Electronic Supplementary Material (ESI) for New Journal of Chemistry.

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

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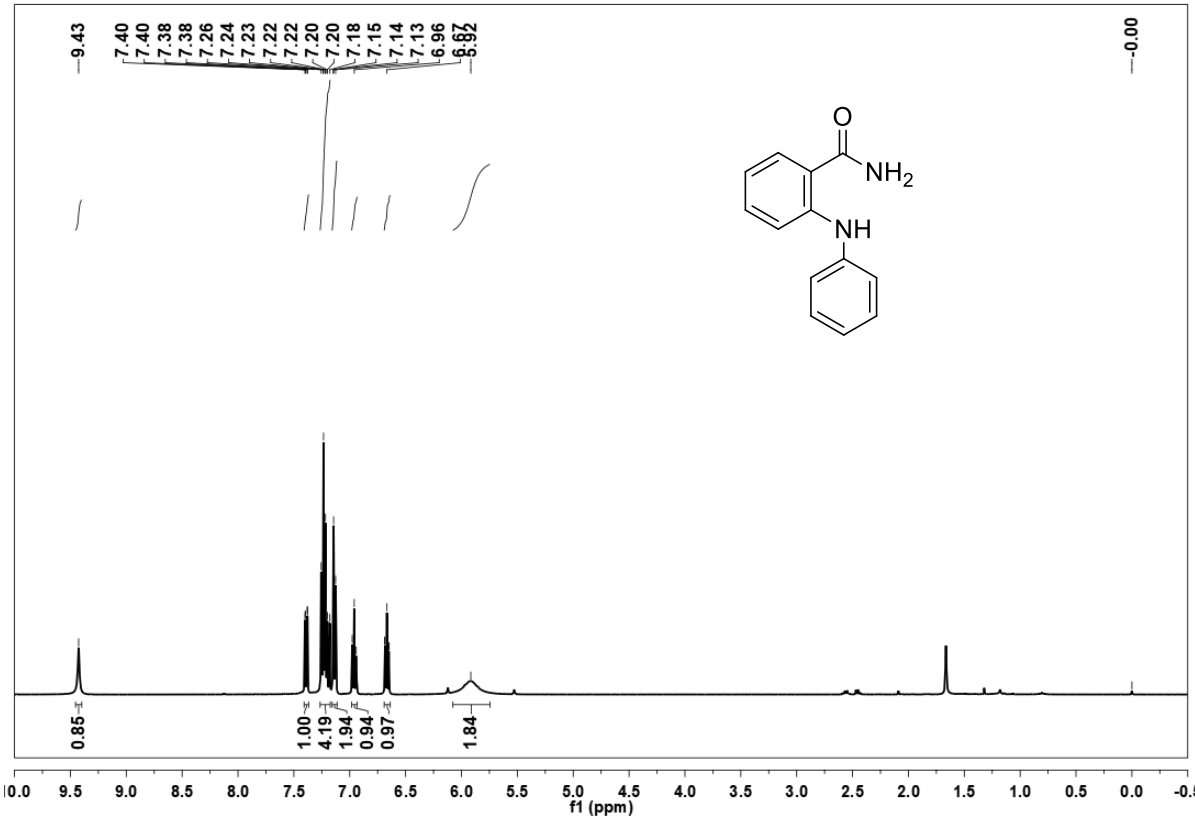
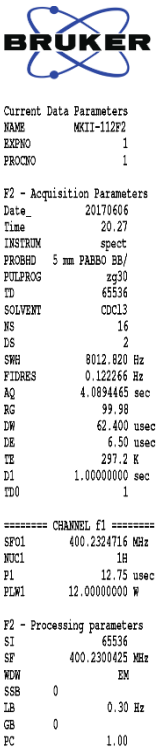
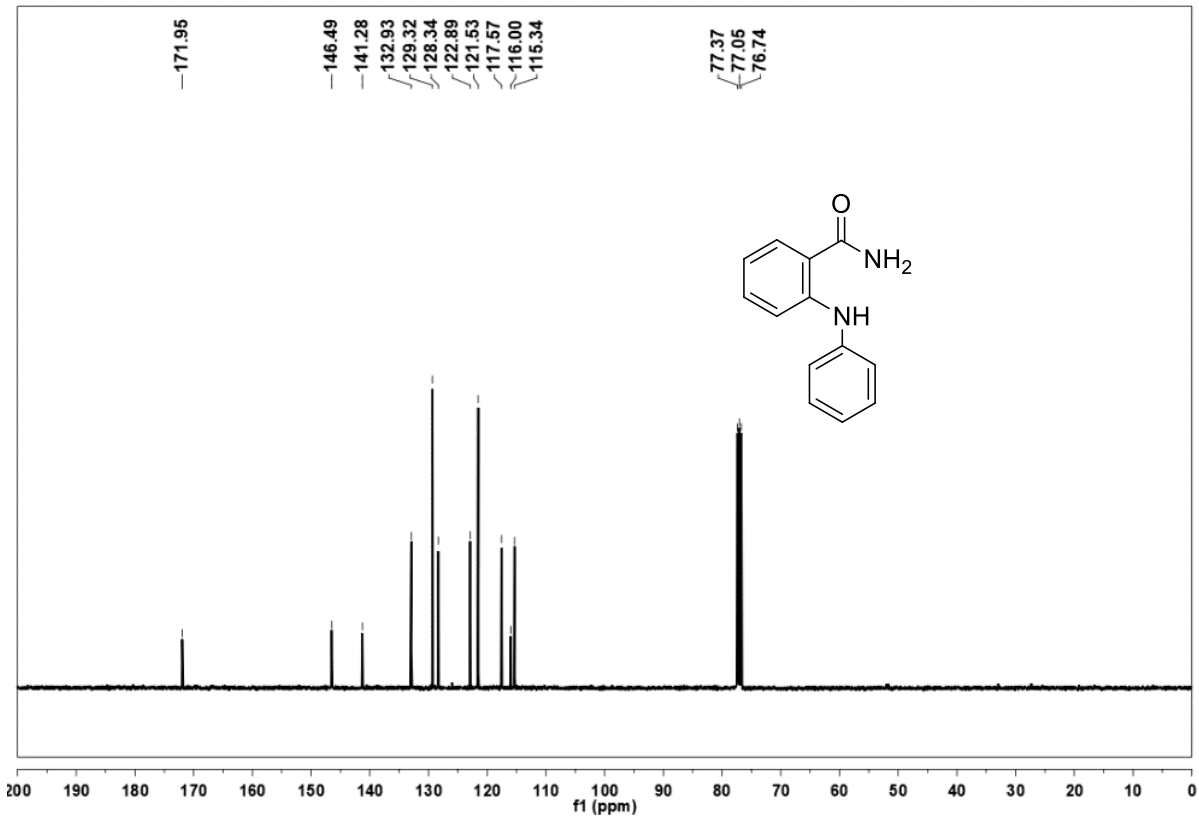
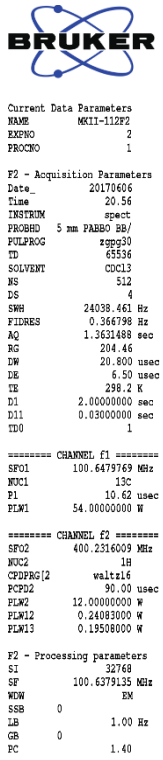
Copies of NMR and HRMS Spectra





^{1}H NMR Spectrum of Compound **3a**





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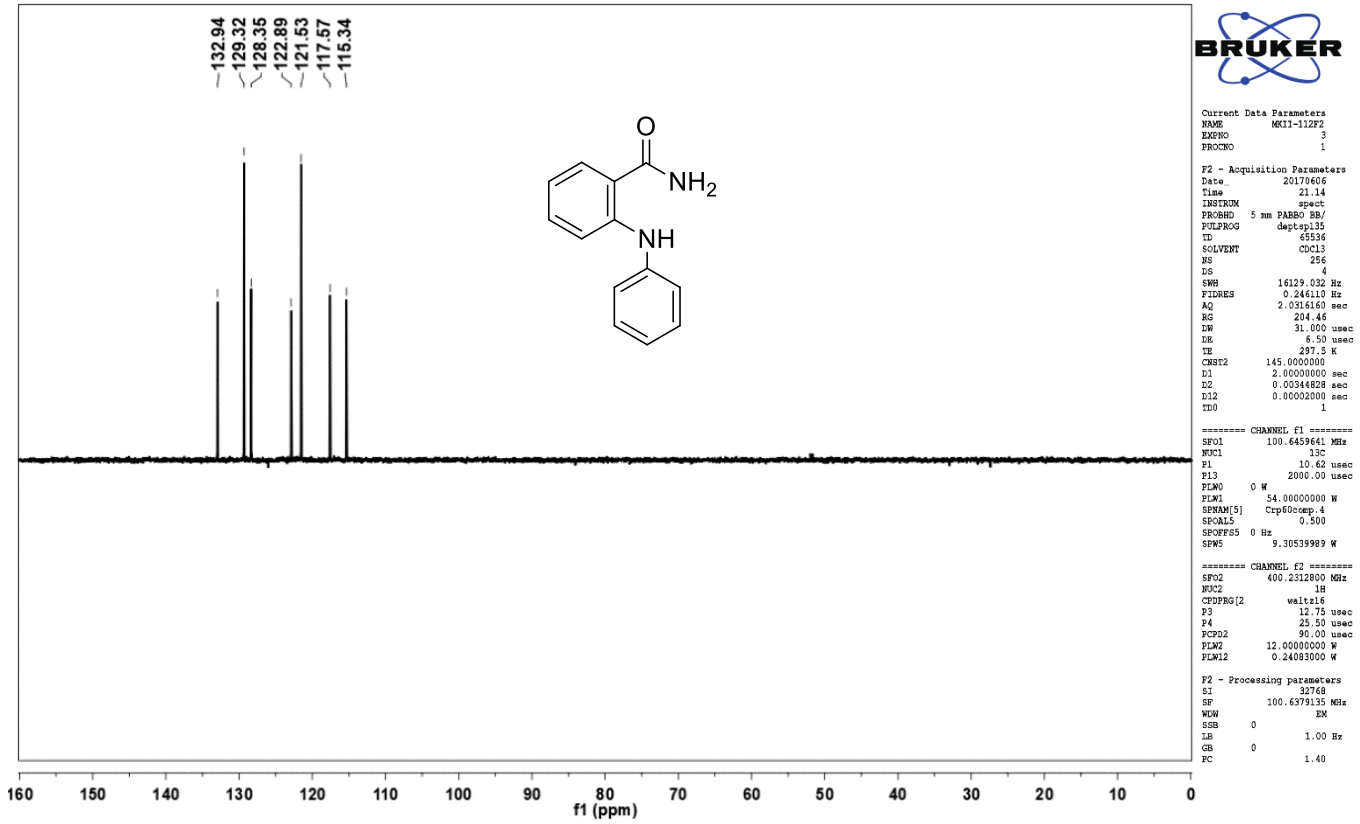

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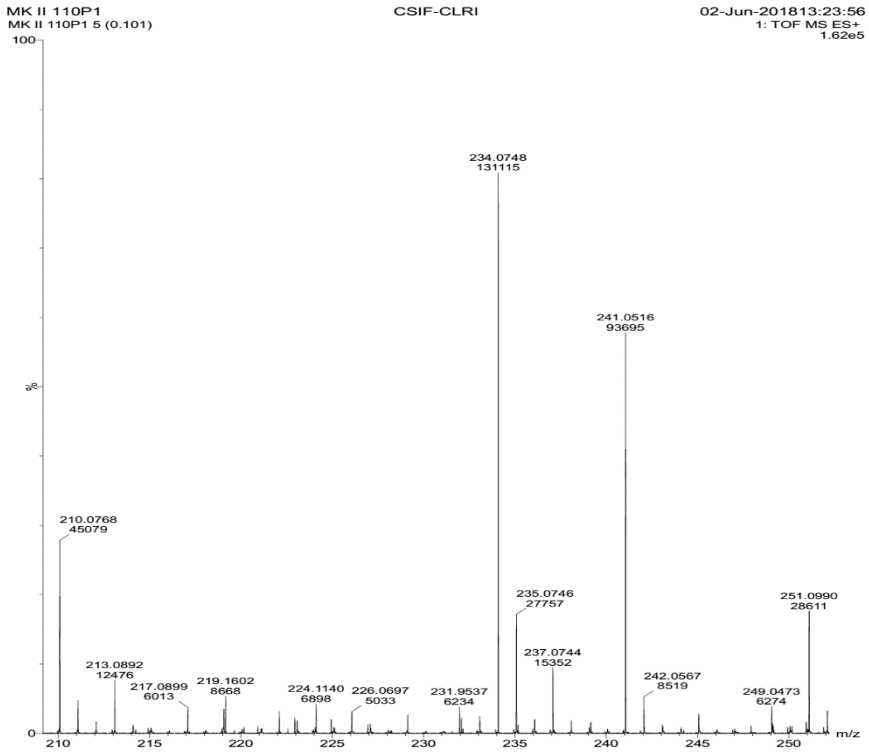

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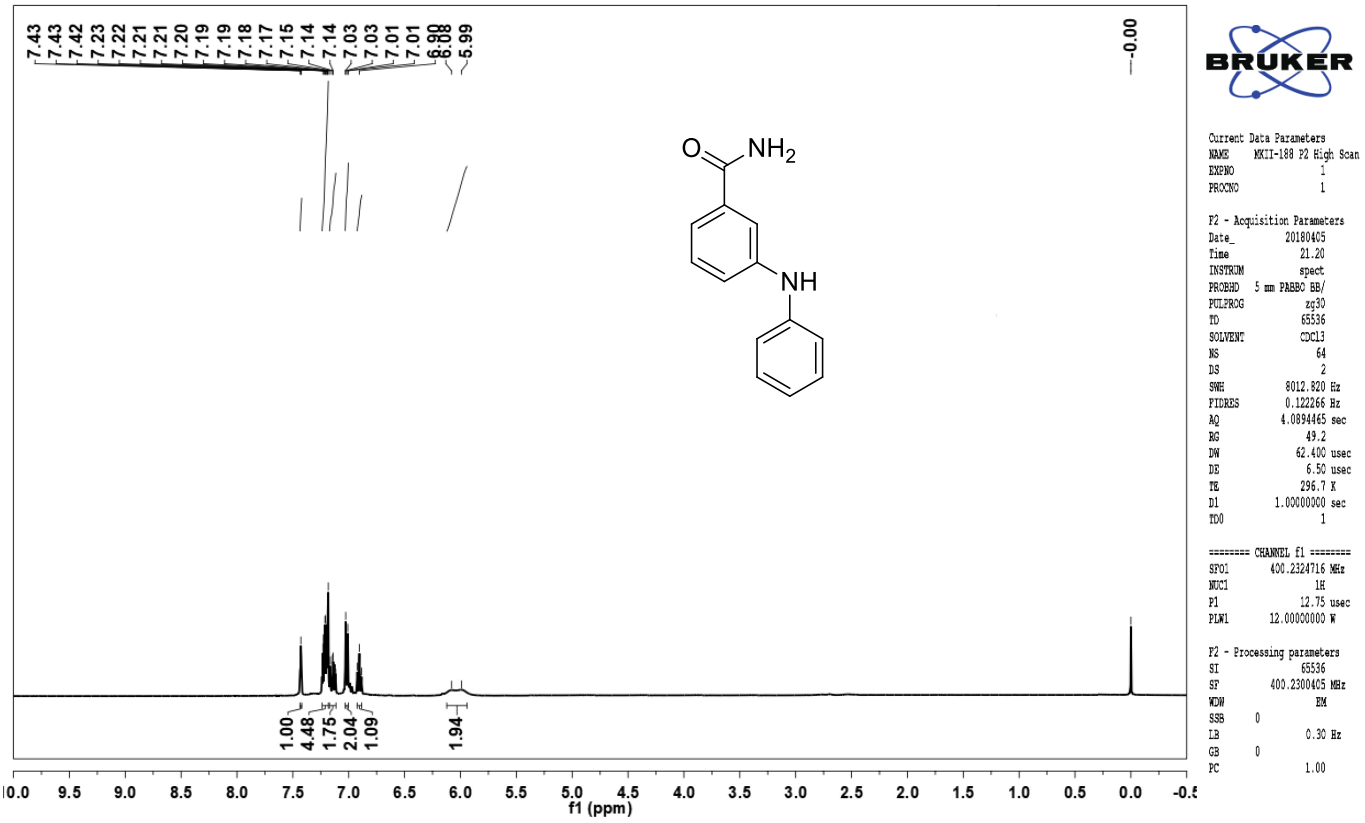

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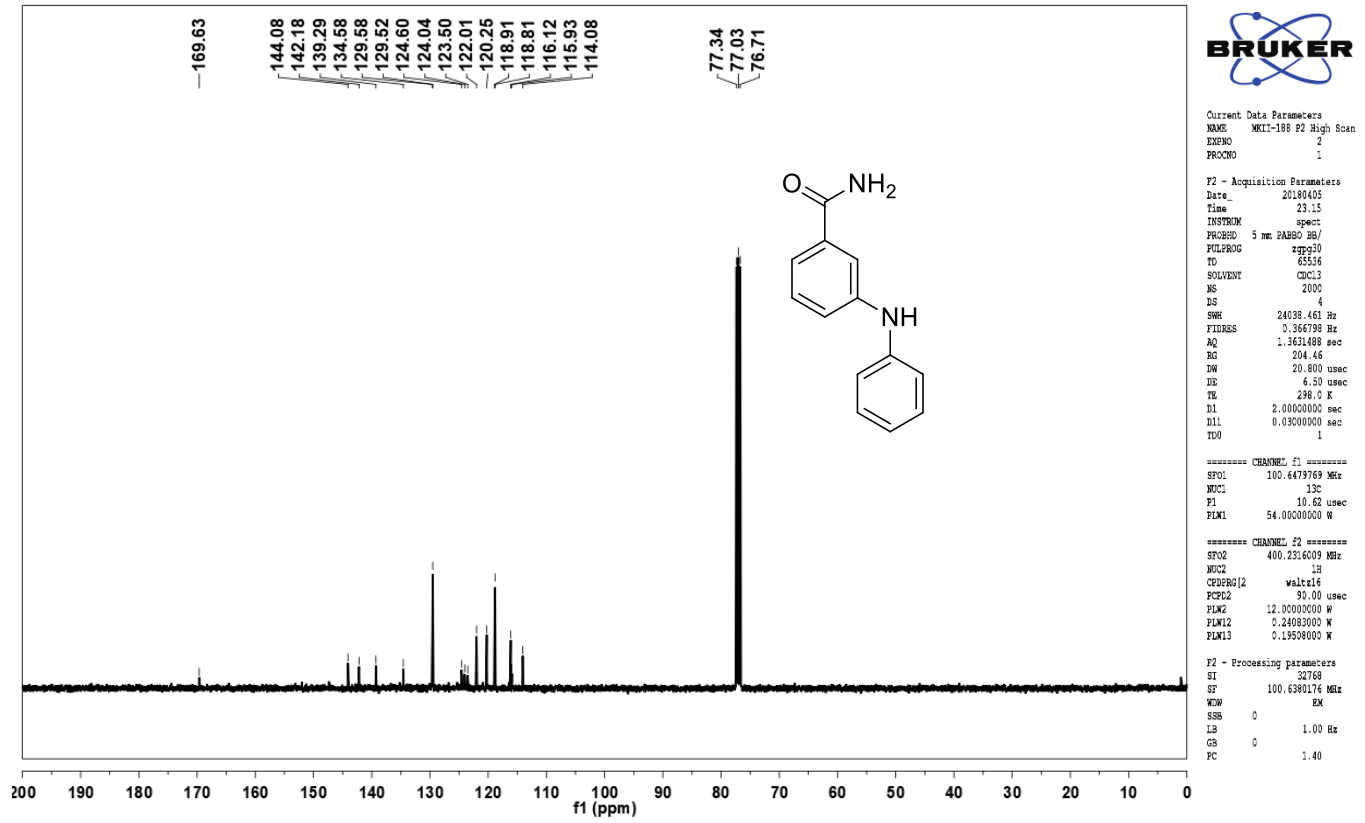

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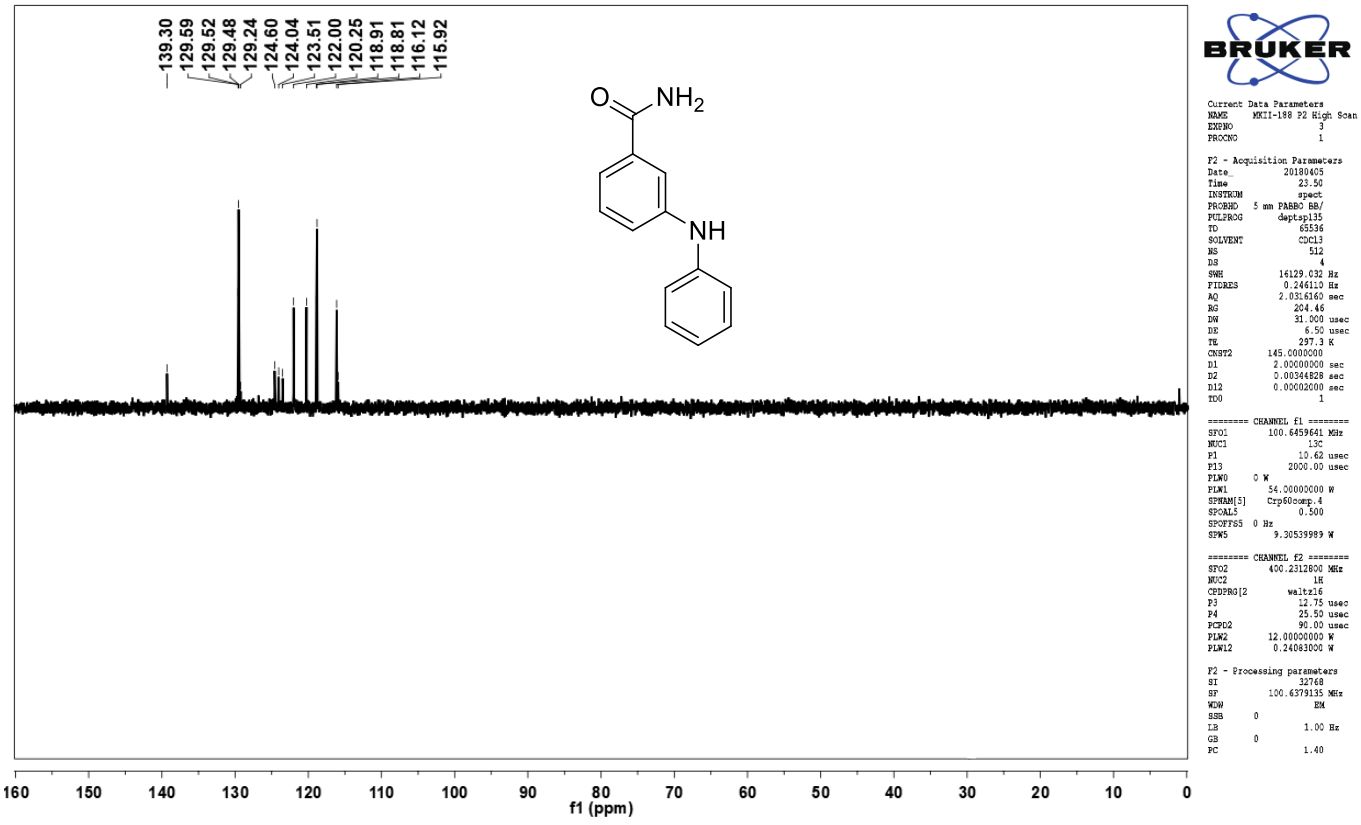

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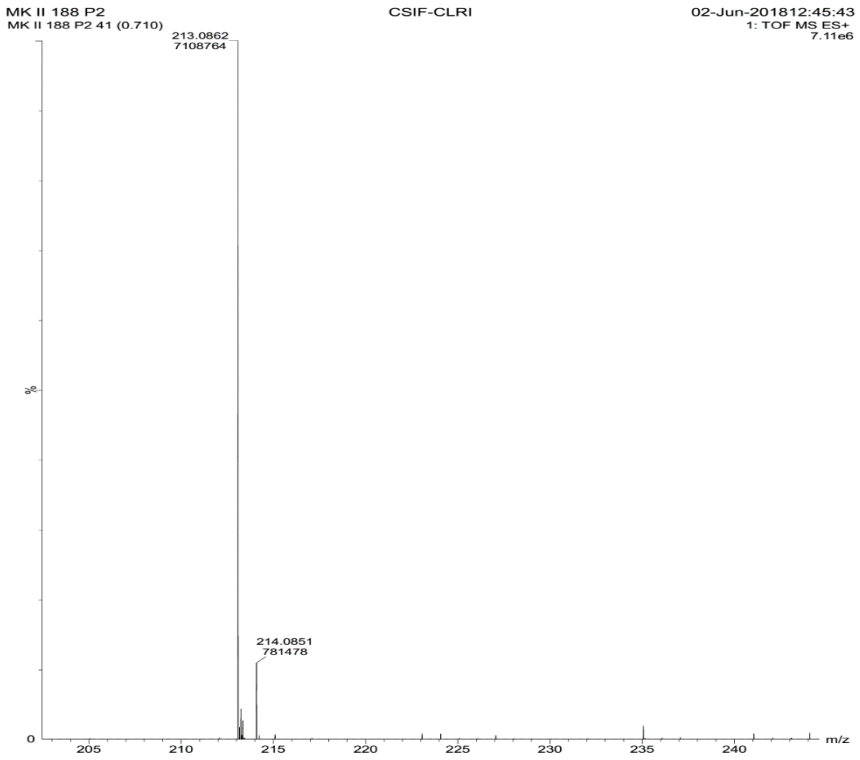

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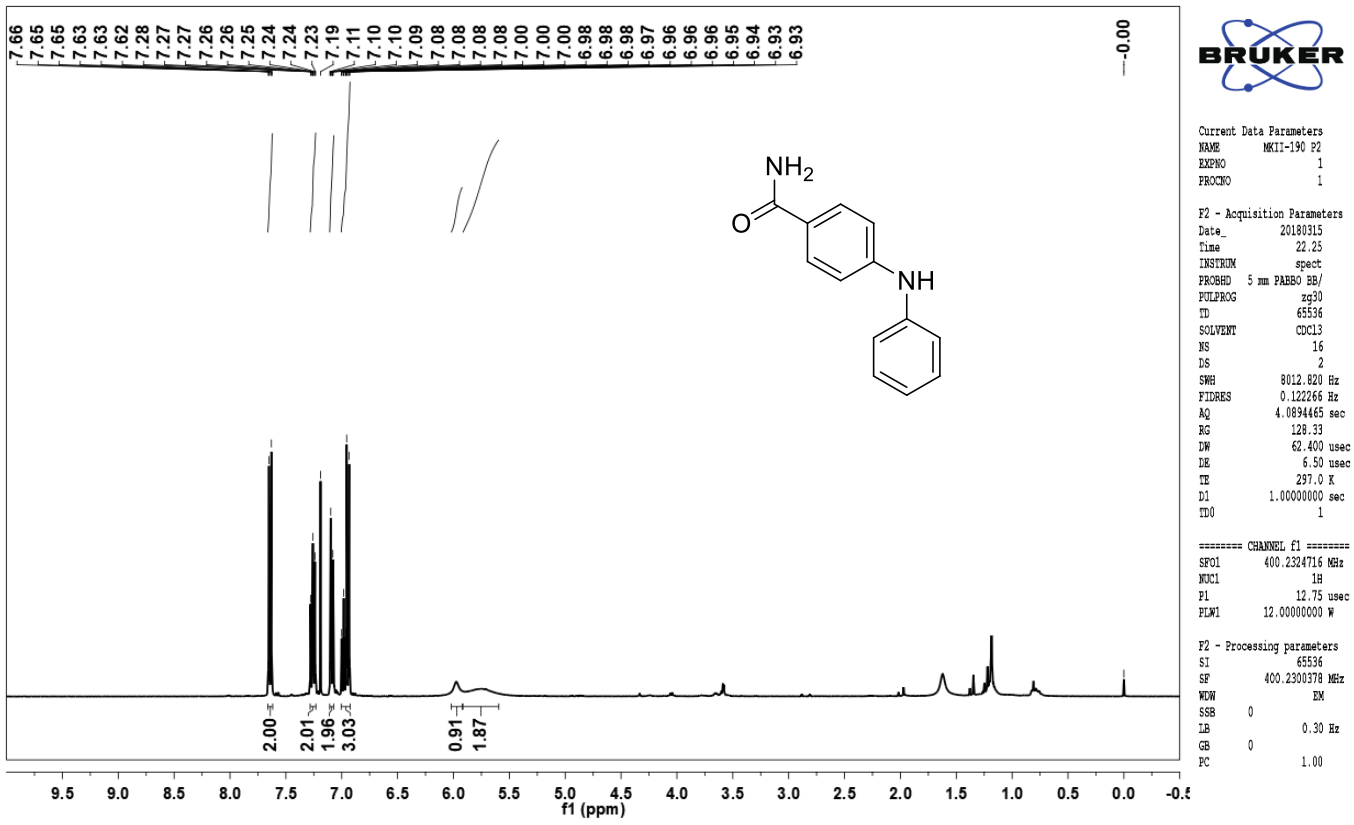

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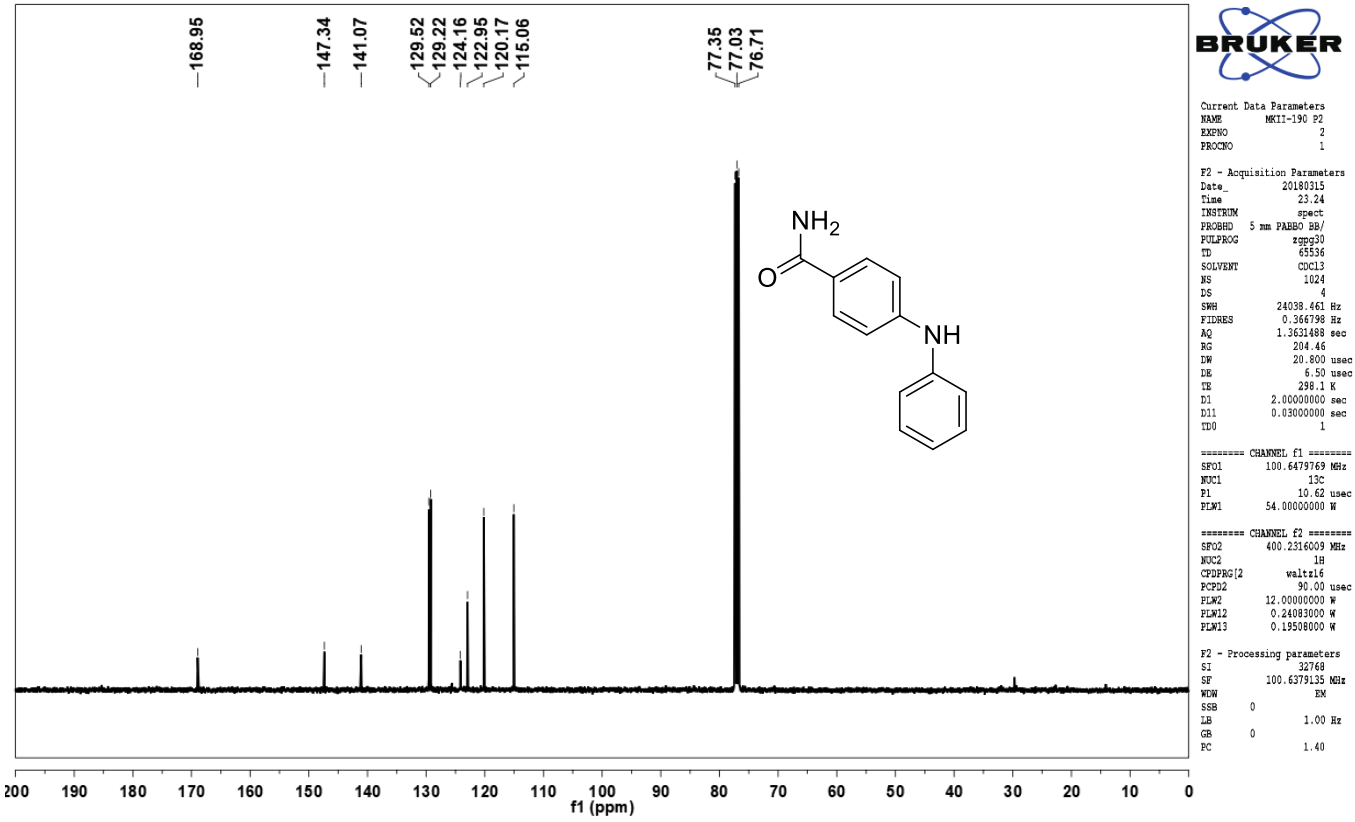

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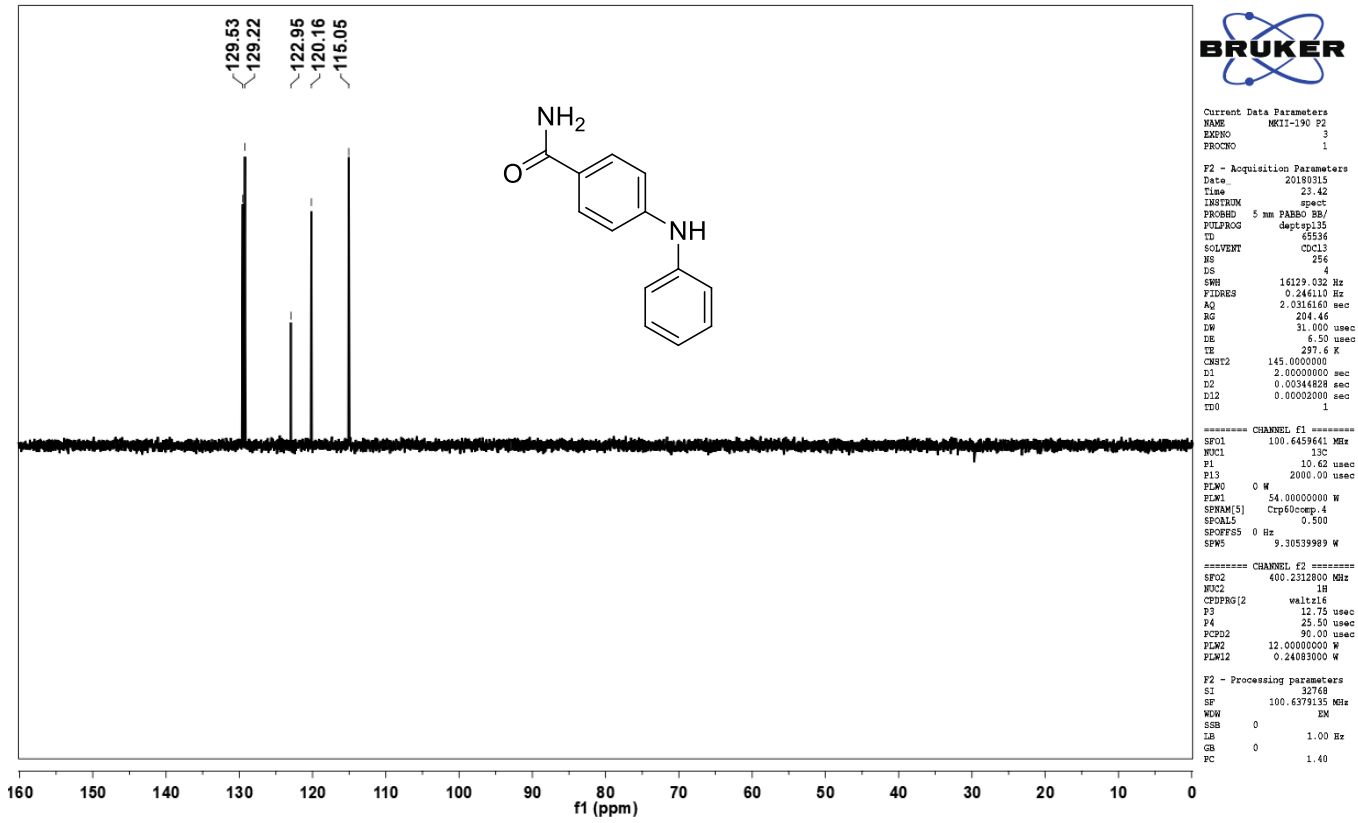

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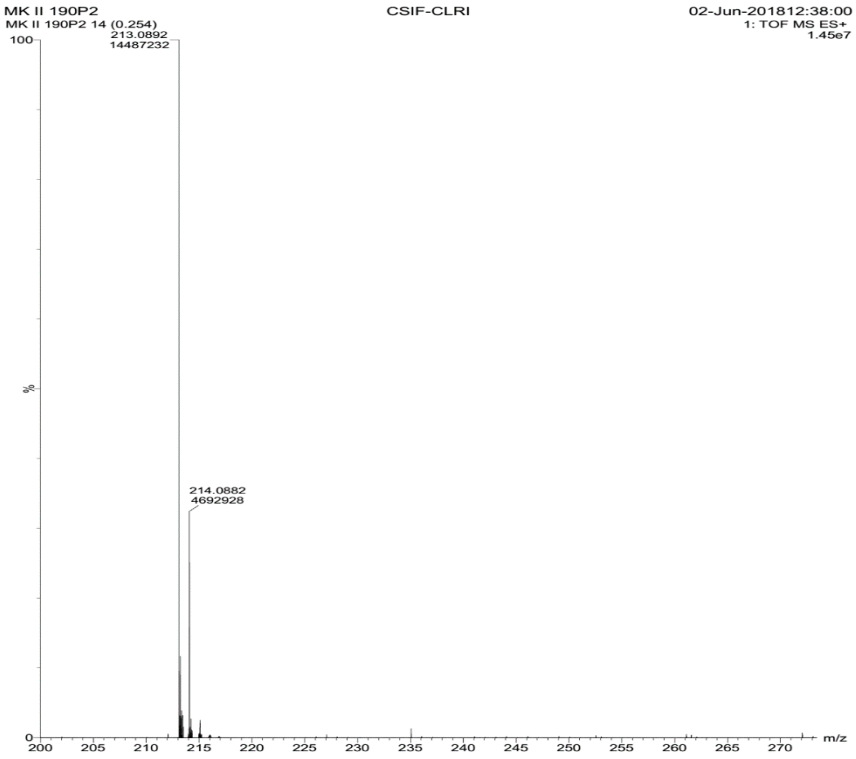

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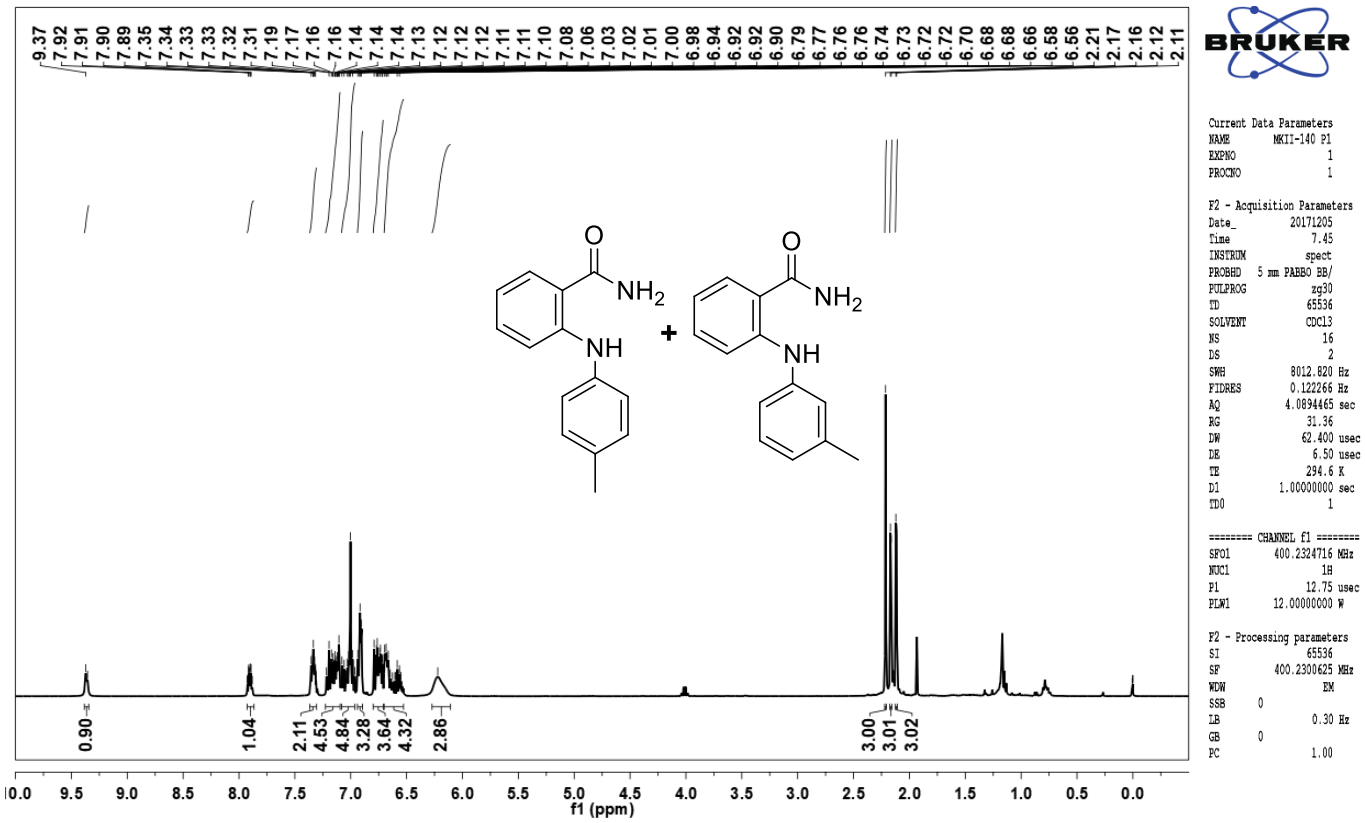

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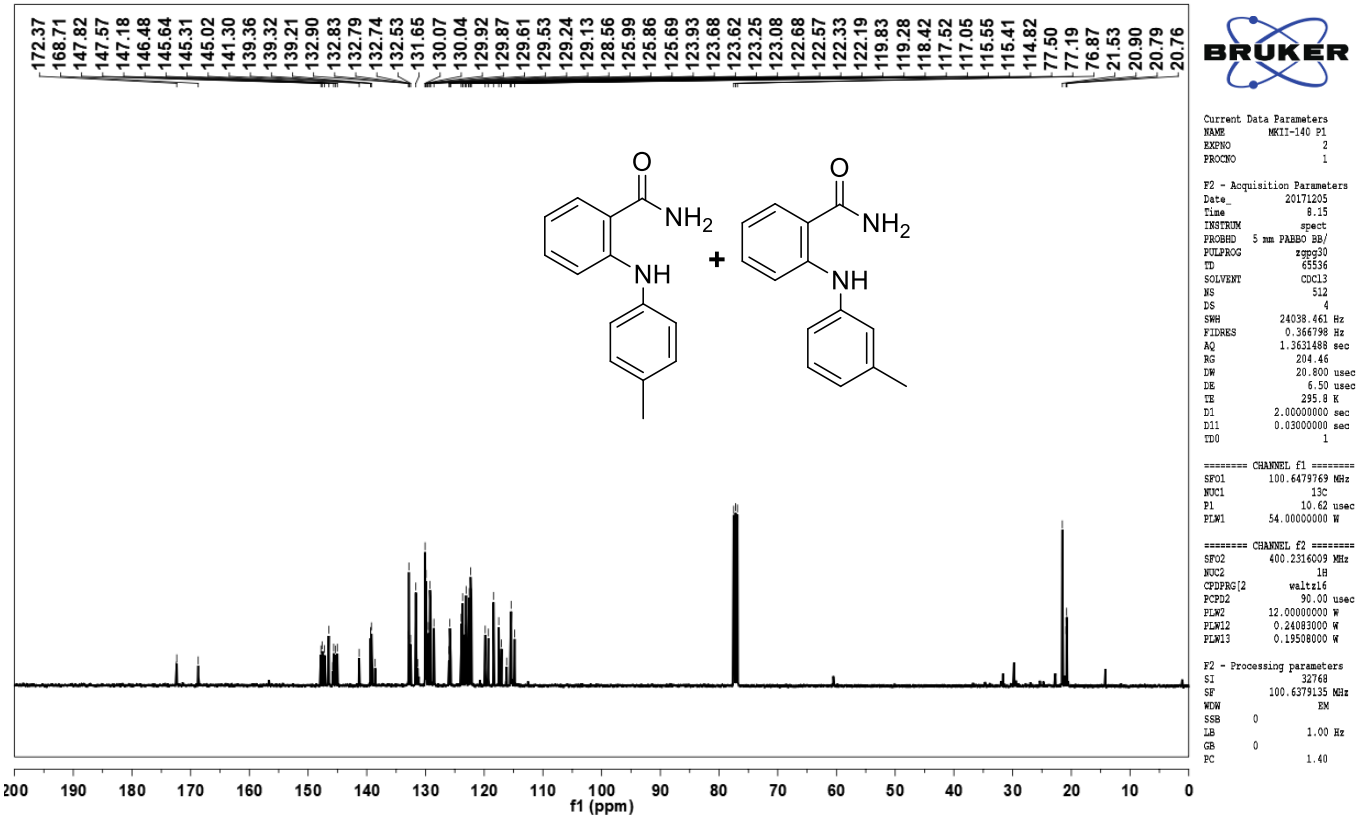

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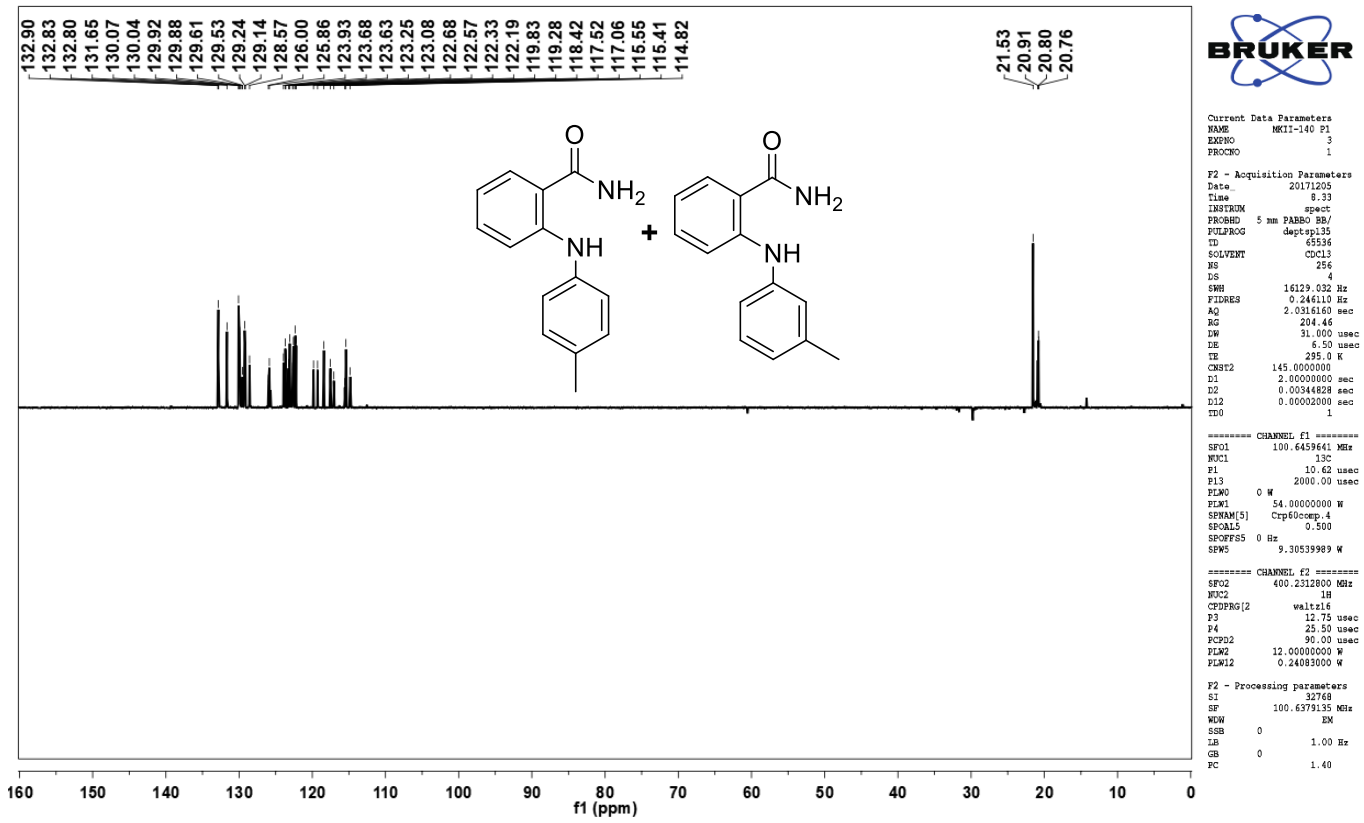

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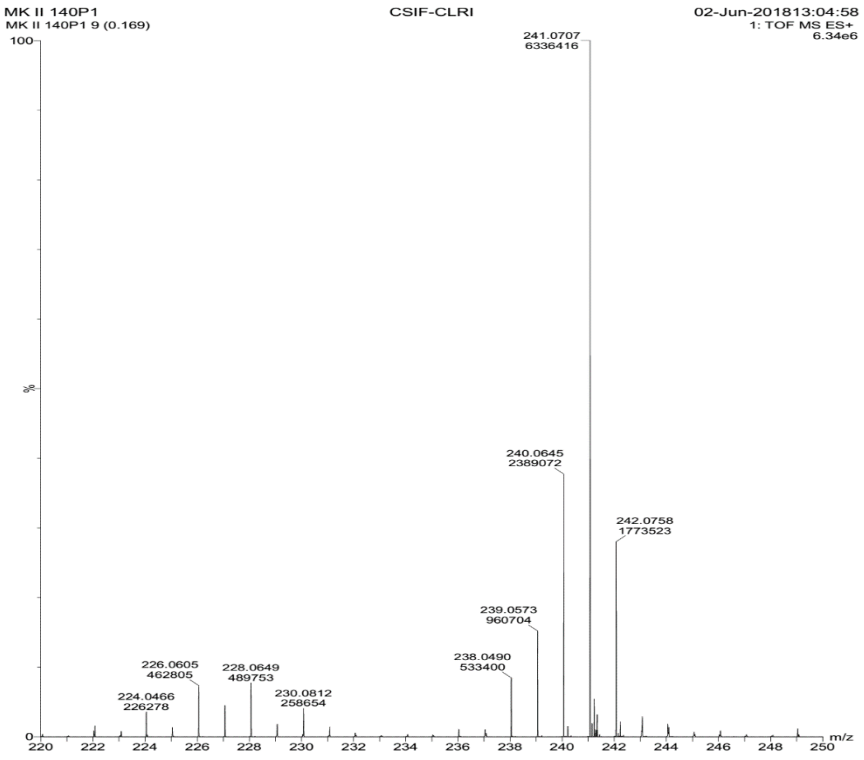

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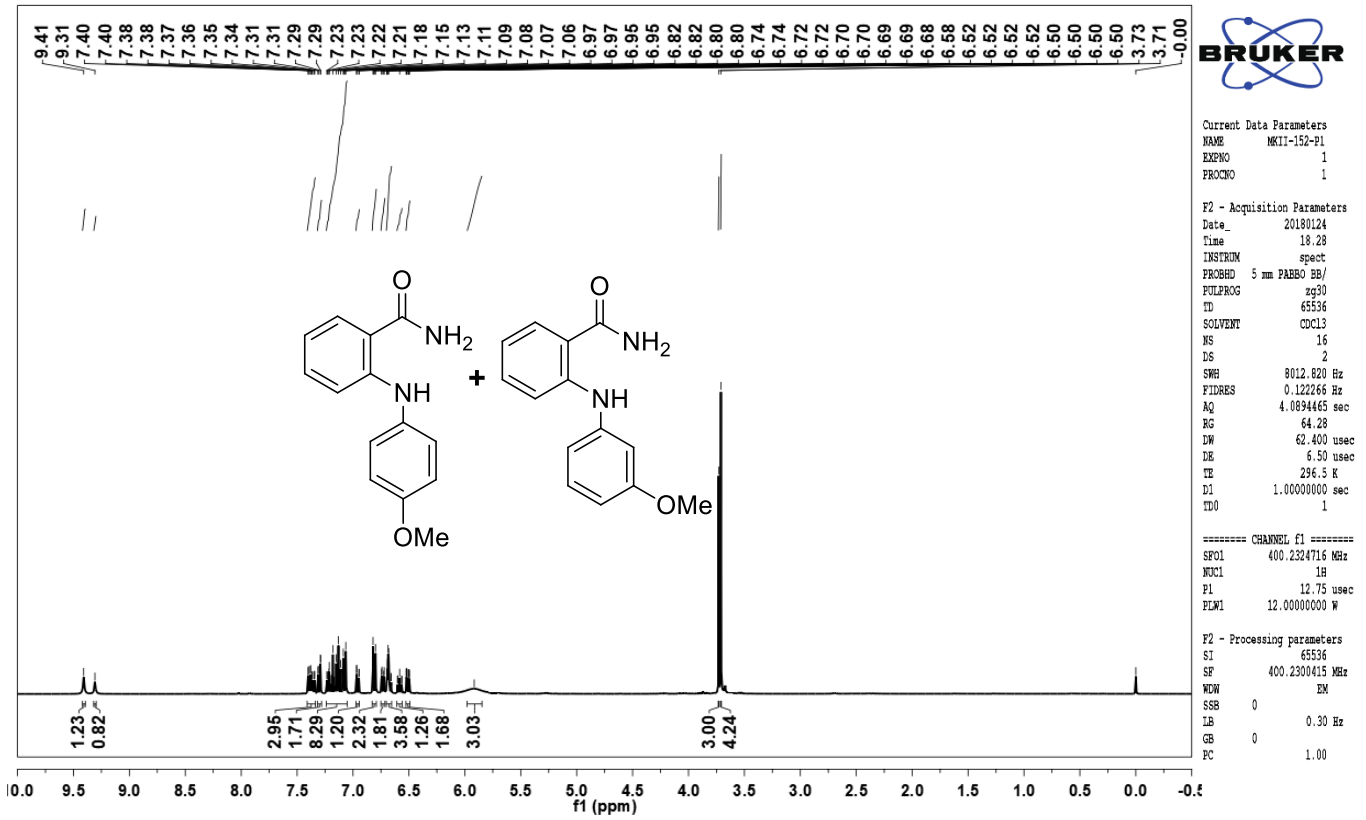

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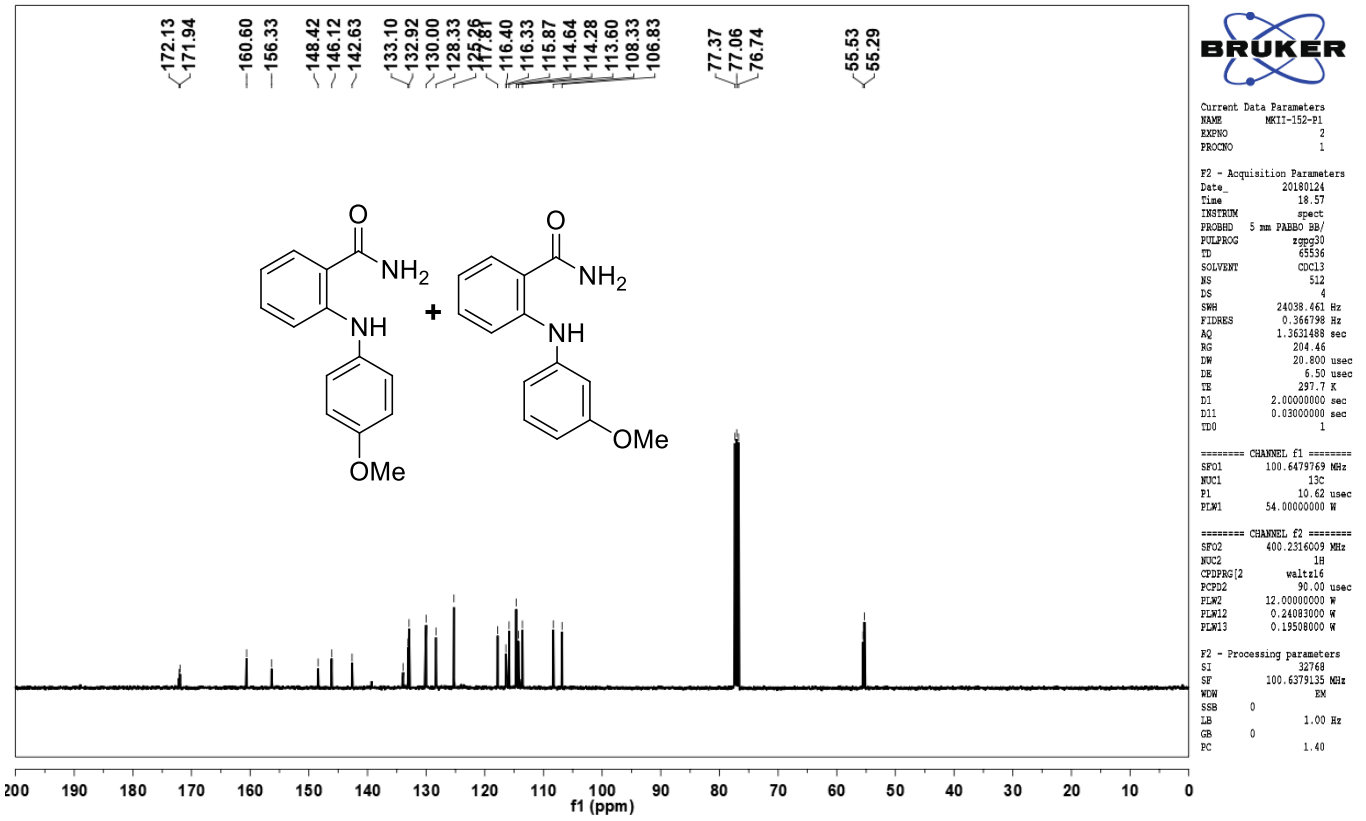

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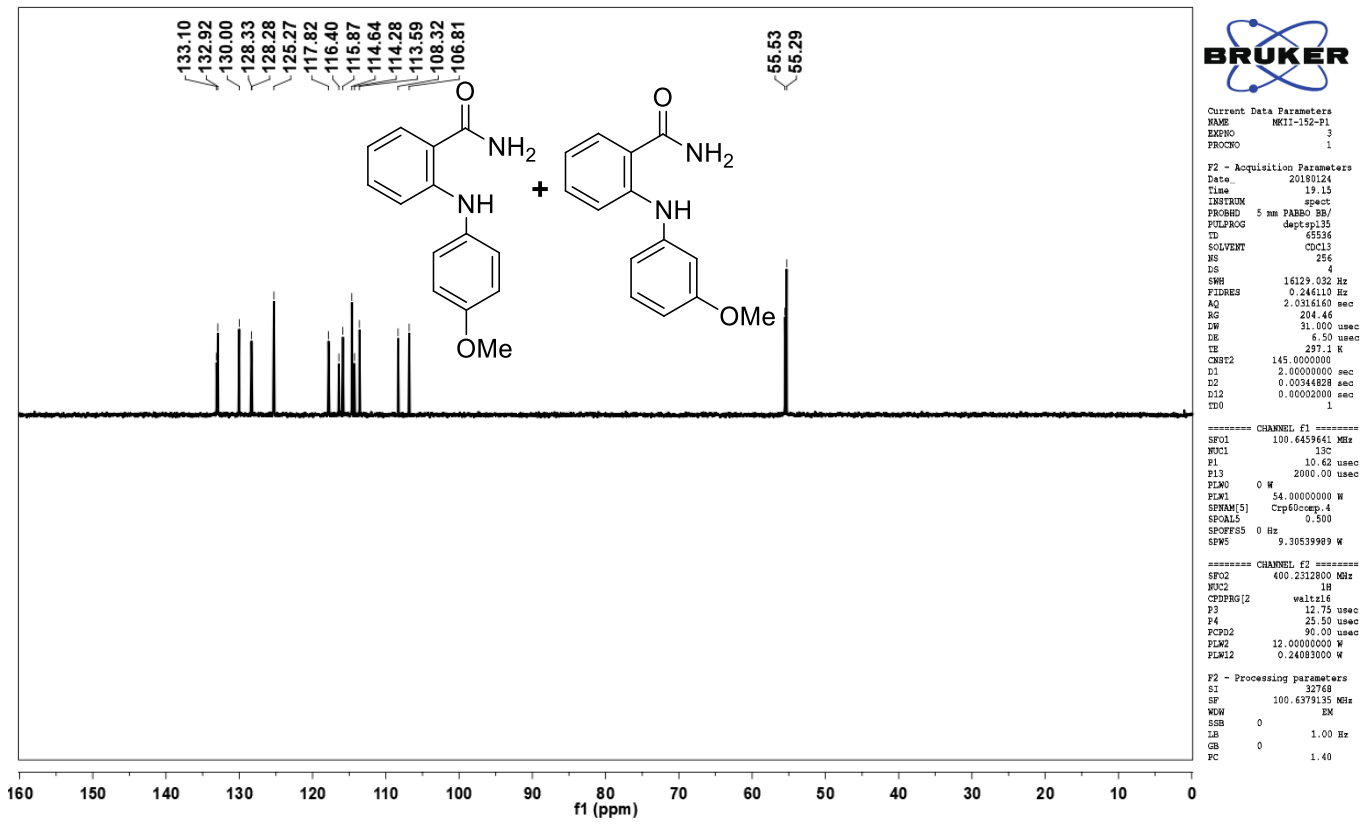

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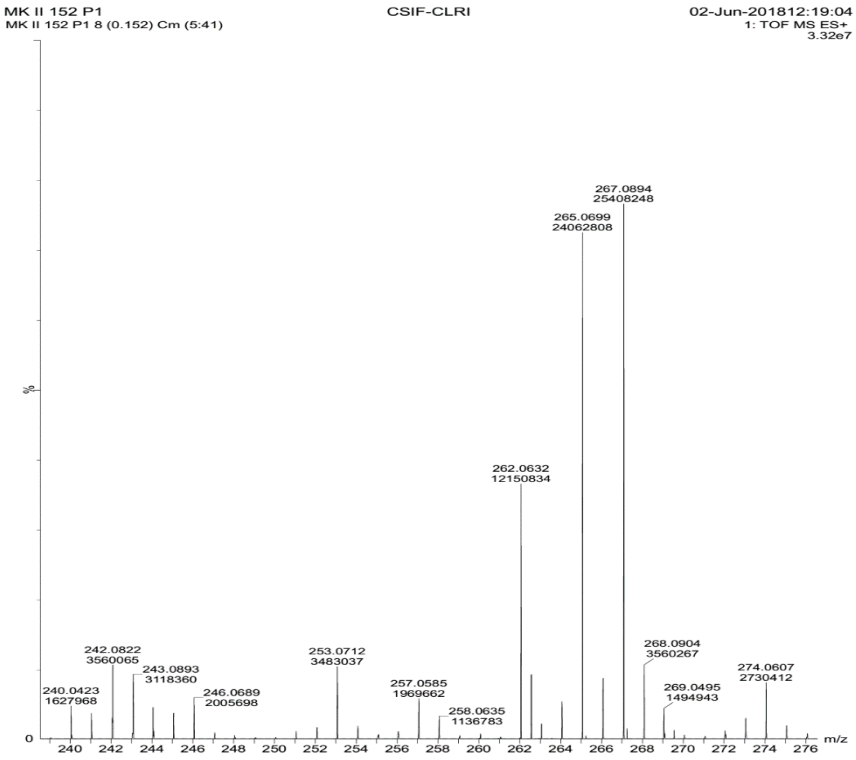

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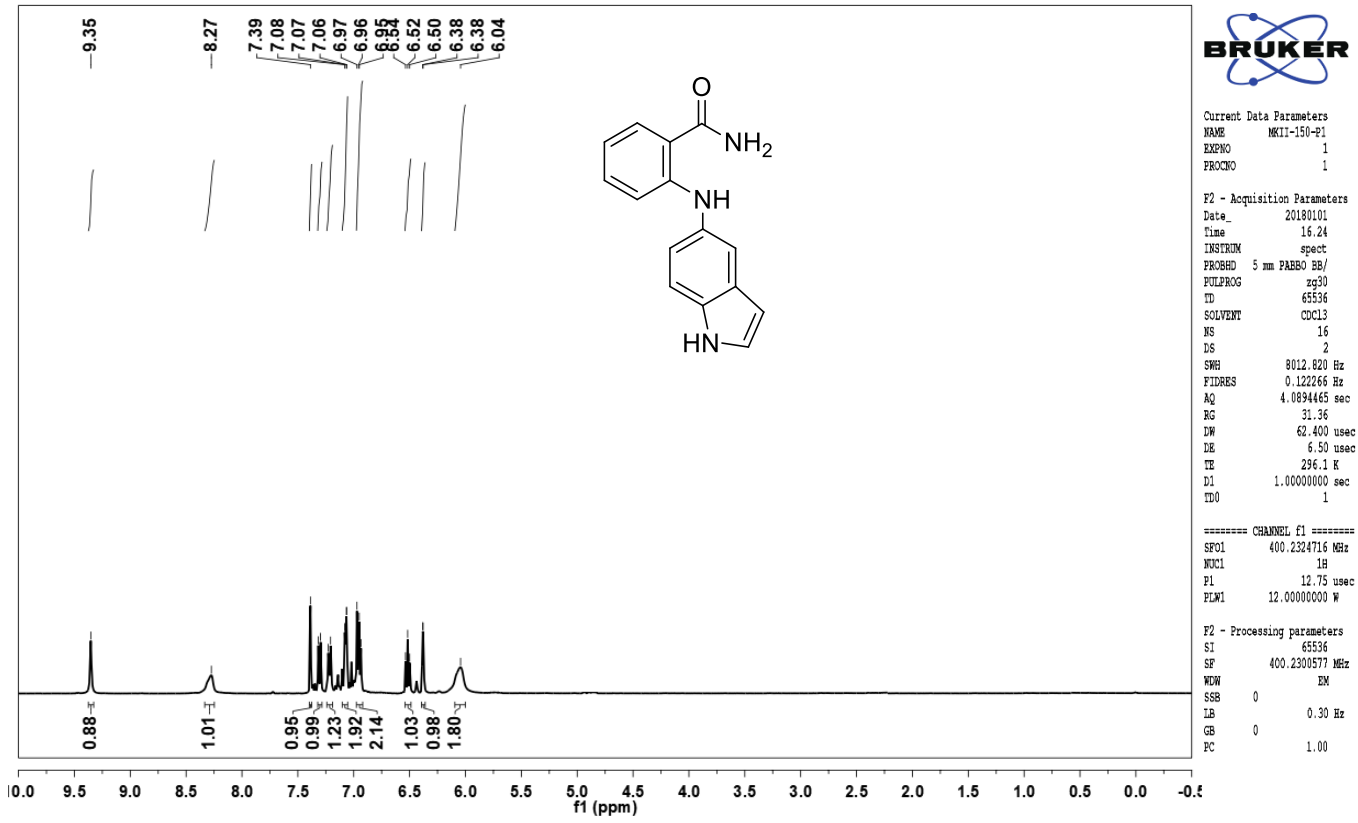

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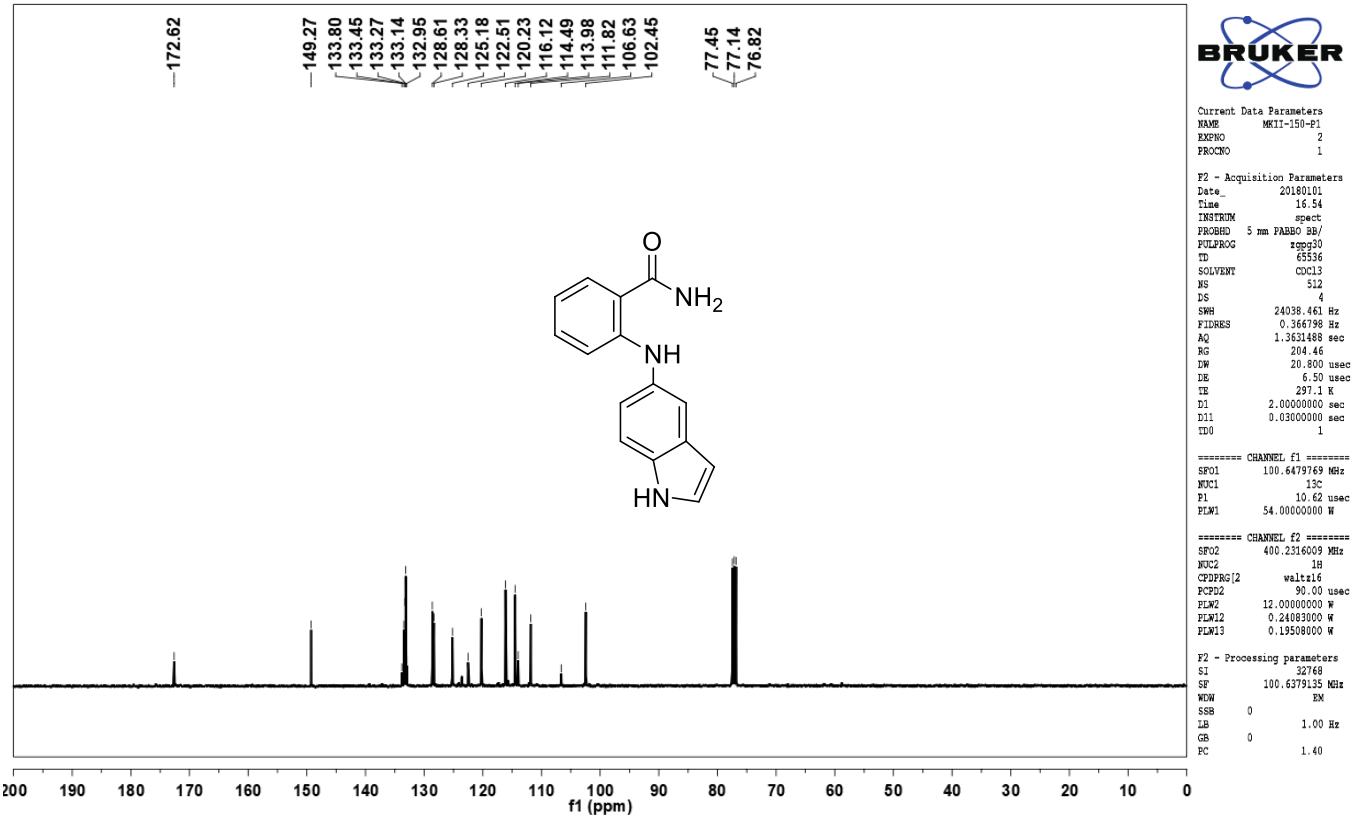

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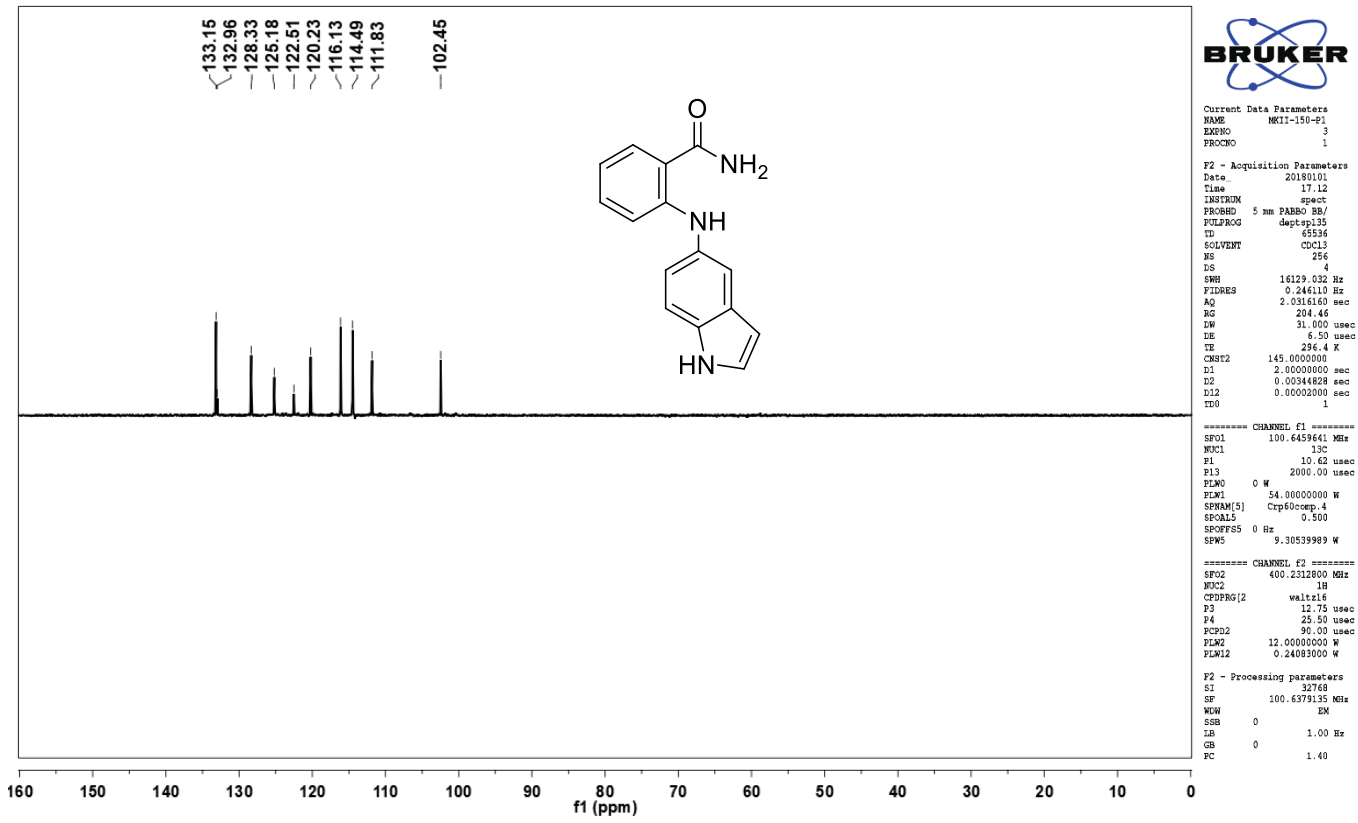

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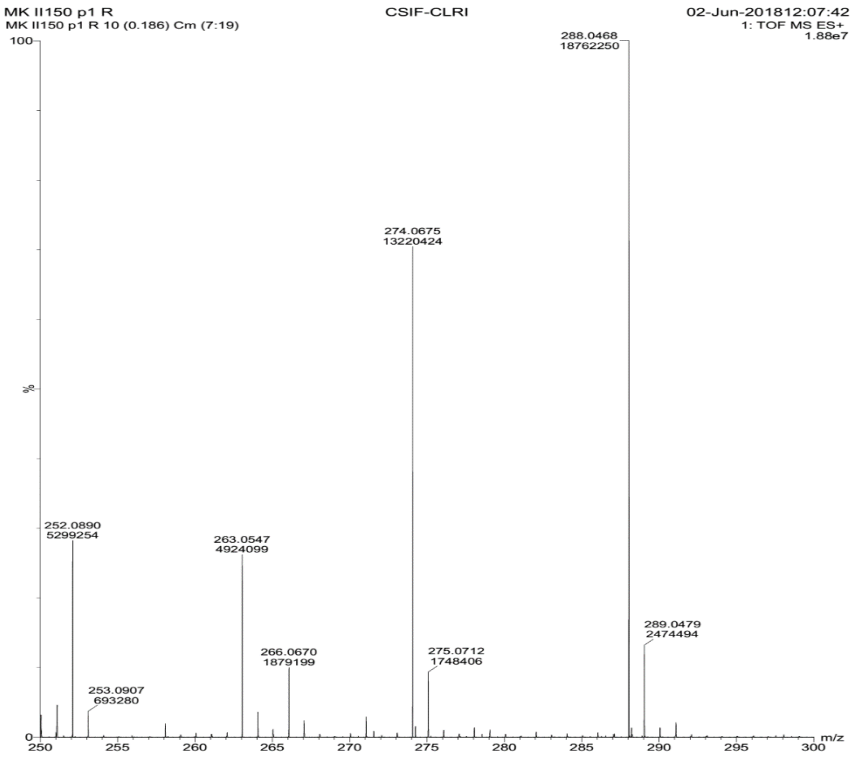

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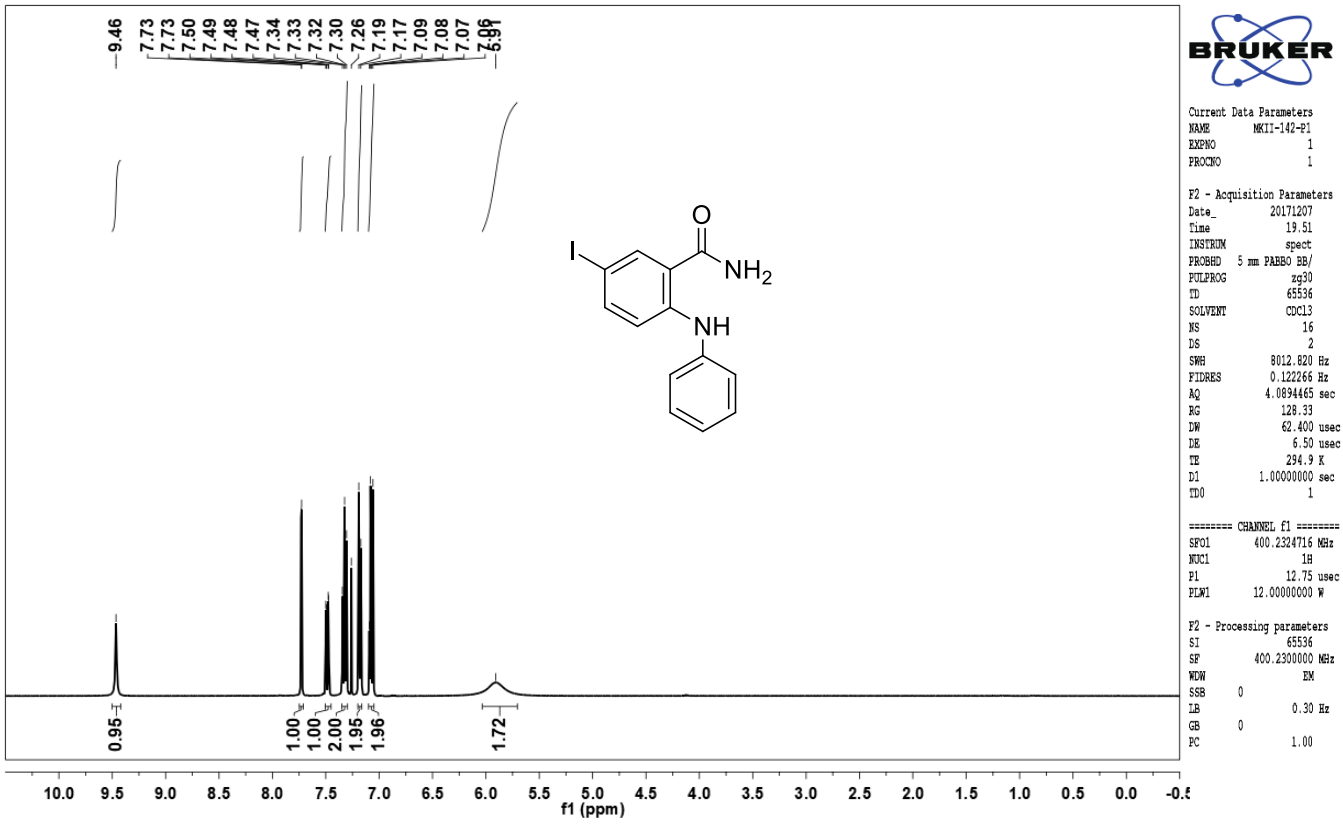

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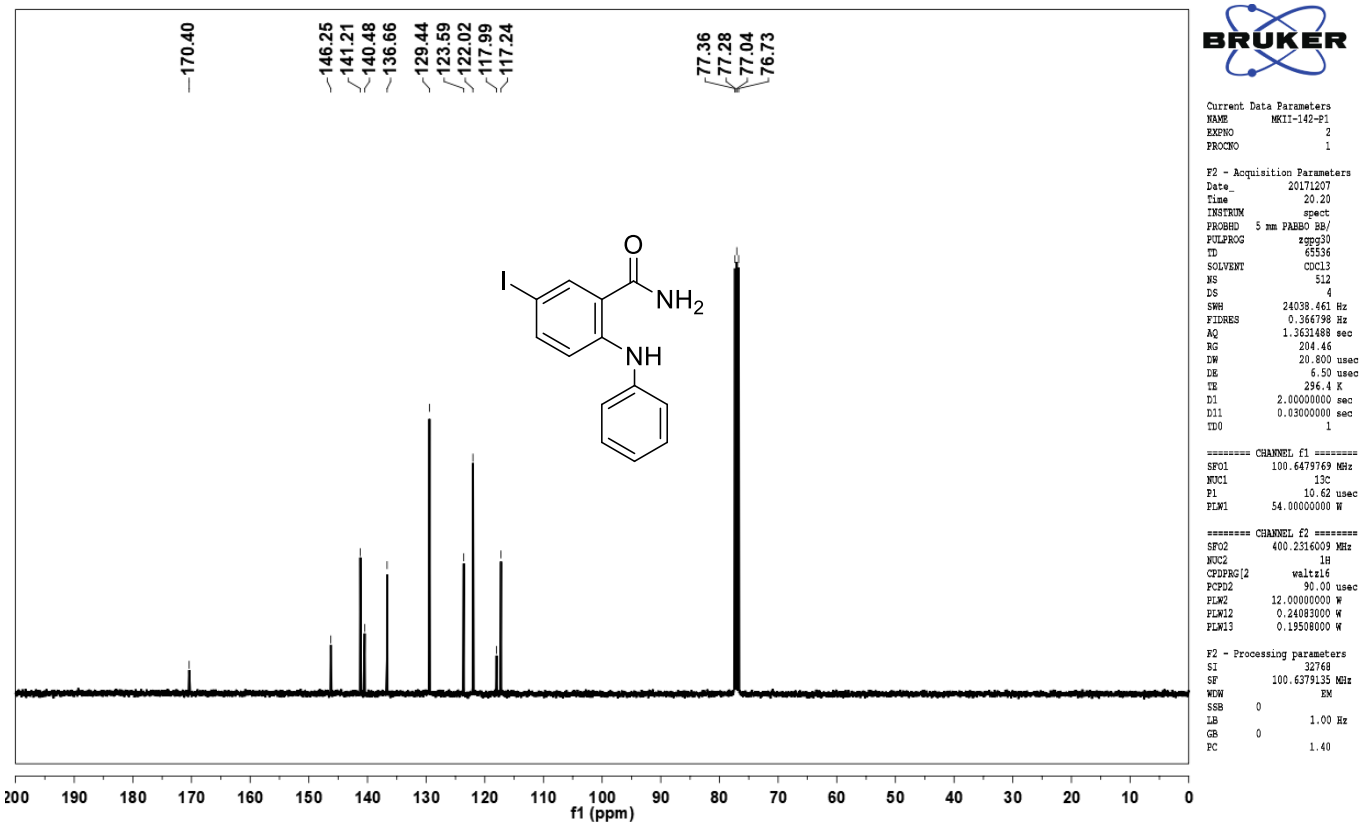

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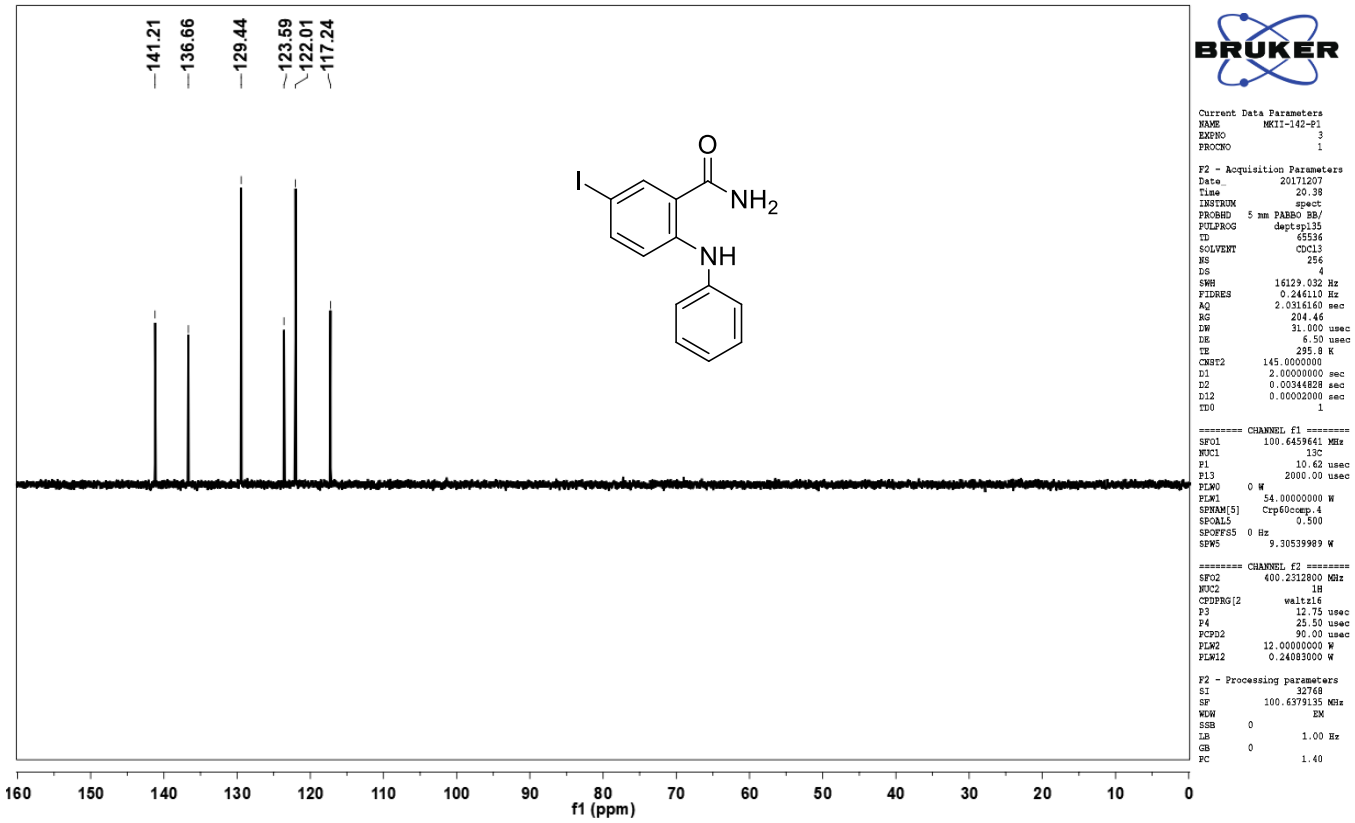

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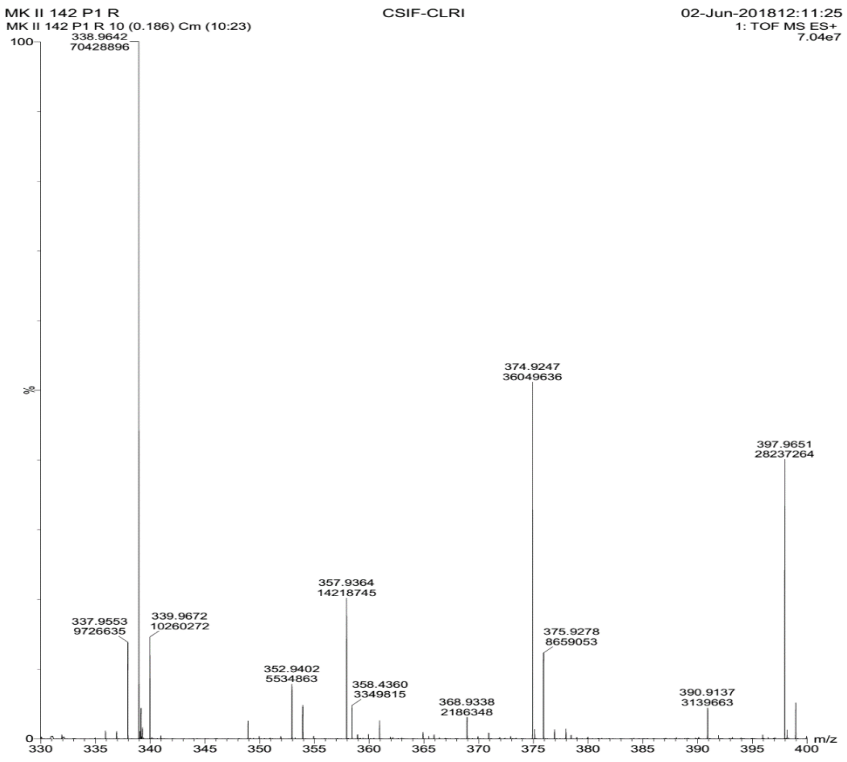

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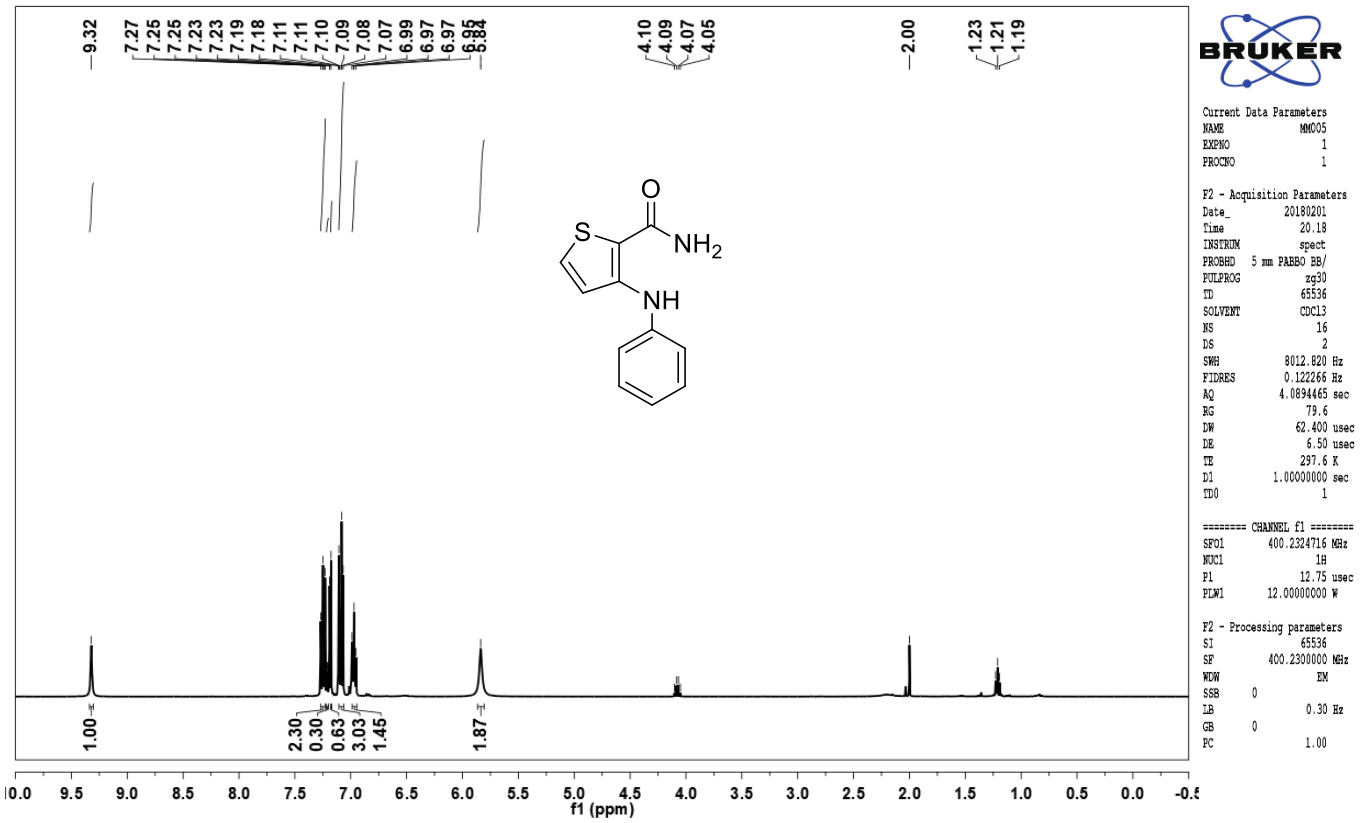

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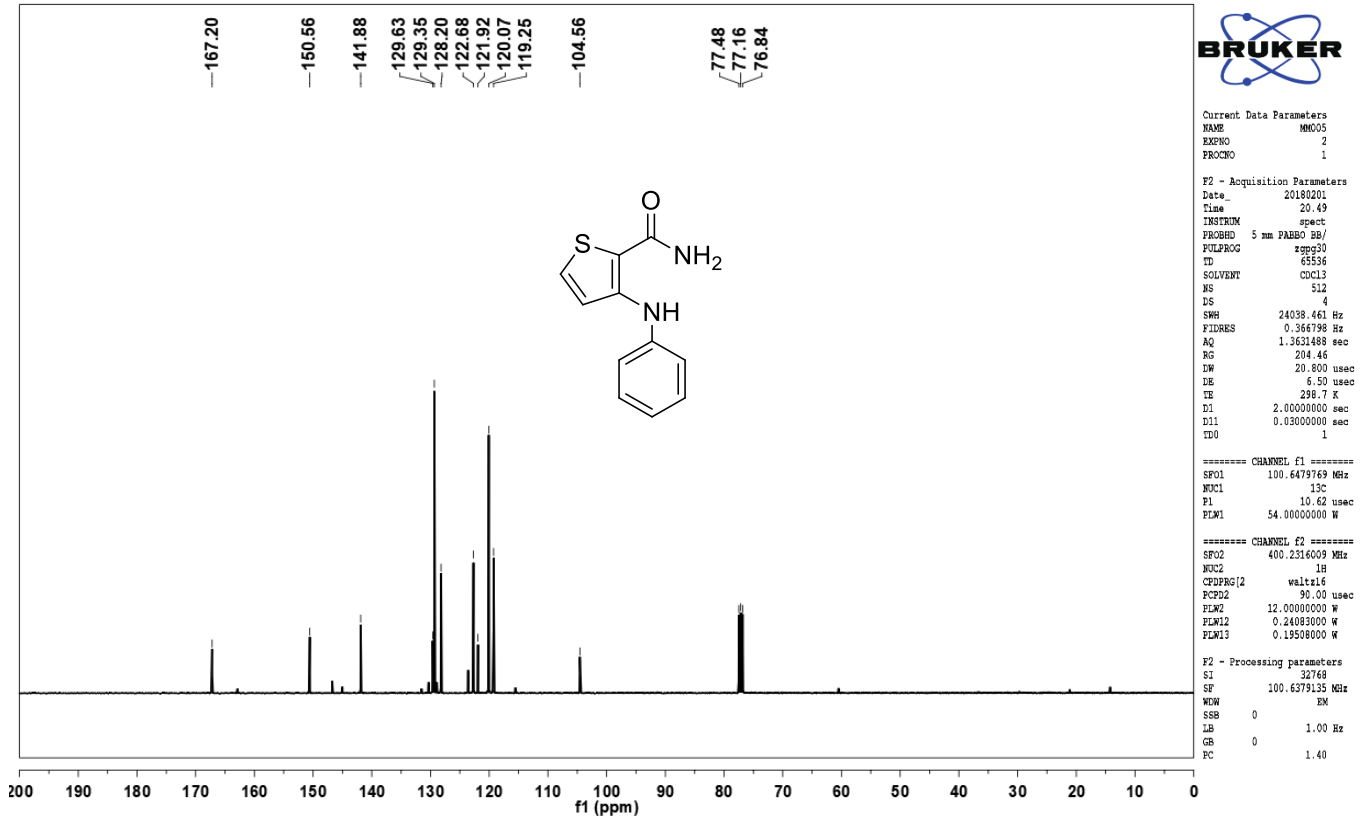

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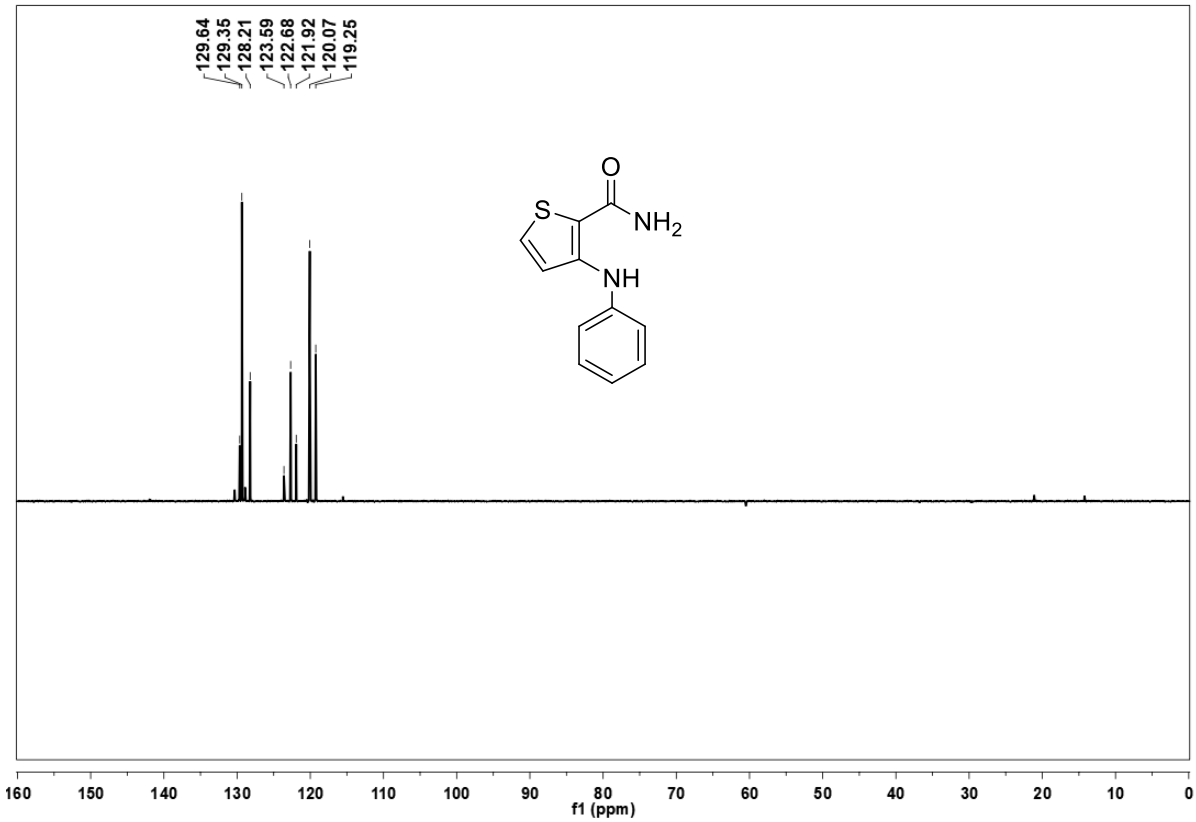

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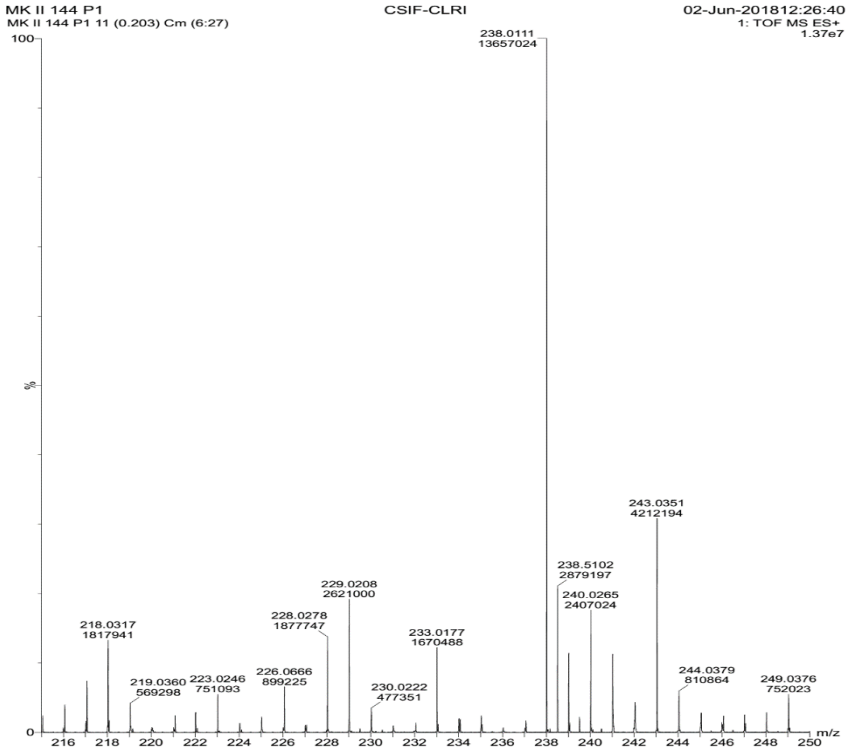

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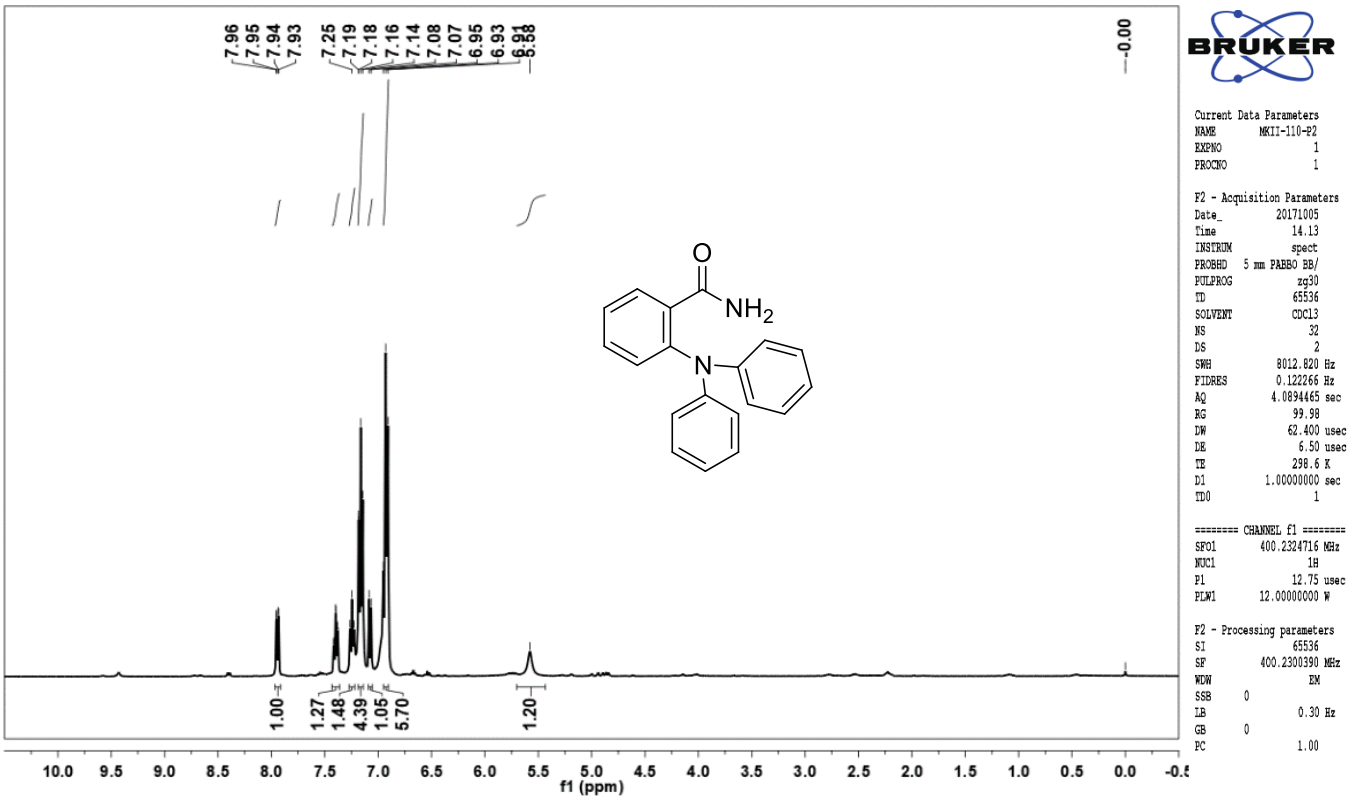

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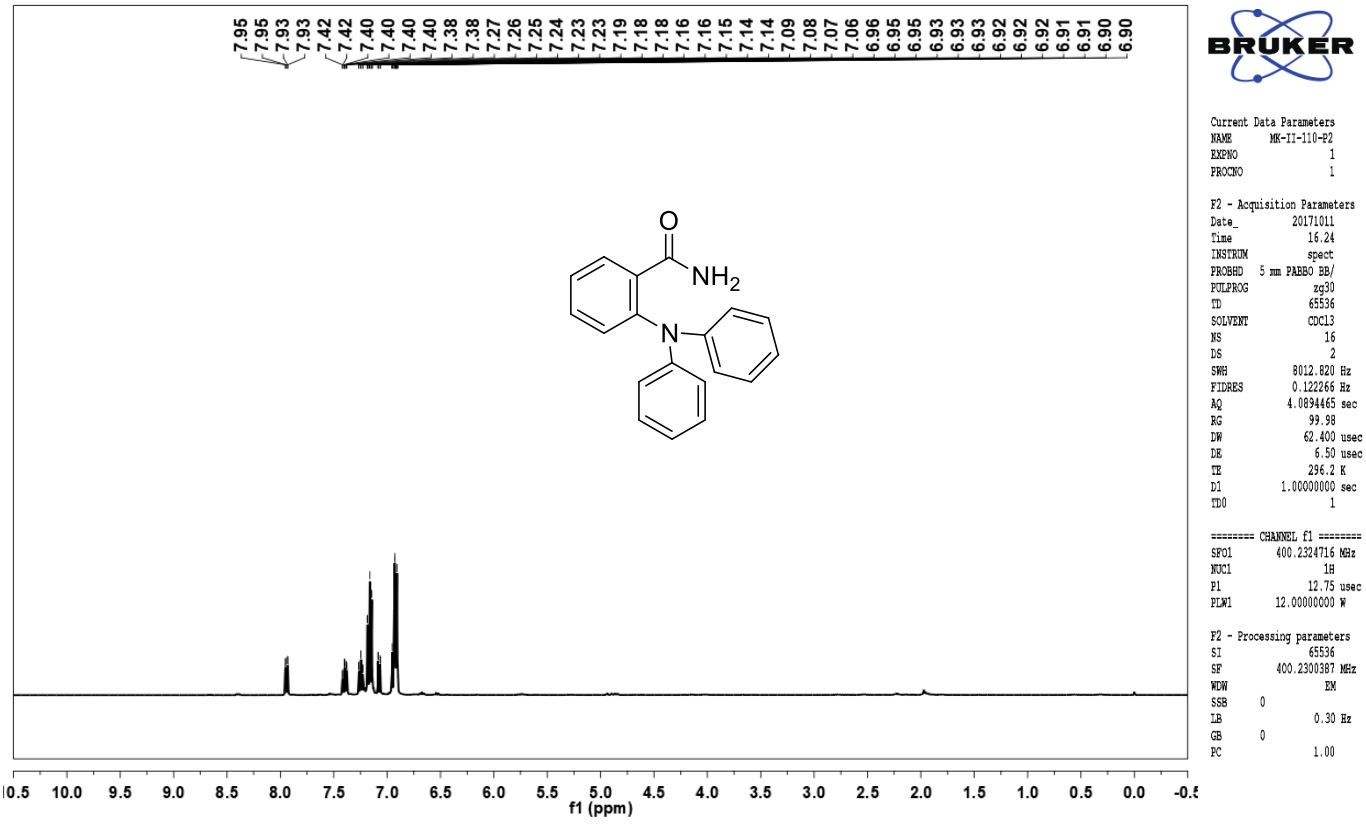
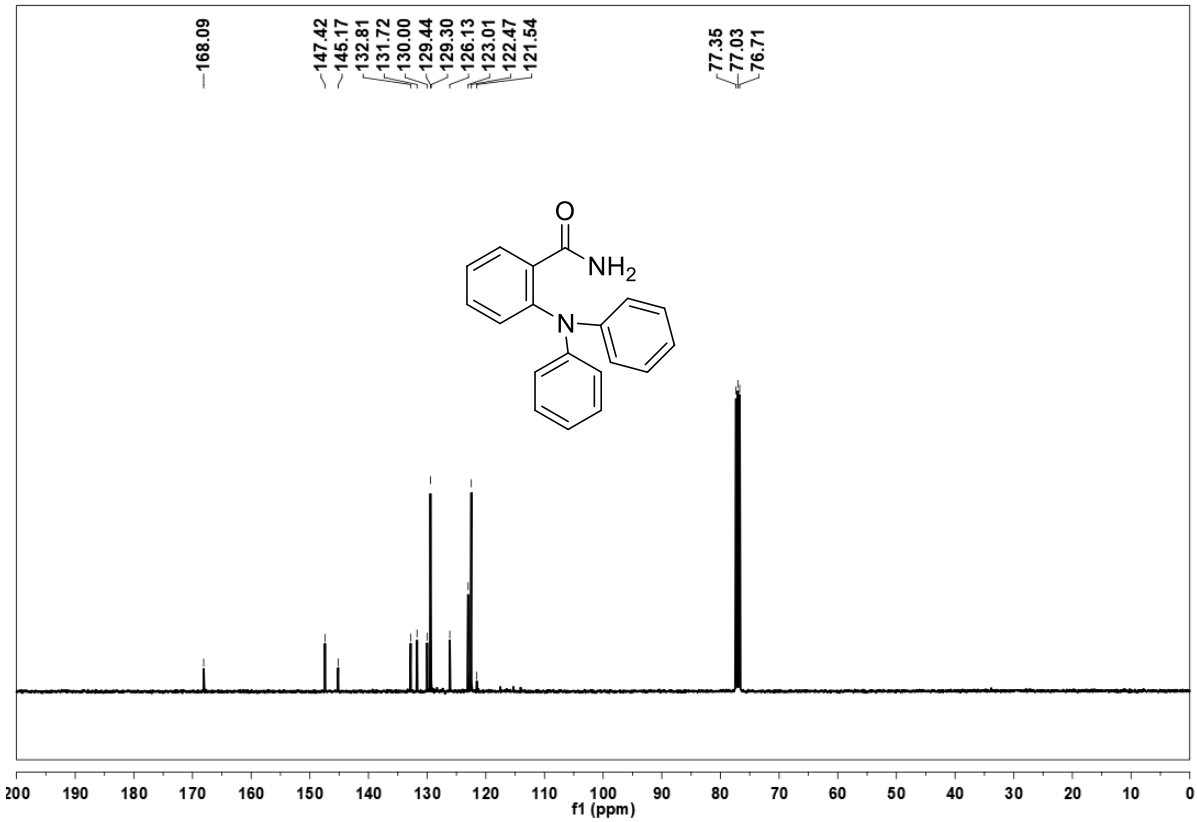


^{1}H NMR Spectrum of Compound **4a** (D_2O exchange experiment)



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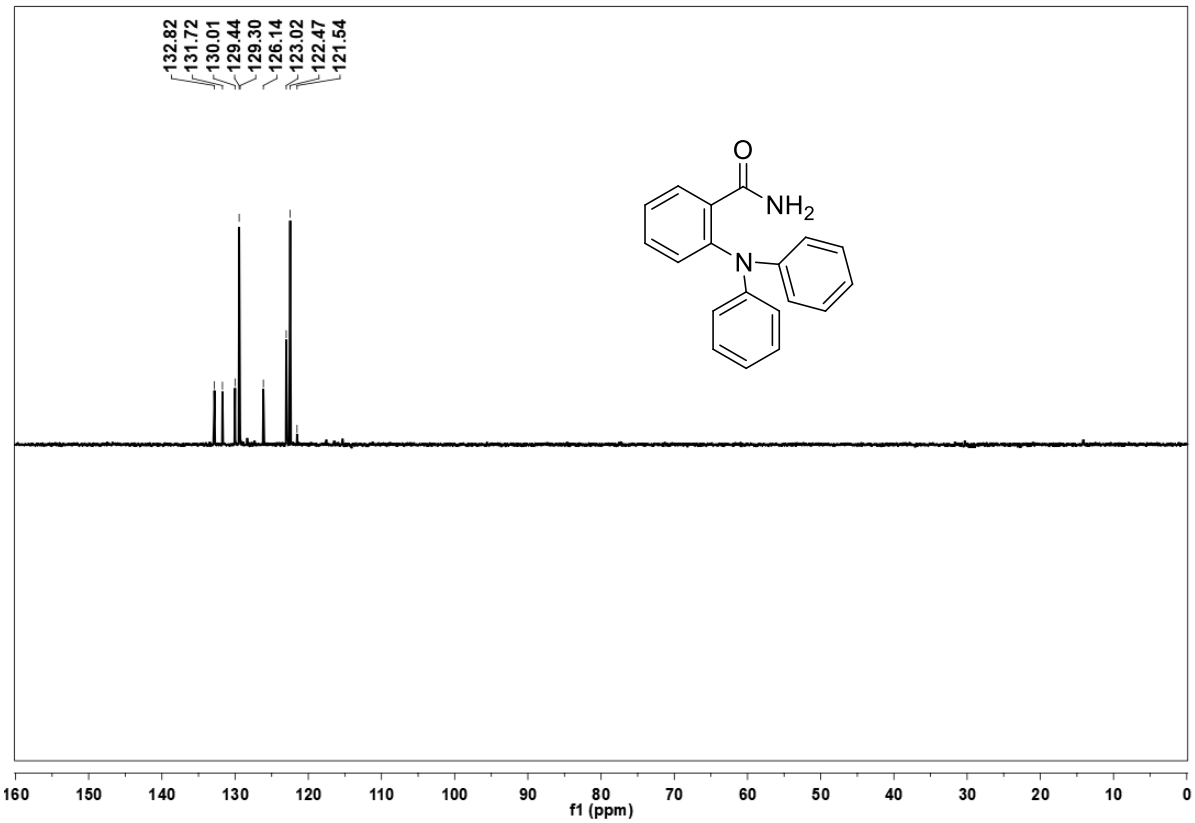

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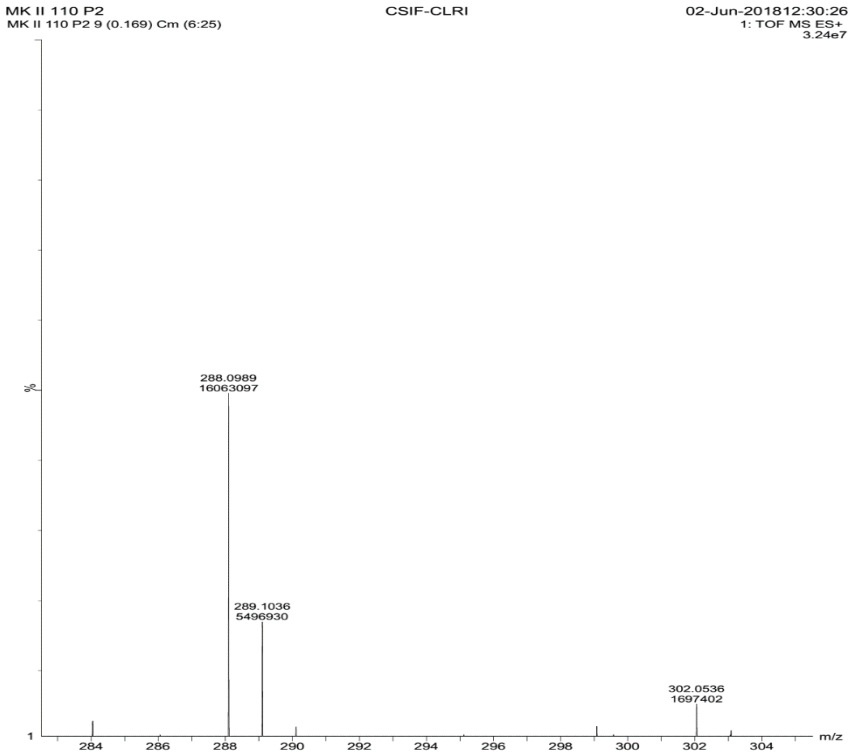

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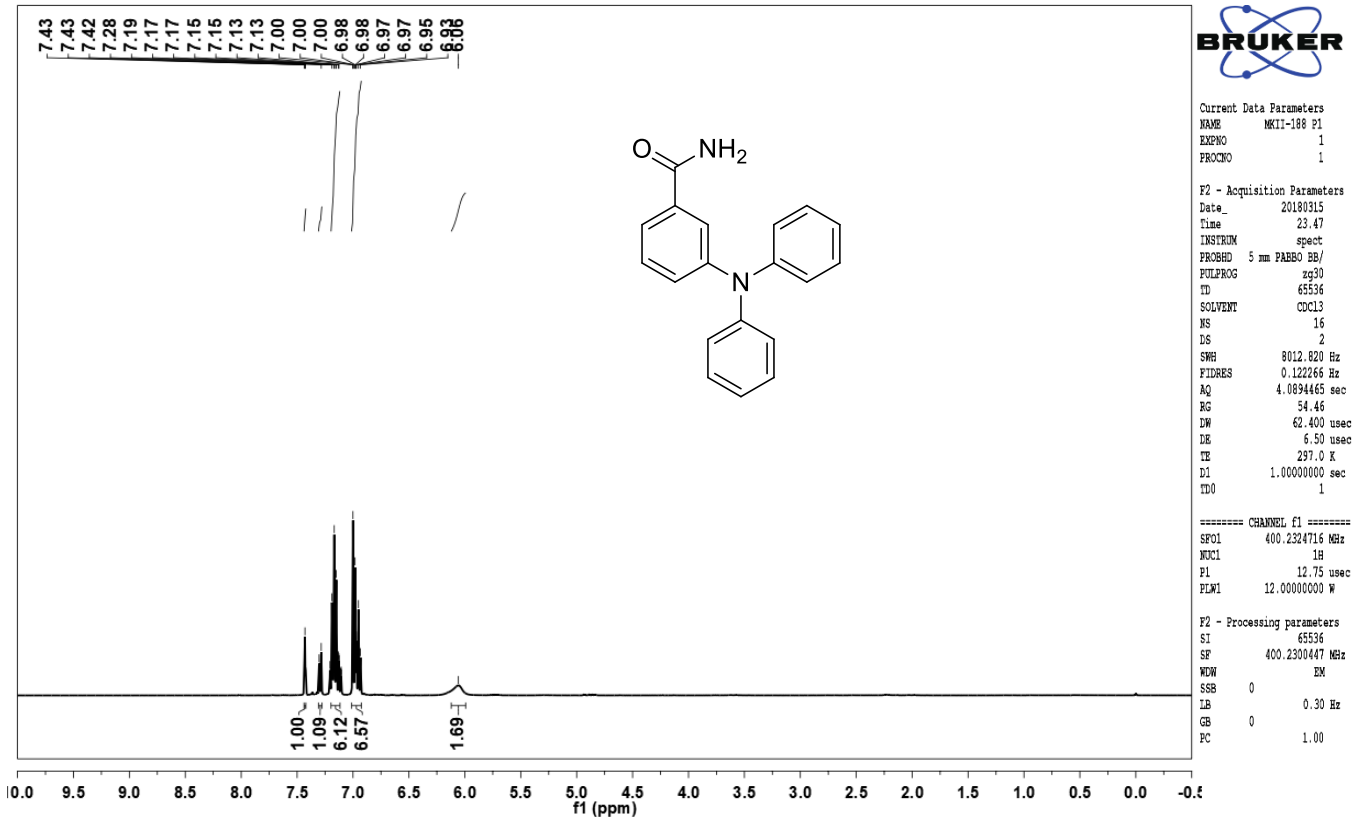

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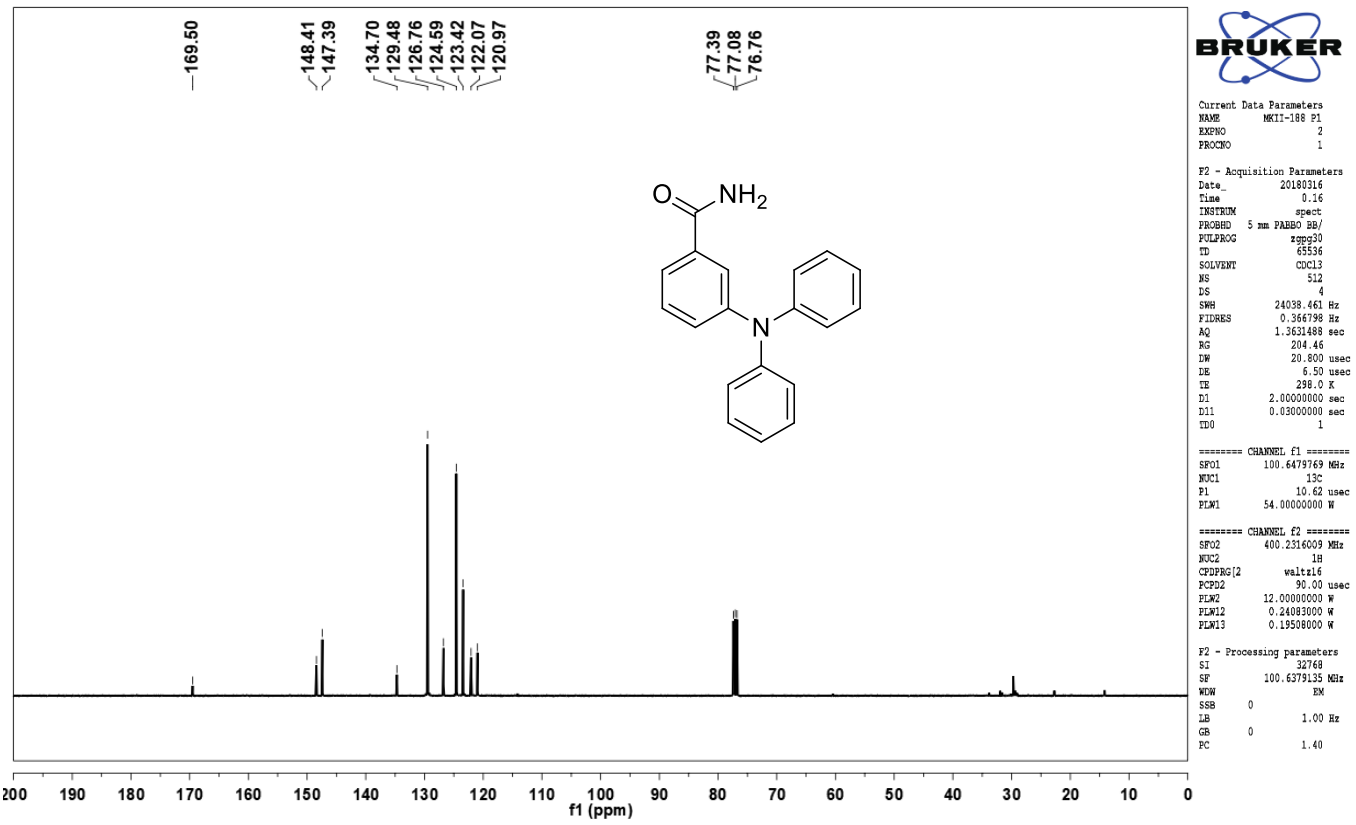

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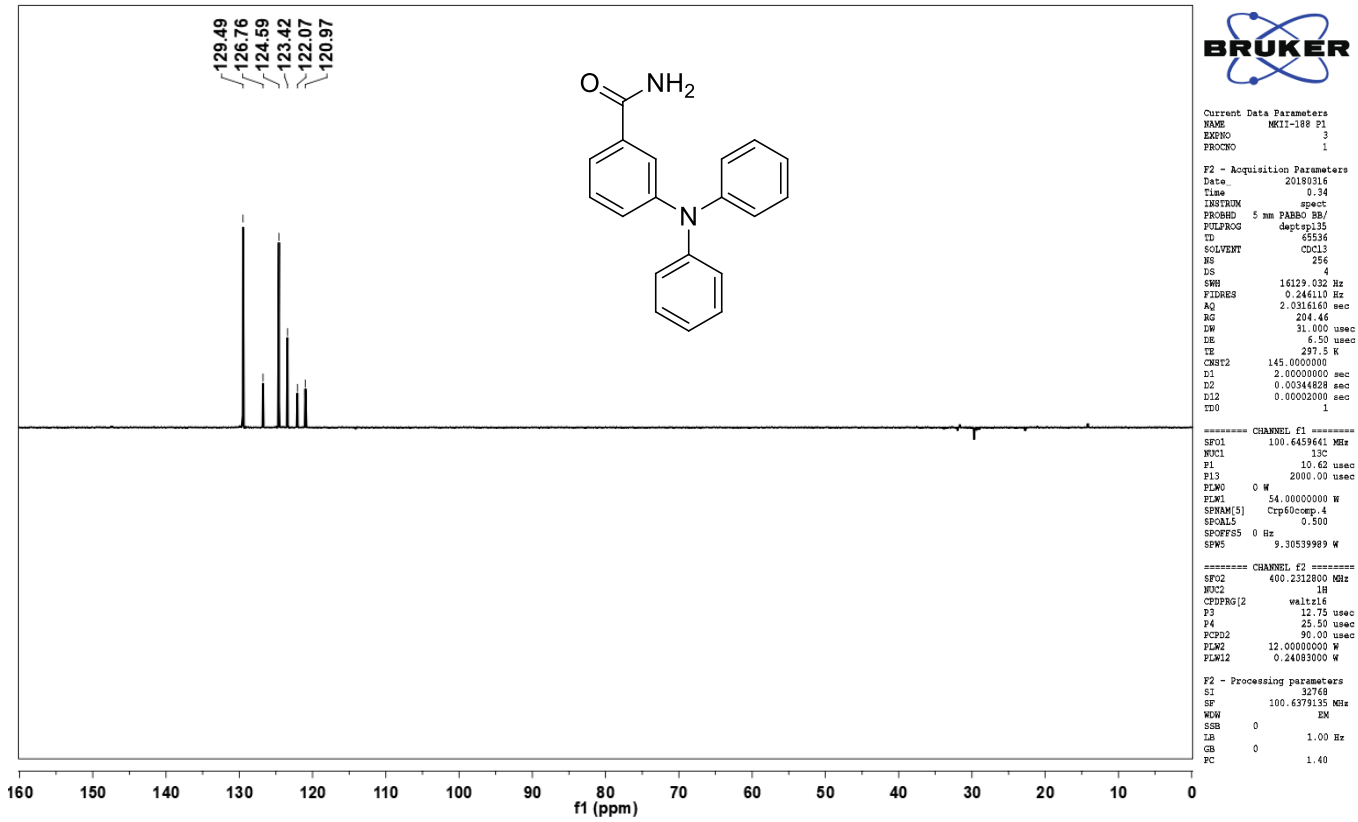

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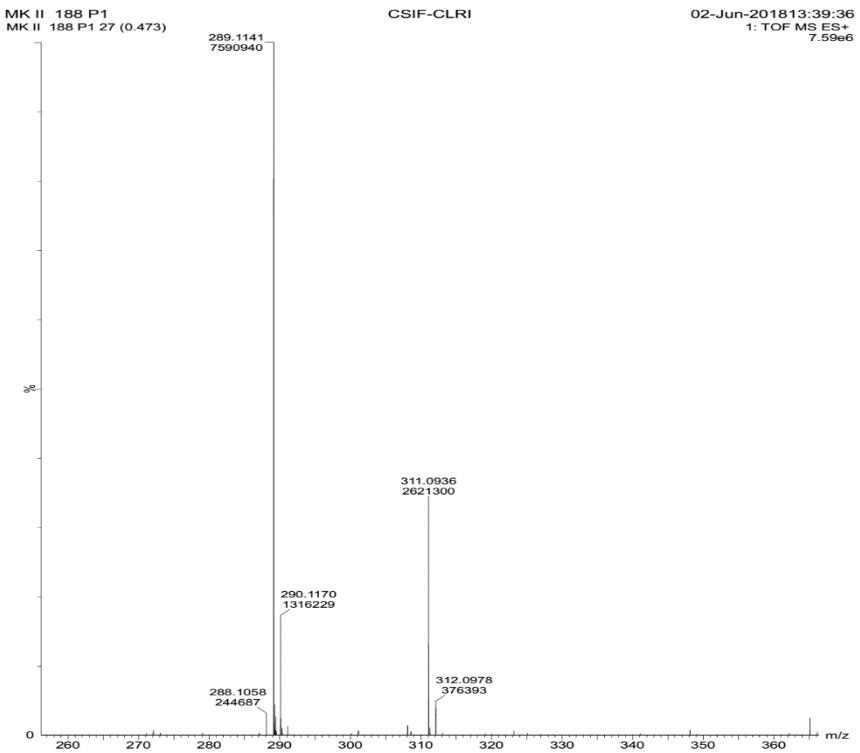

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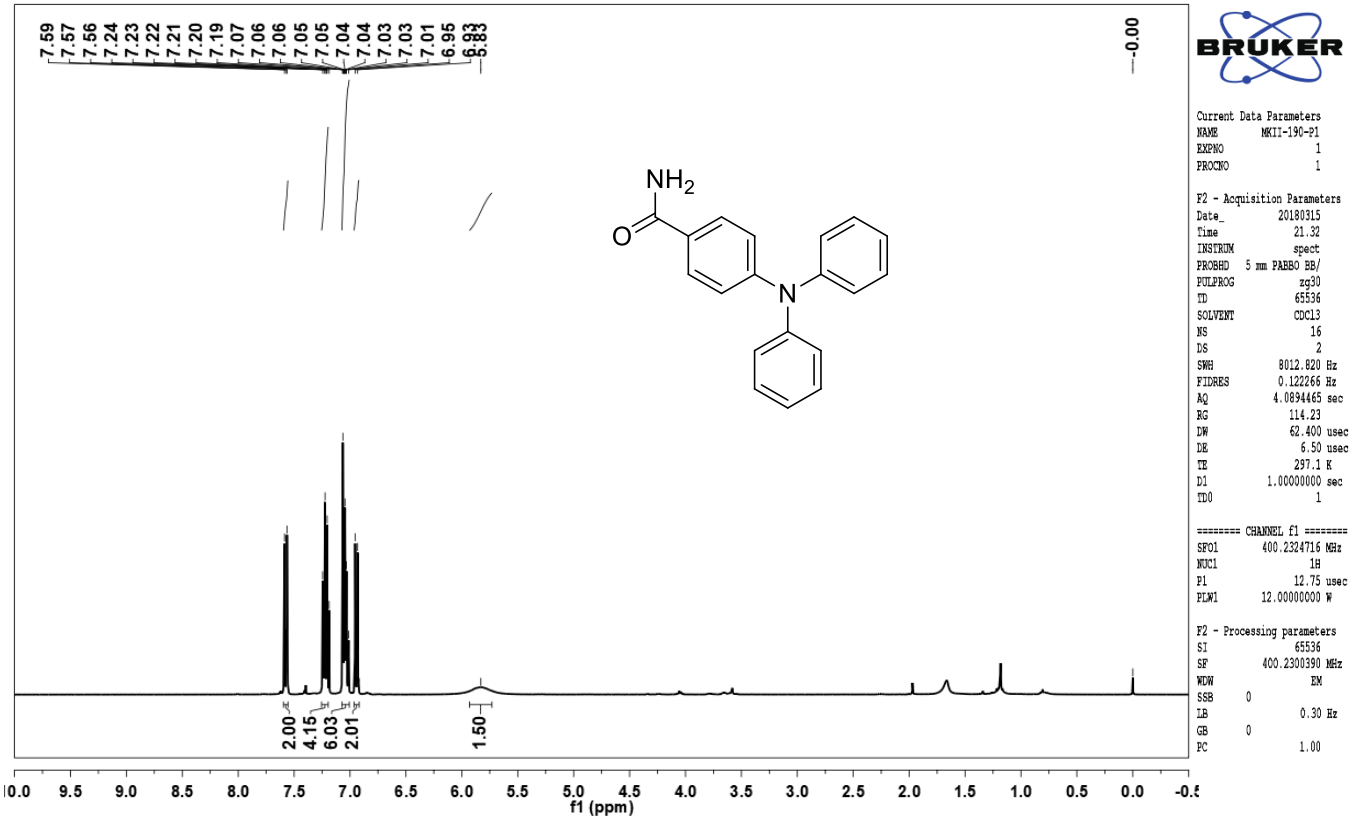

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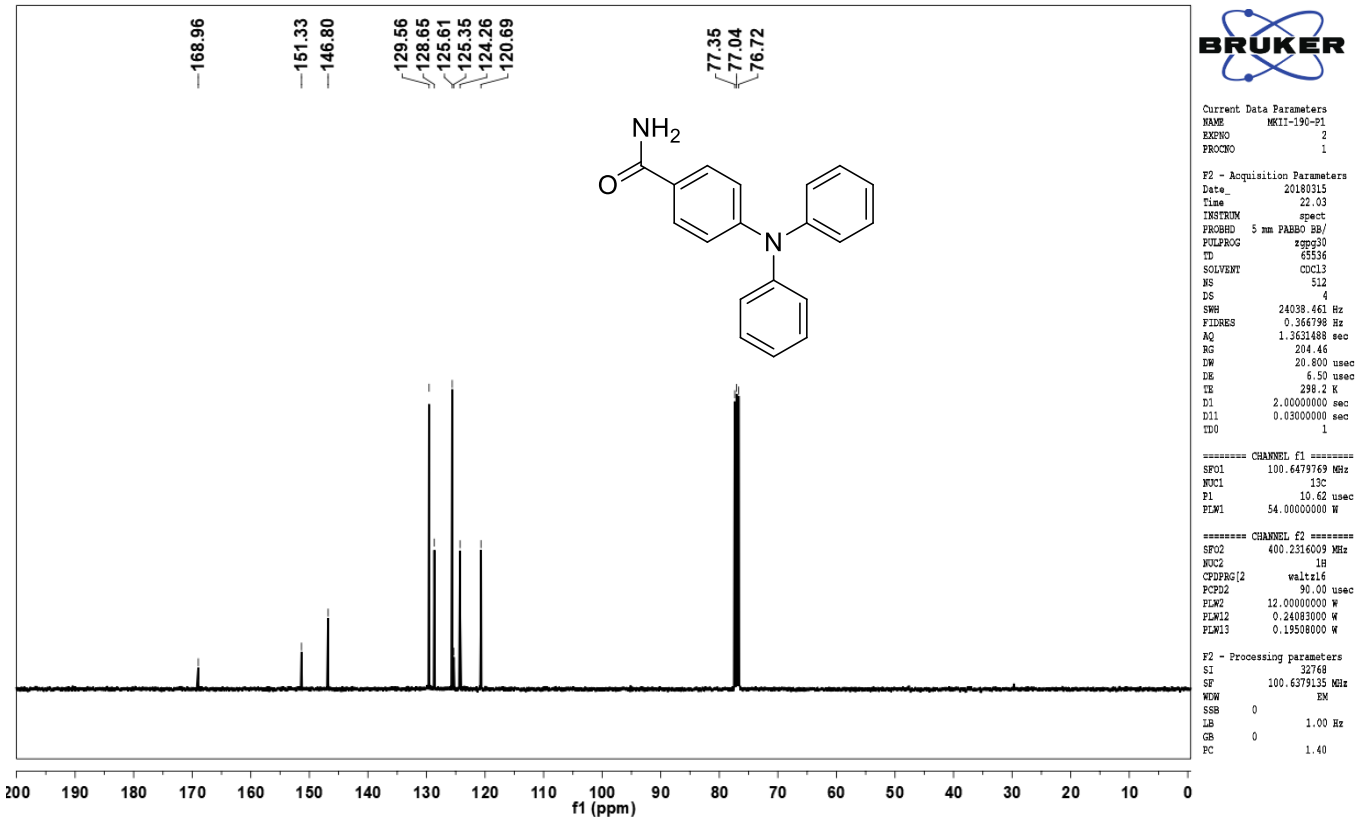

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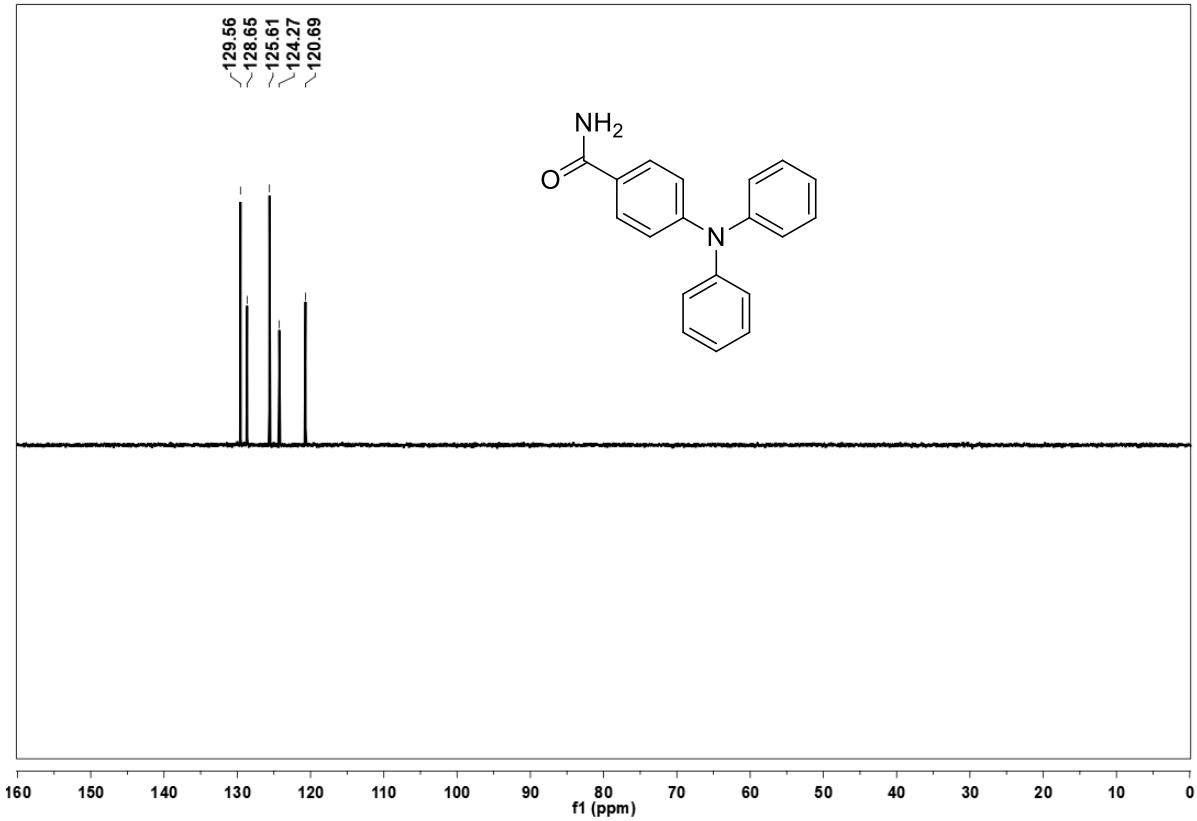

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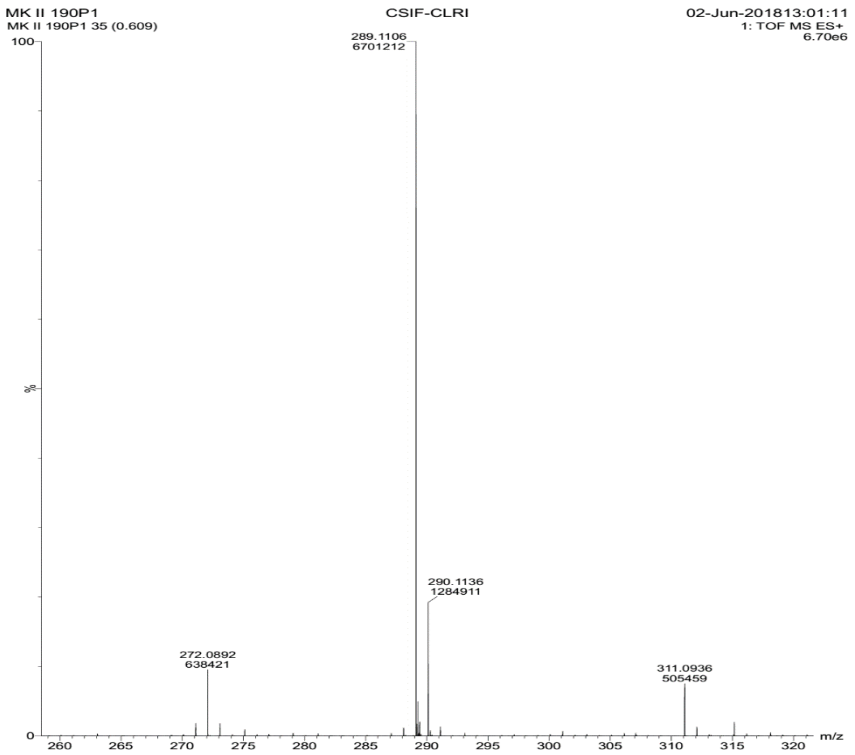

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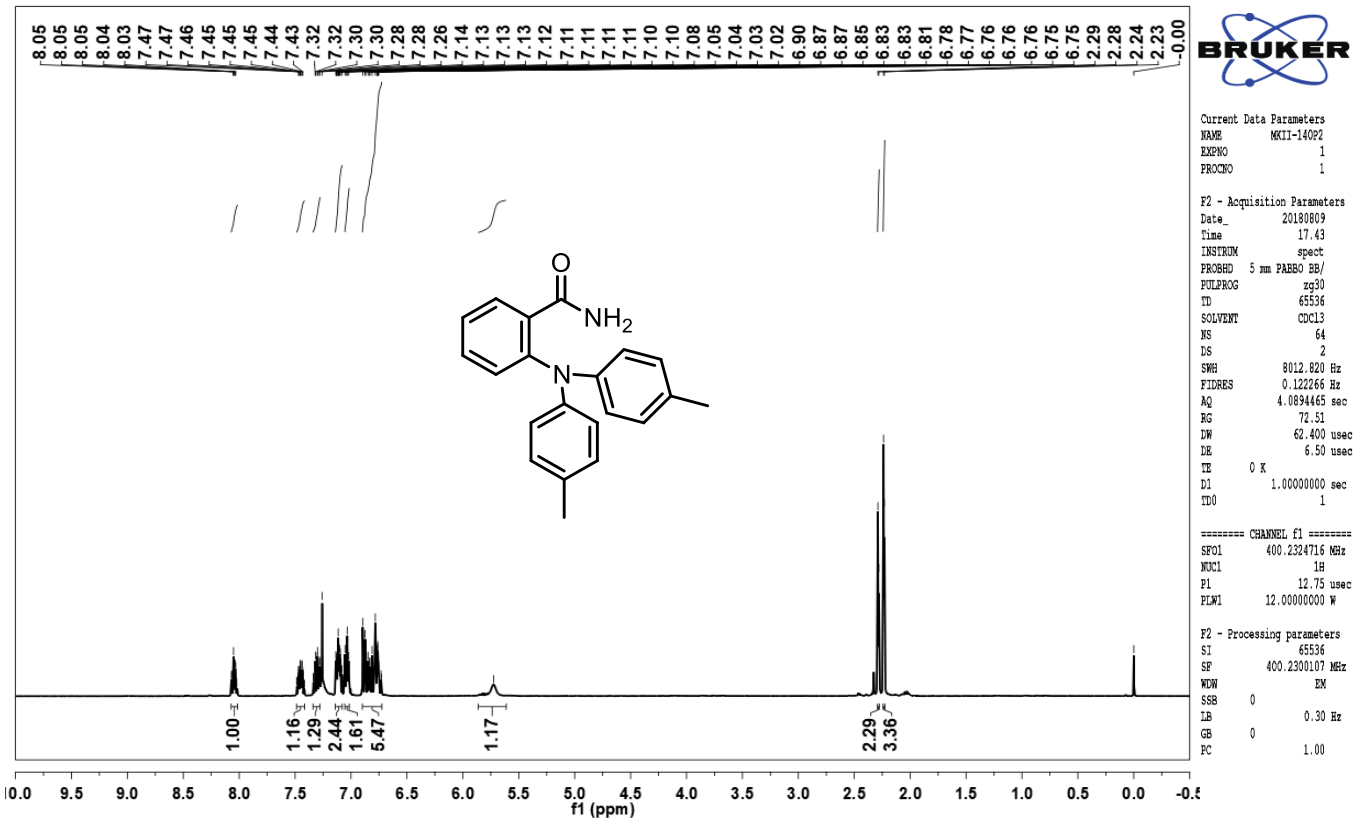

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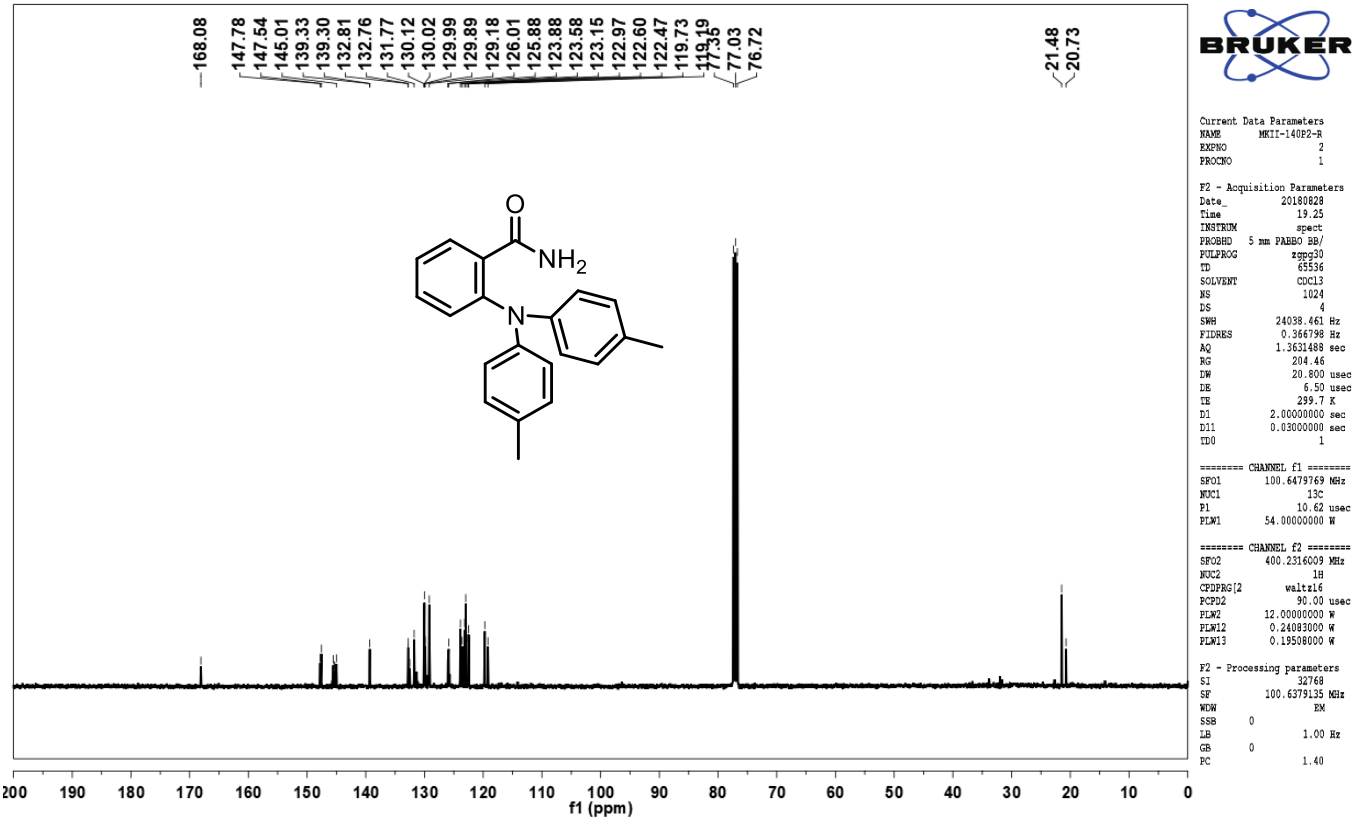

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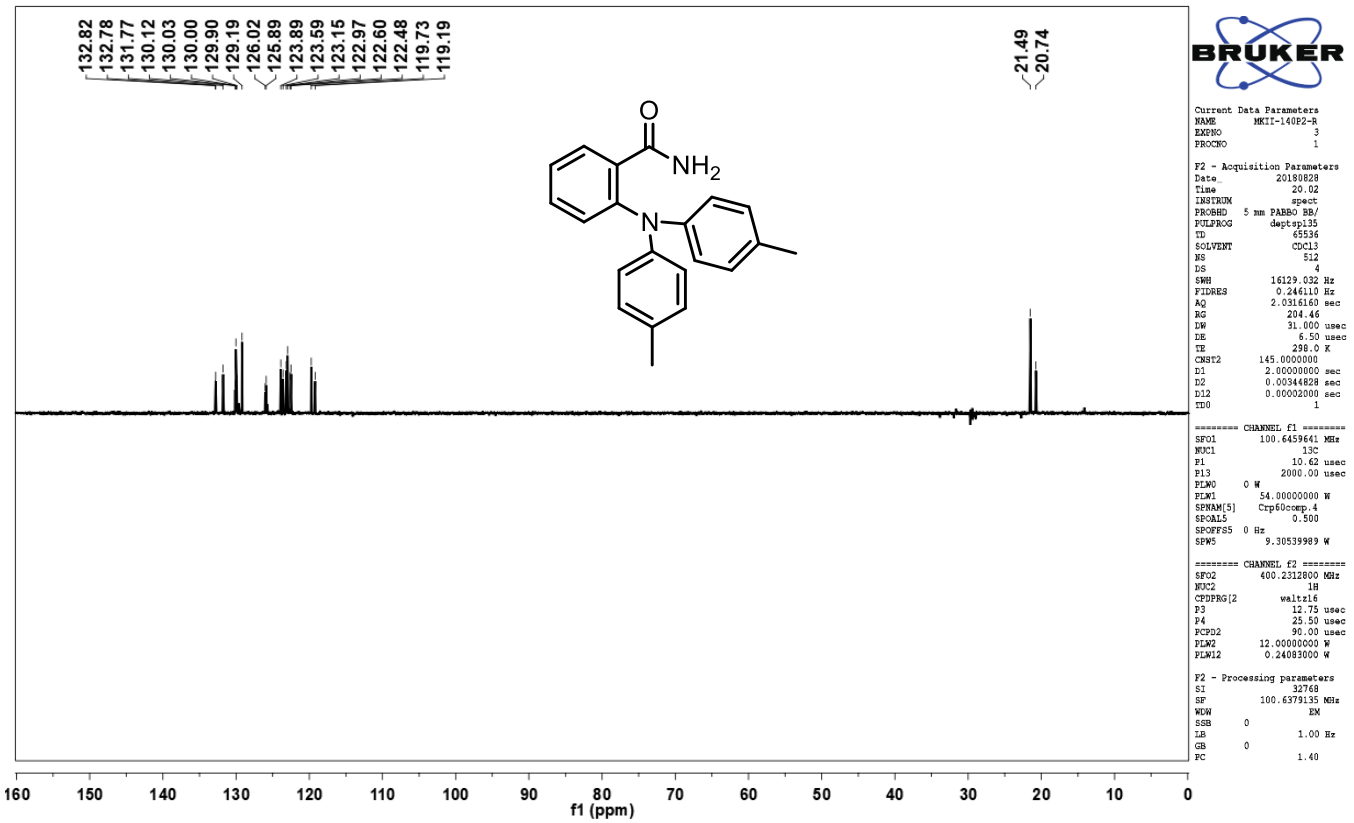

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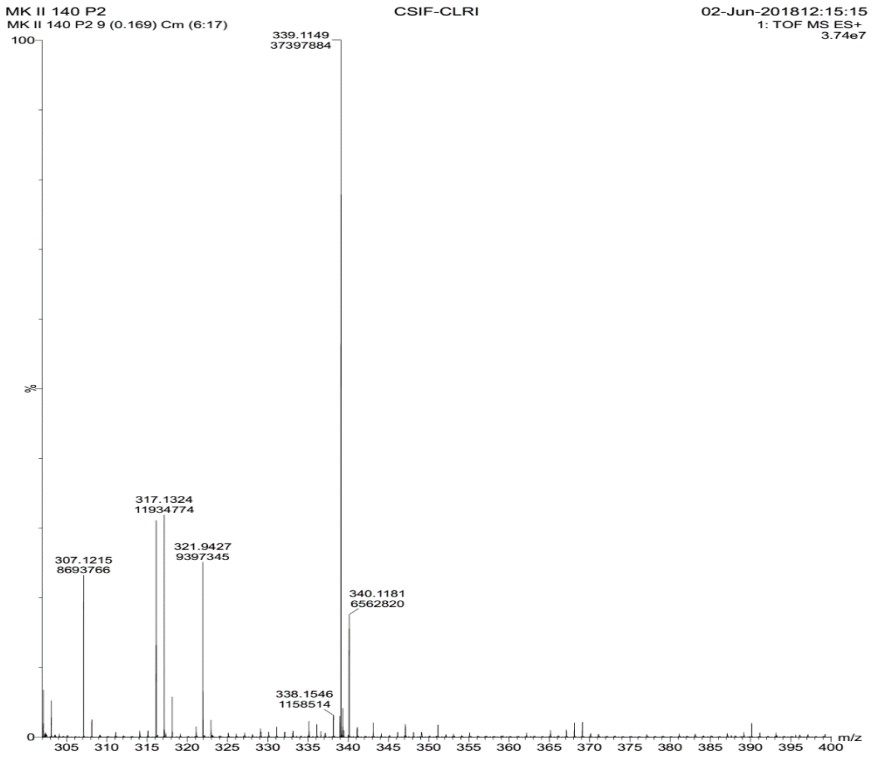

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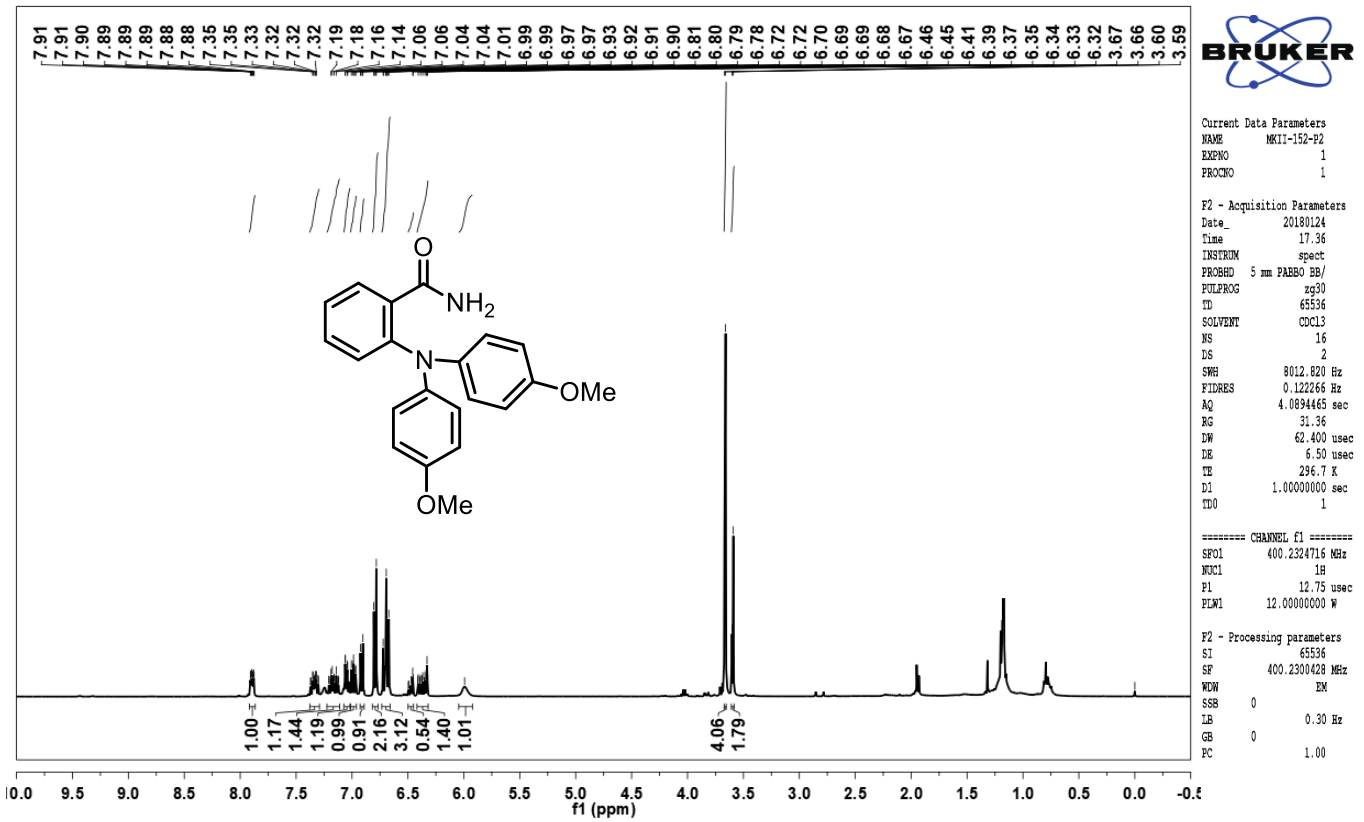
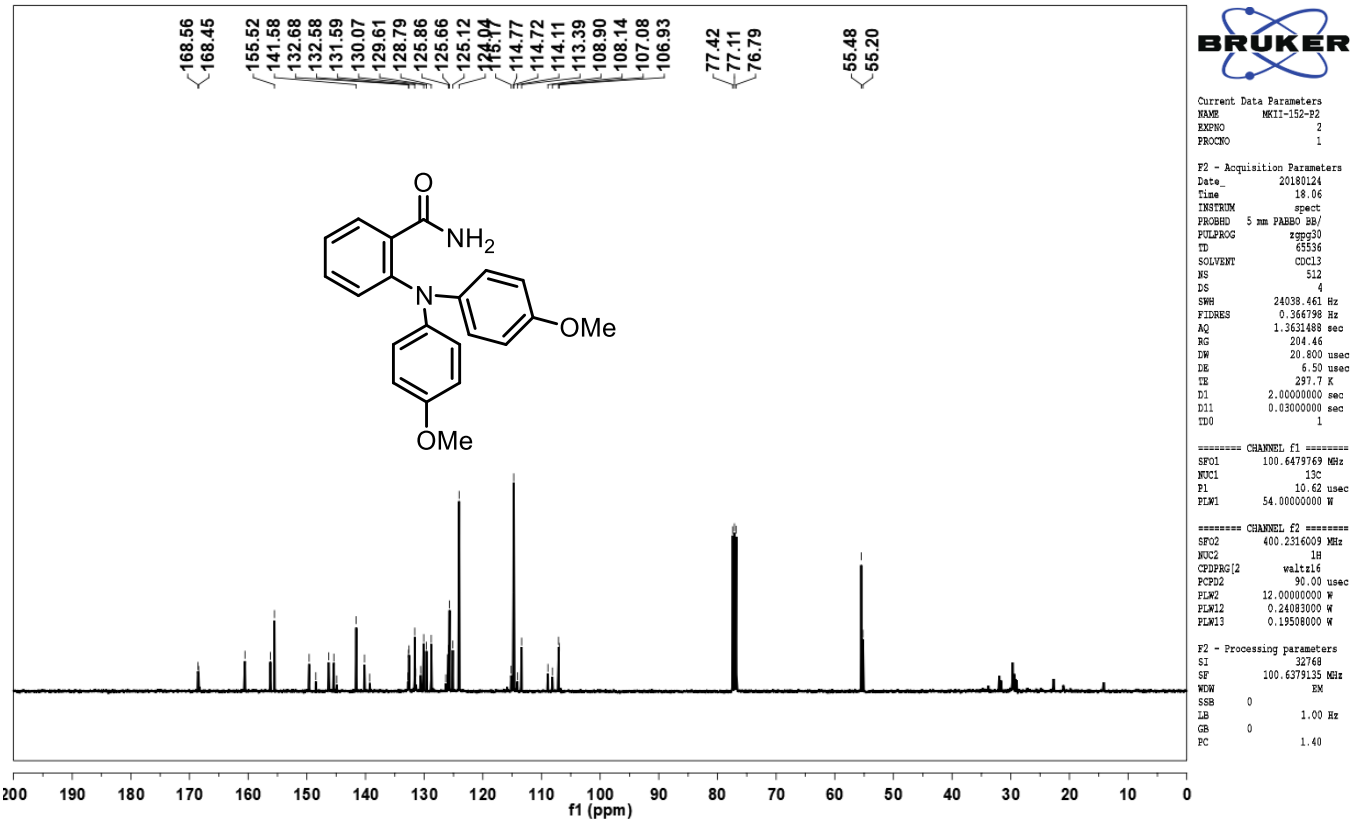
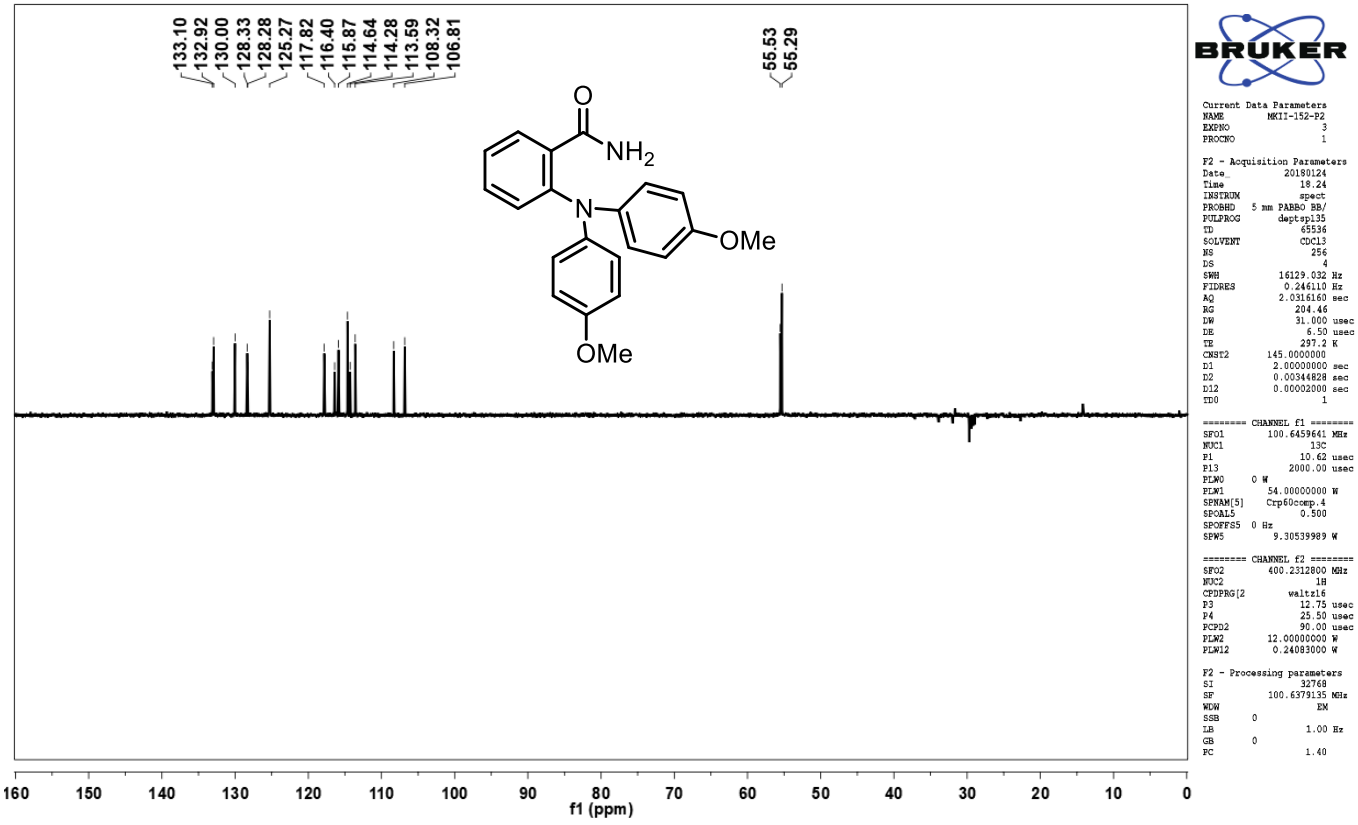


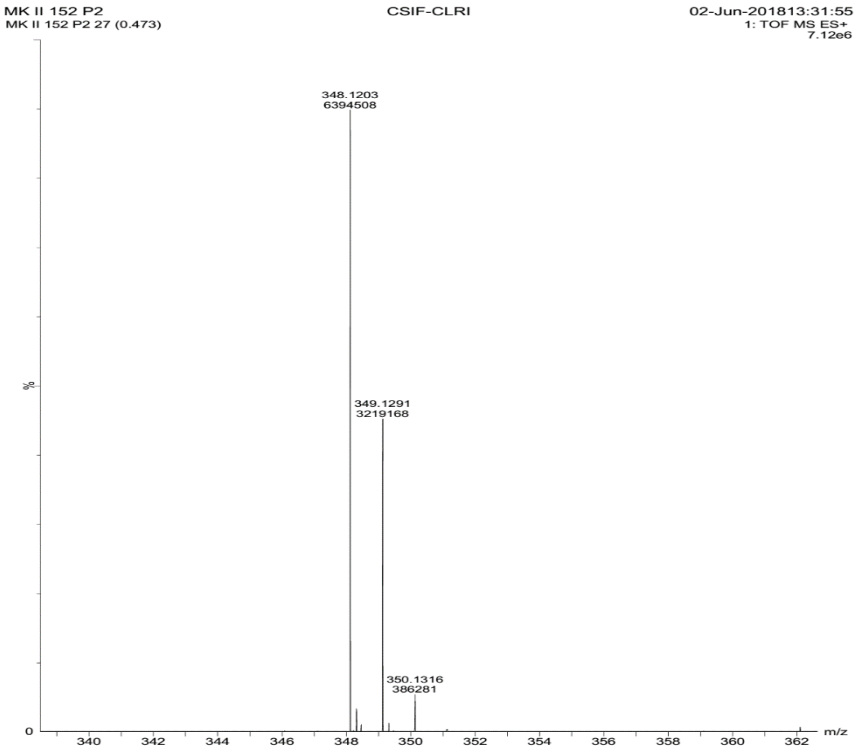
^{1}H NMR Spectrum of Compound **4e**



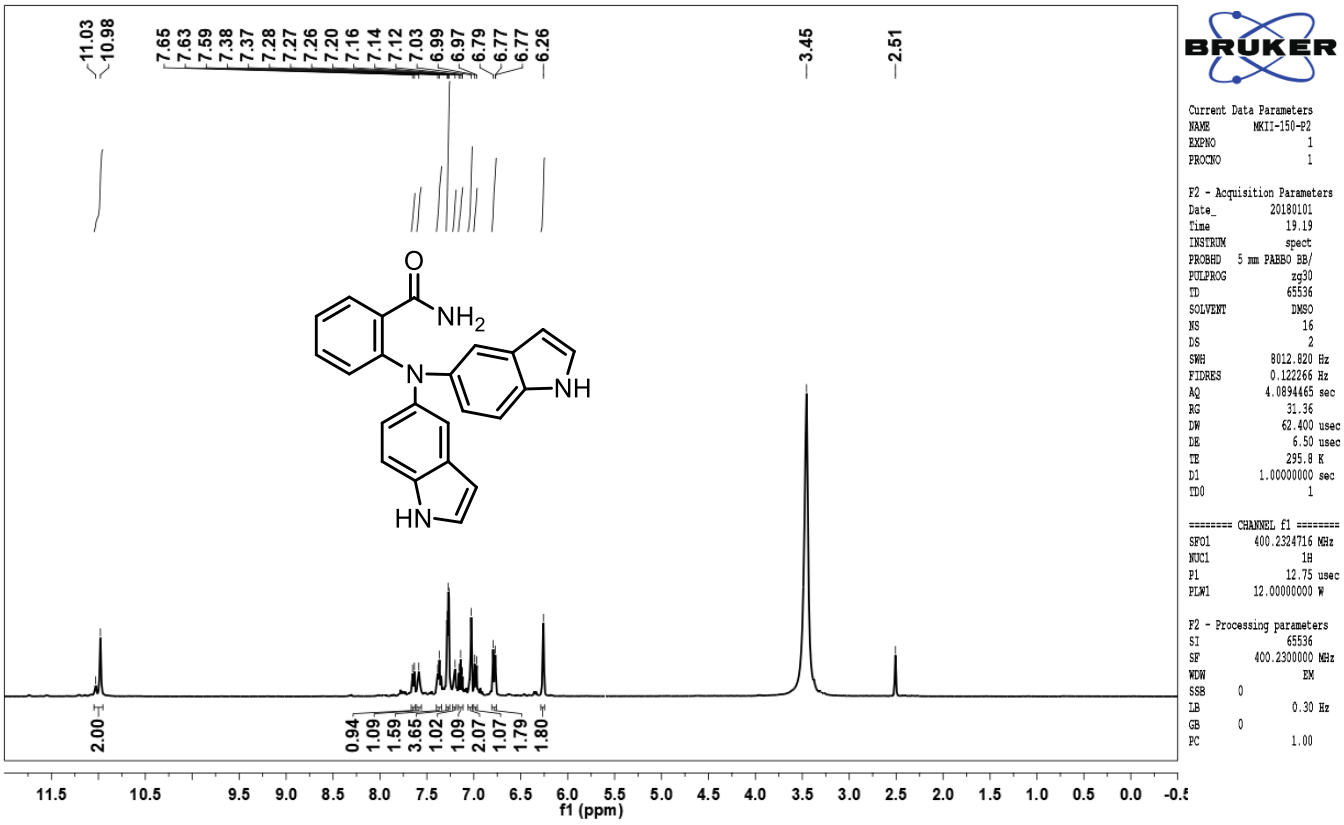
^{13}C NMR Spectrum of Compound **4e**



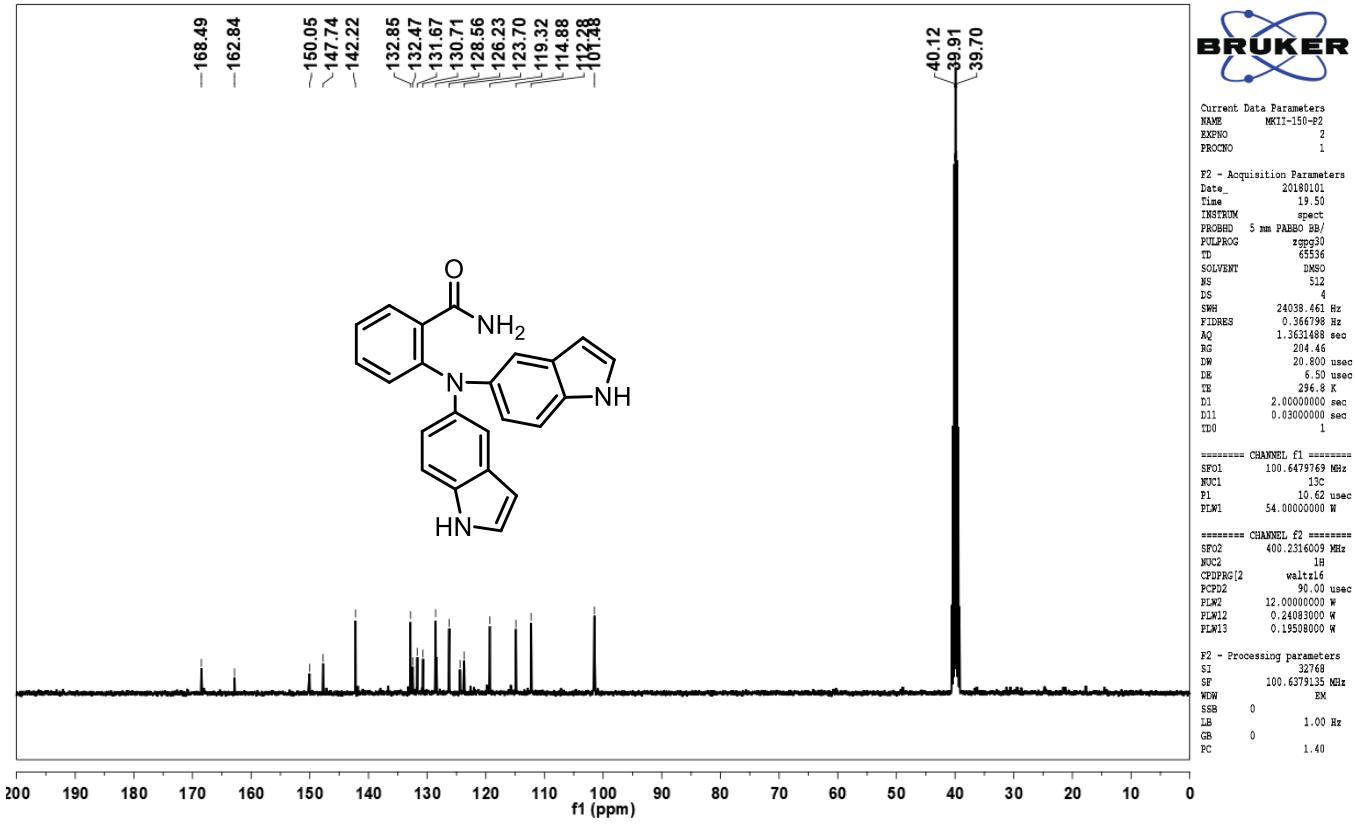
DEPT-135 NMR Spectrum of Compound **4e**



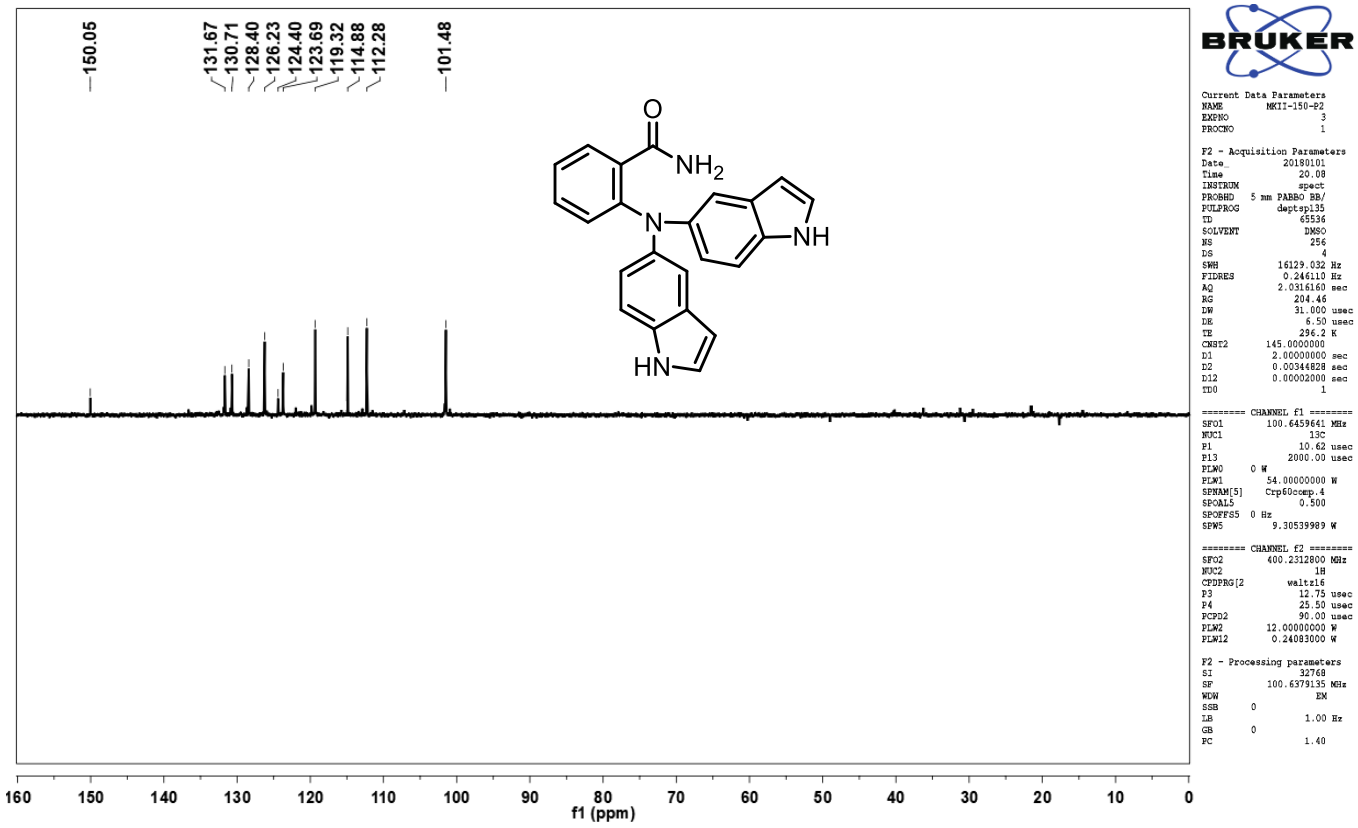
HRMS Spectrum of Compound **4e**



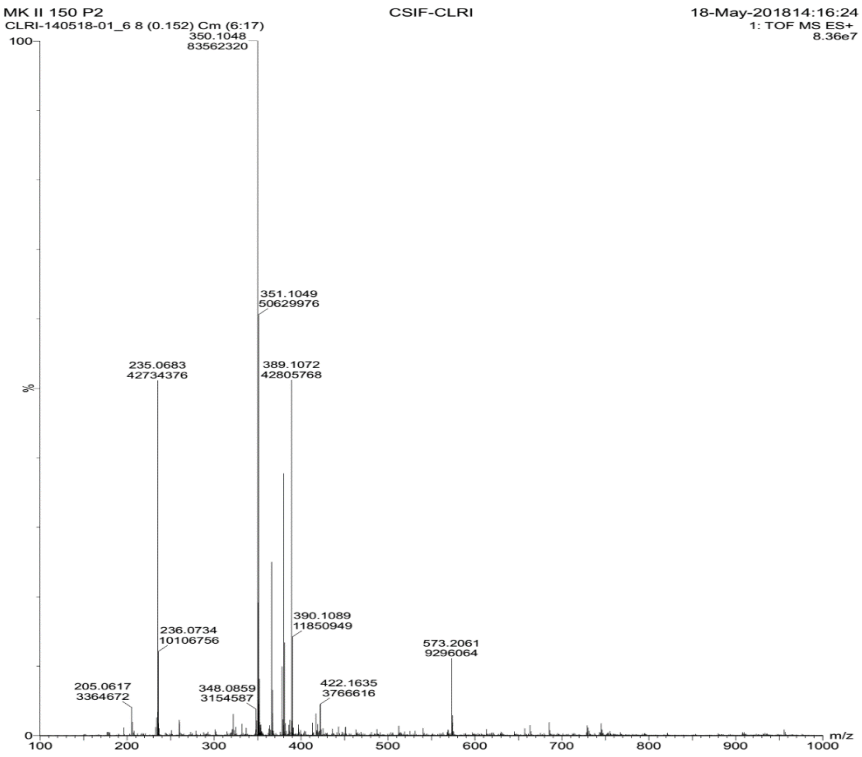
^{1}H NMR Spectrum of Compound **4f**



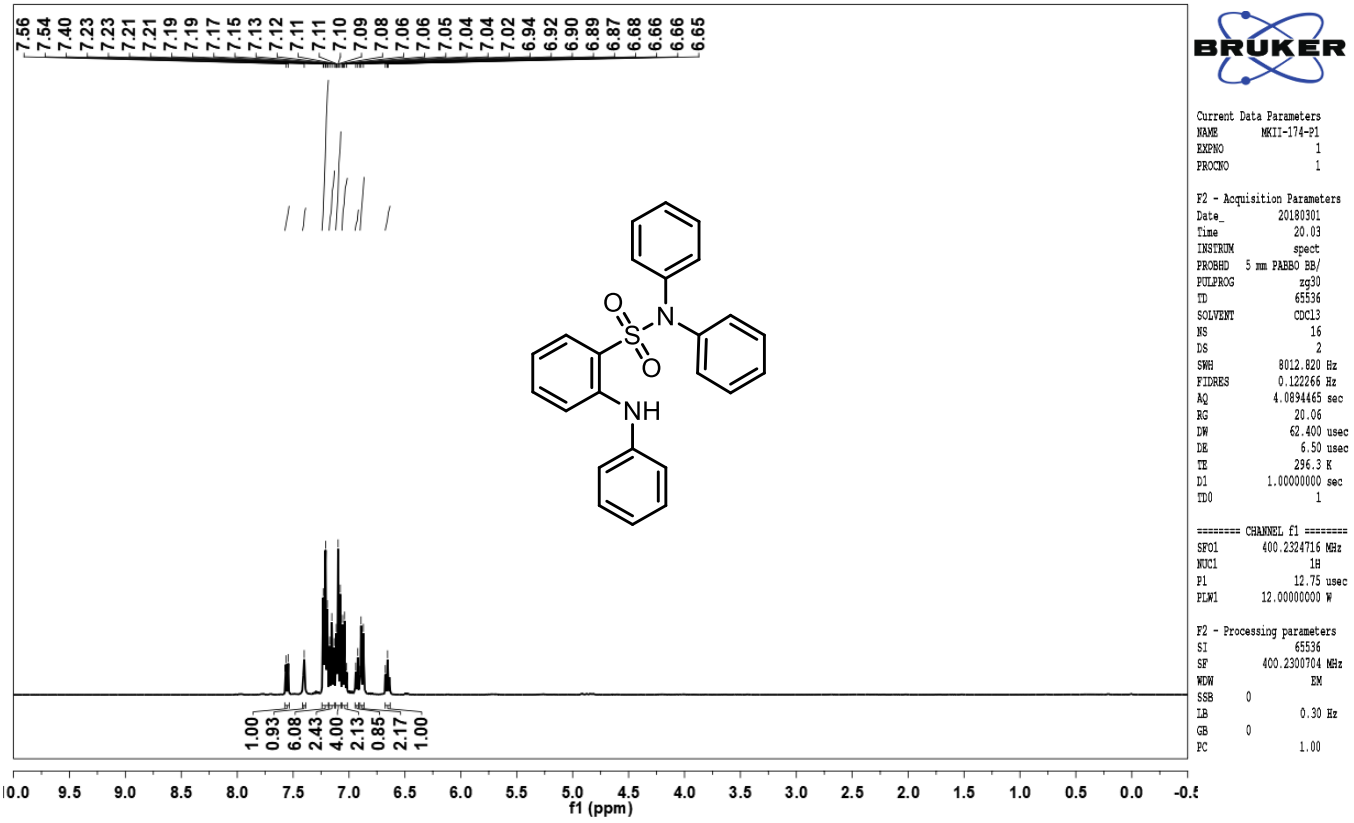
^{13}C NMR Spectrum of Compound **4f**



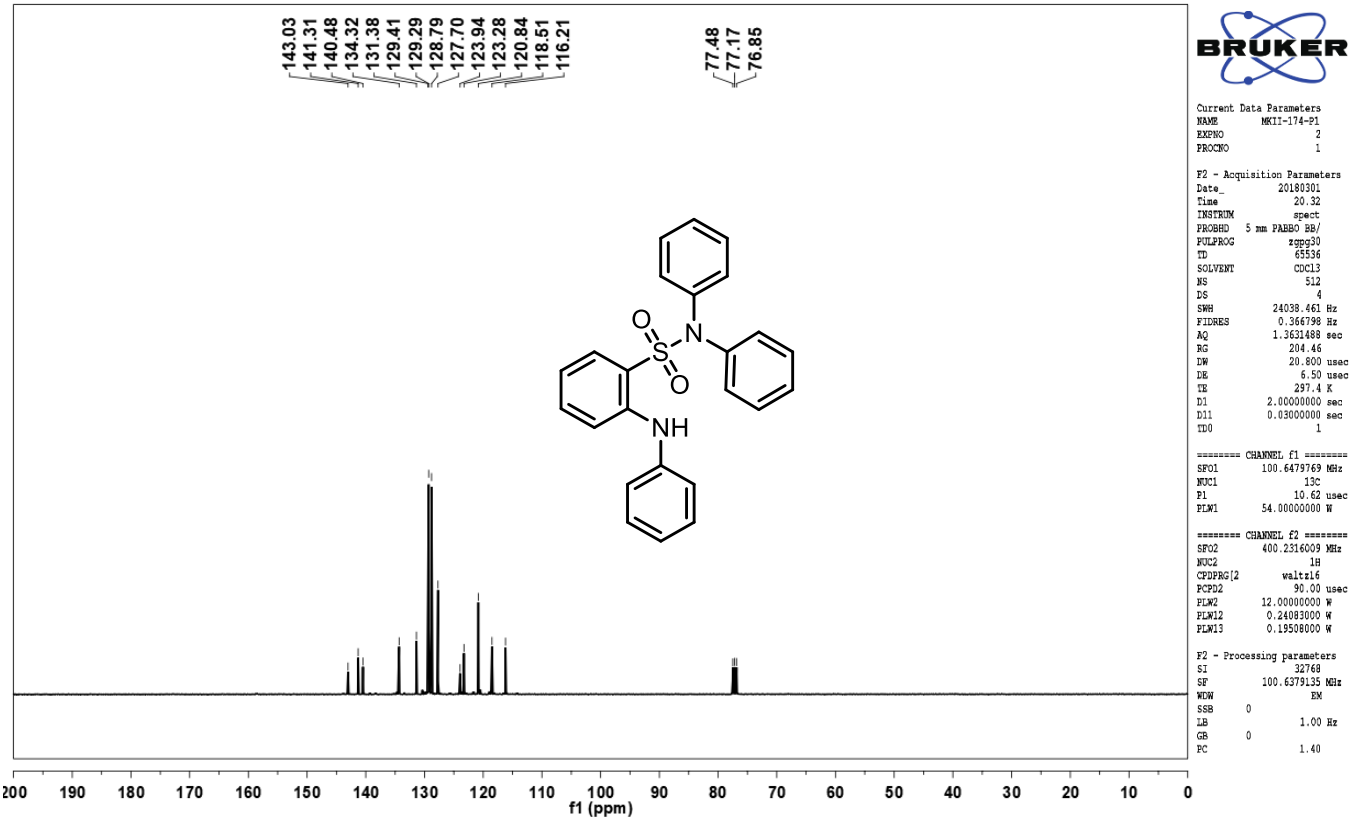
DEPT-135 NMR Spectrum of Compound **4f**



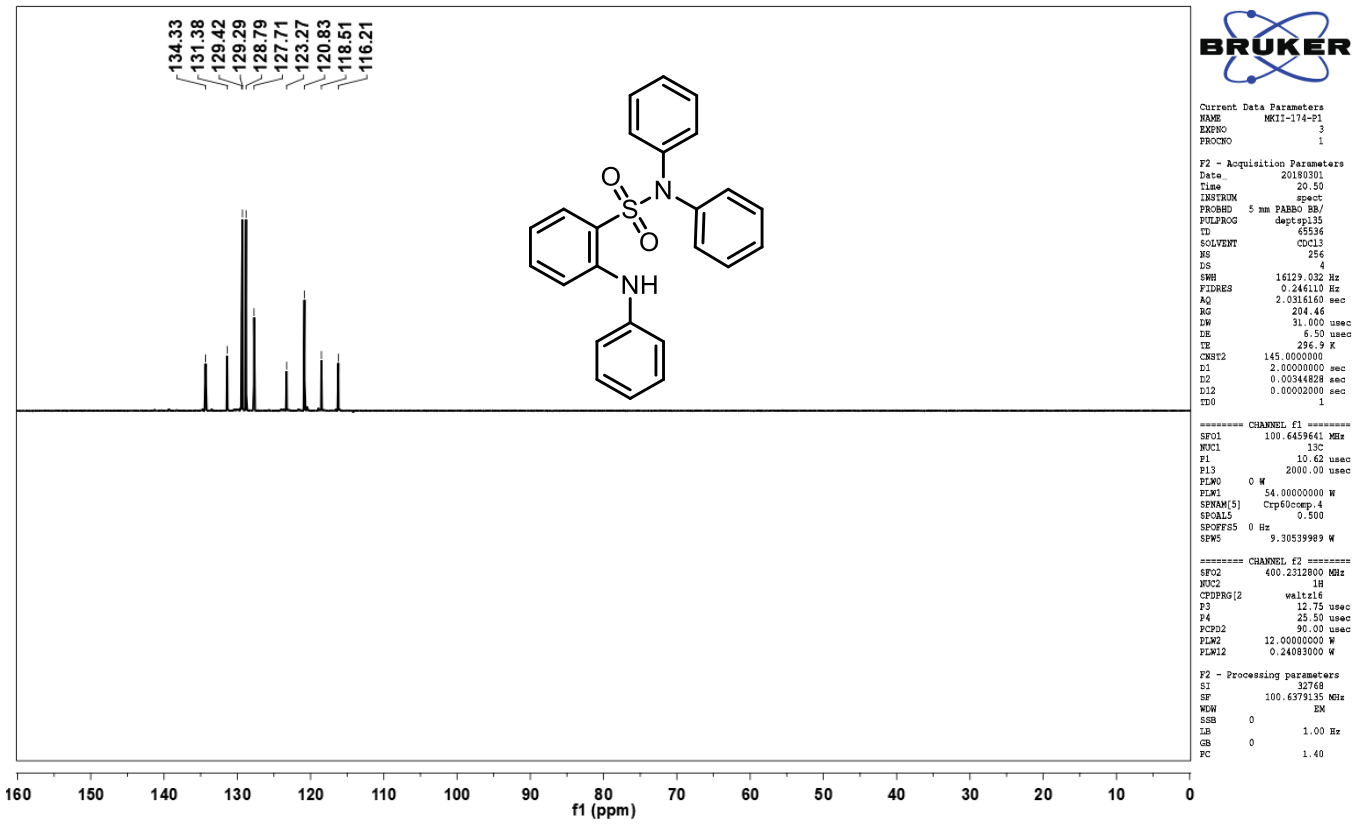
HRMS Spectrum of Compound **4f**



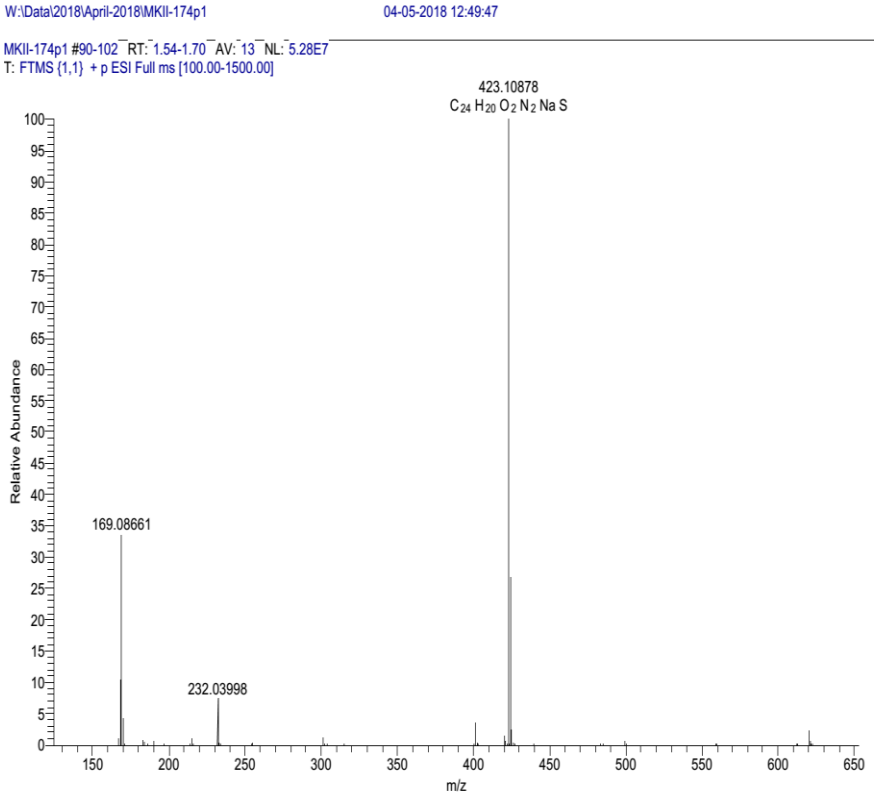
^{1}H NMR Spectrum of Compound **4g**



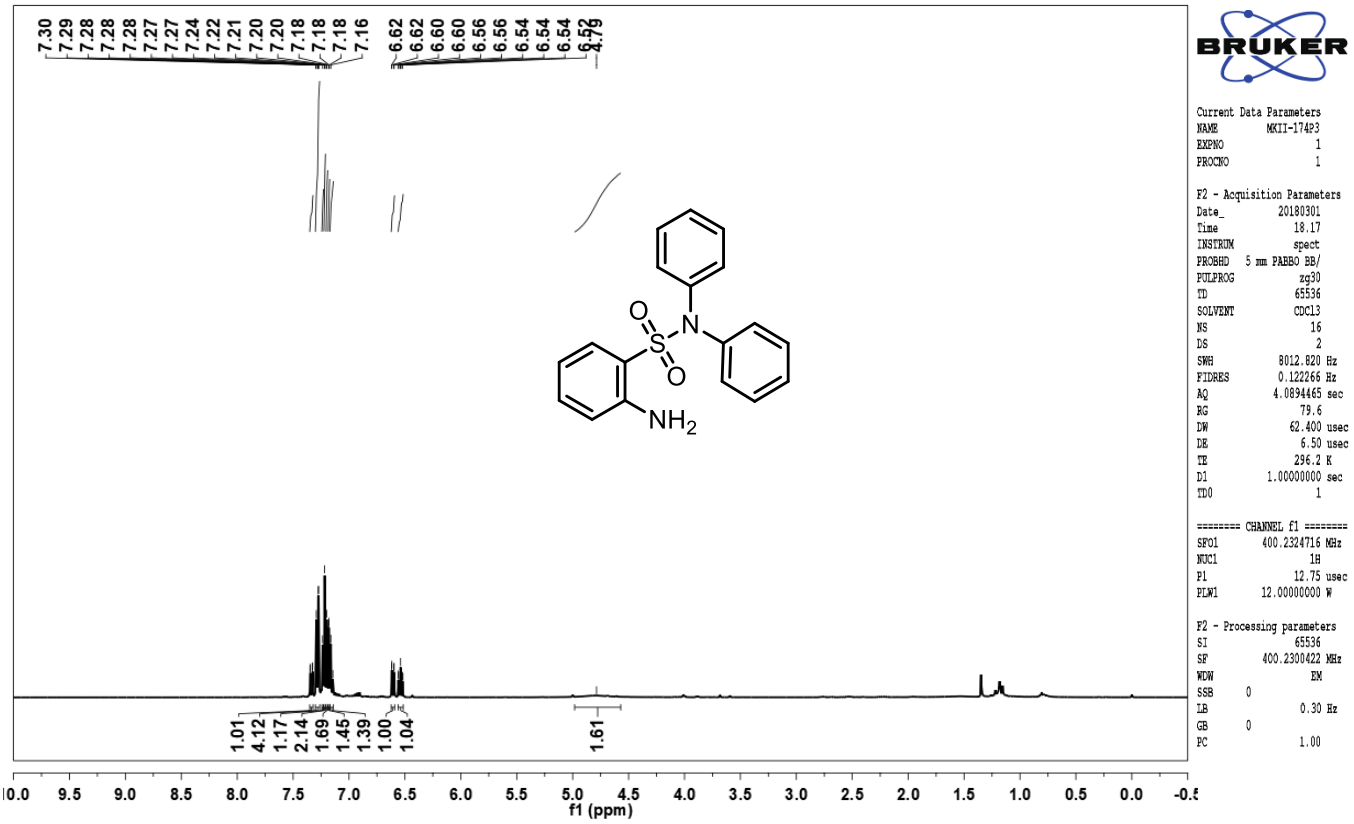
^{13}C NMR Spectrum of Compound **4g**



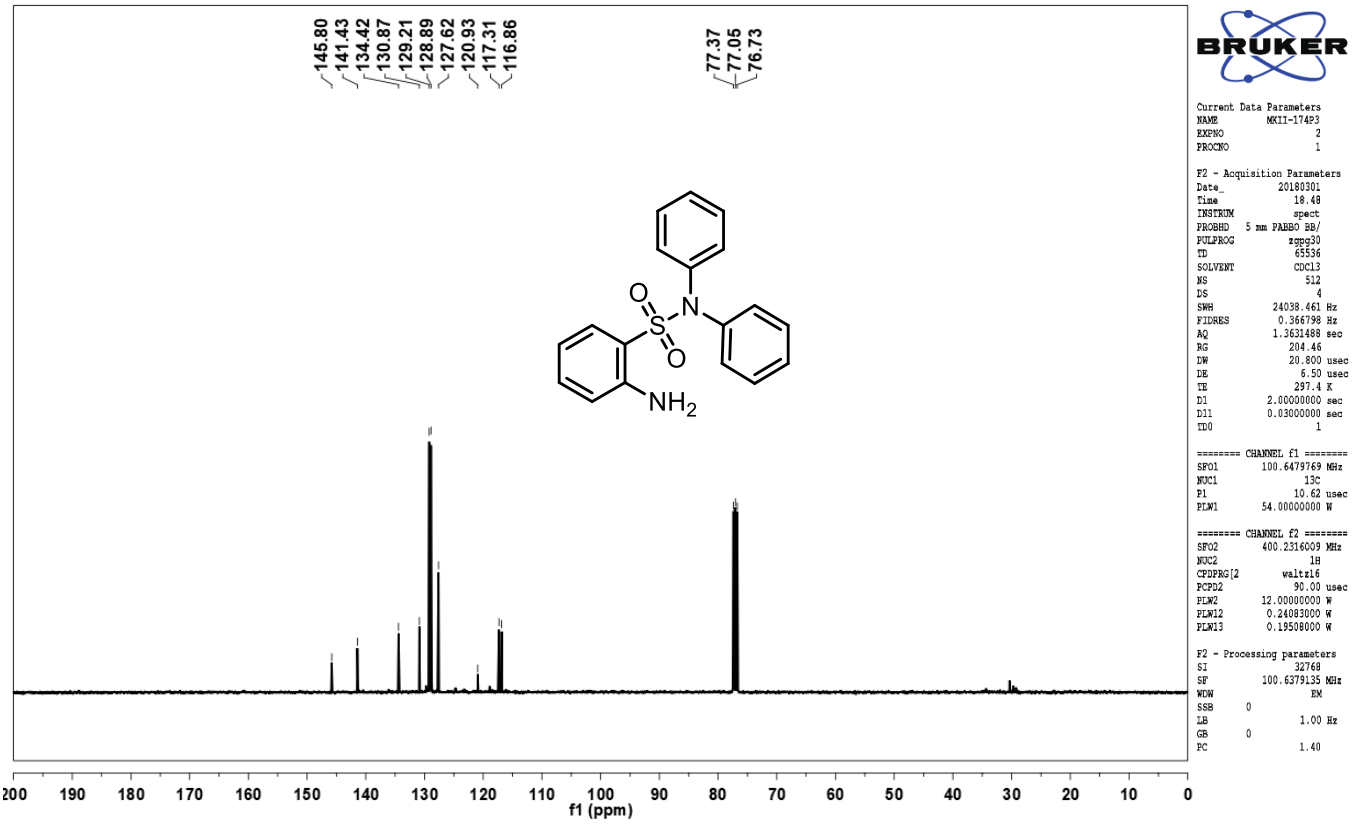
DEPT-135 NMR Spectrum of Compound **4g**



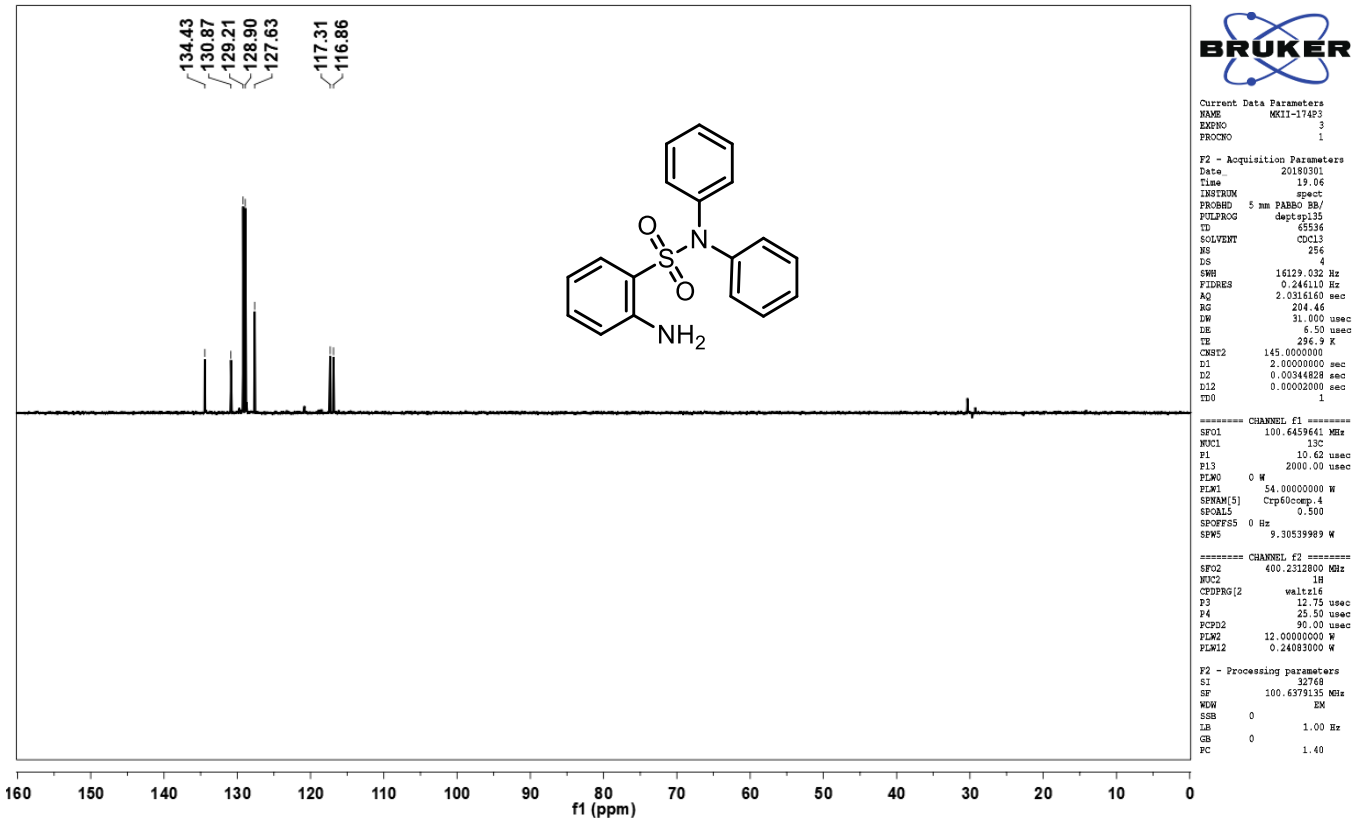
HRMS Spectrum of Compound **4g**



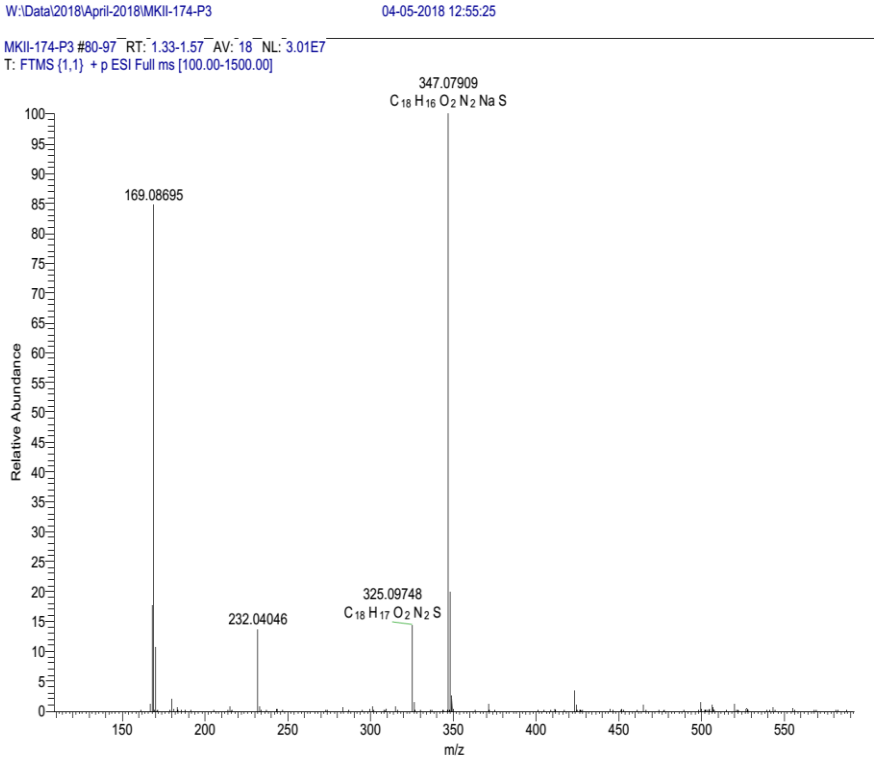
^{1}H NMR Spectrum of Compound **4h**



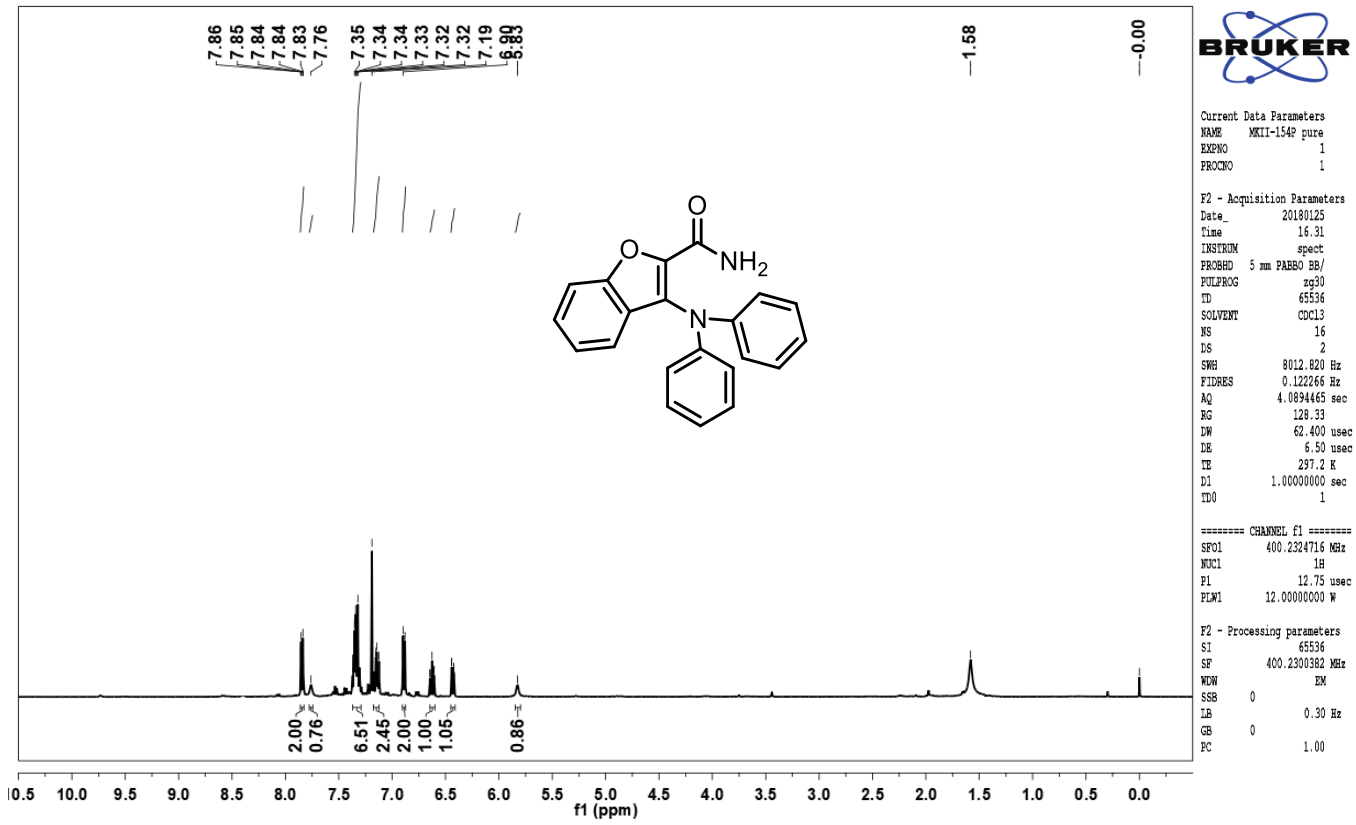
^{13}C NMR Spectrum of Compound **4h**



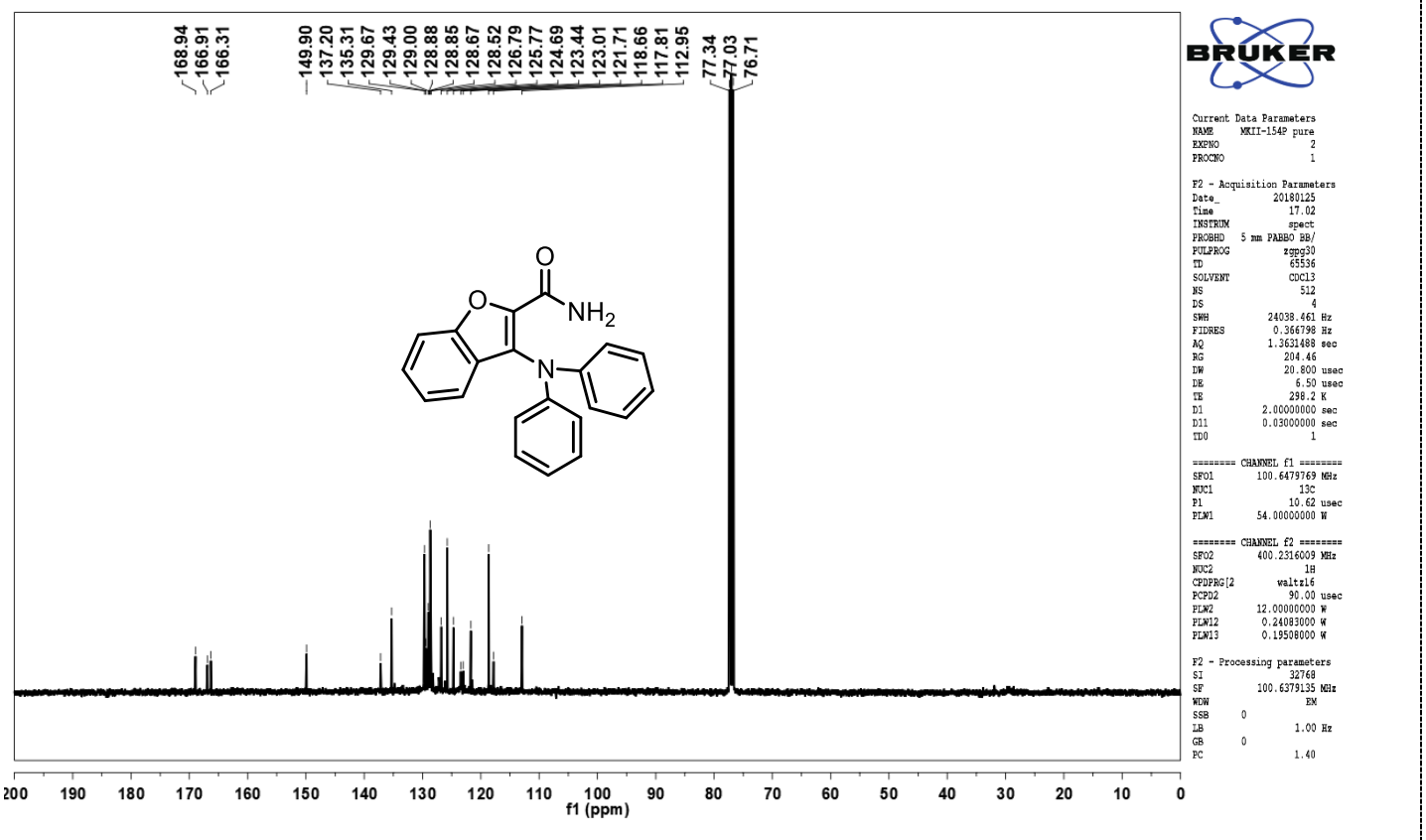
DEPT-135 NMR Spectrum of Compound **4h**



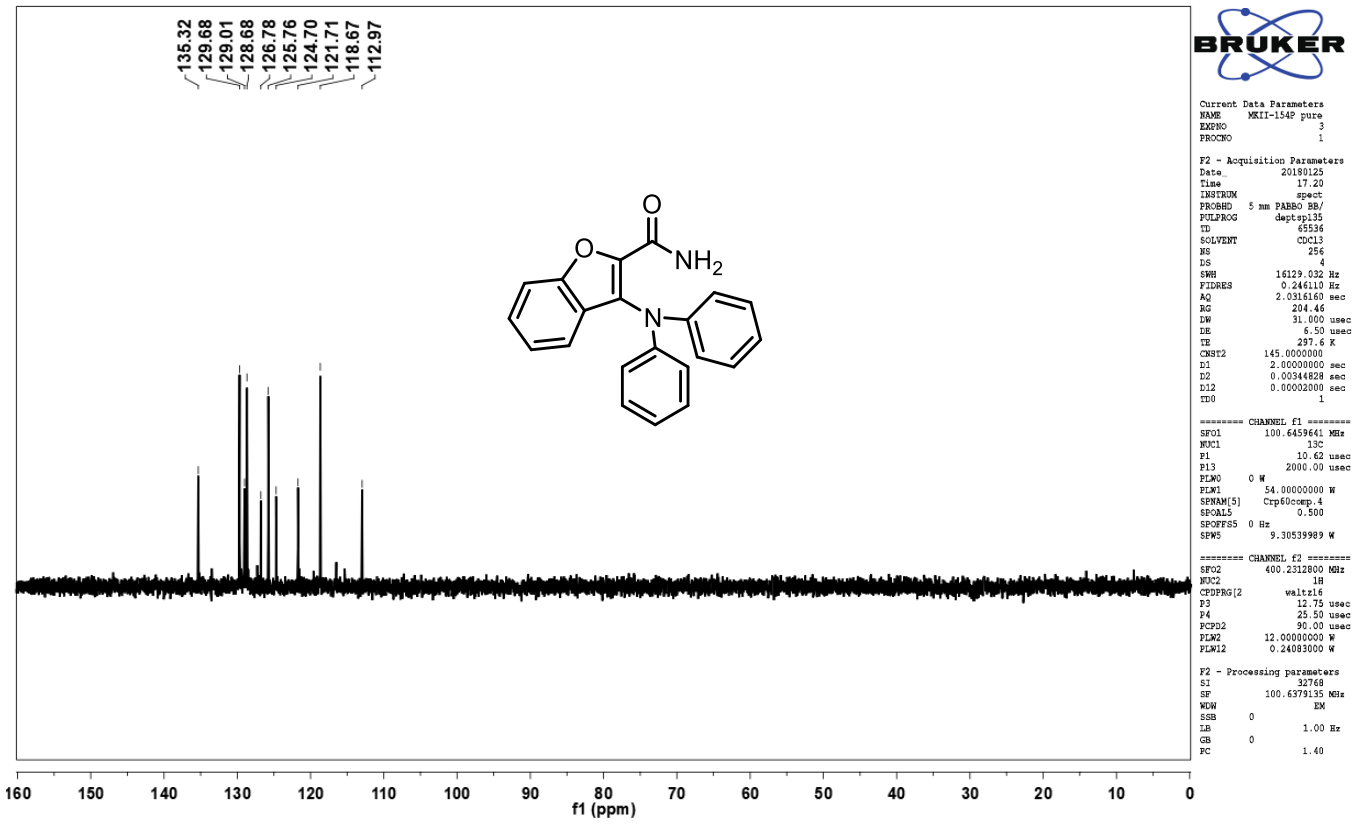
HRMS Spectrum of Compound **4h**



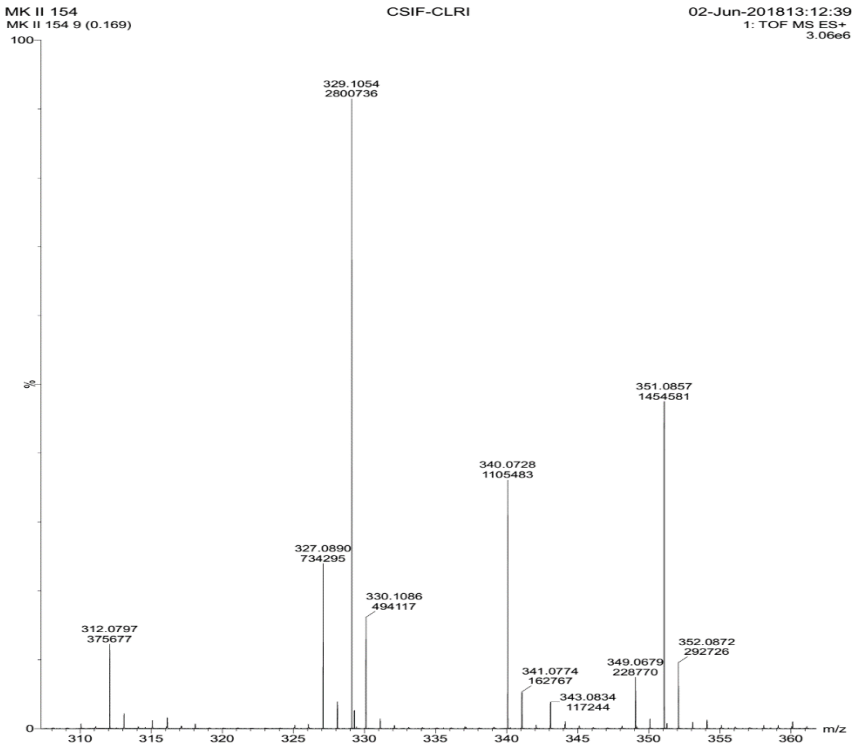
^{1}H NMR Spectrum of Compound **4i**



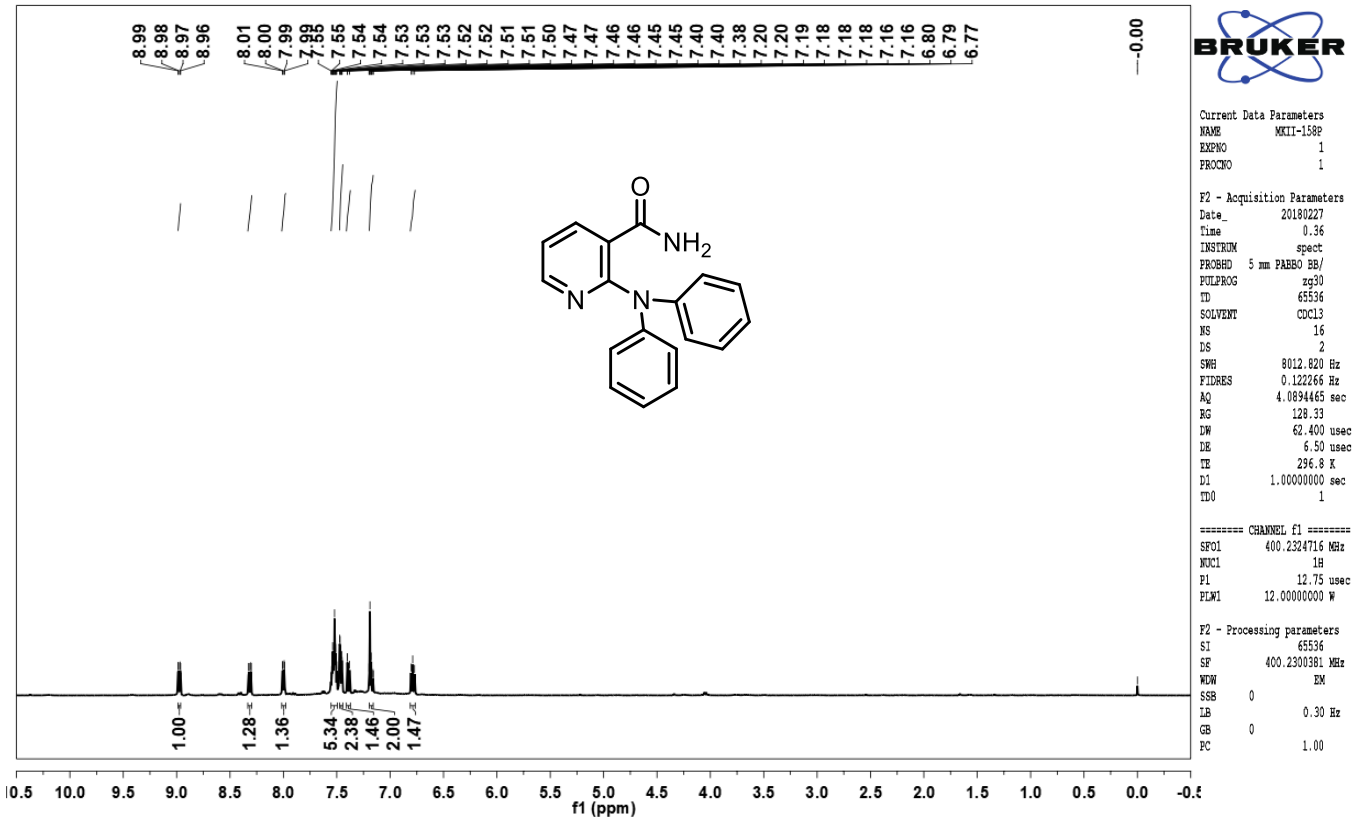
^{13}C NMR Spectrum of Compound **4i**



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



HRMS Spectrum of Compound **4i**



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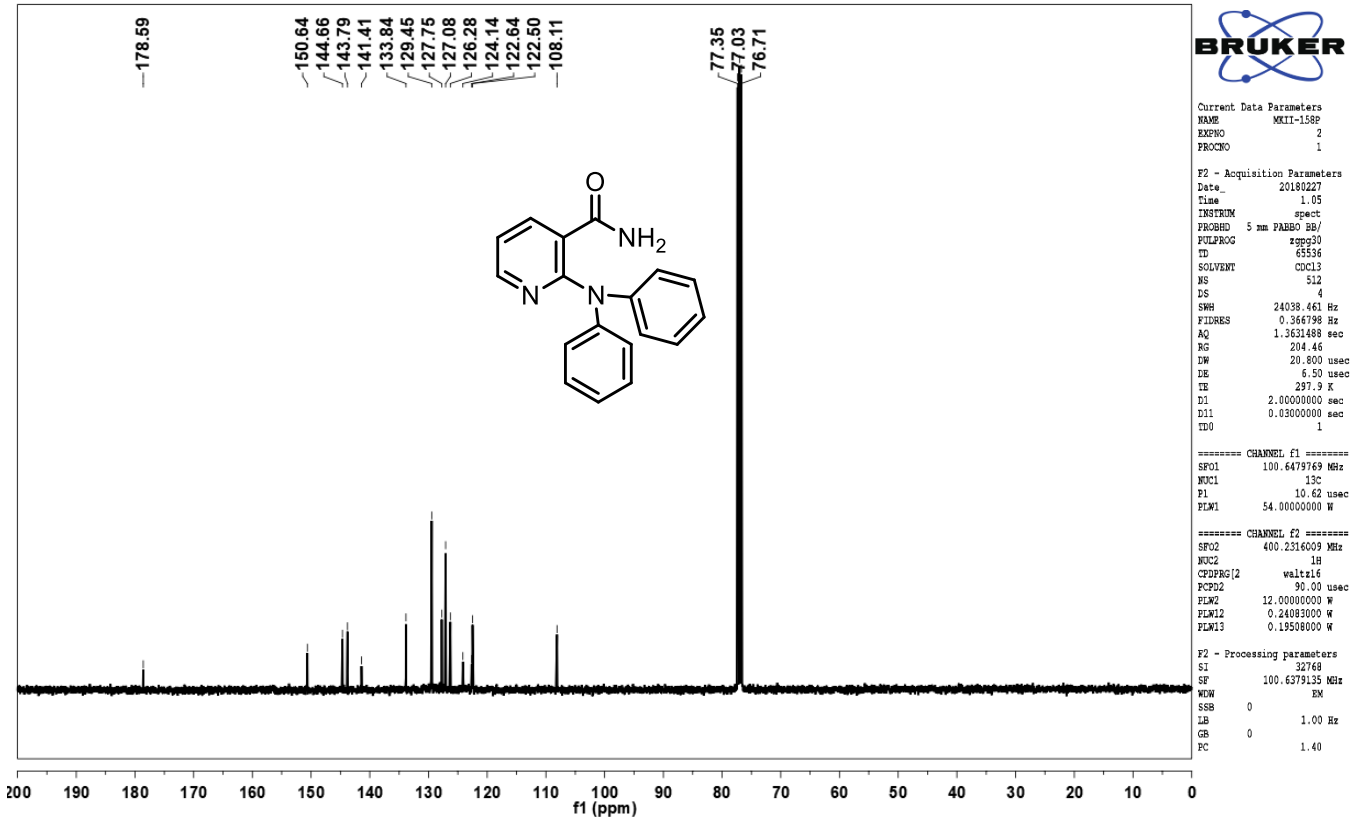
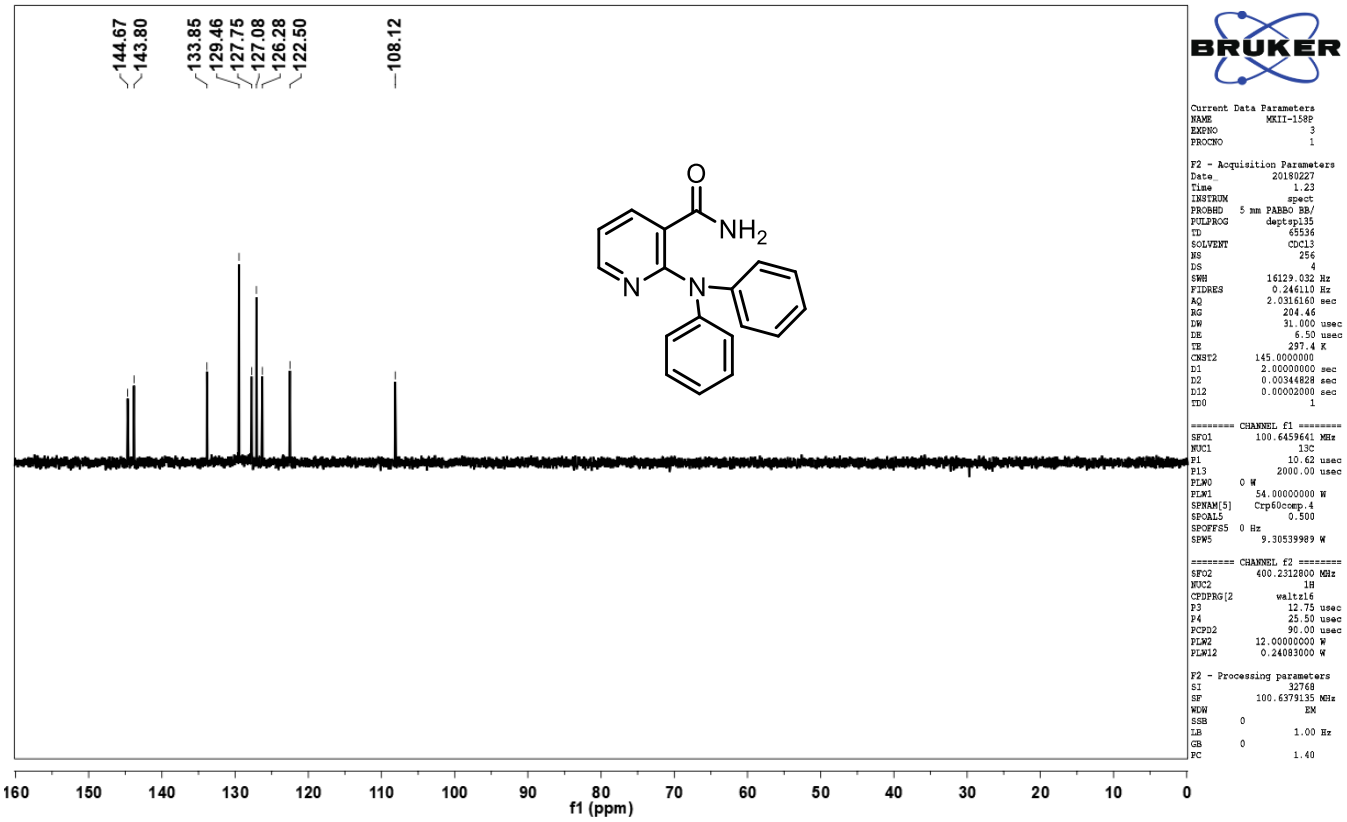
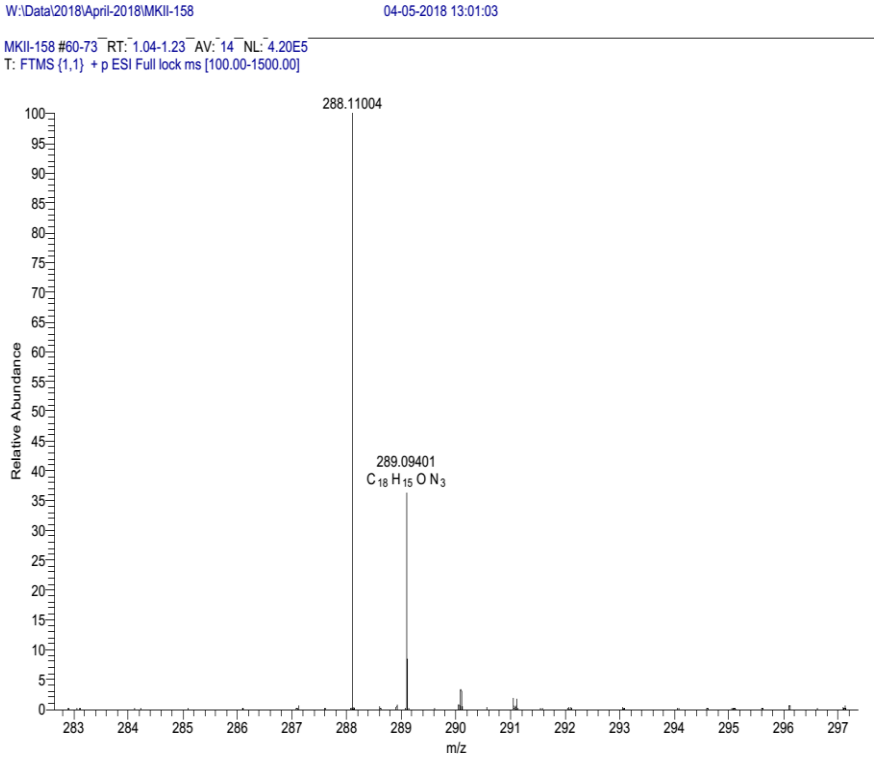


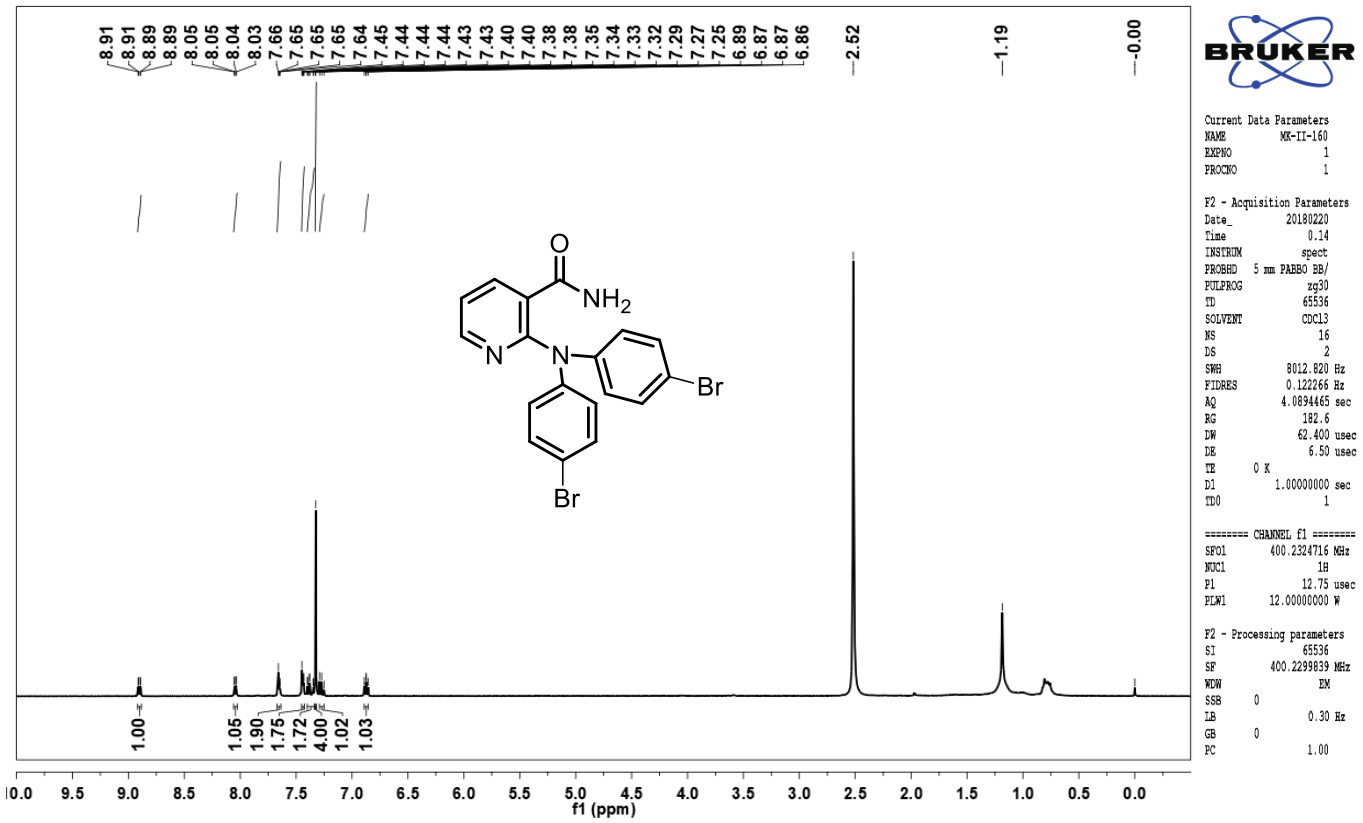
^{13}C NMR Spectrum of Compound **4j**



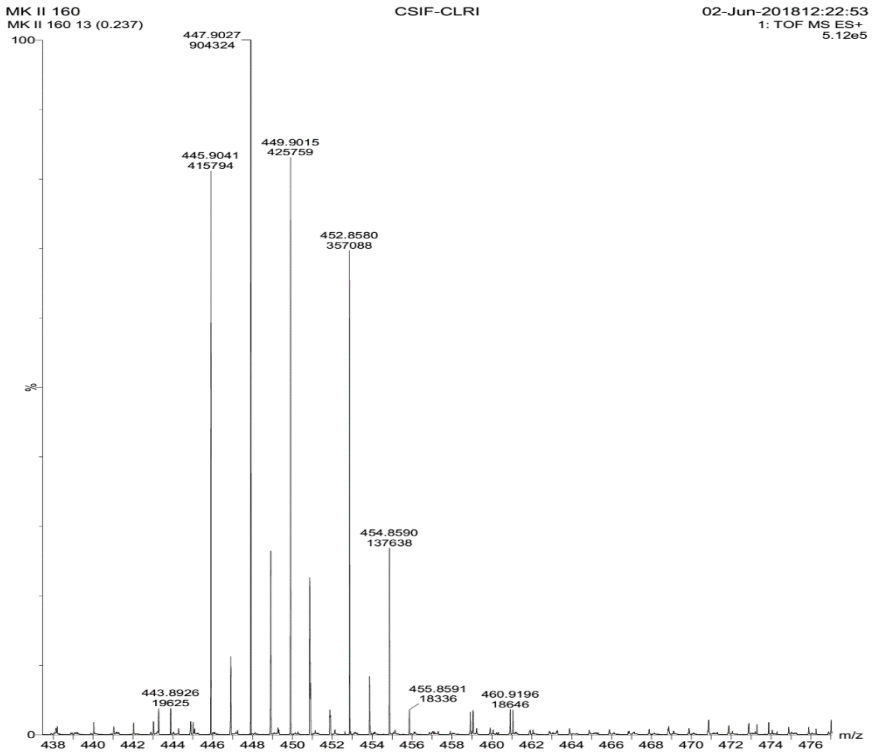
DEPT-135 NMR Spectrum of Compound **4j**



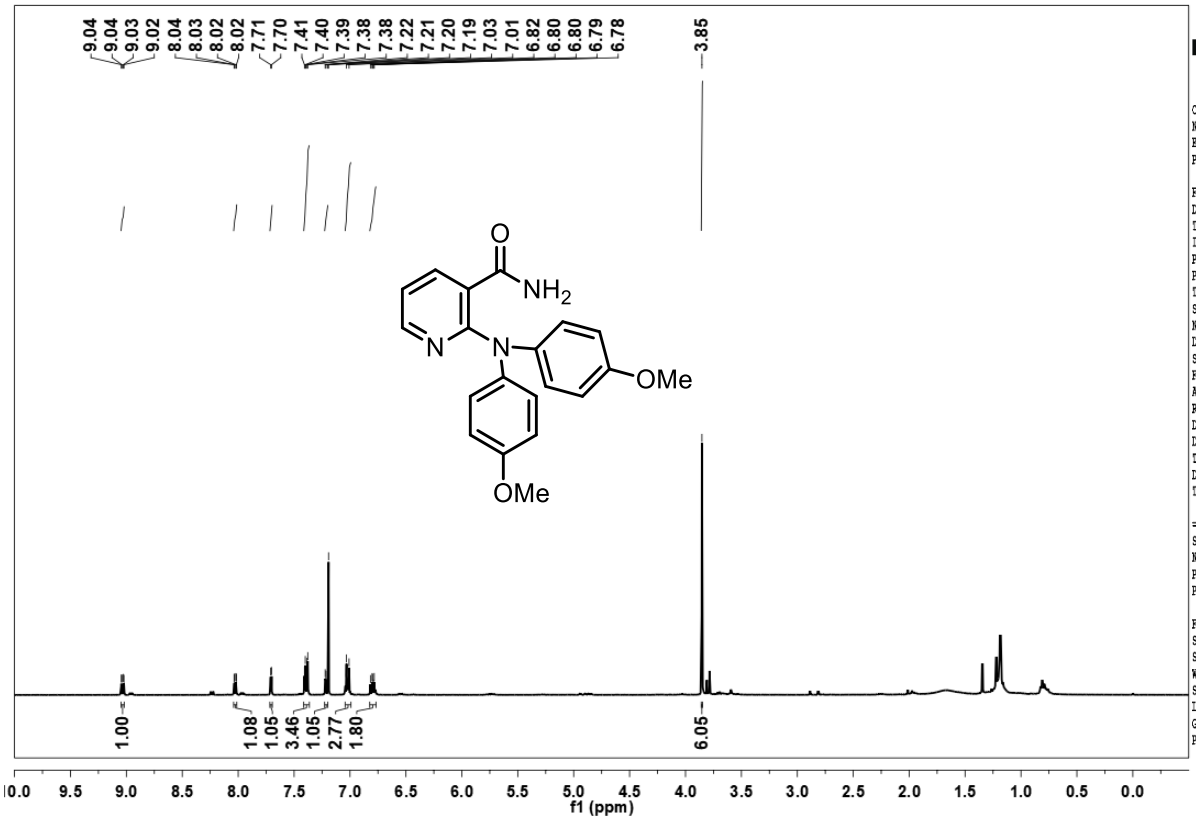
HRMS Spectrum of Compound **4j**



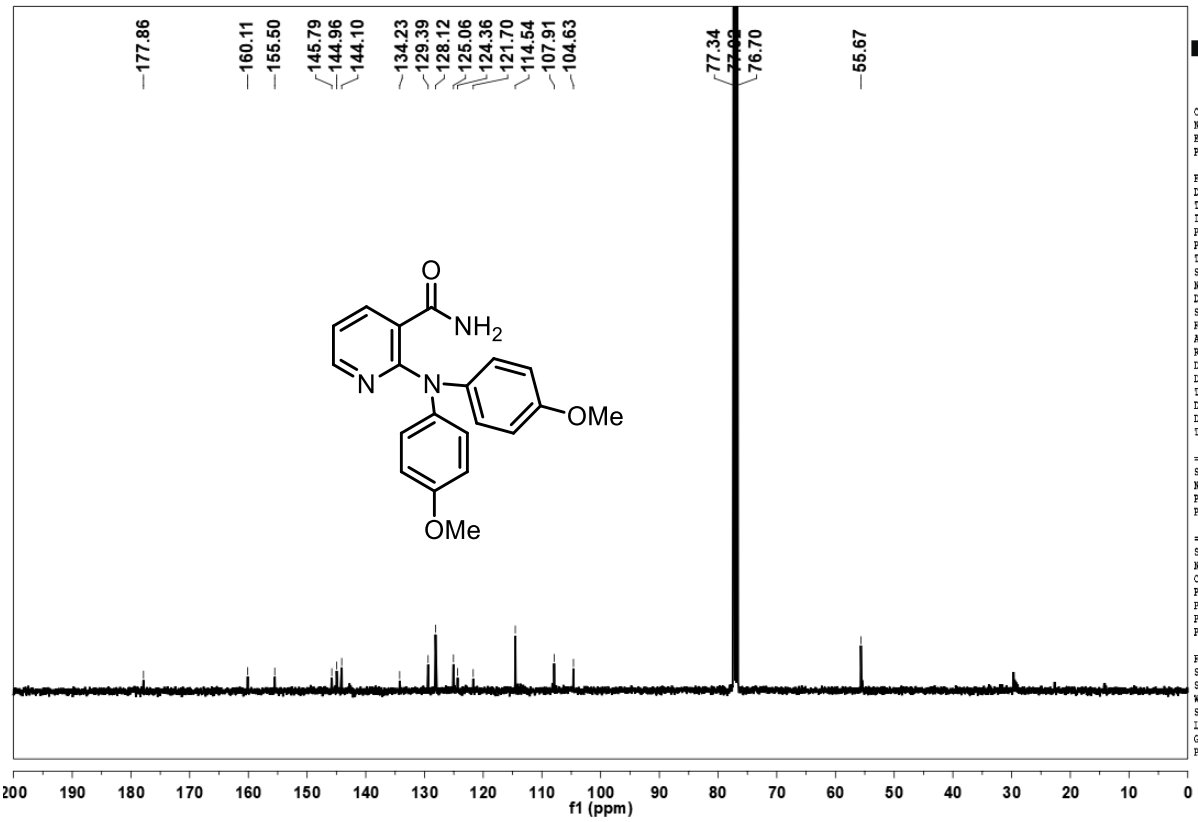
^{1}H NMR Spectrum of Compound **4k**



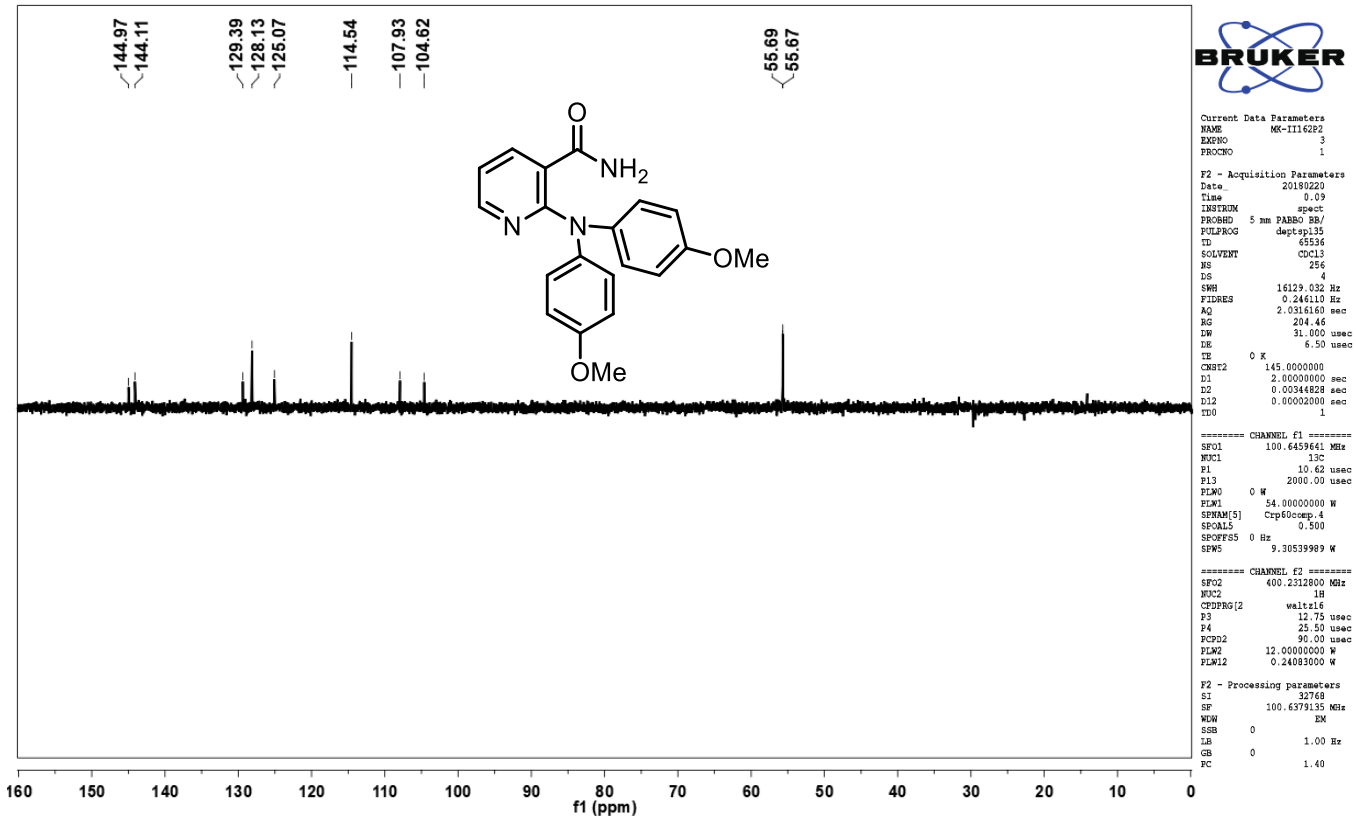
HRMS Spectrum of Compound **4k**



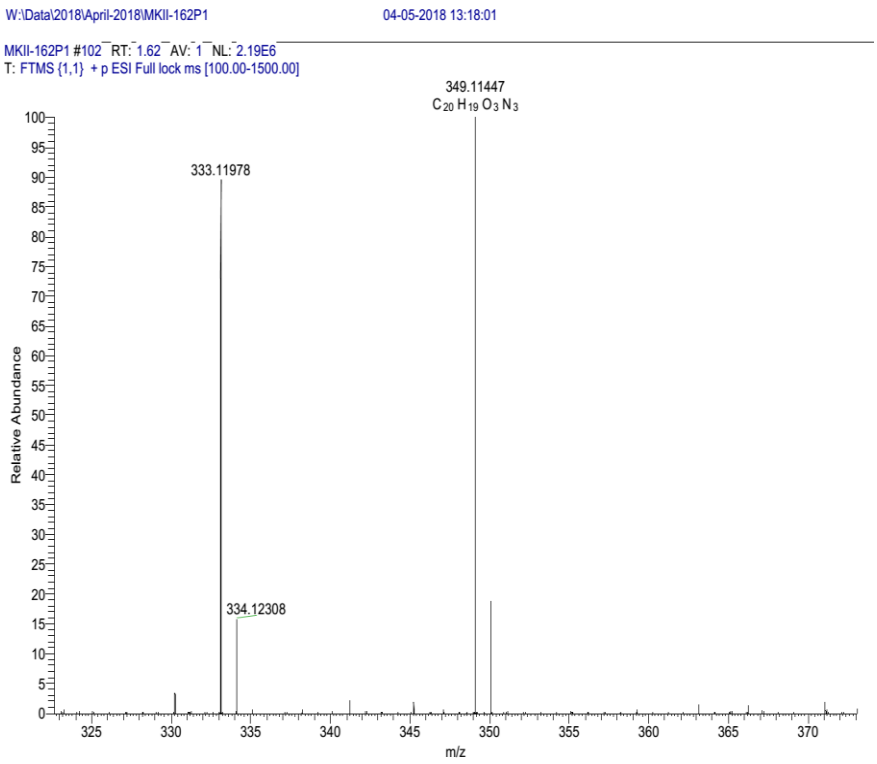
^{1}H NMR Spectrum of Compound **4l**



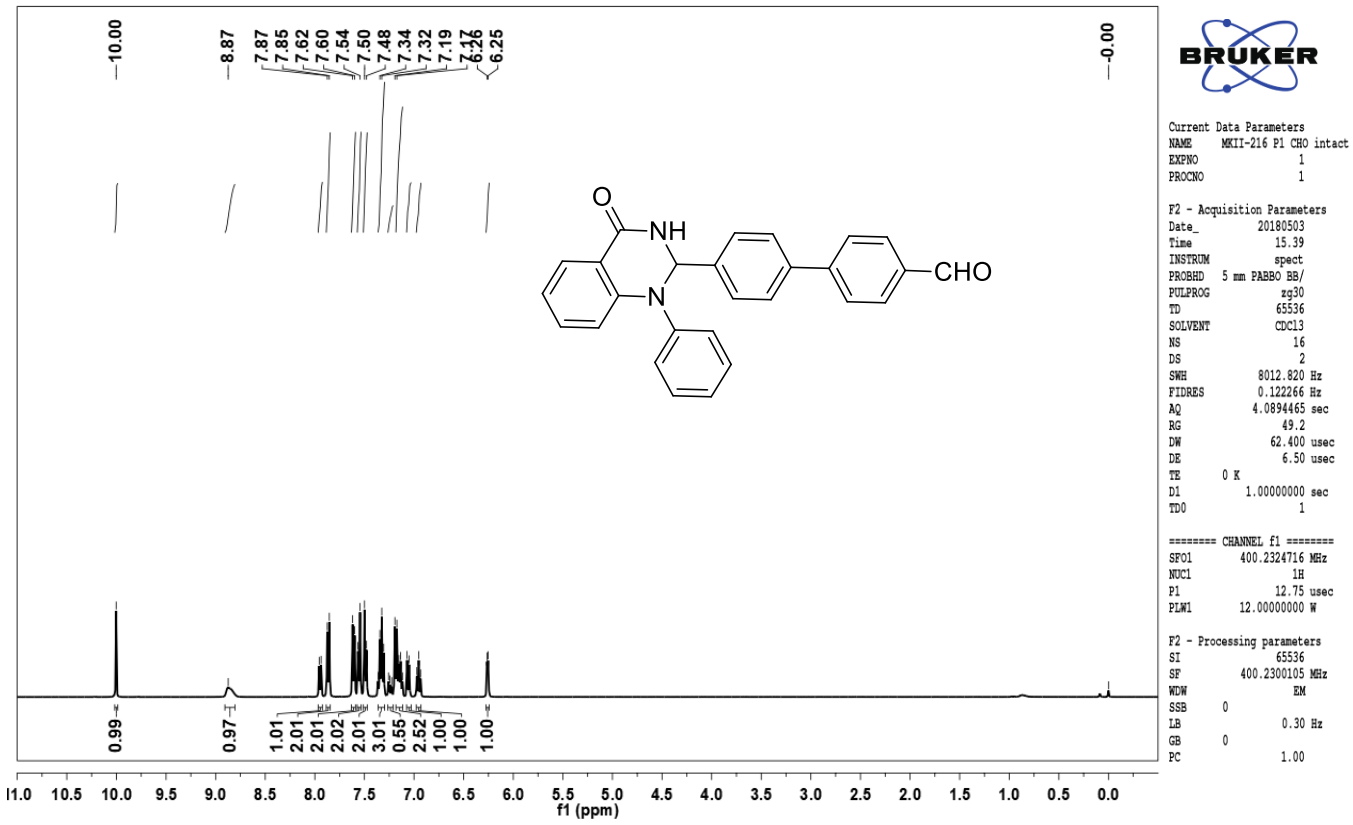
^{13}C NMR Spectrum of Compound **4l**



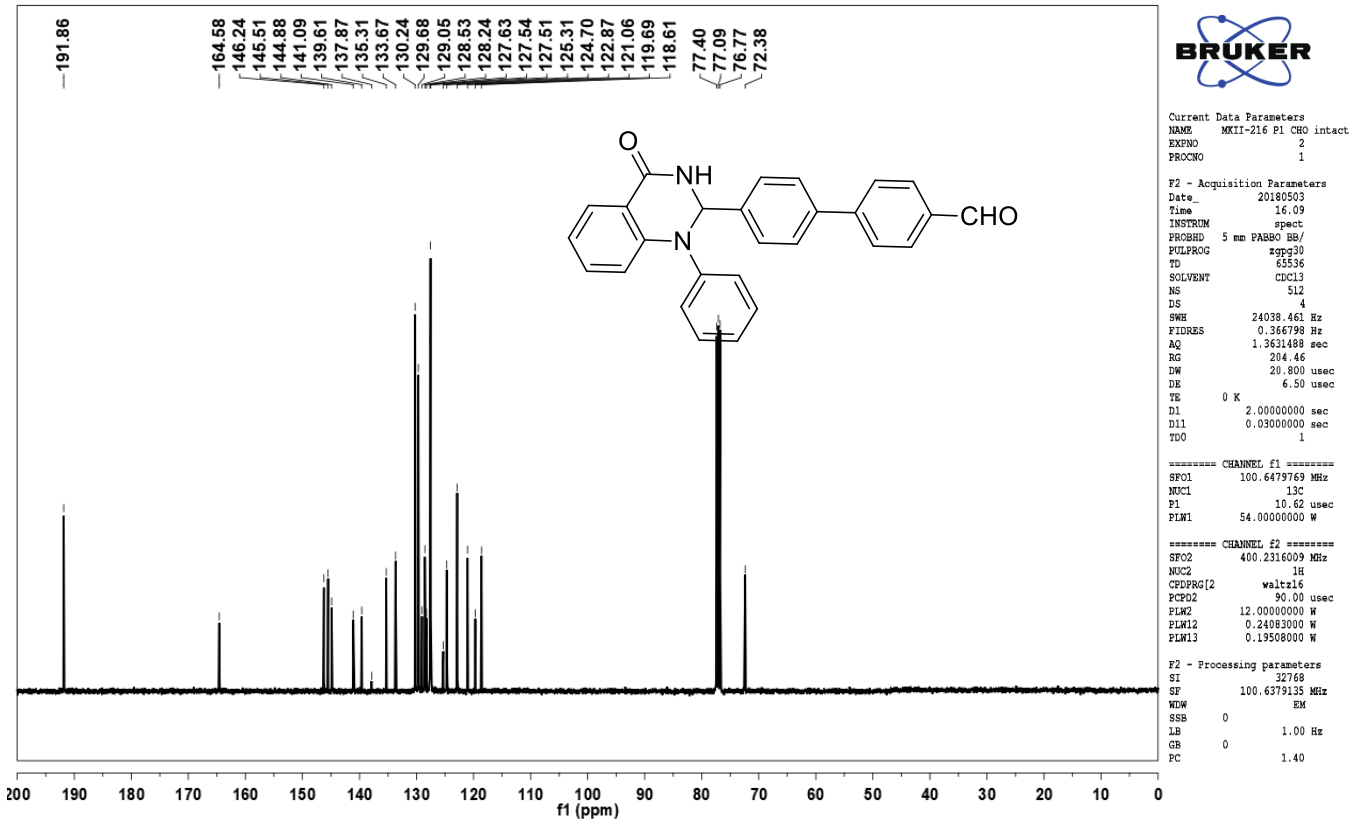
DEPT-135 NMR Spectrum of Compound **4l**



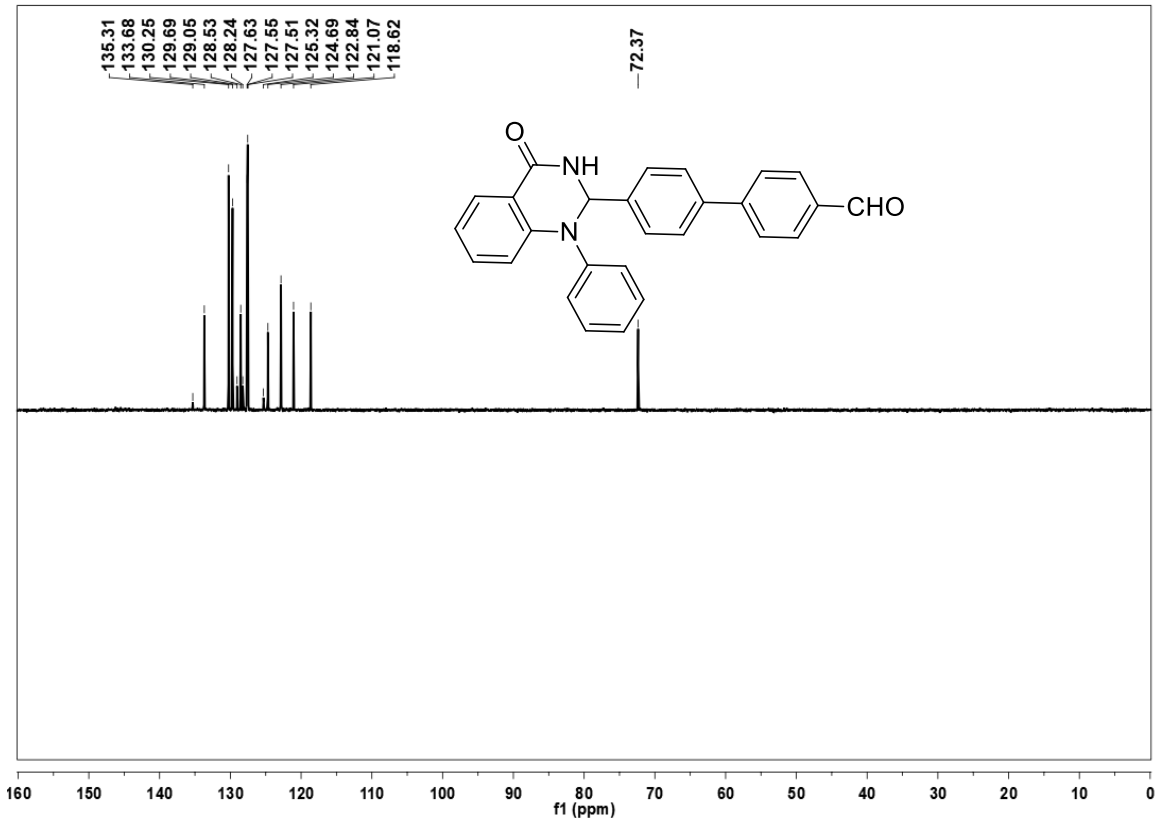
HRMS Spectrum of Compound **4l**



^{1}H NMR Spectrum of Compound **5a**



^{13}C NMR Spectrum of Compound **5a**



BRUKER

Current Data Parameters
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PROCNO 1

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Time 16.27
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PULPROG deptsp135
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SOLVENT CDCl3
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SWH 16129.032 Hz
FIDRES 0.246110 Hz
AQ 2.0316160 sec
RG 204.46
DW 31.000 usec
DE 6.50 usec
TE 0 K
CNST2 145.0000000
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
SPOAL5 0.500
SPOFFS5 0 Hz
SPW5 9.30539989 W

======== CHANNEL f2 ========
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CPDPRG[2 waltz16
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P4 25.50 usec
PCPD2 90.00 usec
PLW2 12.00000000 W
PLW12 0.24083000 W

F2 - Processing parameters
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GB 0
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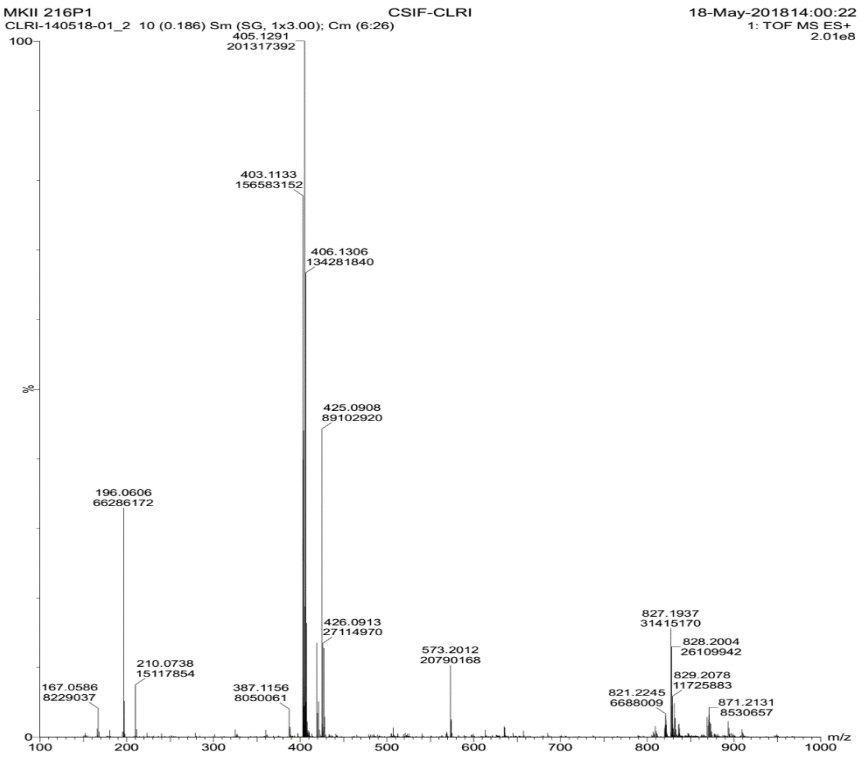
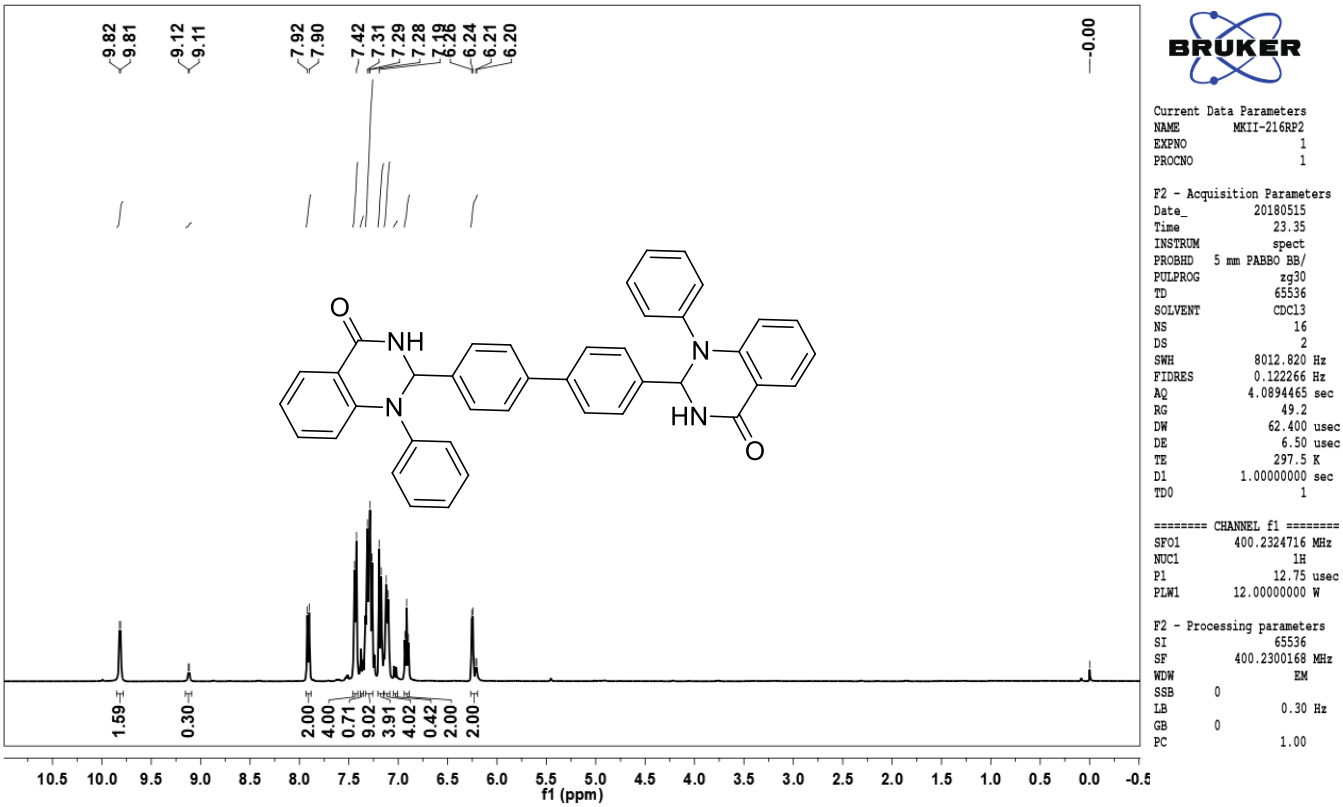
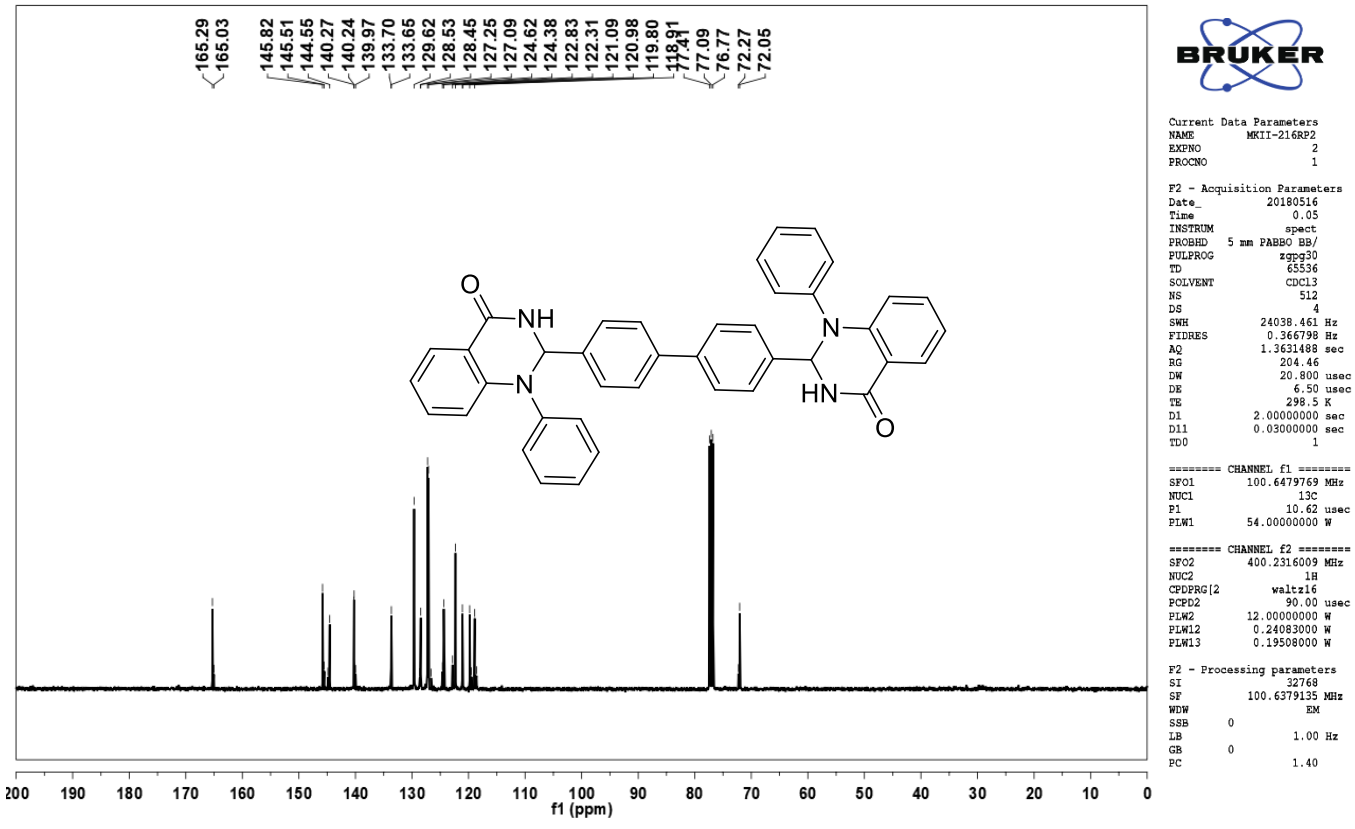
DEPT-135 NMR Spectrum of Compound **5a**



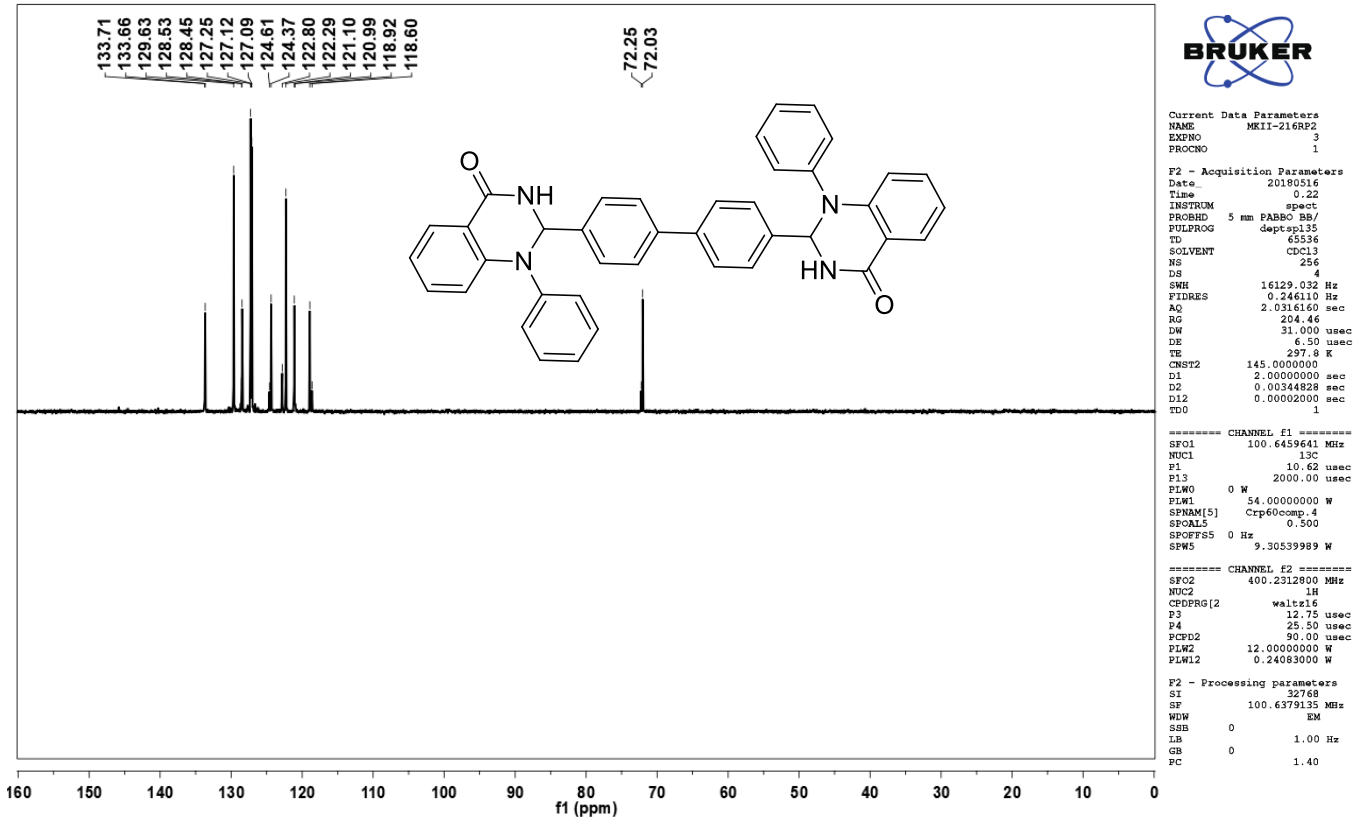
HRMS Spectrum of Compound **5a**



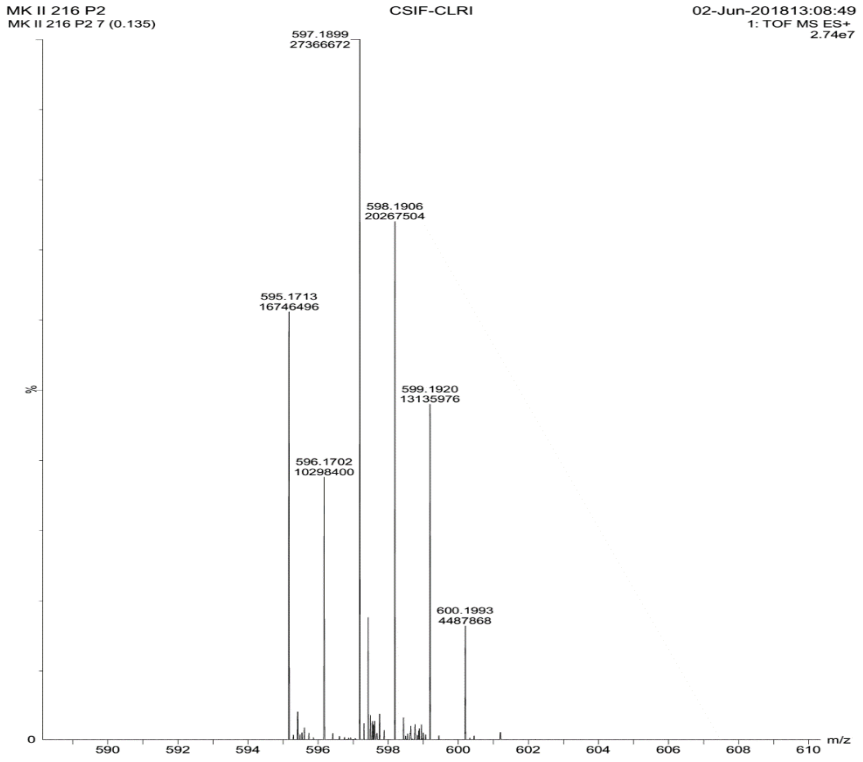
^{1}H NMR Spectrum of Compound **5b**



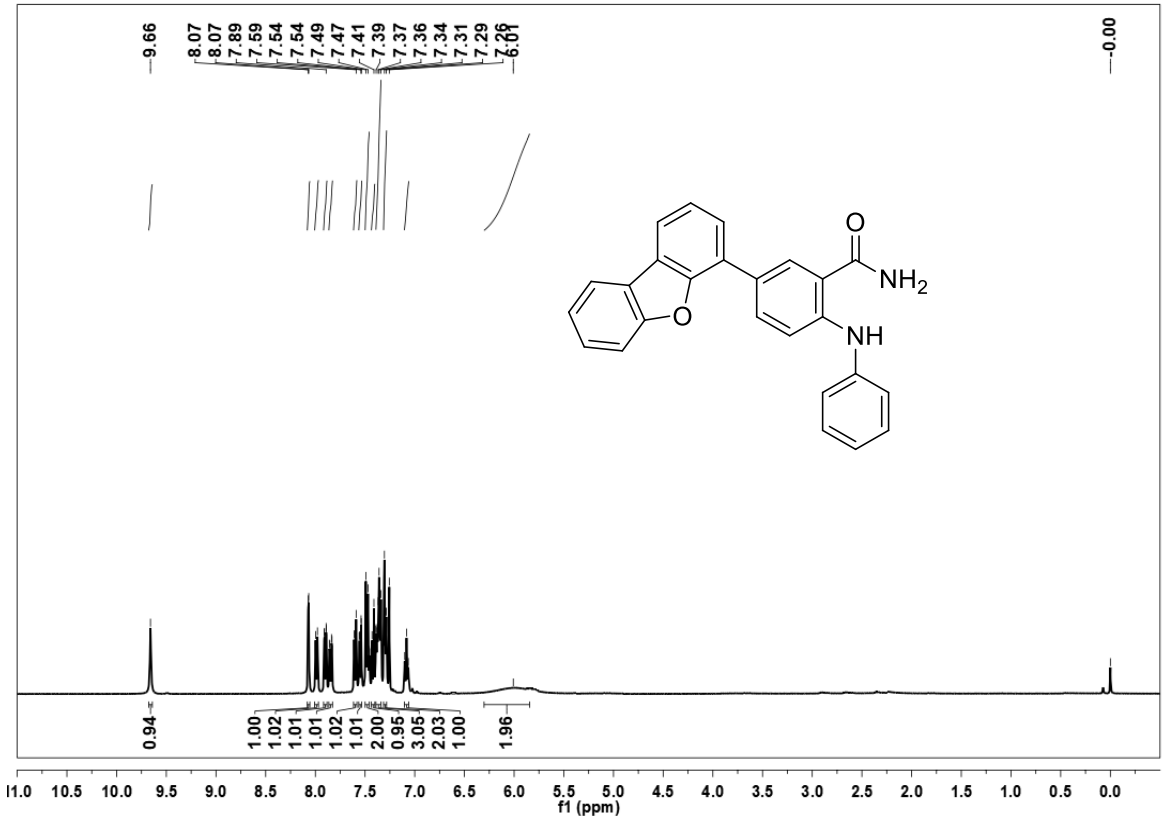
^{13}C NMR Spectrum of Compound **5b**



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



HRMS Spectrum of Compound **5b**



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PROCNO 1

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DS 2
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RG 99.98
DW 62.400 usec
DE 6.50 usec
TE 298.8 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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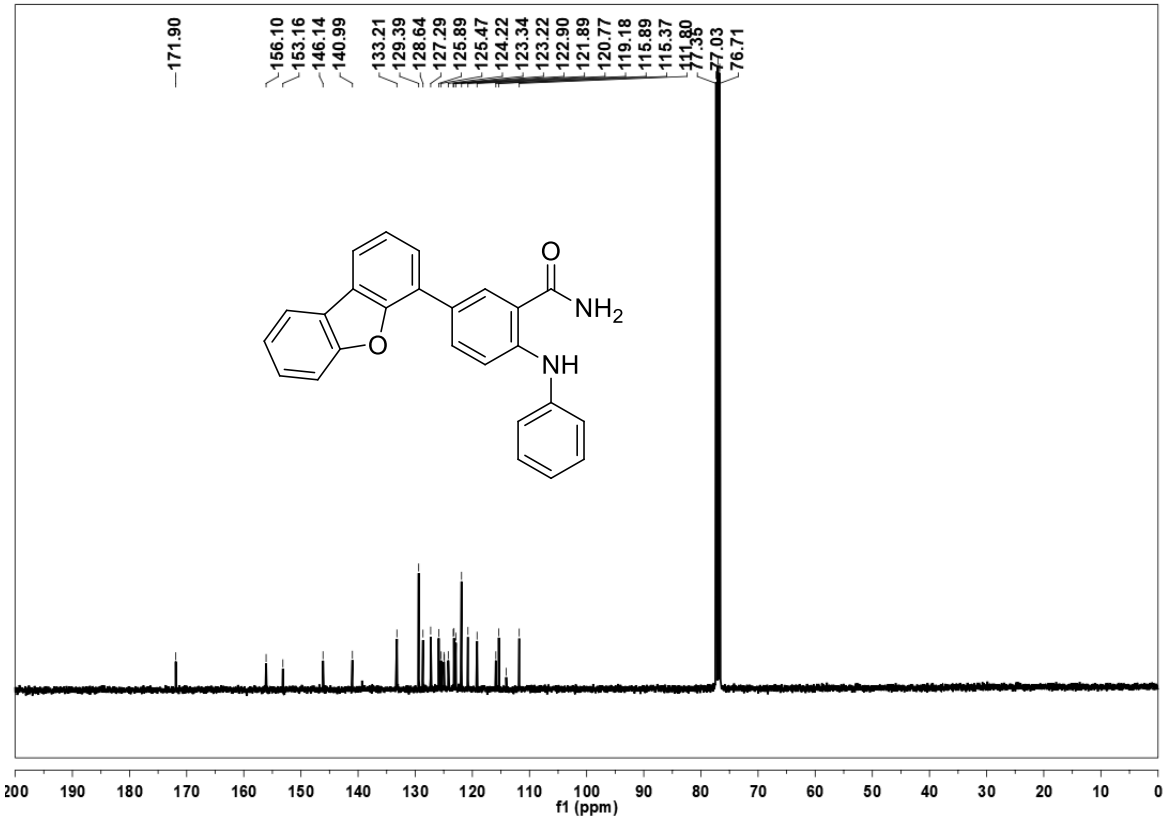
^{1}H NMR Spectrum of Compound **6a**



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PROCNO 1

F2 - Acquisition Parameters
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FIDRES 0.366798 Hz
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RG 204.46
DW 20.800 usec
DE 6.50 usec
TE 300.0 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
CPDPRG[2 waltz16
PCPD2 90.00 usec
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PLW12 0.24083000 W
PLW13 0.19508000 W

F2 - Processing parameters
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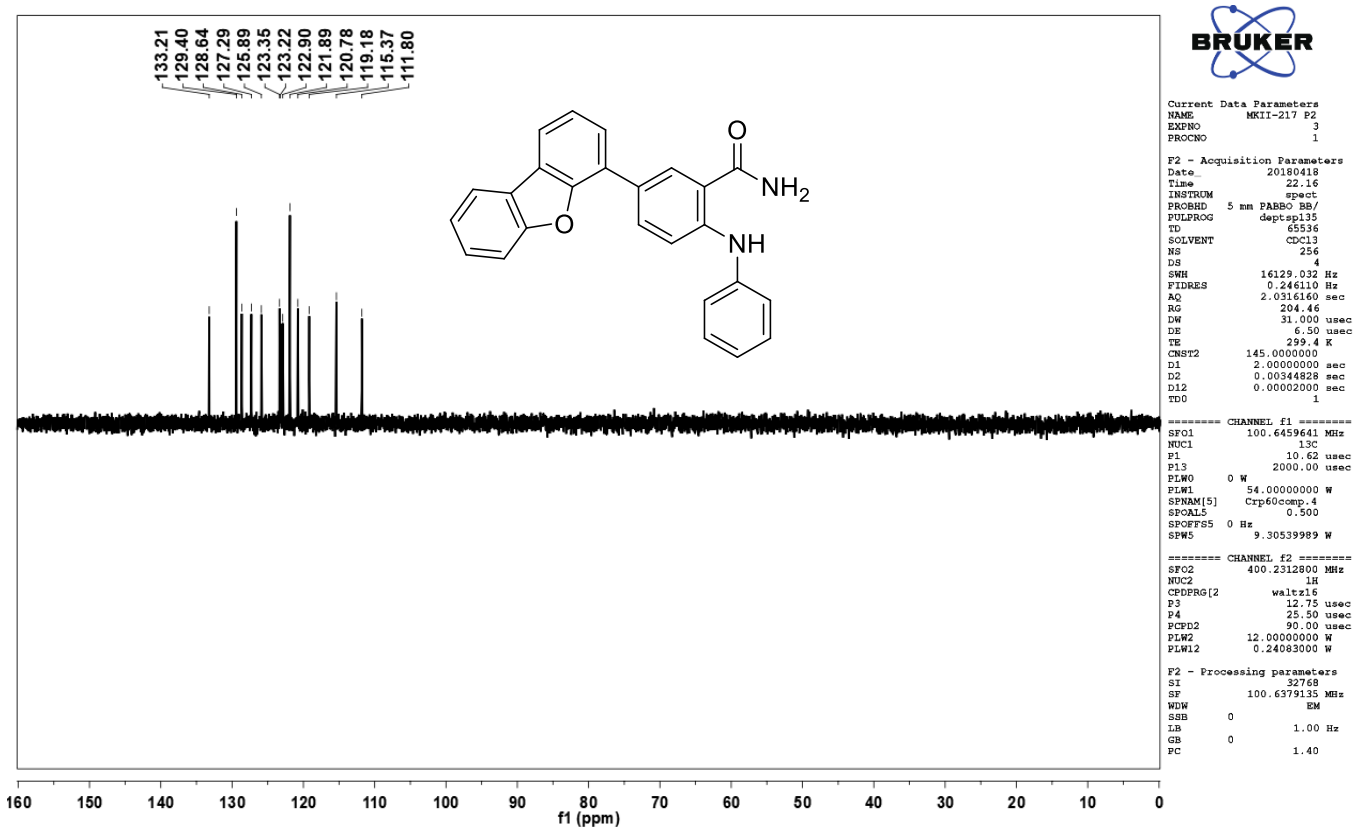
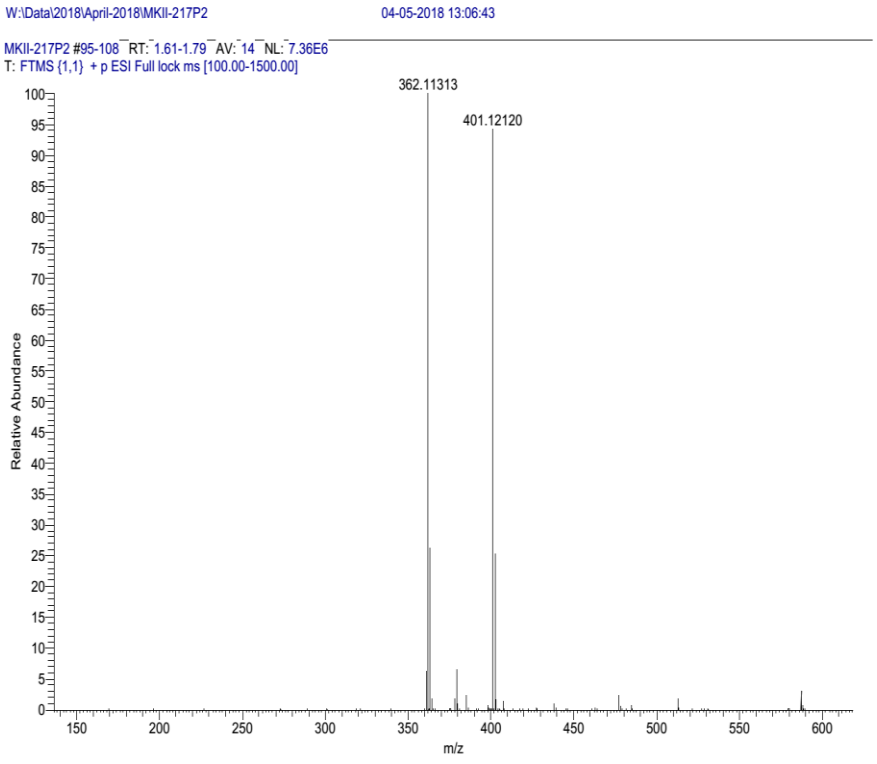
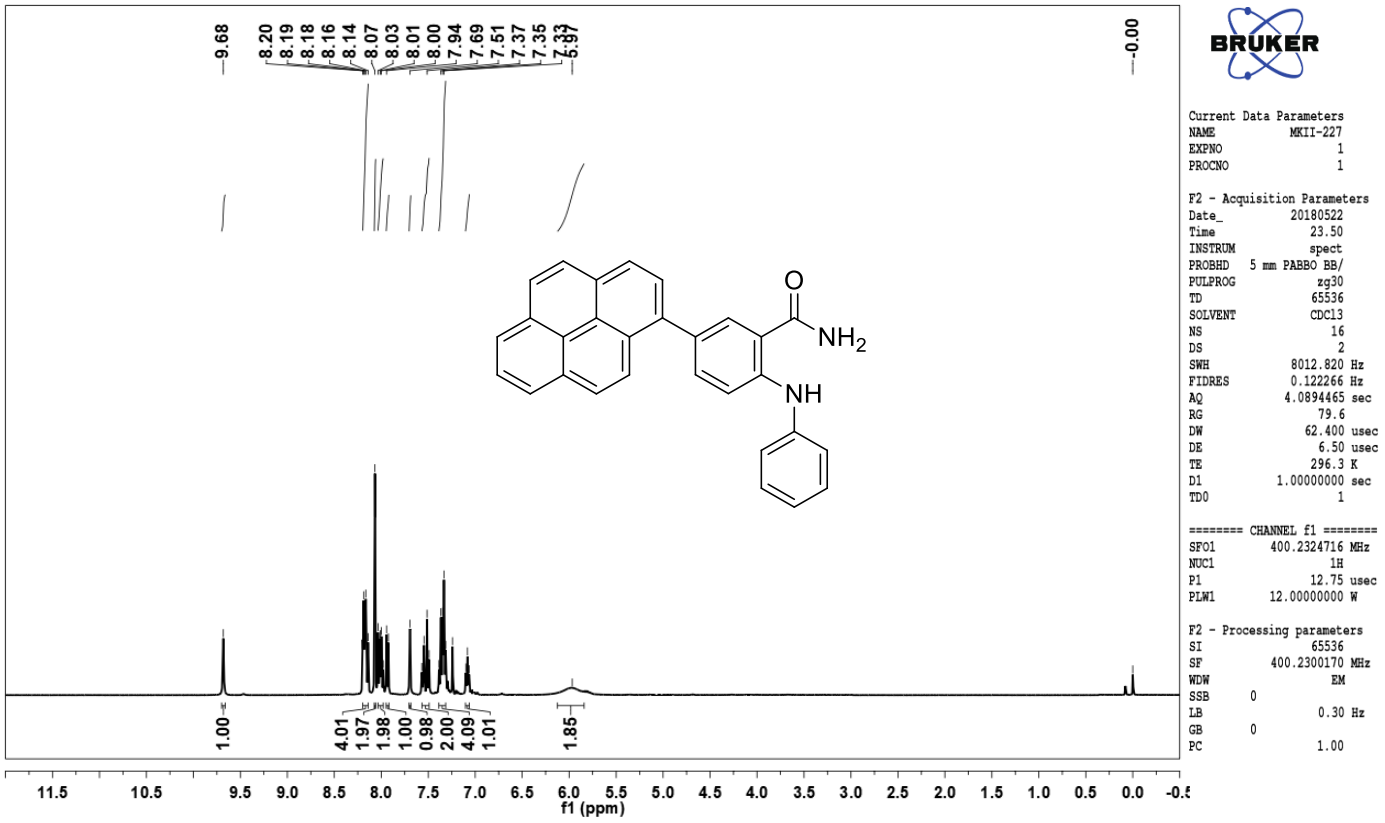
^{13}C NMR Spectrum of Compound **6a**



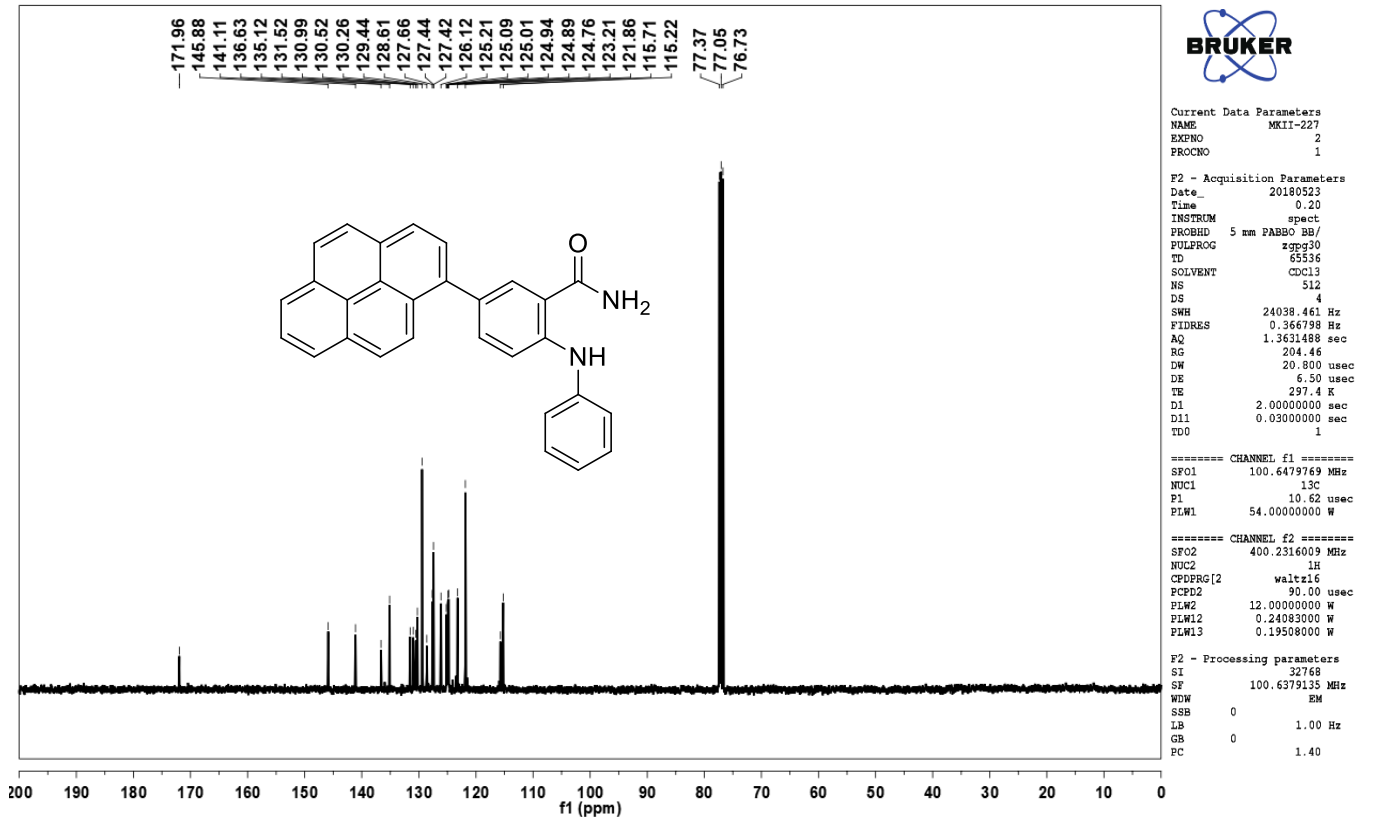
DEPT-135 NMR Spectrum of Compound **6a**



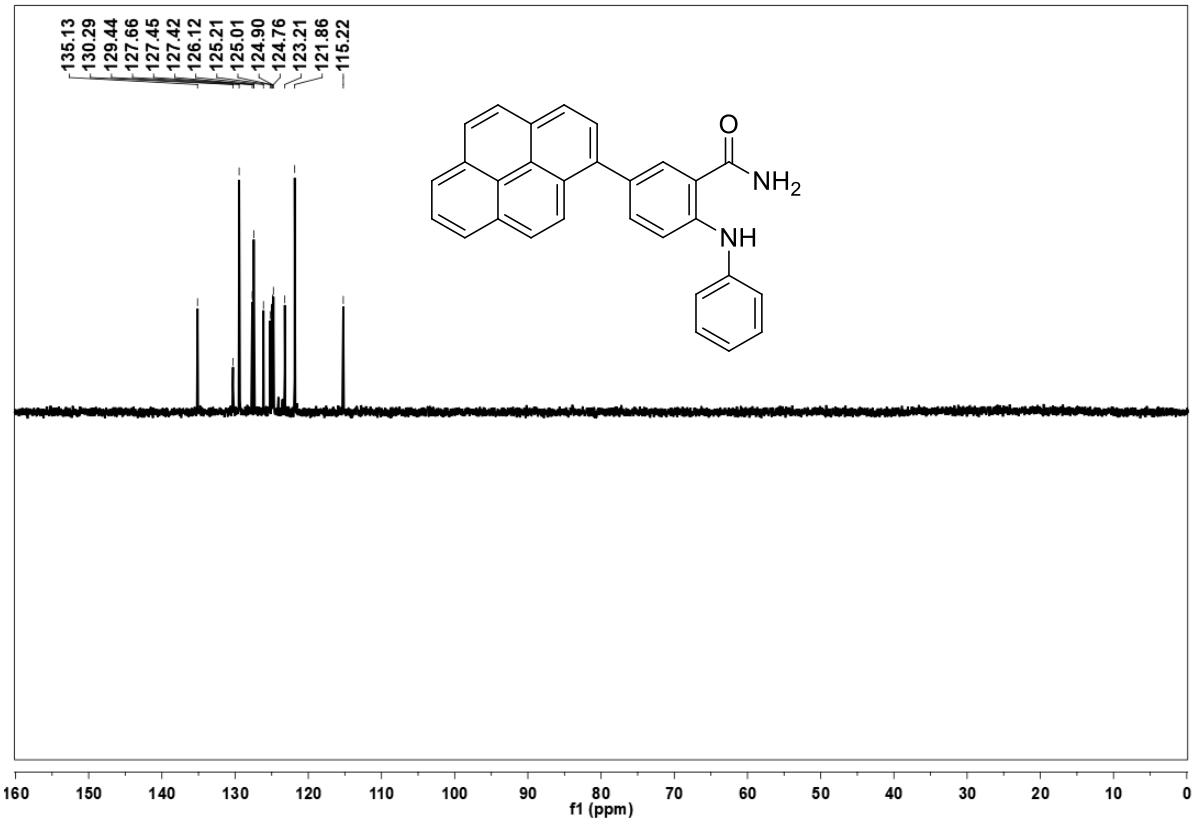
HRMS Spectrum of Compound **6a**



^{1}H NMR Spectrum of Compound **6b**



^{13}C NMR Spectrum of Compound **6b**



BRUKER

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PROCNO                   1

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FIDRES               0.246110 Hz
AQ                2.0316160 sec
RG                   204.46
DW                  31.000 usec
DE                   6.50 usec
TE                  296.9 K
CNST2           145.0000000
D1                2.00000000 sec
D2                0.00344828 sec
D12               0.00002000 sec
TD0                      1

======== CHANNEL f1 ========
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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
SPOAL5               0.500
SPOFFS5    0 Hz
SPW5           9.30539989 W

======== CHANNEL f2 ========
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NUC2                   1H
CPDPRG[2           waltz16
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P4                   25.50 usec
PCPD2                90.00 usec
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PLW12           0.24083000 W

F2 - Processing parameters
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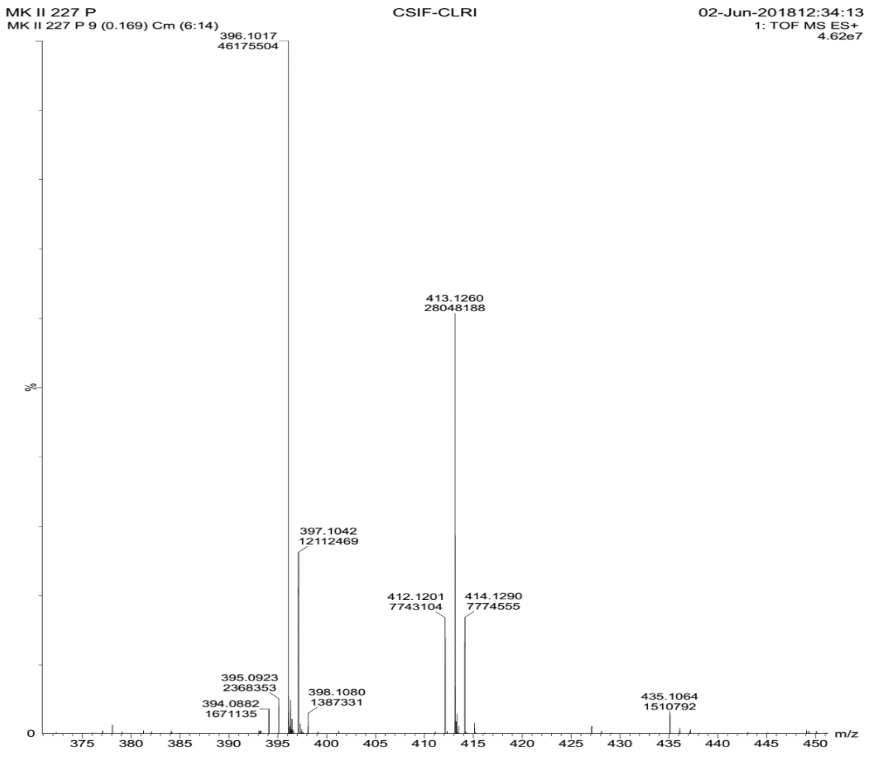
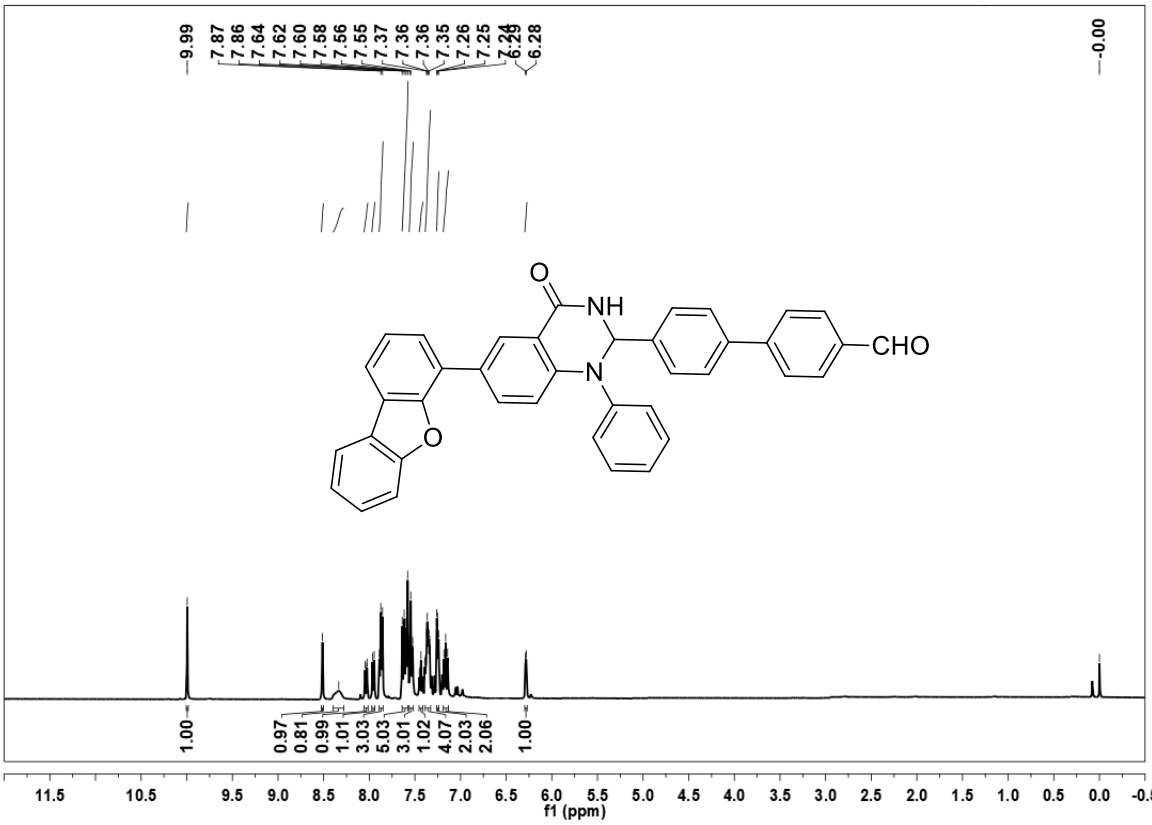
DEPT-135 NMR Spectrum of Compound **6b**



HRMS Spectrum of Compound **6b**

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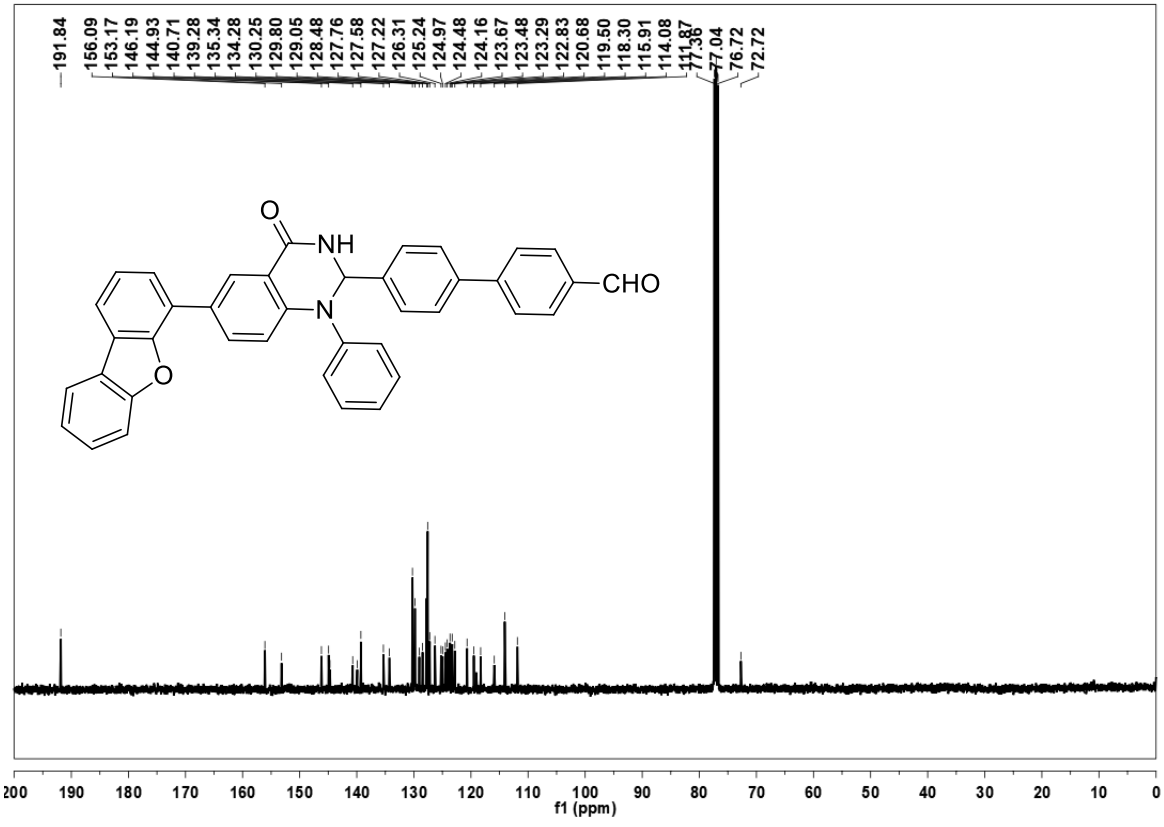
Current Data Parameters
NAME         MKII-221 P1
EXPNO                 1
PROCNO                1

F2 - Acquisition Parameters
Date_          20180503
Time              16.32
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
TD0                   1

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

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

^{1}H NMR Spectrum of Compound **7a**

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Current Data Parameters
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EXPNO                 2
PROCNO                1

F2 - Acquisition Parameters
Date_          20180503
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
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
CPDPRG[2          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
```
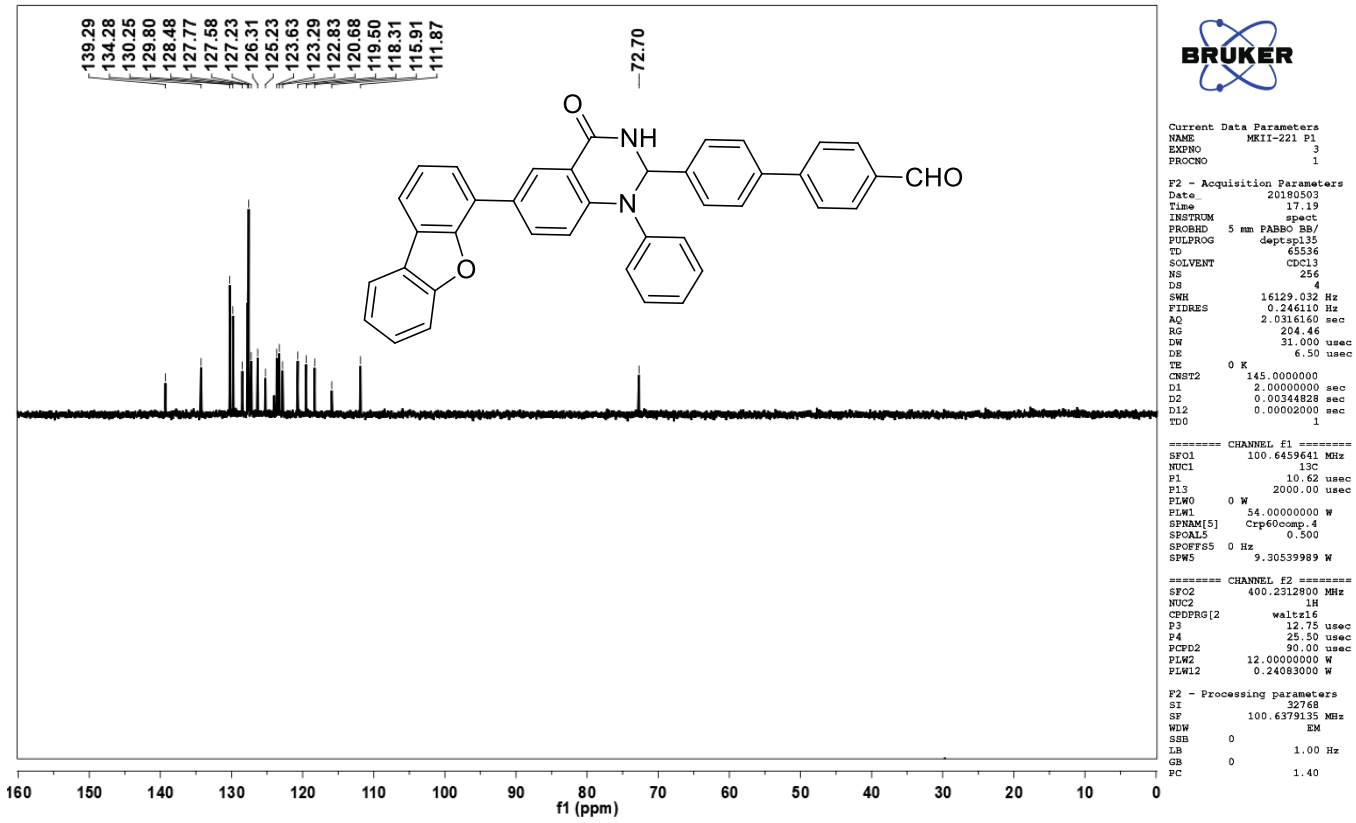
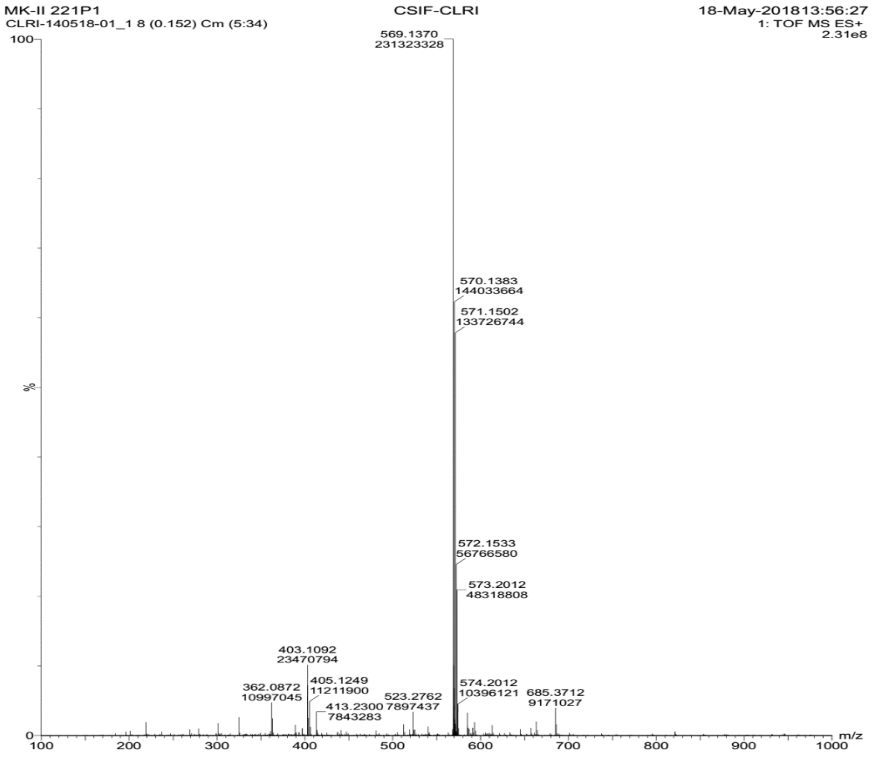
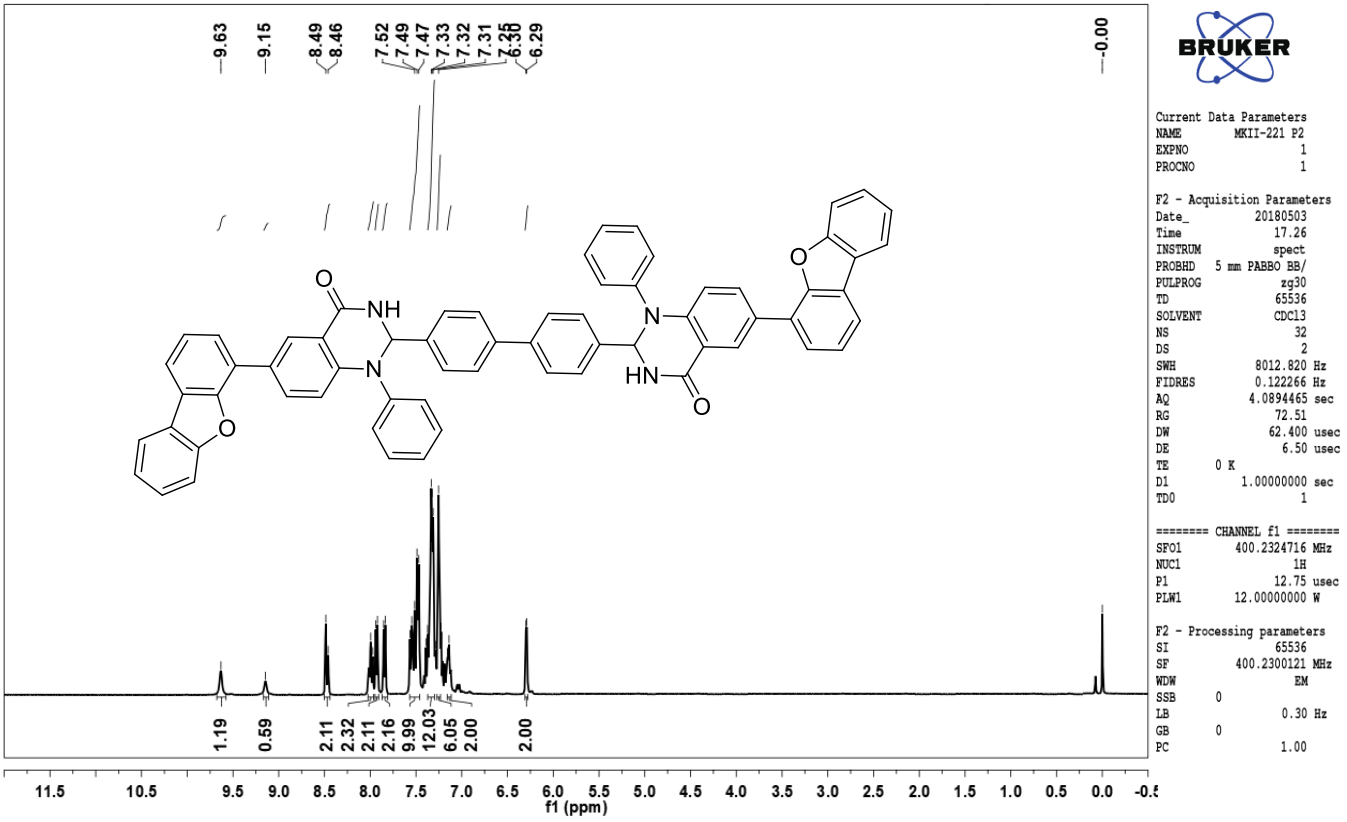

^{13}C NMR Spectrum of Compound **7a**



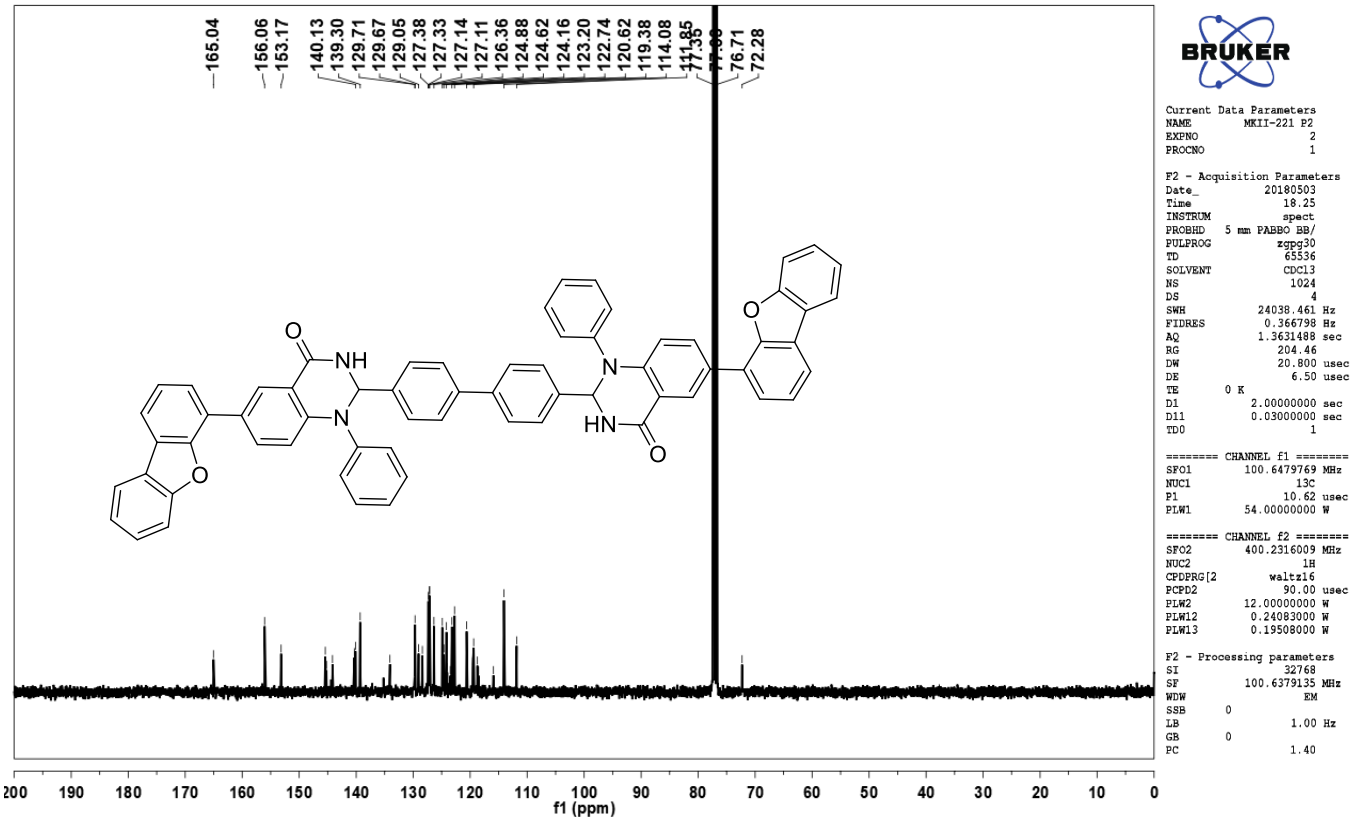
DEPT-135 NMR Spectrum of Compound **7a**



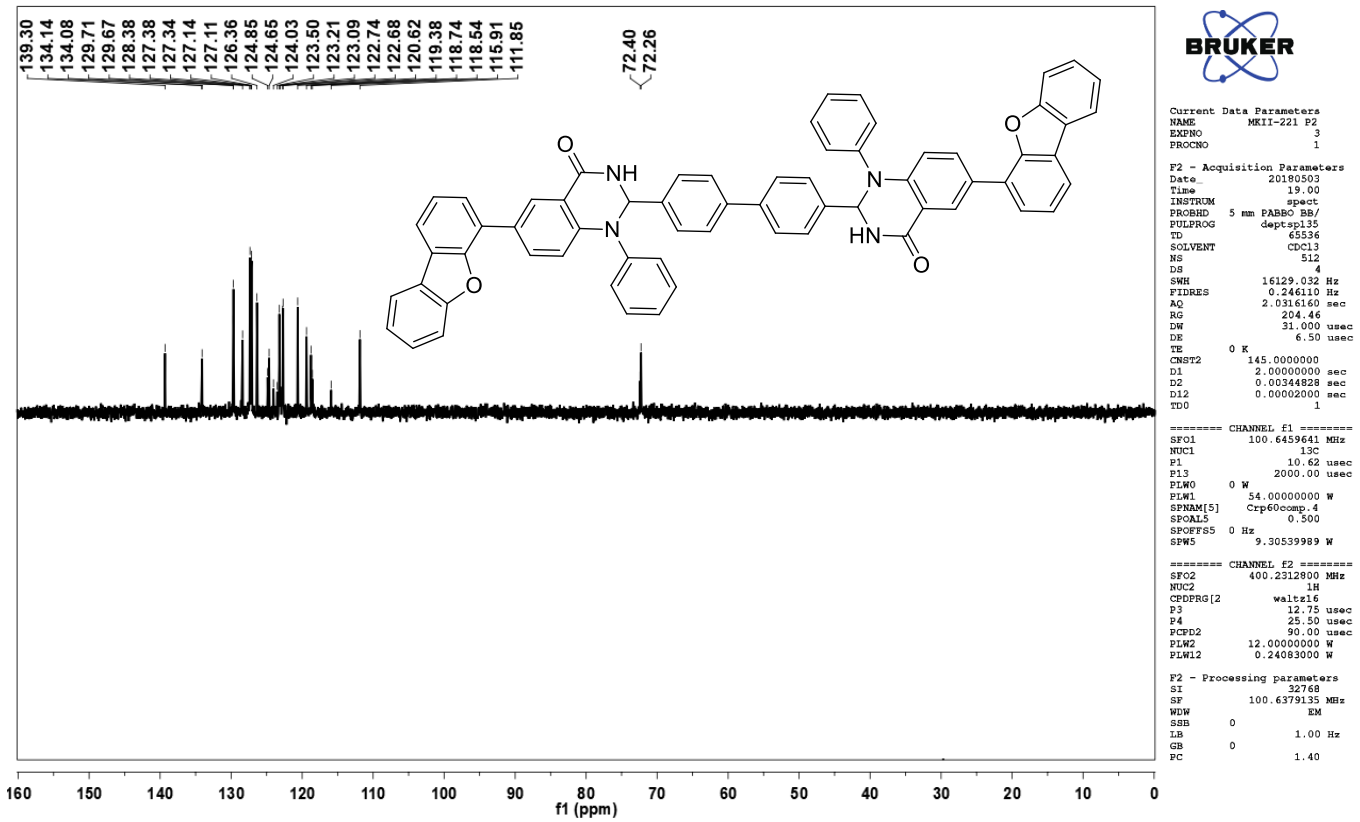
HRMS Spectrum of Compound **7a**



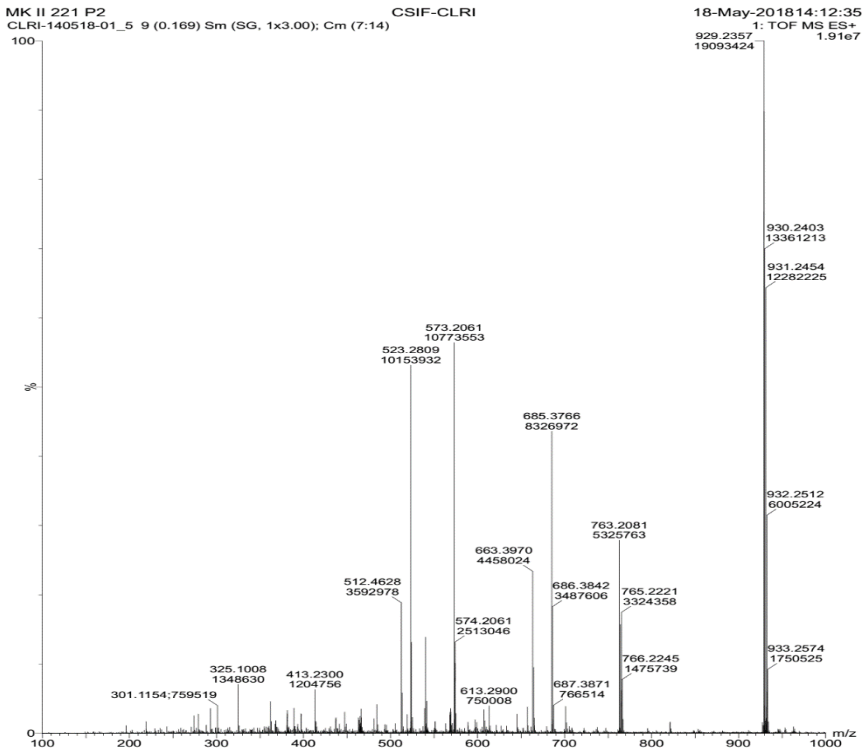
^{1}H NMR Spectrum of Compound **7b**



^{13}C NMR Spectrum of Compound **7b**



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



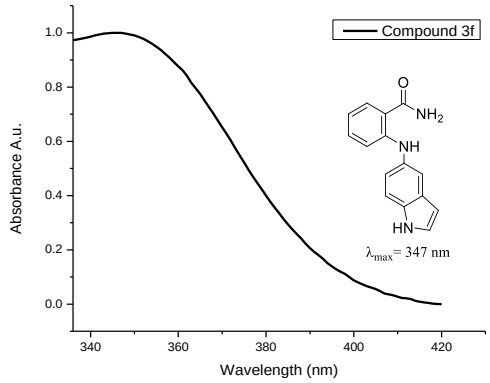
HRMS Spectrum of Compound **7b**

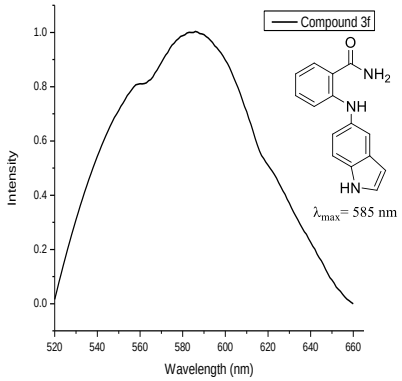
1. Absorption and emission data of compounds

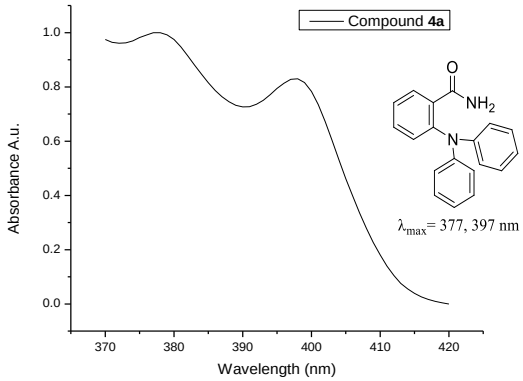
Table 1. Absorption, emission maxima and Stoke shift of the selected synthesized compounds

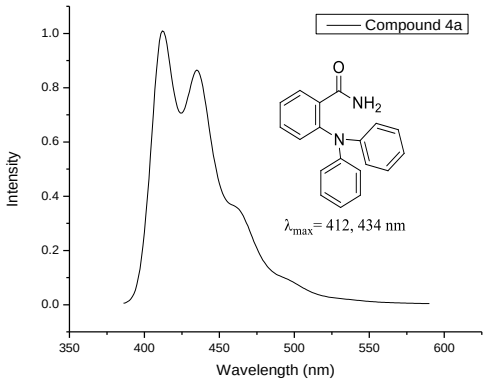
Product	Absorption λ_{max}(nm)	Emission λ_{max}(nm)	$\Delta\bar{\upsilon}$ (cm^{-1})
3f	347	585	11724
4b	295	502	13977
4c	328	492	10162
4g	332	485	9501
4h	318	474	10349
4l	482	584	3622
5a	347	333, 448	4692
7a	289	418	10678
7b	319	449	9076

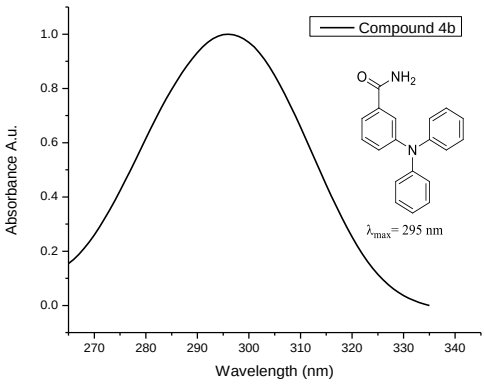
2. Copy of UV-Visible and Emission spectra

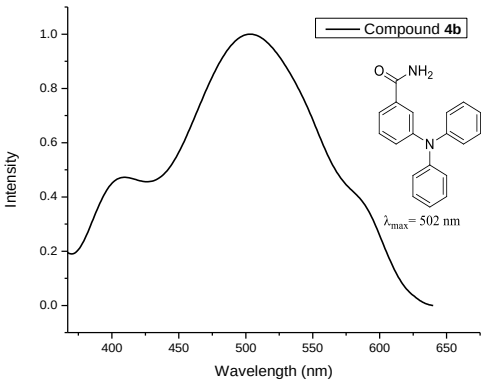


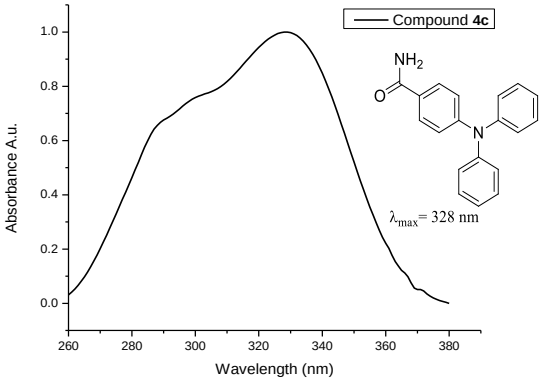


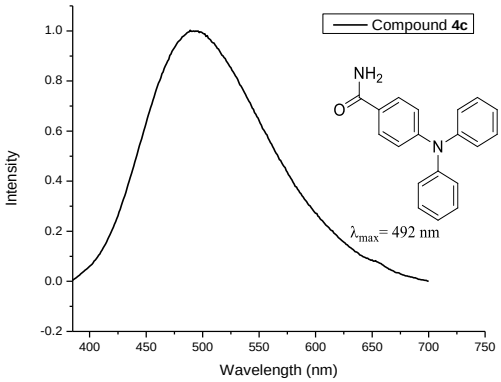


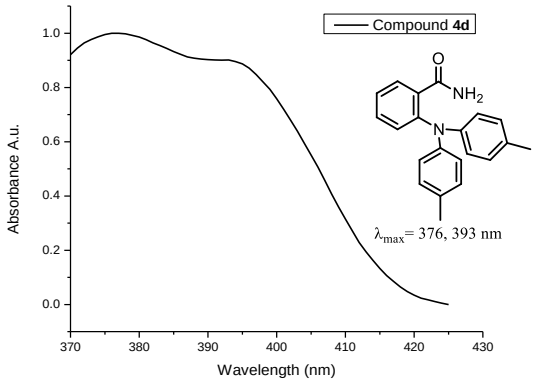


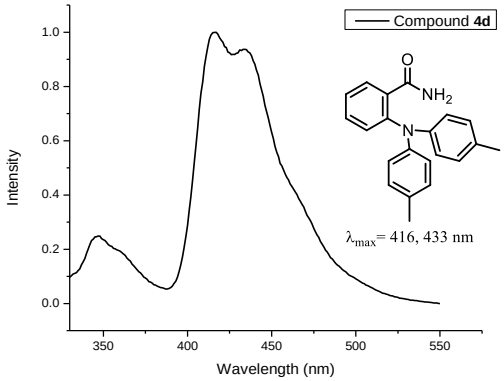

Compound 4b
Absorbance A.u.
Wavelength (nm)
λmax= 295 nm

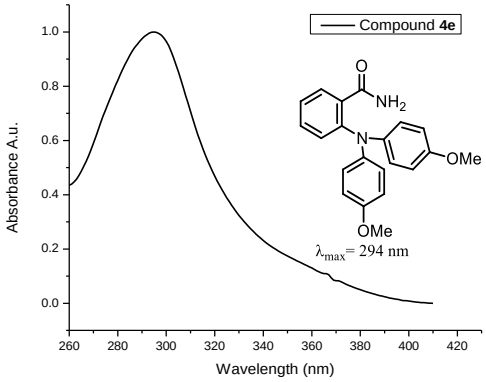

Compound 4b
Intensity
Wavelength (nm)
λmax= 502 nm

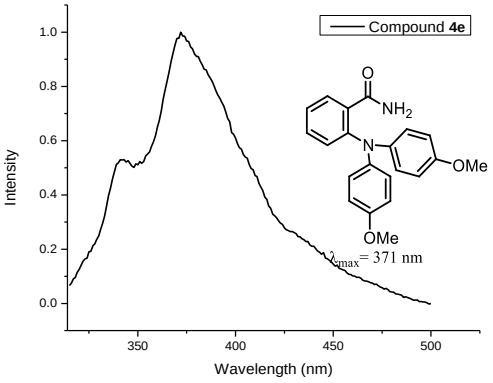

Compound 4c
Absorbance A.u.
Wavelength (nm)
λmax= 328 nm

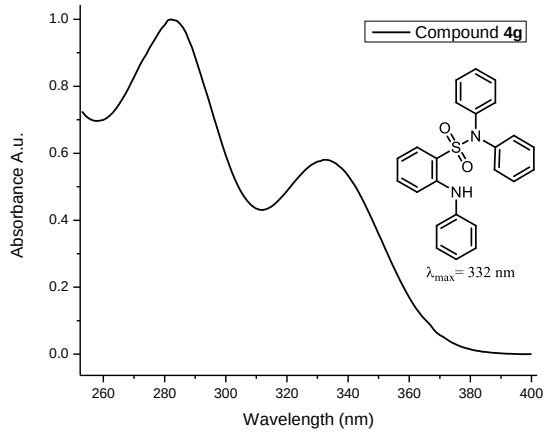

Compound 4c
Intensity
Wavelength (nm)
λmax= 492 nm

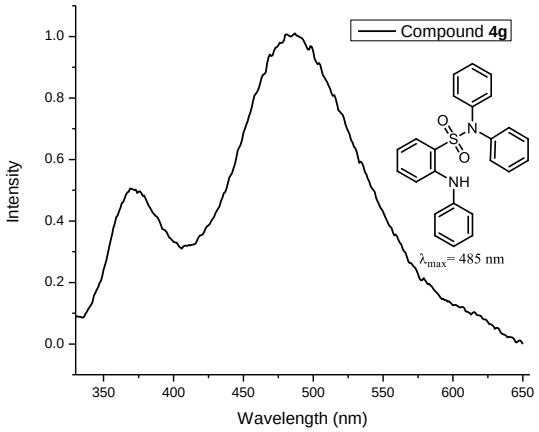

Compound 4d
Absorbance A.u.
Wavelength (nm)
λmax= 376, 393 nm

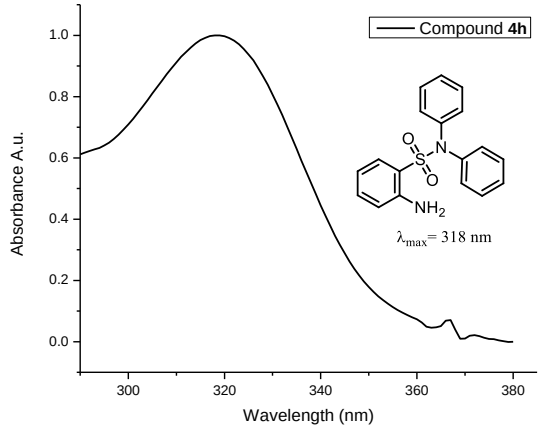

Compound 4d
Intensity
Wavelength (nm)
λmax= 416, 433 nm

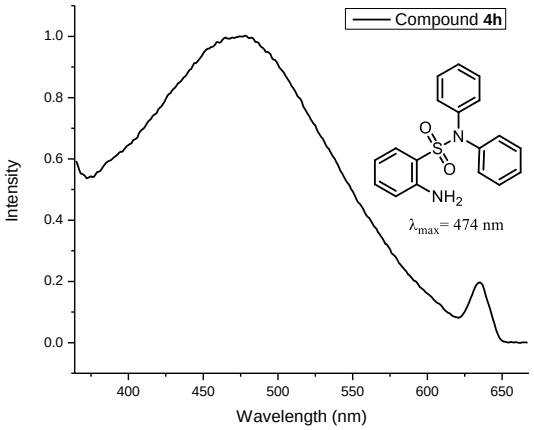

Compound 4e
Absorbance A.u.
Wavelength (nm)
λmax= 294 nm

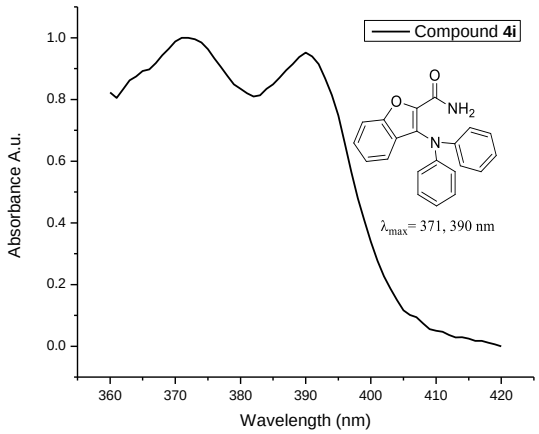

Compound 4e
Intensity
Wavelength (nm)
λmax= 371 nm

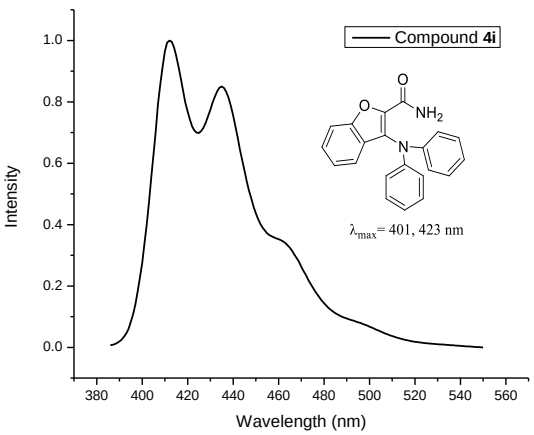

Compound 4g
Absorbance A.u.
Wavelength (nm)
λmax= 332 nm

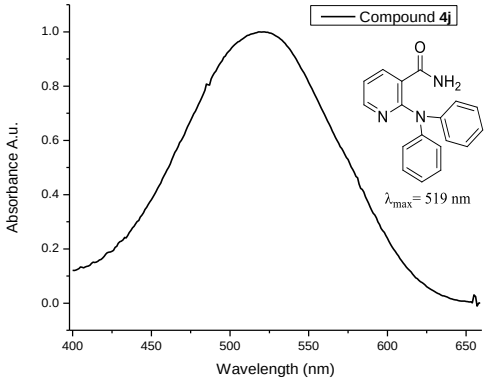

Compound 4g
Intensity
Wavelength (nm)
λmax= 485 nm

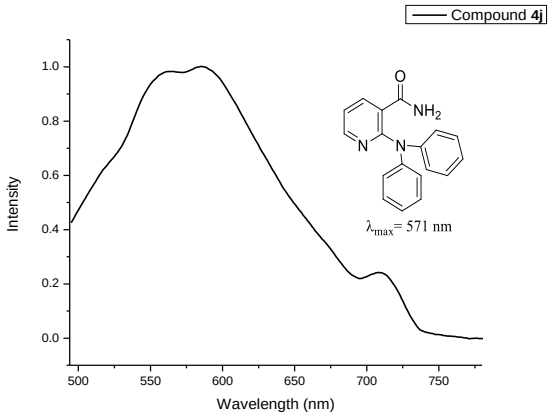

Compound 4h
Absorbance A.u.
Wavelength (nm)
λmax= 318 nm

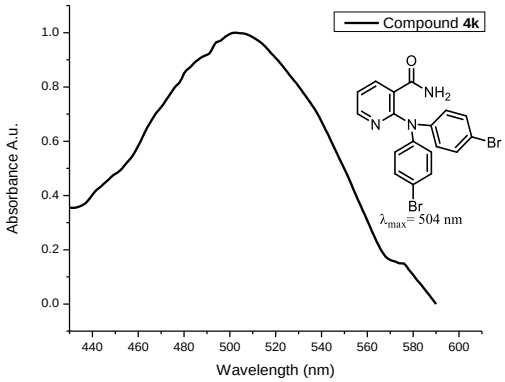

Compound 4h
Intensity
Wavelength (nm)
λmax= 474 nm

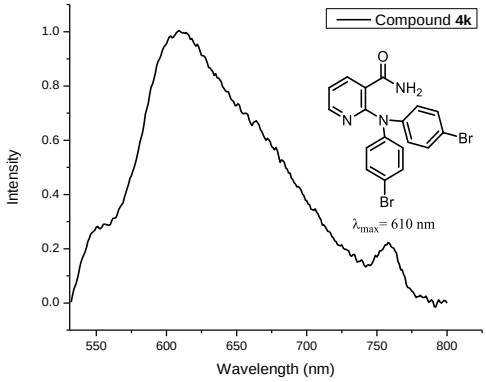

Compound 4i
Absorbance A.u.
Wavelength (nm)
λmax= 371, 390 nm

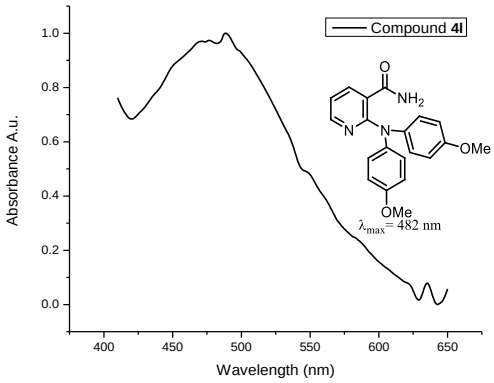

Compound 4i
Intensity
Wavelength (nm)
λmax= 401, 423 nm

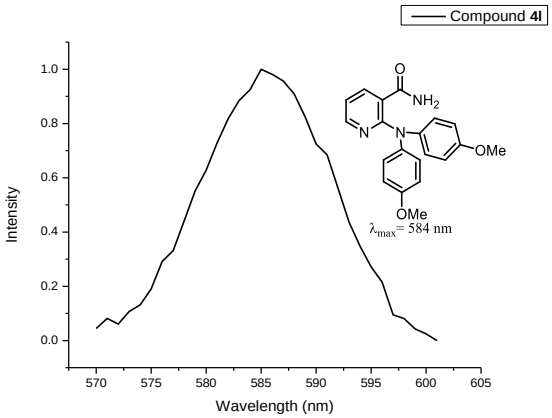

Compound 4j
Absorbance A.u.
Wavelength (nm)
λmax= 519 nm

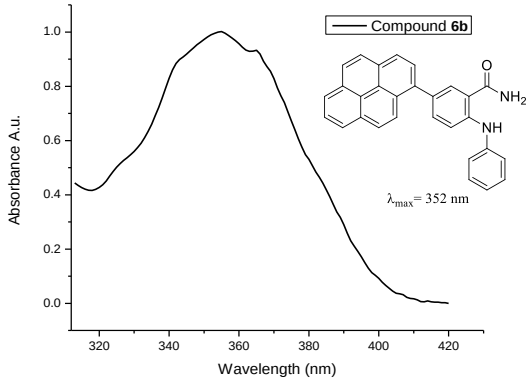

Compound 4j
Intensity
Wavelength (nm)
λmax= 571 nm

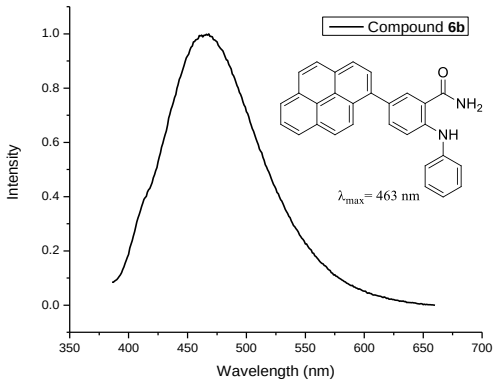

Compound 4k
Absorbance A.u.
Wavelength (nm)
λmax= 504 nm

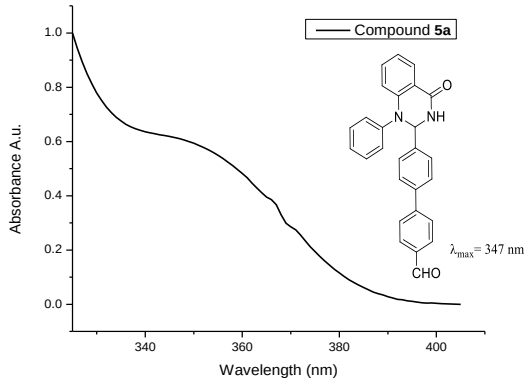

Compound 4k
Intensity
Wavelength (nm)
λmax= 610 nm

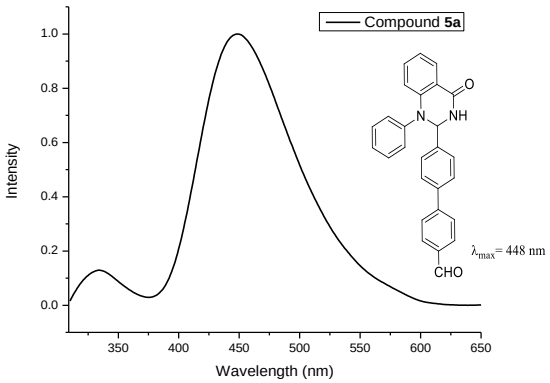

Compound 4l
Absorbance A.u.
Wavelength (nm)
λmax= 482 nm

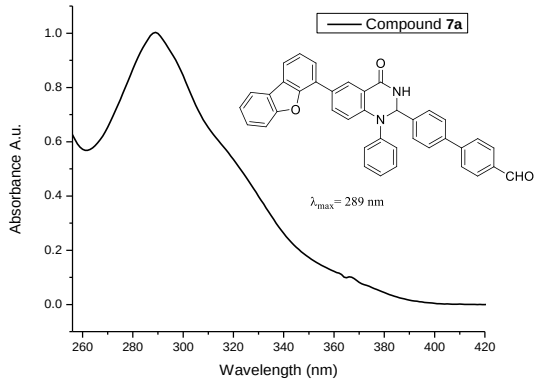

Compound 4l
Intensity
Wavelength (nm)
λmax= 584 nm

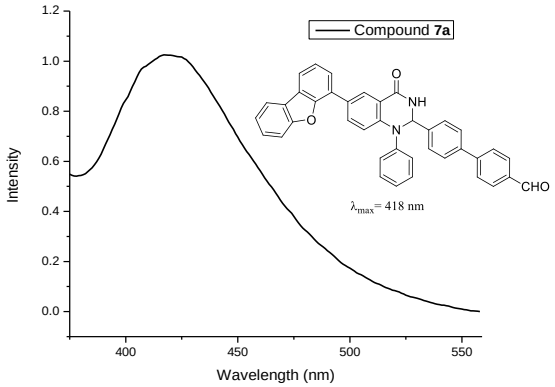

Compound 6b
Absorbance A.u.
Wavelength (nm)
λmax= 352 nm

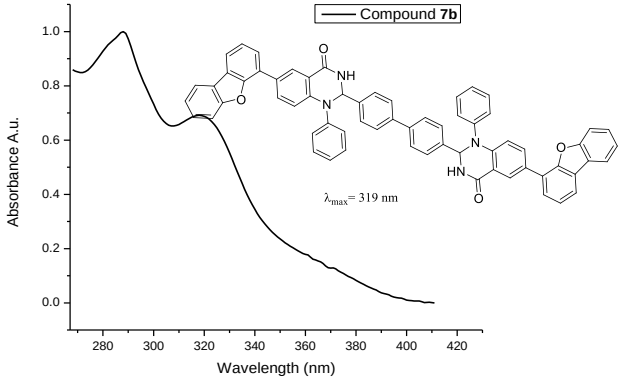

Compound 6b
Intensity
Wavelength (nm)
λmax= 463 nm

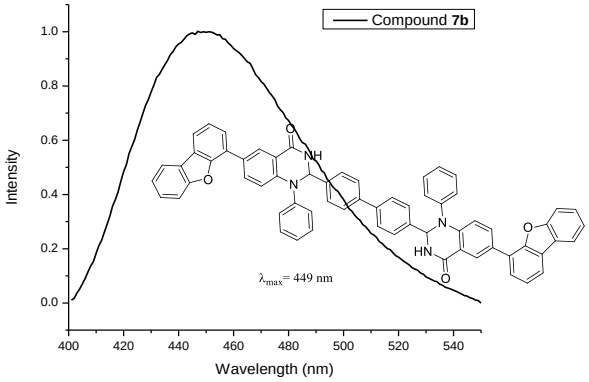

Compound 5a
Absorbance A.u.
Wavelength (nm)
λmax= 347 nm
CHO


Compound 5a
Intensity
Wavelength (nm)
λmax= 448 nm
CHO


Compound 7a
Absorbance A.u.
Wavelength (nm)
λmax= 289 nm
CHO


Compound 7a
Intensity
Wavelength (nm)
λmax= 418 nm
CHO


Compound 7b
Absorbance A.u.
Wavelength (nm)
λmax= 319 nm

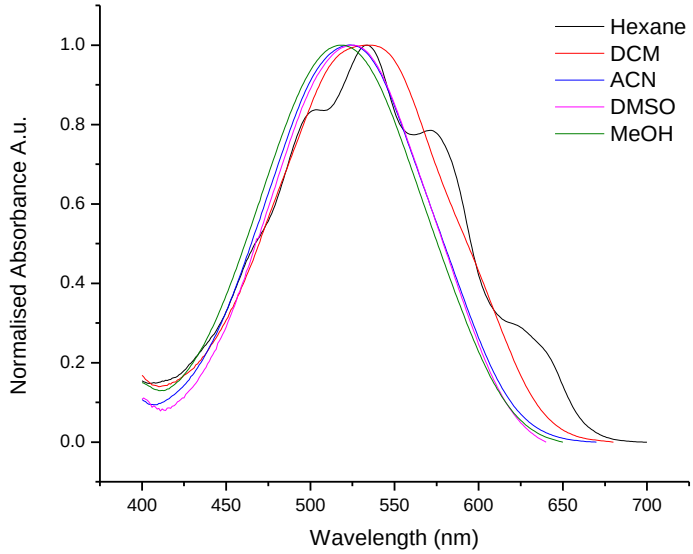

Compound 7b
Intensity
Wavelength (nm)
λmax= 449 nm

3. Crystallographic data of Compound 4a

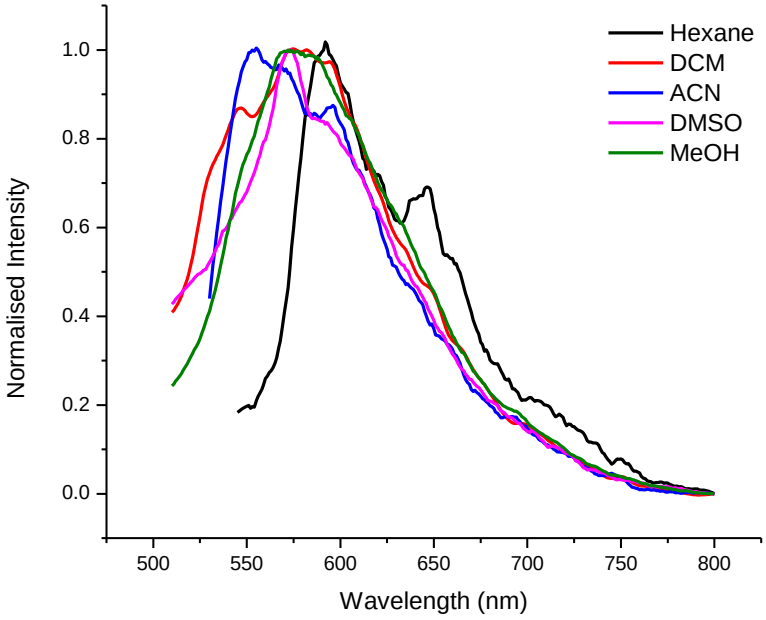
Table 1. Crystal data and structure refinement for Compound **4a**.

Identification code	Compound **4a**	
Empirical formula	C19 H16 N2 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) $Å^3$	
Z	2	
Density (calculated)	1.279 Mg/m^3	
Absorption coefficient	0.080 mm^{-1}	
F(000)	304	
Crystal size	0.150 x 0.150 x 0.100 mm^3	
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^2	
Data / restraints / parameters	2919 / 0 / 208	
Goodness-of-fit on F^2	1.044	
Final R indices [I>2sigma(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 $e.Å^{-3}$	

4. Solvatochromic effect of compound 4j



Solvatochromism of Compound **4j** (Absorption)



Solvatochromism of Compound **4j** (Emission)