

Supplementary data

Synthesis of Flavonols and Assessment of Their Biological Activities as Anticancer Agents

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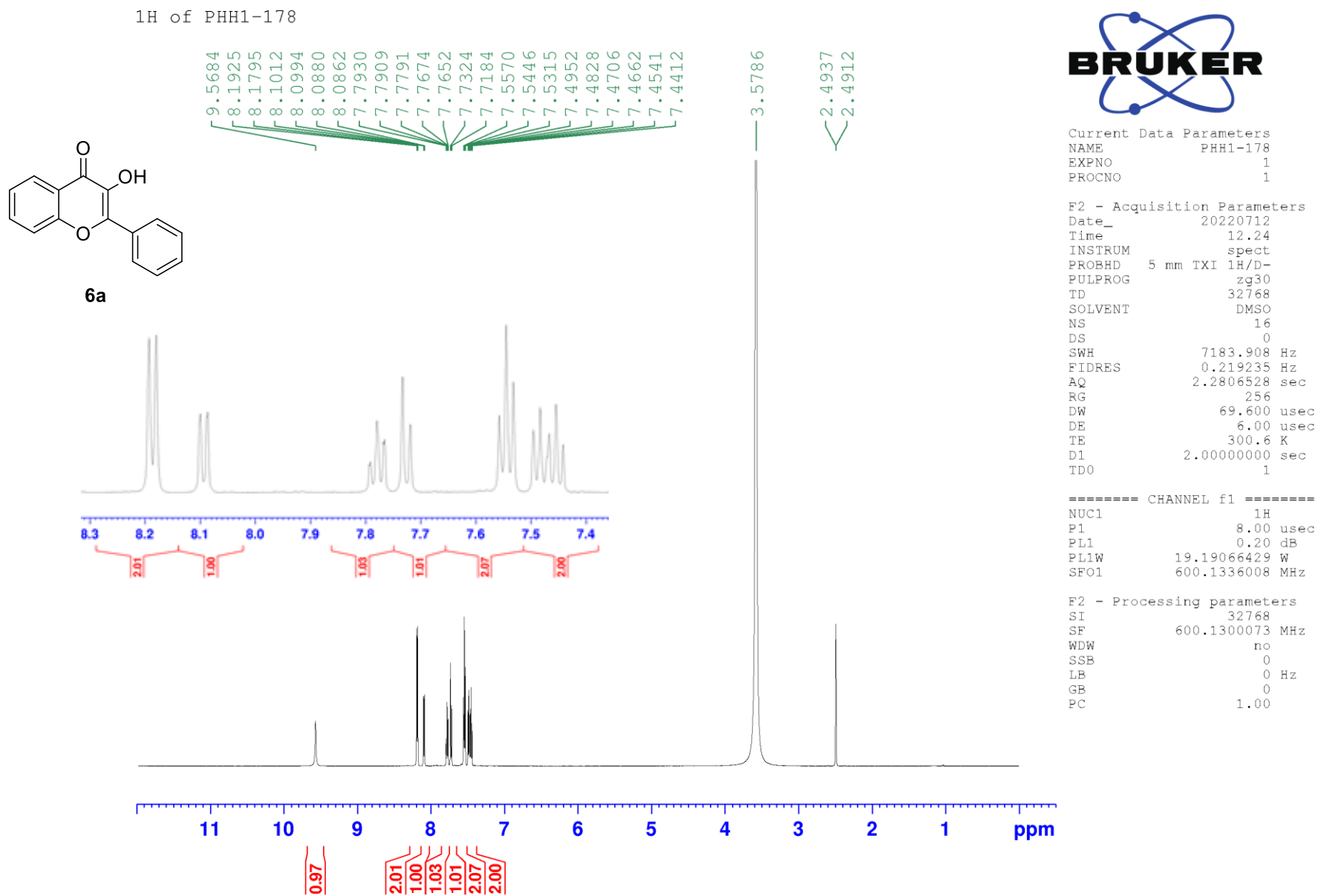
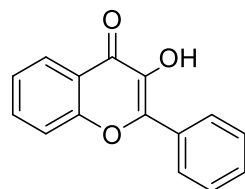
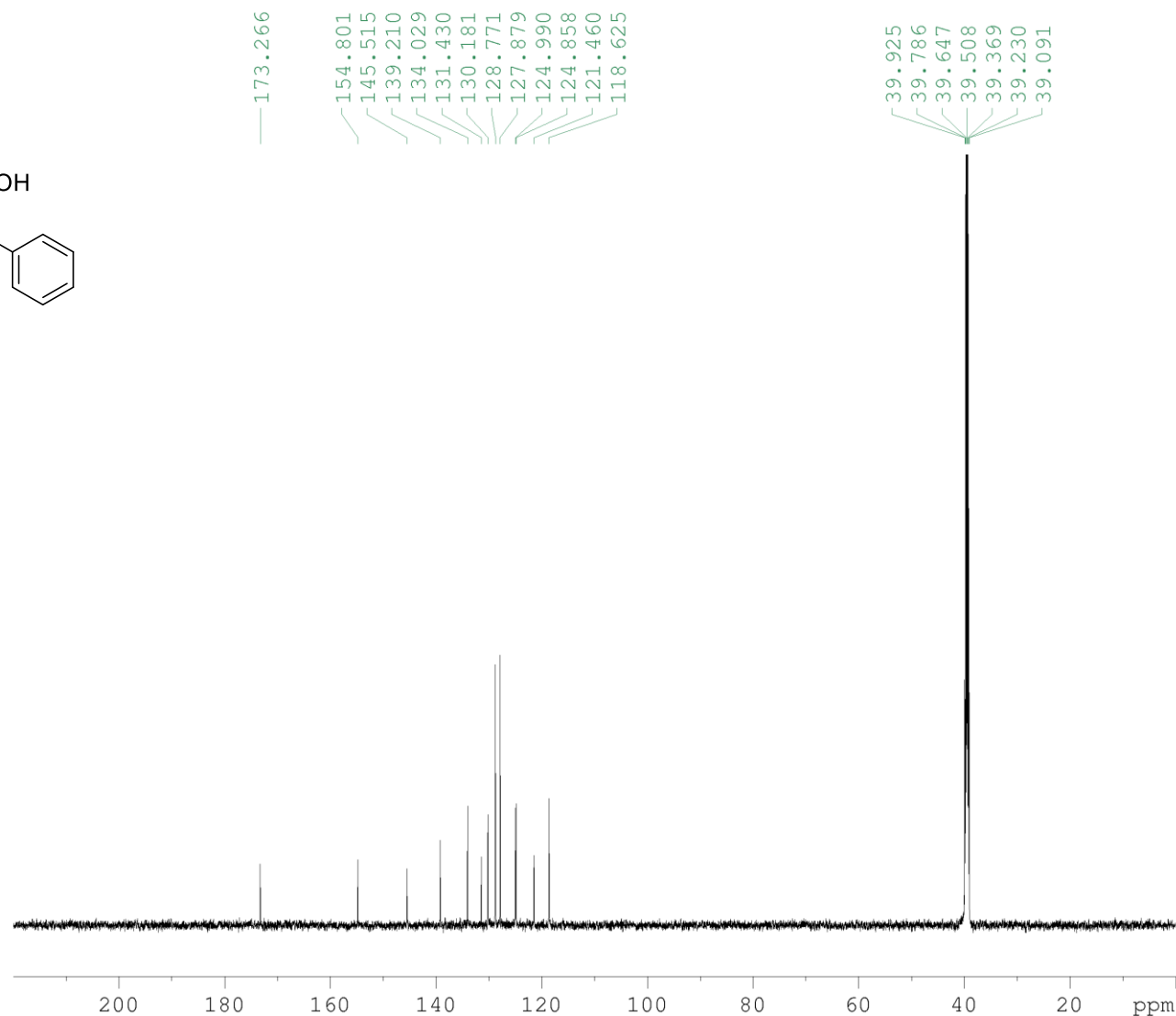


Figure S1. ¹H NMR (600 MHz, DMSO-*d*₆) for compound **6a**.

13C of PHH1-178



6a



Current Data Parameters
NAME PHH1-178
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220624
Time 13.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 200
DS 0
SWH 33333.332 Hz
FIDRES 0.508626 Hz
AQ 0.9830400 sec
RG 46300
DW 15.000 usec
DE 6.00 usec
TE 298.0 K
D1 2.40000010 sec
D11 0.03000000 sec
TD0 1

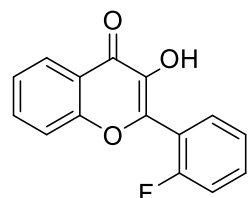
===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.60 dB
PL1W 136.15426636 W
SFO1 150.9194083 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.50 dB
PL12 13.20 dB
PL13 16.20 dB
PL2W 28.38507080 W
PL12W 0.96181160 W
PL13W 0.48204759 W
SFO2 600.1339008 MHz

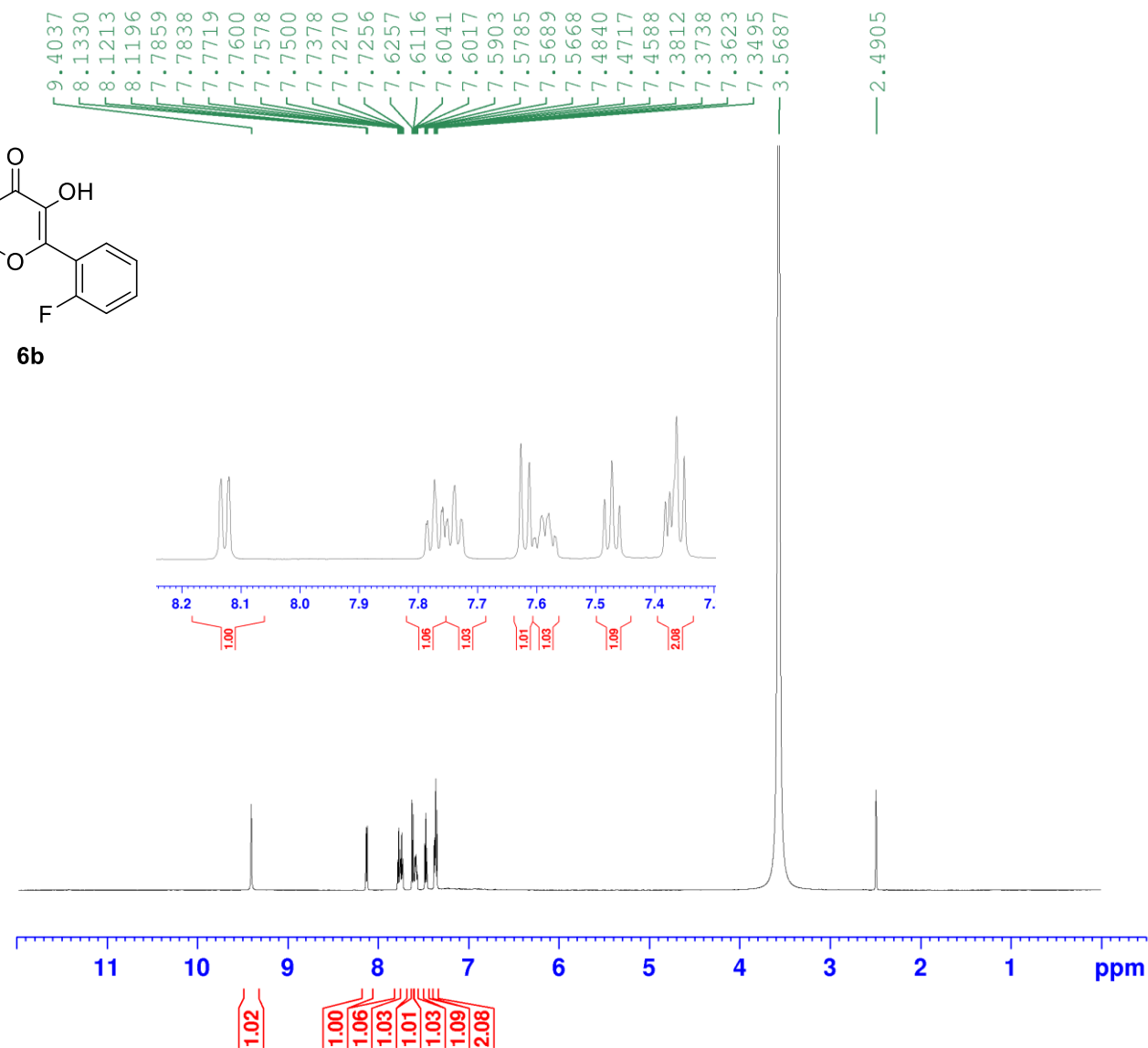
F2 - Processing parameters
SI 32768
SF 150.9028448 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

Figure S2. ^{13}C NMR (150 MHz, $\text{DMSO-}d_6$) for compound **6a**.

¹H of PHH1-205



6b



Current Data Parameters
NAME PHH1-205
EXPNO 1
PROCNO 1

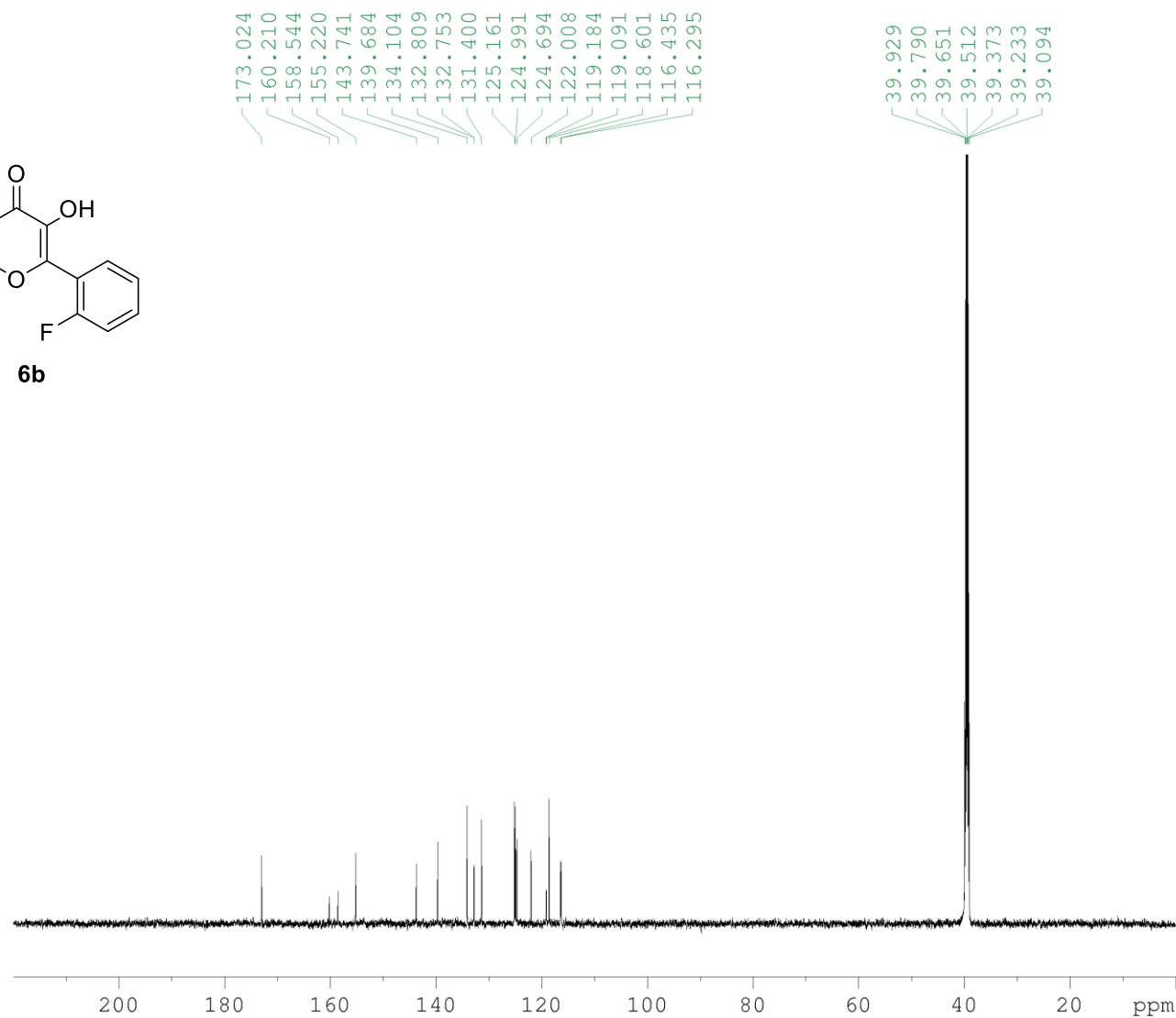
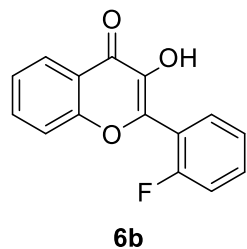
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INSTRUM spect
PROBHD 5 mm TXI 1H/D-
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 16
DS 0
SWH 7183.908 Hz
FIDRES 0.219235 Hz
AQ 2.2806528 sec
RG 161
DW 69.600 usec
DE 6.00 usec
TE 300.9 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.00 usec
PL1 0.20 dB
PL1W 19.19066429 W
SFO1 600.1336008 MHz

F2 - Processing parameters
SI 32768
SF 600.1300073 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

Figure S3. ¹H NMR (600 MHz, DMSO-*d*₆) for compound **6b**.

13C of PHH1-205



Current Data Parameters
NAME PHH1-205
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220624
Time 13.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 215
DS 0
SWH 33333.332 Hz
FIDRES 0.508626 Hz
AQ 0.9830400 sec
RG 46300
DW 15.000 usec
DE 6.00 usec
TE 298.1 K
D1 2.40000010 sec
D11 0.03000000 sec
TD0 1

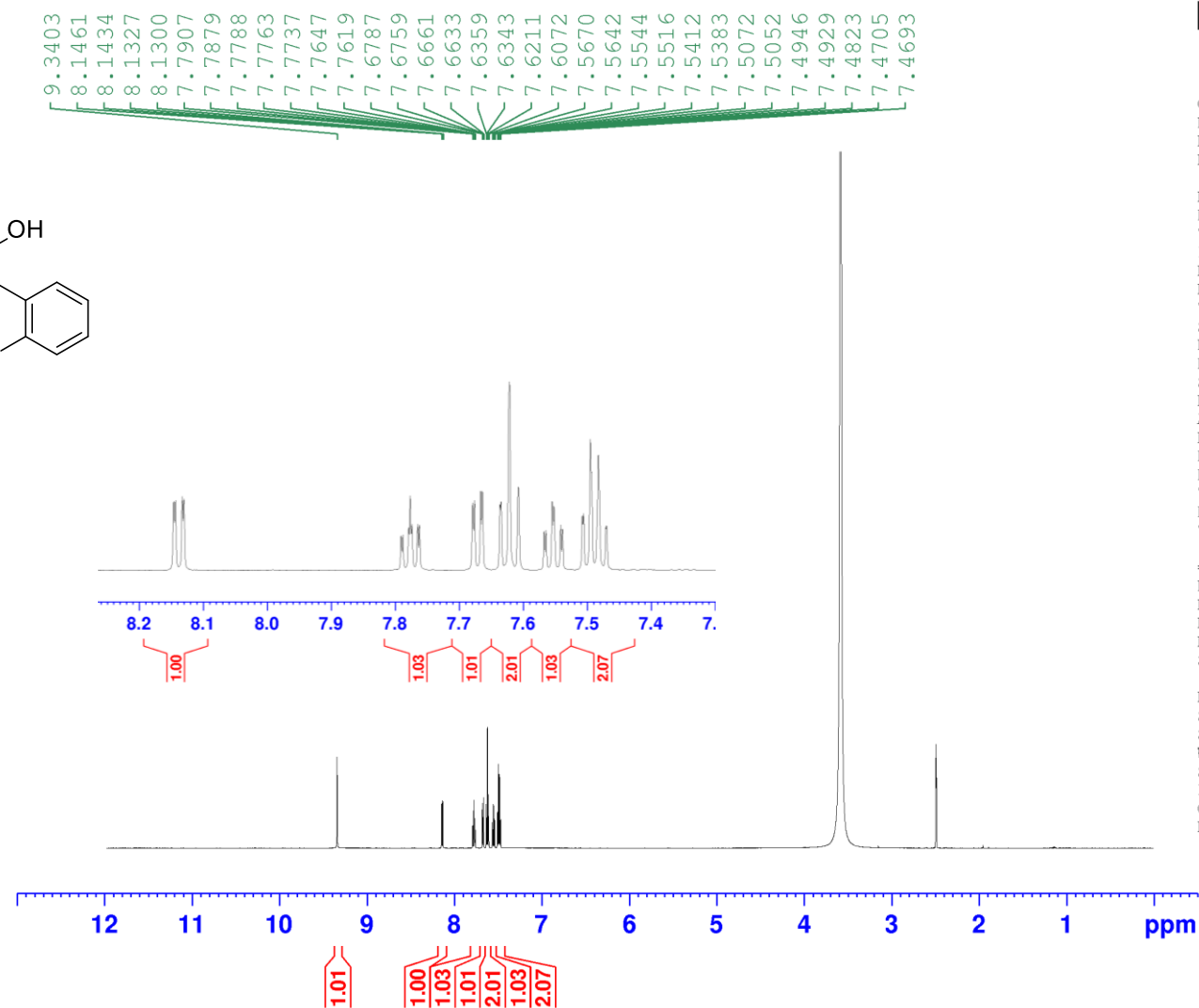
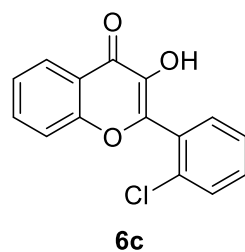
===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.60 dB
PL1W 136.15426636 W
SFO1 150.9194083 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.50 dB
PL12 13.20 dB
PL13 16.20 dB
PL2W 28.38507080 W
PL12W 0.96181160 W
PL13W 0.48204759 W
SFO2 600.1339008 MHz

F2 - Processing parameters
SI 32768
SF 150.9028448 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

Figure S4. ^{13}C NMR (150 MHz, $\text{DMSO-}d_6$) for compound **6b**.

¹H of PHH1-209



Current Data Parameters
NAME PHH1-209
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221012
Time 8.14
INSTRUM spect
PROBHD 5 mm TXI 1H/D-
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 16
DS 0
SWH 7183.908 Hz
FIDRES 0.219235 Hz
AQ 2.2806528 sec
RG 114
DW 69.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.00 usec
PL1 0.20 dB
PL1W 19.19066429 W
SFO1 600.1336008 MHz

F2 - Processing parameters
SI 32768
SF 600.1300073 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

Figure S5. ¹H NMR (600 MHz, DMSO-*d*₆) for compound **6c**.

13C of PHH1-209

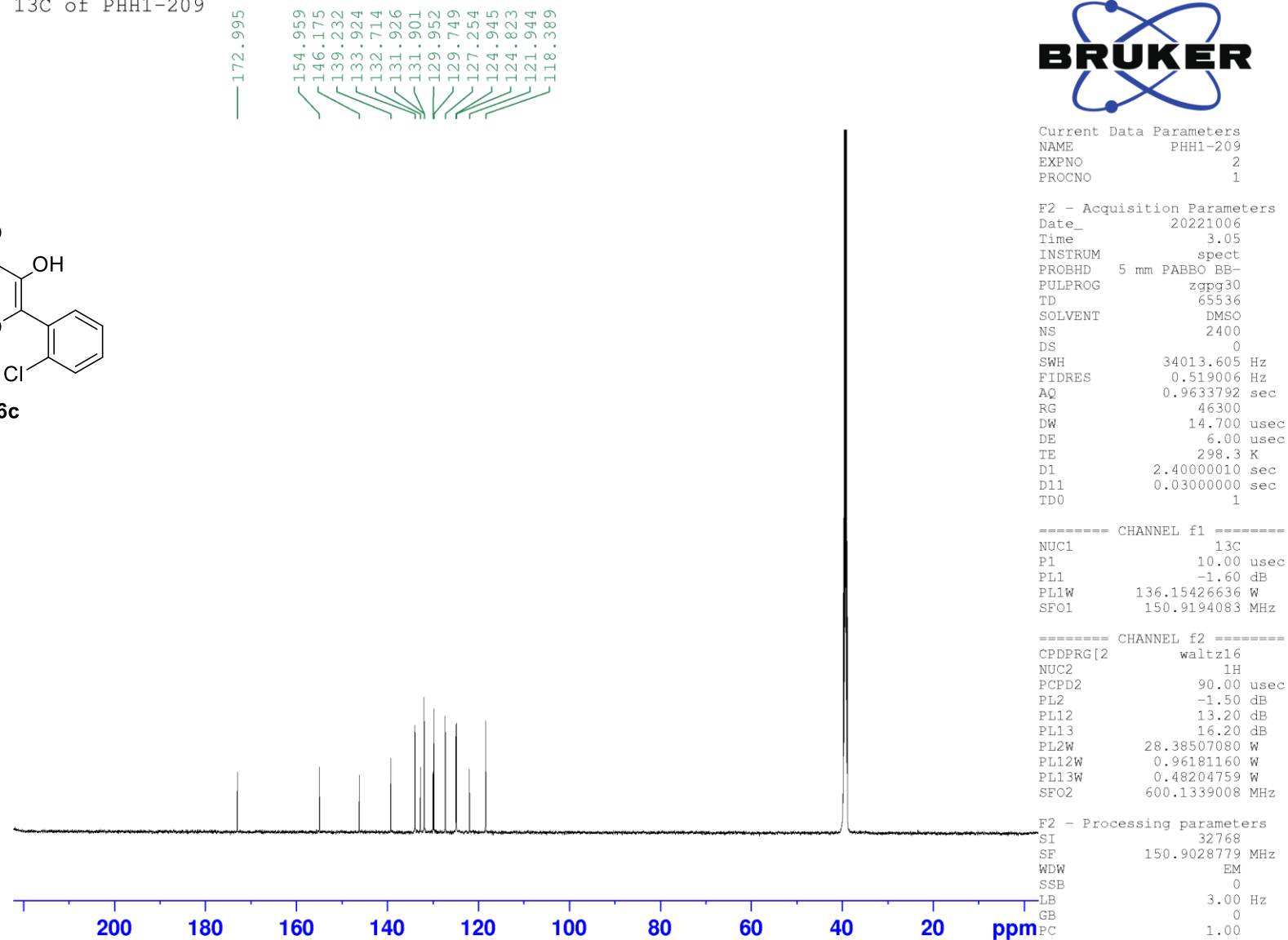
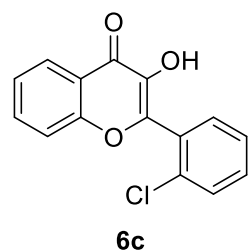


Figure S6. ^{13}C NMR (150 MHz, $\text{DMSO}-d_6$) for compound **6c**.

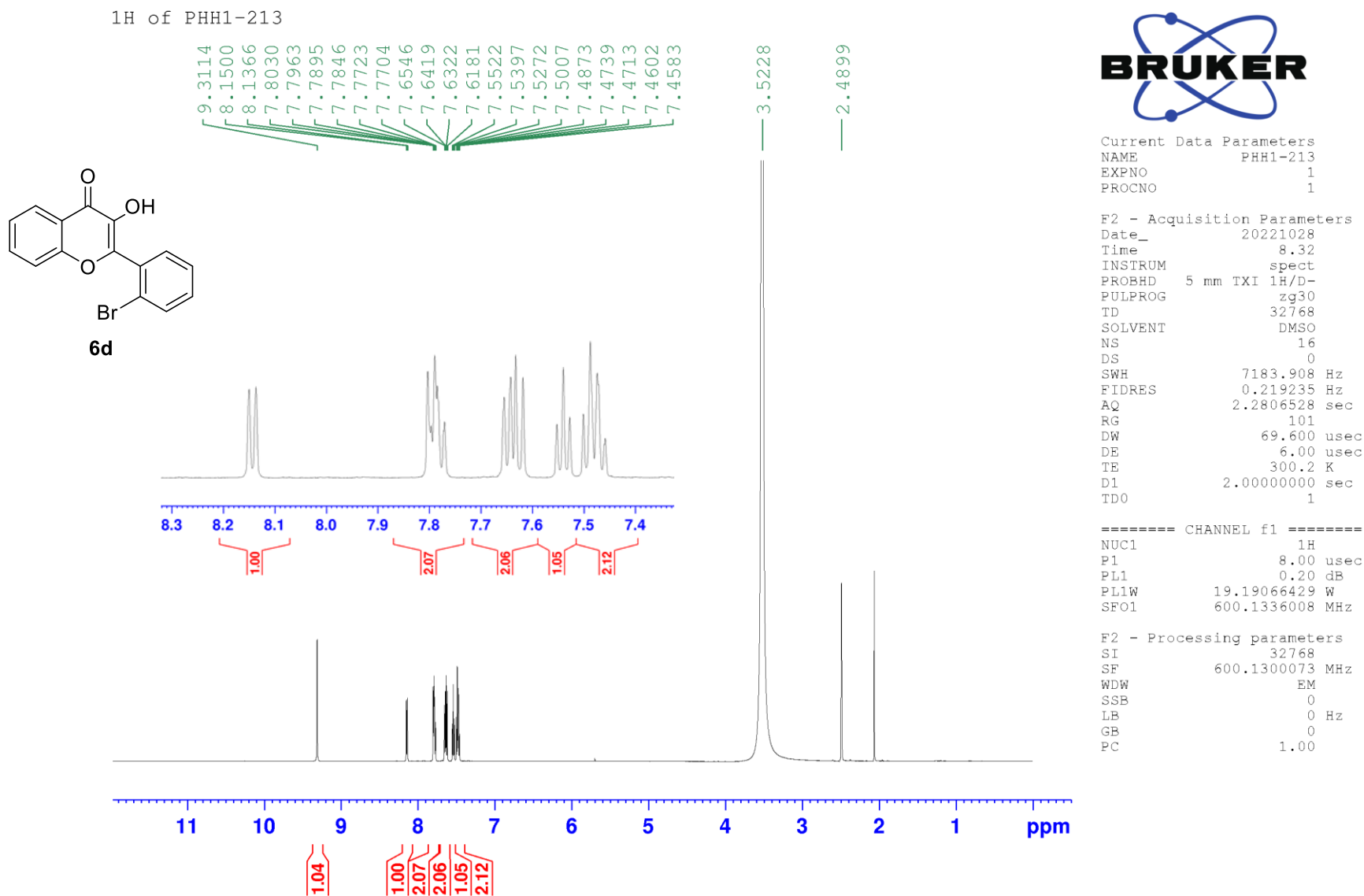


Figure S7. ^1H NMR (600 MHz, $\text{DMSO-}d_6$) for compound **6d**.

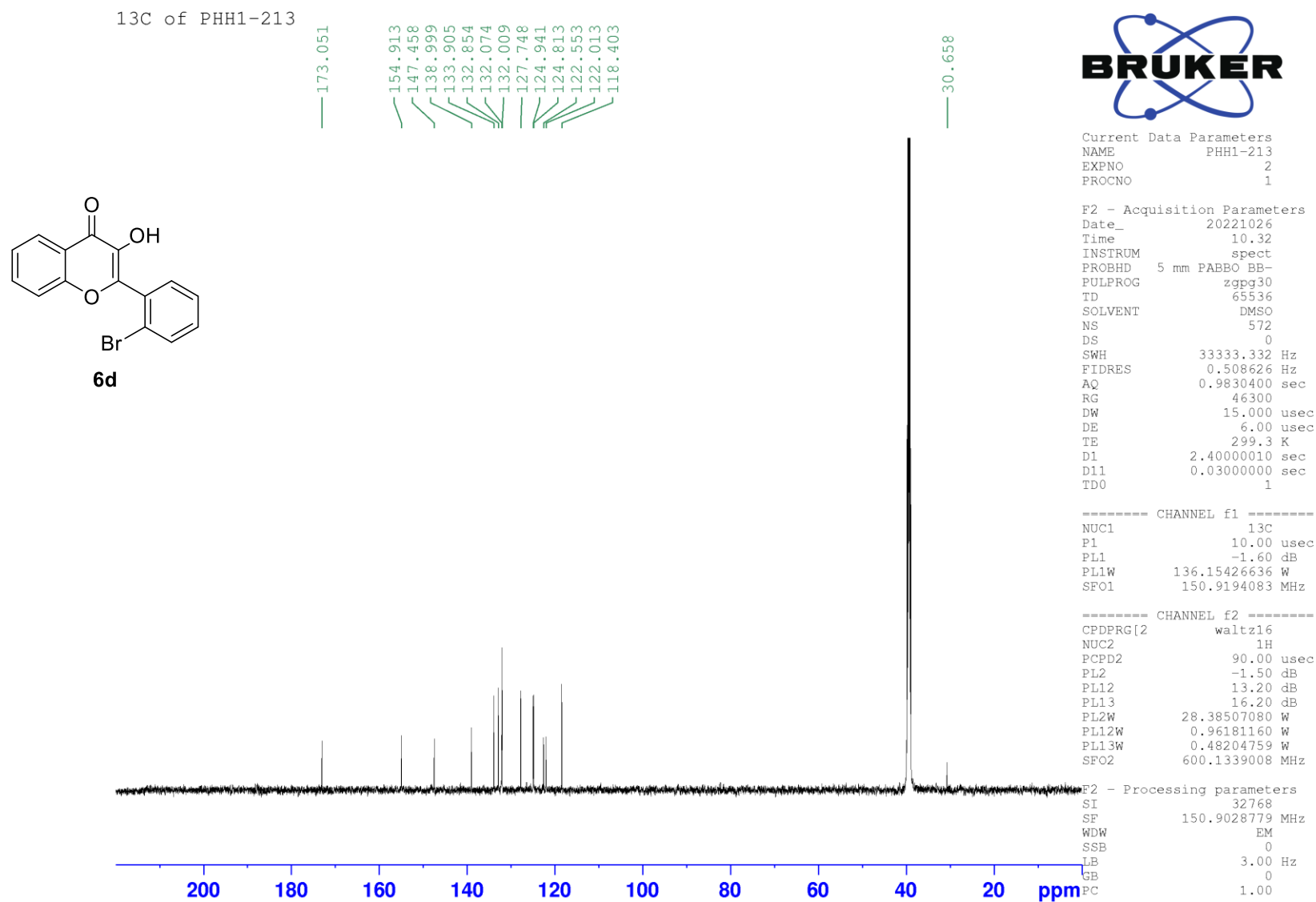
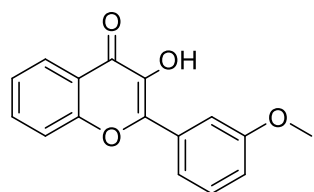
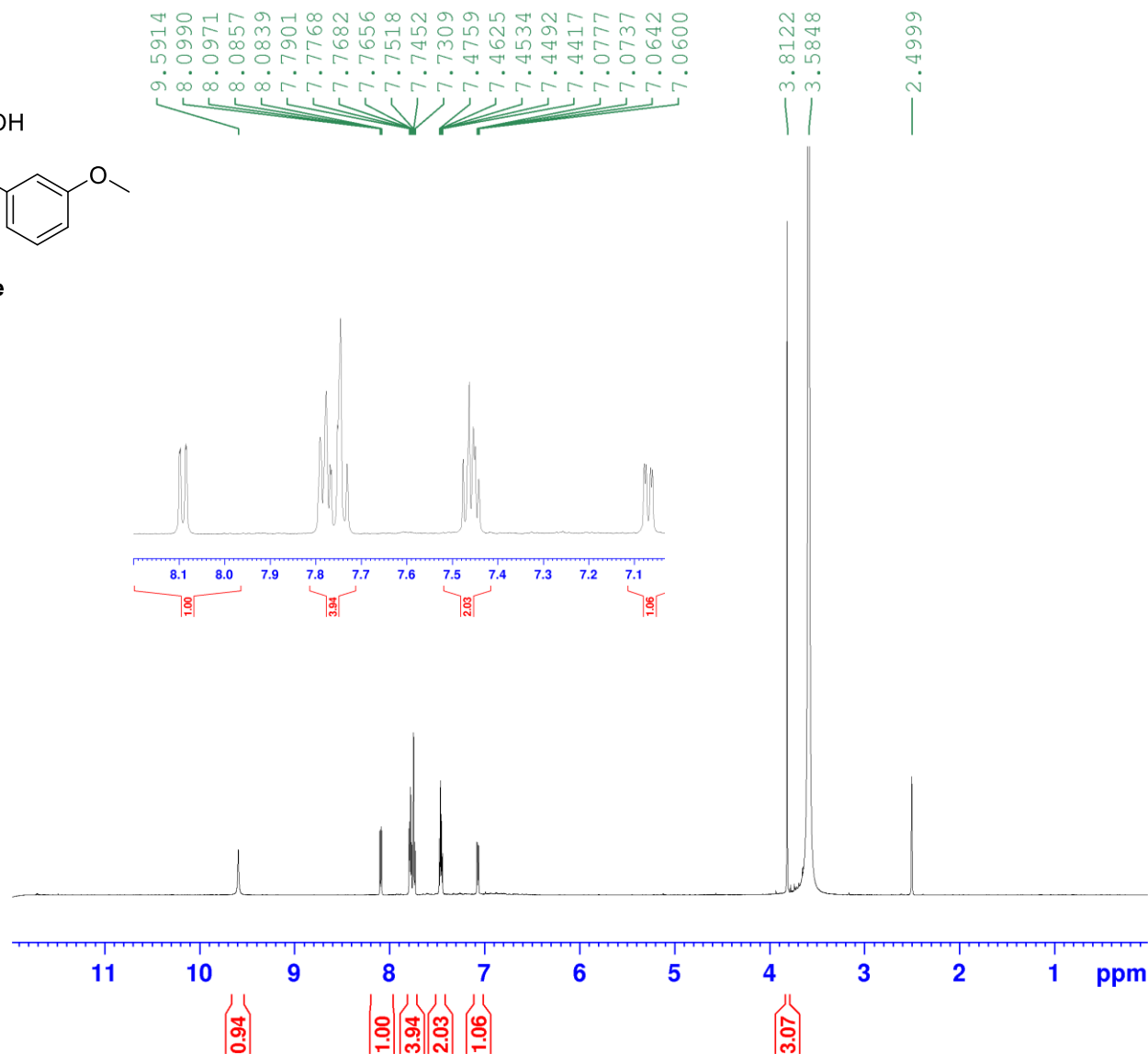


Figure S8. ^{13}C NMR (150 MHz, $\text{DMSO-}d_6$) for compound **6d**.

¹H of PHH1-217



6e



Current Data Parameters
NAME PHH1-217
EXPNO 1
PROCNO 1

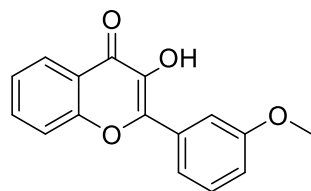
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Time 15.36
INSTRUM spect
PROBHD 5 mm TXI 1H/D-
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 16
DS 0
SWH 7183.908 Hz
FIDRES 0.219235 Hz
AQ 2.2806528 sec
RG 724
DW 69.600 usec
DE 6.00 usec
TE 301.4 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.00 usec
PL1 0.20 dB
PL1W 19.19066429 W
SFO1 600.1336008 MHz

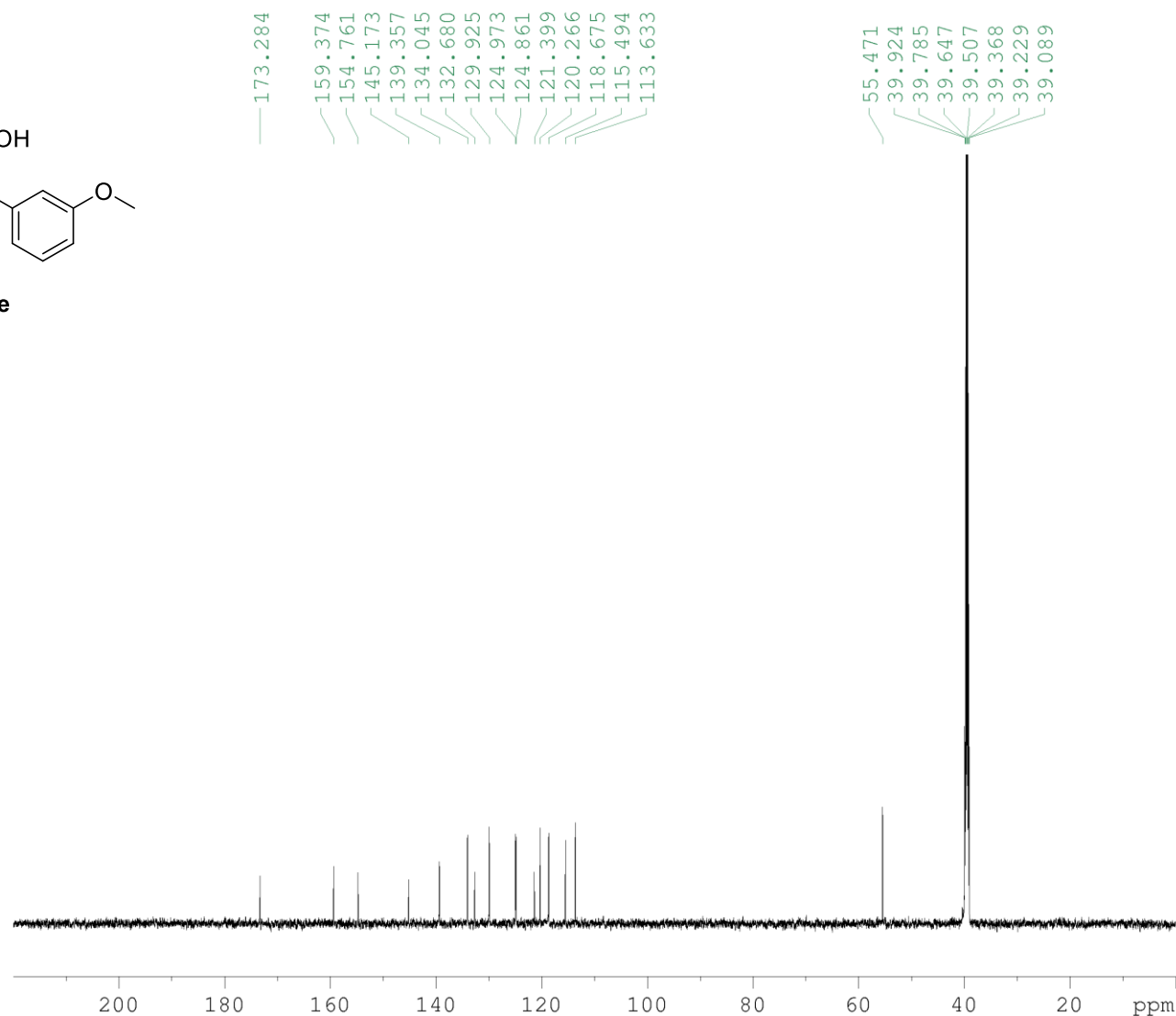
F2 - Processing parameters
SI 32768
SF 600.1300015 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

Figure S9. ¹H NMR (600 MHz, DMSO-*d*₆) for compound **6e**.

13C of PHH1-217



6e



Current Data Parameters
NAME PHH1-217
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220817
Time 14.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 152
DS 0
SWH 33333.332 Hz
FIDRES 0.508626 Hz
AQ 0.9830400 sec
RG 46300
DW 15.000 usec
DE 6.00 usec
TE 298.3 K
D1 2.40000010 sec
D11 0.03000000 sec
TD0 1

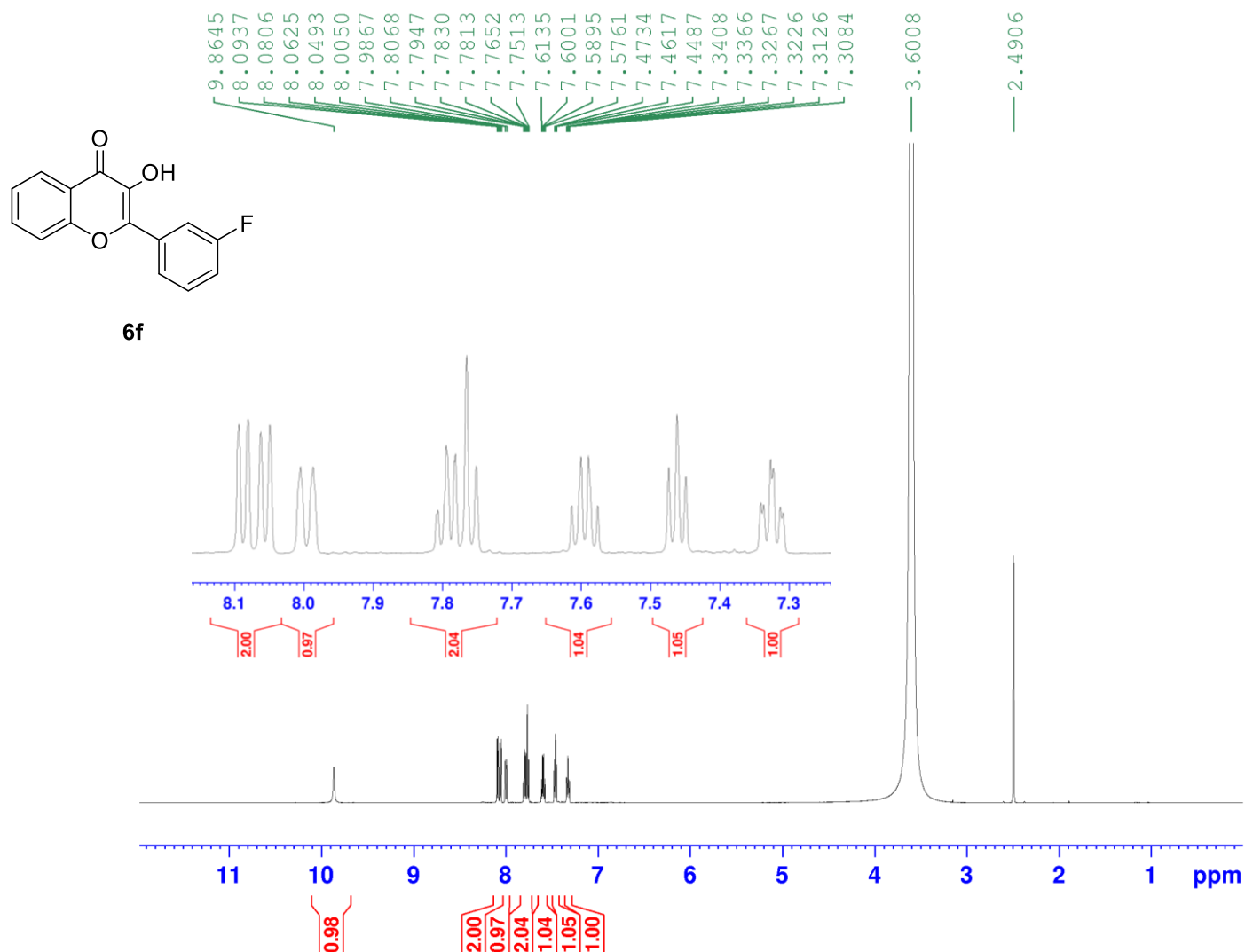
===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.60 dB
PL1W 136.15426636 W
SFO1 150.9194083 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.50 dB
PL12 13.20 dB
PL13 16.20 dB
PL2W 28.38507080 W
PL12W 0.96181160 W
PL13W 0.48204759 W
SFO2 600.1339008 MHz

F2 - Processing parameters
SI 32768
SF 150.9028423 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

Figure S10. ^{13}C NMR (150 MHz, $\text{DMSO}-d_6$) for compound **6e**.
S13

¹H of PHH1-204



Current Data Parameters
NAME PHH1-204
EXPNO 1
PROCNO 1

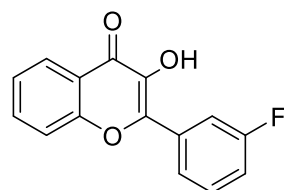
F2 - Acquisition Parameters
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Time 9.21
INSTRUM spect
PROBHD 5 mm TXI 1H/D-
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 16
DS 0
SWH 7183.908 Hz
FIDRES 0.219235 Hz
AQ 2.2806528 sec
RG 114
DW 69.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.00 usec
PL1 0.20 dB
PL1W 19.19066429 W
SFO1 600.1336008 MHz

F2 - Processing parameters
SI 32768
SF 600.1300073 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

Figure S11. ¹H NMR (600 MHz, DMSO-*d*₆) for compound **6f**.

13C of PHH1-204



6f

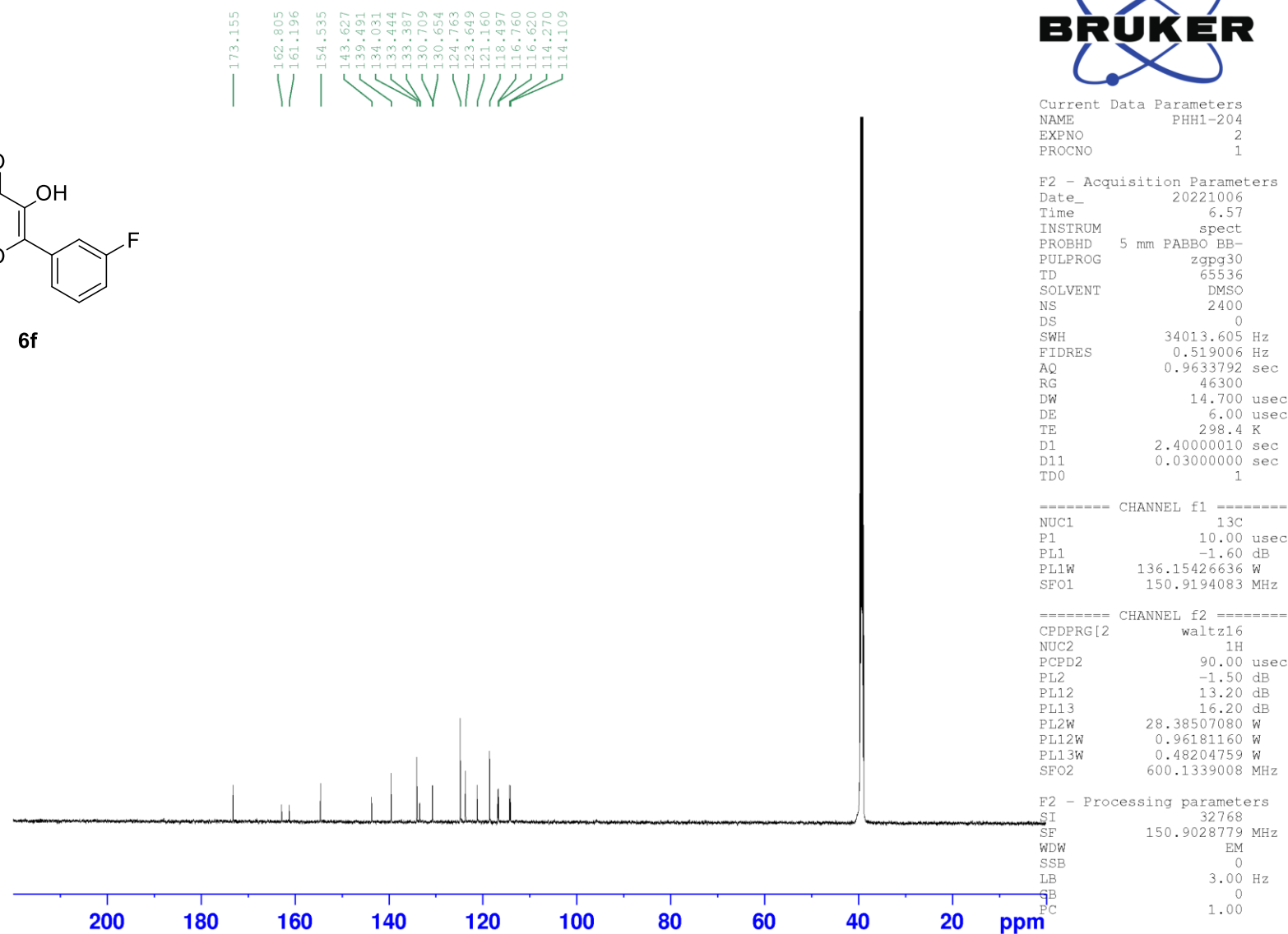
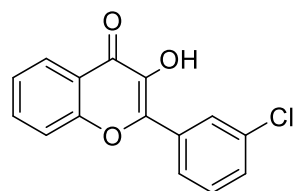
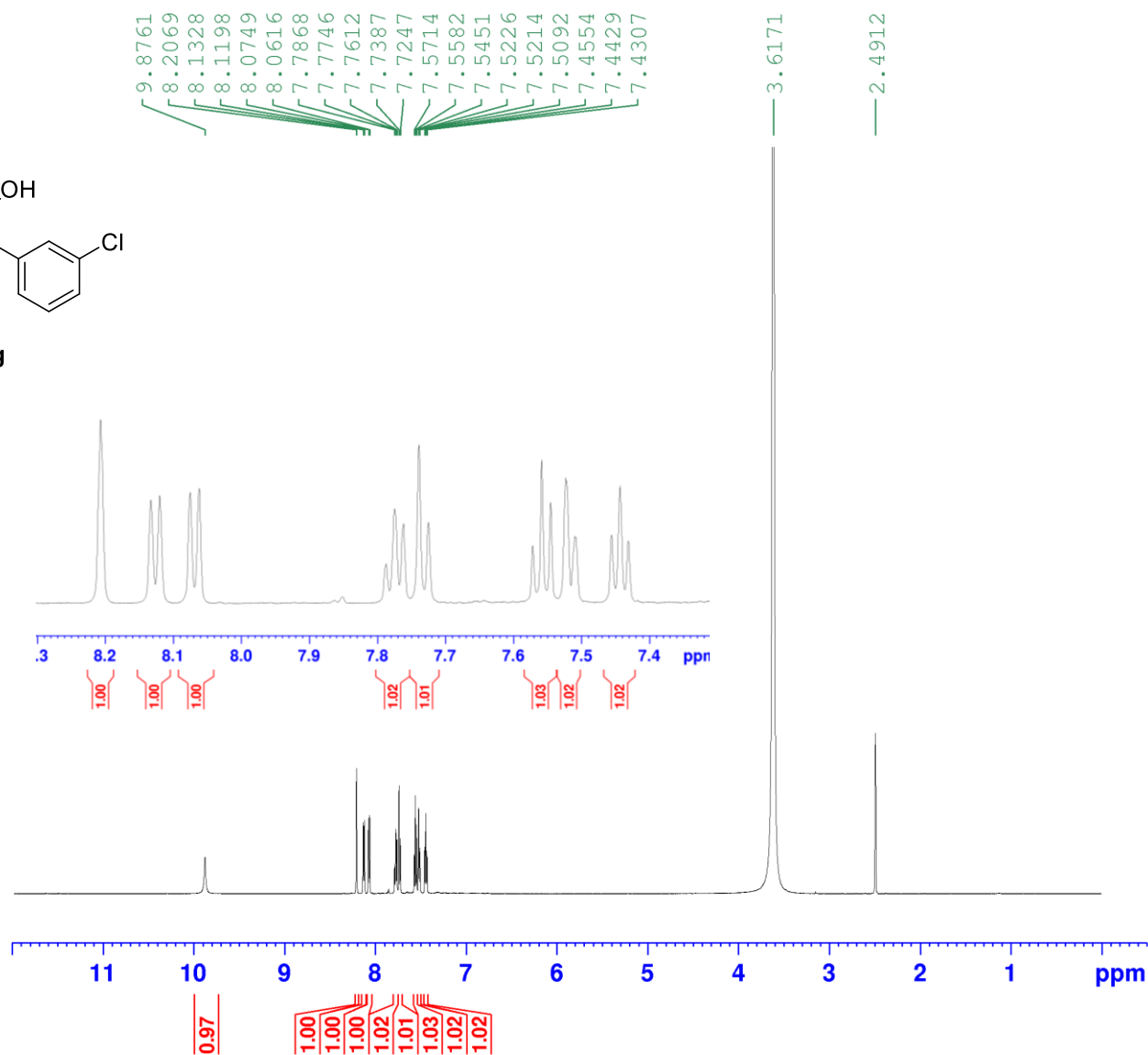


Figure S12. ^{13}C NMR (150 MHz, $\text{DMSO}-d_6$) for compound **6f**.

1H of PHH1-212



6g



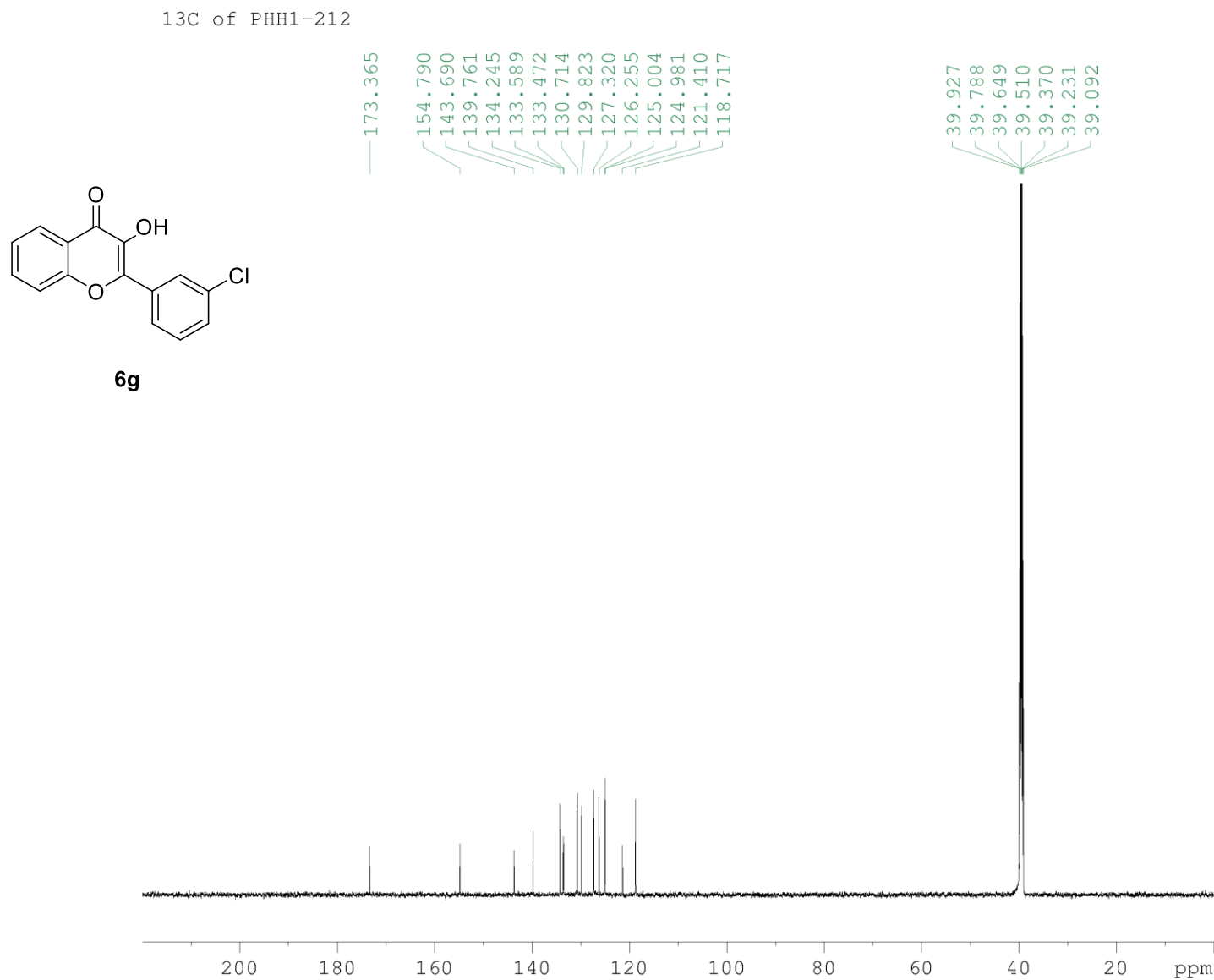
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NAME PHH1-212
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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INSTRUM spect
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PULPROG zg30
TD 32768
SOLVENT DMSO
NS 16
DS 0
SWH 7183.908 Hz
FIDRES 0.219235 Hz
AQ 2.2806528 sec
RG 724
DW 69.600 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.00 usec
PL1 0.20 dB
PL1W 19.19066429 W
SFO1 600.1336008 MHz

F2 - Processing parameters
SI 32768
SF 600.1300073 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

Figure S13. ¹H NMR (600 MHz, DMSO-*d*₆) for compound **6g**.



Current Data Parameters
NAME PHH1-212
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220725
Time 11.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 460
DS 0
SWH 36231.883 Hz
FIDRES 0.552855 Hz
AQ 0.9043968 sec
RG 46300
DW 13.800 usec
DE 6.00 usec
TE 299.9 K
D1 2.40000010 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.60 dB
PL1W 136.15426636 W
SFO1 150.9194083 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.50 dB
PL12 13.20 dB
PL13 16.20 dB
PL2W 28.38507080 W
PL12W 0.96181160 W
PL13W 0.48204759 W
SFO2 600.1339008 MHz

F2 - Processing parameters
SI 32768
SF 150.9028398 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

Figure S14. ¹³C NMR (150 MHz, DMSO-*d*₆) for compound **6g**.

¹H of PHH1-236

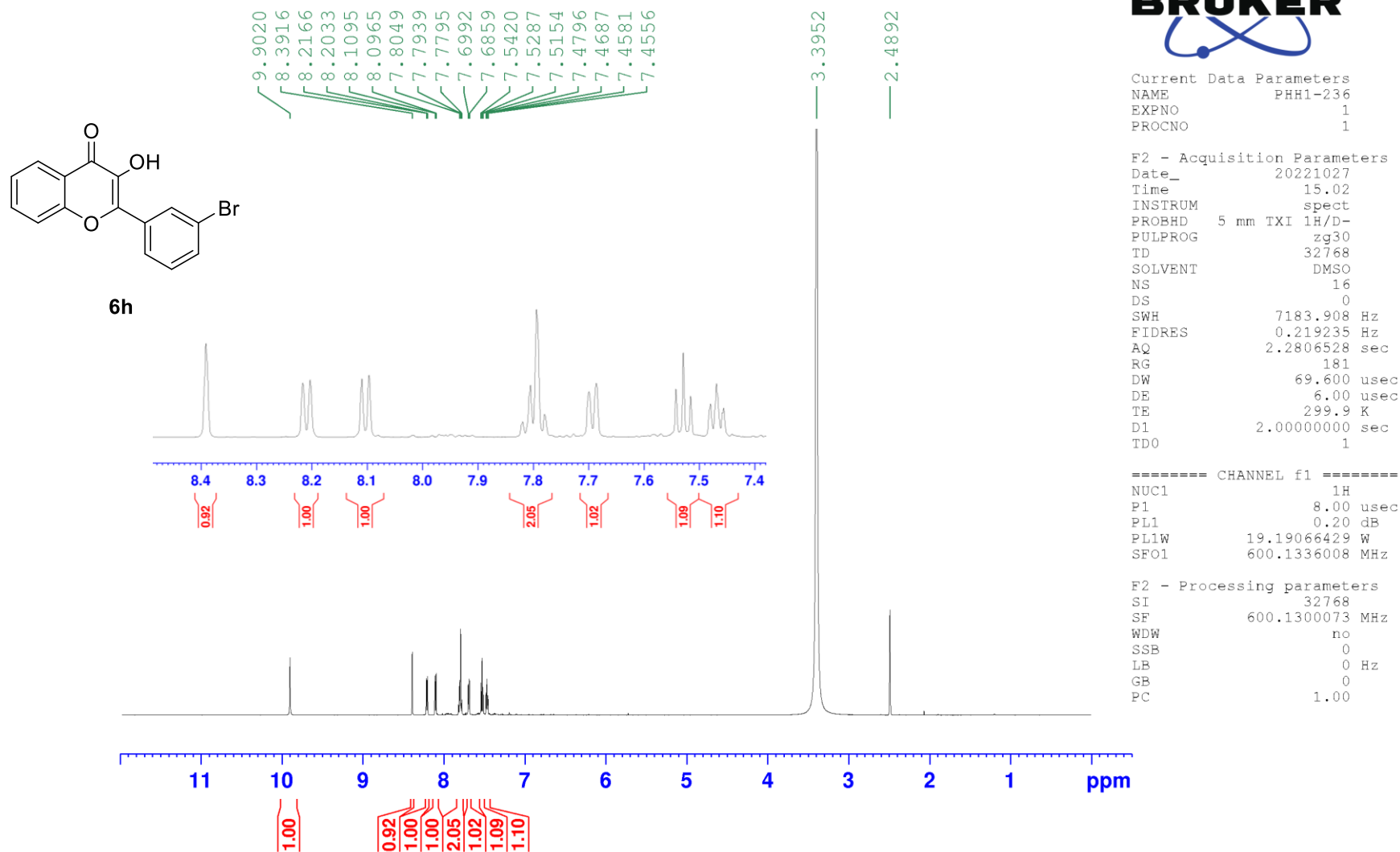


Figure S15. ¹H NMR (600 MHz, DMSO-*d*₆) for compound **6h**.

13C of PHH1-236



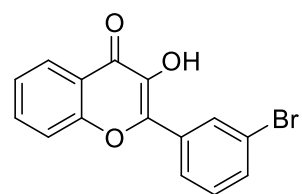
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NAME PHH1-236
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20221026
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INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1691
DS 0
SWH 33333.332 Hz
FIDRES 0.508626 Hz
AQ 0.9830400 sec
RG 46300
DW 15.000 usec
DE 6.00 usec
TE 299.2 K
D1 2.40000010 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.60 dB
PL1W 136.15426636 W
SFO1 150.9194083 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.50 dB
PL12 13.20 dB
PL13 16.20 dB
PL2W 28.38507080 W
PL12W 0.96181160 W
PL13W 0.48204759 W
SFO2 600.1339008 MHz

F2 - Processing parameters
SI 32768
SF 150.9028779 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00



6h

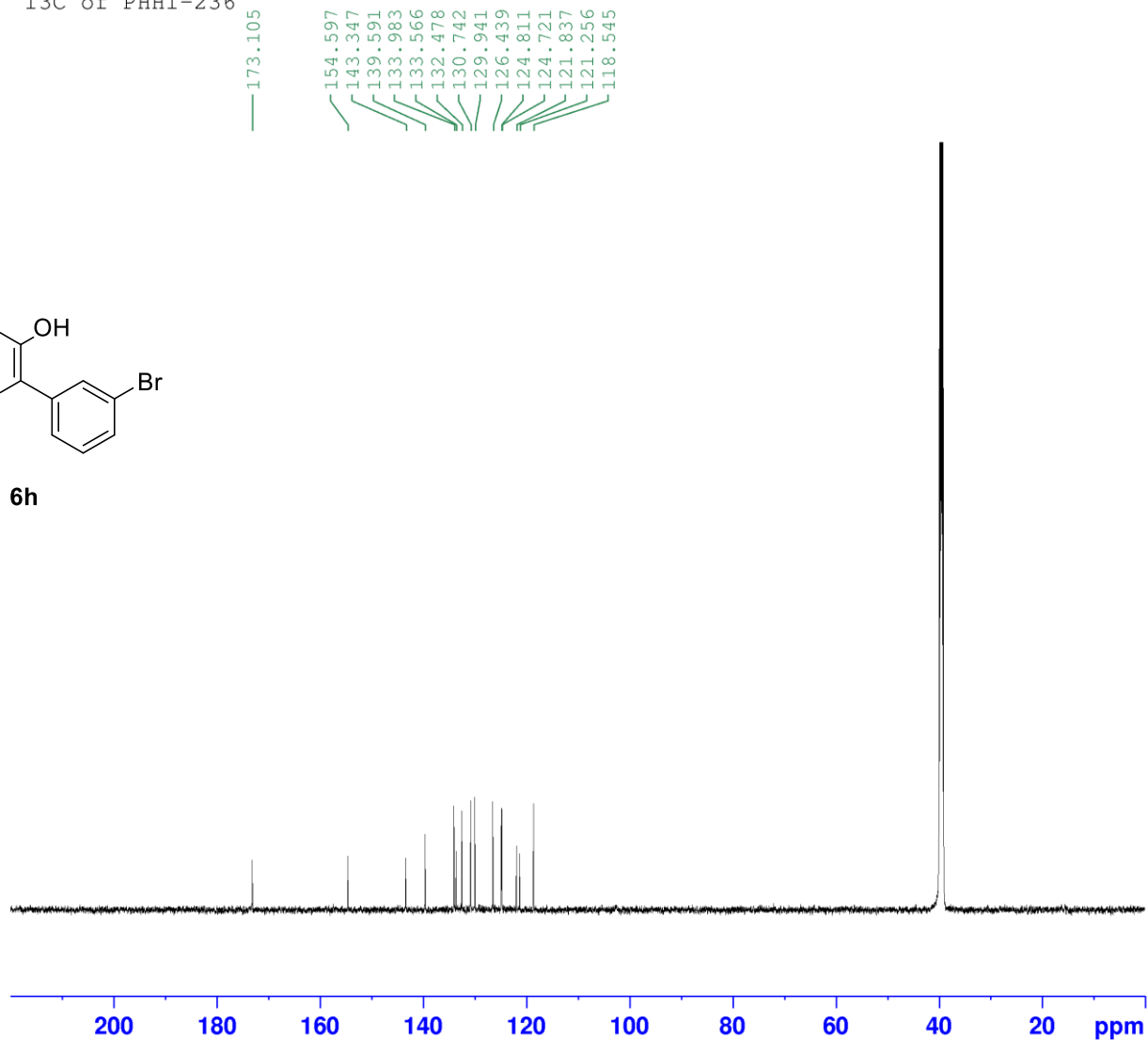
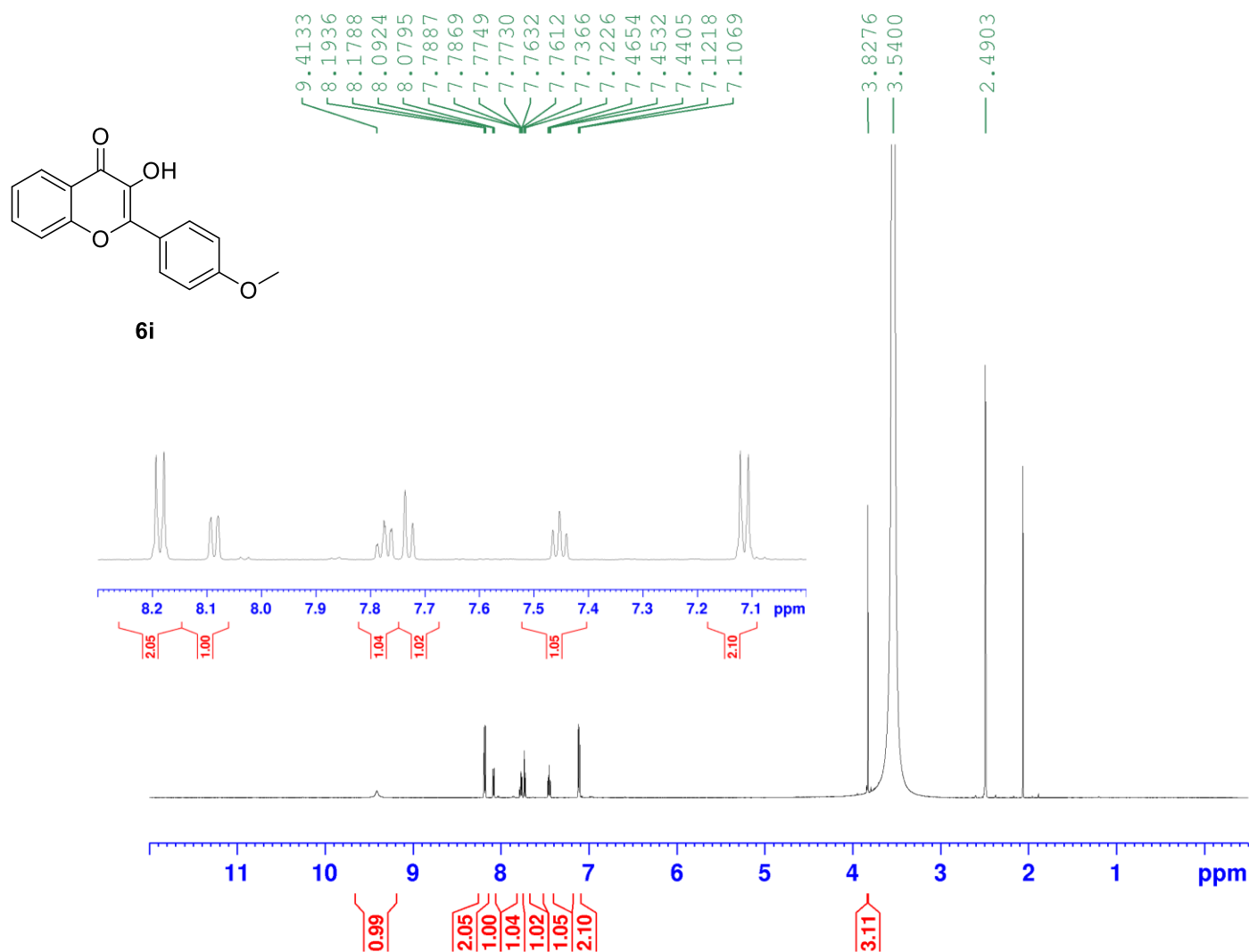


Figure S16. ^{13}C NMR (150 MHz, $\text{DMSO}-d_6$) for compound **6h**.

¹H of PHH1-216



Current Data Parameters
 NAME PHH1-216
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20221101
 Time 8.46
 INSTRUM spect
 PROBHD 5 mm TXI 1H/D-
 PULPROG zg30
 TD 32768
 SOLVENT DMSO
 NS 16
 DS 0
 SWH 7788.162 Hz
 FIDRES 0.237676 Hz
 AQ 2.1037056 sec
 RG 128
 DW 64.200 usec
 DE 6.00 usec
 TE 300.9 K
 D1 2.00000000 sec
 TD0 1

===== CHANNEL f1 =====
 NUC1 1H
 P1 8.00 usec
 PL1 0.20 dB
 PL1W 19.19066429 W
 SFO1 600.1336008 MHz

F2 - Processing parameters
 SI 16384
 SF 600.1300073 MHz
 WDW EM
 SSB 0
 LB 0 Hz
 GB 0
 PC 1.00

Figure S17. ¹H NMR (600 MHz, DMSO-*d*₆) for compound **6i**.

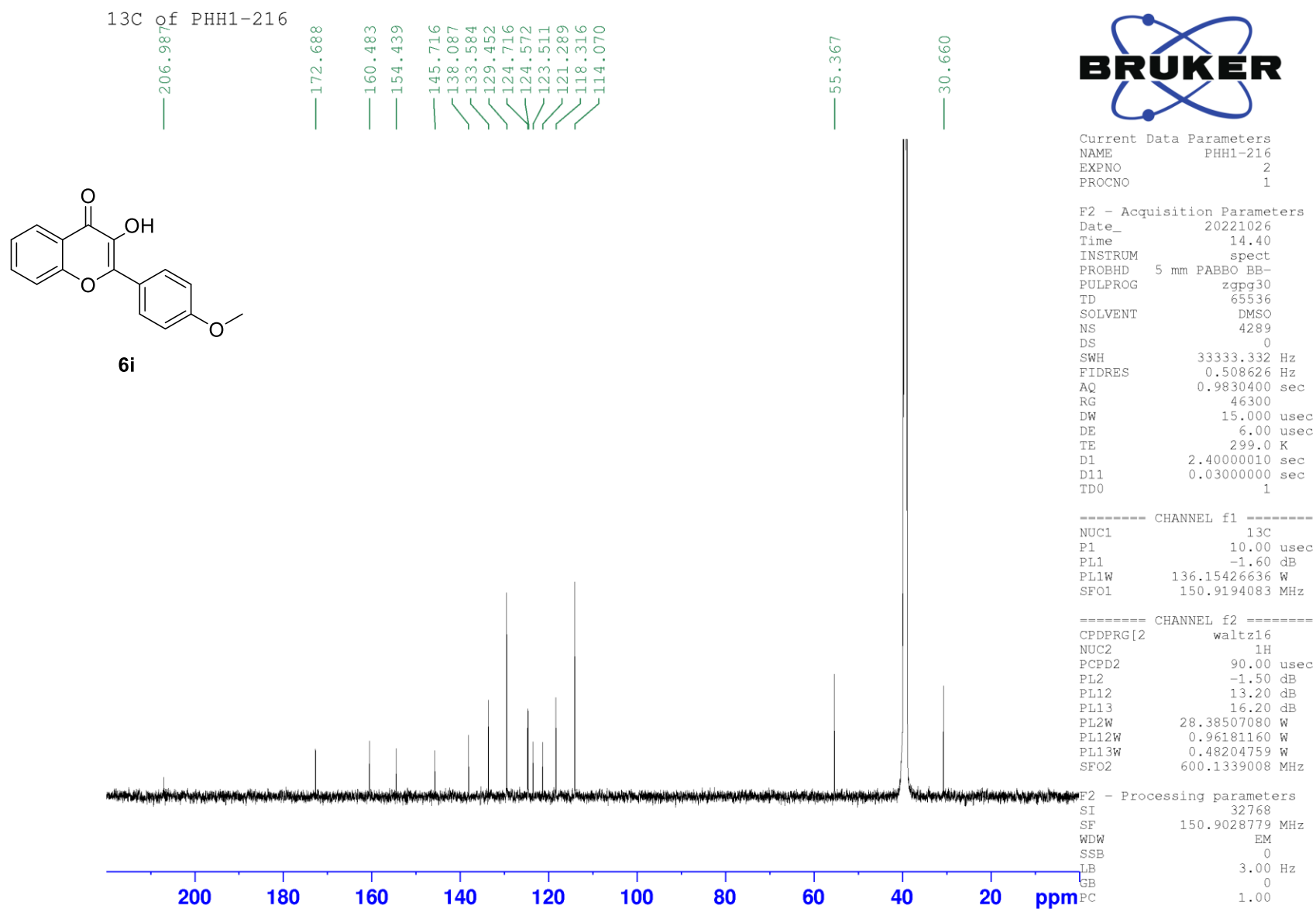
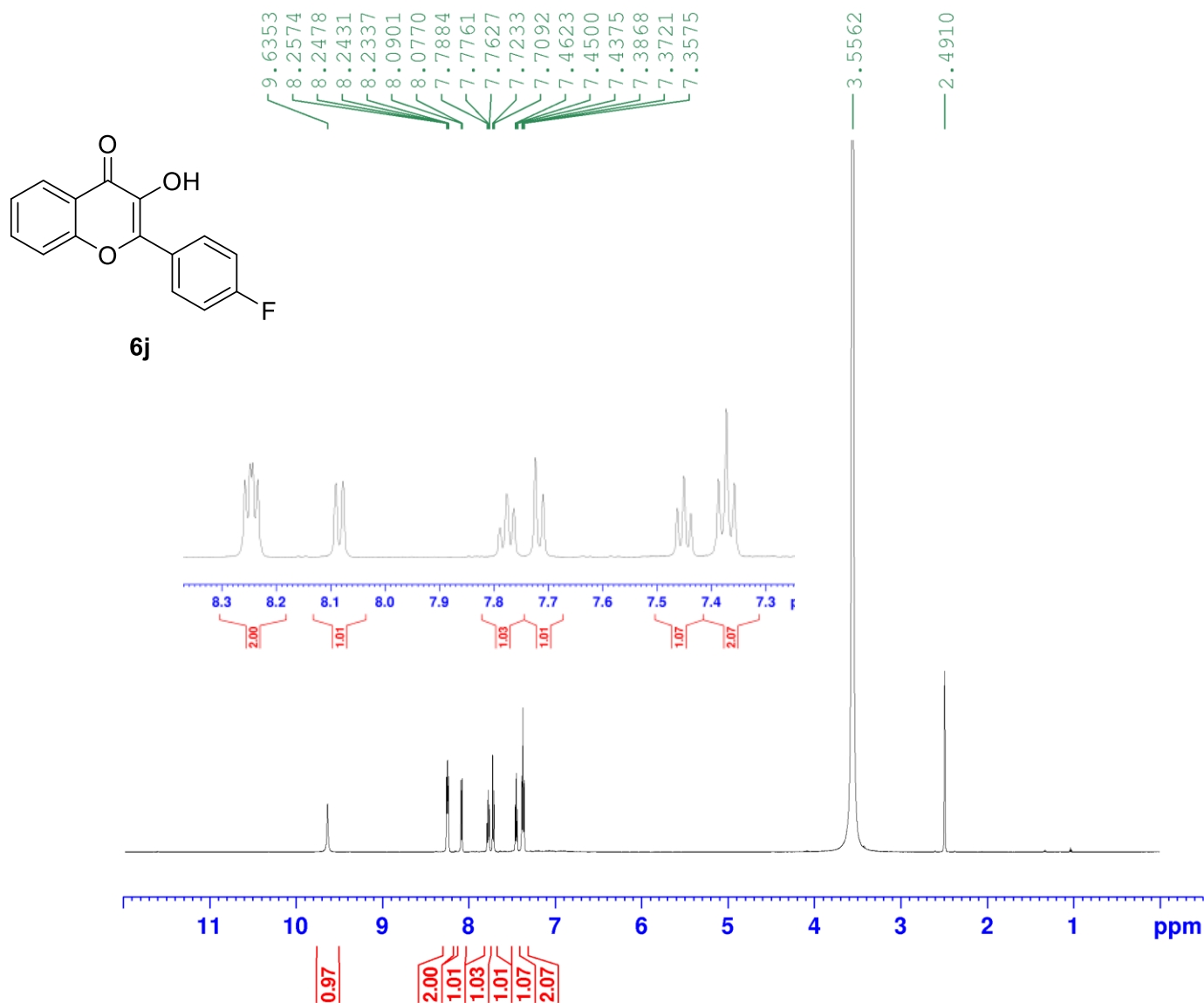


Figure S18. ^{13}C NMR (150 MHz, $\text{DMSO}-d_6$) for compound **6i**.

1H of PHH1-192



Current Data Parameters
NAME PHH1-192
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220627
Time 16.43
INSTRUM spect
PROBHD 5 mm TXI 1H/D-
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 16
DS 0
SWH 7183.908 Hz
FIDRES 0.219235 Hz
AQ 2.2806528 sec
RG 724
DW 69.600 usec
DE 6.00 usec
TE 302.2 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.00 usec
PL1 0.20 dB
PL1W 19.19066429 W
SFO1 600.1336008 MHz

F2 - Processing parameters
SI 32768
SF 600.1300073 MHz
WDW no
SSB 0
LB 0 Hz
GB 0
PC 1.00

Figure S19. ¹H NMR (600 MHz, DMSO-*d*₆) for compound **6j**.
S22

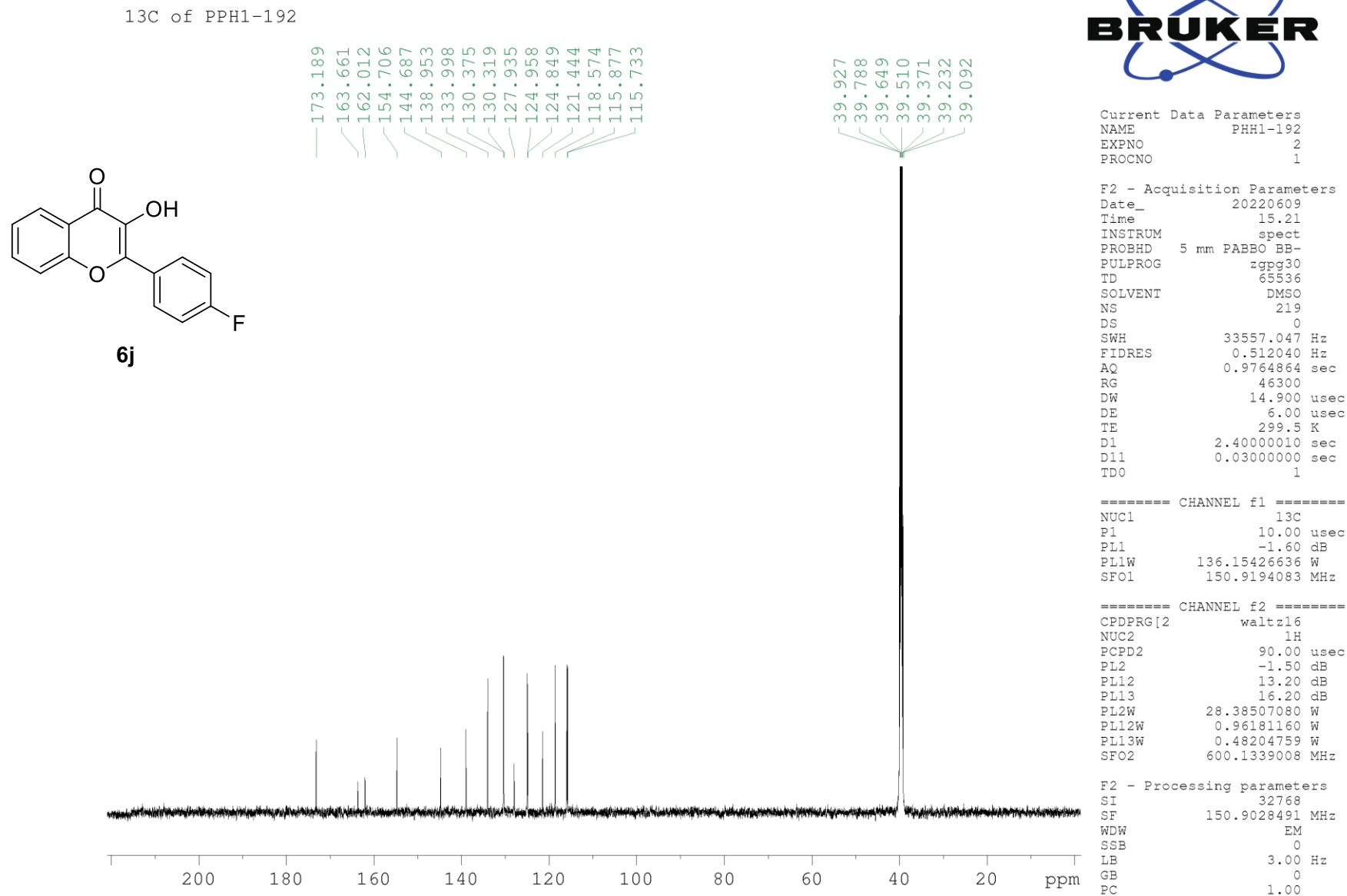


Figure S20. ¹³C NMR (150 MHz, DMSO-*d*₆) for compound **6j**.
 S23

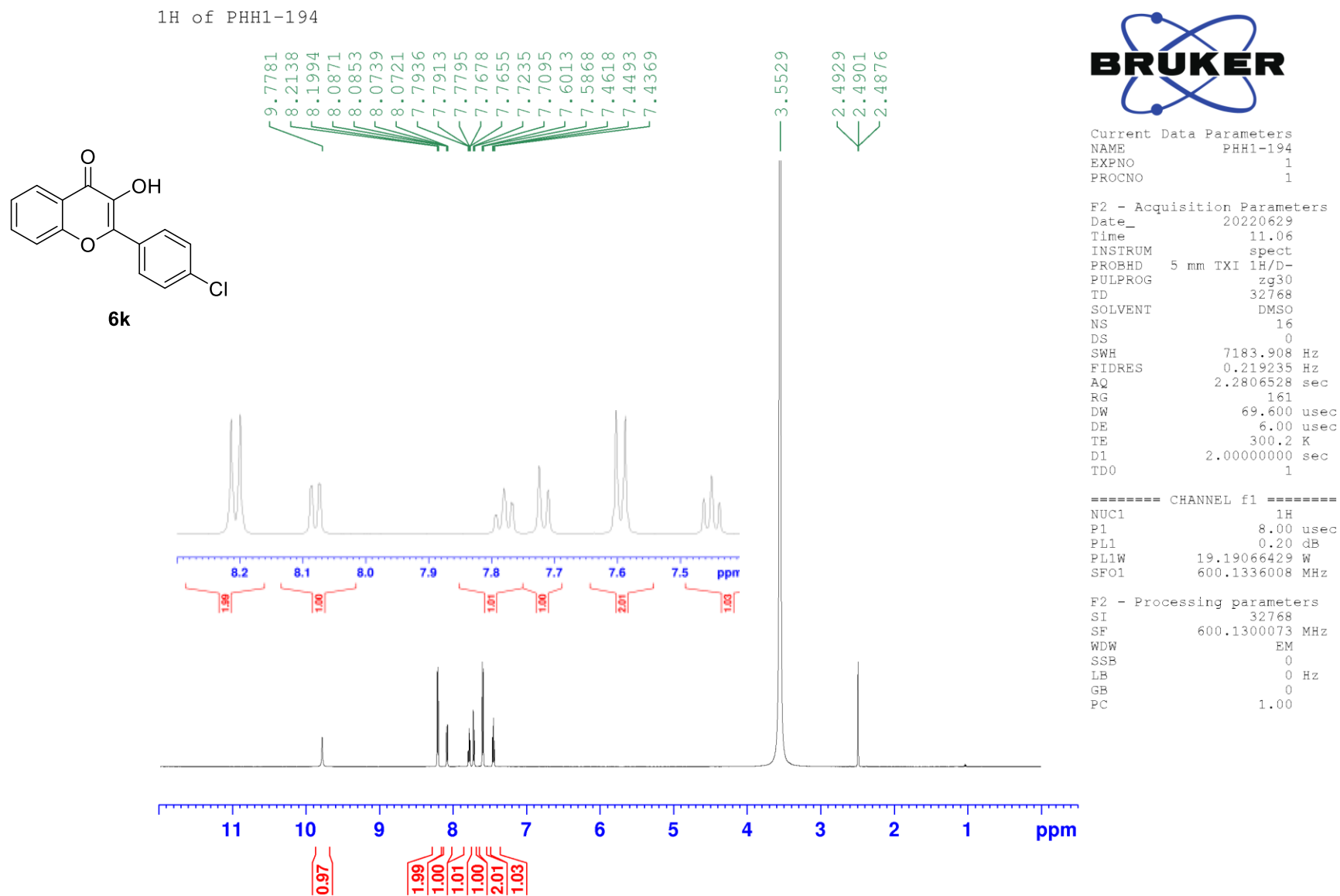


Figure S21. ^1H NMR (600 MHz, $\text{DMSO}-d_6$) for compound **6k**.

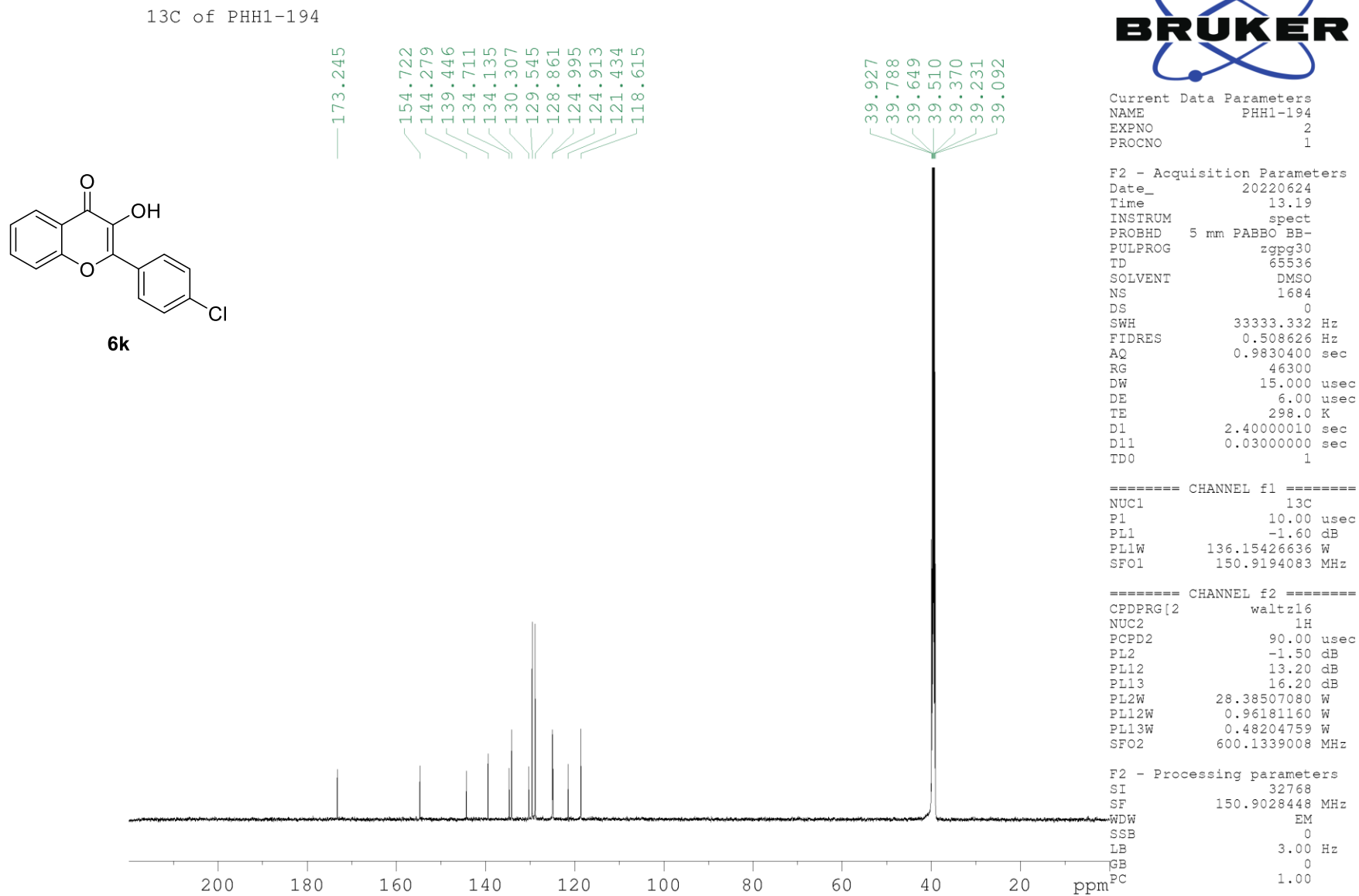
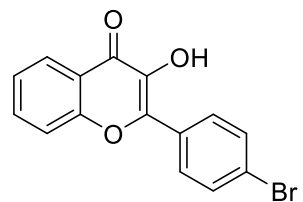
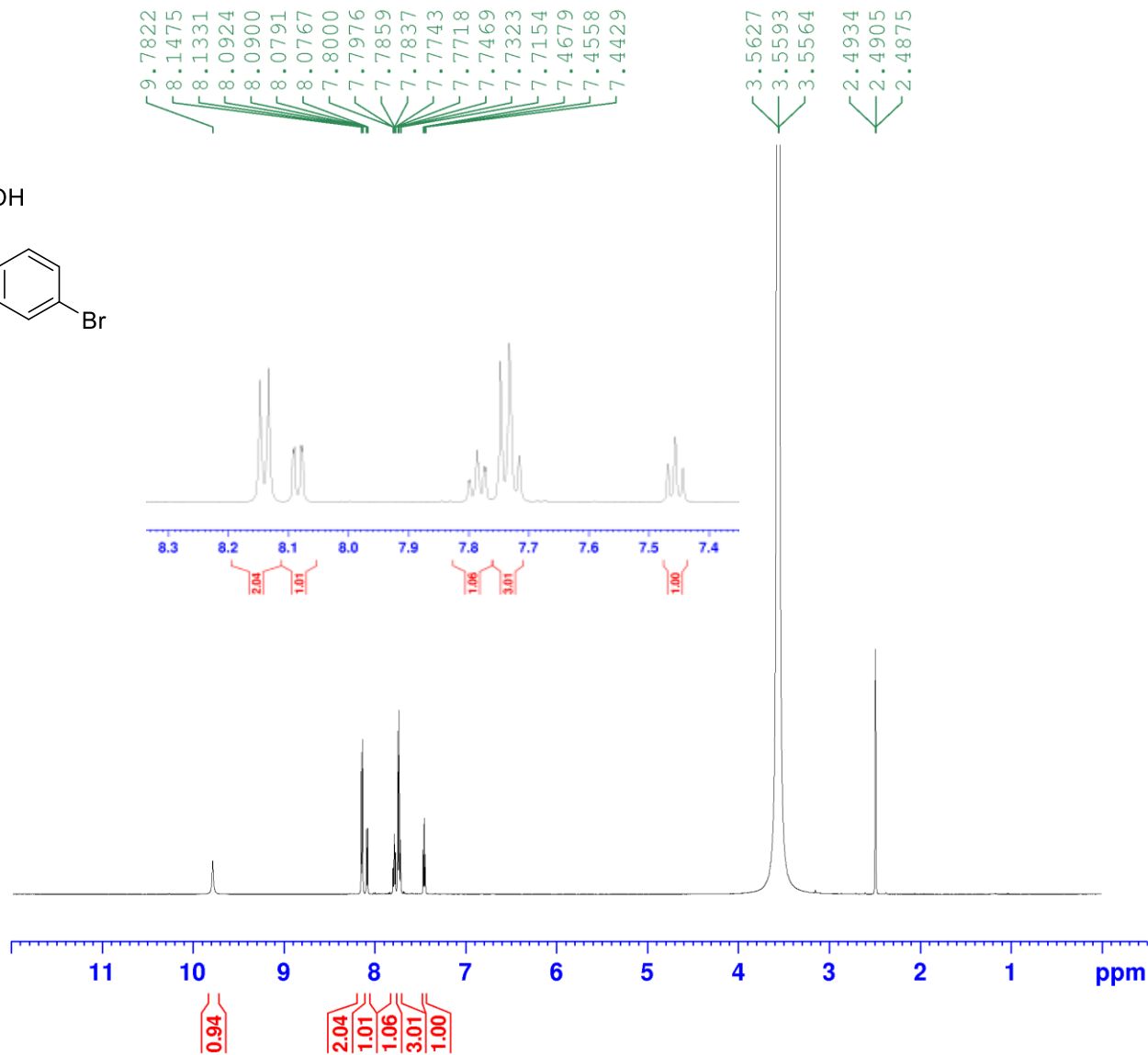


Figure S22. ¹³C NMR (150 MHz, DMSO-*d*₆) for compound **6k**.

¹H of PHH1-191



6I



Current Data Parameters
NAME PHH1-191
EXPNO 1
PROCNO 1

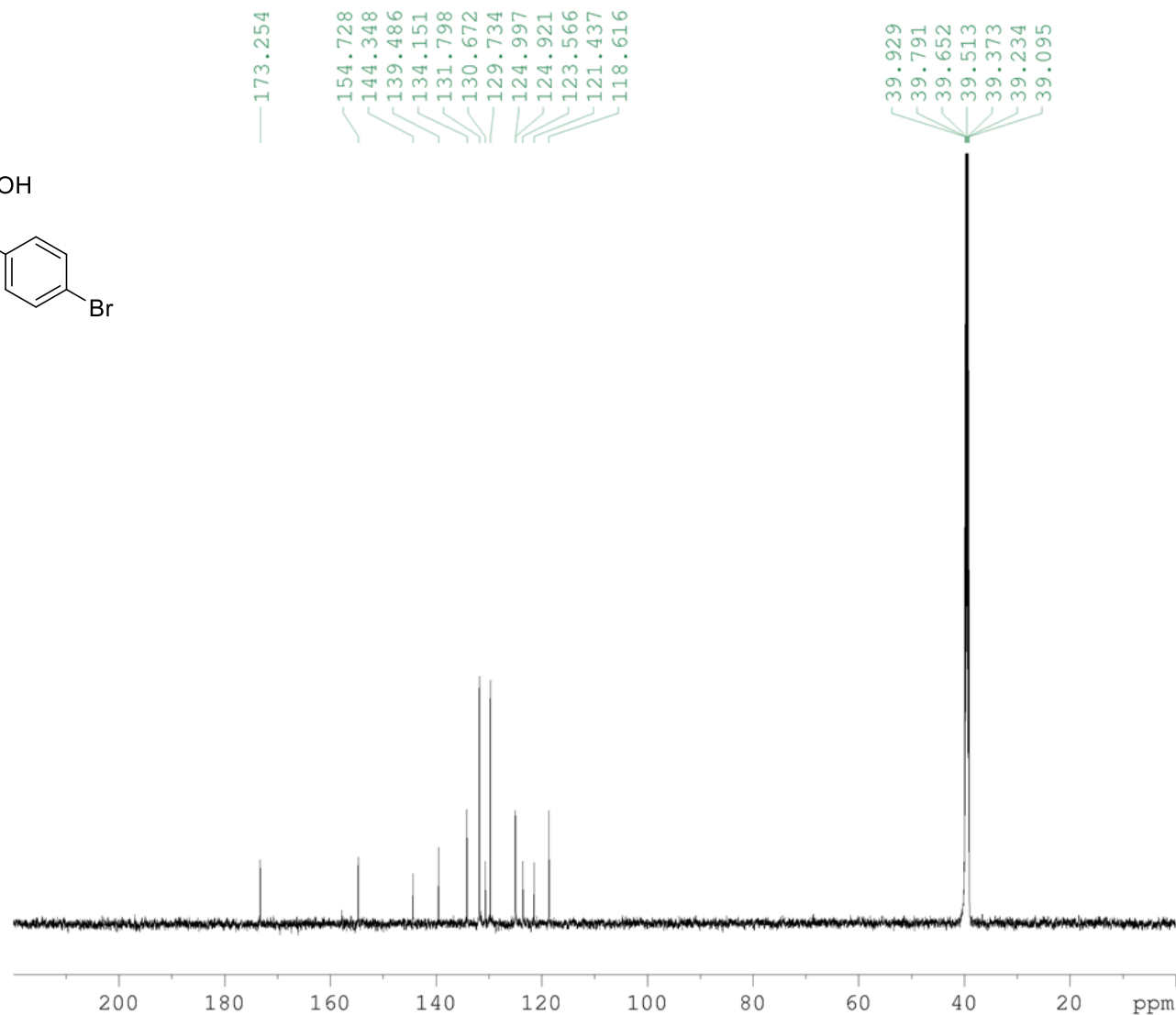
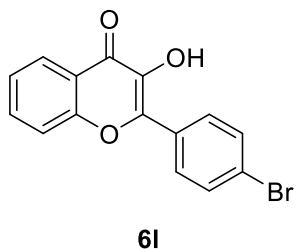
F2 - Acquisition Parameters
Date_ 20220617
Time 16.14
INSTRUM spect
PROBHD 5 mm TXI 1H/D-
PULPROG zg30
TD 32768
SOLVENT DMSO
NS 16
DS 0
SWH 7183.908 Hz
FIDRES 0.219235 Hz
AQ 2.2806528 sec
RG 144
DW 69.600 usec
DE 6.00 usec
TE 301.7 K
D1 2.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 8.00 usec
PL1 0.20 dB
PL1W 19.19066429 W
SFO1 600.1336008 MHz

F2 - Processing parameters
SI 32768
SF 600.1300073 MHz
WDW EM
SSB 0
LB 0 Hz
GB 0
PC 1.00

Figure S23. ¹H NMR (600 MHz, DMSO-*d*₆) for compound **6I**.

13C of PHH1-191



Current Data Parameters
NAME PHH1-191
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220609
Time_ 15.06
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 353
DS 0
SWH 33557.047 Hz
FIDRES 0.512040 Hz
AQ 0.9764864 sec
RG 46300
DW 14.900 usec
DE 6.00 usec
TE 299.6 K
D1 2.40000010 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.60 dB
PL1W 136.15426636 W
SFO1 150.9194083 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.50 dB
PL12 13.20 dB
PL13 16.20 dB
PL2W 28.38507080 W
PL12W 0.96181160 W
PL13W 0.48204759 W
SFO2 600.1339008 MHz

F2 - Processing parameters
SI 32768
SF 150.9028466 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

Figure S24. ^{13}C NMR (150 MHz, $\text{DMSO}-d_6$) for compound **6l**.
S27

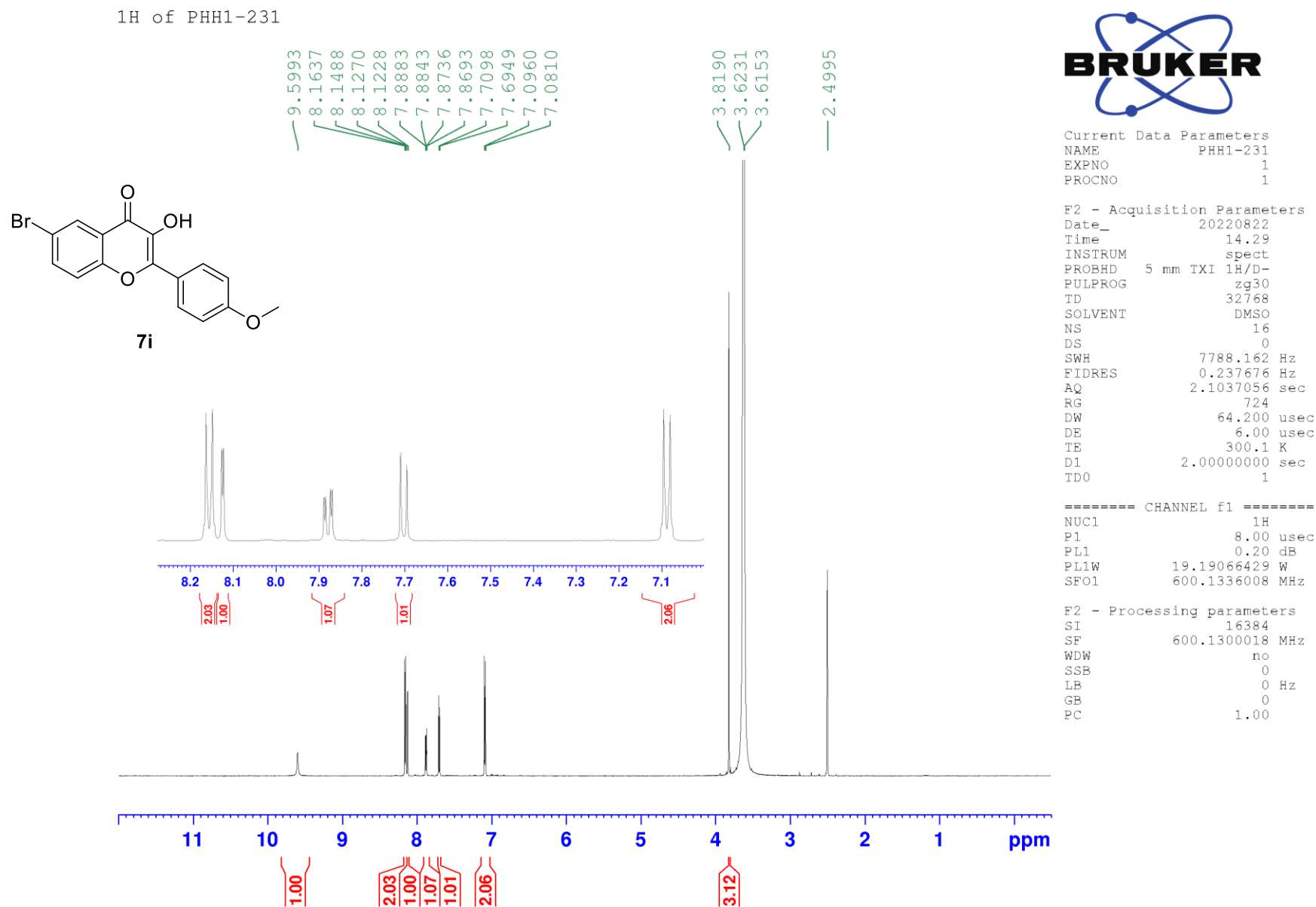
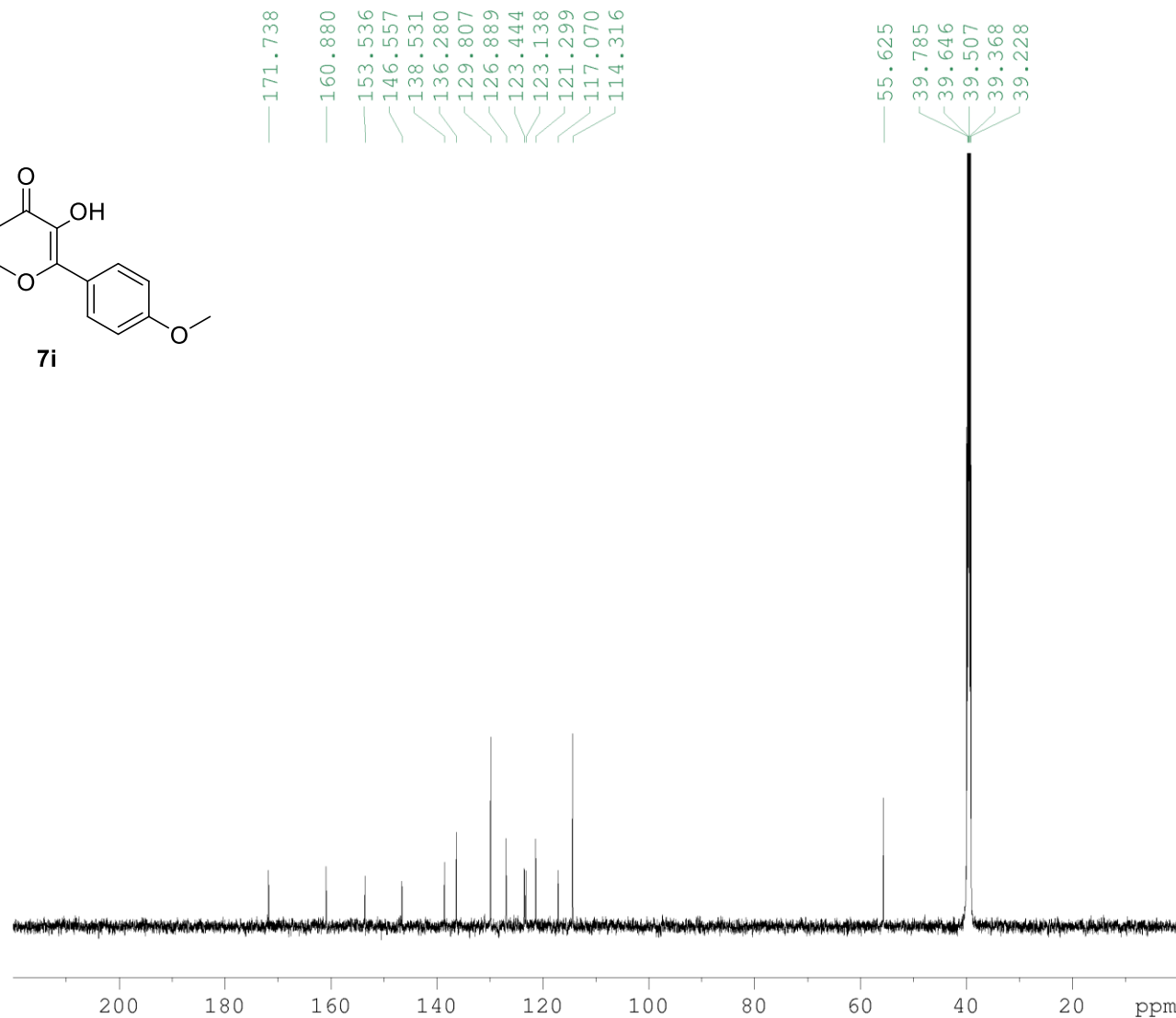
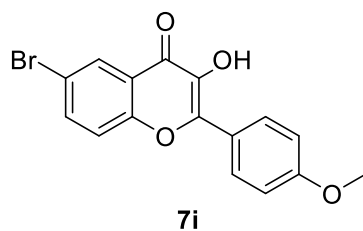


Figure S25. ¹H NMR (600 MHz, DMSO-*d*₆) for compound **7i**.

13C of PHH1-231



Current Data Parameters
NAME PHH1-231
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220817
Time 13.53
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 541
DS 0
SWH 33333.332 Hz
FIDRES 0.508626 Hz
AQ 0.9830400 sec
RG 46300
DW 15.000 usec
DE 6.00 usec
TE 298.4 K
D1 2.40000010 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.60 dB
PL1W 136.15426636 W
SFO1 150.9194083 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.50 dB
PL12 13.20 dB
PL13 16.20 dB
PL2W 28.38507080 W
PL12W 0.96181160 W
PL13W 0.48204759 W
SFO2 600.1339008 MHz

F2 - Processing parameters
SI 32768
SF 150.9028363 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

Figure S26. ¹³C NMR (150 MHz, DMSO-*d*₆) for compound **7i**.
S29

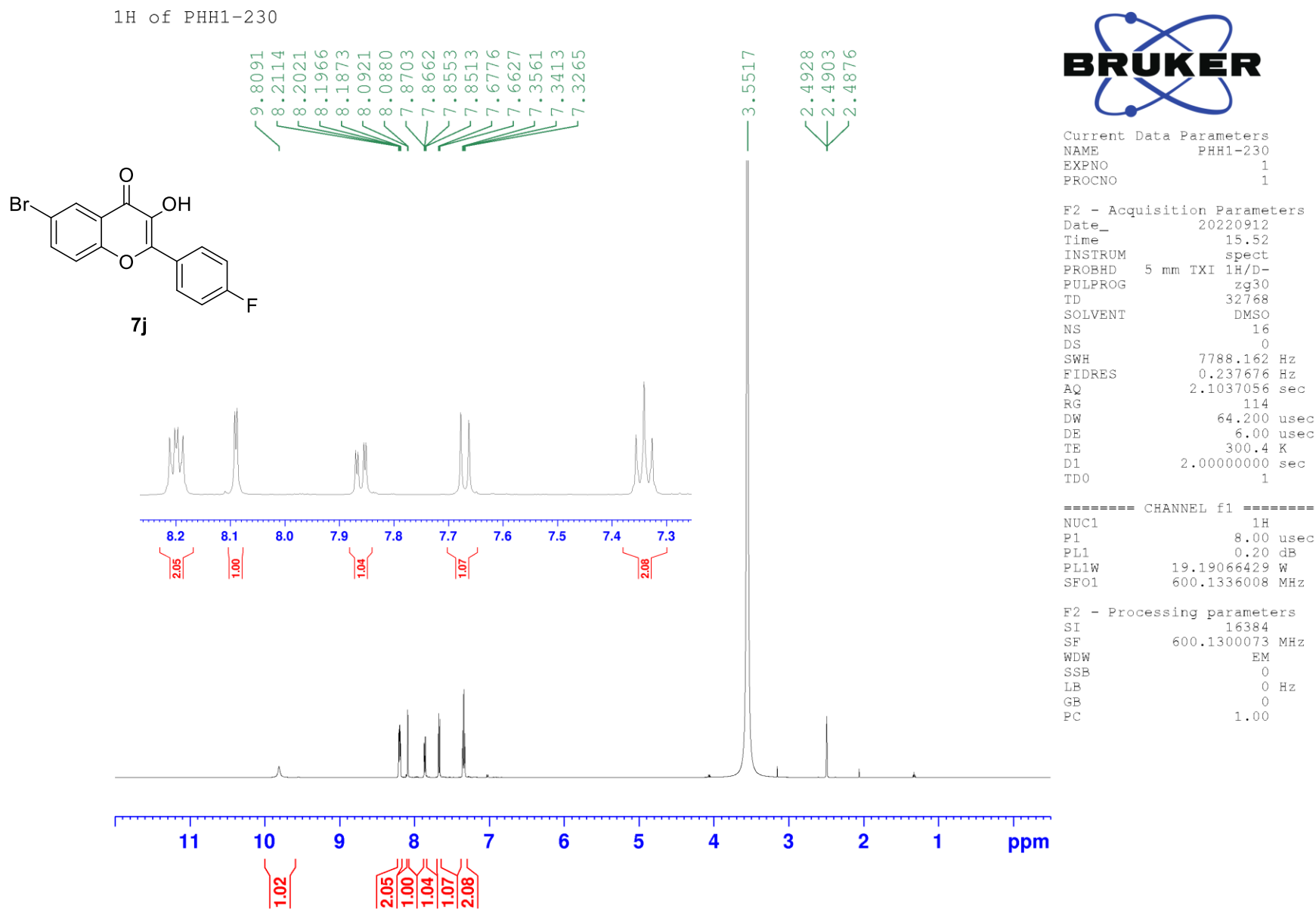
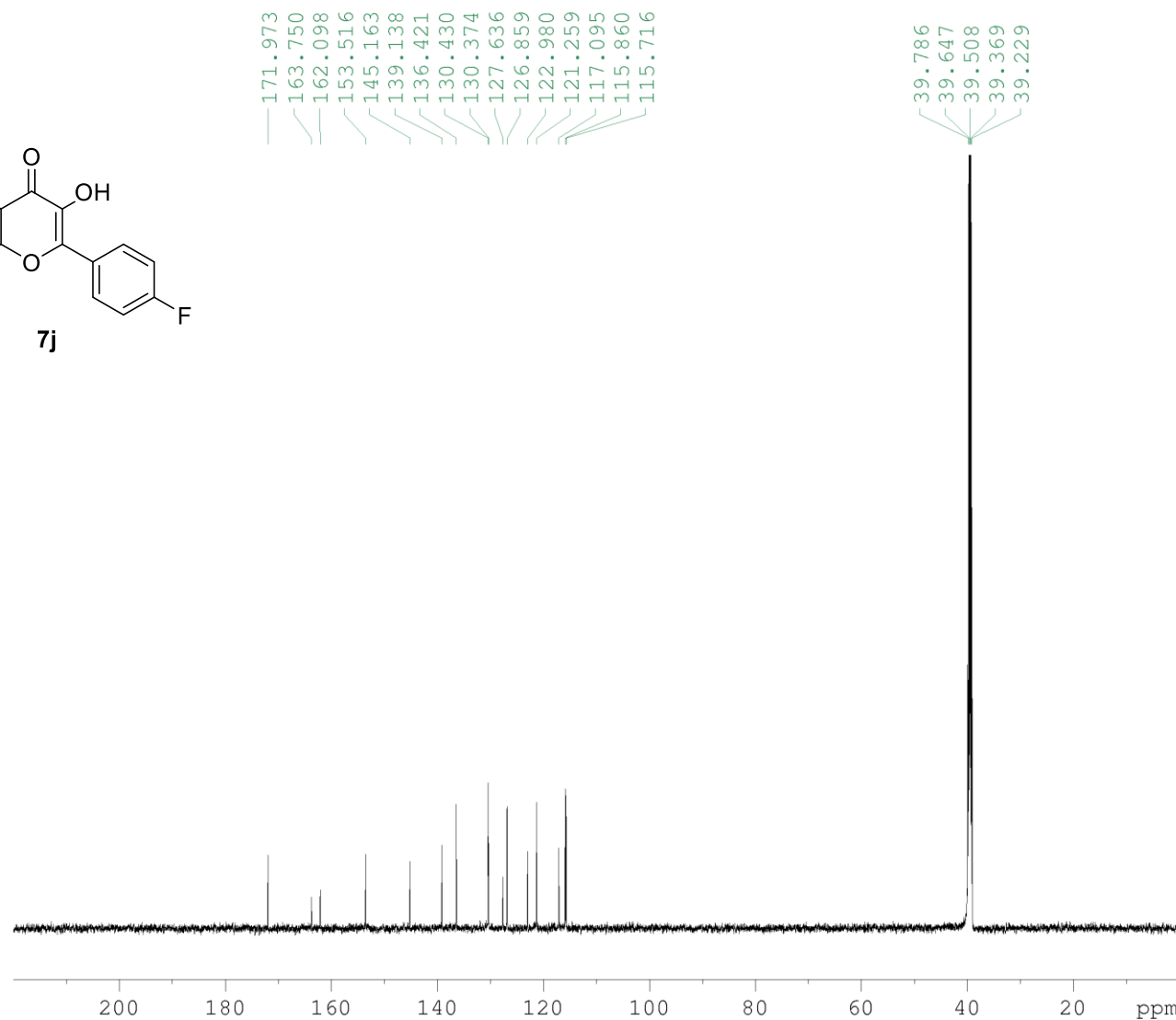
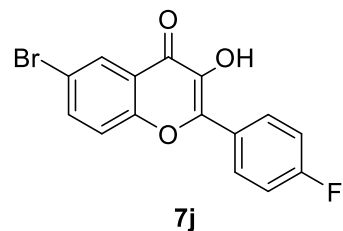


Figure S27. ^1H NMR (600 MHz, $\text{DMSO}-d_6$) for compound **7j**.

13C of PHH1-230



Current Data Parameters
NAME PHH1-230
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220908
Time 16.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 248
DS 0
SWH 33333.332 Hz
FIDRES 0.508626 Hz
AQ 0.9830400 sec
RG 46300
DW 15.000 usec
DE 6.00 usec
TE 299.4 K
D1 2.40000010 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.60 dB
PL1W 136.15426636 W
SFO1 150.9194083 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.50 dB
PL12 13.20 dB
PL13 16.20 dB
PL2W 28.38507080 W
PL12W 0.96181160 W
PL13W 0.48204759 W
SFO2 600.1339008 MHz

F2 - Processing parameters
SI 32768
SF 150.9028466 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

Figure S28. ^{13}C NMR (150 MHz, $\text{DMSO}-d_6$) for compound **7j**.

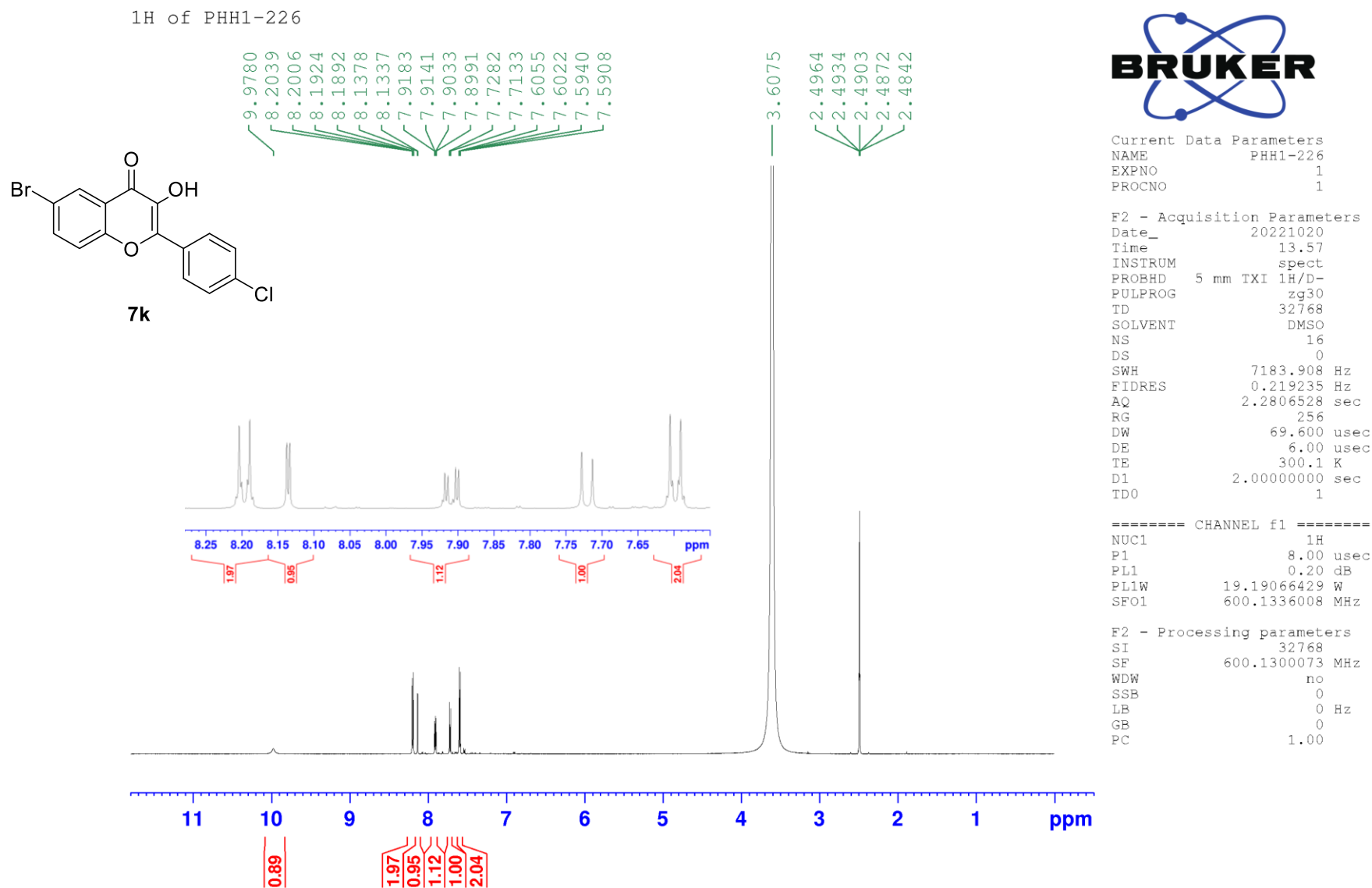


Figure S29. ¹H NMR (600 MHz, DMSO-*d*₆) for compound **7k**.

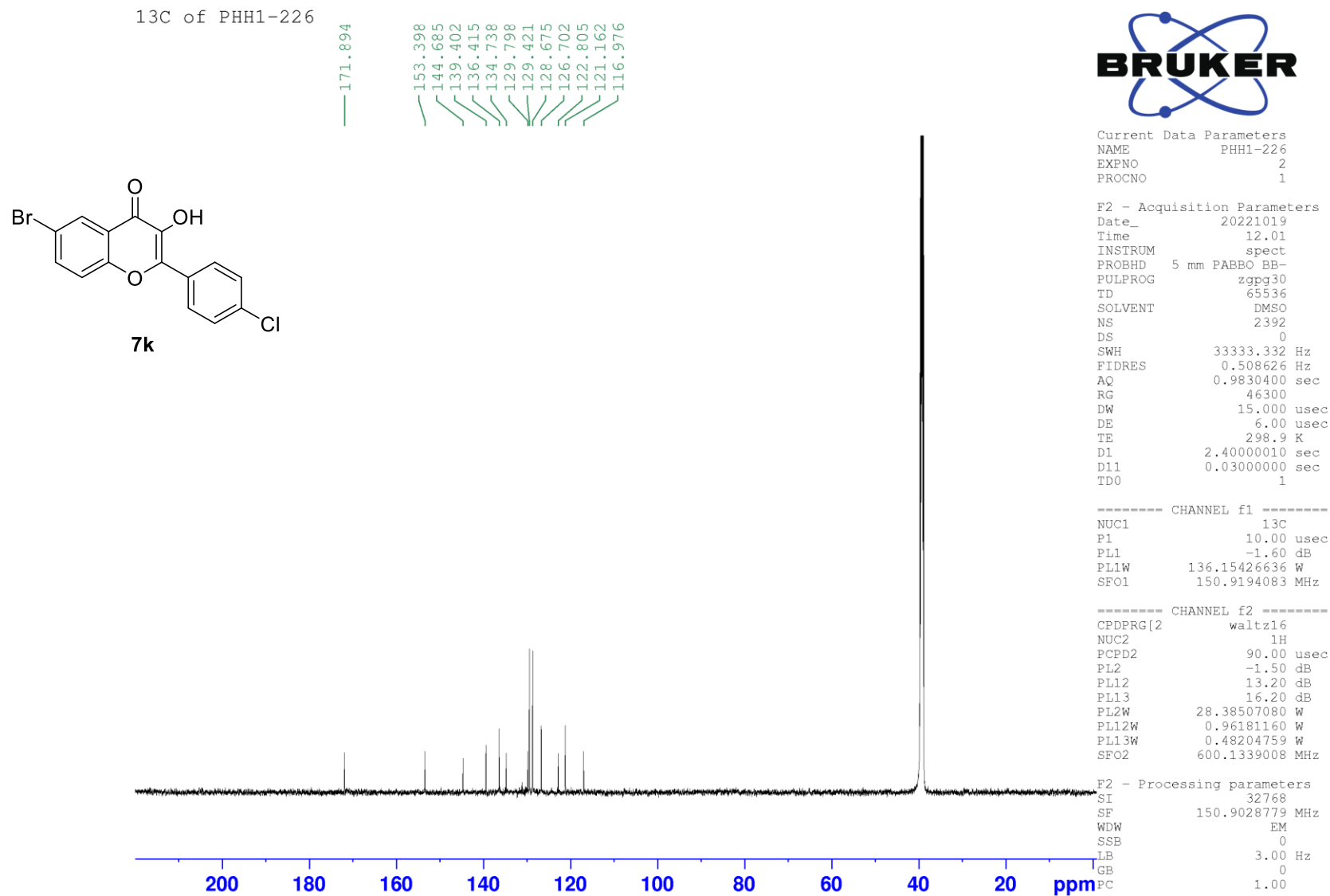


Figure S30. ^{13}C NMR (150 MHz, $\text{DMSO}-d_6$) for compound **7k**.

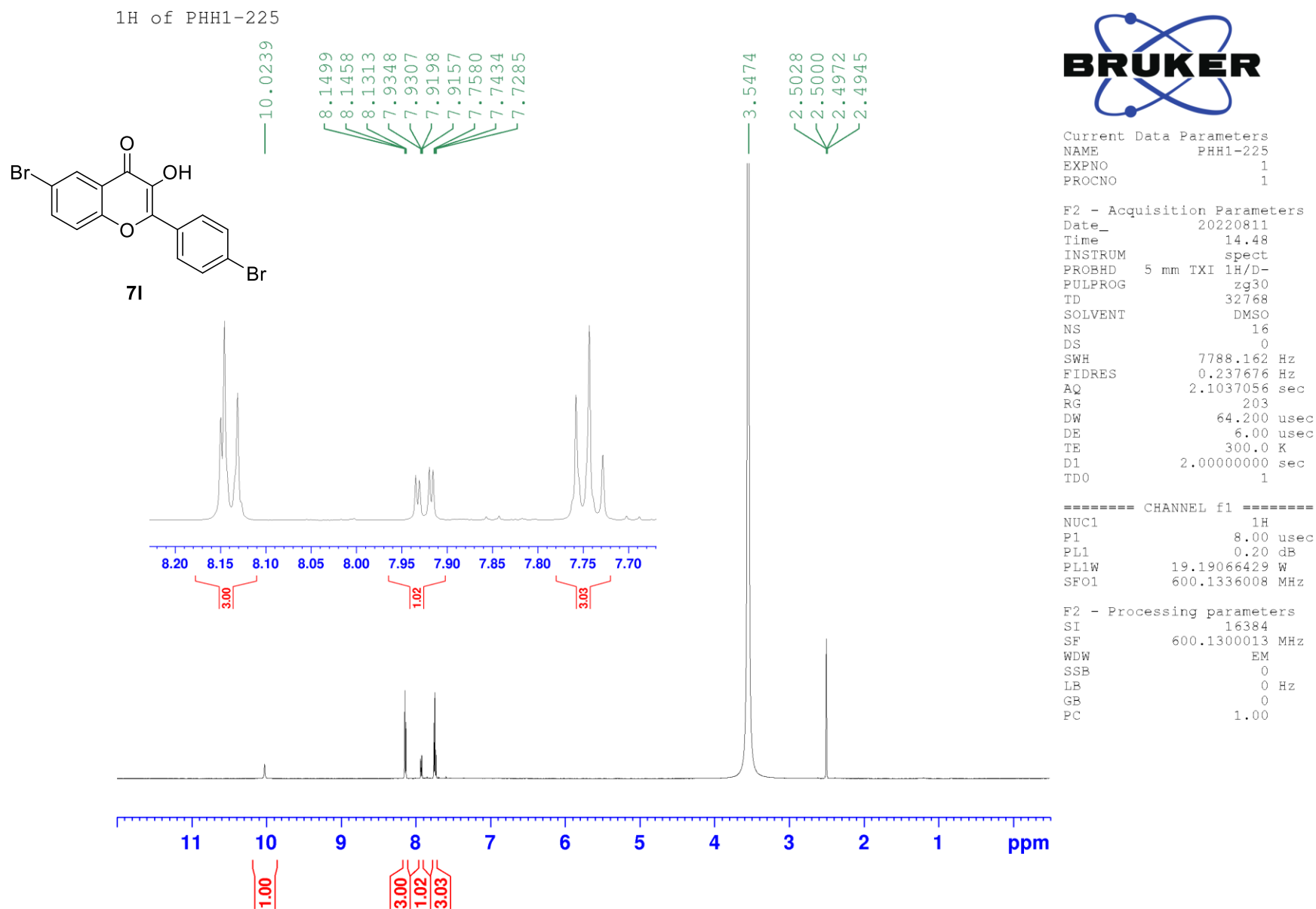
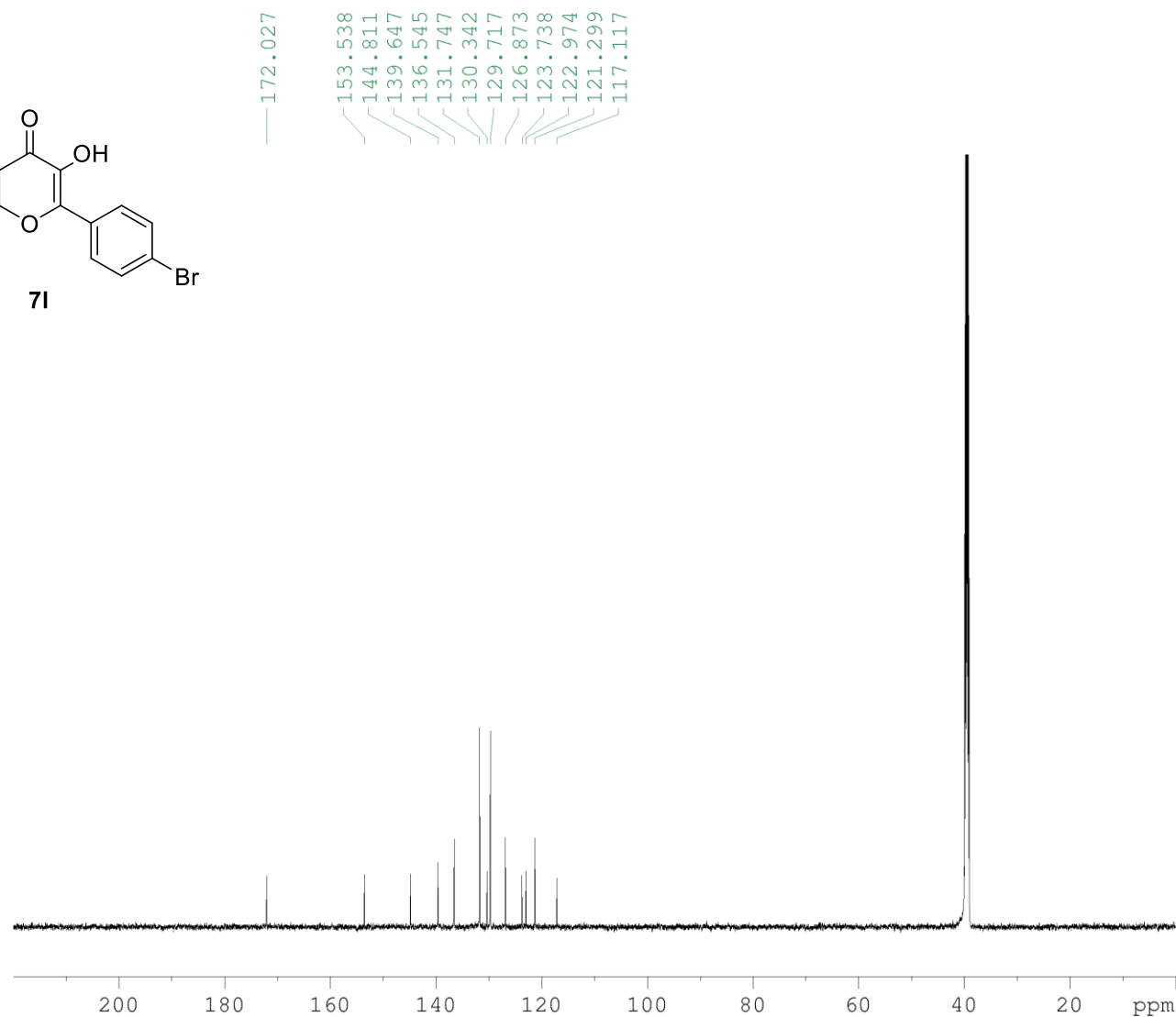
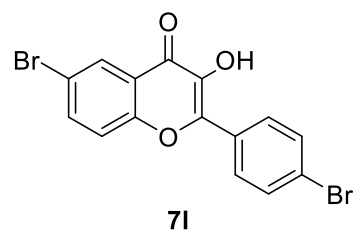


Figure S31. ^1H NMR (600 MHz, $\text{DMSO}-d_6$) for compound **7l**.



13C of PHH1-225



Current Data Parameters
NAME PHH1-225
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20220725
Time 13.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 980
DS 0
SWH 36231.883 Hz
FIDRES 0.552855 Hz
AQ 0.9043968 sec
RG 46300
DW 13.800 usec
DE 6.00 usec
TE 299.9 K
D1 2.40000010 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 13C
P1 10.00 usec
PL1 -1.60 dB
PL1W 136.15426636 W
SFO1 150.9194083 MHz

===== CHANNEL f2 =====
CPDPRG[2] waltz16
NUC2 1H
PCPD2 90.00 usec
PL2 -1.50 dB
PL12 13.20 dB
PL13 16.20 dB
PL2W 28.38507080 W
PL12W 0.96181160 W
PL13W 0.48204759 W
SFO2 600.1339008 MHz

F2 - Processing parameters
SI 32768
SF 150.9028528 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.00

Figure S32. ¹³C NMR (150 MHz, DMSO-*d*₆) for compound 71.