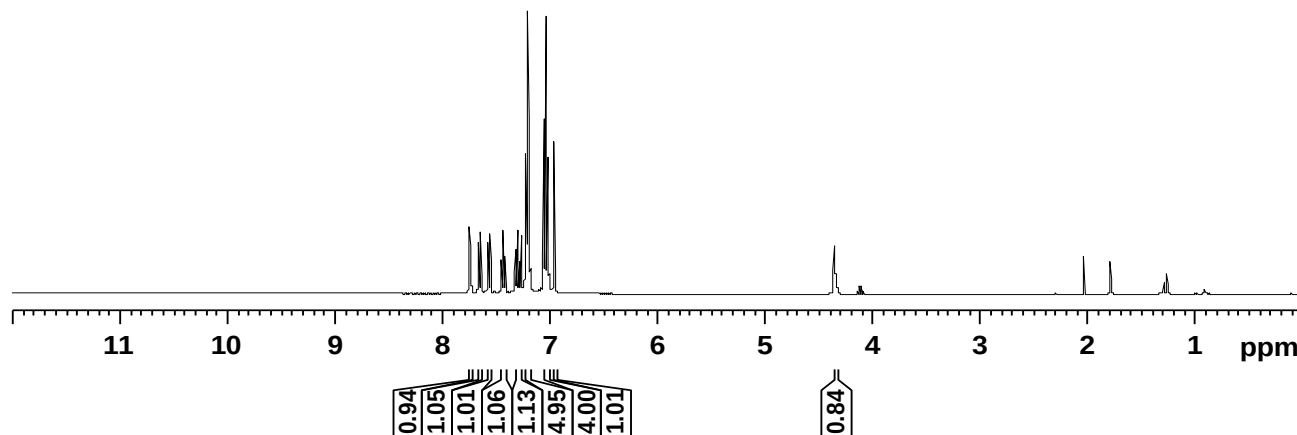
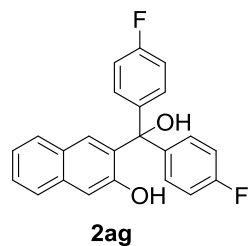
F2 - Processing parameters
SI 32768
SF 100.6127614 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 66: ¹³C-NMR spectra for compound **9f**

PROTON CDC13 {D:\CRR} CIF_NMR 1



7.741
7.657
7.636
7.567
7.547
7.448
7.445
7.431
7.428
7.425
7.411
7.408
7.314
7.312
7.297
7.294
7.291
7.277
7.274
7.260
7.218
7.205
7.196
7.183
7.050
7.029
7.007
6.952
4.346



Current Data Parameters
NAME MK-II-363-F
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190816
Time 9.11
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 144
DW 60.800 usec
DE 6.00 usec
TE 291.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300096 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 67: ¹H-NMR spectra for compound **2ag**

PROTON CDC13 {D:\CRR} CIF_NMR 1

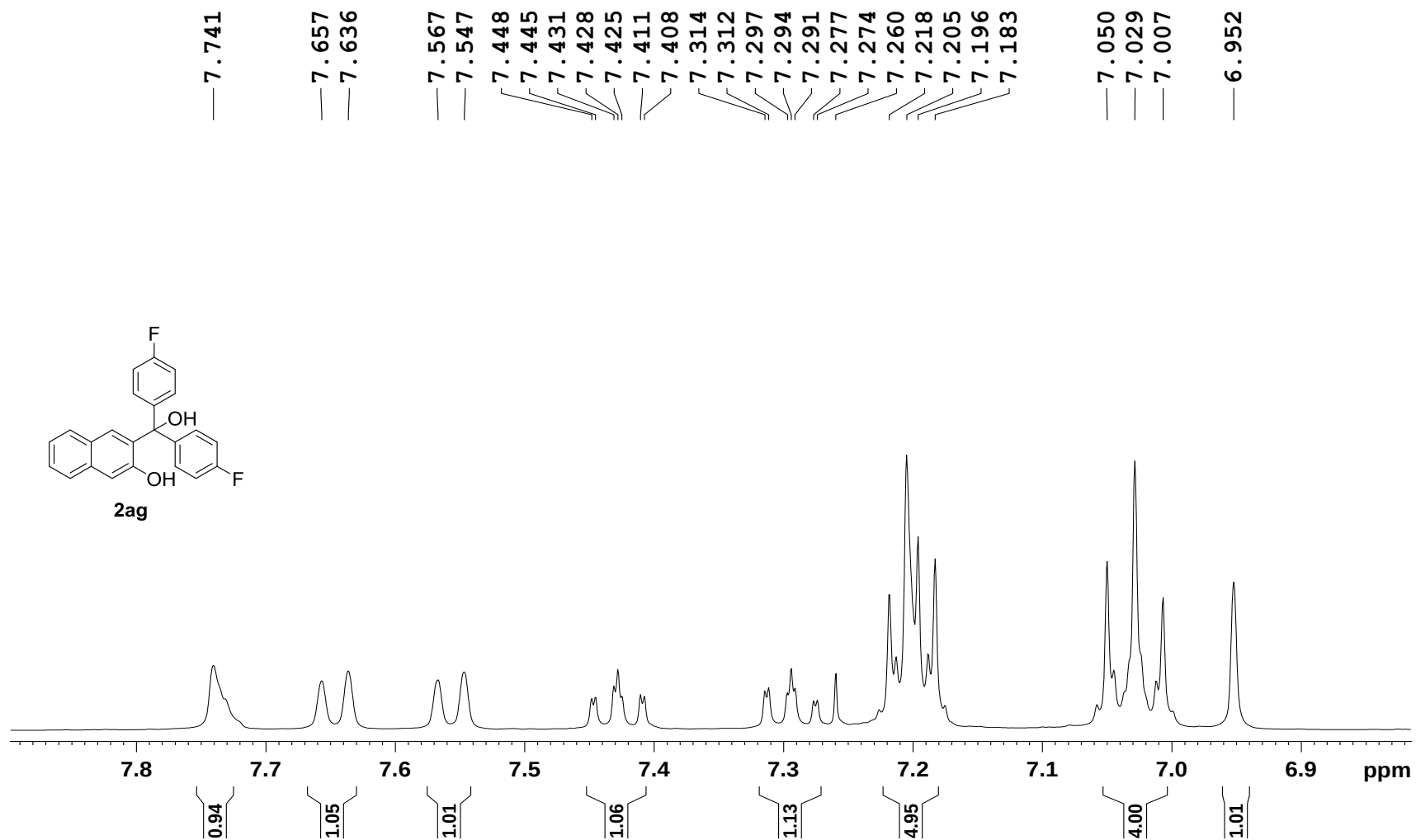
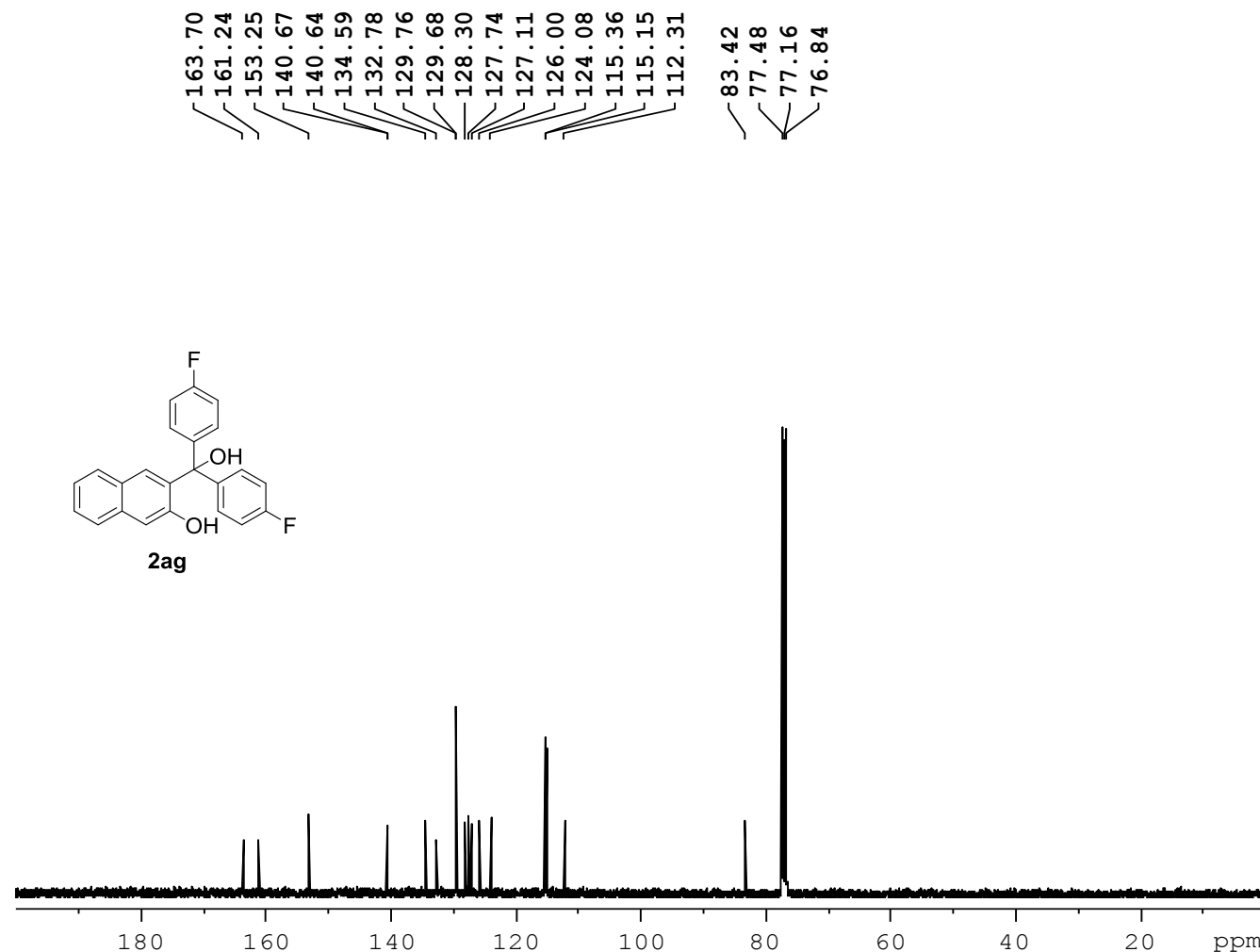


Figure 67a: ^1H -NMR spectra expansion for compound **2ag**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
 NAME MK-II-363-F
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190816
 Time 9.33
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 350
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 36
 DW 20.800 usec
 DE 6.00 usec
 TE 291.5 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

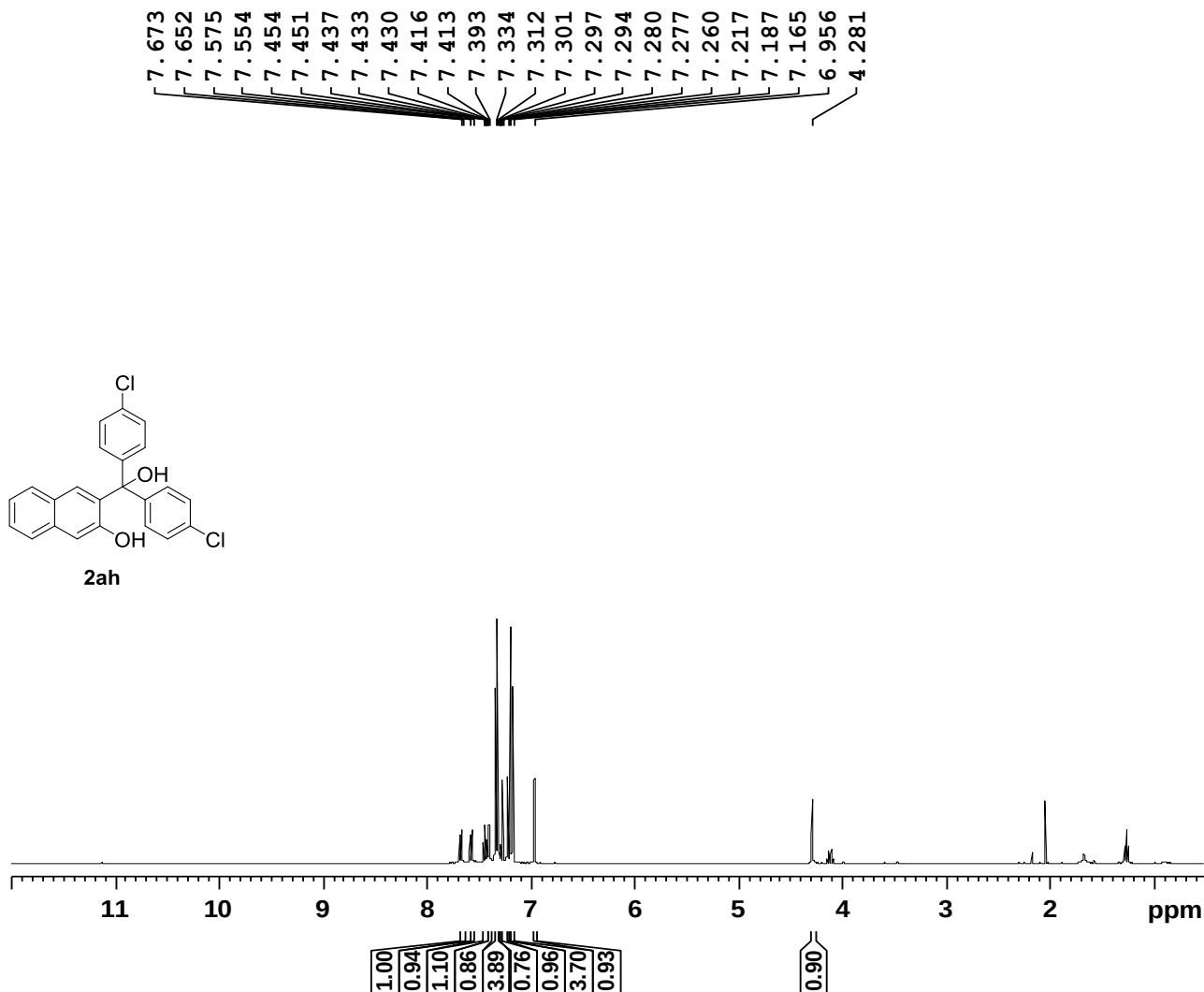
===== CHANNEL f1 =====
 NUC1 13C
 P1 9.95 usec
 PL1 -1.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL12 14.95 dB
 PL13 120.00 dB
 PL2 -1.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127592 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure 68: ¹³C-NMR spectra for compound **2ag**

PROTON CDCl3 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-ED-75-CL
EXPNO 1
PROCNO 1

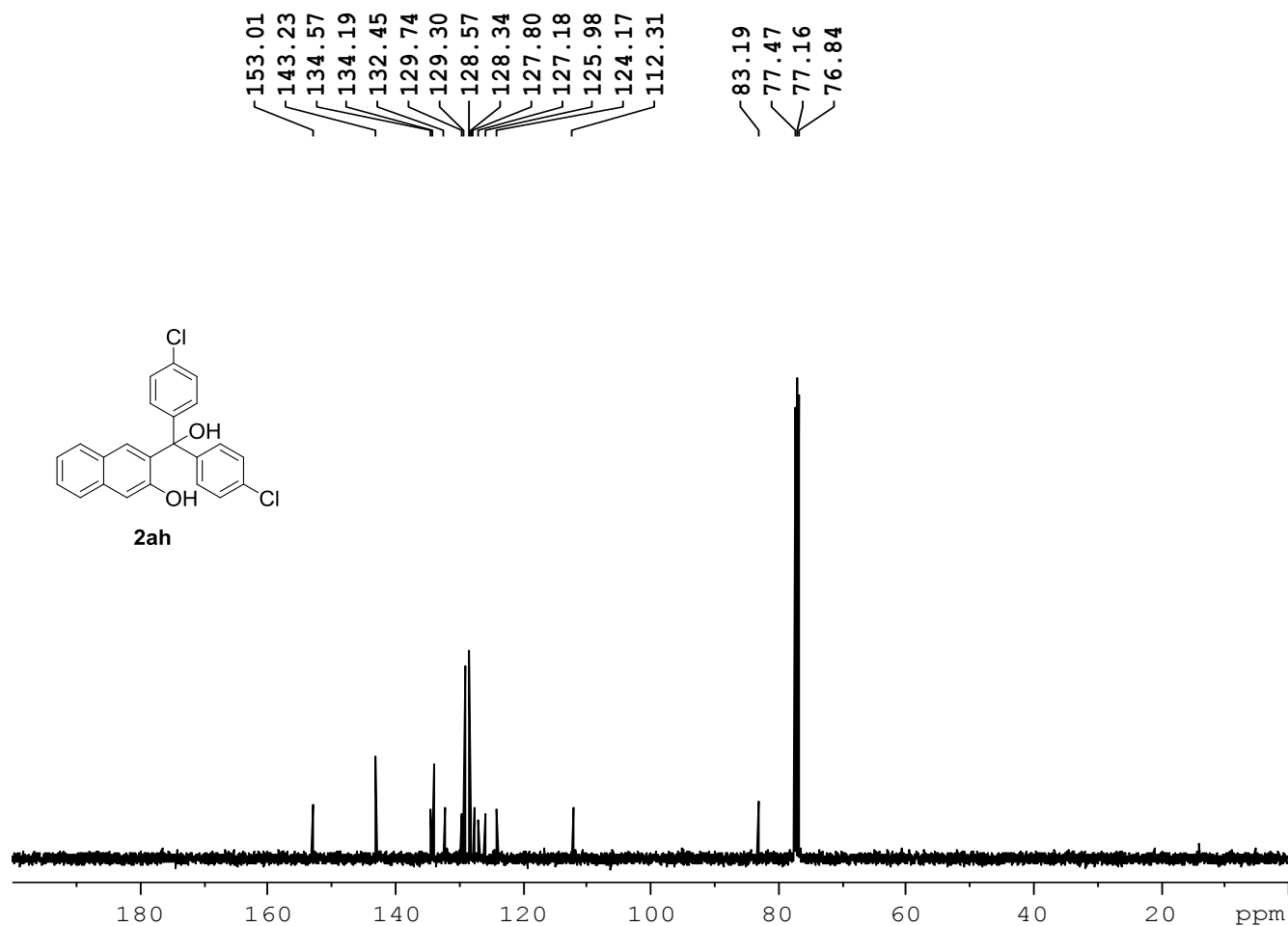
F2 - Acquisition Parameters
Date_ 20190807
Time_ 17.09
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 406
DW 60.800 usec
DE 6.00 usec
TE 294.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 69: ¹H-NMR spectra for compound **2ah**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
 NAME MK-ED-75-CL
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190808
 Time 16.05
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 256
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 40.3
 DW 20.800 usec
 DE 6.00 usec
 TE 293.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 13C
 P1 9.95 usec
 PL1 -1.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL12 14.95 dB
 PL13 120.00 dB
 PL2 -1.00 dB
 SFO2 400.1316005 MHz

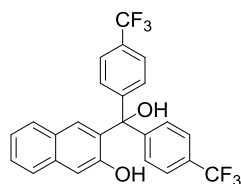
F2 - Processing parameters
 SI 32768
 SF 100.6127586 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure 70: ¹³C-NMR spectra for compound **2ah**

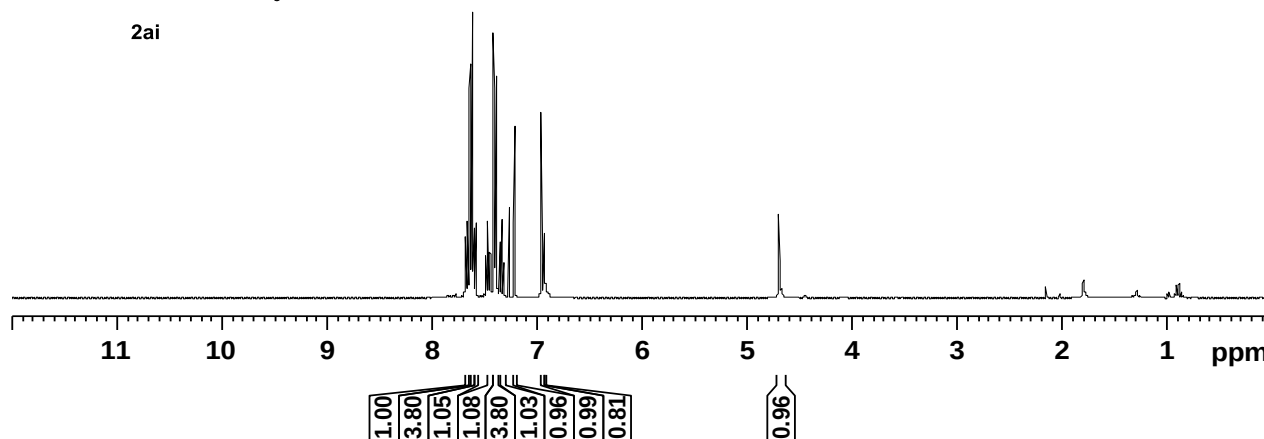
PROTON CDCl3 {D:\CRR} CIF_NMR 1



7.672
7.652
7.631
7.610
7.594
7.573
7.479
7.476
7.462
7.459
7.456
7.441
7.438
7.405
7.385
7.346
7.344
7.329
7.326
7.323
7.309
7.306
7.260
7.208
6.951
6.927
4.691



2ai



Current Data Parameters
NAME MK-ED-34-S
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190807
Time_ 17.14
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 203
DW 60.800 usec
DE 6.00 usec
TE 294.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 71: ¹H-NMR spectra for compound 2ai

PROTON CDCl3 {D:\CRR} CIF_NMR 1

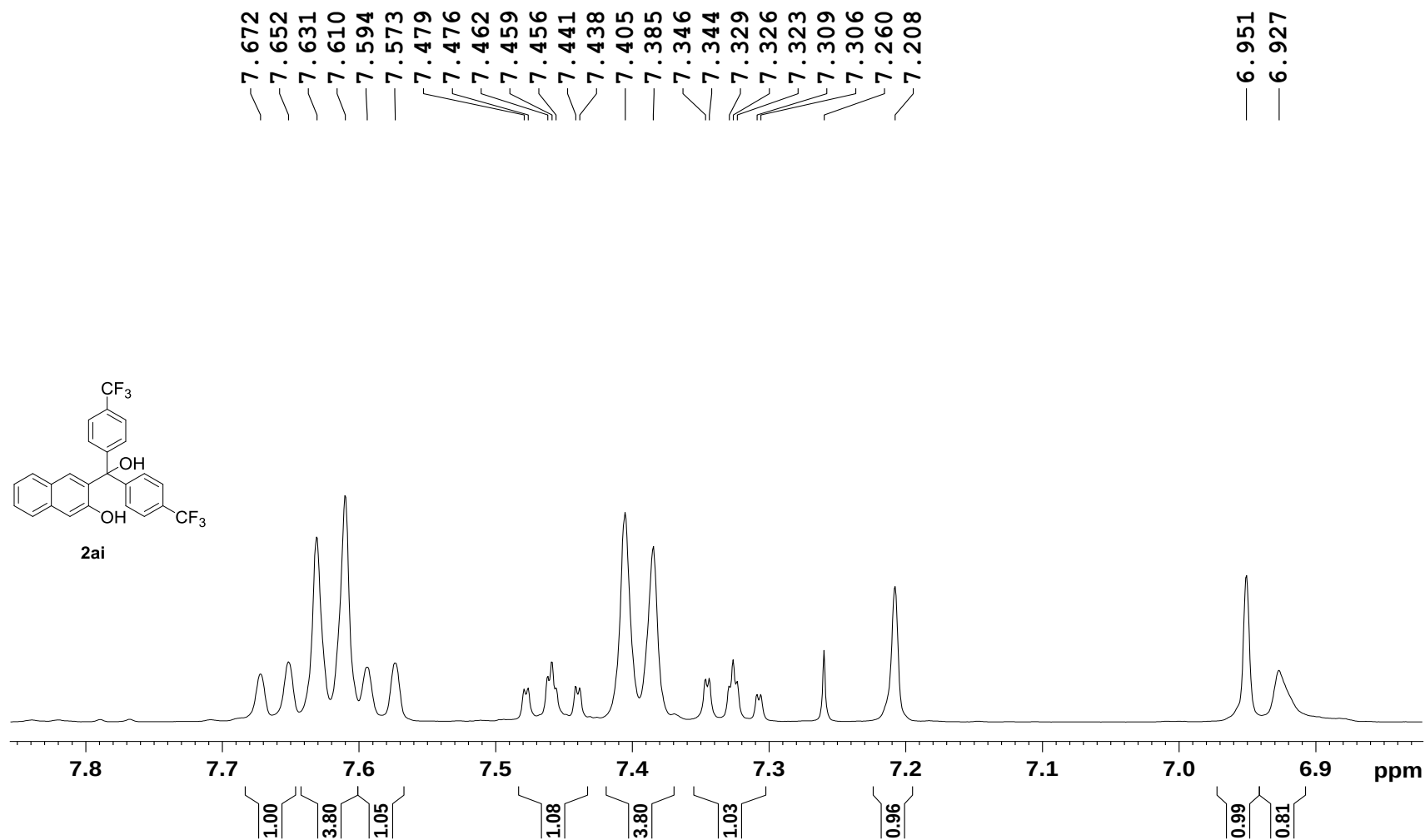
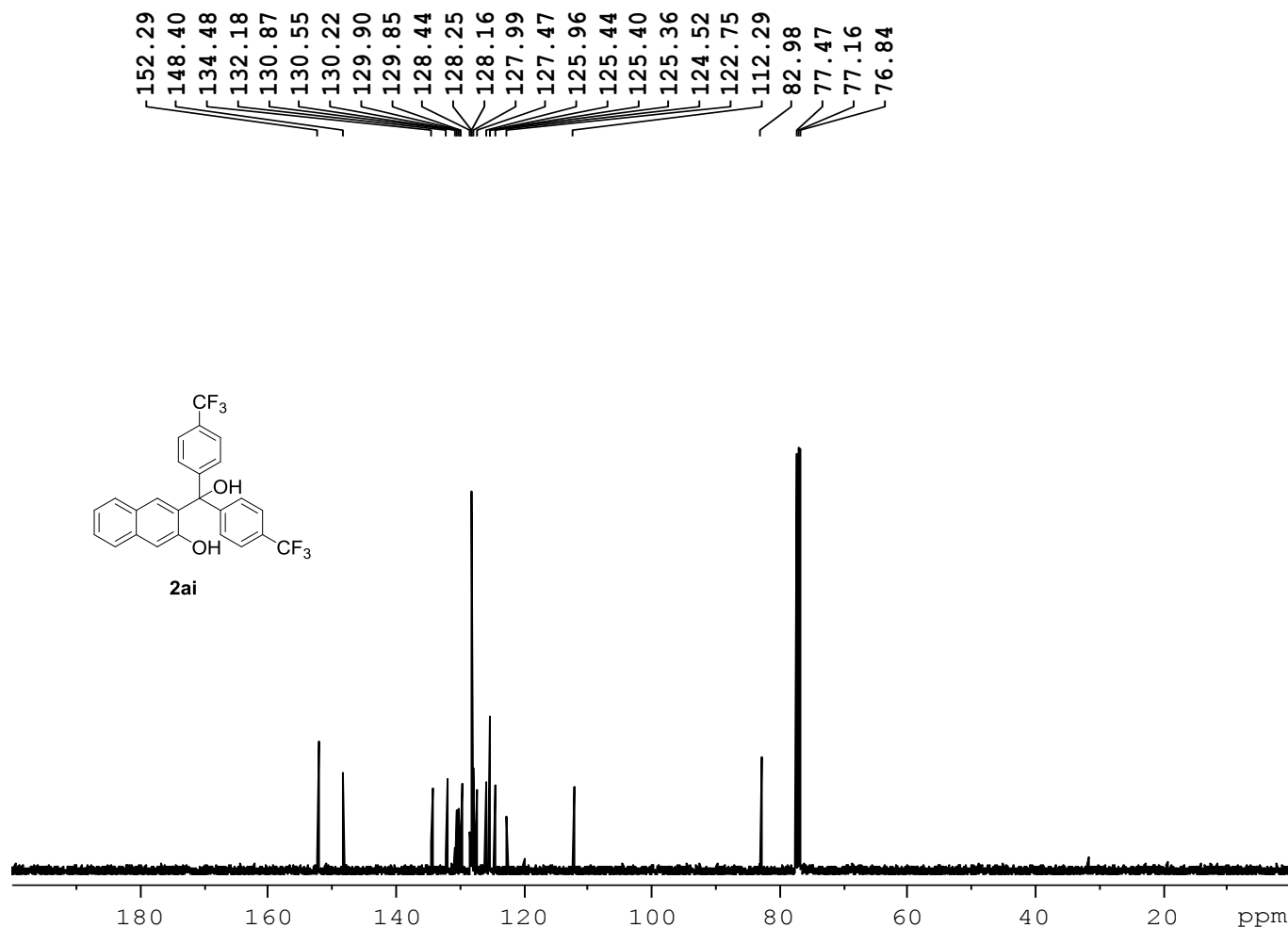


Figure 71a: ¹H-NMR spectra expansion for compound **2ai**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-ED-34-S
EXPNO 2
PROCNO 1

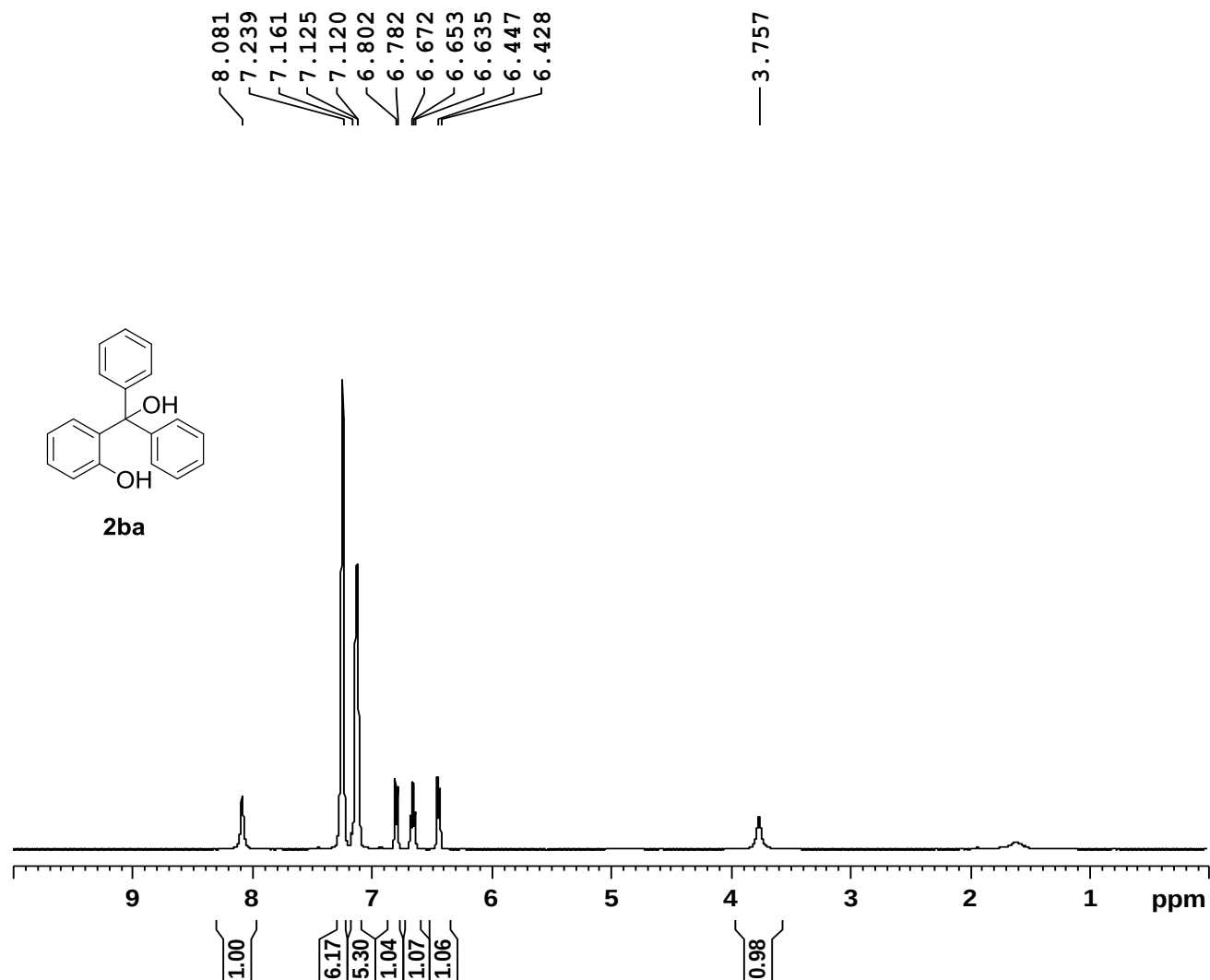
F2 - Acquisition Parameters
Date_ 20190808
Time_ 15.52
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 40.3
DW 20.800 usec
DE 6.00 usec
TE 292.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127593 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 72: ¹H-NMR spectra for compound **2ai**



Current Data Parameters
NAME MK-MM-11
EXPNO 1
PROCNO 1

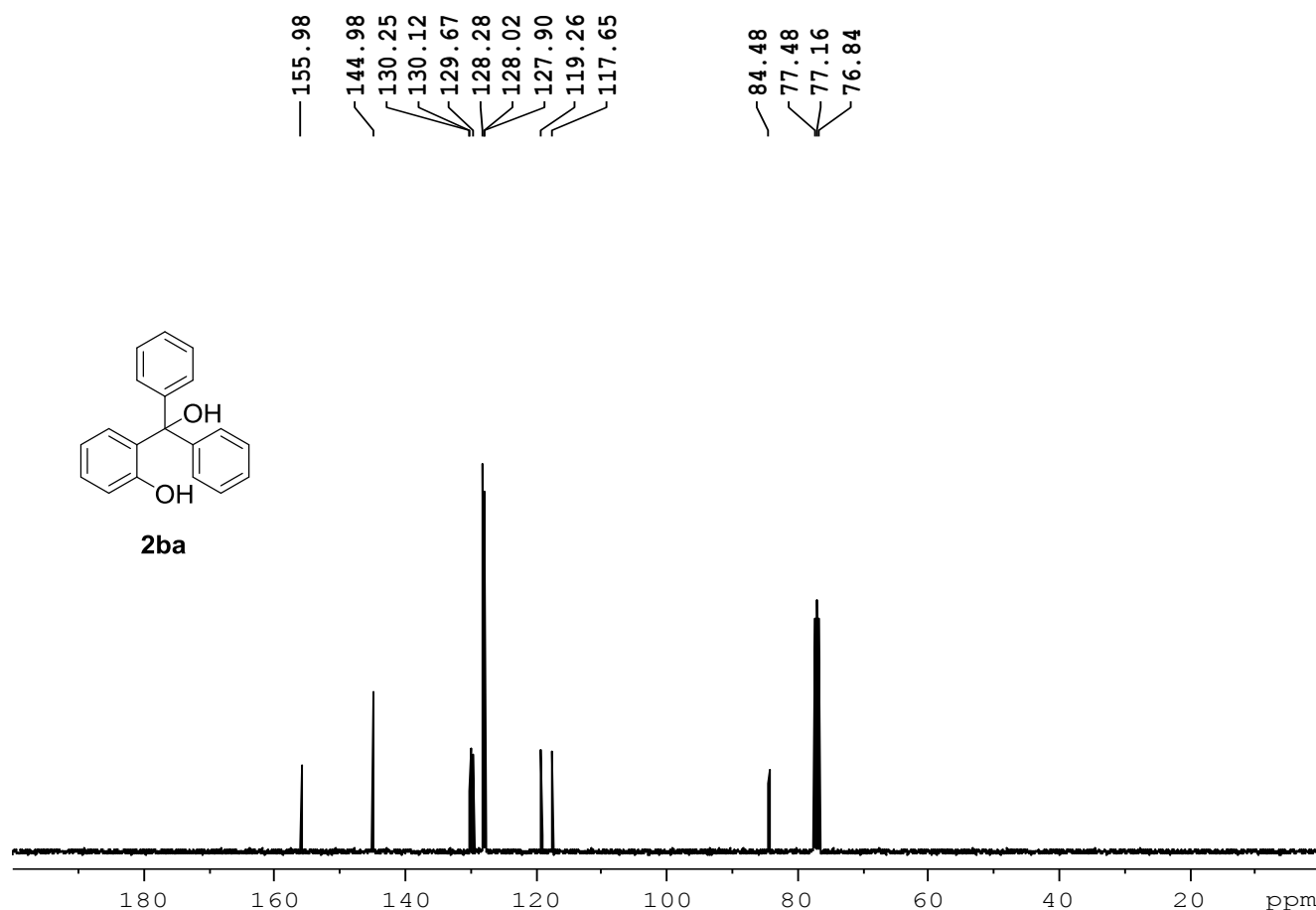
F2 - Acquisition Parameters
Date_ 20190215
Time 23.26
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 512
DW 60.800 usec
DE 6.00 usec
TE 291.9 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300478 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 73: ¹H-NMR spectra for compound **2ba**

C13CPD CDC13 {D:\CRR} KOPAL 1



Current Data Parameters
NAME MK-MM-11
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20181103
Time 15.32
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 362
DW 20.800 usec
DE 6.00 usec
TE 295.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 1

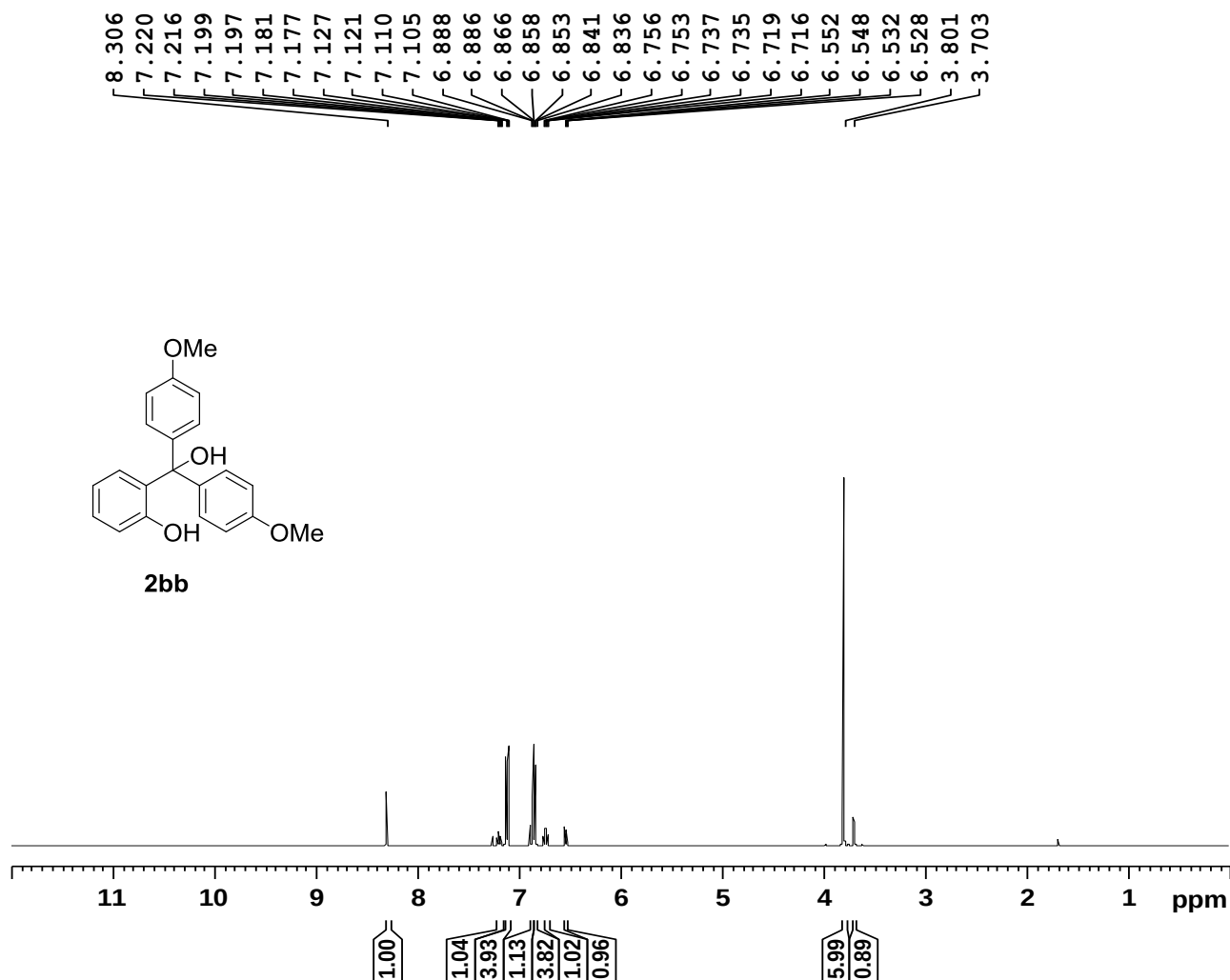
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127611 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 74: ¹³C-NMR spectra for compound **2ba**

PROTON CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-MM-15
EXPNO 1
PROCNO 1

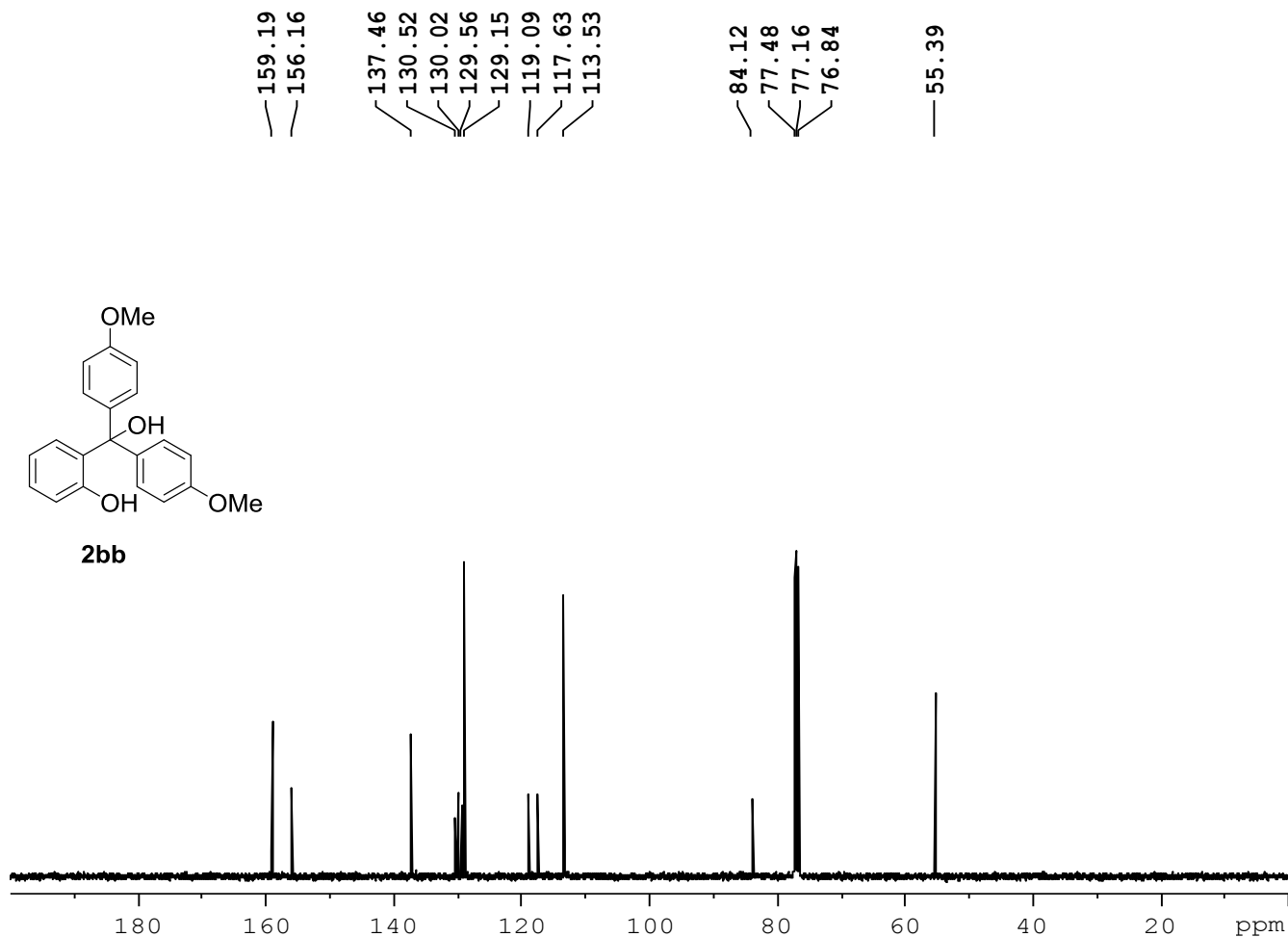
F2 - Acquisition Parameters
Date_ 20190701
Time 16.22
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 144
DW 60.800 usec
DE 6.00 usec
TE 296.2 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.130092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 75: ¹H-NMR spectra for compound **2bb**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
 NAME MK-MM-15
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190701
 Time_ 16.30
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 256
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 322
 DW 20.800 usec
 DE 6.00 usec
 TE 296.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

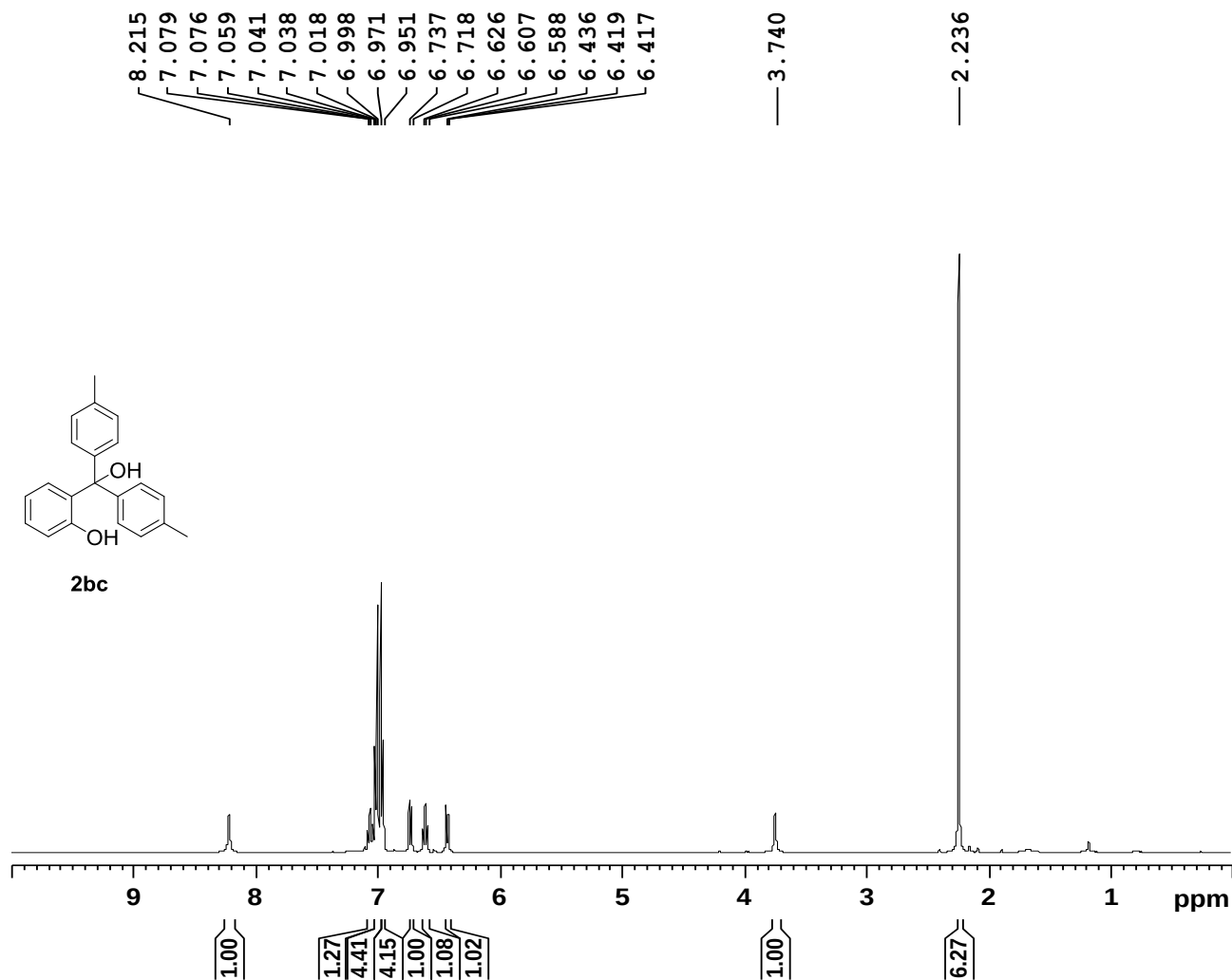
===== CHANNEL f1 =====
 NUC1 13C
 P1 9.95 usec
 PL1 -1.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL12 14.95 dB
 PL13 120.00 dB
 PL2 -1.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127599 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure 76: ^{13}C -NMR spectra for compound **2bb**

PROTON CDCl₃



Current Data Parameters
 NAME MK-MM-16
 EXPNO 1
 PROCNO 1

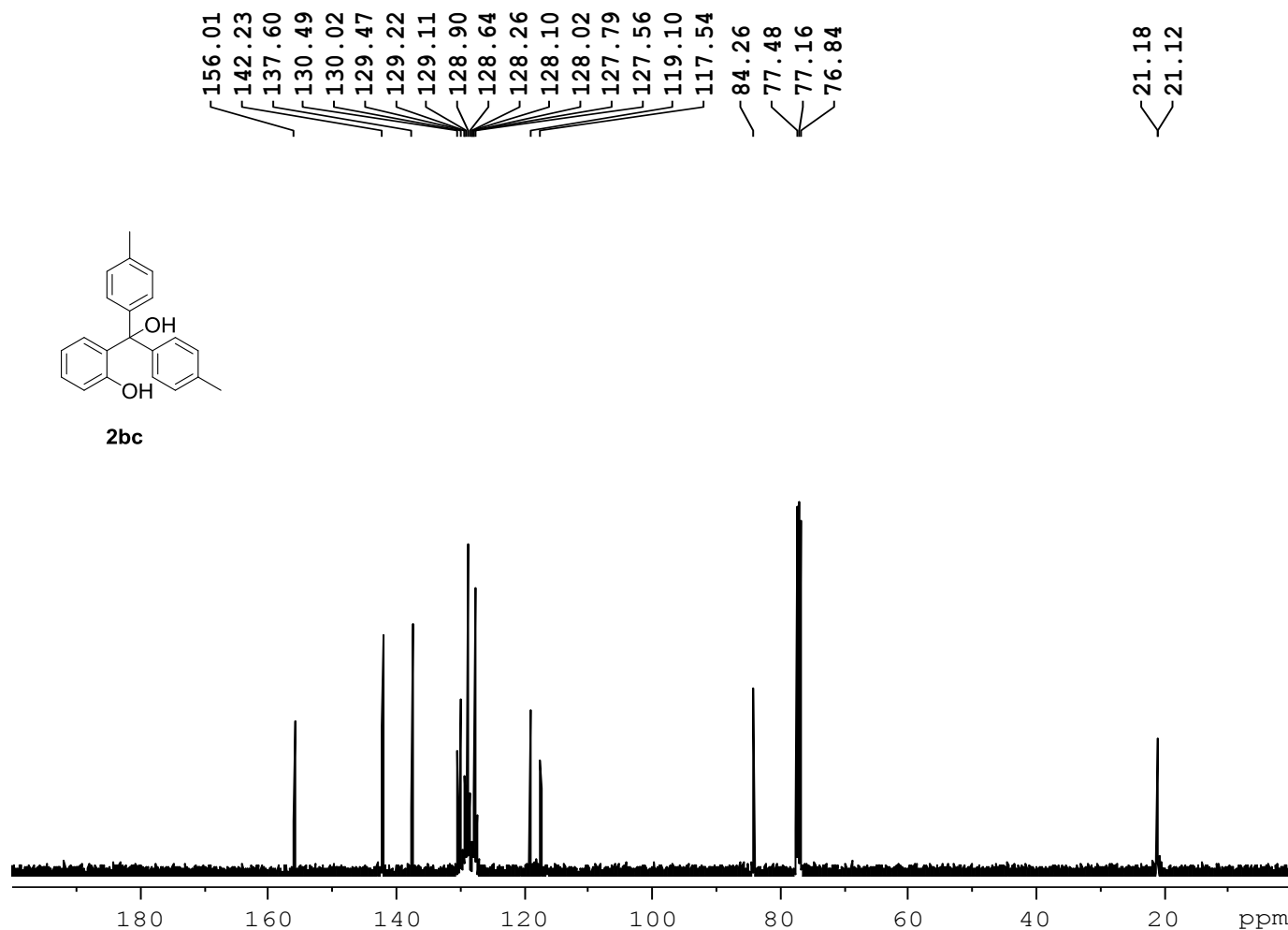
F2 - Acquisition Parameters
 Date_ 20190212
 Time 10.58
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDCl₃
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 57
 DW 60.800 usec
 DE 6.00 usec
 TE 292.8 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.35 usec
 PL1 -1.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300724 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure 77: ¹H-NMR spectra for compound **2bc**

C13CPD CDCL3
M.KARTHICK



```

Current Data Parameters
NAME          MK-MM-16
EXPNO         2
PROCNO        1

F2 - Acquisition Parameters
Date_         20190215
Time_         16.00
INSTRUM       spect
PROBHD        5 mm BBO BB-1H
PULPROG       zgpg30
TD            65536
SOLVENT       DMSO
NS            256
DS            4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG            362
DW            20.800 usec
DE            6.00 usec
TE            296.3 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0           1

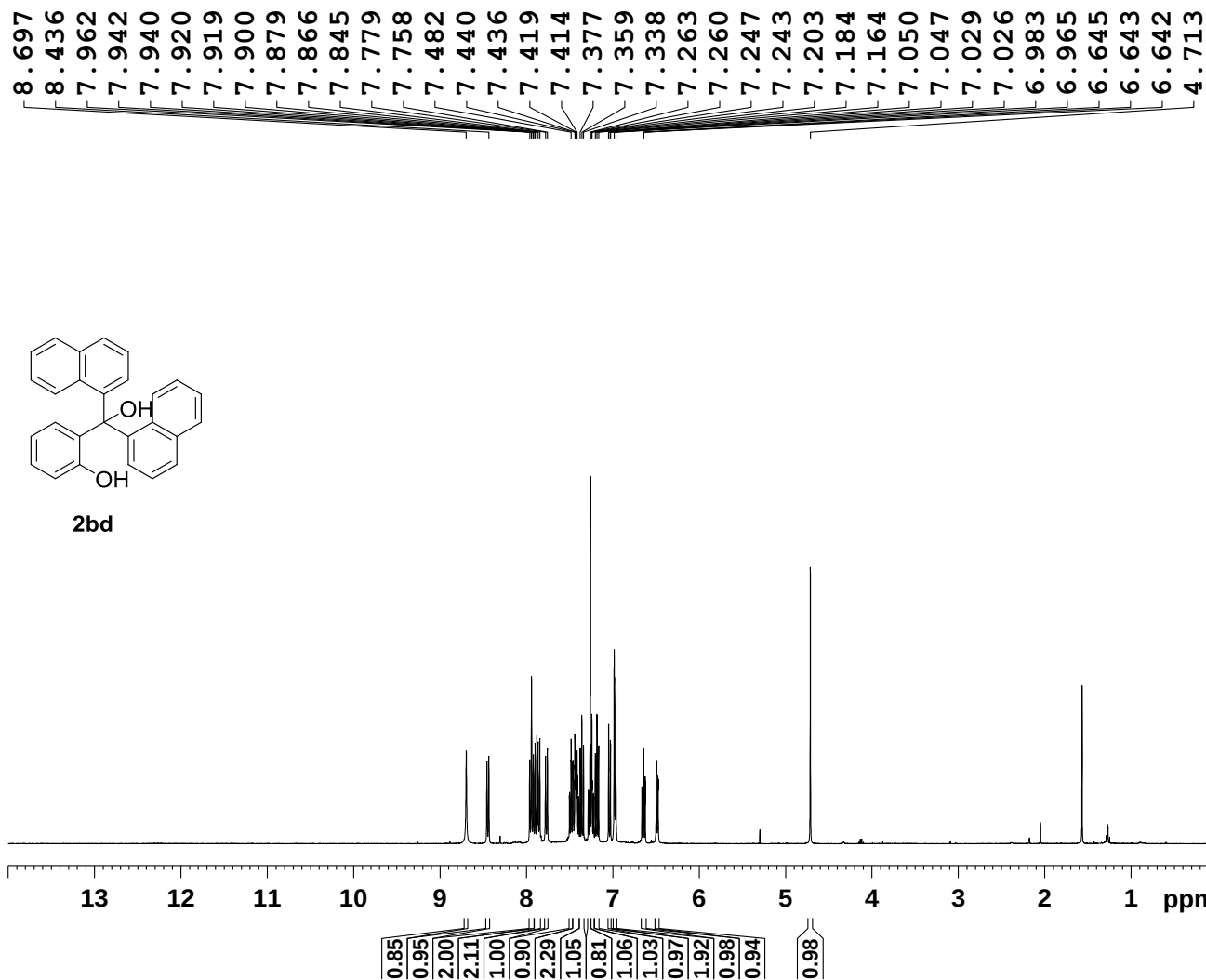
===== CHANNEL f1 =====
NUC1           13C
P1             9.15 usec
PL1            0 dB
SFO1          100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2]     waltz16
NUC2           1H
PCPD2          90.00 usec
PL12           14.90 dB
PL13           14.90 dB
PL2            -3.00 dB
SFO2          400.1316005 MHz

F2 - Processing parameters
SI            32768
SF           100.6126938 MHz
WDW           EM
SSB           0
LB            1.00 Hz
GB            0
PC            1.40
  
```

Figure 78: ¹³C-NMR spectra for compound **2bc**

PROTON CDCl3 {D:\CRR} CIF_NMR 1



Current Data Parameters
 NAME MK-III-433-B
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190710
 Time 11.18
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 256
 DW 60.800 usec
 DE 6.00 usec
 TE 294.6 K
 D1 1.00000000 sec
 TDO 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.35 usec
 PL1 -1.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300096 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure 79: ¹H-NMR spectra for compound **2bd**

PROTON CDC13 {D:\CRR} CIF_NMR 1

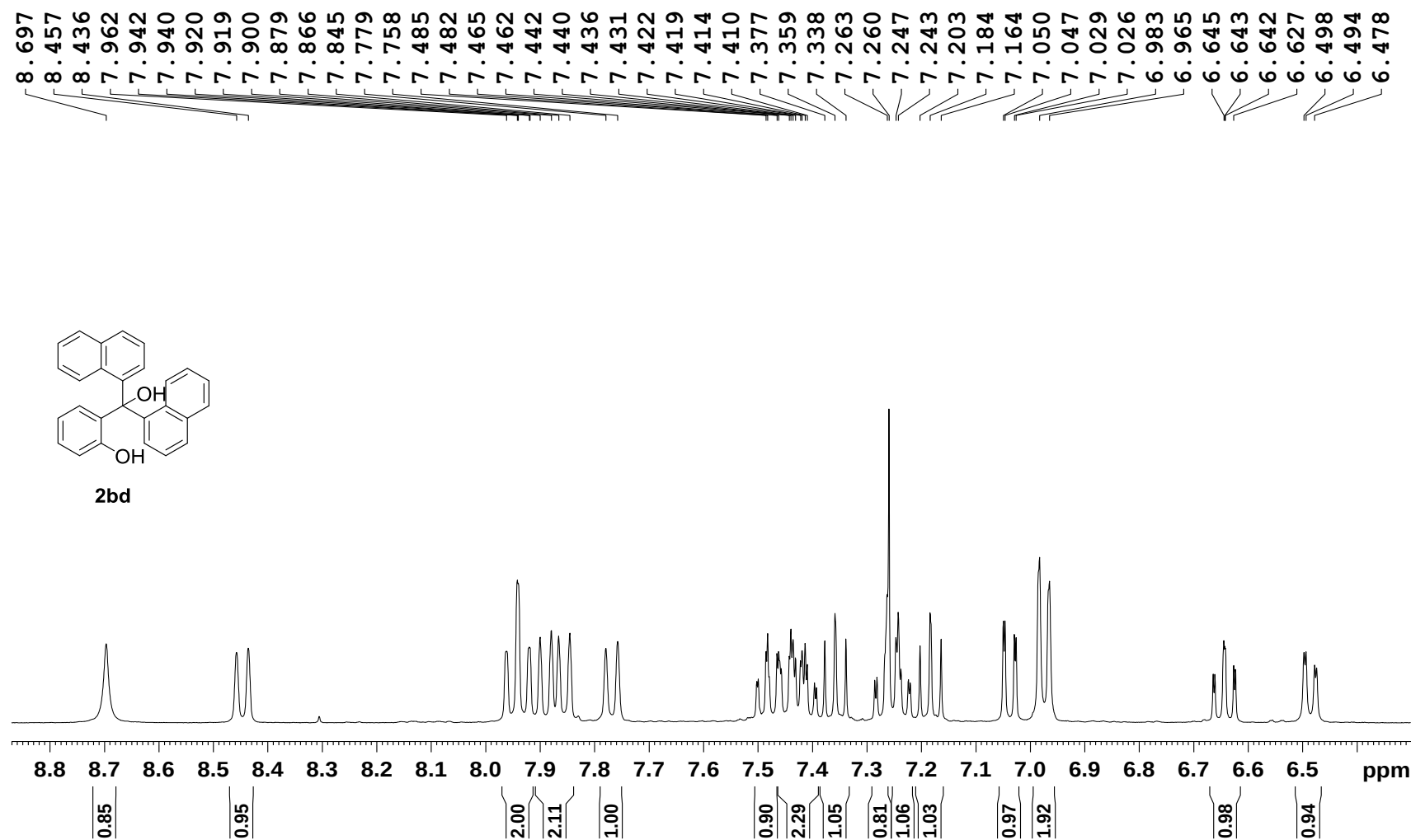
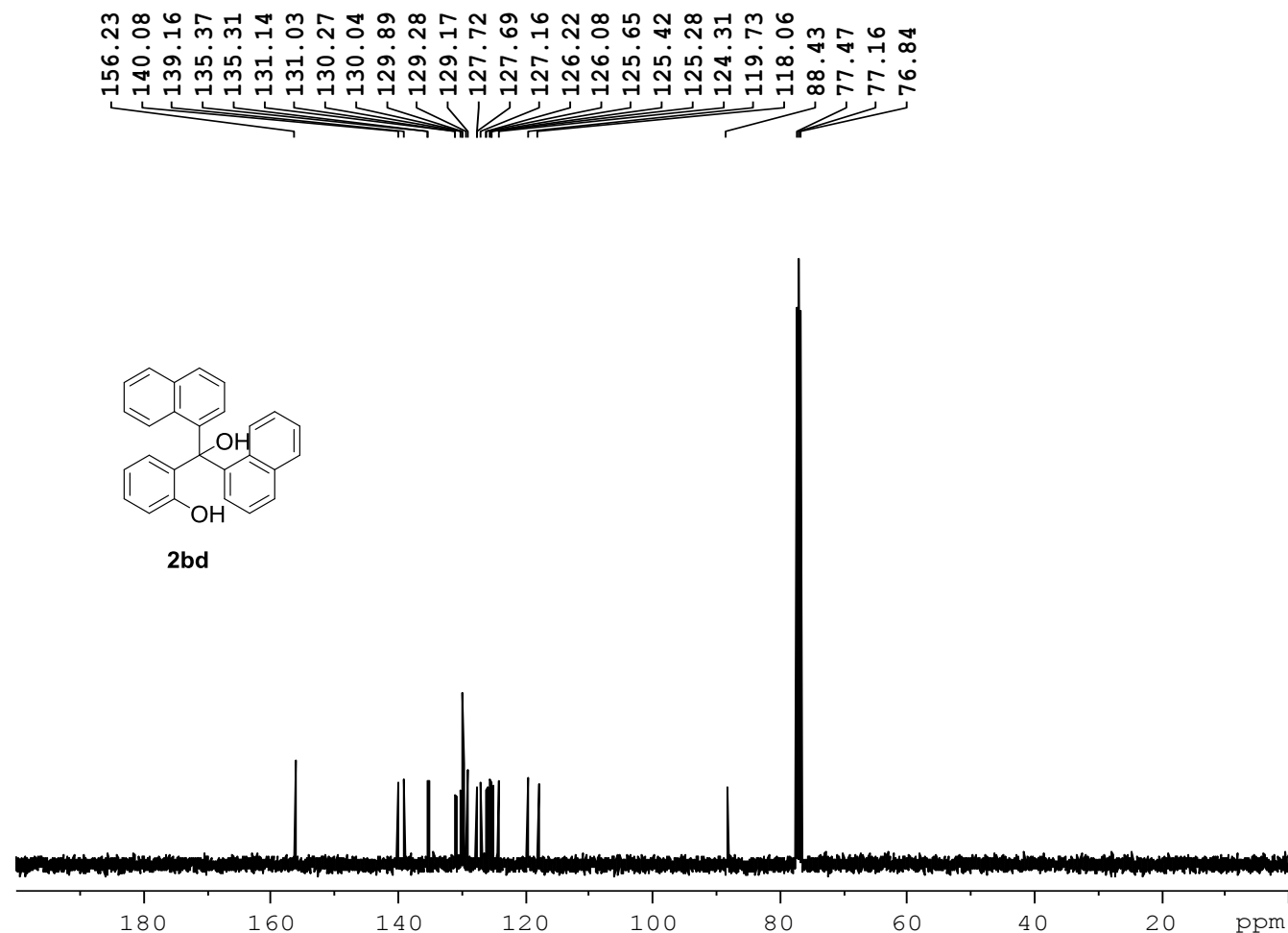


Figure 79a: ^1H -NMR spectra expansion for compound **2bd**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-III-433-B
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190710
Time 16.46
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 158
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 456
DW 20.800 usec
DE 6.00 usec
TE 296.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

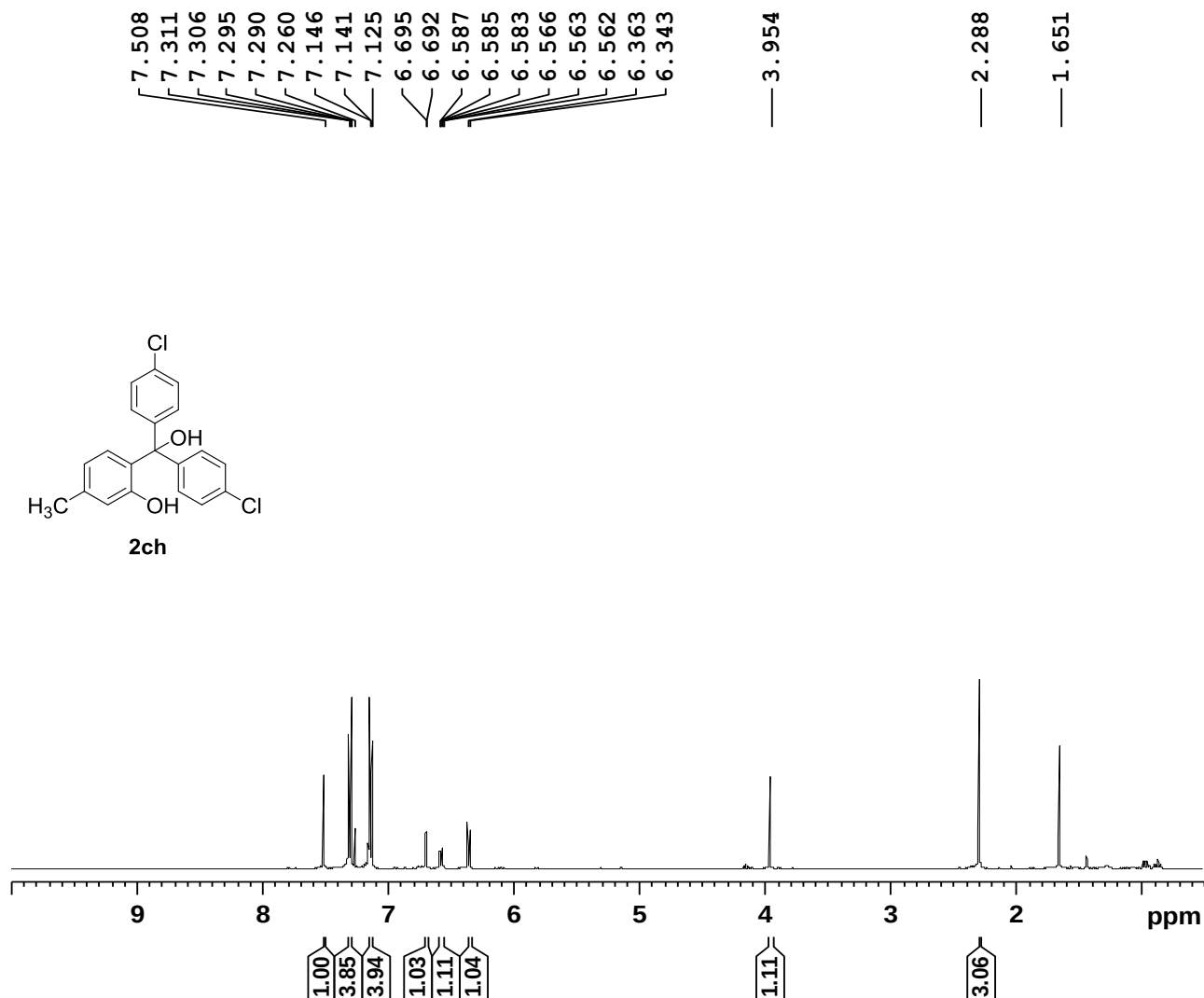
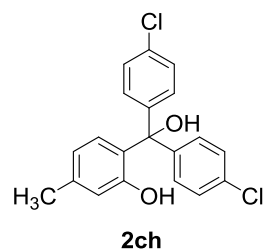
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127601 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 80: ¹³C-NMR spectra for compound **2bd**

PROTON CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-MM-44
EXPNO 1
PROCNO 1

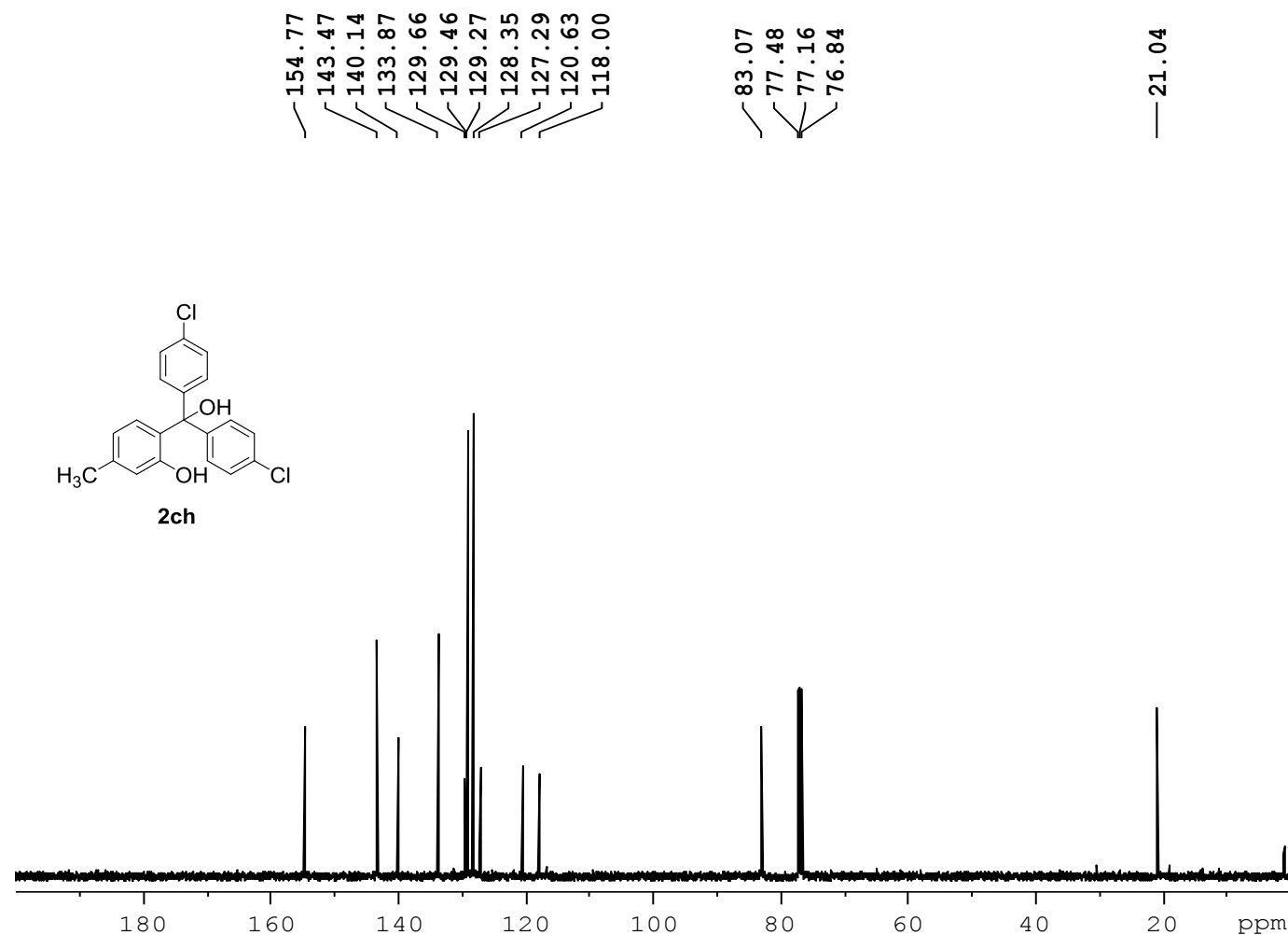
F2 - Acquisition Parameters
Date_ 20190327
Time 14.52
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 228
DW 60.800 usec
DE 6.00 usec
TE 296.4 K
D1 1.0000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 81: ¹H-NMR spectra for compound **2ch**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-MM-44
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190331
Time 11.00
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 87
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 40.3
DW 20.800 usec
DE 6.00 usec
TE 292.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

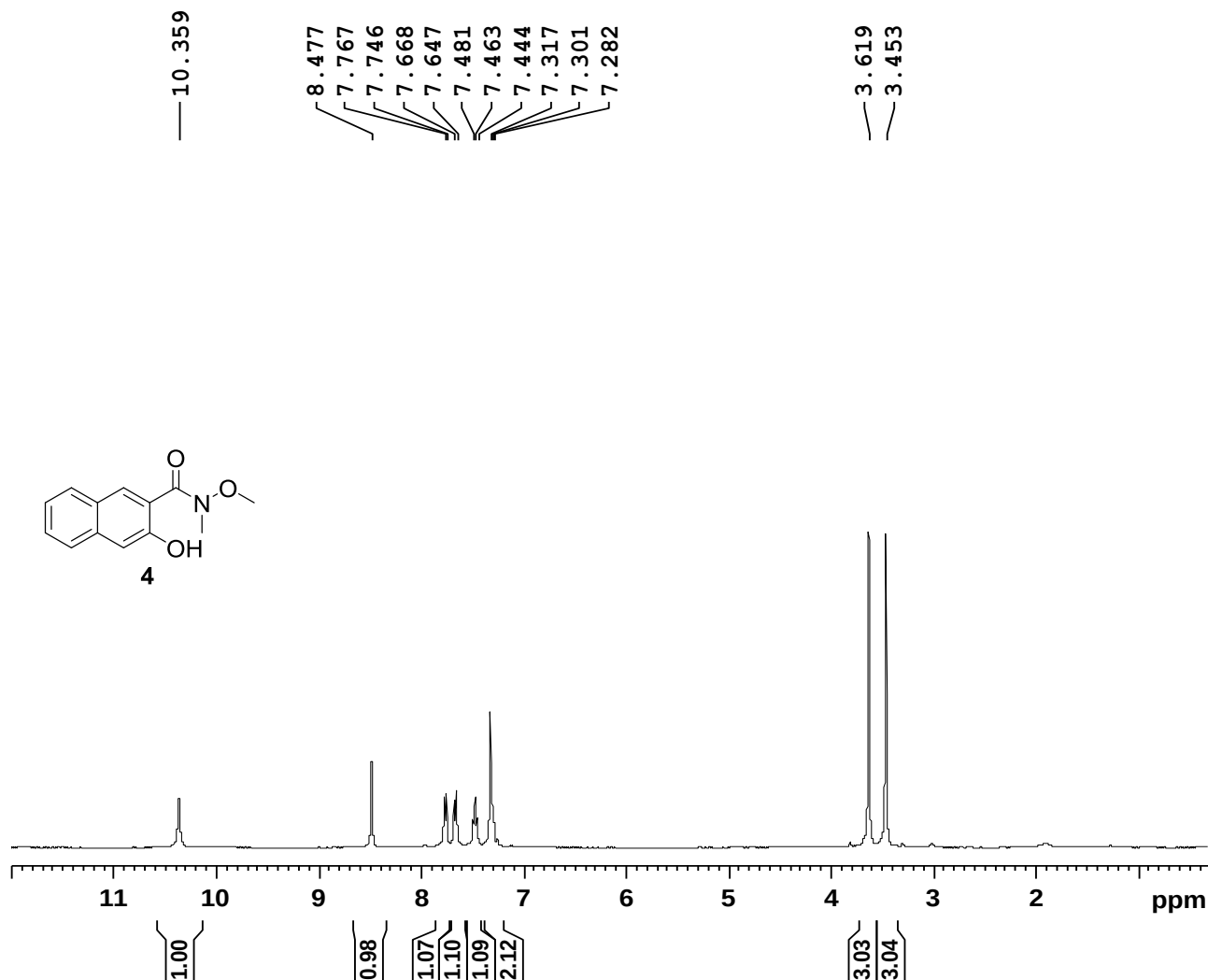
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127688 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 82: ¹³C-NMR spectra for compound **2ch**

PROTON CDCl3 {D:\CRR} CIF_NMR 1



Current Data Parameters
 NAME MK-II-369-F
 EXPNO 1
 PROCNO 1

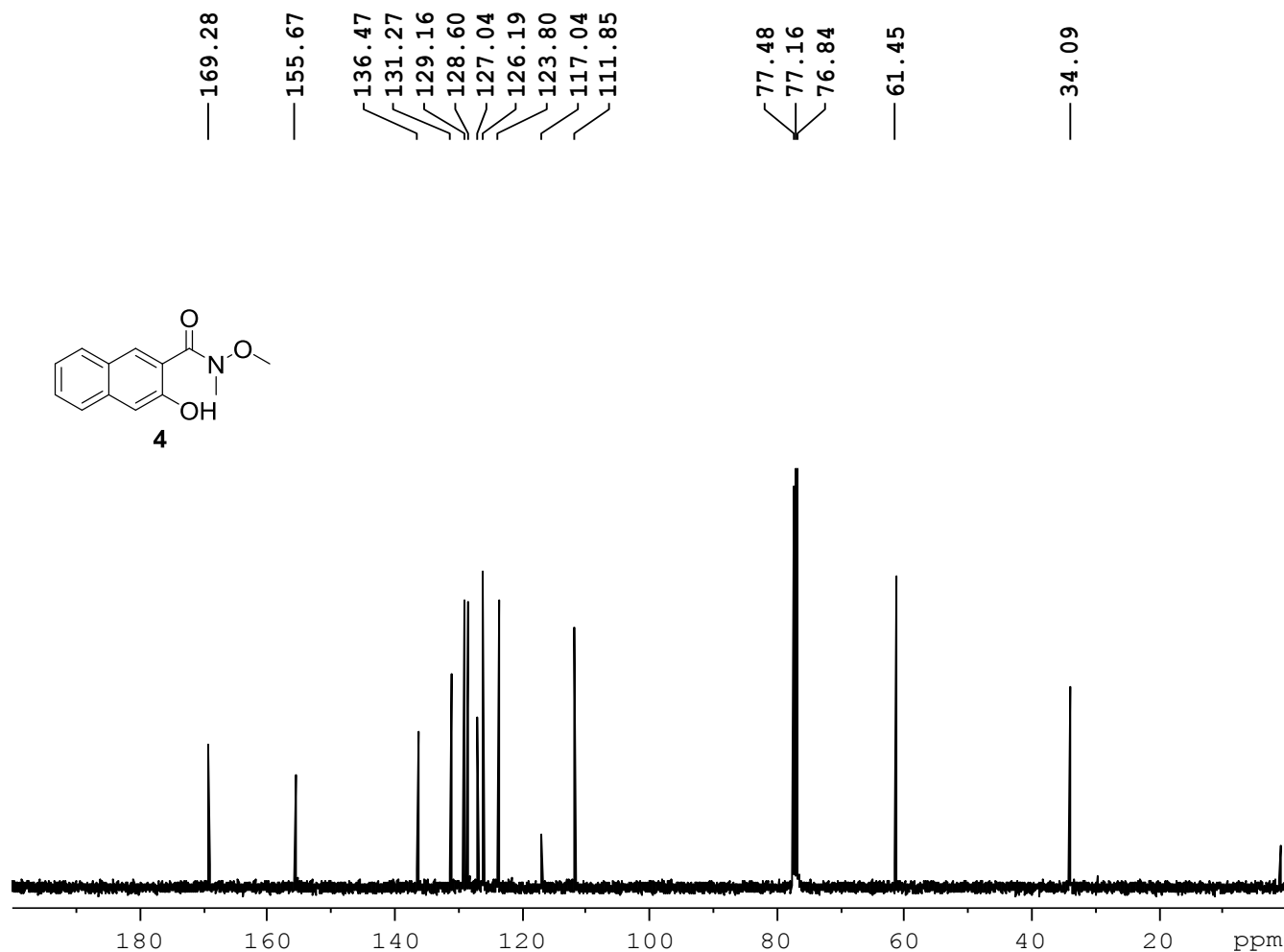
F2 - Acquisition Parameters
 Date_ 20190501
 Time_ 9.45
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 101
 DW 60.800 usec
 DE 6.00 usec
 TE 290.9 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.35 usec
 PL1 -1.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300137 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure 83: ¹H-NMR spectra for compound 4

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
 NAME MK-II-369-F
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters

Date_ 20190501
 Time 10.06
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 350
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 256
 DW 20.800 usec
 DE 6.00 usec
 TE 291.1 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

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

NUC1 13C
 P1 9.95 usec
 PL1 -1.00 dB
 SFO1 100.6228298 MHz

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

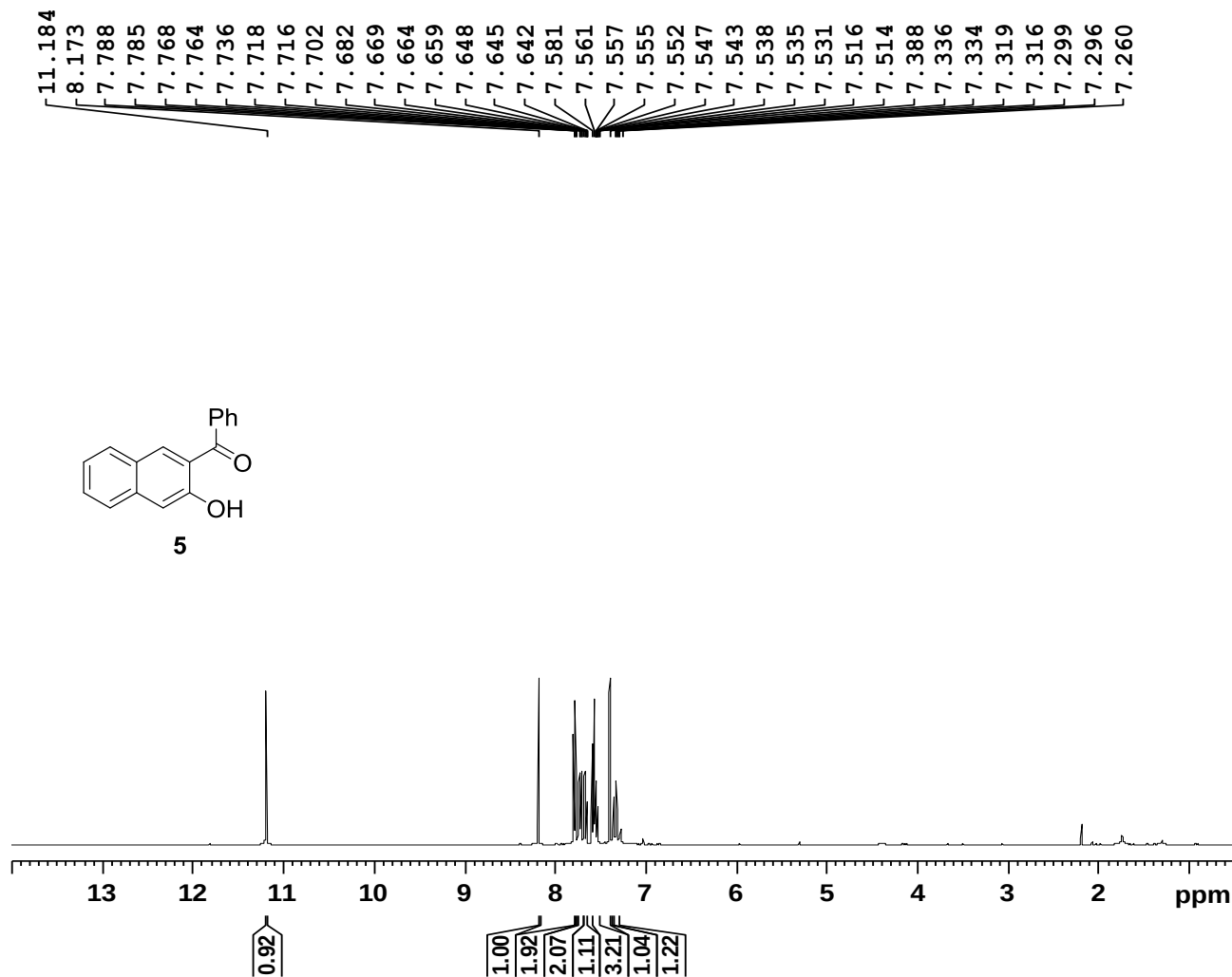
CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL12 14.95 dB
 PL13 120.00 dB
 PL2 -1.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters

SI 32768
 SF 100.6127655 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure 84: ^{13}C -NMR spectra for compound 4

PROTON CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
 NAME MK-II-370-Z
 EXPNO 1
 PROCNO 1

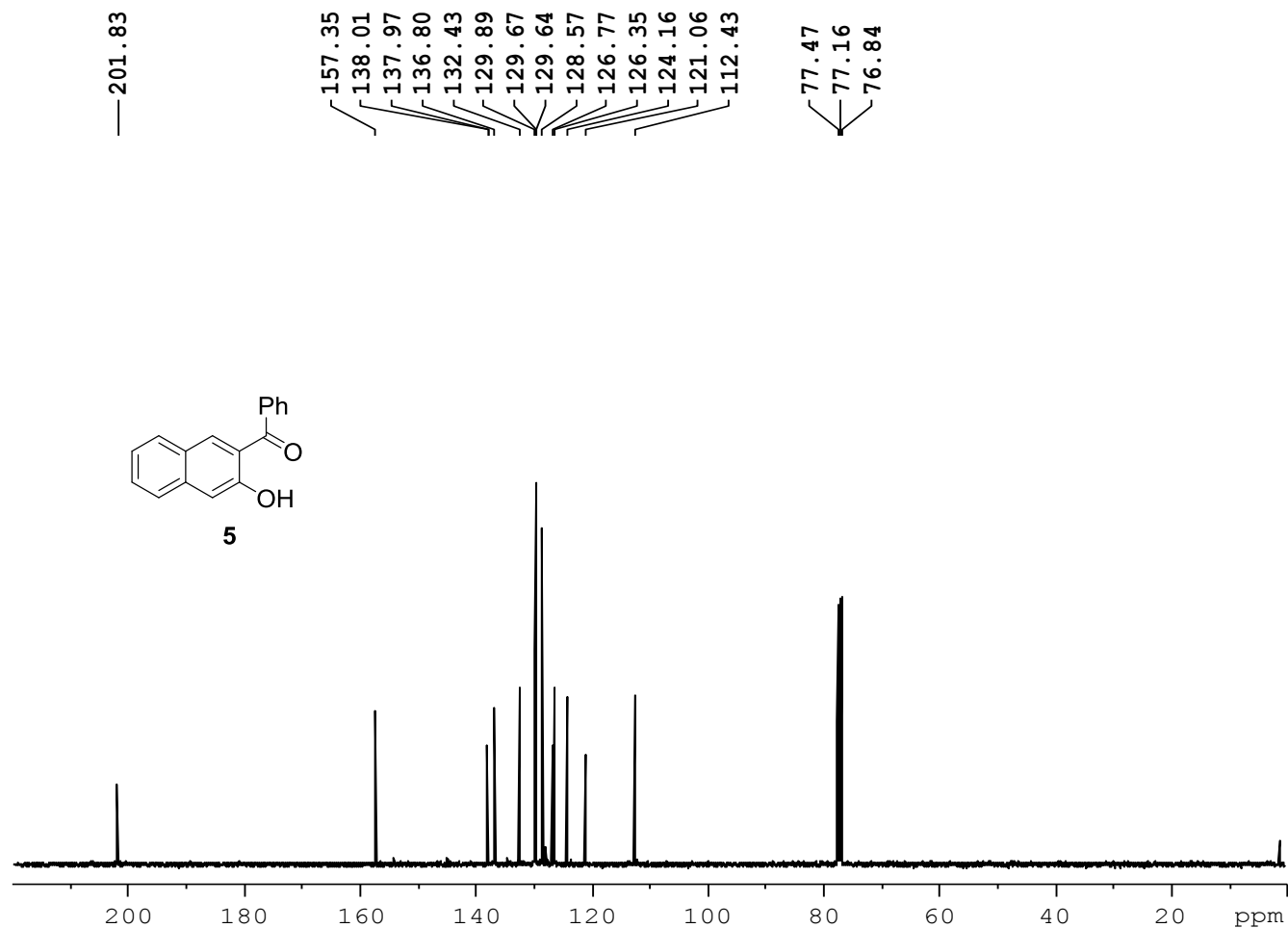
F2 - Acquisition Parameters
 Date_ 20190825
 Time 10.44
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 114
 DW 60.800 usec
 DE 6.00 usec
 TE 290.9 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.35 usec
 PL1 -1.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300092 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure 85: ¹H-NMR spectra for compound 5

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-370-Z
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190825
Time 11.06
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 350
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 362
DW 20.800 usec
DE 6.00 usec
TE 290.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

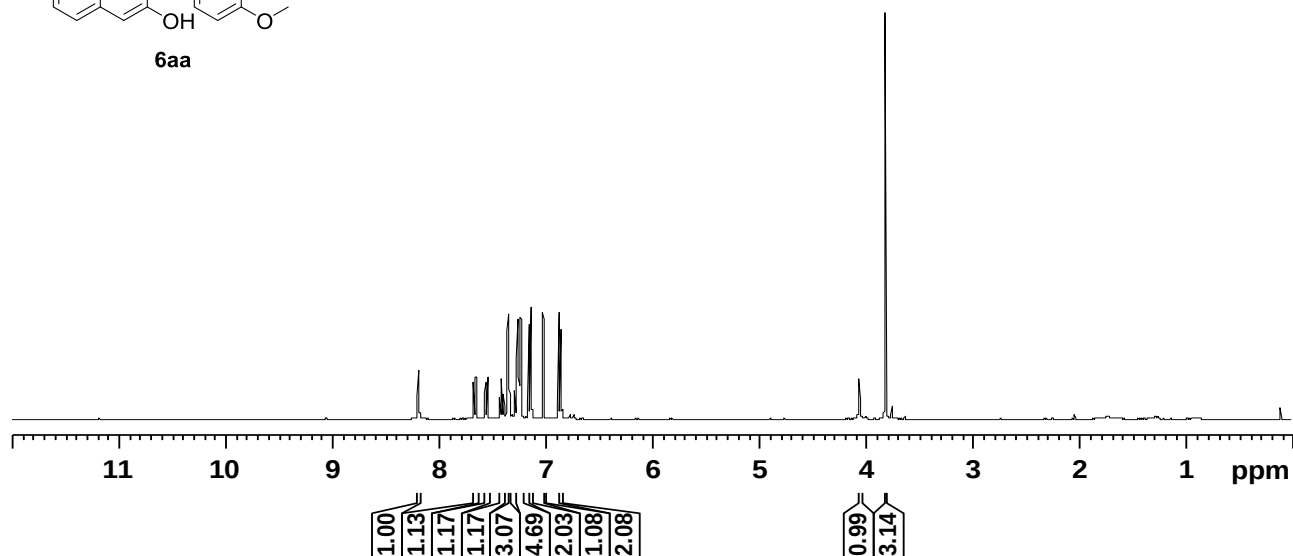
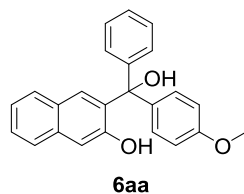
F2 - Processing parameters
SI 32768
SF 100.6127651 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 86: ¹H-NMR spectra for compound 5

PROTON CDCl3 {D:\CRR} CIF_NMR 1



8.189
7.670
7.649
7.559
7.539
7.428
7.426
7.411
7.408
7.390
7.388
7.356
7.348
7.340
7.284
7.282
7.264
7.260
7.253
7.244
7.235
7.228
7.153
7.131
7.018
6.872
6.850
4.058
3.812



Current Data Parameters
NAME MK-II-371-C
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190711
Time 14.19
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 144
DW 60.800 usec
DE 6.00 usec
TE 293.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 87: ¹H-NMR spectra for compound 6aa

PROTON CDCl3 {D:\CRR} CIF_NMR 1

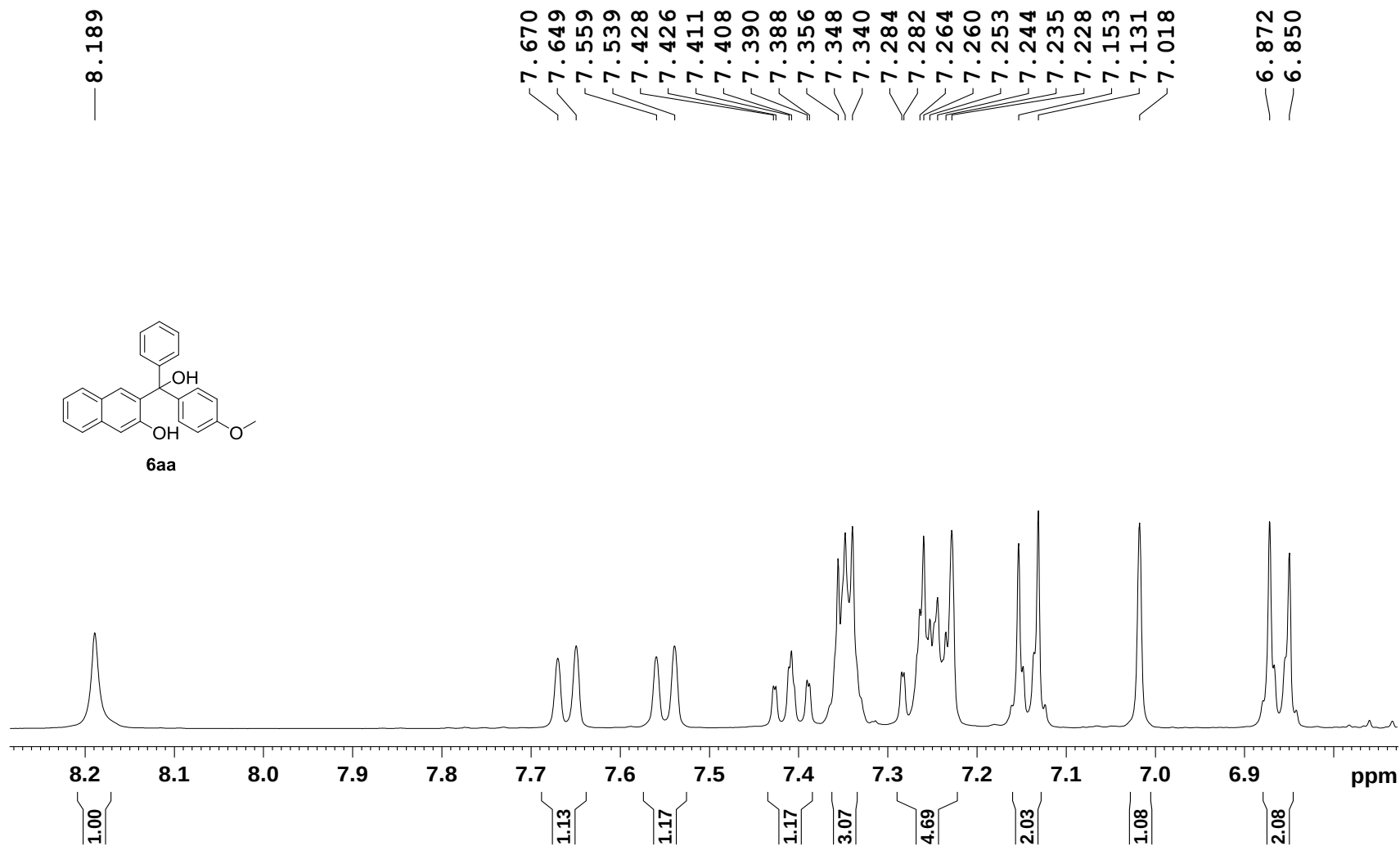
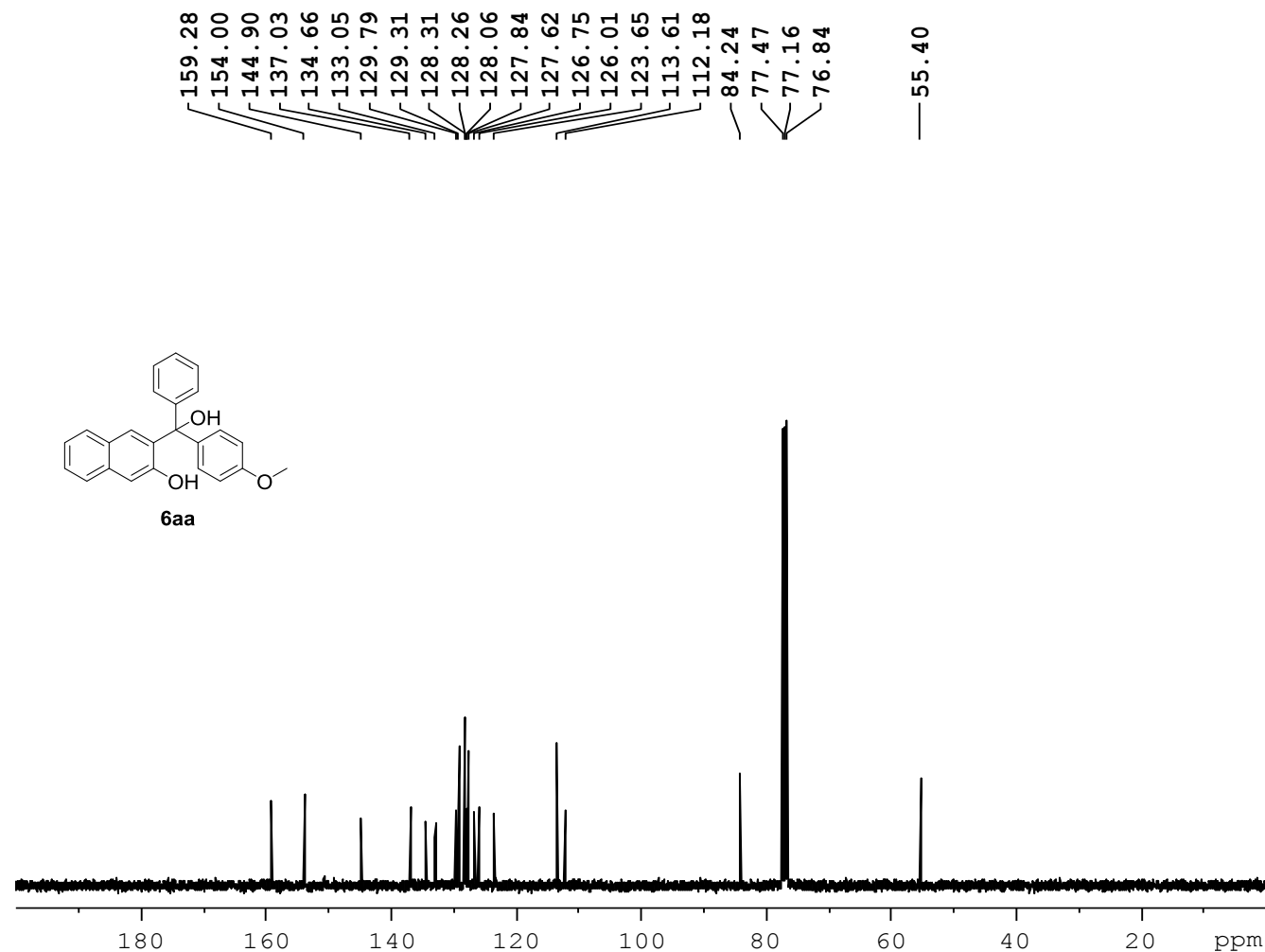


Figure 87a: ¹H-NMR spectra expansion for compound **6aa**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-371-C
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190711
Time 14.24
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 406
DW 20.800 usec
DE 6.00 usec
TE 293.6 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

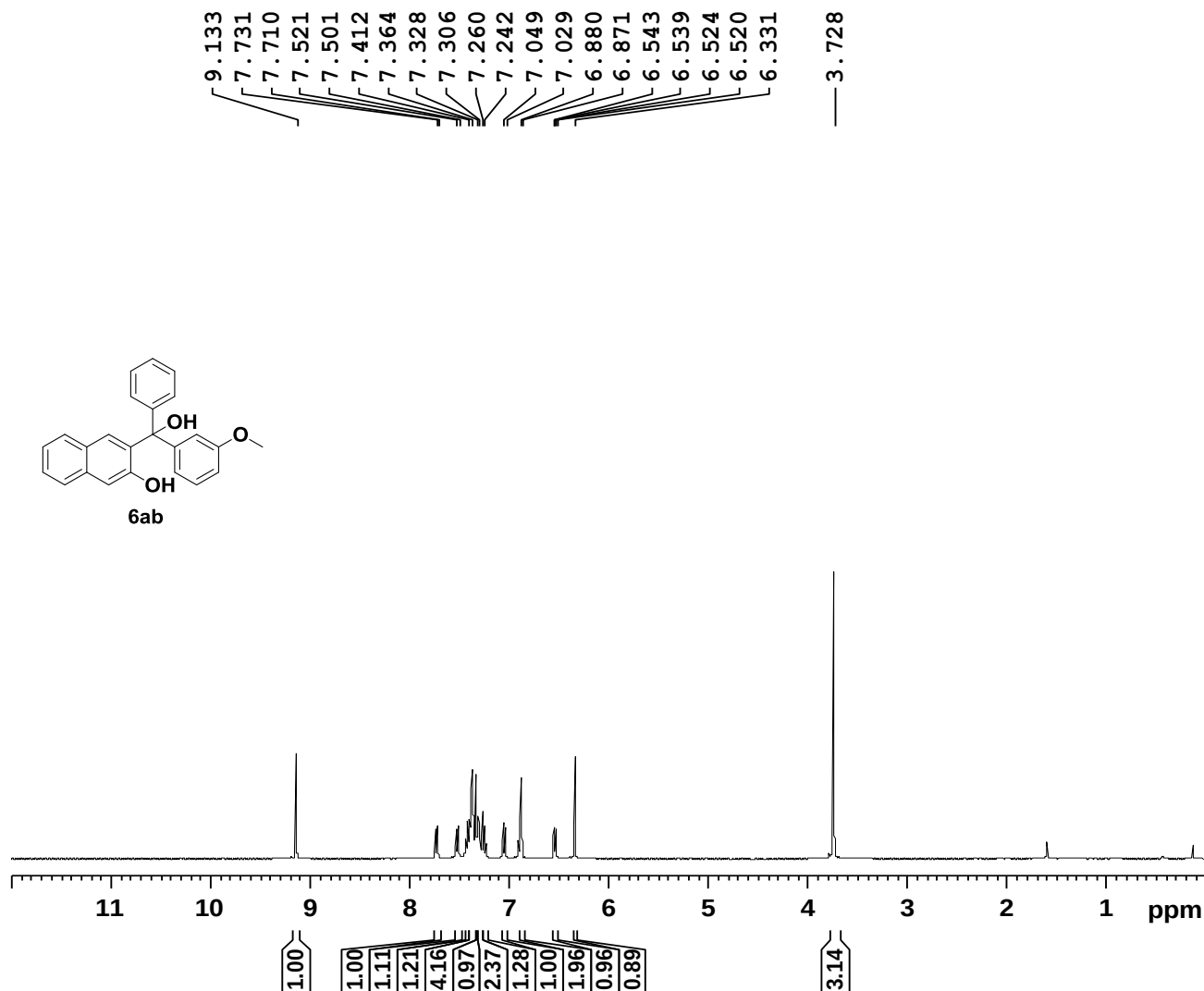
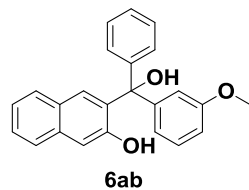
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127614 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 88: ^{13}C -NMR spectra for compound 6aa

PROTON CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
 NAME MK-II-420-A
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190520
 Time 11.31
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 144
 DW 60.800 usec
 DE 6.00 usec
 TE 293.3 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.35 usec
 PL1 -1.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.130093 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure 89: ¹H-NMR spectra for compound **6ab**

PROTON CDCl3 {D:\CRR} CIF_NMR 1

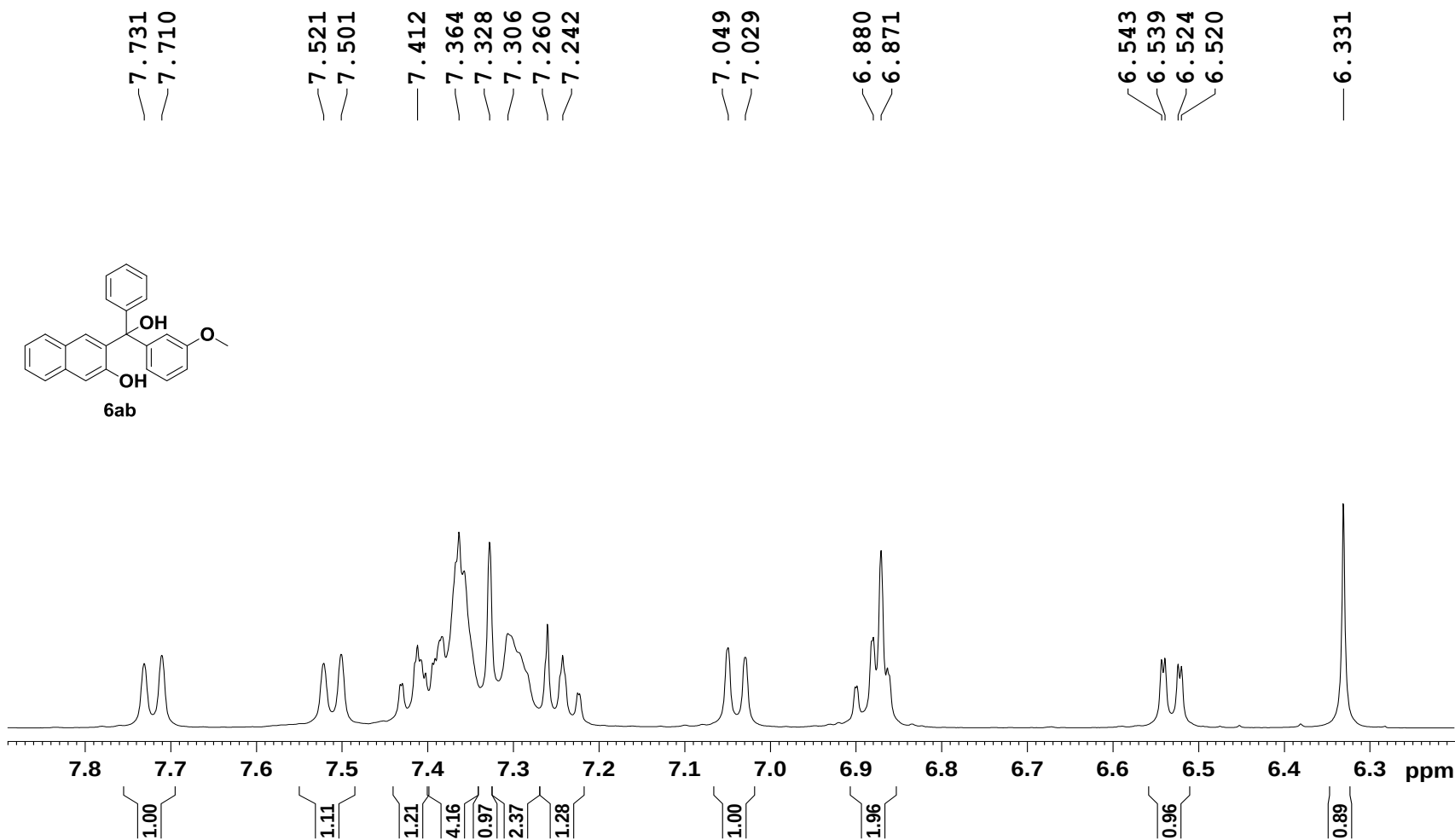
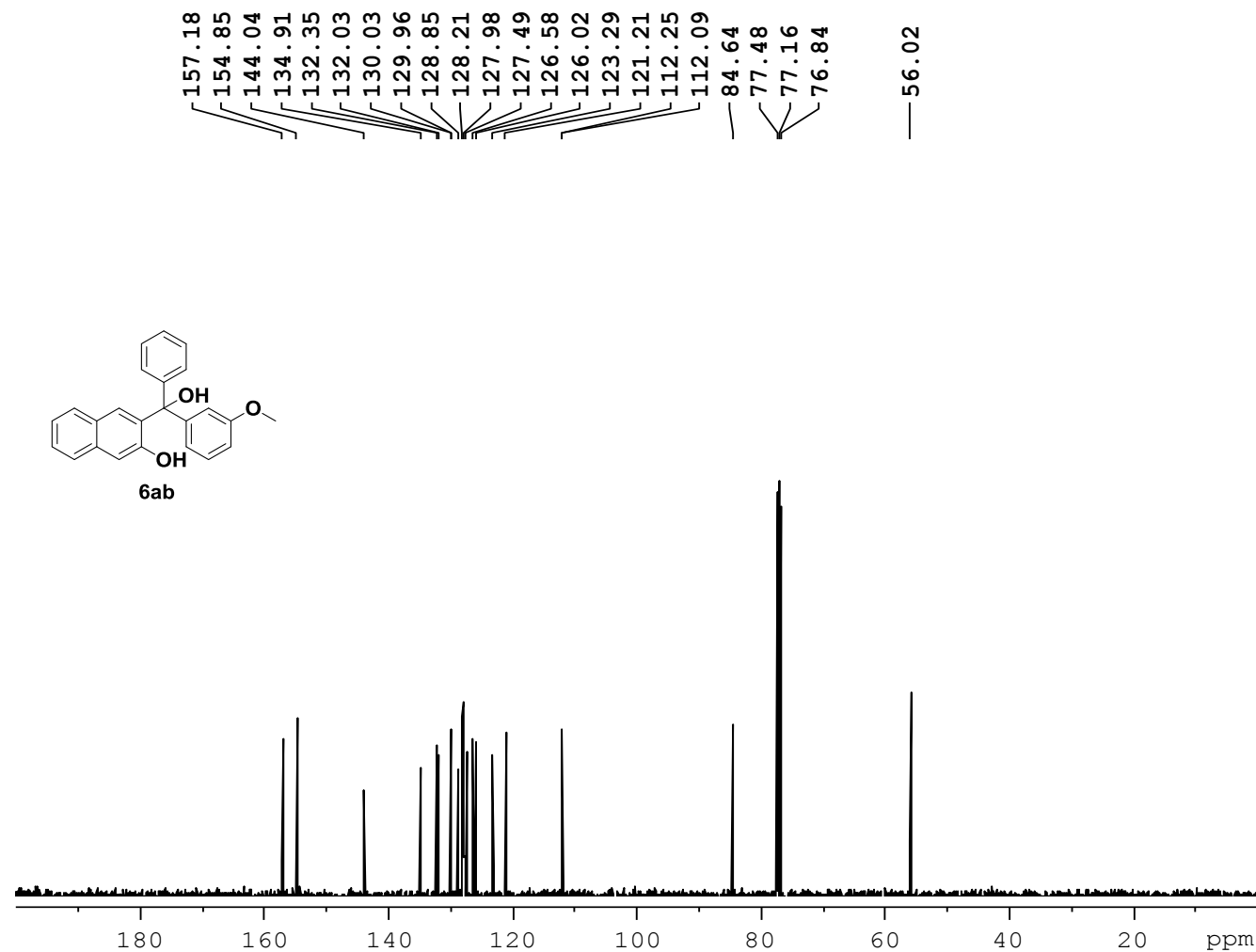


Figure 89a: ¹H-NMR spectra expansion for compound **6ab**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
 NAME MK-II-420-A
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190520
 Time 16.20
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 222
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 40.3
 DW 20.800 usec
 DE 6.00 usec
 TE 293.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

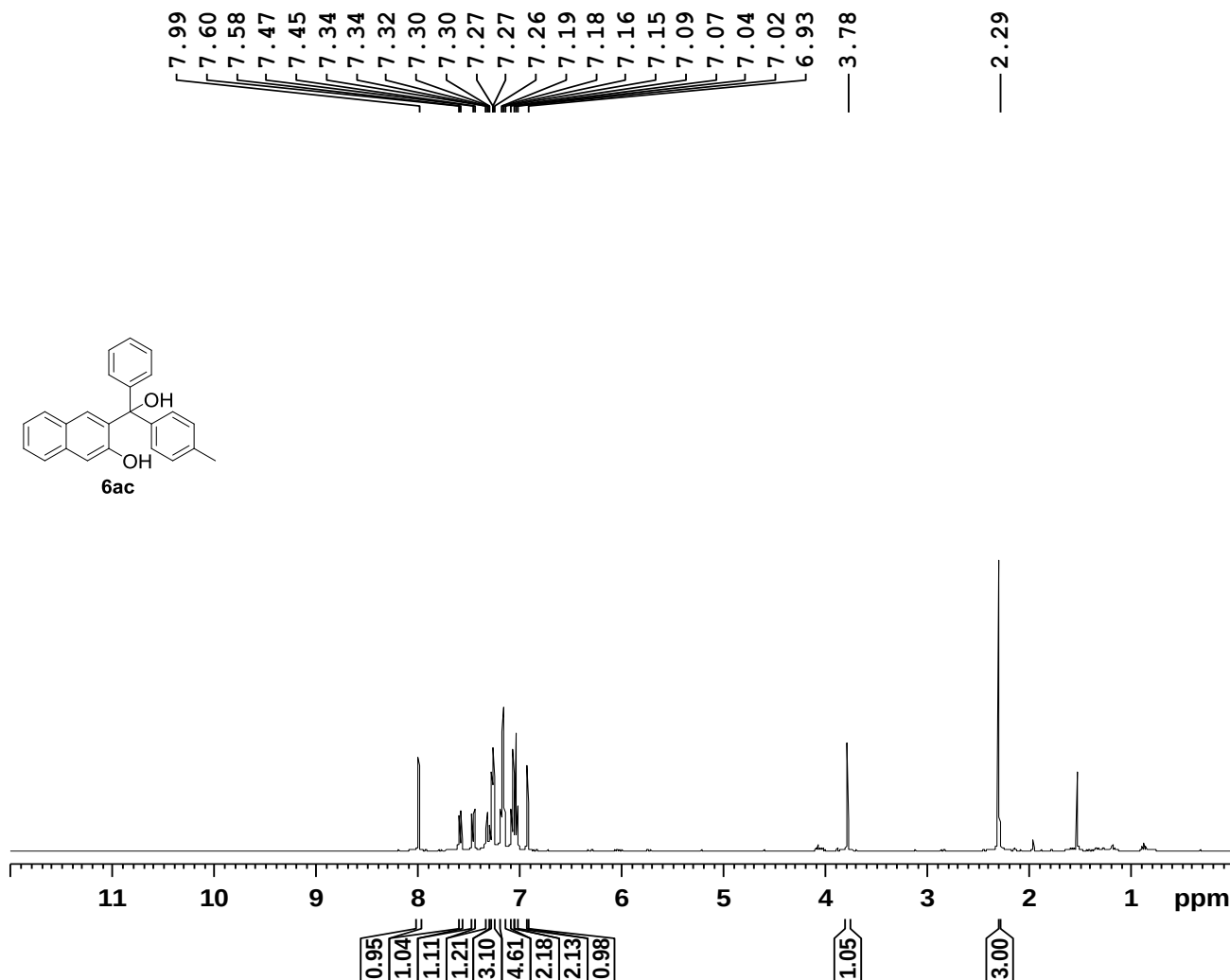
===== CHANNEL f1 =====
 NUC1 13C
 P1 9.95 usec
 PL1 -1.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL12 14.95 dB
 PL13 120.00 dB
 PL2 -1.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127669 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure 90: ¹³C-NMR spectra for compound **6ab**

PROP31DEC CDCl3 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-395
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190405
Time 22.40
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgig
TD 32768
SOLVENT CDCl3
NS 16
DS 2
SWH 8333.333 Hz
FIDRES 0.254313 Hz
AQ 1.9660800 sec
RG 203
DW 60.000 usec
DE 6.00 usec
TE 294.4 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1325018 MHz

===== CHANNEL f2 =====
CPDPRG[2] garp
NUC2 31P
PCPD2 100.00 usec
PL12 120.00 dB
PL2 0 dB
SFO2 161.9760648 MHz

F2 - Processing parameters
SI 32768
SF 400.1300442 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 91: ¹H-NMR spectra for compound **6ac**

PROP31DEC CDC13 {D:\CRR} CIF_NMR 1

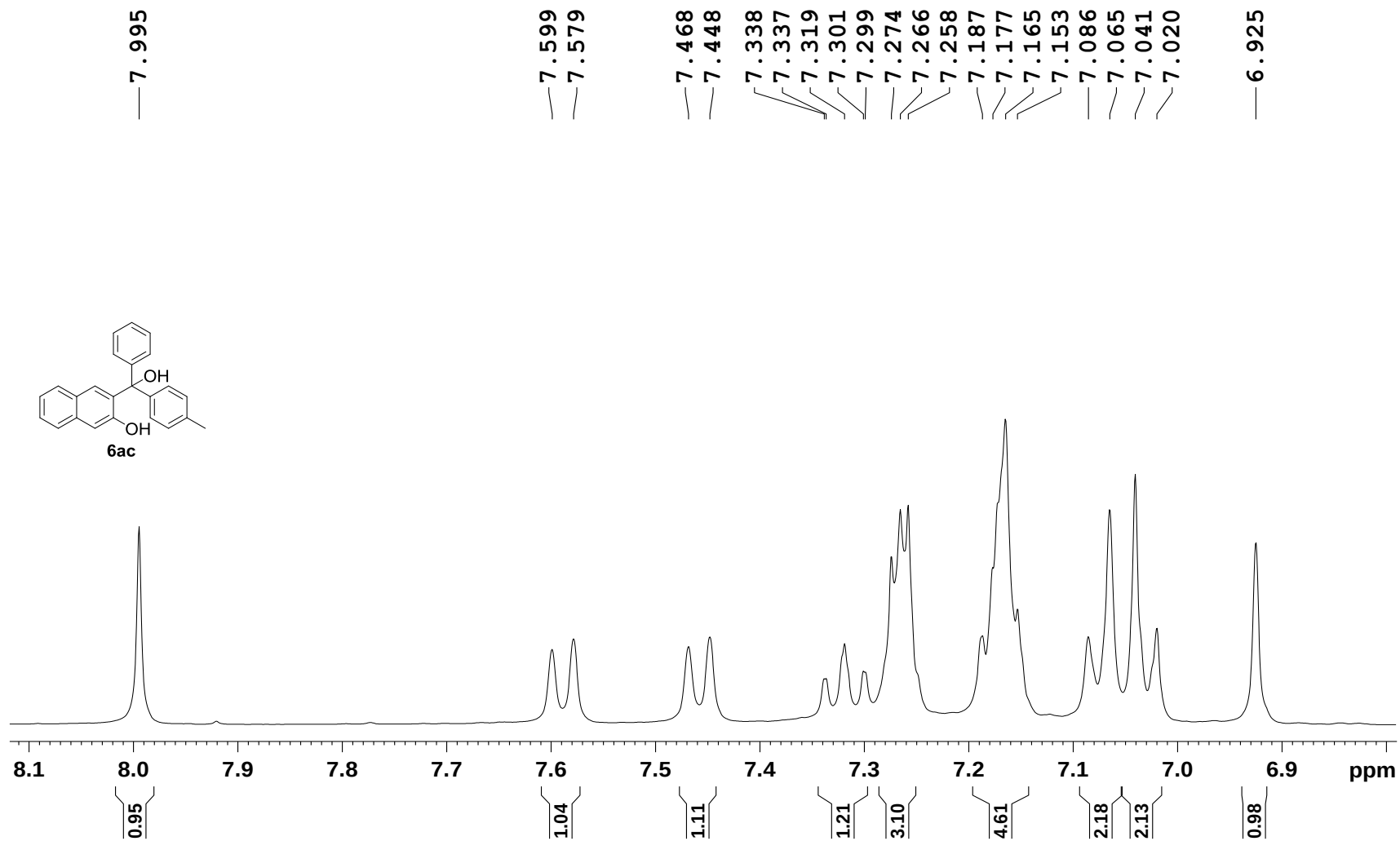
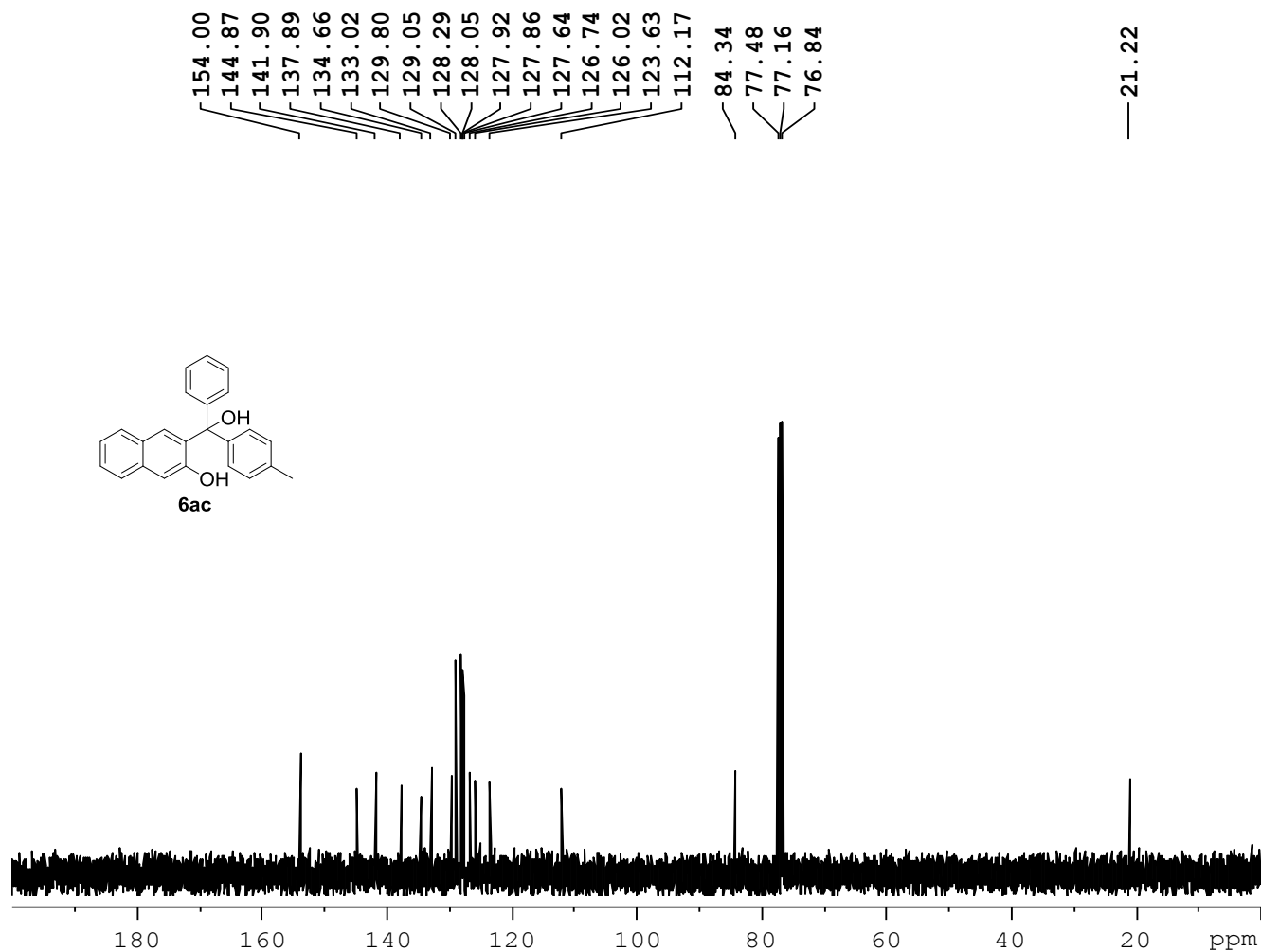


Figure 91a: ¹H-NMR spectra expansion for compound **6ac**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
 NAME MK-II-395
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190406
 Time 0.39
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 77
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 40.3
 DW 20.800 usec
 DE 6.00 usec
 TE 294.4 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

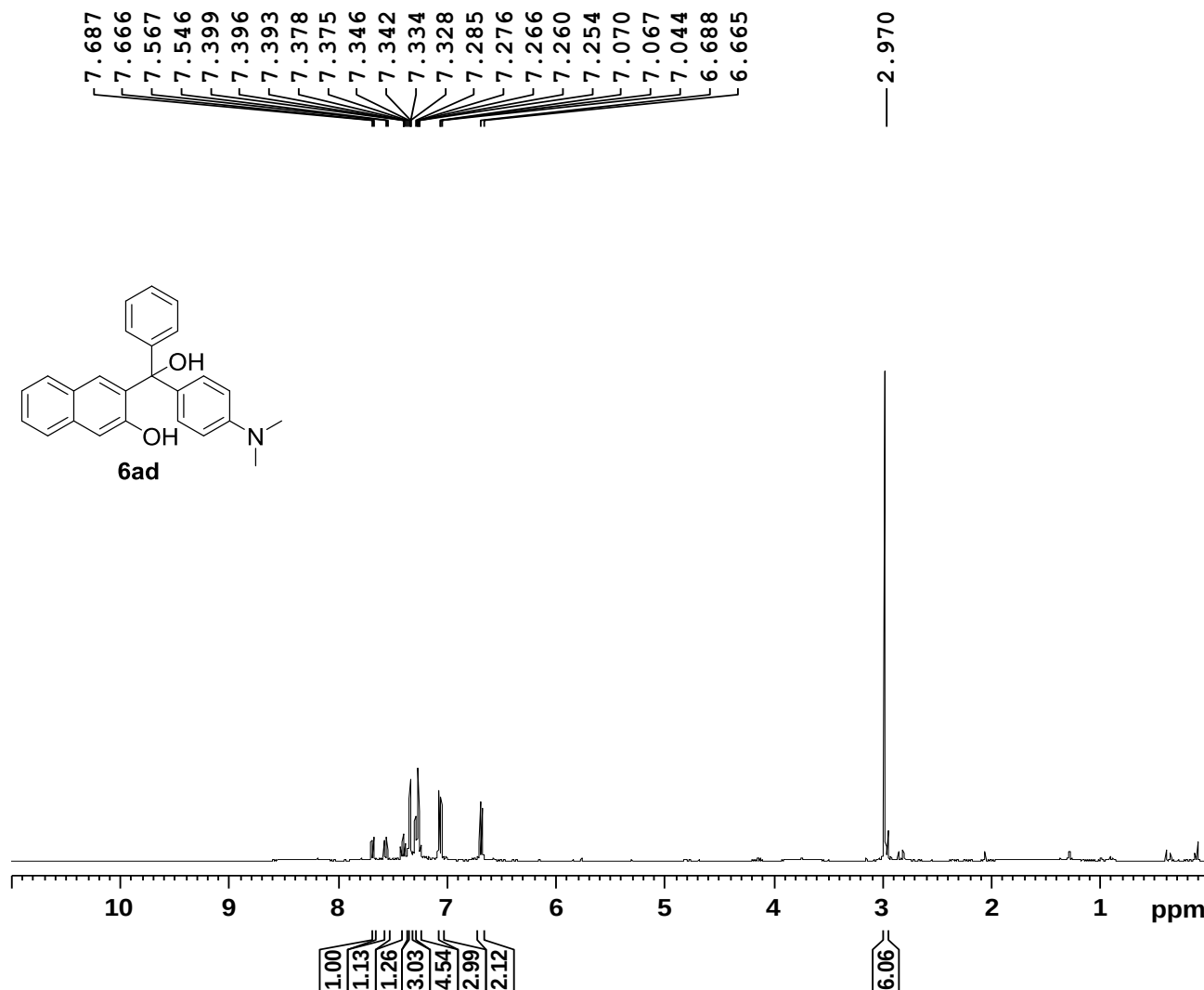
===== CHANNEL f1 =====
 NUC1 13C
 P1 9.95 usec
 PL1 -1.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL12 14.95 dB
 PL13 120.00 dB
 PL2 -1.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127619 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure 92: ¹³C-NMR spectra for compound 6ac

PROTON CDCl3 {D:\CRR} CIF_NMR 1



Current Data Parameters
 NAME MK-II-422
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190527
 Time 14.35
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 228
 DW 60.800 usec
 DE 6.00 usec
 TE 294.6 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.35 usec
 PL1 -1.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.130094 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure 93: ¹H-NMR spectra for compound **6ad**

PROTON CDC13 {D:\CRR} CIF_NMR 1

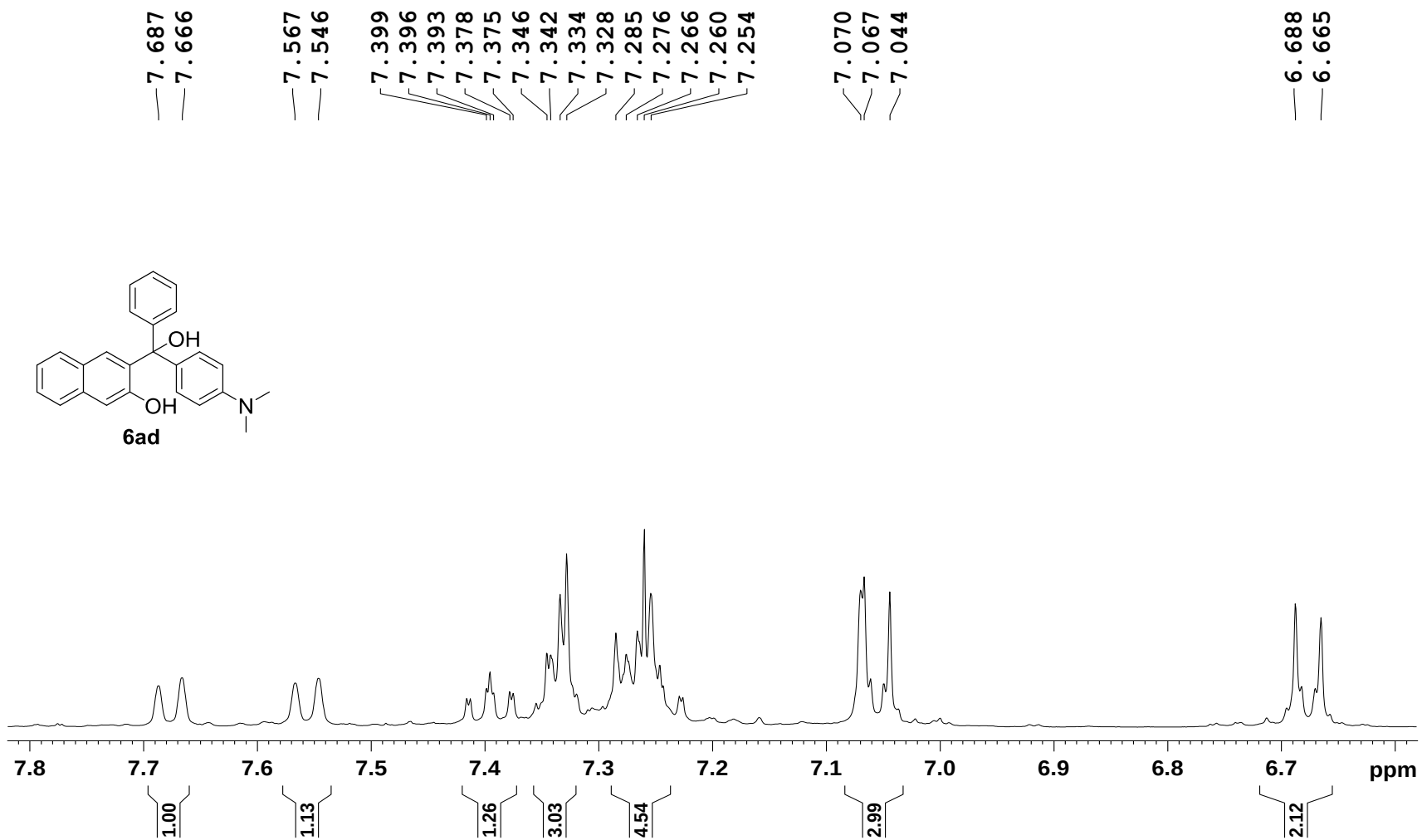
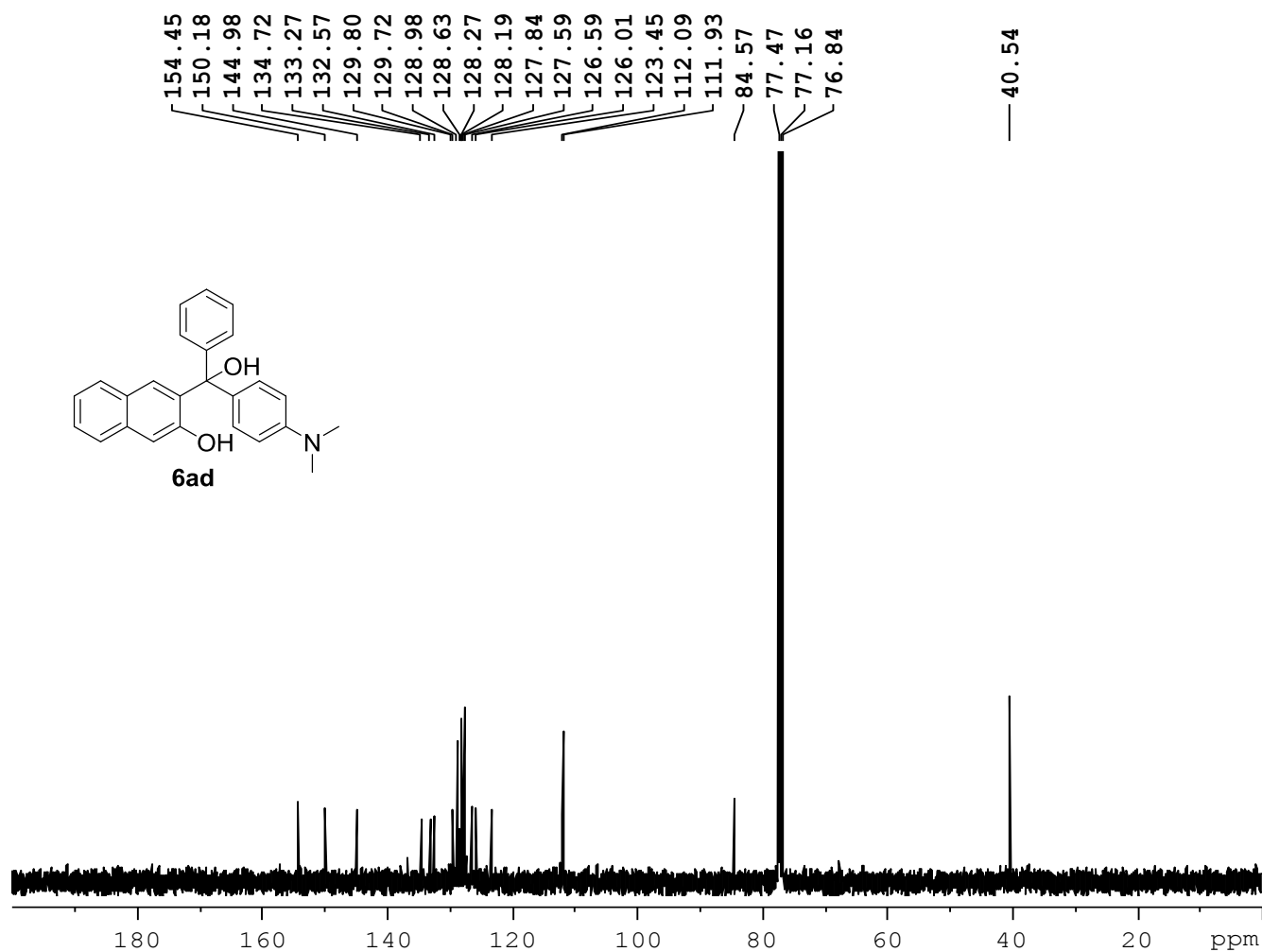


Figure 93a: ^1H -NMR spectra expansion for compound **6ad**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-422
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190530
Time 13.40
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 40.3
DW 20.800 usec
DE 6.00 usec
TE 293.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

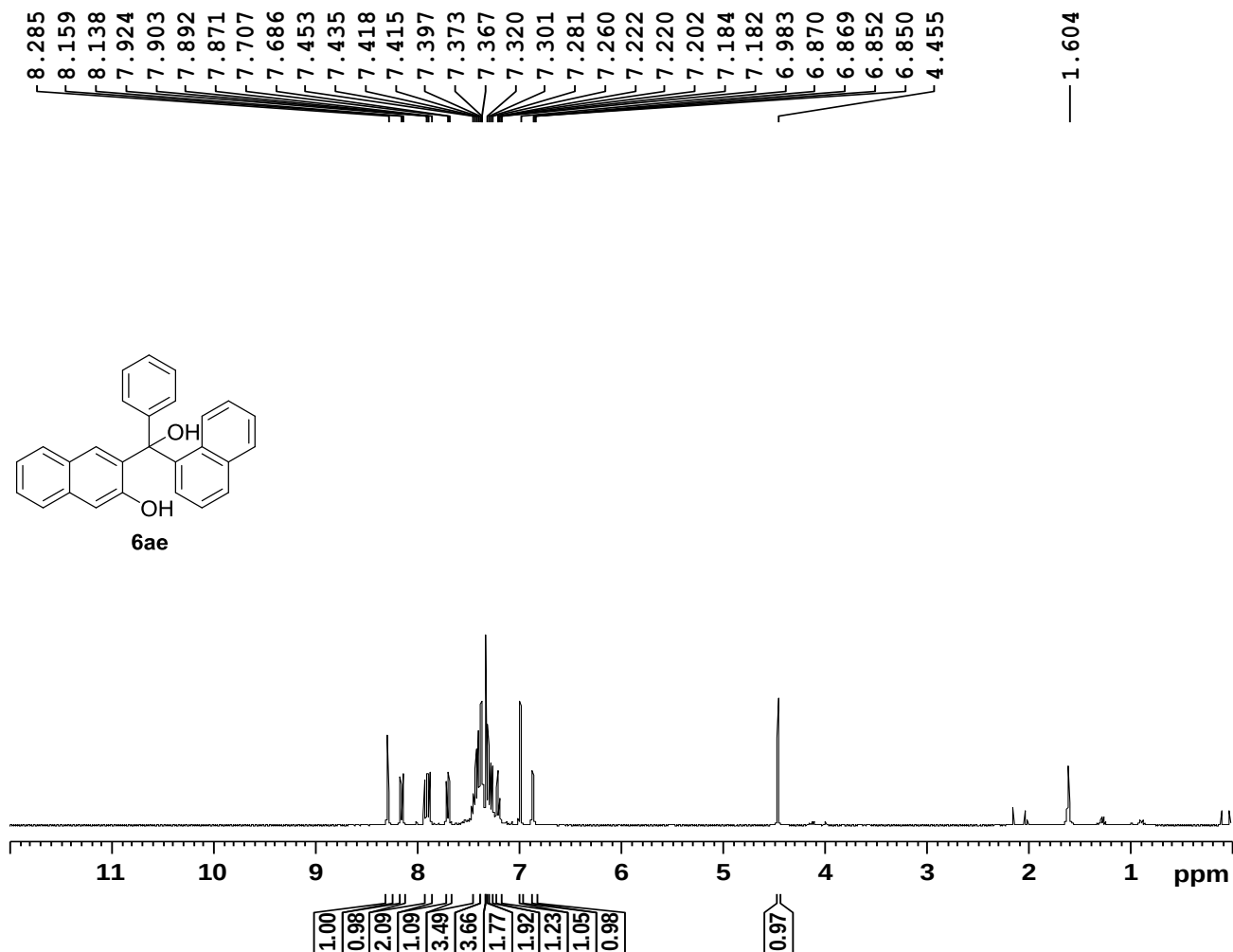
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127590 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 94: ¹³C-NMR spectra for compound 6ad

PROTON CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-402
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190424
Time_ 11.01
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 287
DW 60.800 usec
DE 6.00 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.130093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 95: ¹H-NMR spectra for compound **6ae**

PROTON CDC13 {D:\CRR} CIF_NMR 1

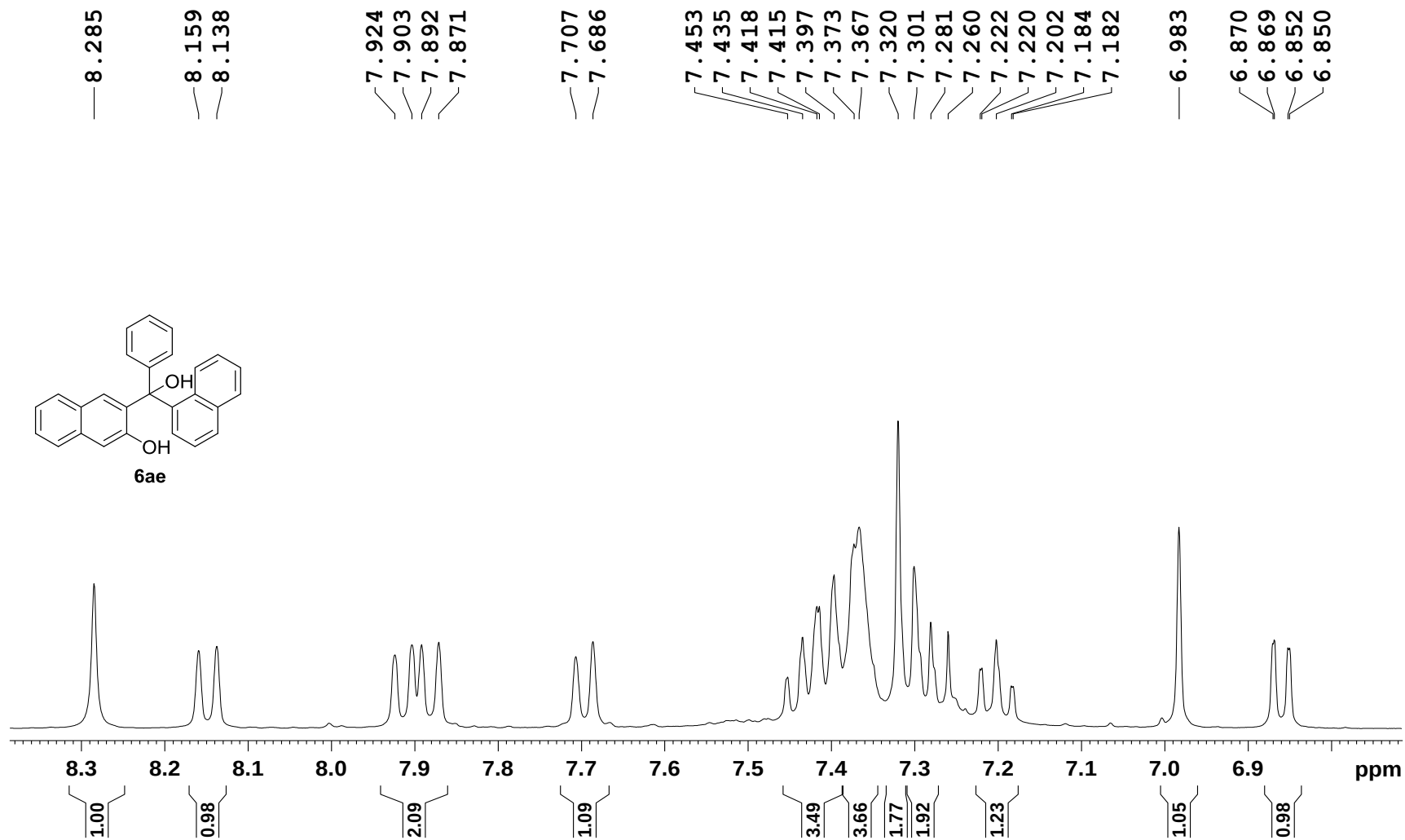
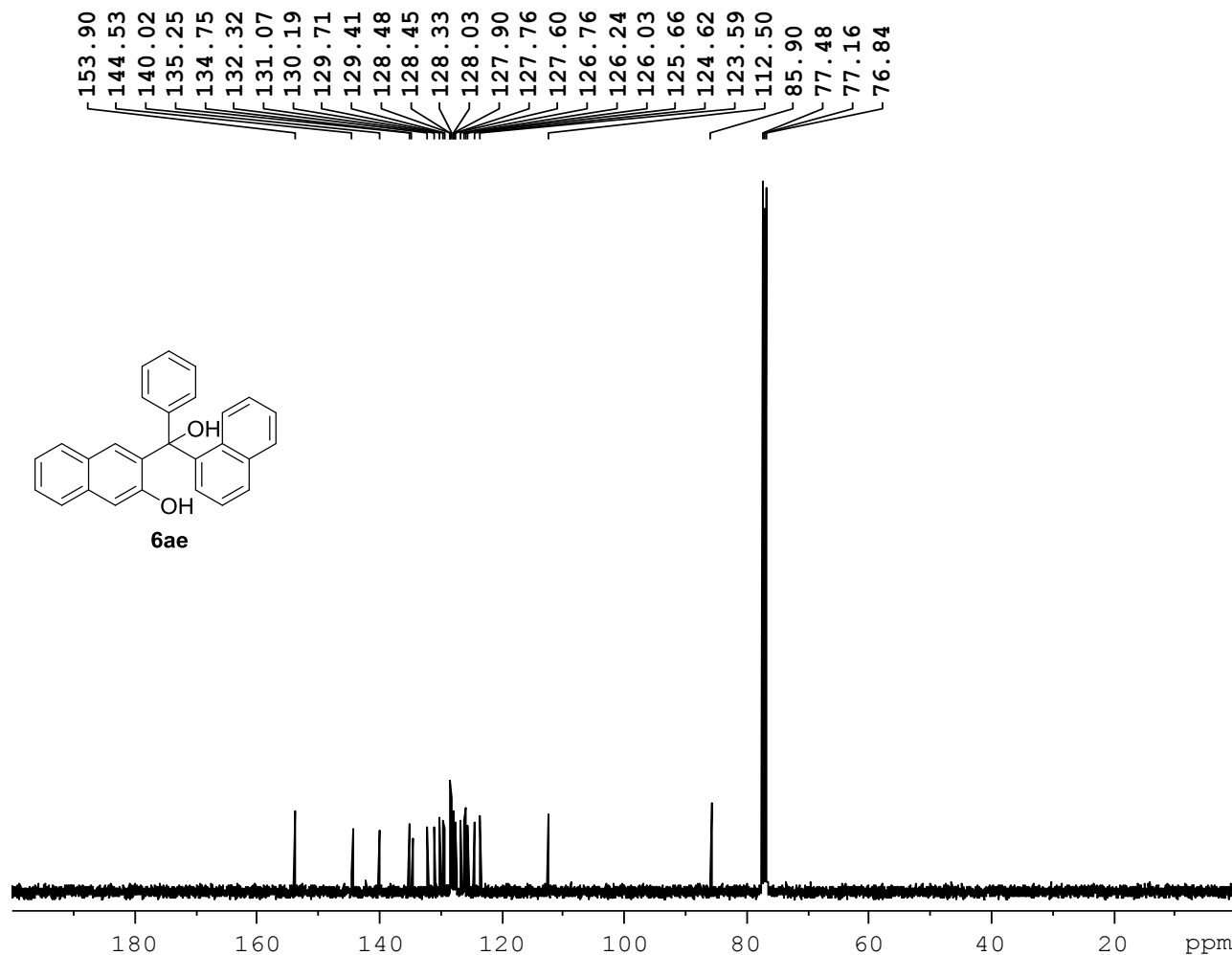


Figure 95a: ¹H-NMR spectra expansion for compound **6ae**



Current Data Parameters
 NAME MK-II-402
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190424
 Time 11.47
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 512
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 45.2
 DW 20.800 usec
 DE 6.00 usec
 TE 296.8 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

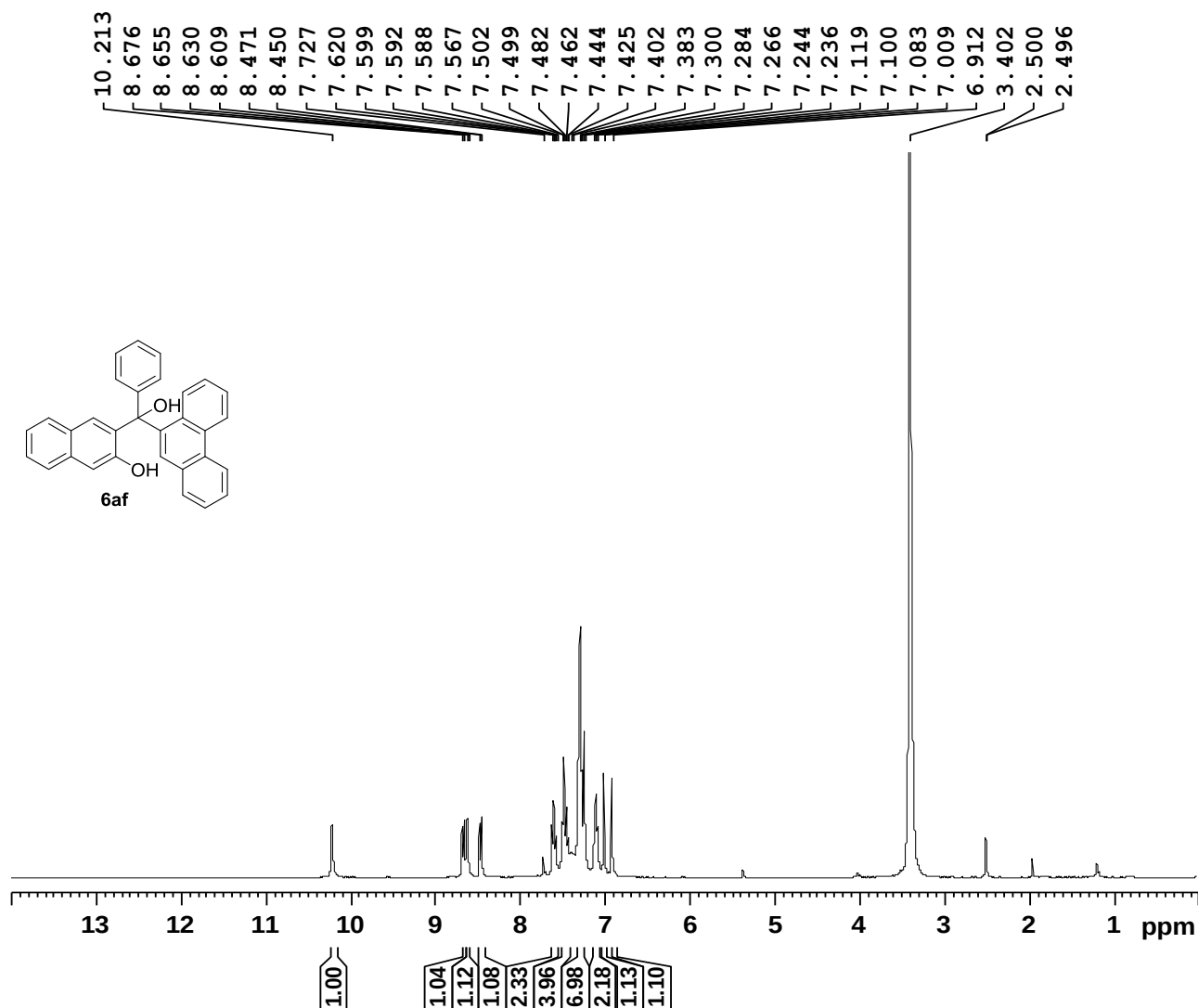
===== CHANNEL f1 =====
 NUC1 13C
 P1 9.95 usec
 PL1 -1.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL12 14.95 dB
 PL13 120.00 dB
 PL2 -1.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127572 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure 96: ^{13}C -NMR spectra for compound **6ae**

PROTON DMSO {D:\CRR} CIF_NMR 1



Current Data Parameters
 NAME MK-UN-04-A
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190702
 Time 12.50
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 128
 DW 60.800 usec
 DE 6.00 usec
 TE 294.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.35 usec
 PL1 -1.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300044 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure 97: ¹H-NMR spectra for compound 6af

PROTON DMSO {D:\CRR} CIF_NMR 1

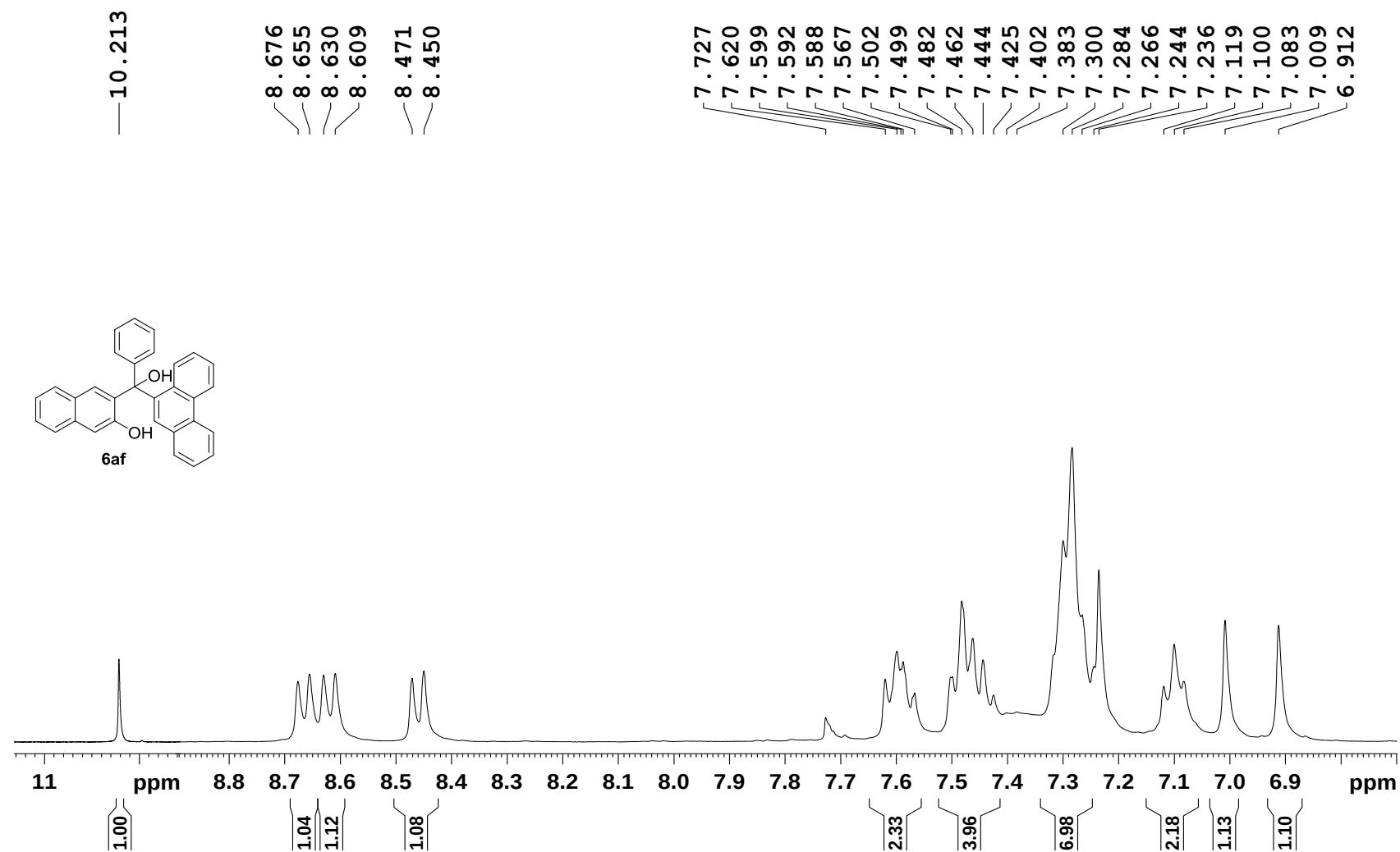
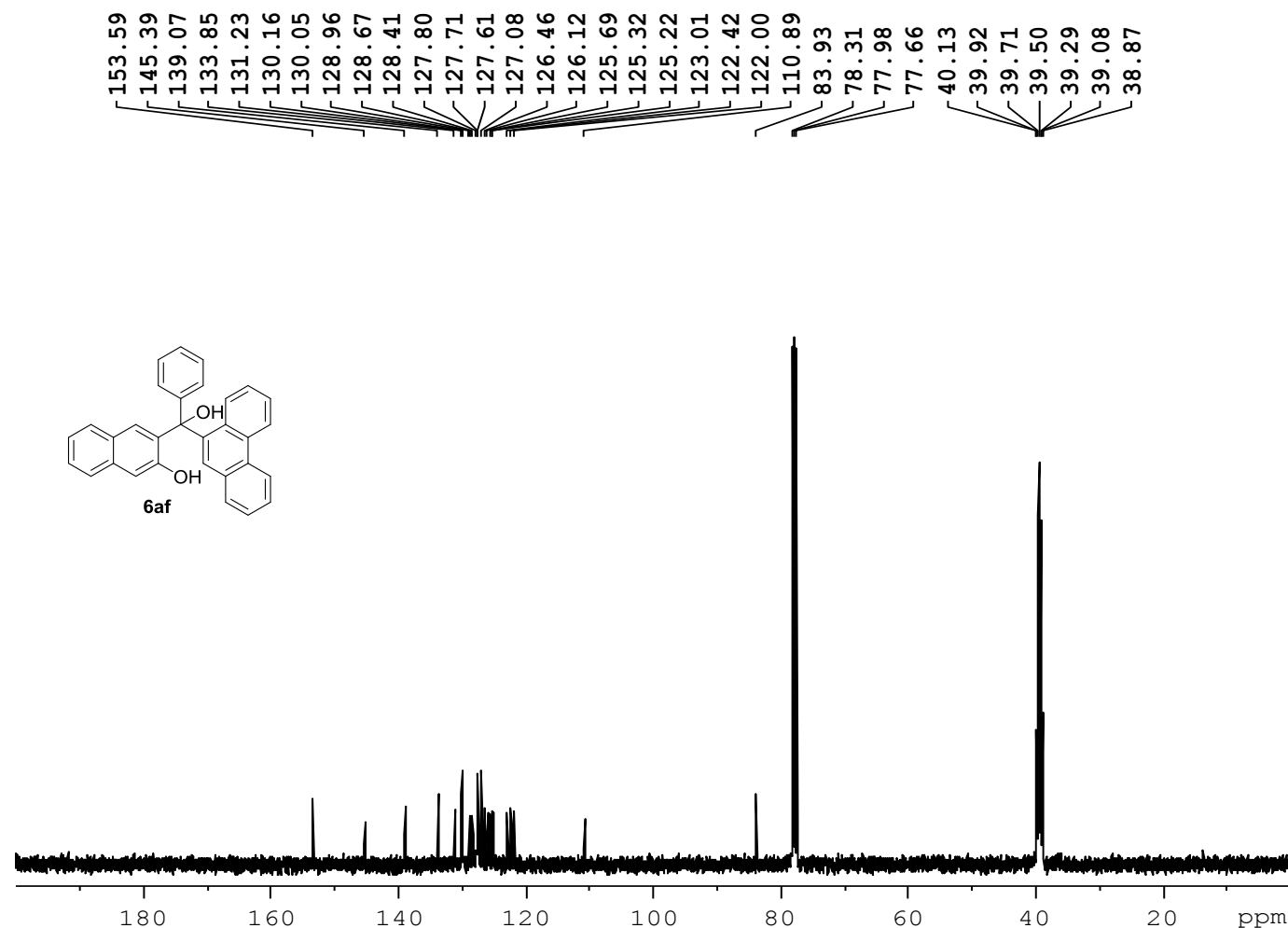


Figure 97a: ^1H -NMR spectra expansion for compound **6af**

C13CPD DMSO {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-UN-04-A
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190703
Time_ 11.19
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 322
DW 20.800 usec
DE 6.00 usec
TE 292.9 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

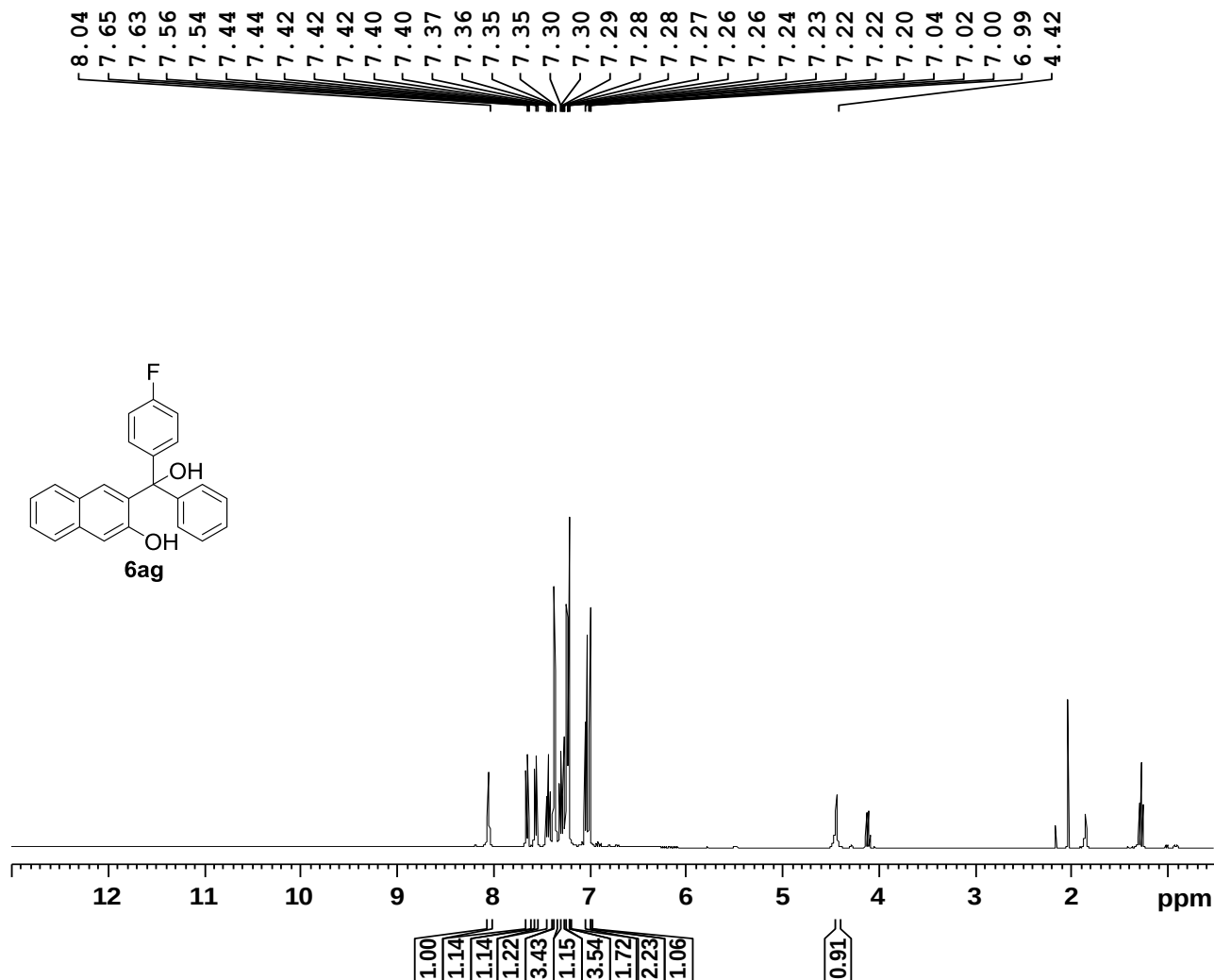
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6128072 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 98: ^{13}C -NMR spectra for compound 6af

PROTON CDCl3 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-378-O
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190815
Time 13.18
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 128
DW 60.800 usec
DE 6.00 usec
TE 291.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.130095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 99: ¹H-NMR spectra for compound **6ag**

PROTON CDC13 {D:\CRR} CIF_NMR 1

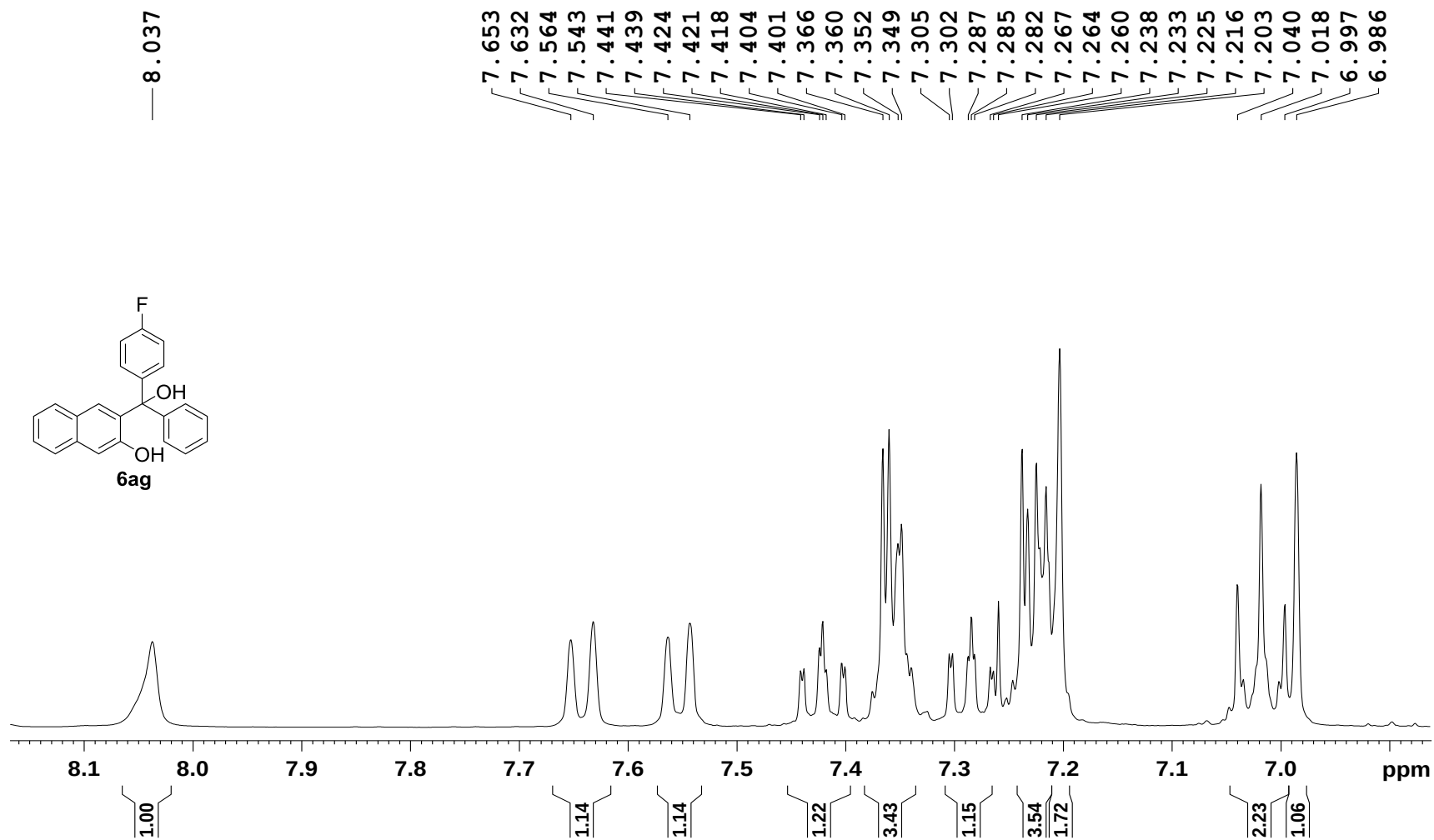
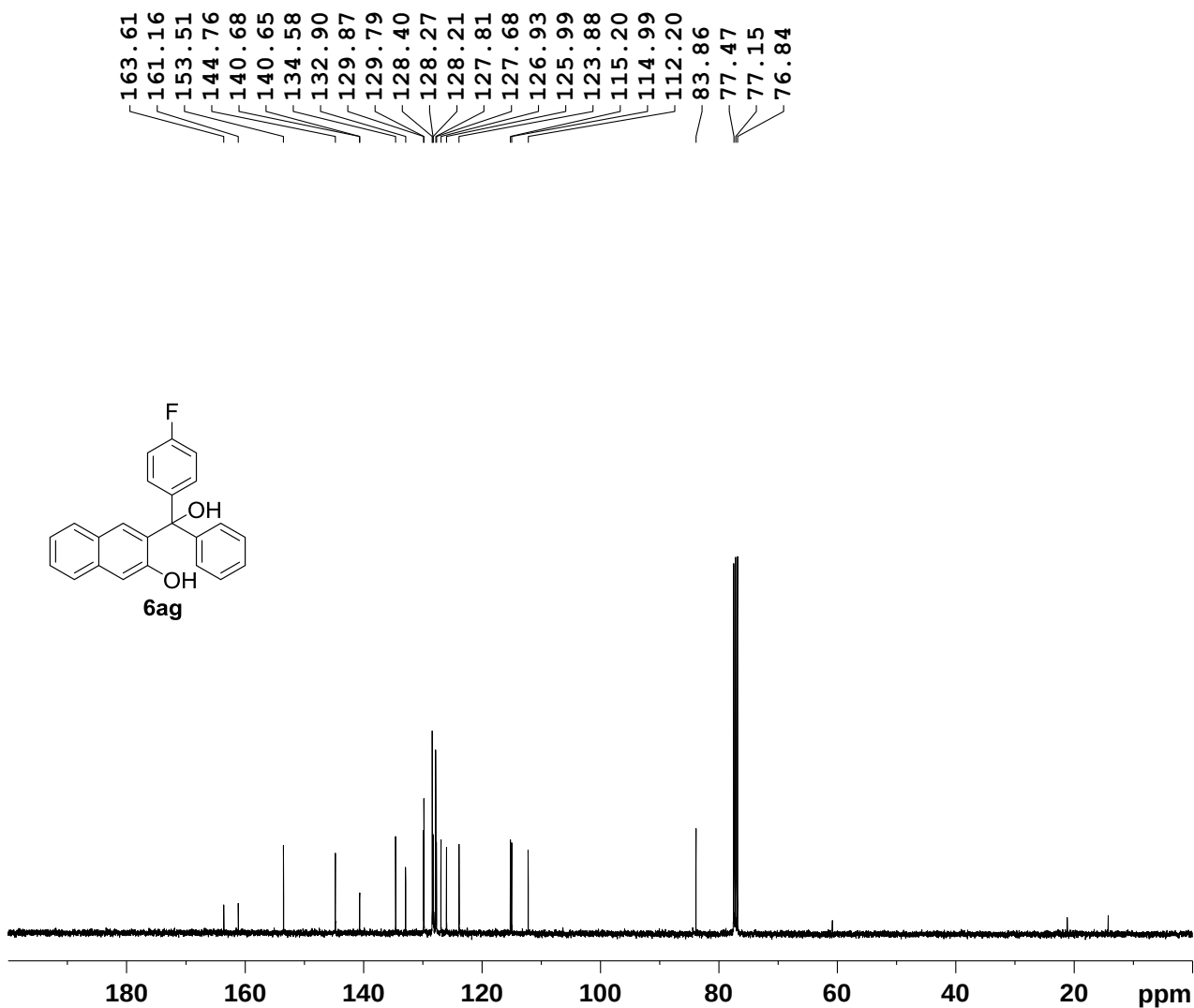


Figure 99a: ¹H-NMR spectra expansion for compound **6ag**



Current Data Parameters

NAME MK-II-378-O
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters

Date_ 20190815
Time_ 13.39
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 350
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 36
DW 20.800 usec
DE 6.00 usec
TE 291.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999999 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters

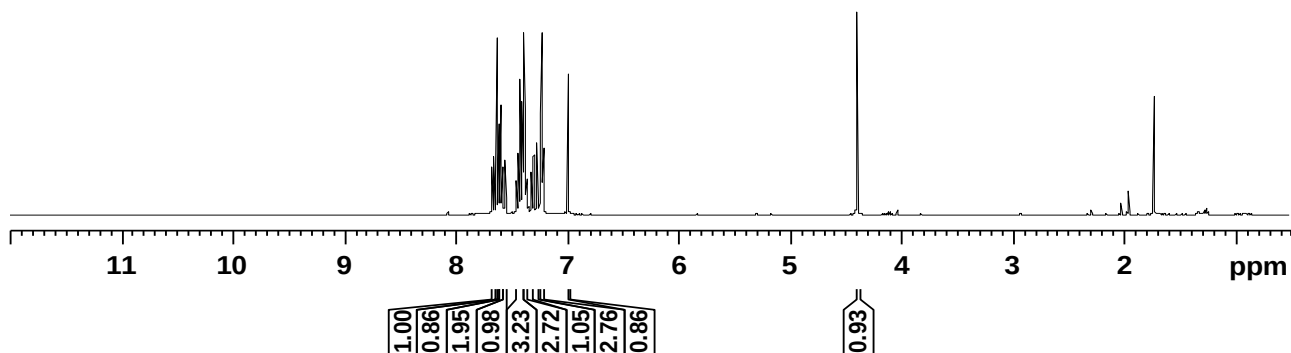
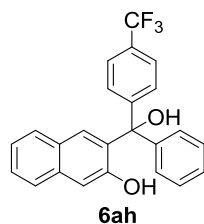
SI 32768
SF 100.6127630 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 100: ^{13}C -NMR spectra for compound **6ag**

PROTON CDCl3 {D:\CRR} CIF_NMR 1



7.649
7.626
7.608
7.587
7.570
7.569
7.549
7.549
7.453
7.450
7.436
7.433
7.429
7.416
7.396
7.386
7.380
7.374
7.372
7.369
7.313
7.310
7.296
7.293
7.290
7.275
7.272
7.260
7.233
7.227
7.221
7.217
7.208
6.984
4.392



Current Data Parameters
NAME MK-II-381
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190401
Time 10.58
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 181
DW 60.800 usec
DE 6.00 usec
TE 292.4 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 101: ¹H-NMR spectra for compound **6ah**

PROTON CDC13 {D:\CRR} CIF_NMR 1

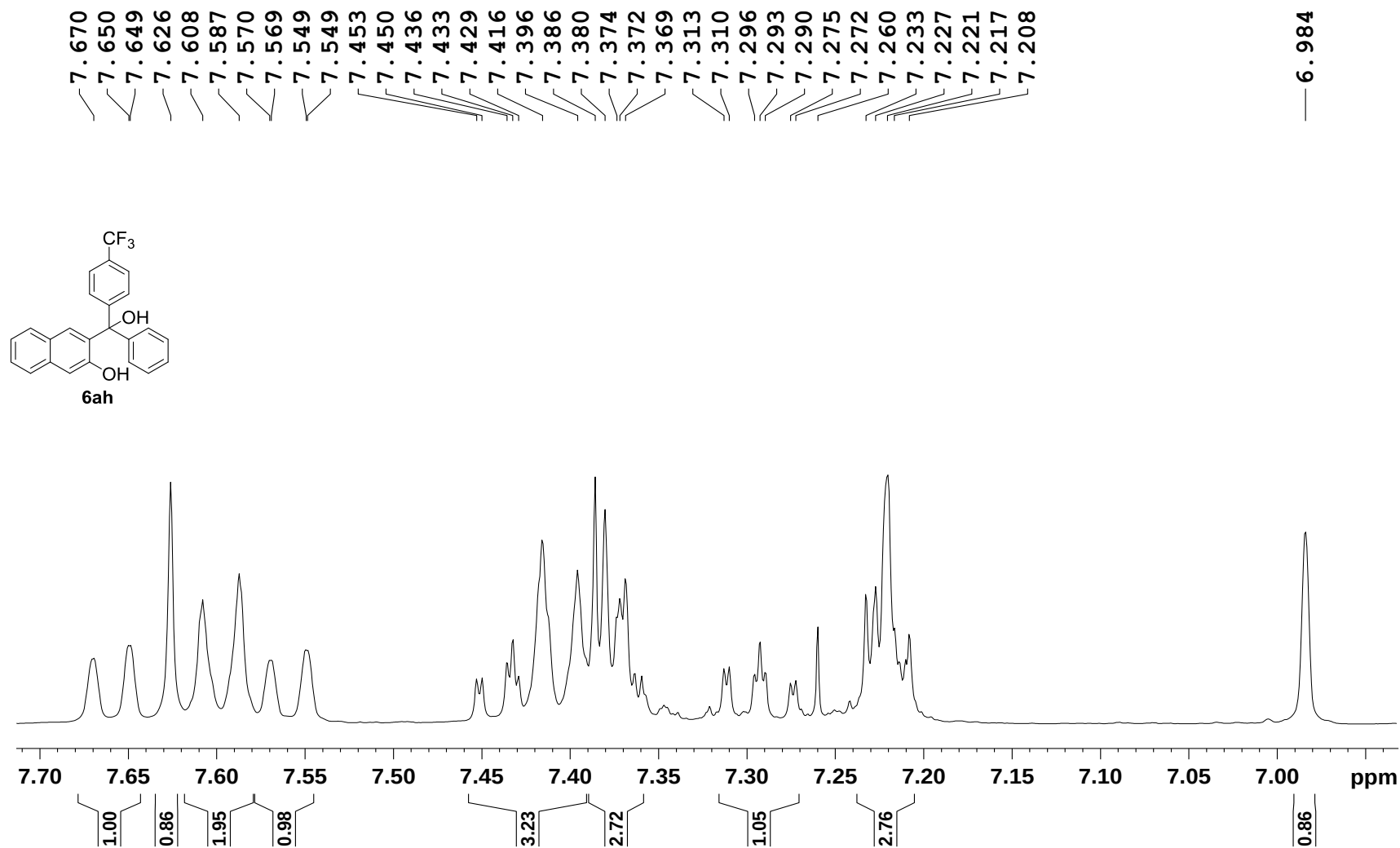
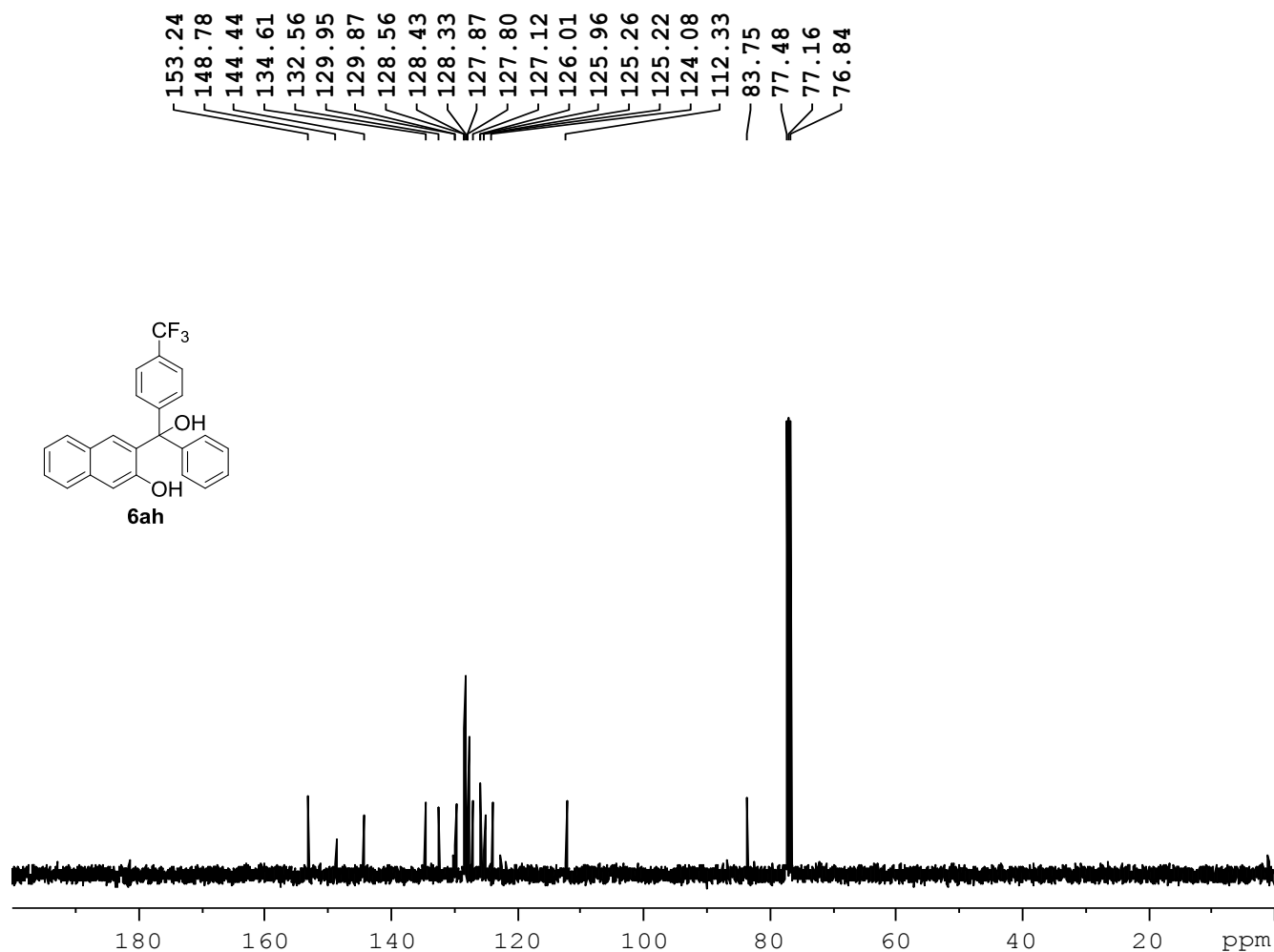


Figure 101a: ¹H-NMR spectra expansion for compound **6ah**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-II-381
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190402
Time 15.39
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 125
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 45.2
DW 20.800 usec
DE 6.00 usec
TE 294.4 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

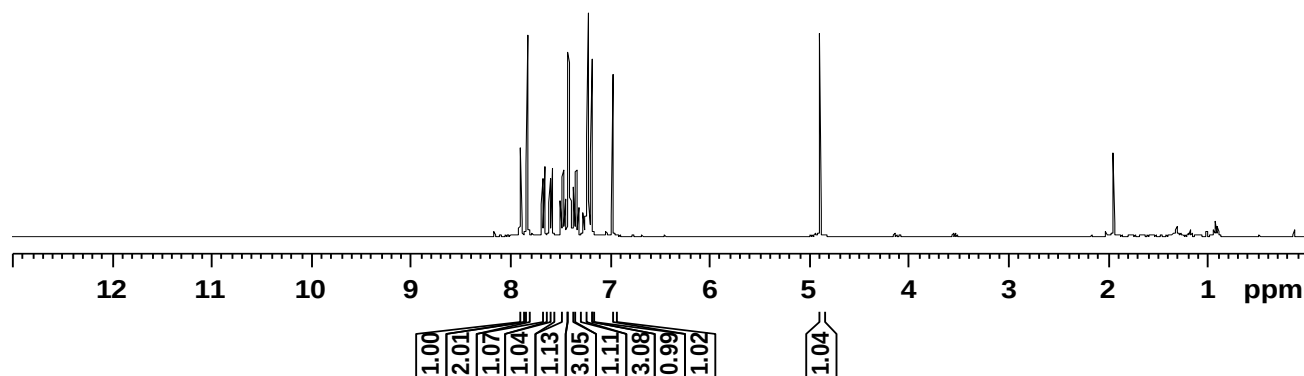
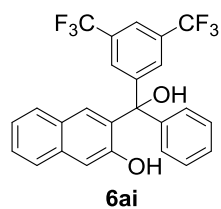
F2 - Processing parameters
SI 32768
SF 100.6127585 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 102: ¹³C-NMR spectra for compound 6ah

PROTON CDCl3 {D:\CRR} CIF_NMR 1



7.888
7.818
7.667
7.647
7.591
7.571
7.481
7.479
7.464
7.461
7.443
7.441
7.407
7.401
7.393
7.391
7.348
7.345
7.328
7.325
7.310
7.308
7.260
7.225
7.220
7.210
7.200
7.173
6.961
4.876



Current Data Parameters
NAME MK-II-384-S
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191104
Time_ 10.17
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 144
DW 60.800 usec
DE 6.00 usec
TE 290.1 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 103: ¹H-NMR spectra for compound 6ai

PROTON CDCl3 {D:\CRR} CIF_NMR 1

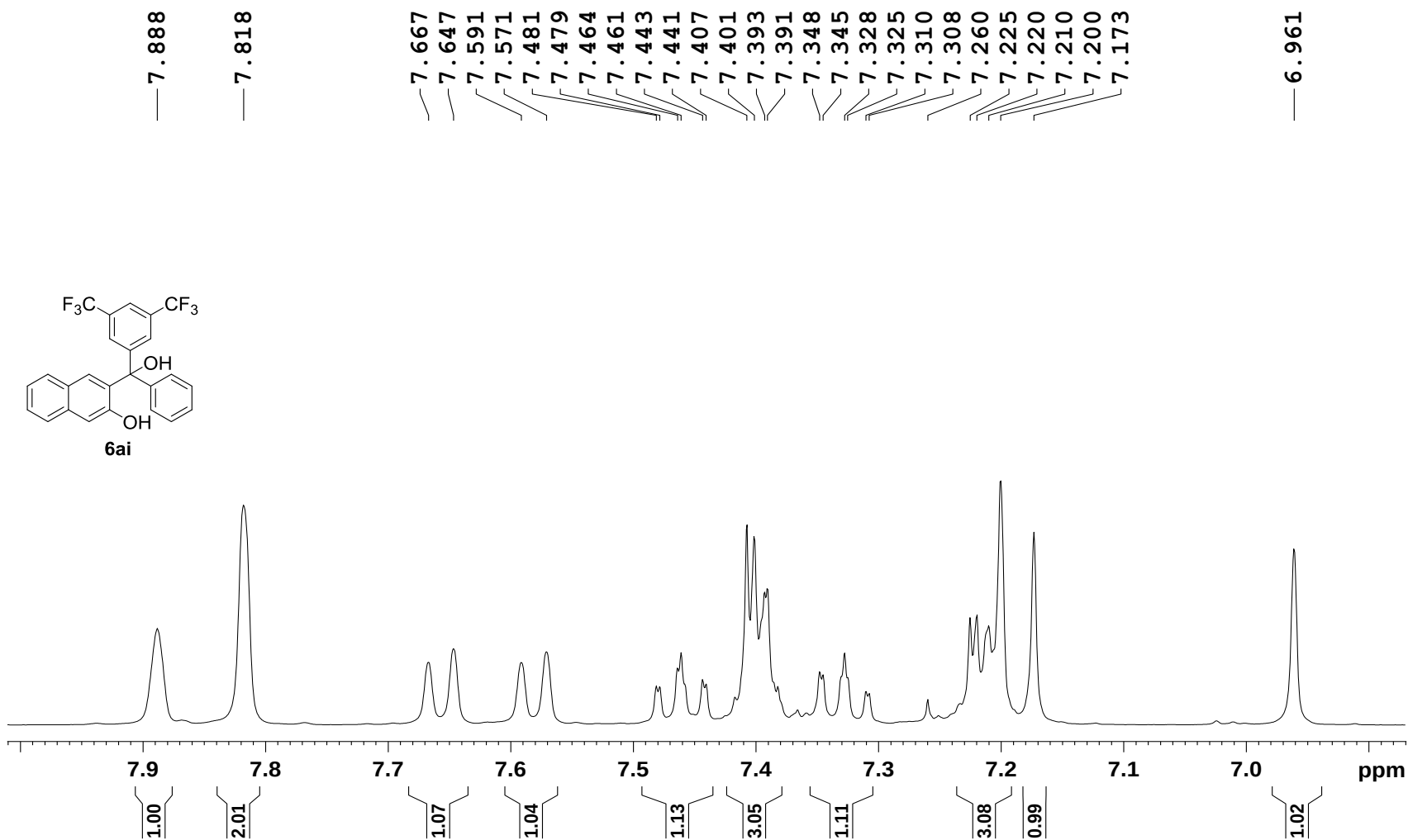
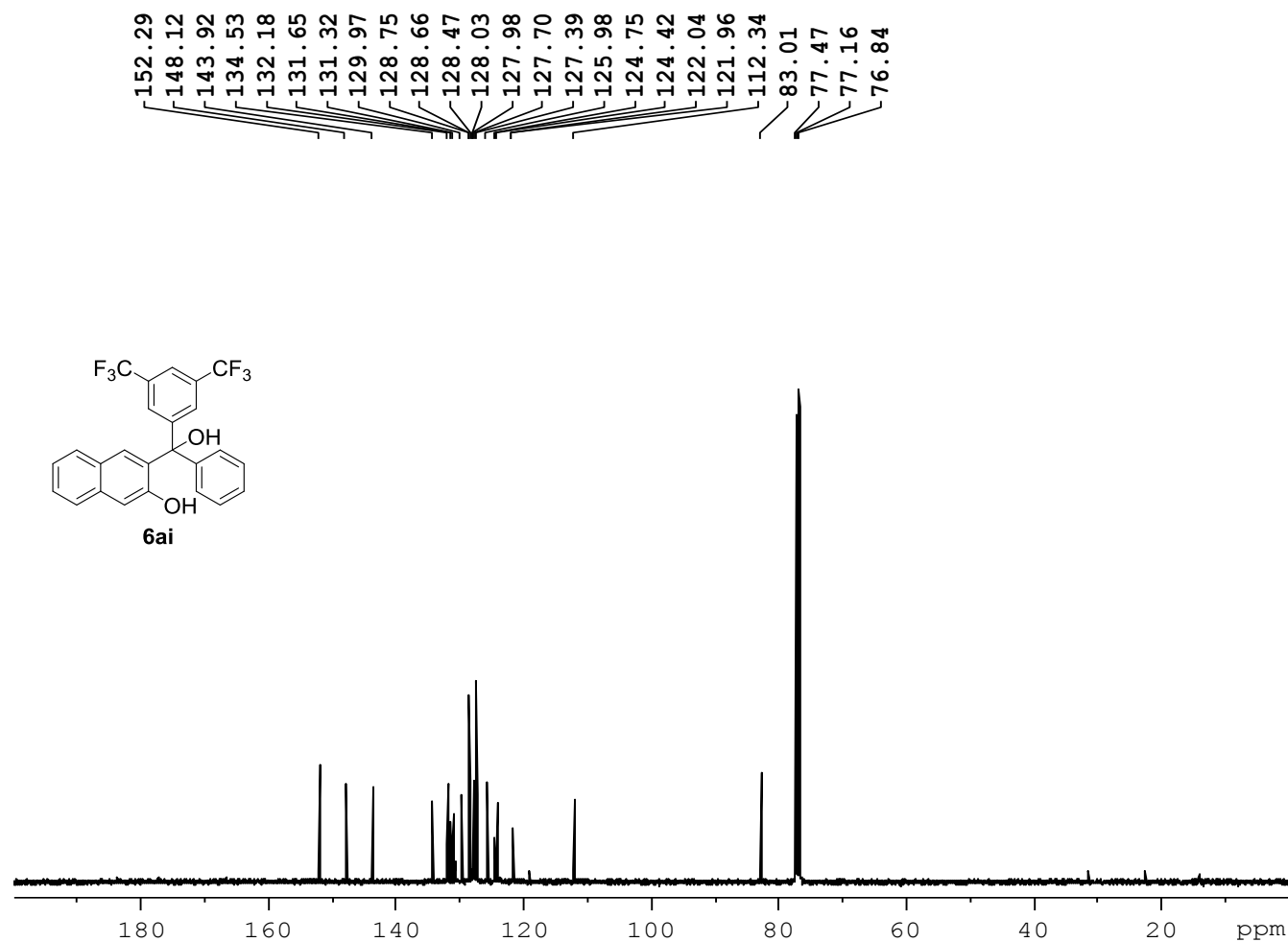


Figure 103a: ^1H -NMR spectra expansion for compound **6ai**



Current Data Parameters
NAME MK-II-384-S
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20191104
Time_ 11.20
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 362
DW 20.800 usec
DE 6.00 usec
TE 291.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

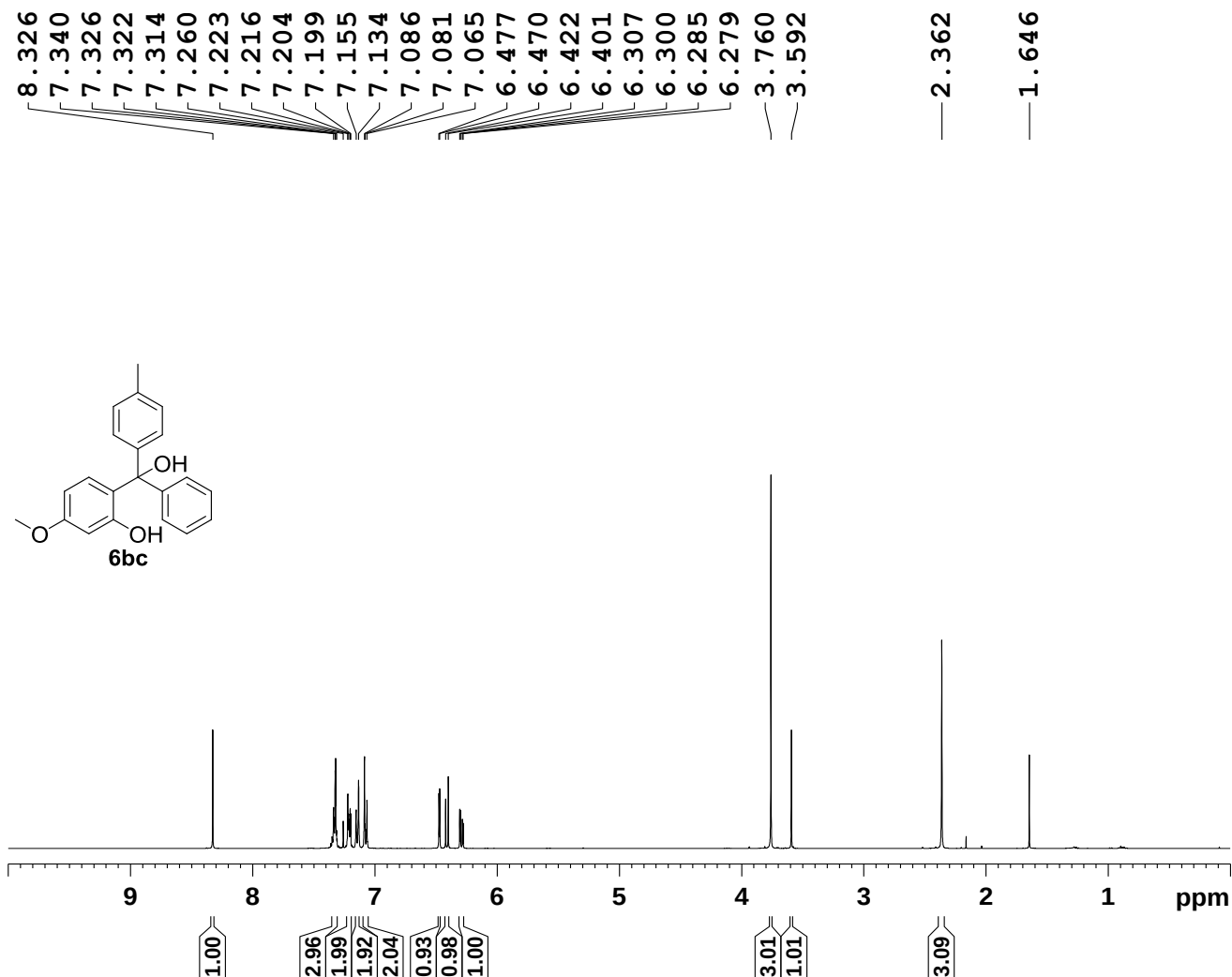
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127592 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 104: ¹³C-NMR spectra for compound **6ai**

PROTON CDCl3 {D:\CRR} CIF_NMR 1



Current Data Parameters
 NAME MK-MM-45
 EXPNO 1
 PROCNO 1

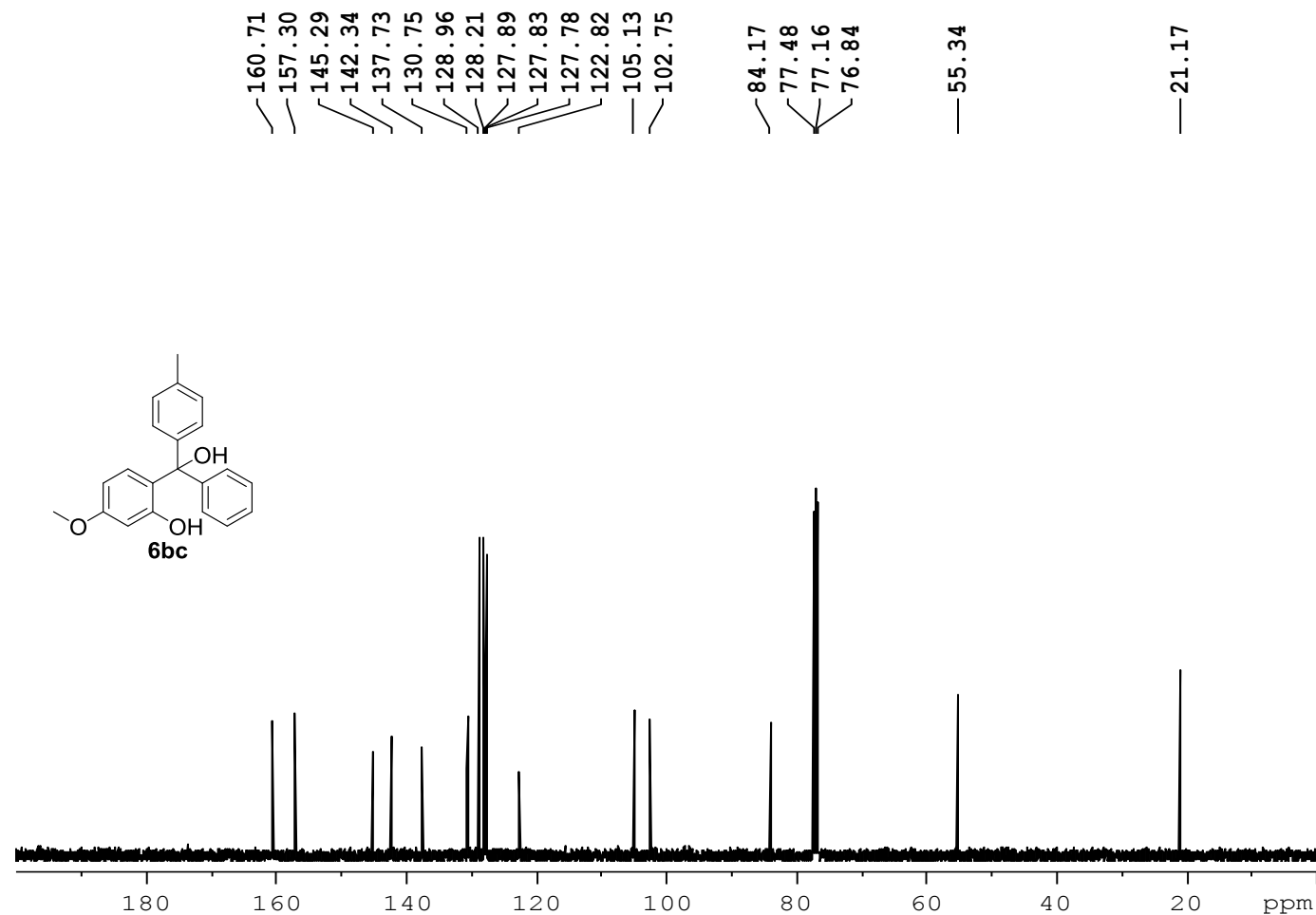
F2 - Acquisition Parameters
 Date_ 20190331
 Time_ 10.15
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 181
 DW 60.800 usec
 DE 6.00 usec
 TE 292.6 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.35 usec
 PL1 -1.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300094 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure 105: ¹H-NMR spectra for compound **6bc**

C13CPD CDCl3 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-MM-45
EXPNO 2
PROCNO 1

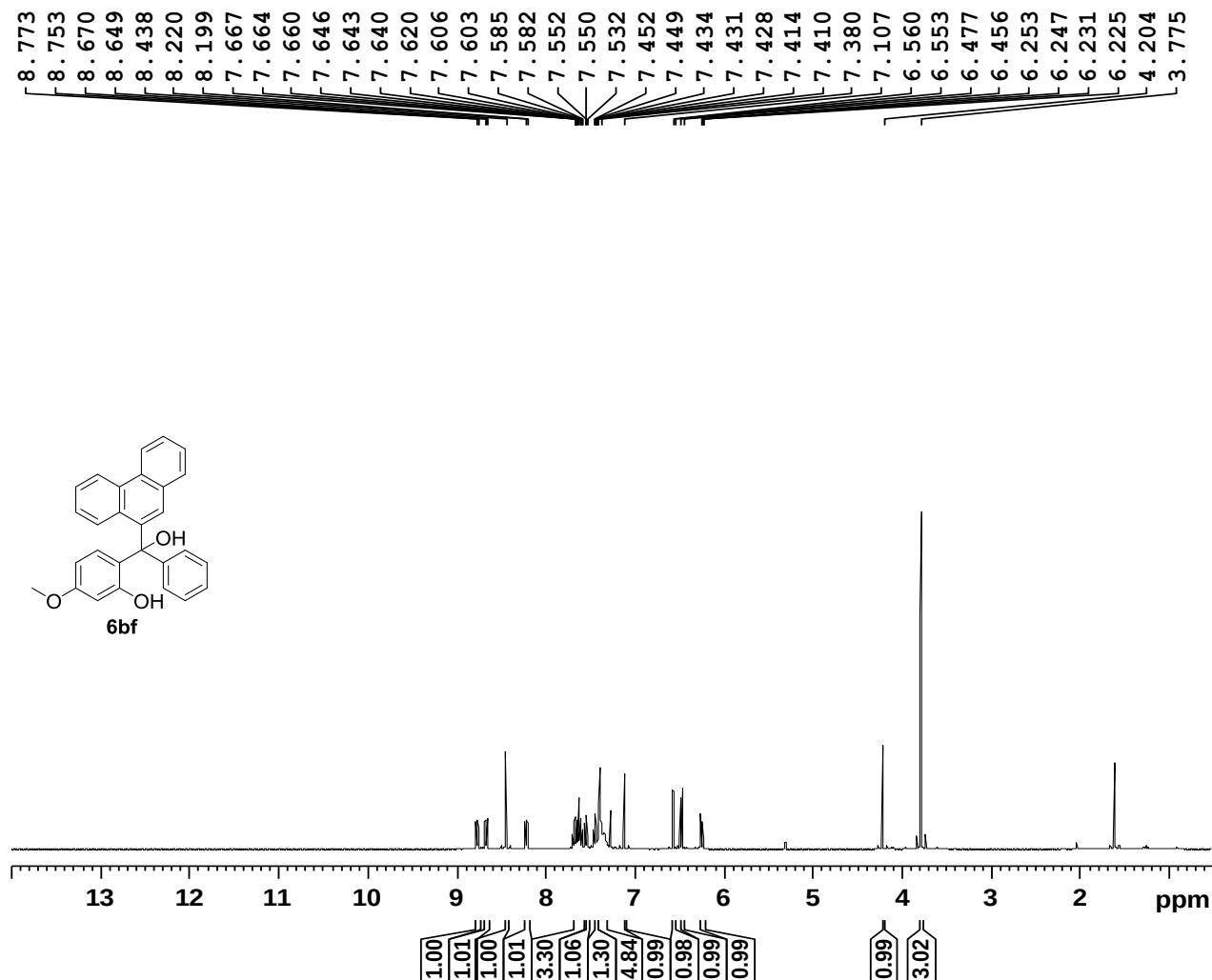
F2 - Acquisition Parameters
Date_ 20190331
Time_ 11.20
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 100
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 40.3
DW 20.800 usec
DE 6.00 usec
TE 292.8 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127633 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 106: ^{13}C -NMR spectra for compound **6bc**



```
Current Data Parameters
NAME          MK-II-415
EXPNO          1
PROCNO         1
```

```

F2 - Acquisition Parameters
Date_                20190507
Time_                15.15
INSTRUM              spect
PROBHD              5 mm BBO BB-1H
PULPROG              zg30
TD                  65536
SOLVENT              CDC13
NS                   16
DS                   2
SWH                  8223.685 Hz
FIDRES               0.125483 Hz
AQ                   3.9845889 sec
RG                   203
DW                   60.800 usec
DE                   6.00 usec
TE                   293.5 K
D1                   1.00000000 sec
TD0                  1

```

```
===== CHANNEL f1 =====
NUC1                      1H
P1                        14.35 usec
PL1                       -1.00 dB
SFO1                     400.1324710 MHz
```

```

F2 - Processing parameters
SI                32768
SF              400.1300094 MHz
WDW                EM
SSB                0
LB                0.30 Hz
GB                0
PC                1.00

```

Figure 107: ^1H -NMR spectra for compound **6bf**

PROTON CDC13 {D:\CRR} CIF_NMR 1

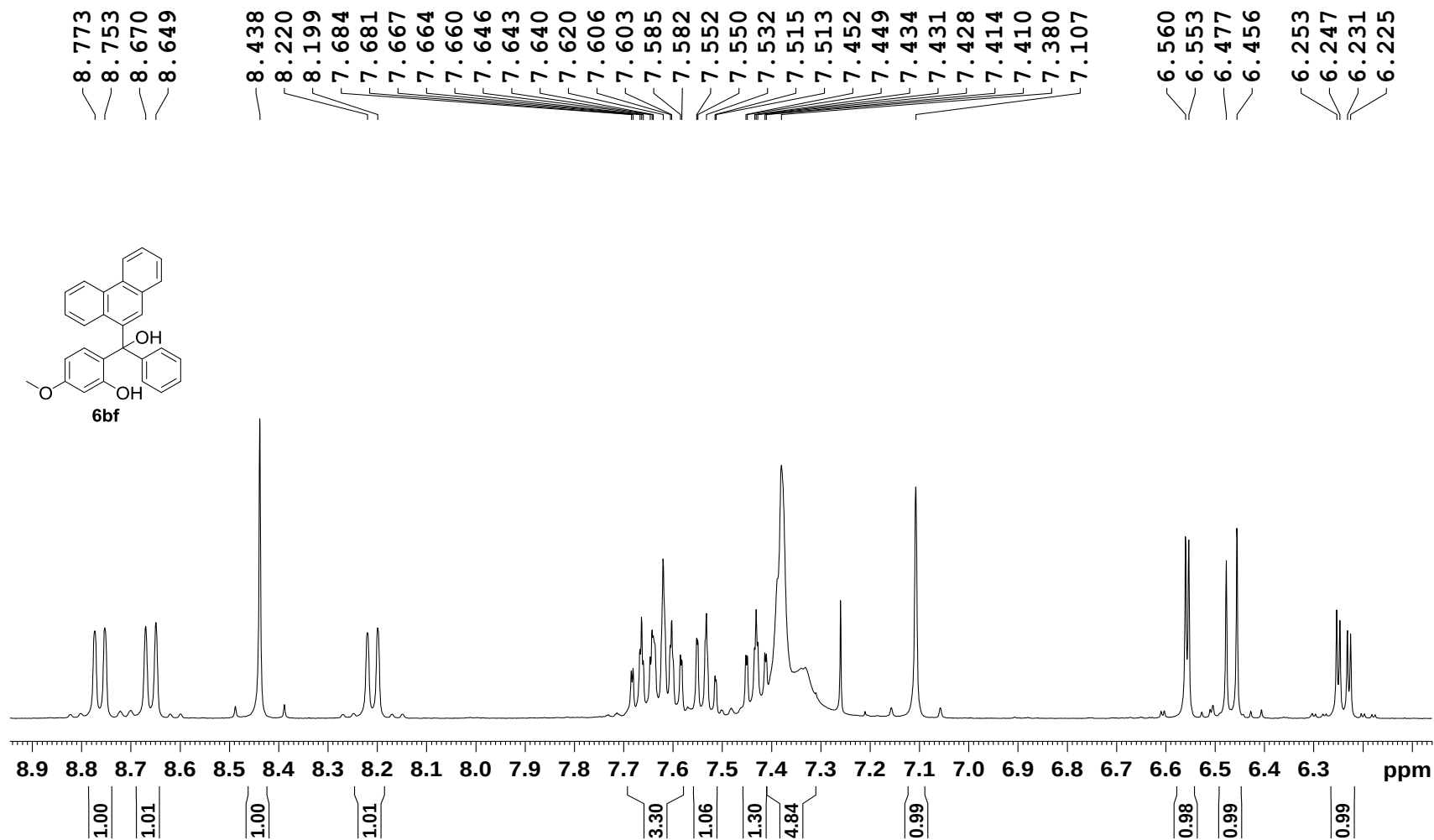
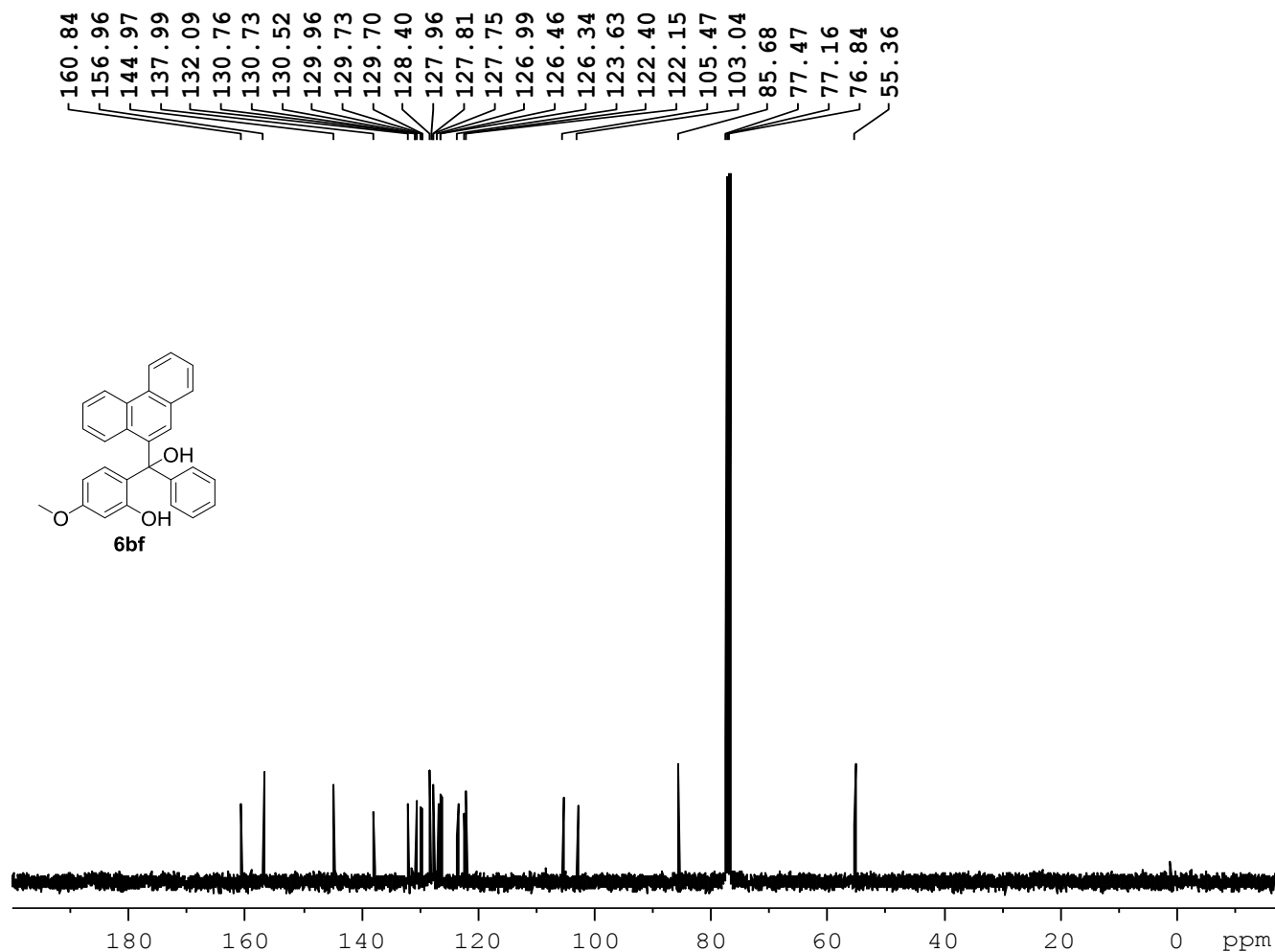


Figure 107a: ^1H -NMR spectra expansion for compound **6bf**



Current Data Parameters
NAME MK-II-415
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190507
Time_ 16.31
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 40.3
DW 20.800 usec
DE 6.00 usec
TE 293.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

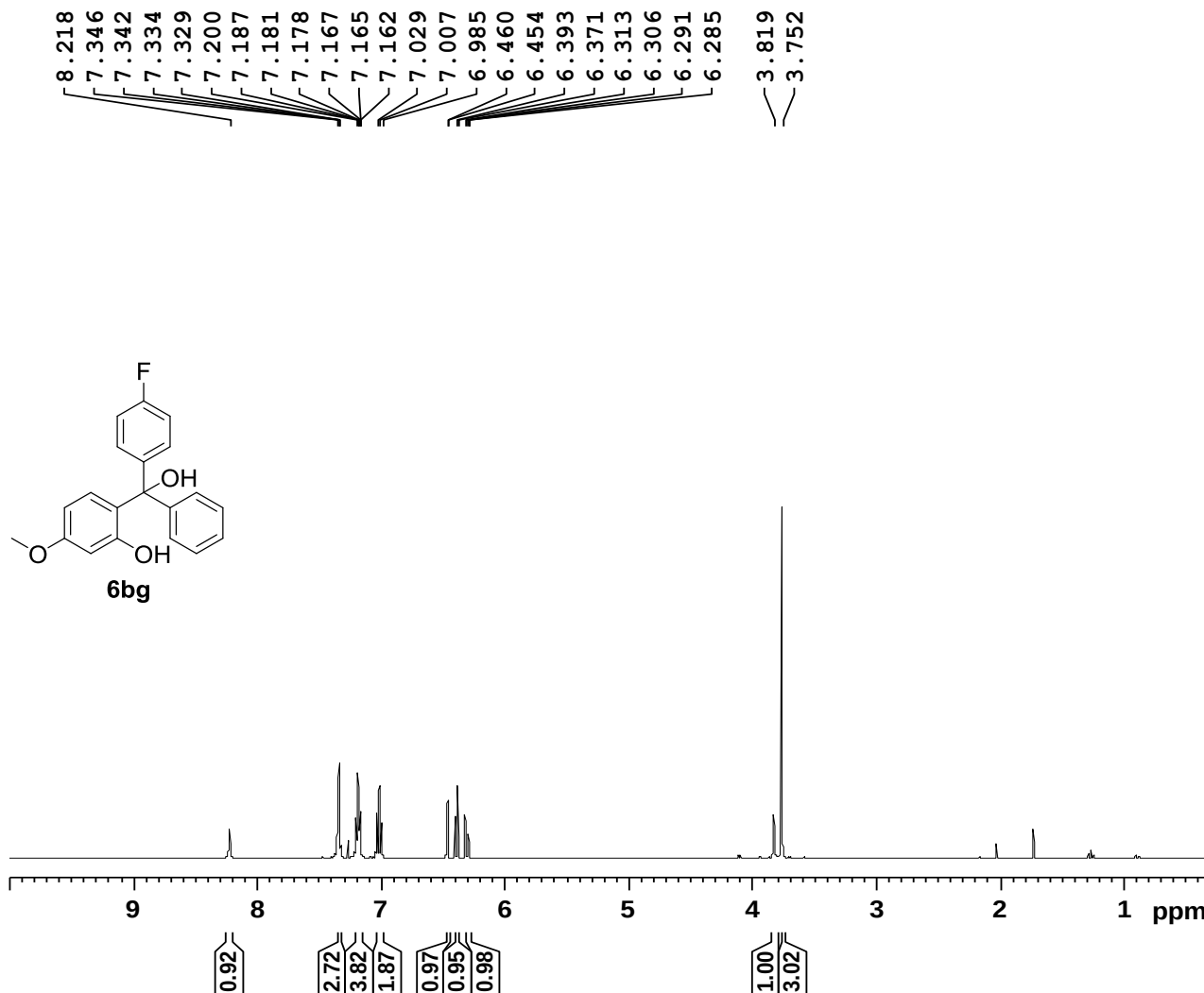
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127598 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 108: ^{13}C -NMR spectra for compound **6bf**

PROTON CDC13 {D:\CRR} CIF_NMR 1



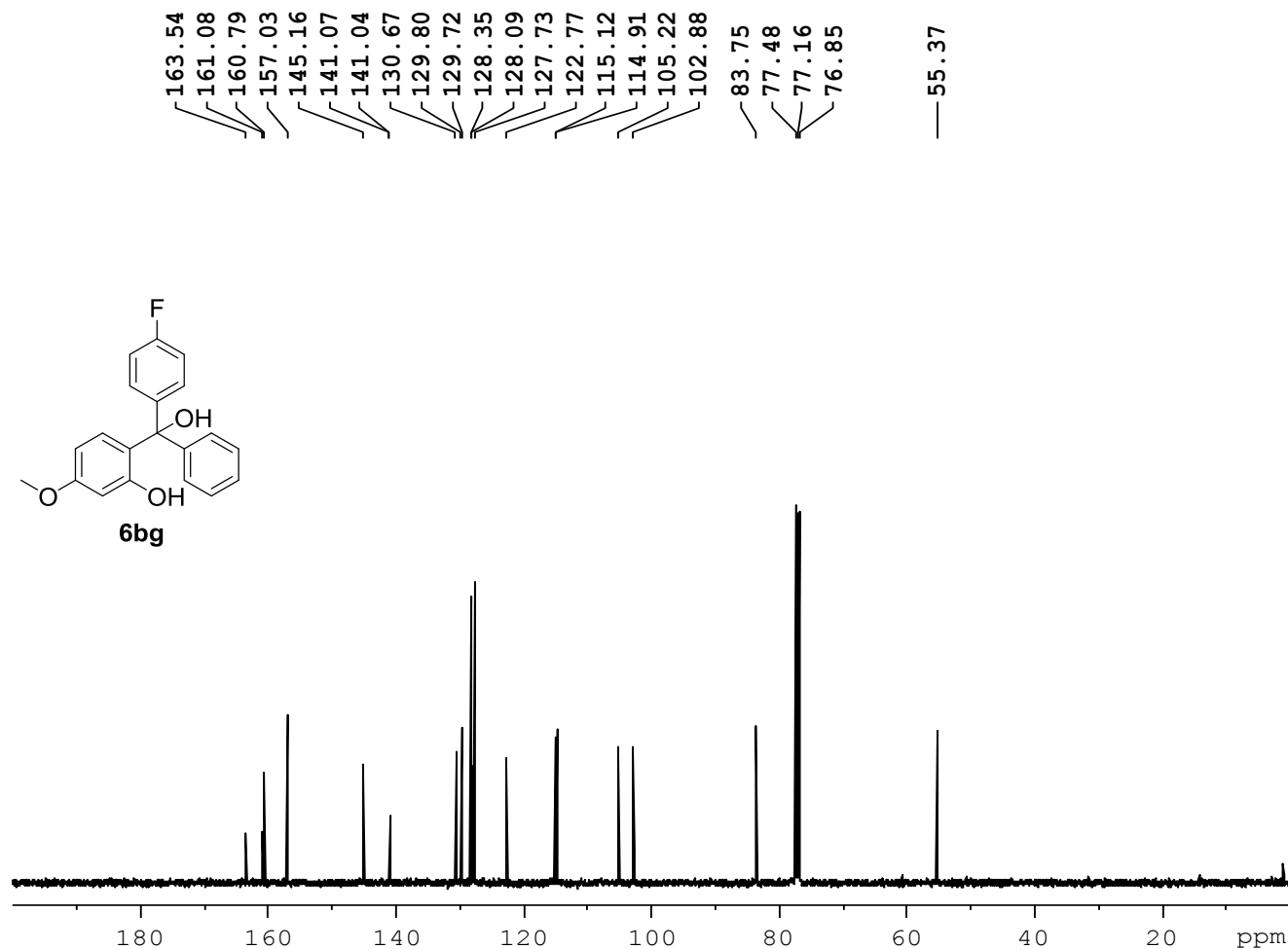
Current Data Parameters
 NAME MK-II-411
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190501
 Time 9.40
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 144
 DW 60.800 usec
 DE 6.00 usec
 TE 290.8 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.35 usec
 PL1 -1.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300093 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure 109: ¹H-NMR spectra for compound **6bg**



Current Data Parameters
 NAME MK-II-411
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190504
 Time 22.51
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 350
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 40.3
 DW 20.800 usec
 DE 6.00 usec
 TE 291.1 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

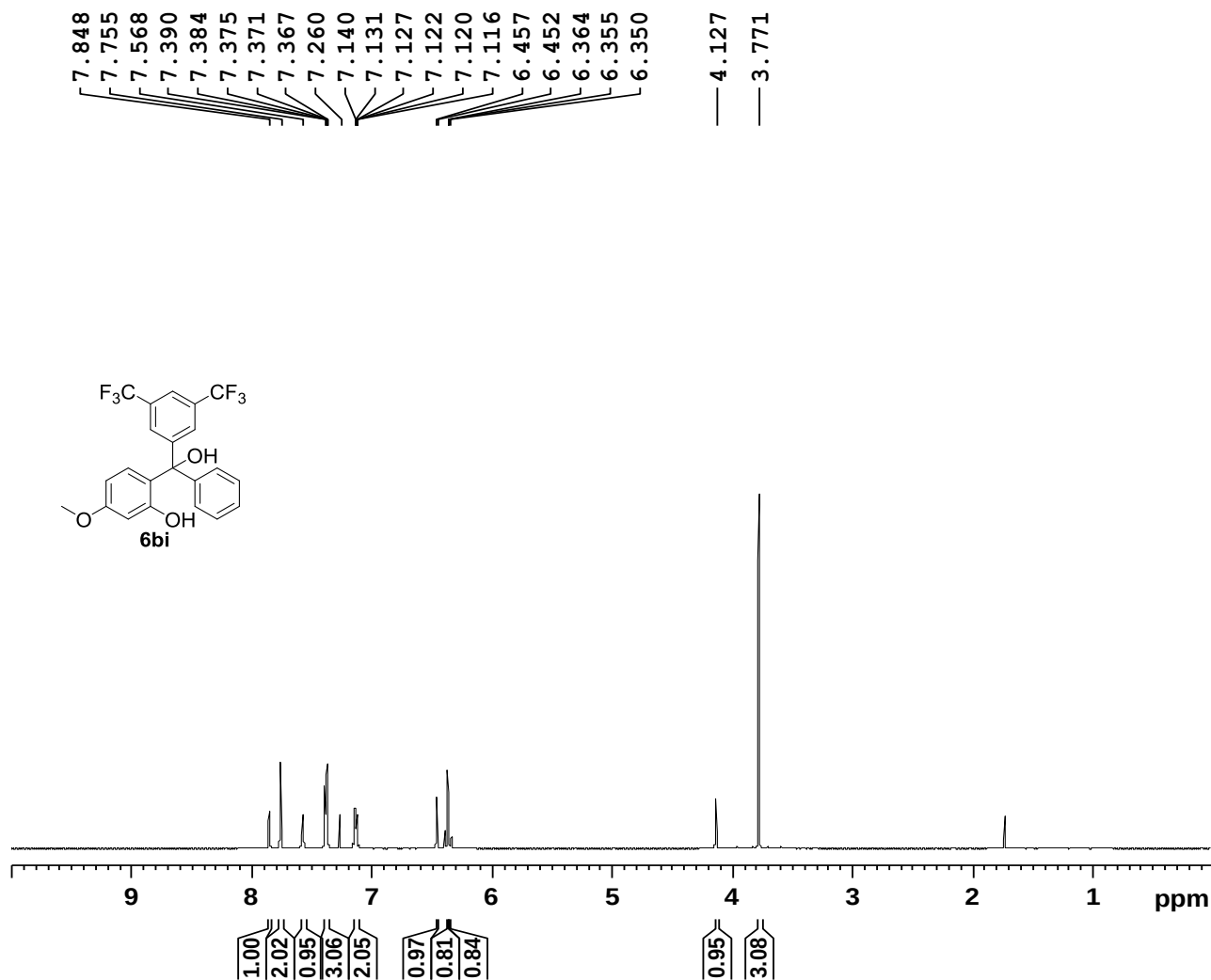
===== CHANNEL f1 =====
 NUC1 13C
 P1 9.95 usec
 PL1 -1.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 1H
 PCPD2 90.00 usec
 PL12 14.95 dB
 PL13 120.00 dB
 PL2 -1.00 dB
 SFO2 400.1316005 MHz

F2 - Processing parameters
 SI 32768
 SF 100.6127619 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure 110: ¹³C-NMR spectra for compound **6bg**

PROTON CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
 NAME MK-MM-46
 EXPNO 1
 PROCNO 1

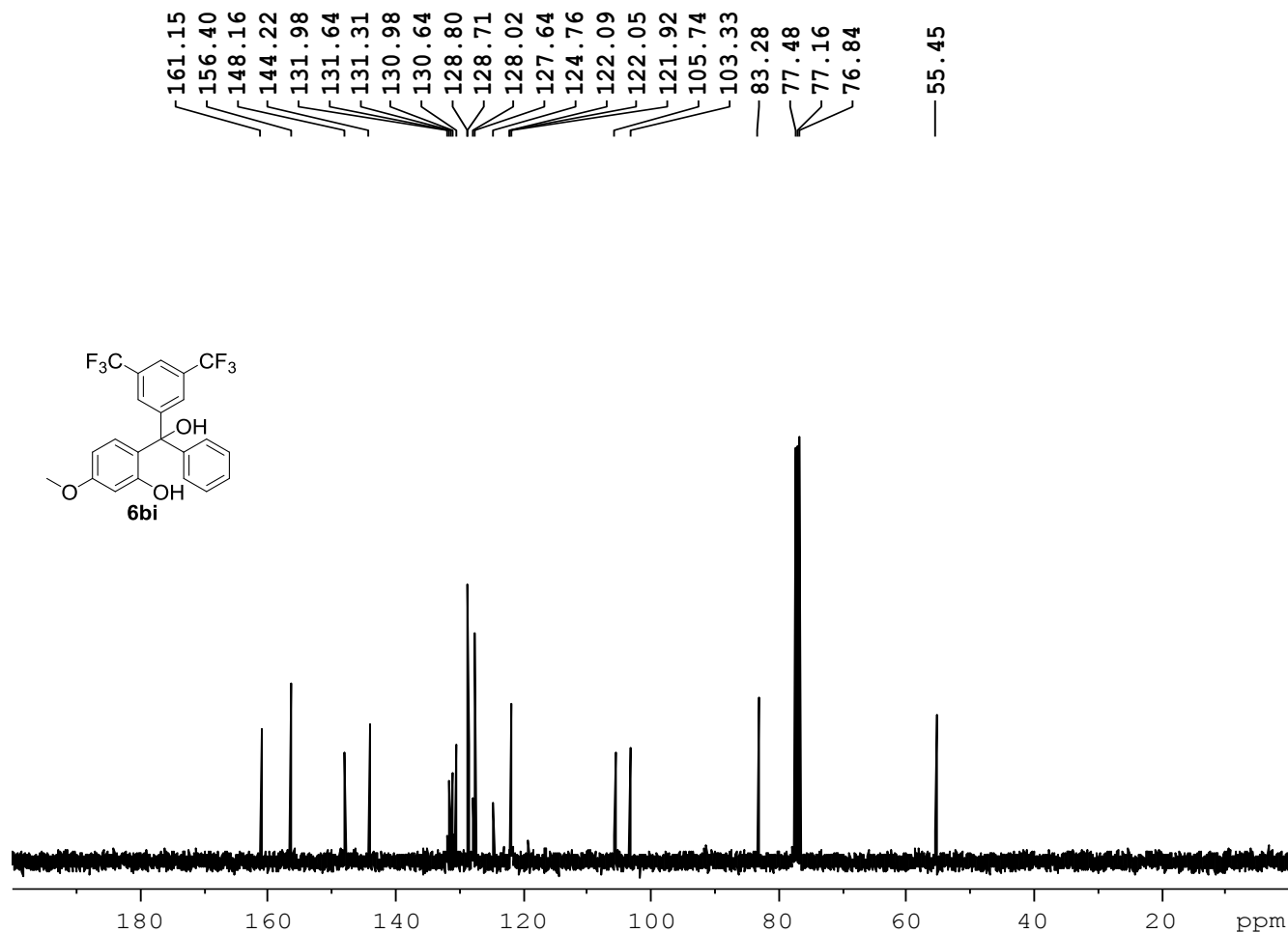
F2 - Acquisition Parameters
 Date_ 20190405
 Time 22.36
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDC13
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 203
 DW 60.800 usec
 DE 6.00 usec
 TE 294.4 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.35 usec
 PL1 -1.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300095 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure 111: ¹H-NMR spectra for compound **6bi**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-MM-46
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190406
Time 0.26
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 134
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 45.2
DW 20.800 usec
DE 6.00 usec
TE 294.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

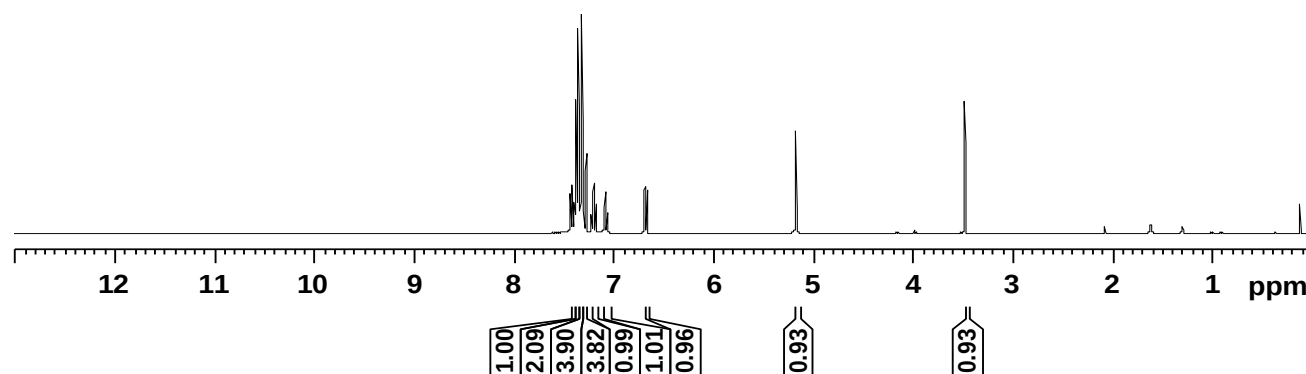
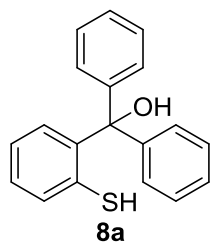
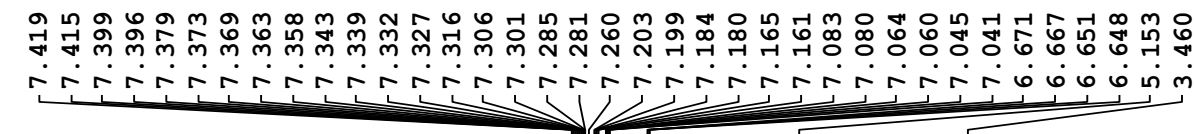
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127565 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 112: ^{13}C -NMR spectra for compound **6bi**

PROTON CDC13 {D:\CRR} CIF_NMR 1



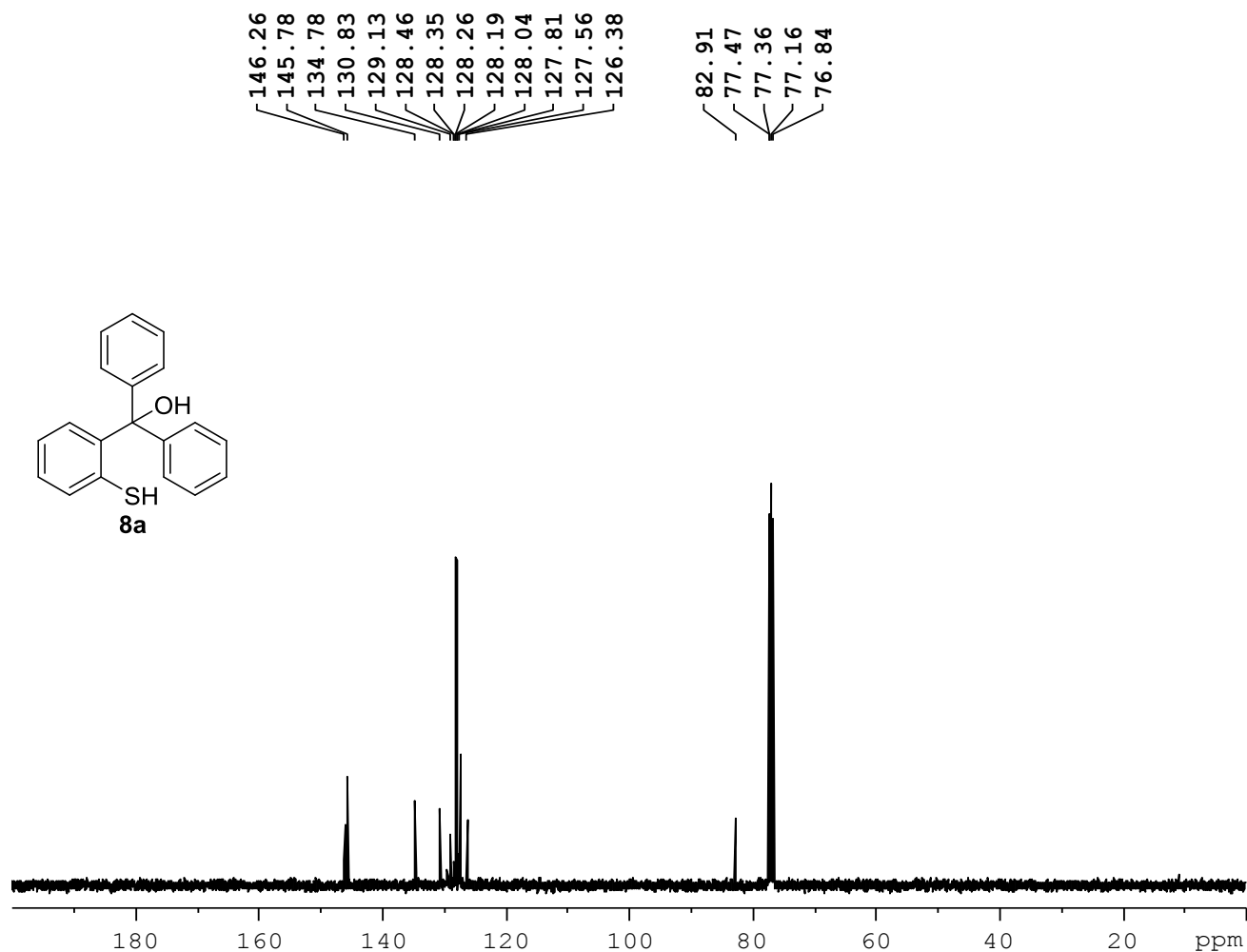
Current Data Parameters
NAME MK-III-434
EXPNO 3
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190817
Time_ 14.56
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 144
DW 60.800 usec
DE 6.00 usec
TE 290.8 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 113: ¹H-NMR spectra for compound **8a**



Current Data Parameters
NAME MK-III-434
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190714
Time 11.51
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 350
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 36
DW 20.800 usec
DE 6.00 usec
TE 291.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

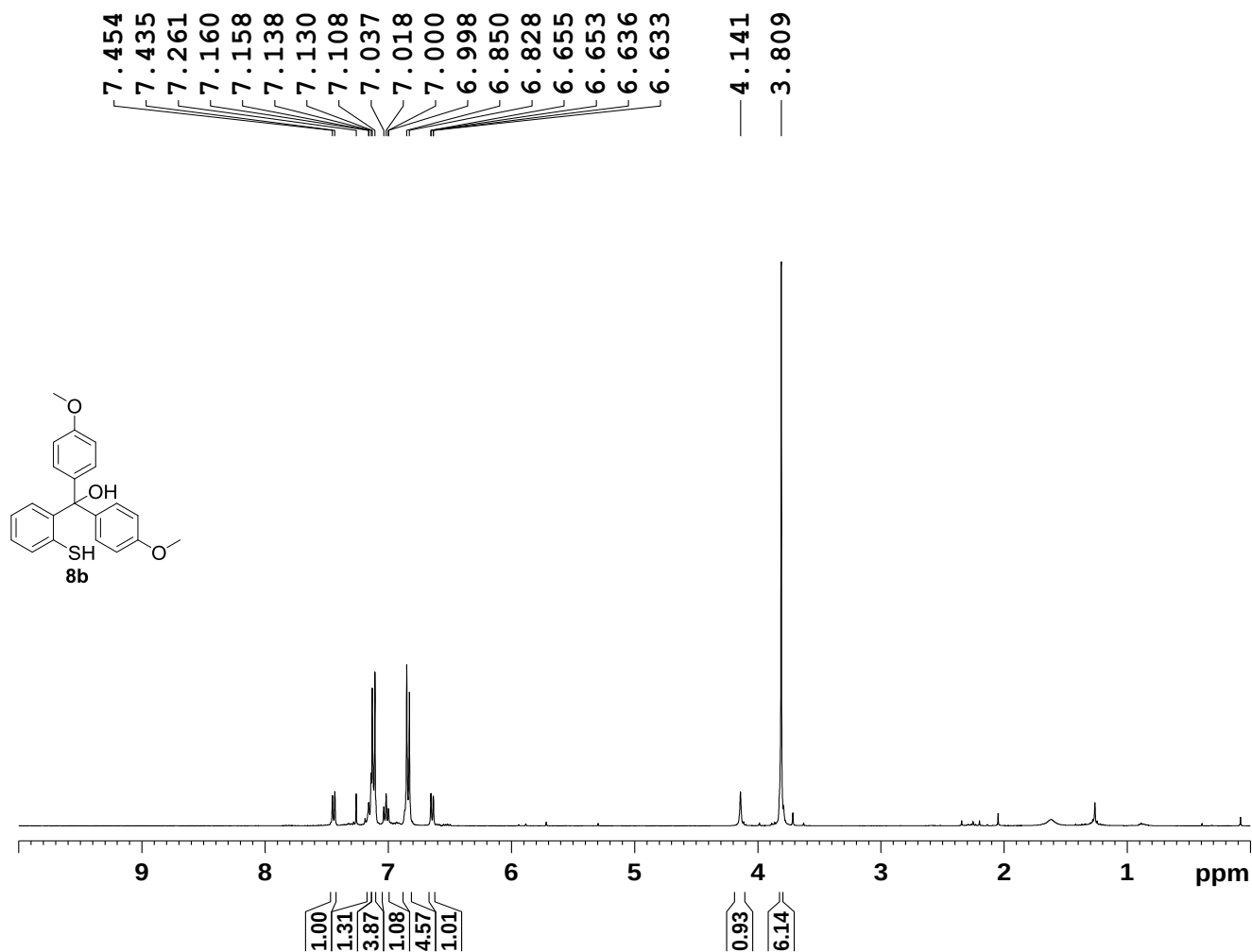
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127587 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 114: ^{13}C -NMR spectra for compound **8a**

PROTON CDC13 {



Current Data Parameters
 NAME MK-MM-26
 EXPNO 1
 PROCNO 1

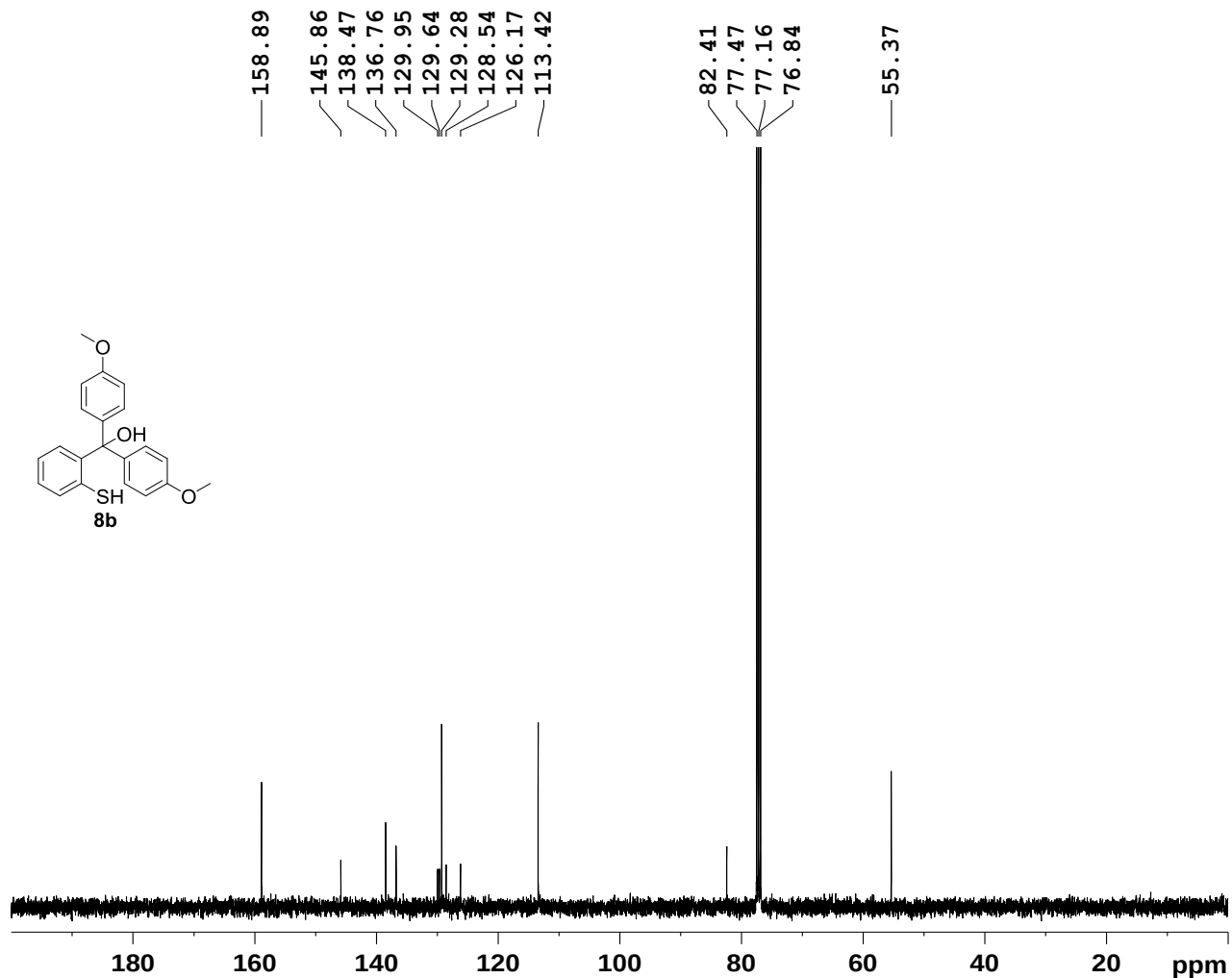
F2 - Acquisition Parameters
 Date_ 20190123
 Time 15.09
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 32
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 287
 DW 60.800 usec
 DE 6.00 usec
 TE 294.2 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.35 usec
 PL1 -1.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300045 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure 115: ¹H-NMR spectra for compound **8b**

C13CPD CDC13 {D:\CRR} nmr 1



Current Data Parameters
NAME MK-MM-26
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190123
Time_ 15.11
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 45.2
DW 20.800 usec
DE 6.00 usec
TE 294.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

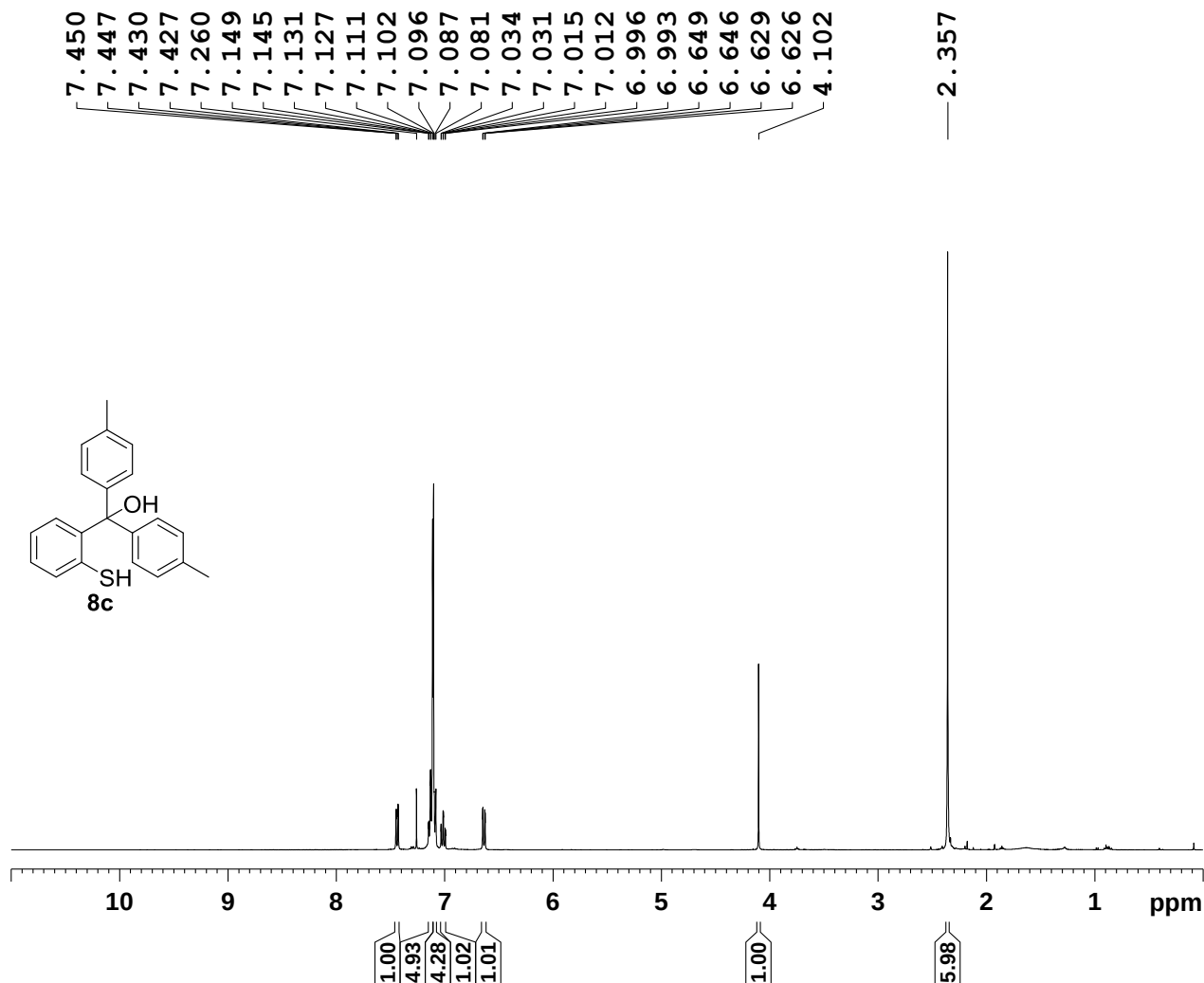
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127564 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 116: ^{13}C -NMR spectra for compound **8b**

PROTON CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters

NAME MK-MM-27
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

Date 20190614
Time 14.50
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 322
DW 60.800 usec
DE 6.00 usec
TE 295.0 K
D1 1.00000000 sec
TD0 1

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

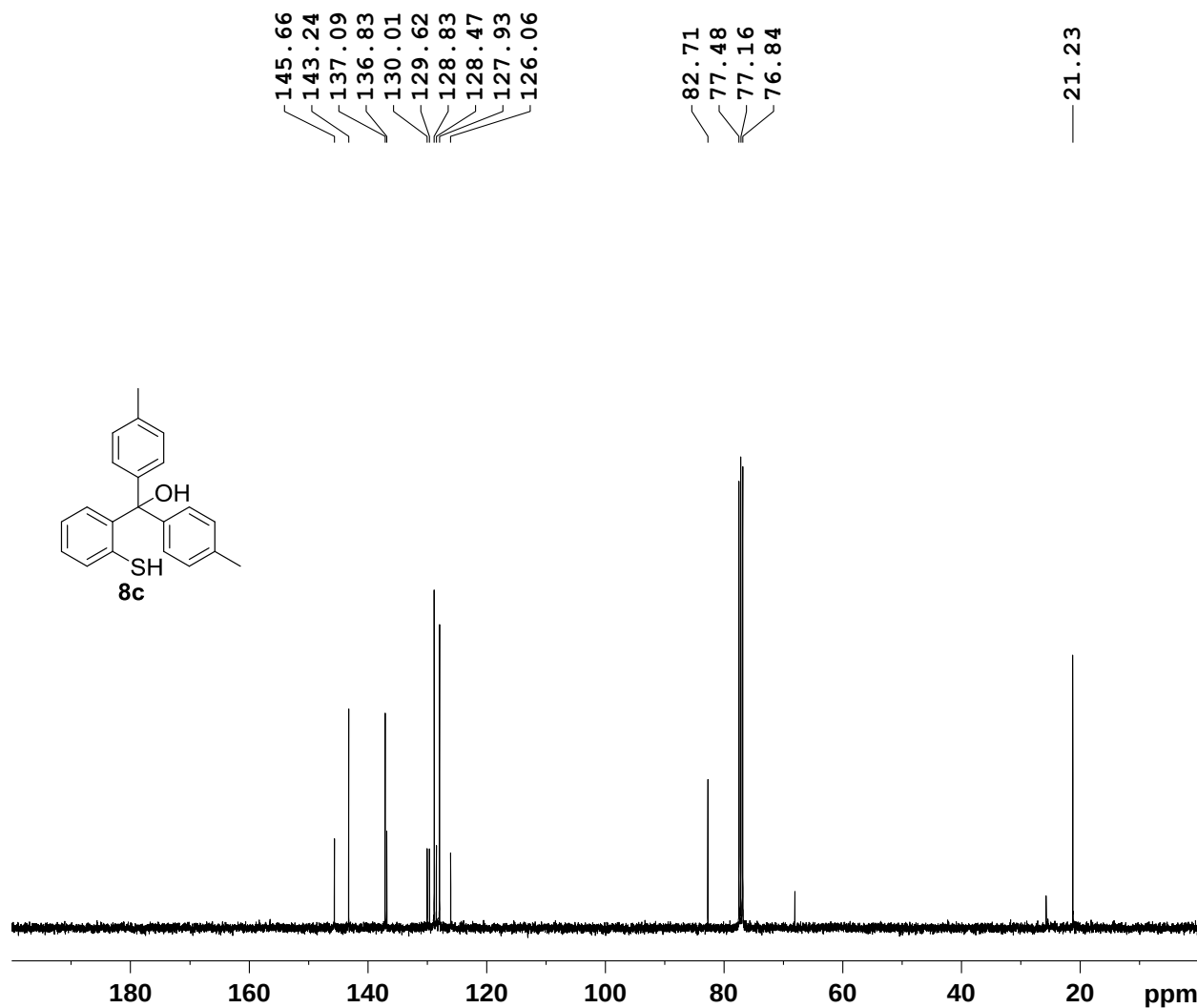
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters

SI 32768
SF 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 117: ¹H-NMR spectra for compound **8c**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-MM-27
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190616
Time 15.10
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 40.3
DW 20.800 usec
DE 6.00 usec
TE 294.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

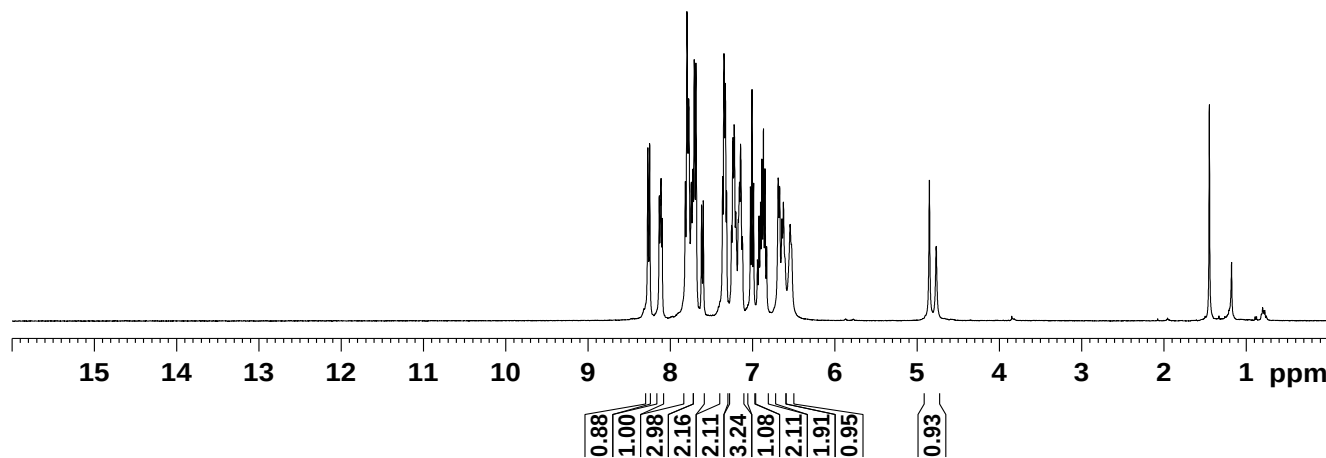
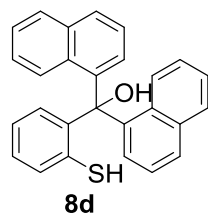
F2 - Processing parameters
SI 32768
SF 100.6127620 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 118: ^{13}C -NMR spectra for compound **8c**

PROP31DEC CDC13 {D:\CRR} CIF_NMR 1



8.271
8.250
8.132
8.119
8.111
8.098
7.816
7.795
7.775
7.743
7.723
7.708
7.687
7.618
7.597
7.363
7.345
7.332
7.314
7.236
7.222
7.202
7.172
7.156
7.145
7.024
7.005
6.985
6.920
6.901
6.885
6.866
6.847
6.687
6.669
6.642
6.623
4.850



Current Data Parameters
NAME MK-III-445-A
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190911
Time_ 15.48
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgig
TD 32768
SOLVENT CDC13
NS 16
DS 2
SWH 8333.333 Hz
FIDRES 0.254313 Hz
AQ 1.9660800 sec
RG 114
DW 60.000 usec
DE 6.00 usec
TE 294.6 K
D1 1.00000000 sec
d11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1325018 MHz

===== CHANNEL f2 =====
CPDPRG[2] garp
NUC2 31P
PCPD2 100.00 usec
PL12 120.00 dB
PL2 0 dB
SFO2 161.9760648 MHz

F2 - Processing parameters
SI 32768
SF 400.1300548 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 119: ¹H-NMR spectra for compound **8d**

PROP31DEC CDC13 {D:\CRR} CIF_NMR 1

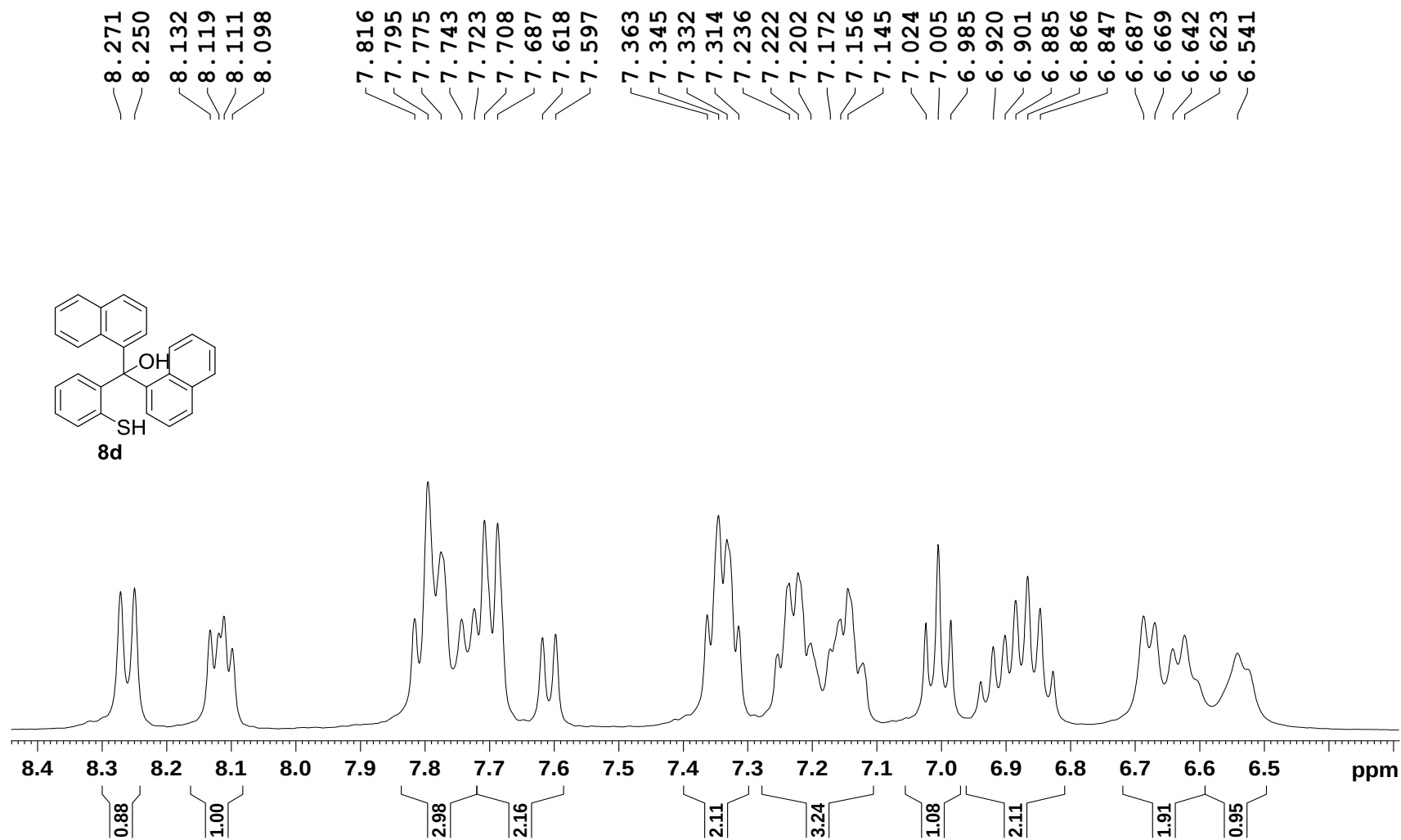
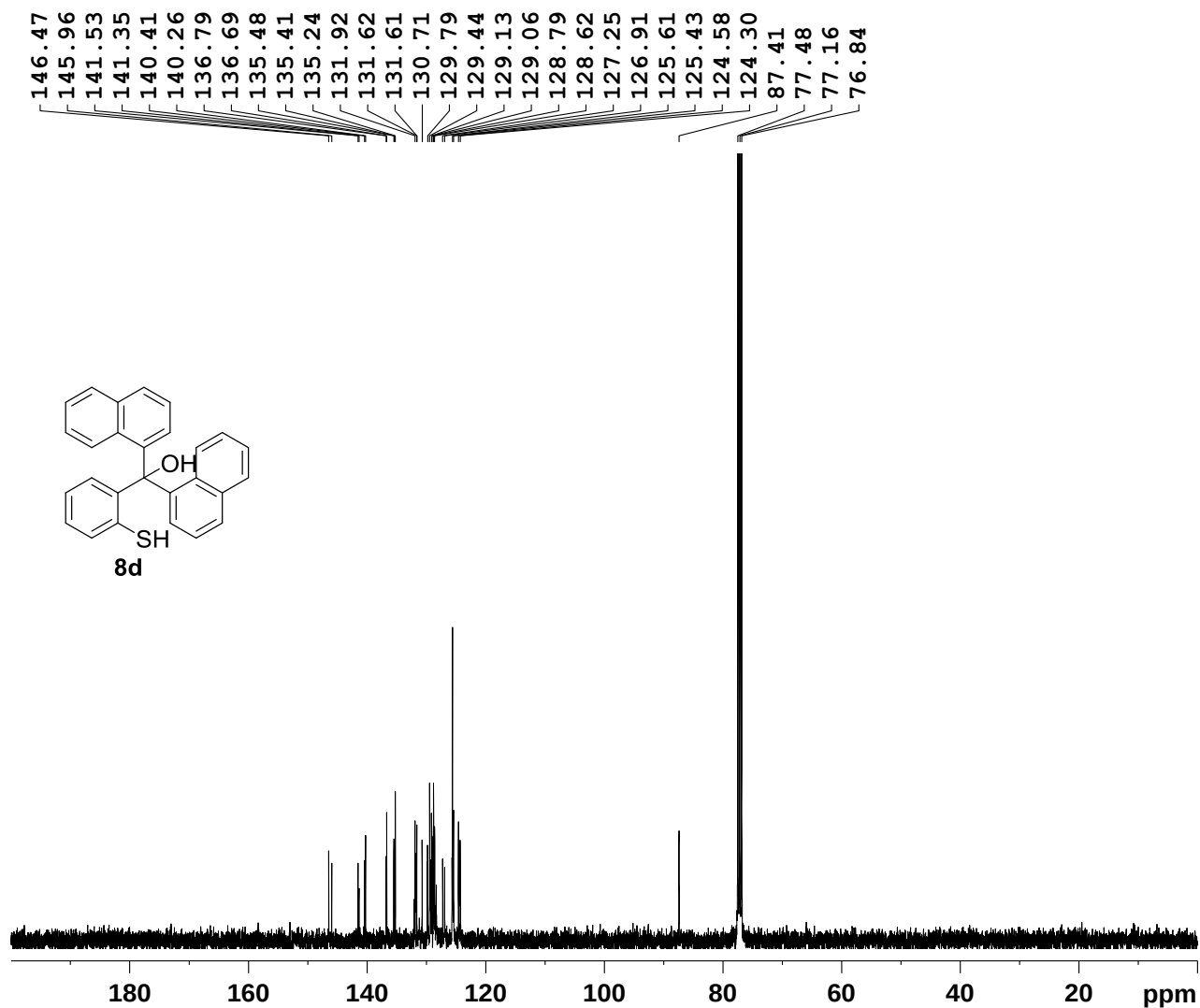


Figure 119a: ¹H-NMR spectra expansion for compound **8d**



Current Data Parameters
 NAME MK-III-445-A
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190911
 Time_ 22.37
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zgpg30
 TD 65536
 SOLVENT CDC13
 NS 602
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 322
 DW 20.800 usec
 DE 6.00 usec
 TE 298.8 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 ^{13}C
 P1 9.95 usec
 PL1 -1.00 dB
 SFO1 100.6228298 MHz

===== CHANNEL f2 =====
 CPDPRG[2] waltz16
 NUC2 ^1H
 PCPD2 90.00 usec
 PL12 14.95 dB
 PL13 120.00 dB
 PL2 -1.00 dB
 SFO2 400.1316005 MHz

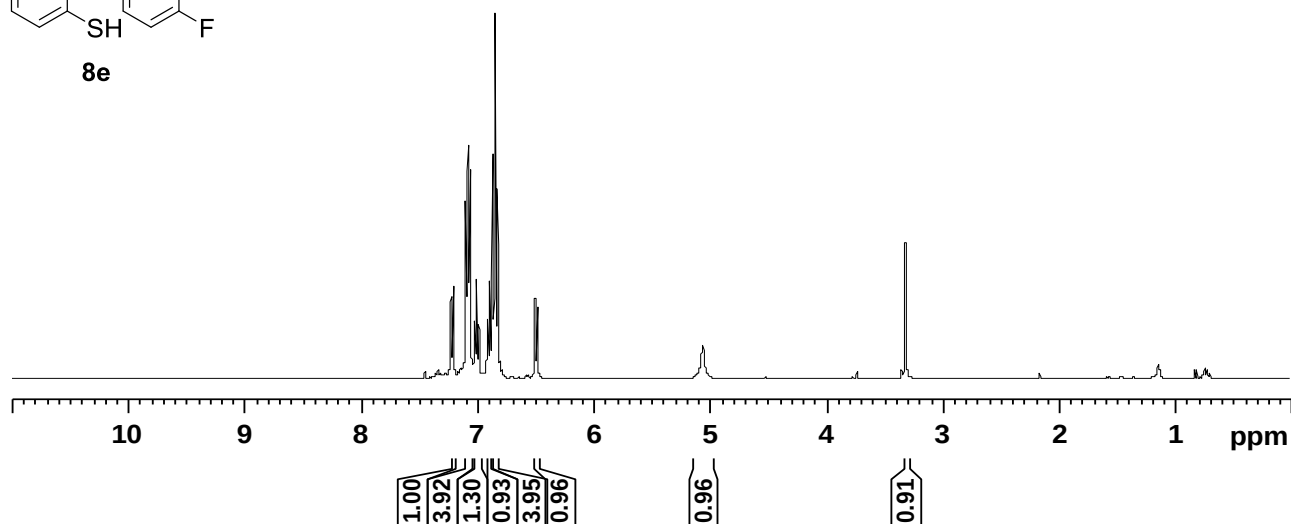
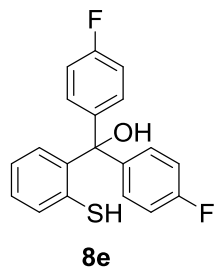
F2 - Processing parameters
 SI 32768
 SF 100.6127587 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

Figure 120: ^{13}C -NMR spectra for compound **8d**

PROTON CDC13 {D:\CRR} CIF_NMR 1



7.220
7.218
7.201
7.199
7.093
7.088
7.079
7.071
7.063
7.057
7.020
7.016
7.001
6.998
6.982
6.979
6.910
6.907
6.891
6.889
6.863
6.858
6.842
6.825
6.820
6.500
6.497
6.480
6.477
5.057
3.313



Current Data Parameters
NAME MK-III-448-A
EXPNO 1
PROCNO 1

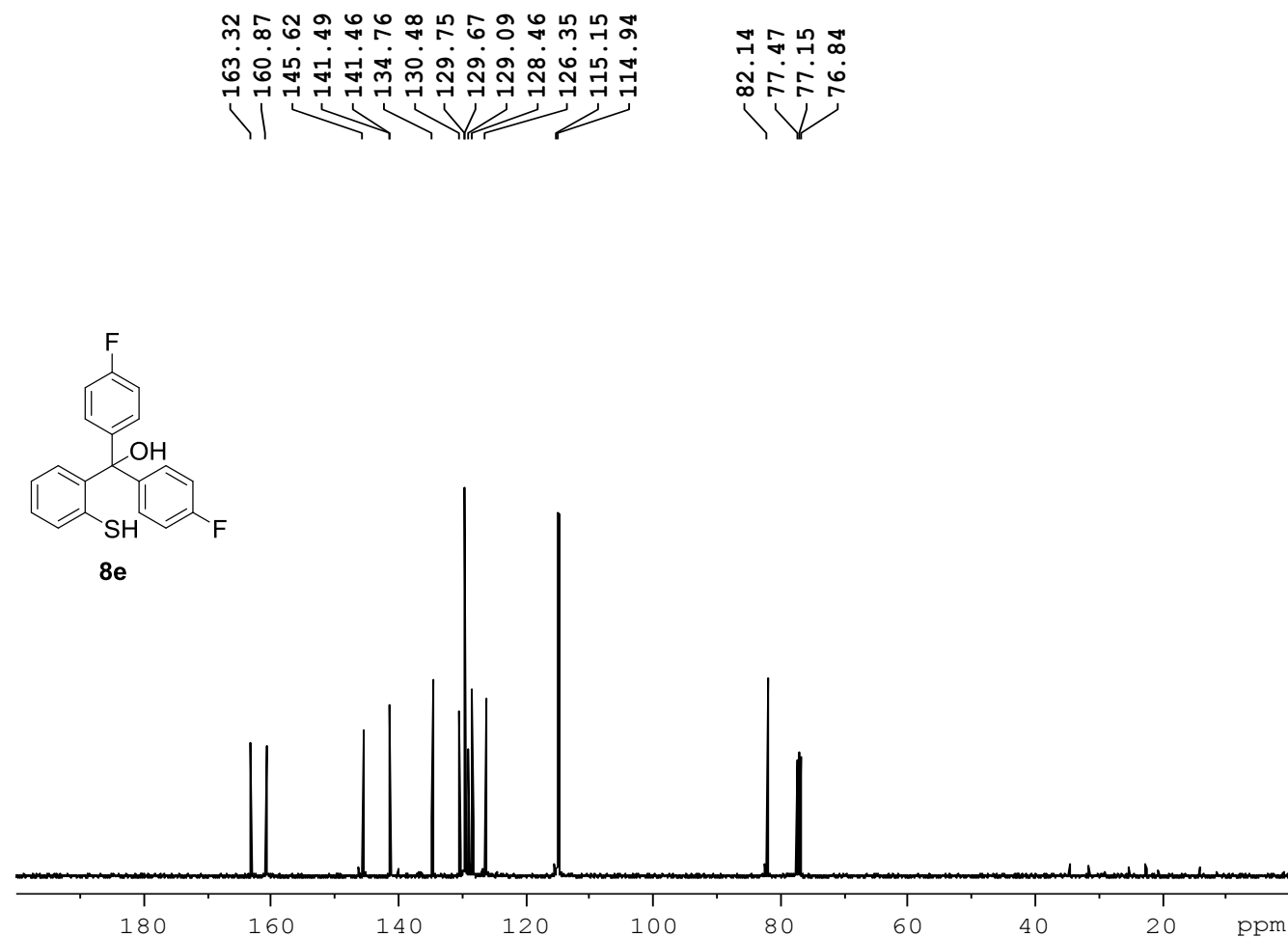
F2 - Acquisition Parameters
Date_ 20190910
Time 10.51
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9845889 sec
RG 45.2
DW 60.800 usec
DE 6.00 usec
TE 296.5 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 14.35 usec
PL1 -1.00 dB
SFO1 400.1324710 MHz

F2 - Processing parameters
SI 32768
SF 400.1300934 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 121: ^1H -NMR spectra for compound **8e**

C13CPD CDC13 {D:\CRR} CIF_NMR 1



Current Data Parameters
NAME MK-III-448-A
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190910
Time 11.07
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 406
DW 20.800 usec
DE 6.00 usec
TE 296.7 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

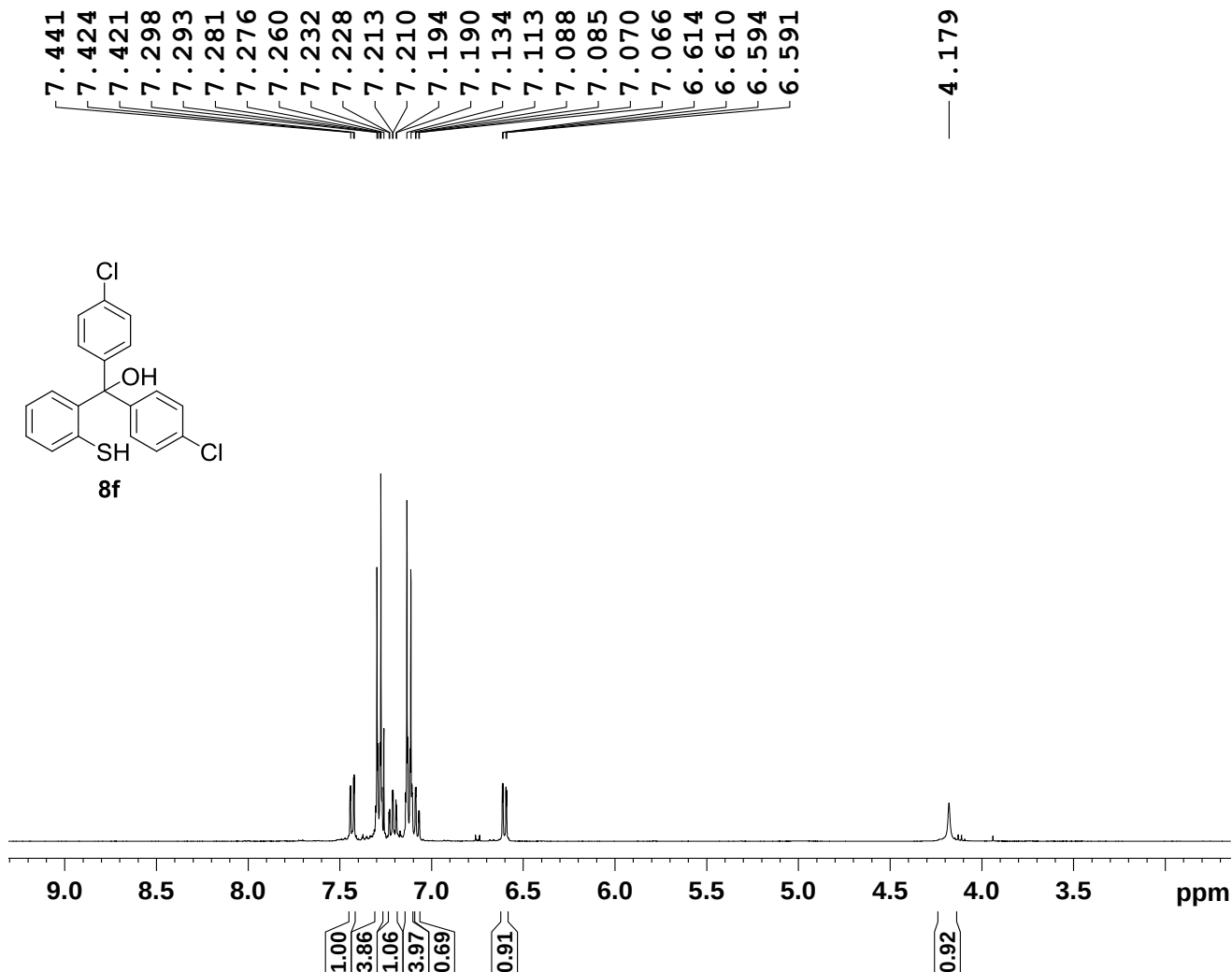
===== CHANNEL f1 =====
NUC1 13C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127741 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 122: ¹³C-NMR spectra for compound **8e**

PROTON CDCl3 {D:\CRR} CIF_NMR 1



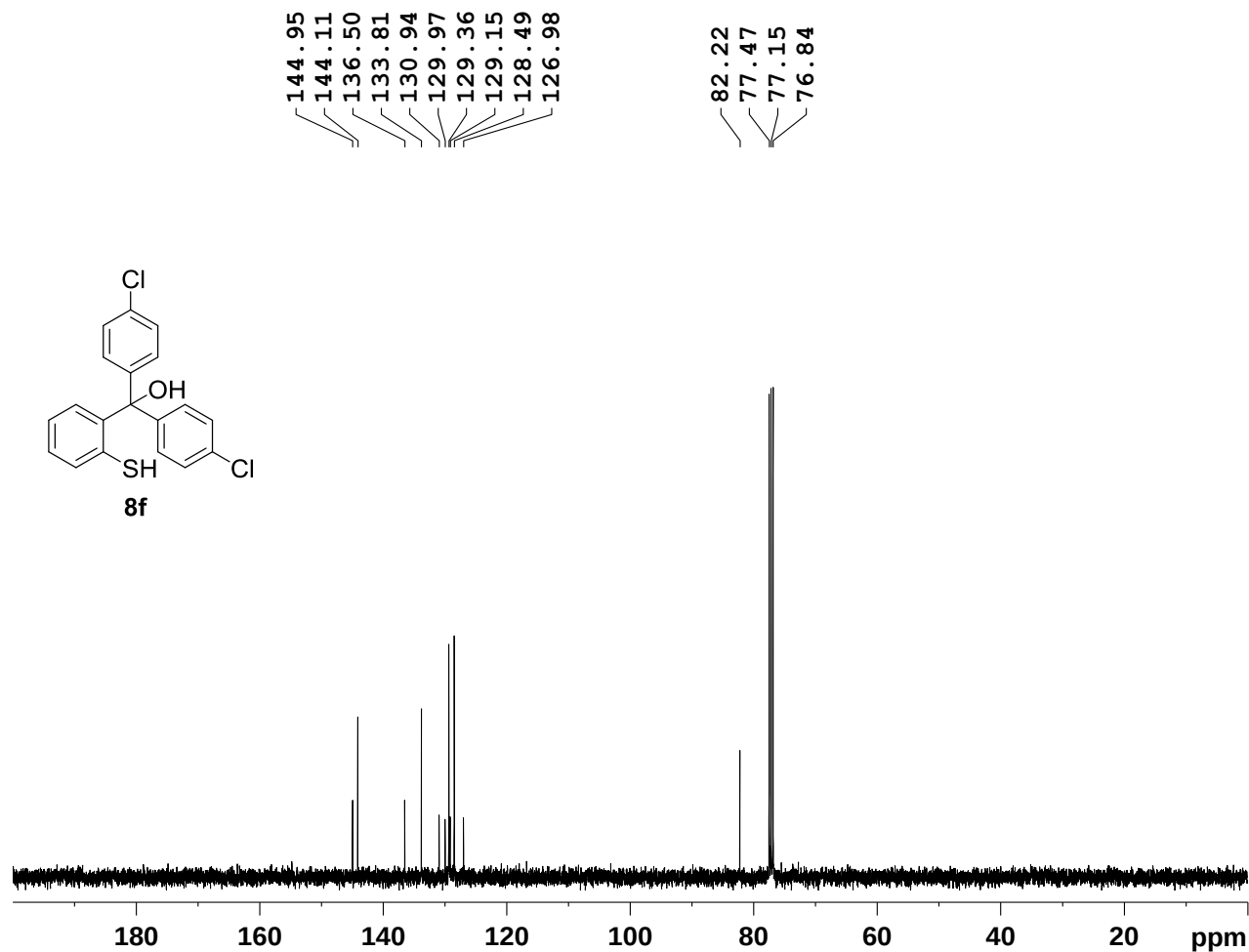
Current Data Parameters
 NAME MK-II-423-N
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20190612
 Time 12.47
 INSTRUM spect
 PROBHD 5 mm BBO BB-1H
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 16
 DS 2
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9845889 sec
 RG 362
 DW 60.800 usec
 DE 6.00 usec
 TE 295.1 K
 D1 1.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 14.35 usec
 PL1 -1.00 dB
 SFO1 400.1324710 MHz

F2 - Processing parameters
 SI 32768
 SF 400.1300095 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure 123: ¹H-NMR spectra for compound **8f**



Current Data Parameters
NAME MK-II-423-N
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20190614
Time 14.57
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 196
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 40.3
DW 20.800 usec
DE 6.00 usec
TE 295.2 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

===== CHANNEL f1 =====
NUC1 ^{13}C
P1 9.95 usec
PL1 -1.00 dB
SFO1 100.6228298 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 ^1H
PCPD2 90.00 usec
PL12 14.95 dB
PL13 120.00 dB
PL2 -1.00 dB
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127586 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

Figure 124: ^{13}C -NMR spectra for compound **8f**

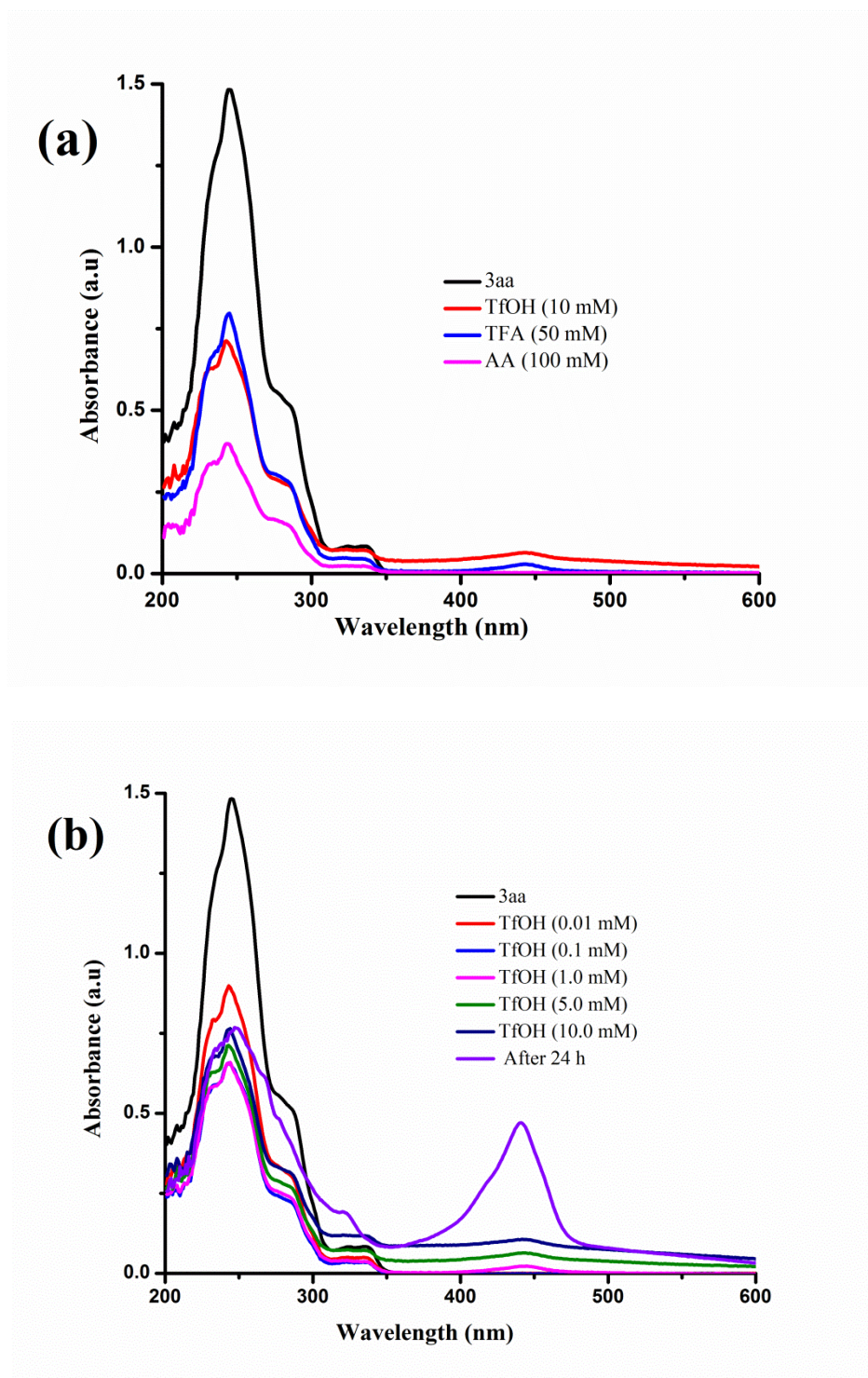


Fig. S1. (a) Absorption spectra of **3aa** in different acid medium (b) Absorption spectra of **3aa** with various concentration of TfOH in CHCl_3

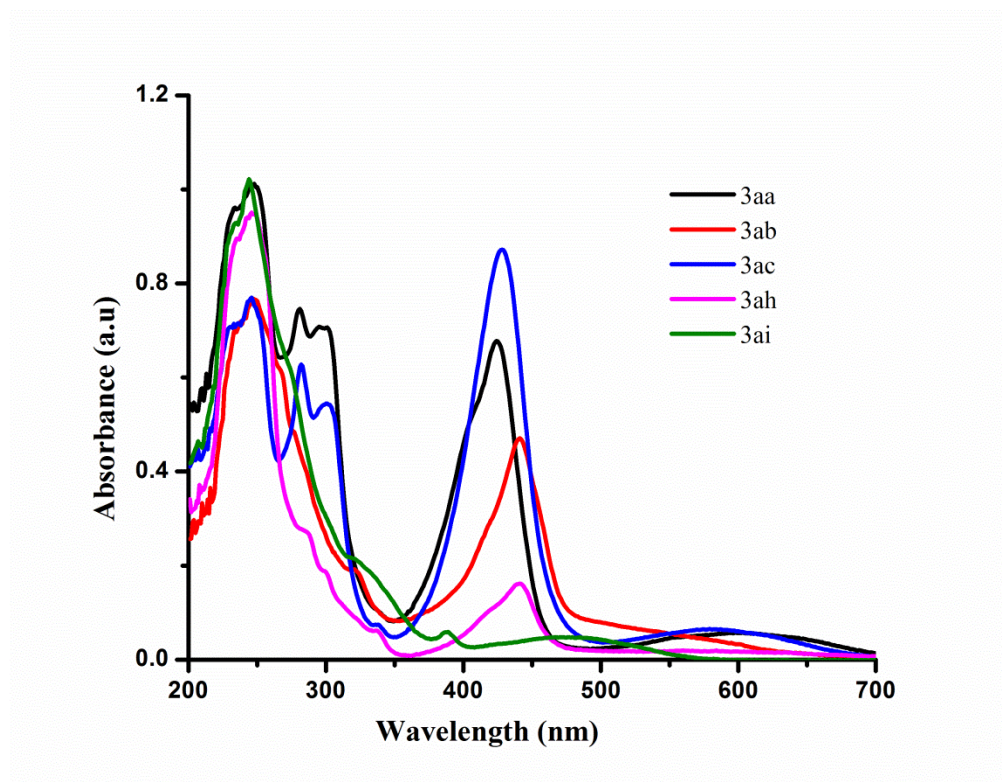


Fig. S2. Absorption spectra of **3aa**, **3ab**, **3ac**, **3ah**, and **3ai** with TfOH in CHCl_3

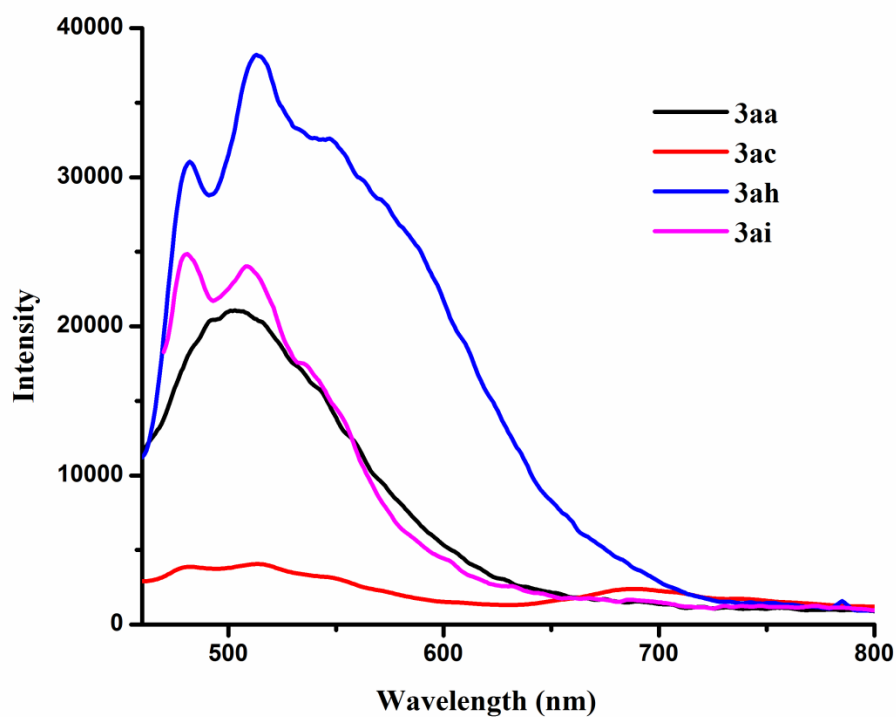


Fig. S3. Fluorescence spectra of **3aa**, **3ac**, **3ah**, and **3i** with TfOH in CHCl_3

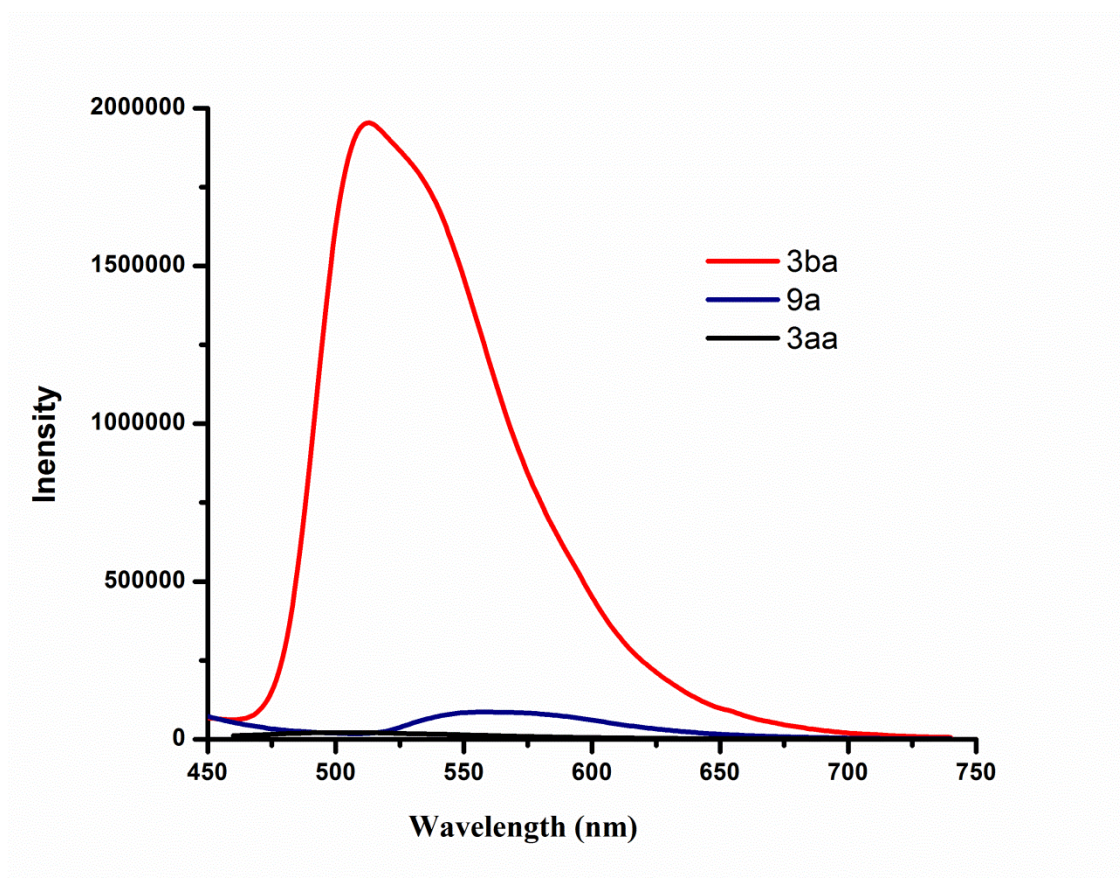


Fig. S4. Fluorescence spectra of **3a**, **11a**, and **13a** with TfOH in CHCl_3