

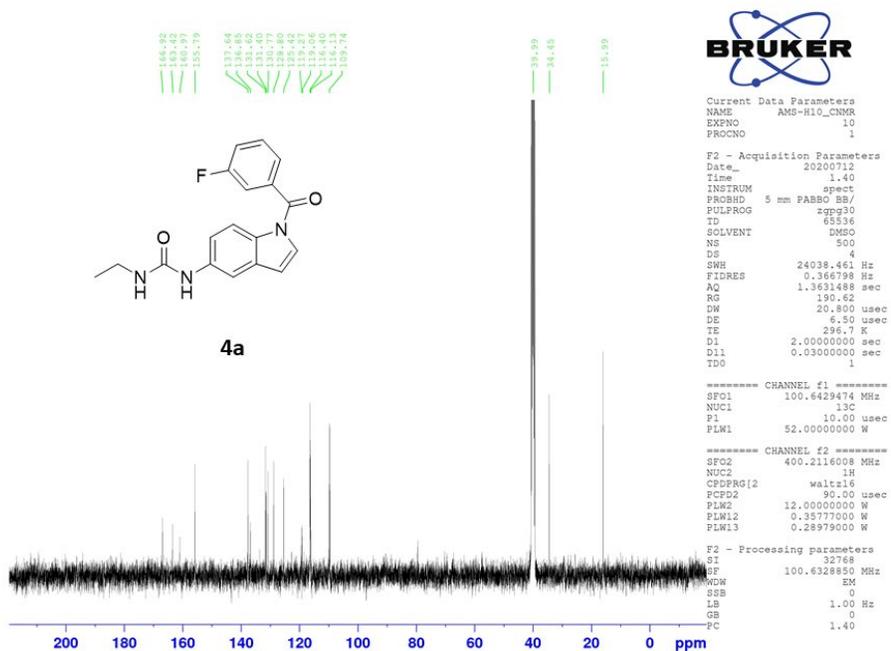
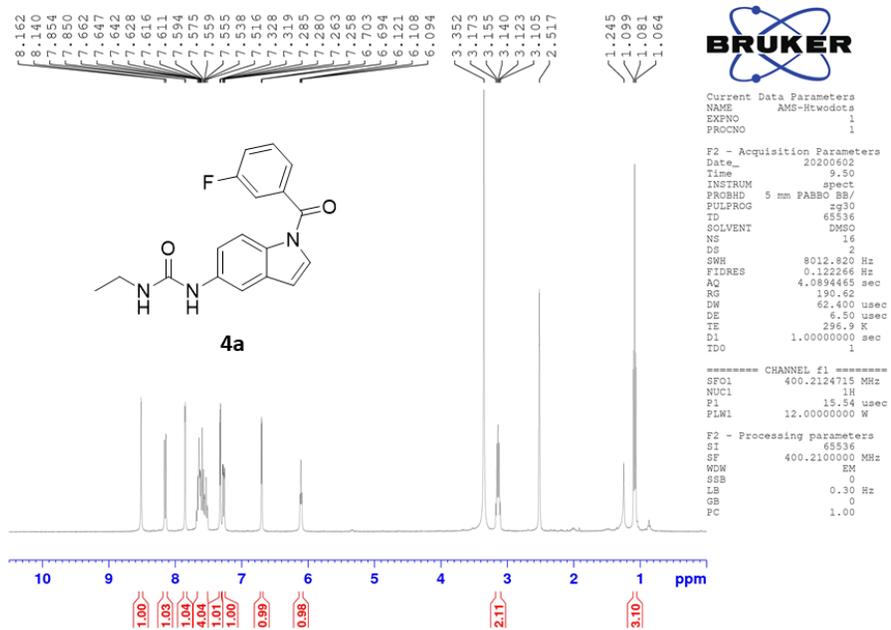
## Supplementary material

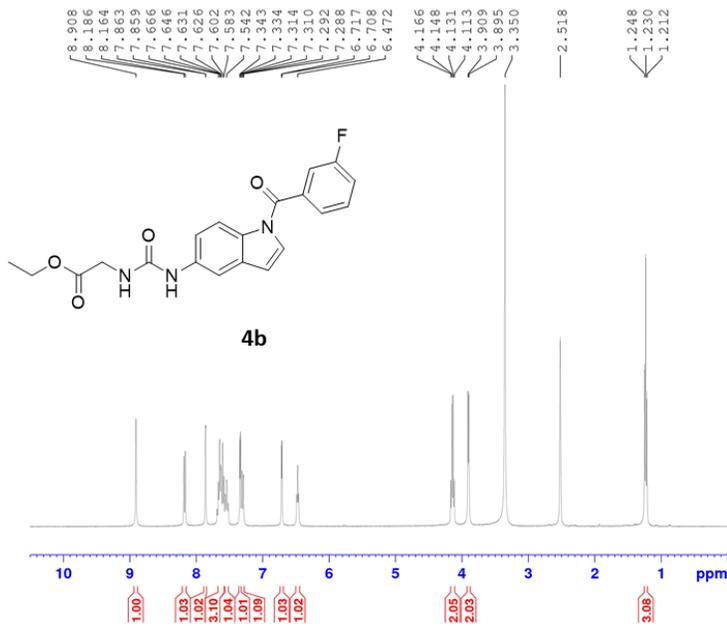
# Highly Potent, Selective, and Competitive Indole-Based MAO-B Inhibitors Protect PC12 Cells against 6-Hydroxydopamine- and Rotenone-Induced Oxidative Stress

### Contents

1.  $^1\text{H}$ NMR and  $^{13}\text{C}$ NMR data of compounds **4a–n**, **5a–j**, **6a–e**, **7a**, **7b**, and **8a–e**
2. HPLC purity data
3. HRMS data
4. Molecular modelling supplementary material

# 1. <sup>1</sup>HNMR and <sup>13</sup>CNMR data of compounds 4a–n, 5a–j, 6a–e, 7a, 7b, and 8a–e



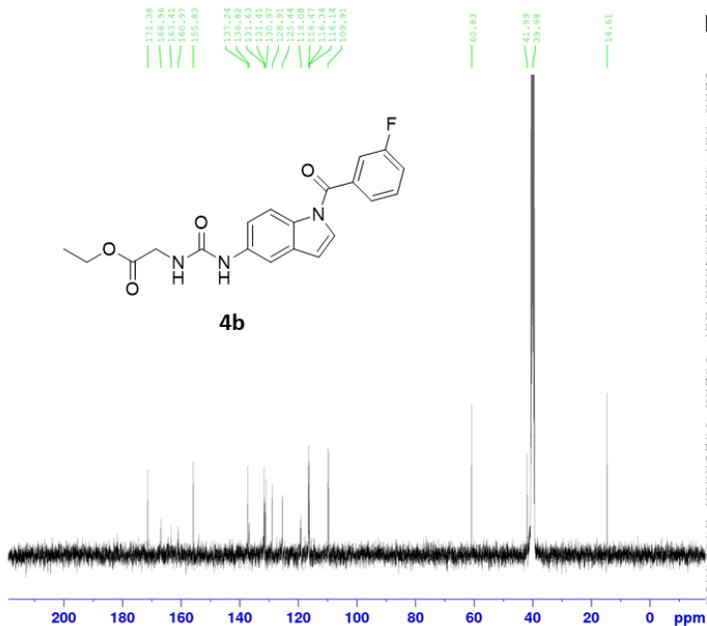


Current Data Parameters  
 NAME AMS-H14  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200407  
 Time 16.01  
 INSTRUM spect  
 PROBHD 5 mm FAPBBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 190.62  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



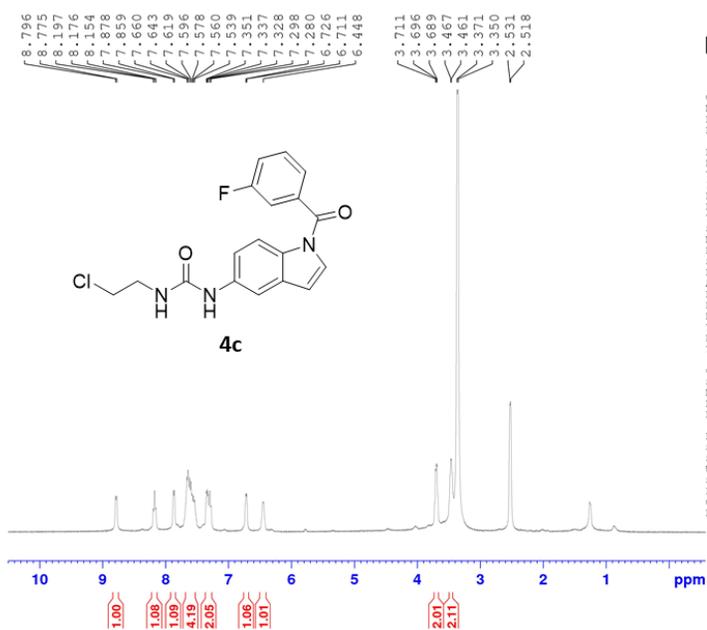
Current Data Parameters  
 NAME AMS-H14\_CNMR  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200712  
 Time 2.11  
 INSTRUM spect  
 PROBHD 5 mm FAPBBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 500  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.7 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.2116008 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

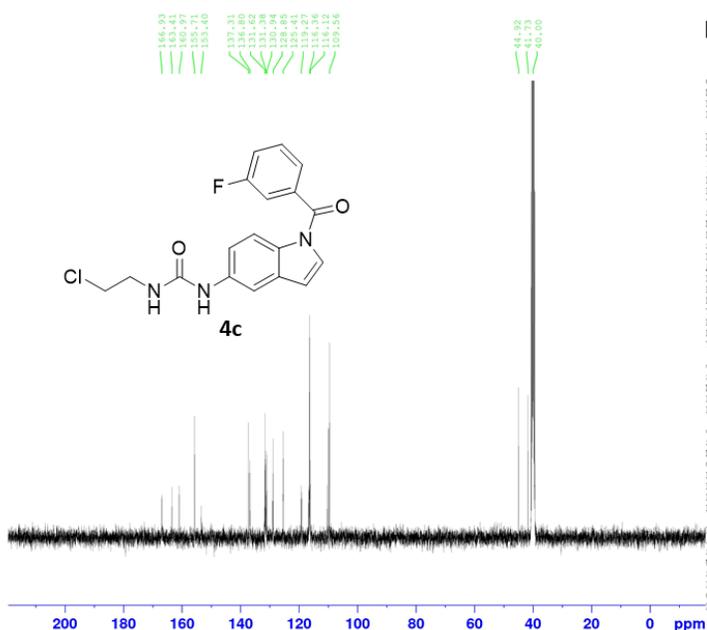


Current Data Parameters  
 NAME AMS-H28F  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200526  
 Time 19.53  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 190.62  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 297.2 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



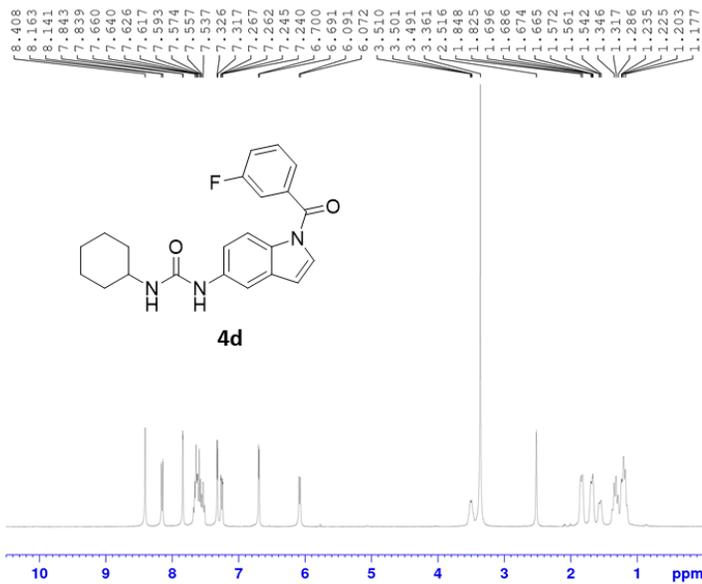
Current Data Parameters  
 NAME AMS-H28\_CNMR  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200429  
 Time 21.57  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 256  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.9 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.2116008 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328860 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

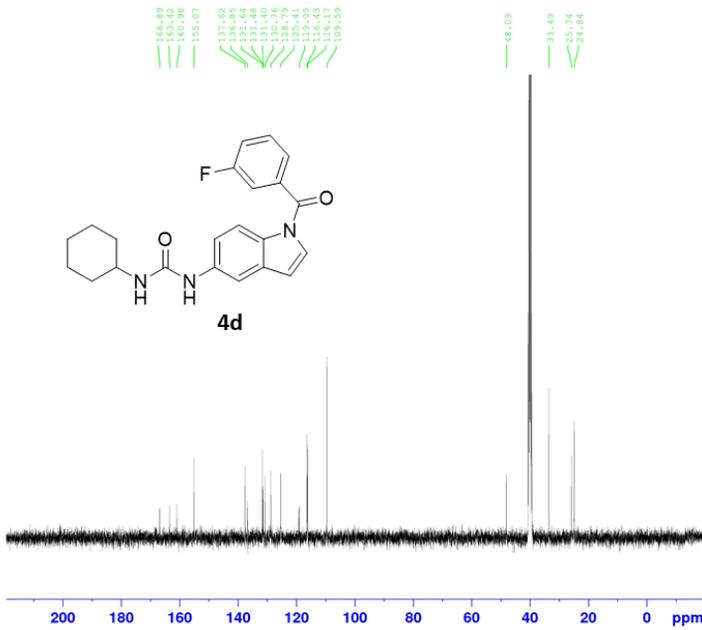


Current Data Parameters  
 NAME AMS-Horedot  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200602  
 Time 9.46  
 INSTRUM spect  
 PROBHD 5 mm FAPBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 133.17  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 296.8 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



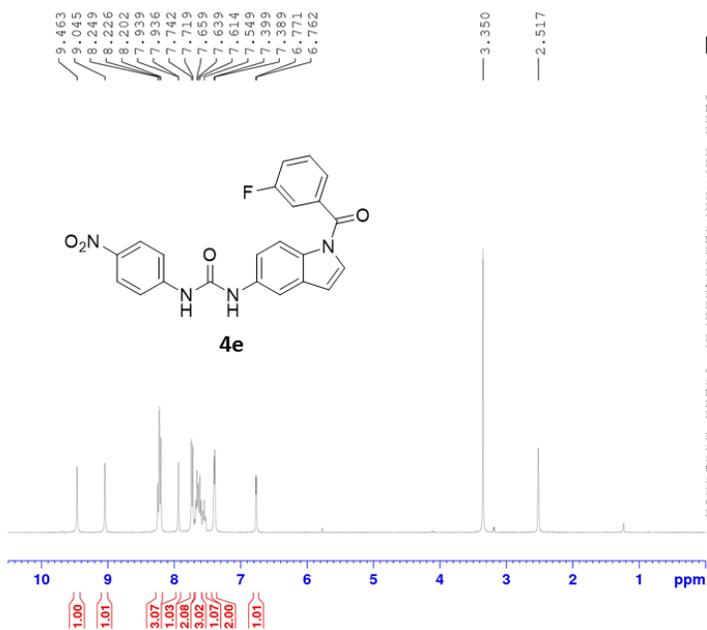
Current Data Parameters  
 NAME AMS-Horedot-CNMR  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200623  
 Time 12.41  
 INSTRUM spect  
 PROBHD 5 mm FAPBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 220  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 299.4 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.2116008 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

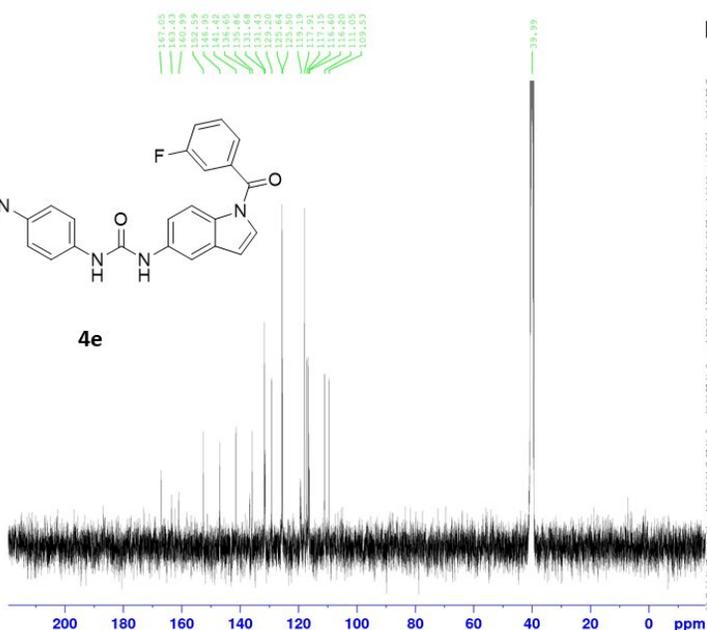


Current Data Parameters  
 NAME AMS-H11  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200402  
 Time 12.27  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 190.62  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



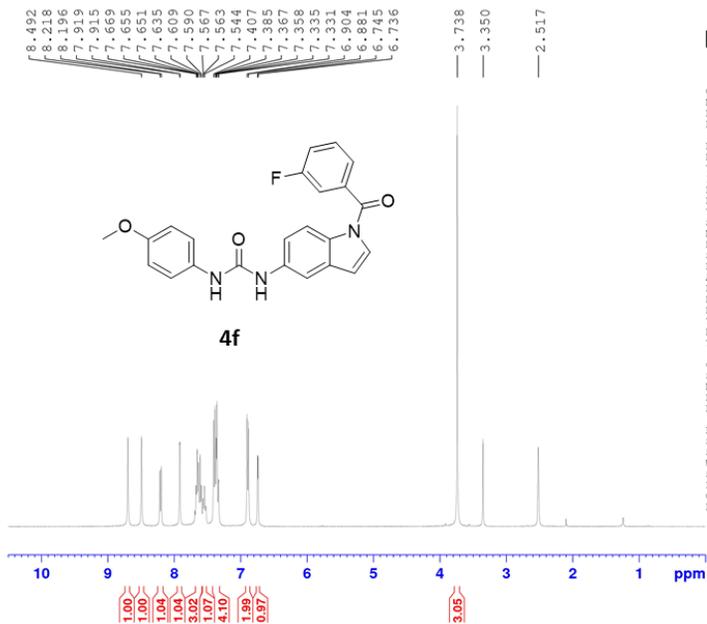
Current Data Parameters  
 NAME AMS-H11\_CNRR  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200711  
 Time 23.36  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 500  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.7 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.2116008 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

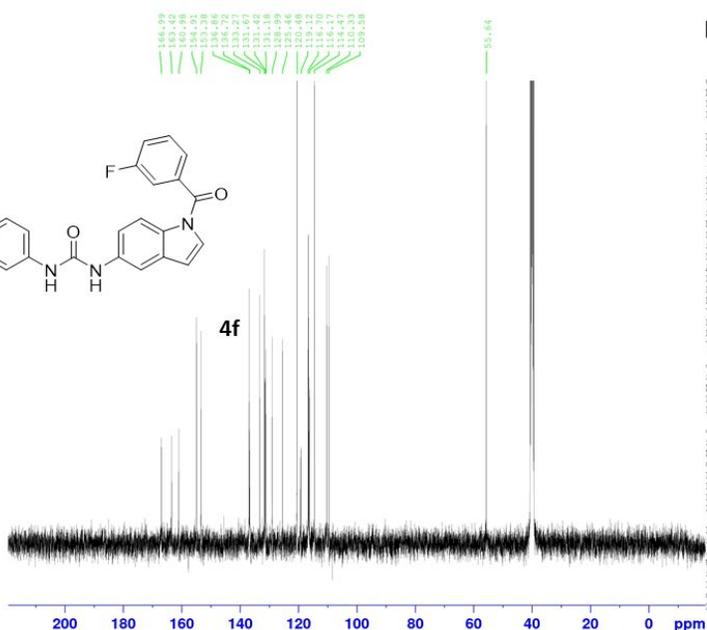


Current Data Parameters  
 NAME AMS-H25  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200408  
 Time 18.59  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 190.62  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.1 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



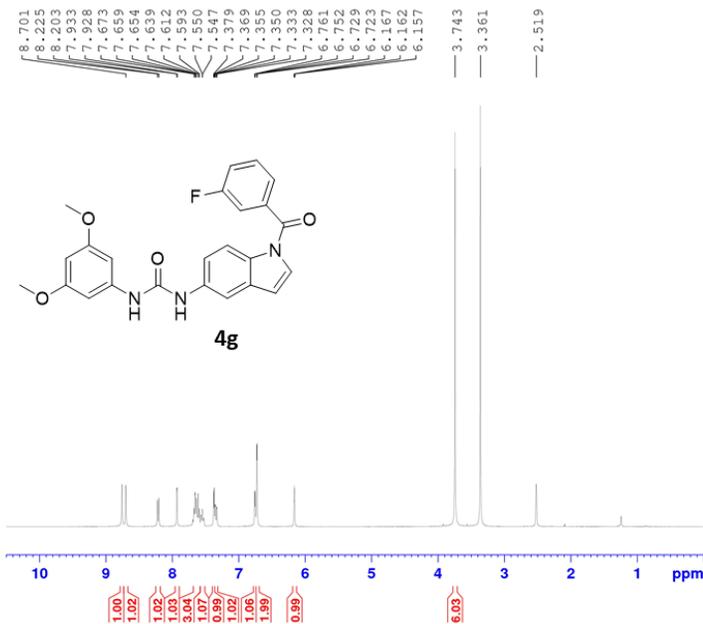
Current Data Parameters  
 NAME AMS-H25\_CNMR  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200711  
 Time 22.33  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 500  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.7 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.2116008 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

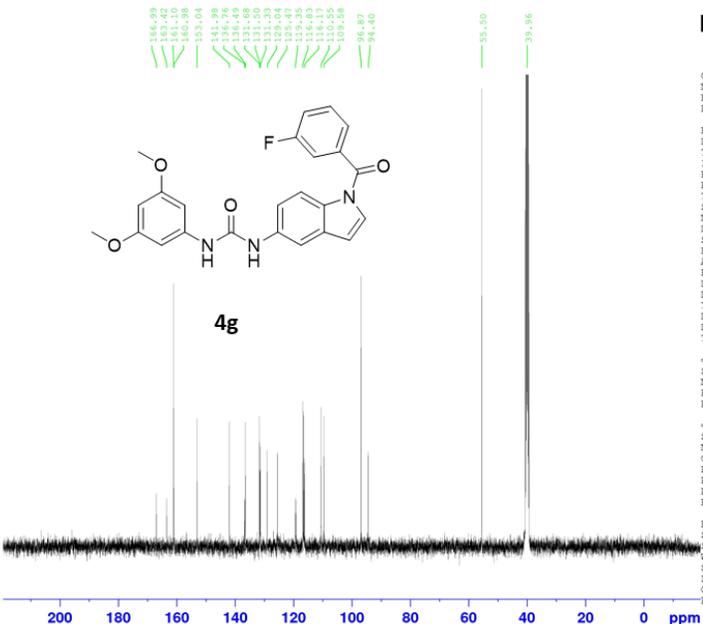


Current Data Parameters  
 NAME AMS-H13  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200402  
 Time 18.59  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.894465 sec  
 RG 190.62  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 297.8 K  
 D1 1.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.0000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



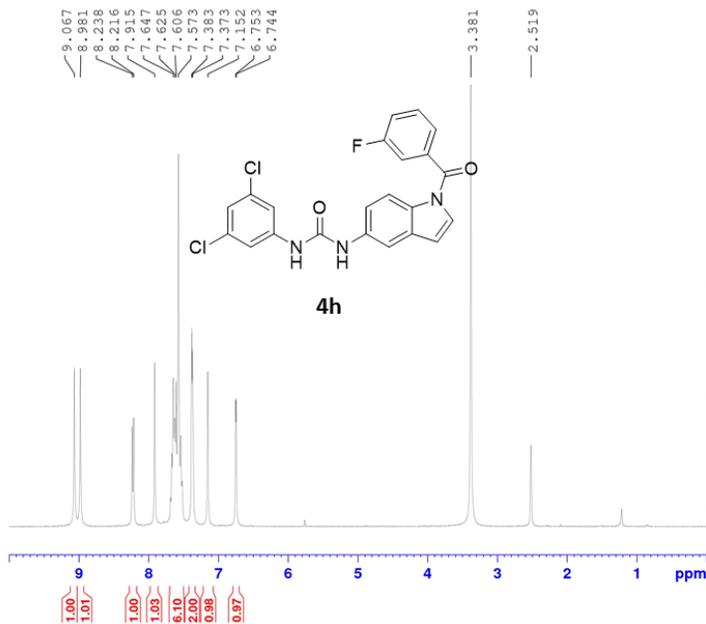
Current Data Parameters  
 NAME AMS-H13\_CNMR  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200712  
 Time 4.16  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 500  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.2631488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.7 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.0000000 W

===== CHANNEL f2 =====  
 SFO2 400.2116008 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.0000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

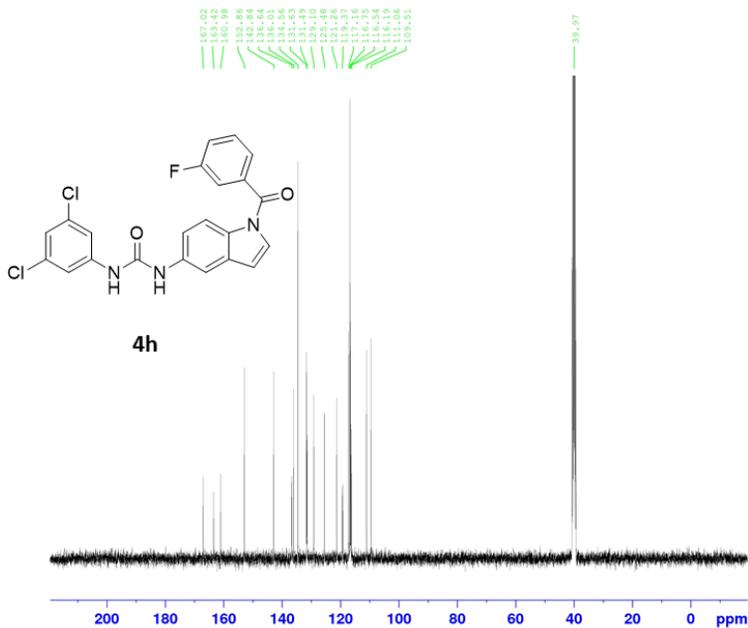


Current Data Parameters  
 NAME AMS-H19  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200421  
 Time 18.42  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 103.95  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 299.2 K  
 D1 1.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



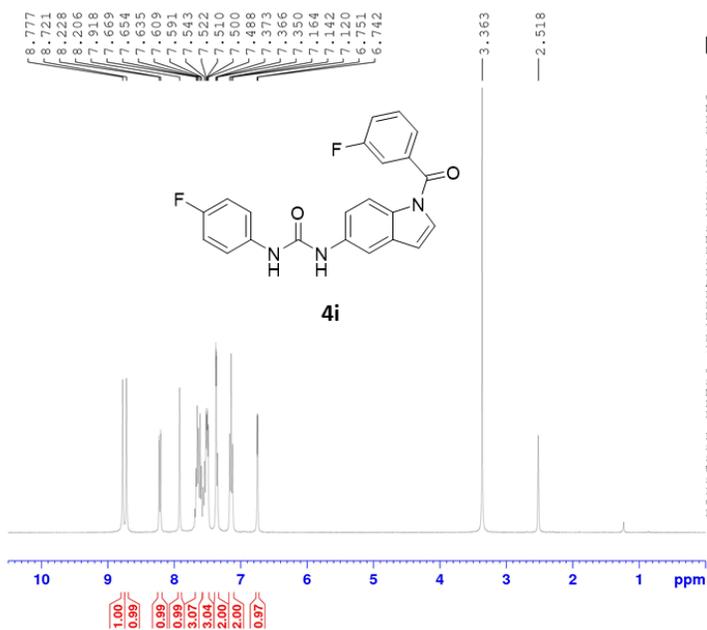
Current Data Parameters  
 NAME AMS-H19\_CNMR  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200712  
 Time 0.07  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 500  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3651488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.7 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.2116008 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



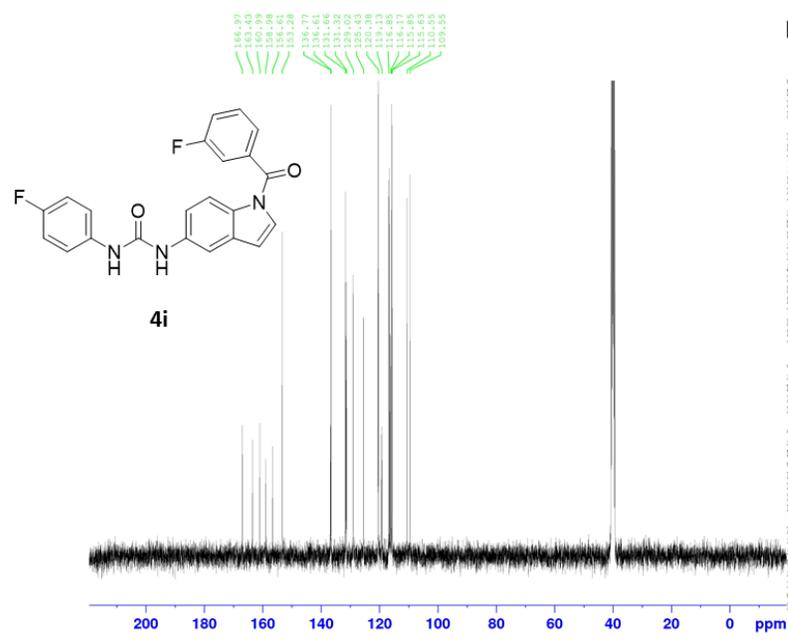
**BRUKER**

Current Data Parameters  
 NAME AMS\_H18  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200429  
 Time 17.35  
 INSTRUM spect  
 PROBHD 5 mm FAPBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 190.62  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 SFO1 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



**BRUKER**

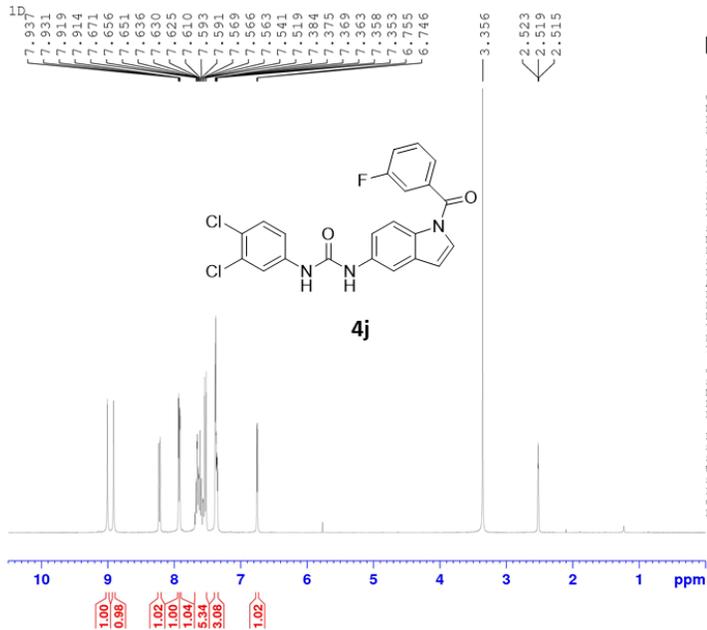
Current Data Parameters  
 NAME AMS-H18\_CNMR  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200713  
 Time 22.37  
 INSTRUM spect  
 PROBHD 5 mm FAPBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 600  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.6 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 SFO1 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

==== CHANNEL f2 =====  
 SFO2 400.2116008 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

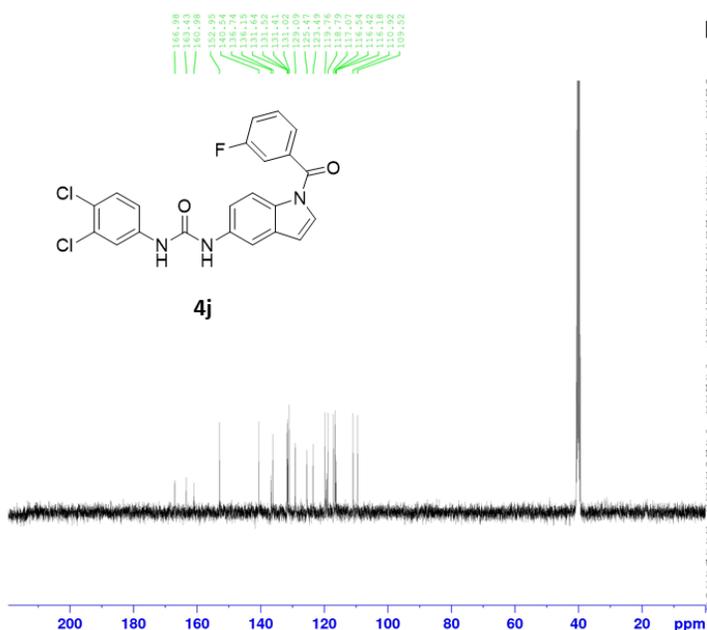


Current Data Parameters  
 NAME AMS-HY  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200622  
 Time 17.52  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 146.31  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 300.3 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



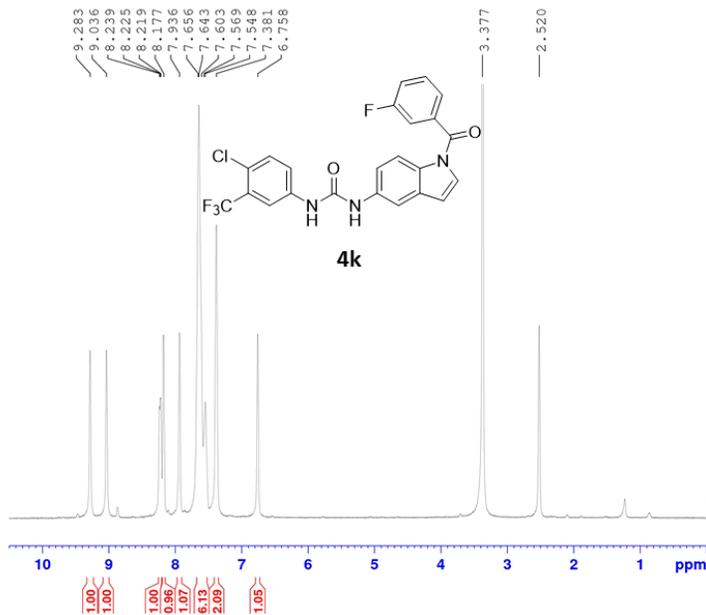
Current Data Parameters  
 NAME AMS-HY  
 EXPNO 20  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200622  
 Time 19.26  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 128  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3651488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 299.9 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.2116008 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

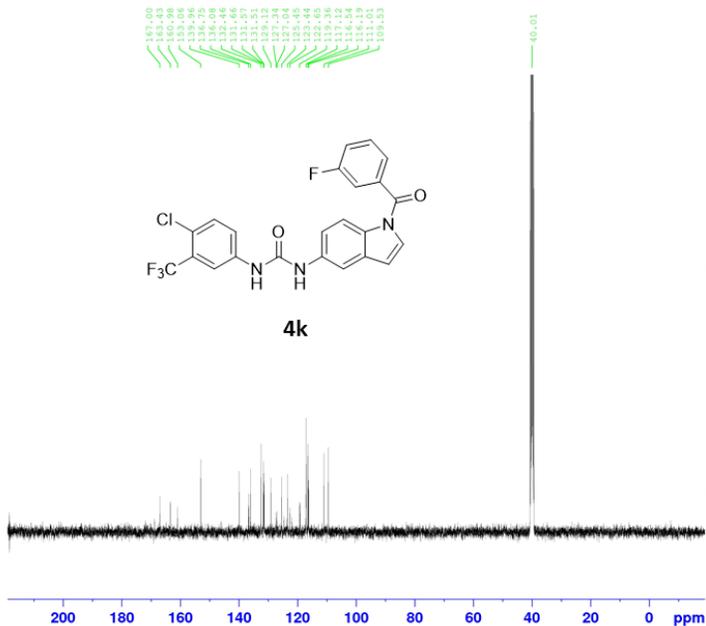


Current Data Parameters  
 NAME AMS-89  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200526  
 Time 19.59  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 190.62  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 297.6 K  
 D1 1.00000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 SFO1 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



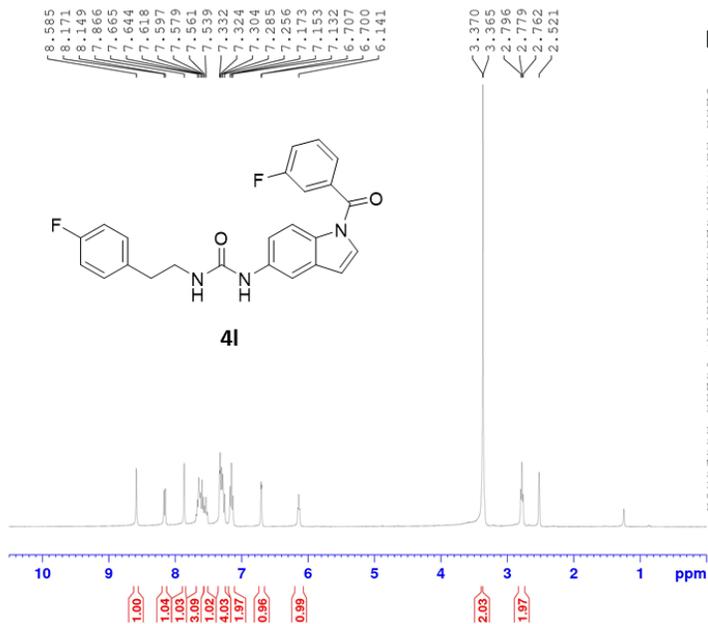
Current Data Parameters  
 NAME 4k\_CNMR  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20201231  
 Time 22.59  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 1000  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 299.3 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 SFO1 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

==== CHANNEL f2 =====  
 SFO2 400.2116008 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

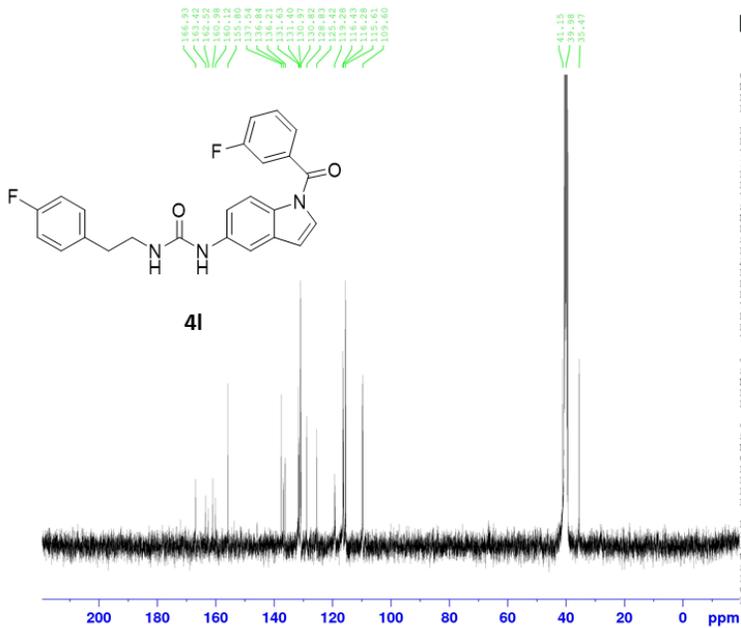


Current Data Parameters  
 NAME AMS-H27F  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200407  
 Time 19.14  
 INSTRUM spect  
 PROBHD 5 mm FAPBBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 190.62  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.1 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



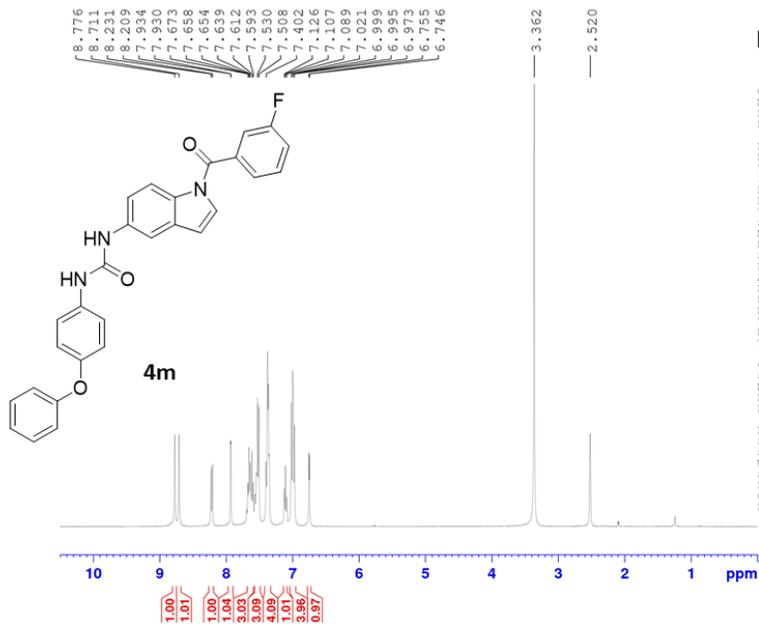
Current Data Parameters  
 NAME AMS-H27\_CNMR  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200711  
 Time 23.05  
 INSTRUM spect  
 PROBHD 5 mm FAPBBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 500  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.7 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.2116008 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

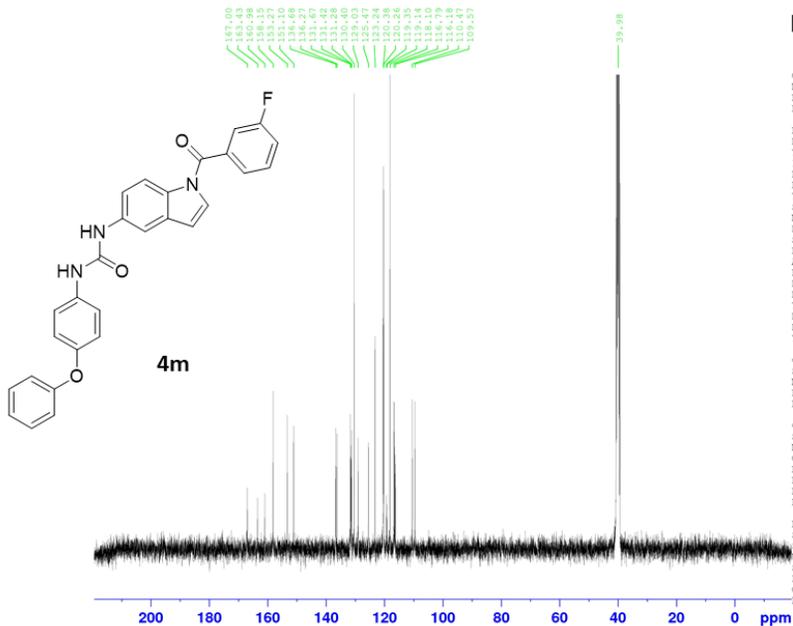


Current Data Parameters  
 NAME AMS-H26  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200407  
 Time 19.08  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 190.62  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.2 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
 NAME AMS-H26\_CNMR  
 EXPNO 10  
 PROCNO 1

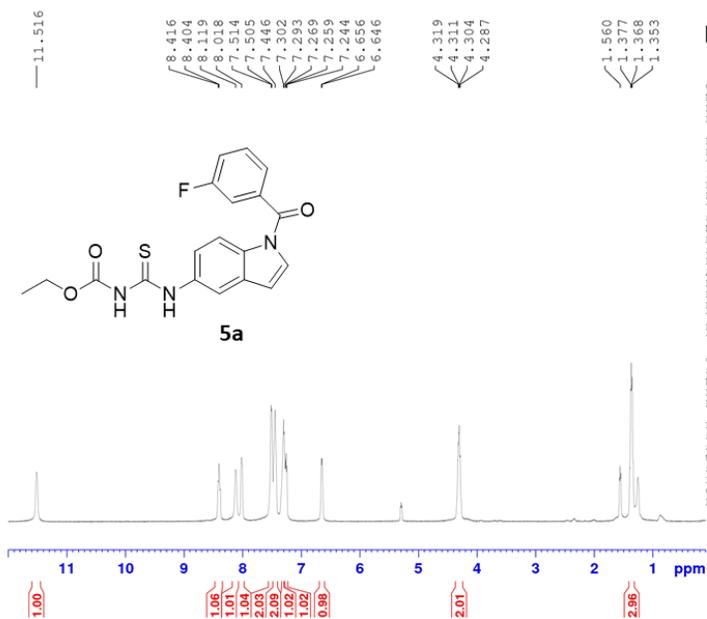
F2 - Acquisition Parameters  
 Date\_ 20200712  
 Time 0.38  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 500  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.2631488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.7 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.2116008 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



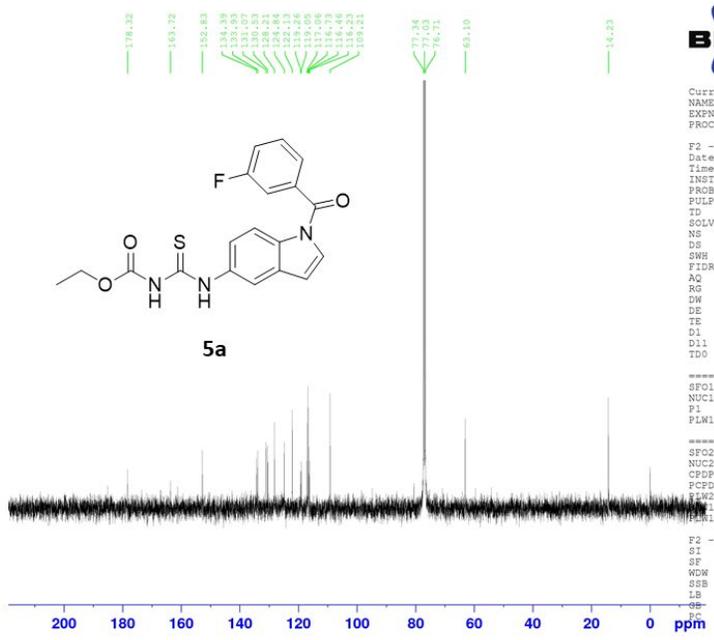


Current Data Parameters  
 NAME AMS-H22.F  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200406  
 Time 20.10  
 INSTRUM spect  
 PROBHD 5 mm FAPBBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 190.62  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 302.0 K  
 D1 1.00000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 SFO1 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100190 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



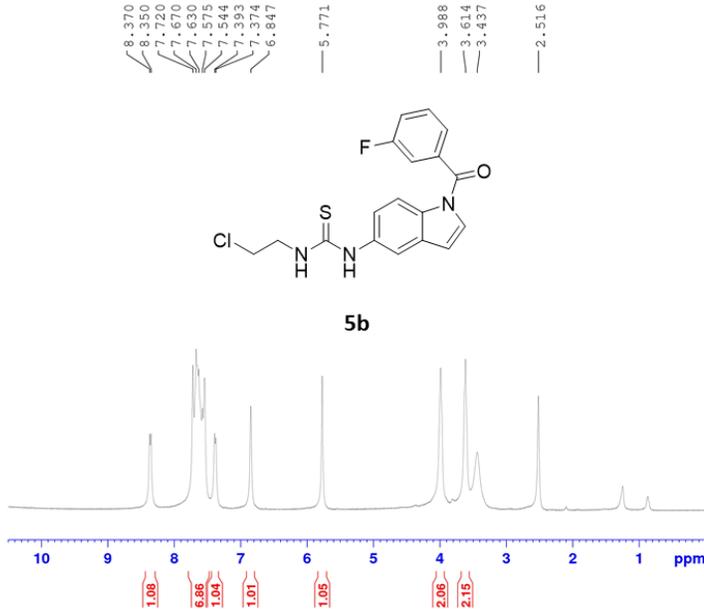
Current Data Parameters  
 NAME AMS-H22\_CNMR  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200713  
 Time 23.58  
 INSTRUM spect  
 PROBHD 5 mm FAPBBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 600  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3651488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 301.5 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 SFO1 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

==== CHANNEL f2 =====  
 SFO2 400.2116008 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 P1W2 12.00000000 W  
 P1W12 0.35777000 W  
 P1W13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

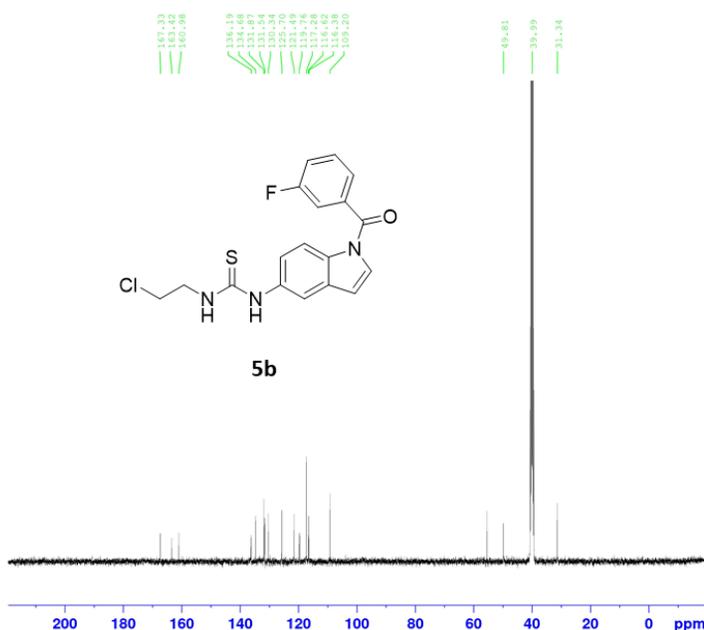


Current Data Parameters  
 NAME AMS-H29  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200423  
 Time 20.07  
 INSTRUM spect  
 PROBHD 5 mm FAPBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 190.62  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.8 K  
 D1 1.0000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 SF01 400.214715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.0000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



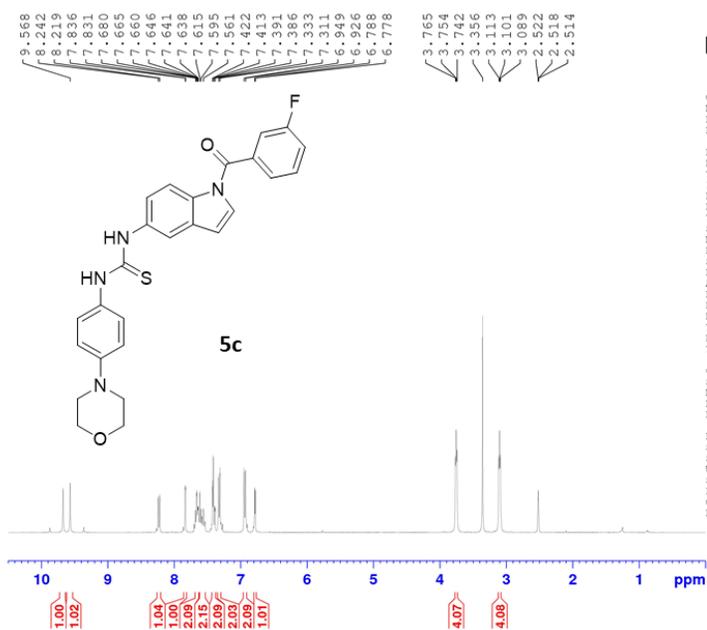
Current Data Parameters  
 NAME AMS-H29\_CNMR  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200712  
 Time 3.14  
 INSTRUM spect  
 PROBHD 5 mm FAPBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 500  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.2631488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.7 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TDO 1

==== CHANNEL f1 =====  
 SF01 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.0000000 W

==== CHANNEL f2 =====  
 SF02 400.2116008 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.0000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

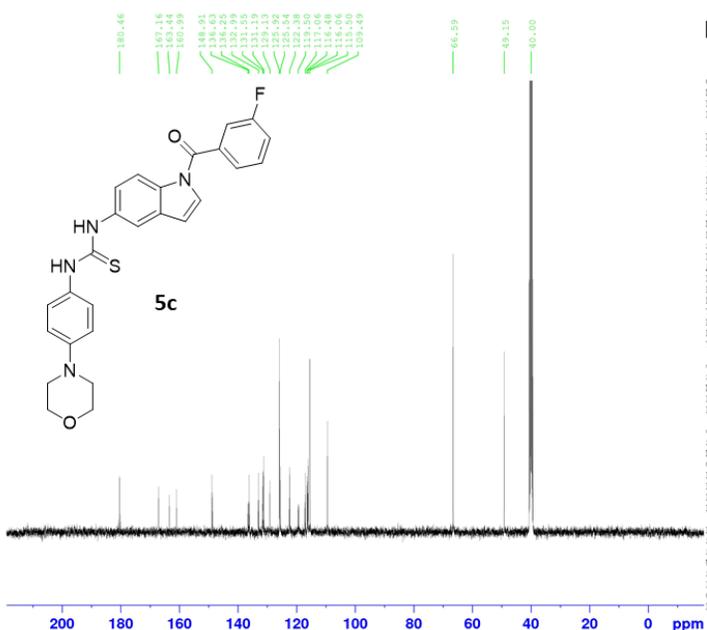


Current Data Parameters  
 NAME AMS\_H30  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200429  
 Time 17.30  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 119.61  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.2 K  
 D1 1.00000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 SFO1 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



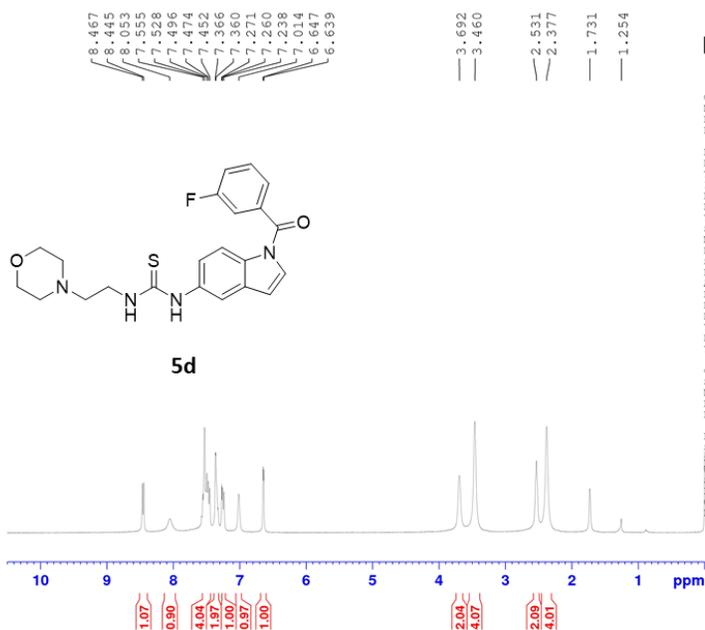
Current Data Parameters  
 NAME AMS-H30\_CNMR  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200712  
 Time 1.09  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 500  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.2631488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.7 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 SFO1 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

==== CHANNEL f2 =====  
 SFO2 400.2116008 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

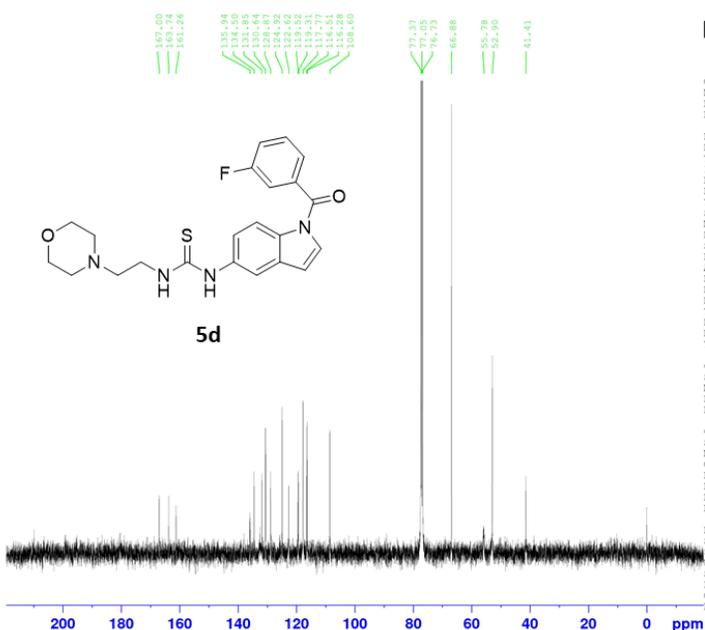


Current Data Parameters  
 NAME AMS-H32(CDCl3)  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200518  
 Time 18.03  
 INSTRUM spect  
 PROBHD 5 mm FAPBBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 190.62  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.0 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100086 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
 NAME AMS-H32\_CNMR  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200714  
 Time 0.37  
 INSTRUM spect  
 PROBHD 5 mm FAPBBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 600  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3651488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 300.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

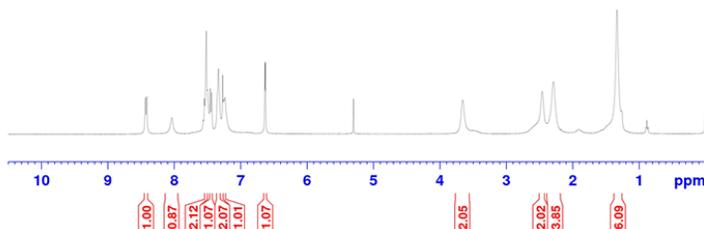
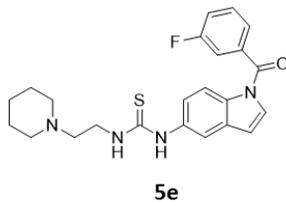
===== CHANNEL f2 =====  
 SFO2 400.2116008 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

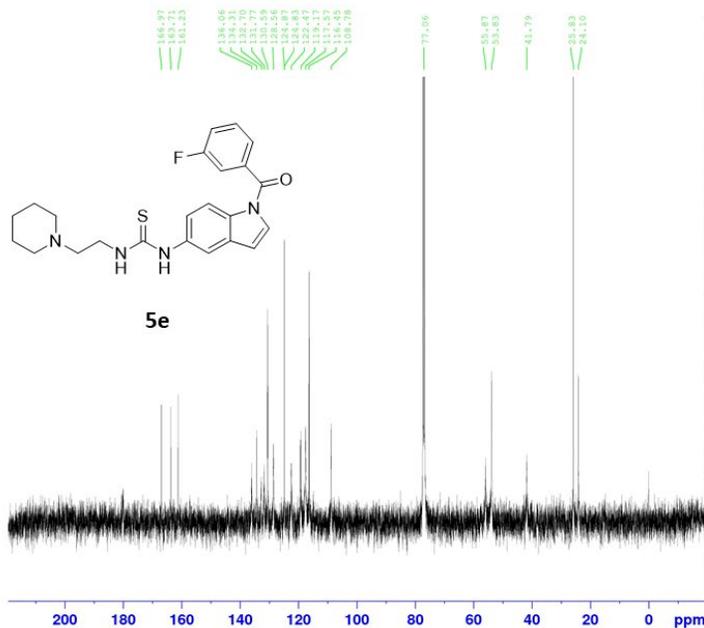
8.435  
8.414  
8.037  
7.545  
7.516  
7.501  
7.459  
7.437  
7.334  
7.272  
7.256  
7.237  
6.635  
6.626  
— 5.301  
— 3.655  
— 2.457  
— 2.289  
— 1.332  
— 1.264  
— 0.882



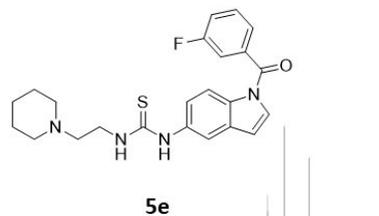
Current Data Parameters  
NAME AMS-H33  
EXPNO 1  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20200527  
Time 19.07  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 133.17  
DM 62.400 usec  
DE 6.50 usec  
TE 297.1 K  
D1 1.00000000 sec  
TDO 1



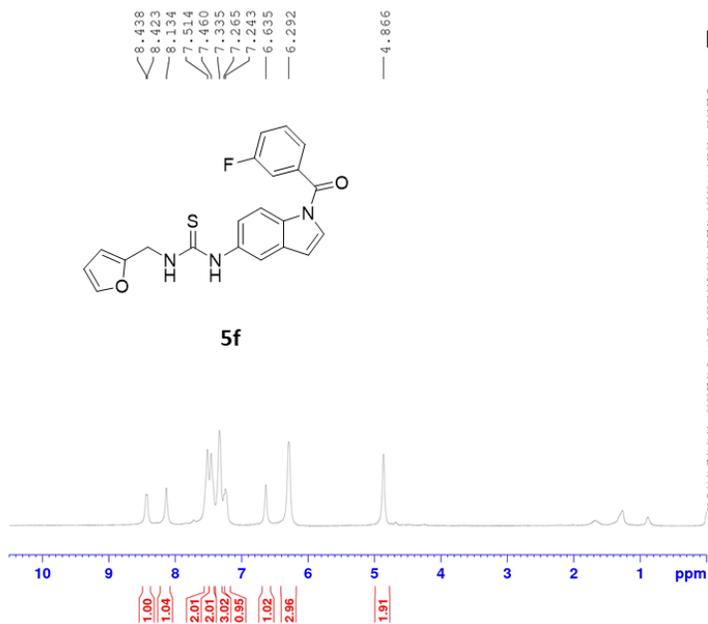
===== CHANNEL f1 =====  
SFO1 400.2124715 MHz  
NUC1 1H  
P1 15.54 usec  
PLW1 12.00000000 W  
F2 - Processing parameters  
SI 65536  
SF 400.2100090 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00



Current Data Parameters  
NAME AMS-H33\_CNMR  
EXPNO 10  
PROCNO 1  
F2 - Acquisition Parameters  
Date\_ 20200714  
Time 1.53  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 600  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 190.62  
DM 20.800 usec  
DE 6.50 usec  
TE 302.4 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1



===== CHANNEL f1 =====  
SFO1 100.6429474 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 52.00000000 W  
===== CHANNEL f2 =====  
SFO2 400.2116008 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 12.00000000 W  
PLW12 0.35777000 W  
PLW13 0.28979000 W  
F2 - Processing parameters  
SI 32768  
SF 100.6328850 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

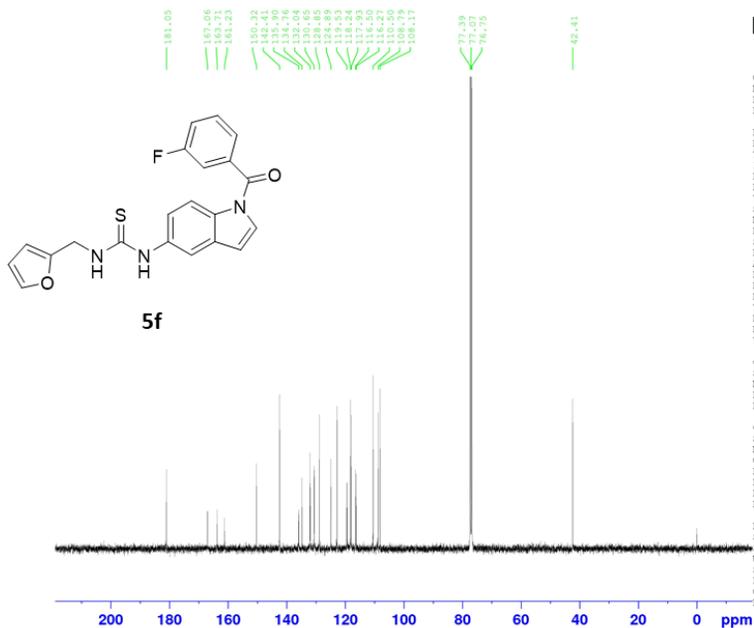


Current Data Parameters  
 NAME AMS-H16  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200410  
 Time 12.43  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 133.17  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.2 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100120 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



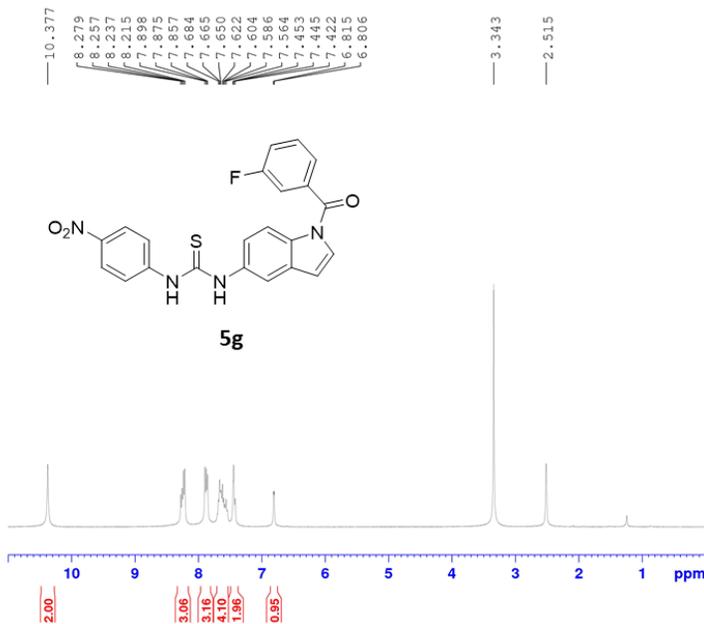
Current Data Parameters  
 NAME AMS-H16\_CNMR  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200713  
 Time 23.15  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 600  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.2631488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.8 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.2116008 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

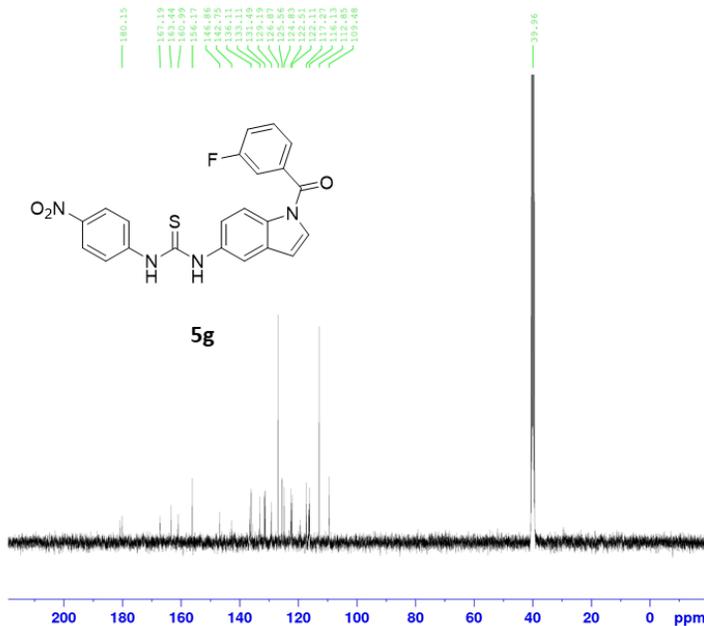


Current Data Parameters  
 NAME AMS-H17  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200423  
 Time 20.02  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 190.62  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 299.0 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SF01 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



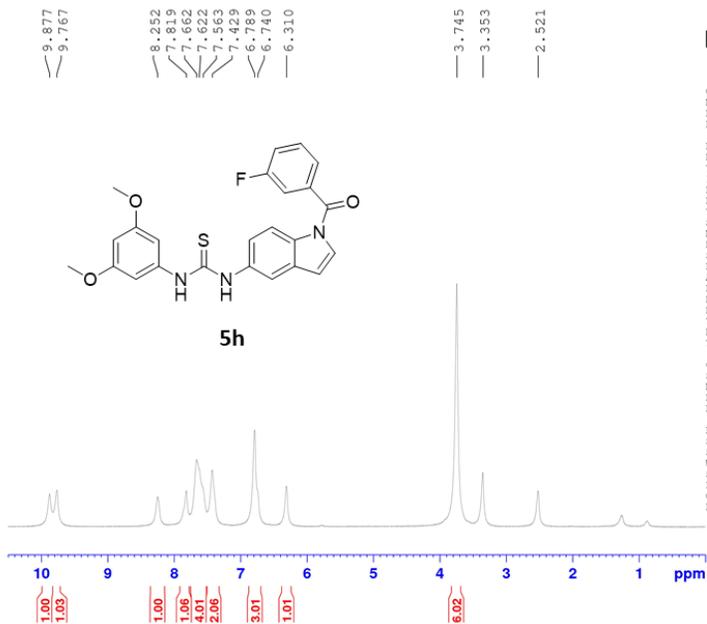
Current Data Parameters  
 NAME AMS-H17\_CNMR  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200711  
 Time 20.13  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 500  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.7 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SF01 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

===== CHANNEL f2 =====  
 SF02 400.2116008 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

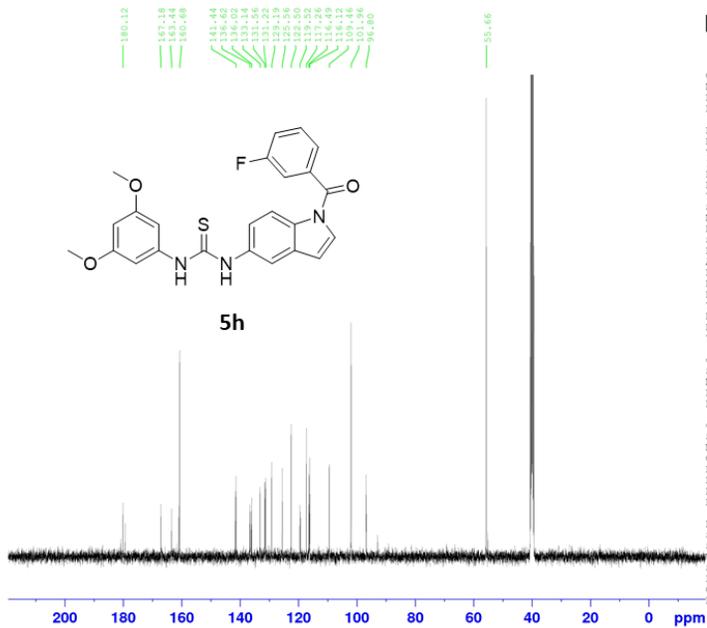


Current Data Parameters  
 NAME AMS-H24  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200410  
 Time 12.53  
 INSTRUM spect  
 PROBHD 5 mm FAPBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 133.17  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.1 K  
 D1 1.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



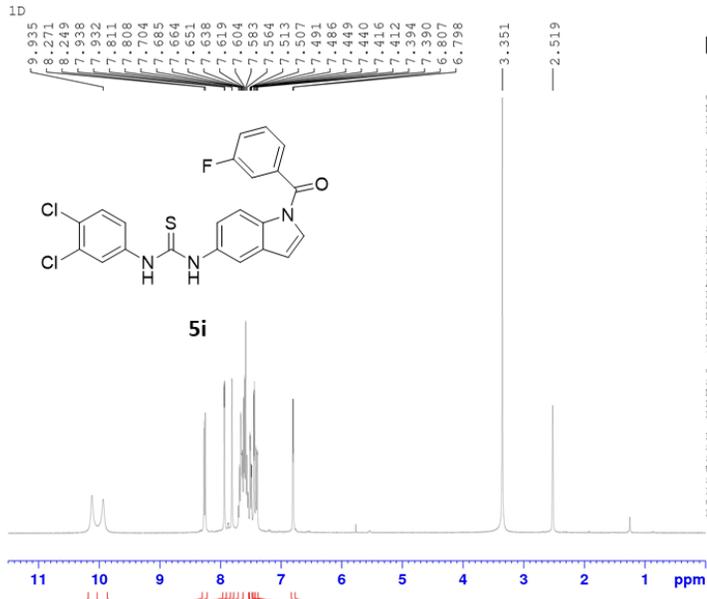
Current Data Parameters  
 NAME AMS-H24\_CNMR  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200712  
 Time 2.42  
 INSTRUM spect  
 PROBHD 5 mm FAPBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 500  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.2631488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.7 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.2116008 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

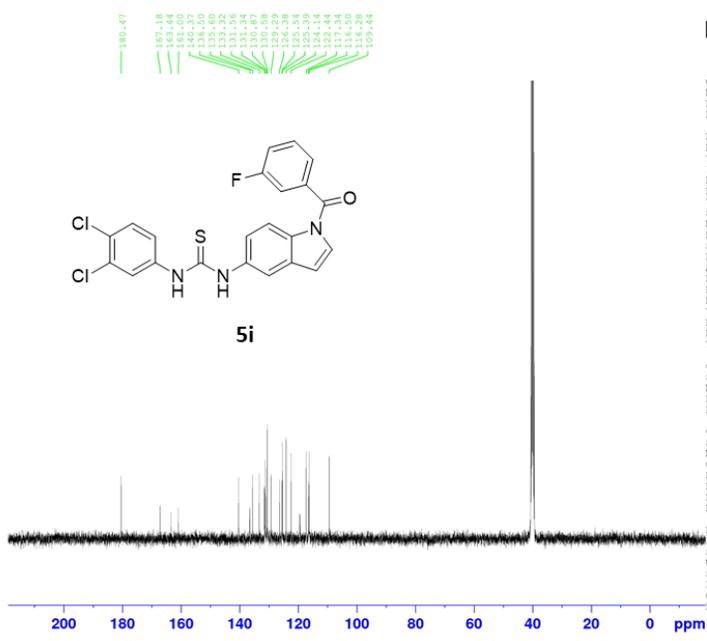


Current Data Parameters  
 NAME AMS-HZ  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200622  
 Time 17.49  
 INSTRUM spect  
 PROBHD 5 mm FAPBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 146.31  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 300.3 K  
 D1 1.00000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 SFO1 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
 NAME AMS-HZ  
 EXPNO 20  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200622  
 Time 19.14  
 INSTRUM spect  
 PROBHD 5 mm FAPBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 256  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 300.3 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 SFO1 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

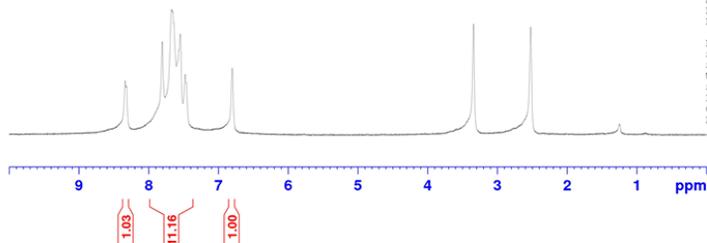
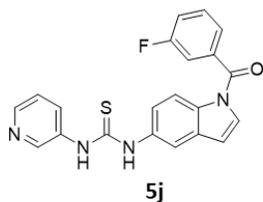
==== CHANNEL f2 =====  
 SFO2 400.2116008 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

8.339  
8.321  
7.806  
7.671  
7.548  
7.478  
6.802

3.341

2.523



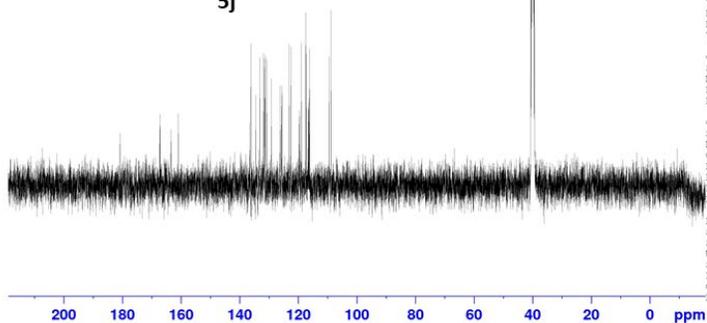
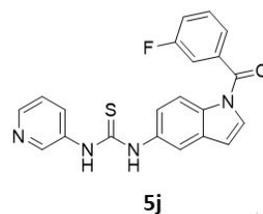
Current Data Parameters  
NAME AMS-H23-F  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20200421  
Time 18.35  
INSTRUM spect  
PROBHD 5 mm F4BBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT DMSO  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 190.62  
DM 62.400 usec  
DE 6.50 usec  
TE 298.9 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 400.2124715 MHz  
NUC1 1H  
P1 15.54 usec  
PLW1 12.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.2100000 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

180.82  
162.18  
161.44  
161.00  
136.12  
134.48  
133.80  
131.80  
130.77  
128.19  
125.56  
122.48  
117.55  
117.46  
116.66  
109.48  
108.84  
40.00



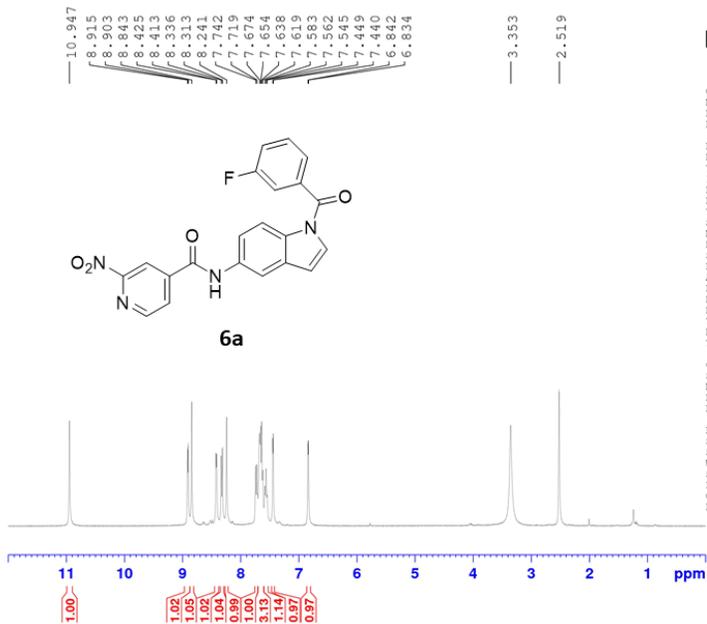
Current Data Parameters  
NAME AMS-H23\_CNMR  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20200711  
Time 21.31  
INSTRUM spect  
PROBHD 5 mm F4BBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT DMSO  
NS 500  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 190.62  
DM 20.800 usec  
DE 6.50 usec  
TE 296.7 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 100.6429474 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 52.00000000 W

===== CHANNEL f2 =====  
SFO2 400.2116008 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 12.00000000 W  
PLW12 0.35777000 W  
PLW13 0.28979000 W

F2 - Processing parameters  
SI 32768  
SF 100.6328850 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



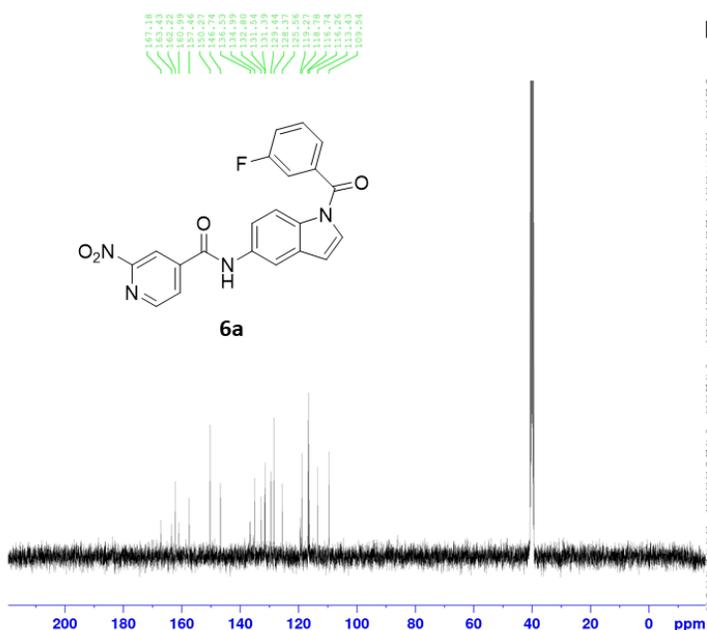
**BRUKER**

Current Data Parameters  
 NAME AMS-H1  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200421  
 Time 18.29  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 190.62  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.4 K  
 D1 1.00000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 SFO1 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



**BRUKER**

Current Data Parameters  
 NAME AMS-H1\_CNMR  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20201130  
 Time 12.48  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 500  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 299.2 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

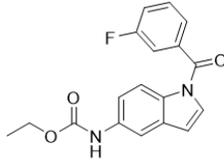
==== CHANNEL f1 =====  
 SFO1 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

==== CHANNEL f2 =====  
 SFO2 400.2116008 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

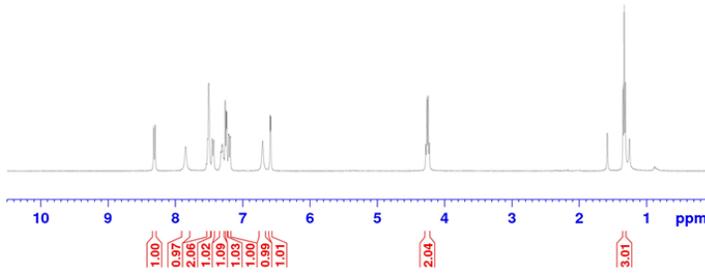
F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

8.322  
8.300  
7.848  
7.520  
7.505  
7.451  
7.431  
7.323  
7.307  
7.300  
7.291  
7.260  
7.245  
7.236  
7.210  
7.206  
7.188  
7.184  
6.705  
6.592  
6.583  
4.281  
4.264  
4.246  
4.228

1.585  
1.351  
1.333  
1.315



6b



Current Data Parameters  
NAME AMS-HT-F  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20200408  
Time 19.54  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.089465 sec  
RG 190.62  
DW 62.400 usec  
DE 6.50 usec  
TE 298.0 K  
D1 1.00000000 sec  
TDO 1

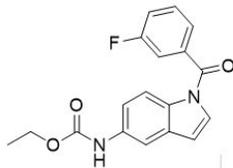
===== CHANNEL f1 =====  
SFO1 400.2124715 MHz  
NUC1 1H  
P1 15.54 usec  
PLW1 12.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.2100132 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

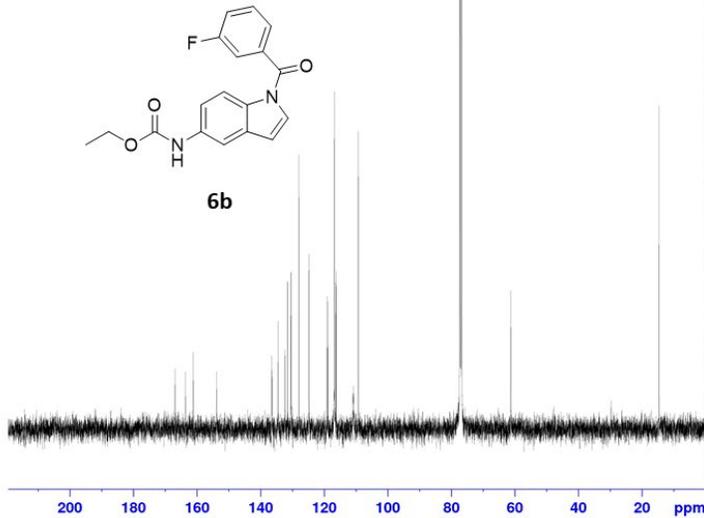
166.91  
163.69  
161.21  
153.87  
136.48  
134.50  
133.52  
133.38  
132.77  
127.06  
117.12  
116.83  
107.27

77.85  
77.03  
76.72  
61.26

14.61



6b



Current Data Parameters  
NAME AMS-HT\_CNRR  
EXPNO 10  
PROCNO 1

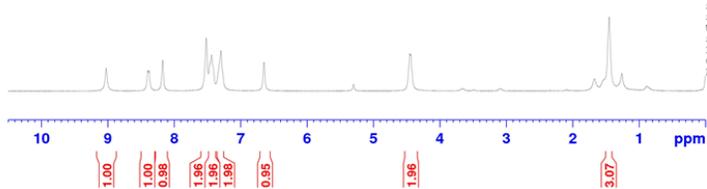
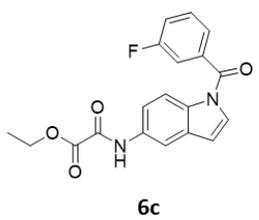
F2 - Acquisition Parameters  
Date\_ 20200714  
Time 1.16  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 600  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3651488 sec  
RG 190.62  
DW 20.800 usec  
DE 6.50 usec  
TE 301.4 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 100.6429474 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 52.00000000 W

===== CHANNEL f2 =====  
SFO2 400.2116008 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 12.00000000 W  
PLW12 0.35777000 W  
PLW13 0.28979000 W

F2 - Processing parameters  
SI 32768  
SF 100.6328850 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

9.025  
8.397  
8.378  
8.174  
7.518  
7.438  
7.297  
6.649  
4.452  
4.438  
1.670  
1.449  
1.258



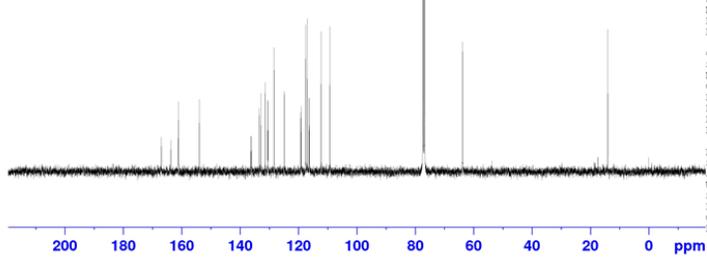
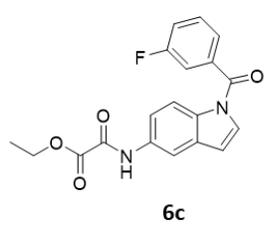
Current Data Parameters  
NAME AMS-H8  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20200515  
Time 17.44  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zg30  
TD 65536  
SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 190.62  
DM 62.400 usec  
DE 6.50 usec  
TE 298.0 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 400.2124715 MHz  
NUC1 1H  
P1 15.54 usec  
PLW1 12.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.2101116 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

167.00  
165.69  
161.12  
153.92  
135.16  
133.39  
132.81  
132.53  
130.35  
128.35  
119.04  
117.51  
116.44  
115.21  
109.26  
77.37  
77.06  
76.74  
63.77  
14.04



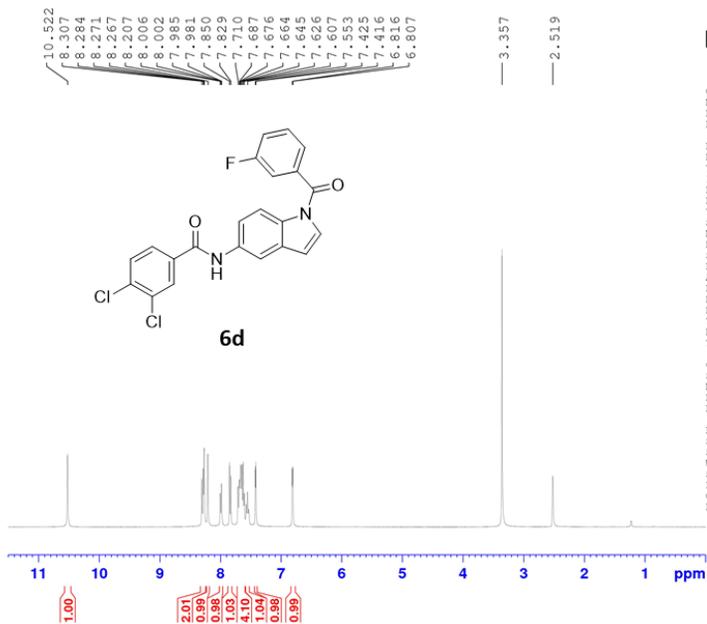
Current Data Parameters  
NAME AMS-H8\_CNMR  
EXPNO 10  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20200713  
Time 21.55  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 450  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 190.62  
DM 20.800 usec  
DE 6.50 usec  
TE 299.1 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

===== CHANNEL f1 =====  
SFO1 100.6429474 MHz  
NUC1 13C  
P1 10.00 usec  
PLW1 52.00000000 W

===== CHANNEL f2 =====  
SFO2 400.2116008 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
PCPD2 90.00 usec  
PLW2 12.00000000 W  
PLW12 0.35777000 W  
PLW13 0.28979000 W

F2 - Processing parameters  
SI 32768  
SF 100.6328850 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

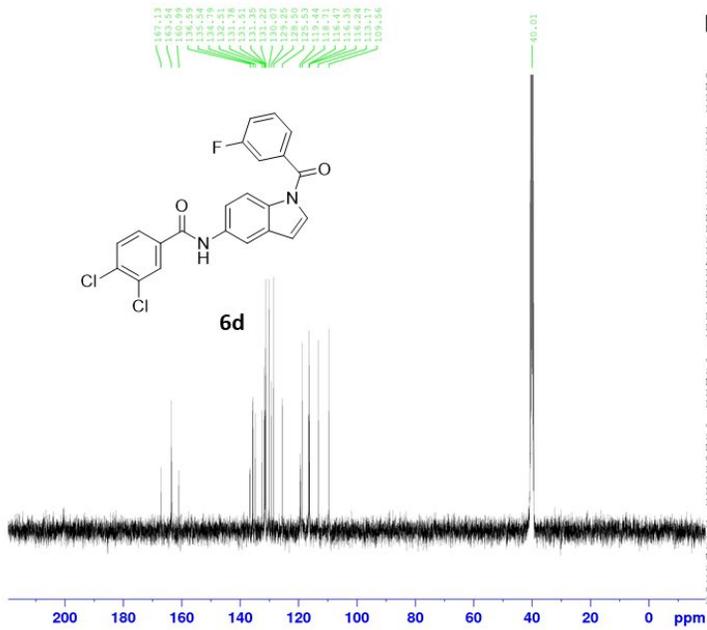


Current Data Parameters  
 NAME AMS-HX  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200623  
 Time 11.56  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 146.31  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.4 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SF01 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
 NAME AMS-HX  
 EXPNO 11  
 PROCNO 1

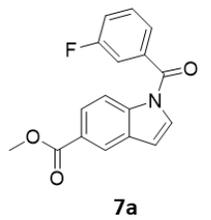
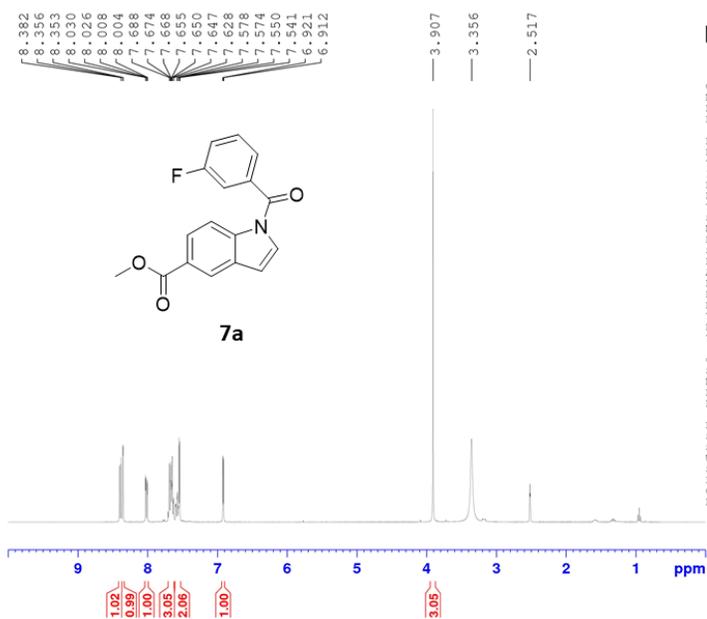
F2 - Acquisition Parameters  
 Date\_ 20200623  
 Time 12.13  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 256  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 299.8 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SF01 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

===== CHANNEL f2 =====  
 SF02 400.2116008 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



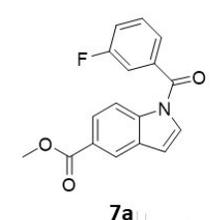
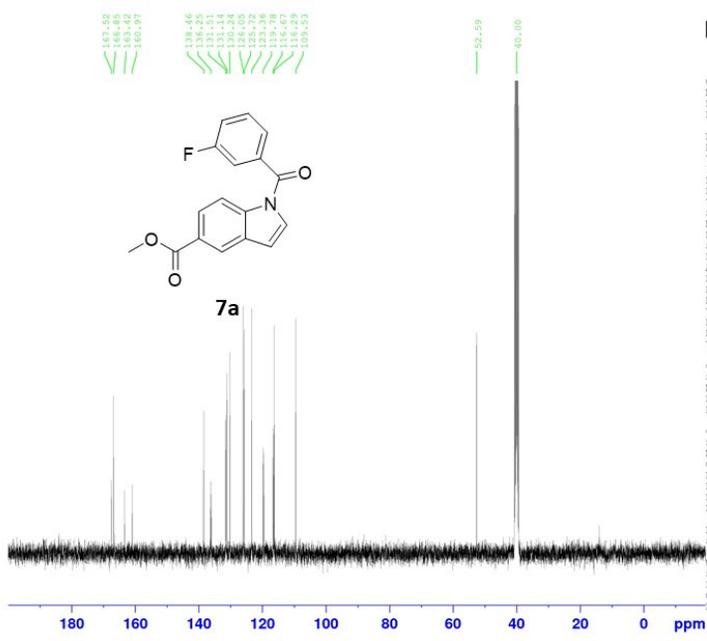


Current Data Parameters  
 NAME AMS-38  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200831  
 Time 16.49  
 INSTRUM spect  
 PROBHD 5 mm FABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 171.62  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 297.9 K  
 D1 1.00000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 SFO1 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



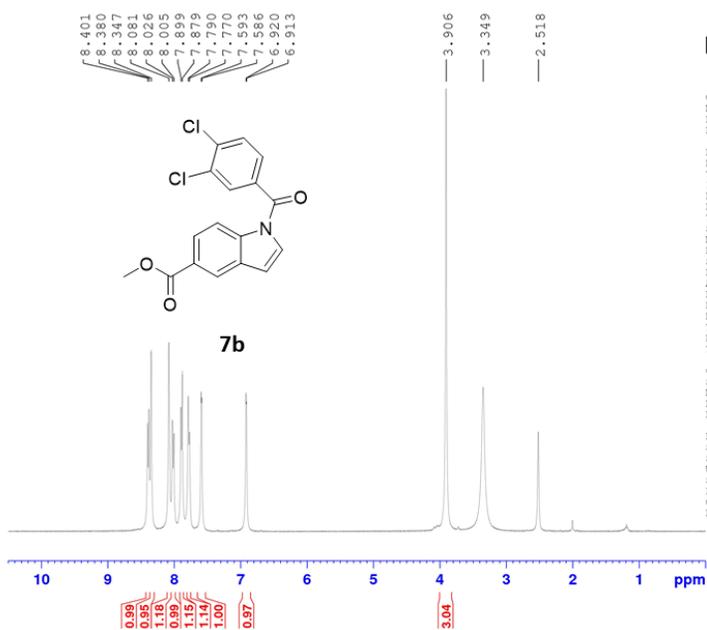
Current Data Parameters  
 NAME AMS-38  
 EXPNO 11  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200831  
 Time 17.13  
 INSTRUM spect  
 PROBHD 5 mm FABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 400  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.6 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 SFO1 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

==== CHANNEL f2 =====  
 SFO2 400.2116008 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

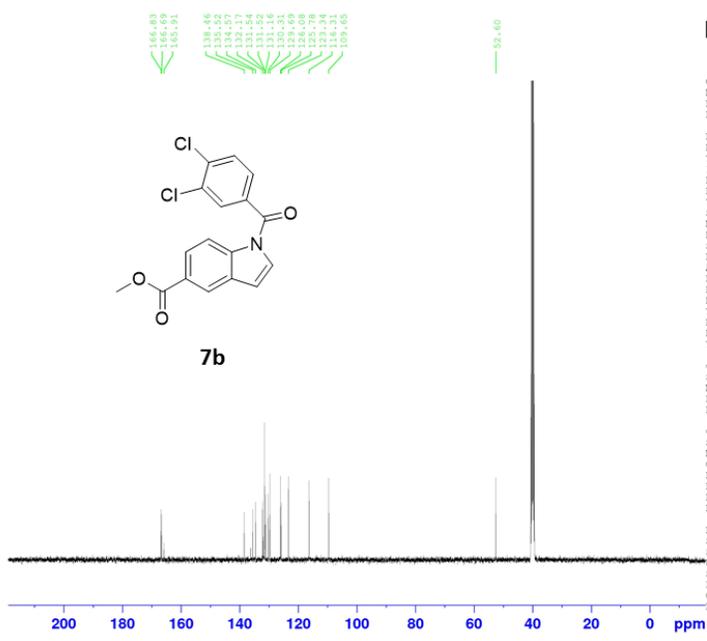


Current Data Parameters  
 NAME AMS-H49  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200925  
 Time 18.08  
 INSTRUM spect  
 PROBHD 5 mm FAPBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 190.62  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 297.7 K  
 D1 1.00000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 SF01 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



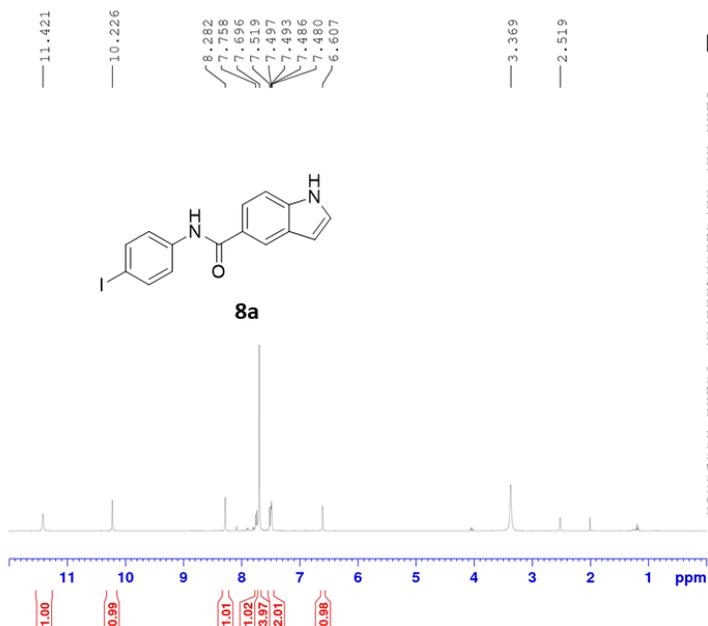
Current Data Parameters  
 NAME AMS-H49-CNMR  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20200925  
 Time 23.00  
 INSTRUM spect  
 PROBHD 5 mm FAPBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 1024  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.2651488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.7 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 SF01 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

==== CHANNEL f2 =====  
 SF02 400.2116008 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40



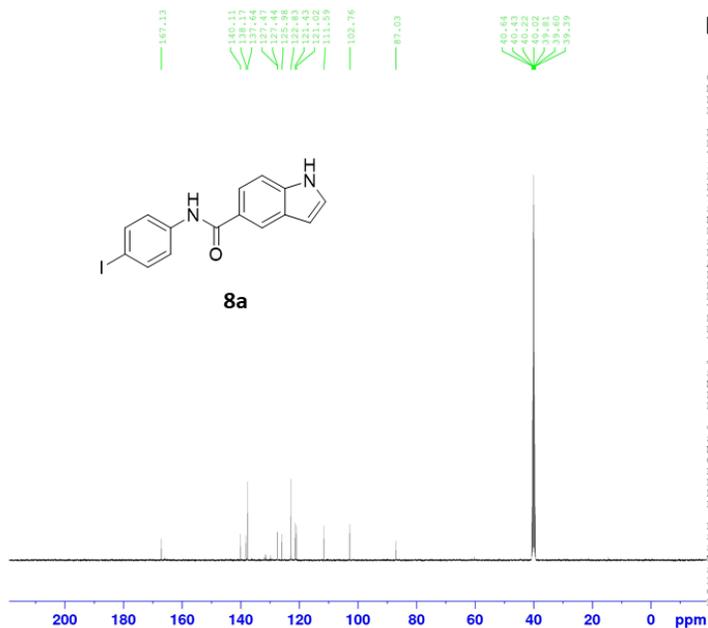
```

Current Data Parameters
NAME      A-H41 (2nd)
EXPNO    10
PROCNO   1

F2 - Acquisition Parameters
Date_    20201020
Time     20.05
INSTRUM spect
PROBHD   5 mm PABBO BB/
PULPROG zg30
TD       65536
SOLVENT  DMSO
NS       16
DS       2
SWH      8012.820 Hz
FIDRES   0.122266 Hz
AQ       4.0894465 sec
RG       146.31
DM       62.400 usec
DE       6.50 usec
TE       298.1 K
D1       1.00000000 sec
TDO      1

===== CHANNEL f1 =====
SFO1    400.2124715 MHz
NUC1    1H
P1      15.54 usec
PLW1    12.00000000 W

F2 - Processing parameters
SI      65536
SF      400.2100000 MHz
WDW     EM
SSB     0
LB      0.30 Hz
GB      0
PC      1.00
  
```



```

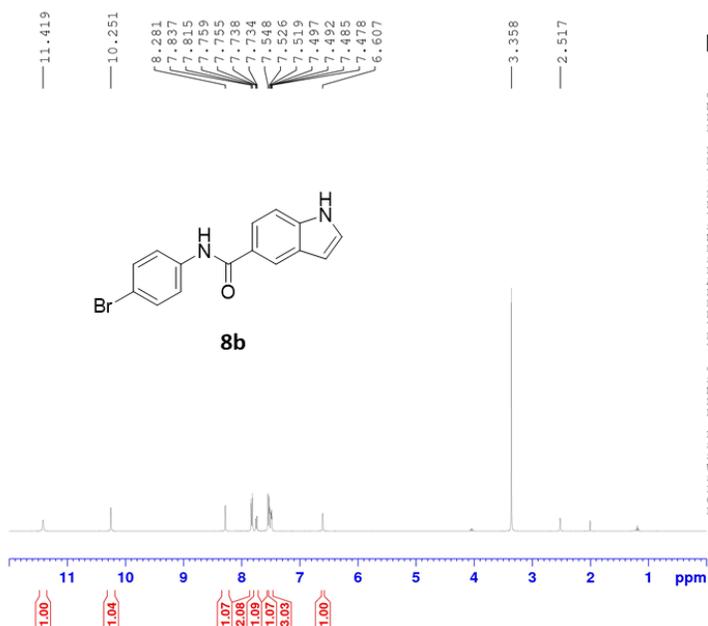
Current Data Parameters
NAME      A-H41_CNMR
EXPNO    10
PROCNO   1

F2 - Acquisition Parameters
Date_    20201022
Time     22.42
INSTRUM spect
PROBHD   5 mm PABBO BB/
PULPROG zgpg30
TD       65536
SOLVENT  DMSO
NS       700
DS       4
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ       1.3631488 sec
RG       190.62
DM       20.800 usec
DE       6.50 usec
TE       299.6 K
D1       2.00000000 sec
D11      0.03000000 sec
TDO      1

===== CHANNEL f1 =====
SFO1    100.6429474 MHz
NUC1    13C
P1      10.00 usec
PLW1    52.00000000 W

===== CHANNEL f2 =====
SFO2    400.2116008 MHz
NUC2    1H
CPDPRG2 waltz16
PCPD2   90.00 usec
PLW2    12.00000000 W
PLW12   0.35777000 W
PLW13   0.28979000 W

F2 - Processing parameters
SI      32768
SF      100.6328850 MHz
WDW     EM
SSB     0
LB      1.00 Hz
GB      0
PC      1.40
  
```

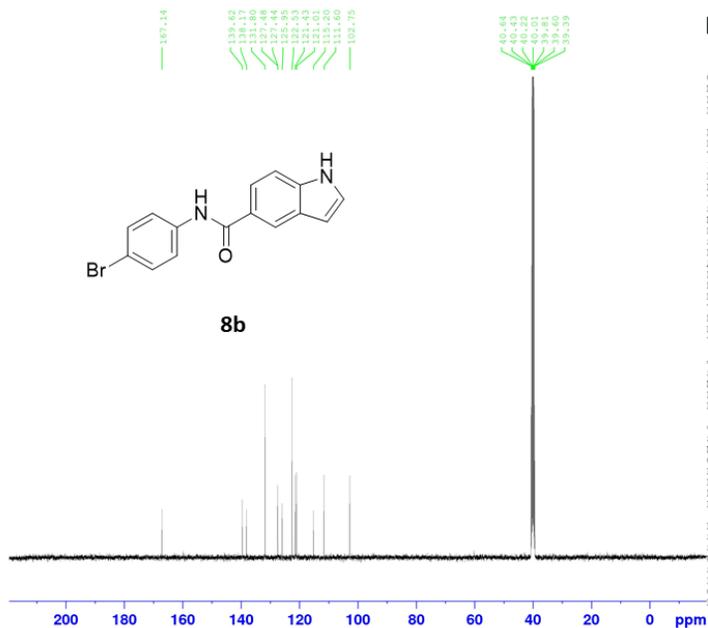


Current Data Parameters  
 NAME H-42  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20201022  
 Time 10.53  
 INSTRUM spect  
 PROBHD 5 mm FABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 171.62  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.7 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



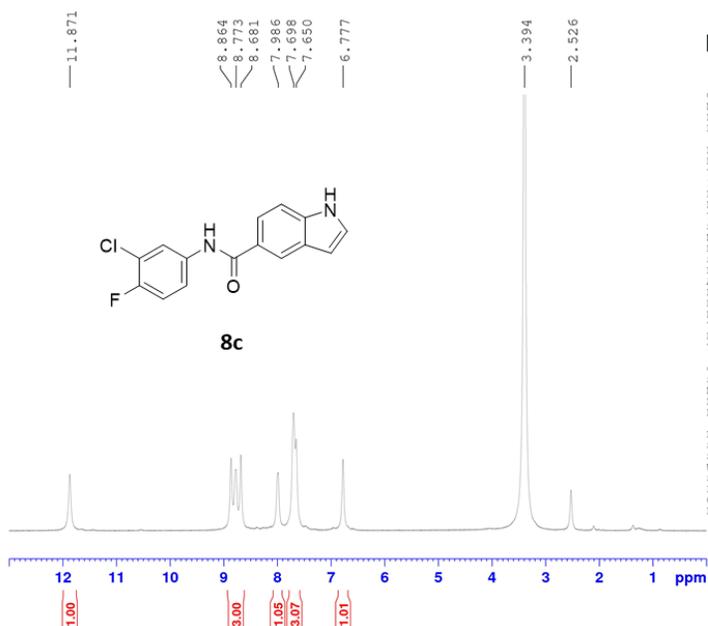
Current Data Parameters  
 NAME A-H42\_CNMR  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20201022  
 Time 23.28  
 INSTRUM spect  
 PROBHD 5 mm FABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 700  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.2631488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 299.5 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.2116008 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

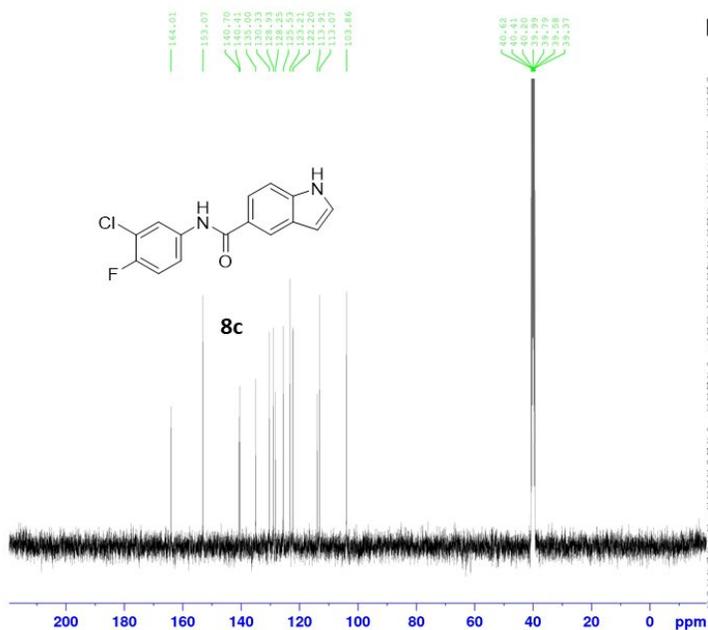


Current Data Parameters  
 NAME A-H43\_HNMR  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20201029  
 Time 19.10  
 INSTRUM spect  
 PROBHD 5 mm F4BBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 133.17  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.3 K  
 D1 1.0000000 sec  
 TDO 1

==== CHANNEL f1 =====  
 SF01 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



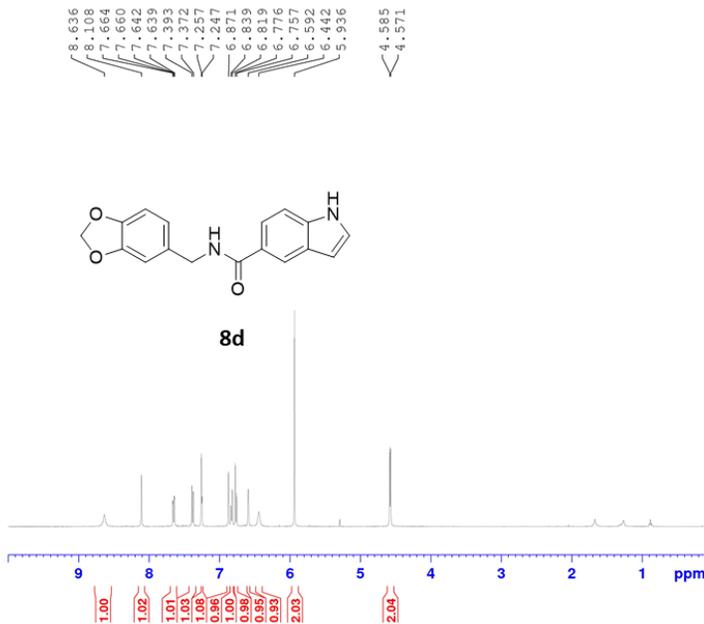
Current Data Parameters  
 NAME A-H43\_CNMR  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20201029  
 Time 19.58  
 INSTRUM spect  
 PROBHD 5 mm F4BBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 450  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 299.4 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TDO 1

==== CHANNEL f1 =====  
 SF01 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

==== CHANNEL f2 =====  
 SF02 400.2116008 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

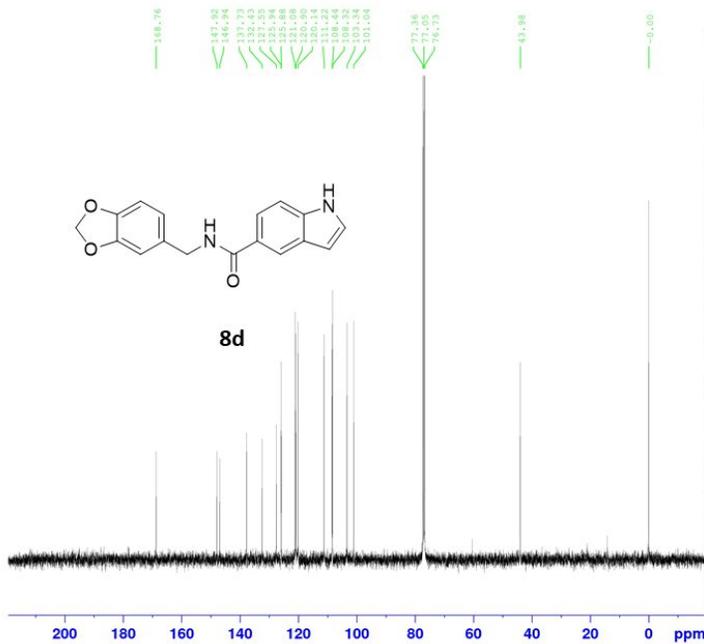


Current Data Parameters  
 NAME A-H57f\_BNMR  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20201023  
 Time 18.09  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 190.62  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 298.4 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100146 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



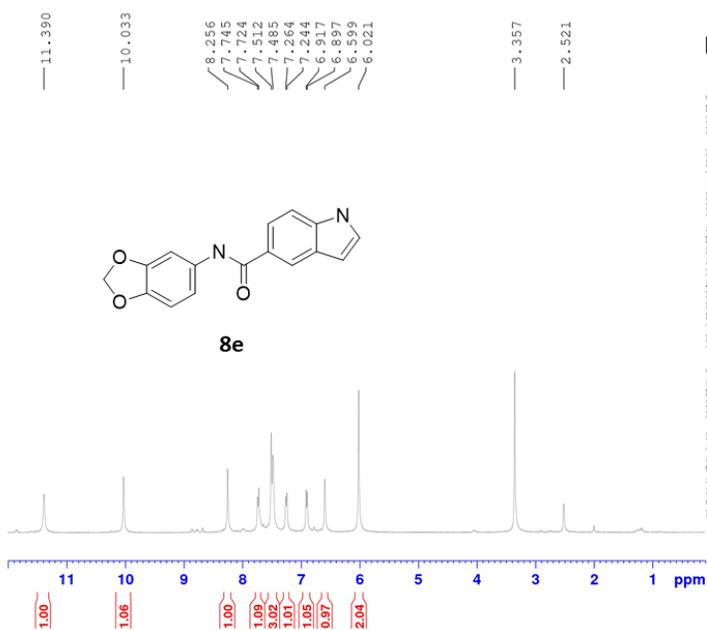
Current Data Parameters  
 NAME AMS-H57  
 EXPNO 11  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20201008  
 Time 20.50  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 250  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 300.1 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.2116008 MHz  
 NUC2 1H  
 CPDPRG[2] waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6328876 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

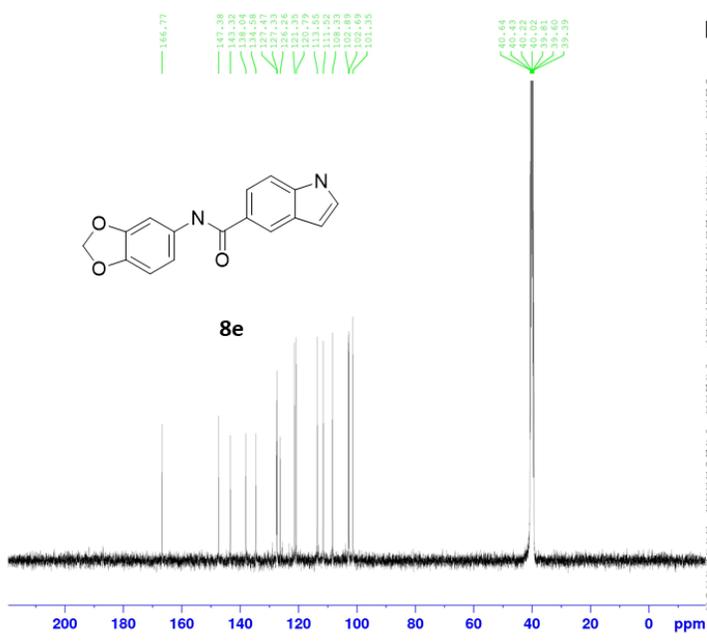


Current Data Parameters  
 NAME H58  
 EXPNO 10  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20201009  
 Time 0.27  
 INSTRUM spect  
 PROBHD 5 mm FAPBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT DMSO  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 146.31  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 300.3 K  
 D1 1.00000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 400.2124715 MHz  
 NUC1 1H  
 P1 15.54 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2100000 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00



Current Data Parameters  
 NAME H58  
 EXPNO 11  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20201009  
 Time 1.53  
 INSTRUM spect  
 PROBHD 5 mm FAPBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 1500  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 190.62  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 299.8 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TDO 1

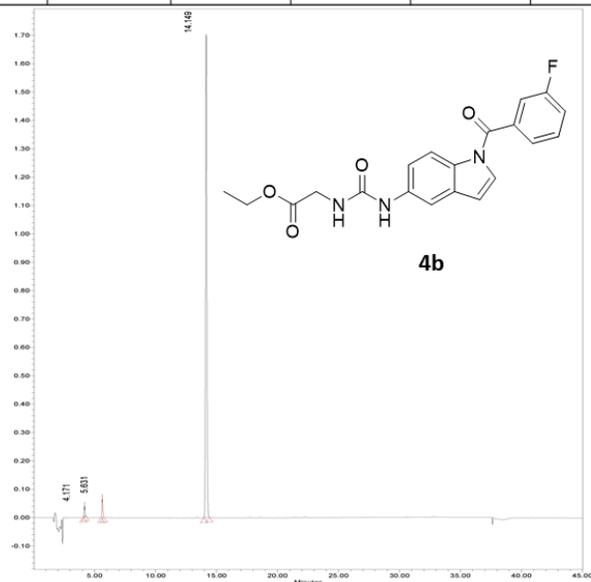
===== CHANNEL f1 =====  
 SFO1 100.6429474 MHz  
 NUC1 13C  
 P1 10.00 usec  
 PLW1 52.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.2116008 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.35777000 W  
 PLW13 0.28979000 W

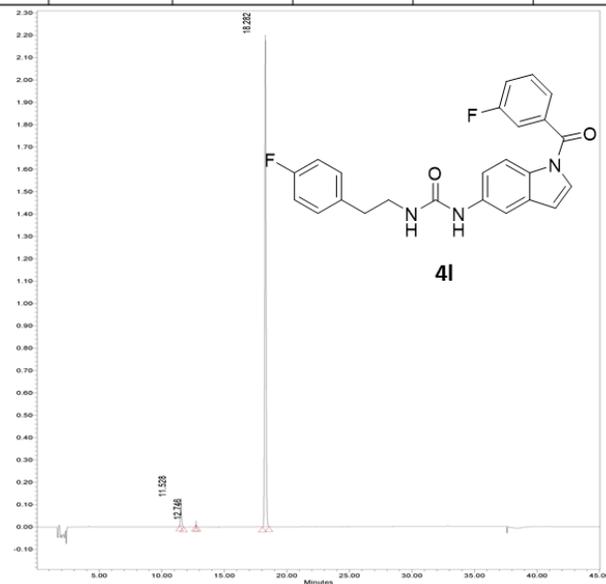
F2 - Processing parameters  
 SI 32768  
 SF 100.6328850 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

## 2. Representative HPLC purity data of the compounds

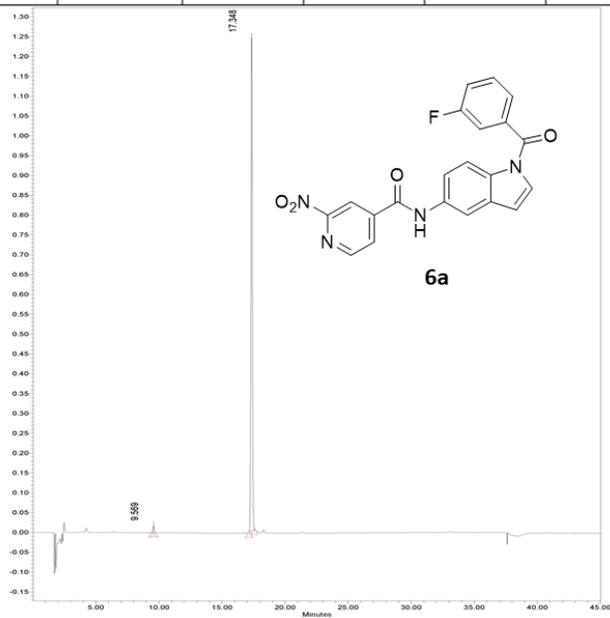
Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area ( $\mu\text{V}\cdot\text{sec}$ )	% Area	Height ( $\mu\text{V}$ )	Int Type	Amount
1	4.171							182884	1.44	36389	bb	
2	5.631							362117	2.86	67497	bb	
3	14.149							12135189	95.70	1702752	bb	



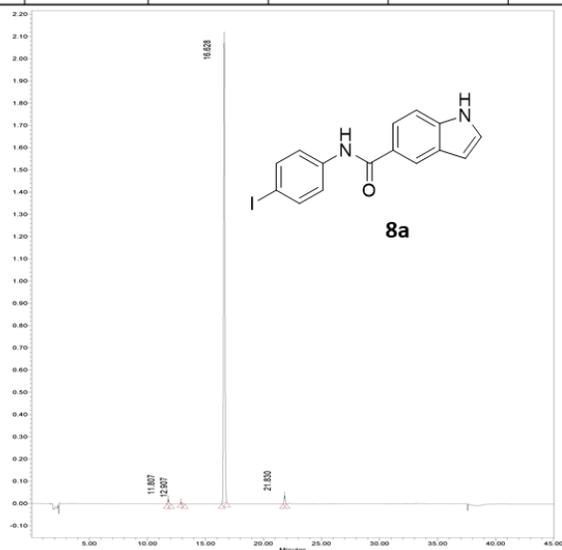
Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area ( $\mu\text{V}\cdot\text{sec}$ )	% Area	Height ( $\mu\text{V}$ )	Int Type	Amount
1	11.528							722618	4.30	108944	bb	
2	12.746							34035	0.20	6370	bb	
3	18.282							16041627	95.50	2201606	bb	



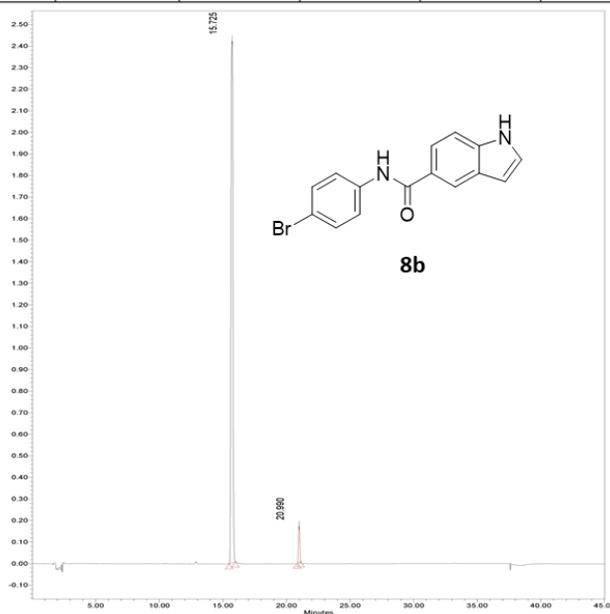
Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area ( $\mu\text{V}\cdot\text{sec}$ )	% Area	Height ( $\mu\text{V}$ )	Int Type	Amount
1	9.569							84076	0.88	14431	bb	
2	17.348							9455947	99.12	1252820	bb	



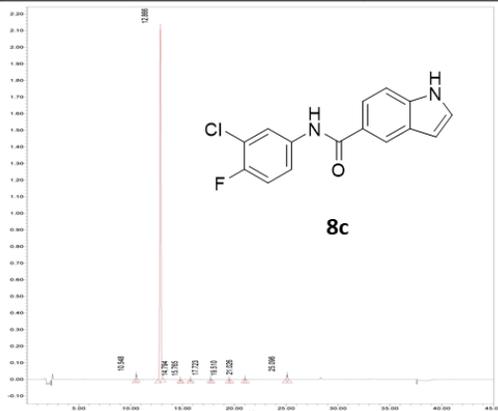
Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area ( $\mu\text{V}\cdot\text{sec}$ )	% Area	Height ( $\mu\text{V}$ )	Int Type	Amount
1	11.807							143417	0.85	20959	bb	
2	12.907							36312	0.21	4101	bb	
3	16.628							16480558	97.34	2106271	bb	
4	21.830							271366	1.60	37619	bb	



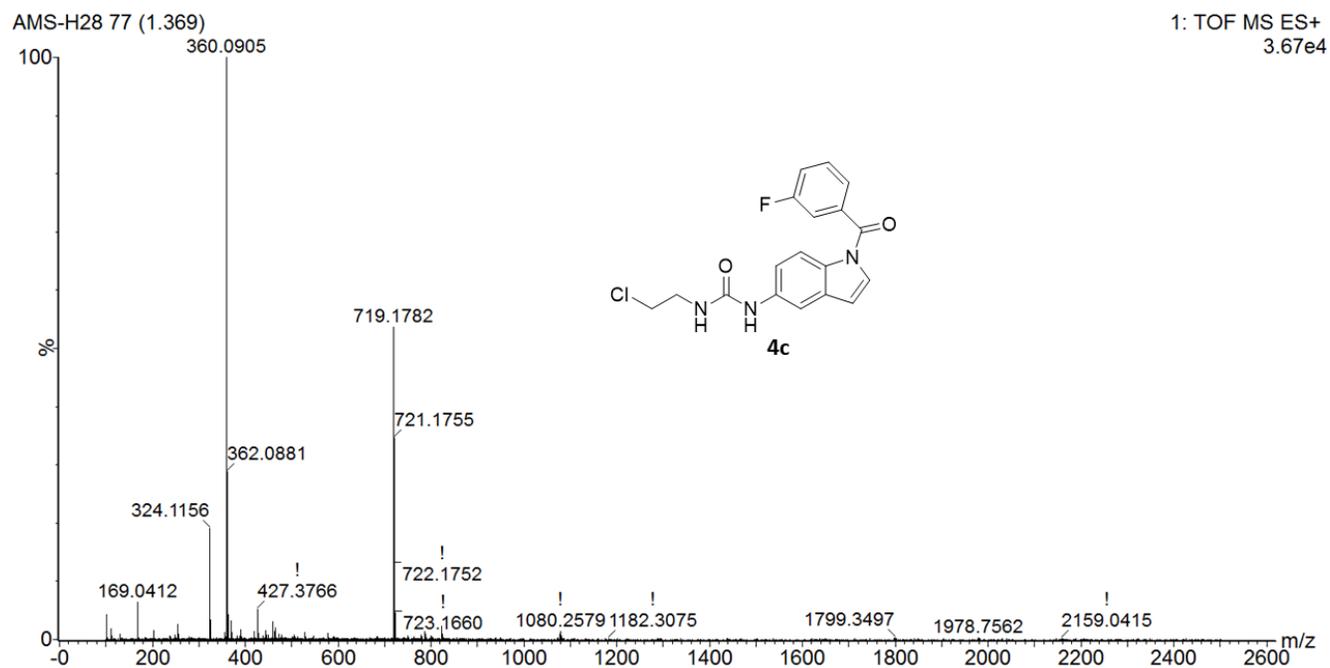
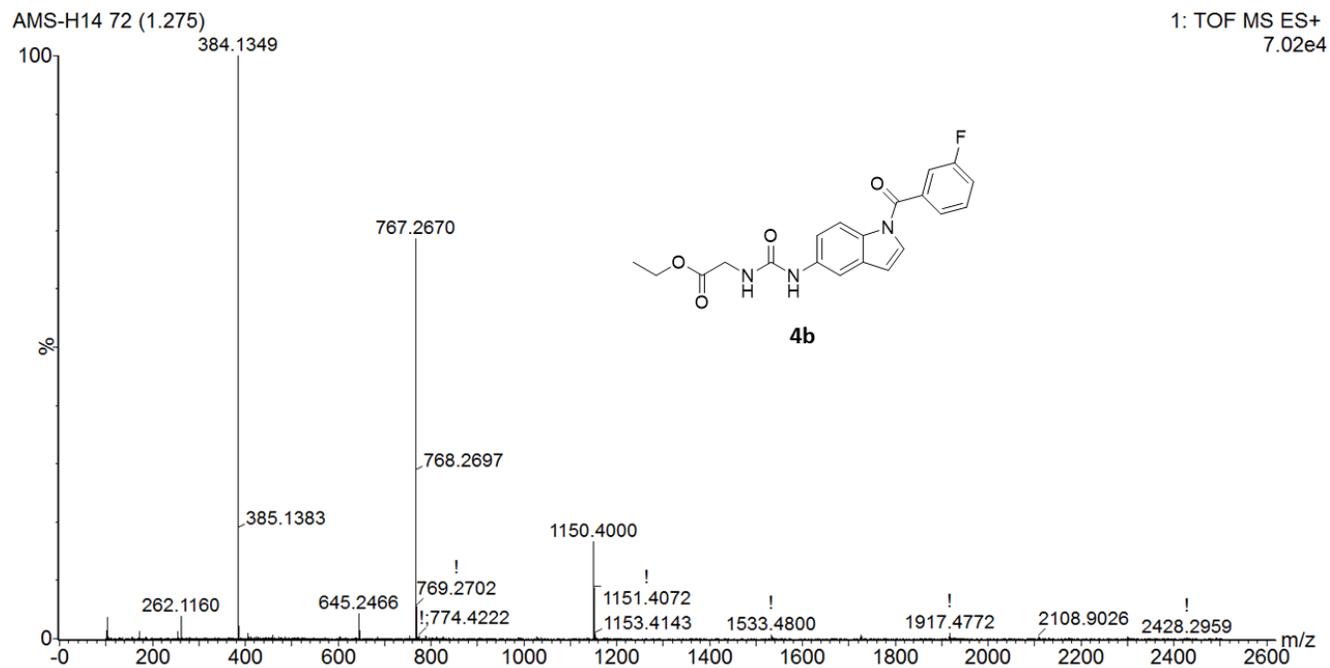
	Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area ( $\mu\text{V}\cdot\text{sec}$ )	% Area	Height ( $\mu\text{V}$ )	Int Type	Amount
1		15.725							26481219	95.64	2461374	bb	
2		20.990							1206129	4.36	174283	bb	



	Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area ( $\mu\text{V}\cdot\text{sec}$ )	% Area	Height ( $\mu\text{V}$ )	Int Type	Amount
1		10.548							173366	1.05	27024	bb	
2		12.866							16023703	97.28	2134594	bb	
3		14.794							3519	0.02	838	bb	
4		15.765							2730	0.02	573	bb	
5		17.723							14939	0.09	2821	bb	
6		19.510							15872	0.10	2458	bb	
7		21.026							41357	0.25	6726	bb	
8		25.096							196114	1.19	27752	bb	

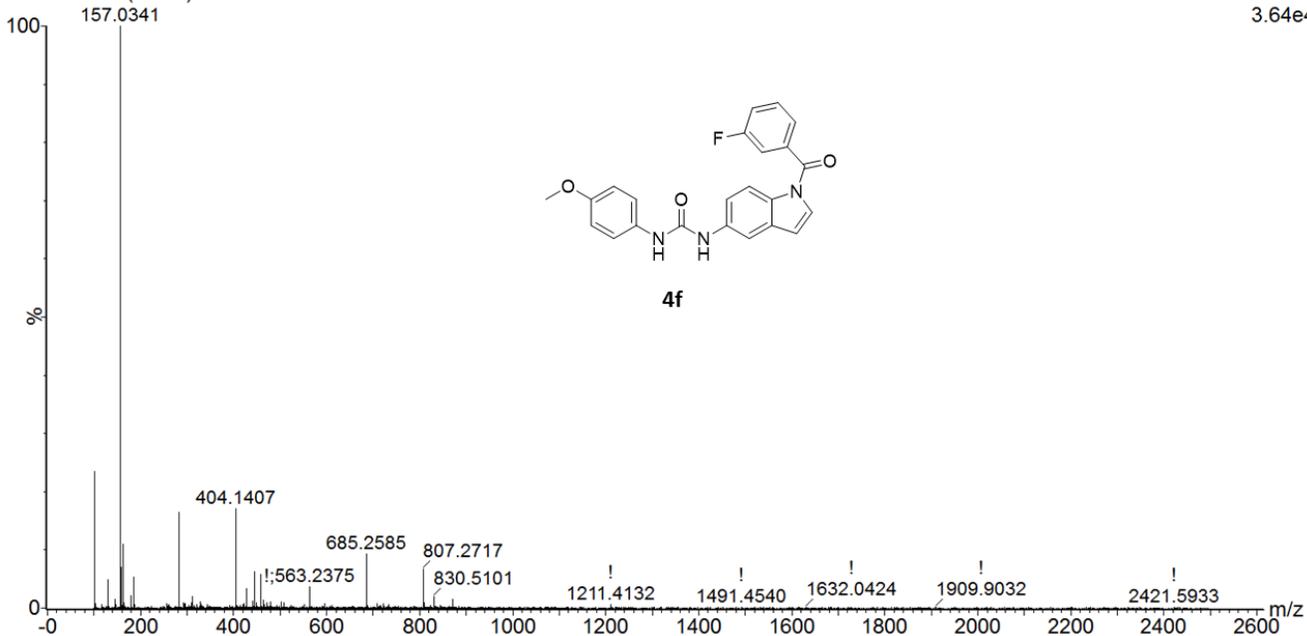


### 3. Representative HRMS data of the compounds



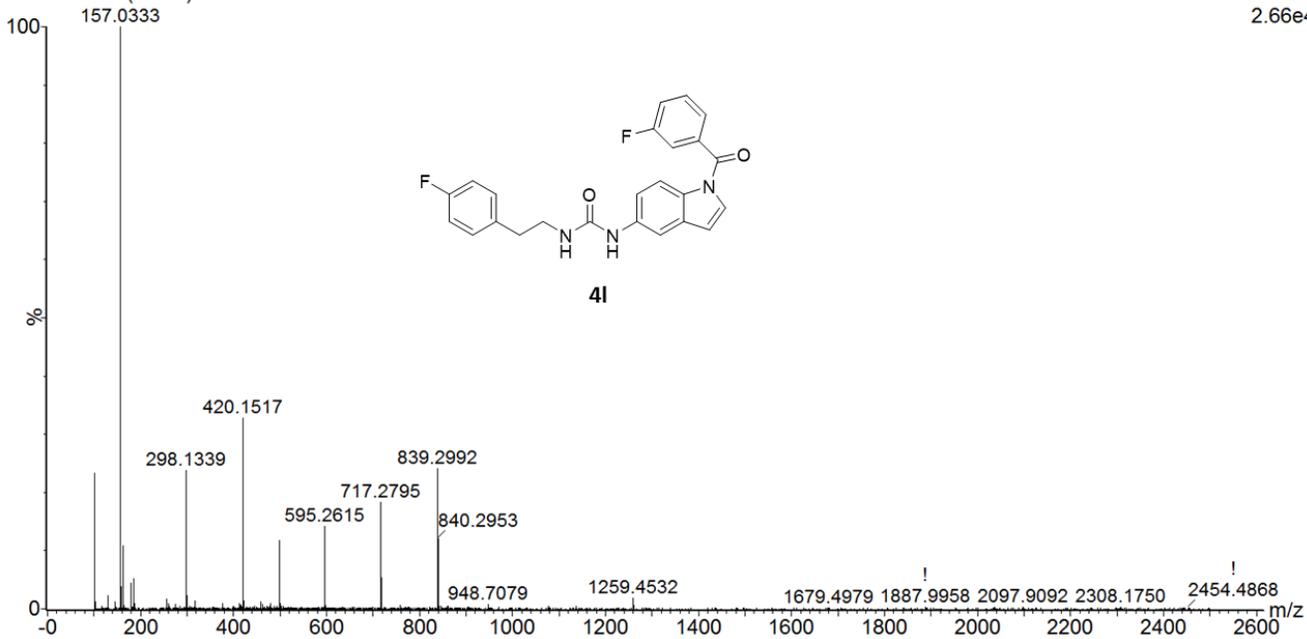
AMS-H25 79 (1.403)

1: TOF MS ES+  
3.64e4



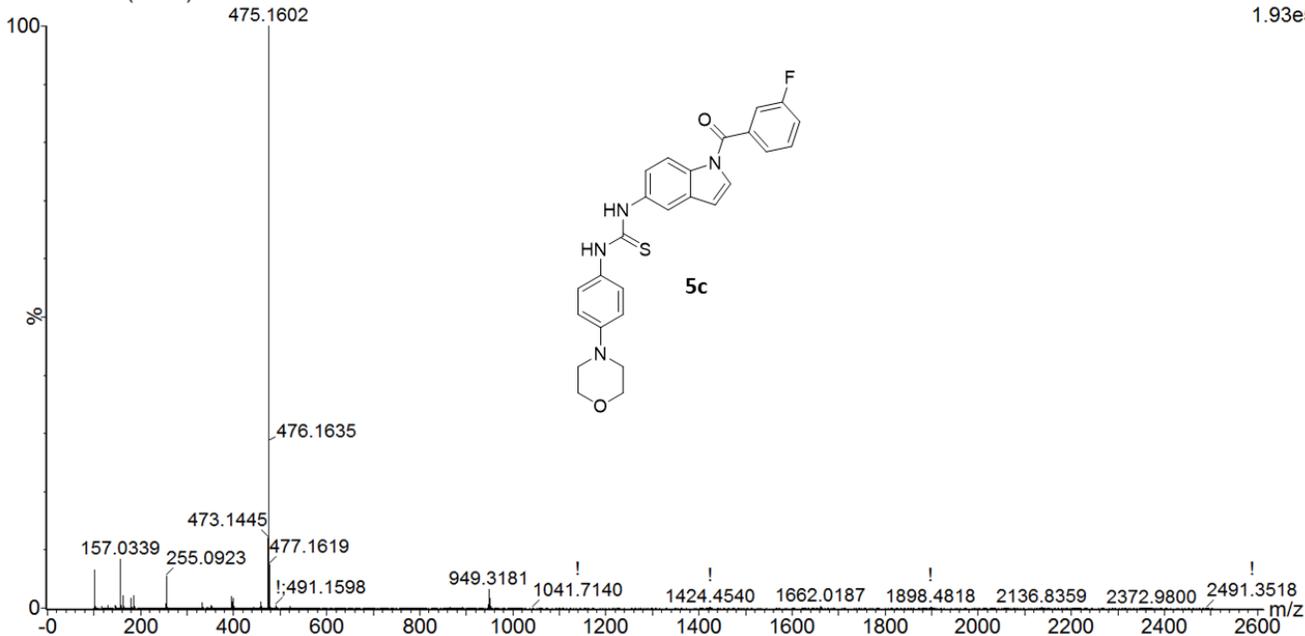
AMS-H27 78 (1.386)

1: TOF MS ES+  
2.66e4



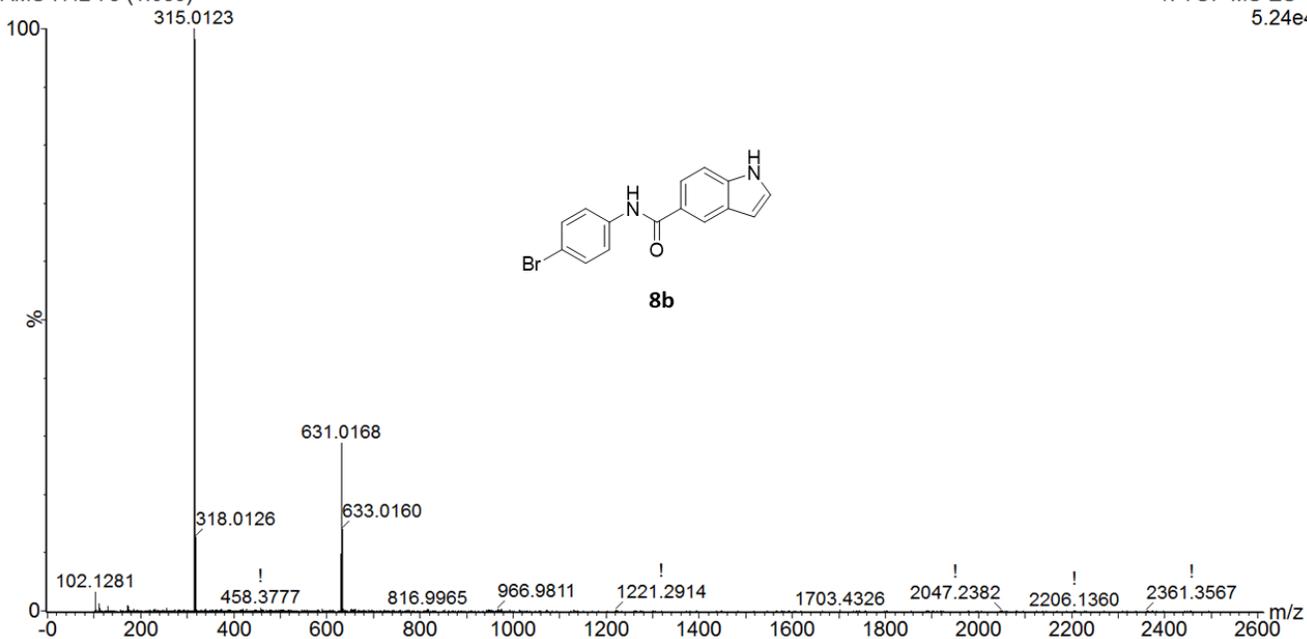
AMS-H30 74 (1.310)

1: TOF MS ES+  
1.93e5

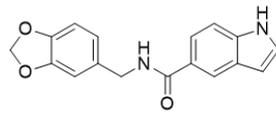


AMS-H42 78 (1.386)

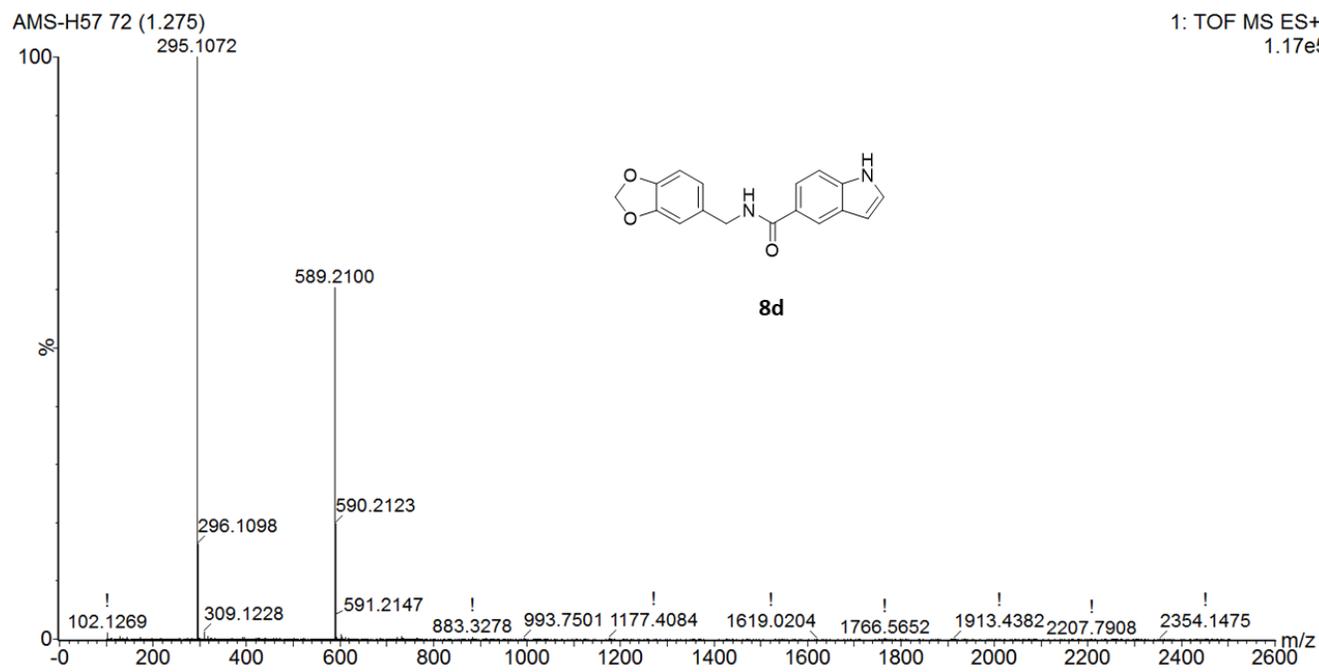
1: TOF MS ES+  
5.24e4



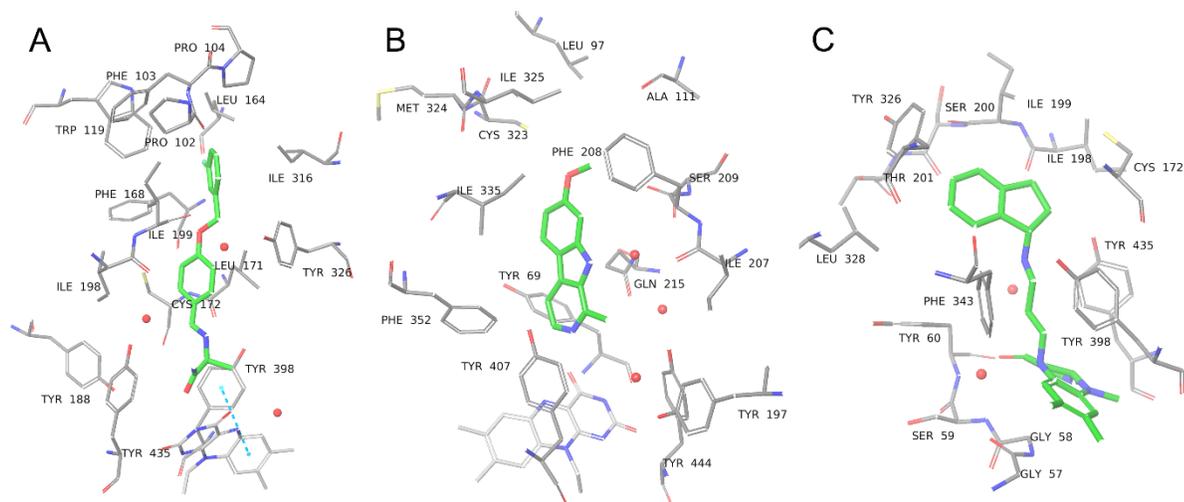
1: TOF MS ES+  
1.17e5



8d



#### 4. Molecular modelling supplementary material



**Figure S1.** Binding modes of reference reversible inhibitors (A) safinamide bound to MAO-B (PDB ID: 2V5Z), (B) harmine bound to MAO-A (PDB ID: 2Z5X) and covalent irreversible inhibitor (C) rasagiline bound to MAO-B (PDB ID: 1S2Y). Ligands are presented as green thick sticks, pocket atoms – gray thin sticks and crucial water molecules - red spheres. Hydrogen atoms omitted for clarity.