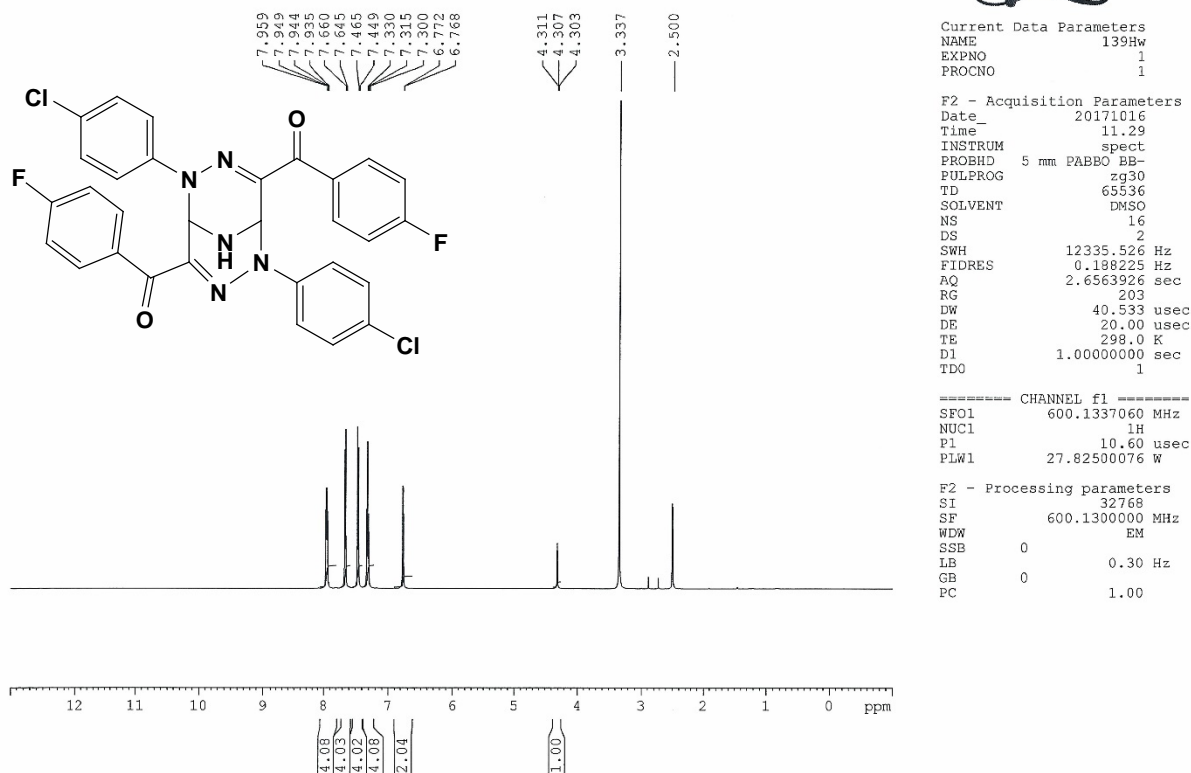


Supporting Information on

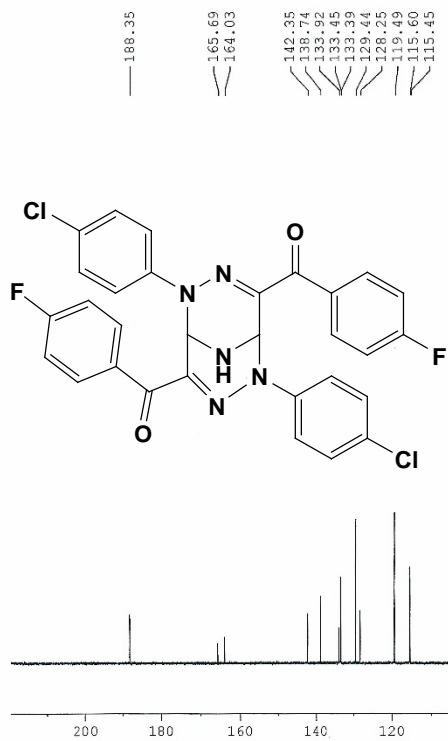
Facile assembling of novel 2,3,6,7,9-pentaazabicyclo[3.3.1]nona-3,7-diene derivatives under microwave and ultrasound platforms

Hamad M. Al-Matar^{a*}, Kamal M. Dawood^b, Wael M. Tohamy^c and Mona A. Shalaby^a

¹H NMR spectrum of compound 2a



¹³C NMR spectrum of compound 2a



Current Data Parameters
 NAME 139fw
 EXPNO 2
 PROCNO 1

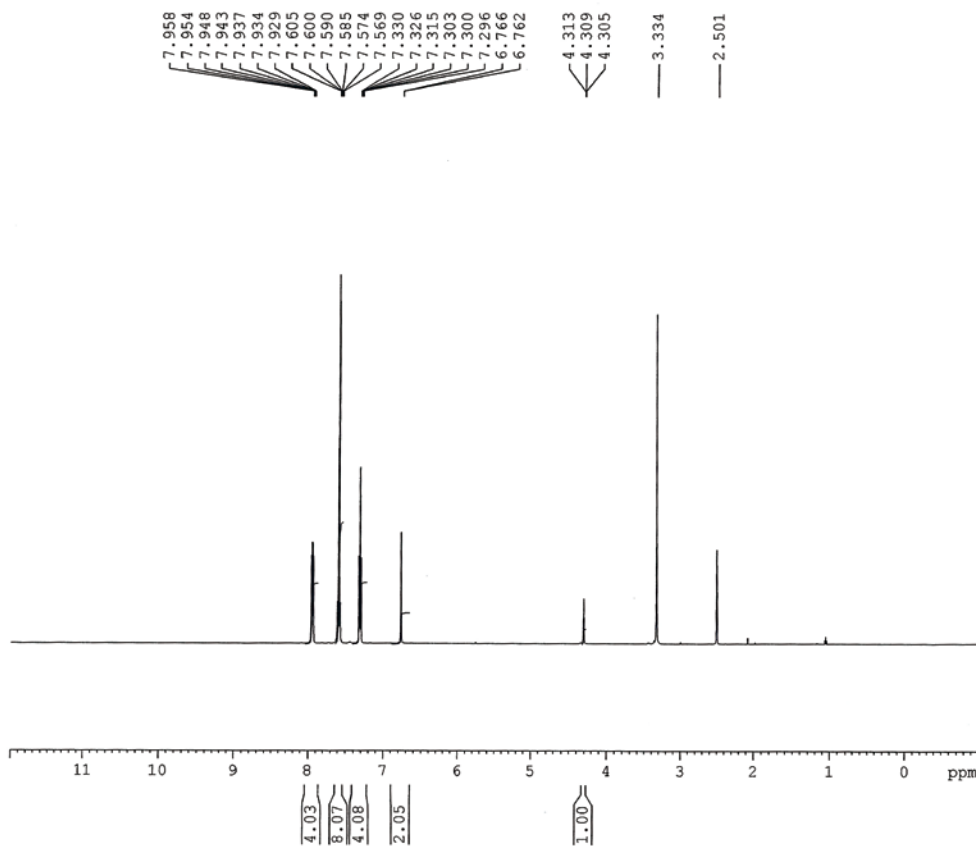
F2 - Acquisition Parameters
 Date_ 20171016
 Time_ 12.33
 INSTRUM spect
 PROBHD 5 mm PABEO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 1374
 DS 4
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 203
 DW 13.867 usec
 DE 50.00 usec
 TE 298.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TDO 1

===== CHANNEL f1 =====
 SFO1 150.9178979 MHz
 NUC1 13C
 P1 8.80 usec
 PLW1 78.13500214 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 70.00 usec
 PLW2 27.82500076 W
 PLW12 0.63804001 W
 PLW13 0.31264001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028090 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

¹H NMR spectrum of compound **2b**

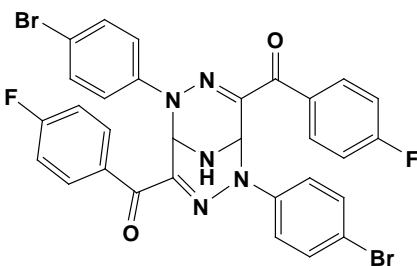


Current Data Parameters
 NAME 137HW-1H
 EXPNO 1
 PROCNO 1

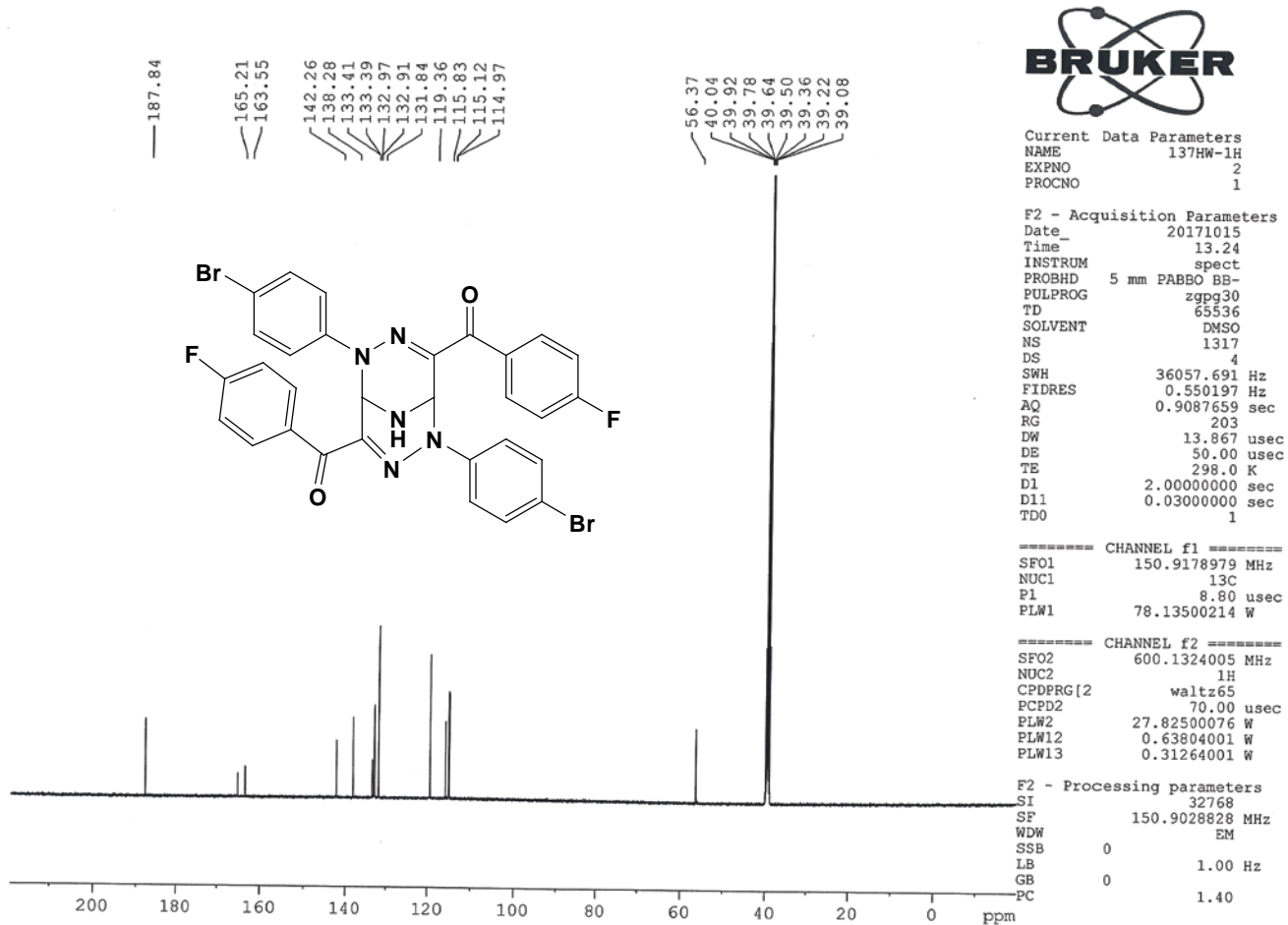
F2 - Acquisition Parameters
 Date_ 20171015
 Time_ 12.36
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 16
 DS 2
 SWH 12335.526 Hz
 FIDRES 0.188225 Hz
 AQ 2.6563926 sec
 RG 203
 DW 40.533 usec
 DE 20.00 usec
 TE 298.0 K
 D1 1.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 SF01 600.1337060 MHz
 NUC1 1H
 P1 10.60 usec
 PLW1 27.82500076 W

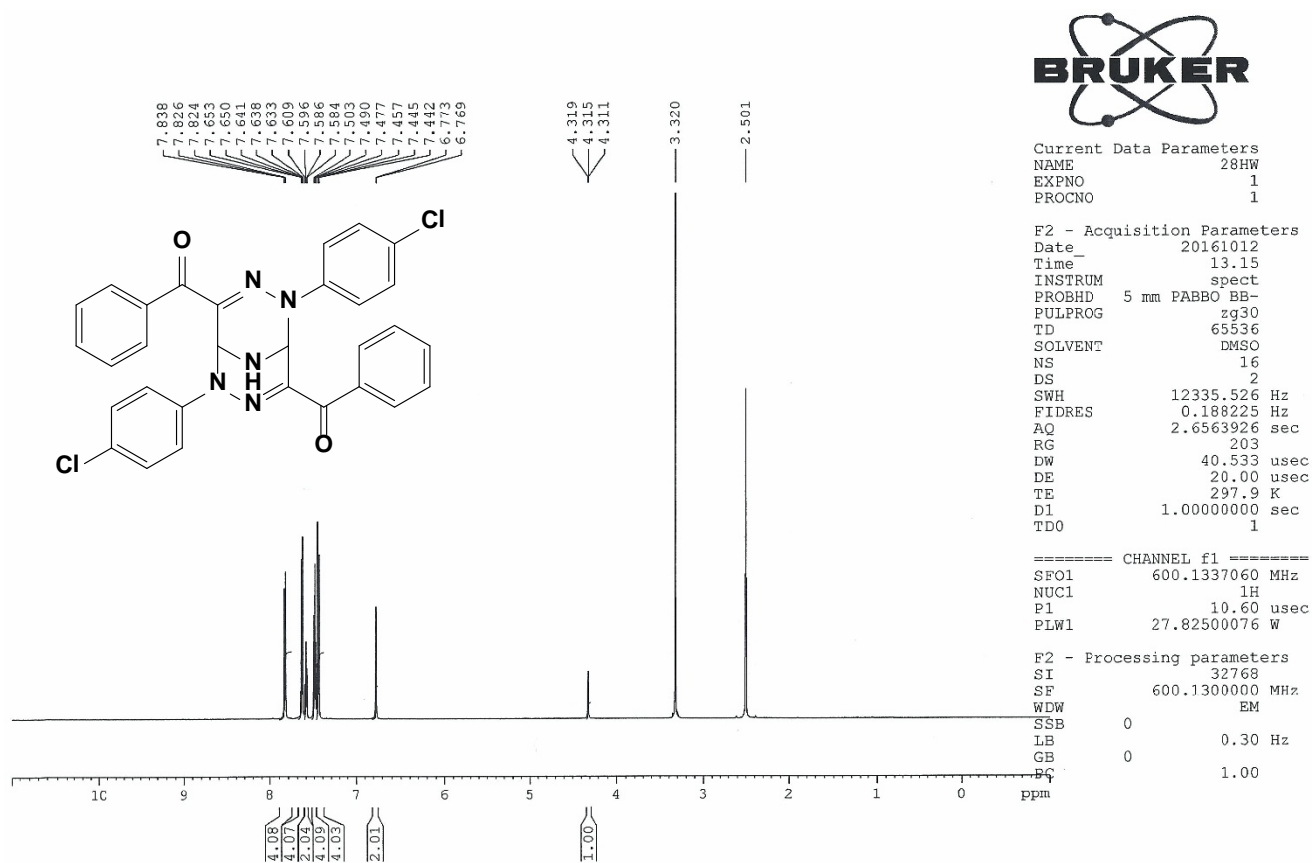
F2 - Processing parameters
 SI 32768
 SF 600.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00



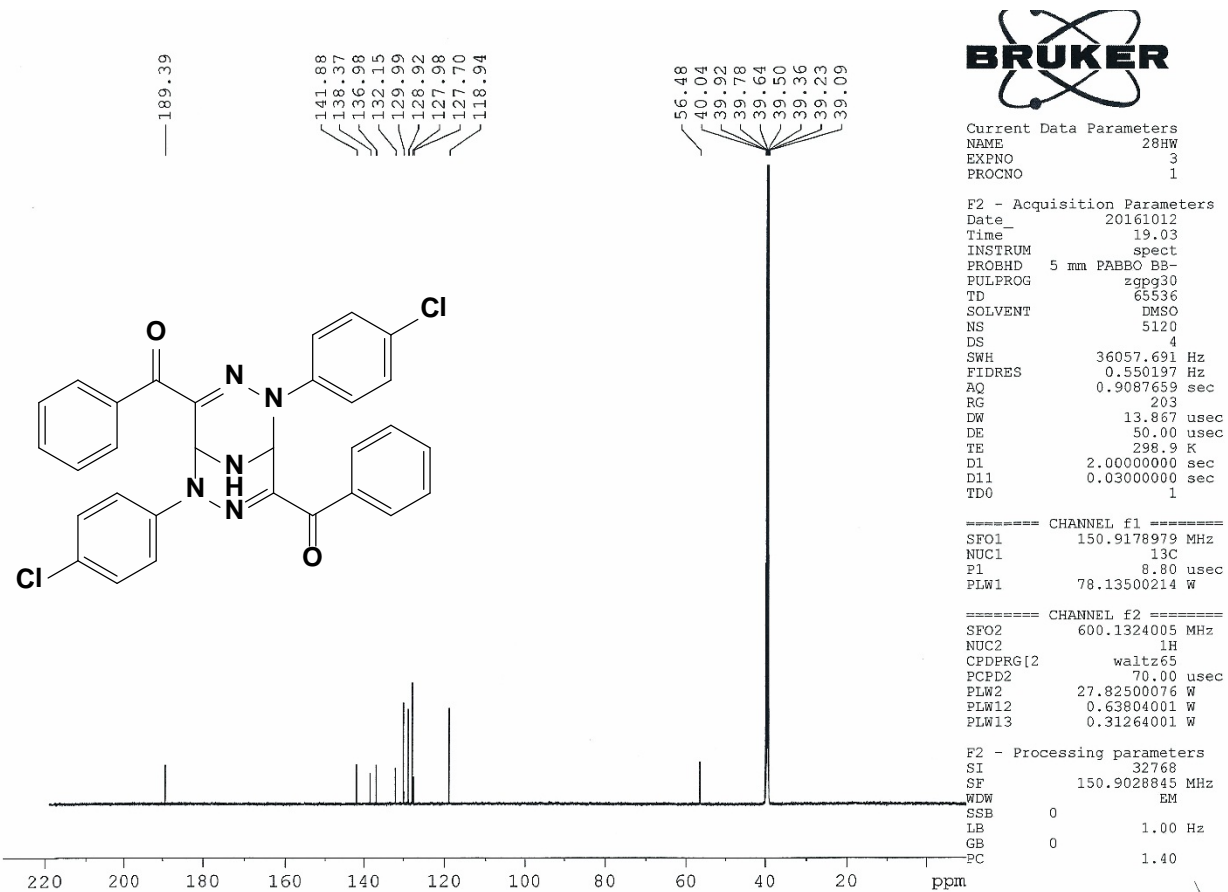
¹³C NMR spectrum of compound **2b**



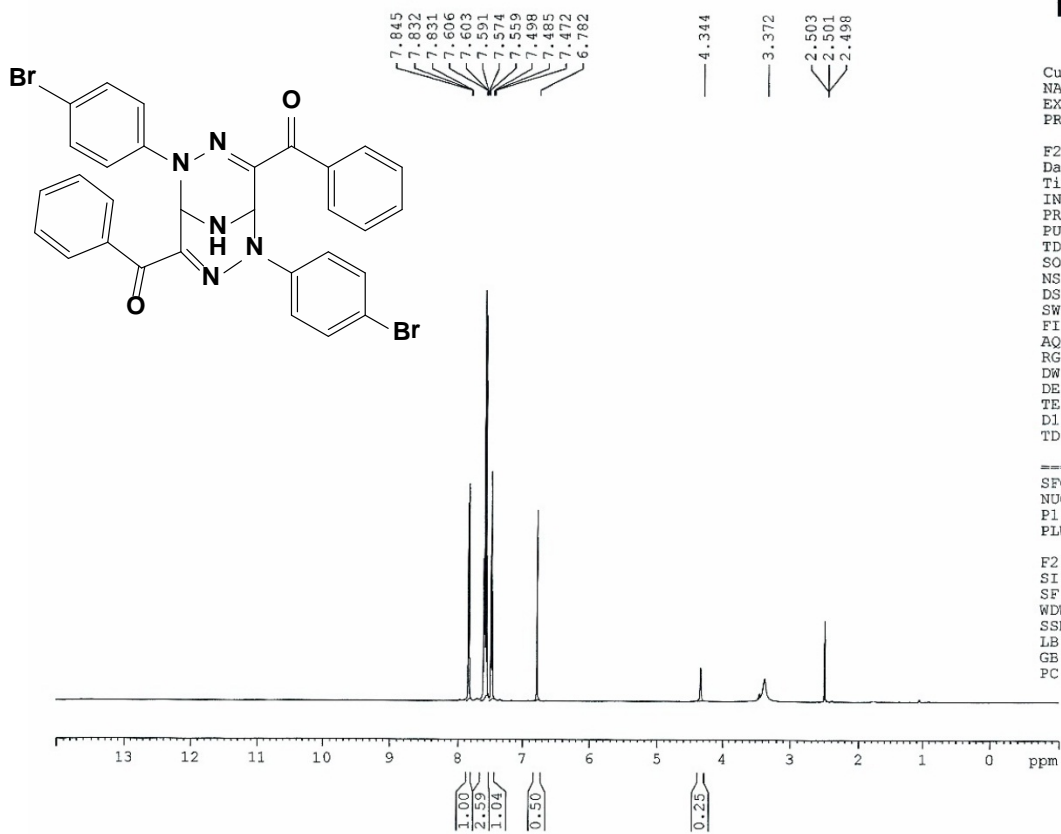
¹H NMR spectrum of compound **2c**



¹³C NMR spectrum of compound **2c**



¹H NMR spectrum of compound **2d**



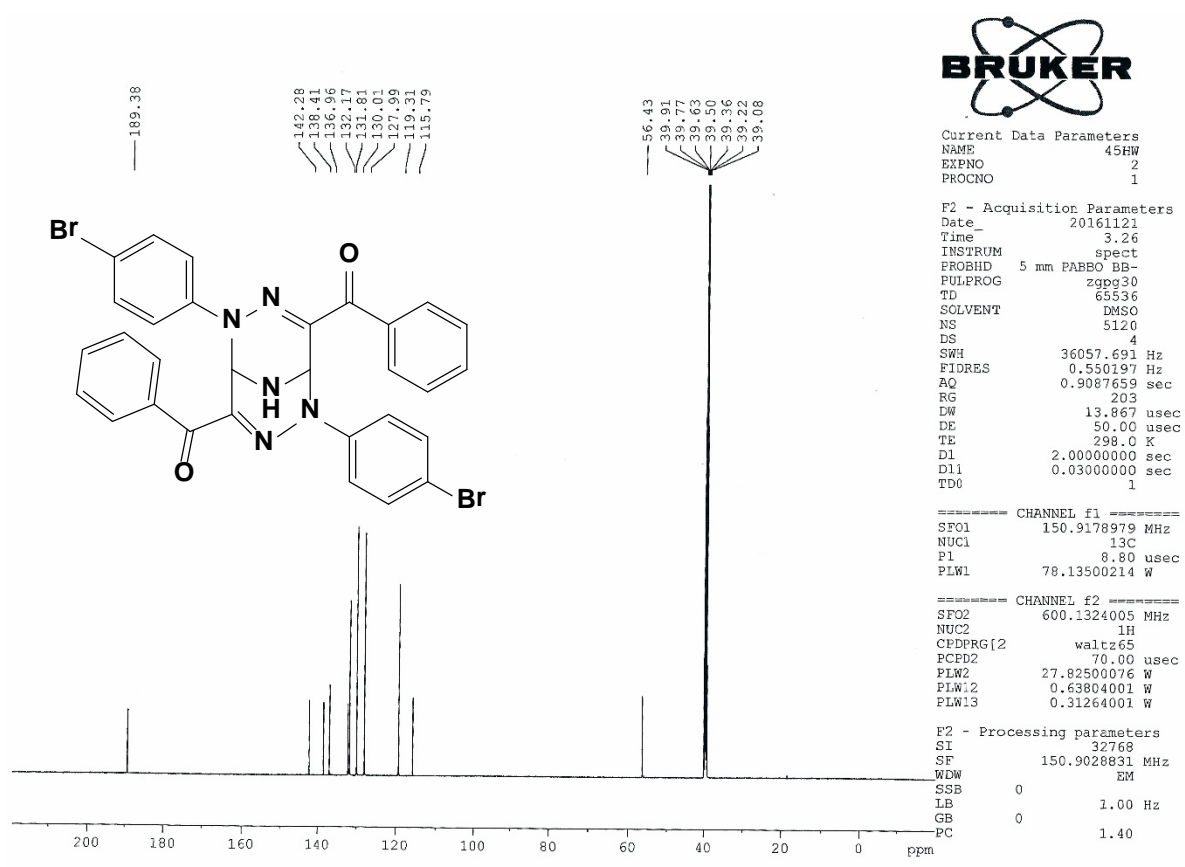
Current Data Parameters
 NAME 45HW
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20161114
 Time_ 11.12
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zg30
 TD 65536
 SOLVENT DMSO
 NS 8
 DS 2
 SWH 12335.526 Hz
 FIDRES 0.188225 Hz
 AQ 2.6563926 sec
 RG 161
 DW 40.533 usec
 DE 20.00 usec
 TE 295.3 K
 D1 1.00000000 sec
 TD0 1

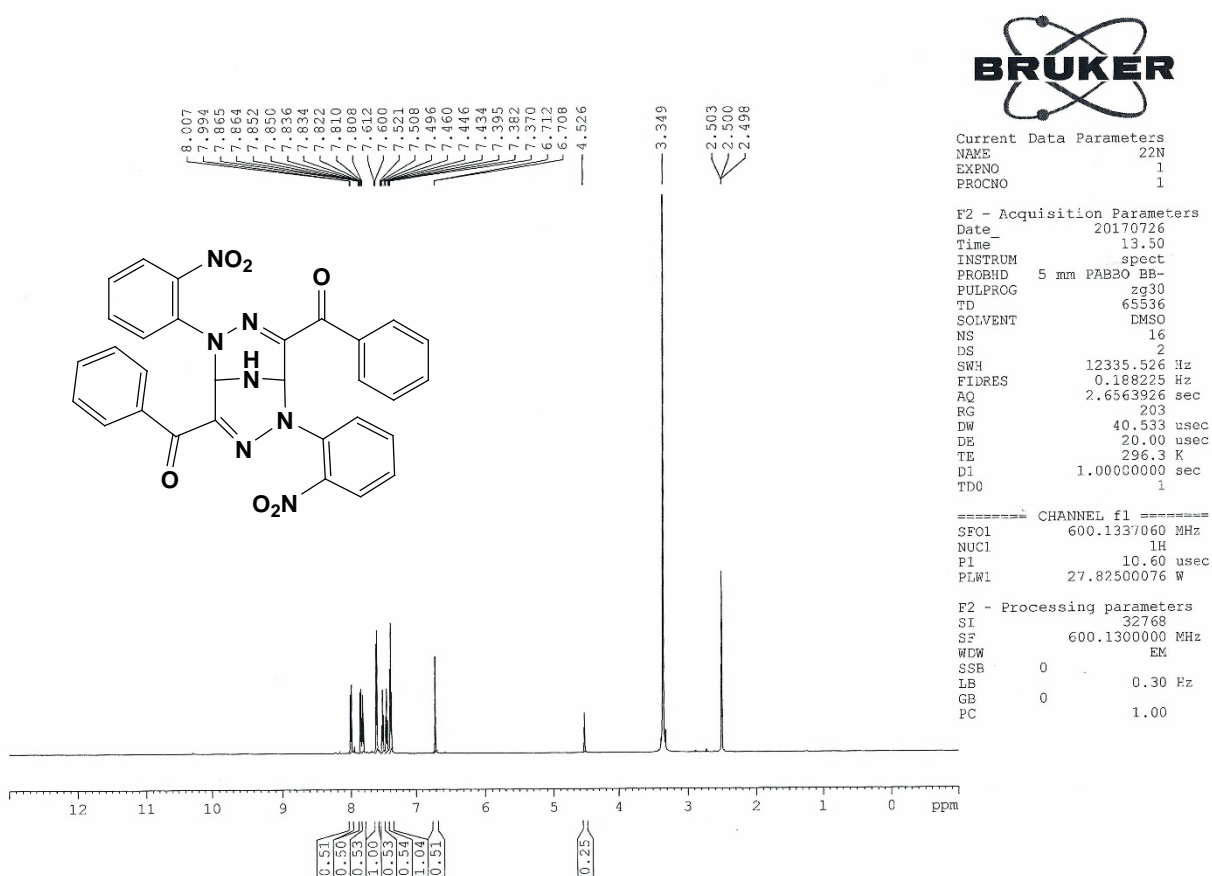
==== CHANNEL f1 =====
 SFO1 600.1337060 MHz
 NUC1 1H
 P1 10.60 usec
 PLW1 27.82500076 W

F2 - Processing parameters
 SI 32768
 SF 600.1300000 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

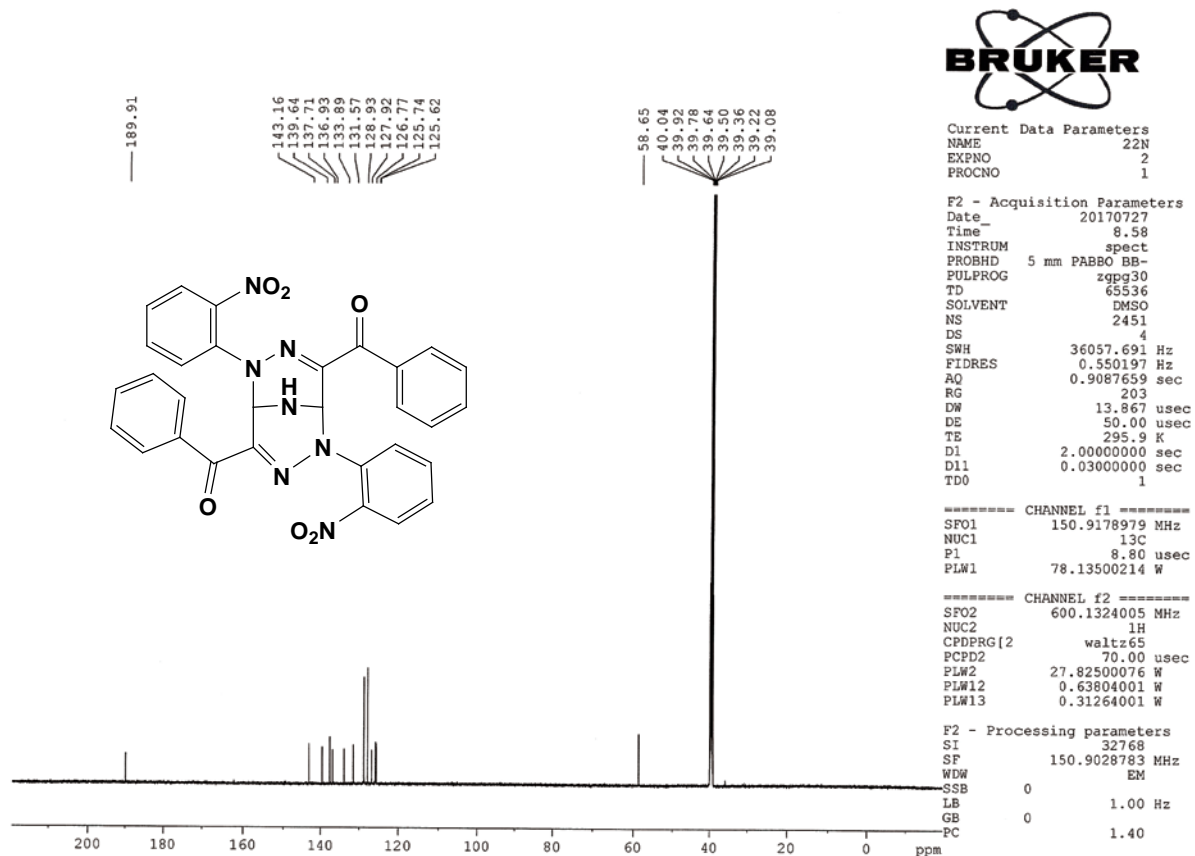
¹³C NMR spectrum of compound 2d



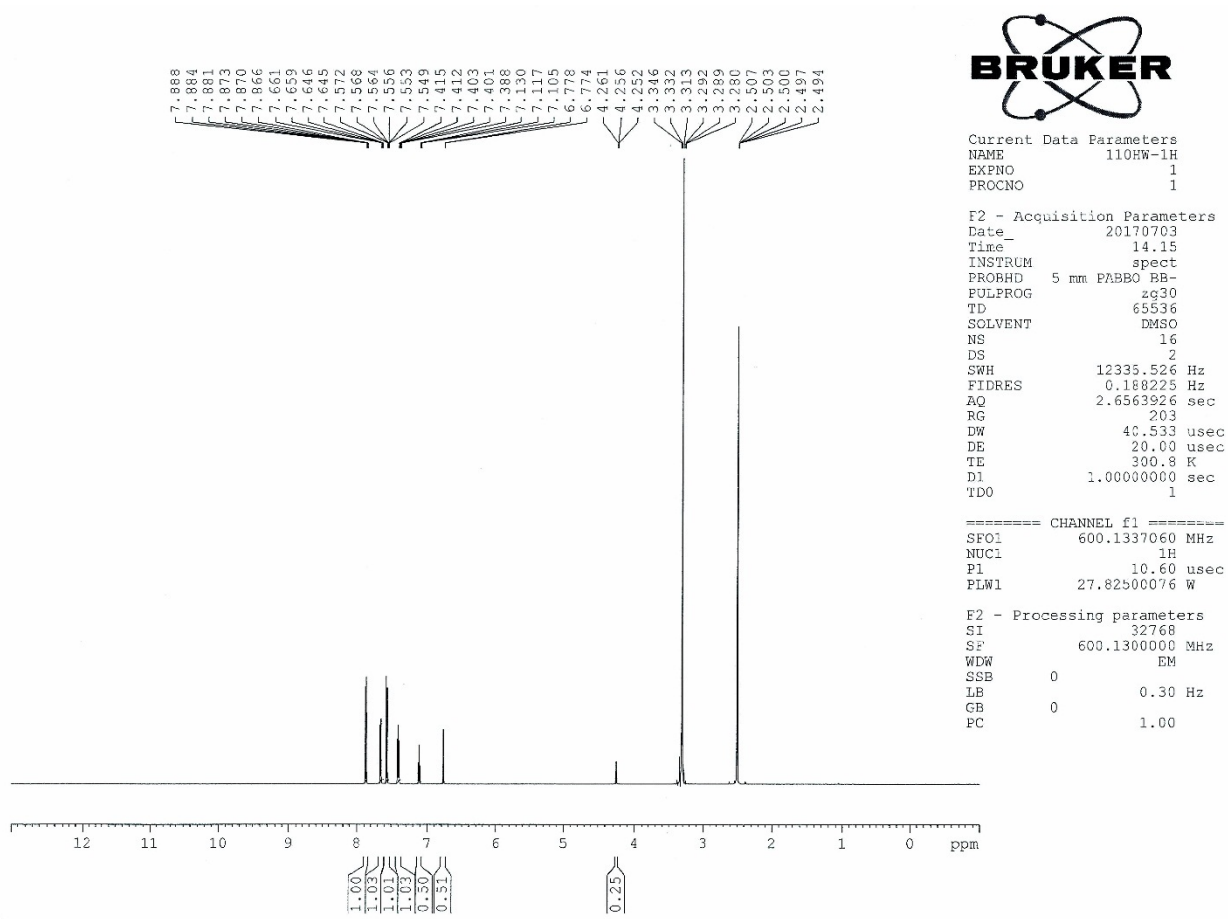
¹H NMR spectrum of compound **2e**



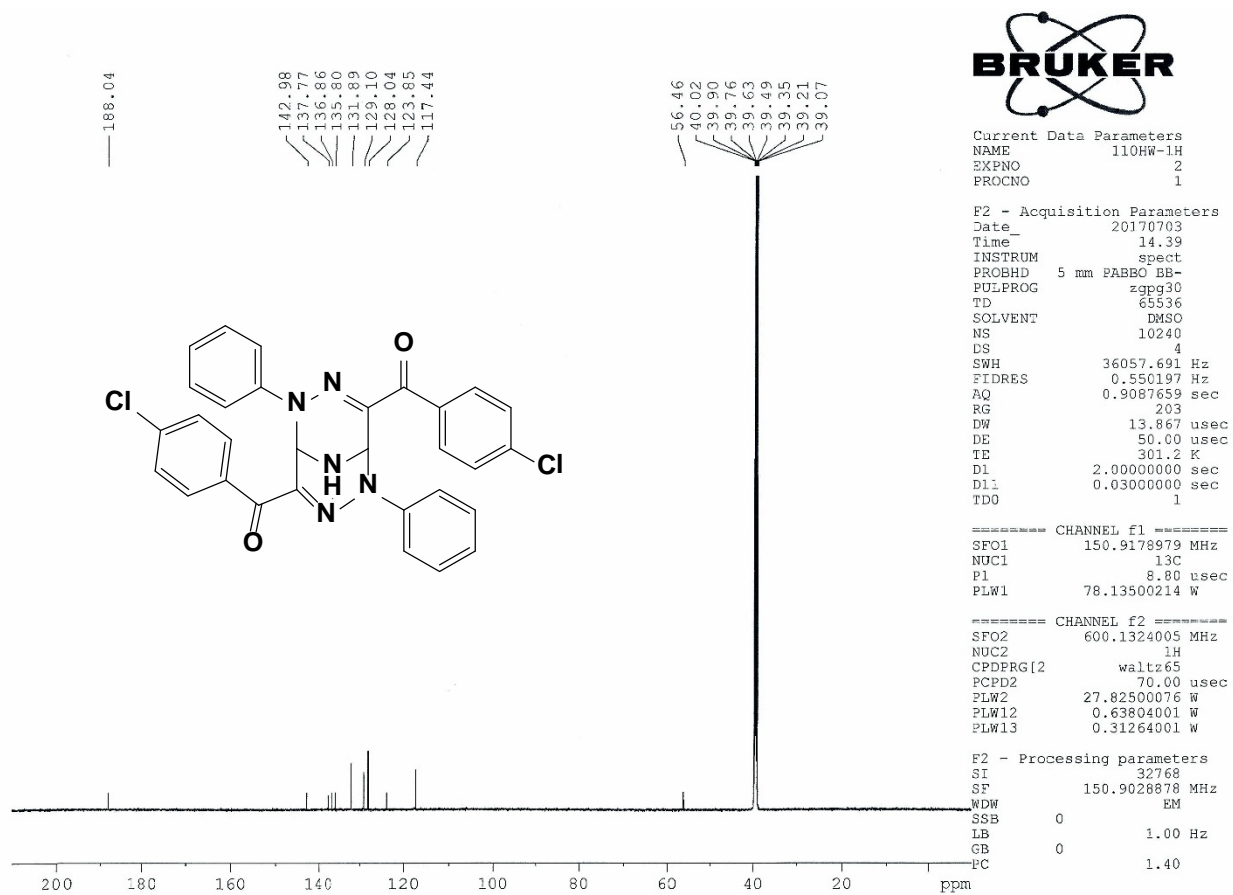
¹³C NMR spectrum of compound 2e



¹H NMR spectrum of compound **2f**



¹³C NMR spectrum of compound **2f**



Current Data Parameters
 NAME 110HW-1H
 EXPNO 2
 PROCNO 1

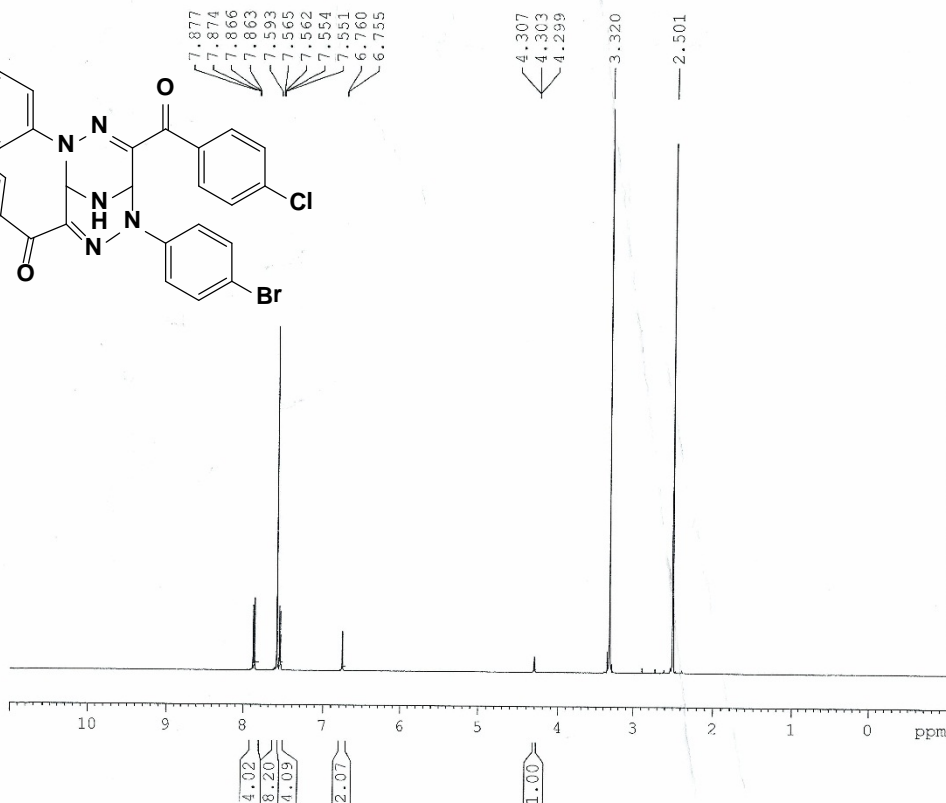
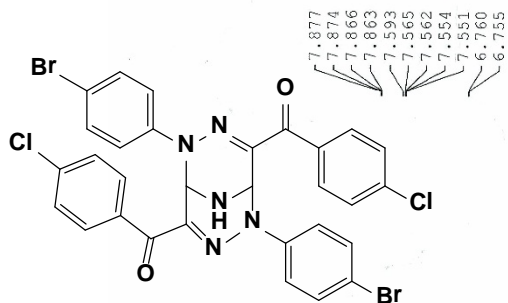
F2 - Acquisition Parameters
 Date 20170703
 Time 14.39
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 10240
 DS 4
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 203
 DW 13.867 usec
 DE 50.00 usec
 TE 301.2 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178979 MHz
 NUC1 13C
 P1 8.80 usec
 PLW1 78.13500214 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 70.00 usec
 PLW2 27.82500076 W
 PLW12 0.63804001 W
 PLW13 0.31264001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028878 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

¹H NMR spectrum of compound 2g



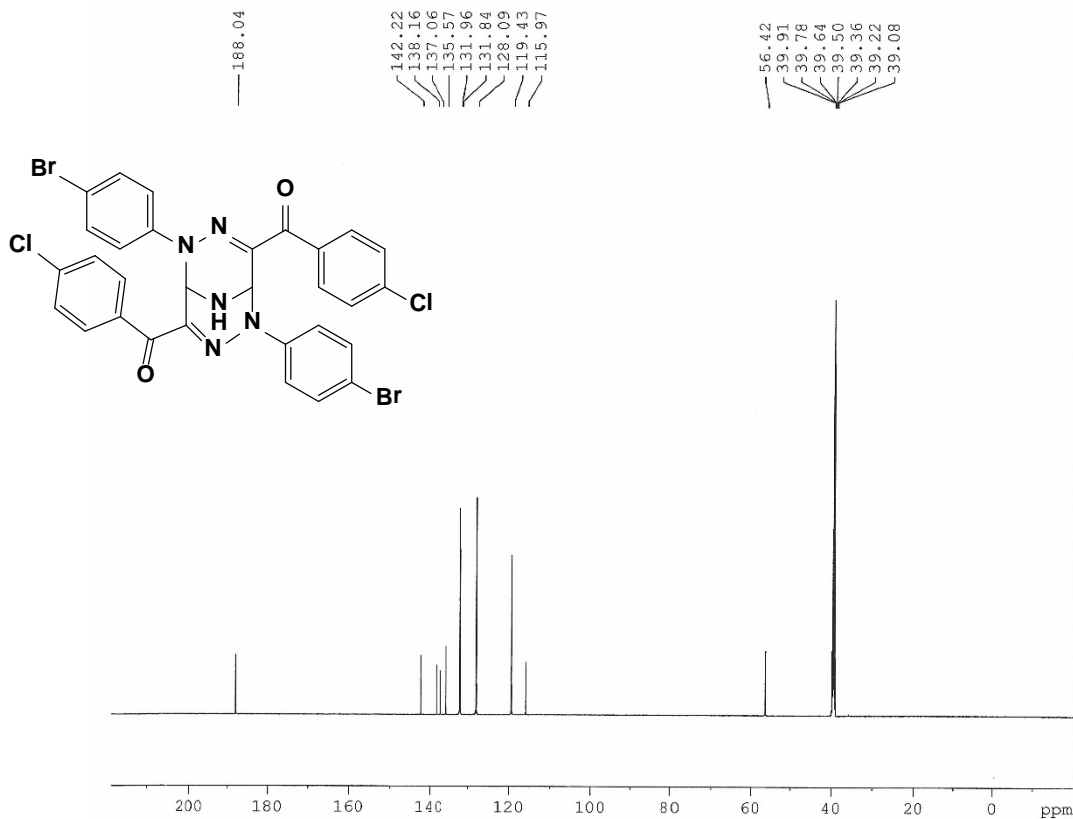
Current Data Parameters
NAME 107HW-1H
EXPNO 5
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170620
Time 17.12
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6563926 sec
RG 203
DW 40.533 usec
DE 20.00 usec
TE 298.0 K
D1 1.0000000 sec
TD0 1

==== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 10.60 usec
PLW1 27.82500076 W

F2 - Processing parameters
SI 32768
SF 600.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR spectrum of compound 2g



Current Data Parameters
 NAME 107HW-1H
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20170618
 Time_ 19.45
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 7168
 DS 4
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 203
 DW 13.867 usec
 DE 50.00 usec
 TE 298.0 K
 D1 2.00000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178979 MHz
 NUC1 13C
 P1 8.80 usec
 PLW1 78.13500214 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 70.00 usec
 PLW2 27.82500076 W
 PLW12 0.63804001 W
 PLW13 0.31264001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028839 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

¹H NMR spectrum of compound **2h**



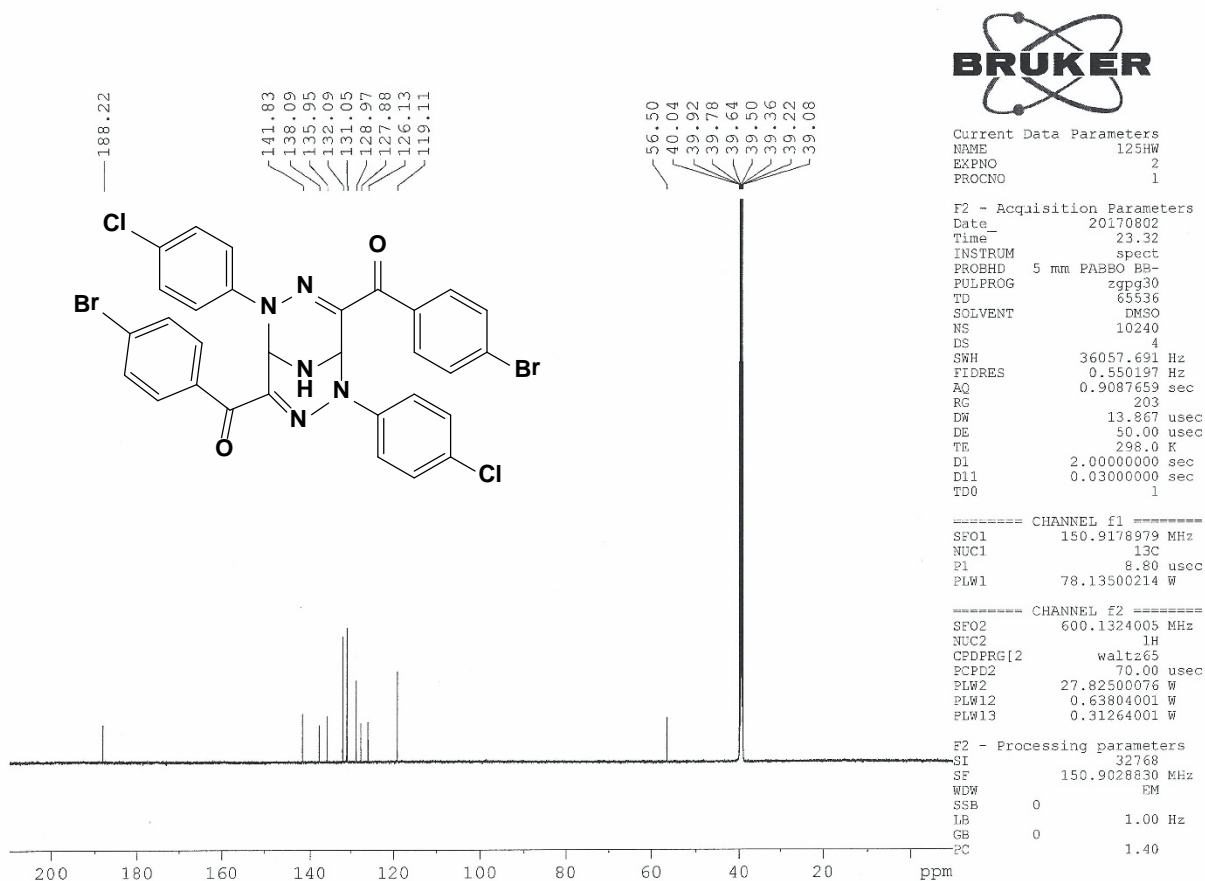
Current Data Parameters
NAME 125HW
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170802
Time 8.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6563926 sec
RG 203
DW 40.533 usec
DE 20.00 usec
TE 298.0 K
D1 1.0000000 sec
TDO 1

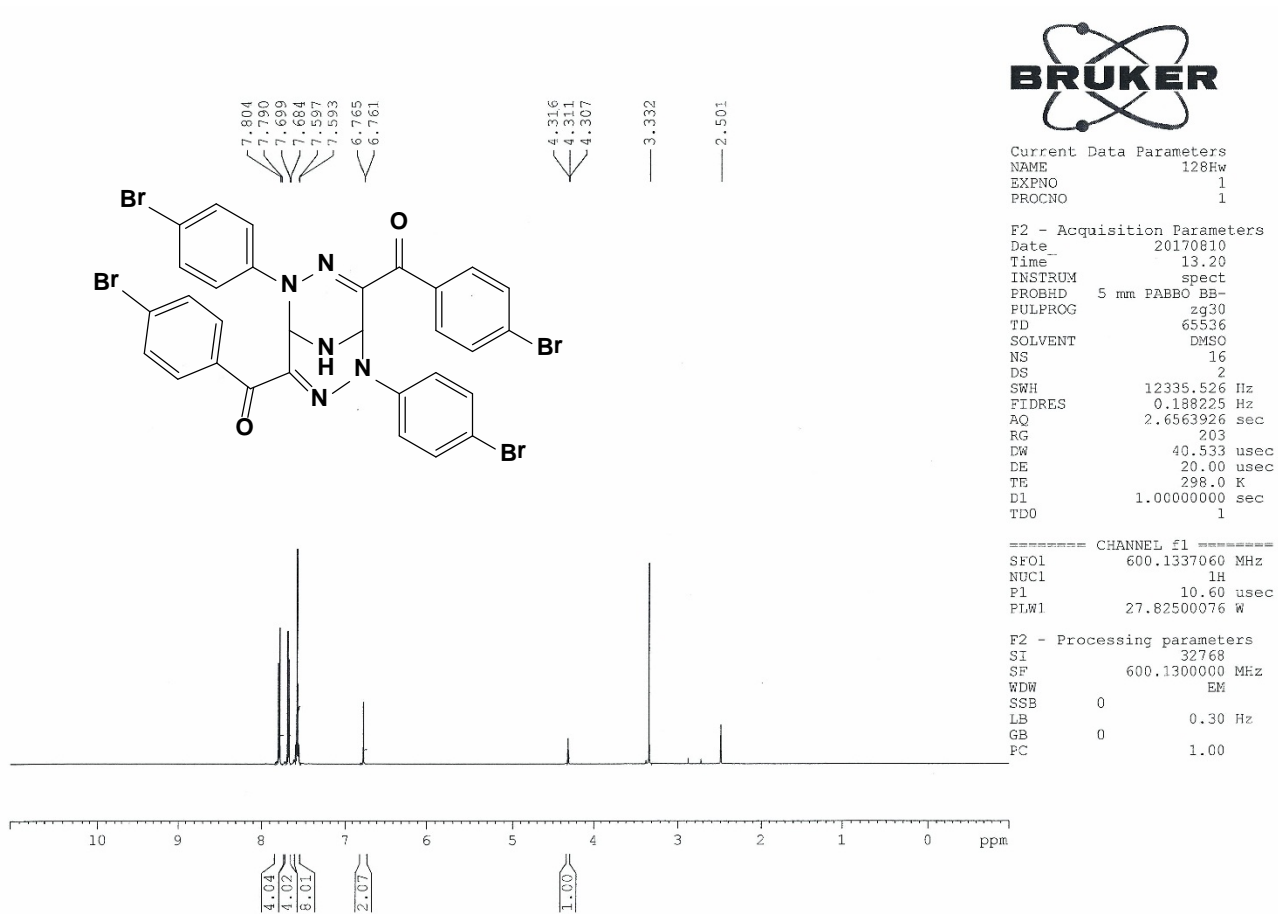
==== CHANNEL f1 =====
SF01 600.1337060 MHz
NUC1 1H
P1 10.60 usec
PLW1 27.82500076 W

F2 - Processing parameters
SI 32768
SF 600.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

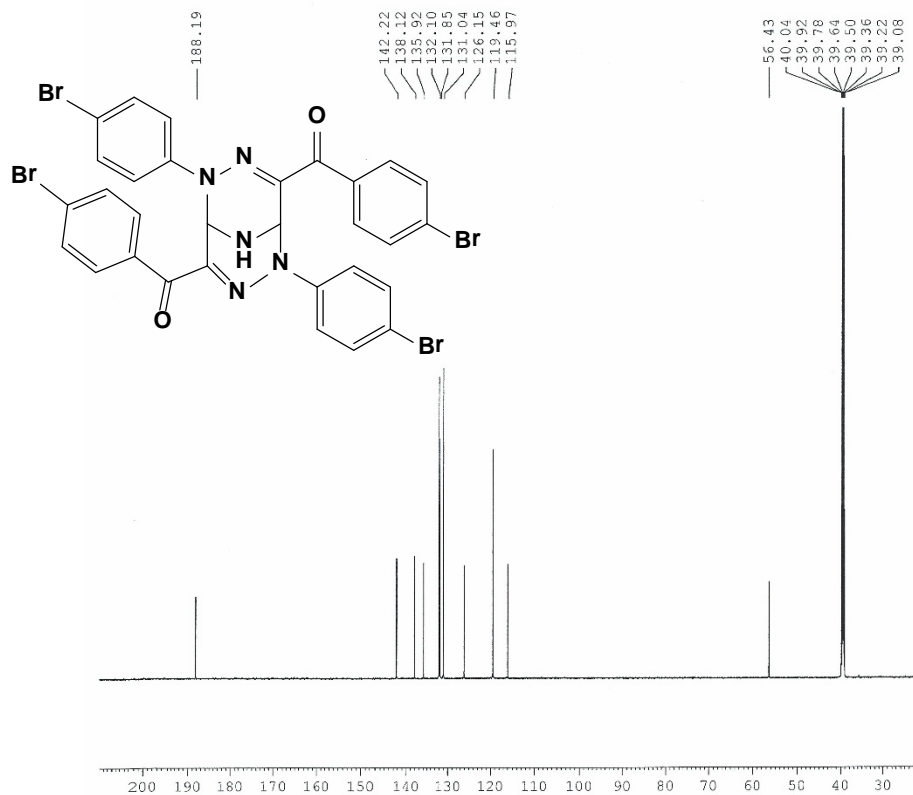
¹³C NMR spectrum of compound **2h**



¹H NMR spectrum of compound **2i**



¹³C NMR spectrum of compound 2i



Current Data Parameters
NAME 128HW
EXPNO 2
PROCNO 1

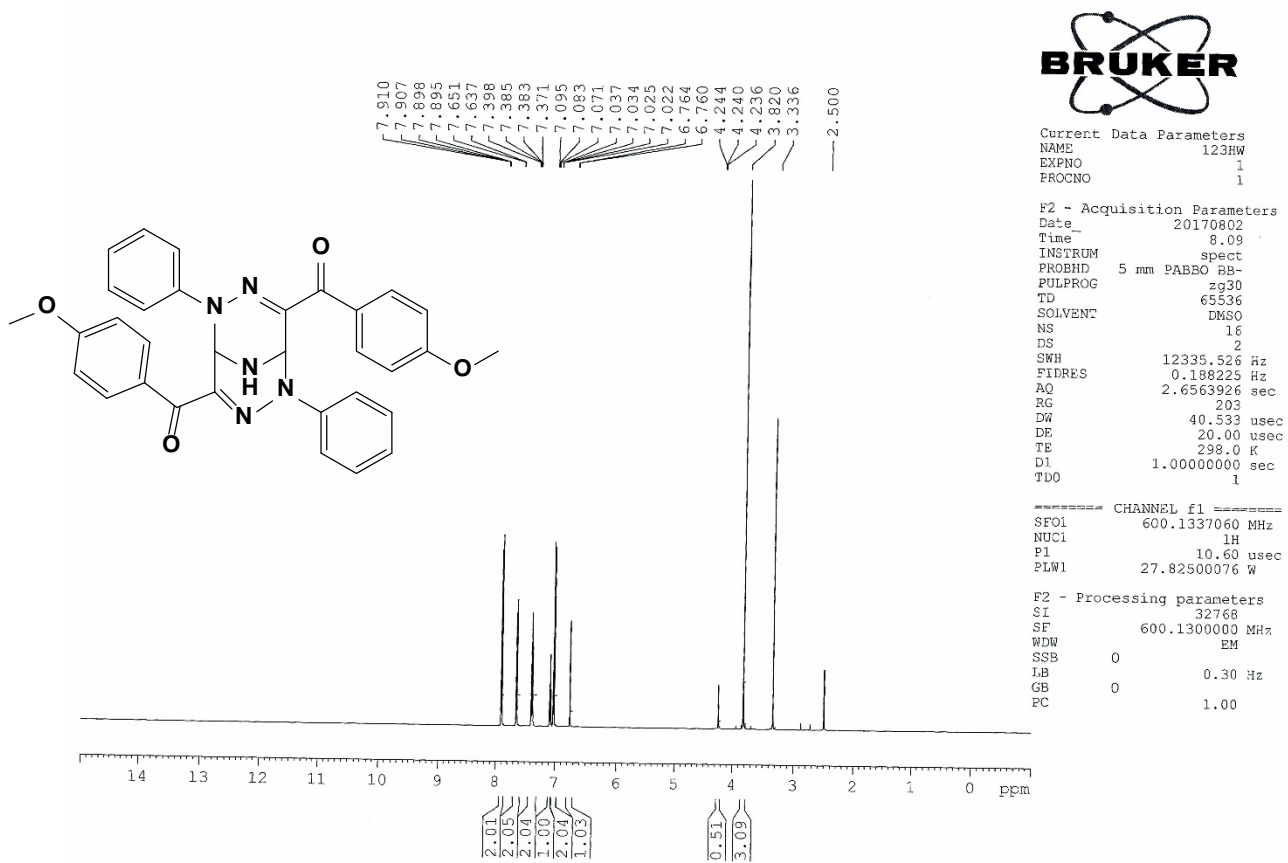
F2 - Acquisition Parameters
Date_ 20170812
Time_ 6.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 5120
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 203
DW 13.867 usec
DE 50.00 usec
TE 298.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TDO 1

===== CHANNEL f1 =====
SFO1 150.9178979 MHz
NUC1 13C
P1 8.80 usec
PLW1 78.13500214 W

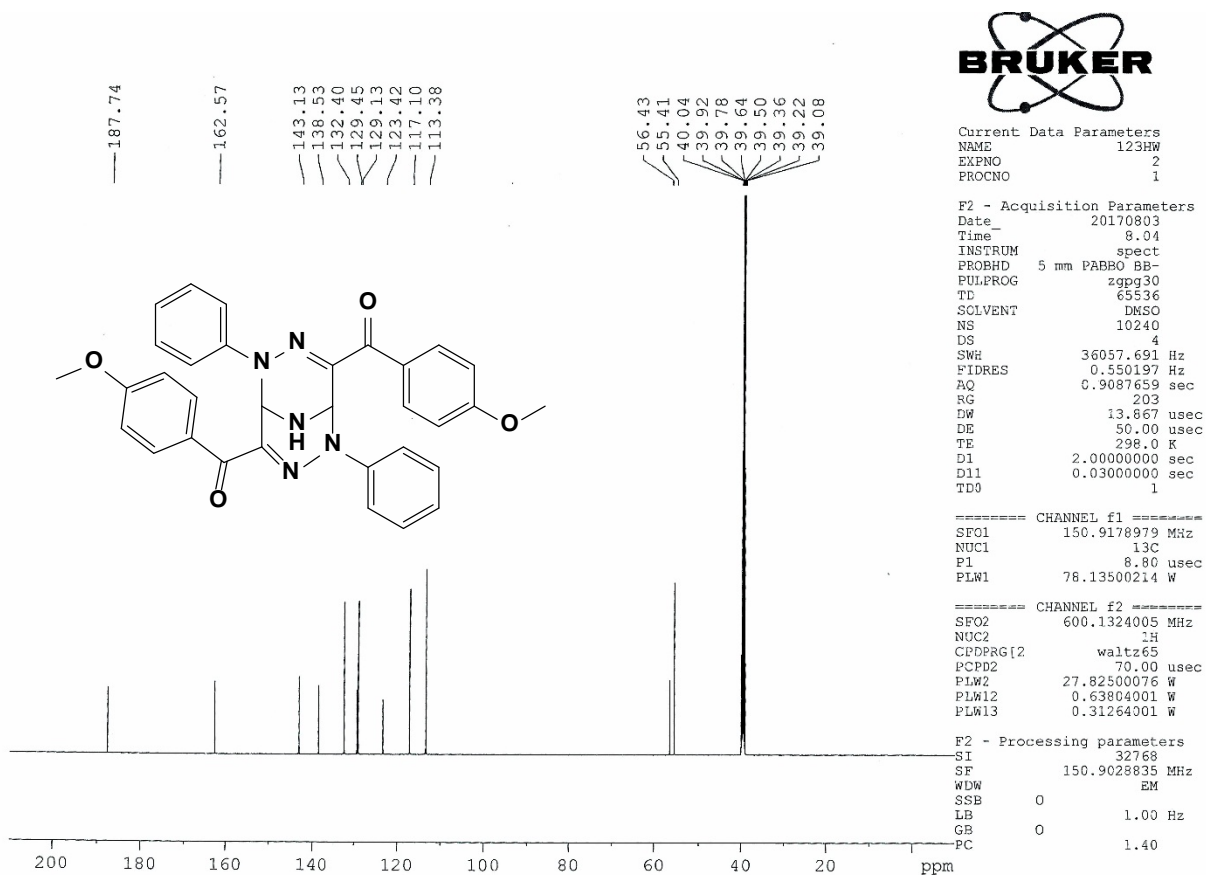
===== CHANNEL f2 =====
SFO2 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 70.00 usec
PLW2 27.82500076 W
PLW12 0.63804001 W
PLW13 0.31264001 W

F2 - Processing parameters
SI 32768
SF 150.9028837 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

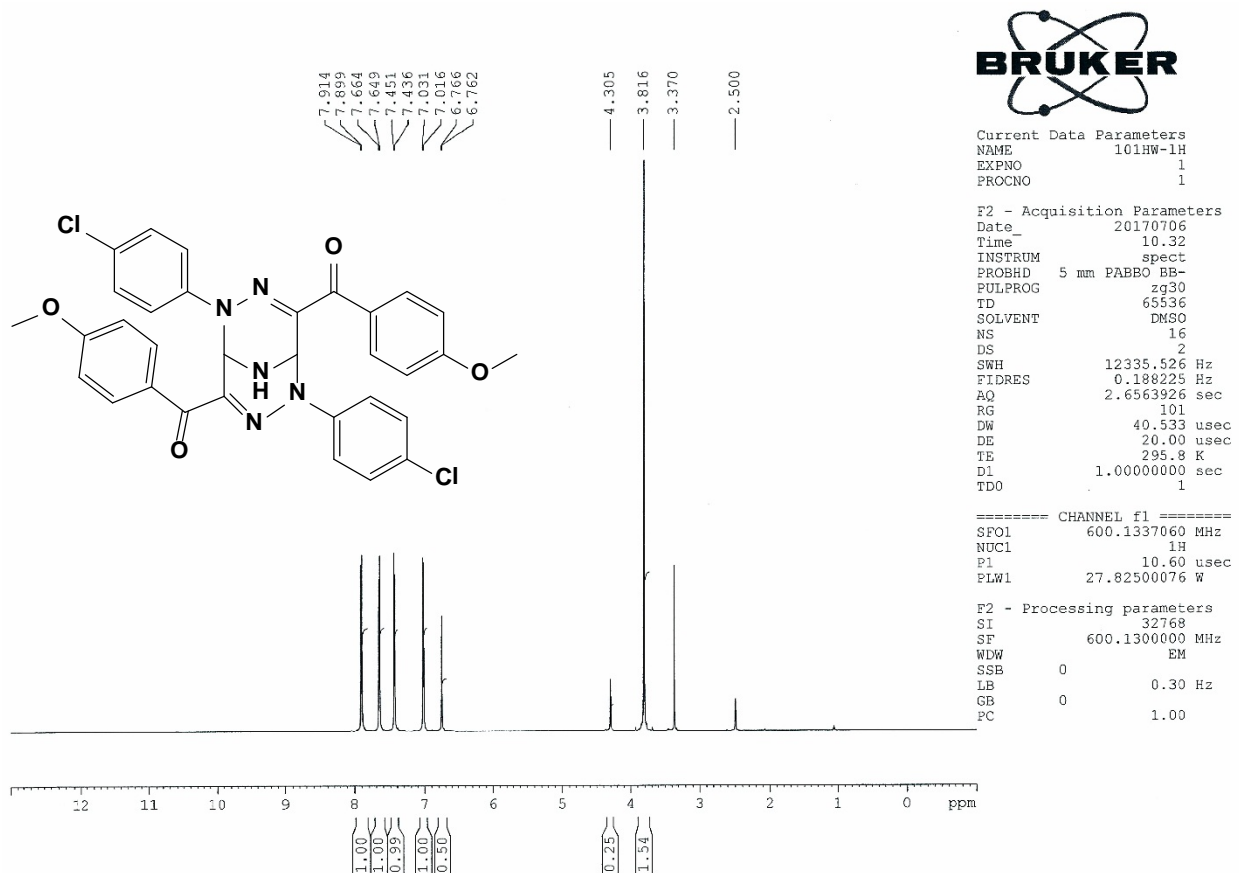
¹H NMR spectrum of compound 2j



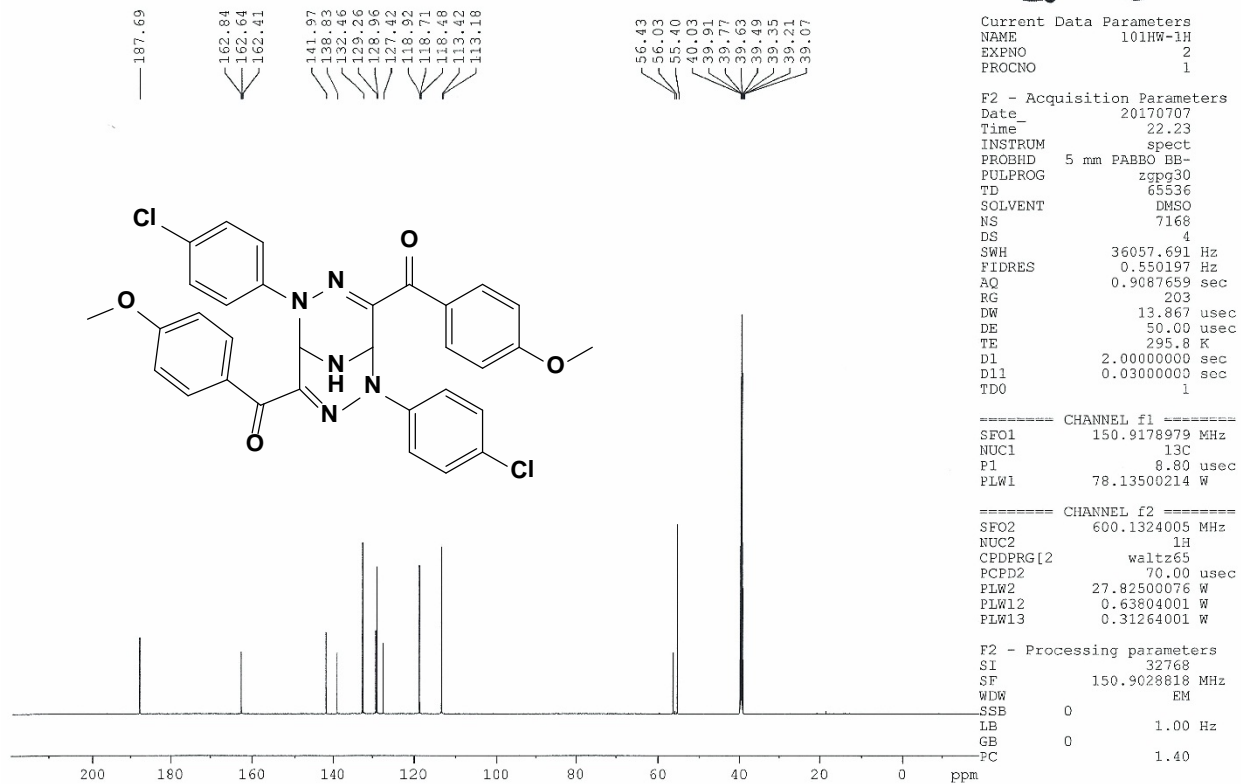
¹³C NMR spectrum of compound 2j



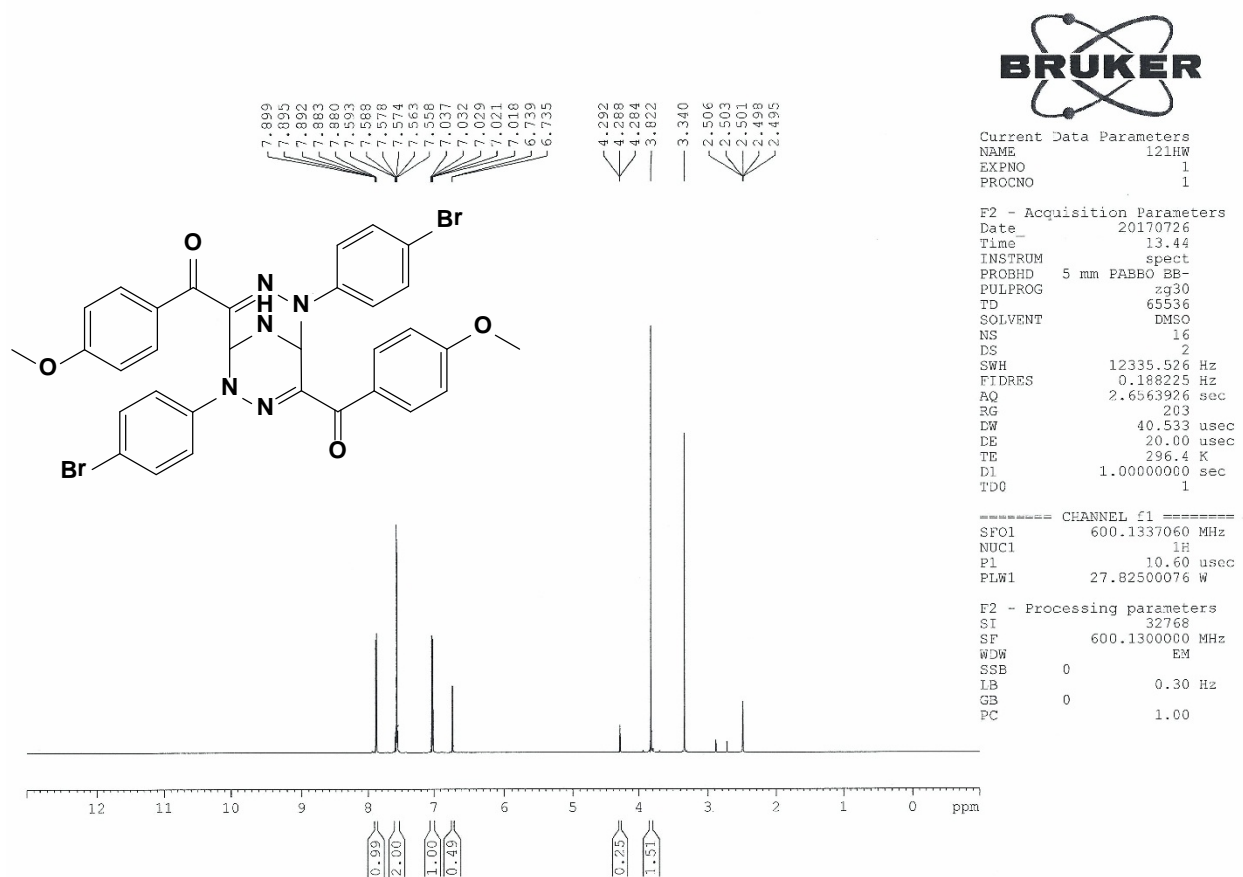
¹H NMR spectrum of compound **2k**



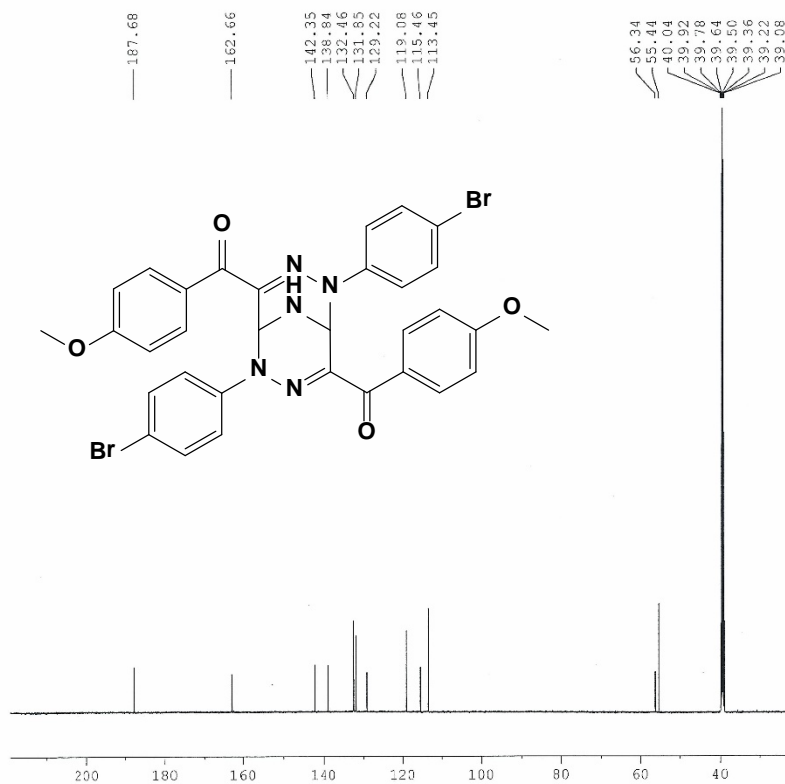
¹³C NMR spectrum of compound **2k**



¹H NMR spectrum of compound **2l**



¹³C NMR spectrum of compound **21**



Current Data Parameters
NAME 121HW
EXPNO 2
PROCNO 1

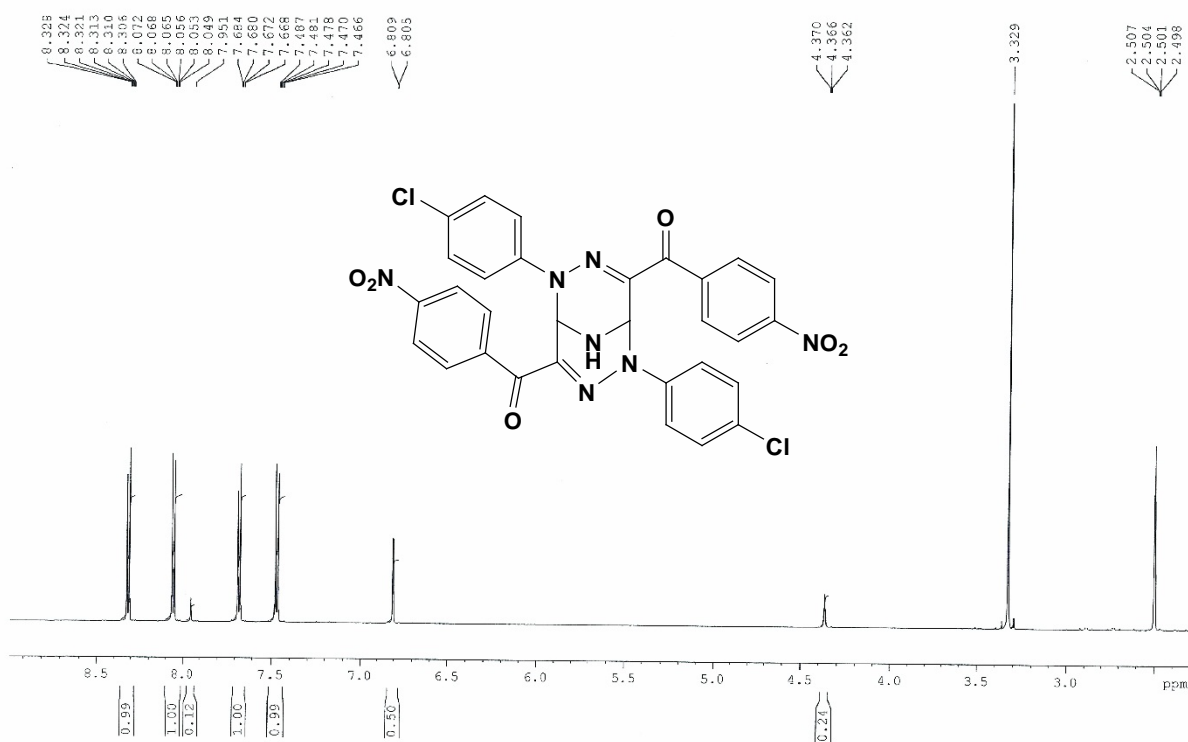
F2 - Acquisition Parameters
Date_ 20170727
Time 8.43
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1145
DS 4
SWH 36057.691 Hz
FIDRES 0.550197 Hz
AQ 0.9087659 sec
RG 203
DW 13.867 usec
DE 50.00 usec
TE 296.0 K
D1 2.0000000 sec
D11 0.0300000 sec
TD0 1

===== CHANNEL f1 =====
SF01 150.9178979 MHz
NUC1 13C
P1 8.80 usec
PLW1 78.13500214 W

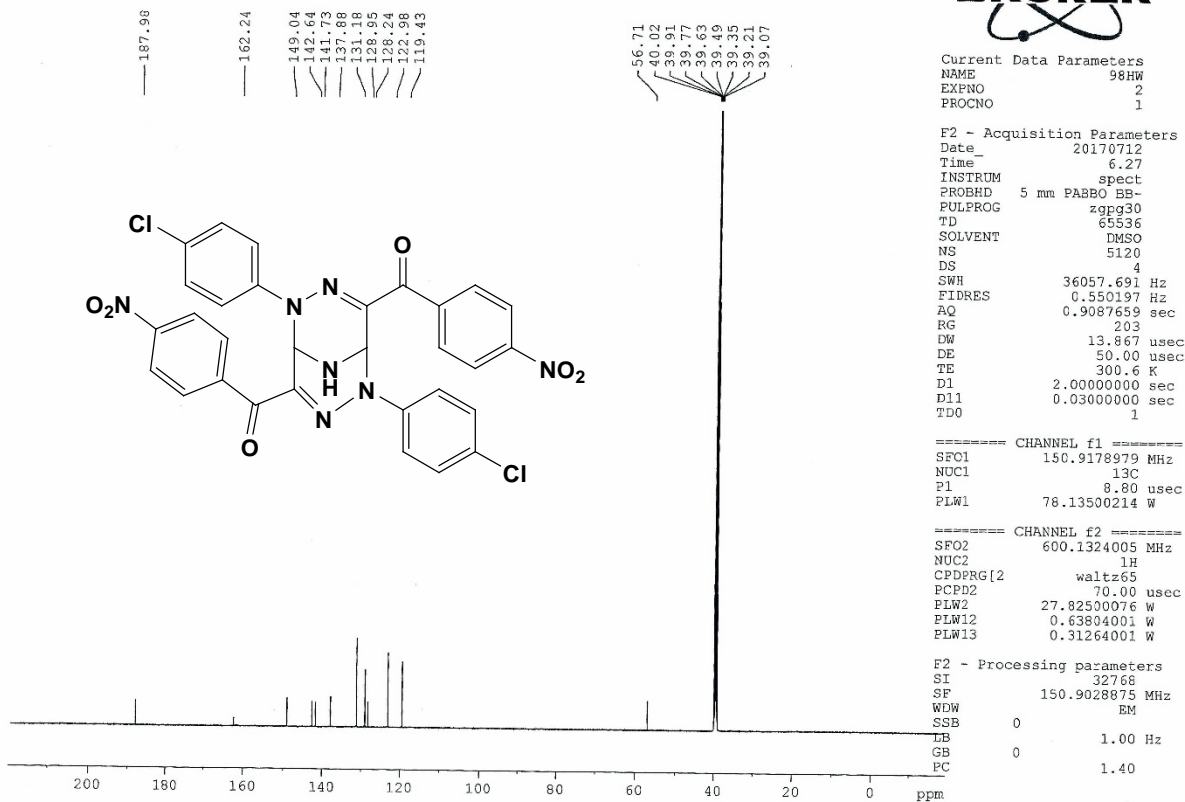
===== CHANNEL f2 =====
SF02 600.1324005 MHz
NUC2 1H
CPDPRG[2] waltz65
PCPD2 70.00 usec
PLW2 27.82500076 W
PLW12 0.63804001 W
PLW13 0.31264001 W

F2 - Processing parameters
SI 32768
SF 150.9028809 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
SC 1.40

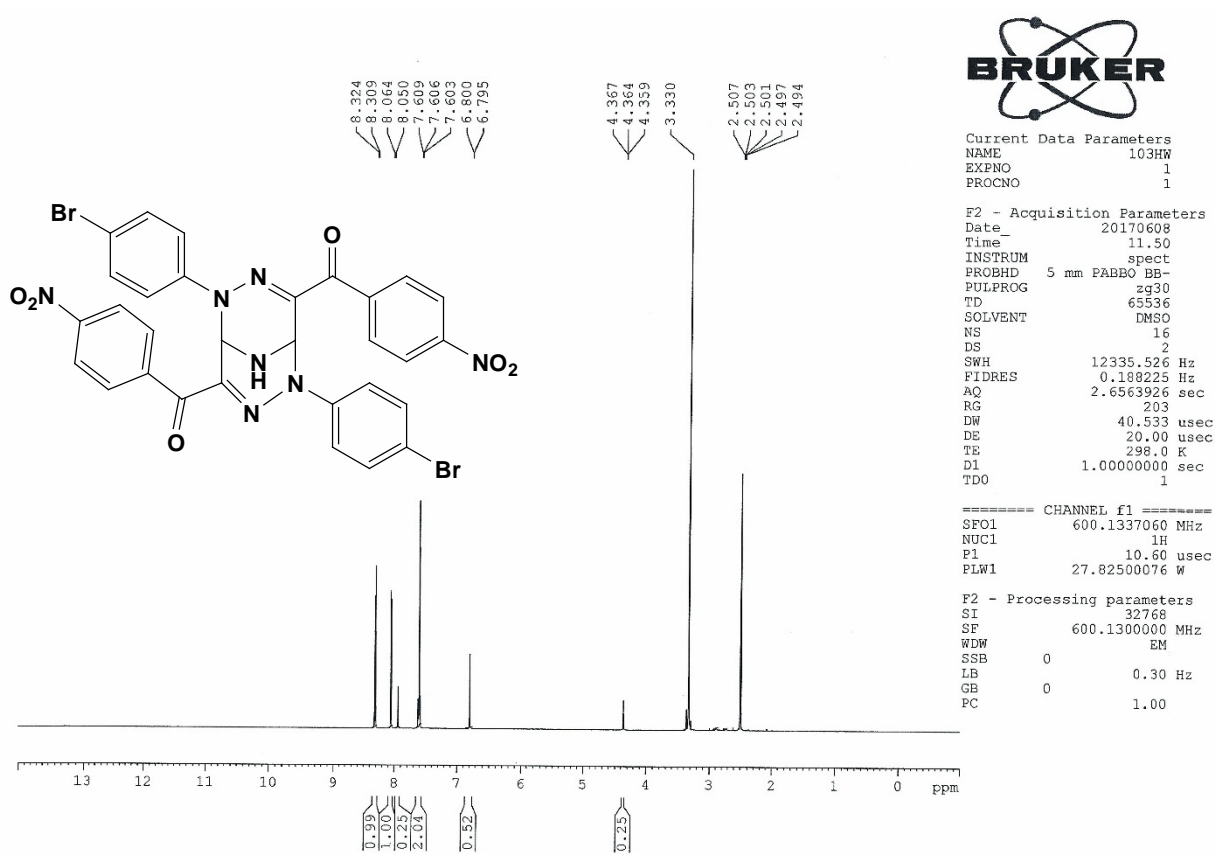
¹H NMR spectrum of compound **2m**



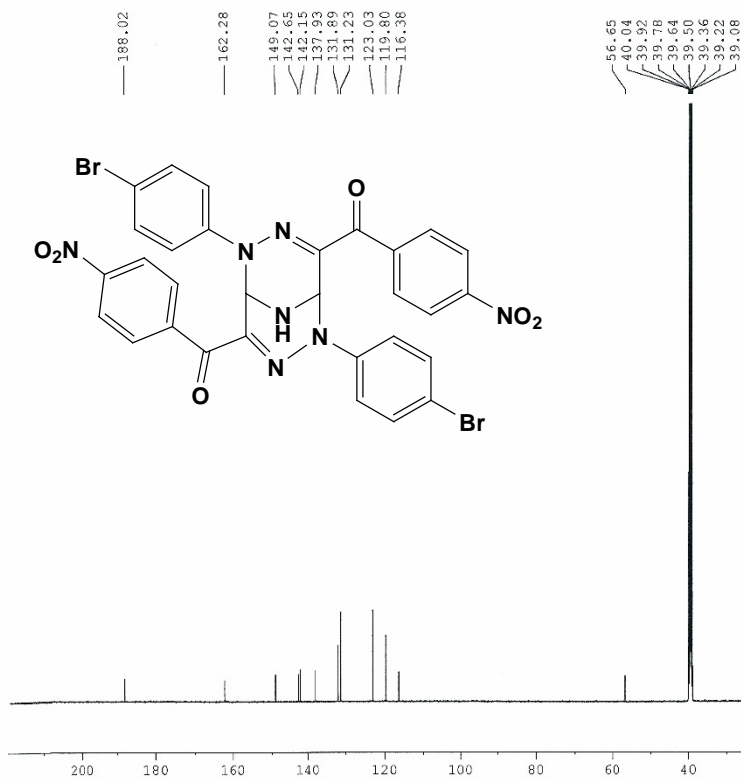
¹³C NMR spectrum of compound 2m



¹H NMR spectrum of compound **2n**



¹³C NMR spectrum of compound **2n**



Current Data Parameters
 NAME 103HW
 EXPNO 2
 PROCNO 1

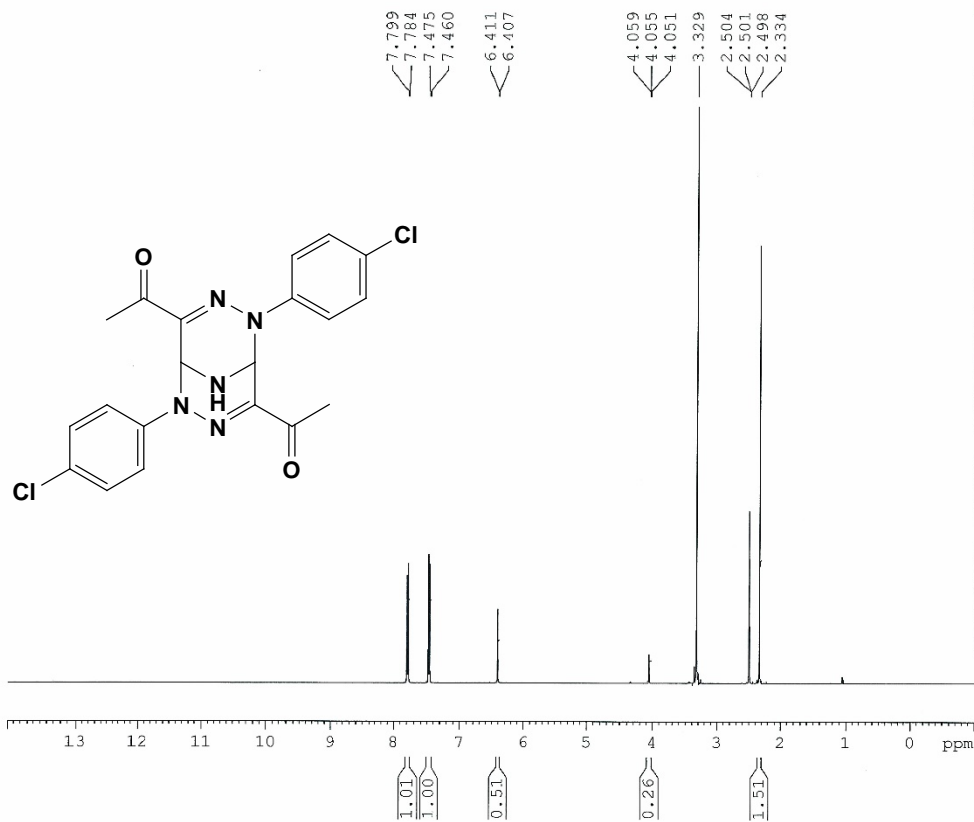
F2 - Acquisition Parameters
 Date_ 20170609
 Time 23.24
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 10240
 DS 4
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 203
 DW 13.867 usec
 DE 50.00 usec
 TR 298.0 K
 D1 2.0000000 sec
 D11 0.0300000 sec
 TDO 1

==== CHANNEL f1 =====
 SFO1 150.9178979 MHz
 NUC1 13C
 P1 8.80 usec
 PLW1 78.13500214 W

==== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG[2] waltz65
 PCPD2 70.00 usec
 PLW2 27.82500076 W
 PLW12 0.63804001 W
 PLW13 0.31264001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028818 MHz
 WDR EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

¹H NMR spectrum of compound **2o**



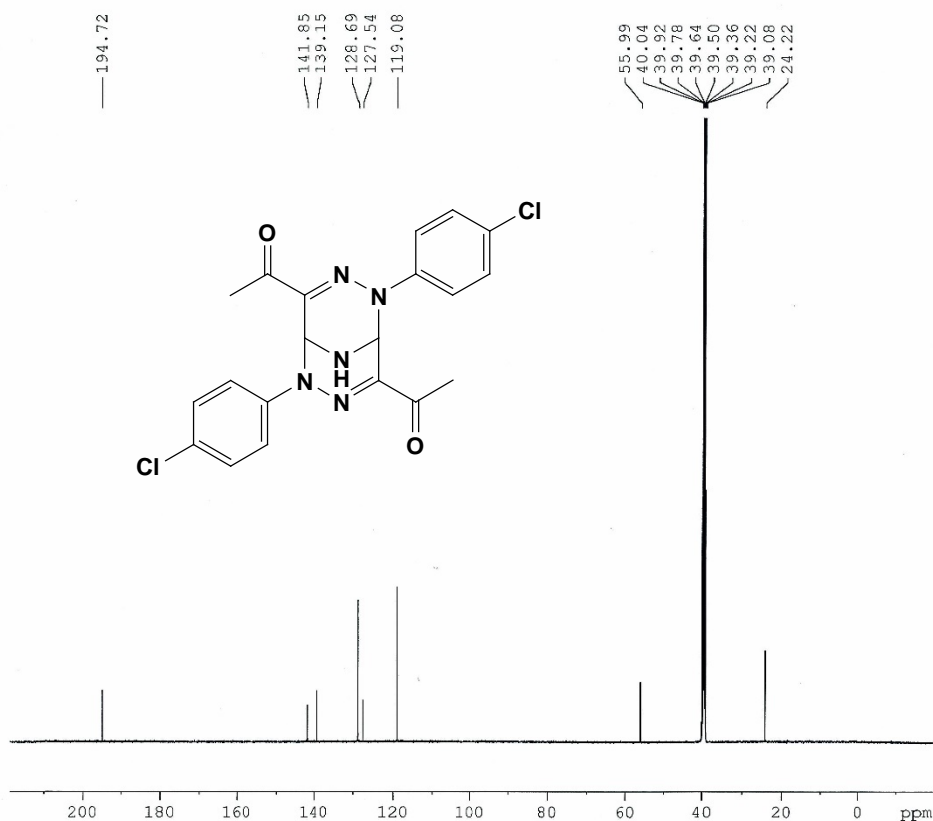
Current Data Parameters
NAME 8HW-1H
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160830
Time_ 12.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 12335.526 Hz
FIDRES 0.188225 Hz
AQ 2.6563926 sec
RG 203
DW 40.533 usec
DE 20.00 usec
TE 298.3 K
DL 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 600.1337060 MHz
NUC1 1H
P1 10.60 usec
PLW1 27.82500076 W

F2 - Processing parameters
SI 32768
SF 600.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

¹³C NMR spectrum of compound **2o**



Current Data Parameters
 NAME 8HW-1H
 EXPNO 2
 PROCNO 1

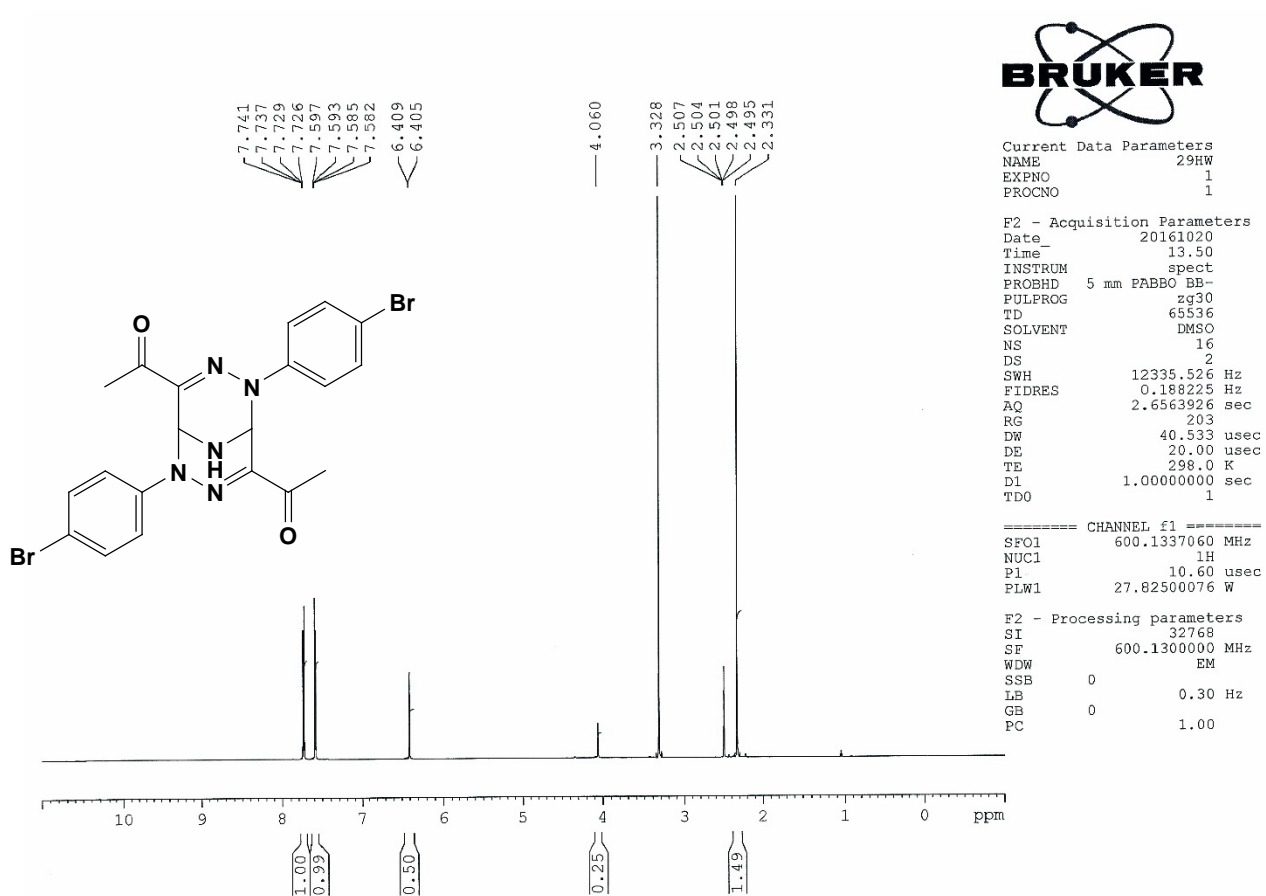
F2 - Acquisition Parameters
 Date 20160830
 Time 14.33
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT DMSO
 NS 10240
 DS 4
 SWH 36057.691 Hz
 FIDRES 0.550197 Hz
 AQ 0.9087659 sec
 RG 203
 DW 13.867 usec
 DE 50.00 usec
 TE 301.2 K
 D1 2.0000000 sec
 D11 0.03000000 sec
 TD0 1

===== CHANNEL f1 =====
 SFO1 150.9178979 MHz
 NUC1 13C
 P1 8.80 usec
 PLW1 78.13500214 W

===== CHANNEL f2 =====
 SFO2 600.1324005 MHz
 NUC2 1H
 CPDPRG2 waltz65
 PCPD2 70.00 usec
 PLW2 27.82500076 W
 PLW12 0.63804001 W
 PLW13 0.31264001 W

F2 - Processing parameters
 SI 32768
 SF 150.9028893 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

¹H NMR spectrum of compound 2p



¹³C NMR spectrum of compound 2p

