

# Synthesis of Blue-Red Emissive Amido Substituted Di(het)aryl and Tri(het)aryl Amine Derivatives via Chemoselective *N*-Mono and *N, N*-Diarylation of (Het) Aryl Amino Amides Using Benzyne/Arynes

Ramakrishnan Suseela Meerakrishna and Ponnusamy Shanmugam\*

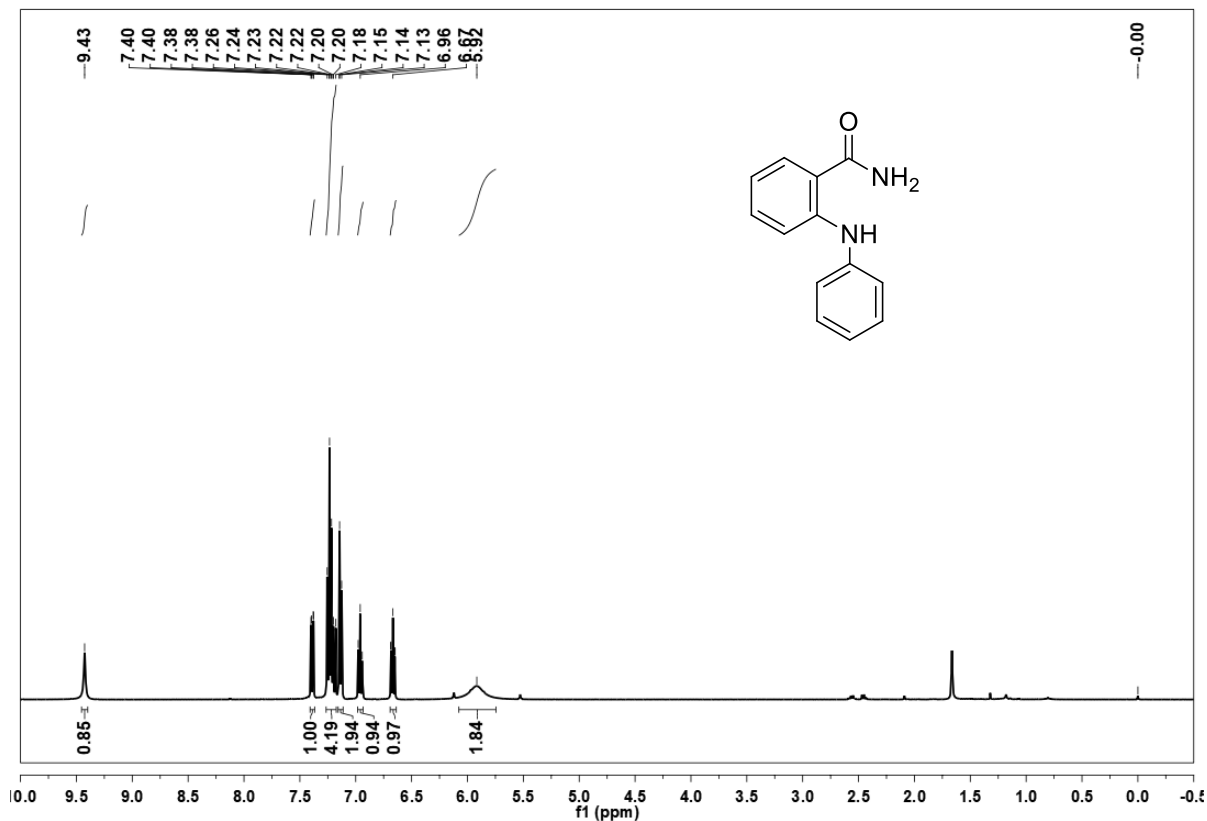
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Email: shanmu196@rediffmail.com

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# Copies of NMR and HRMS Spectra



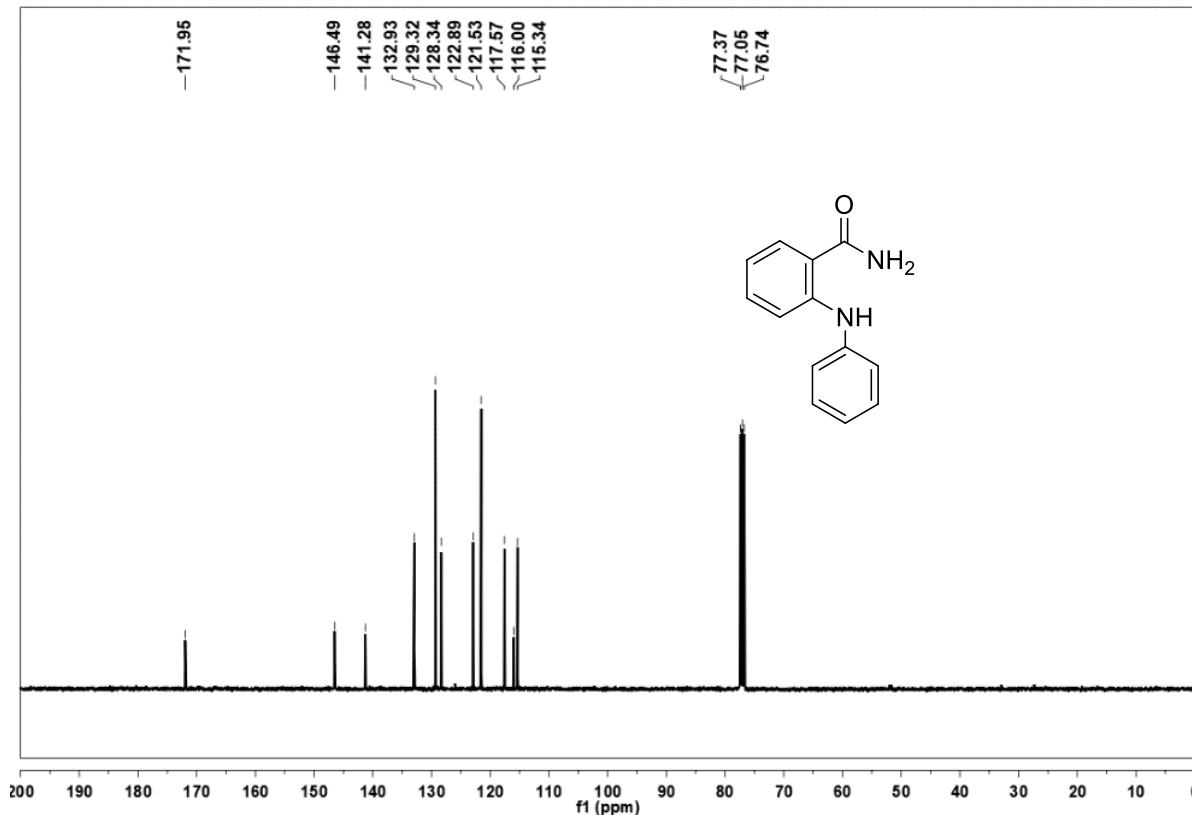
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 NS 16  
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 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
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 RG 99.98  
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 TE 297.2 K  
 D1 1.0000000 sec  
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<sup>1</sup>H NMR Spectrum of Compound 3a



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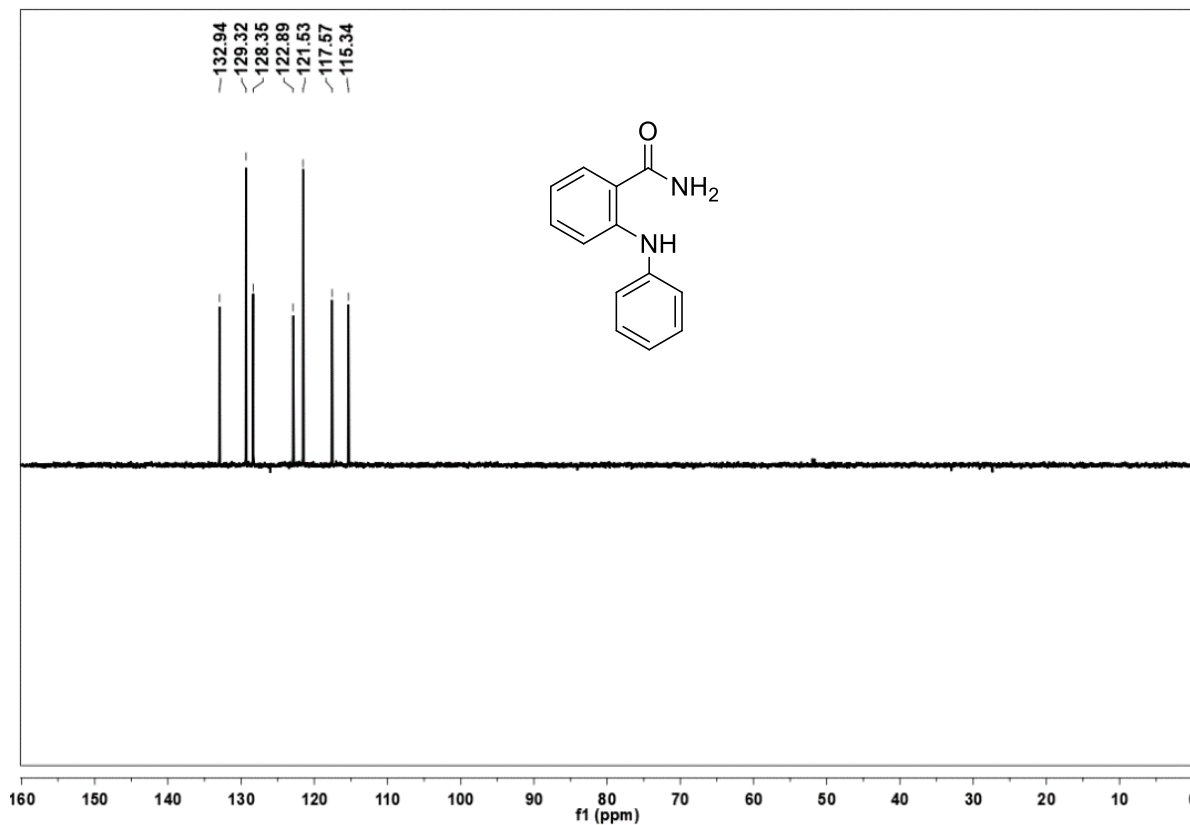
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 NS 512  
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 FIDRES 0.366798 Hz  
 Aq 1.3631488 sec  
 RG 204.46  
 LW 20.800 usec  
 DE 6.50 usec  
 TE 298.2 K  
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 NUC2 1H  
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F2 - Processing parameters  
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<sup>13</sup>C NMR Spectrum of Compound 3a



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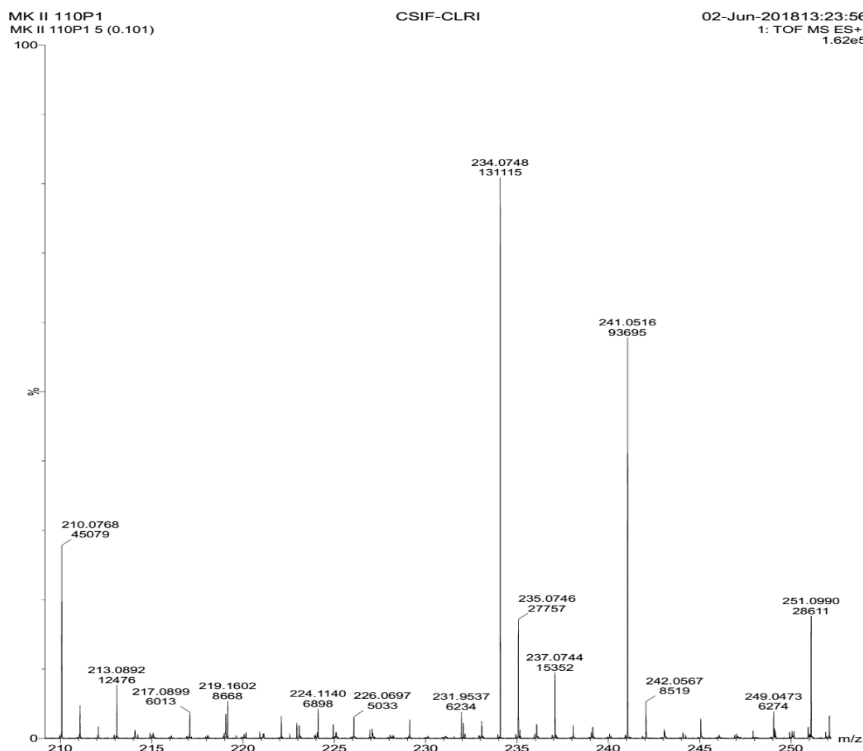
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 RG: 204.46  
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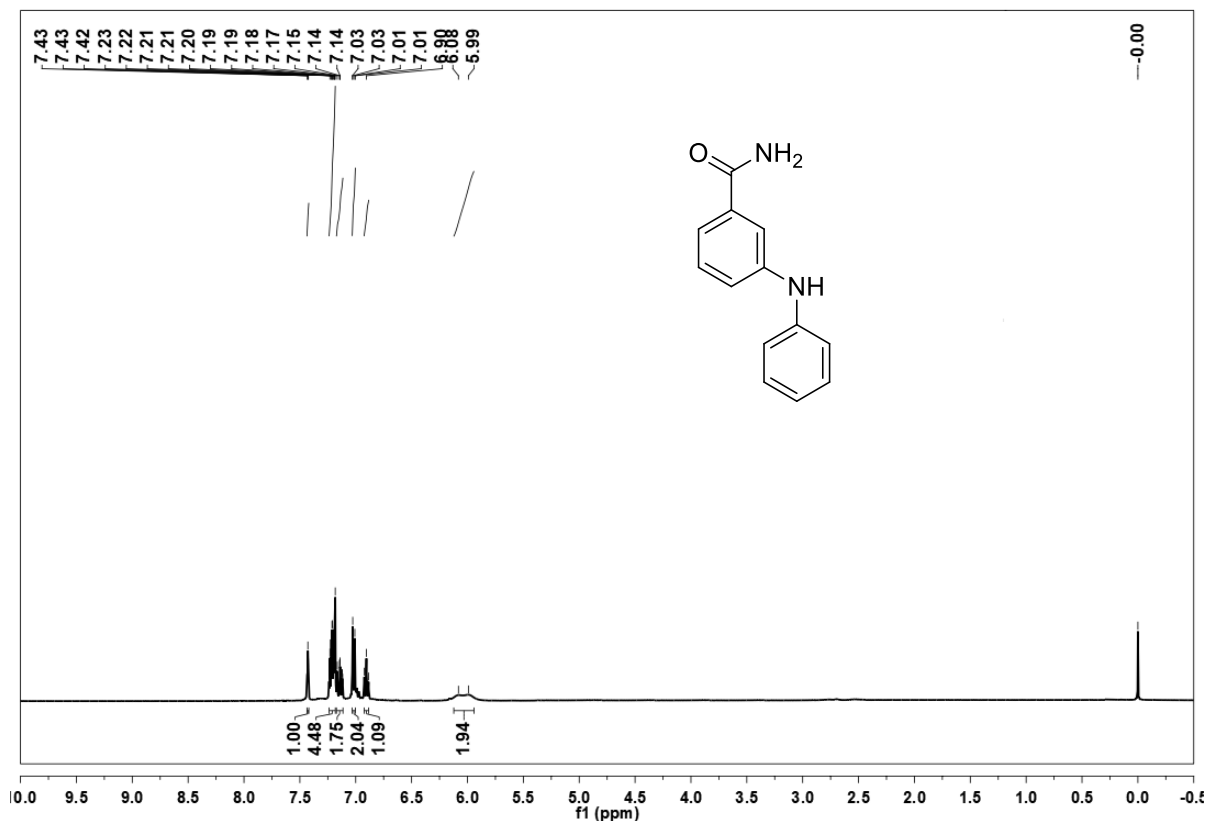
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DEPT-135 NMR Spectrum of Compound 3a



HRMS Spectrum of Compound 3a



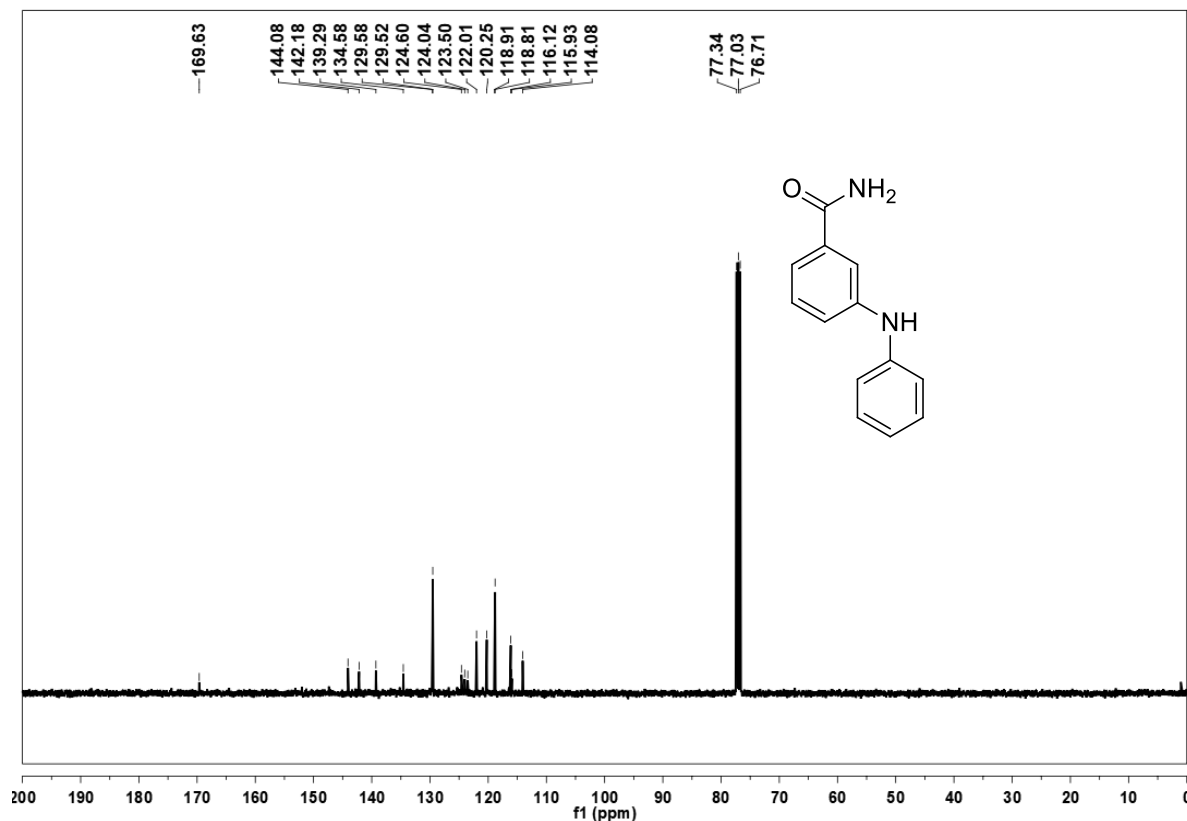
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 SWE 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 49.2  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 296.7 K  
 D1 1.0000000 sec  
 TD0 1

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 PLW1 12.00000000 W

F2 - Processing parameters  
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<sup>1</sup>H NMR Spectrum of Compound 3b



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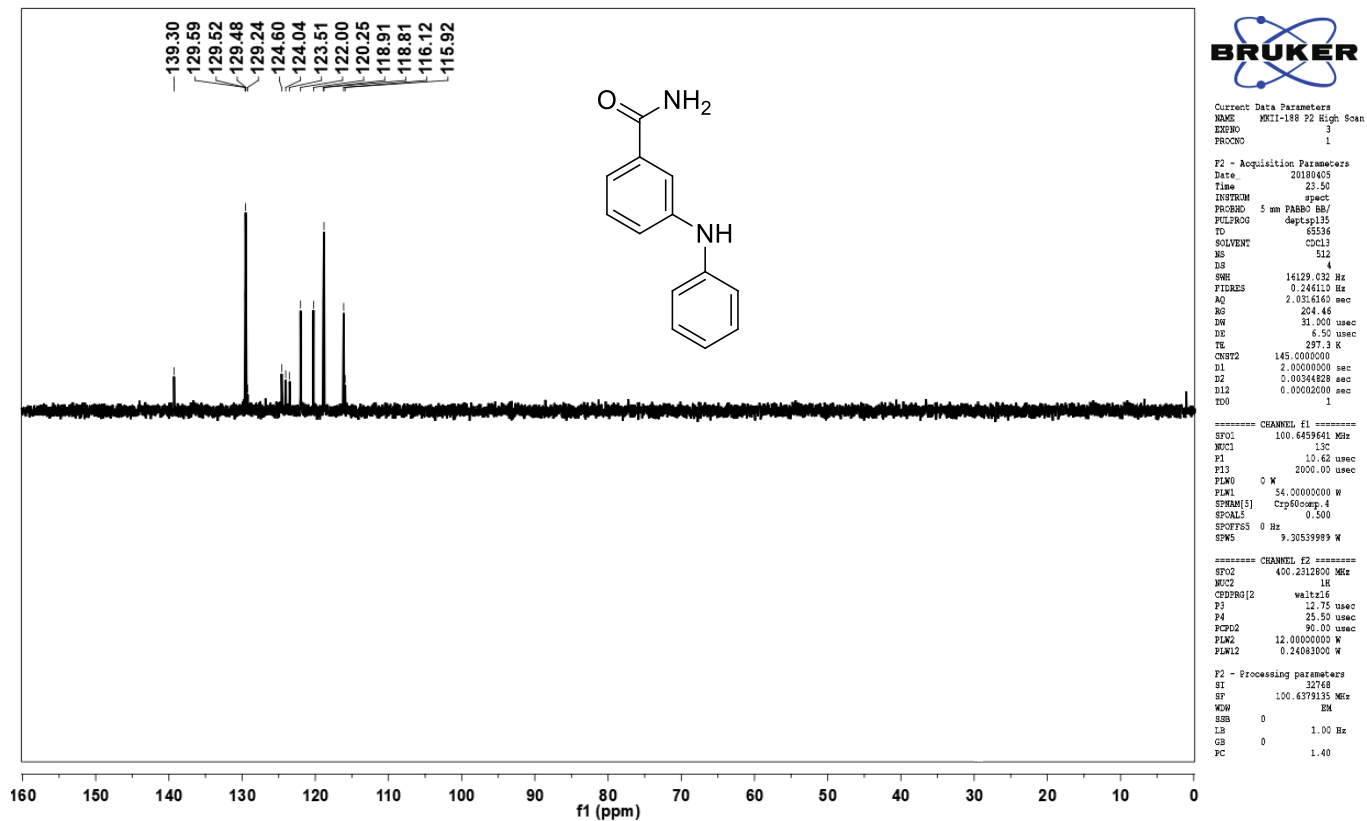
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 DS 4  
 SWE 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 204.46  
 DW 20.800 usec  
 DE 4.50 usec  
 TE 298.0 K  
 D1 2.0000000 sec  
 D11 0.03000000 sec  
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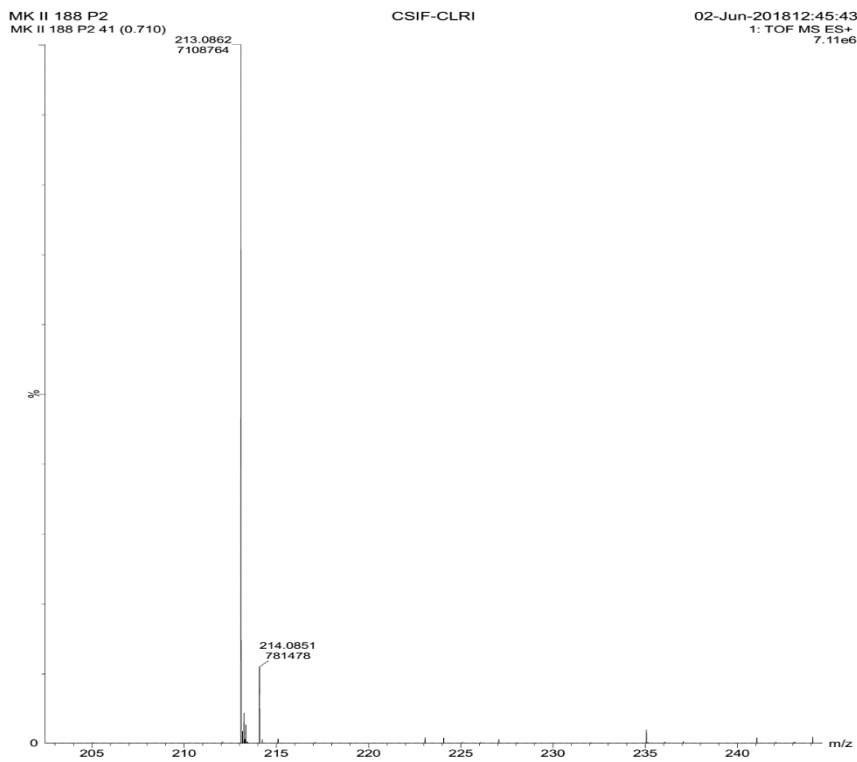
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 PLW12 0.24083000 W  
 PLW13 0.19598000 W

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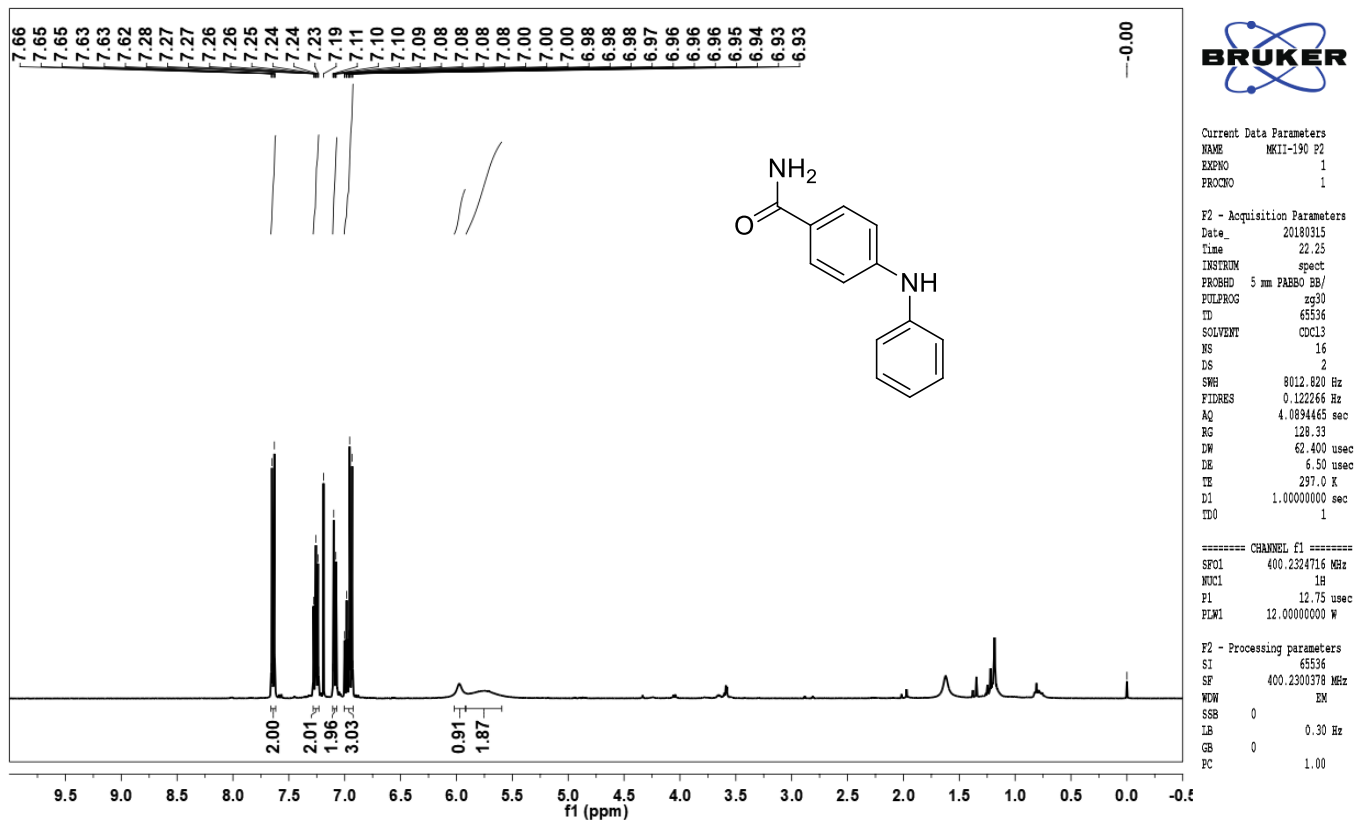
<sup>13</sup>C NMR Spectrum of Compound 3b



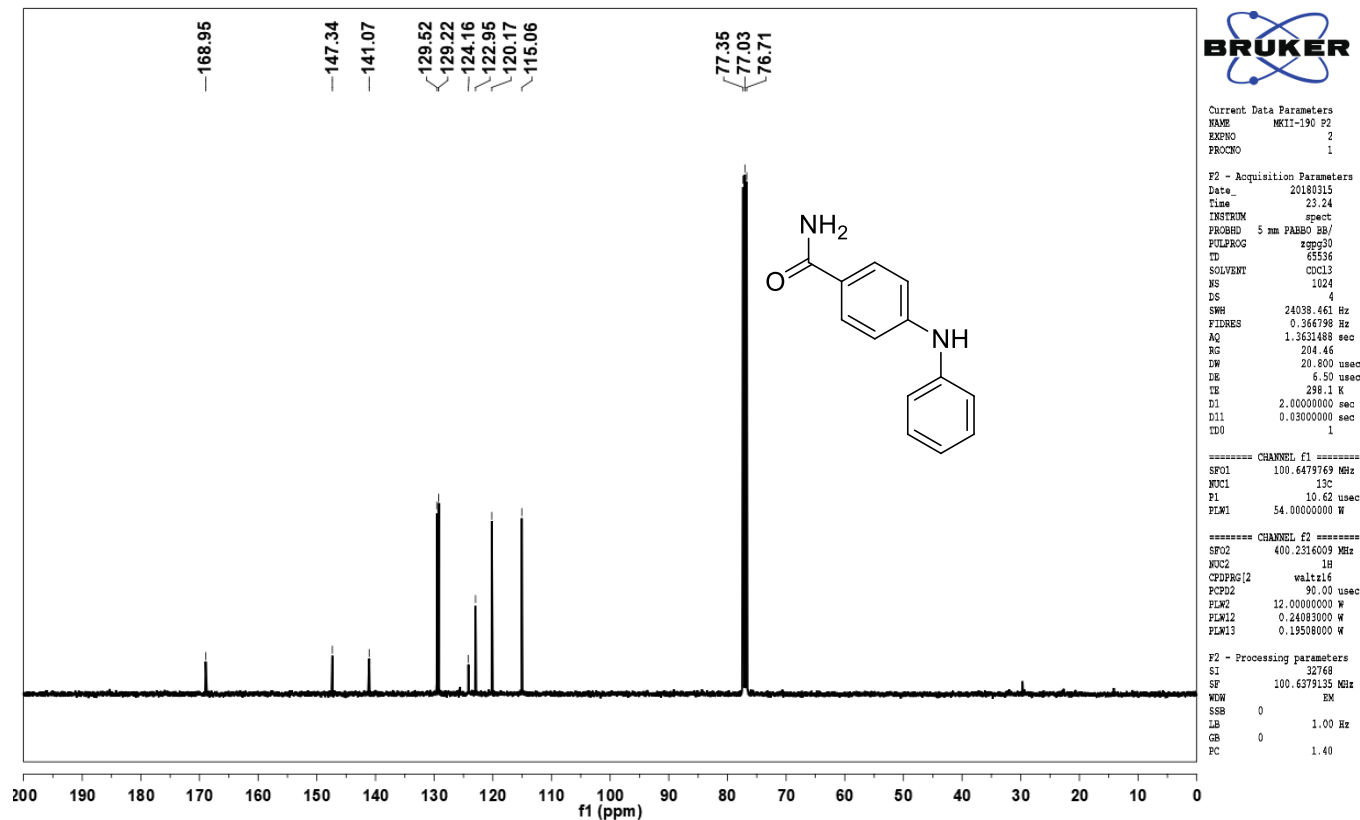
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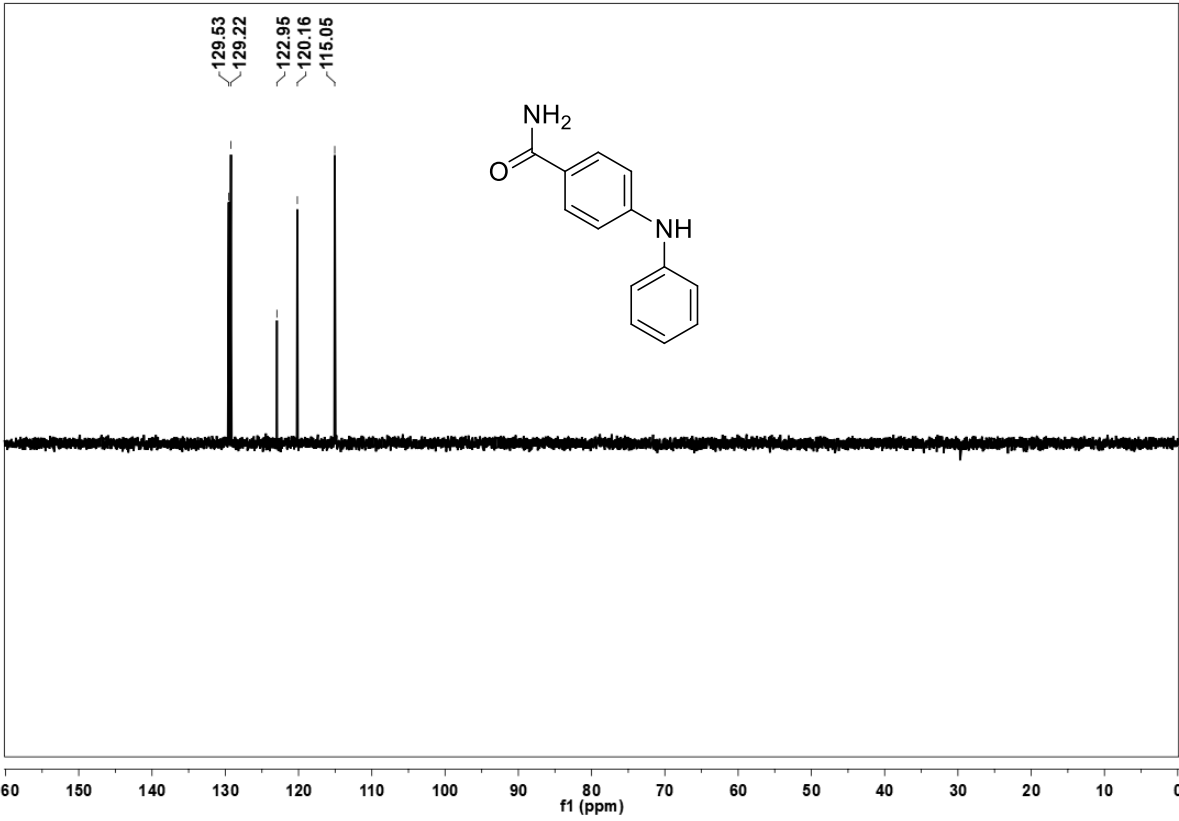
HRMS Spectrum of Compound **3b**



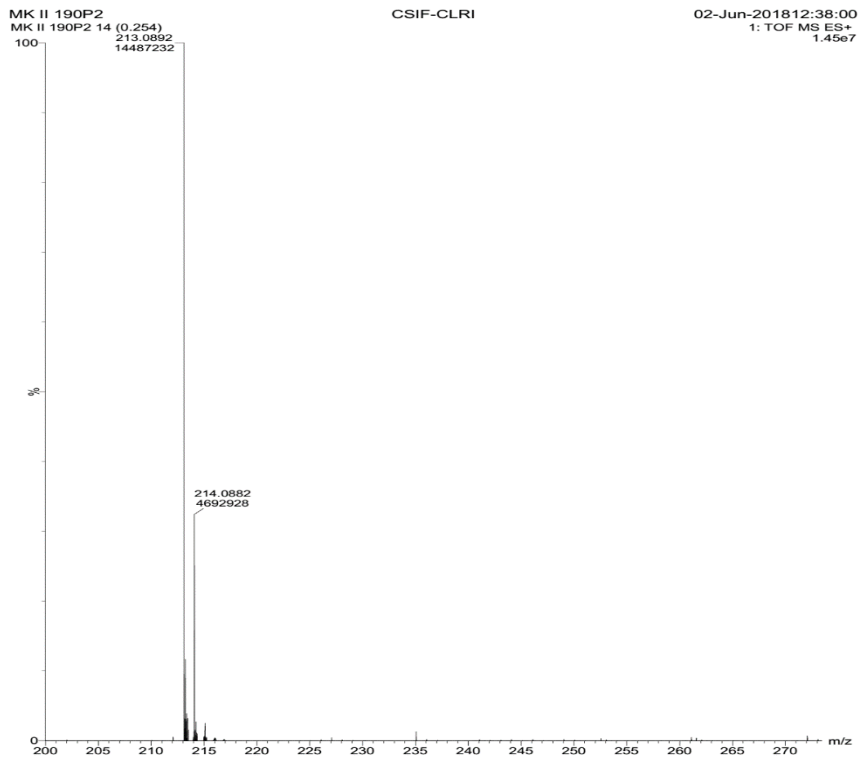
**<sup>1</sup>H NMR Spectrum of Compound 3c**



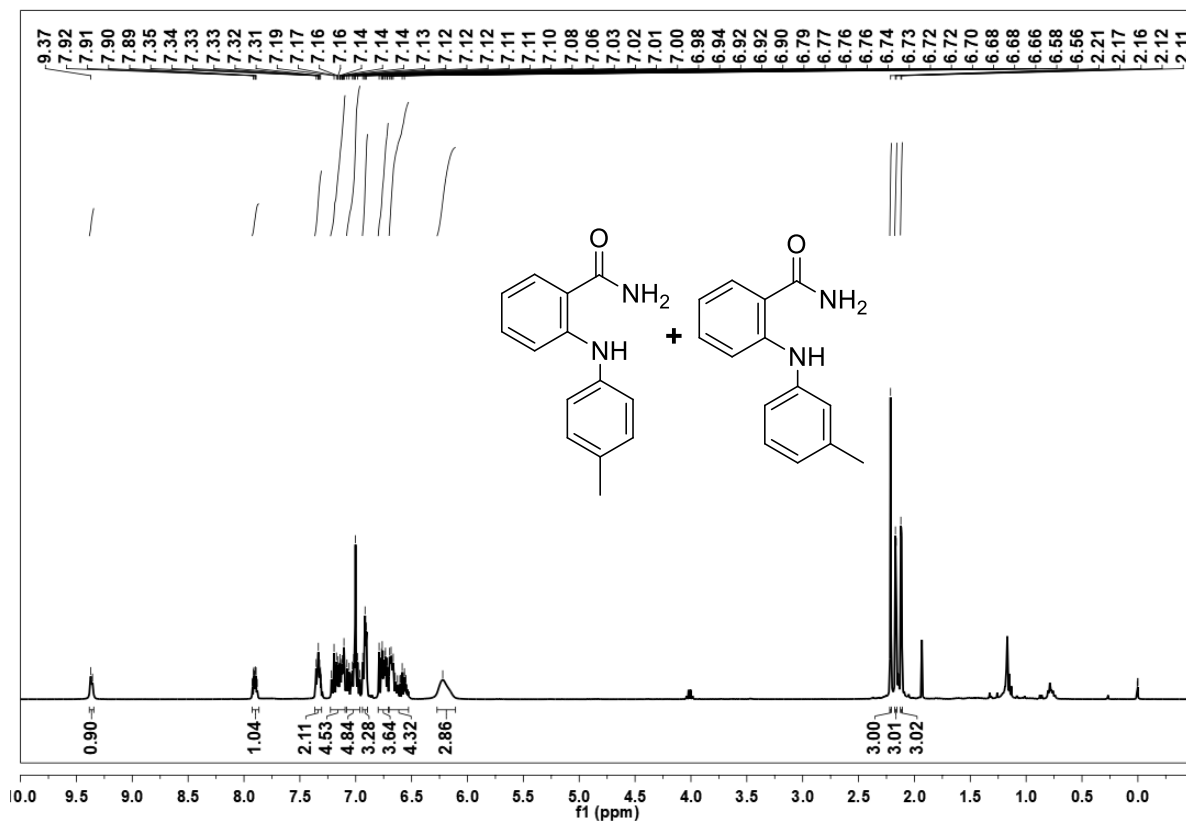
**<sup>13</sup>C NMR Spectrum of Compound 3c**



DEPT-135 NMR Spectrum of Compound 3c



HRMS Spectrum of Compound 3c



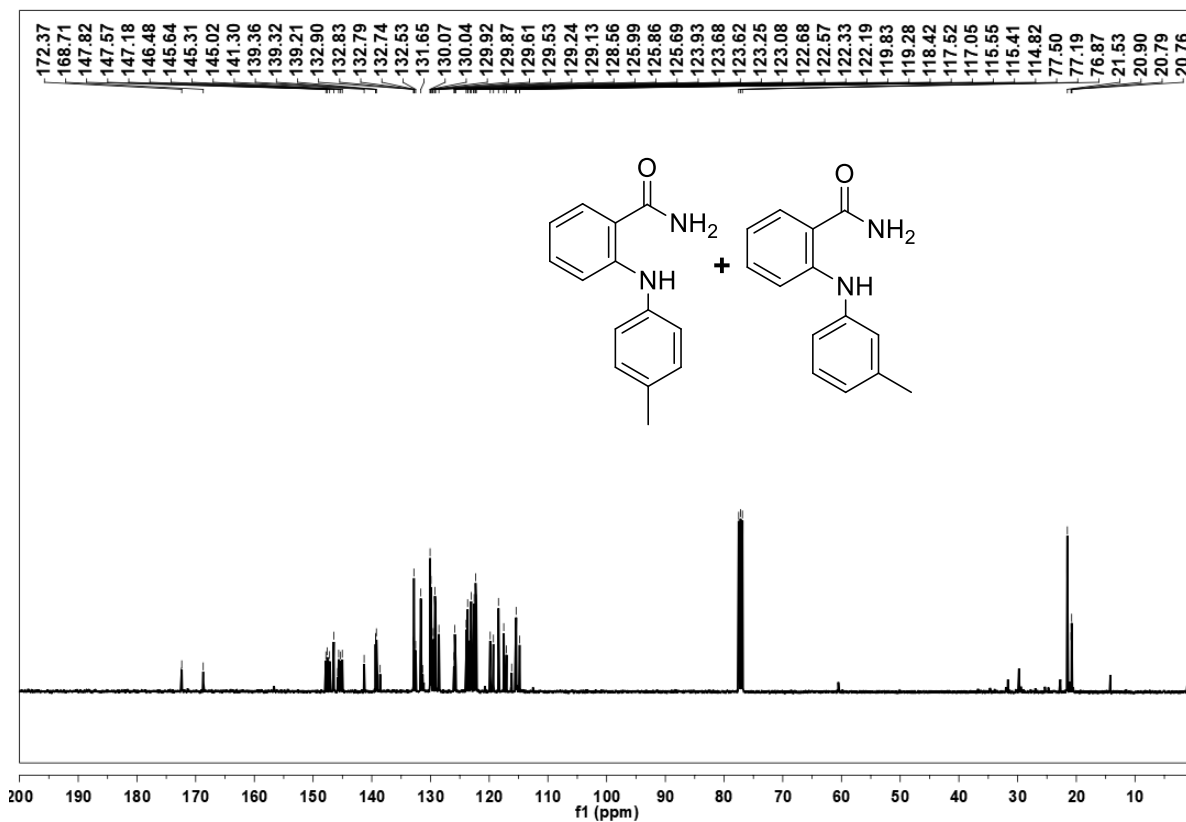
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SOLVENT CDCl3  
NS 16  
DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 31.36  
LW 62.400 usec  
DE 6.50 usec  
TE 294.6 K  
D1 1.00000000 sec  
TD0 1

===== CHANNEL f1 =====  
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NUC1 1H  
P1 12.75 usec  
PLW1 12.00000000 W

F2 - Processing parameters  
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SF 400.2300625 MHz  
WDW EM  
SSB 0  
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GB 0  
PC 1.00

**<sup>1</sup>H NMR Spectrum of Compound 3d**



BRUKER

Current Data Parameters  
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EXPHO 2  
PROCNO 1

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INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
ID 65536  
SOLVENT CDCl3  
NS 512  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
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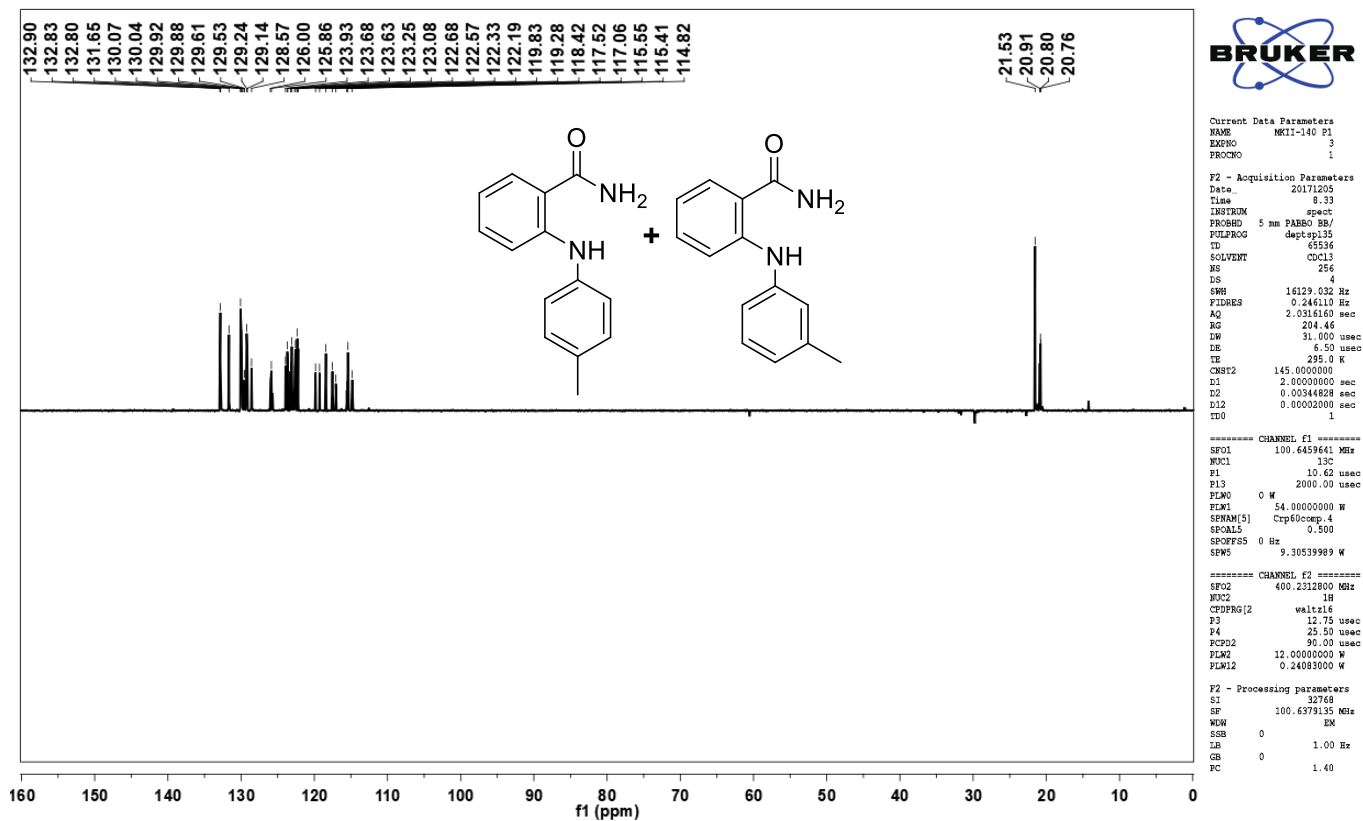
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NUC1 13C  
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PLW13 0.19580000 W

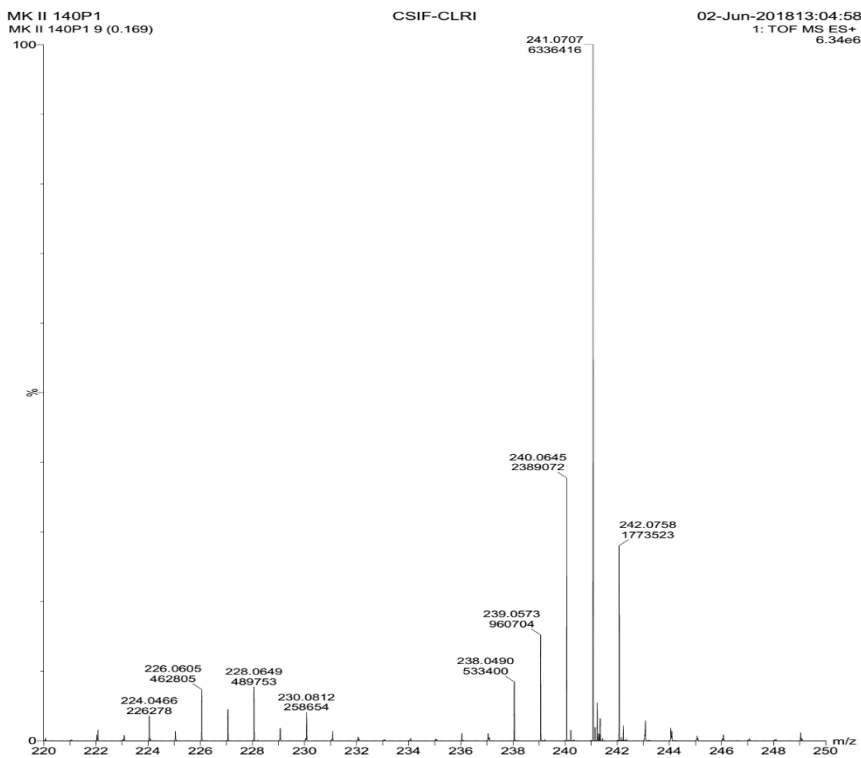
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**<sup>13</sup>C NMR Spectrum of Compound 3d**

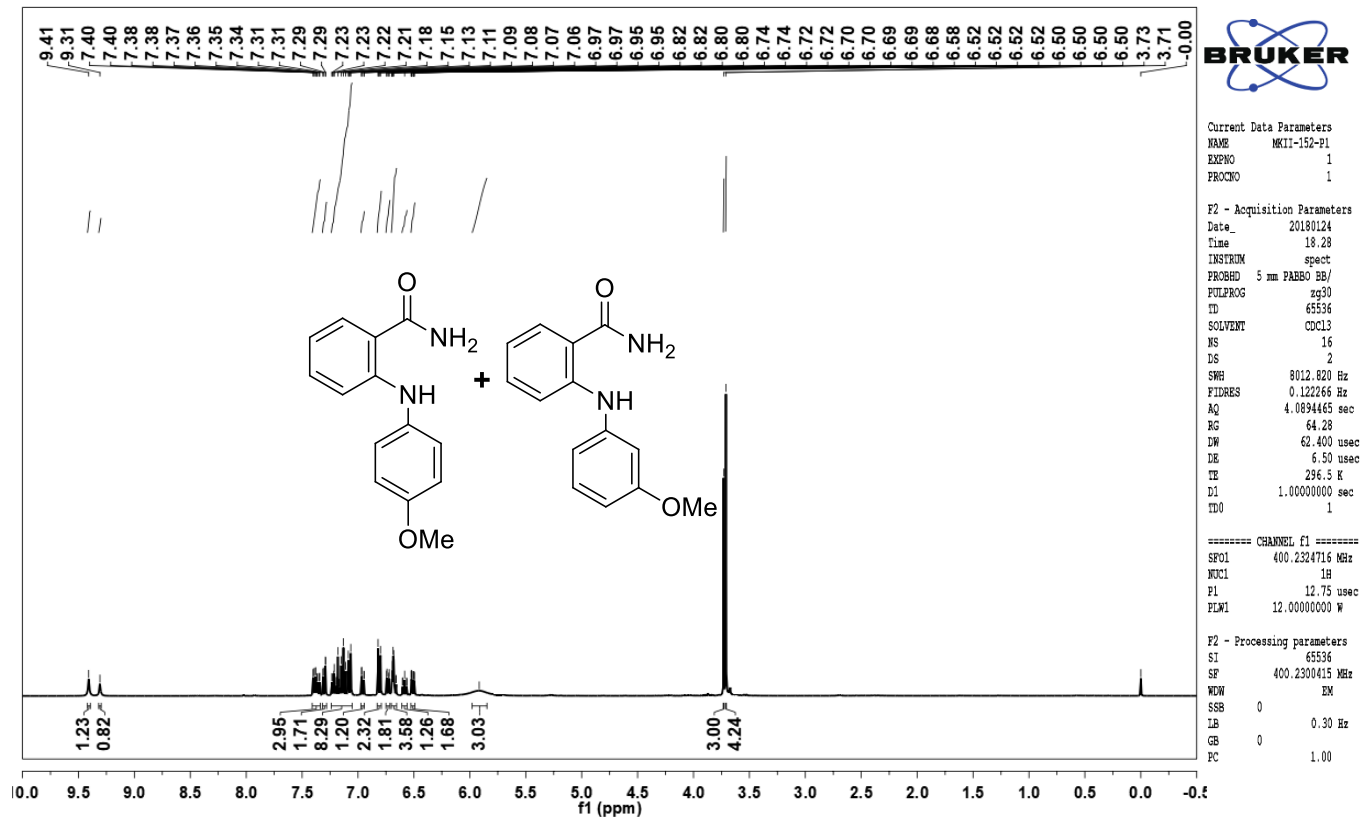




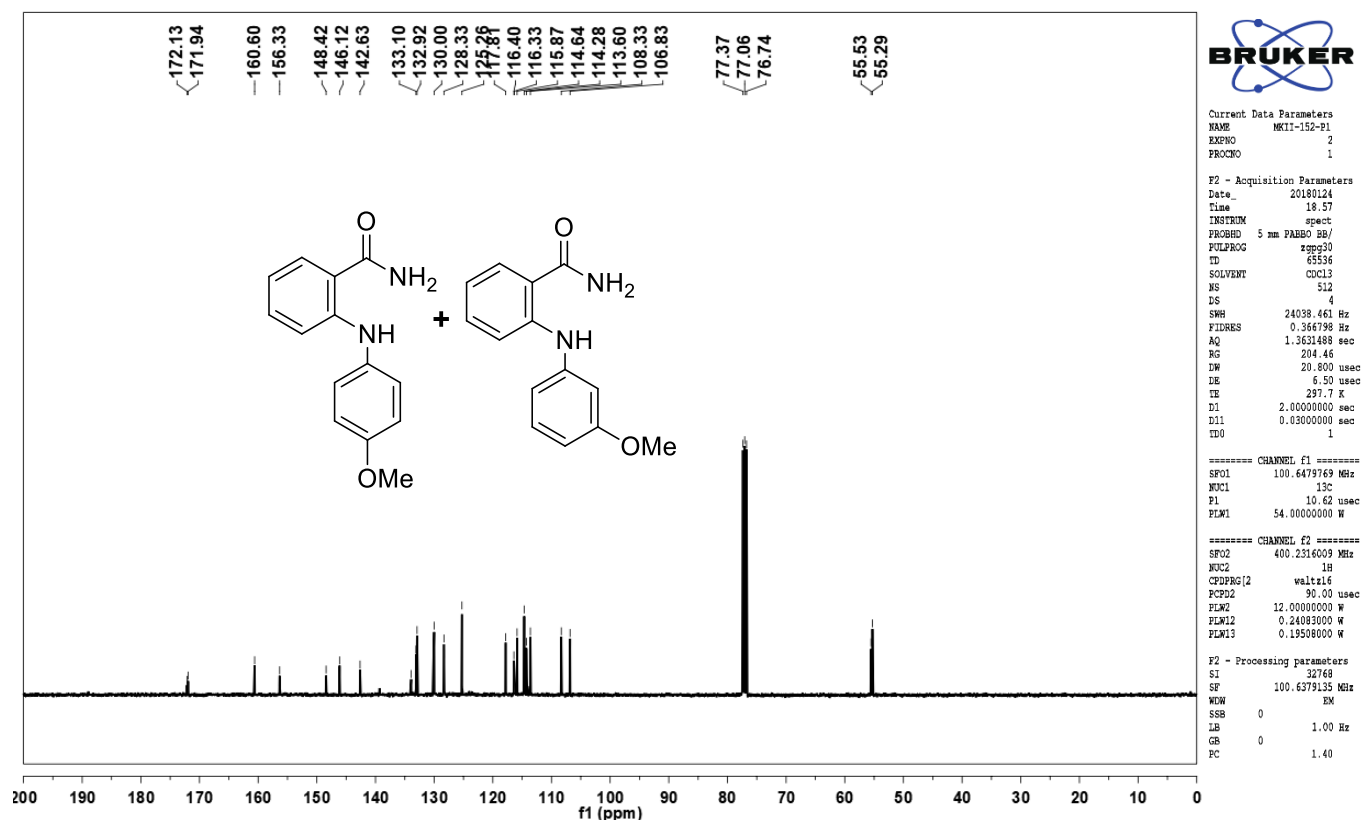
DEPT-135 NMR Spectrum of Compound 3d



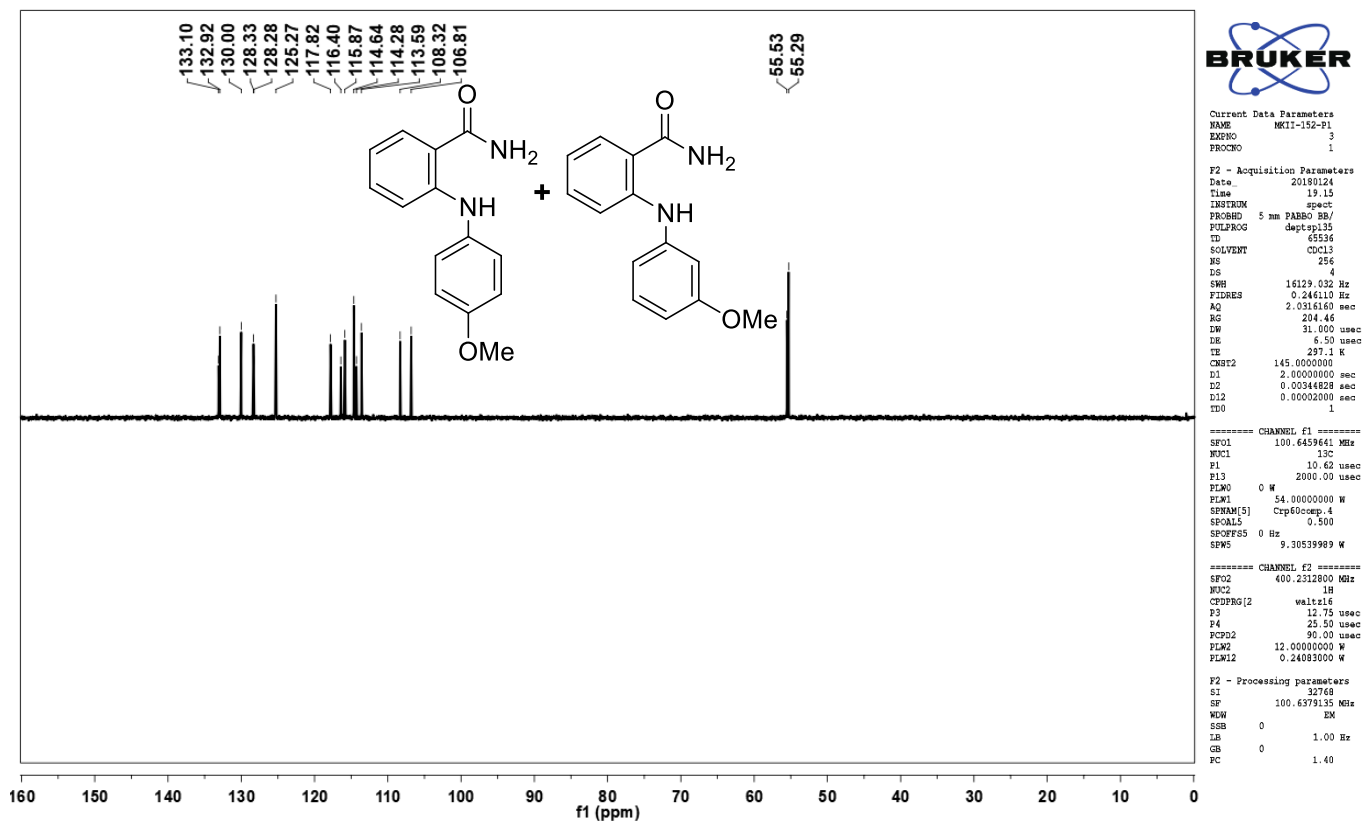
HRMS Spectrum of Compound 3d



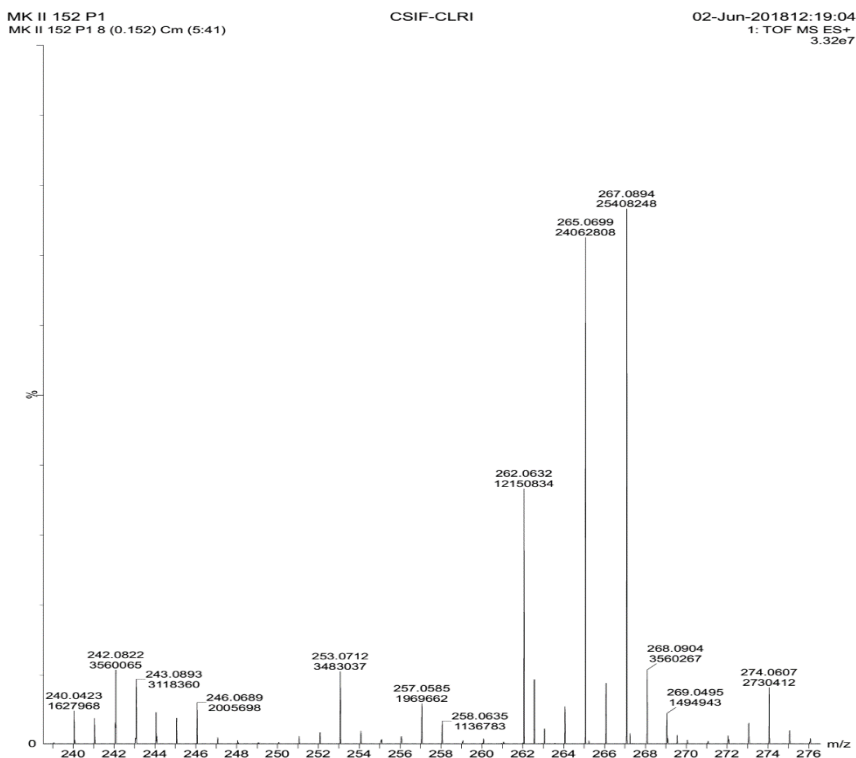
<sup>1</sup>H NMR Spectrum of Compound 3e



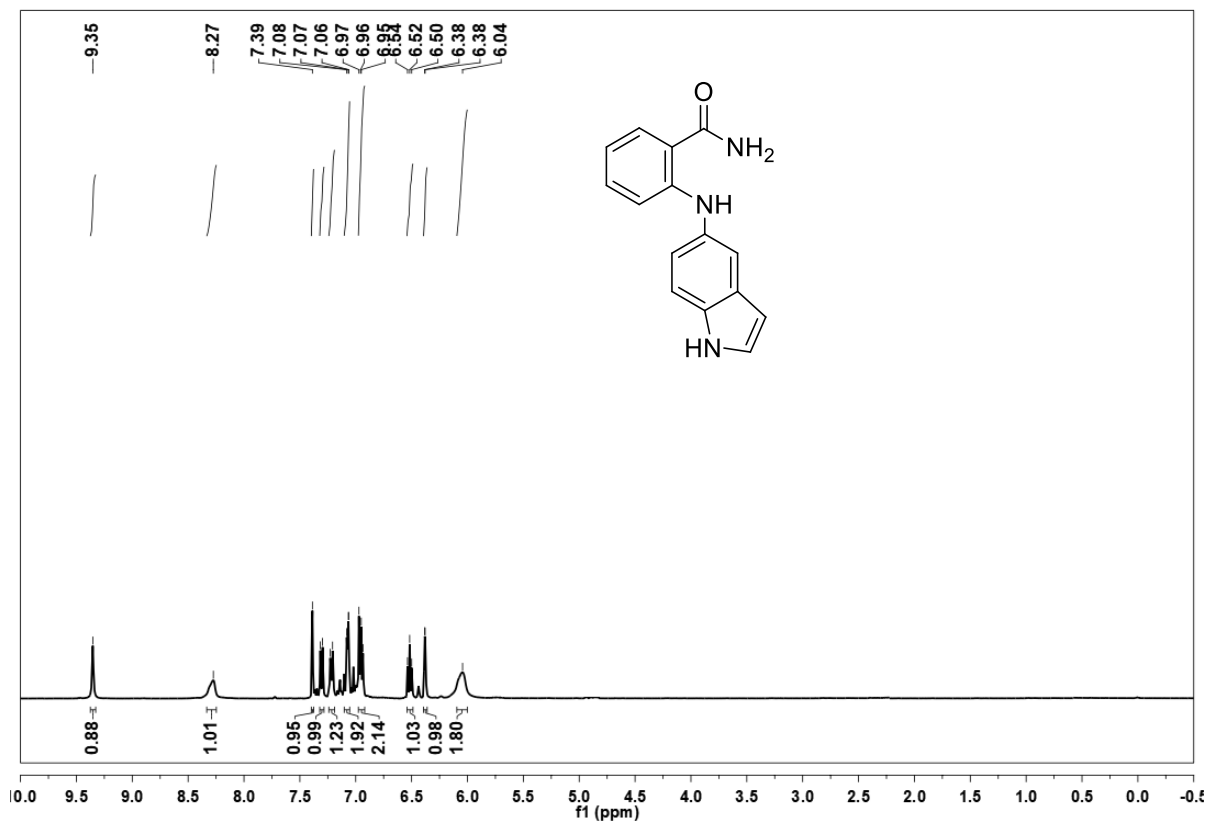
<sup>13</sup>C NMR Spectrum of Compound 3e



DEPT-135 NMR Spectrum of Compound 3e



HRMS Spectrum of Compound 3e



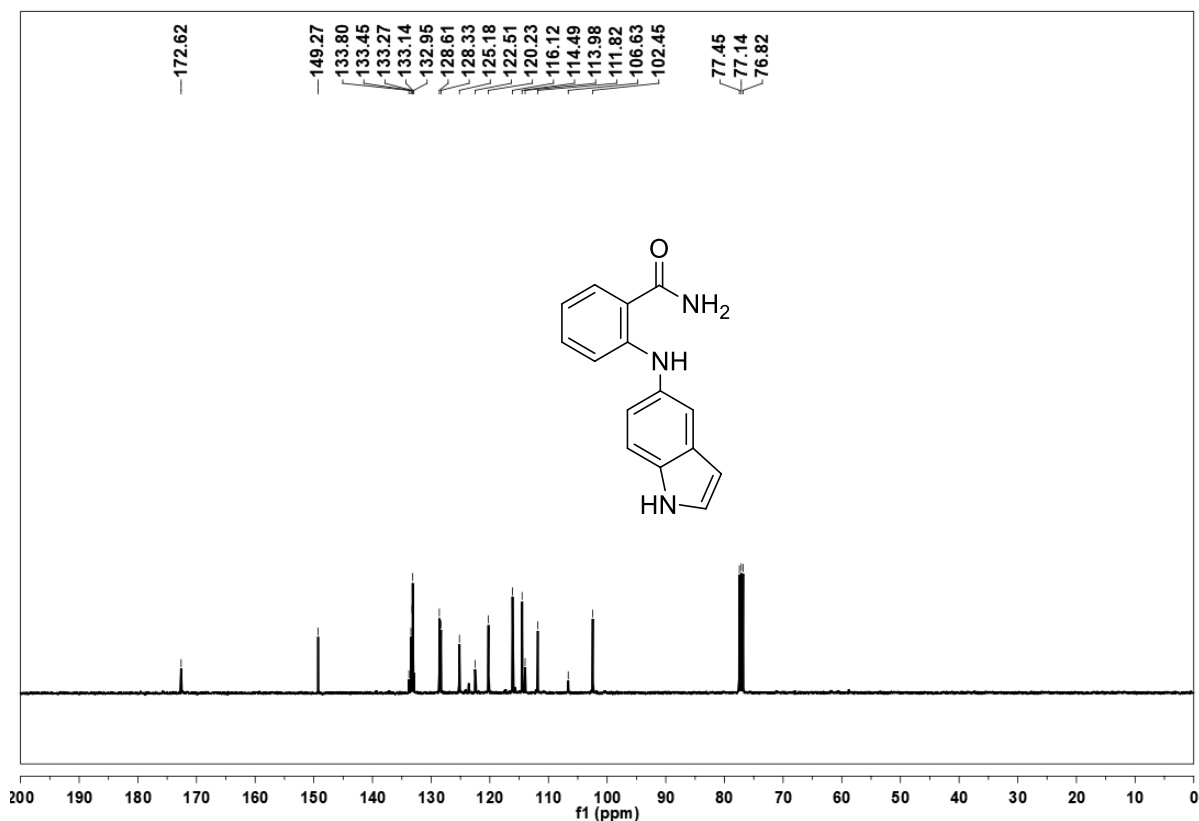
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SOLVENT CDCl3  
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DS 2  
SWH 8012.820 Hz  
FIDRES 0.122266 Hz  
AQ 4.0894465 sec  
RG 31.36  
DW 62.400 usec  
DE 6.50 usec  
TE 296.1 K  
D1 1.0000000 sec  
TD0 1

===== CHANNEL f1 =====  
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NUC1 1H  
P1 12.75 usec  
PLW1 12.0000000 W

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<sup>1</sup>H NMR Spectrum of Compound 3f



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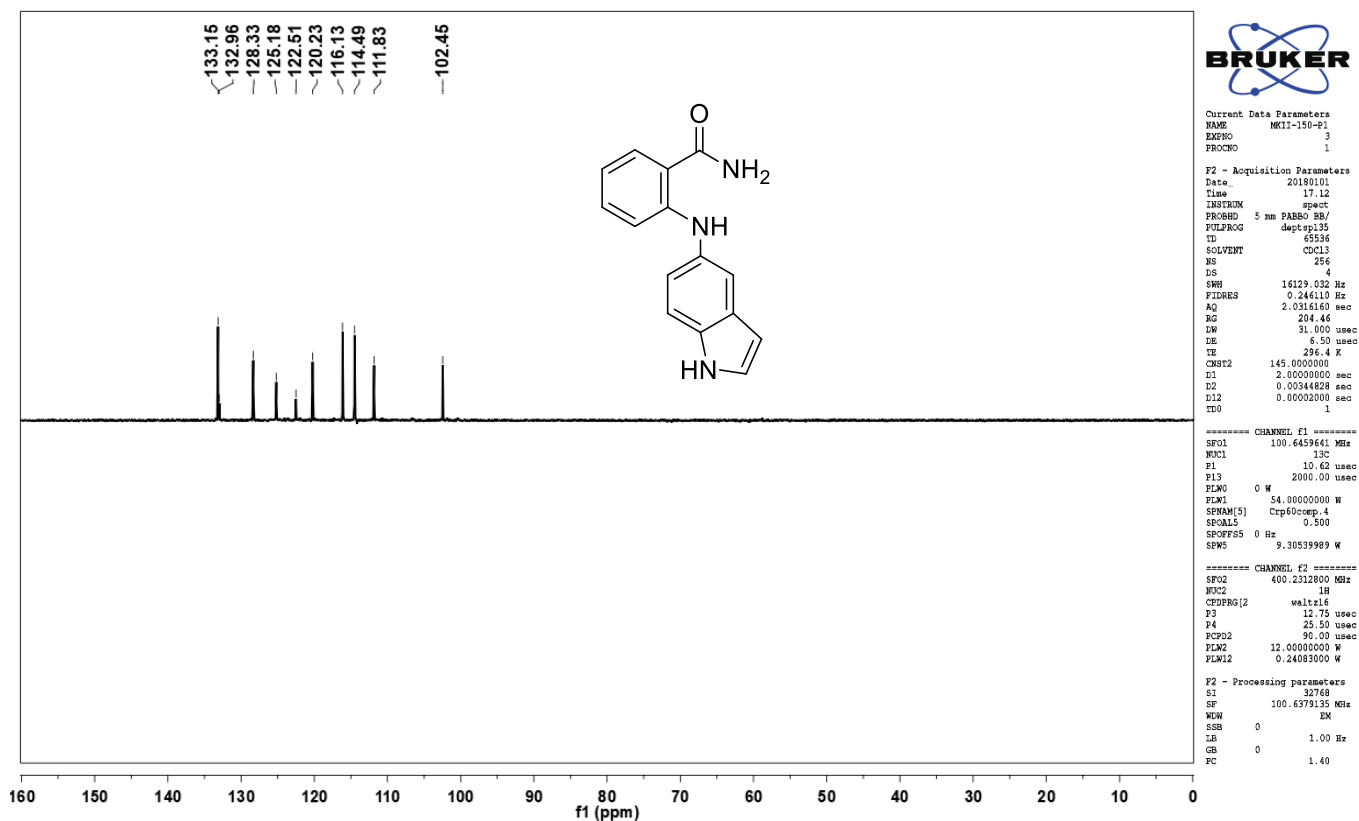
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DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 204.46  
LW 20.800 usec  
DE 6.50 usec  
TE 297.1 K  
D1 2.0000000 sec  
D11 0.0300000 sec  
TD0 1

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P1 10.62 usec  
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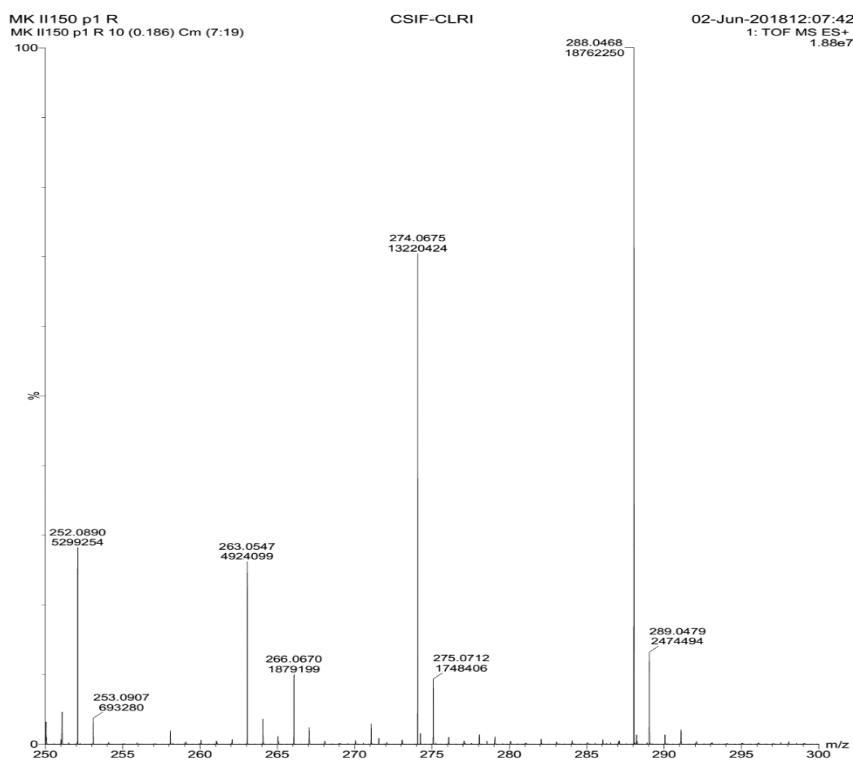
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PLW12 0.24083000 W  
PLW13 0.15508000 W

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GB 0  
PC 1.40

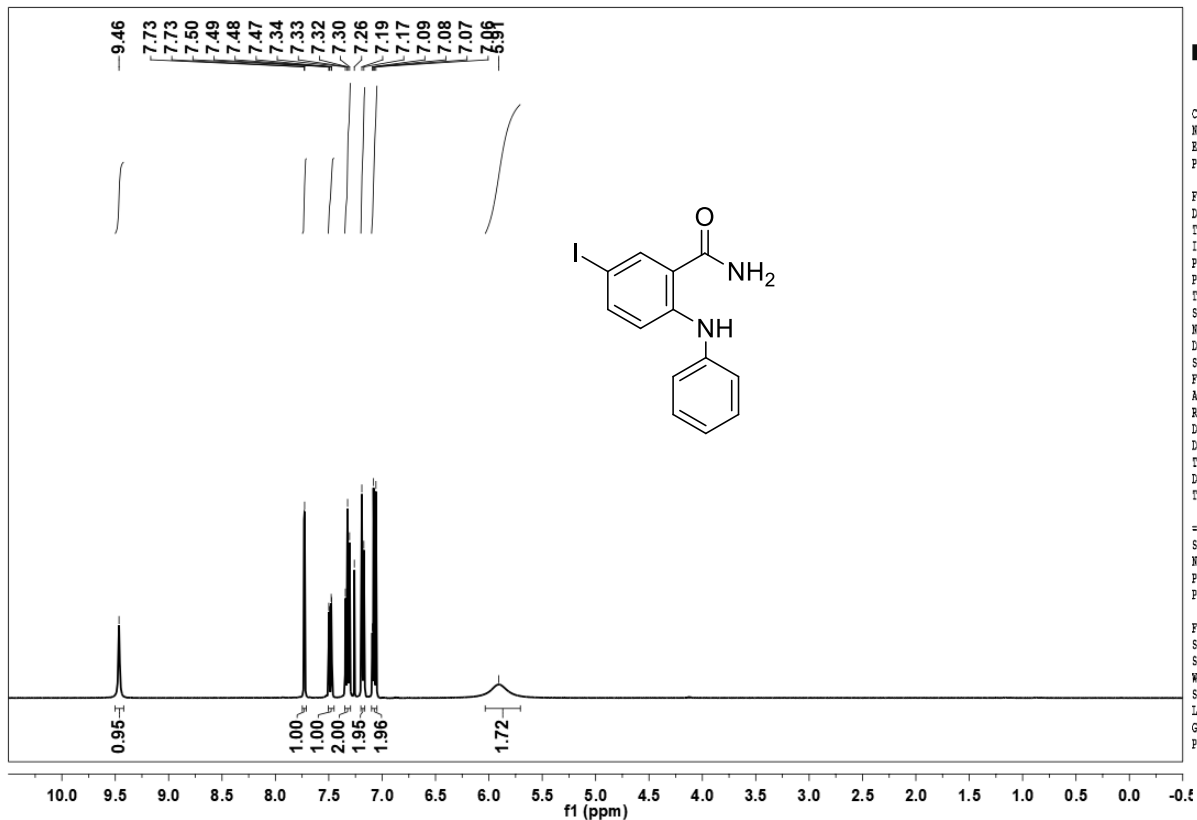
<sup>13</sup>C NMR Spectrum of Compound 3f



DEPT-135 NMR Spectrum of Compound 3f



HRMS Spectrum of Compound 3f



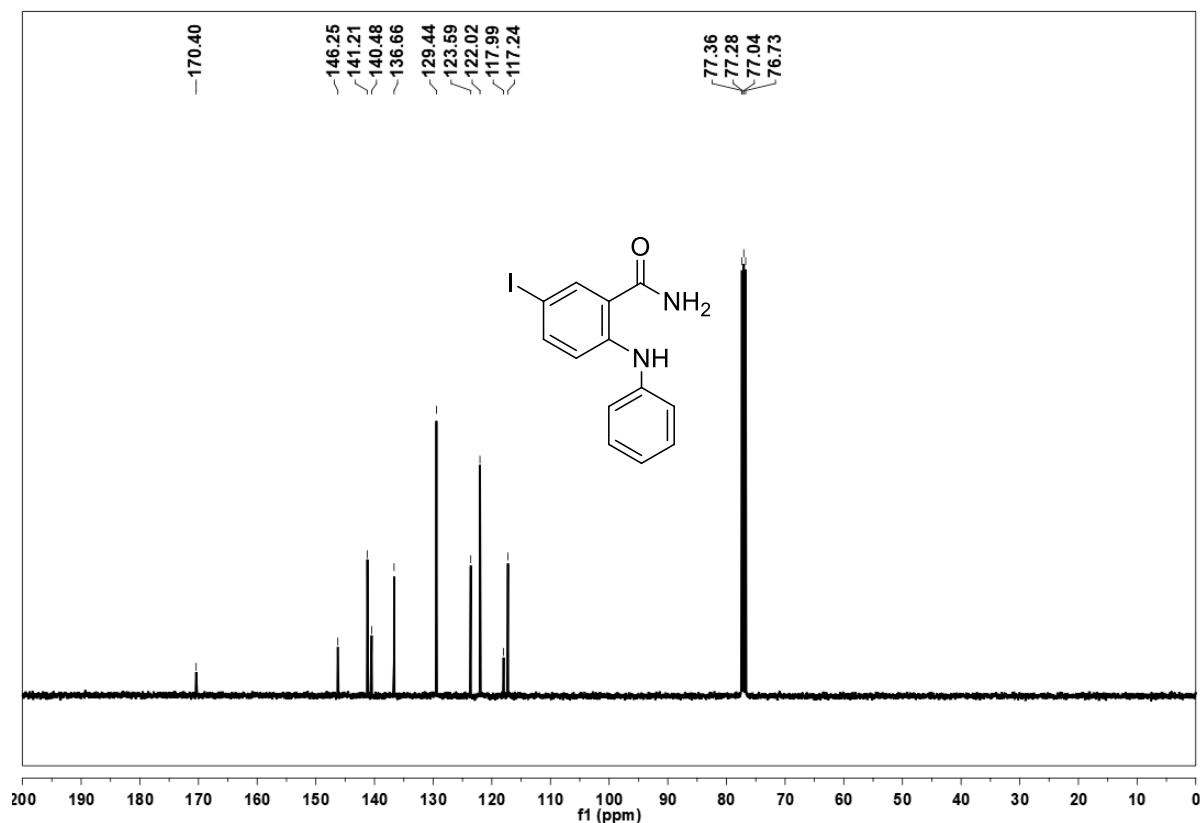
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 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 128.33  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 294.9 K  
 D1 1.0000000 sec  
 TDO 1

==== CHANNEL f1 =====  
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 NUC1 1H  
 P1 12.75 usec  
 PLW1 12.0000000 W

F2 - Processing parameters  
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 SF 400.2300000 MHz  
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**1H NMR Spectrum of Compound 3g**



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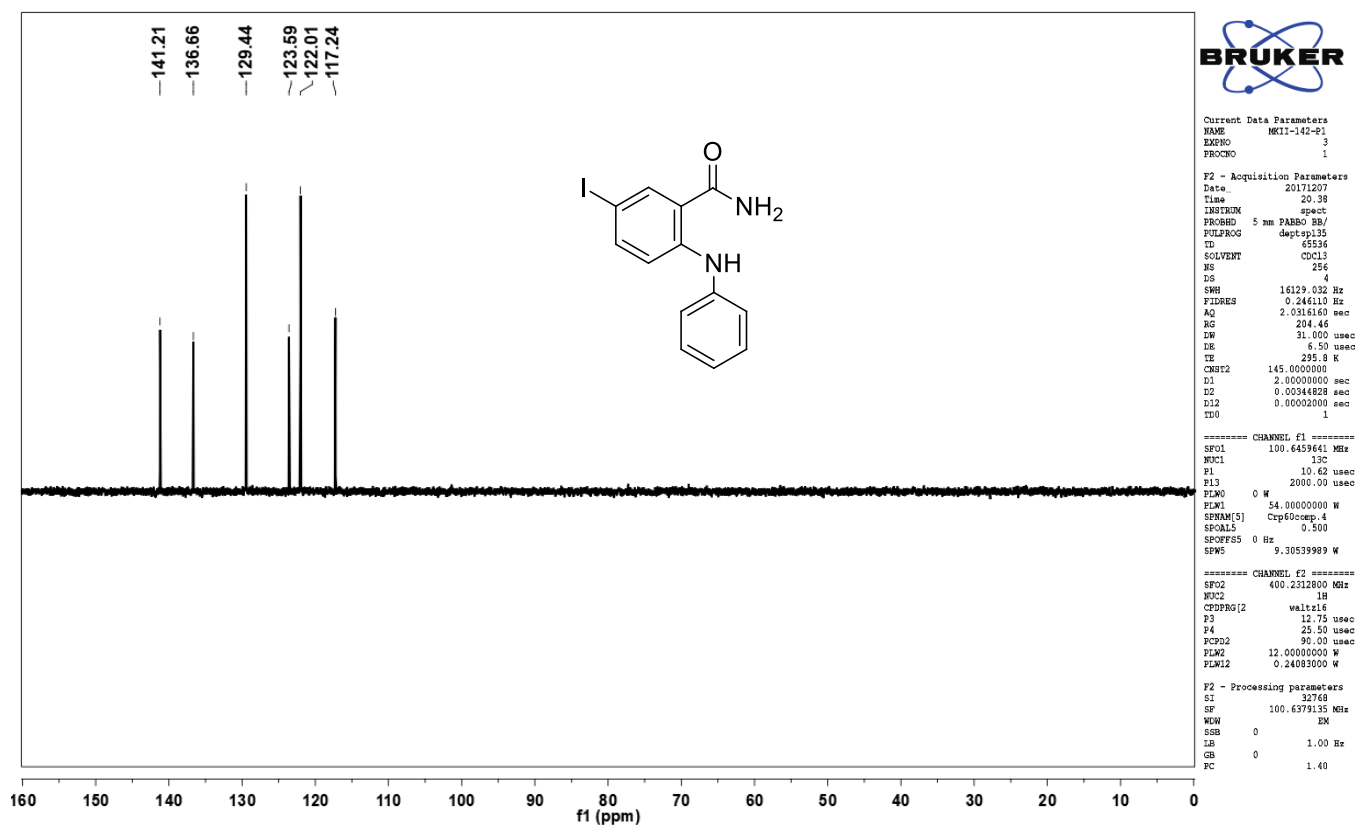
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 TD 65536  
 SOLVENT CDCl3  
 NS 512  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 204.46  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.4 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TDO 1

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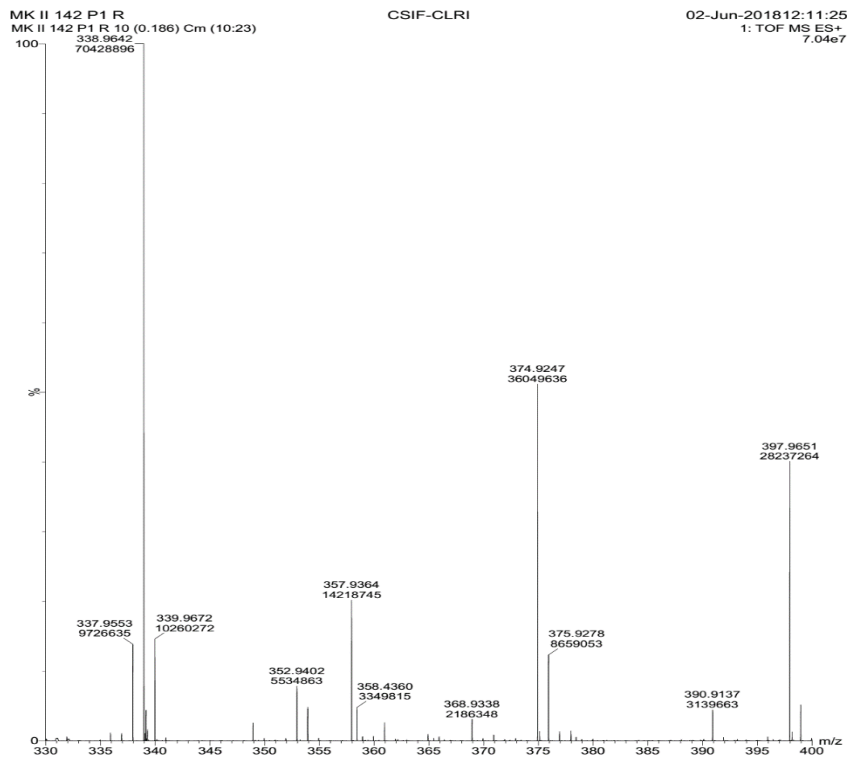
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 NUC2 1H  
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 PLW12 0.24083000 W  
 PLW13 0.19508000 W

F2 - Processing parameters  
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 GB 0  
 PC 1.40

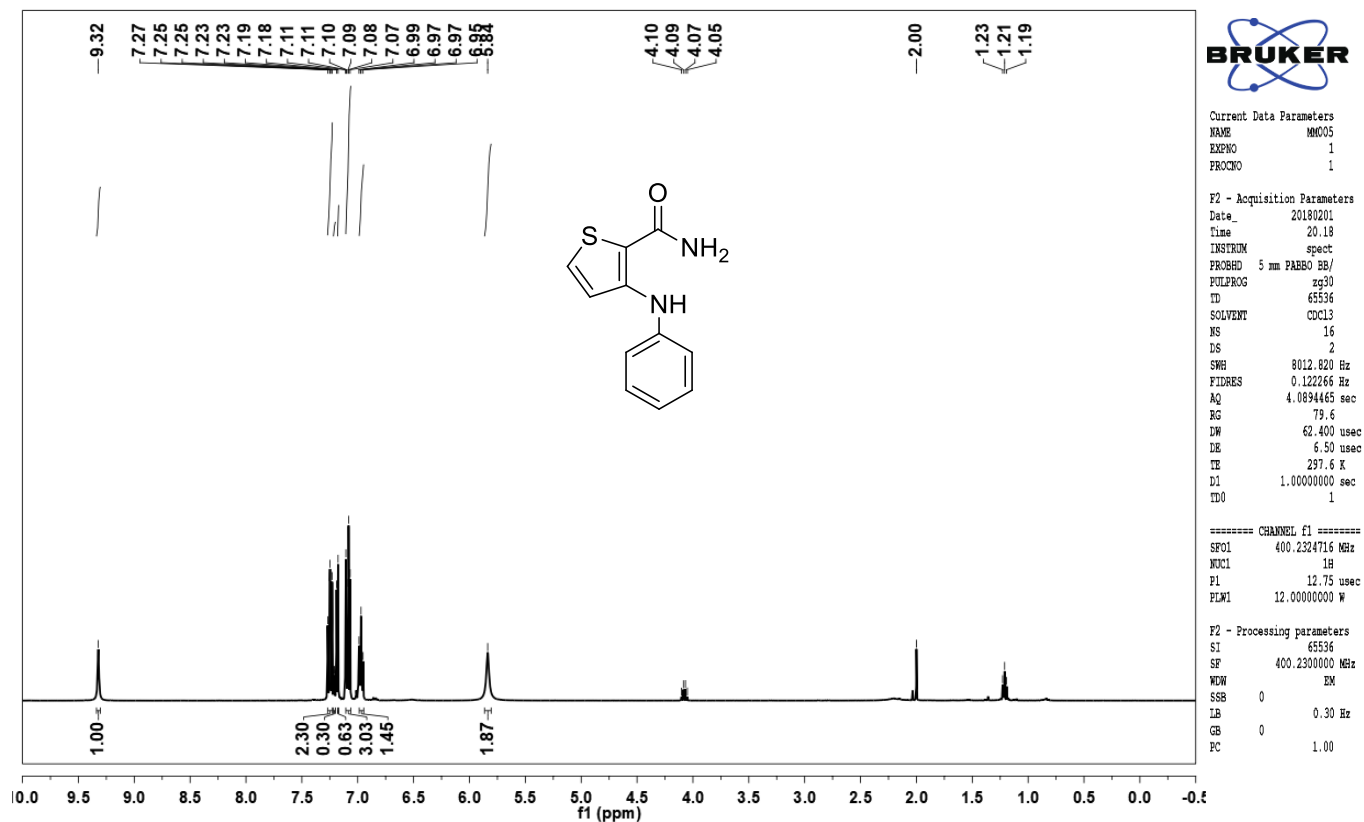
**13C NMR Spectrum of Compound 3g**



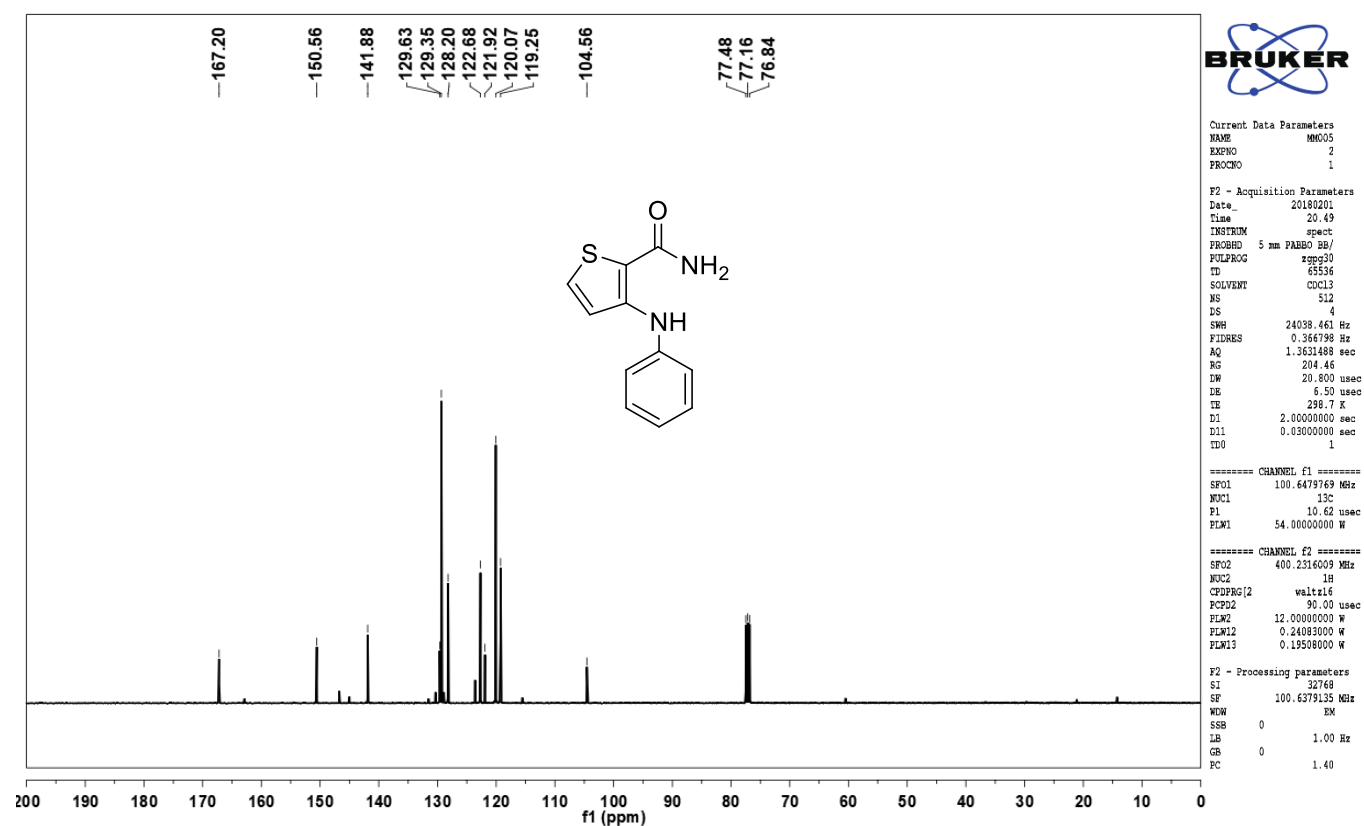
DEPT-135 NMR Spectrum of Compound 3g



HRMS Spectrum of Compound 3g

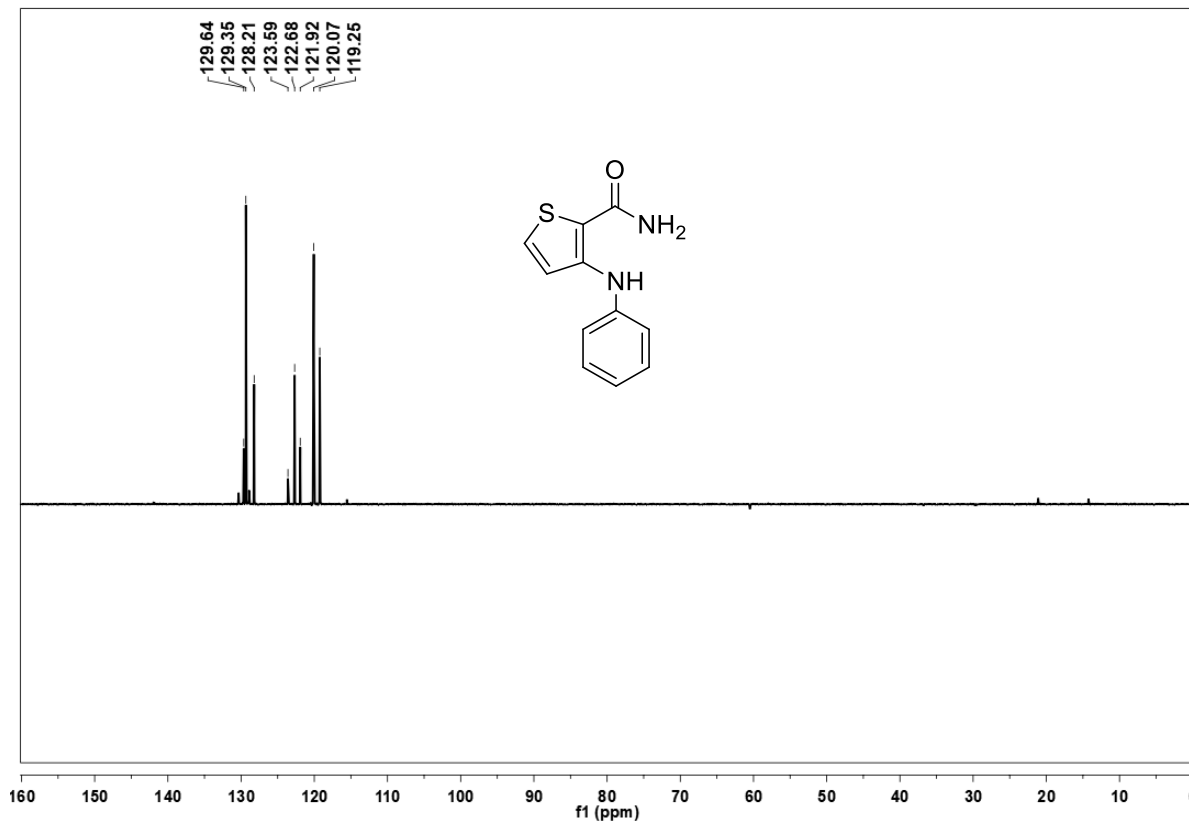


**<sup>1</sup>H NMR Spectrum of Compound 3h**

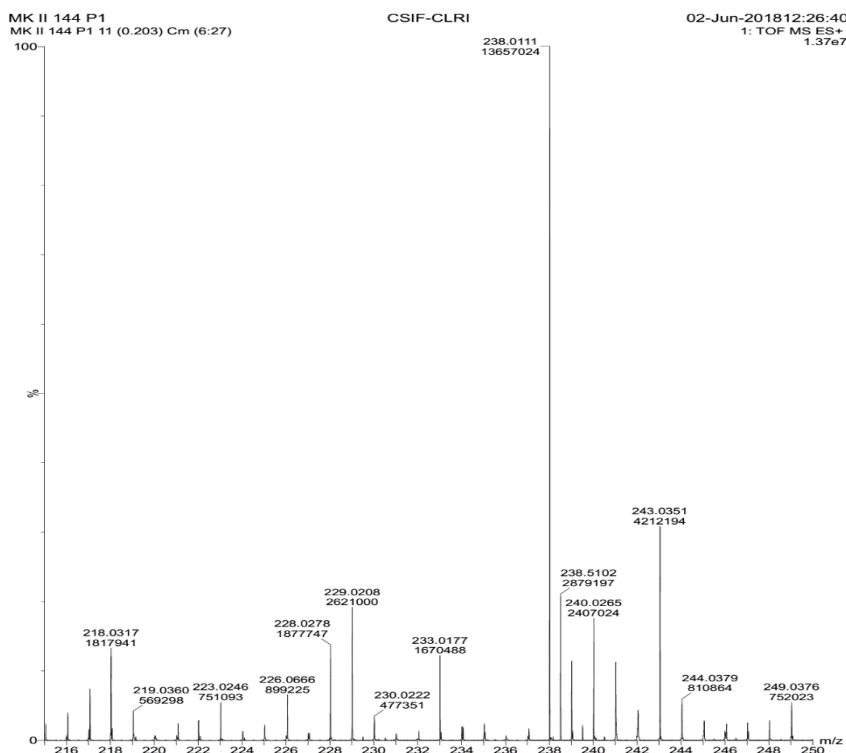


**<sup>13</sup>C NMR Spectrum of Compound 3h**

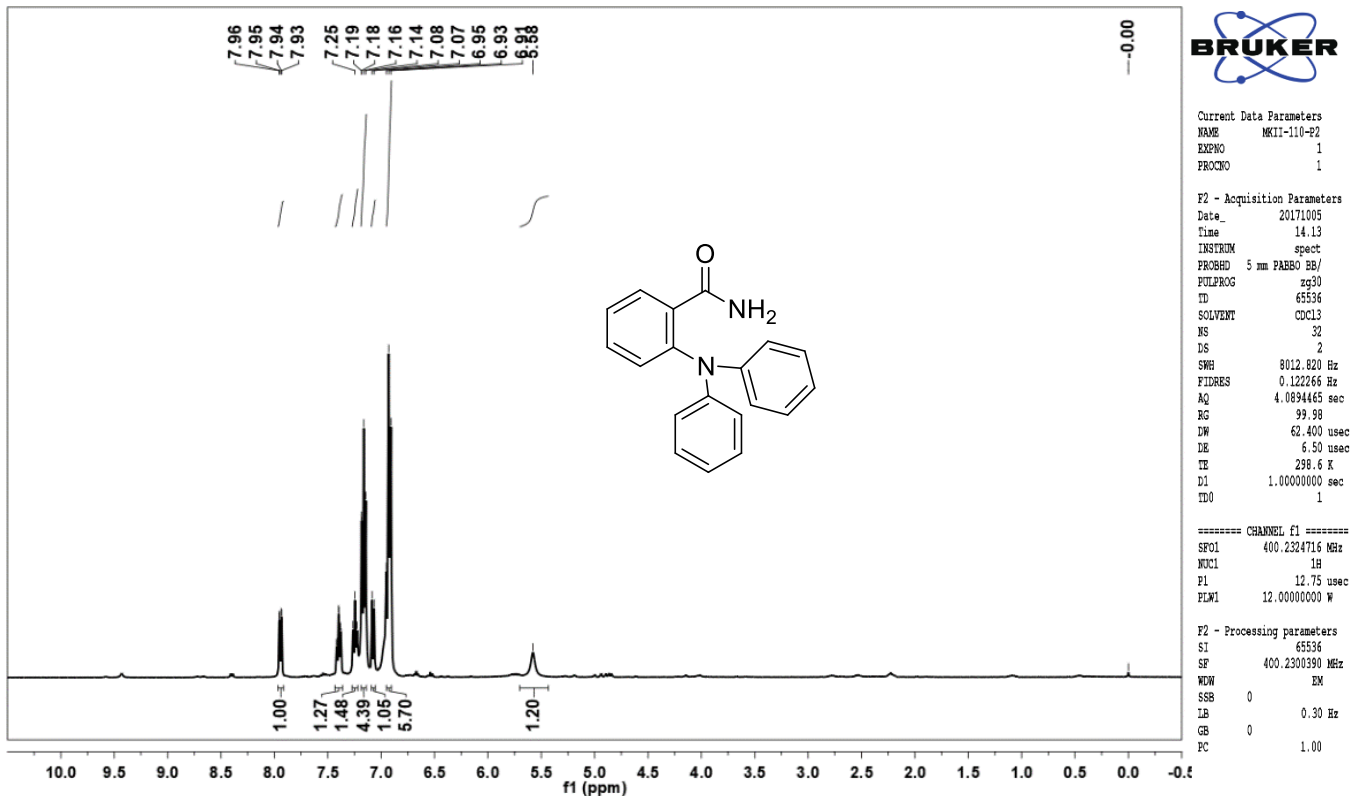




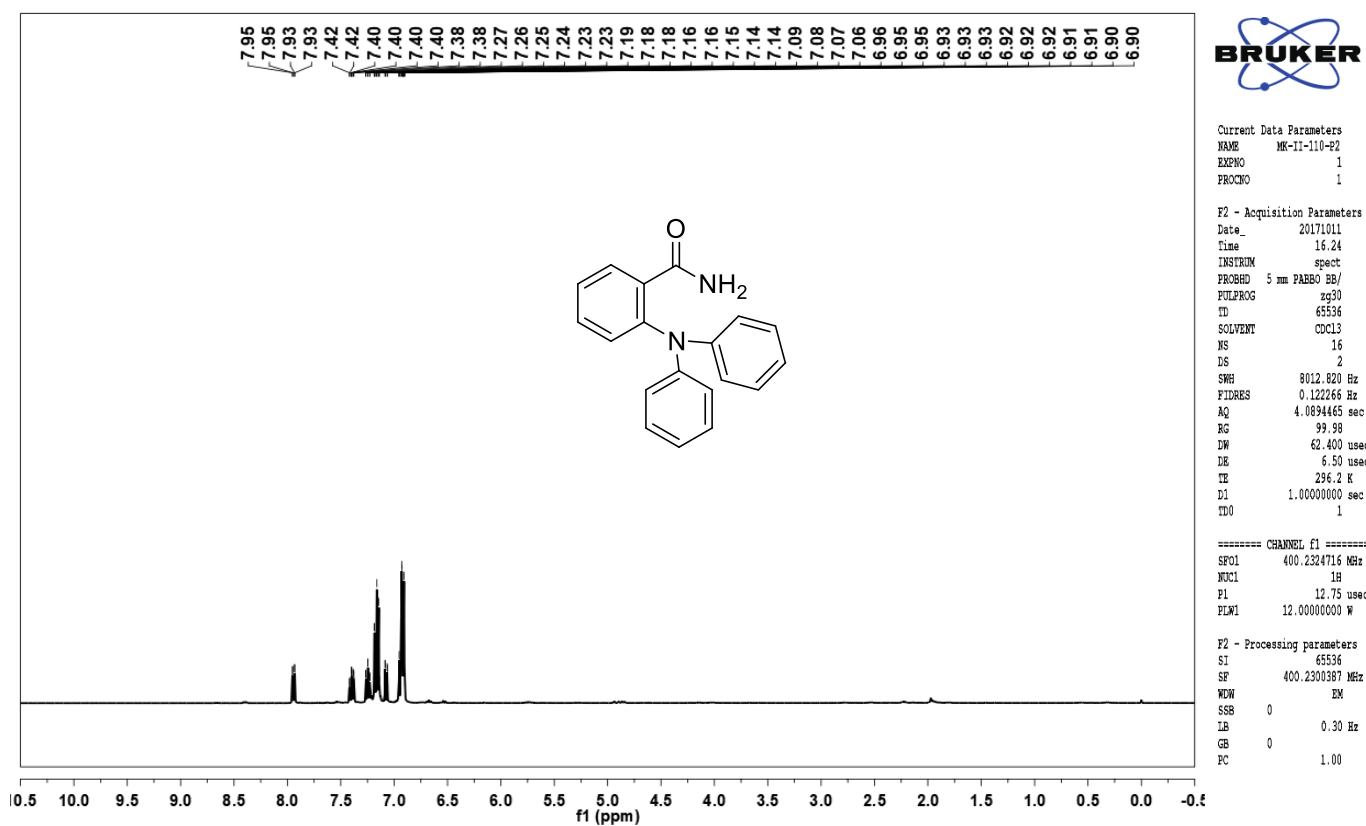
DEPT-135 NMR Spectrum of Compound **3h**



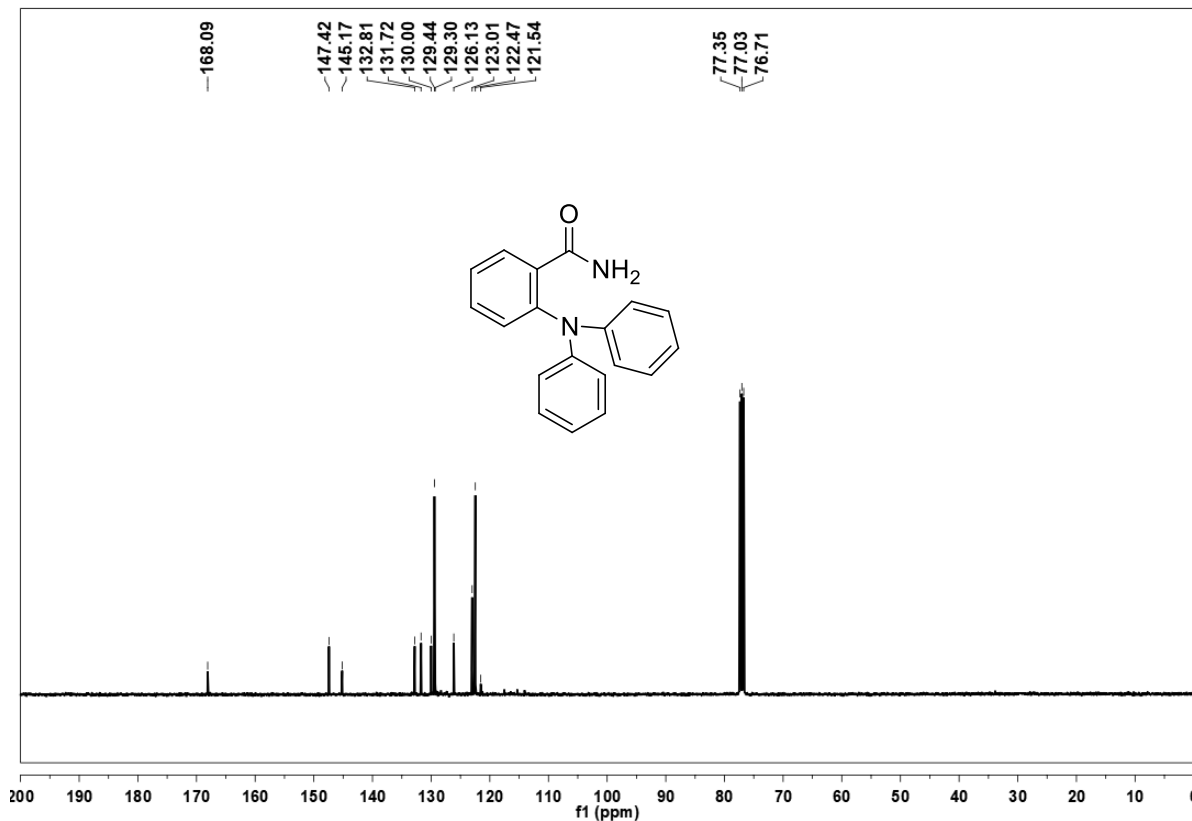
HRMS Spectrum of Compound **3h**



<sup>1</sup>H NMR Spectrum of Compound **4a**



<sup>1</sup>H NMR Spectrum of Compound **4a** (D<sub>2</sub>O exchange experiment)



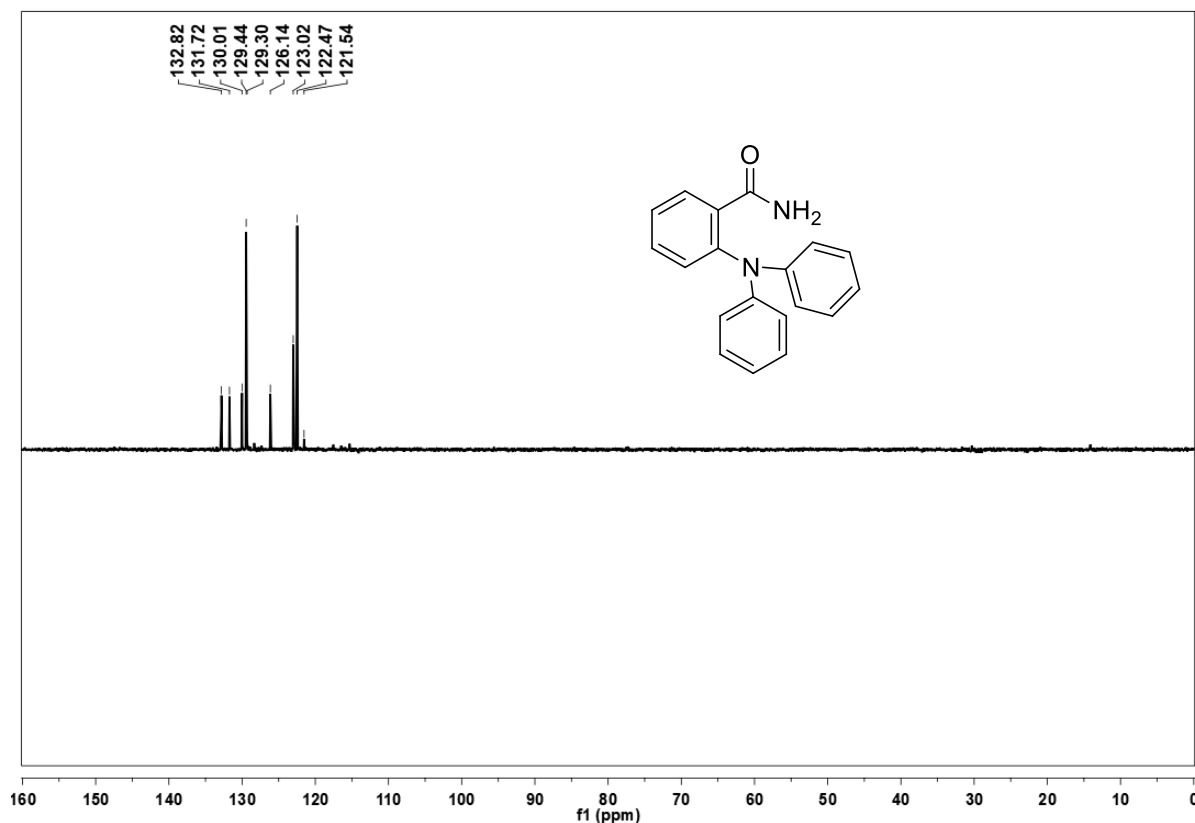
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 SOLVENT cdcl3  
 NS 1024  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3621488 sec  
 RG 204.46  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.1 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SF01 100.6479769 MHz  
 NUC1 13C  
 P1 10.62 usec  
 PLW1 54.0000000 W  
 ===== CHANNEL f2 =====  
 SF02 400.2316009 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.0000000 W  
 PLW3 0.24083000 W  
 PLW13 0.19508000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6379135 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 FC 1.40

<sup>13</sup>C NMR Spectrum of Compound 4a



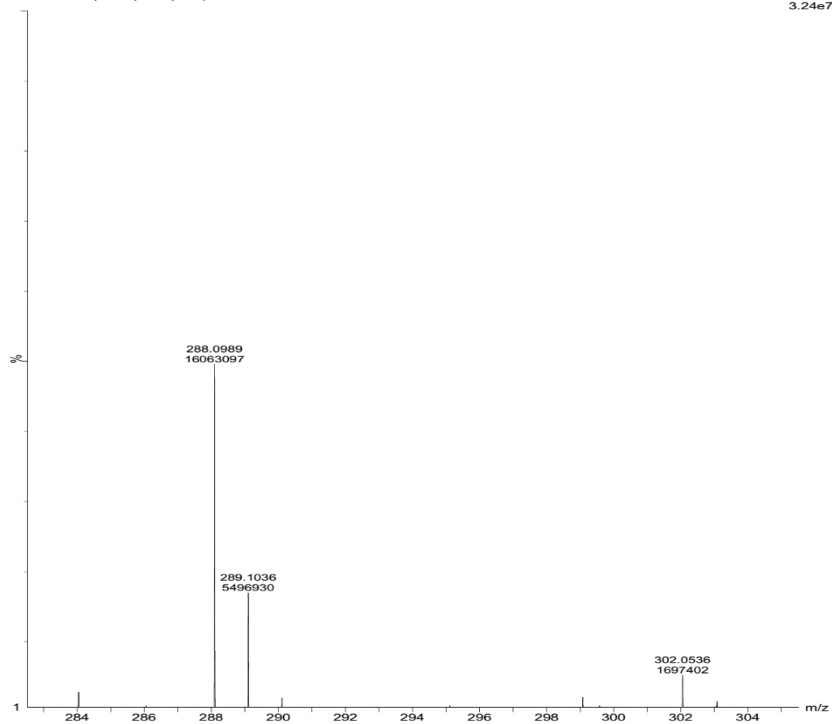
Current Data Parameters  
 NAME MKII-110-P2  
 EXPHO 3  
 PROCNO 1

F2 - Acquisition Parameters  
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 Time 15.48  
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 PROBHD 5 mm PABBO BB/  
 PULPROG deptcp135  
 TD 65536  
 SOLVENT cdcl3  
 NS 512  
 DS 4  
 SWH 16129.032 Hz  
 FIDRES 0.246110 Hz  
 AQ 2.0316160 sec  
 RG 204.46  
 DW 31.000 usec  
 DE 6.50 usec  
 TE 297.4 K  
 CMBE2 145.000000  
 D1 2.0000000 sec  
 D2 0.03344808 sec  
 D12 0.00002000 sec  
 TD0 1

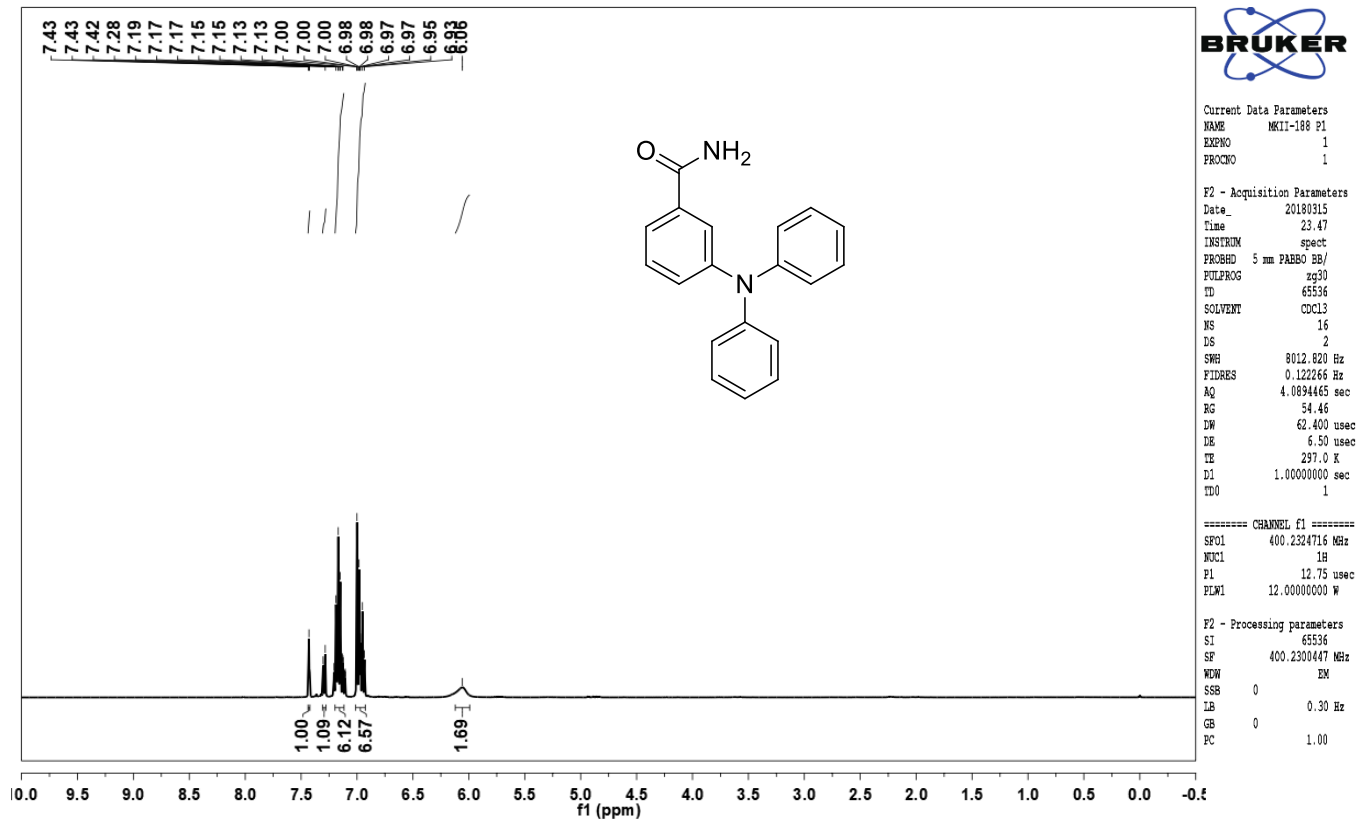
==== CHANNEL f1 =====  
 SF01 100.6459641 MHz  
 NUC1 13C  
 P1 10.62 usec  
 P13 2000.00 usec  
 PLW0 0 W  
 PLW1 54.0000000 W  
 SENAM[5] Ctp50comp.4  
 SFOALS 0.500  
 SFOFFS 0 Hz  
 SWS 9.30539989 W  
 ===== CHANNEL f2 =====  
 SF02 400.2312000 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 P3 12.75 usec  
 P4 25.50 usec  
 PCPD2 90.00 usec  
 PLW2 12.0000000 W  
 PLW3 0.24083000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6379135 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 FC 1.40

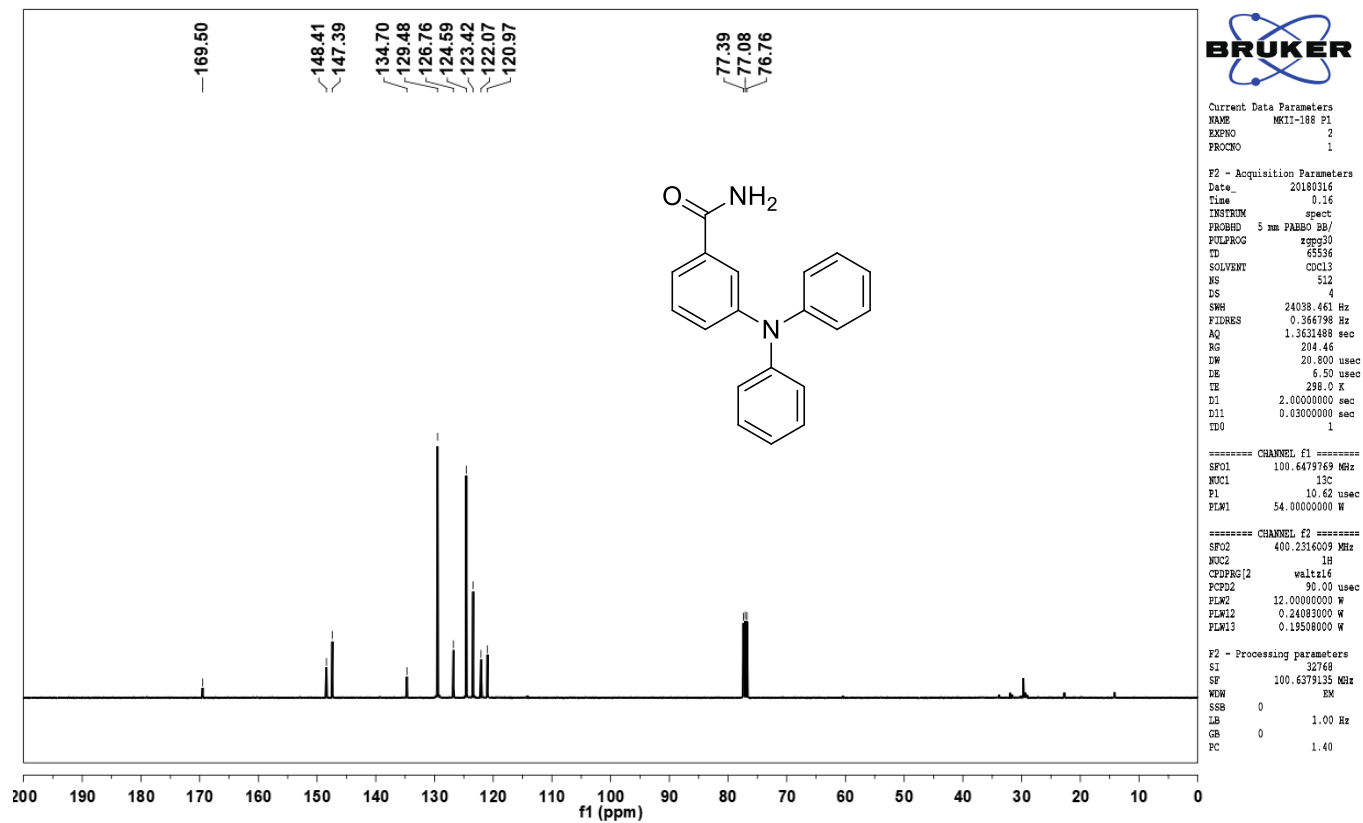
DEPT-135 NMR Spectrum of Compound 4a



HRMS Spectrum of Compound **4a**



**1H NMR Spectrum of Compound 4b**



**13C NMR Spectrum of Compound 4b**



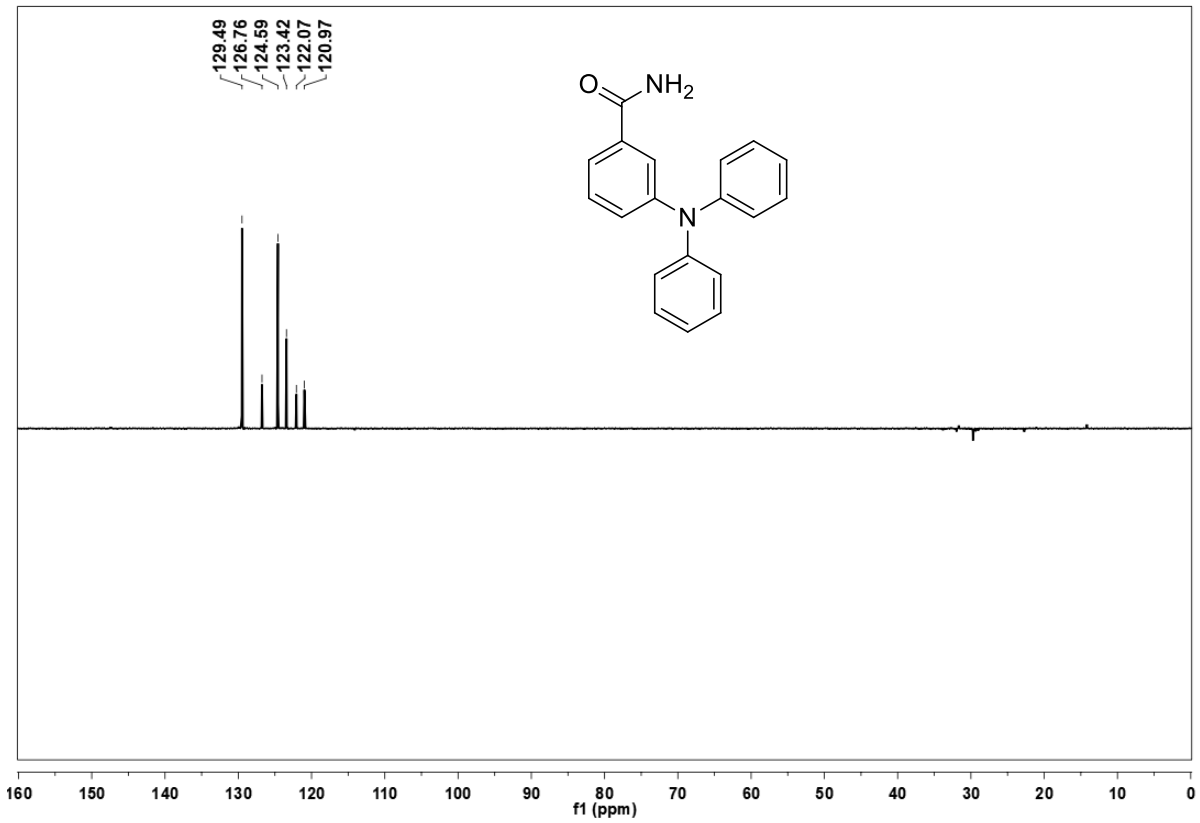
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NAME MK11-188 P1  
EXPO 3  
PROCNO 1

F2 - Acquisition Parameters  
Date 20180316  
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INSTRUM spect  
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PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 256  
DS 4  
SWH 16129.032 Hz  
FIDRES 0.246110 Hz  
AQ 2.0316160 sec  
RG 204.46  
DW 31.000 usec  
DE 6.50 usec  
TE 297.5 K  
CNS2 145.0000000  
D1 2.0000000 sec  
D2 0.00344828 sec  
D12 0.00002000 sec  
TD0 1

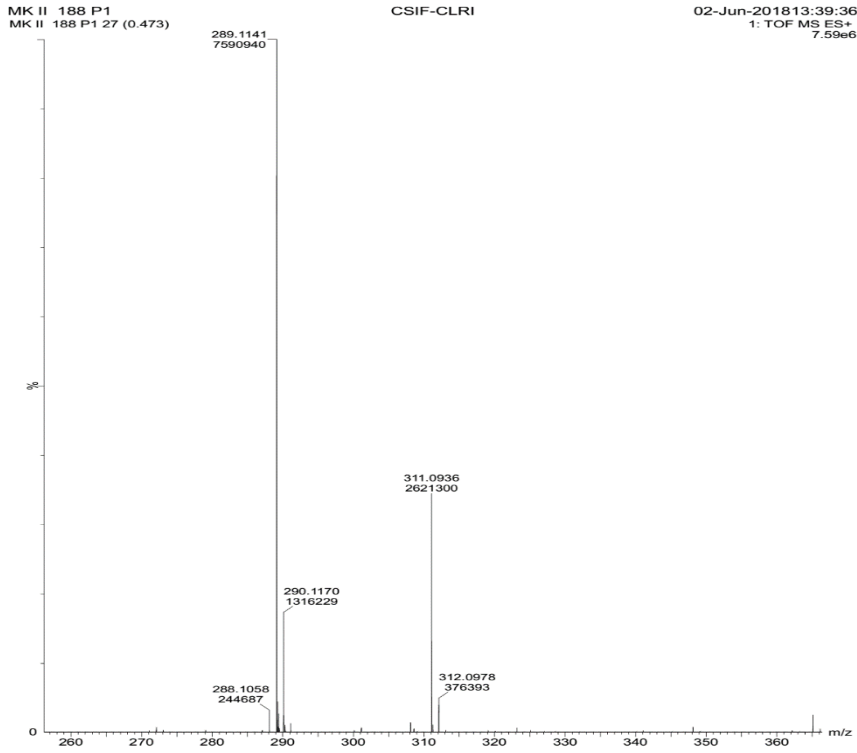
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P1 10.62 usec  
P13 2000.00 usec  
PLM0 0 W  
PLM1 54.00000000 W  
SPNAM[5] Crp60comp.4  
SFOA15 0.500  
SFOF55 0 Hz  
SEMS 9.30539989 W

===== CHANNEL f2 =====  
SF02 400.2312800 MHz  
NUC2 1H  
CPDPRG2 waltz16  
P3 12.75 usec  
P4 25.50 usec  
PCPD2 50.00 usec  
PLM2 12.00000000 W  
PLM12 0.24083000 W

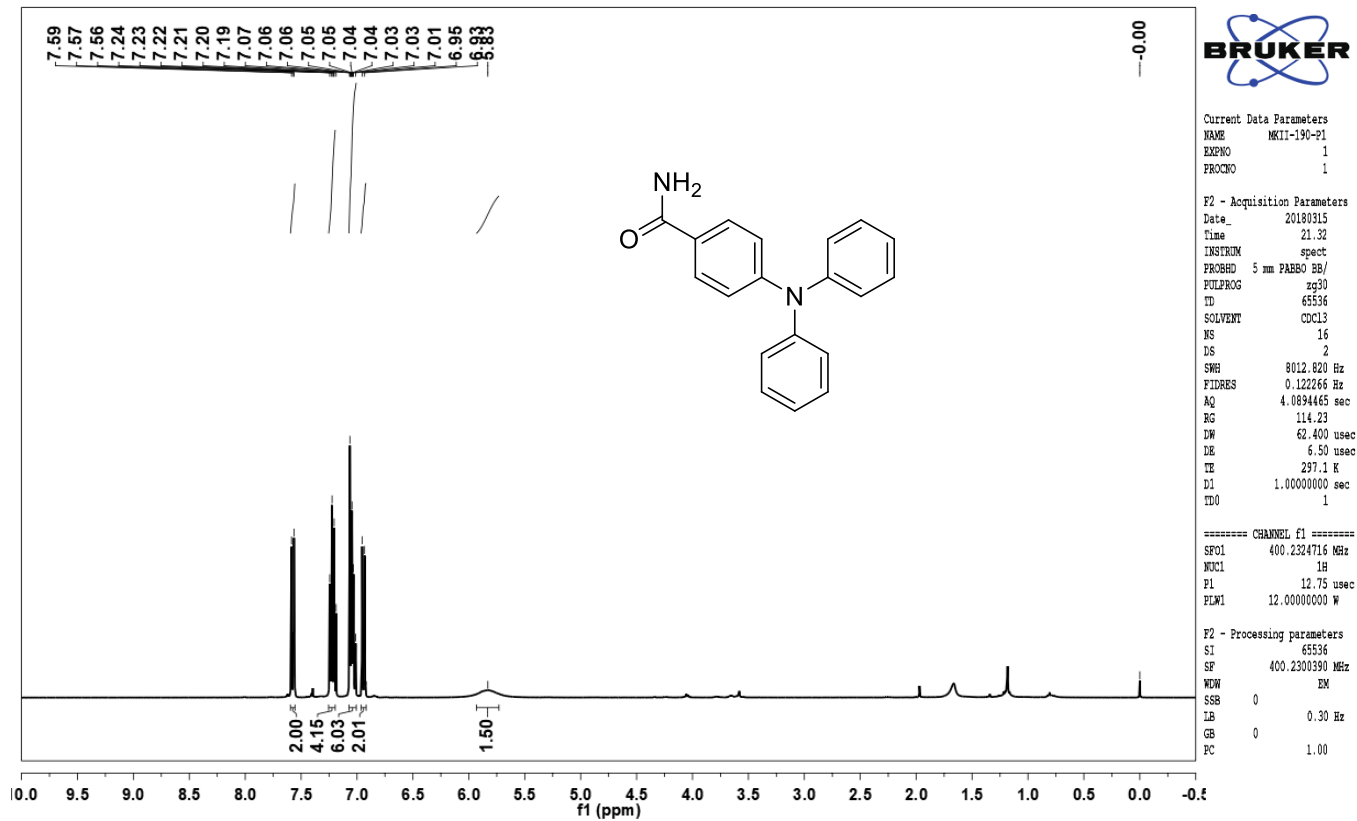
F2 - Processing parameters  
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SF 100.6379135 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
FC 1.40



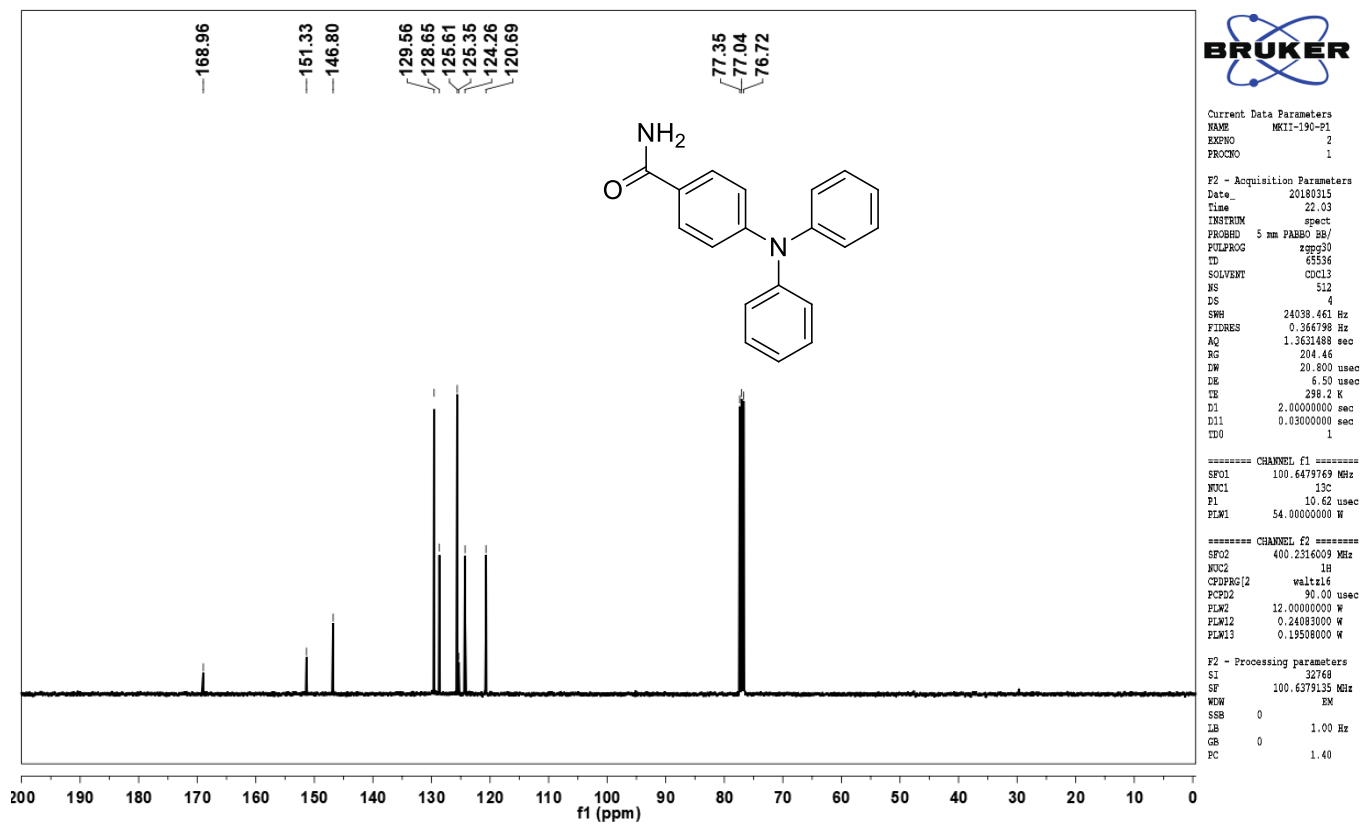
DEPT-135 NMR Spectrum of Compound 4b



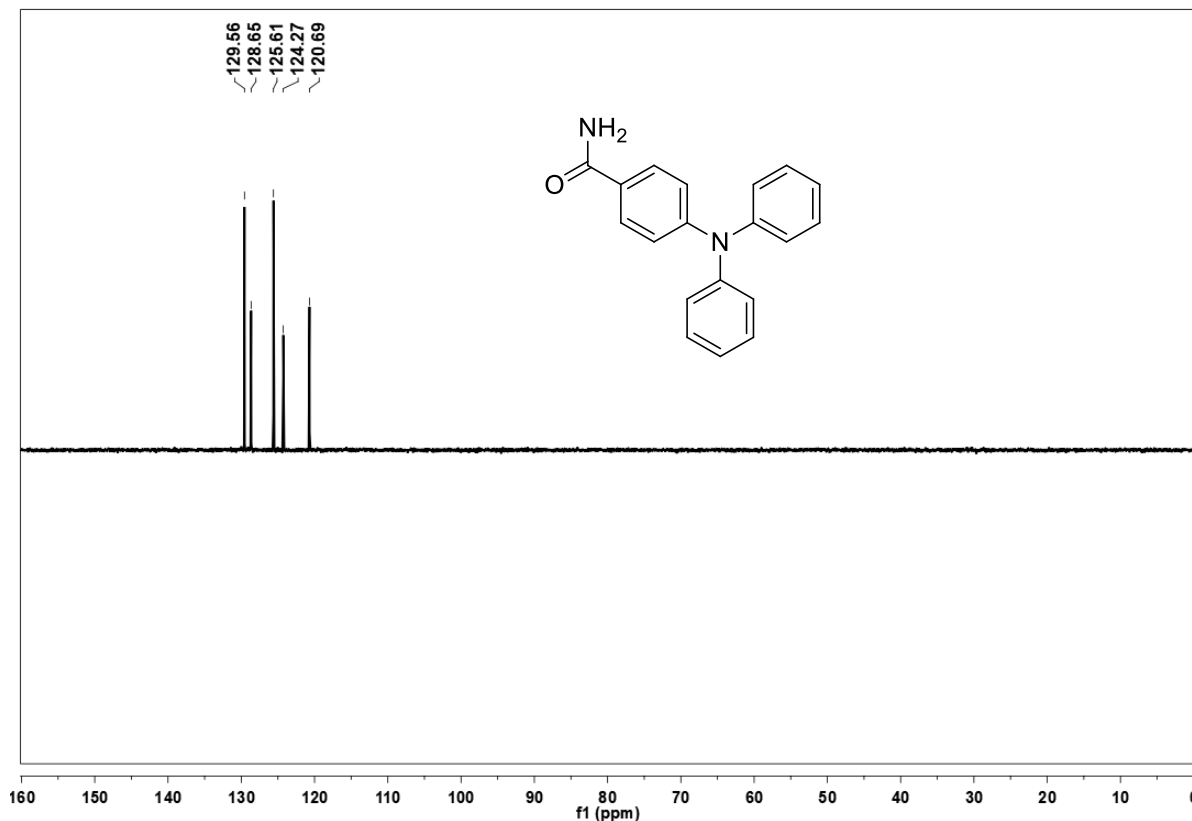
HRMS Spectrum of Compound 4b



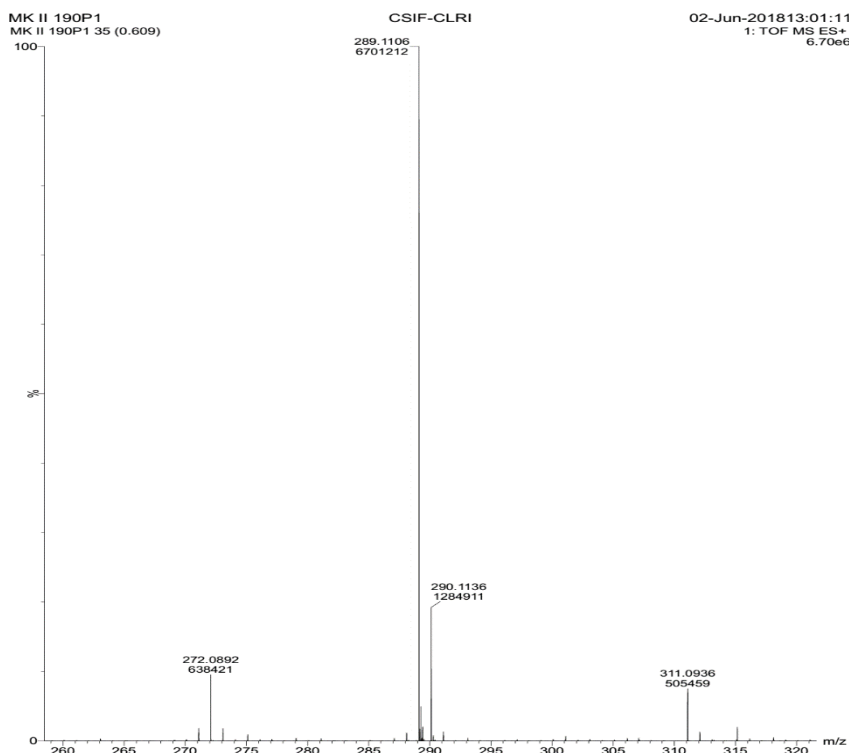
**<sup>1</sup>H NMR Spectrum of Compound 4c**



**<sup>13</sup>C NMR Spectrum of Compound 4c**

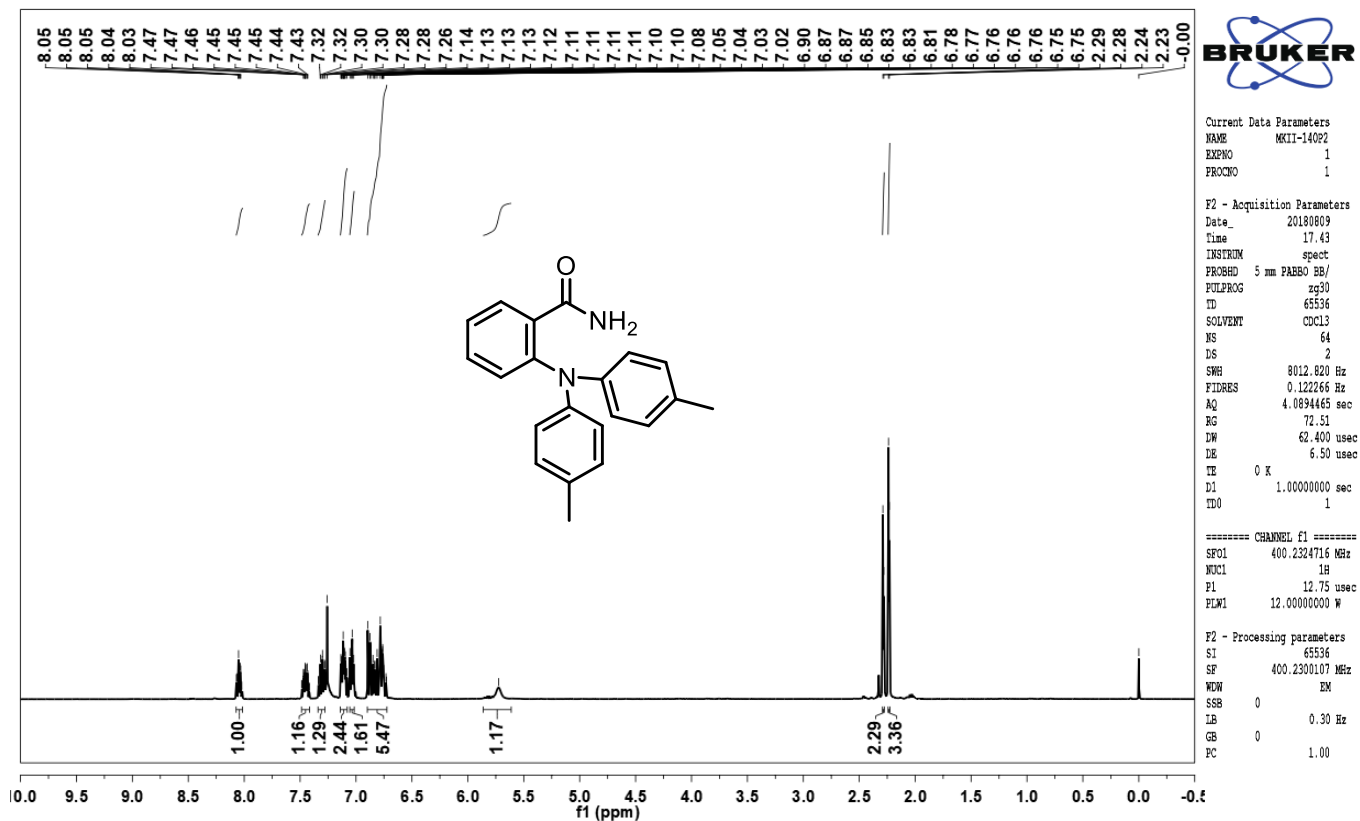


DEPT-135 NMR Spectrum of Compound **4c**

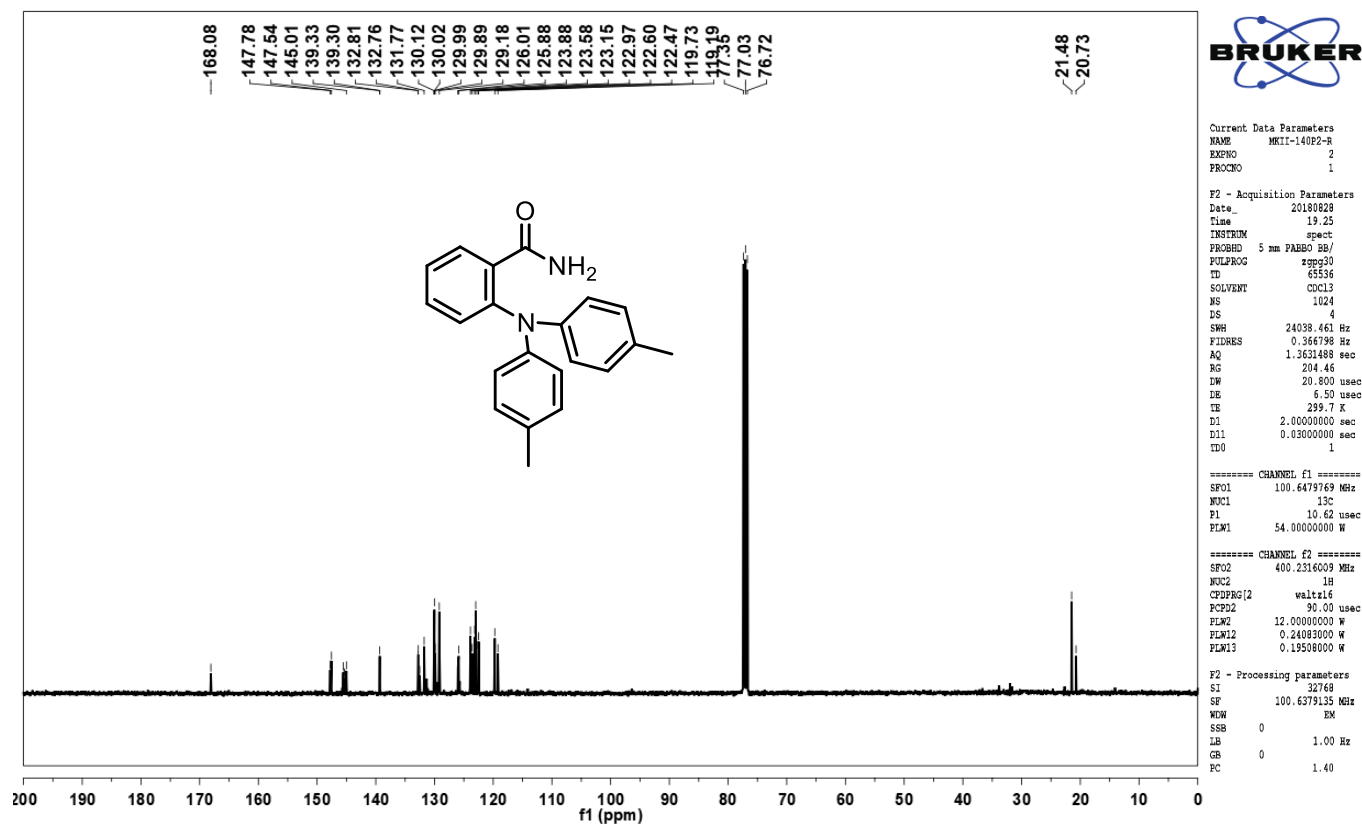


HRMS Spectrum of Compound **4c**

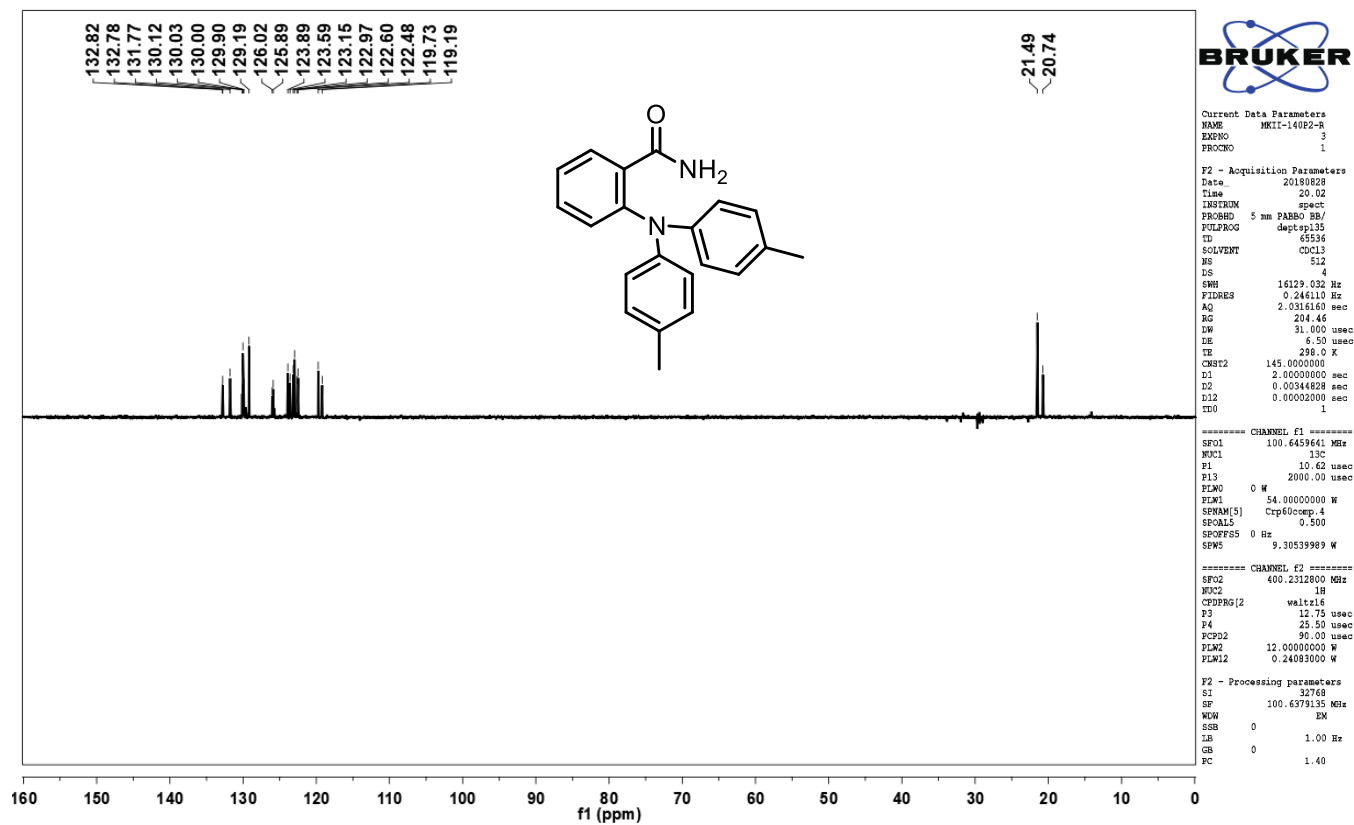




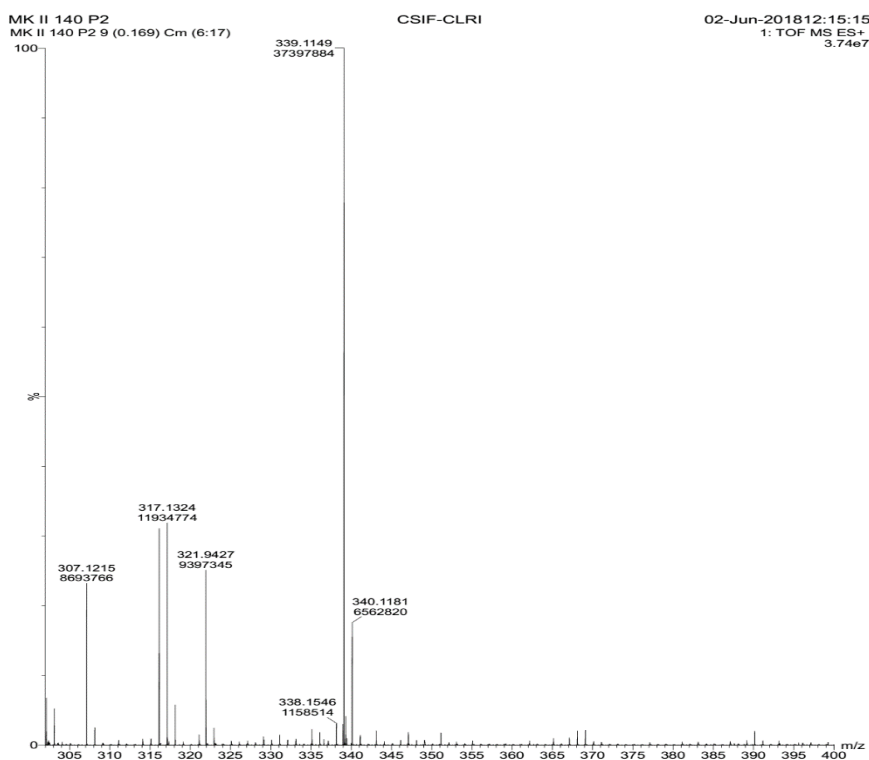
**<sup>1</sup>H NMR Spectrum of Compound 4d**



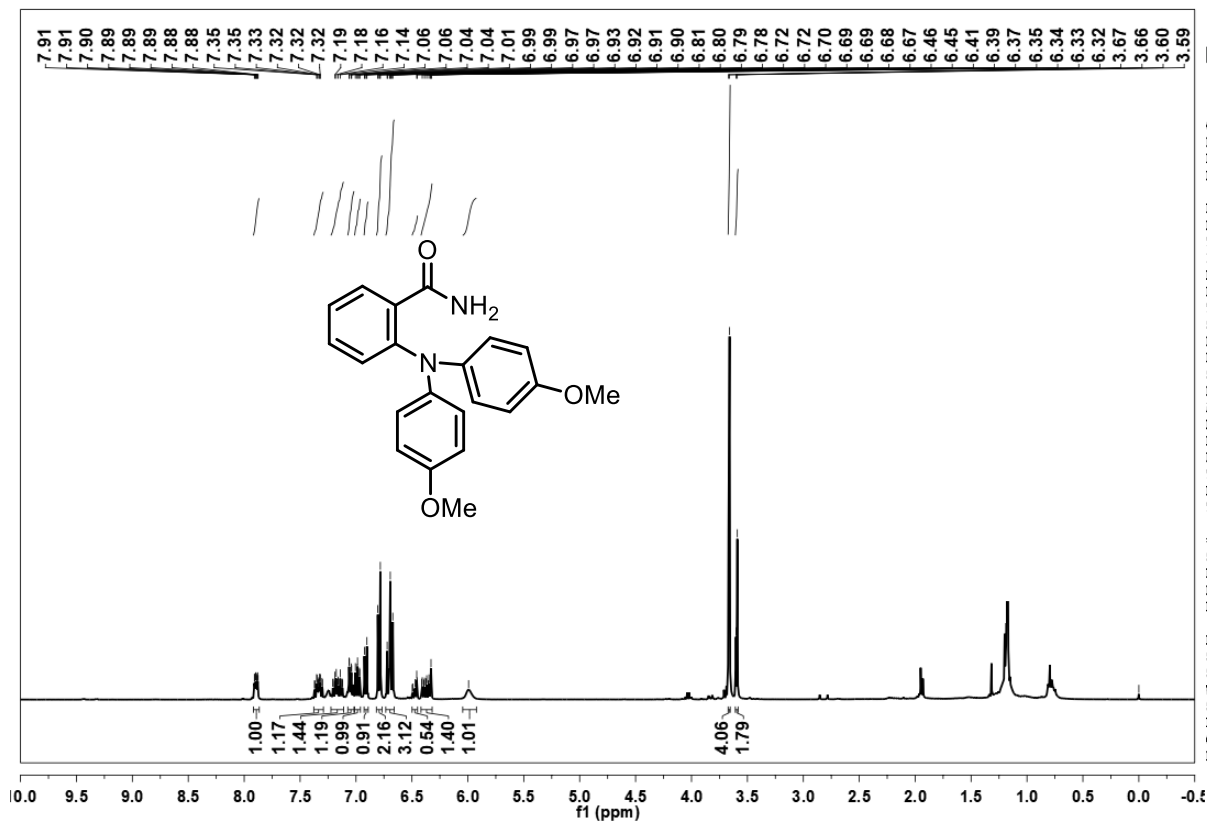
**<sup>13</sup>C NMR Spectrum of Compound 4d**



DEPT-135 NMR Spectrum of Compound 4d



HRMS Spectrum of Compound 4d



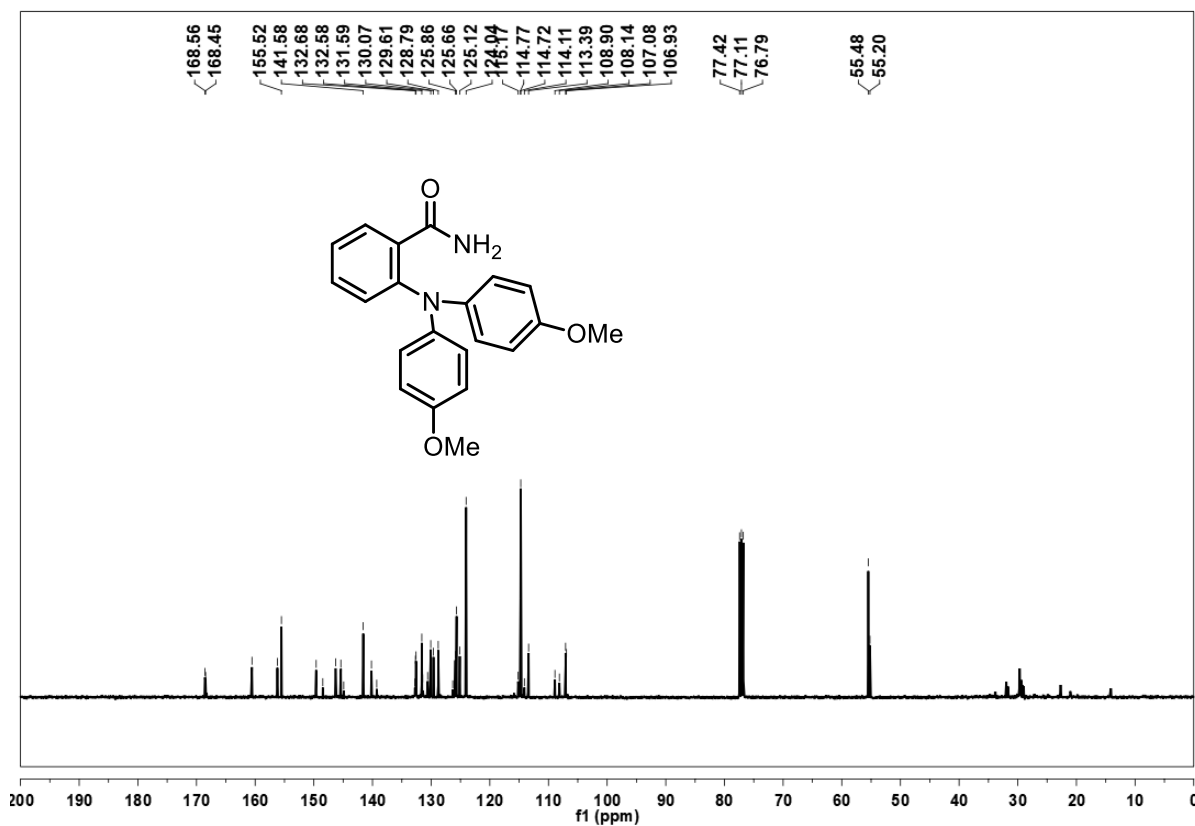
Current Data Parameters  
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 EXNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20180124  
 Time 17.36  
 INSTRUM spect  
 PROBD 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 31.36  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 296.7 K  
 D1 1.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 400.2324716 MHz  
 NUCL1 1H  
 P1 12.75 usec  
 PLW1 12.0000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2300428 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

**1H NMR Spectrum of Compound 4e**



Current Data Parameters  
 NAME MK11-152-p2  
 EXNO 2  
 PROCNO 1

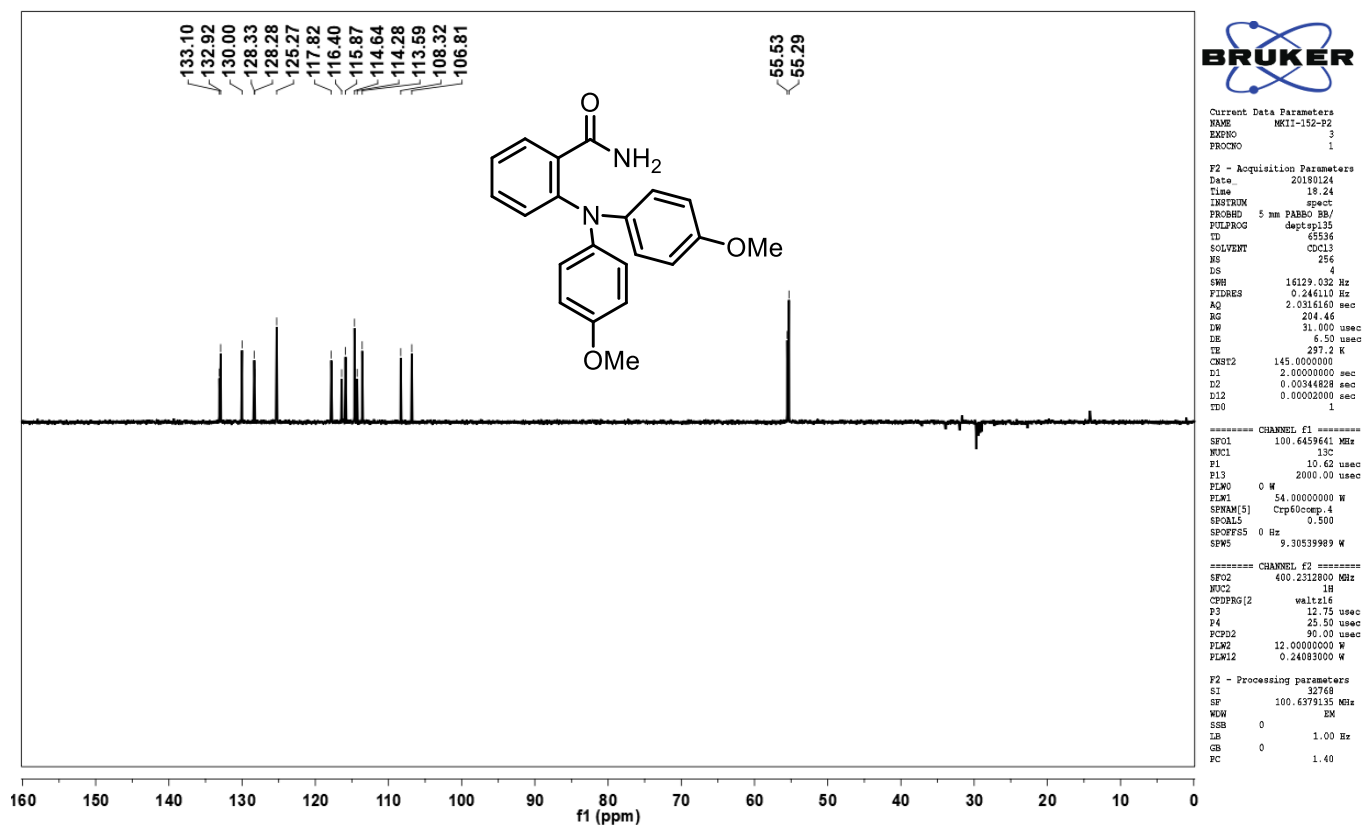
F2 - Acquisition Parameters  
 Date\_ 20180124  
 Time 18.06  
 INSTRUM spect  
 PROBD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 512  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 204.46  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.7 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6273769 MHz  
 NUCL1 13C  
 P1 10.62 usec  
 PLW1 54.0000000 W

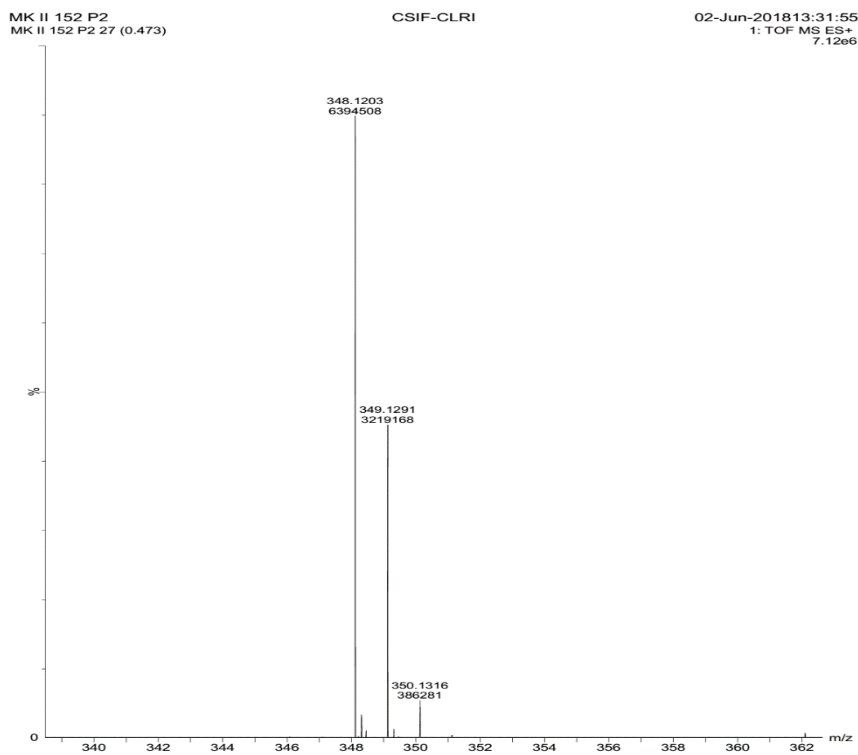
===== CHANNEL f2 =====  
 SFO2 400.2316009 MHz  
 NUCL2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.0000000 W  
 PLW12 0.24083000 W  
 PLW13 0.19508000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6379135 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

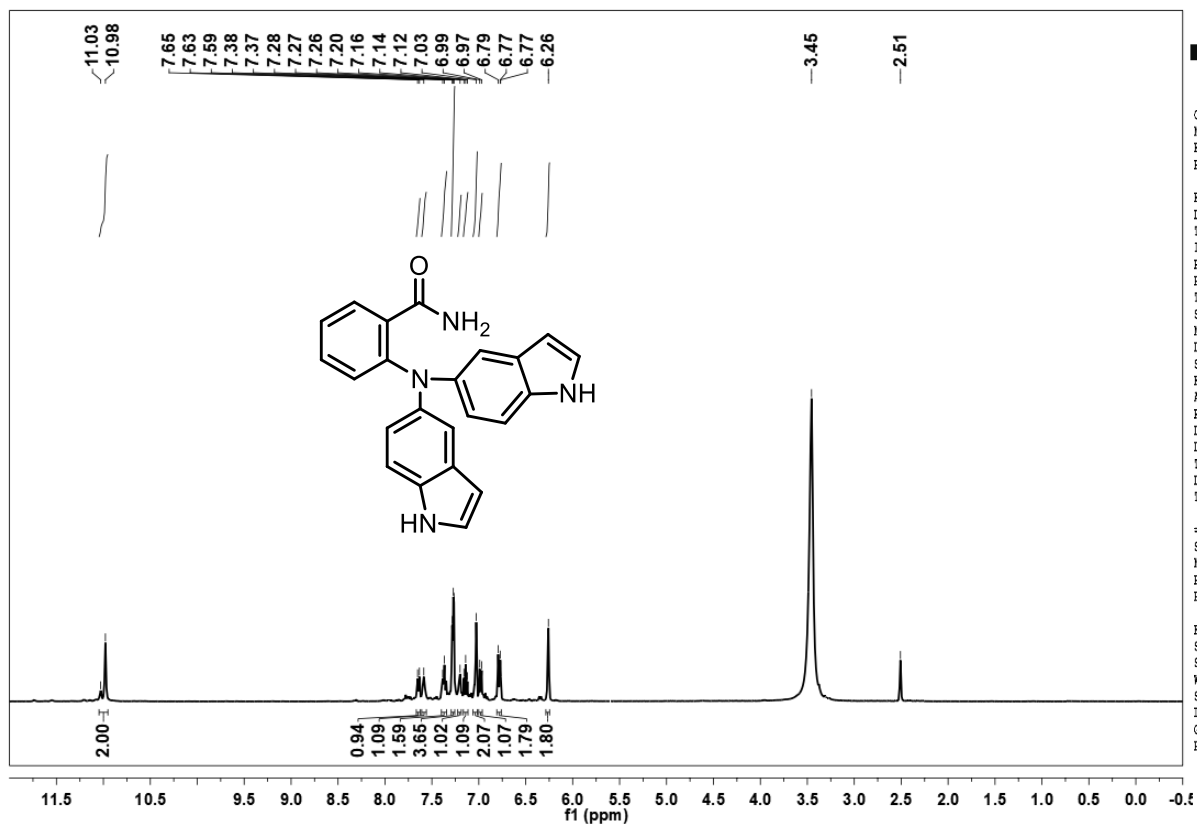
**13C NMR Spectrum of Compound 4e**



DEPT-135 NMR Spectrum of Compound 4e



HRMS Spectrum of Compound 4e



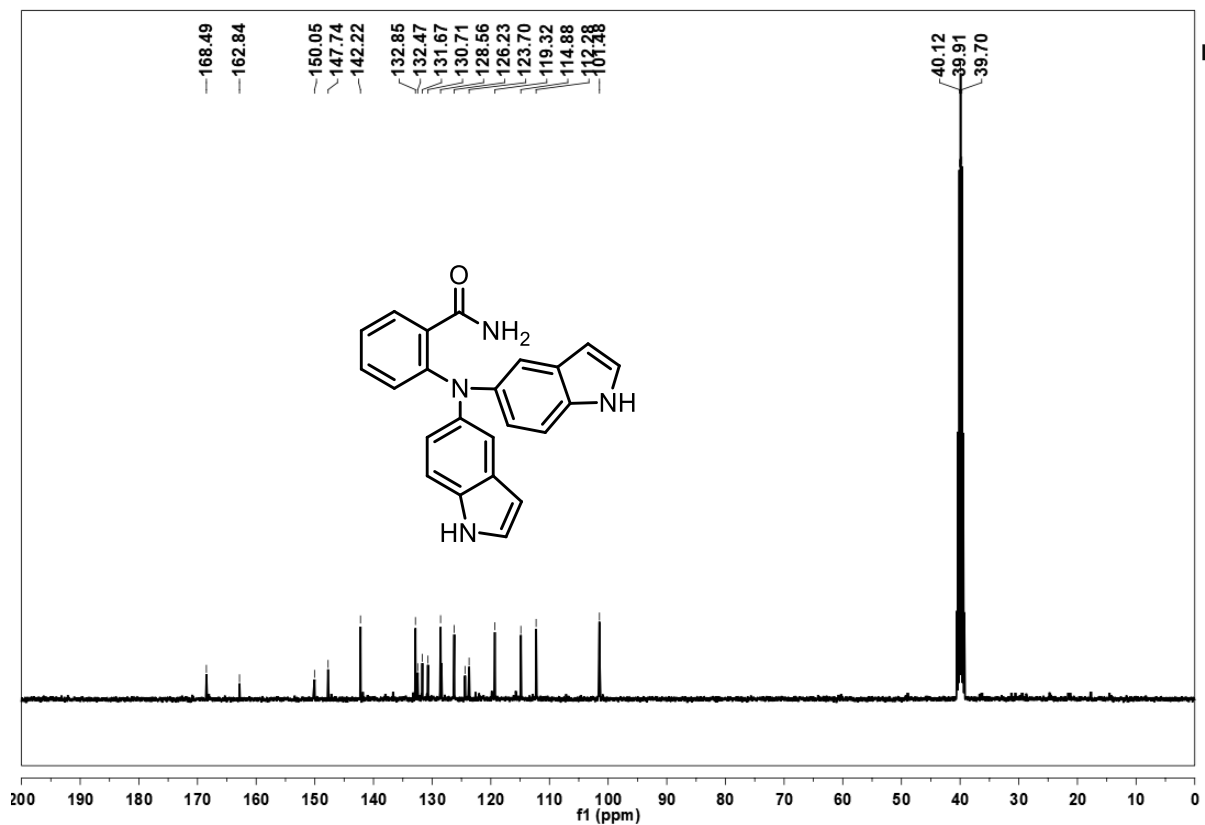
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 NAME MKII-150-P2  
 EXEWO 1  
 PROCNO 1

F2 - Acquisition Parameters  
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 Time 19.19  
 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 31.36  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 295.8 K  
 D1 1.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 400.2324716 MHz  
 NUC1 1H  
 P1 12.75 usec  
 PLW1 12.0000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2300000 MHz  
 MW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

<sup>1</sup>H NMR Spectrum of Compound 4f



Current Data Parameters  
 NAME MKII-150-P2  
 EXEWO 2  
 PROCNO 1

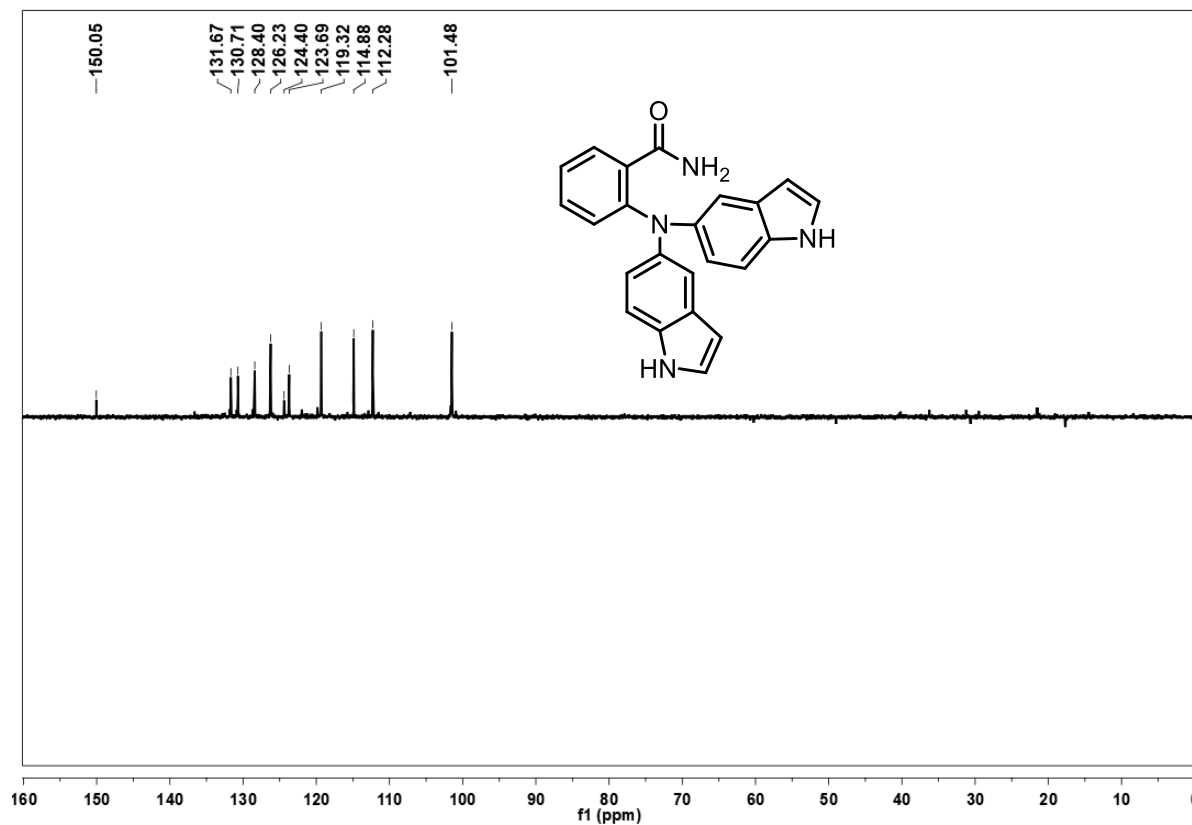
F2 - Acquisition Parameters  
 Date\_ 20180101  
 Time 19.50  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT DMSO  
 NS 512  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 204.46  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 296.8 K  
 D1 2.0000000 sec  
 D11 0.0300000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6479769 MHz  
 NUC1 13C  
 P1 10.62 usec  
 PLW1 54.0000000 W

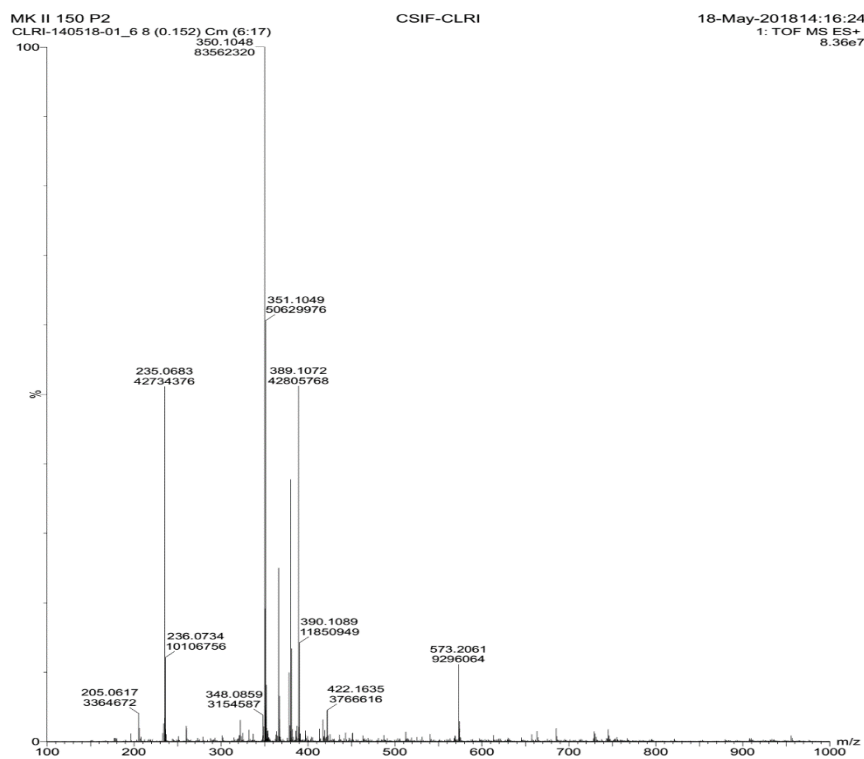
===== CHANNEL f2 =====  
 SFO2 400.2316009 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.0000000 W  
 PLW12 0.24083000 W  
 PLW13 0.19508000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6379135 MHz  
 MW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

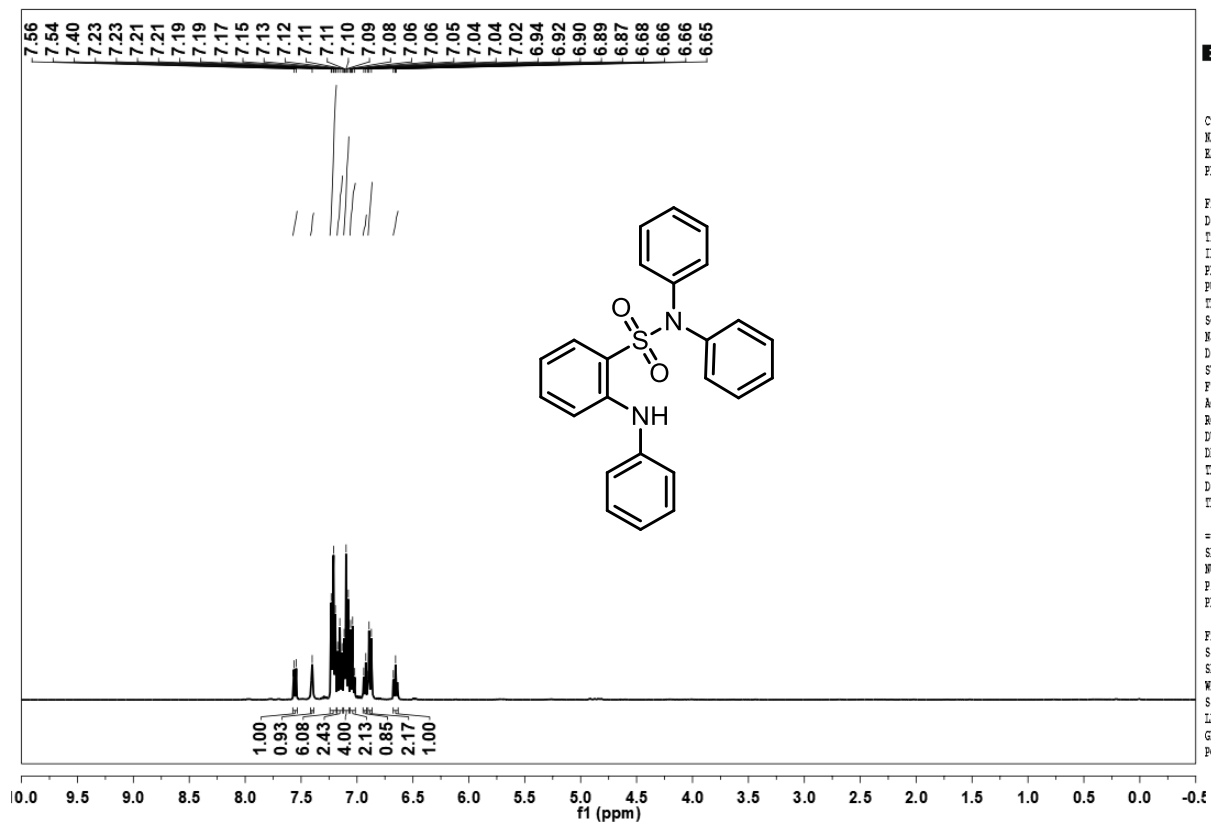
<sup>13</sup>C NMR Spectrum of Compound 4f



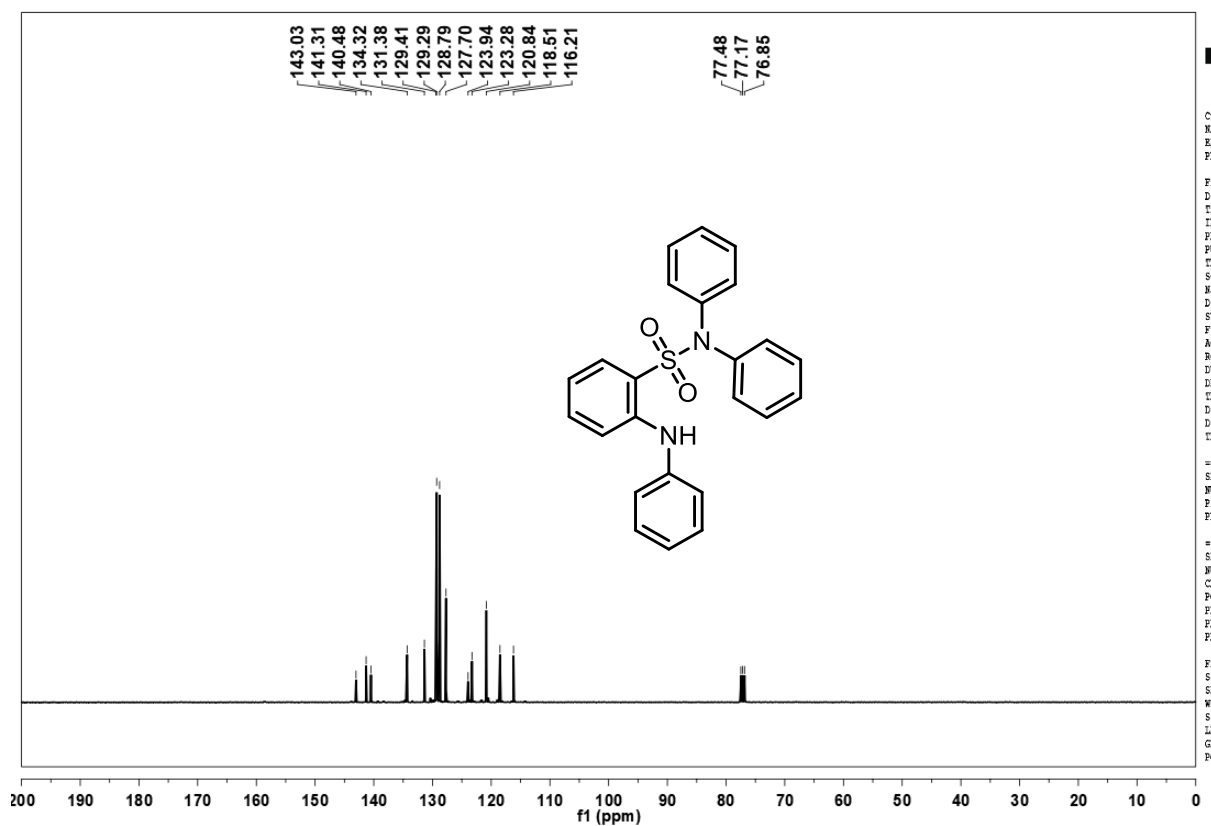
DEPT-135 NMR Spectrum of Compound 4f



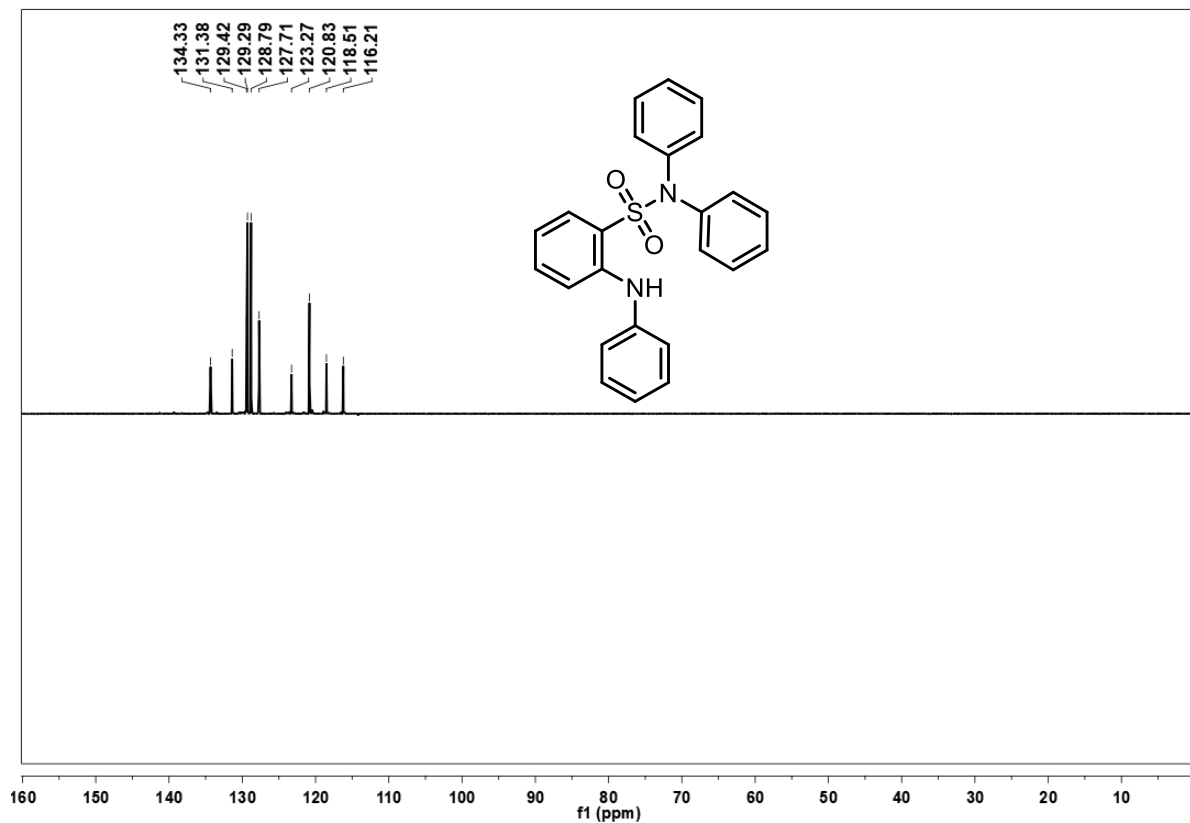
HRMS Spectrum of Compound 4f



**<sup>1</sup>H NMR Spectrum of Compound 4g**



**<sup>13</sup>C NMR Spectrum of Compound 4g**

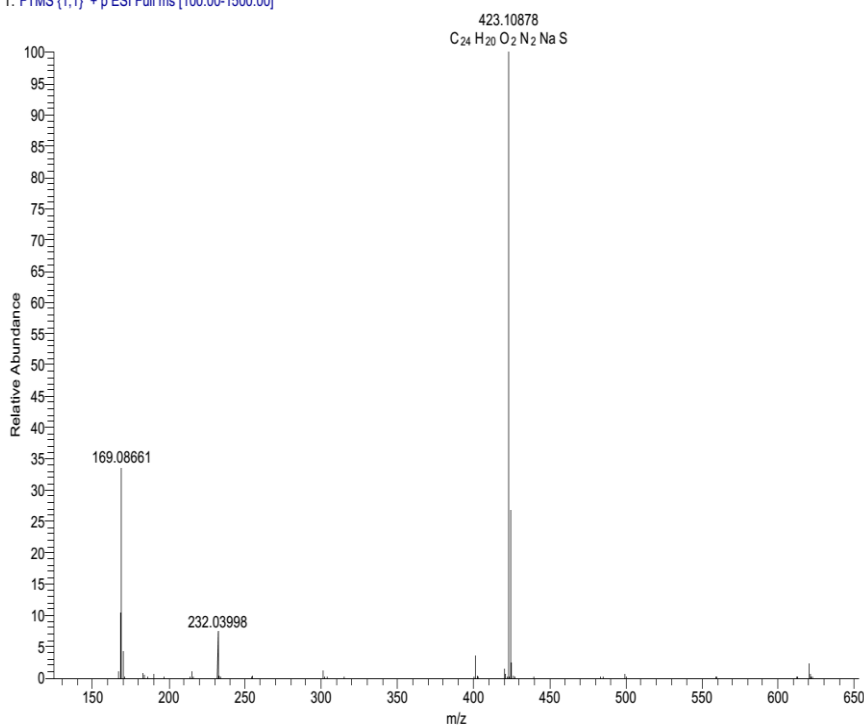


DEPT-135 NMR Spectrum of Compound **4g**

W:\Data\2018\April-2018\MKII-174p1

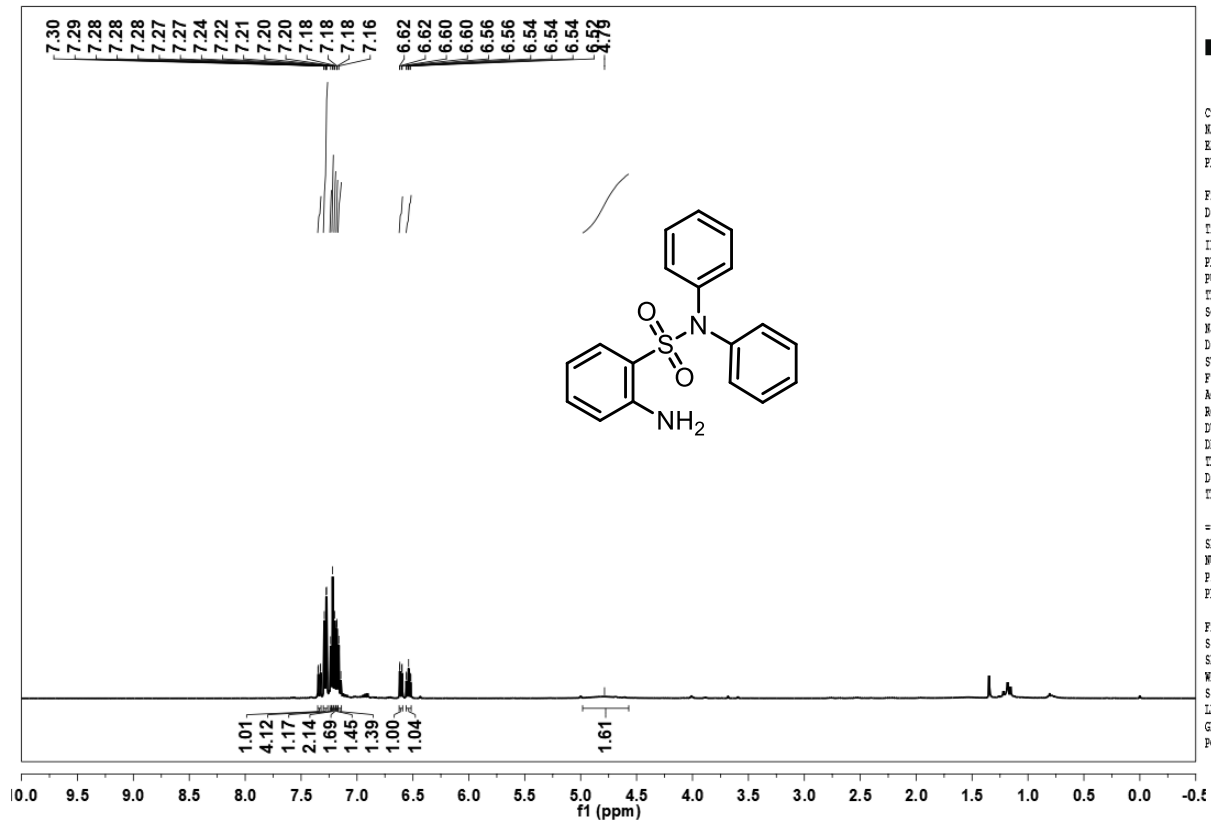
04-05-2018 12:49:47

MKII-174p1 #90-102 RT: 1.54-1.70 AV: 13 NL: 5.28E7  
T: FTMS (1,1) + p ESI Full ms [100.00-1500.00]



HRMS Spectrum of Compound **4g**





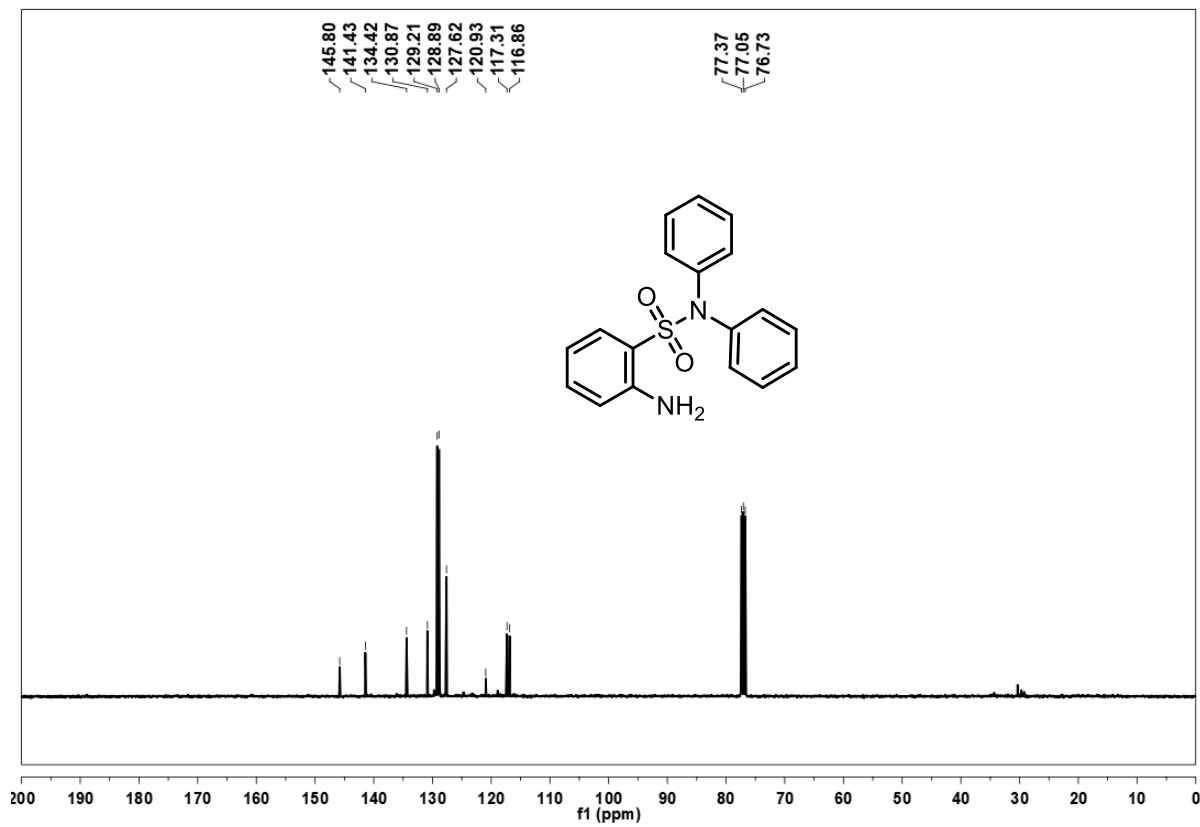
Current Data Parameters  
 NAME MKII-174P3  
 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
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 Time 18.17  
 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 79.6  
 EW 62.400 usec  
 DE 6.50 usec  
 TE 296.2 K  
 D1 1.0000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 400.2324716 MHz  
 NUCL1 1H  
 P1 12.75 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2300422 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

**1H NMR Spectrum of Compound 4h**



Current Data Parameters  
 NAME MKII-174P3  
 EXPNO 2  
 PROCNO 1

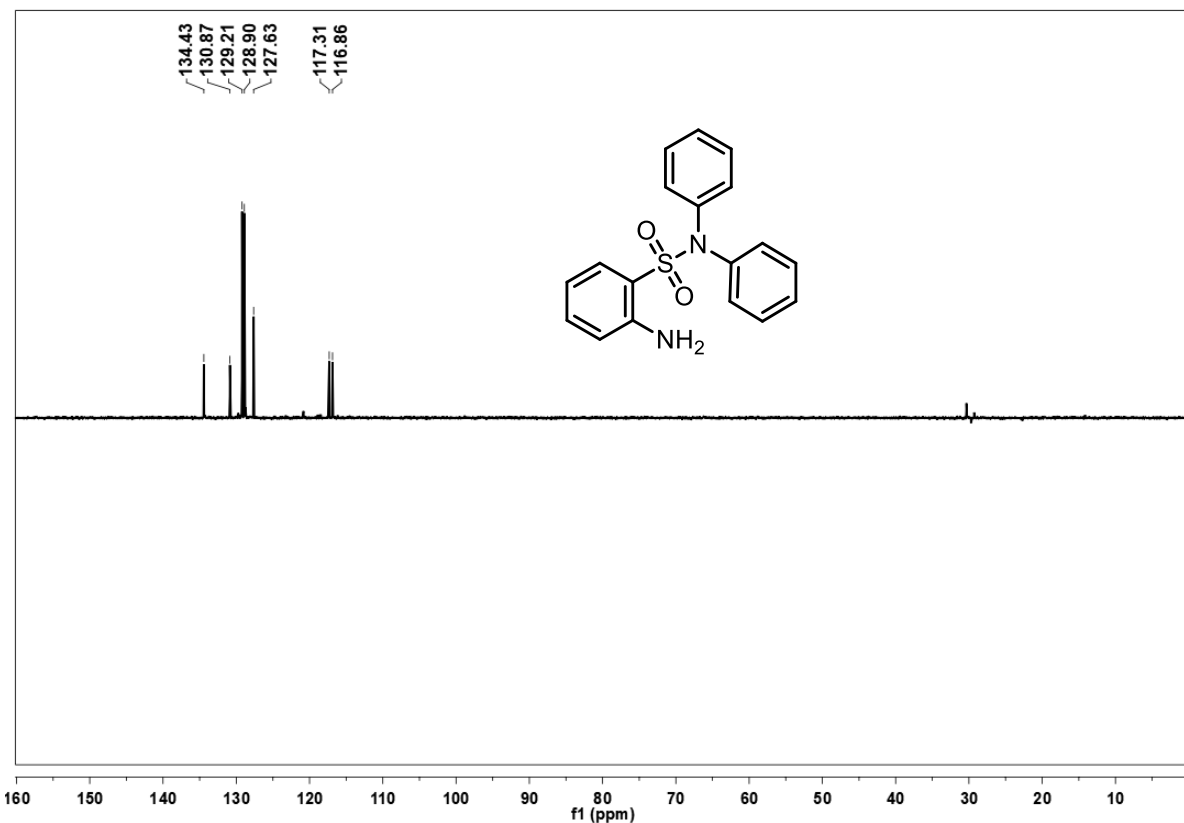
F2 - Acquisition Parameters  
 Date\_ 20180301  
 Time 18.48  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 512  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.364798 Hz  
 AQ 1.3631488 sec  
 RG 204.46  
 EW 20.800 usec  
 DE 6.50 usec  
 TE 297.4 K  
 D1 2.0000000 sec  
 D11 0.03000000 sec  
 TDO 1

===== CHANNEL f1 =====  
 SFO1 100.6479769 MHz  
 NUCL1 13C  
 P1 10.62 usec  
 PLW1 54.00000000 W

===== CHANNEL f2 =====  
 SFO2 400.2316009 MHz  
 NUCL2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.24083000 W  
 PLW13 0.19598000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6379135 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

**13C NMR Spectrum of Compound 4h**

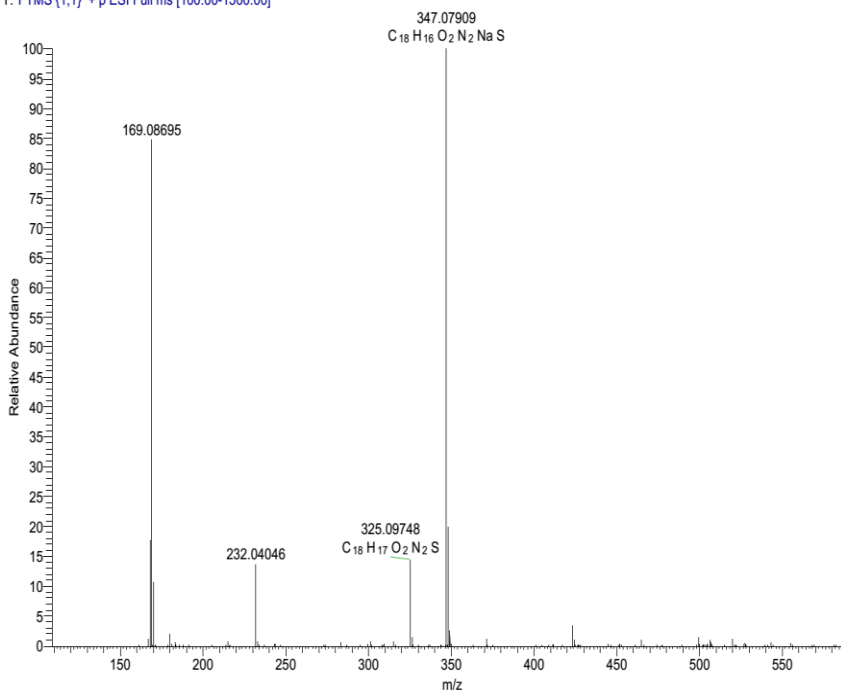


DEPT-135 NMR Spectrum of Compound **4h**

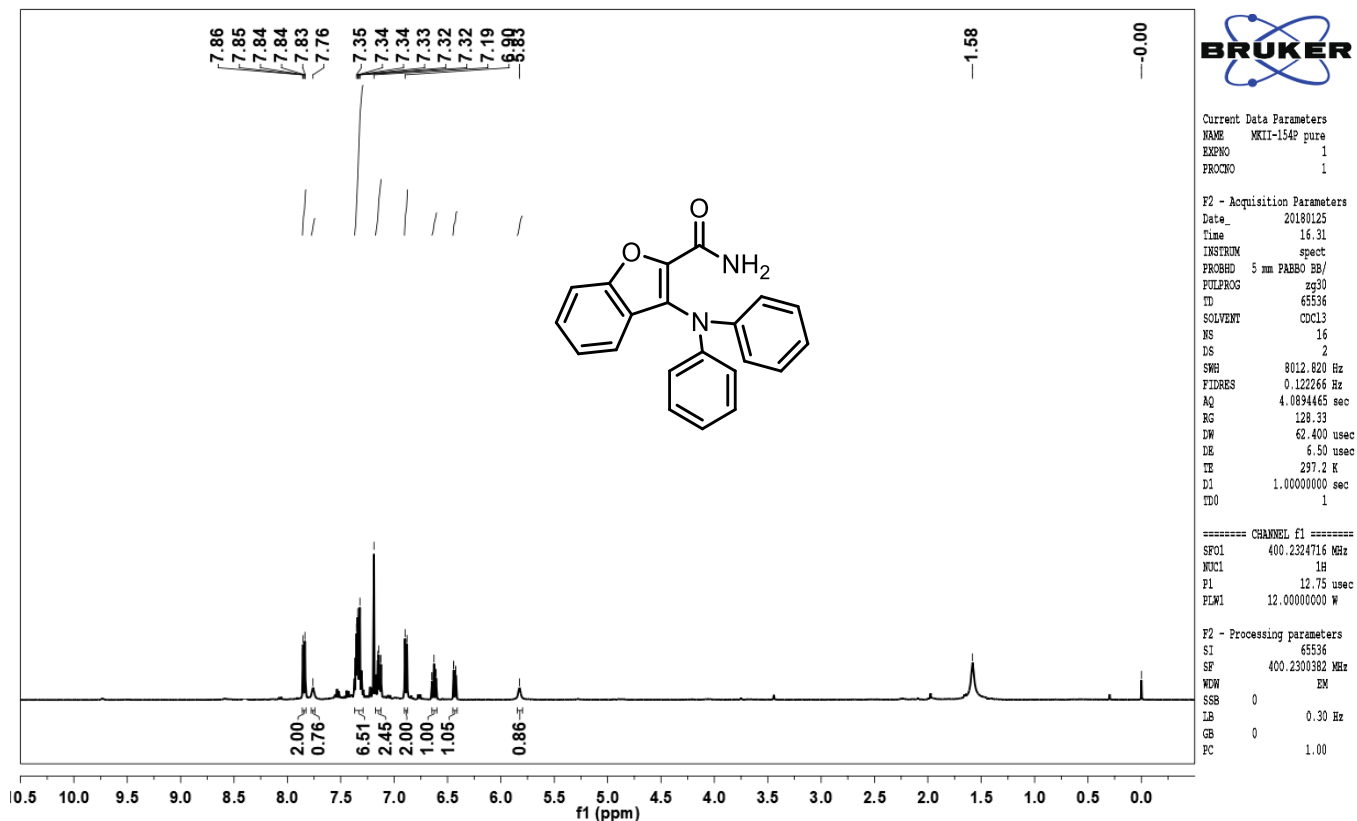
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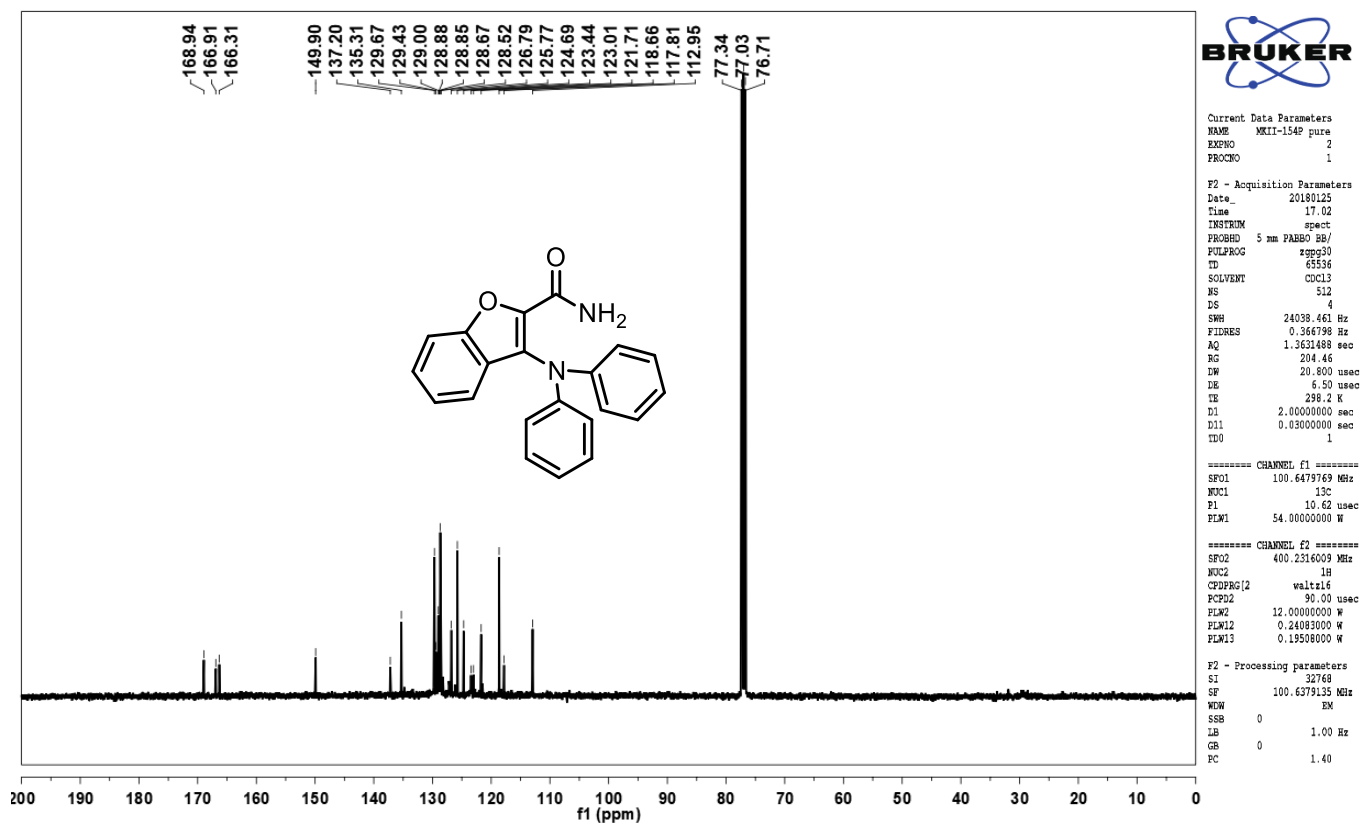
MKII-174-P3 #80-97 RT: 1.33-1.57 AV: 18 NL: 3.01E7  
T: FTMS (1,1) + p ESI Full ms [100.00-1500.00]



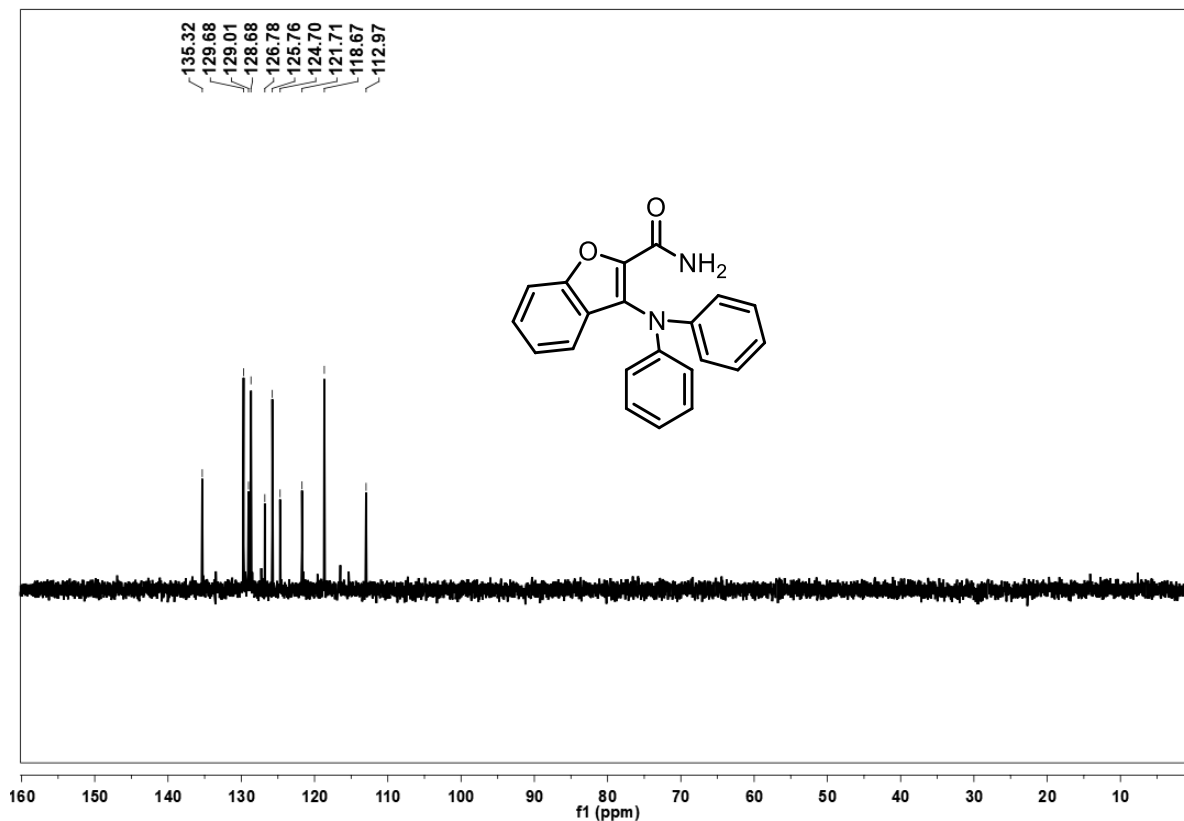
HRMS Spectrum of Compound **4h**



**<sup>1</sup>H NMR Spectrum of Compound 4i**



**<sup>13</sup>C NMR Spectrum of Compound 4i**



Current Data Parameters  
NAME MKII-154 pure  
EXPRO 3  
PROCNO 1

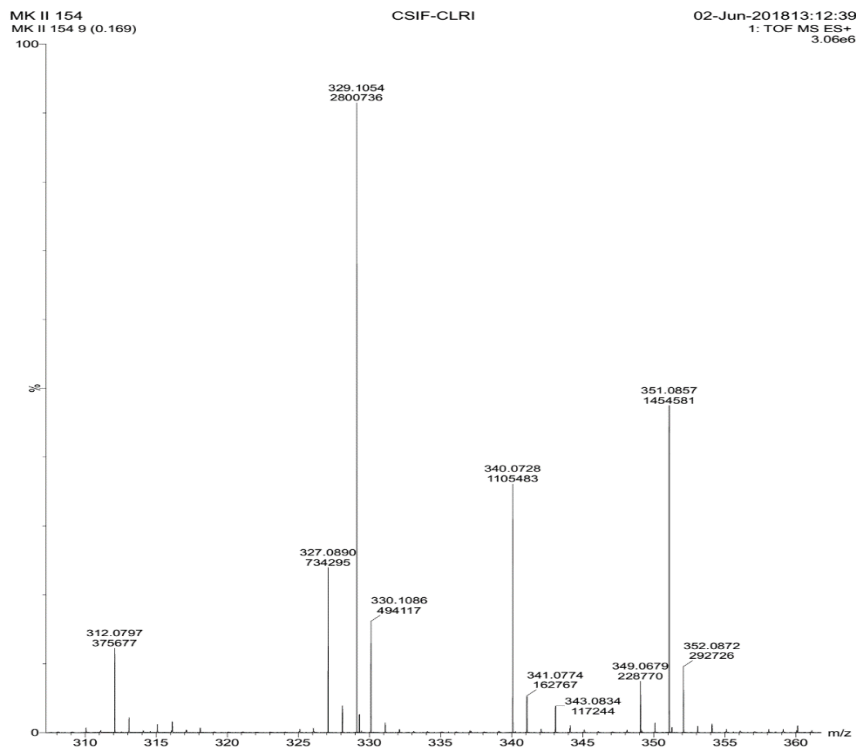
F2 - Acquisition Parameters  
Date\_ 20180125  
Time 17.20  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG deptpi135  
TD 45536  
SOLVENT CDCL3  
NS 256  
DS 4  
SWH 16129.032 Hz  
FIDRES 0.246110 Hz  
AQ 2.0316160 sec  
RG 204.46  
DW 31.000 usec  
DE 6.50 usec  
TE 297.6 K  
CNS2 145.000000  
D1 2.00000000 sec  
D2 0.00344828 sec  
D12 0.00002000 sec  
TD0 1

===== CHANNEL f1 =====  
SF01 100.6459641 Mhz  
NUC1 13C  
F1 10.62 usec  
P13 2000.00 usec  
PLW0 0 W  
FLW1 54.00000000 W  
SFOFF5 Cmp4  
SFOAL5 0.500  
SFOFFSS 0 Hz  
SFOVS 9.30539989 W

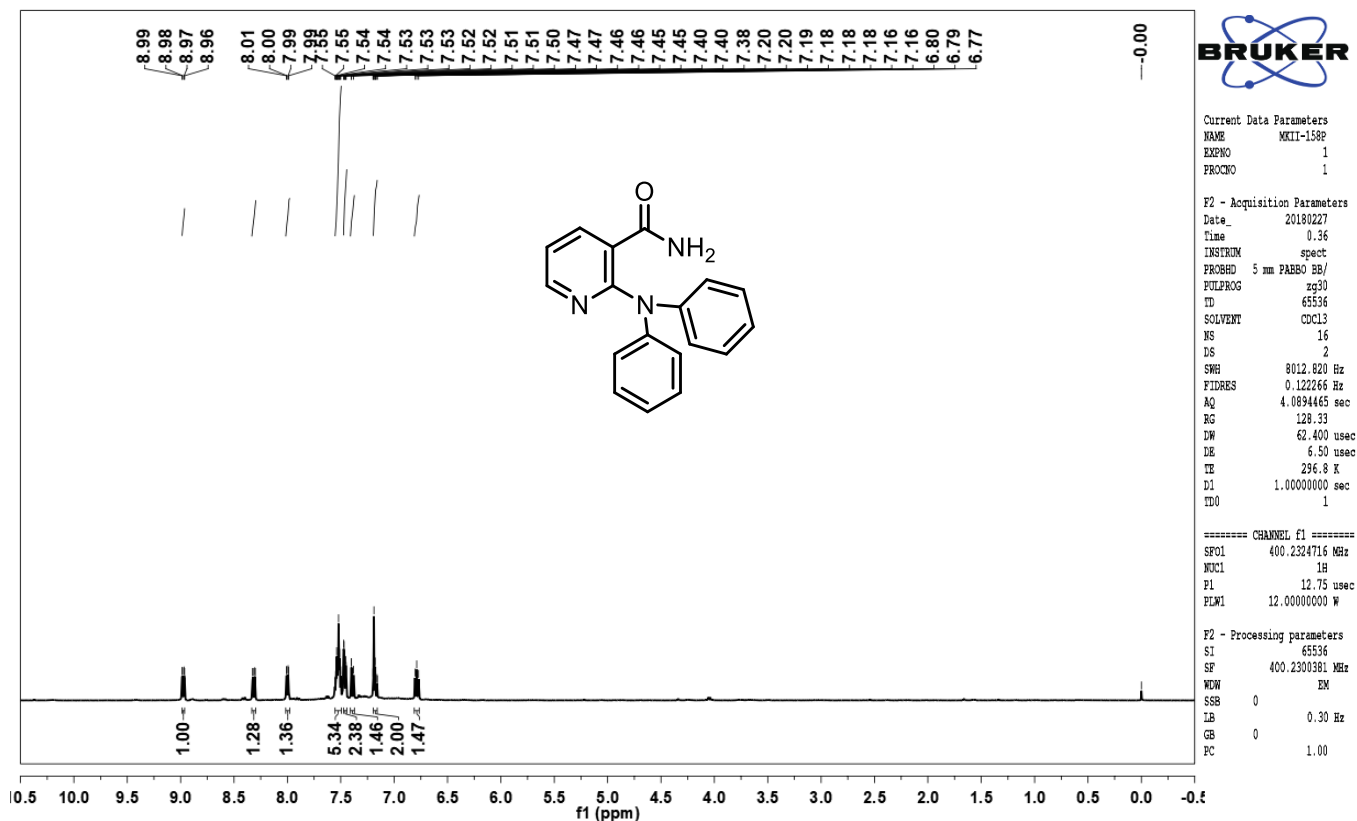
===== CHANNEL f2 =====  
SF02 400.2312800 Mhz  
NUC2 1H  
CPDPRG2 waltz16  
P3 12.75 usec  
P4 25.50 usec  
PCPD2 90.00 usec  
PLW2 12.00000000 W  
FLW2 0.24083000 W

F2 - Processing parameters  
SI 32768  
SF 100.6379135 Mhz  
WUN EM  
SSB 0  
LB 1.00 Hz  
GB 0  
FC 1.40

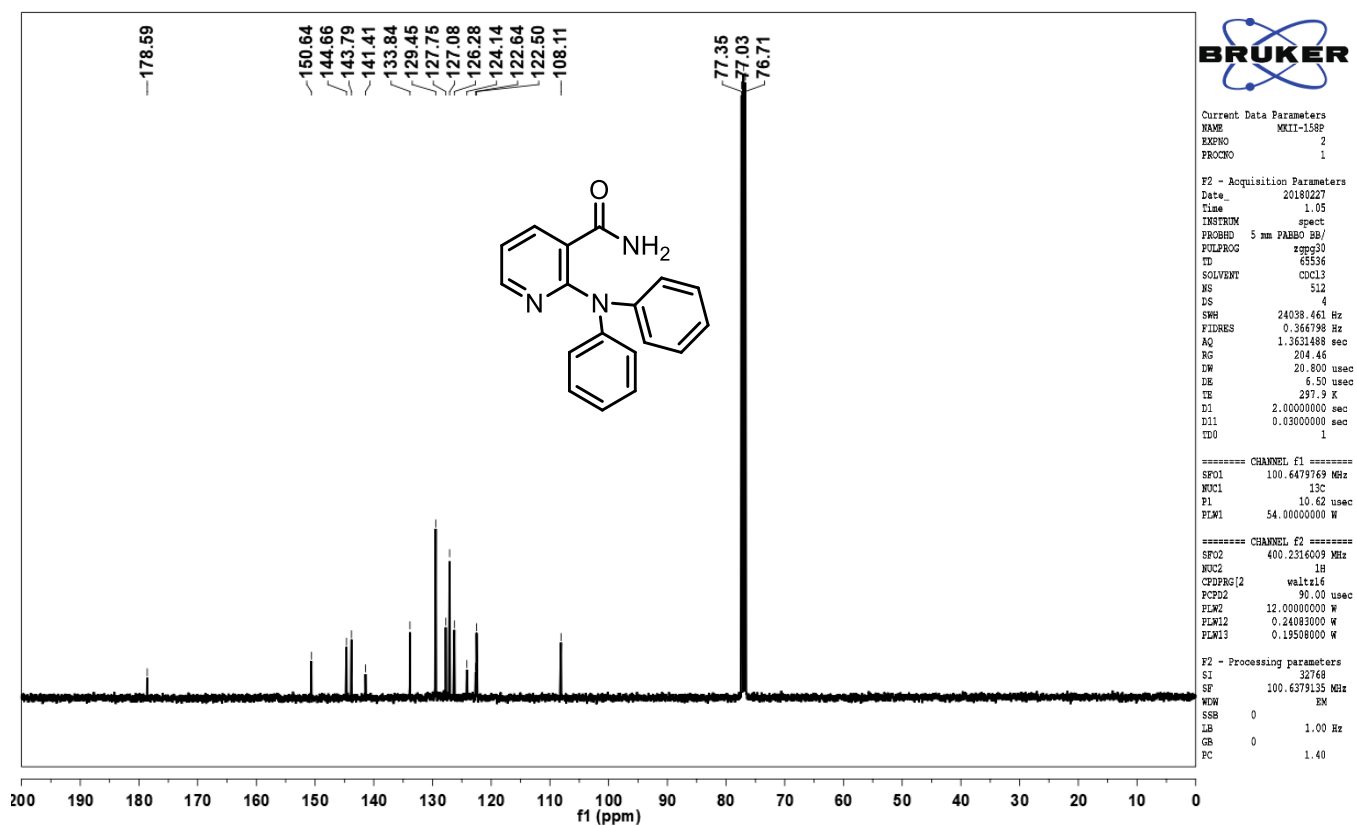
DEPT-135 NMR Spectrum of Compound 4i



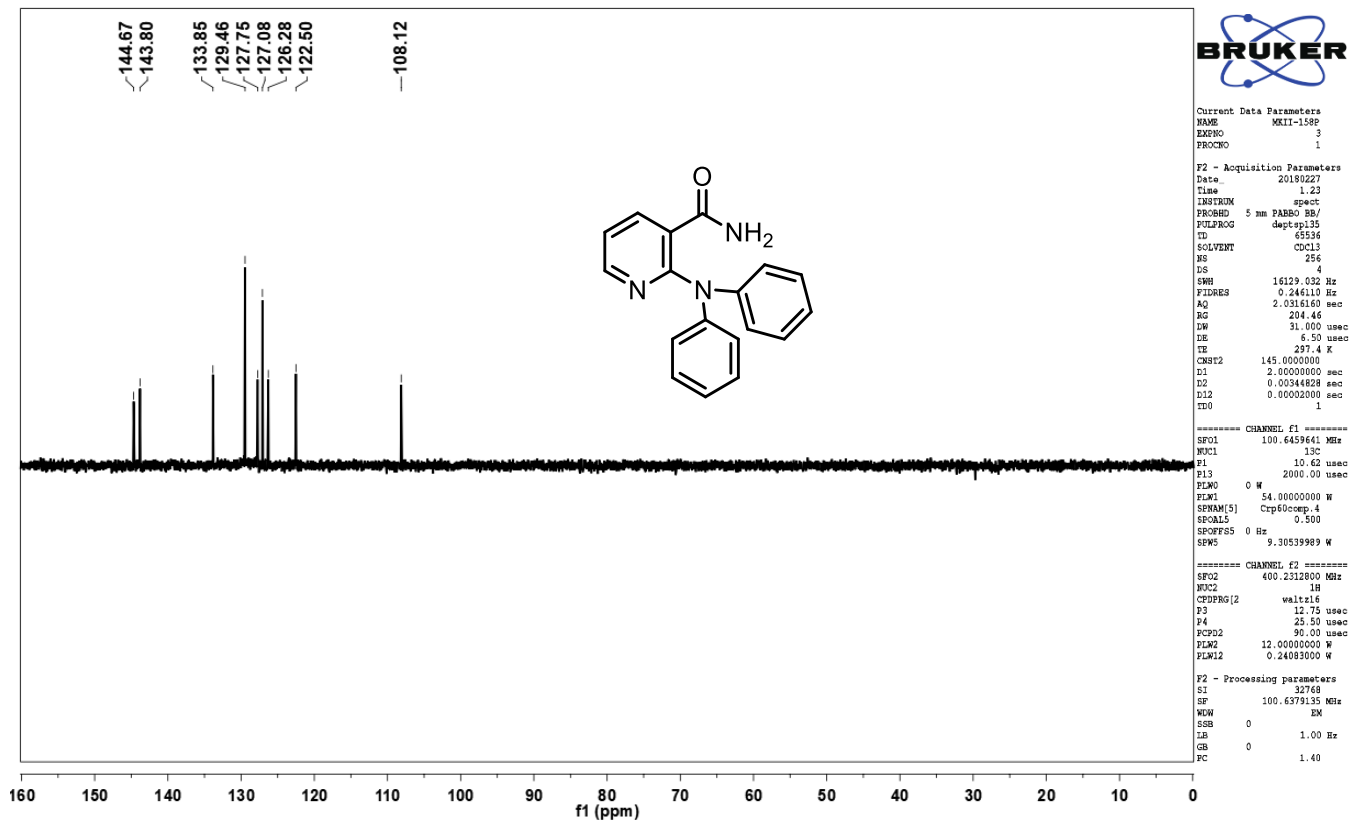
HRMS Spectrum of Compound 4i



**<sup>1</sup>H NMR Spectrum of Compound 4j**



**<sup>13</sup>C NMR Spectrum of Compound 4j**

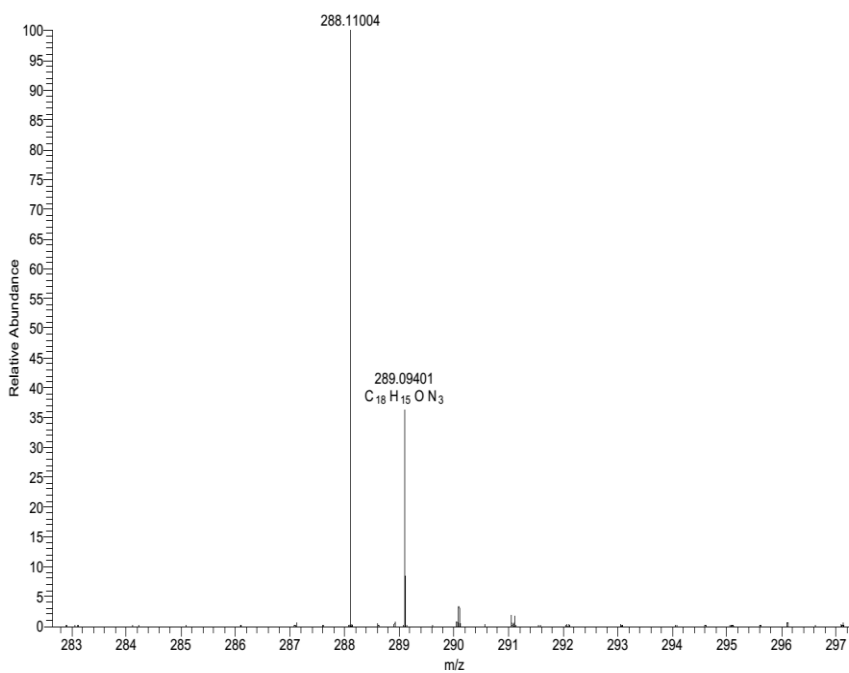


DEPT-135 NMR Spectrum of Compound **4j**

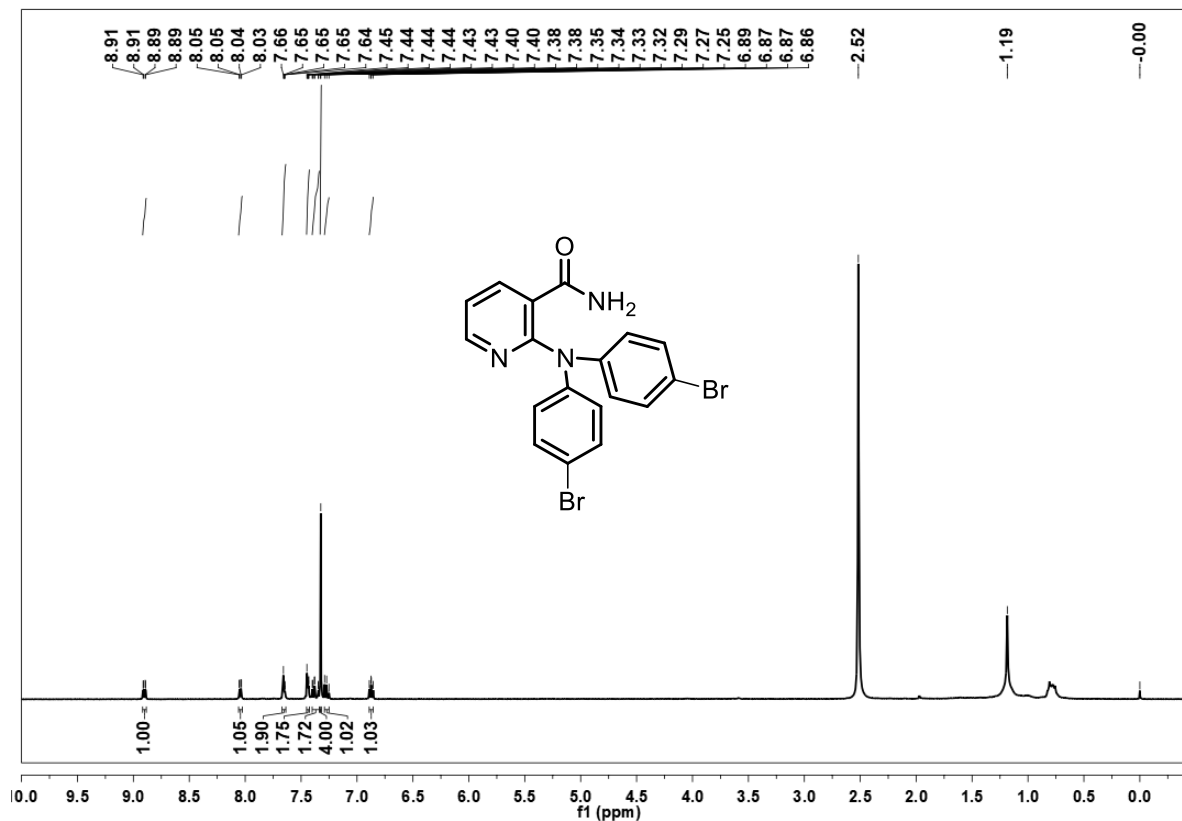
W:\Data\2018\April-2018\MKII-158

04-05-2018 13:01:03

MKII-158 #60-73 RT: 1.04-1.23 AV: 14 NL: 4.20E5  
 T: FTMS (1,1) + p ESI Full lock ms [100.00-1500.00]



HRMS Spectrum of Compound **4j**



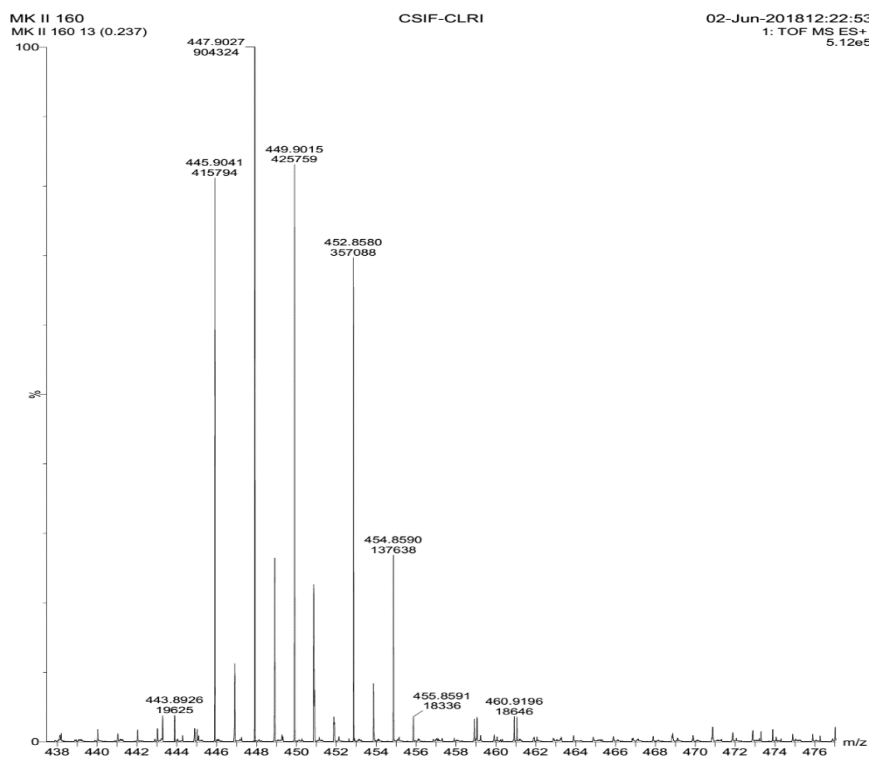
Current Data Parameters  
NAME MK-II-160  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20180220  
Time 0.14  
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 182.6  
LW 62.400 usec  
DE 6.50 usec  
TE 0 K  
D1 1.0000000 sec  
TD0 1

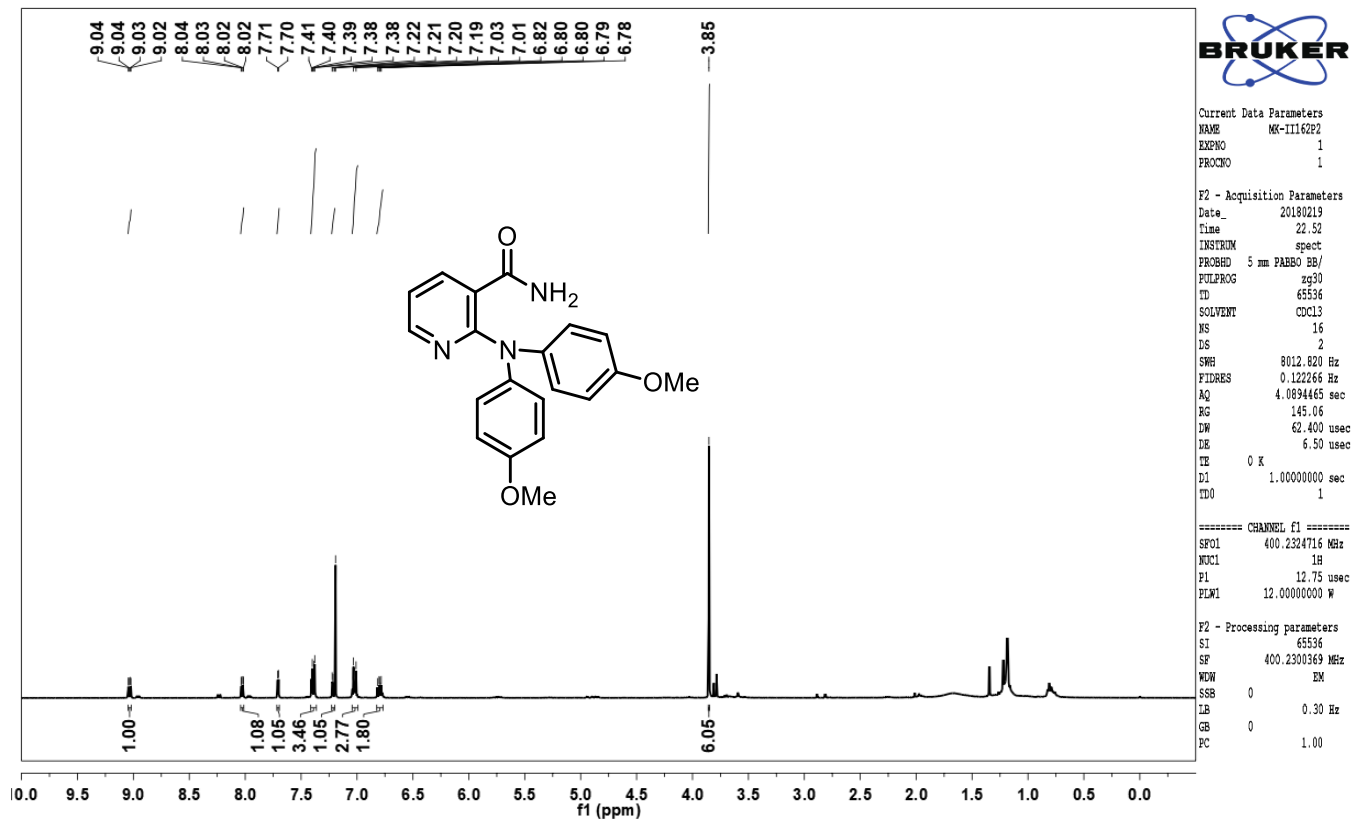
==== CHANNEL f1 =====  
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NUC1 1H  
P1 12.75 usec  
PLW1 12.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.2298839 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

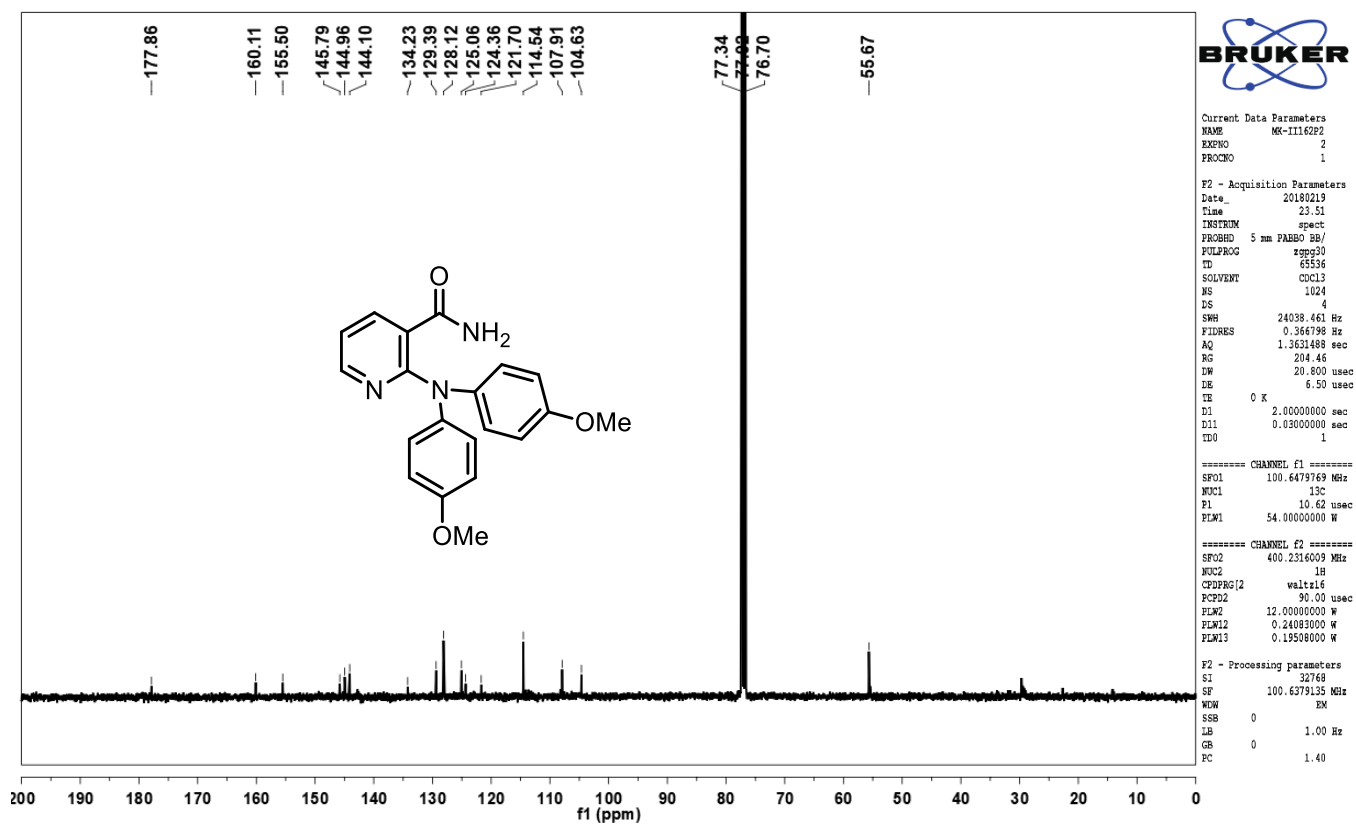
<sup>1</sup>H NMR Spectrum of Compound 4k



HRMS Spectrum of Compound 4k

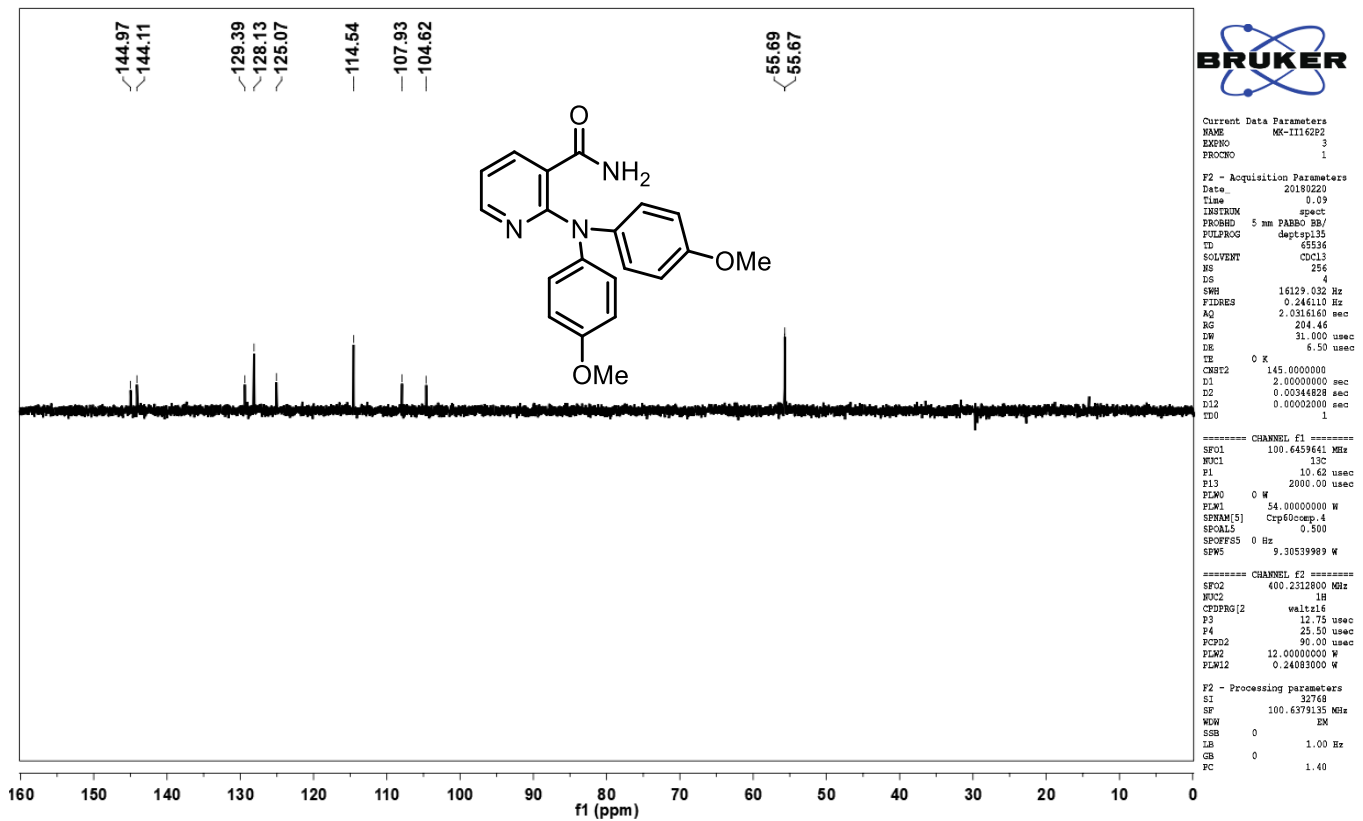


**<sup>1</sup>H NMR Spectrum of Compound 4I**



**<sup>13</sup>C NMR Spectrum of Compound 4I**



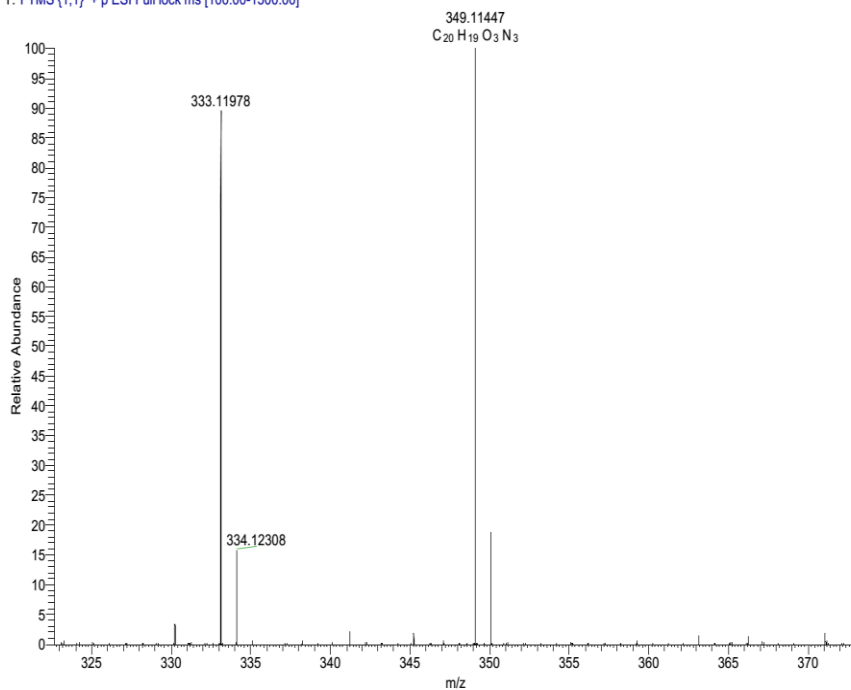


DEPT-135 NMR Spectrum of Compound **4I**

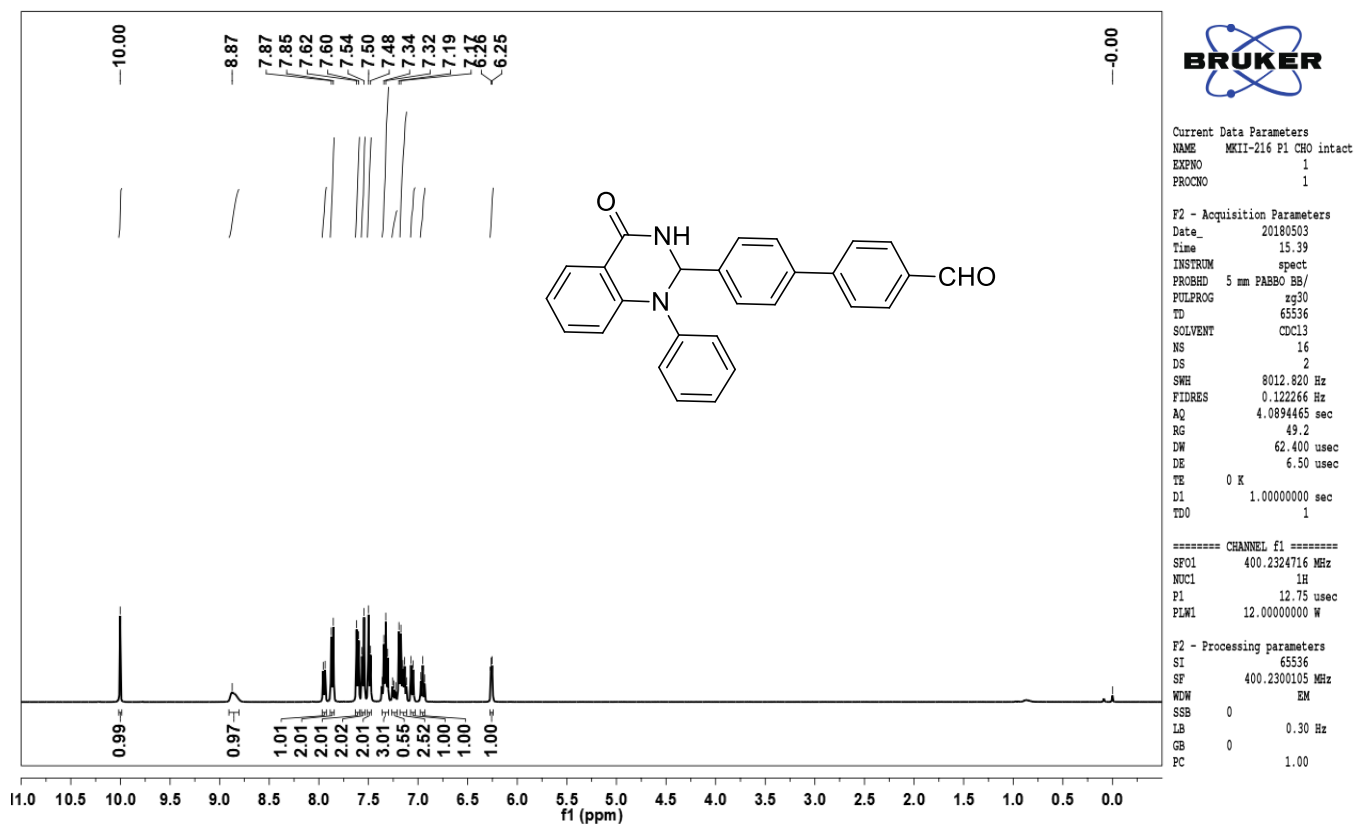
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04-05-2018 13:18:01

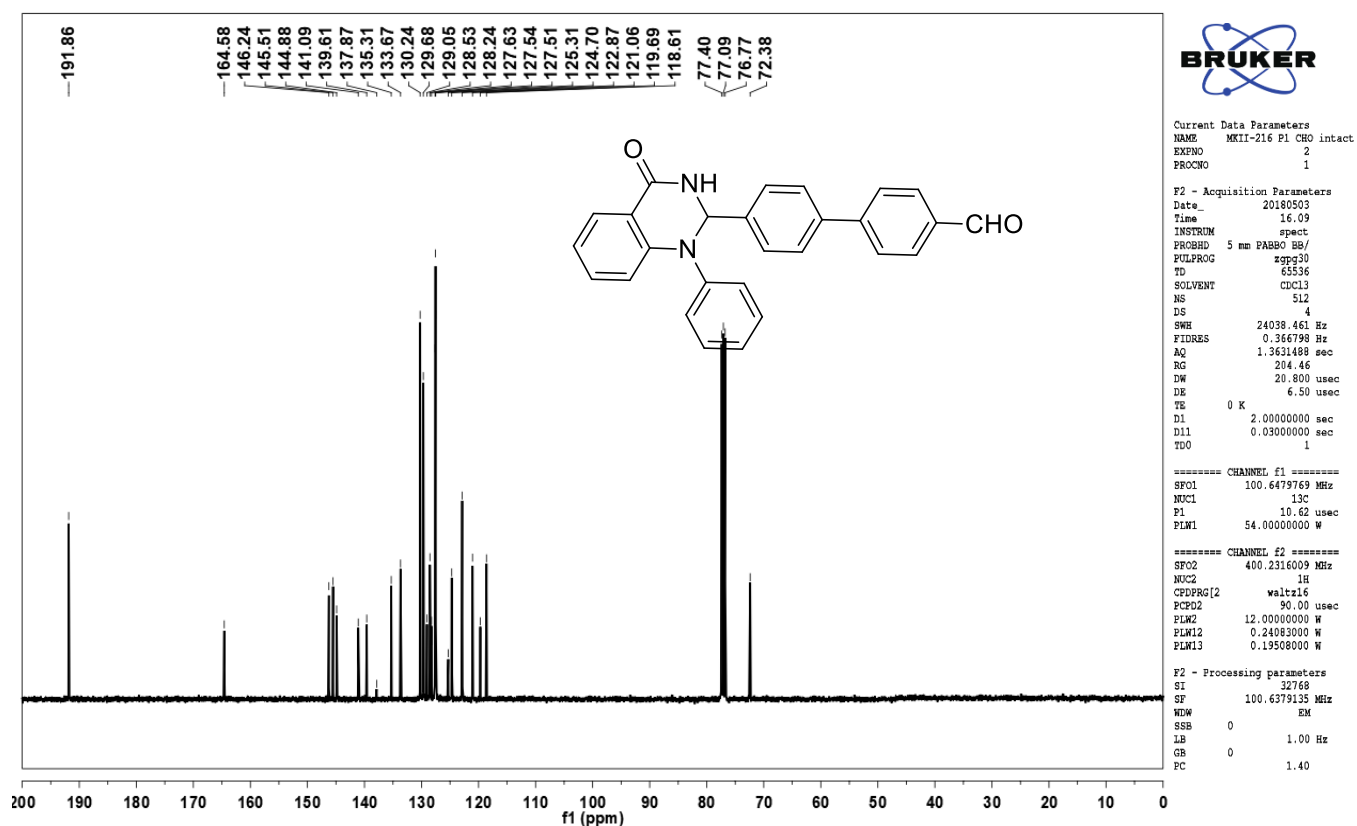
MKII-162P1 #102 RT: 1.62 AV: 1 NL: 2.19E6  
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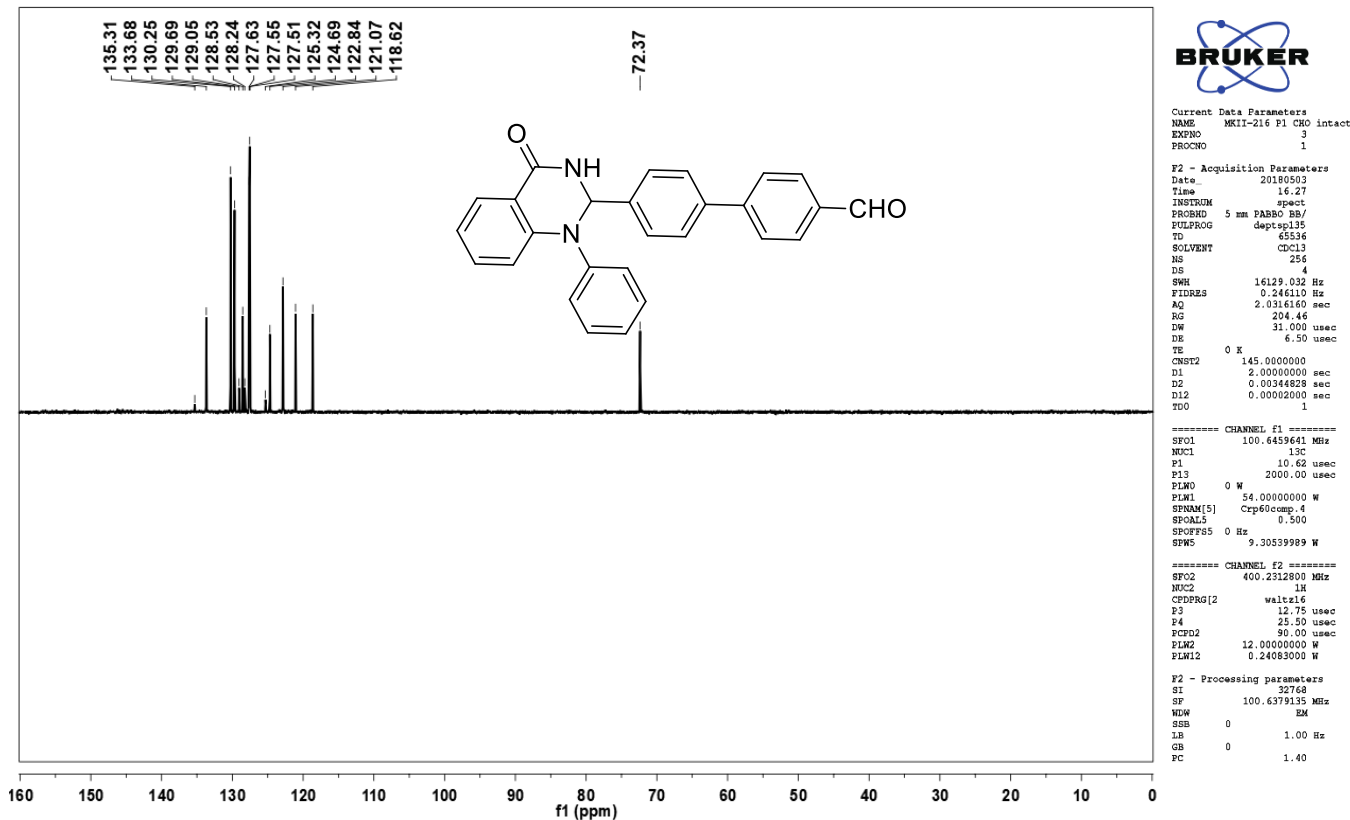
HRMS Spectrum of Compound **4I**



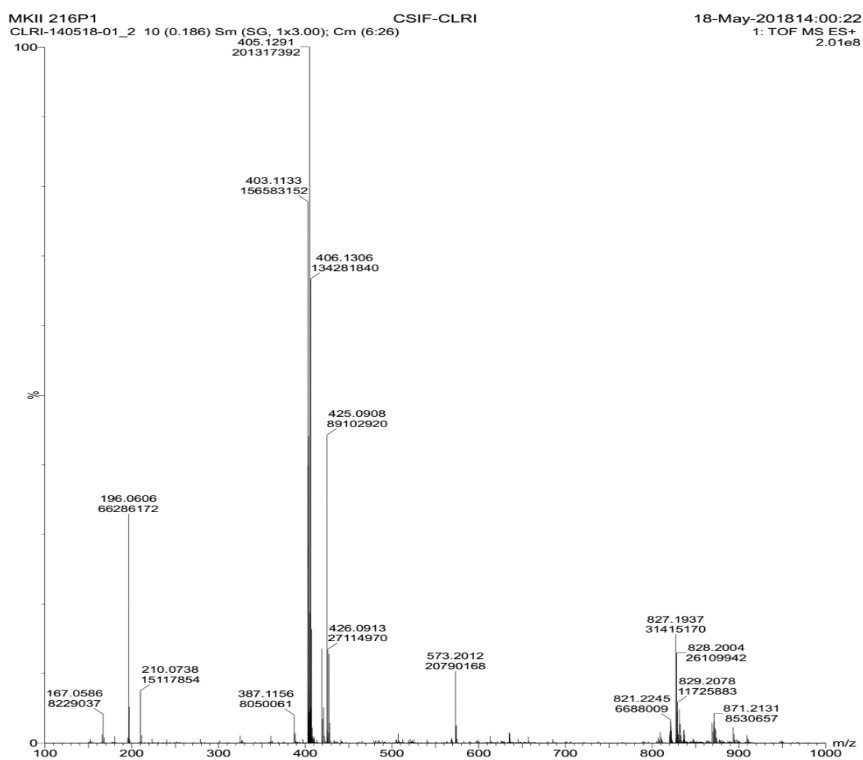
**<sup>1</sup>H NMR Spectrum of Compound 5a**



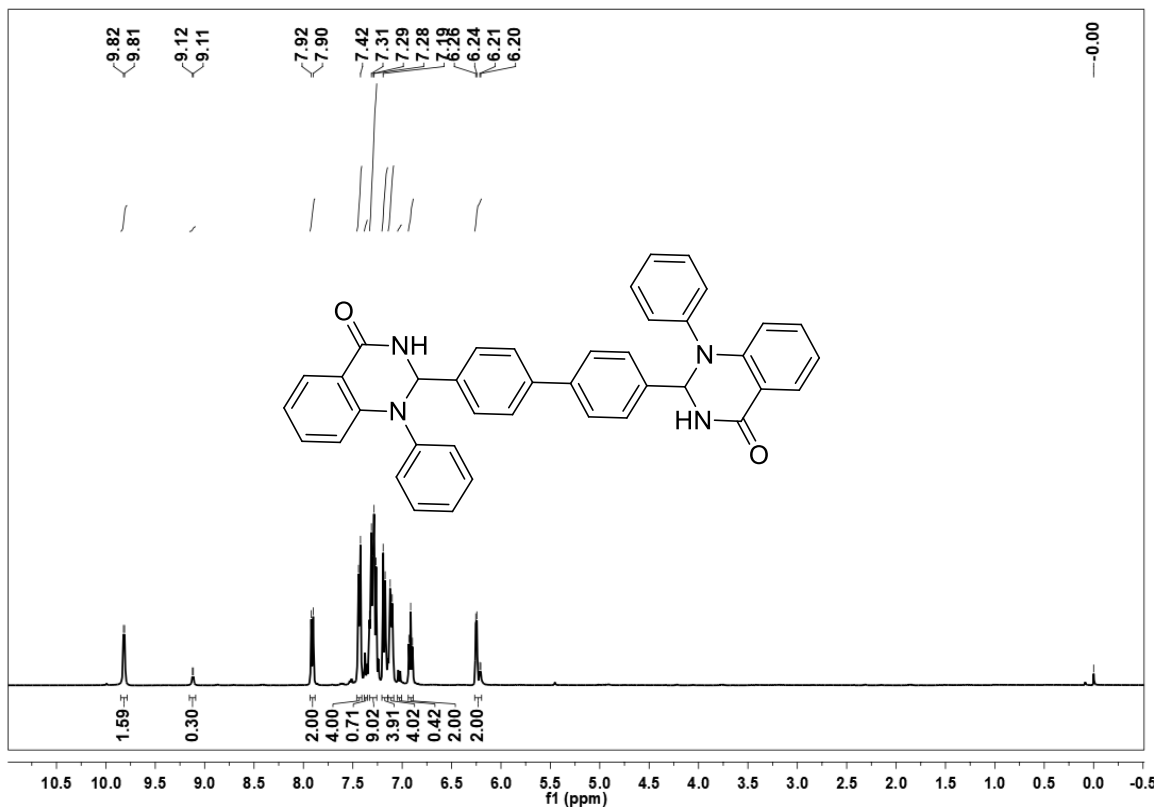
**<sup>13</sup>C NMR Spectrum of Compound 5a**



DEPT-135 NMR Spectrum of Compound 5a



HRMS Spectrum of Compound 5a



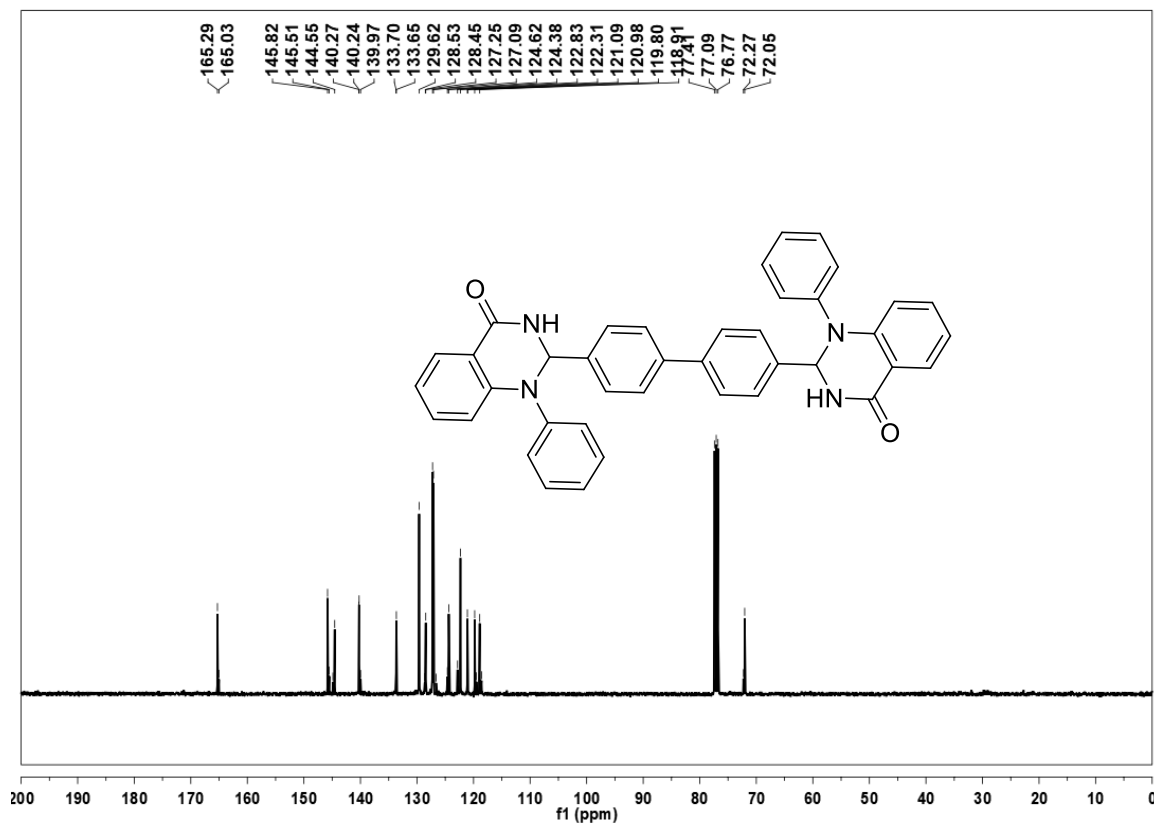
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 EXPNO 1  
 PROCNO 1

F2 - Acquisition Parameters  
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 Time 23.35  
 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 49.2  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 297.5 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SF01 400.2324716 MHz  
 NUC1 1H  
 P1 12.75 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2300168 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

**<sup>1</sup>H NMR Spectrum of Compound 5b**



Current Data Parameters  
 NAME MKII-216RP2  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20180516  
 Time 0.05  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 512  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 204.46  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 298.5 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SF01 100.6479769 MHz  
 NUC1 13C  
 P1 10.62 usec  
 PLW1 54.00000000 W

==== CHANNEL f2 =====  
 SF02 400.2316009 MHz  
 NUC2 1H  
 CDDPRG(2) waltz16  
 FCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.24083000 W  
 PLW13 0.19508000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6379135 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

**<sup>13</sup>C NMR Spectrum of Compound 5b**



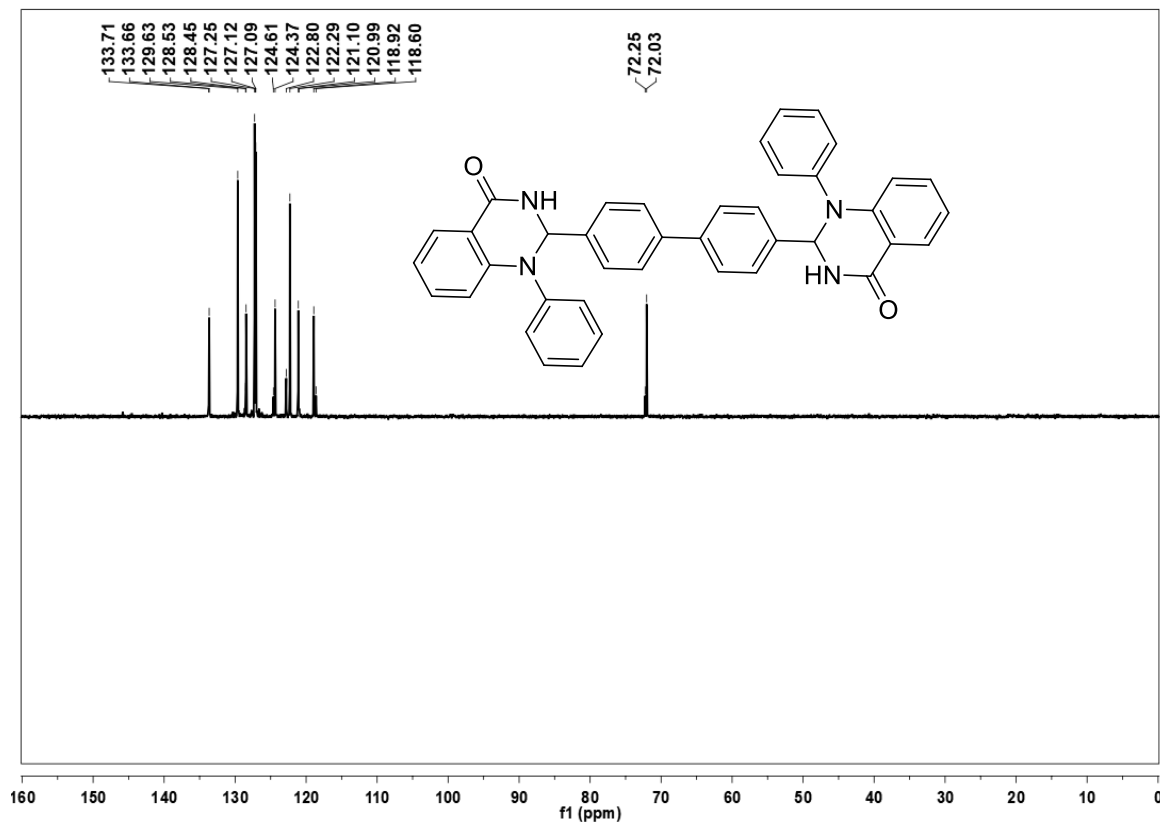
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PROCNO 1

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PULPROG deptsp135  
TD 65536  
SOLVENT cdc13  
NS 256  
DS 4  
SWH 16129.032 Hz  
FIDRES 0.246110 Hz  
AQ 2.0316160 sec  
RG 204.46  
DW 31.000 usec  
DE 6.50 usec  
TE 297.8 K  
CNS2 145.000000  
D1 2.00000000 sec  
D2 0.00344828 sec  
D12 0.00002000 sec  
TD0 1

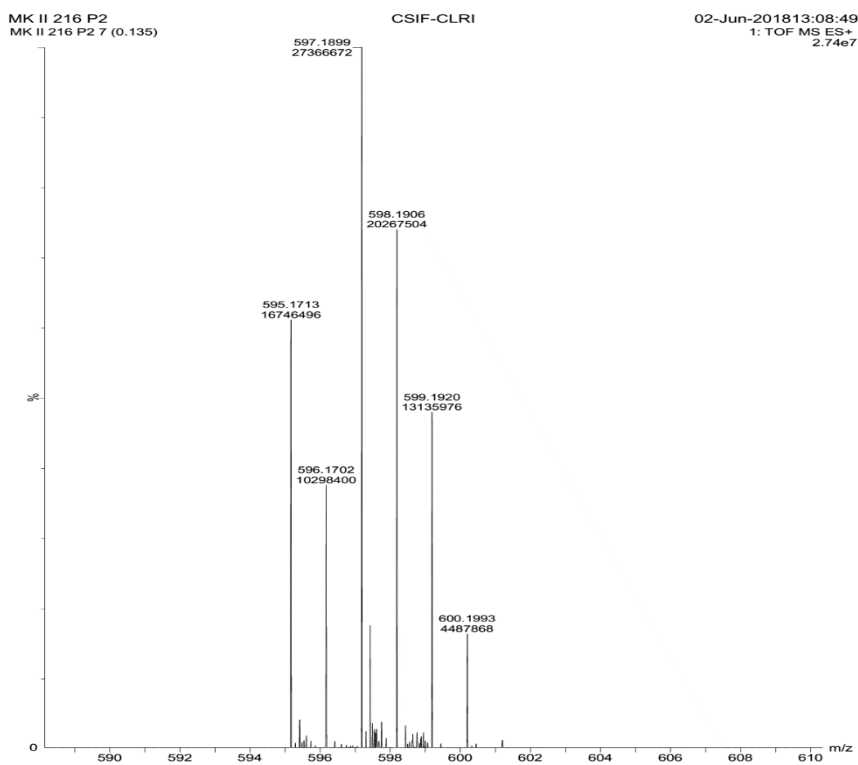
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NUC1 13C  
P1 10.62 usec  
P13 2000.00 usec  
PLW0 0 W  
PLW1 54.00000000 W  
SPNAM[5] Crp60comp\_4  
SFOAL5 0.500  
SPOFFS5 0 Hz  
SPW5 9.30539989 W

==== CHANNEL F2 =====  
SFO2 400.2312800 MHz  
NUC2 1H  
CDEPRG[2] waltz16  
P3 12.75 usec  
P4 25.50 usec  
PCPD2 90.00 usec  
PLW2 12.00000000 W  
PLW12 0.24083000 W

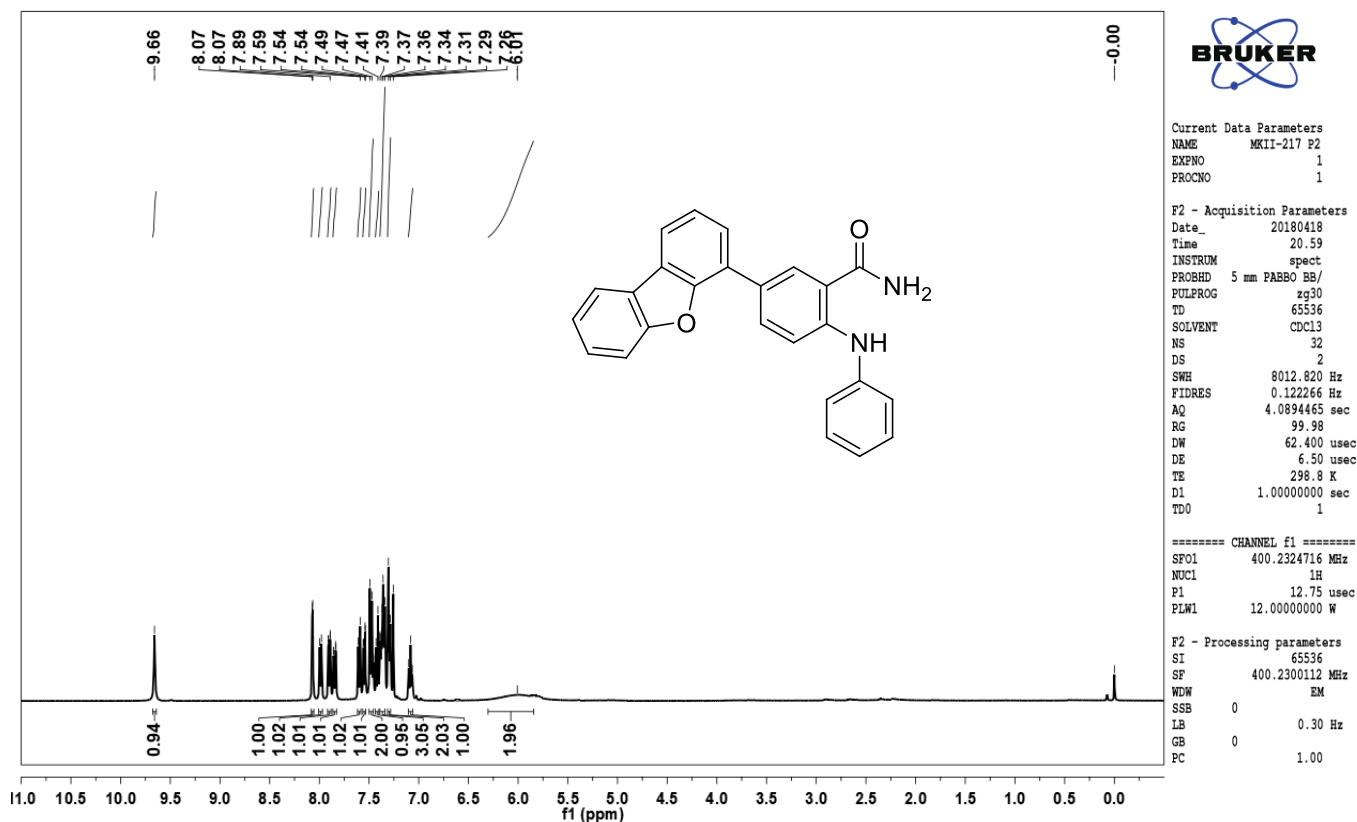
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SF 100.6379135 MHz  
WDW EM  
SBB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



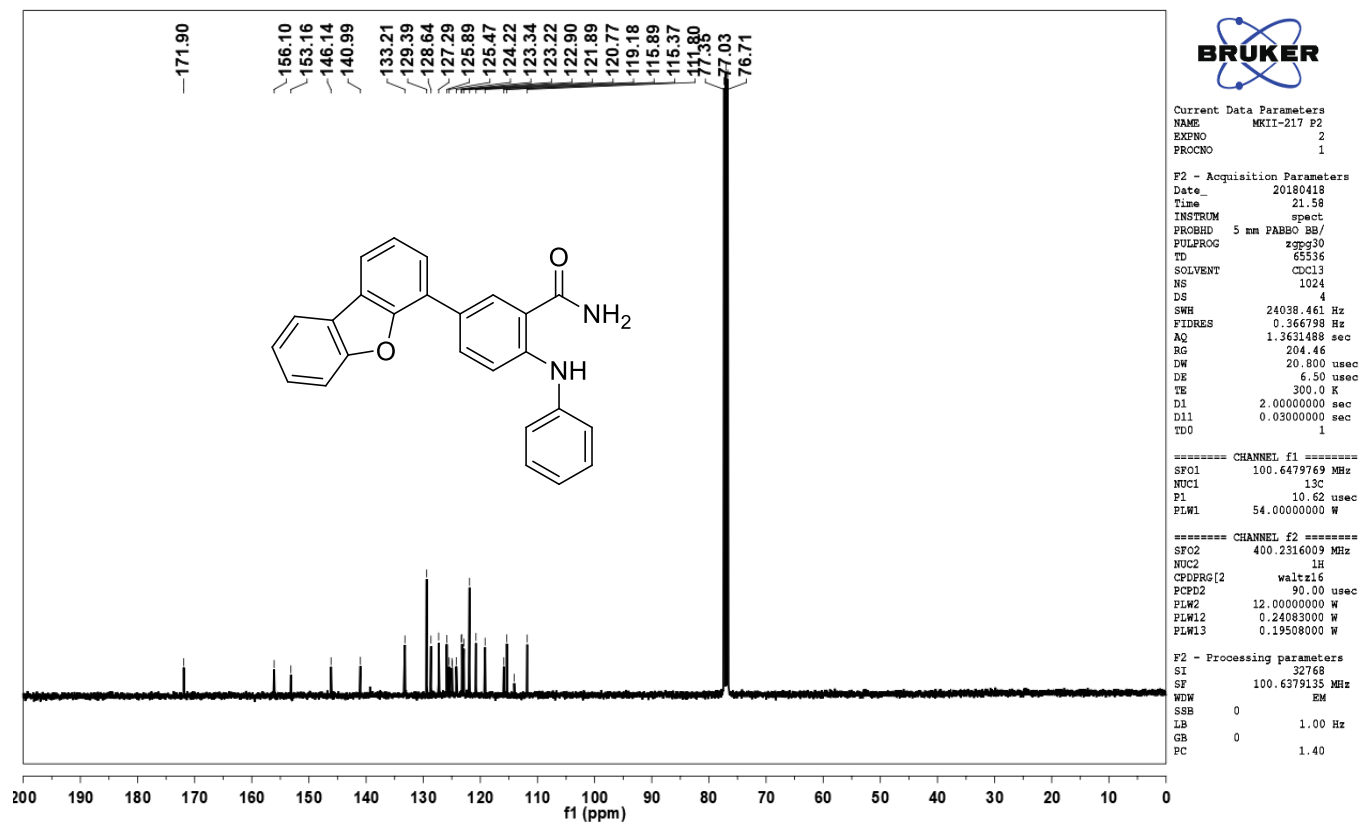
DEPT-135 NMR Spectrum of Compound **5b**



HRMS Spectrum of Compound **5b**



**1H NMR Spectrum of Compound 6a**



**13C NMR Spectrum of Compound 6a**



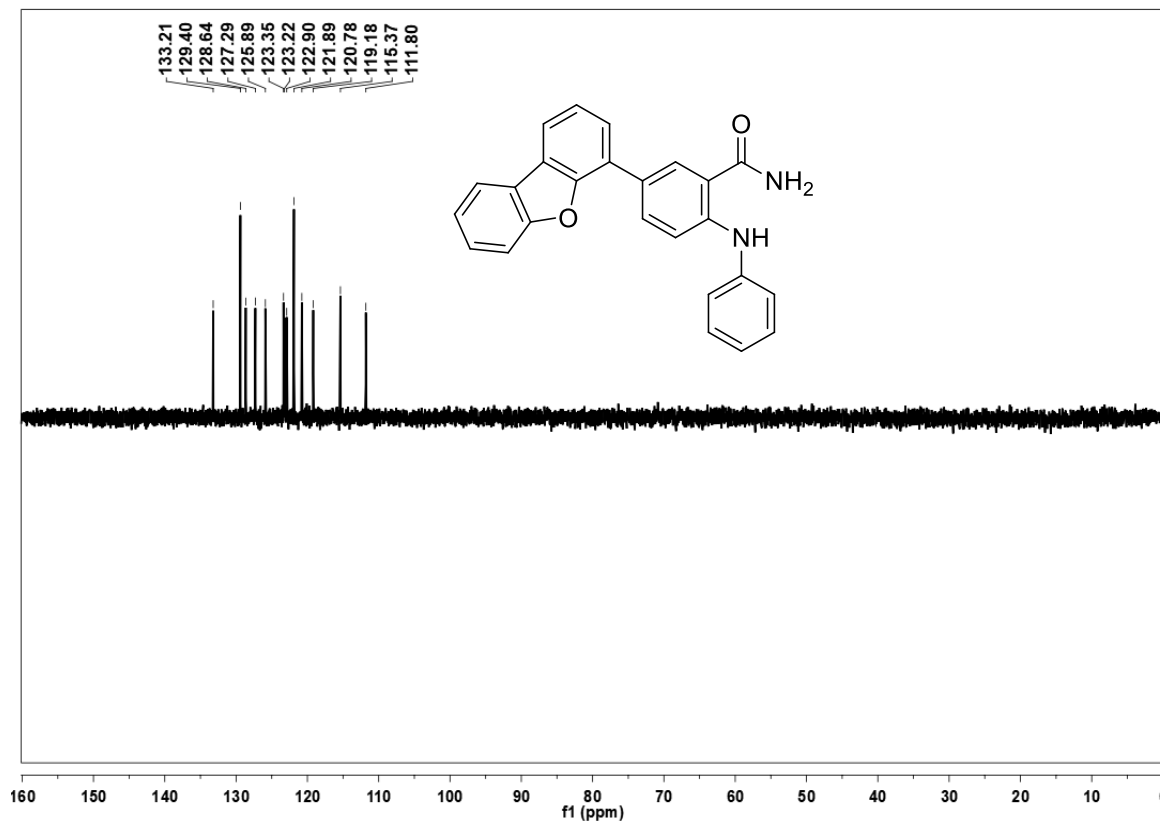
Current Data Parameters  
NAME MKII-217 F2  
EXNO 3  
PROCNO 1

F2 - Acquisition Parameters  
Date 20180418  
Time 22.16  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG deptsp135  
TD 65536  
SOLVENT CDCl3  
NS 256  
DS 4  
SWH 16129.032 Hz  
FIDRES 0.246110 Hz  
AQ 2.0316160 sec  
RG 204.46  
DW 31.000 usec  
DE 6.50 usec  
TE 299.4 K  
CNS2 145.000000  
D1 2.0000000 sec  
D2 0.00344828 sec  
D12 0.00002000 sec  
TD 1

===== CHANNEL f1 =====  
SFO1 100.6459641 MHz  
NUC1 13C  
P1 10.62 usec  
P13 2000.00 usec  
PLW0 0 W  
PLW1 54.00000000 W  
SPNAM[5] Crp60comp.4  
SFOALS 0.500  
SPOFFS5 0 Hz  
SPW5 9.30539989 W

===== CHANNEL f2 =====  
SFO2 400.2312800 MHz  
NUC2 1H  
CPDPRG[2] waltz16  
P3 12.75 usec  
P4 25.50 usec  
PCPD2 90.00 usec  
PLW2 12.00000000 W  
PLW12 0.24083000 W

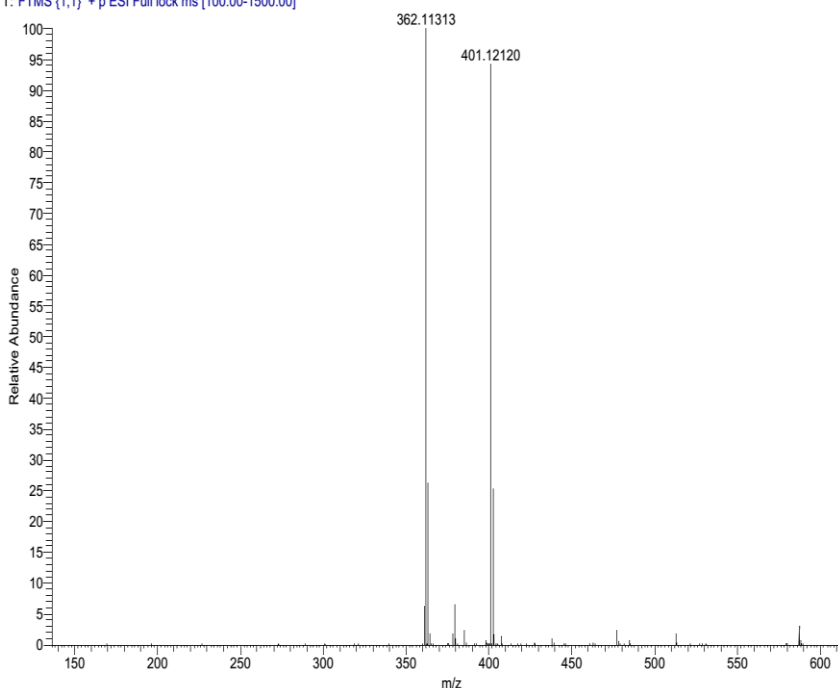
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SF 100.6379135 MHz  
WDW EM  
SBB 0  
LB 1.00 Hz  
GB 0  
PC 1.40



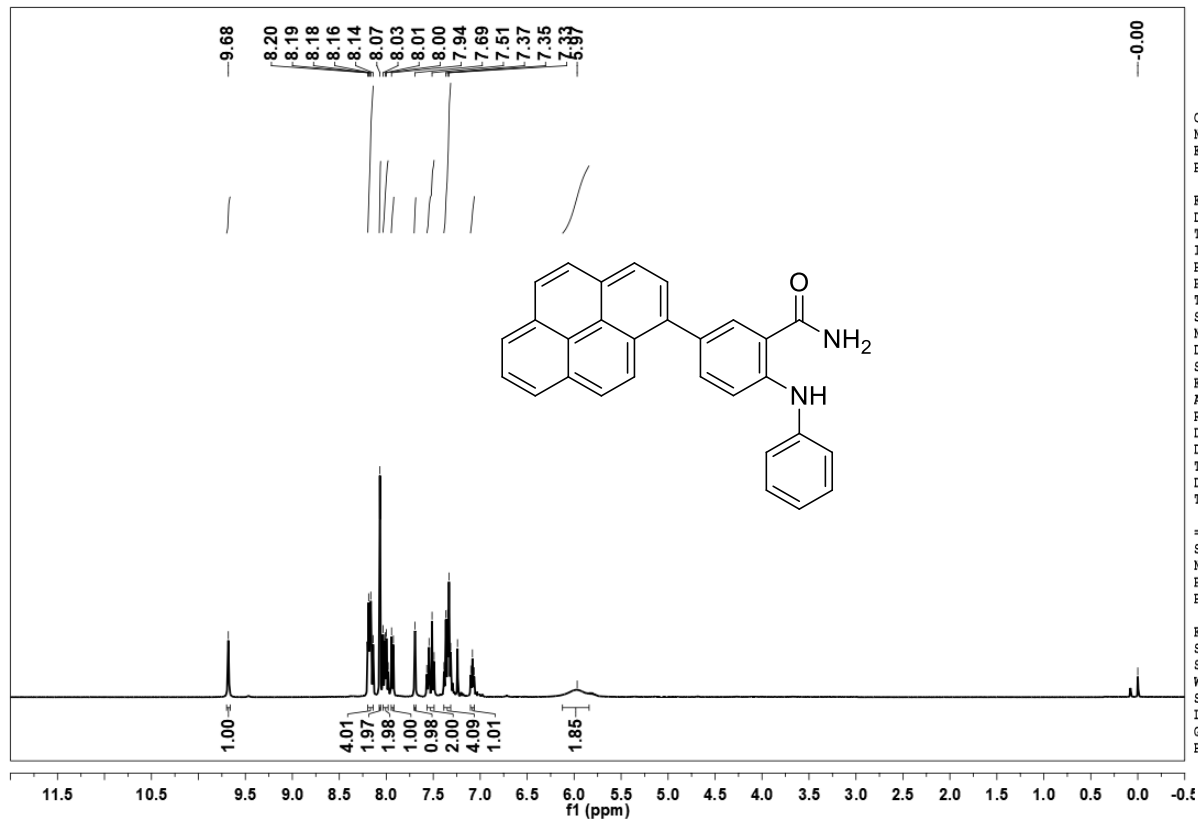
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04-05-2018 13:06:43

MKII-217P2 #95-108 RT: 1.61-1.79 AV: 14 NL: 7.36E6  
T: FTMS (1,1) + p ESI Full lock ms [100.00-1500.00]



HRMS Spectrum of Compound 6a



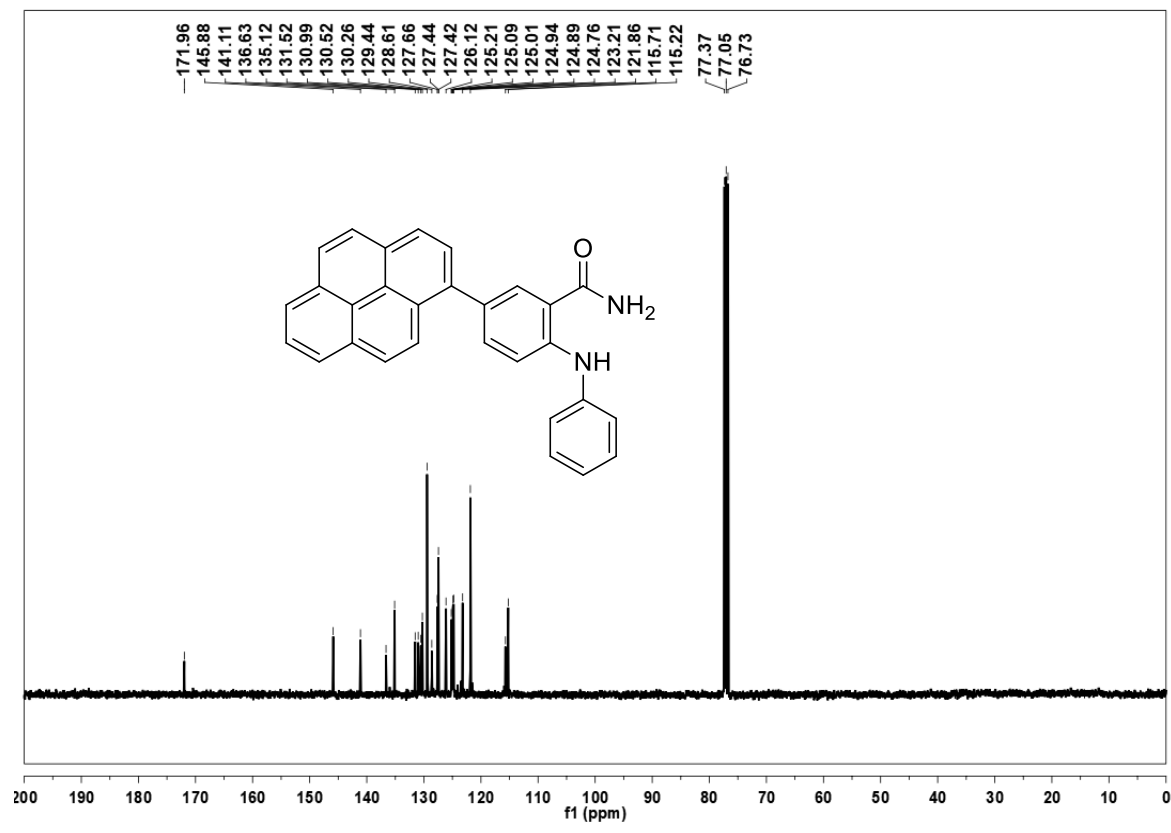
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 PROCNO 1

F2 - Acquisition Parameters  
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 Time 23.50  
 INSTRUM spect  
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 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 16  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 79.6  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 296.3 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SFO1 400.2324716 MHz  
 NUC1 1H  
 P1 12.75 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2300170 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

<sup>1</sup>H NMR Spectrum of Compound 6b



Current Data Parameters  
 NAME MKII-227  
 EXPNO 2  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20180523  
 Time 0.20  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 512  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 204.46  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 297.4 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

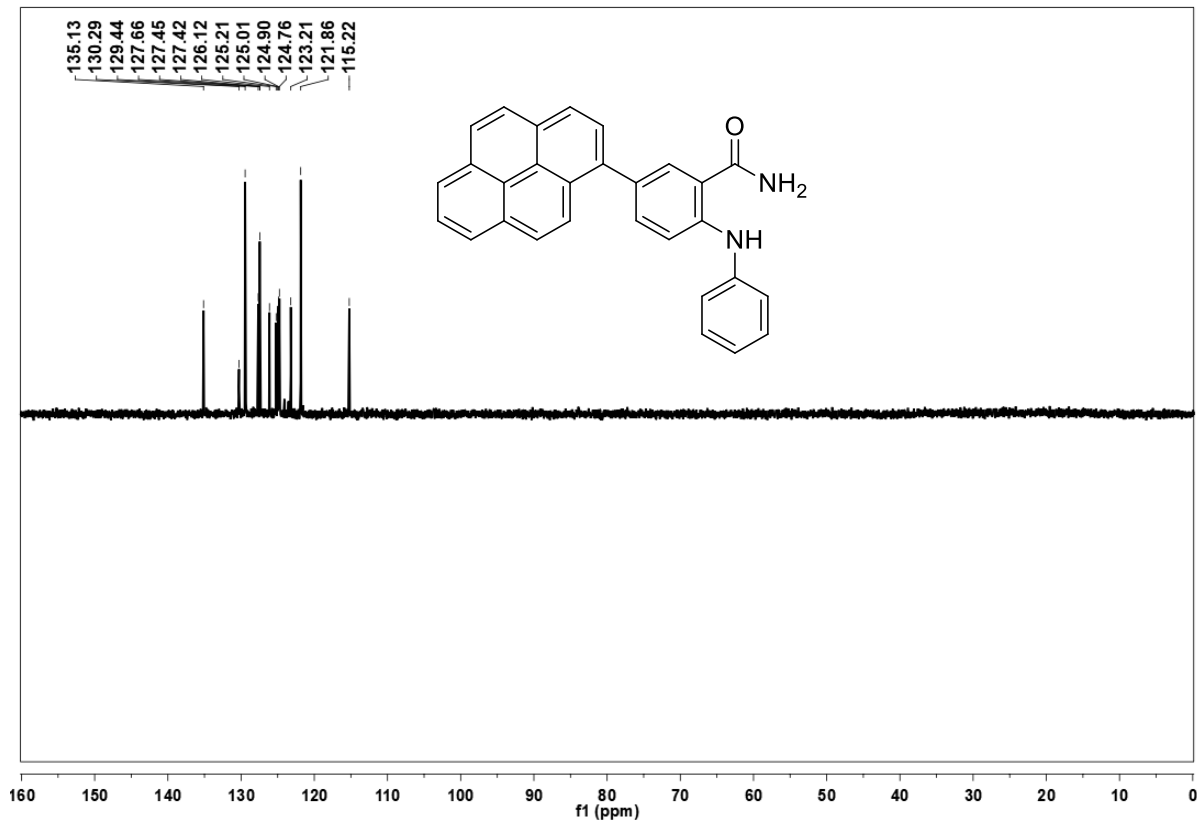
==== CHANNEL f1 =====  
 SFO1 100.6479769 MHz  
 NUC1 13C  
 P1 10.62 usec  
 PLW1 54.00000000 W

==== CHANNEL f2 =====  
 SFO2 400.2316009 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.24083000 W  
 PLW13 0.19508000 W

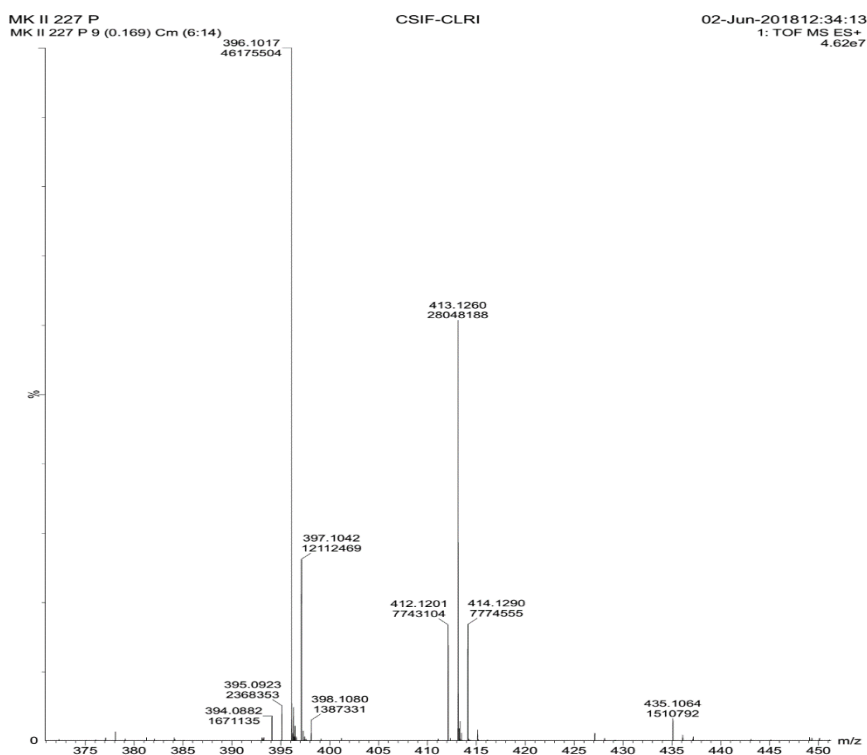
F2 - Processing parameters  
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 SF 100.6379135 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

<sup>13</sup>C NMR Spectrum of Compound 6b

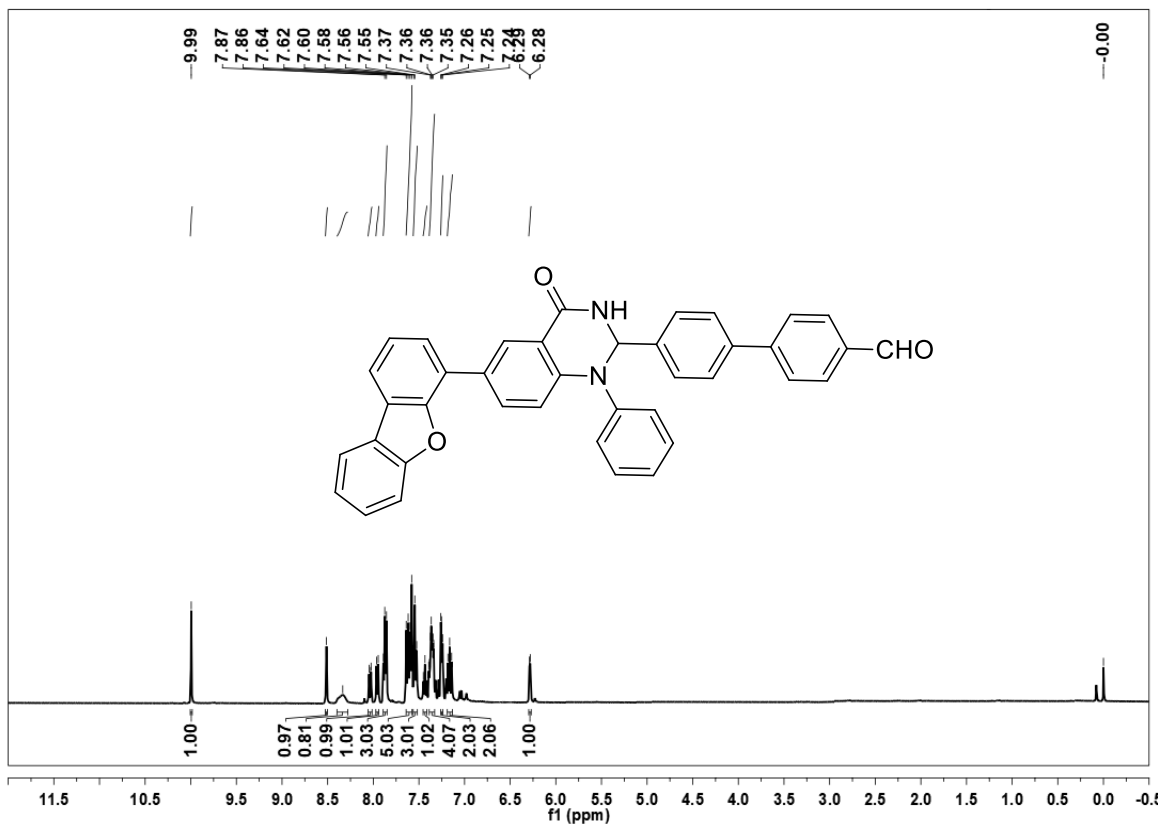




### DEPT-135 NMR Spectrum of Compound 6b



### HRMS Spectrum of Compound 6b



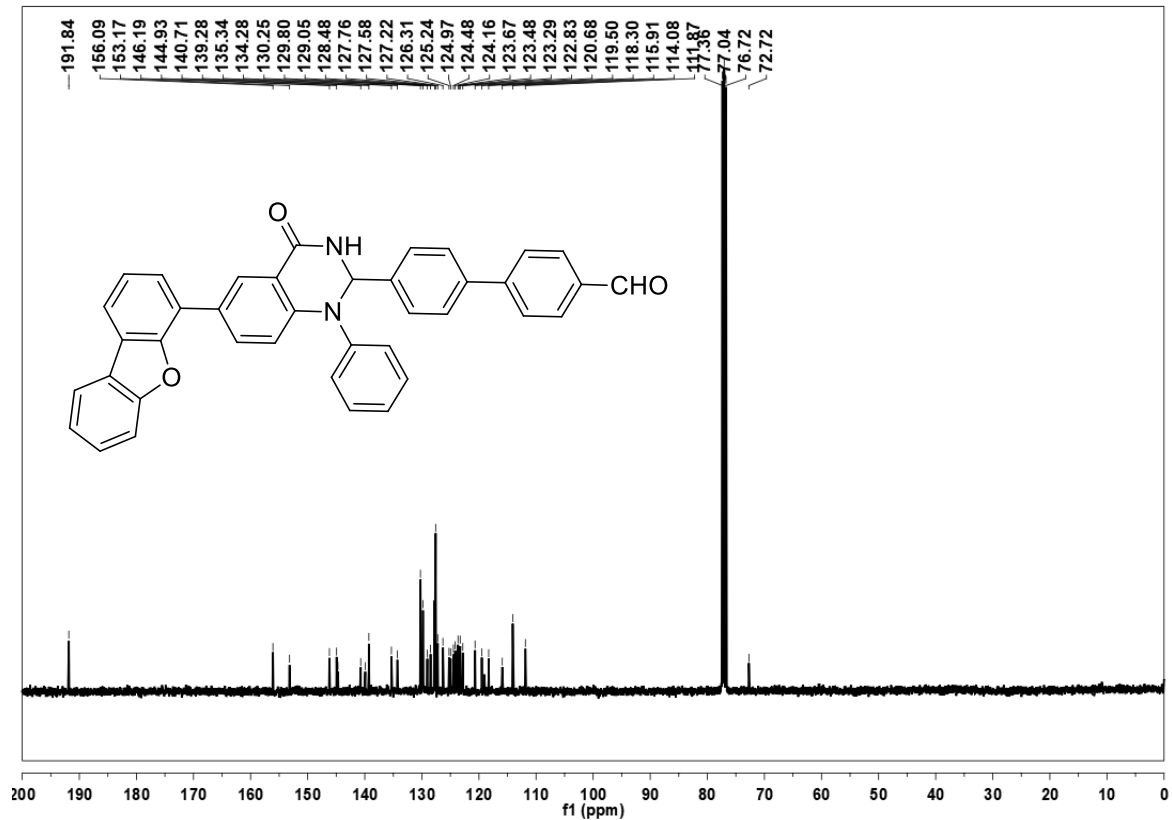
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NAME MKII-221 P1  
EXPNO 1  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20180503  
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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 31.36  
DW 62.400 usec  
DE 6.50 usec  
TE 0 K  
D1 1.00000000 sec  
TDO 1

===== CHANNEL f1 =====  
SF01 400.2324716 MHz  
NUC1 1H  
P1 12.75 usec  
PLW1 12.00000000 W

F2 - Processing parameters  
SI 65536  
SF 400.2300128 MHz  
WDW EM  
SSB 0  
LB 0.30 Hz  
GB 0  
PC 1.00

<sup>1</sup>H NMR Spectrum of Compound 7a



Current Data Parameters  
NAME MKII-221 P1  
EXPNO 2  
PROCNO 1

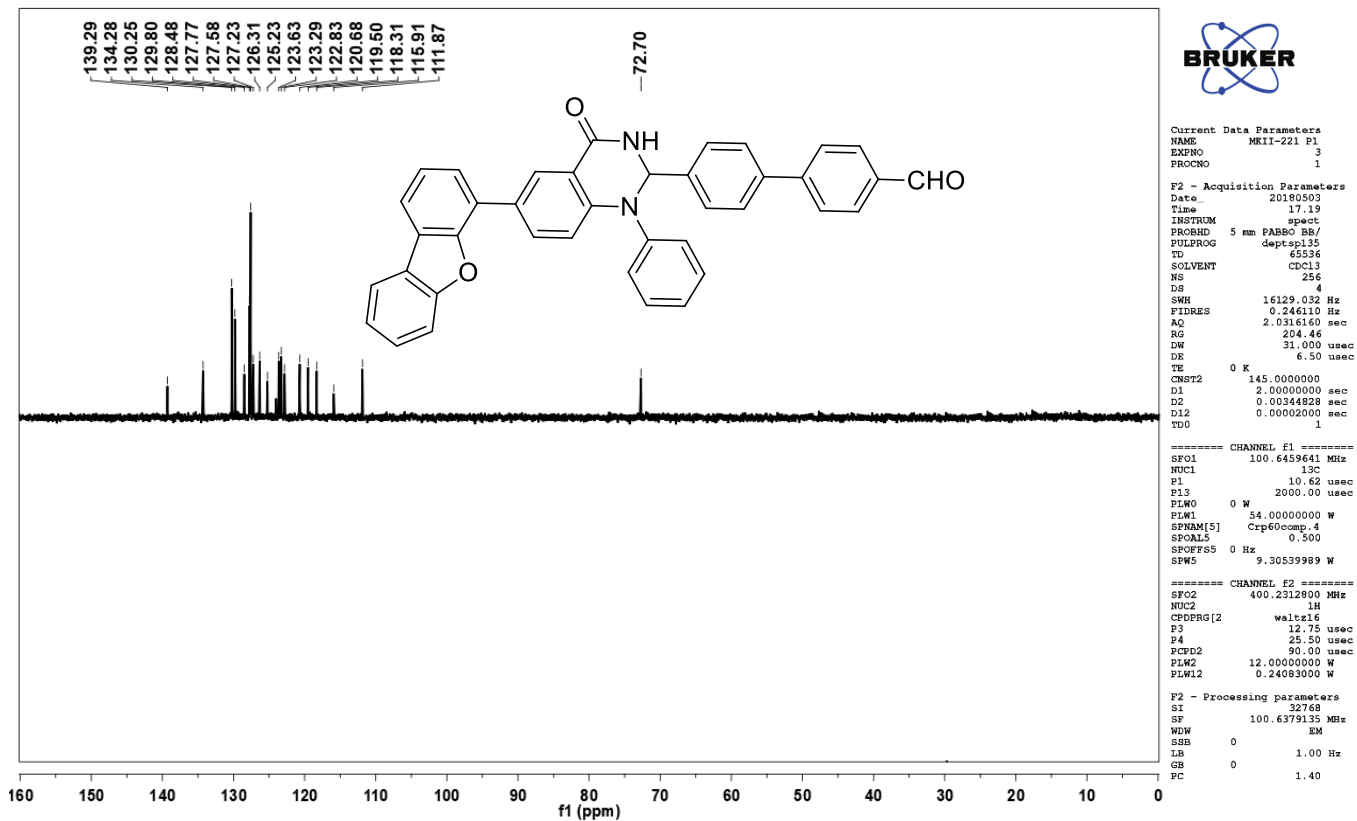
F2 - Acquisition Parameters  
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Time 17.01  
INSTRUM spect  
PROBHD 5 mm PABBO BB/  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 512  
DS 4  
SWH 24038.461 Hz  
FIDRES 0.366798 Hz  
AQ 1.3631488 sec  
RG 204.46  
DW 20.800 usec  
DE 6.50 usec  
TE 0 K  
D1 2.00000000 sec  
D11 0.03000000 sec  
TDO 1

===== CHANNEL f1 =====  
SF01 100.6479769 MHz  
NUC1 13C  
P1 10.62 usec  
PLW1 54.00000000 W

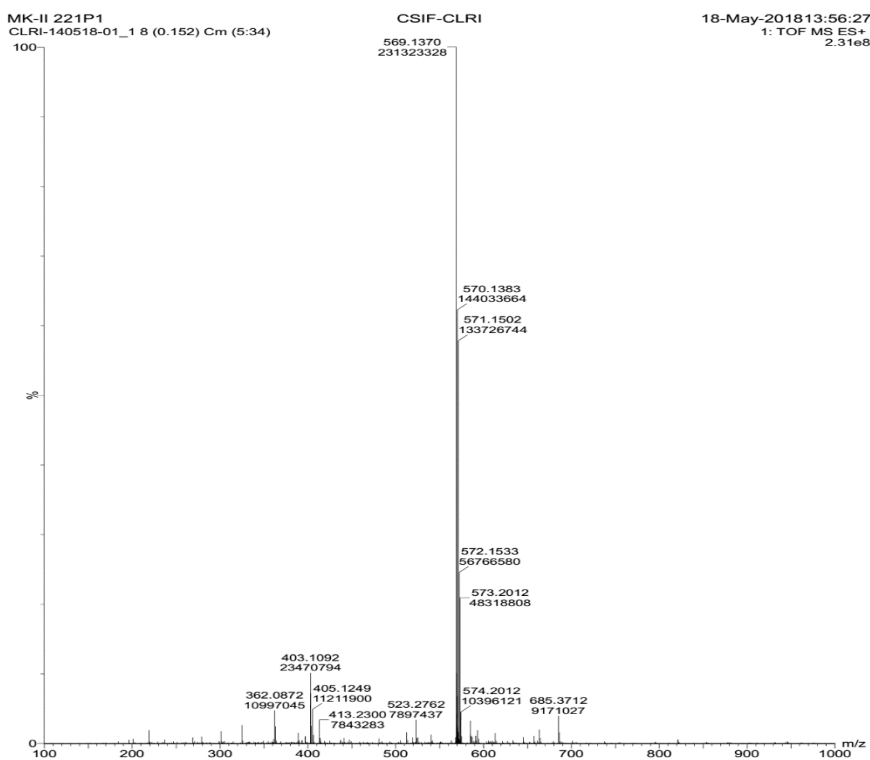
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SF02 400.2316009 MHz  
NUC2 1H  
PCPD2 waltz16  
PCPD2 90.00 usec  
PLW2 12.00000000 W  
PLW12 0.24983000 W  
PLW13 0.19508000 W

F2 - Processing parameters  
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SF 100.6379135 MHz  
WDW EM  
SSB 0  
LB 1.00 Hz  
GB 0  
PC 1.40

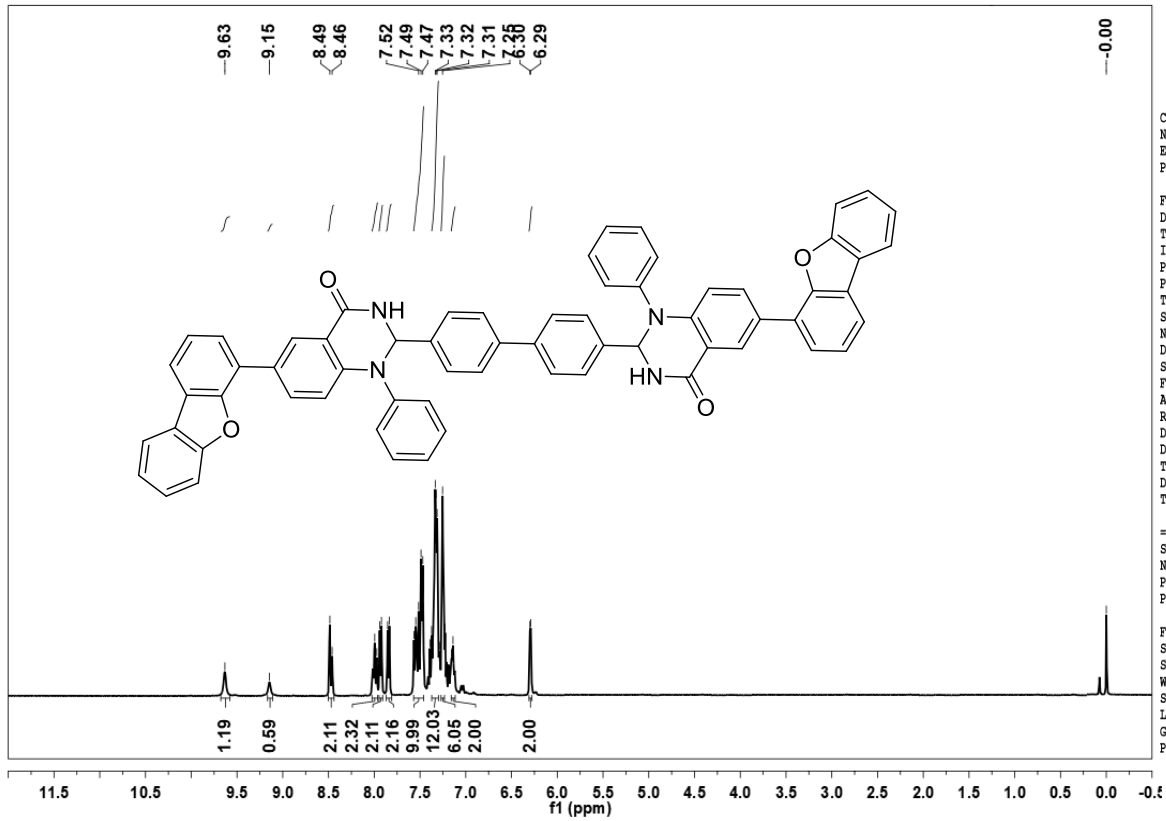
<sup>13</sup>C NMR Spectrum of Compound 7a



DEPT-135 NMR Spectrum of Compound **7a**



HRMS Spectrum of Compound **7a**



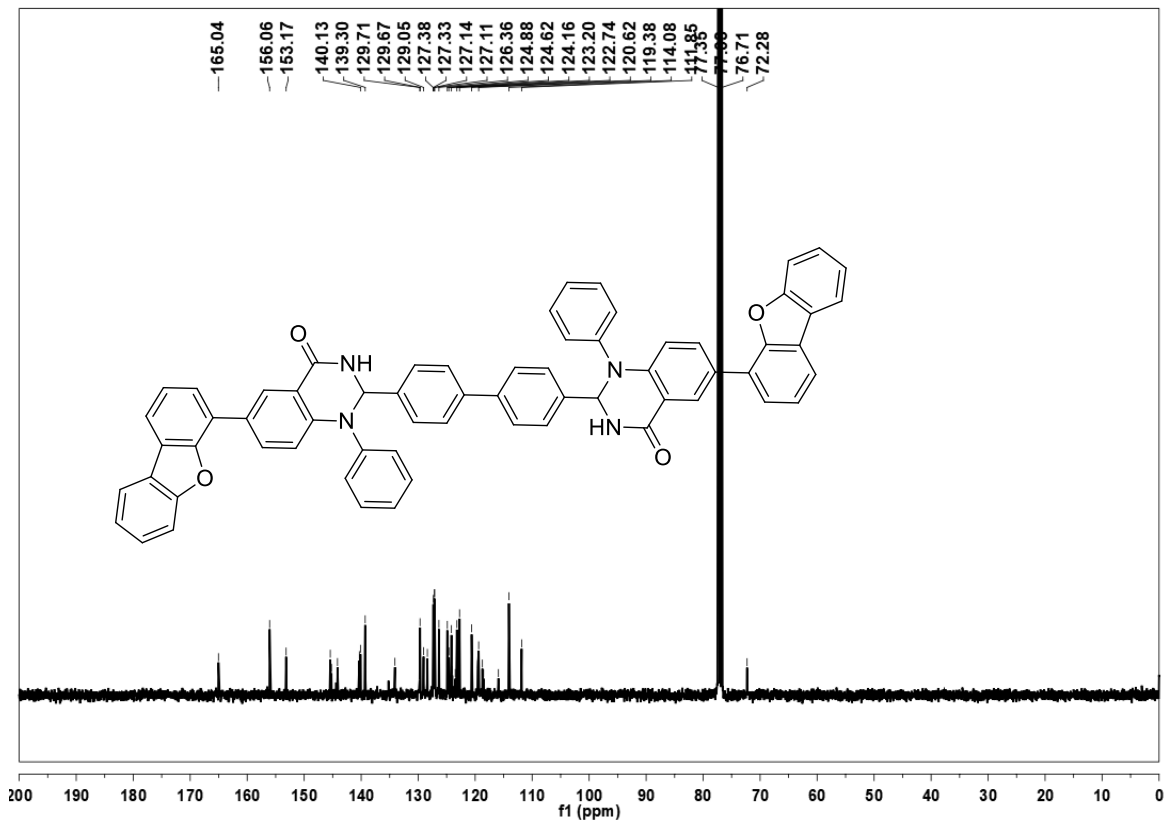
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 PROCNO 1

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 PROBHD 5 mm PABBO BB/  
 PULPROG zg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 32  
 DS 2  
 SWH 8012.820 Hz  
 FIDRES 0.122266 Hz  
 AQ 4.0894465 sec  
 RG 72.51  
 DW 62.400 usec  
 DE 6.50 usec  
 TE 0 K  
 D1 1.00000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SF01 400.2324716 MHz  
 NUC1 1H  
 P1 12.75 usec  
 PLW1 12.00000000 W

F2 - Processing parameters  
 SI 65536  
 SF 400.2300121 MHz  
 WDW EM  
 SSB 0  
 LB 0.30 Hz  
 GB 0  
 PC 1.00

**<sup>1</sup>H NMR Spectrum of Compound 7b**



Current Data Parameters  
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 PROCNO 1

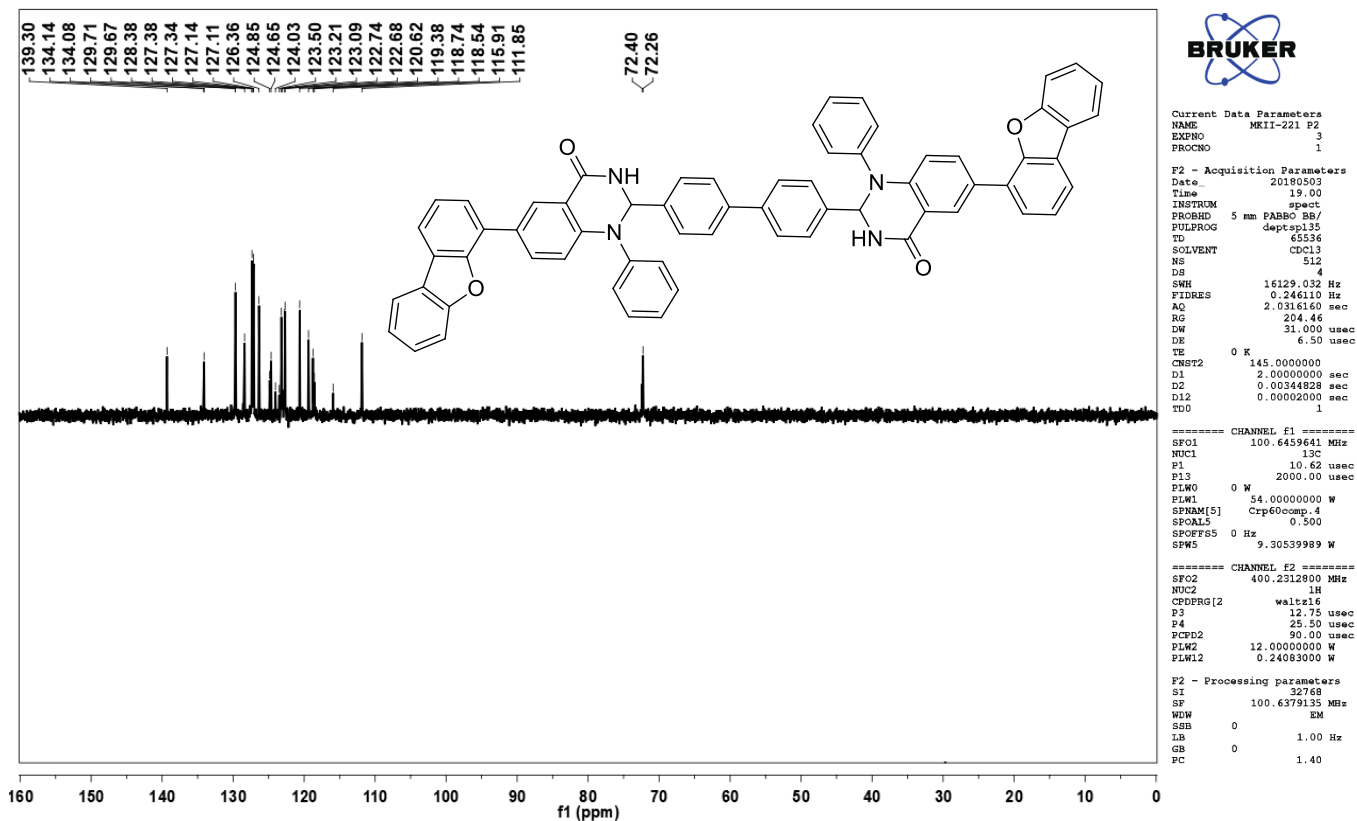
F2 - Acquisition Parameters  
 Date\_ 20180503  
 Time 18.25  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB/  
 PULPROG zgpg30  
 TD 65536  
 SOLVENT CDCl3  
 NS 1024  
 DS 4  
 SWH 24038.461 Hz  
 FIDRES 0.366798 Hz  
 AQ 1.3631488 sec  
 RG 204.46  
 DW 20.800 usec  
 DE 6.50 usec  
 TE 0 K  
 D1 2.00000000 sec  
 D11 0.03000000 sec  
 TD0 1

==== CHANNEL f1 =====  
 SF01 100.6479769 MHz  
 NUC1 13C  
 P1 10.62 usec  
 PLW1 54.00000000 W

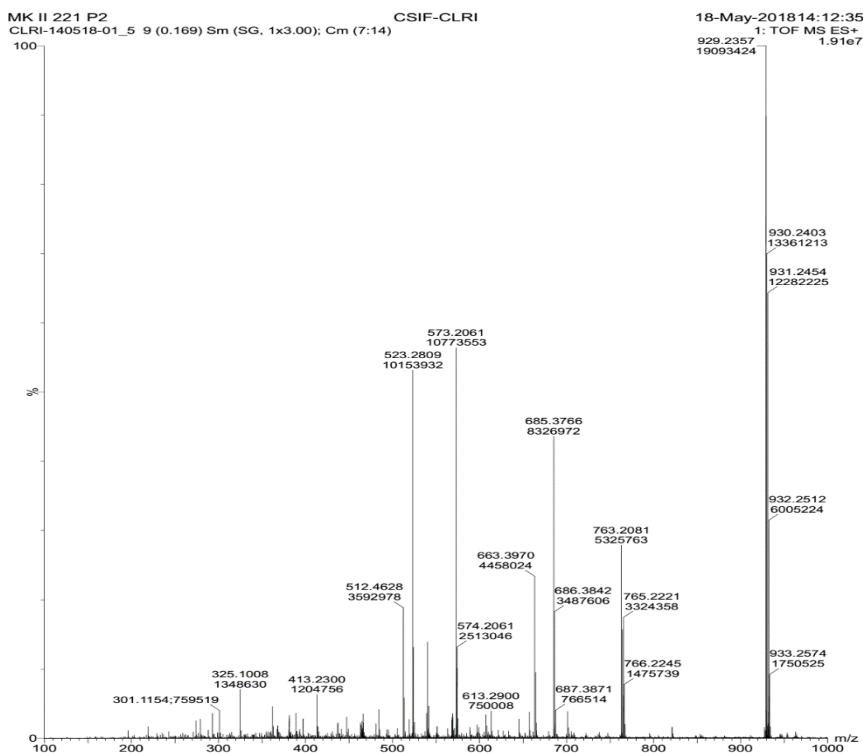
==== CHANNEL f2 =====  
 SF02 400.2316009 MHz  
 NUC2 1H  
 CPDPRG2 waltz16  
 PCPD2 90.00 usec  
 PLW2 12.00000000 W  
 PLW12 0.24083000 W  
 PLW13 0.19508000 W

F2 - Processing parameters  
 SI 32768  
 SF 100.6379135 MHz  
 WDW EM  
 SSB 0  
 LB 1.00 Hz  
 GB 0  
 PC 1.40

**<sup>13</sup>C NMR Spectrum of Compound 7b**



DEPT-135 NMR Spectrum of Compound 7b



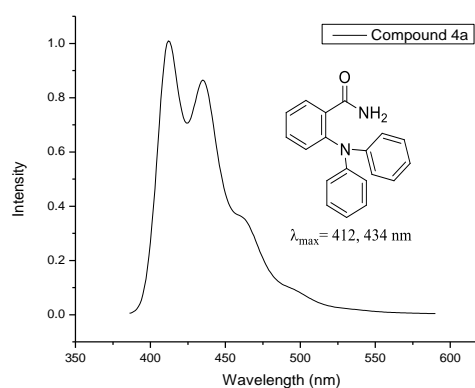
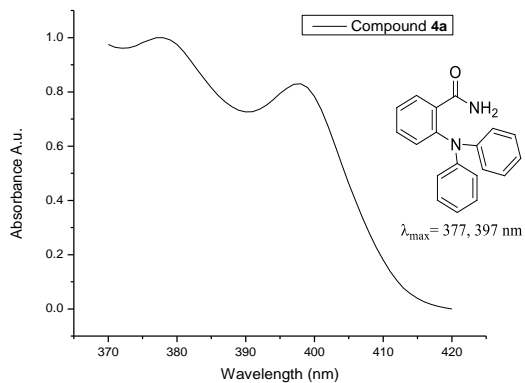
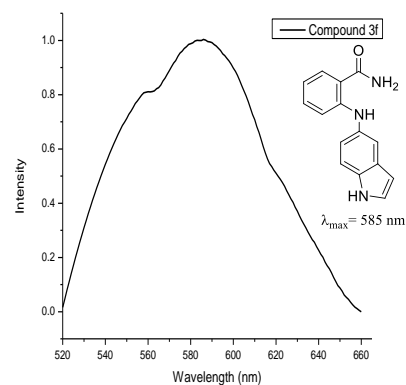
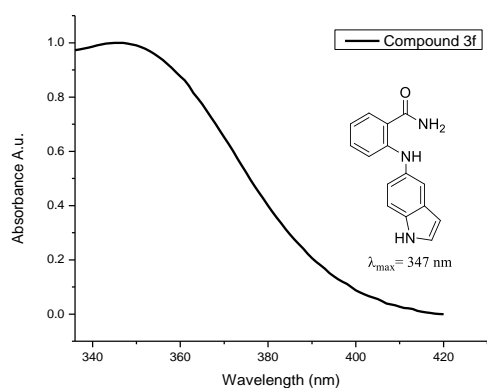
HRMS Spectrum of Compound 7b

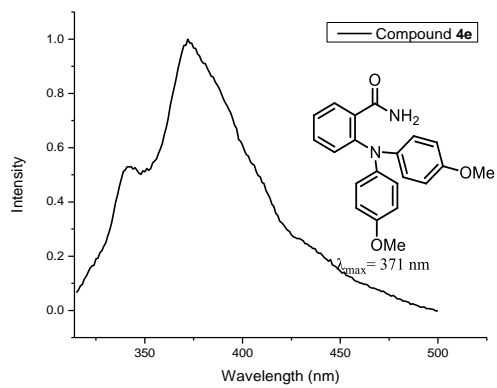
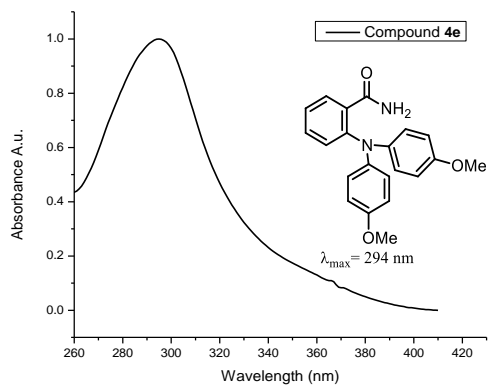
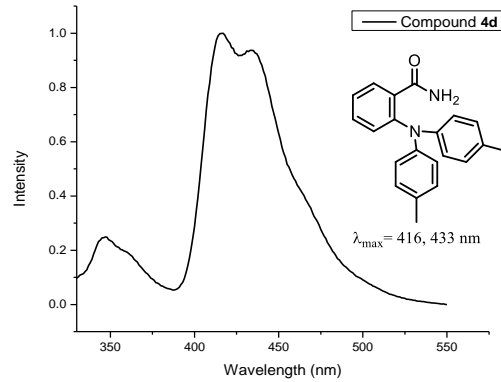
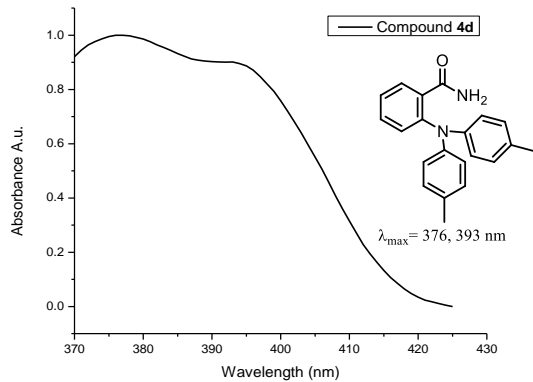
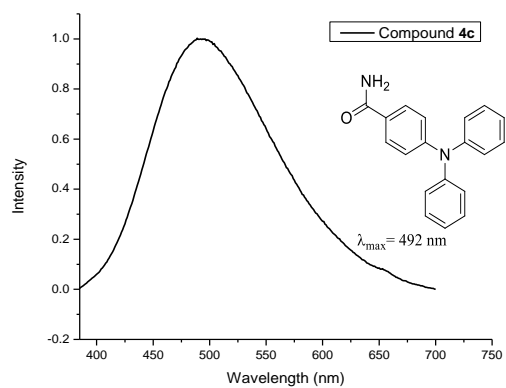
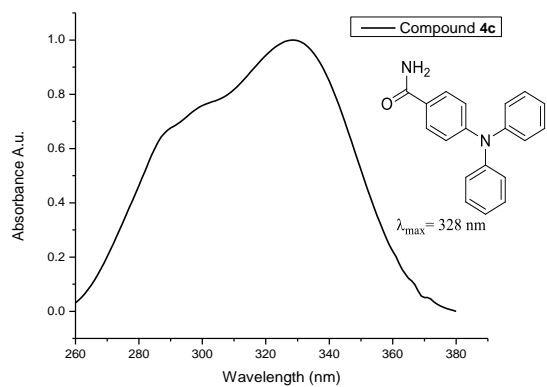
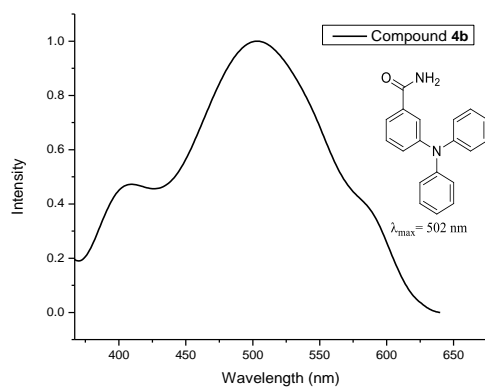
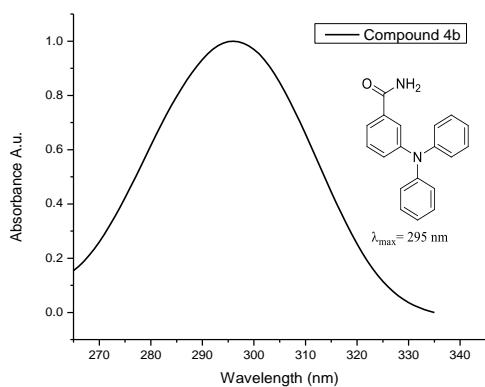
## 1. Absorption and emission data of compounds

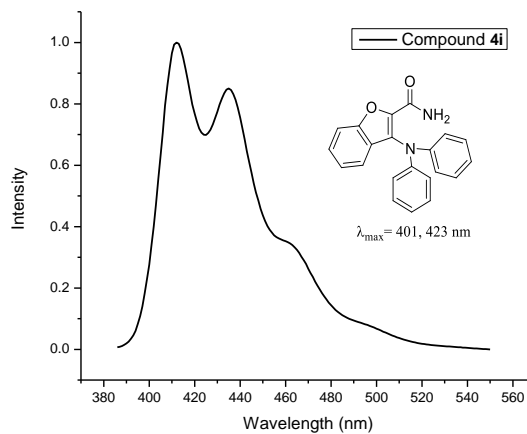
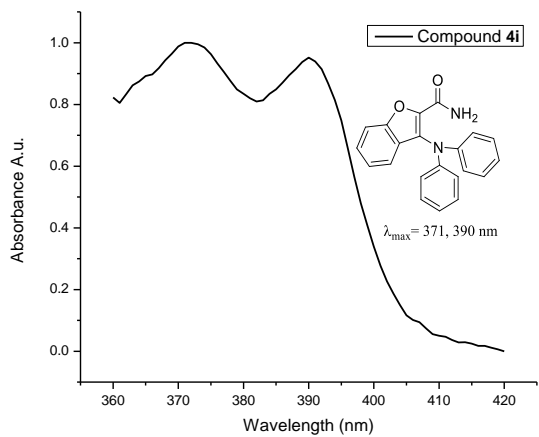
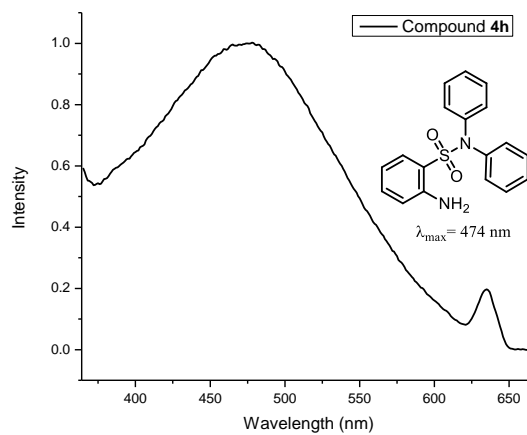
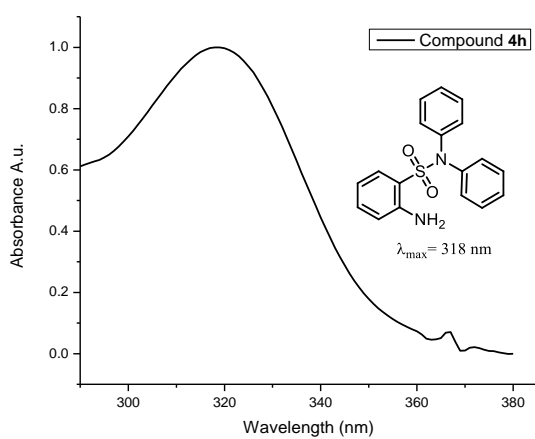
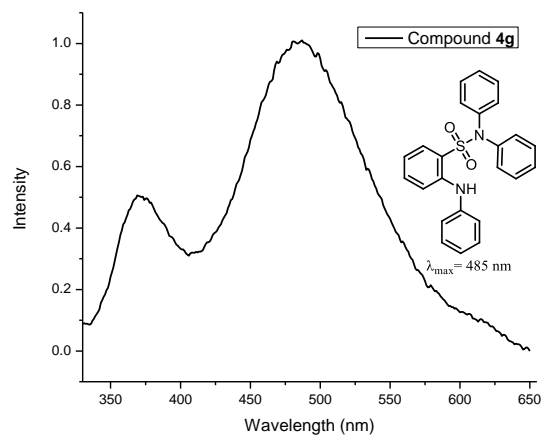
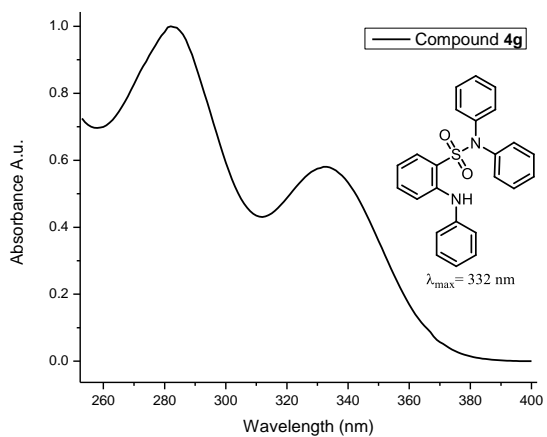
**Table 1.** Absorption, emission maxima and Stoke shift of the selected synthesized compounds

Product	Absorption $\lambda_{\max}$ (nm)	Emission $\lambda_{\max}$ (nm)	$\Delta\bar{\nu}$ ( $\text{cm}^{-1}$ )
3f	347	585	11724
4b	295	502	13977
4c	328	492	10162
4g	332	485	9501
4h	318	474	10349
4l	482	584	3622
5a	347	333, 448	4692
7a	289	418	10678
7b	319	449	9076

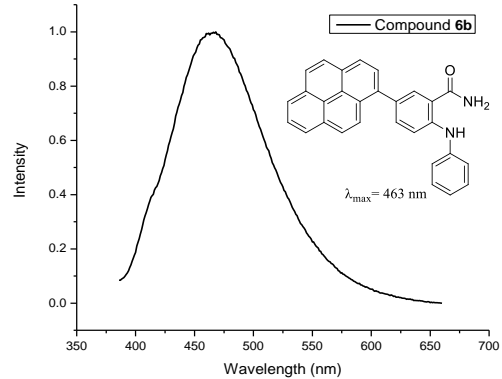
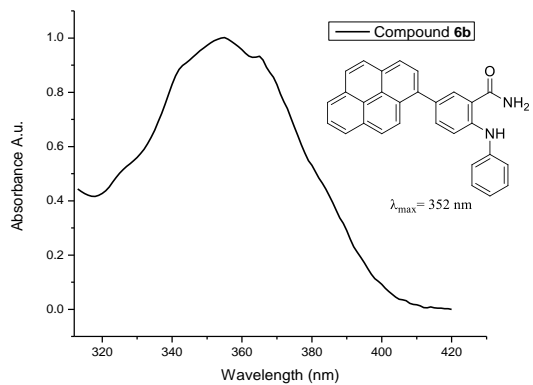
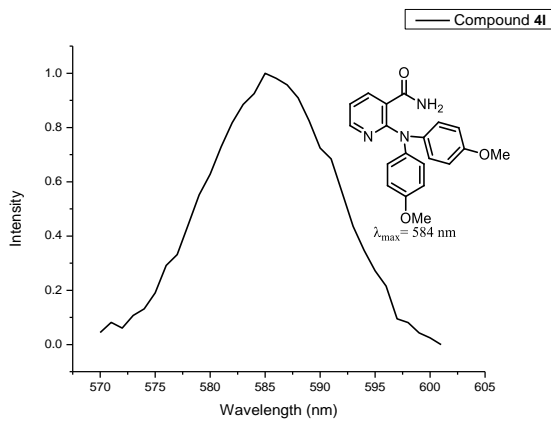
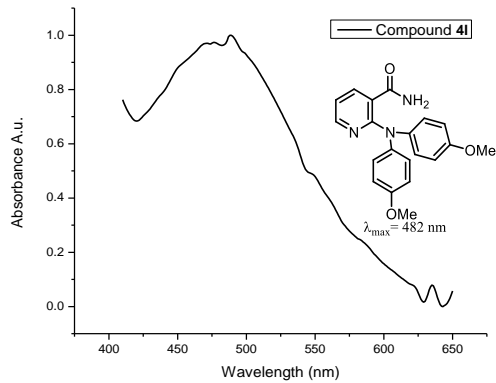
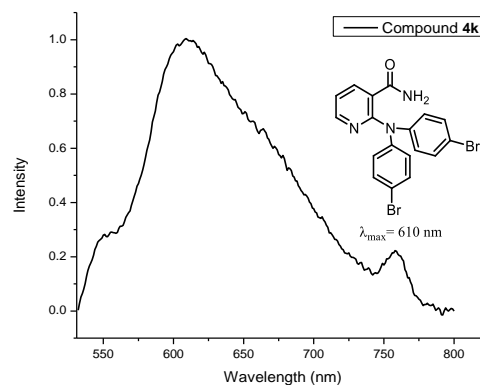
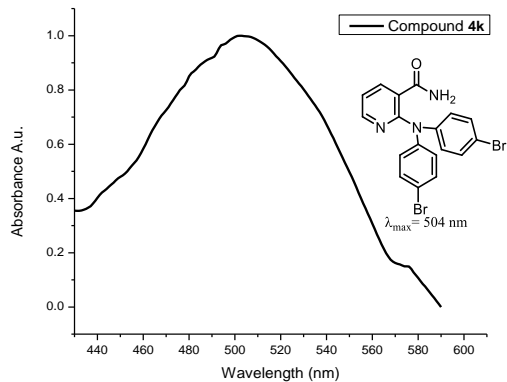
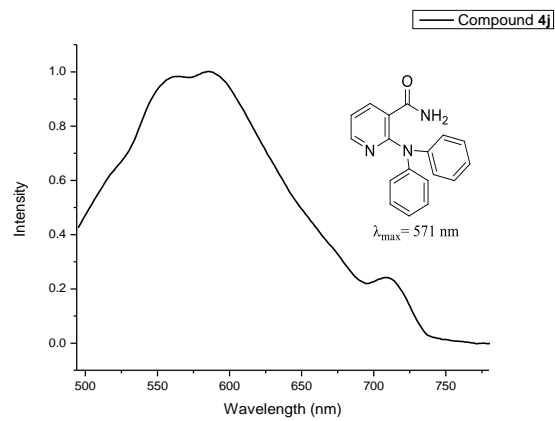
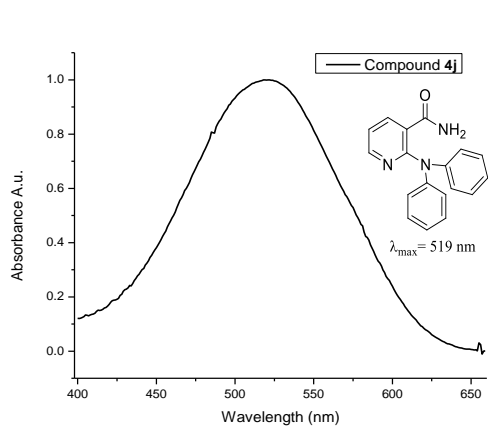
## 2. Copy of UV-Visible and Emission spectra

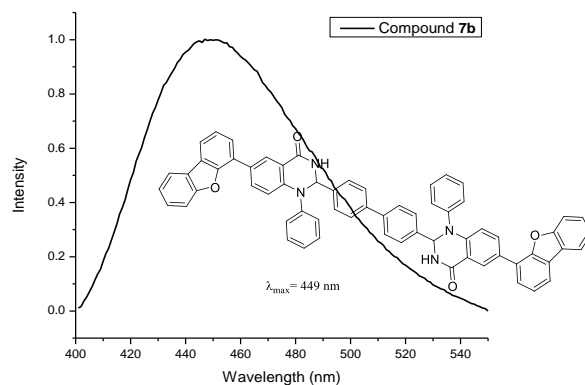
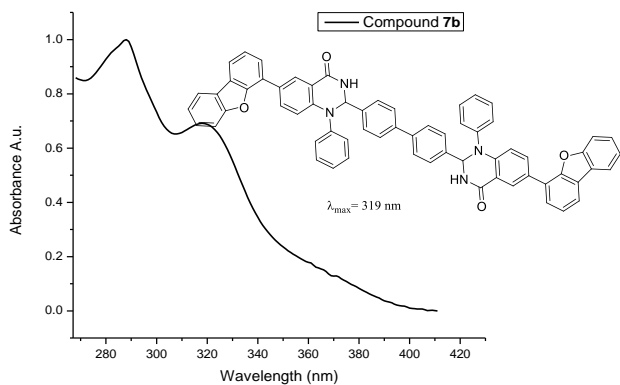
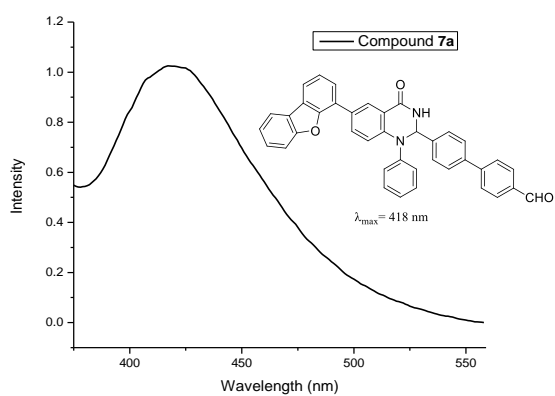
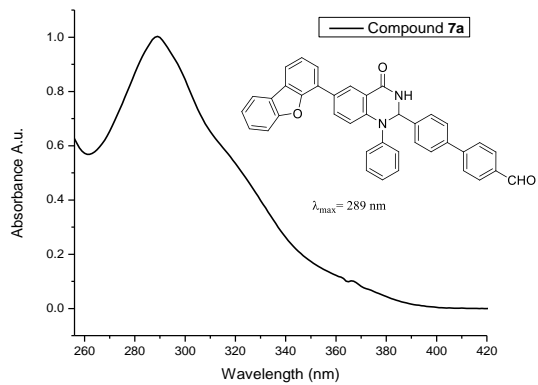
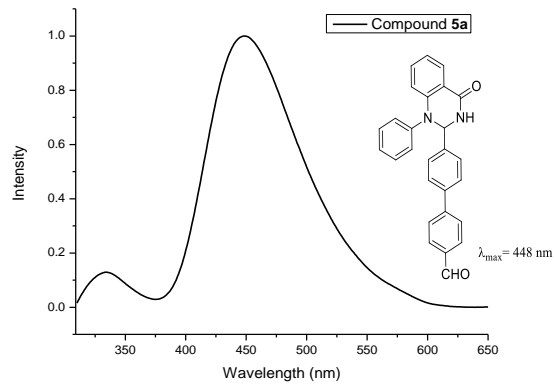
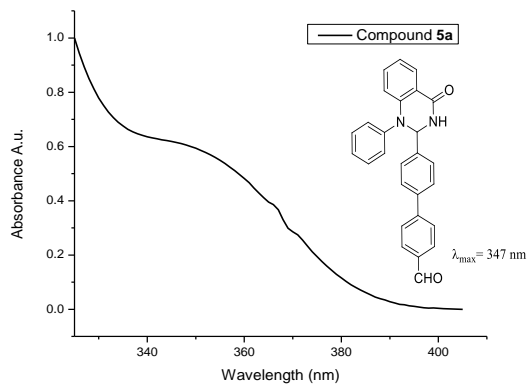










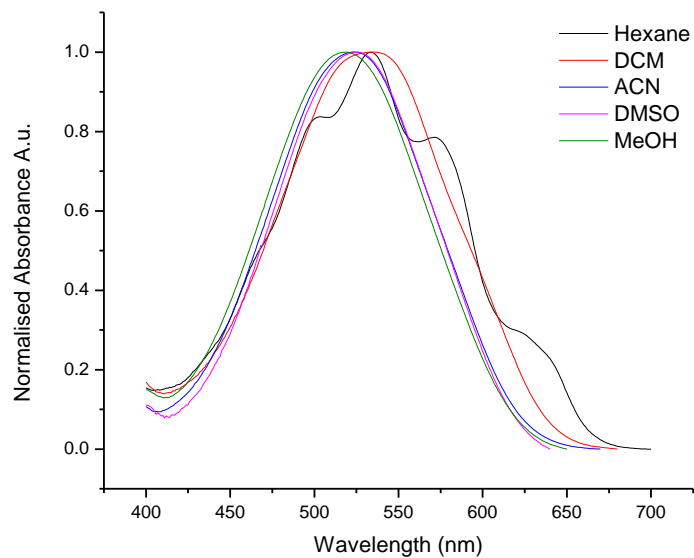


### 3. Crystallographic data of Compound 4a

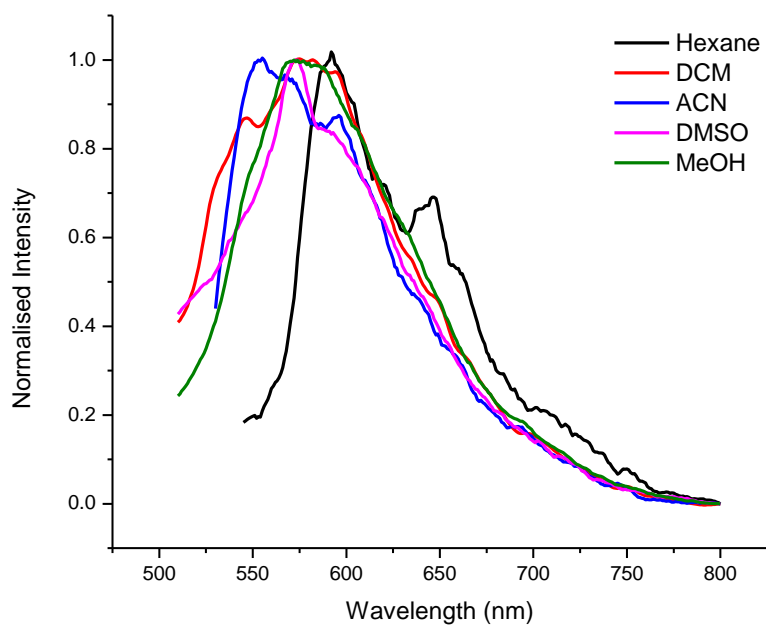
Table 1. Crystal data and structure refinement for Compound 4a.

Identification code	Compound 4a	
Empirical formula	C <sub>19</sub> H <sub>16</sub> N <sub>2</sub> O	
Formula weight	288.34	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.1292(7) Å	α = 84.328(3)°.
	b = 9.3744(7) Å	β = 88.471(3)°.
	c = 10.0457(6) Å	γ = 61.065(3)°.
Volume	748.50(9) Å <sup>3</sup>	
Z	2	
Density (calculated)	1.279 Mg/m <sup>3</sup>	
Absorption coefficient	0.080 mm <sup>-1</sup>	
F(000)	304	
Crystal size	0.150 x 0.150 x 0.100 mm <sup>3</sup>	
Theta range for data collection	2.495 to 25.999°.	
Index ranges	-11 ≤ h ≤ 11, -11 ≤ k ≤ 11, -12 ≤ l ≤ 12	
Reflections collected	21188	
Independent reflections	2919 [R(int) = 0.0351]	
Completeness to theta = 25.242°	99.2 %	
Absorption correction	Multi-scan	
Max. and min. transmission	0.7462 and 0.7122	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	2919 / 0 / 208	
Goodness-of-fit on F <sup>2</sup>	1.044	
Final R indices [I > 2σ(I)]	R1 = 0.0394, wR2 = 0.0925	
R indices (all data)	R1 = 0.0624, wR2 = 0.1126	
Extinction coefficient	0.034(4)	
Largest diff. peak and hole	0.230 and -0.184 e.Å <sup>-3</sup>	

#### 4. Solvatochromic effect of compound 4j



Solvatochromism of Compound 4j (Absorption)



Solvatochromism of Compound 4j (Emission)