

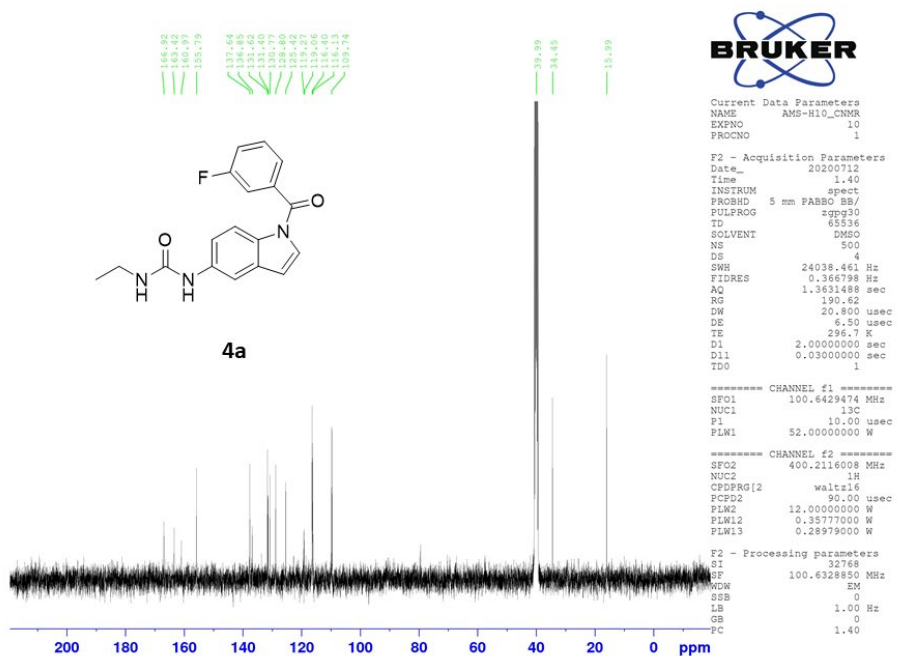
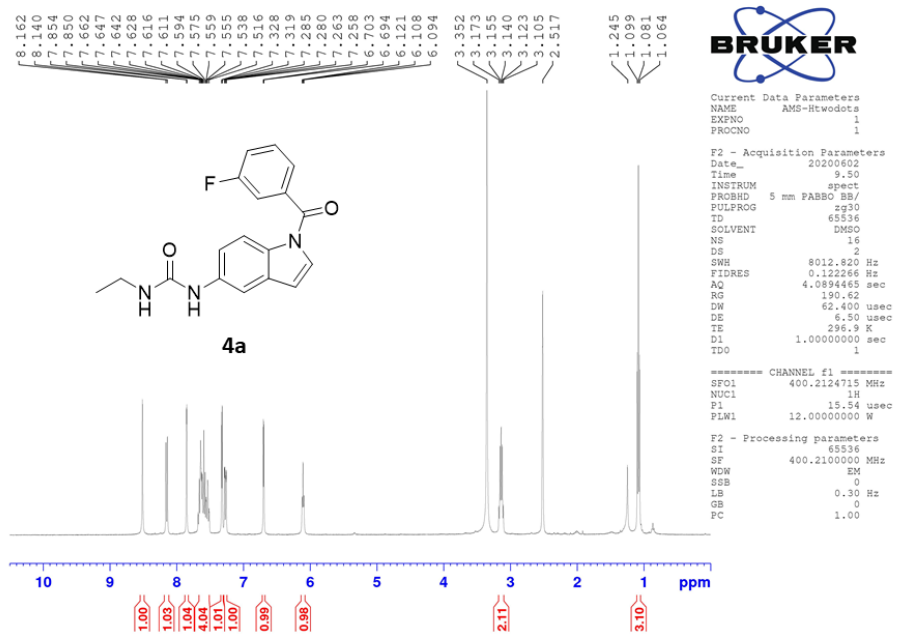
Supplementary material

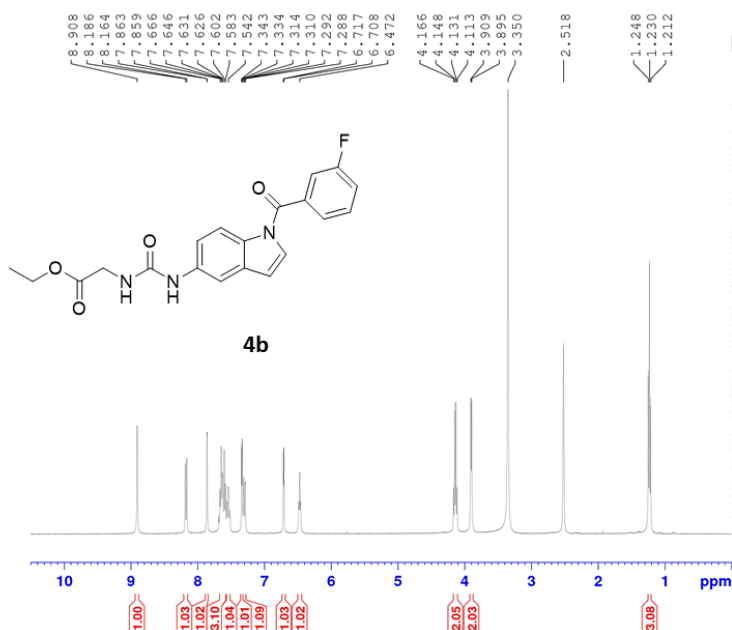
Highly Potent, Selective, and Competitive Indole-Based MAO-B Inhibitors Protect PC12 Cells against 6-Hydroxydopamine- and Rotenone-Induced Oxidative Stress

Contents

1. ^1H NMR and ^{13}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. ¹HNMR and ¹³CNMR data of compounds 4a–n, 5a–j, 6a–e, 7a, 7b, and 8a–e



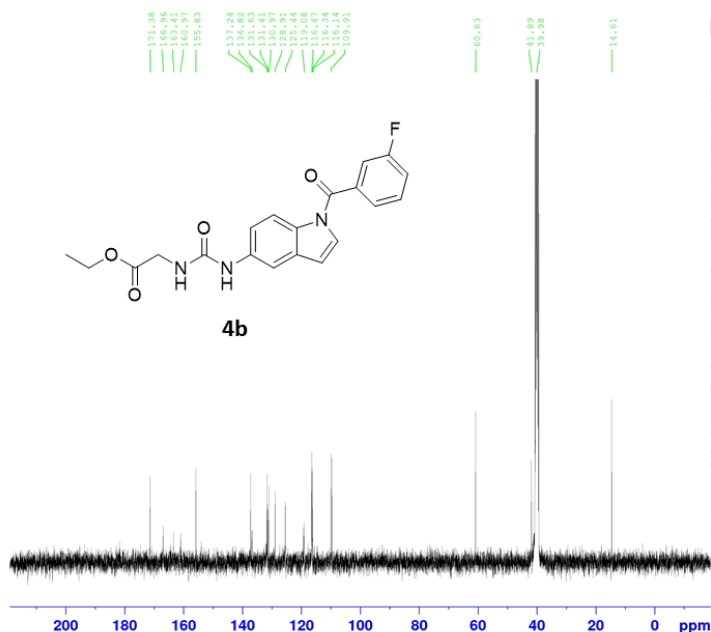


Current Data Parameters
NAME AMS-H14
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200407
Time 16.01
INSTRUM spect
PROBHD 5 mm 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
DM 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

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

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



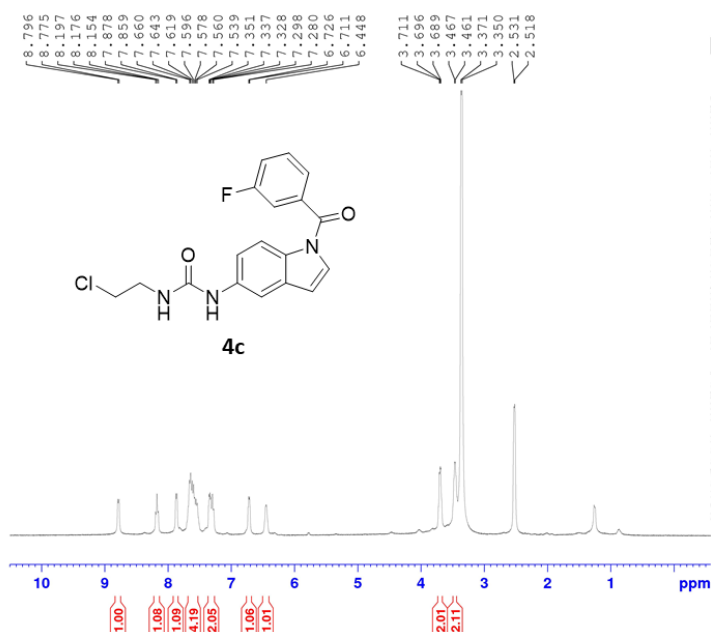
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NAME AMS-H14_CNMR
EXPNO 10
PROCNO 1

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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
TD0 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
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SF 100.6328850 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

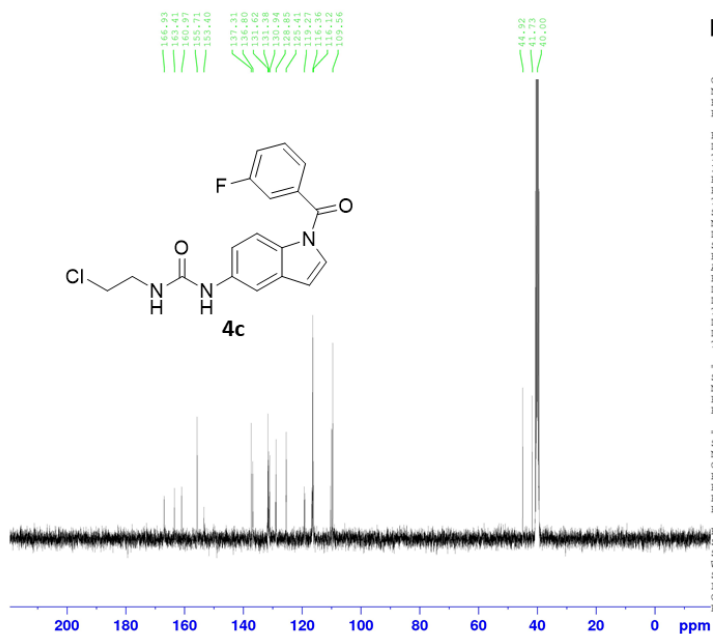


Current Data Parameters
NAME AMS-H28F
EXPNO 1
PROCNO 1

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
TD0 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



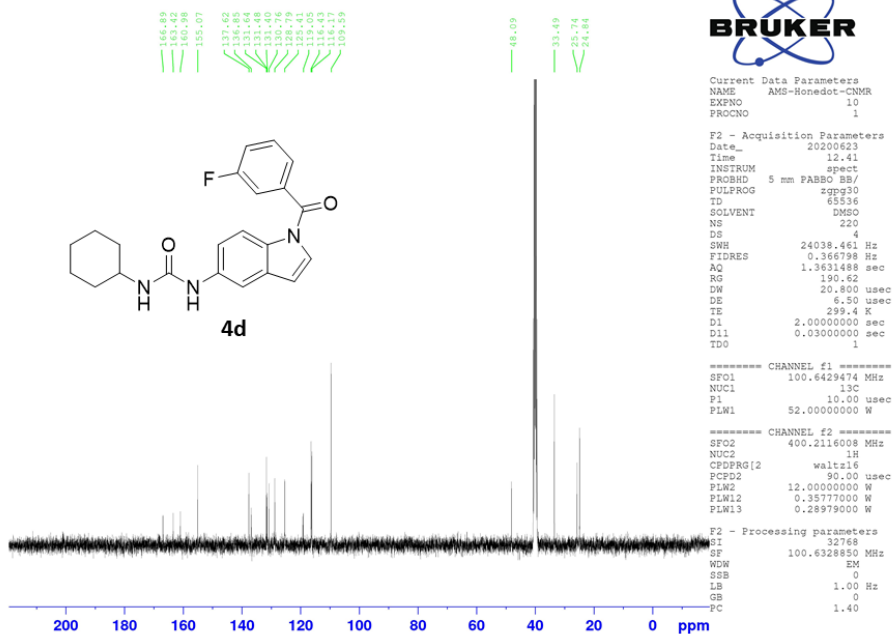
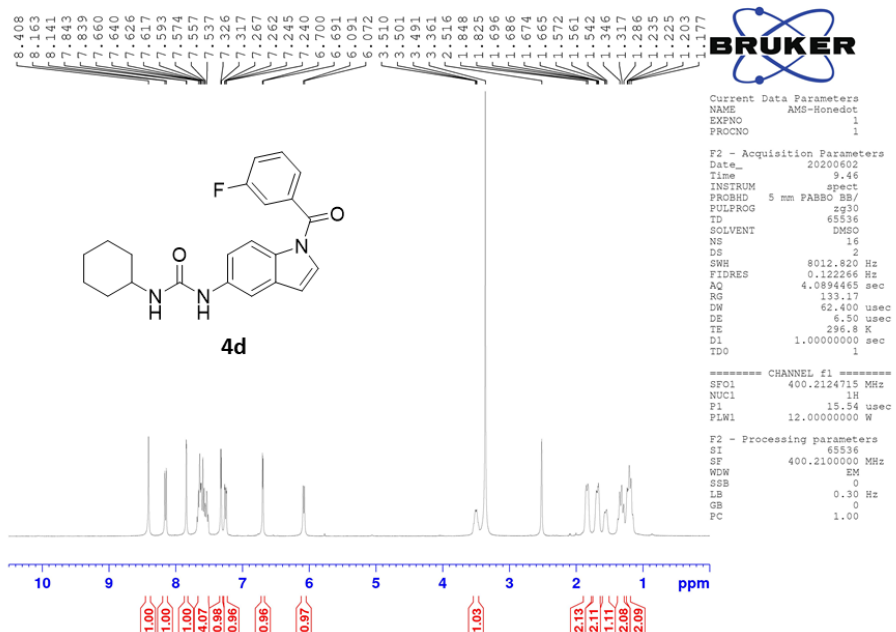
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EXPNO 1
PROCNO 1

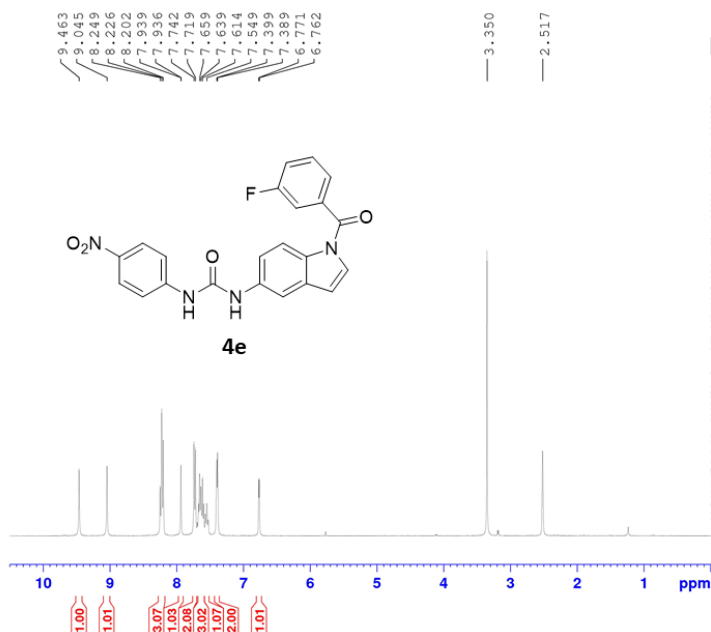
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PROBHD 5 mm PABBO BB/
PULPROG zgpg30
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SOLVENT DMSO
NS 256
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 190.62
DW 20.800 usec
DE 6.50 usec
TE 298.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 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





BRUKER

Current Data Parameters

NAME AMS-H11
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters

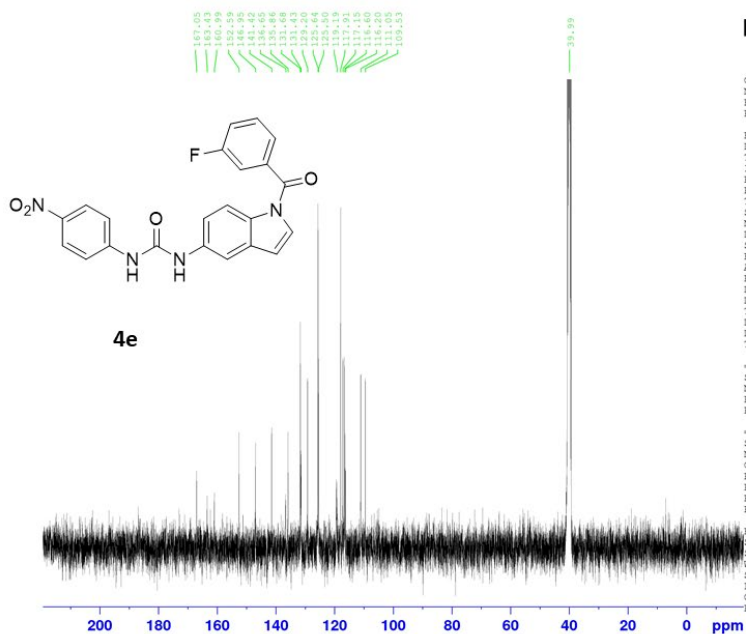
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PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 190.62
DW 62.400 usec
DE 6.50 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1

===== 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-H11_CNMR
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
TD0 1

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

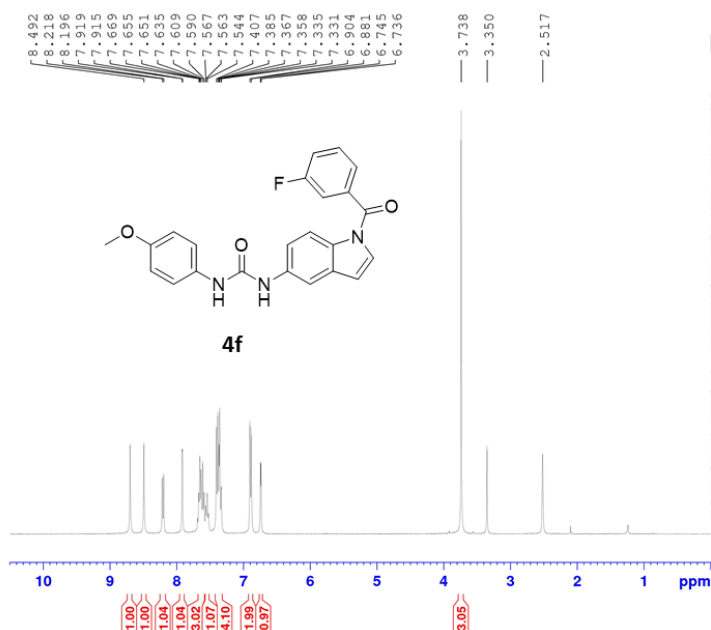
SFO1 100.6429474 MHz
NUC1 13C
P1 10.00 usec
PLW1 52.00000000 W

===== 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

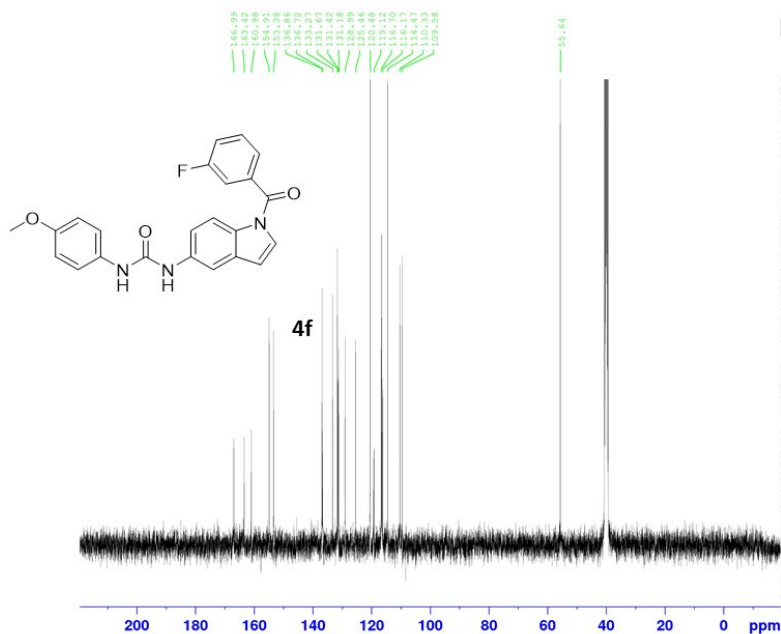


Current Data Parameters
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
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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
TD0 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



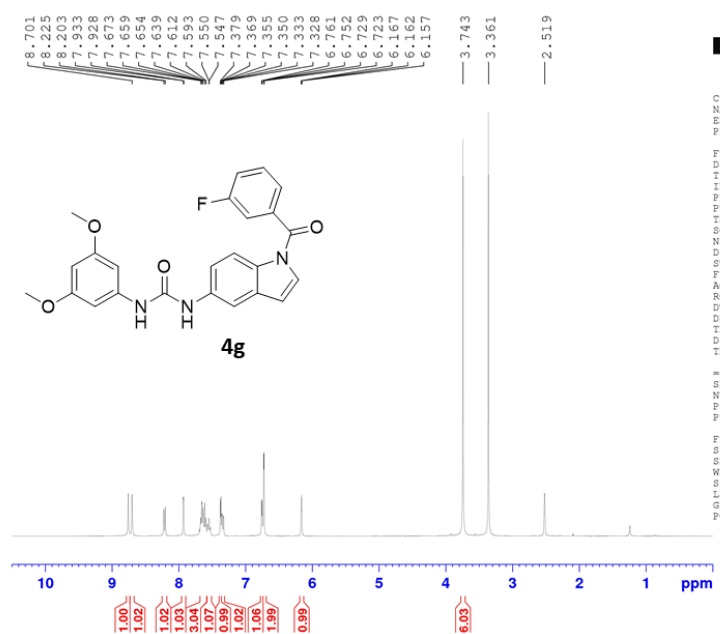
Current Data Parameters
NAME AMS-H25_CNMR
EXPNO 10
PROCNO 1

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
TD0 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

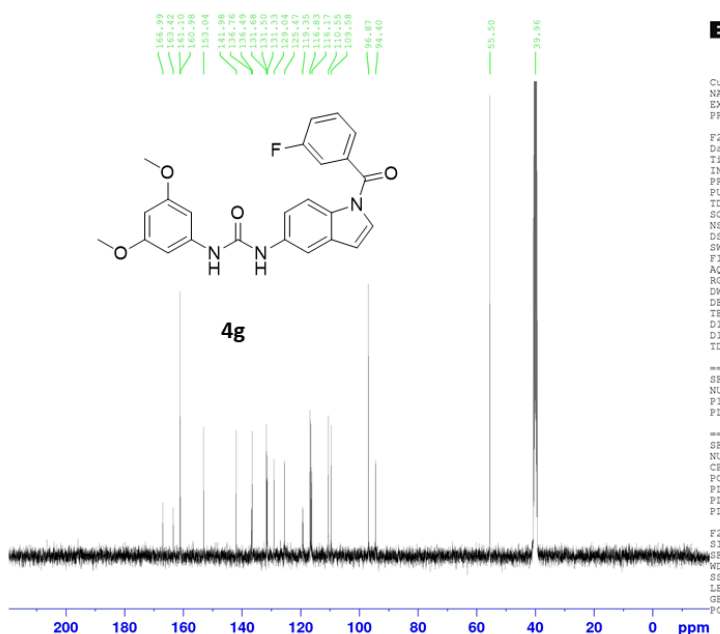


Current Data Parameters
NAME AMS-H13
EXPNO 1
PROCNO 1

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 4.8894465 sec
RG 190.62
DW 62.400 usec
DE 6.50 usec
TE 297.8 K
D1 1.00000000 sec
TD0 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
SBB 0
LB 0.30 Hz
GB 0
PC 1.00



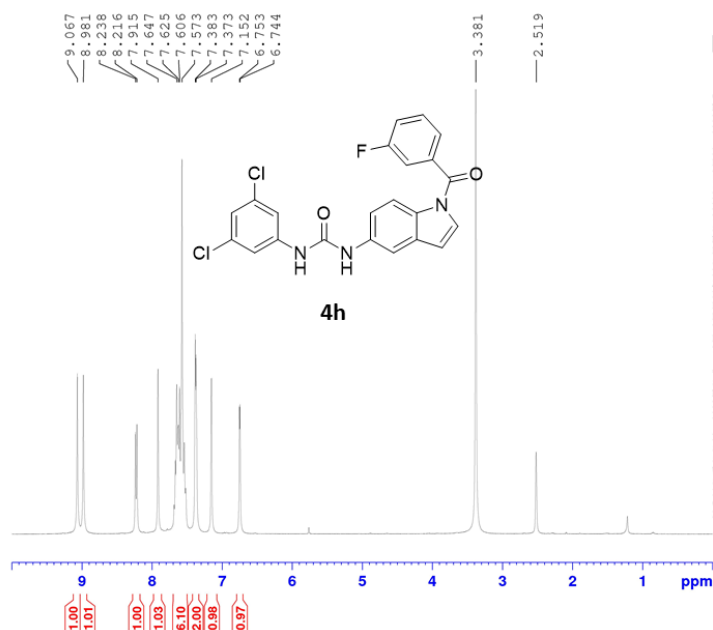
Current Data Parameters
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EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
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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 1.3631488 sec
RG 190.62
DW 20.800 usec
DE 6.50 usec
TE 296.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 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
SBB 0
LB 1.00 Hz
GB 0
PC 1.40

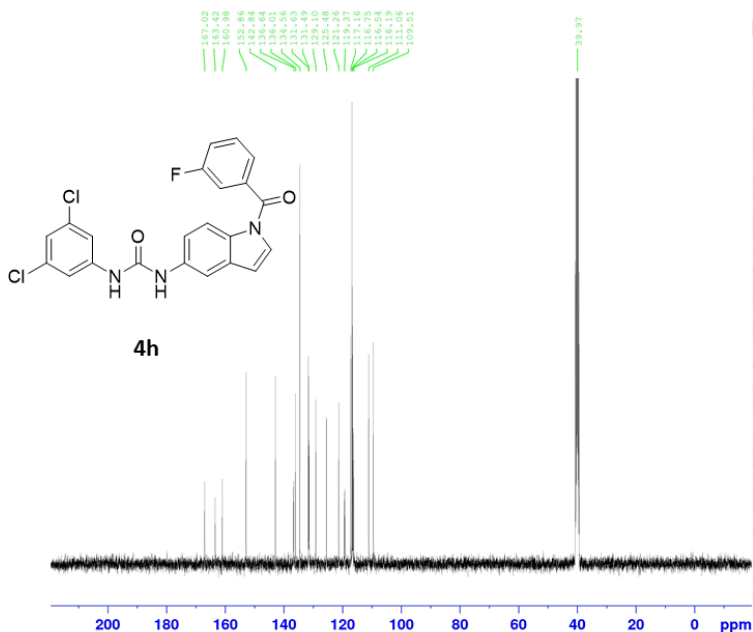


Current Data Parameters
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EXPNO 1
PROCNO 1

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 1.00000000 sec
TD0 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



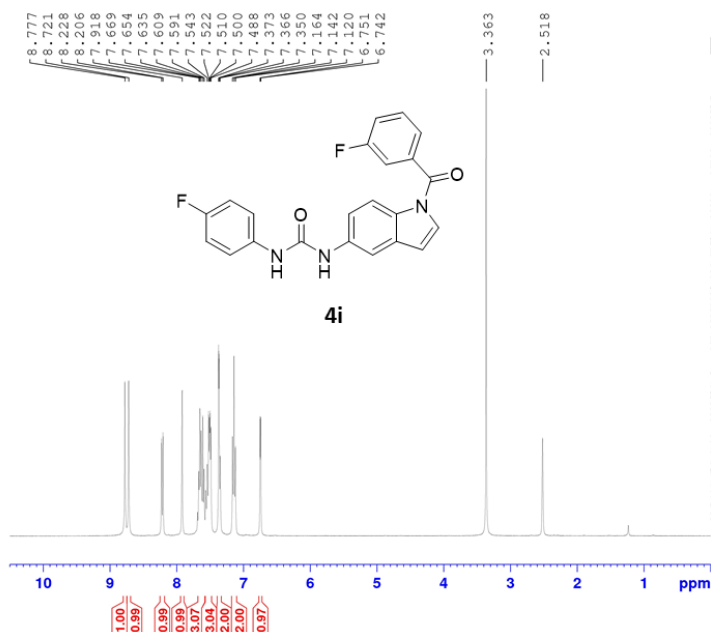
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NAME AMS-H19_CNMR
EXPNO 10
PROCNO 1

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 1.3631488 sec
RG 190.62
DW 20.800 usec
DE 6.50 usec
TE 296.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.629474 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 100.628850 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

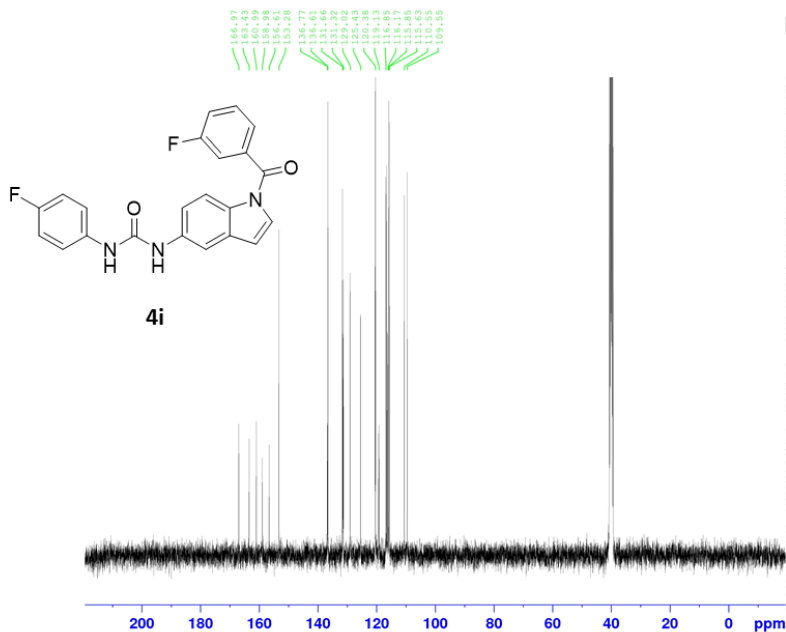


Current Data Parameters
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EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200429
Time 17.35
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
TD0 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



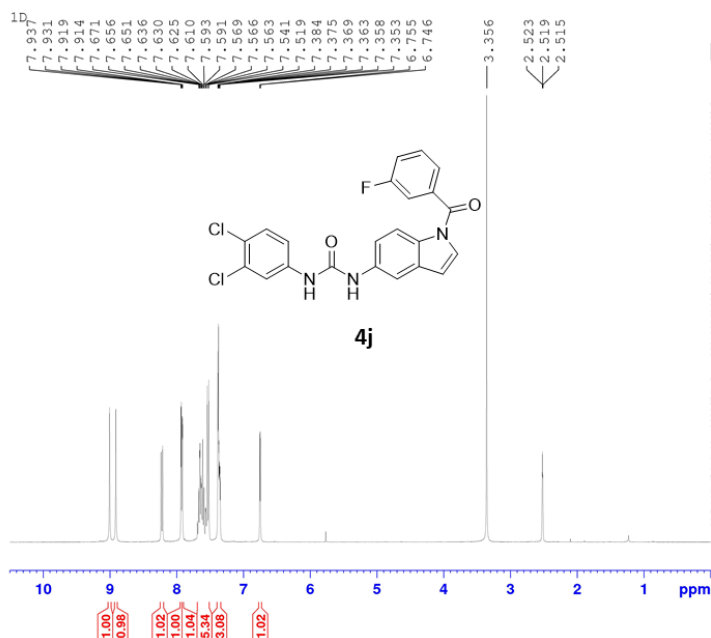
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EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
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Time 22.37
INSTRUM spect
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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
TD0 1

===== CHANNEL f1 =====
SFO1 100.629474 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 100.628850 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

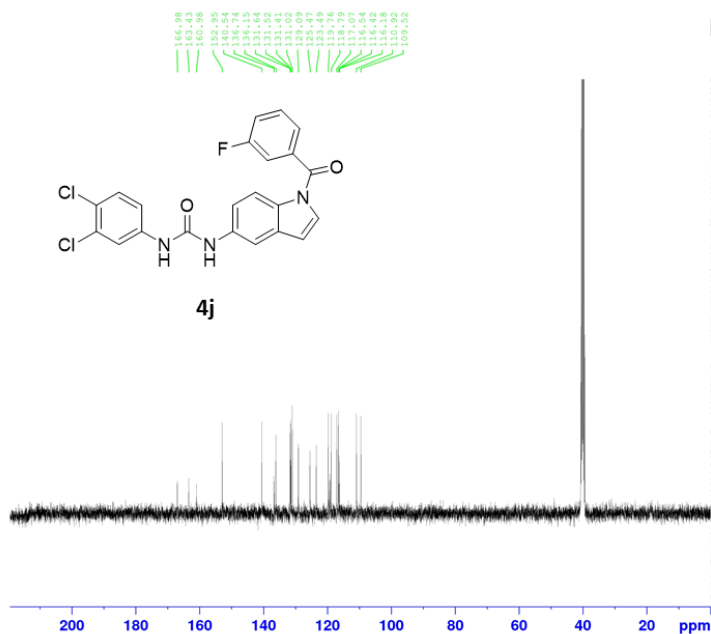


Current Data Parameters
NAME AMS-HY
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200622
Time 17.52
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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
TD0 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



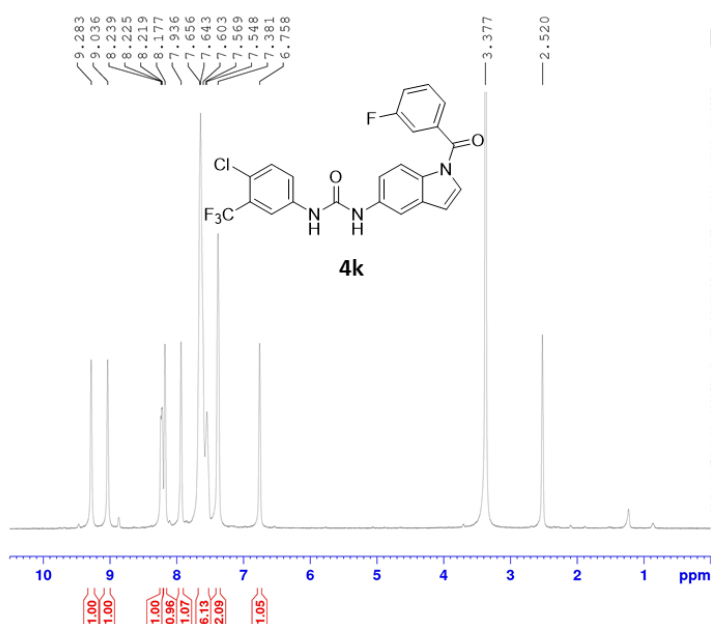
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EXPNO 20
PROCNO 1

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Time 18.26
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PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 128
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 299.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 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

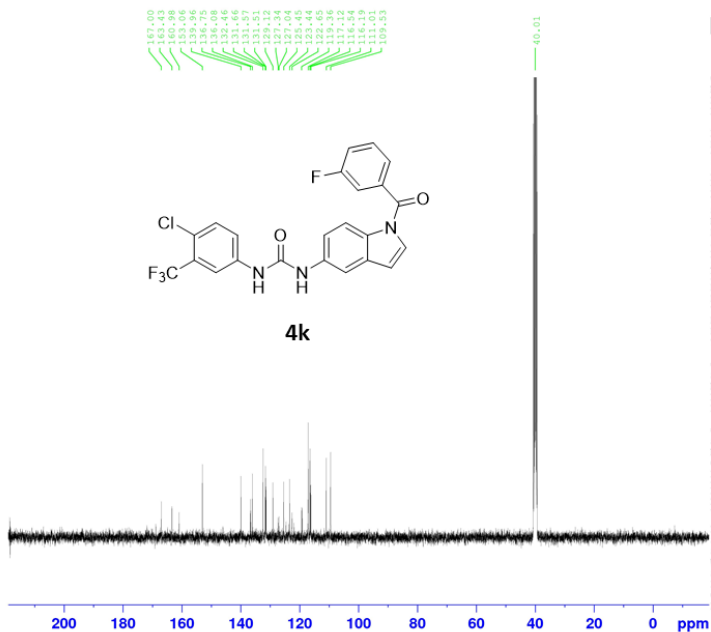


Current Data Parameters
NAME 4k_CNMR
EXPNO 10
PROCNO 1

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
TD0 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



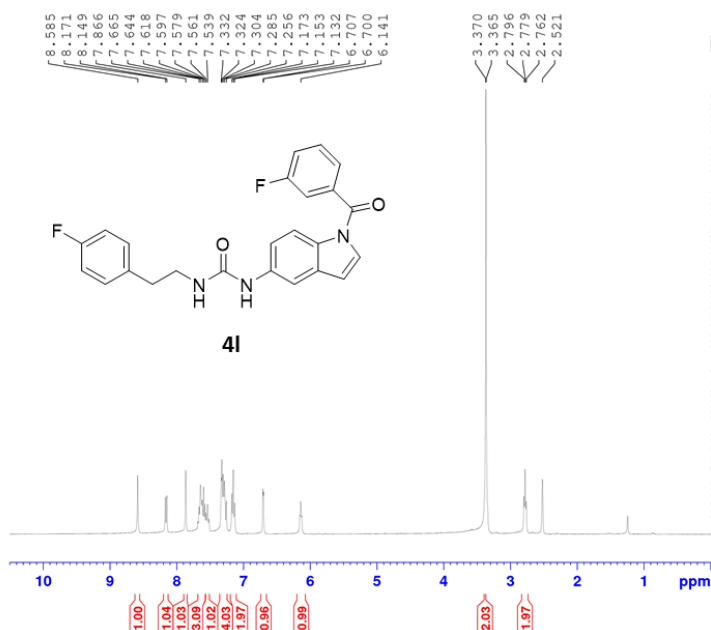
Current Data Parameters
NAME 4k_CNMR
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201231
Time 22.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
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
TD0 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

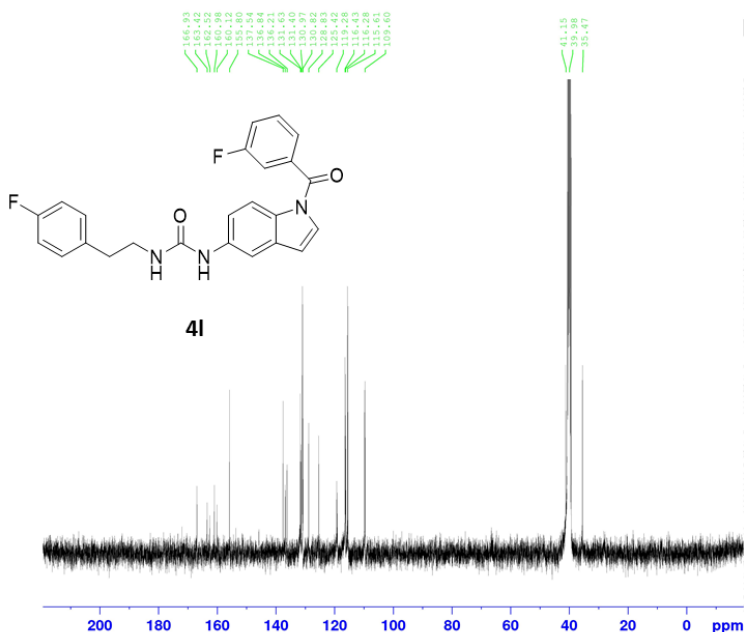


Current Data Parameters
NAME AMS-H27
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200407
Time 19.14
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
TD0 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



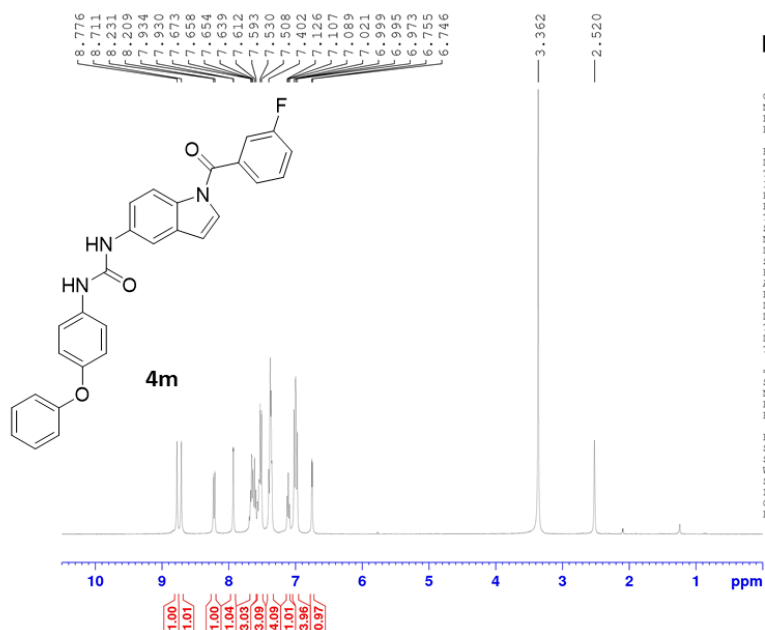
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NAME AMS-H27_CNMR
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200711
Time 23.05
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
TD0 1

===== CHANNEL f1 =====
SFO1 100.629474 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 100.628850 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

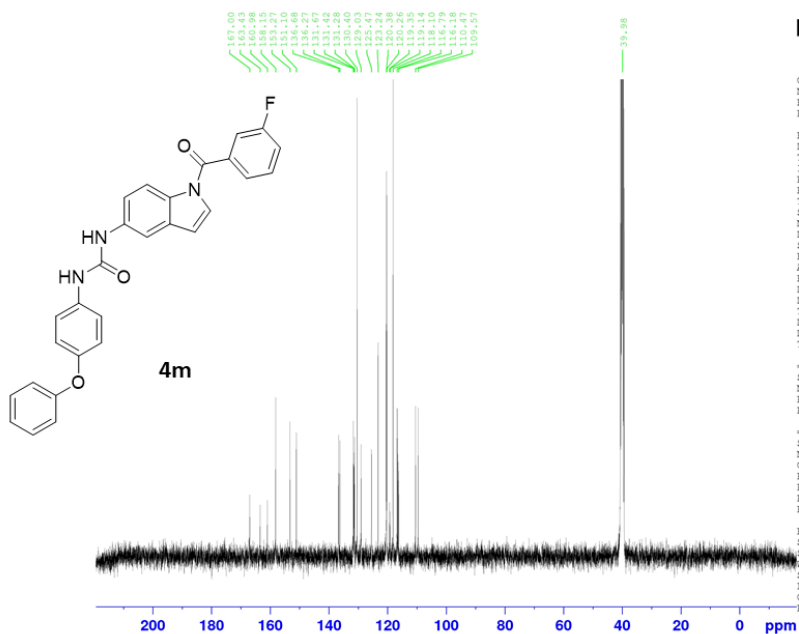


Current Data Parameters
NAME AMS-H26
EXPNO 1
PROCNO 1

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
TD0 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



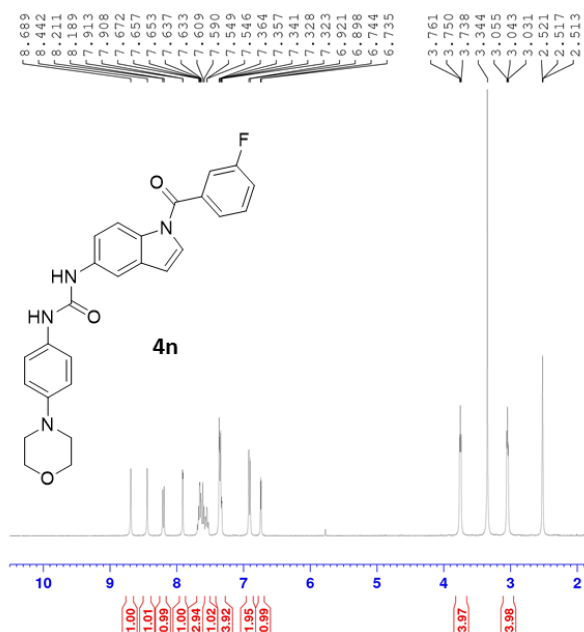
Current Data Parameters
NAME AMS-H26_CNMR
EXPNO 10
PROCNO 1

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 1.3631488 sec
RG 190.62
DW 20.800 usec
DE 6.50 usec
TE 296.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 100.629474 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 100.628850 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

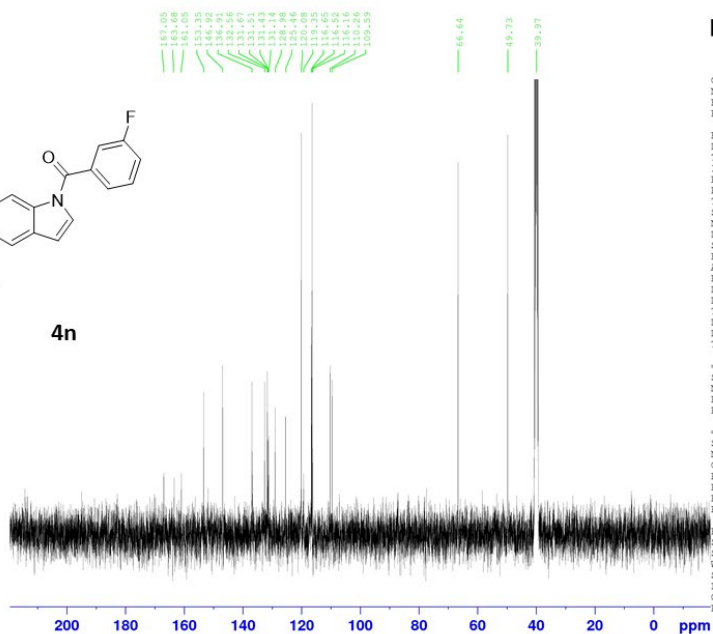


Current Data Parameters
NAME AMS-H31-F
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200414
Time 16.29
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 298.0 K
D1 1.00000000 sec
TD0 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



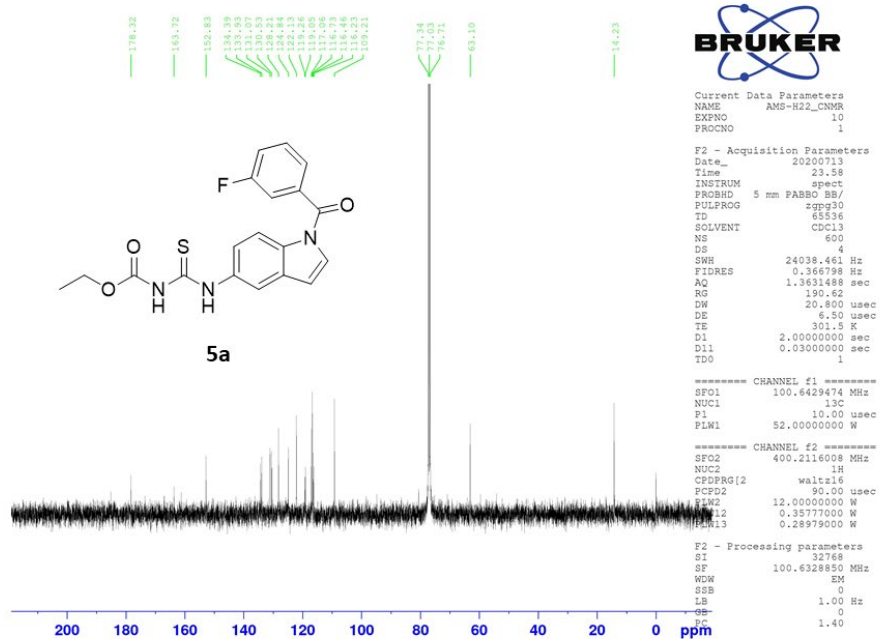
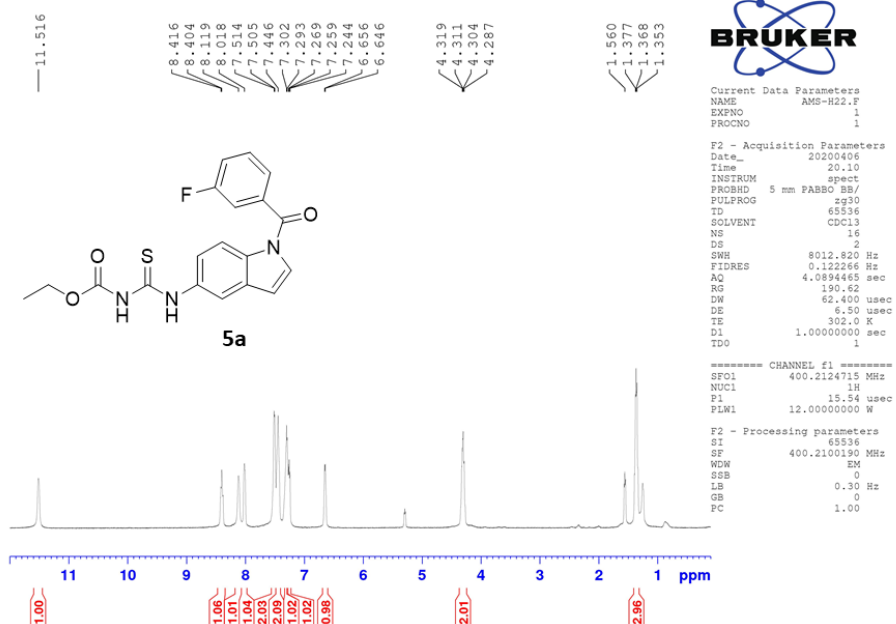
Current Data Parameters
NAME AMS-H31_CNMR
EXPNO 10
PROCNO 1

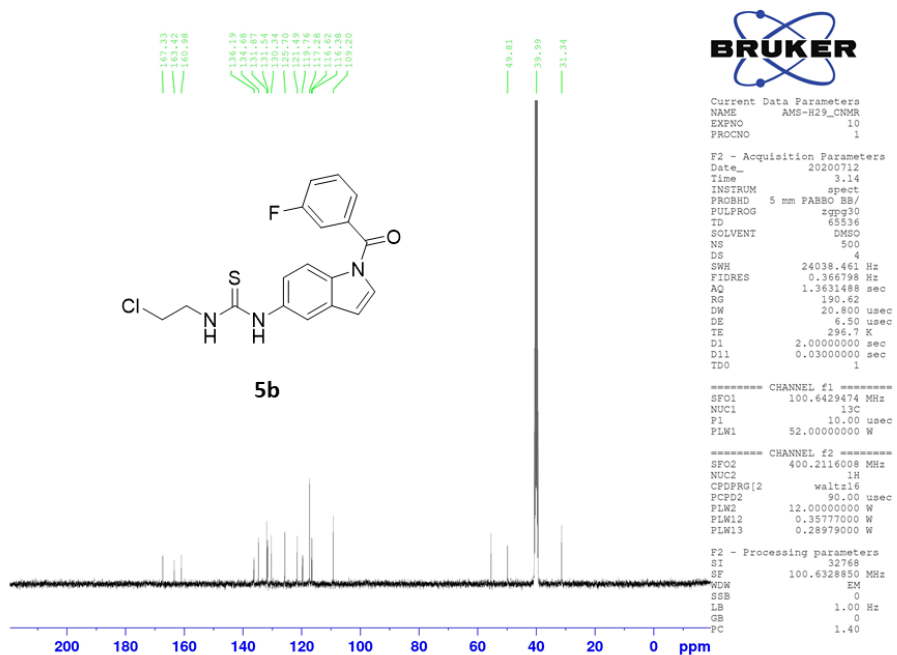
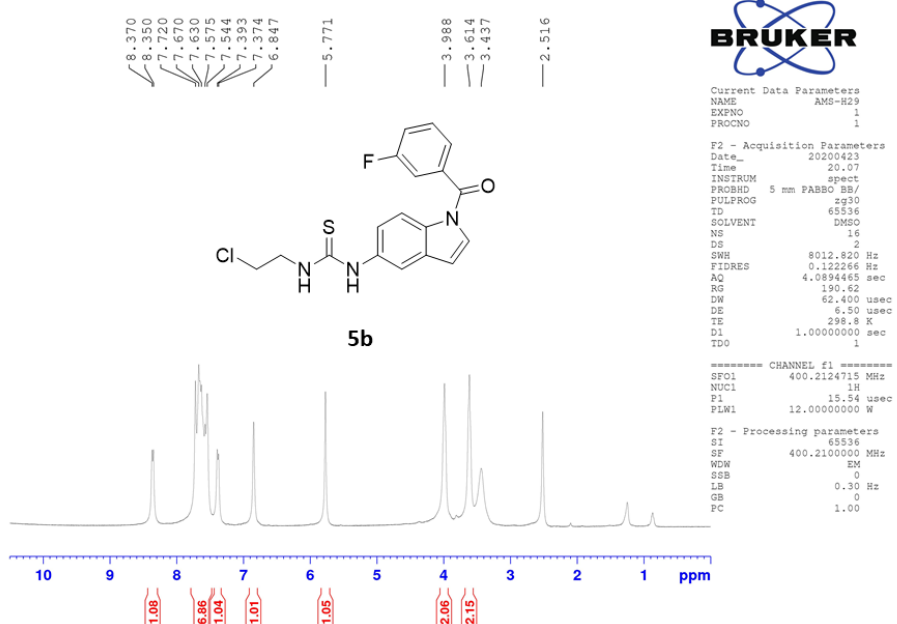
F2 - Acquisition Parameters
Date_ 20200711
Time 22.02
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 190.62
DW 20.800 usec
DE 6.50 usec
TE 296.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

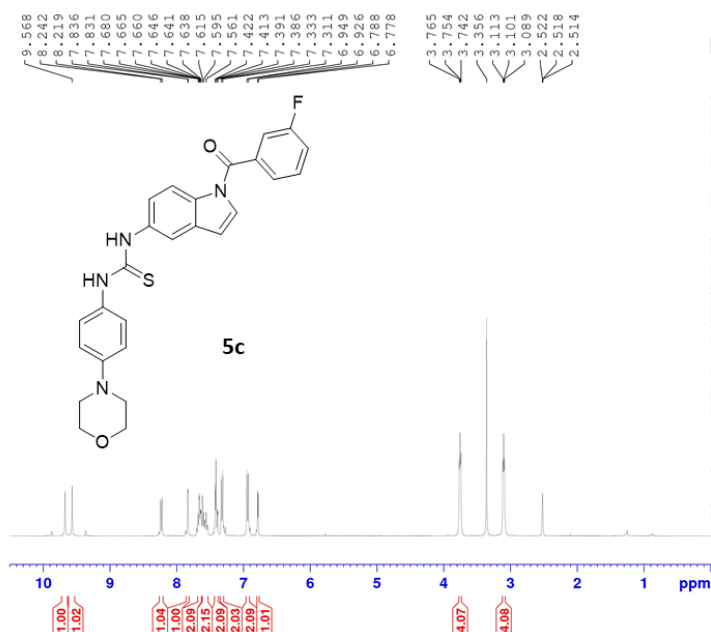
===== CHANNEL f1 =====
SFO1 100.6429474 MHz
NUC1 13C
P1 10.00 usec
PLW1 52.00000000 W

===== 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





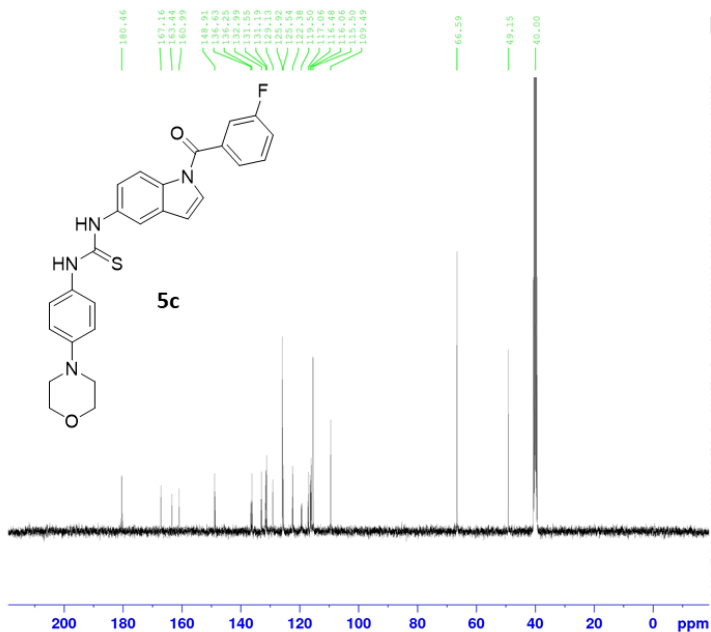


Current Data Parameters
 NAME AMS_H3O
 EXPNO 1
 PROCNO 1

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



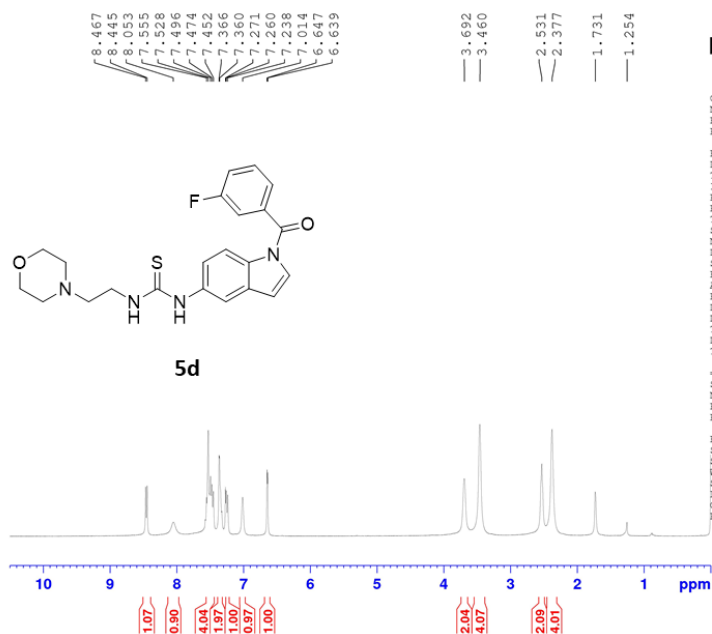
Current Data Parameters
 NAME AMS-H3O_CNMR
 EXPNO 10
 PROCNO 1

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 1.3631488 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



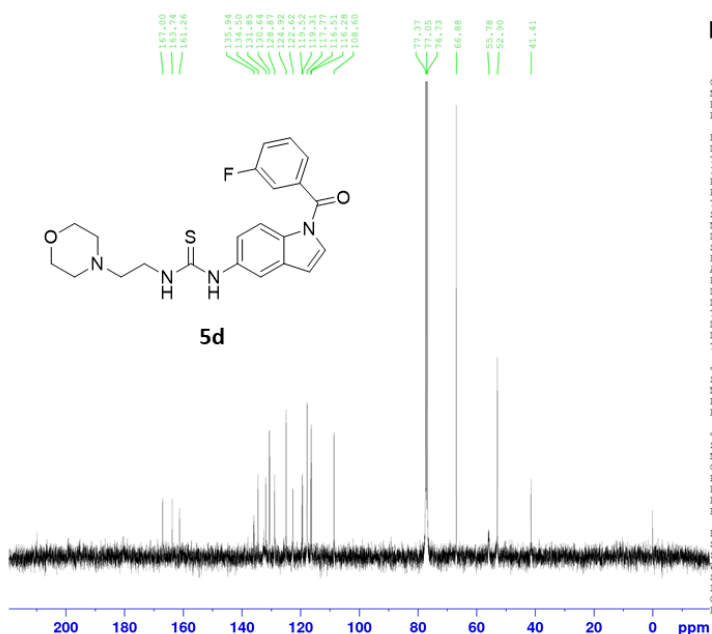
BRUKER

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

F2 - Acquisition Parameters
Date_ 20200518
Time 18.03
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 298.0 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



BRUKER

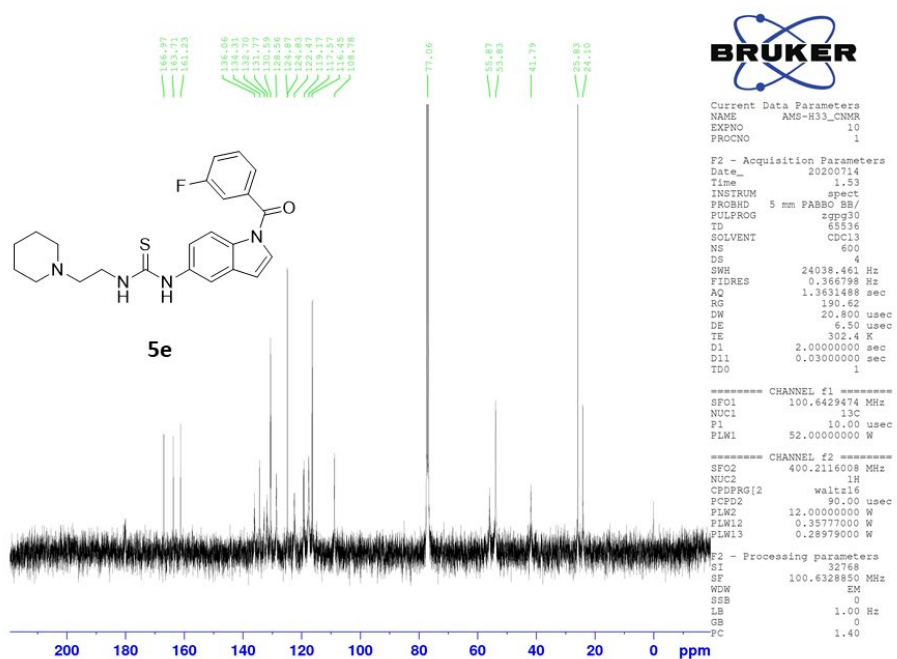
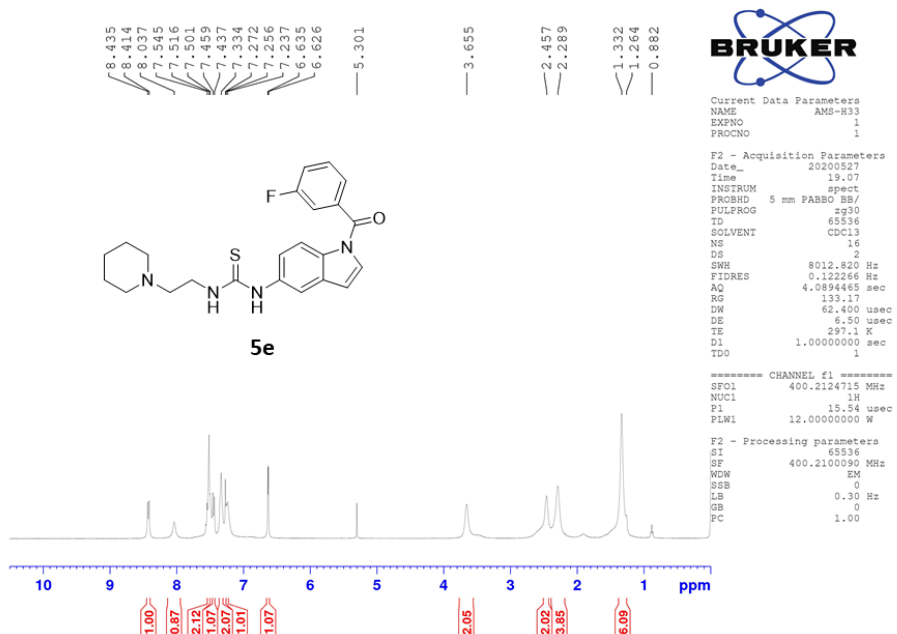
Current Data Parameters
NAME AMS-H32_CNMR
EXPNO 10
PROCNO 1

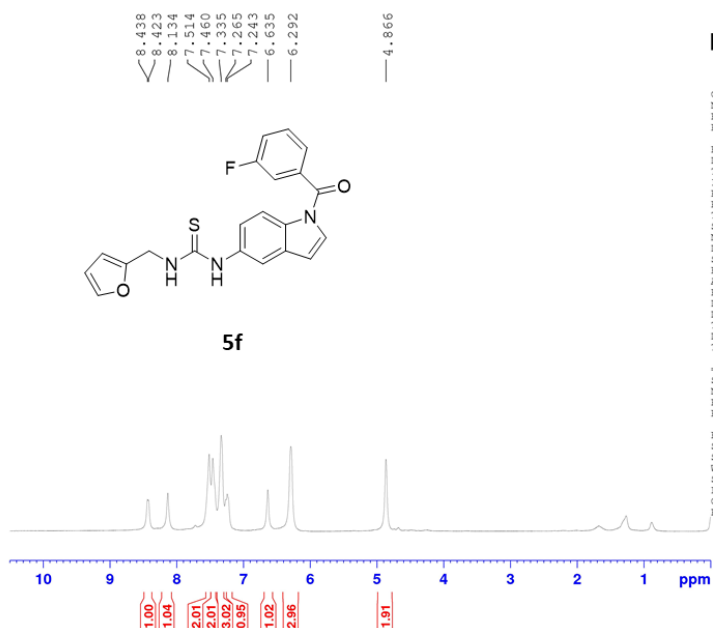
F2 - Acquisition Parameters
Date_ 20200714
Time 0.37
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 600
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 190.62
DW 20.800 usec
DE 6.50 usec
TE 300.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TDO 1

===== 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



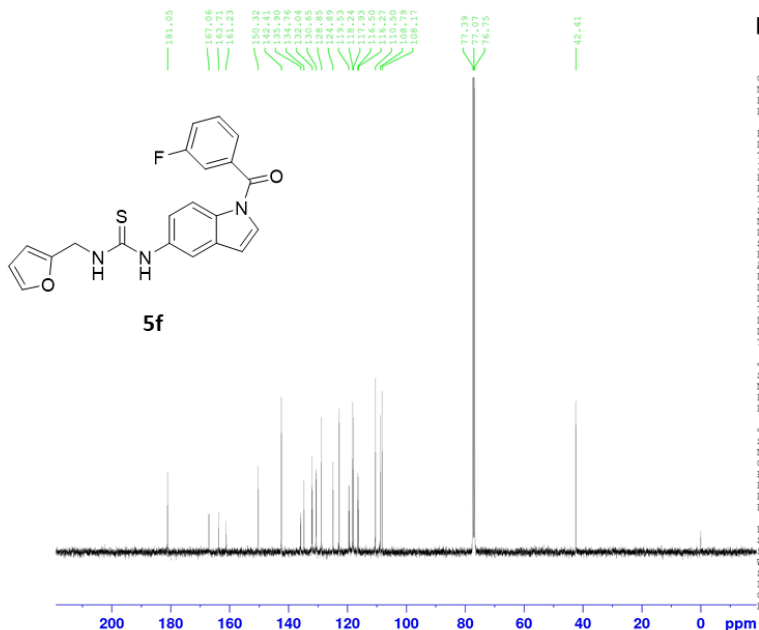


Current Data Parameters
NAME AMS-H16
EXPNO 1
PROCNO 1

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



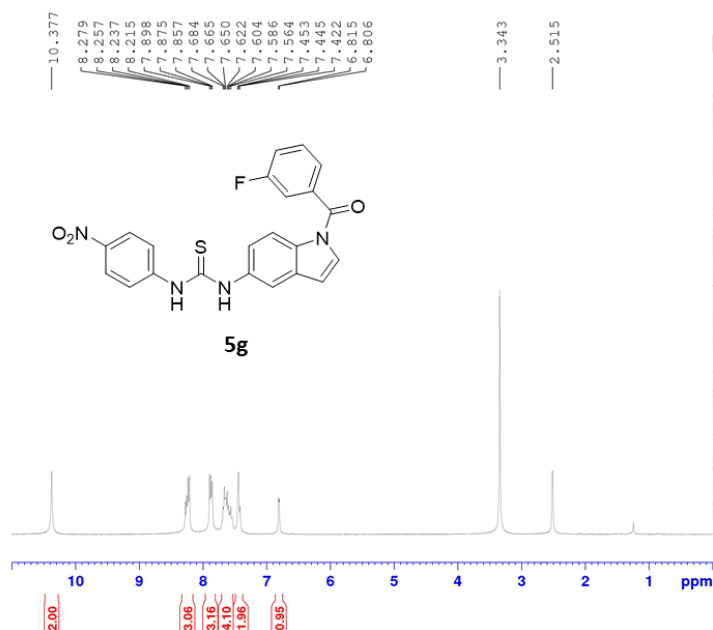
Current Data Parameters
NAME AMS-H16_CNMR
EXPNO 10
PROCNO 1

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 1.3631488 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

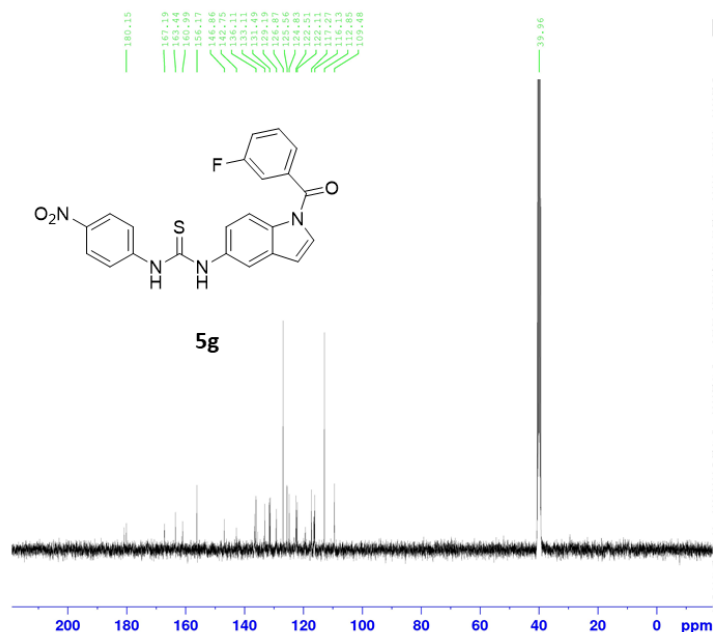


Current Data Parameters
NAME AMS-H17
EXPNO 1
PROCNO 1

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
TD0 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



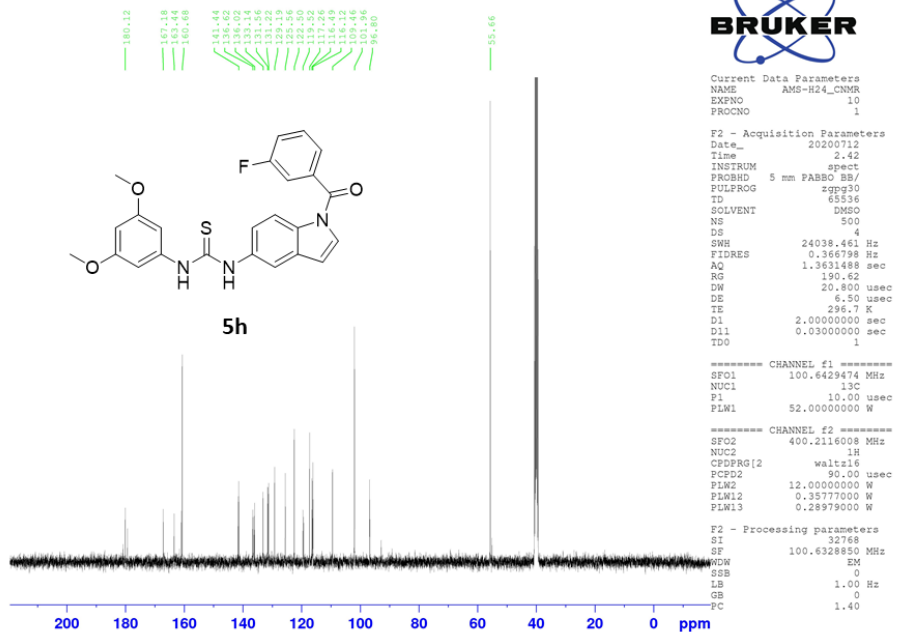
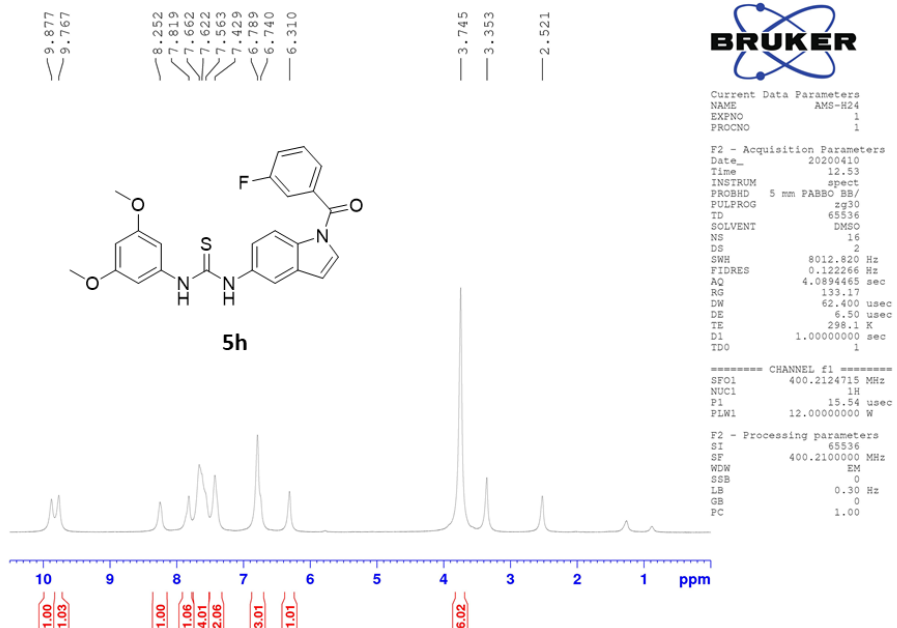
Current Data Parameters
NAME AMS-H17_CNMR
EXPNO 10
PROCNO 1

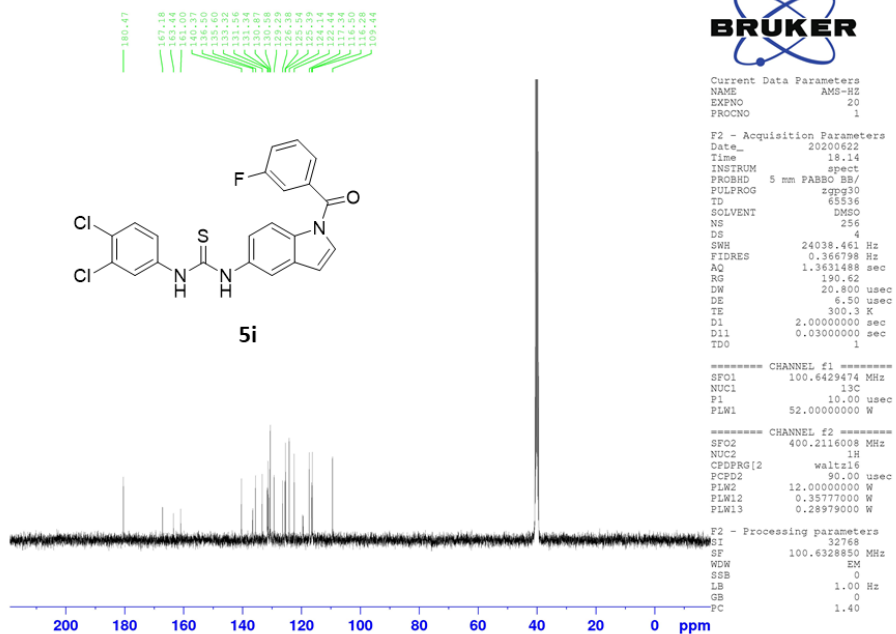
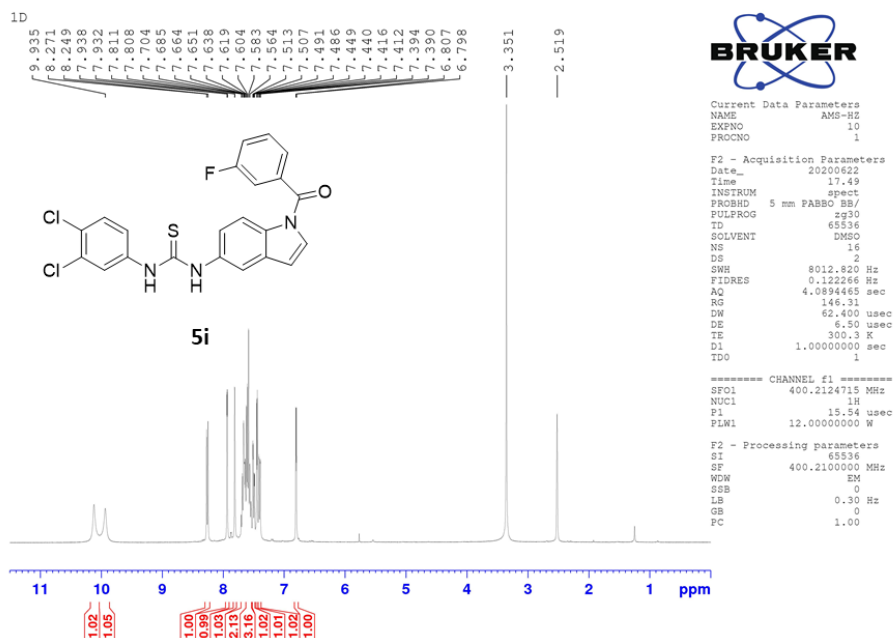
F2 - Acquisition Parameters
Date_ 20200711
Time 20.13
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 500
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 190.62
DW 20.800 usec
DE 6.50 usec
TE 296.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

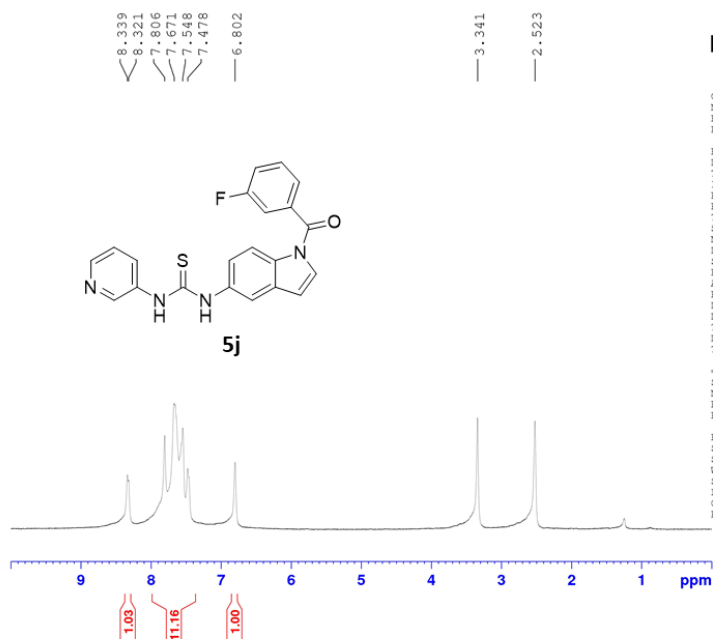
===== CHANNEL f1 =====
SFO1 100.6429474 MHz
NUC1 13C
P1 10.00 usec
PLW1 52.00000000 W

===== 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





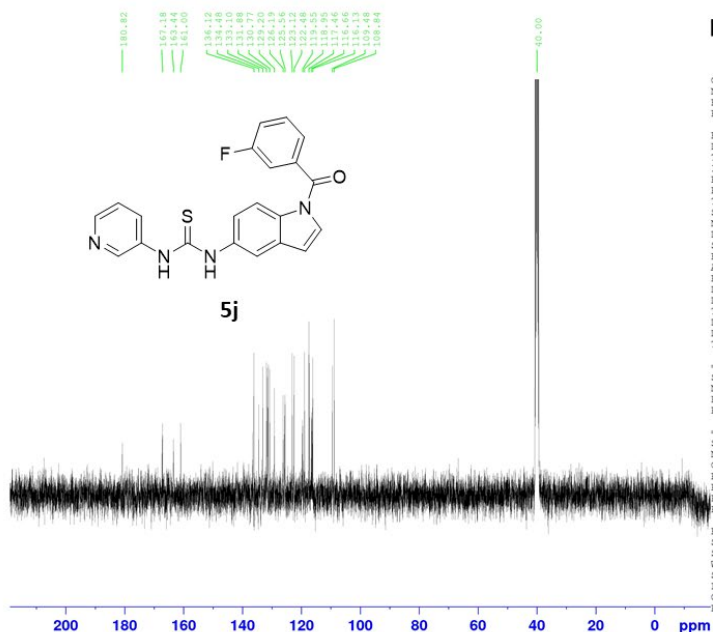


Current Data Parameters
NAME AMS-H23-F
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200421
Time 18.35
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 298.9 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



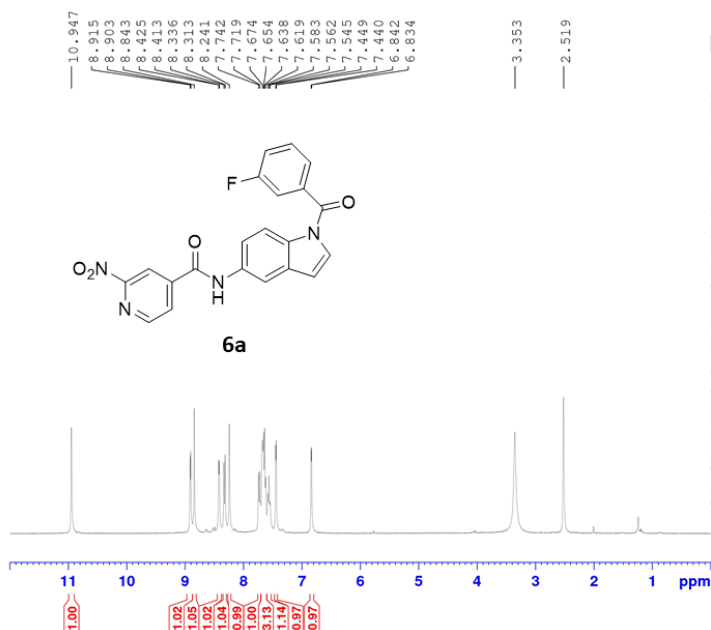
Current Data Parameters
NAME AMS-H23_CNMR
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20200711
Time 21.31
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 100.629474 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

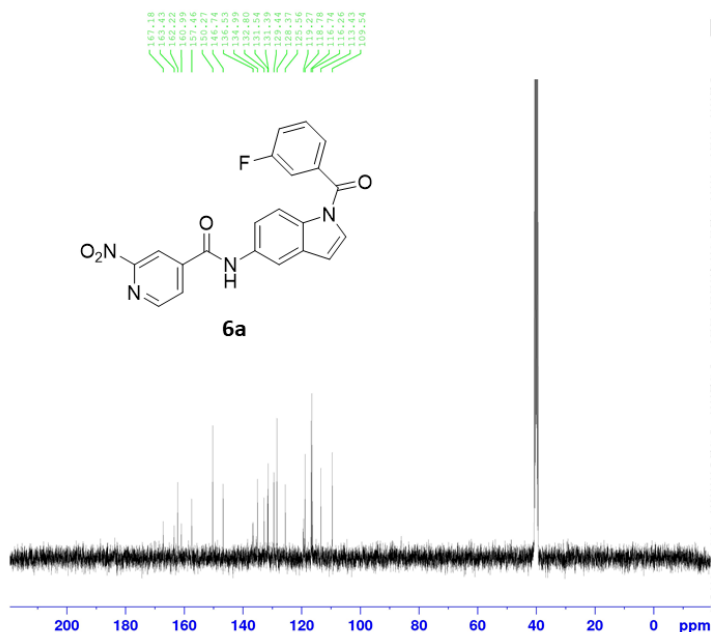


Current Data Parameters
 NAME AMS-H1
 EXPNO 1
 PROCNO 1

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



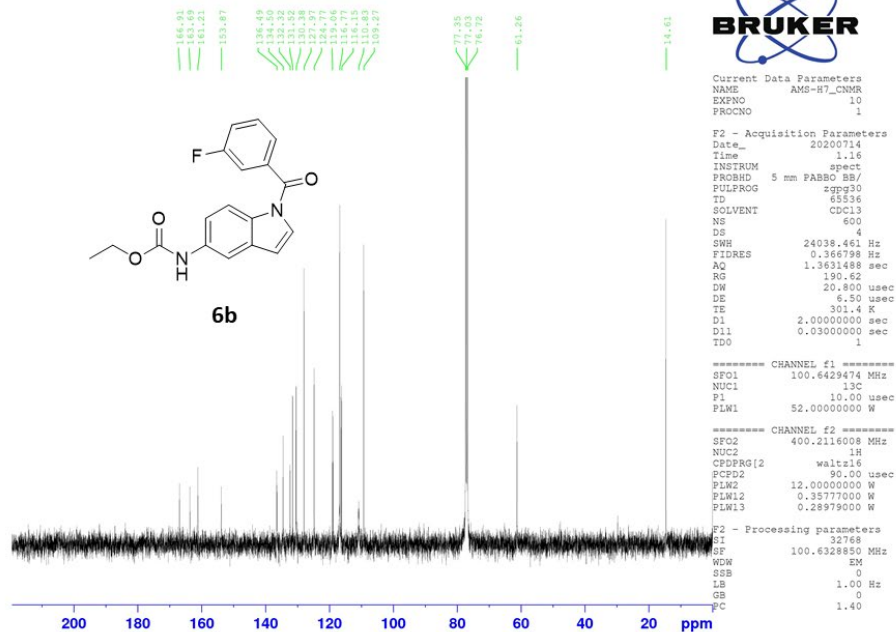
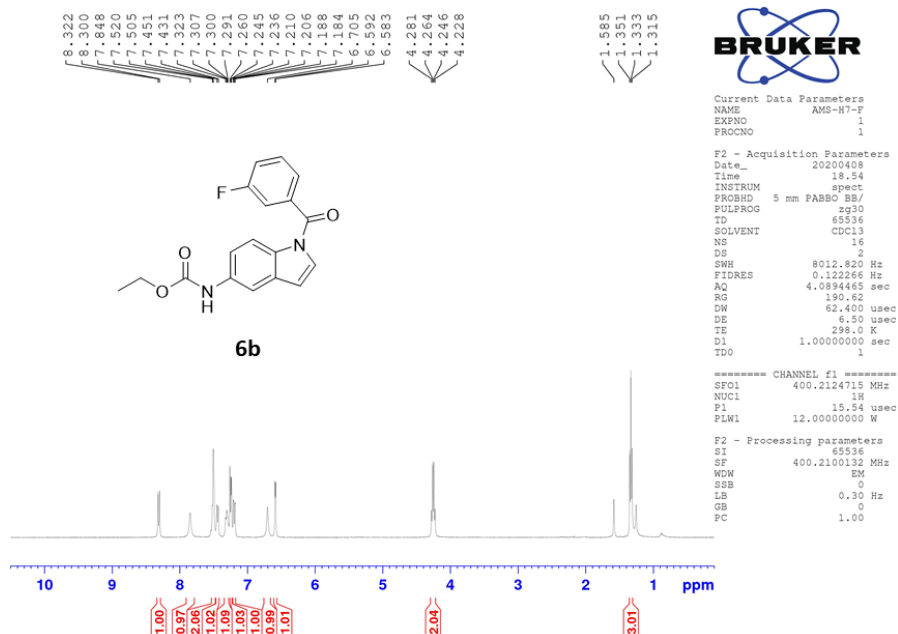
Current Data Parameters
 NAME AMS-H1_CNMR
 EXPNO 10
 PROCNO 1

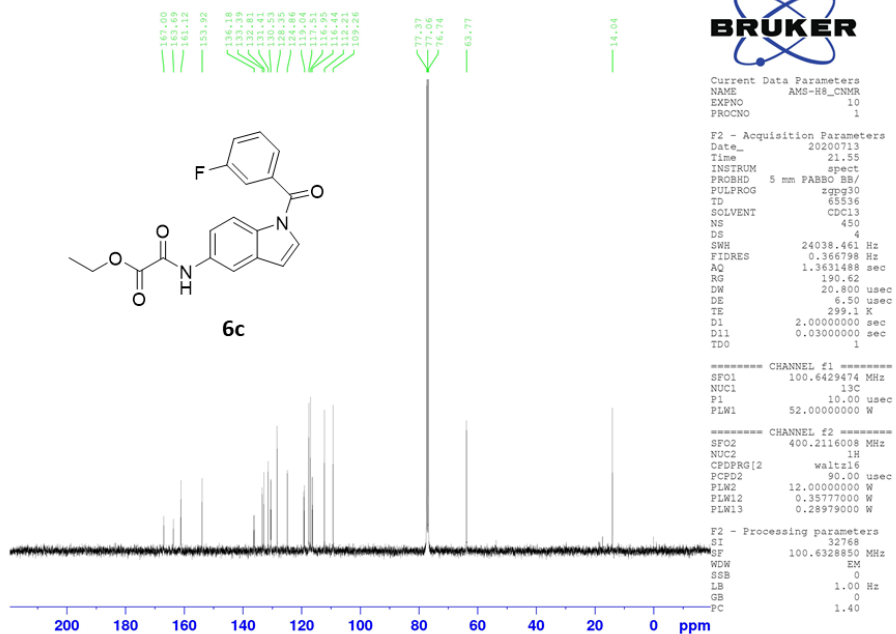
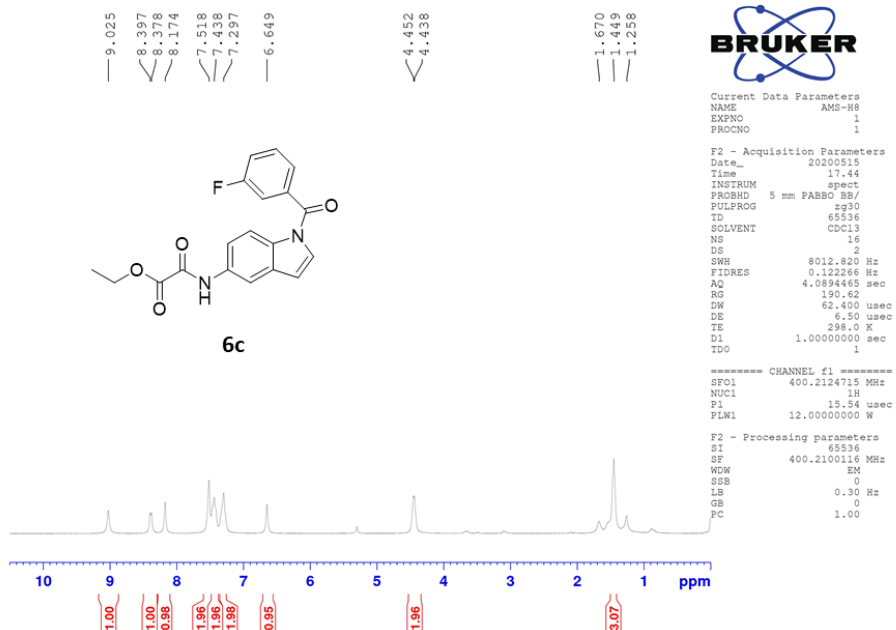
F2 - Acquisition Parameters
 Date_ 20201130
 Time 12.48
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 500
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631488 sec
 RG 190.62
 DW 20.800 usec
 DE 6.50 usec
 TE 299.2 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TDO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

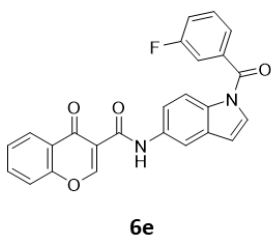
===== CHANNEL f1 =====
 SFO1 100.6429474 MHz
 NUC1 13C
 P1 10.00 usec
 PLW1 52.00000000 W

===== CHANNEL f2 =====
 SFO2 400.2116008 MHz
 NUC2 1H
 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-H111_conc
EXPNO      10
PROCNO     1
```

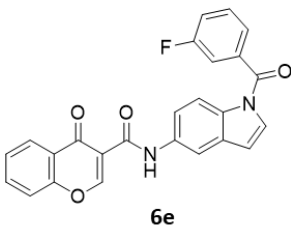
```

F2 - Acquisition Parameters
Date_      20200903
Time       16.34
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
DE          62.400 usec
DW          6.50 usec
TE         297.5 K
D1         1.00000000 sec
ID0        .1

```

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

```
F2 - Processing parameters
SI          65536
SF          400.210000 MHz
WDW          EM
SSB          0
LB          0.30 Hz
GB          0
PC          1.00
```



```
Current Data Parameters
NAME          4e_CNMR
EXPNO          10
PROCNO         1
```

```

F2 - Acquisition Parameters
Date_   20101010
Time    2.50
INSTRUM spect
PROBHD  5 mm PABBO BE/
PULPROG zgpg30
TD       65536
SOLVENT DMSO
NS       4000
DS       4
SWH      24038.461 Hz
FIDRES   0.366798 Hz
AQ       1.3631488 sec
RG       190.62
DW       20.800 use
DE       6.50 use
TE       299.8 K
D1       2.000000000
D11      0.030000000 sec
TD0      1

```

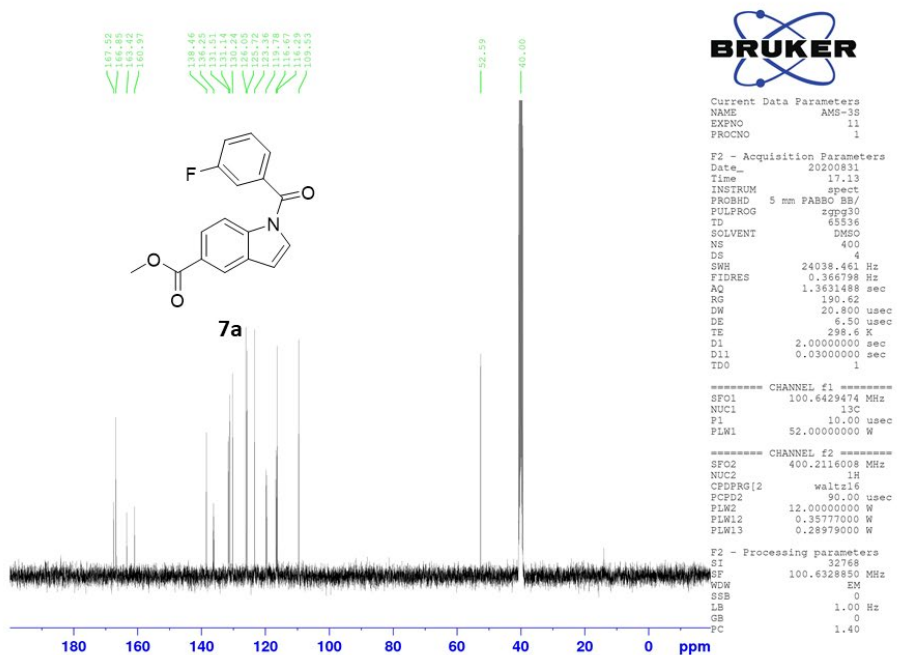
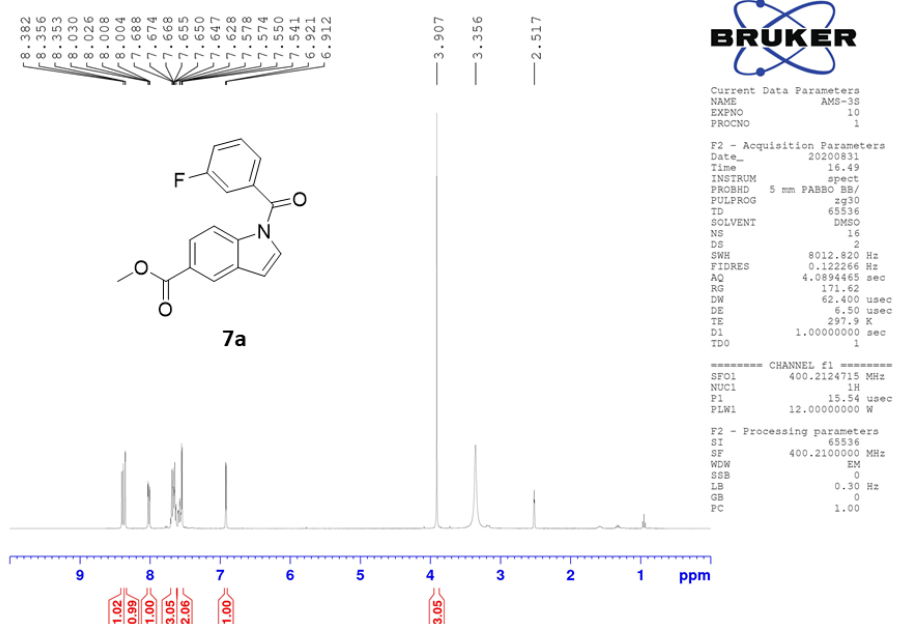
```
===== CHANNEL f1 =====
SFO1      100.6429474 MHz
NUC1      13C
P1         10.00 usec
PLW1      52.00000000 W
```

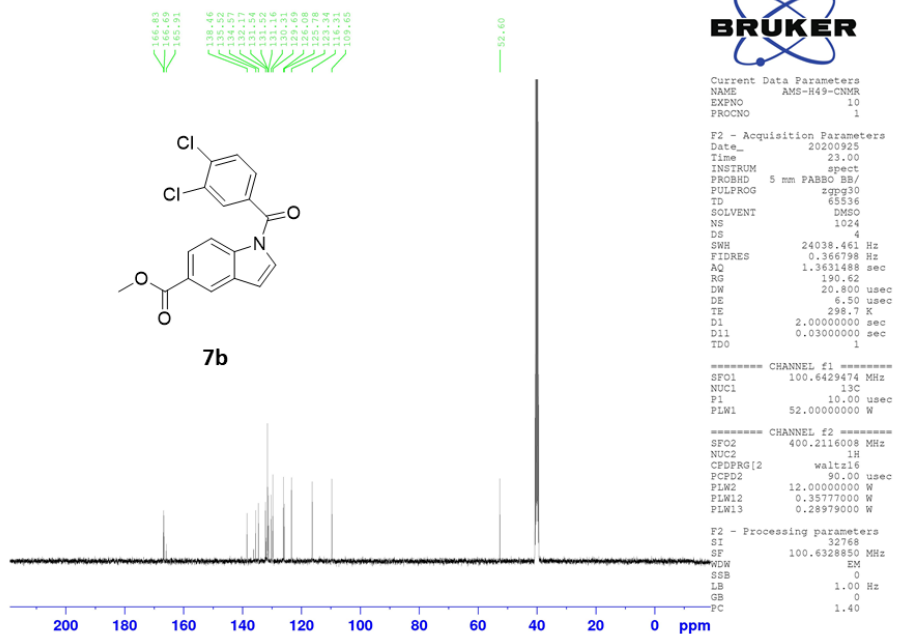
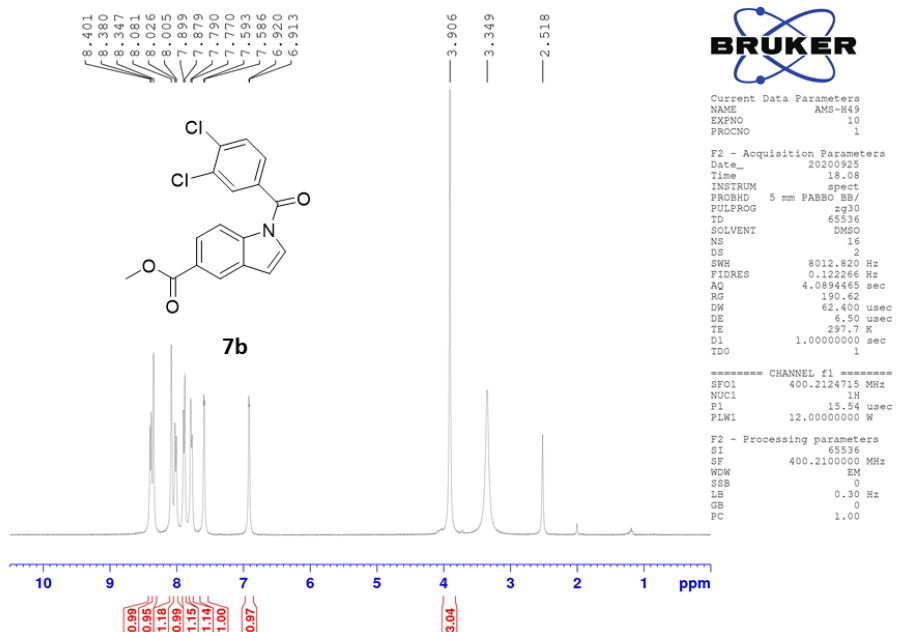
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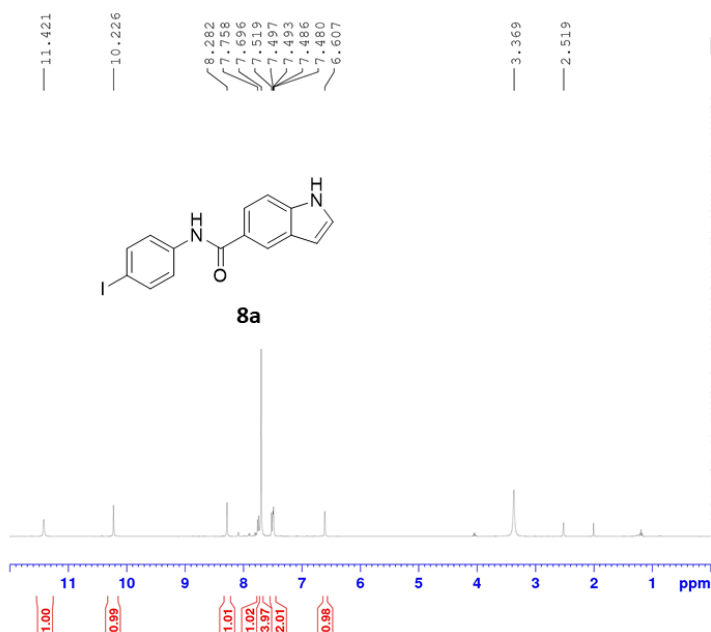
SFO2      400.2116008 MHz
NUC2      1H
CPDPRG[2  waltz16
PCPD2     90.00 usec
PLW2      12.00000000 W
PLW12     0.35777000 W
PLW13     0.28979000 W

```

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





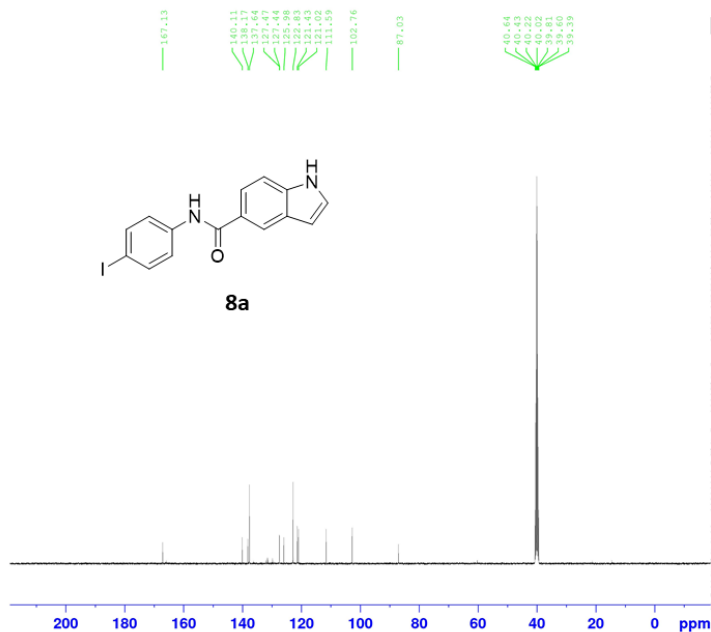


Current Data Parameters
NAME A-H41 (2nd)
EXPNO 10
PROCNO 1

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
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 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



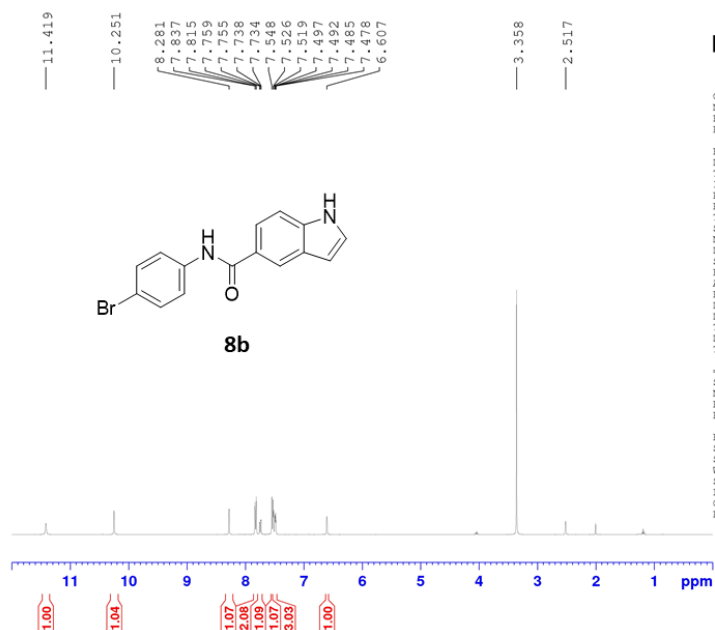
Current Data Parameters
NAME A-H41_CNMR
EXPNO 10
PROCNO 1

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
DW 20.800 usec
DE 6.50 usec
TE 299.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 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

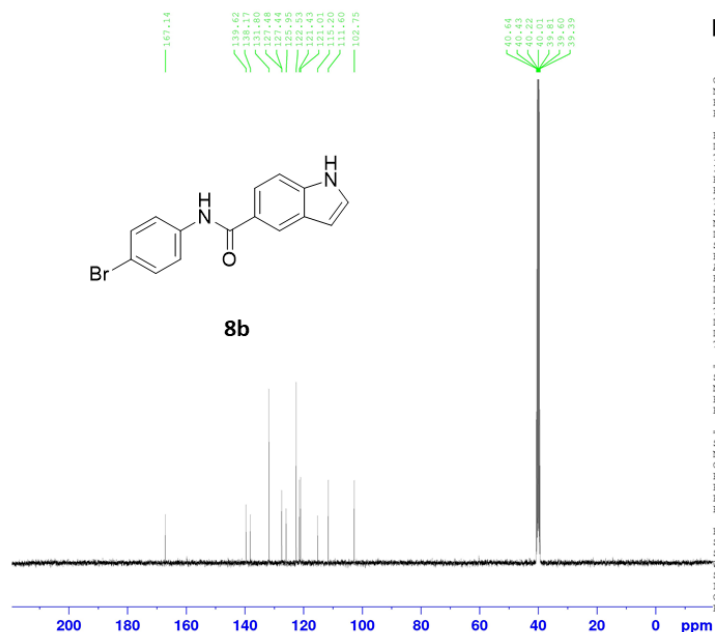


Current Data Parameters
NAME H-42
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201022
Time 10.53
INSTRUM spect
PROBHD 5 mm 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 171.62
DW 62.400 usec
DE 6.50 usec
TE 298.7 K
D1 1.00000000 sec
TD0 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



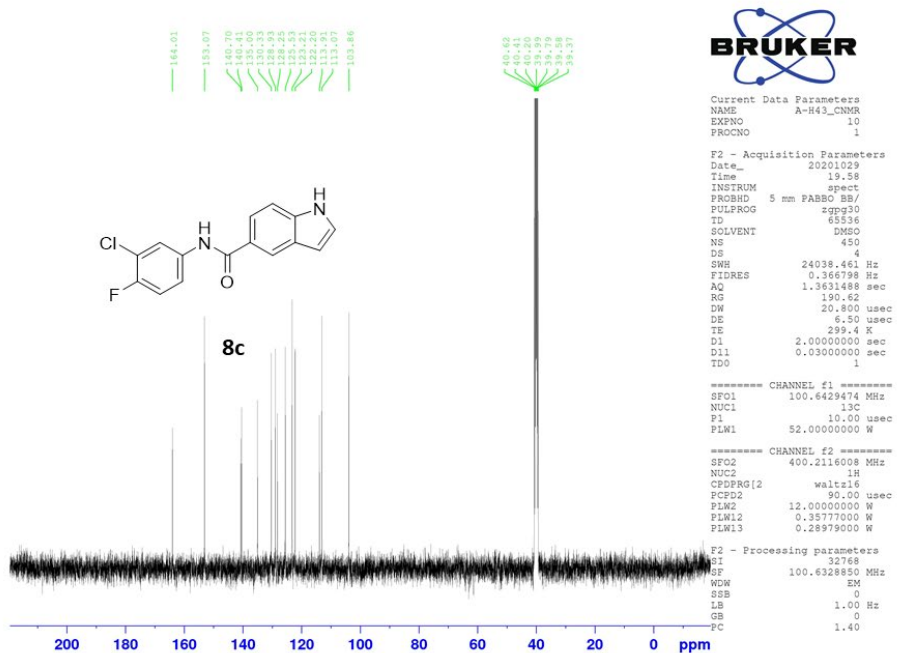
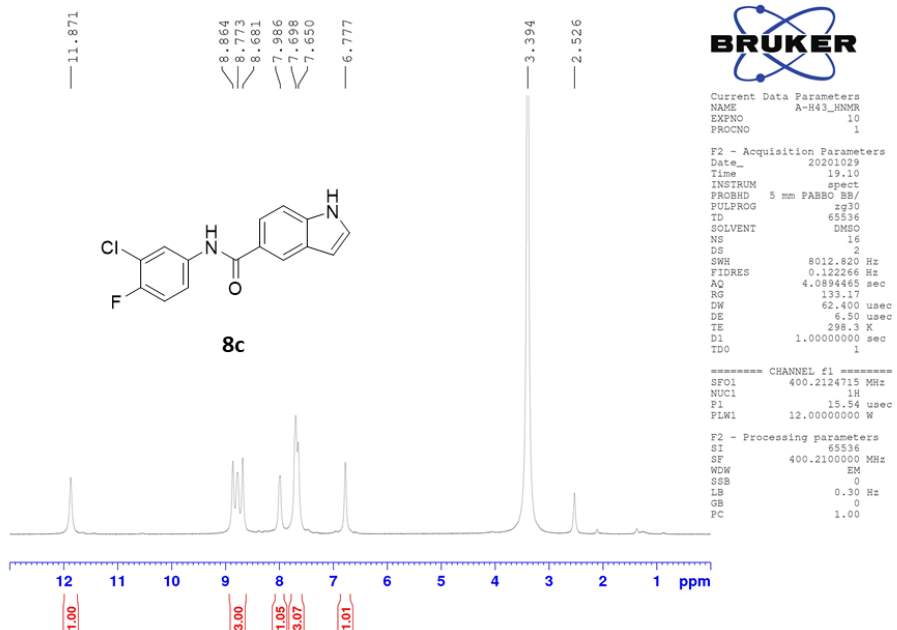
Current Data Parameters
NAME A-H42_CNMR
EXPNO 10
PROCNO 1

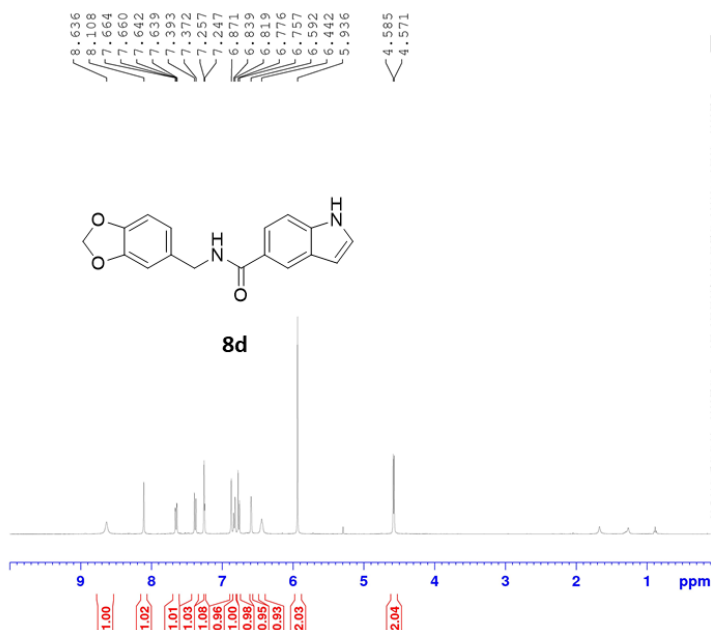
F2 - Acquisition Parameters
Date_ 20201022
Time 23.28
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 700
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 190.62
DW 20.800 usec
DE 6.50 usec
TE 299.5 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

===== 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



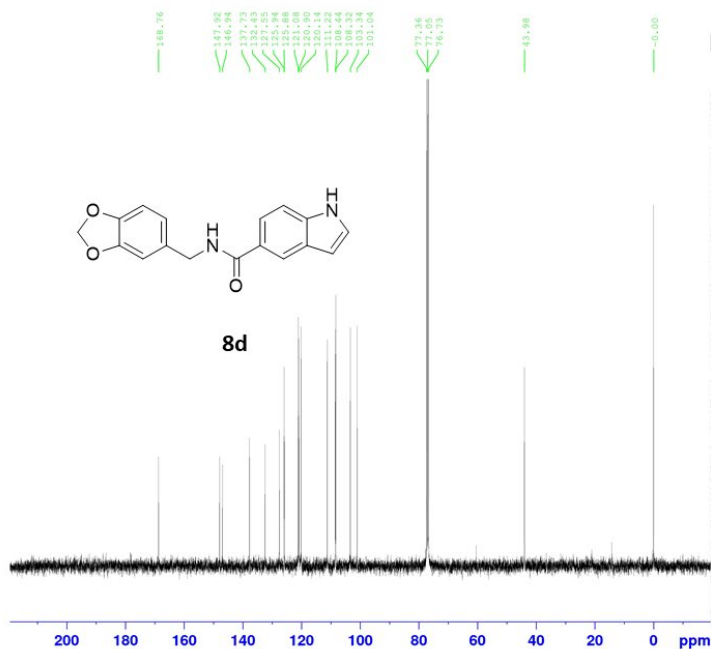


Current Data Parameters
 NAME A-H57f_NMR
 EXPNO 10
 PROCNO 1

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



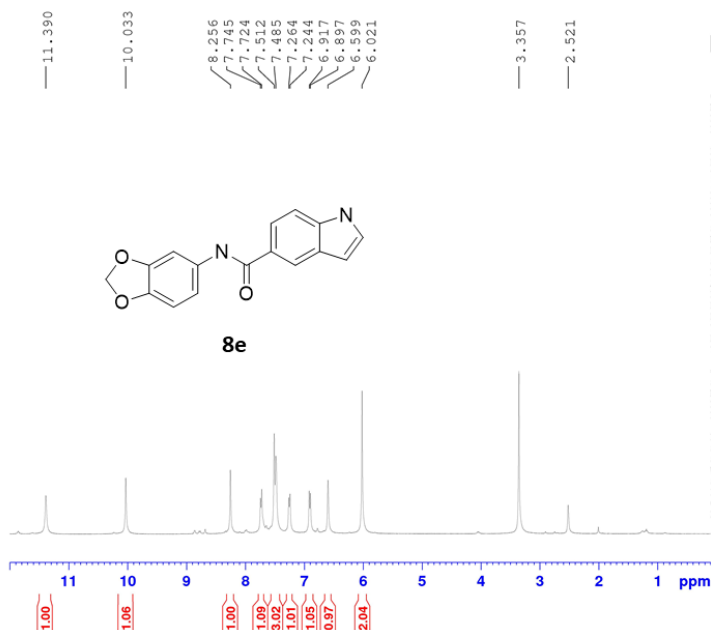
Current Data Parameters
 NAME AMS-H57
 EXPNO 11
 PROCNO 1

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
 CPDPRG2 waltz16
 PCPD2 90.00 usec
 PLW2 12.00000000 W
 PLW12 0.35777000 W
 PLW13 0.28979000 W

F2 - Processing parameters
 SI 32768
 SF 100.6328876 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

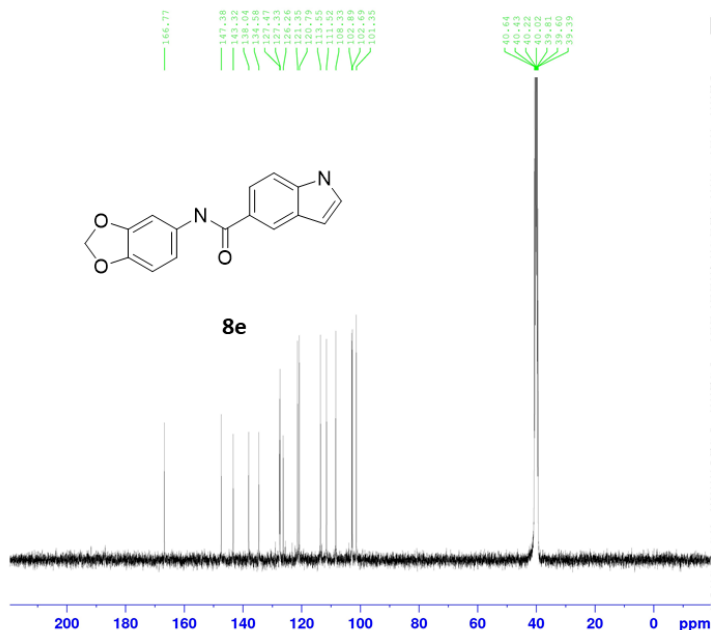
Date_	20201009
Time	0.27
INSTRUM	spect
PROBHD	5 mm PABBO BB/
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	8012.820 Hz
FIDRES	0.122266 Hz
AQ	4.0894465 sec
RG	146.31
DW	62.400 usec
DE	6.50 usec
TE	300.3 K
D1	1.00000000 sec
TD0	1

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

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

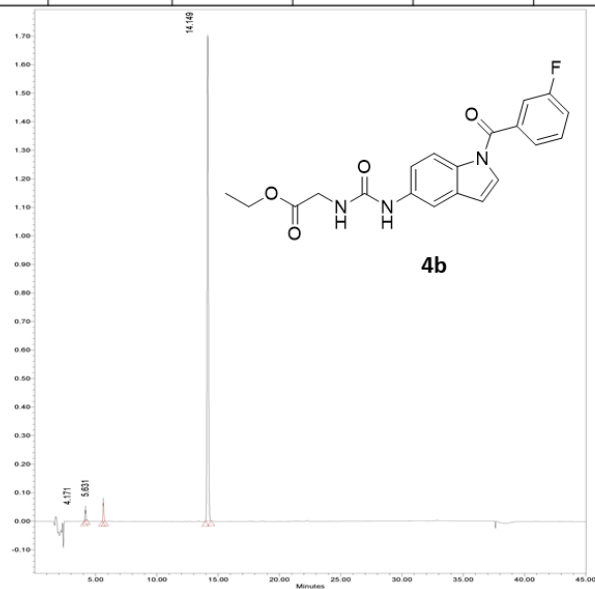
F2 - Processing parameters

SI	65536
SF	400.2100000 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

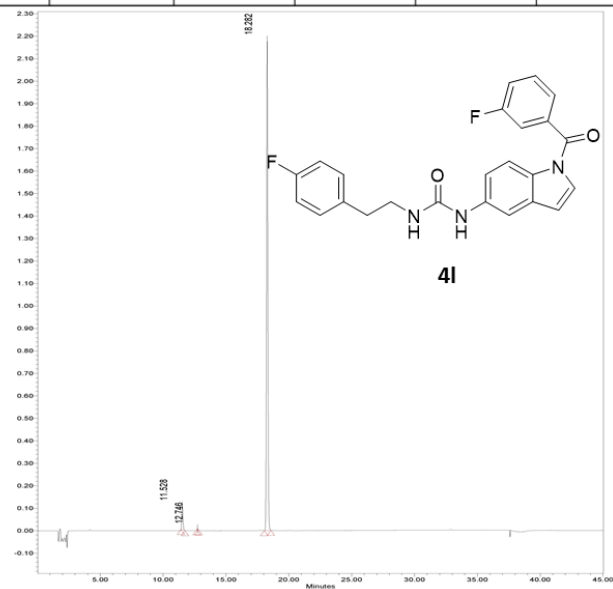


2. Representative HPLC purity data of the compounds

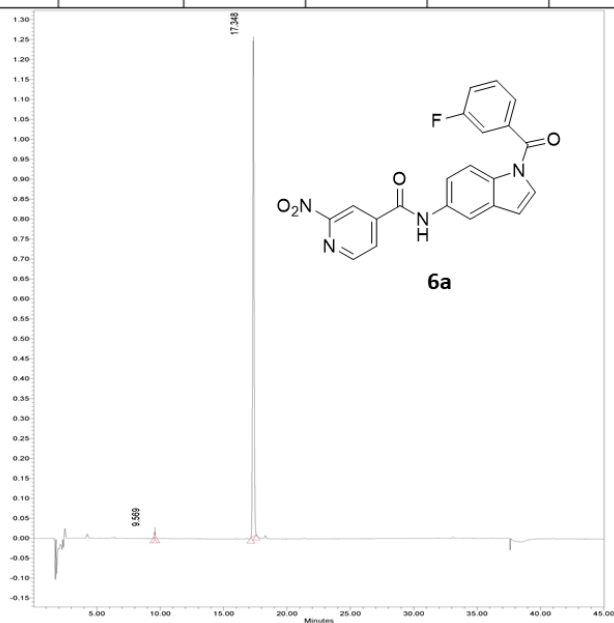
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1		4.171							182884	1.44	36389	bb	
2		5.631							362117	2.86	67497	bb	
3		14.149							12135189	95.70	1702752	bb	



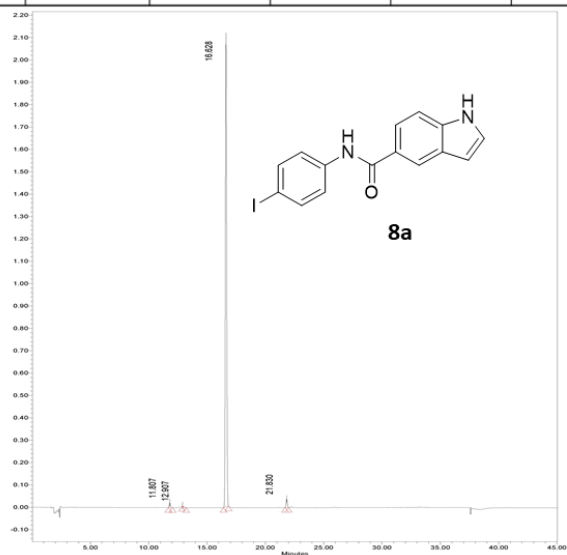
	Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (μV*sec)	% Area	Height (μV)	Int Type	Amount
1		11.528							722618	4.30	108944	bb	
2		12.746							34035	0.20	6370	bb	
3		18.282							16041627	95.50	2201606	bb	



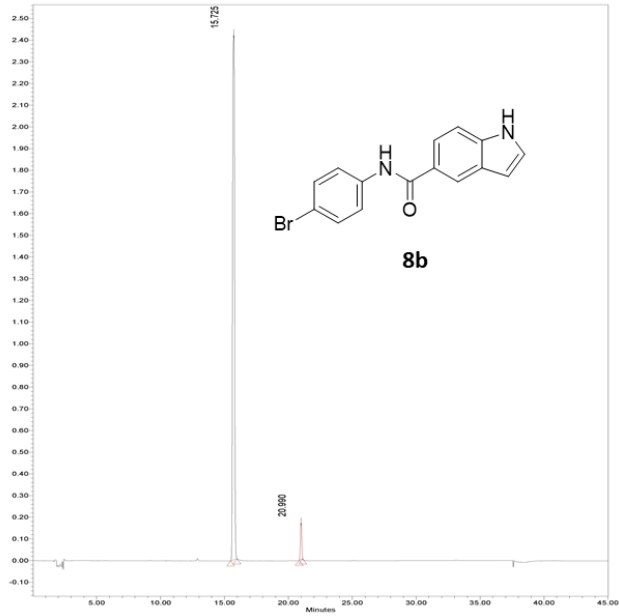
	Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (μV*sec)	% Area	Height (μV)	Int Type	Amount
1		9.569							84076	0.88	14431	bb	
2		17.348							9455947	99.12	1252820	bb	



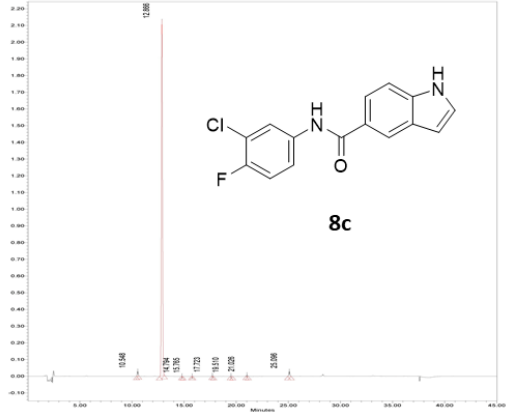
	Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (μV*sec)	% Area	Height (μV)	Int Type	Amount
1		11.807							143417	0.85	20959	bb	
2		12.907							36312	0.21	4101	bb	
3		16.628							16480558	97.34	2106271	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 (μV*sec)	% Area	Height (μV)	Int Type	Amount
1		15.725							26481219	95.64	2461374	bb	
2		20.990							1206129	4.36	174283	bb	



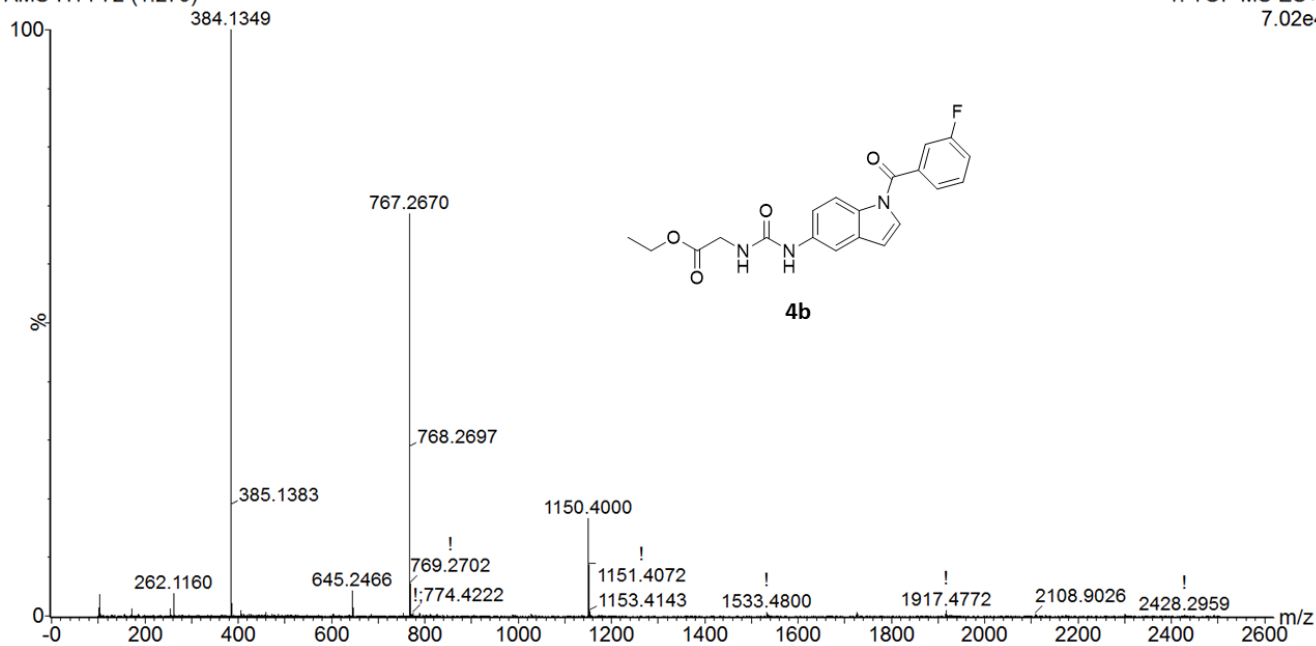
	Name	Retention Time (min)	Purity1 Angle	Purity1 Threshold	PDA Match1 Spect. Name	PDA Match1 Angle	PDA Match1 Threshold	PDA Match1 Lib. Name	Area (μV*sec)	% Area	Height (μV)	Int Type	Amount
1		10.548							173366	1.05	27024	bb	
2		12.866							16023703	97.28	2134594	bb	
3		14.794							3519	0.02	838	bb	
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

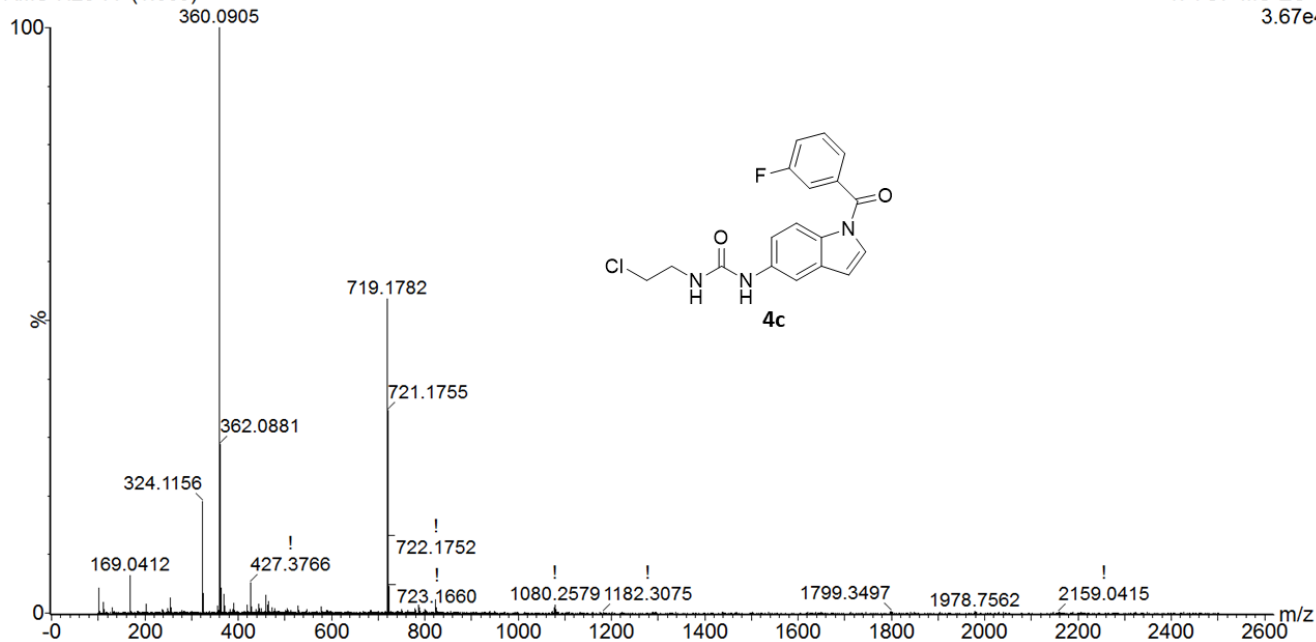
AMS-H14 72 (1.275)

1: TOF MS ES+
7.02e4

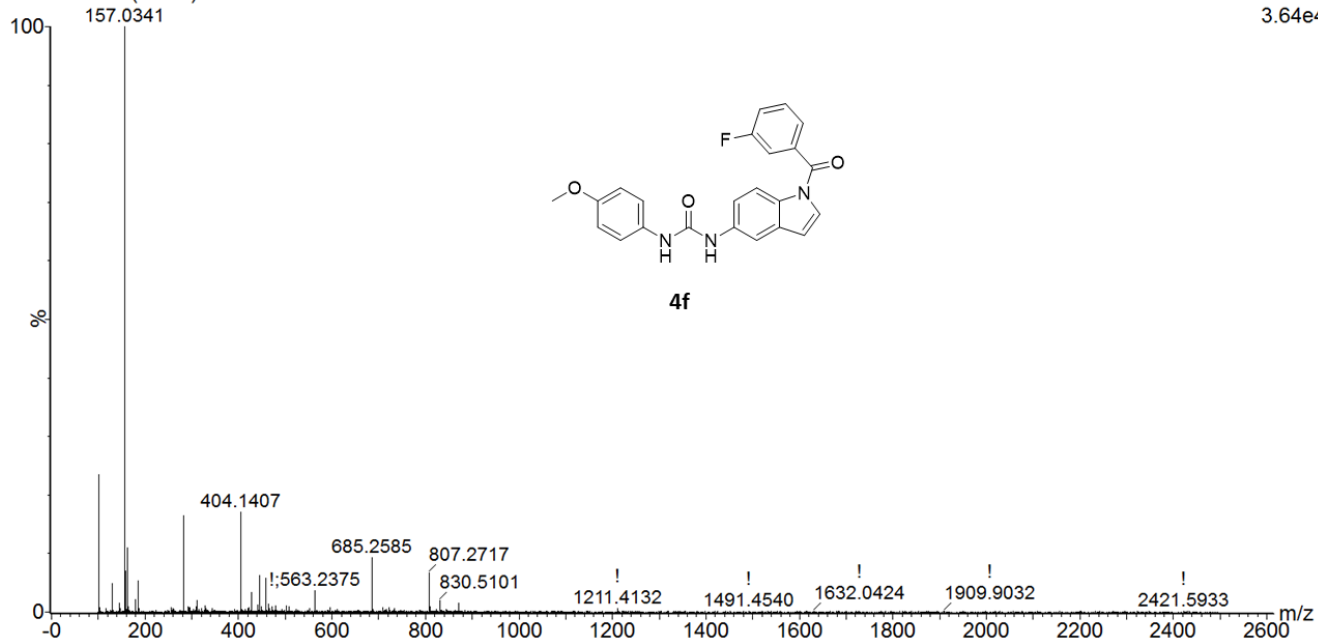


AMS-H28 77 (1.369)

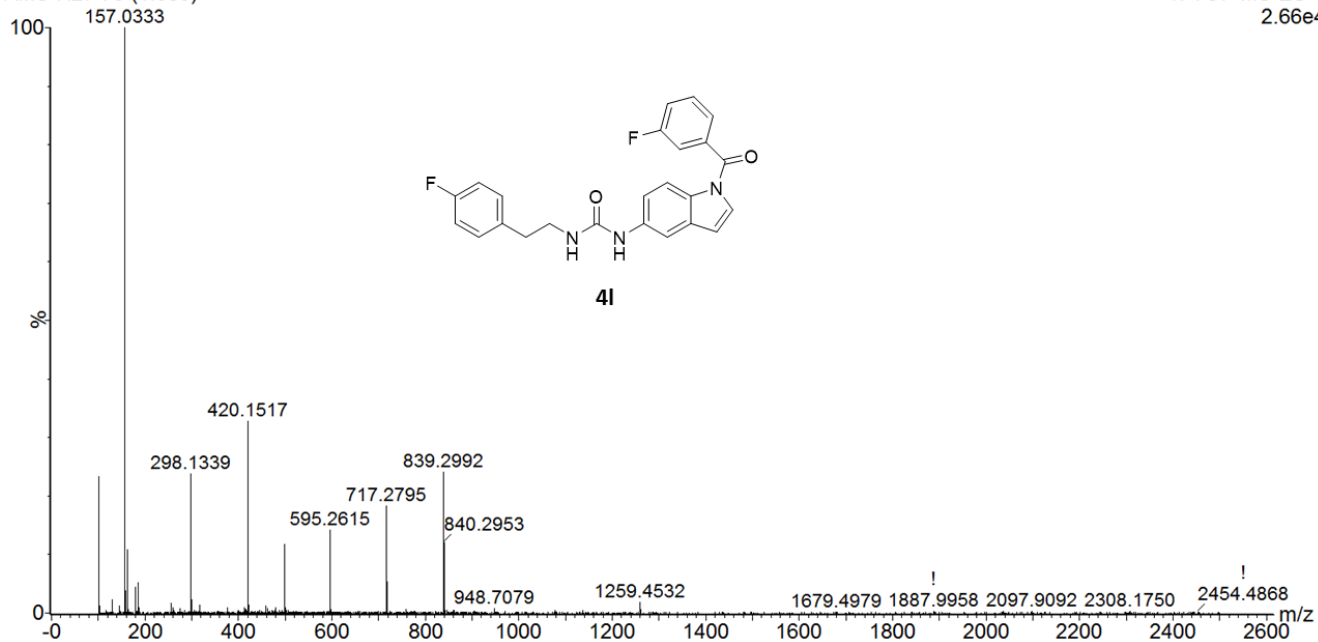
1: TOF MS ES+
3.67e4



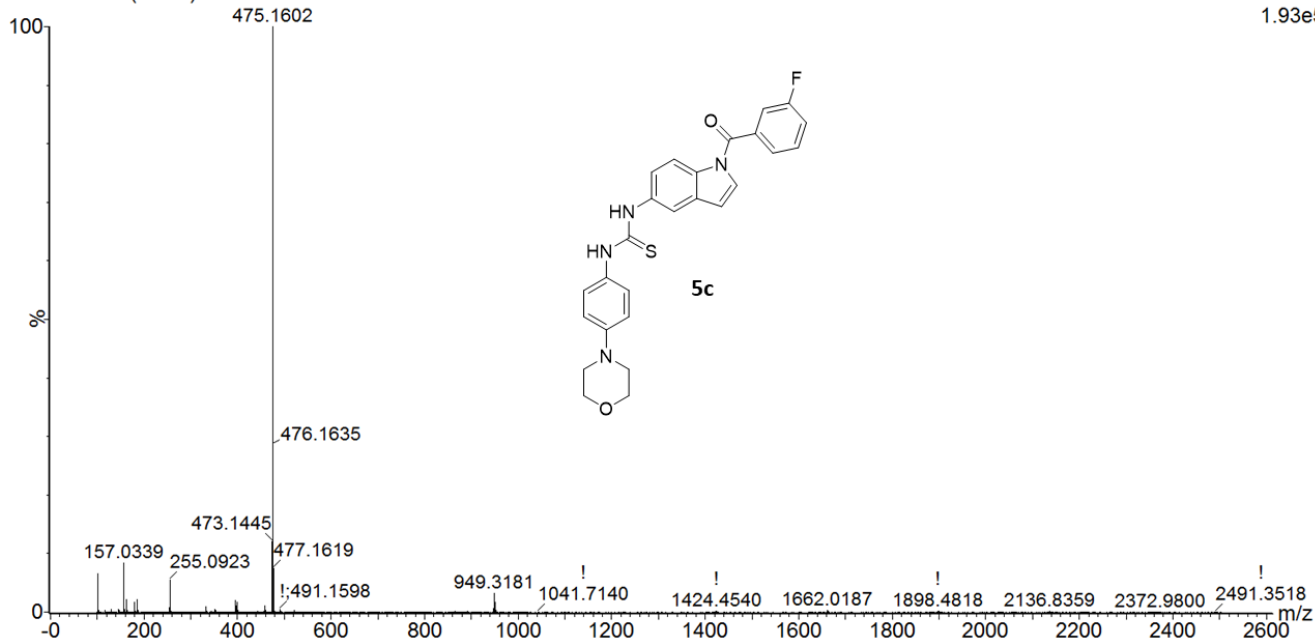
AMS-H25 79 (1.403)

1: TOF MS ES+
3.64e4

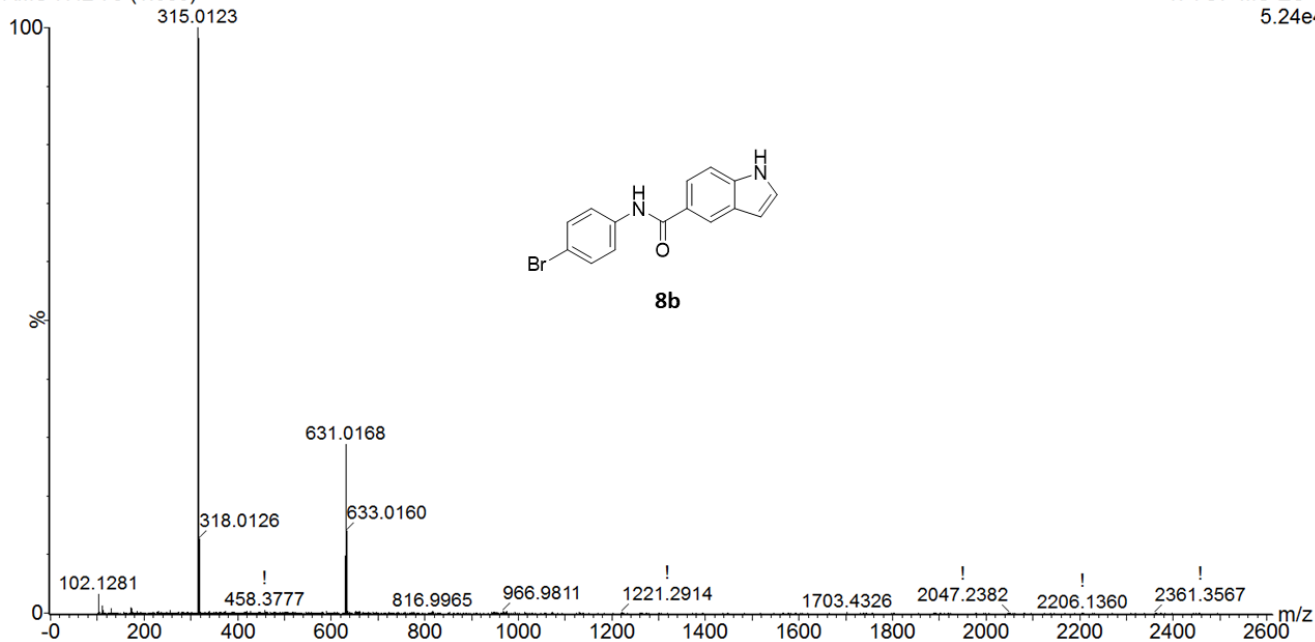
AMS-H27 78 (1.386)

1: TOF MS ES+
2.66e4

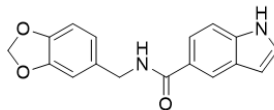
AMS-H30 74 (1.310)

1: TOF MS ES+
1.93e5

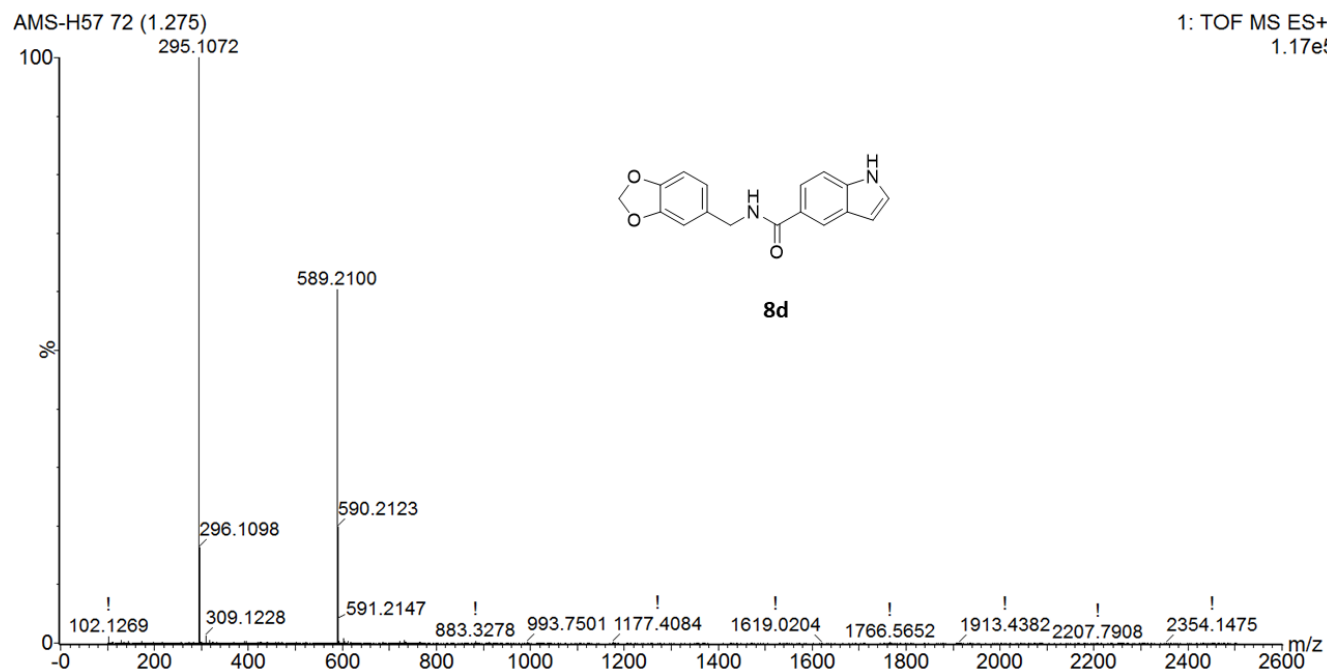
AMS-H42 78 (1.386)

1: TOF MS ES+
5.24e4

1: TOF MS ES+
1.17e5



8d



4. Molecular modelling supplementary material

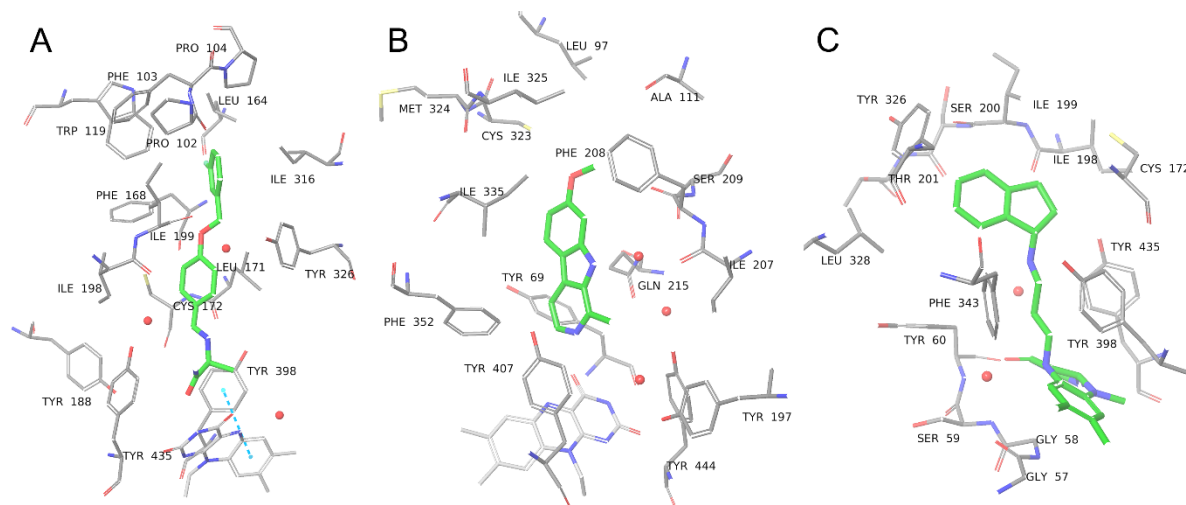


Figure S1. Binding modes of reference reversible inhibitors (A) safinamide bound to MAO-B (PDB ID: 2V5Z), (B) harmine bound to MAO-A (PDB ID: 2Z5X) and covalent irreversible inhibitor (C) rasagiline bound to MAO-B (PDB ID: 1S2Y). Ligands are presented as green thick sticks, pocket atoms – gray thin sticks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