

An Expedited Microwave Assisted One-Pot Sequential Route to Pyrido fused Imidazo[4,5-*c*] quinolines in Green Media

R.Nishanth Rao, Kaushik Chanda*

Department of Chemistry, School of Advanced Science, Vellore Institute of Technology,
Vellore-632014, India.

Email: chandakaushik1@gmail.com

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Experimental Section

General Procedure

Unless otherwise indicated all common reagents and solvents were used as obtained from commercial suppliers without further purification. ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) were recorded on a Bruker DRX400 spectrometer. Chemical shifts are reported in ppm relative to the internal solvent peak. Coupling constants, J , are given in Hz. Multiplicities of peaks are given as: d (doublet), m (multiplet), s (singlet), and t (triplet). Mass spectra were recorded on a Perkin Elmer Calrus 600 GC-MS spectrometer. IR spectra were recorded on a Bomen DA8 3FTS spectrometer. Microwave assisted reactions were carried out in a Catalyst Scientific Microwave oven system (Model No: CATA R (Catalyst System, Pune) operating at 2450 MHz equipped with glass vial extension by a condenser was used for performing the reaction. The microwave was equipped with a temperature control system (external probe).

2-(2-nitrophenyl)imidazo[1,2-*a*]pyridine 3a.

Yield = 0.36 g, 95%; Yellow solid; R_f = 0.5 (20%EtOAc/*n*-hexane); ^1H NMR (400 MHz, CDCl_3) δ 8.10 (d, J = 6.76 Hz, 1H), 7.99 (d, J = 7.8 Hz, 1H), 7.76 (s, 1H), 7.71(d, J = 8.04 Hz, 1H), 7.62 (t, J = 6.9 Hz, 2H), 7.45 (t, J = 7.8 Hz, 1H), 7.19 (t, J = 7.24 Hz, 1H), 6.80 (t, J = 6.76 Hz, 1H); ^{13}C NMR (100 MHz, CDCl_3) δ 144.0, 140.0, 134.9, 126.5, 126.1, 123.2, 122.4, 120.5, 120.0, 118.2, 112.6, 107.6, 105.3; MS (GC-MS): 239; HRMS (EI, m/z) calcd for $\text{C}_{13}\text{H}_9\text{N}_3\text{O}_2$: m/z 239.0695; Found 239.0697; IR (cm^{-1} , KBr) 3149, 3020, 1519, 1354, 1276, 1193.

2-(imidazo[1,2-*a*]pyridin-2-yl)aniline 4a.

Yield = 0.415 g, 93%; white solid; R_f = 0.4 (20%EtOAc/*n*-hexane); ^1H NMR (400 MHz, CDCl_3) δ 8.12 (d, J = 6.6 Hz, 1H), 7.80 (s, 1H), 7.57 (d, J = 9 Hz, 1H), 7.51 (d, J = 7.68 Hz, 1H), 7.16-7.09 (m, 2H) 6.79-6.70 (m, 3H); ^{13}C NMR (100MHz, CDCl_3) δ 146.6, 145.8, 144.5, 128.9, 128.2, 125.2, 124.1, 117.3, 117.2, 116.8, 112.4, 108.3; MS (GC-MS) 209;

HRMS (EI, m/z) calcd for C₁₃H₁₁N₃: m/z 209.0953; Found 209.0950; IR (cm⁻¹, KBr) 3448, 3296, 1595, 1315, 937, 731.

8-methyl-2-(2-nitrophenyl)imidazo[1,2-*a*]pyridine 3b.

Yield = 0.435 g, 92%; white solid; R_f = 0.5 (20%EtOAc/n-hexane); ¹H NMR (400 MHz, CDCl₃) δ 8.01-7.90 (m, 2H), 7.71 (d, J = 8.8 Hz, 2H), 7.61 (t, J = 6.8 Hz, 1H), 7.45 (t, J = 7.6 Hz, 1H), 6.97 (d, J = 6.8 Hz, 1H), 6.71 (t, J = 6.8 Hz, 1H), 2.61 (3H); ¹³C NMR (100MHz,CDCl₃) δ 149.3, 145.9, 139.6, 131.8, 131.5, 128.3, 128.1, 127.9, 123.7, 123.5, 123.4, 112.8, 110.9, 16.9 MS (GC-MS) 253; HRMS (EI, m/z)calcd for C₁₄H₁₁N₃O₂: m/z 253.0851; Found 253.0835; IR (cm⁻¹, KBr) 3059, 1658, 1554, 1315, 1423, 778.

2-(8-methylimidazo[1,2-*a*]pyridin-2-yl)aniline 4b.

Yield = 0.39 g, 95%; white solid; R_f = 0.48 (20%EtOAc/n-hexane); ¹H NMR (400 MHz, CDCl₃) δ 7.90 (d, J = 8 Hz, 1H), 7.70 (s, 1H), 7.44 (d, J = 7.6 Hz, 1H), 7.03 (t, J = 8 Hz, 1H), 6.86 (d, J = 8.4 Hz, 1H), 6.68 (d, J = 8.4 Hz, 1H), 6.67-6.58 (m, 2H), 2.53 (3H); ¹³C NMR (100MHz,CDCl₃) δ 145.9, 145.0, 128.7, 128.0, 127.1, 123.0, 122.9, 117.2, 116.8, 116.8, 112.4, 108.6, 16.9; MS (GC-MS) 223; HRMS (EI, m/z)calcd for C₁₄H₁₃N₃: m/z 223.1109; Found 223.1109; IR (cm⁻¹, KBr) 3057, 1604, 1463, 773, 729.

7-methyl-2-(2-nitrophenyl)imidazo[1,2-*a*]pyridine 3c

Yield = 0.43 g, 91%; white solid; R_f = 0.51 (20%EtOAc/n-hexane); ¹H NMR (400 MHz, CDCl₃) δ 8.20 (d, J = 8 Hz, 1H), 7.89 (d, J = 7.2 Hz, 1H), 7.88-7.76 (m, 2H), 7.68 (d, J = 7.2 Hz, 1H) 7.51 (d, J = 6.8 Hz, 1H), 7.31 (d, J = 6.8 Hz, 1H), 6.68 (d, J = 6.91 Hz, 1H), 2.83 (3H); ¹³C NMR(100MHz,CDCl₃) δ 148.1, 146.8, 134.2, 131.7, 130.6, 128.8, 128.4, 126.8, 125.2, 123.5, 122.9, 122.0, 112.6, 17.6; MS (GC-MS) 253; HRMS (EI, m/z)calcd for C₁₄H₁₁N₃O₂: m/z 253.0851; Found 253.0841; IR (cm⁻¹, KBr) 3057, 1718, 1589, 1460, 796.

2-(7-methylimidazo[1,2-*a*]pyridin-2-yl)aniline 4c.

Yield: 0.372 g, 90%; white solid; R_f = 0.45 (20%EtOAc/*n*-hexane); ^1H NMR (400 MHz, CDCl₃) δ 8.0 (d, *J* = 6.8 Hz, 1H), 7.72 (s, 1H), 7.50 (d, *J* = 7.6 Hz, 1H), 7.34 (s, 1H), 7.10 (t, *J* = 8.4 Hz, 1H), 6.72 (t, *J* = 6.1 Hz, 2H), 6.62 (d, *J* = 6.8 Hz, 1H), 2.39 (3H); ^{13}C NMR(100MHz,CDCl₃) δ 135.2, 128.7, 128.1, 124.4, 117.3, 116.9, 116.7, 115.6, 115.1, 107.7, 21.3; MS (GC-MS) 223; HRMS (EI, m/z) calcd for C₁₄H₁₃N₃: m/z 223.1109; Found 223.1101; IR (cm⁻¹, KBr) 3414, 1712, 1604, 1456, 769.

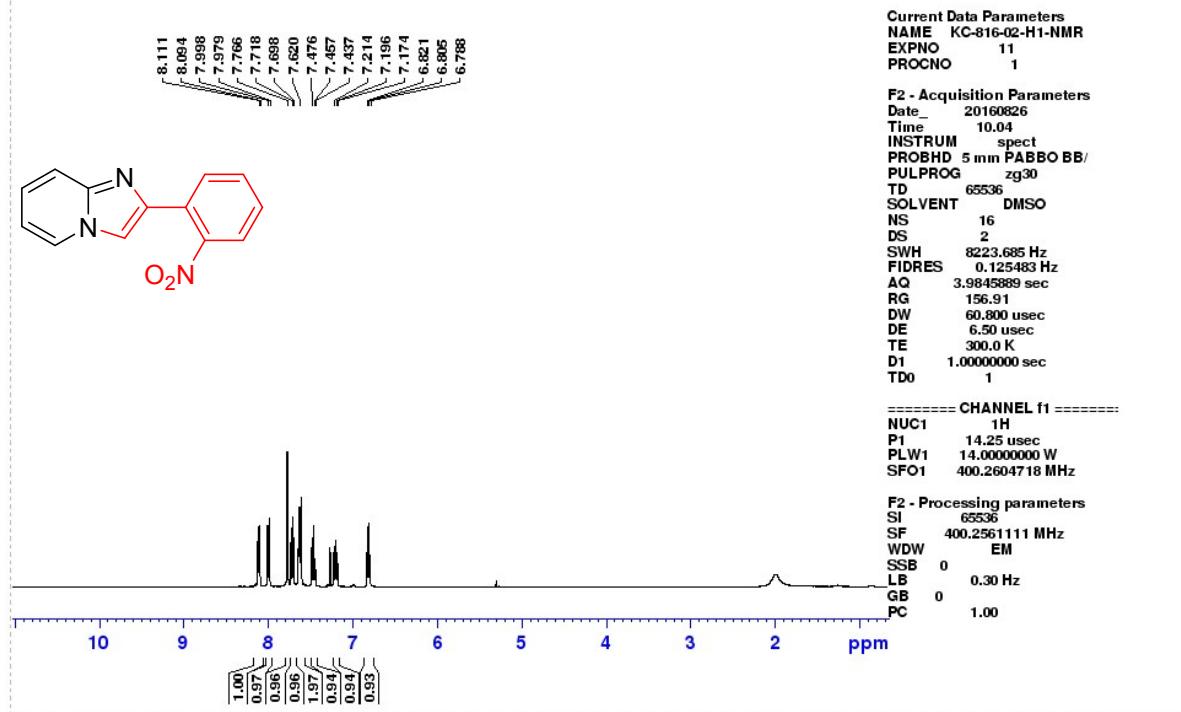
6,8-difluoro-2-(2-nitrophenyl)imidazo[1,2-*a*]pyridine 3d.

Yield = 0.375 g, 89 %; white solid; R_f = 0.4 (20%EtOAc/*n*-hexane); ^1H NMR (400 MHz, CDCl₃) δ Yield = 0.375 g, 89 %; white solid; R_f = 0.4 (20%EtOAc/*n*-hexane); ^1H NMR (400 MHz, CDCl₃) δ 8.14 (d, *J* = 8.32 Hz, 2H), 7.72 (t, *J* = 7.48 Hz, 2H), 7.61 (t, *J* = 7.32 Hz, 1H), 7.43 (d, *J* = 7.4 Hz, 2H); ^{13}C NMR (100MHz,CDCl₃) δ 158.1, 156.5, 145.3, 135.1, 134.9, 134.7, 131.8, 129.1, 128.1, 127.8, 124.8, 124.4; MS (GC-MS) 275; HRMS (EI, m/z)calcd for C₁₃H₇F₂N₃O₂: m/z 275.0506; Found 275.0500; IR (cm⁻¹, KBr) 2814, 1627, 147, 1180, 781.

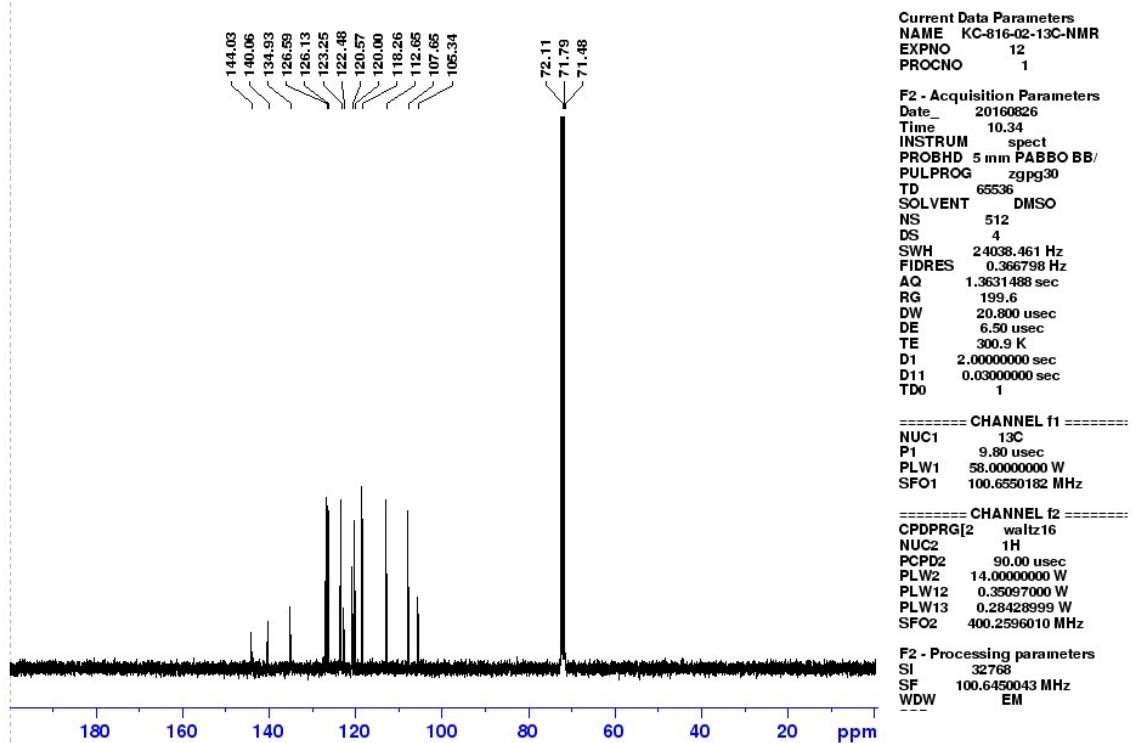
2-(6,8-difluoroimidazo[1,2-*a*]pyridin-2-yl)aniline 4d.

Yield = 0.345 g, 91%; white solid; R_f = 0.42 (20%EtOAc/*n*-hexane); ^1H NMR (400 MHz, CDCl₃) δ 8.01 (d, *J* = 6.4 Hz, 2H), 7.95 (s, 2H), 7.68-7.64 (m, 1H), 7.36 (t, *J* = 7.2 Hz, 1H), 6.89 (t, *J* = 8 Hz, 1H); ^{13}C NMR (100MHz,CDCl₃) δ 149.5, 146.9, 139.9, 132.0, 131.4, 130.1, 129.4, 128.1, 124.6, 110.7; MS (GC-MS) 245; HRMS (EI, m/z)calcd for C₁₄H₁₃N₃: m/z 245.0765; Found 245.0750; IR(cm⁻¹, KBr) 3369, 2872, 1618, 1435, 769, 750.

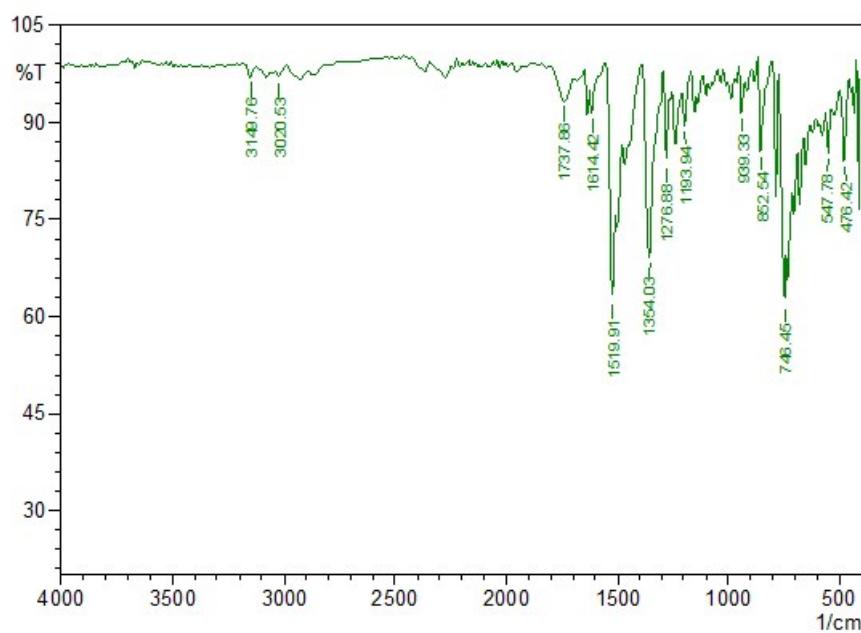
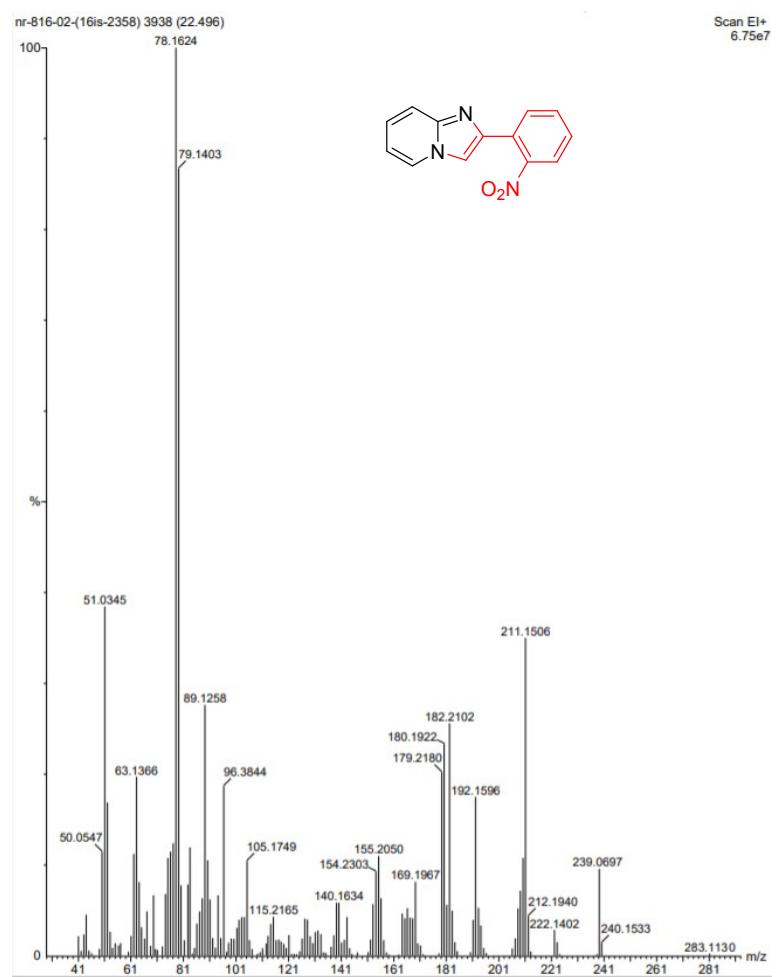
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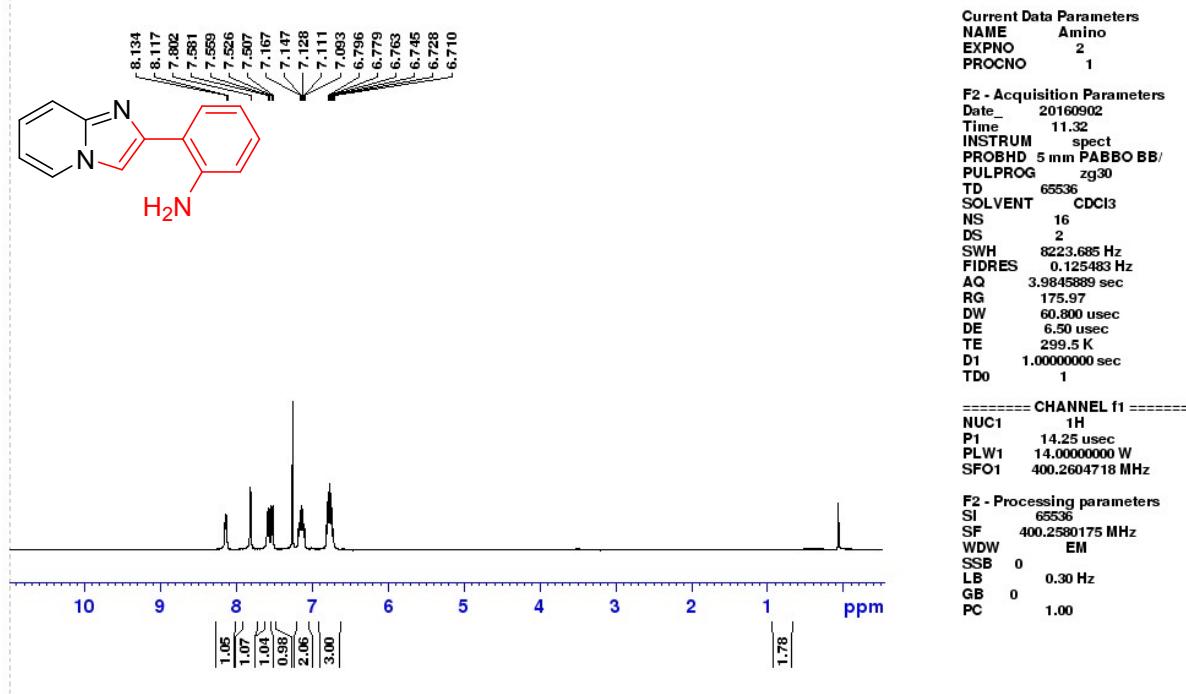


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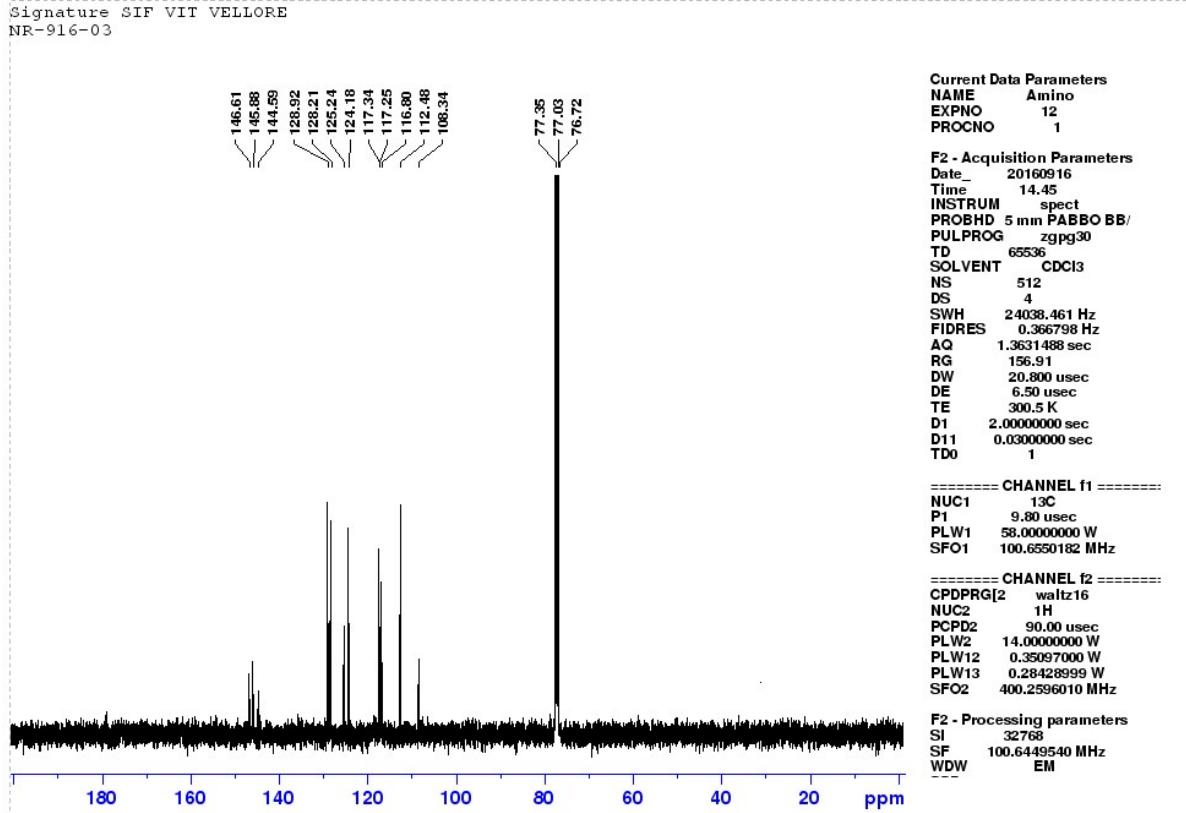


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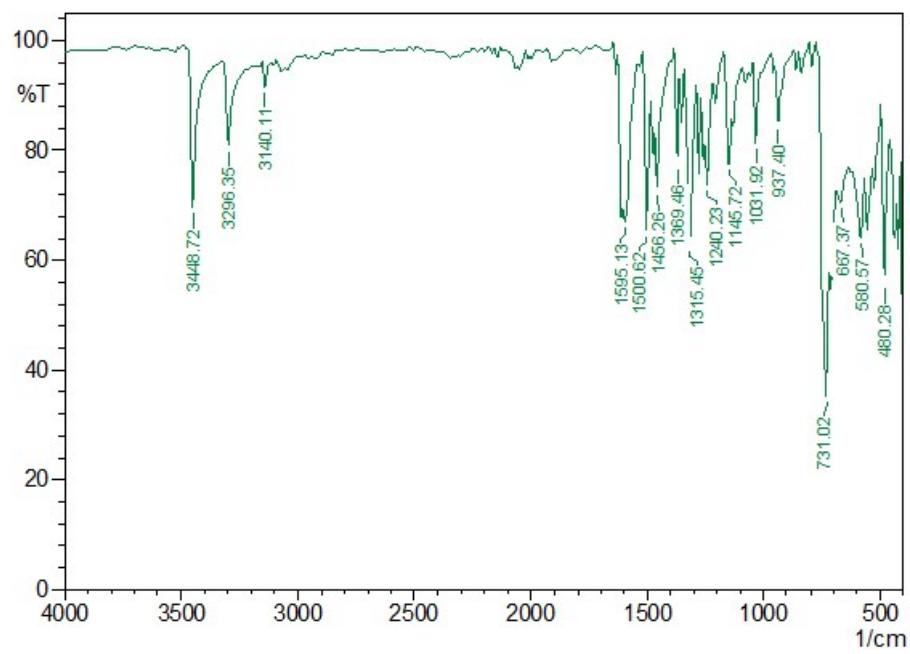
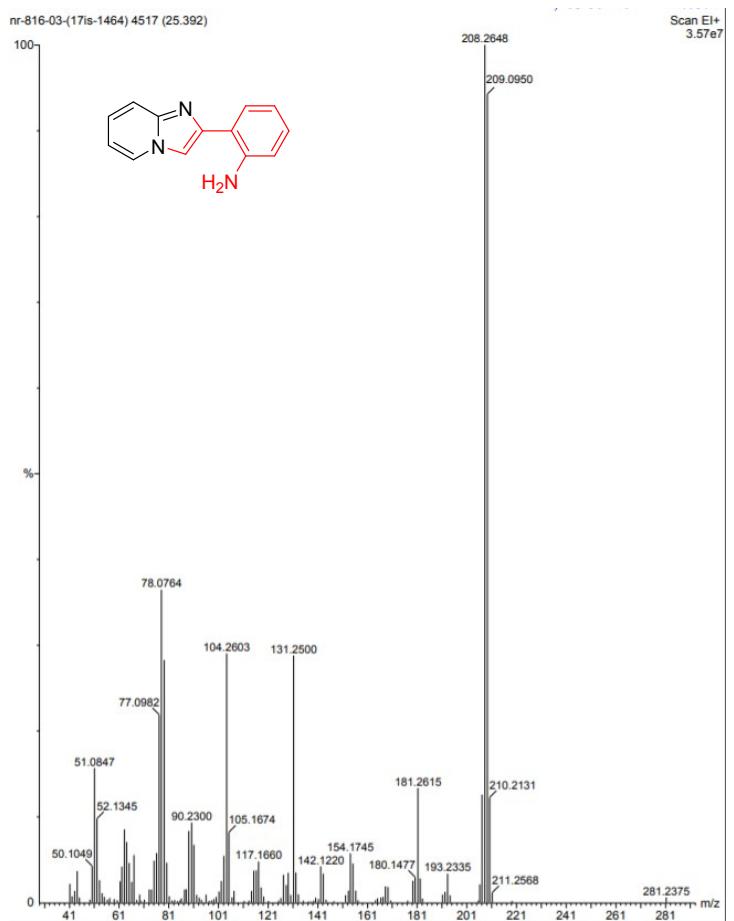
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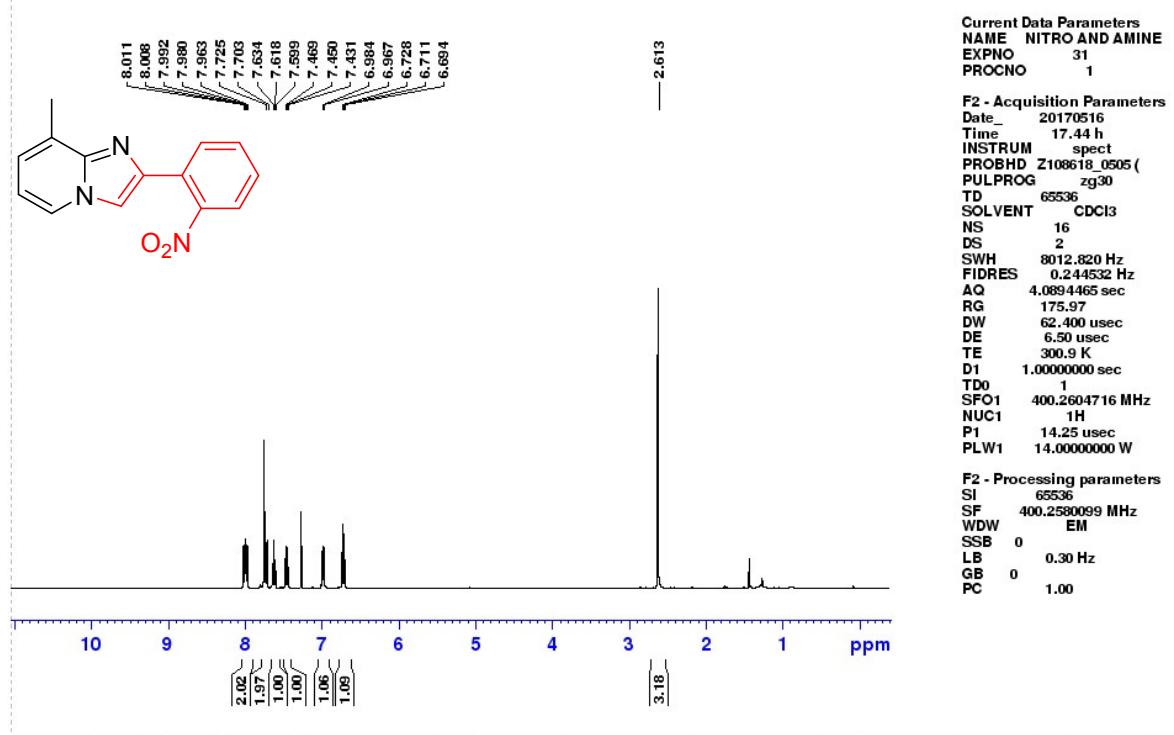


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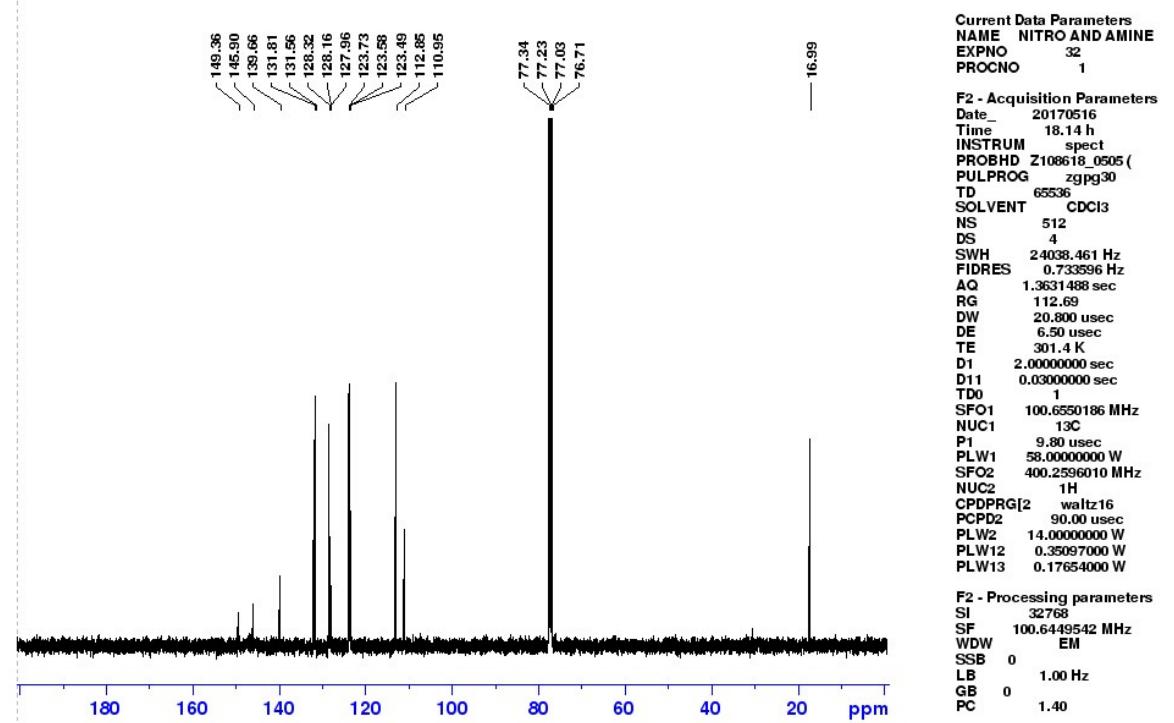


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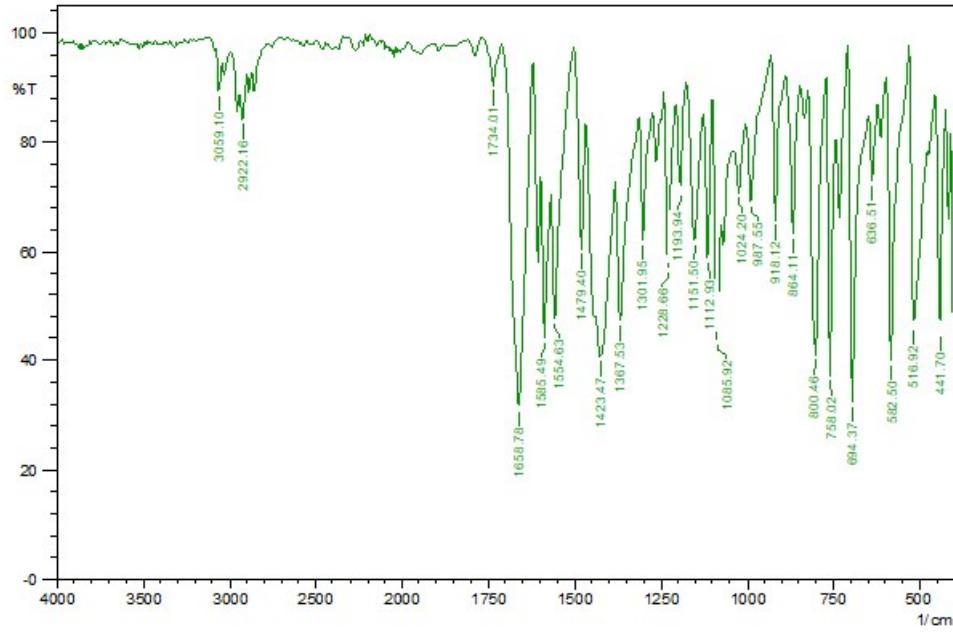
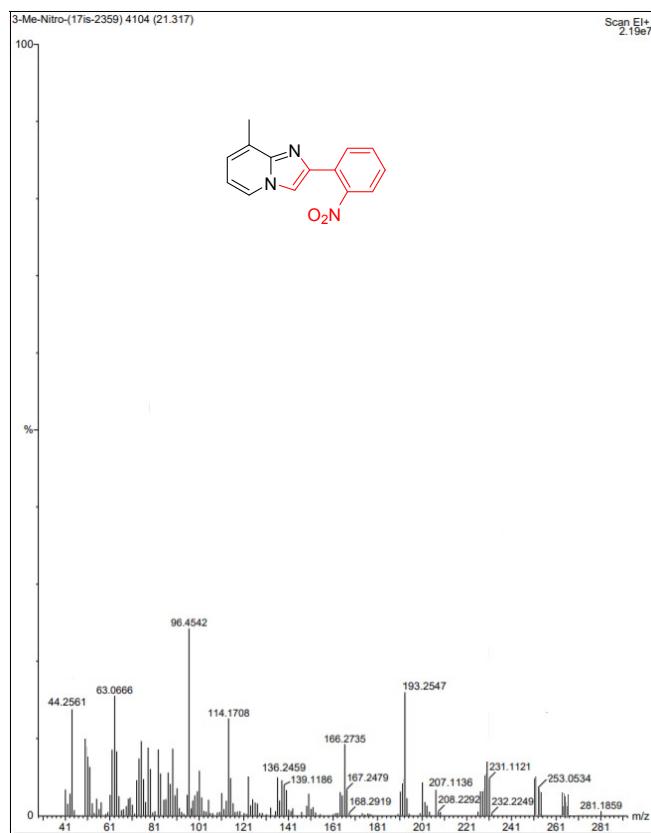
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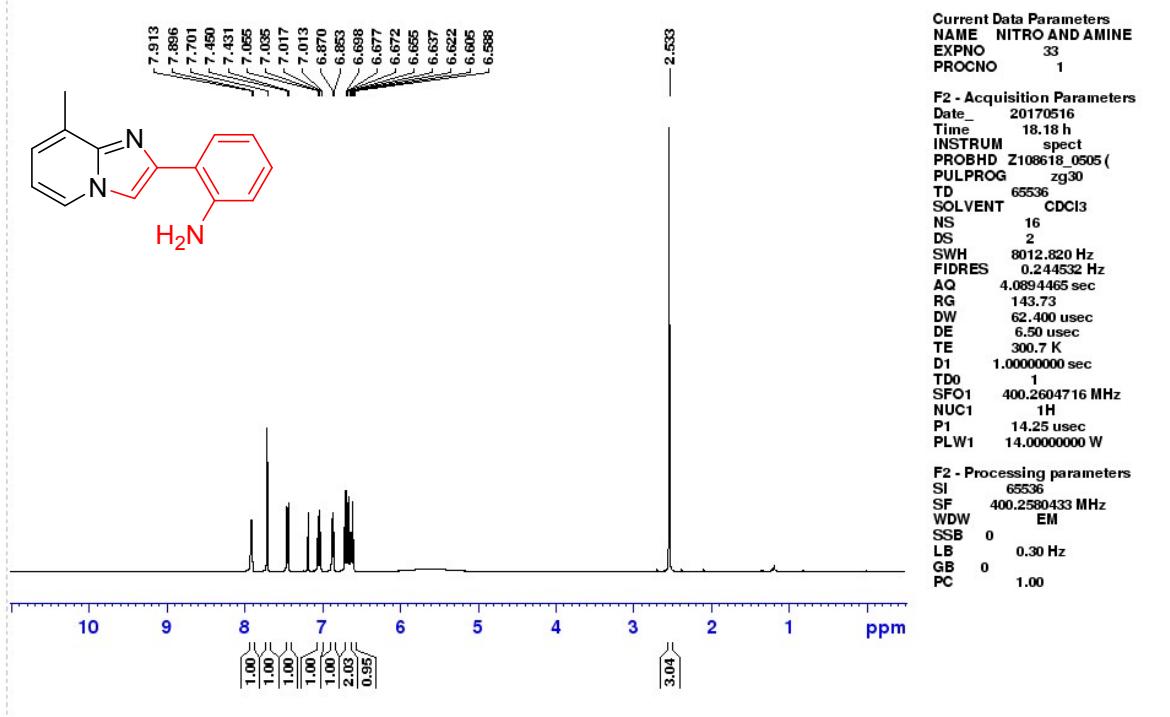


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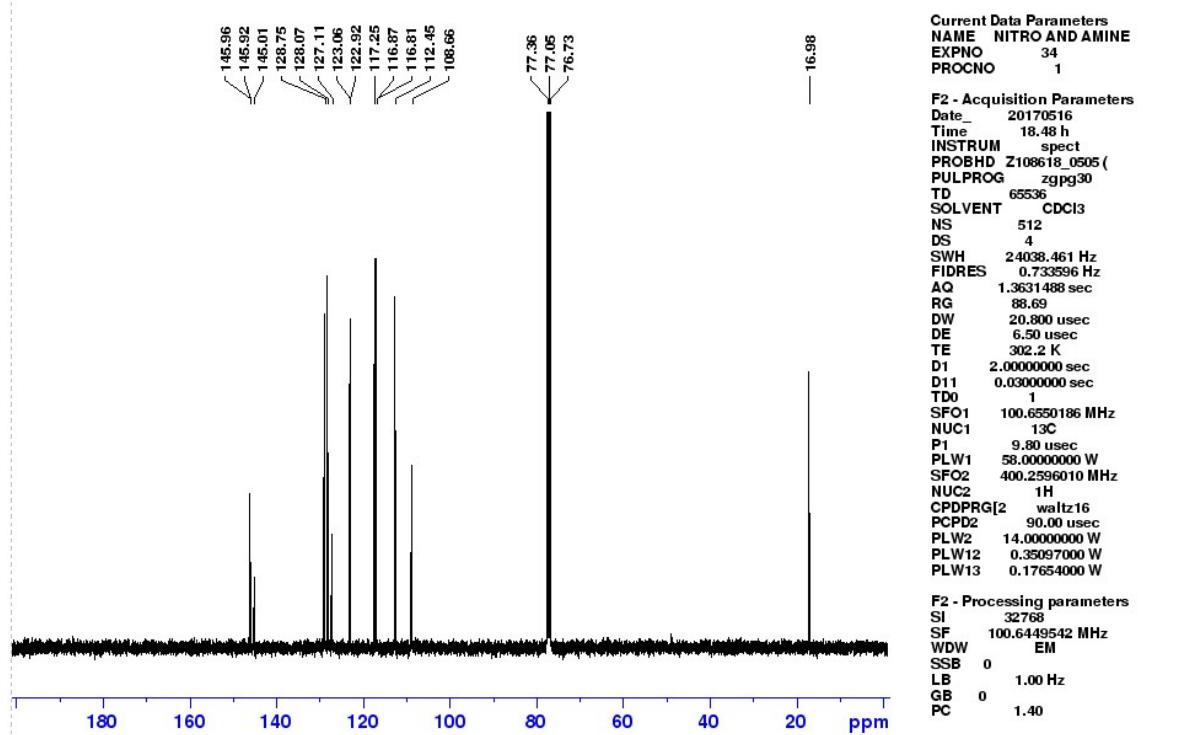


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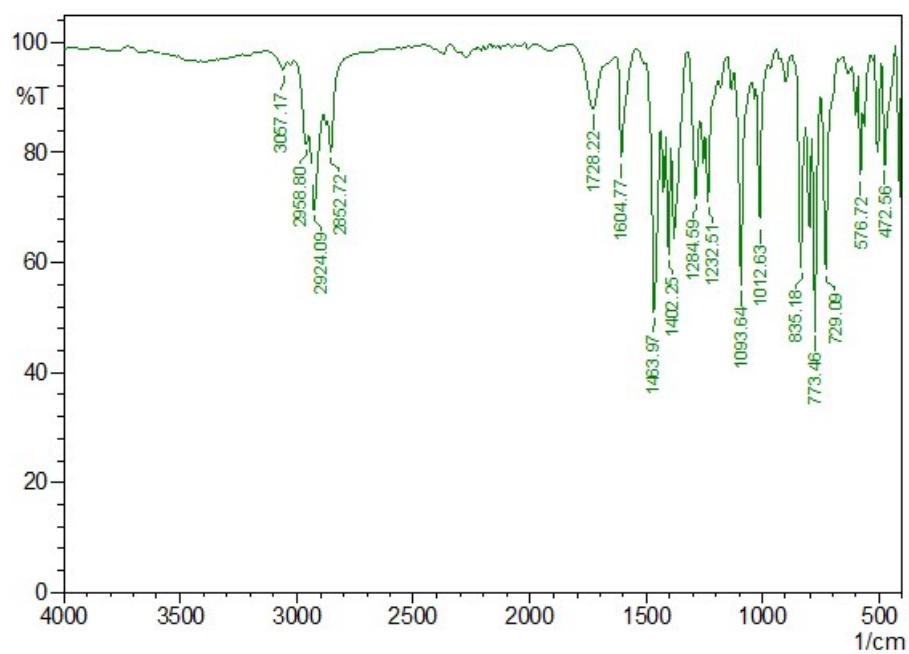
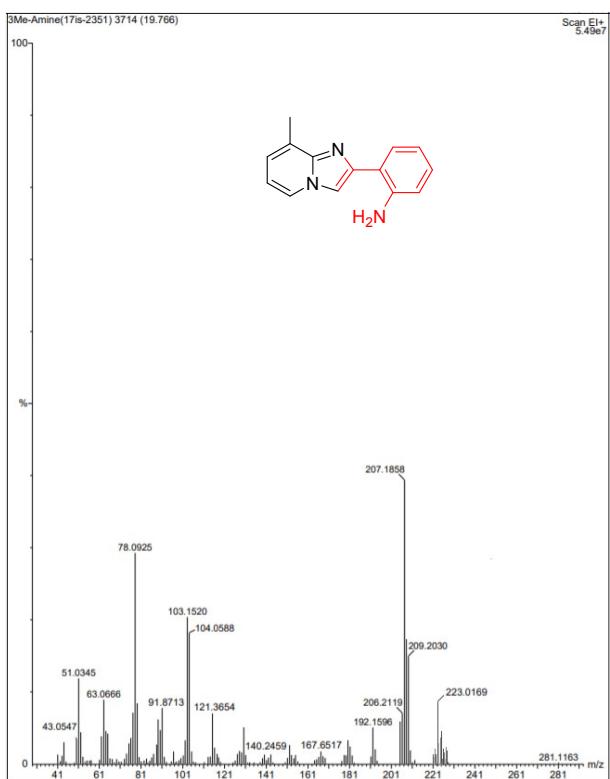
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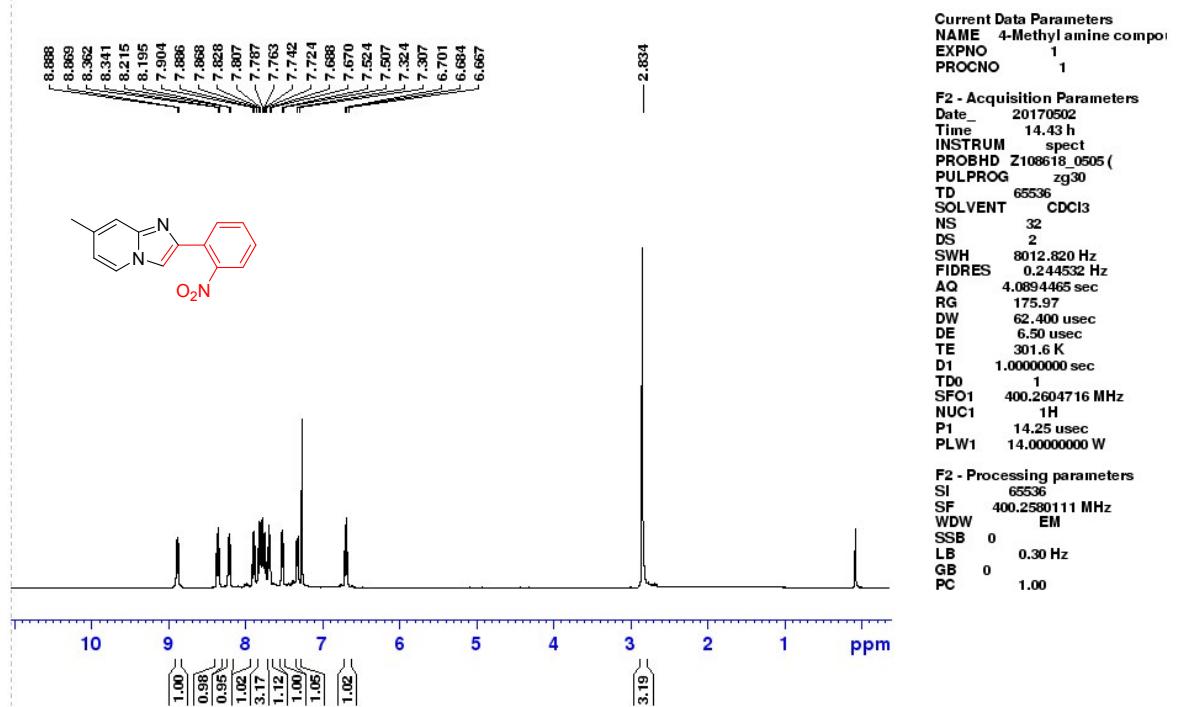


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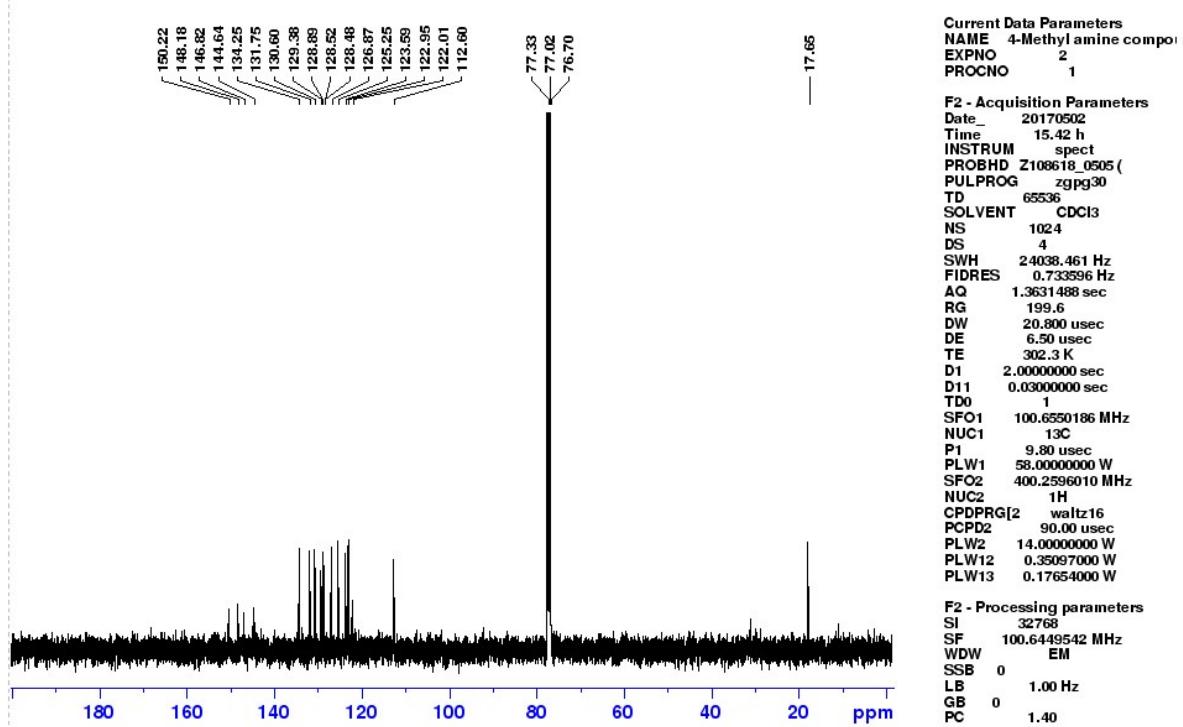


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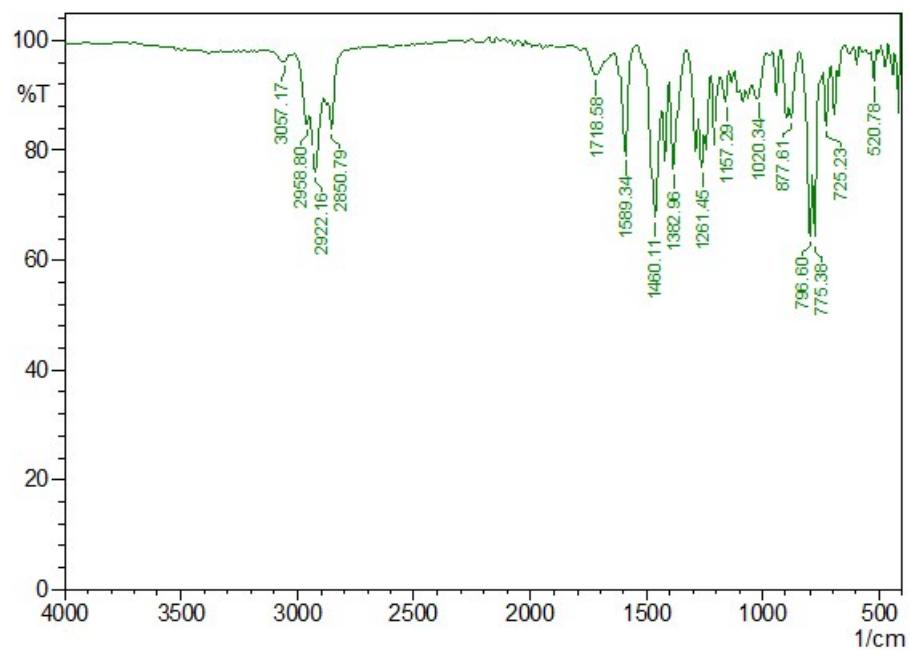
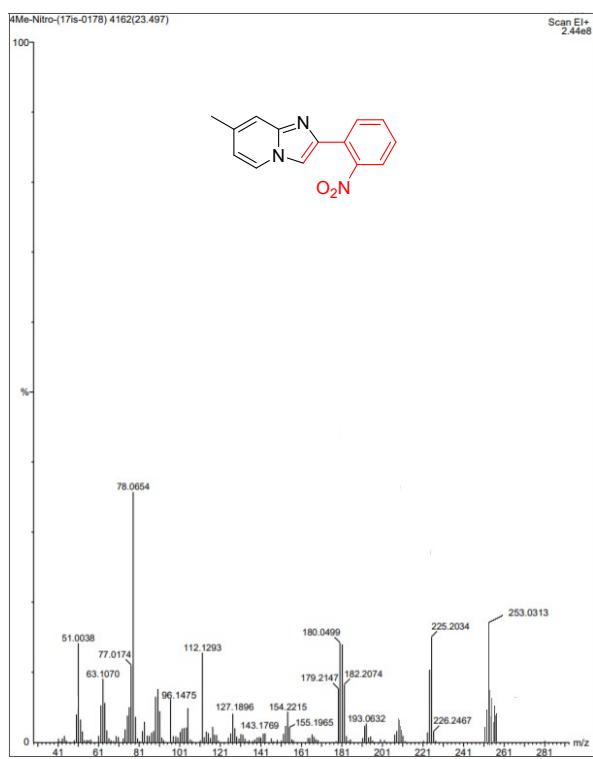
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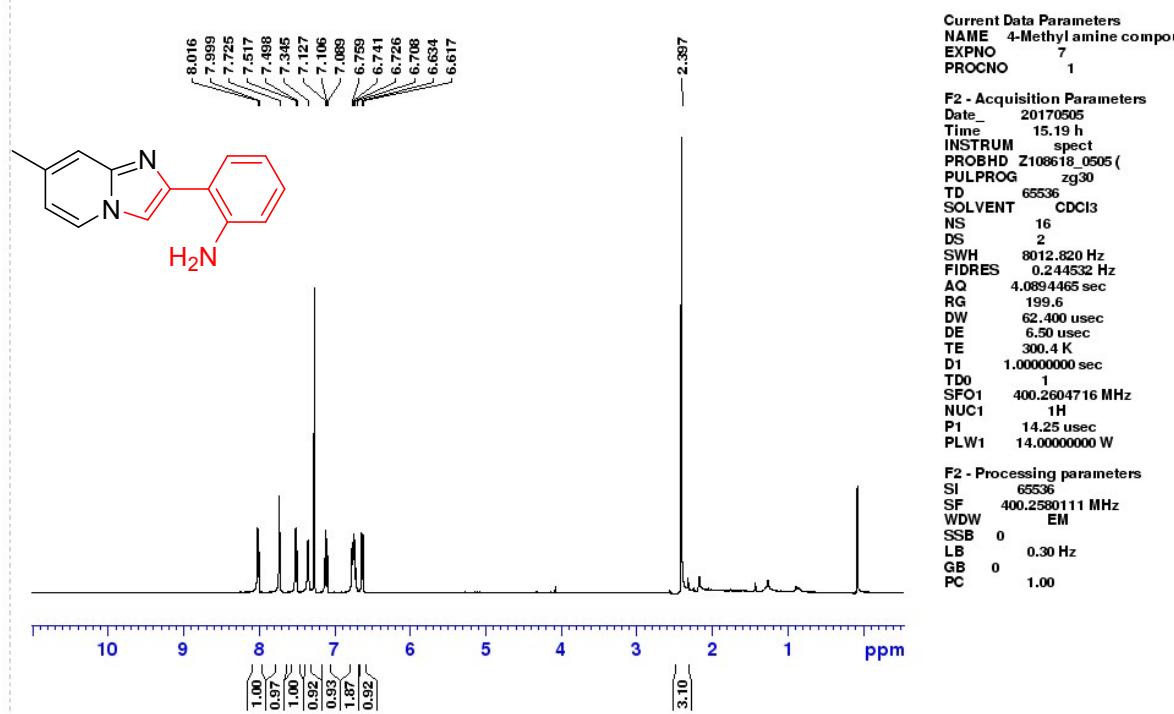


¹H-NMR and ¹³C-NMR of compound 3c in CDCl₃.

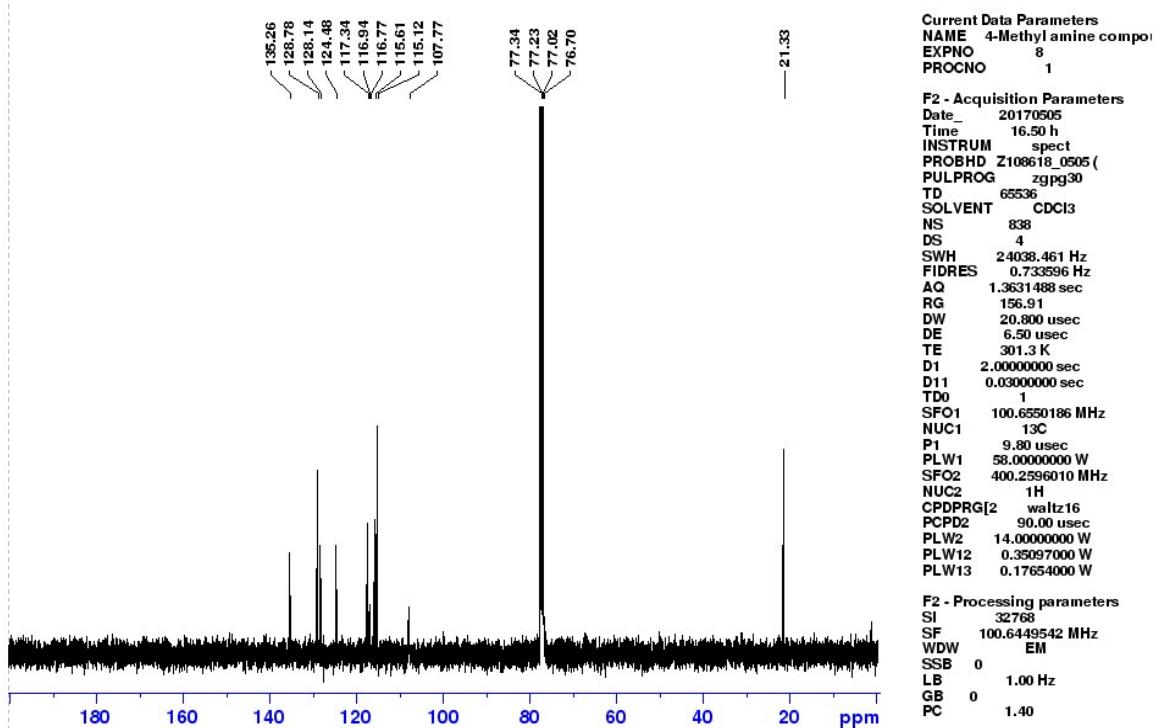


Mass and IR of Compound 3c.

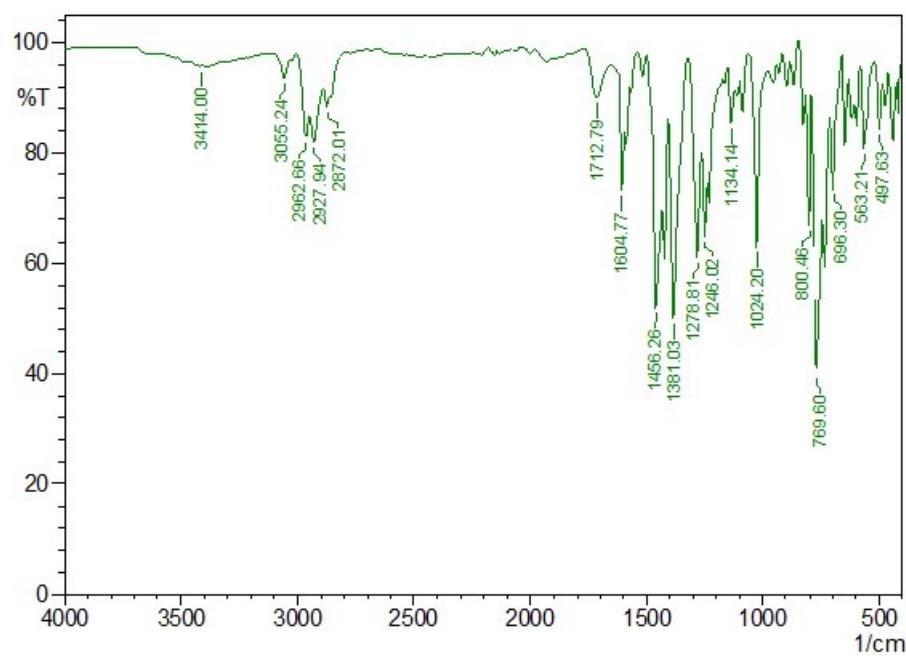
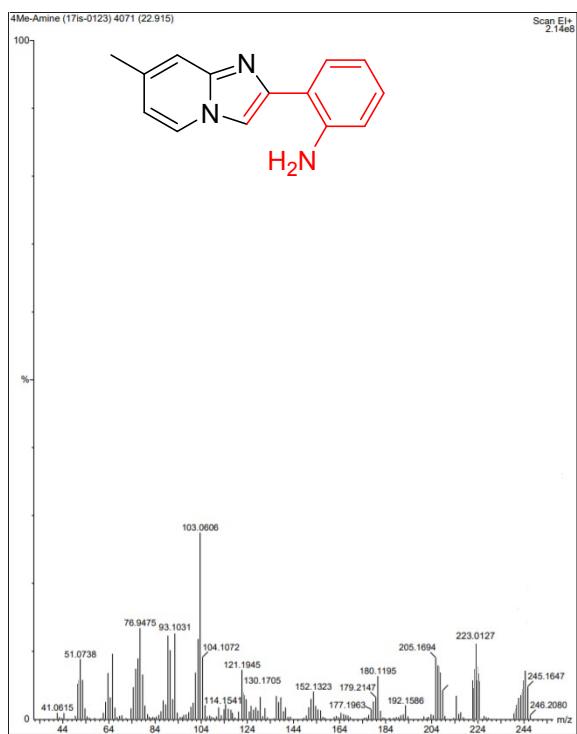
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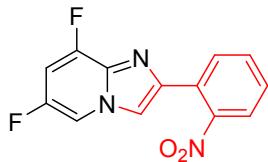
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Mass and IR of Compound 4c.

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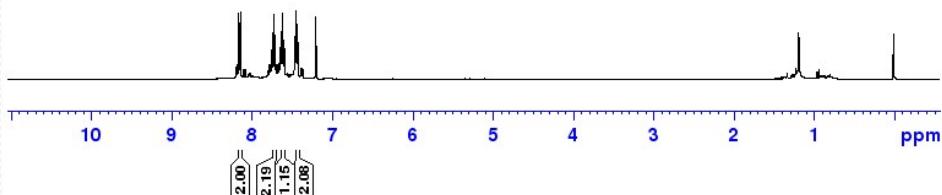
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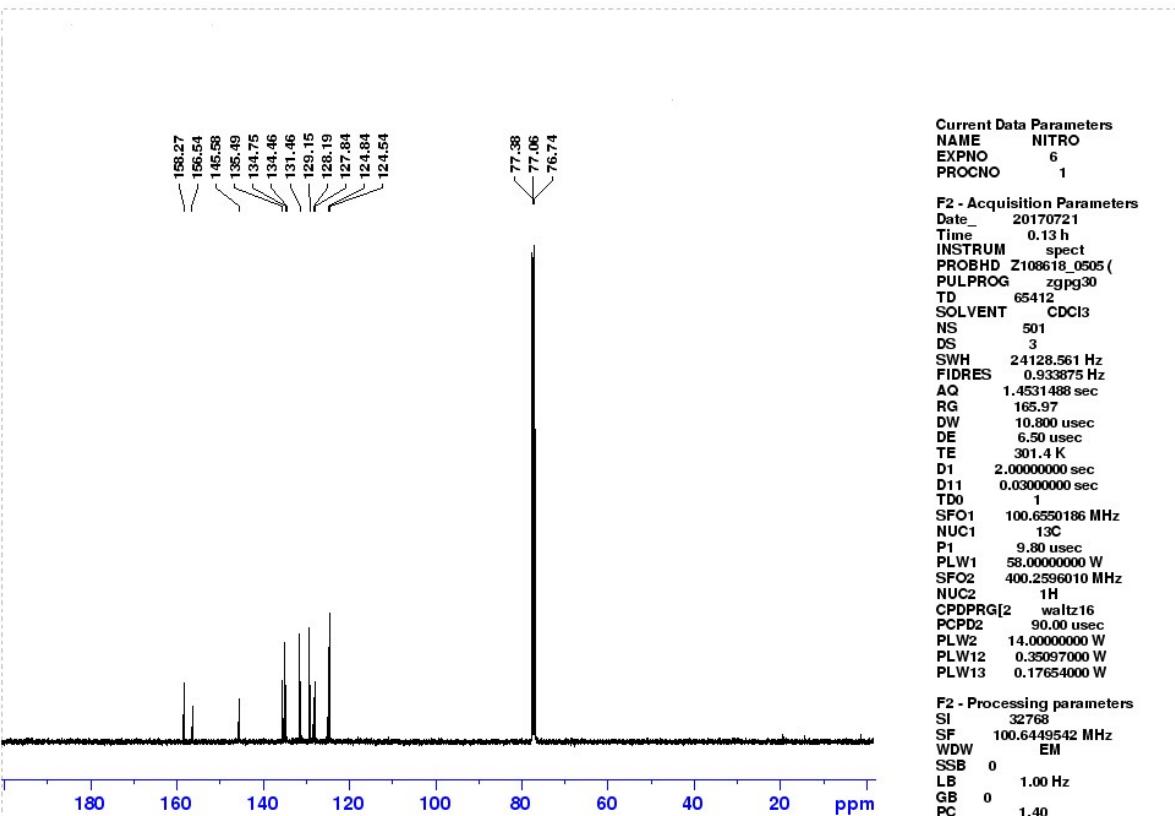
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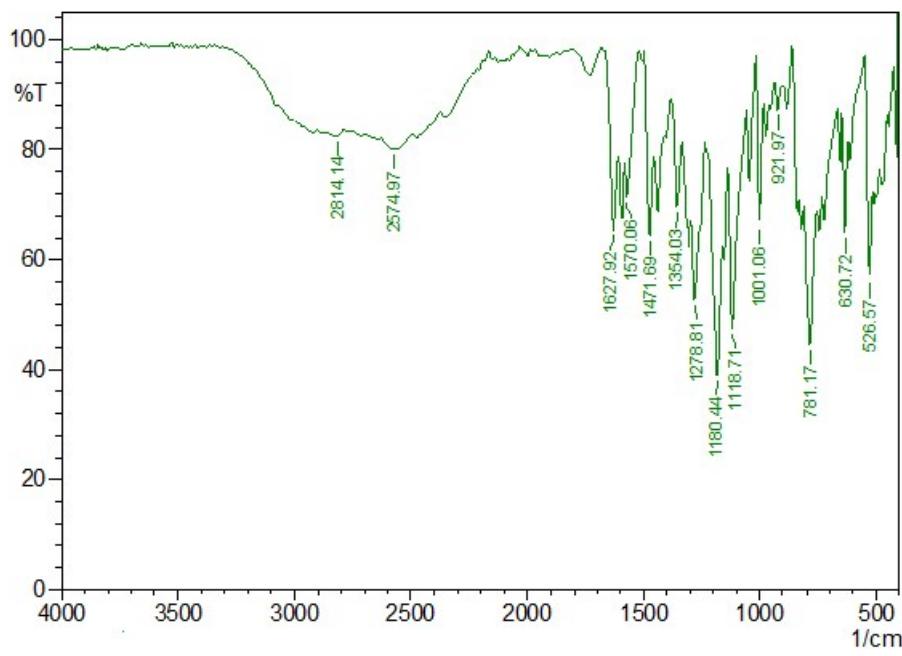
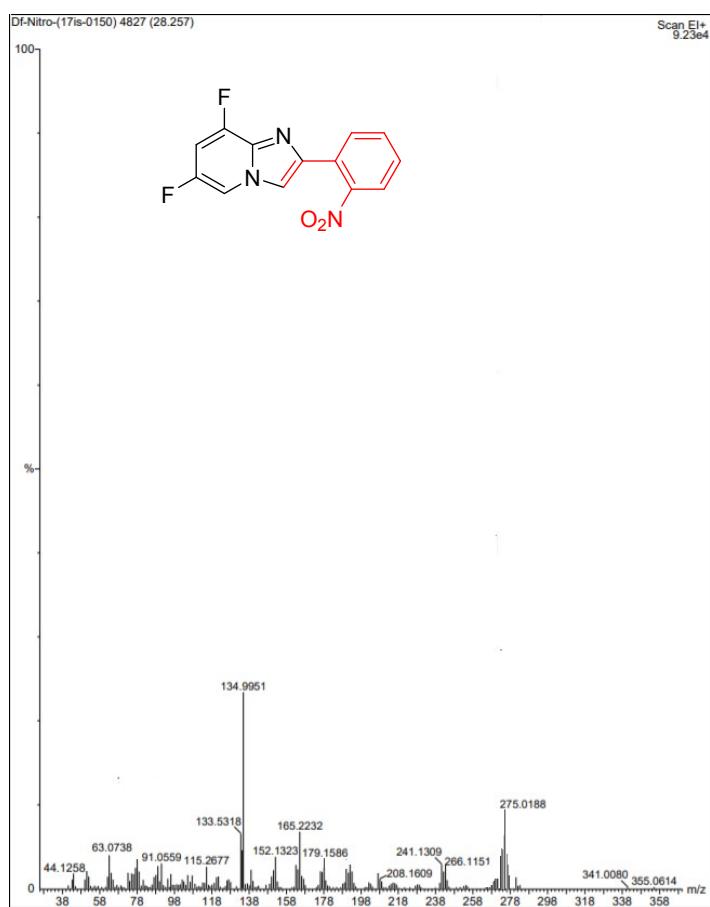
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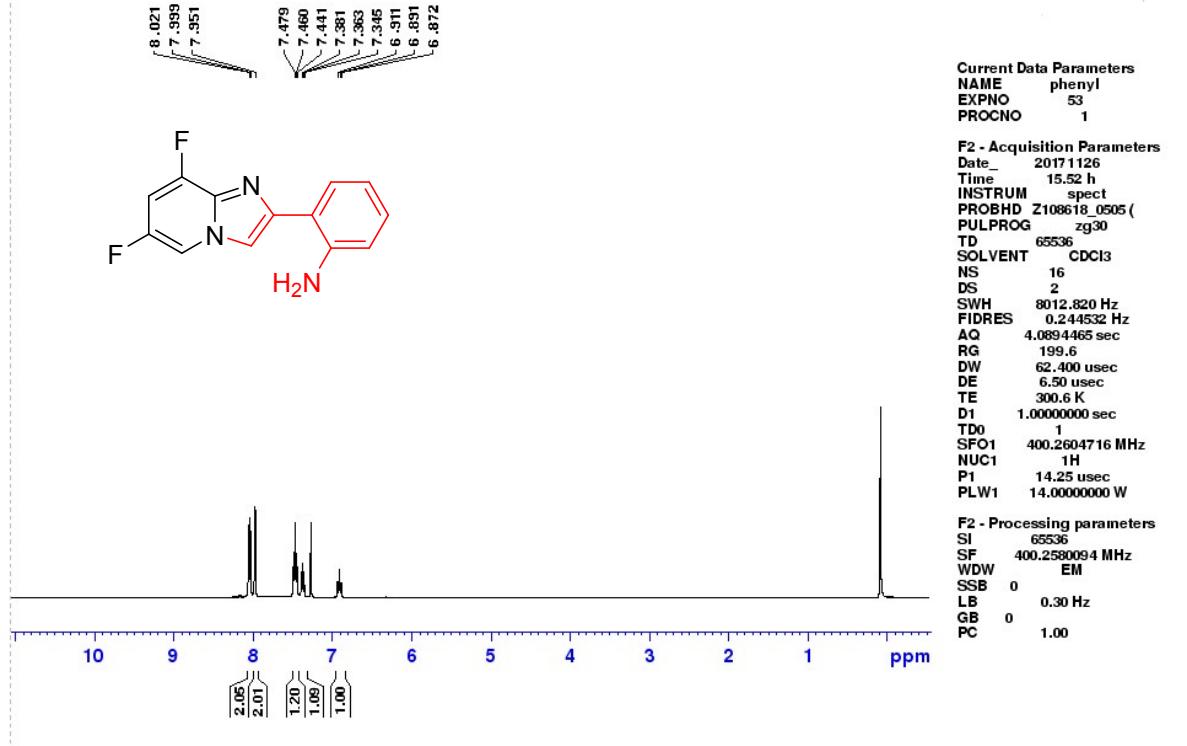


¹H-NMR and ¹³C-NMR of compound 3d in CDCl₃.

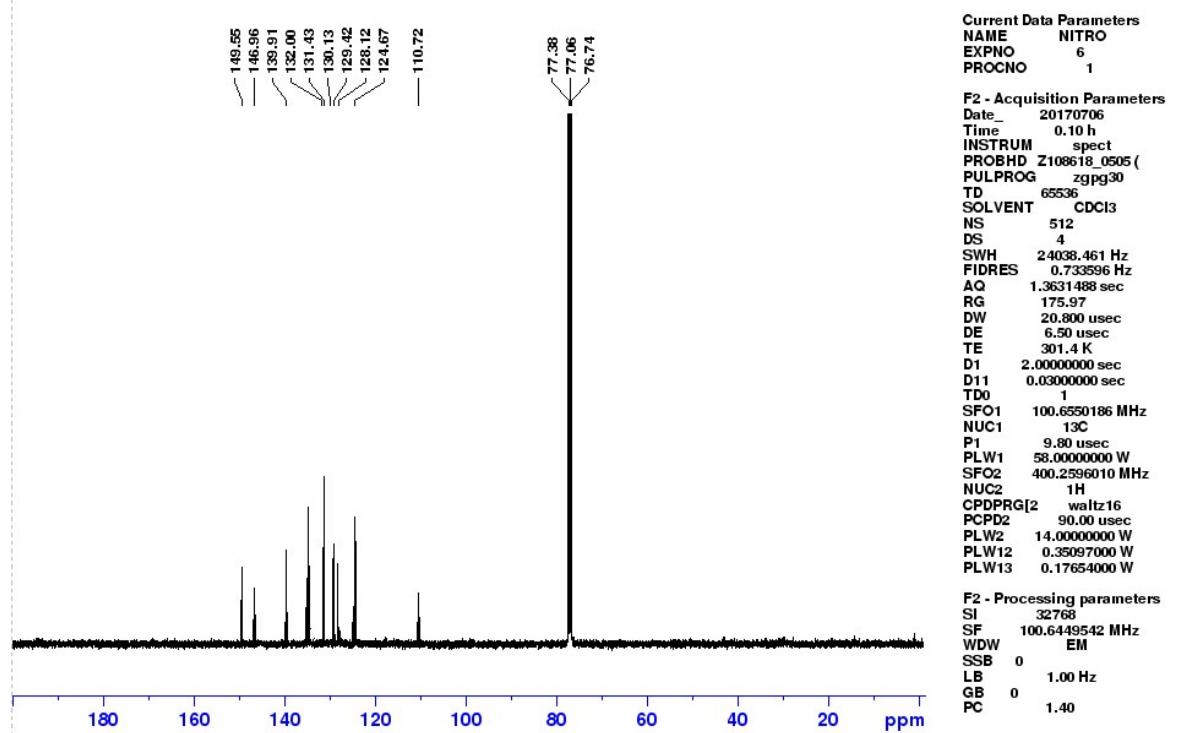


Mass and IR of Compound **3d**.

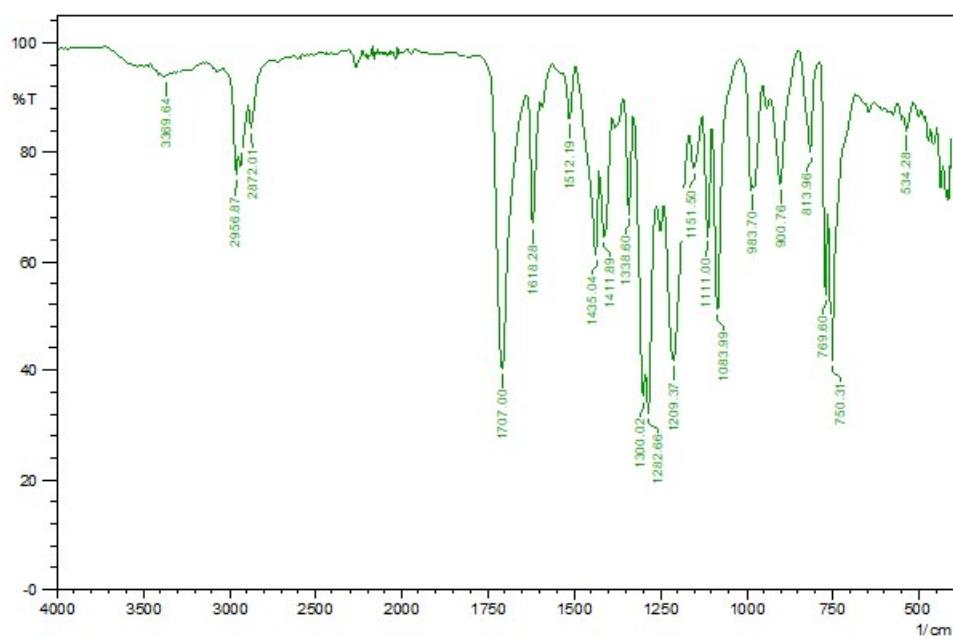
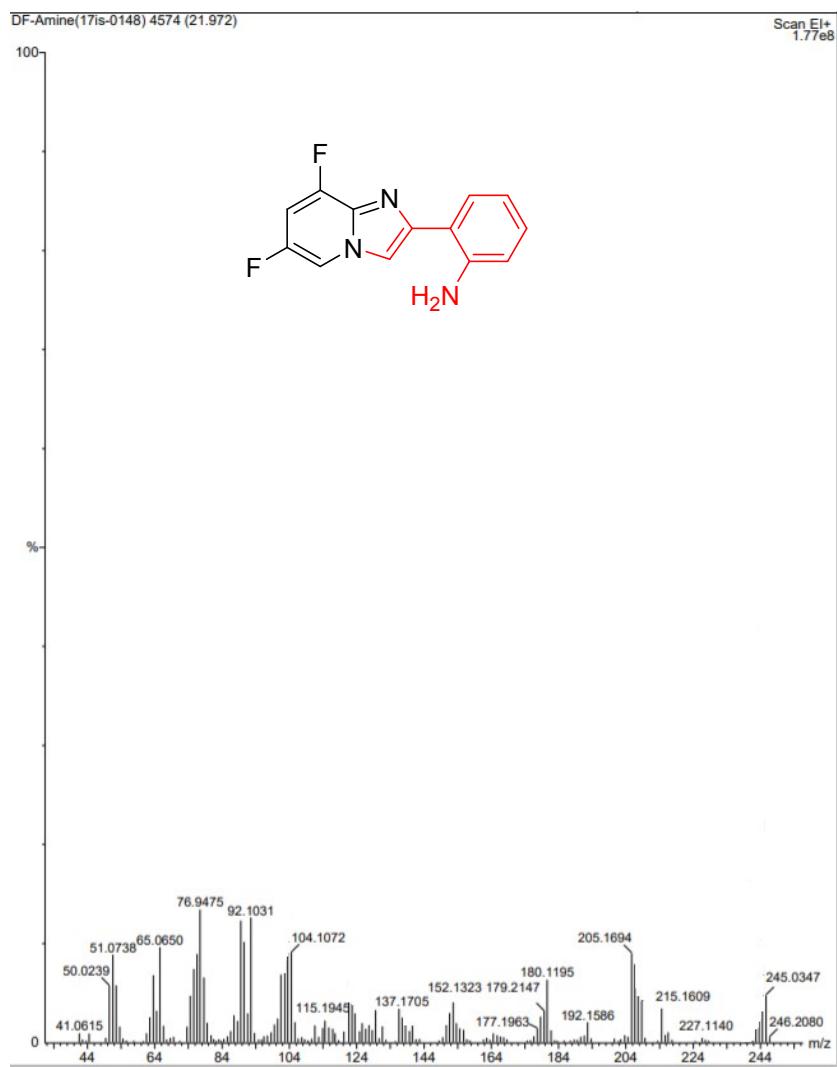
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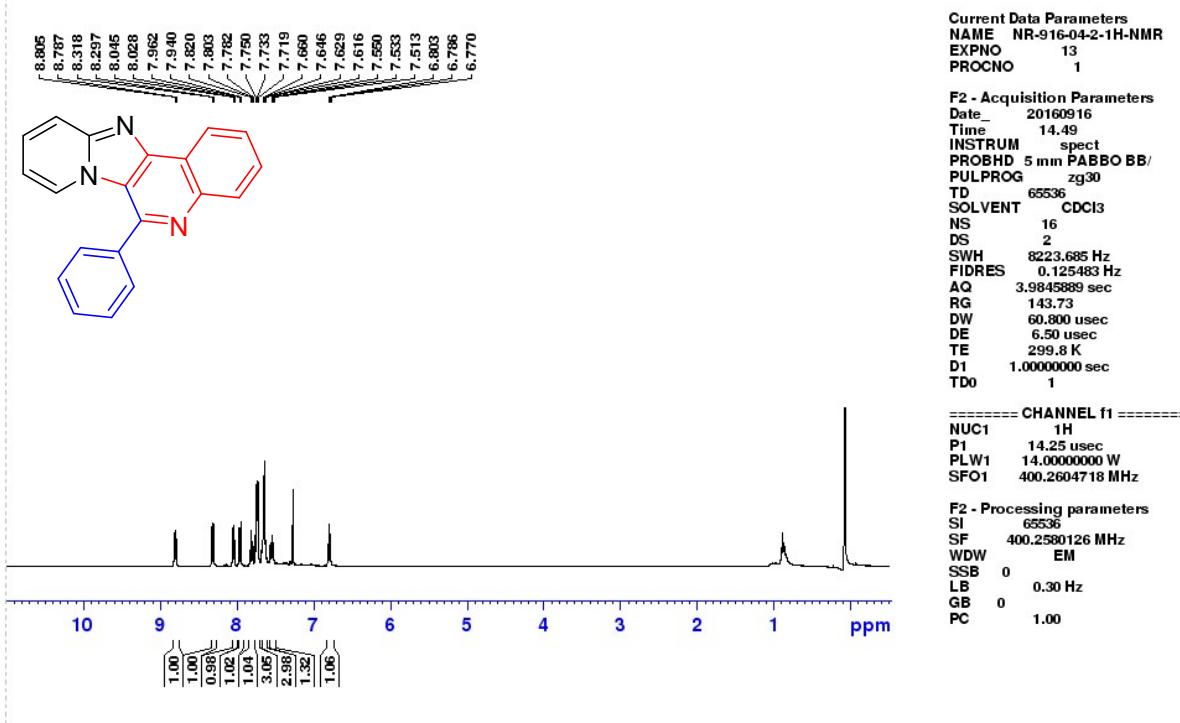


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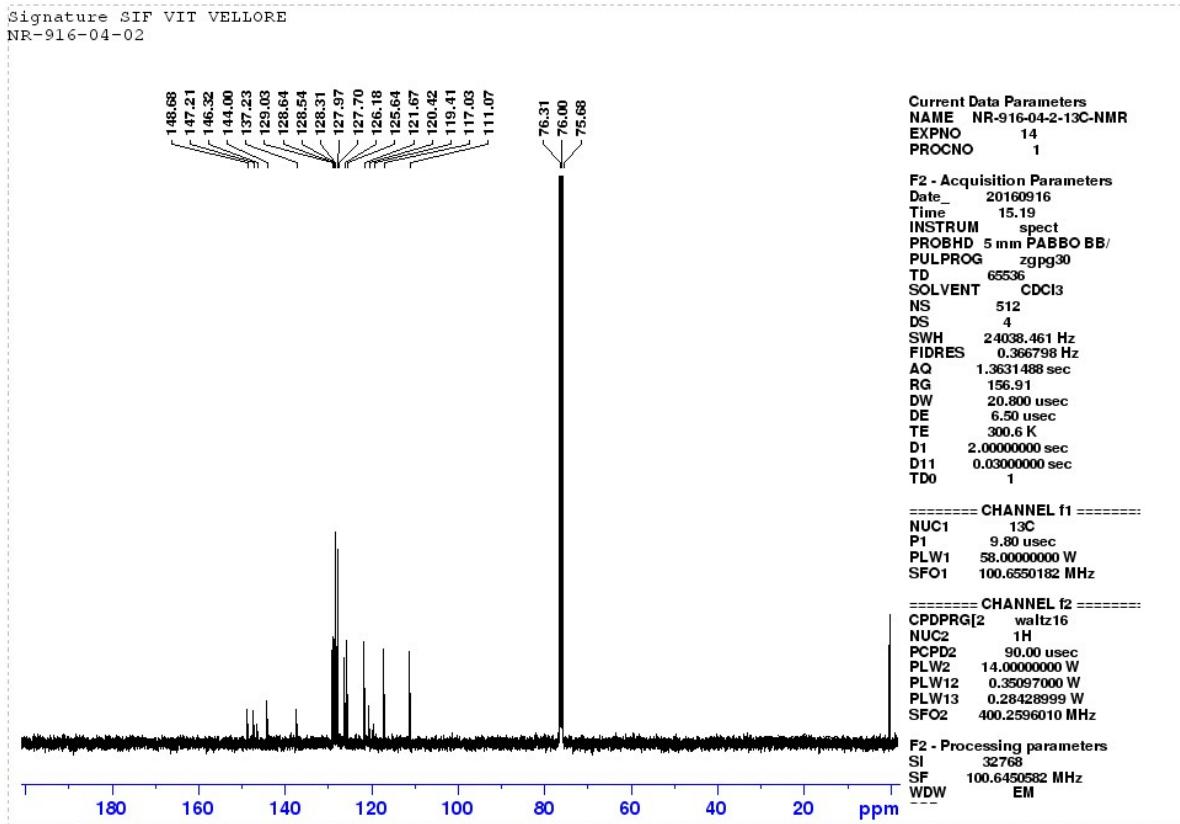


Mass and IR of Compound 4d.

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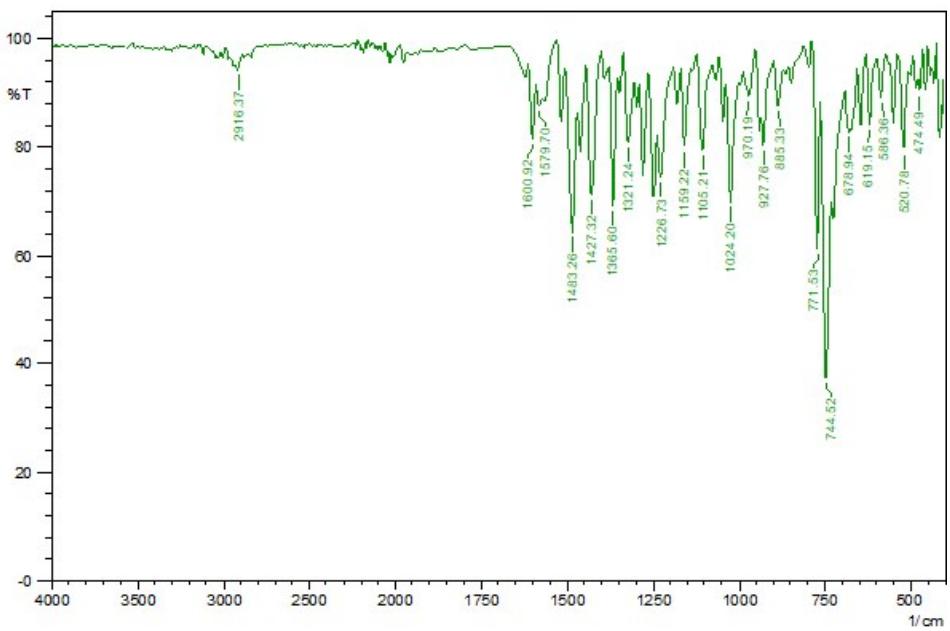
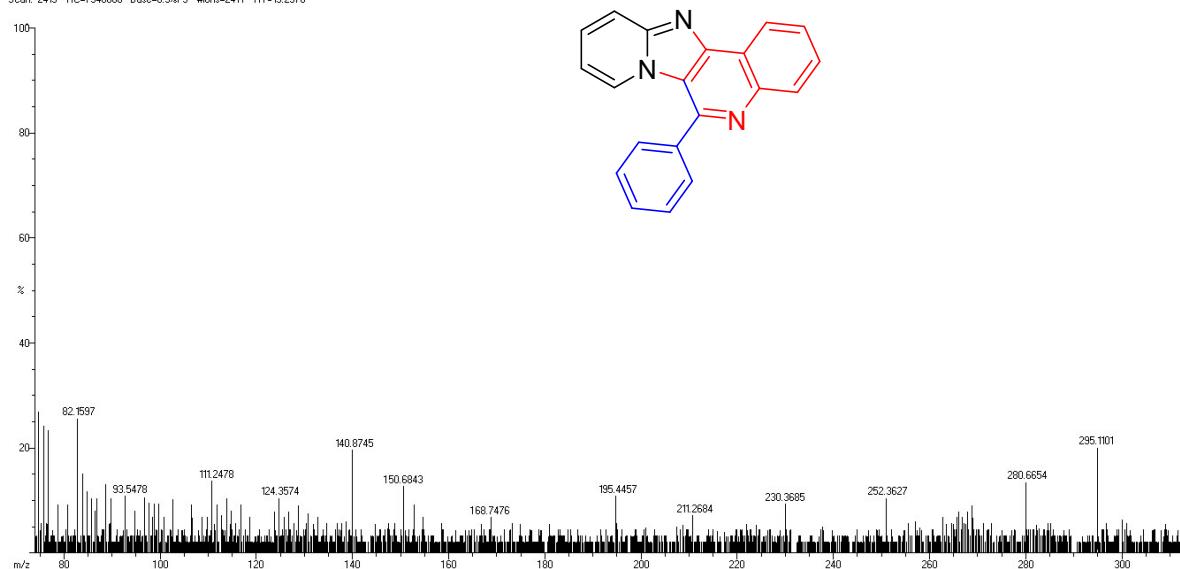


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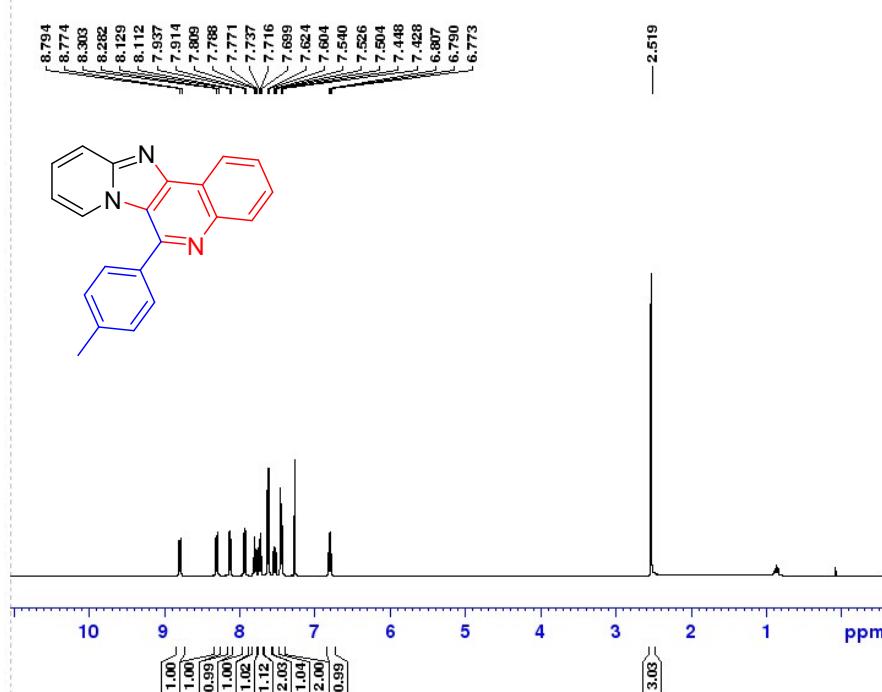
¹H-NMR and ¹³C-NMR of compound 6a in CDCl₃.

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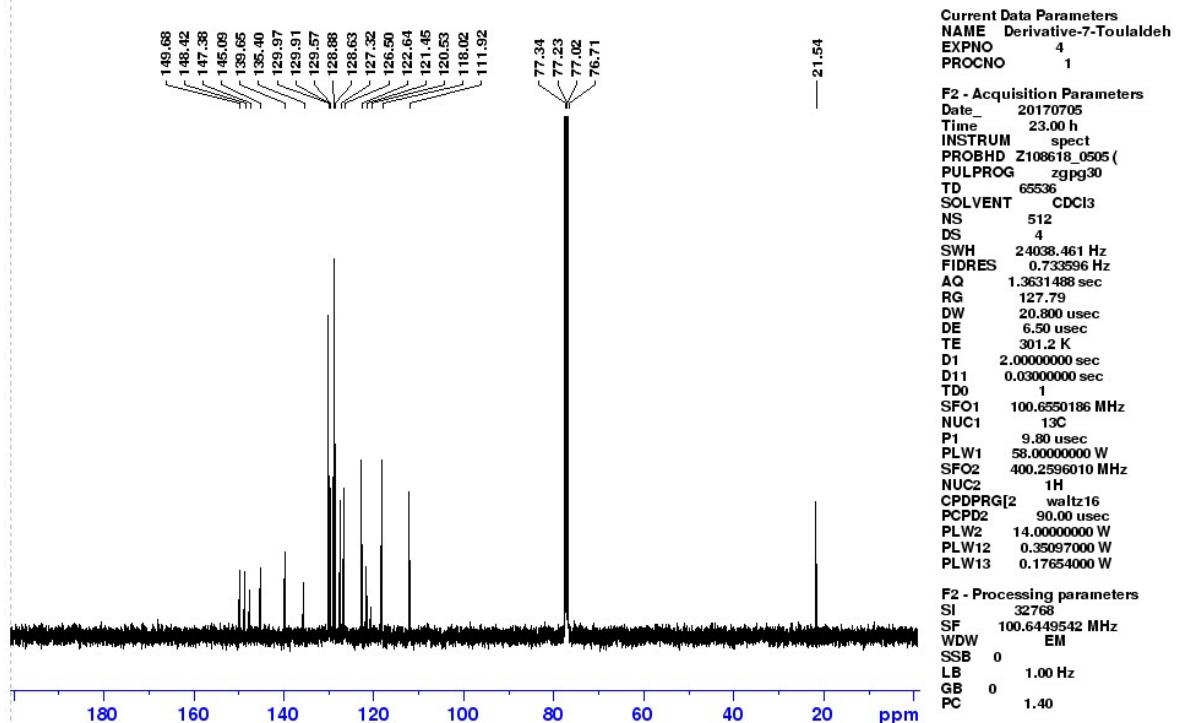


IR and HRMS of compound **6a**

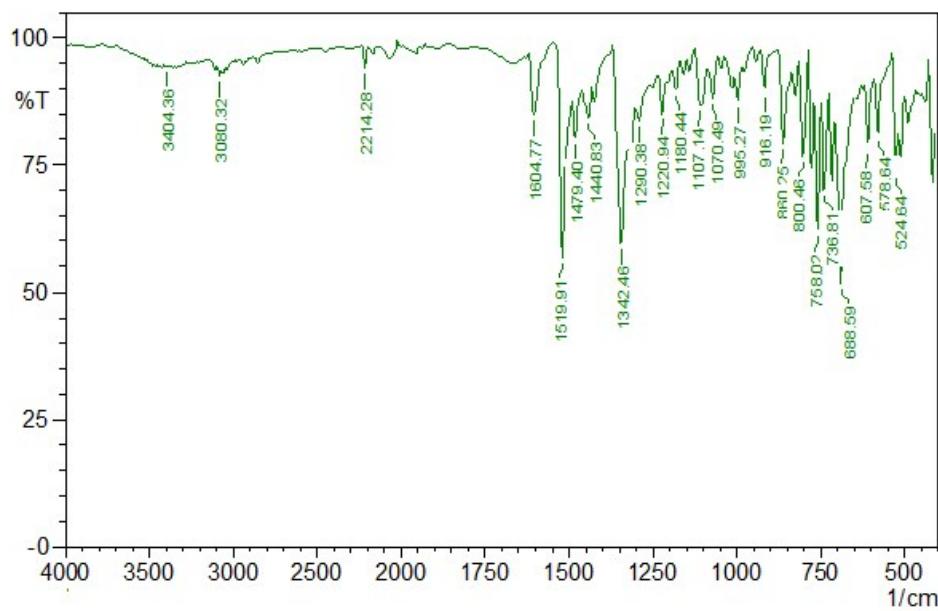
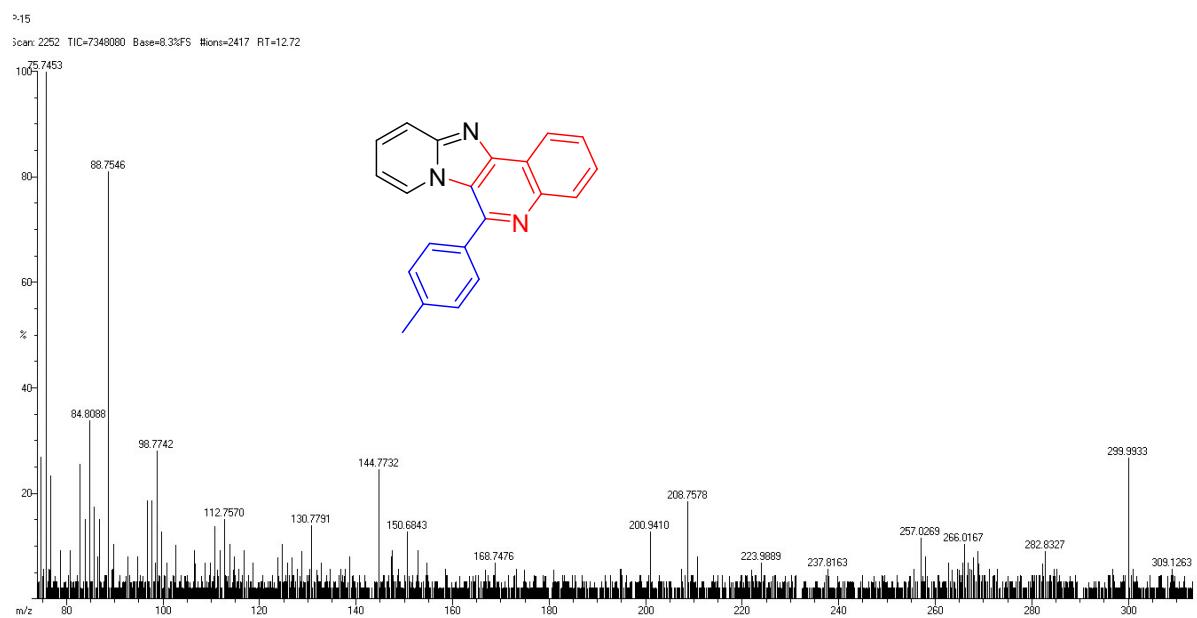
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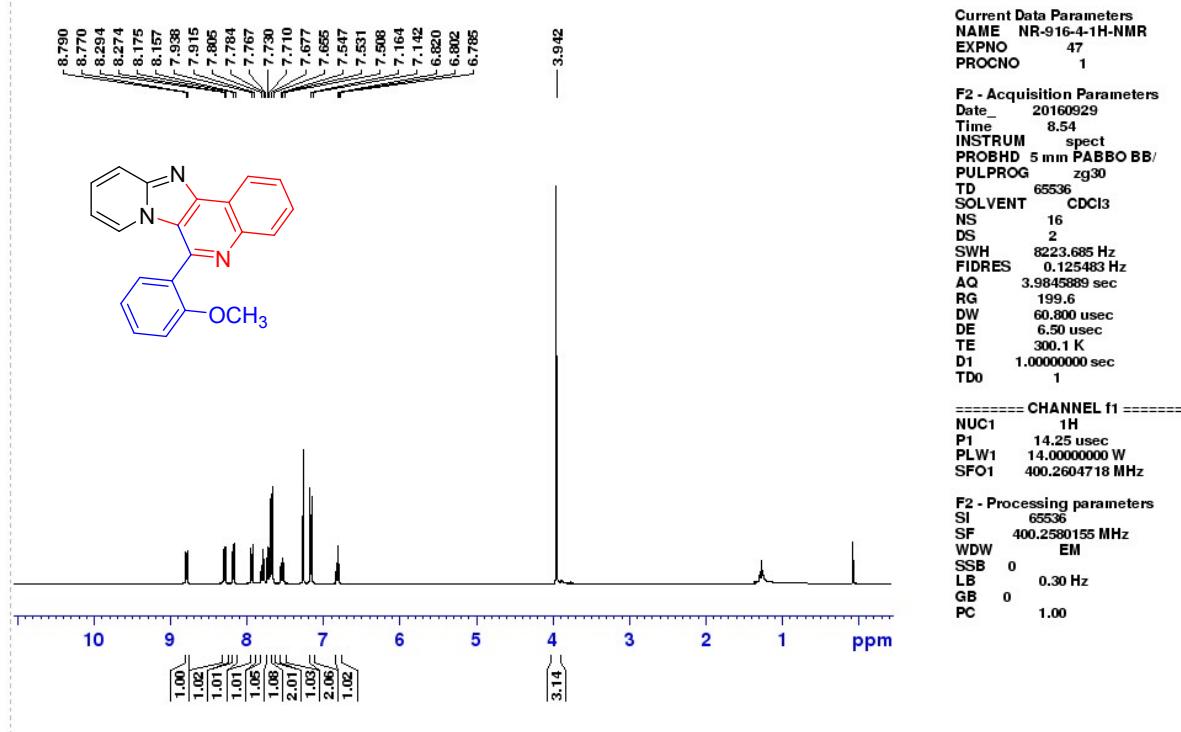


¹H-NMR and ¹³C-NMR of compound 6b in CDCl₃

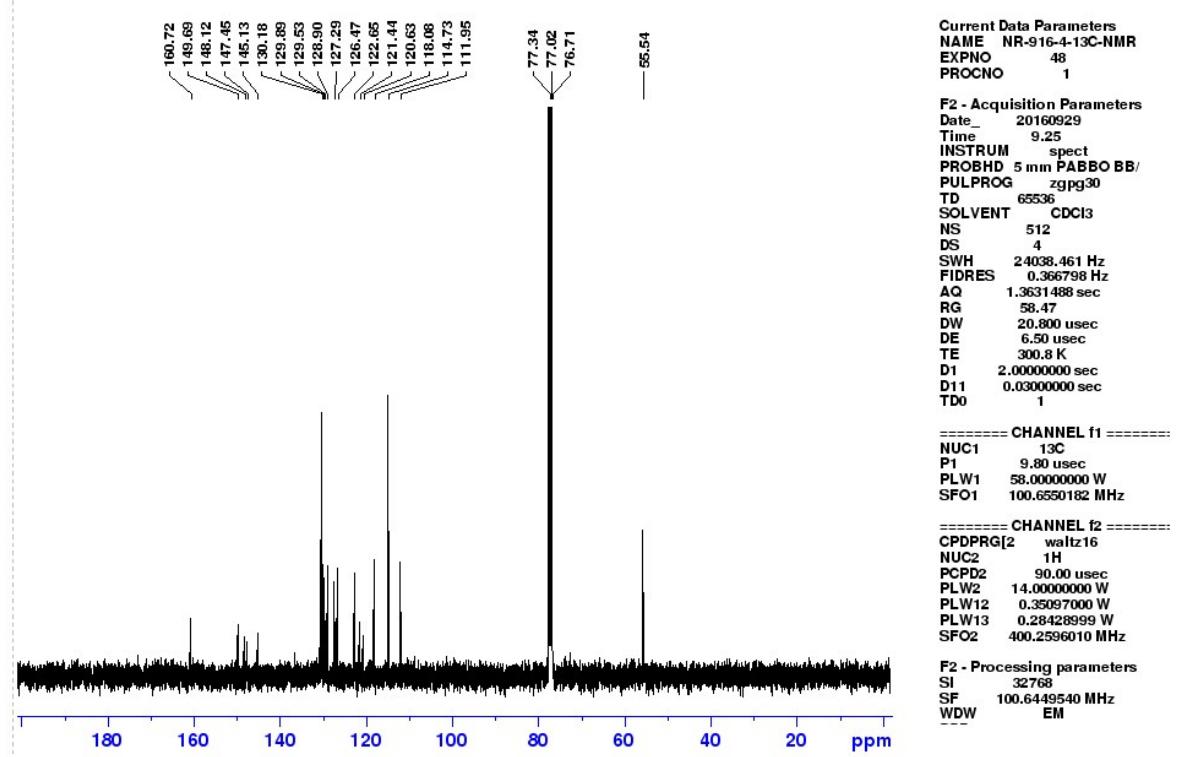


IR and HRMS of compound **6b**

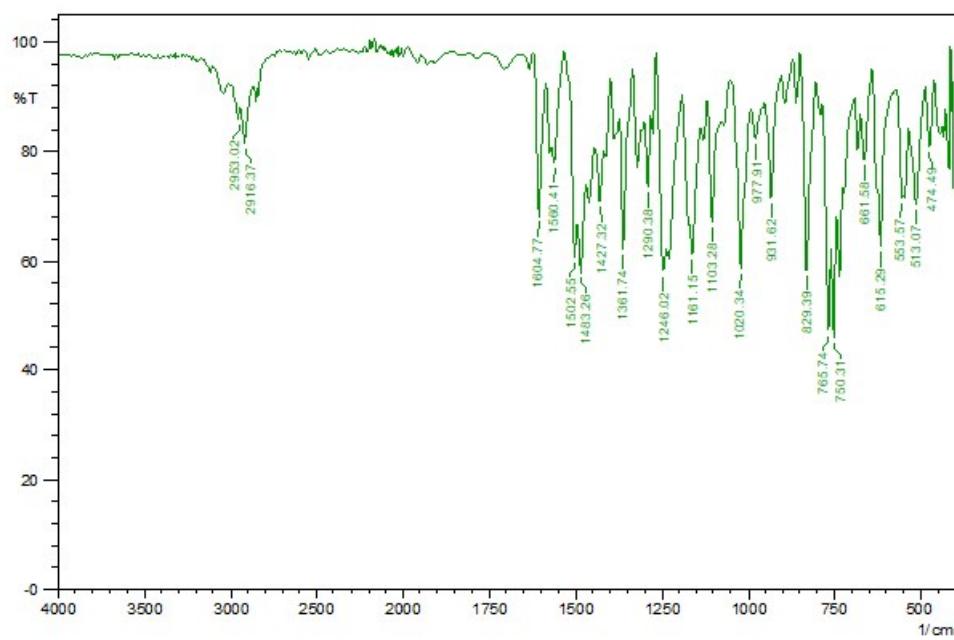
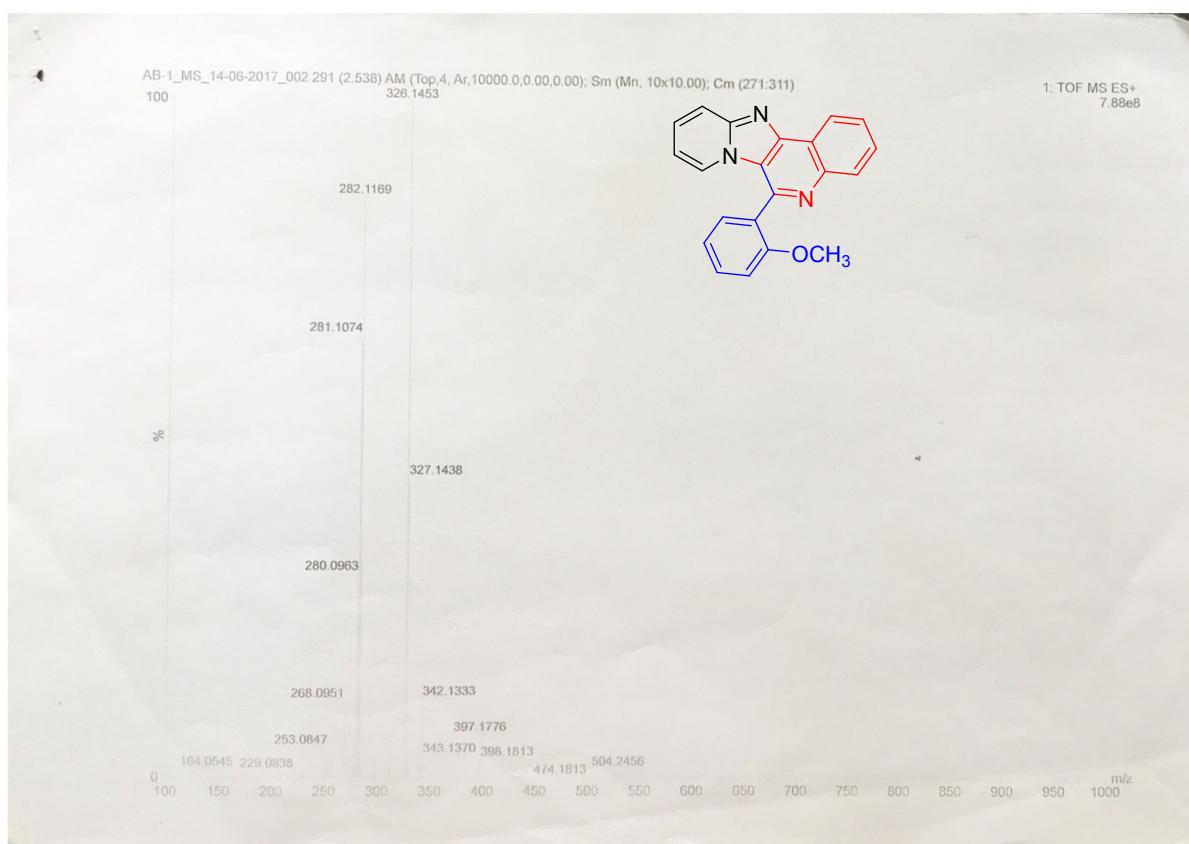
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NR-916-4



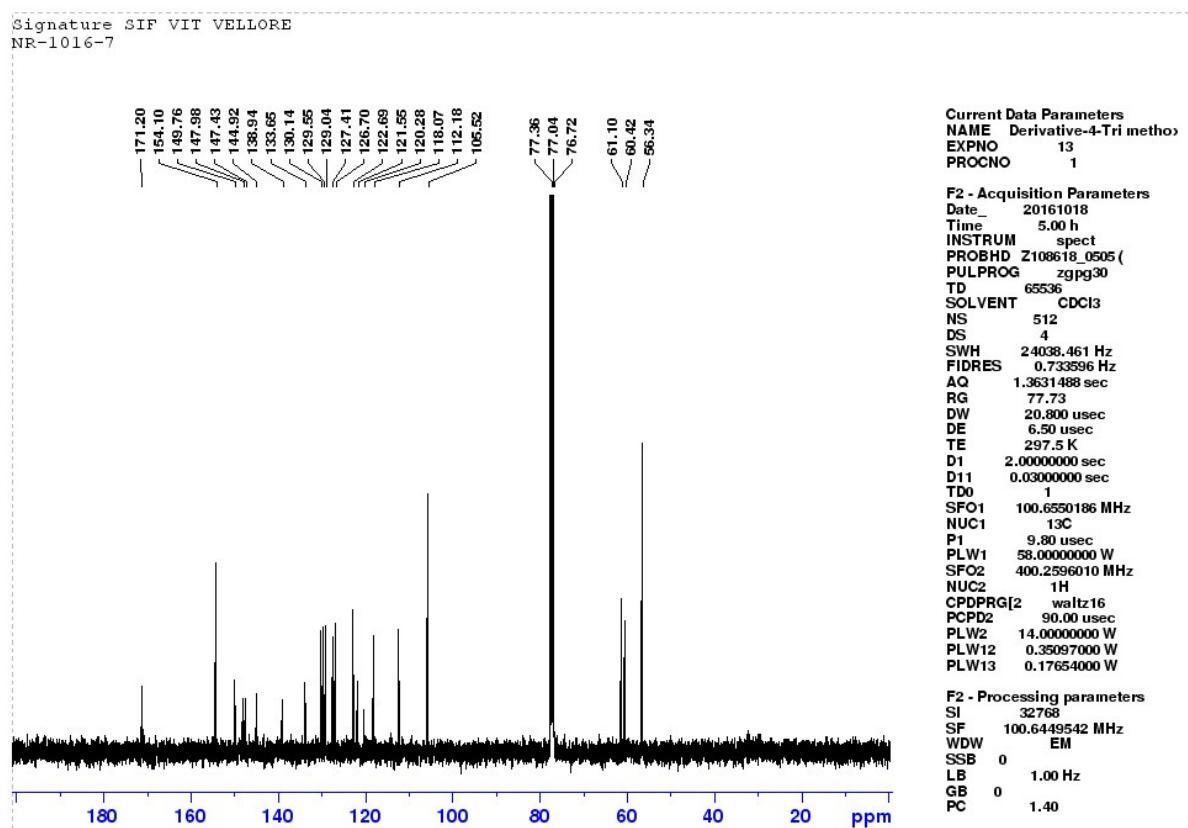
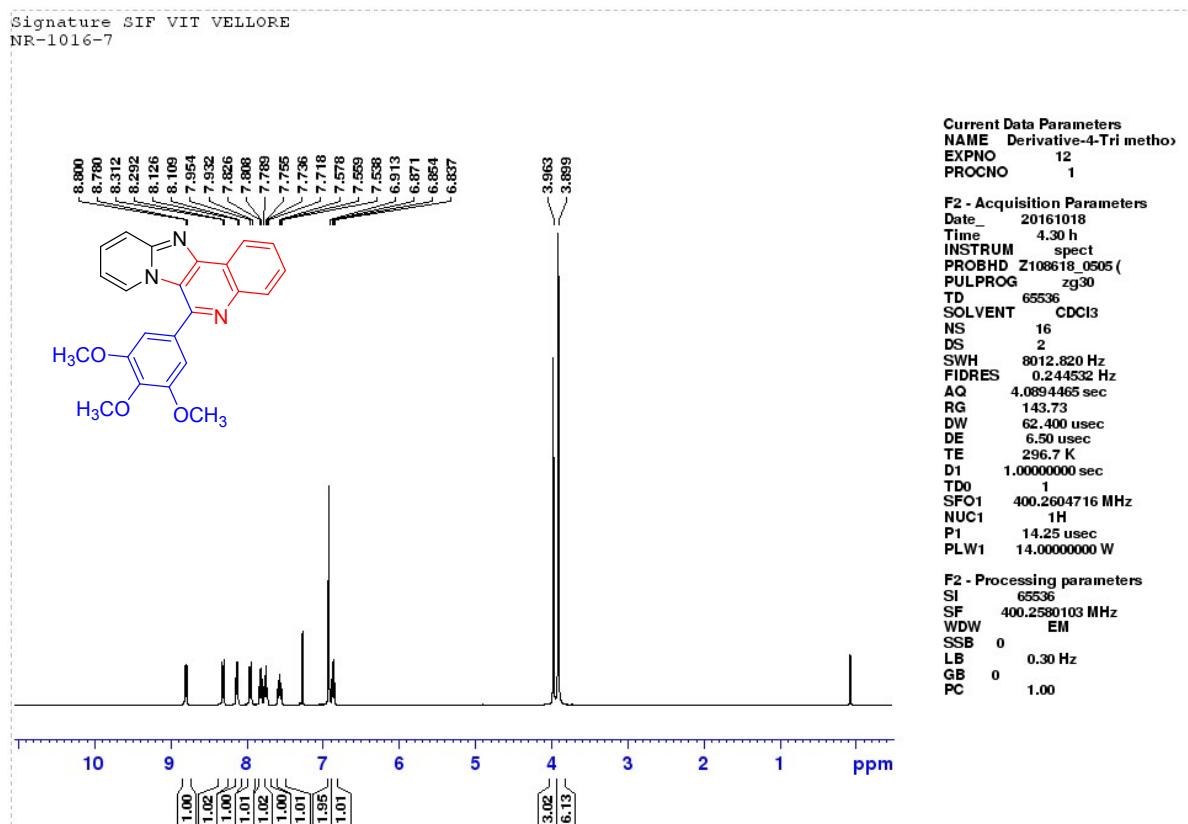
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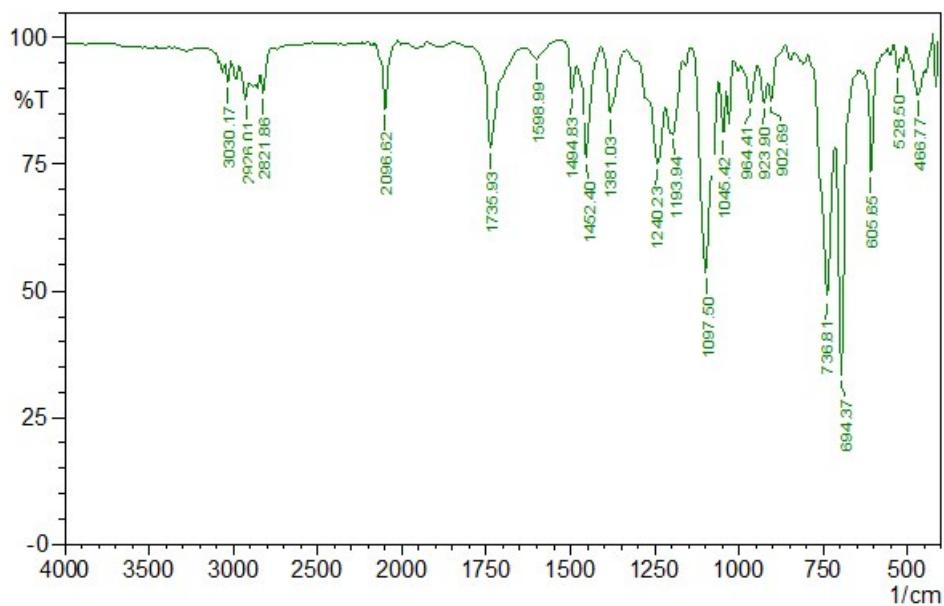
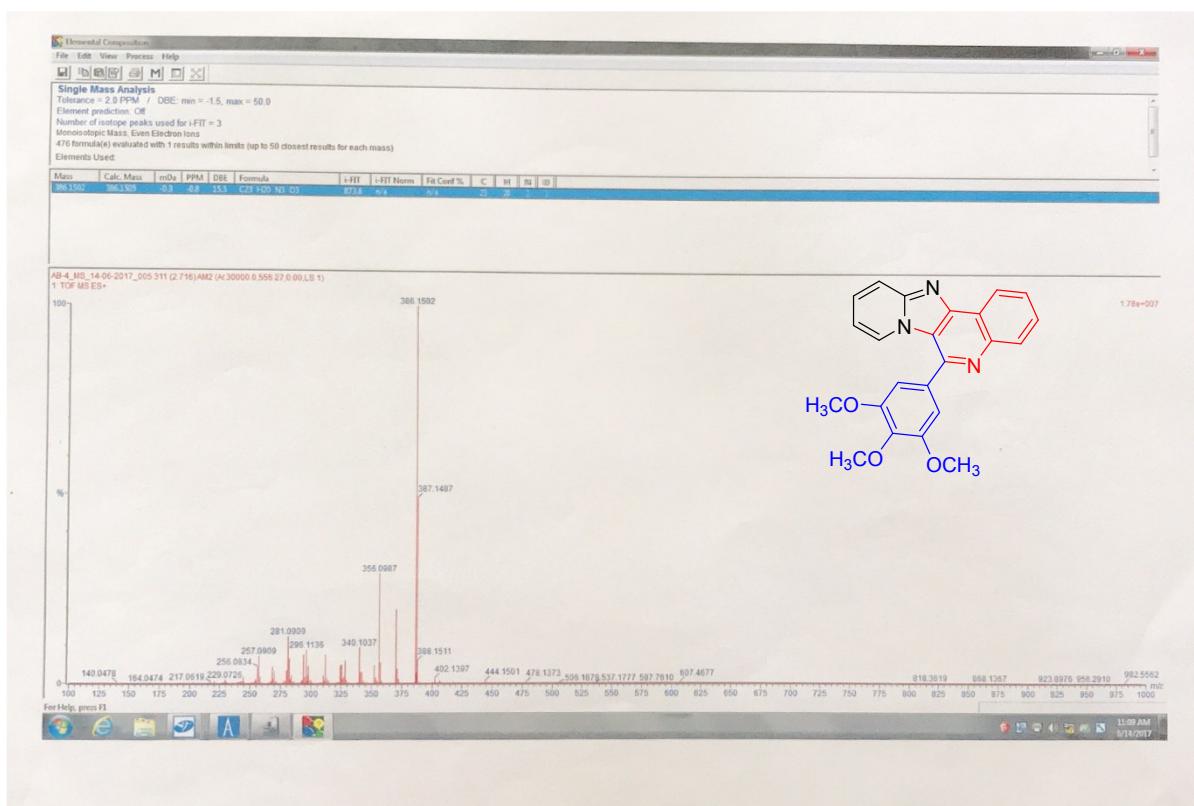
¹H-NMR and ¹³C-NMR of compound **6c** in CDCl₃.



IR and HRMS of compound **6c**

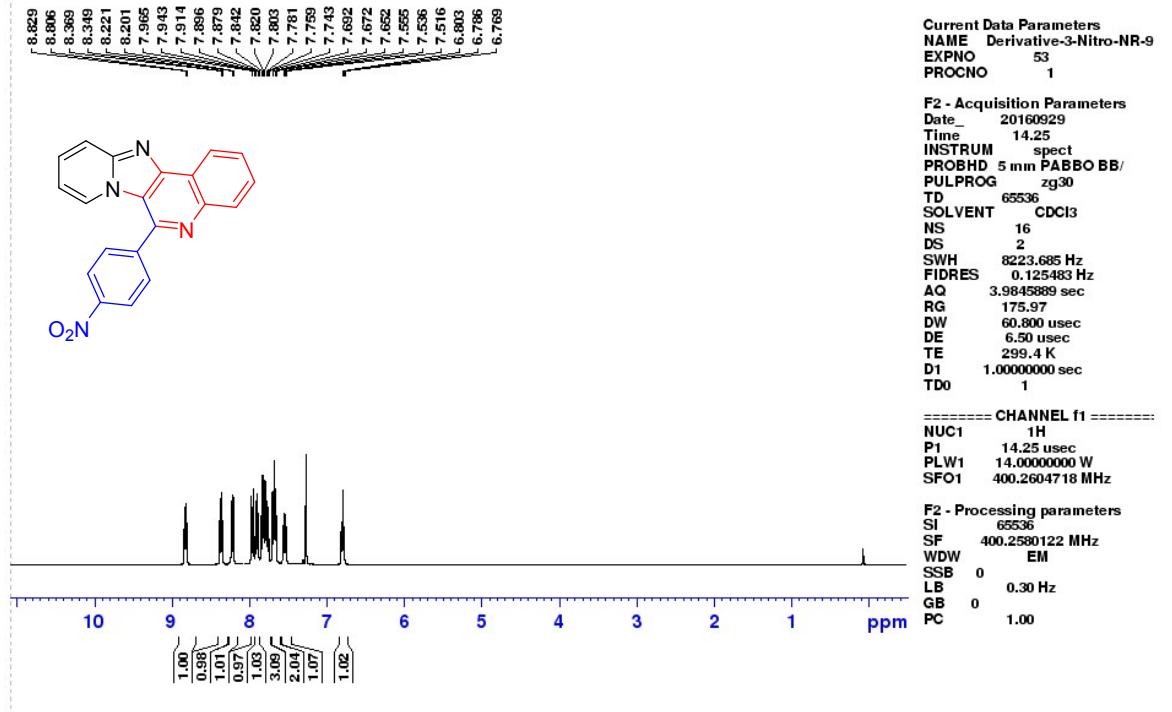


¹H-NMR and ¹³C-NMR of compound **6d** in CDCl₃

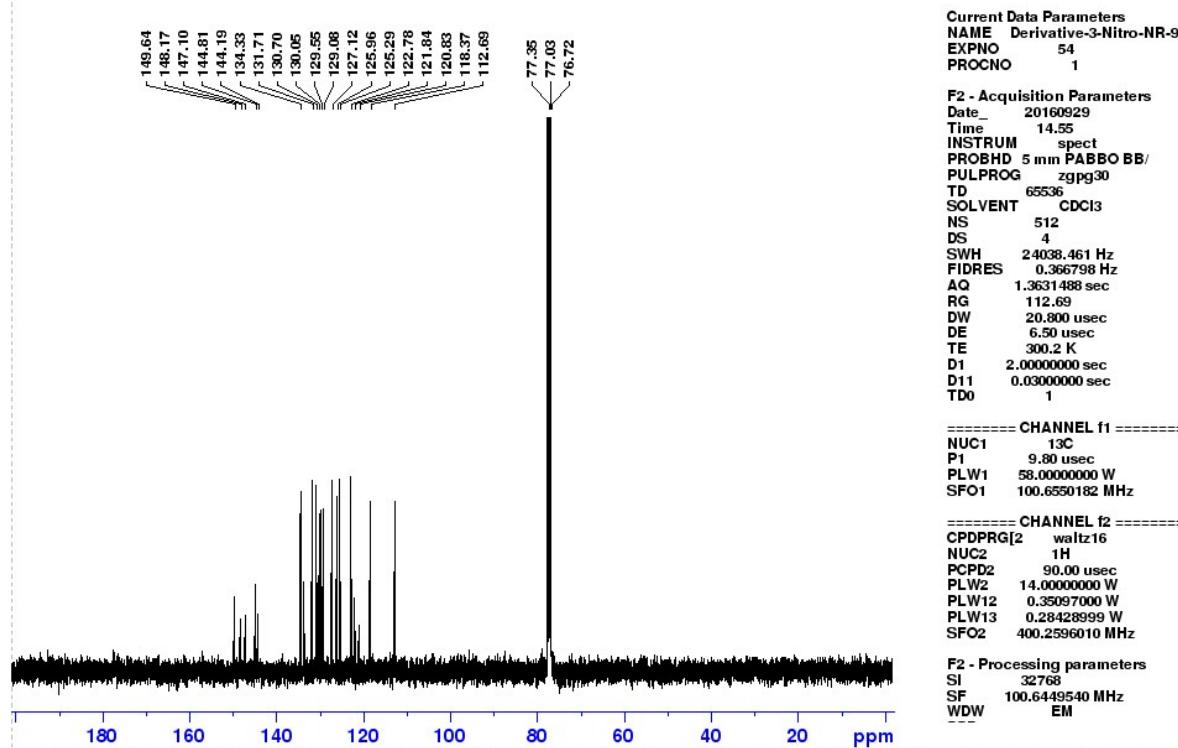


IR and HRMS of compound **6d**

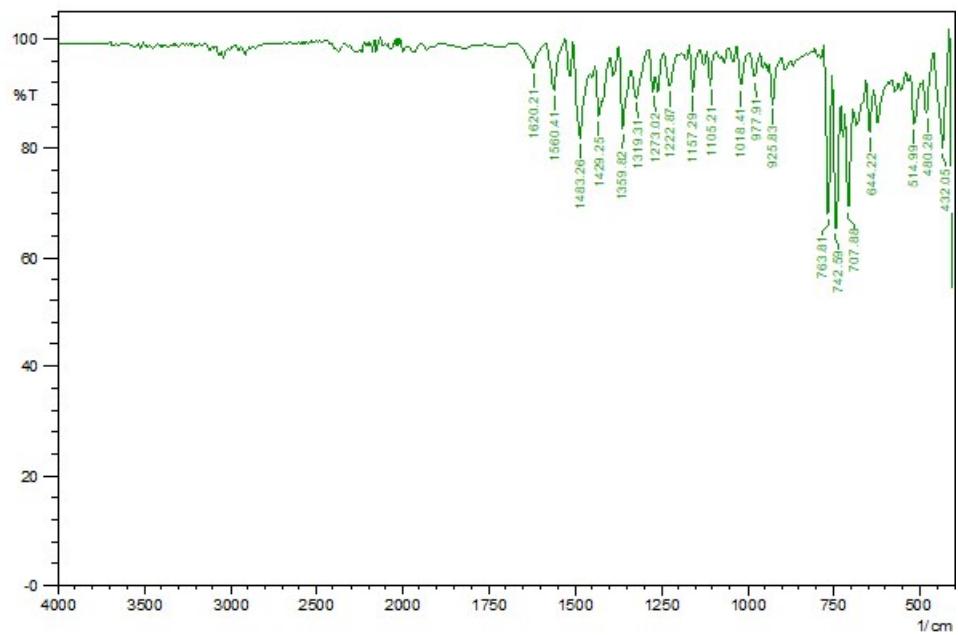
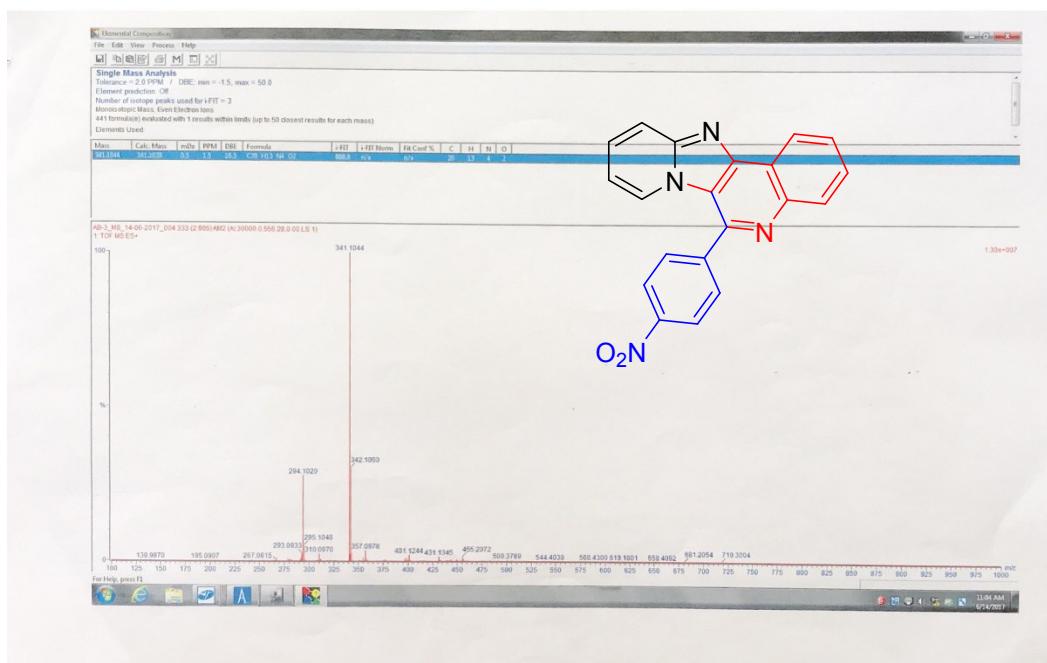
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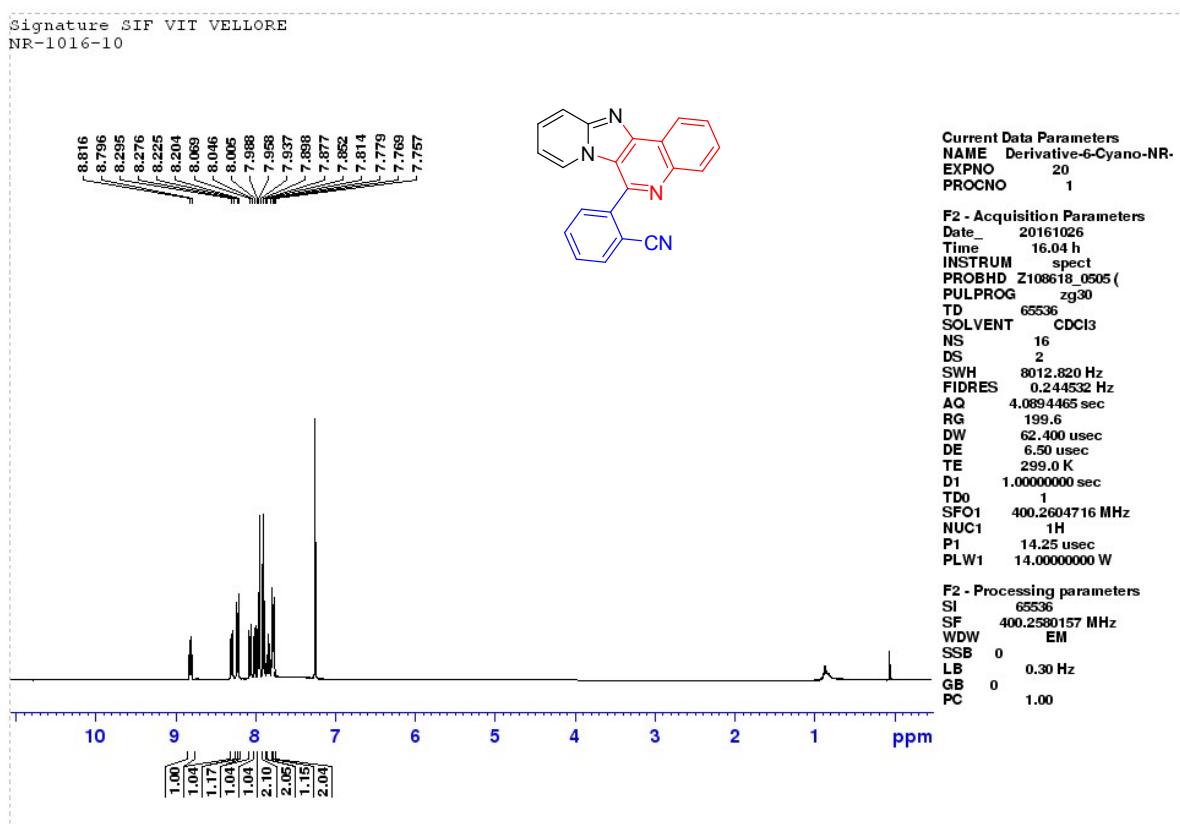


¹H-NMR and ¹³C-NMR of compound 6e in CDCl₃

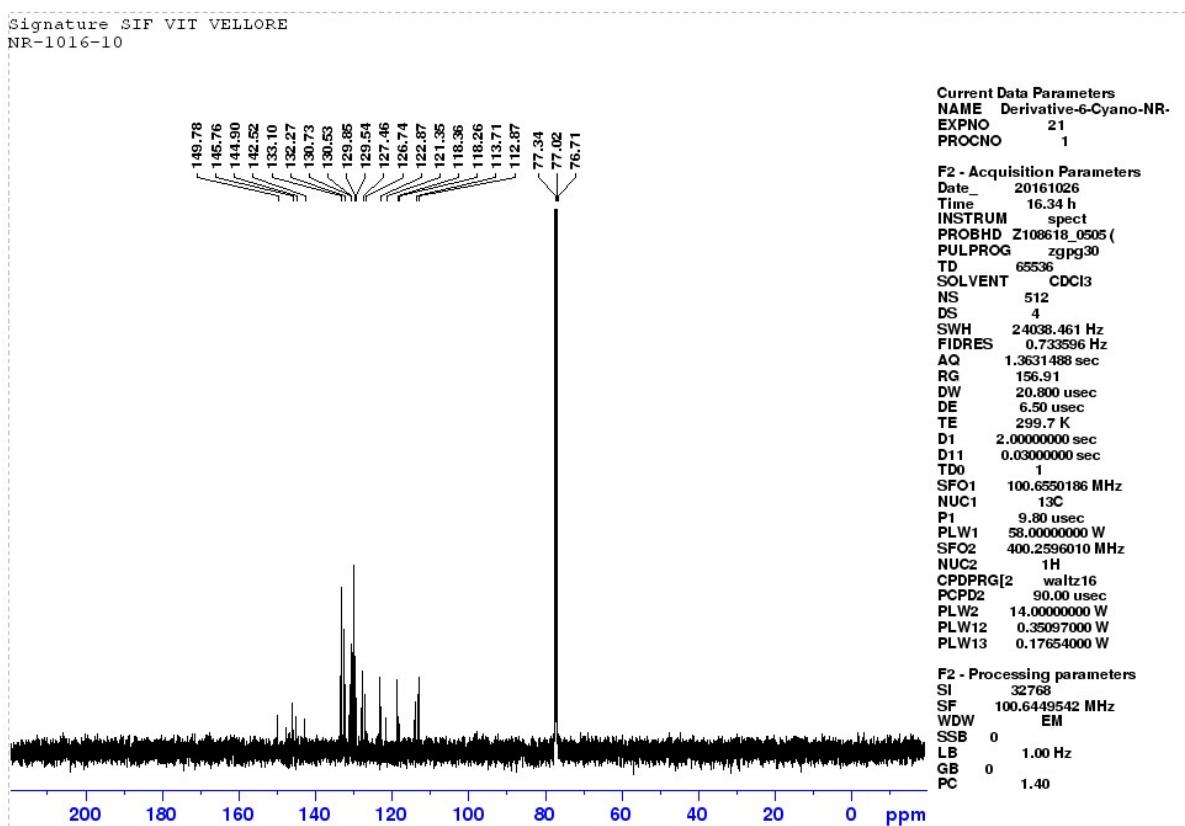


IR and HRMS of compound **6e**

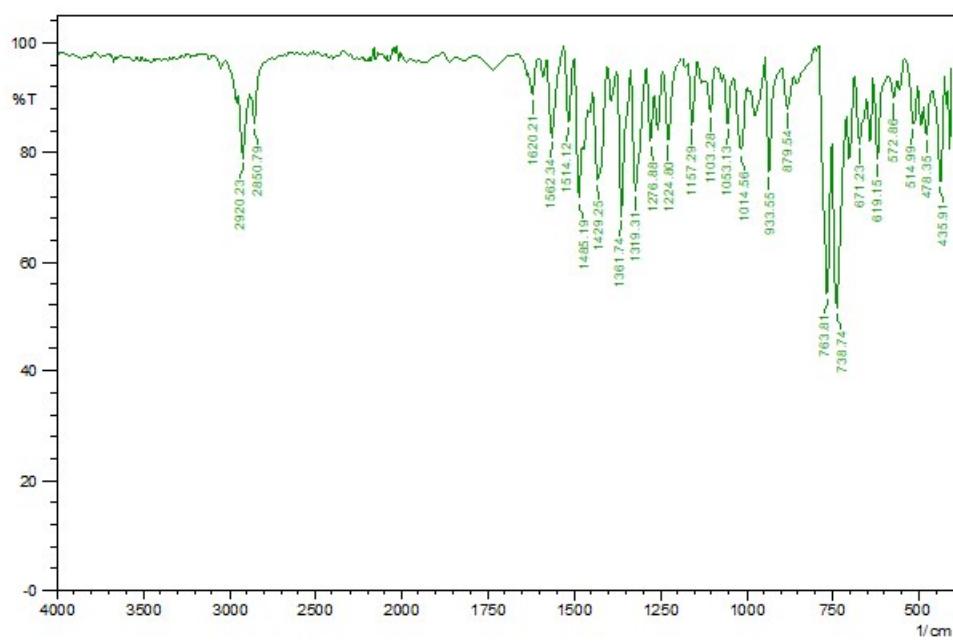
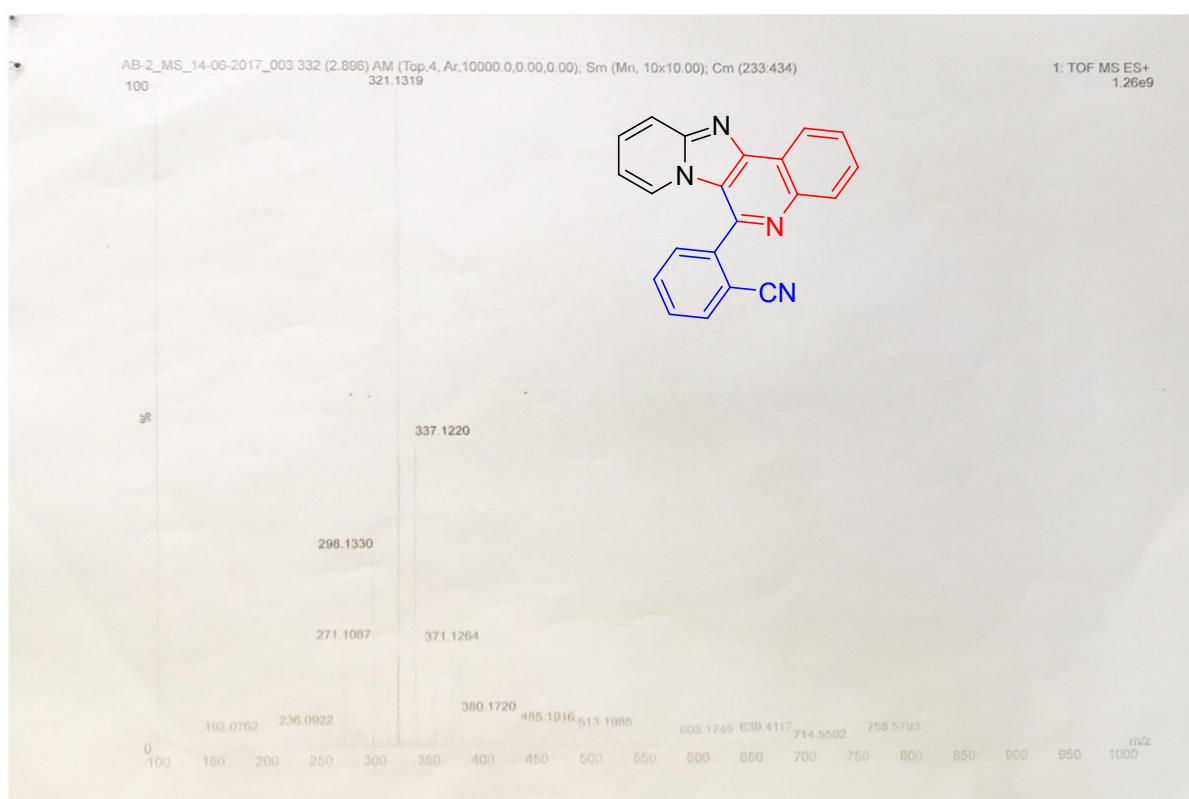
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NR-1016-10



Signature SIF VIT VELLORE
NR-1016-10

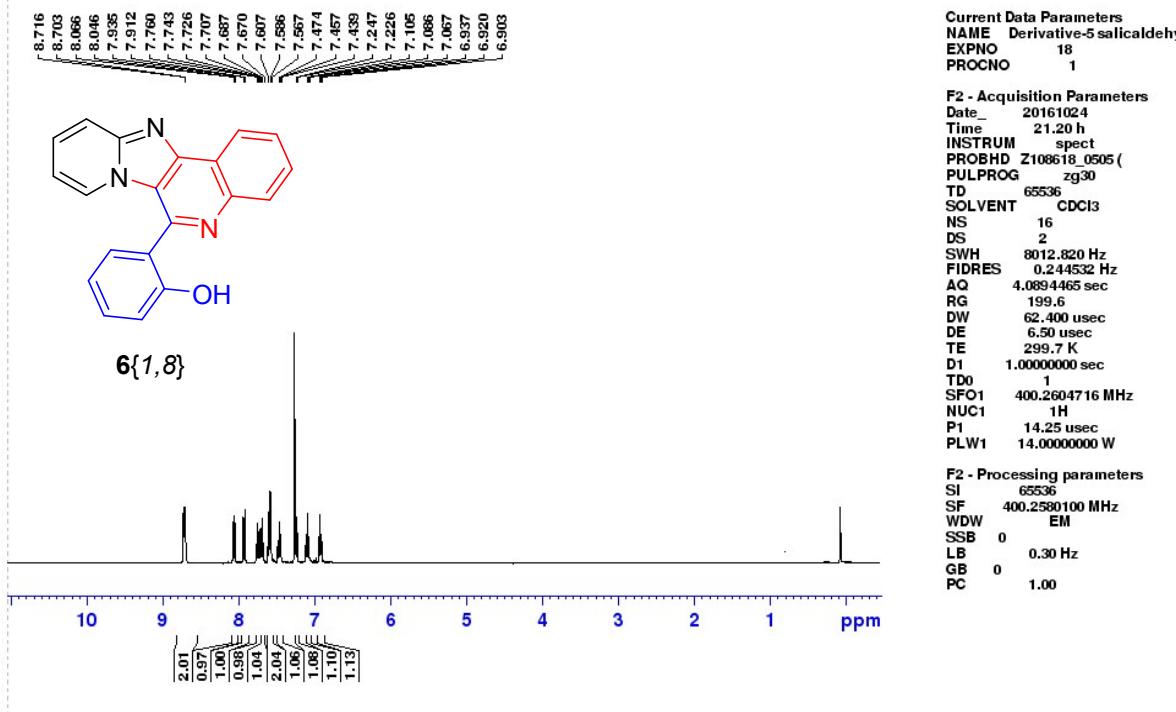


¹H-NMR and ¹³C-NMR of compound 6f in CDCl₃

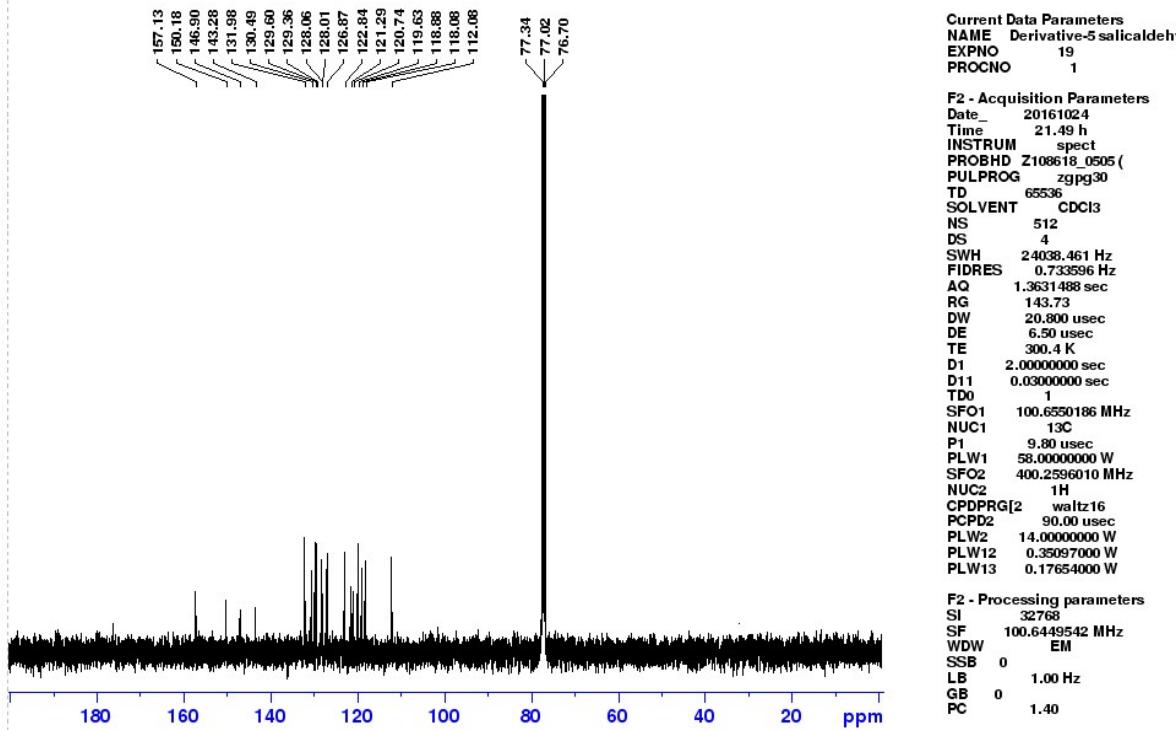


IR and HRMS of compound **6f**

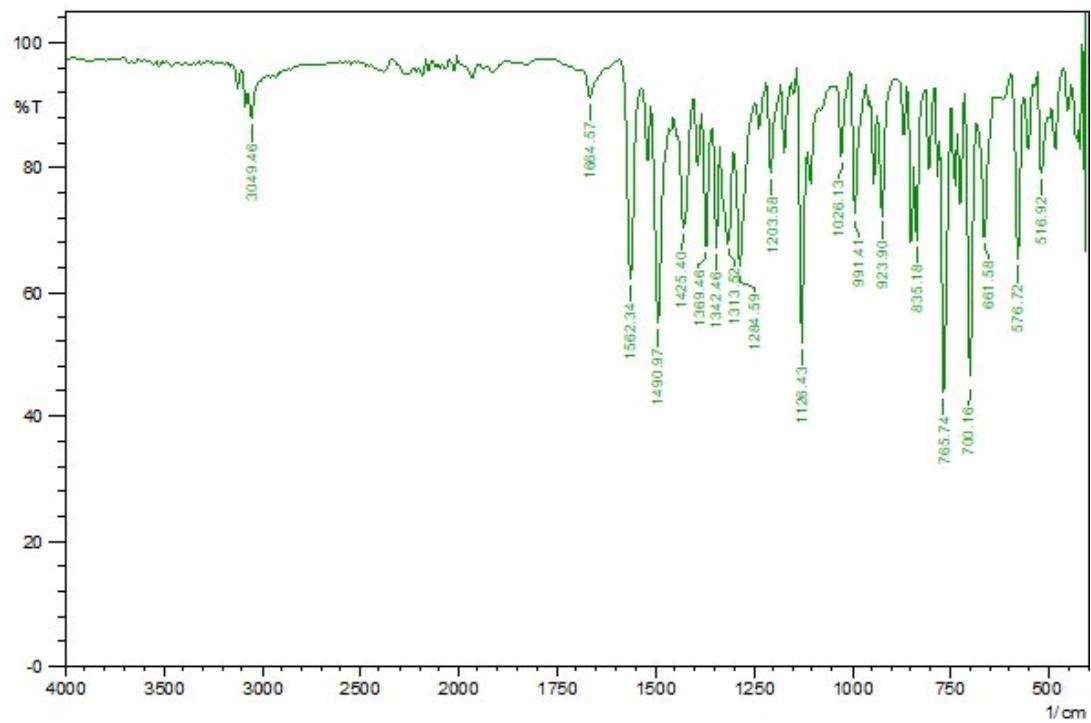
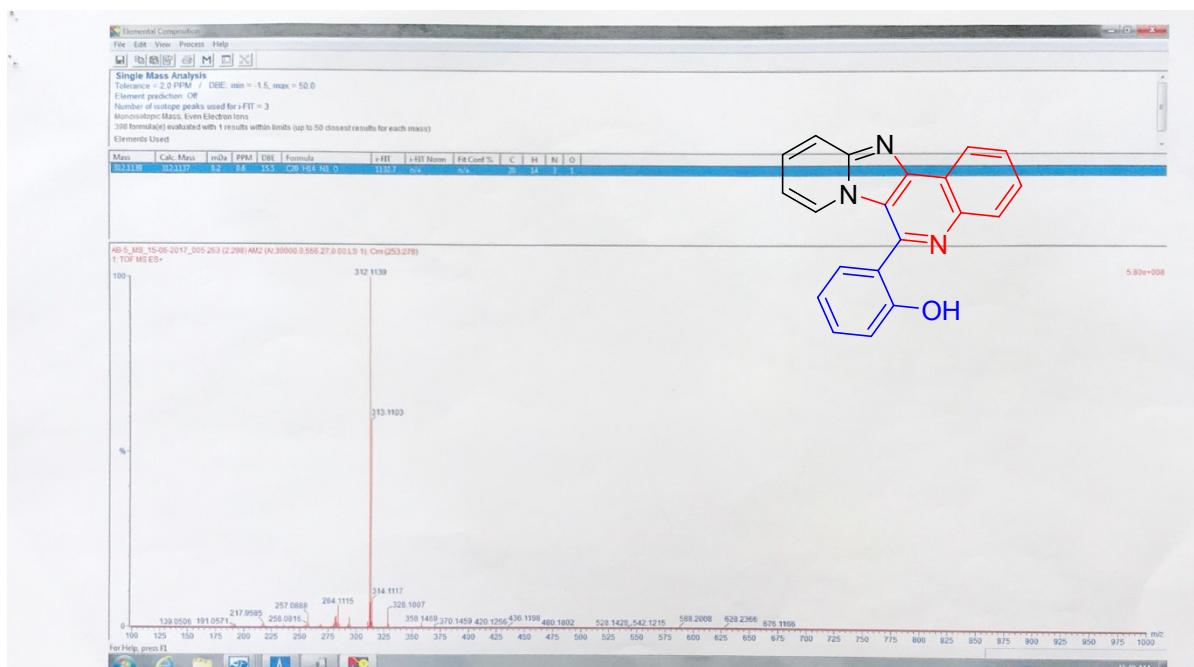
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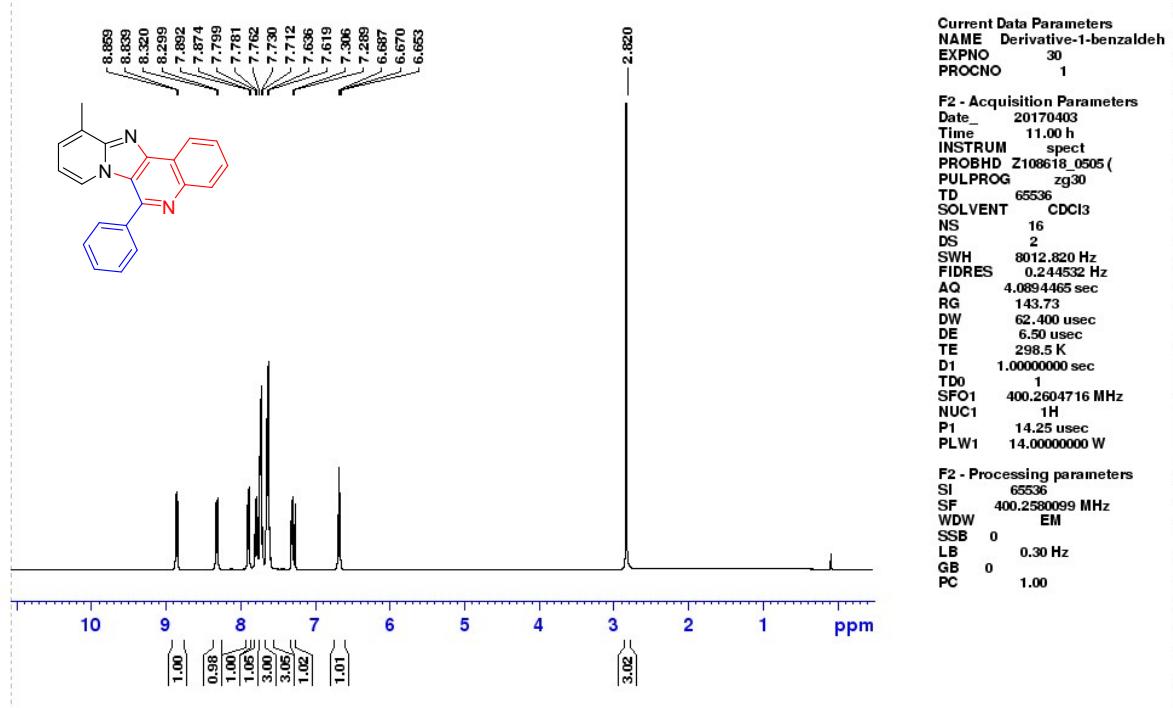


¹H-NMR and ¹³C-NMR of compound 6g in CDCl₃

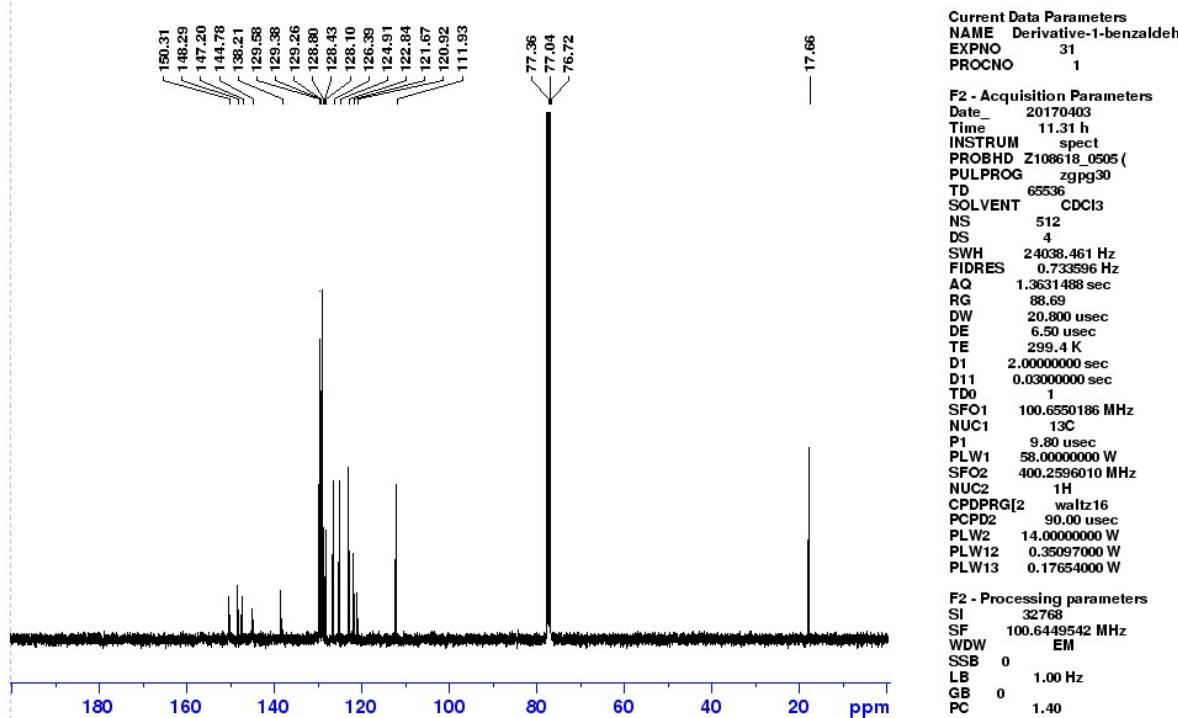


IR and HRMS of compound **6g**

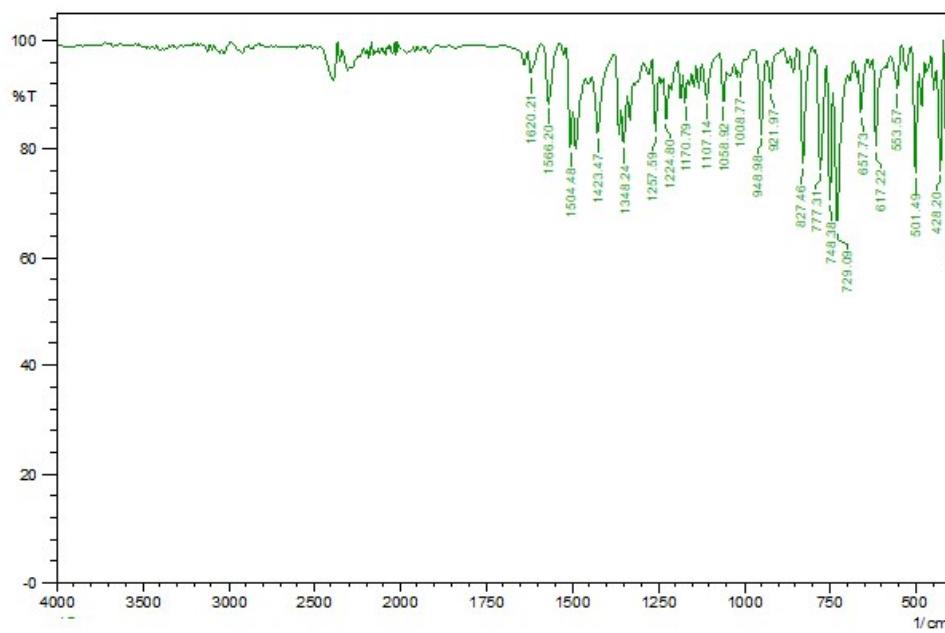
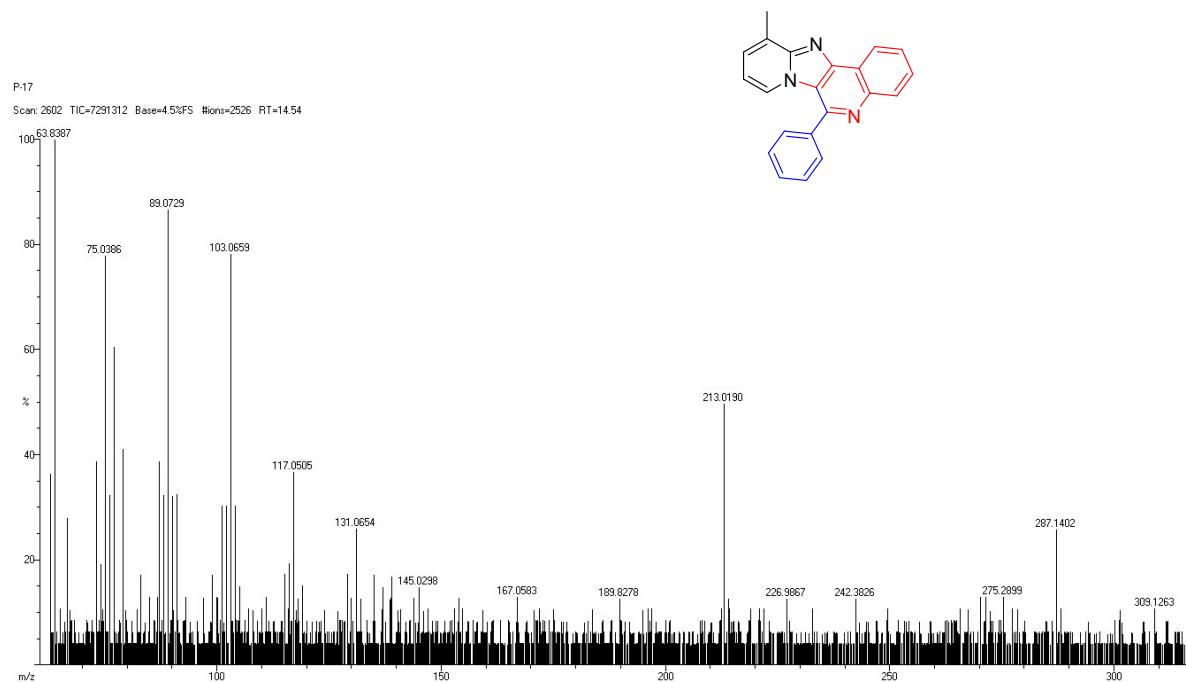
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NR-417-PCT-3



Signature SIF VIT VELLORE
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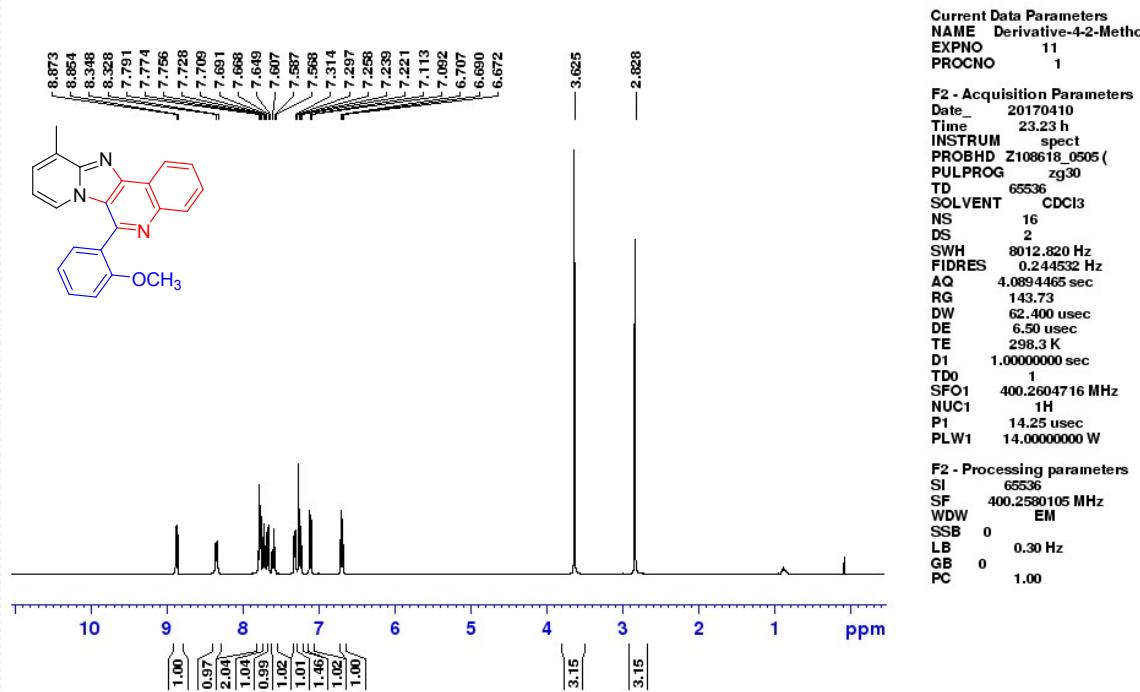


¹H-NMR and ¹³C-NMR of compound **6h** in CDCl₃.

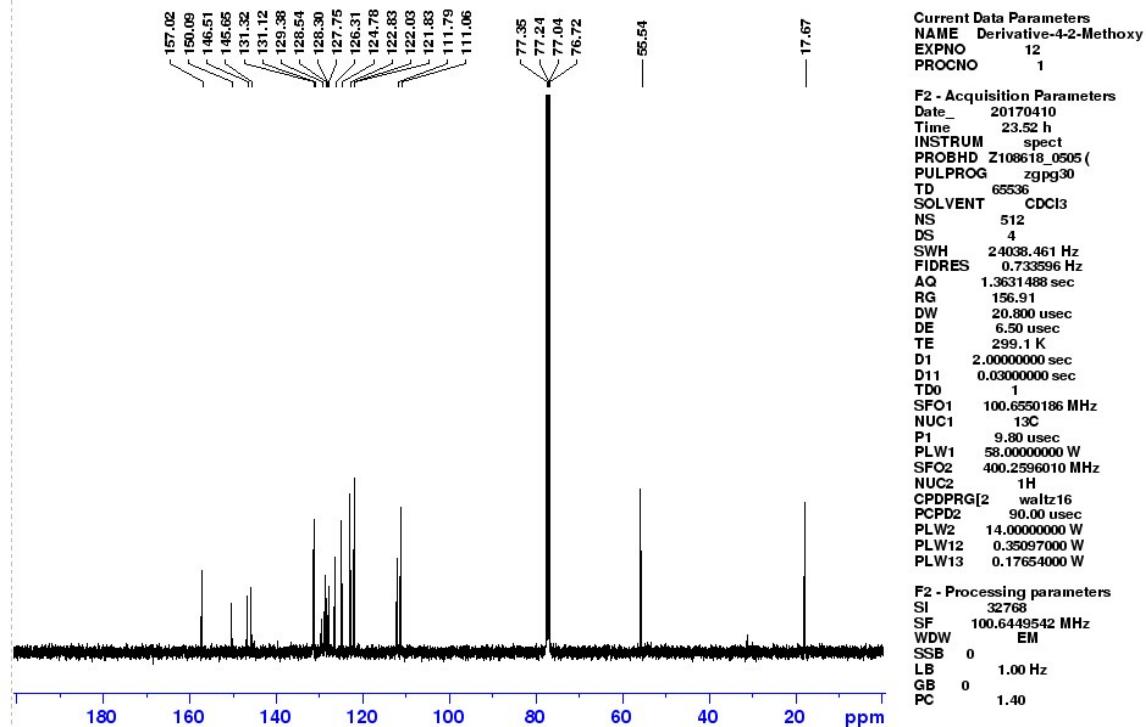


HRMS and IR of compound **6h**.

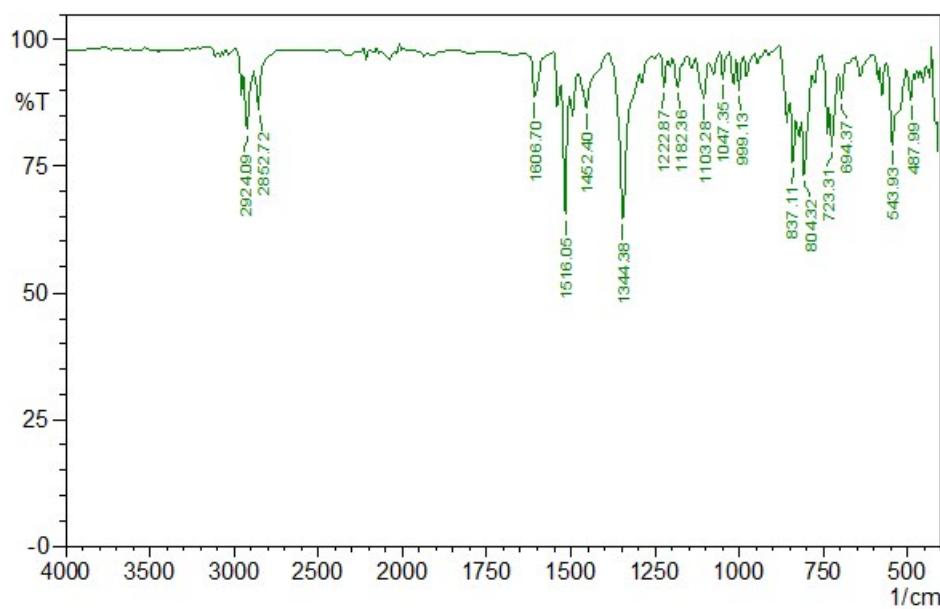
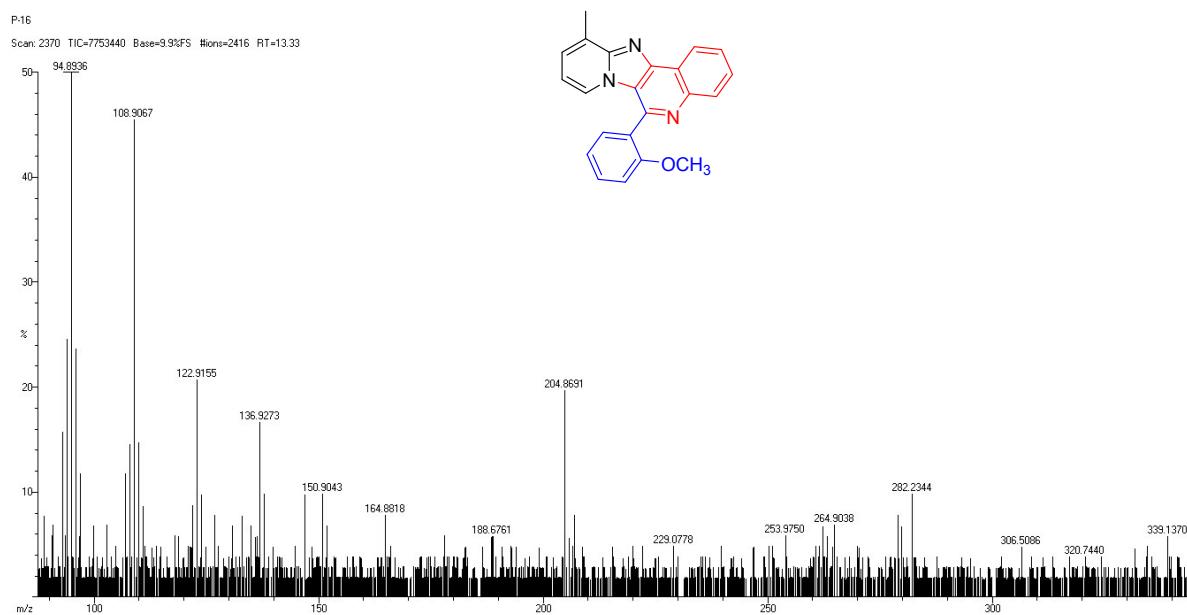
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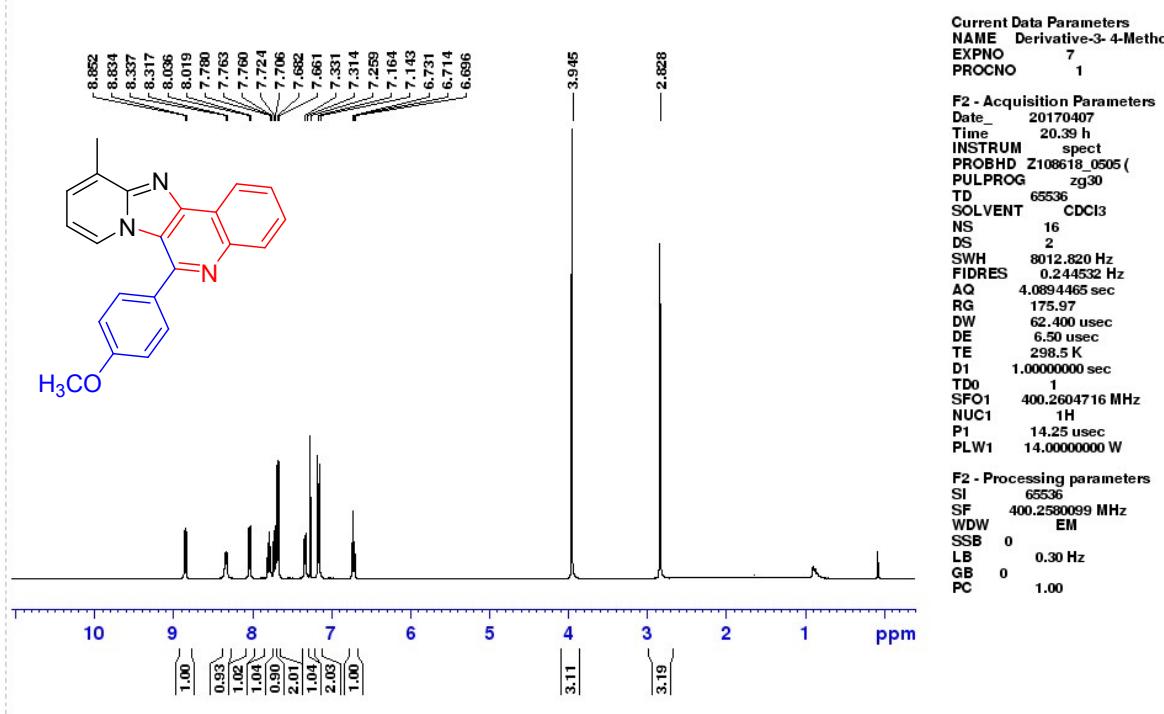


¹H-NMR and ¹³C-NMR of compound 6i in CDCl₃

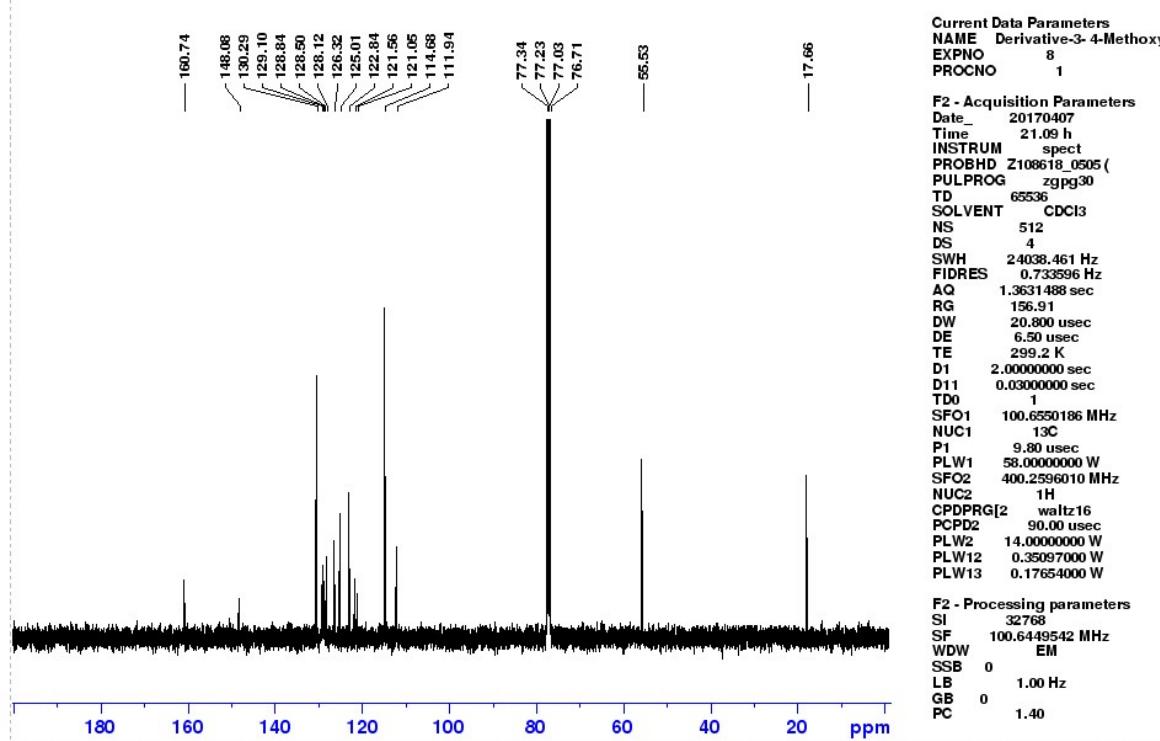


HRMS and IR of compound **6i**

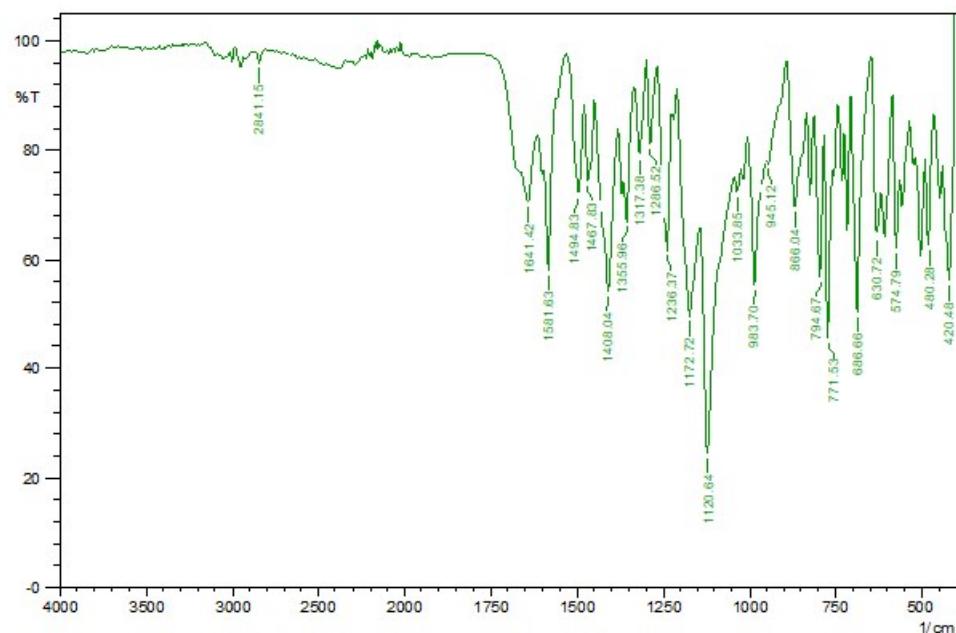
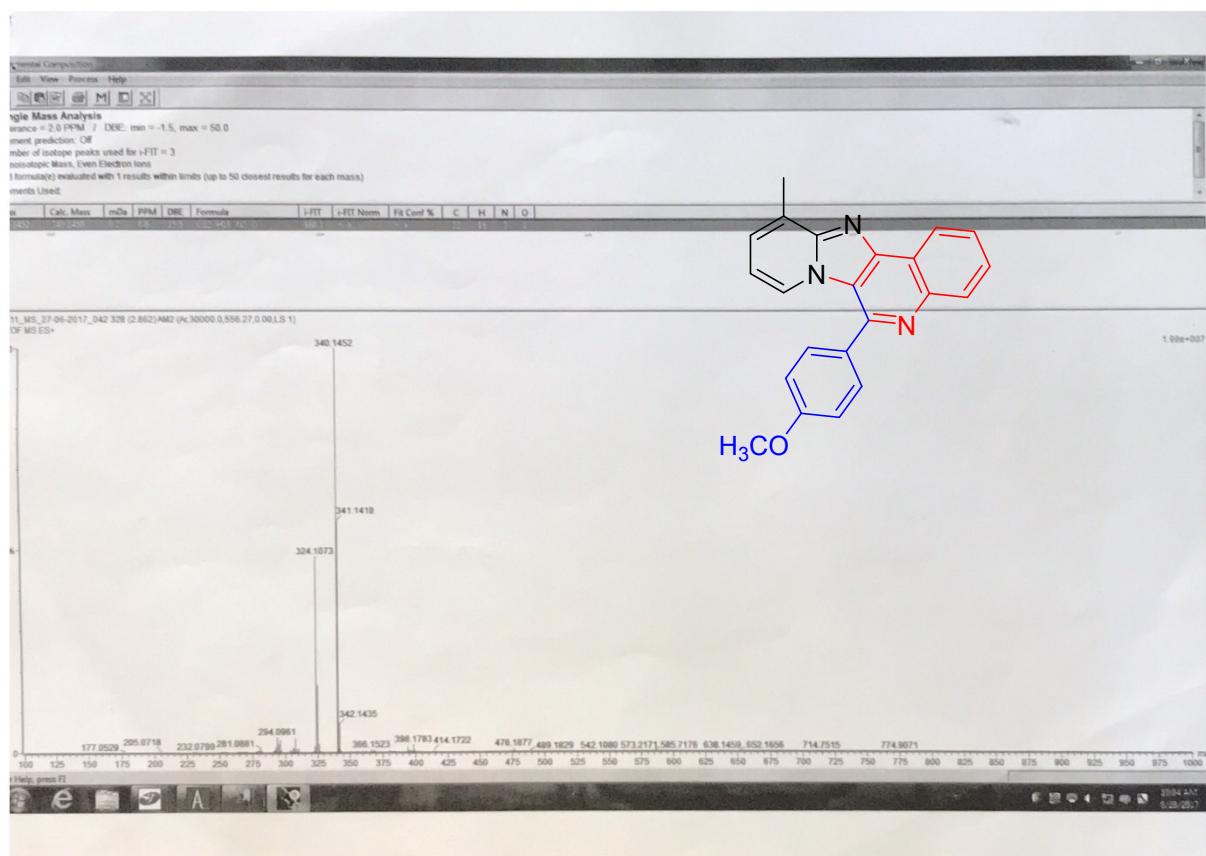
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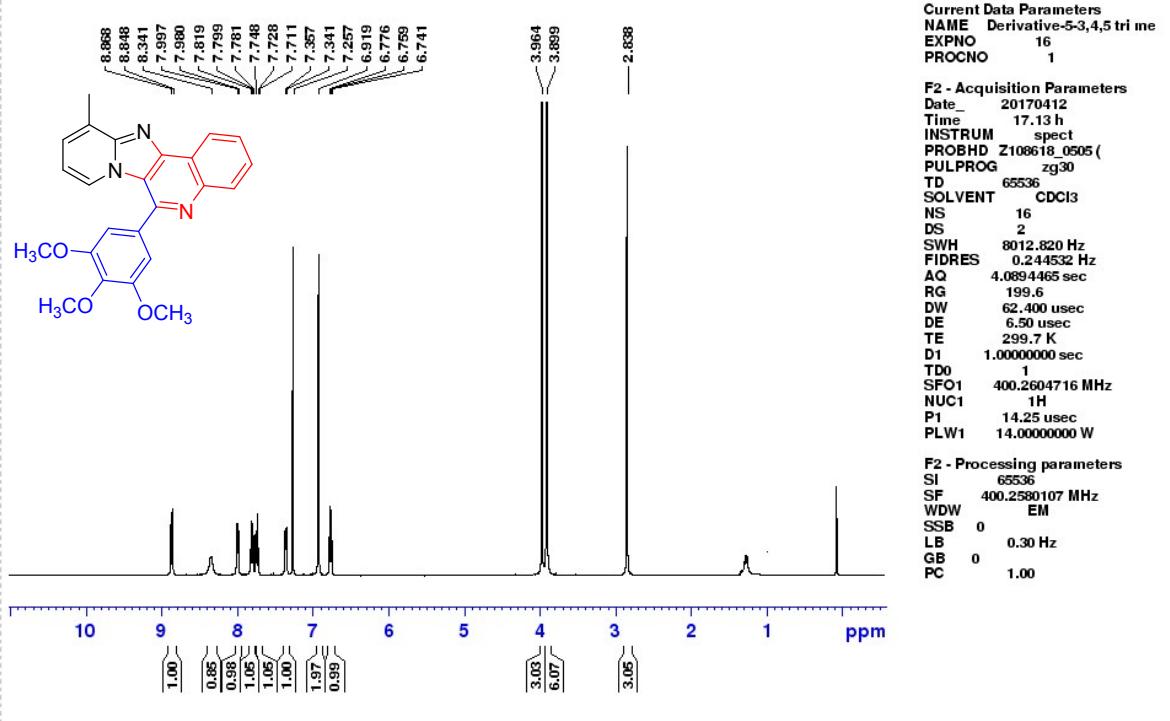


¹H-NMR and ¹³C-NMR of compound 6jin CDCl₃

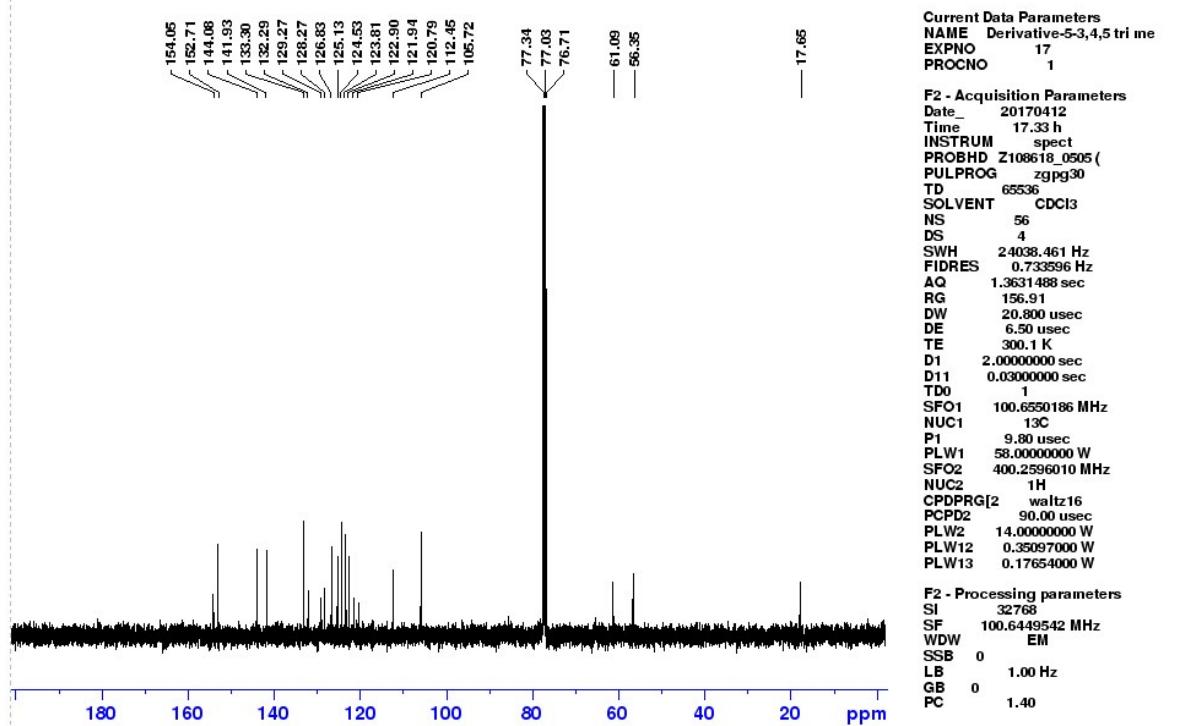


HRMS and IR of compound **6j**.

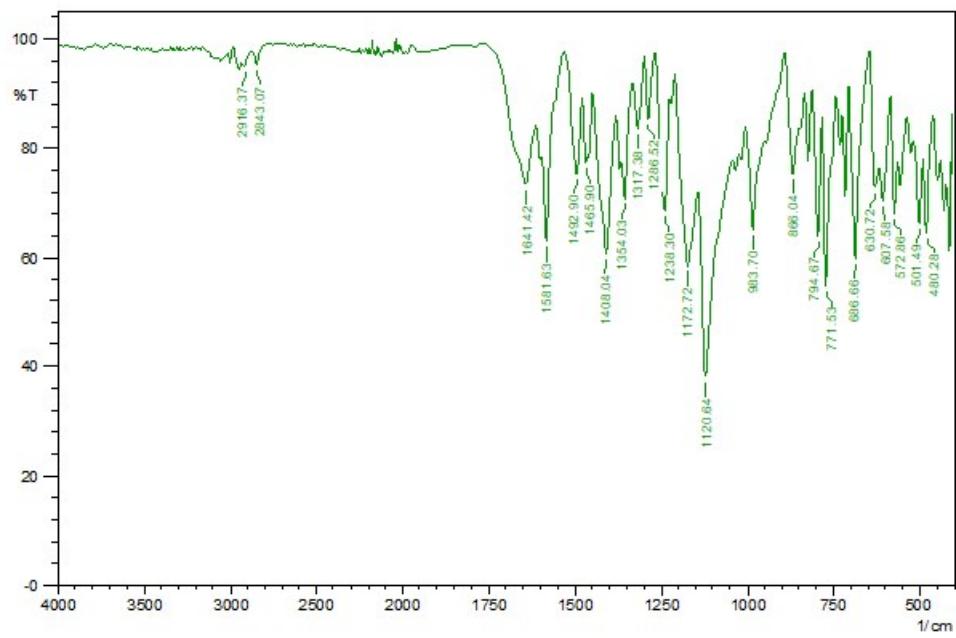
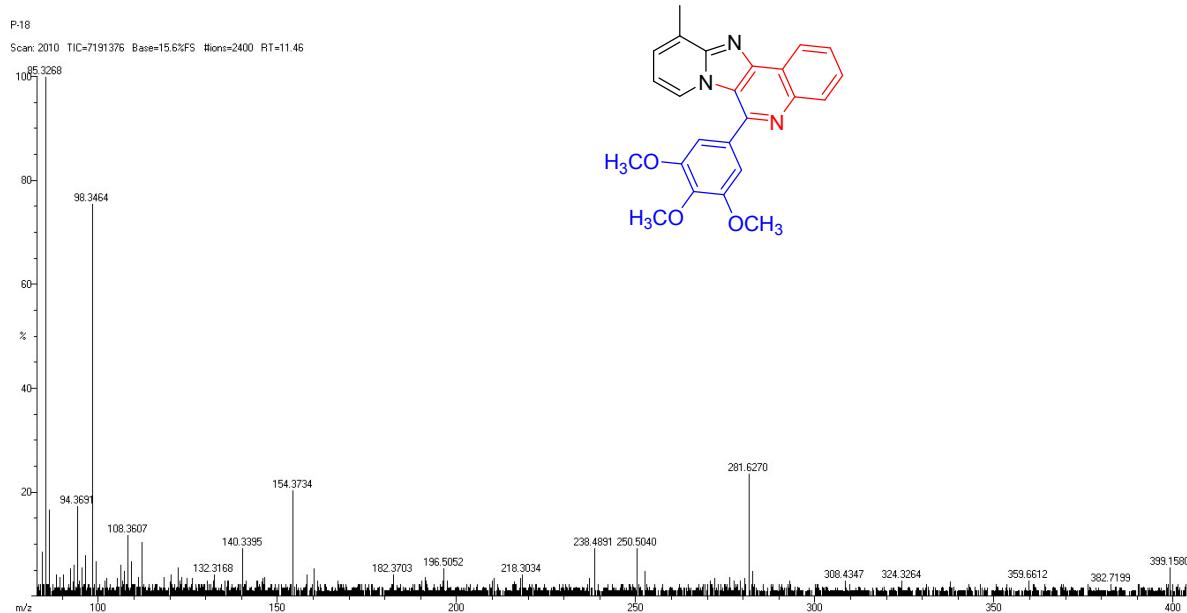
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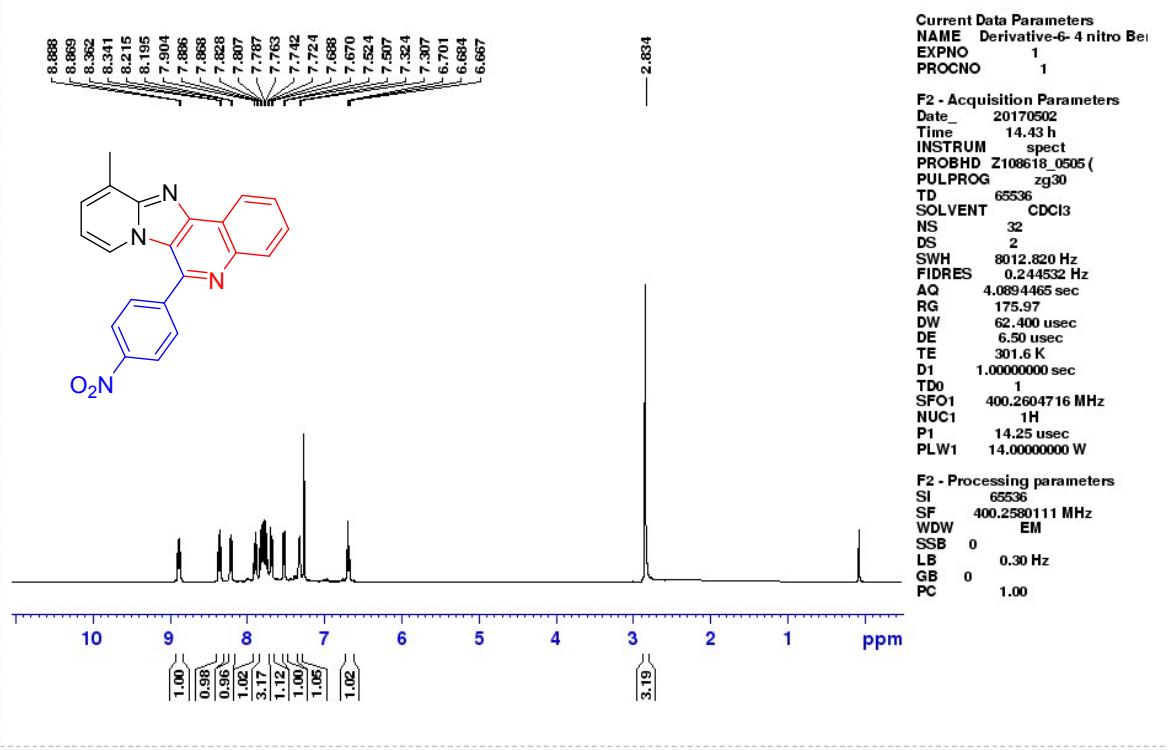


¹H-NMR and ¹³C-NMR of compound 6k in CDCl₃

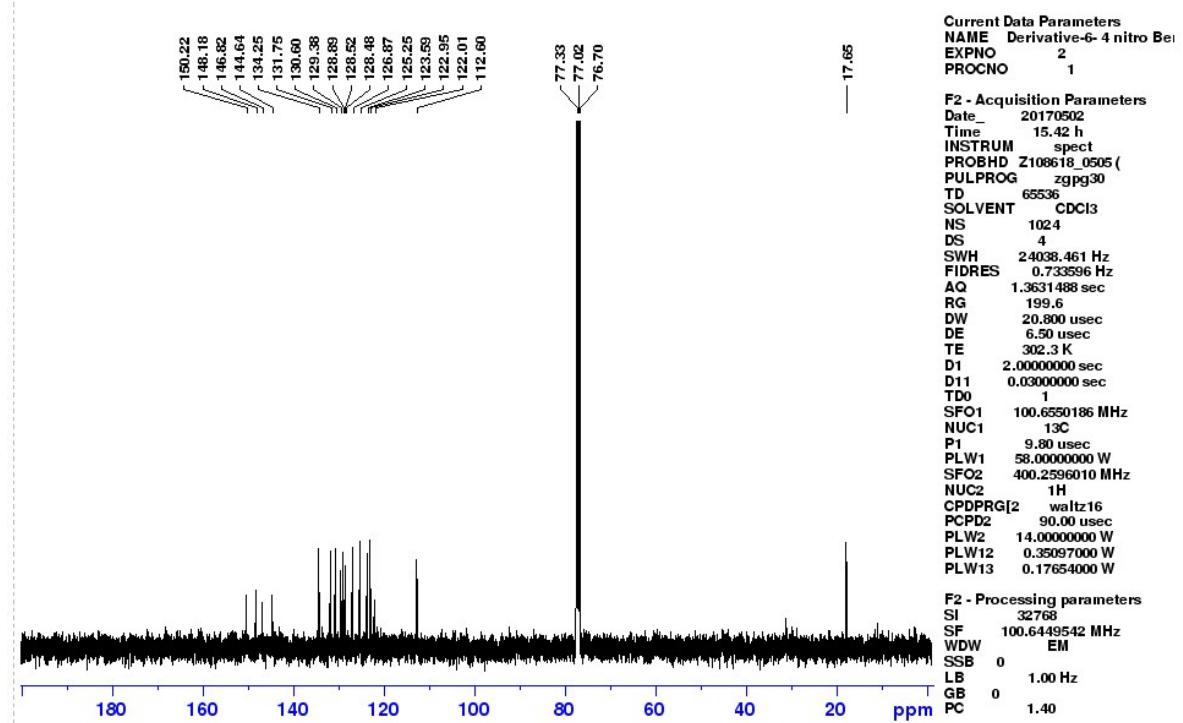


HRMS and IR of compound **6k**

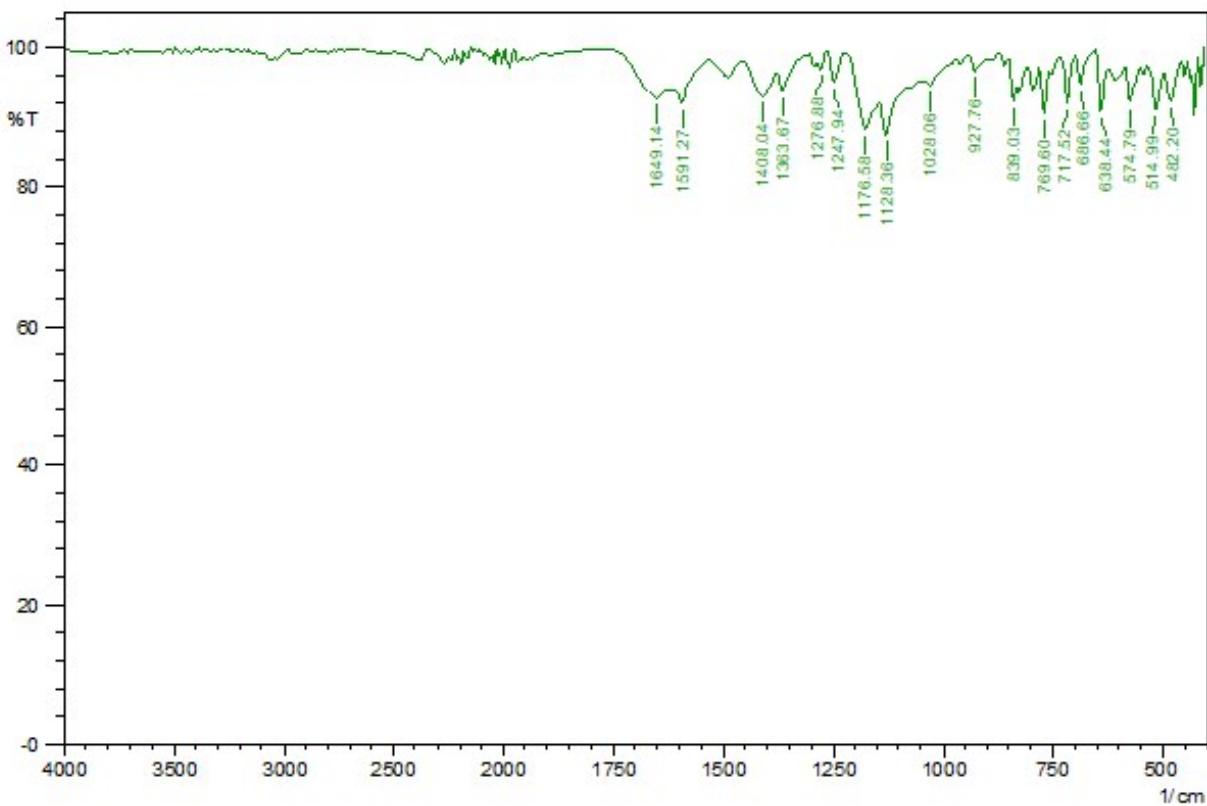
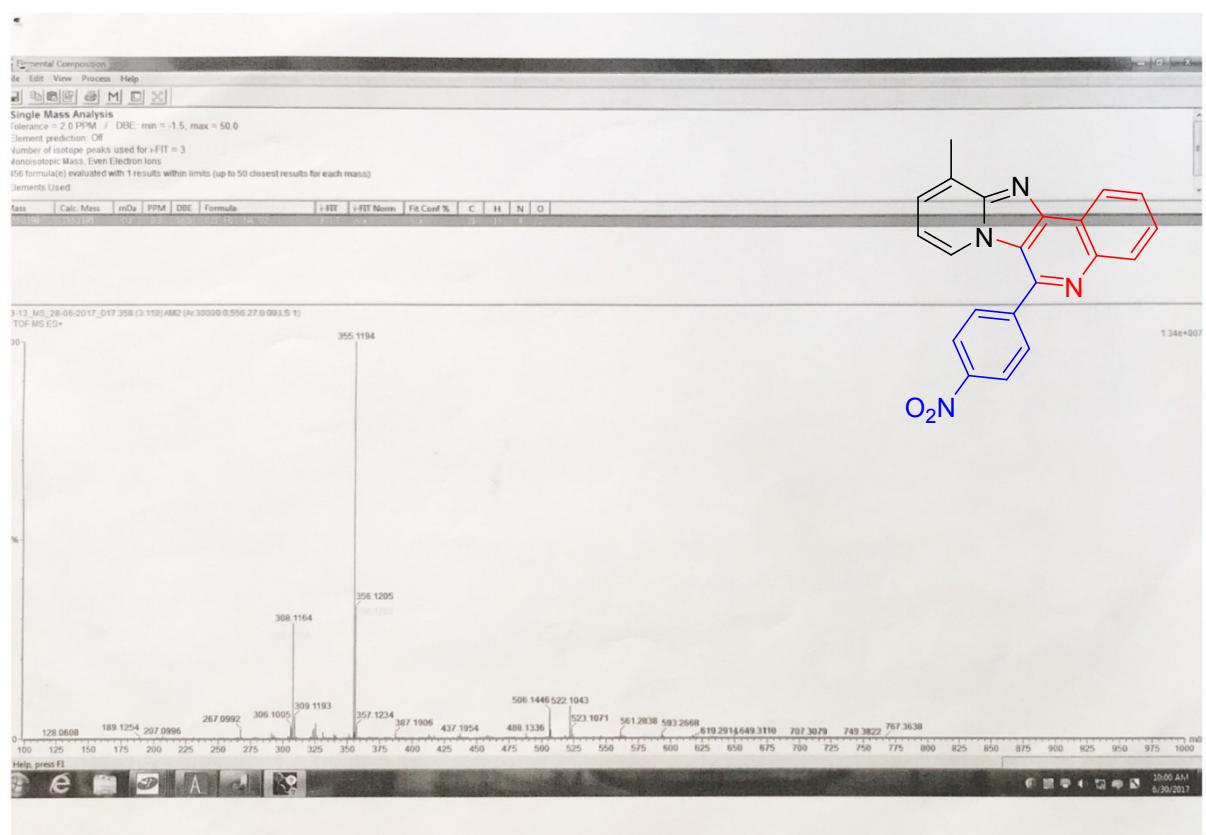
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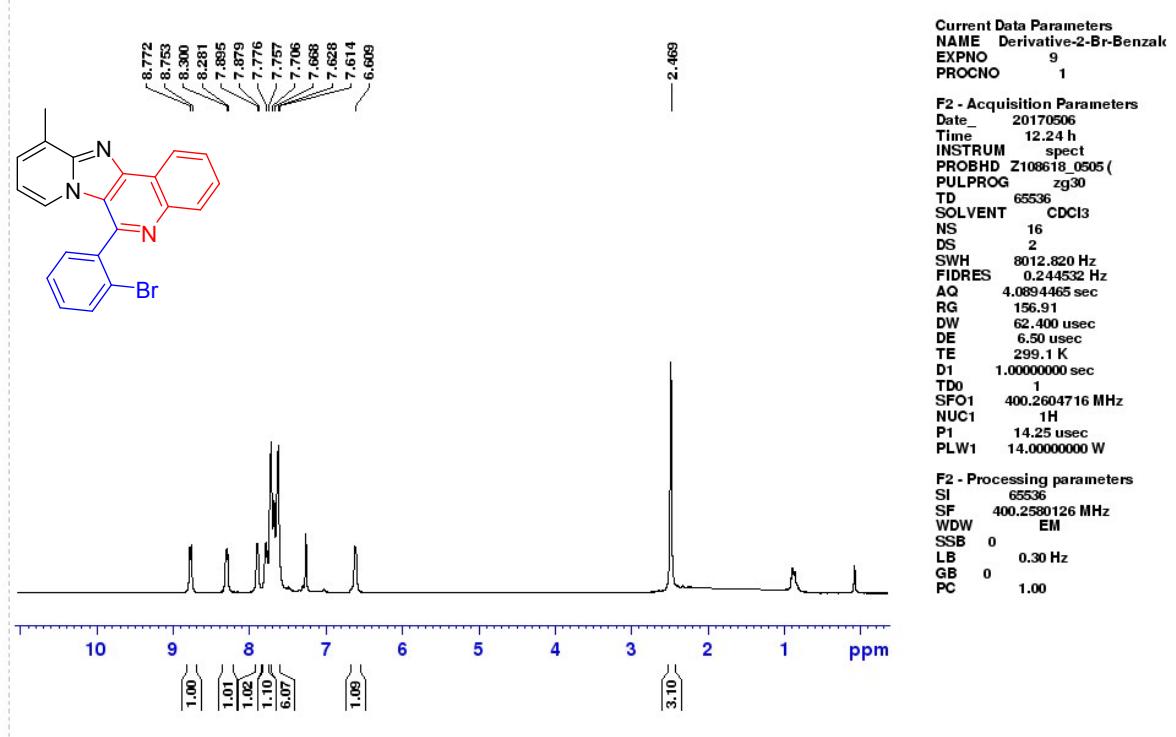


¹H-NMR and ¹³C-NMR of compound 6I in CDCl₃

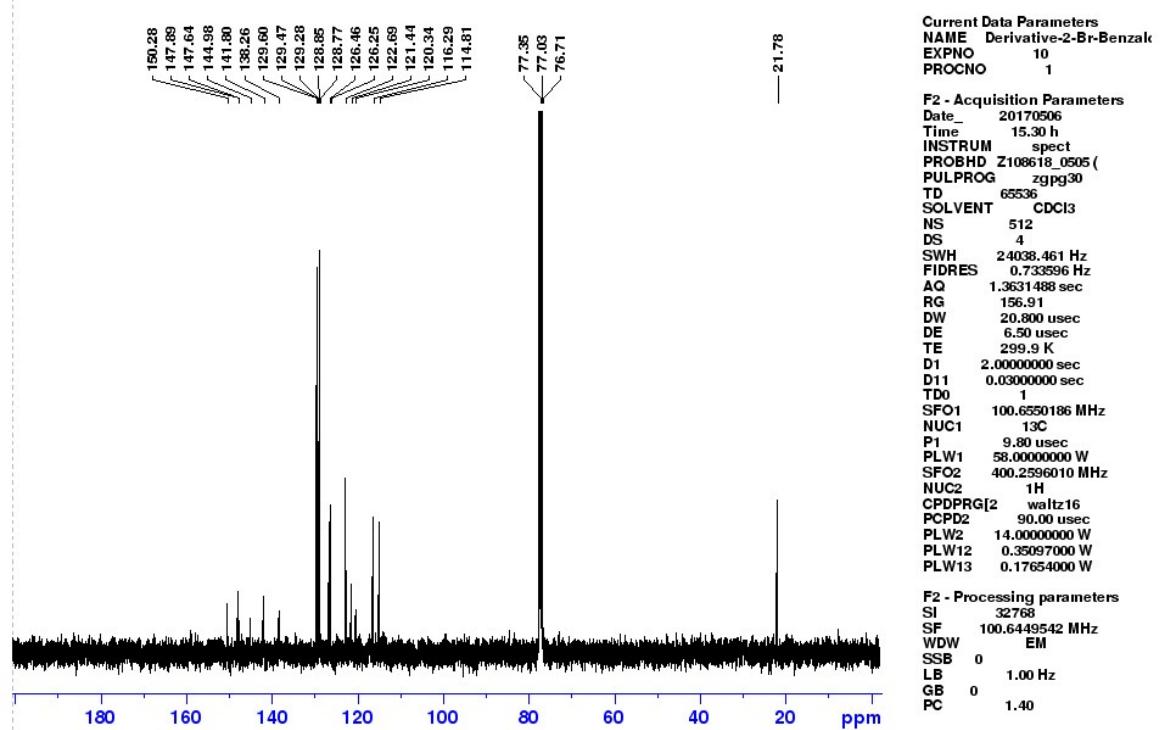


HRMS and IR of compound **61**

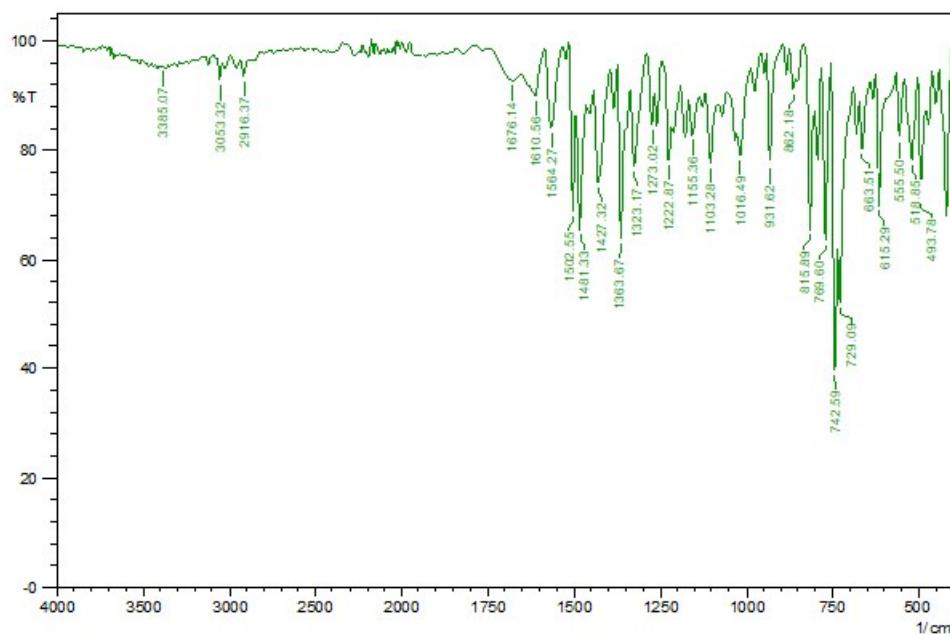
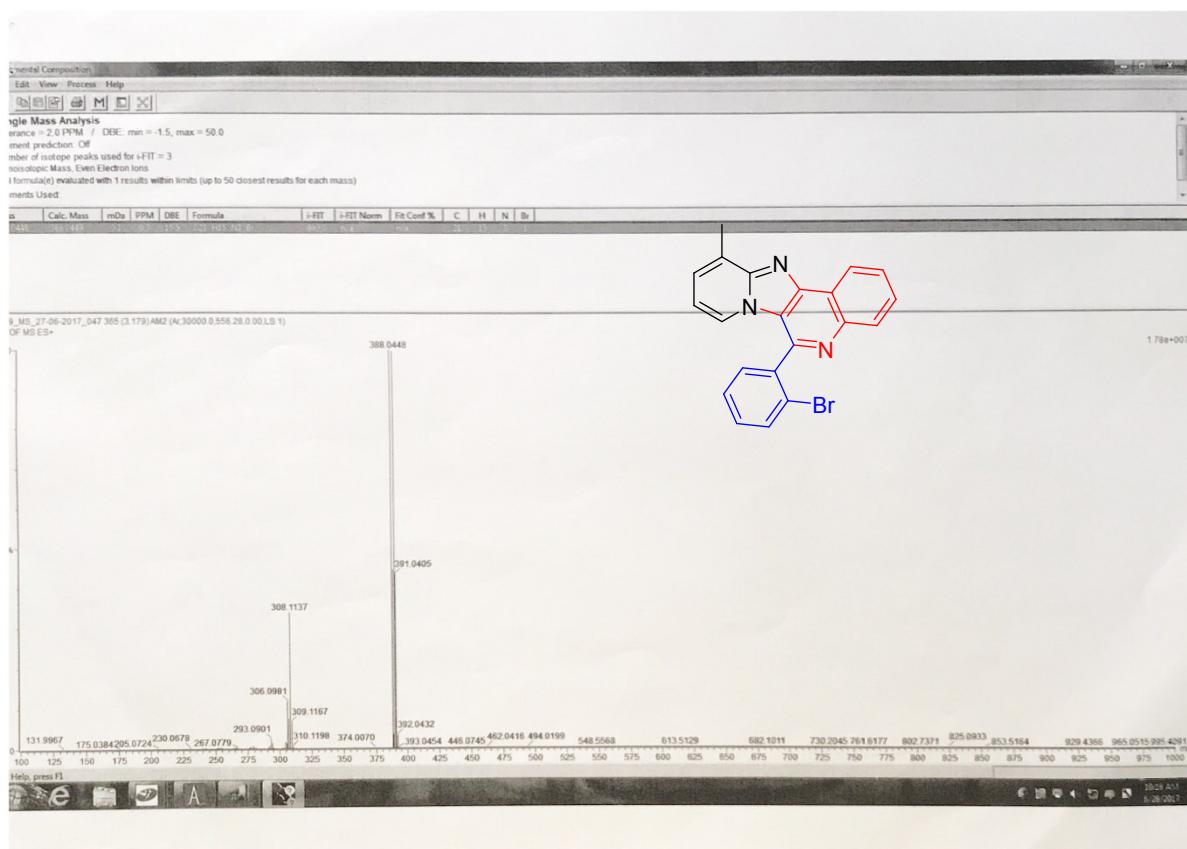
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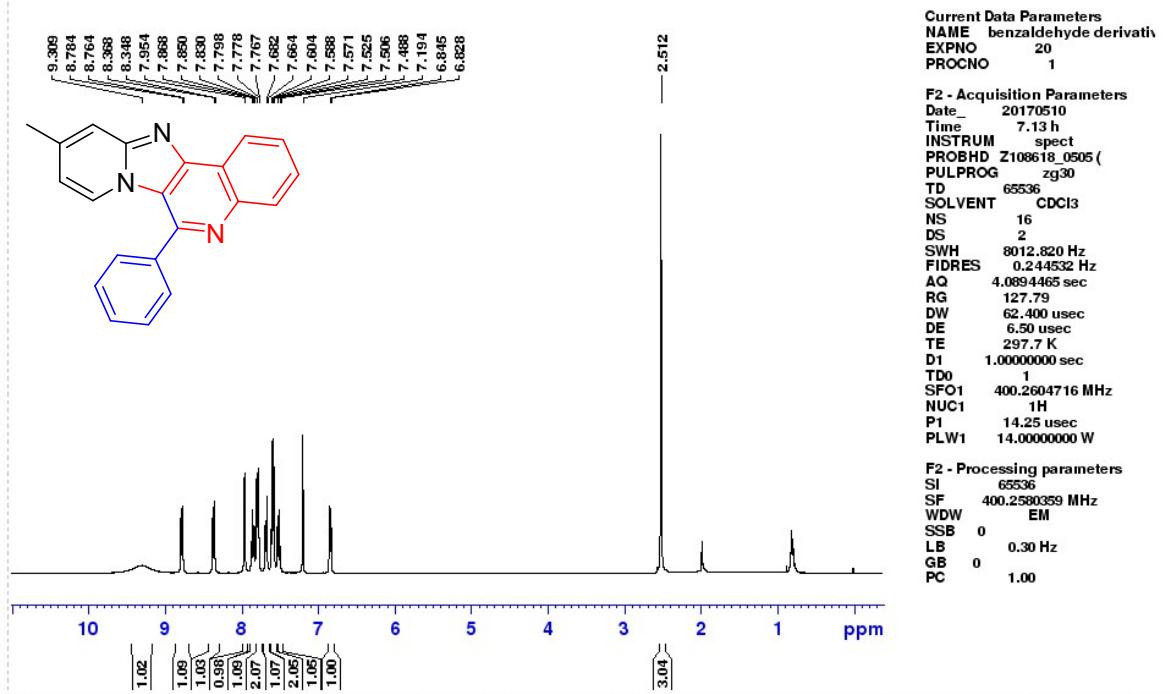


¹H-NMR and ¹³C-NMR of compound **6m** in CDCl₃.

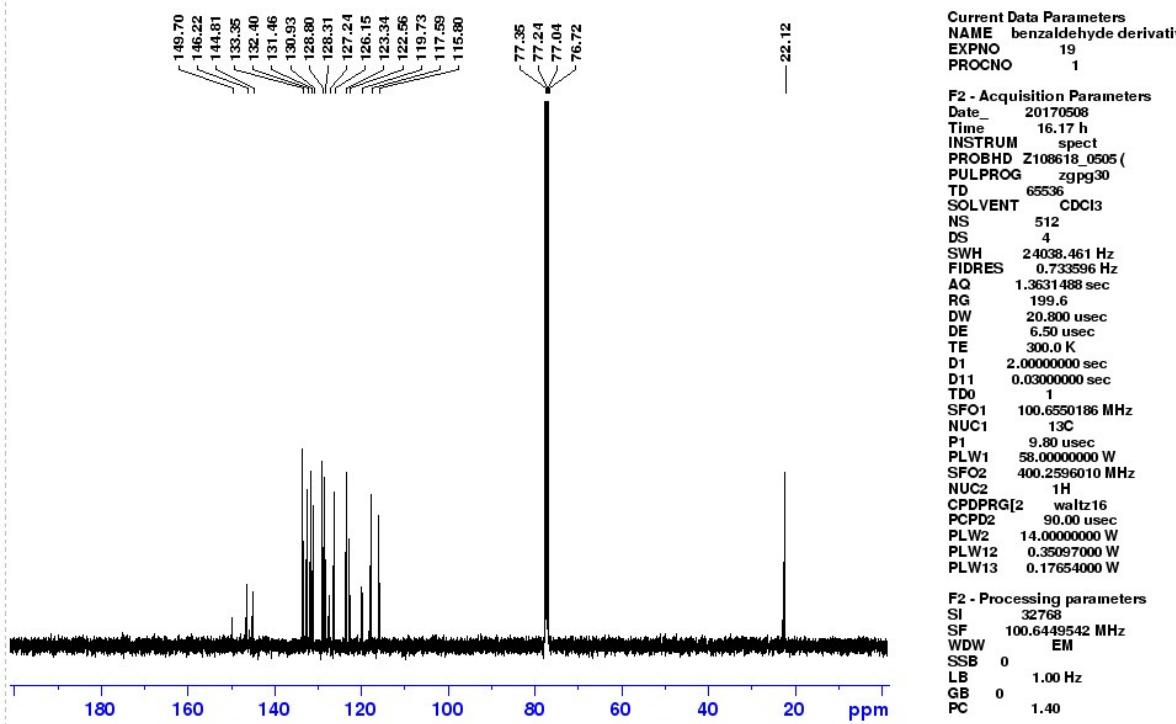


HRMS and IR of compound **6m**.

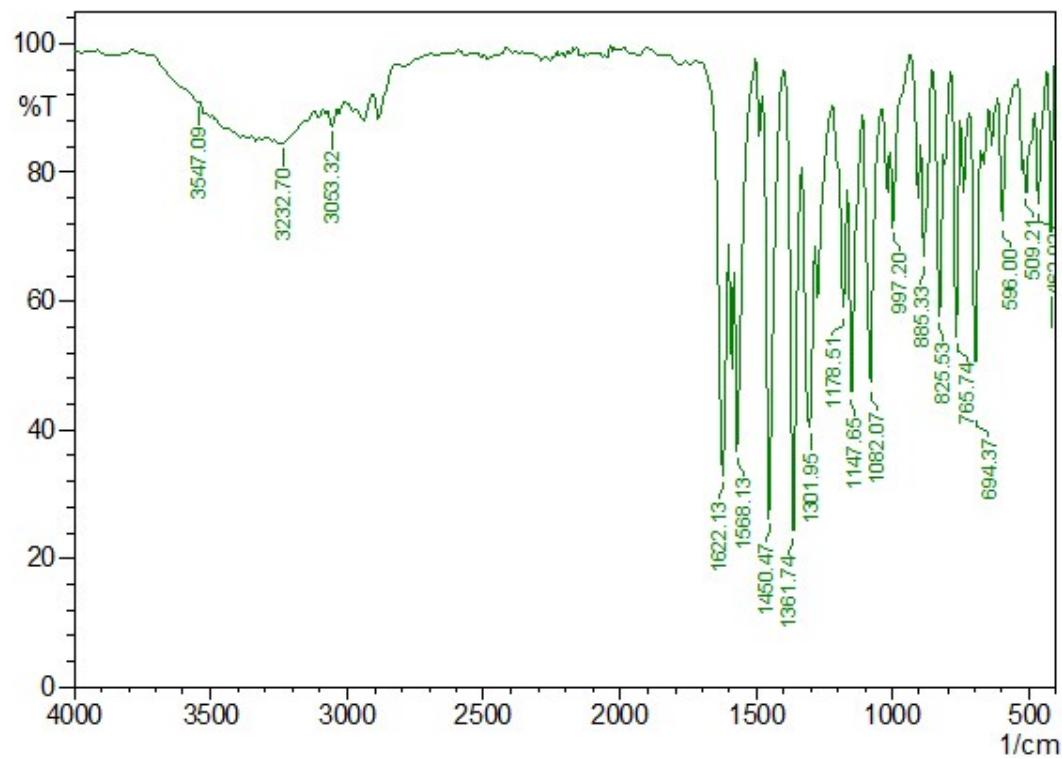
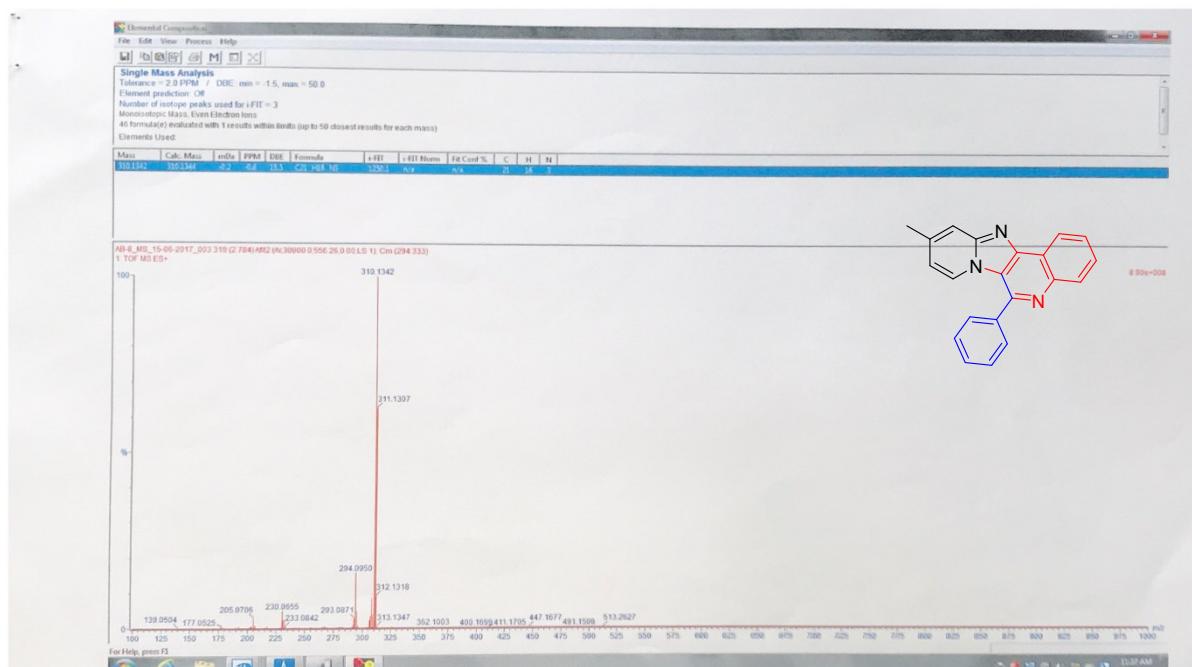
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Signature SIF VIT VELLORE
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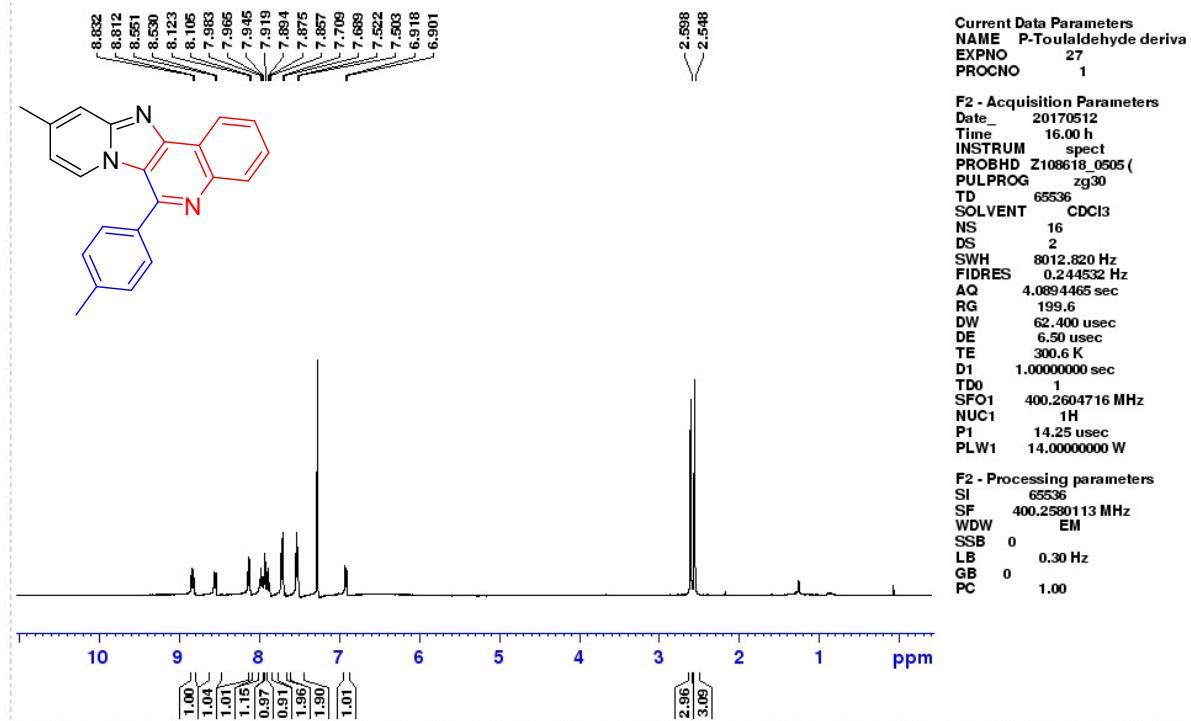


¹H-NMR and ¹³C-NMR of compound **6n** in CDCl₃.

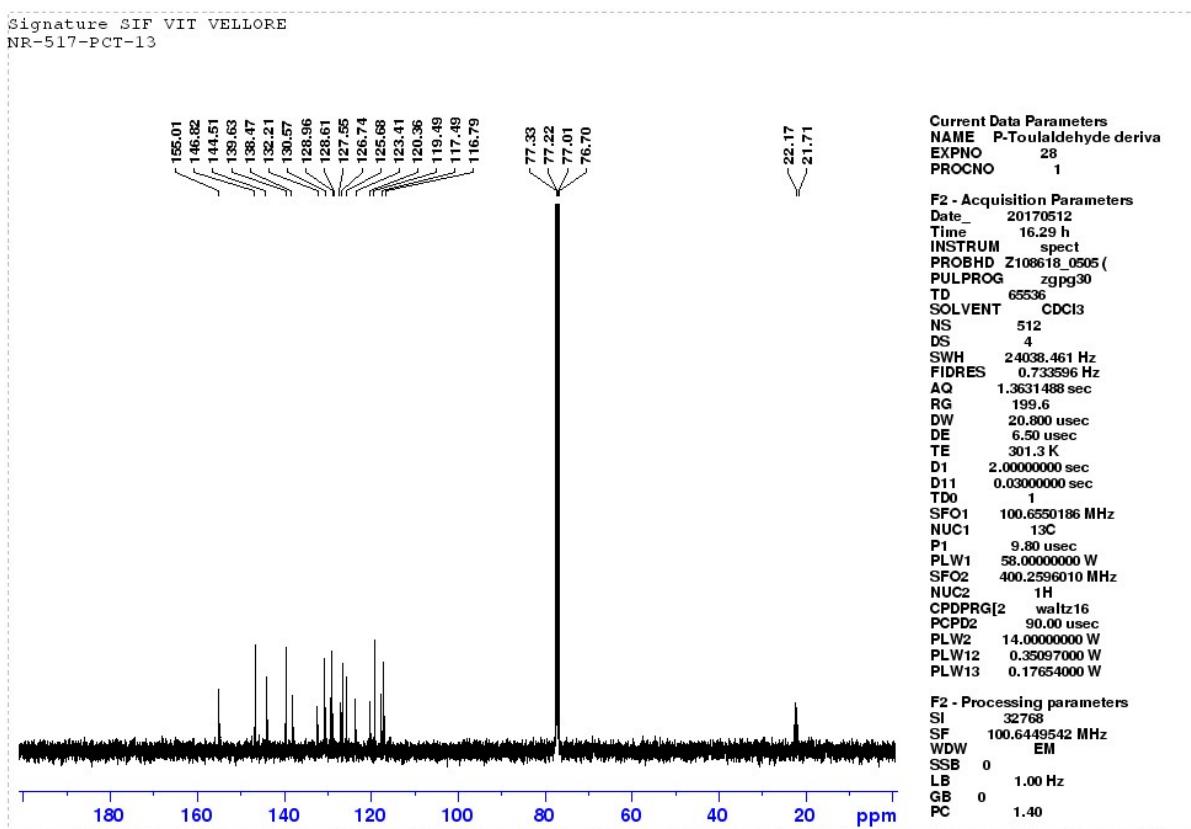


HRMS and IR of compound **6n**.

Signature SIF VIT VELLORE
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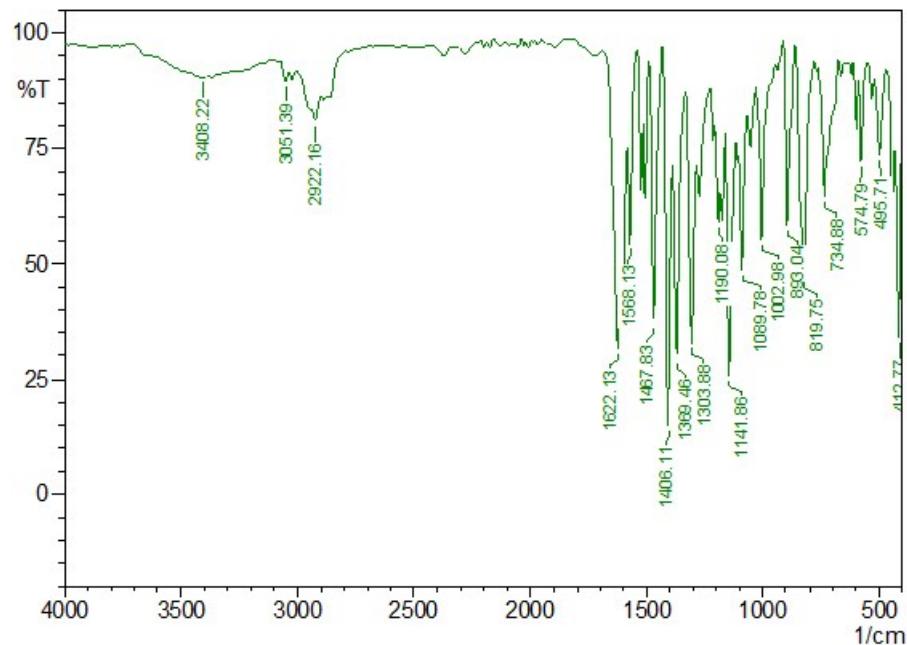
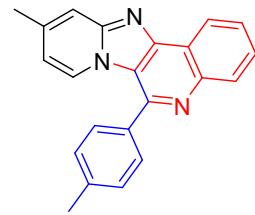
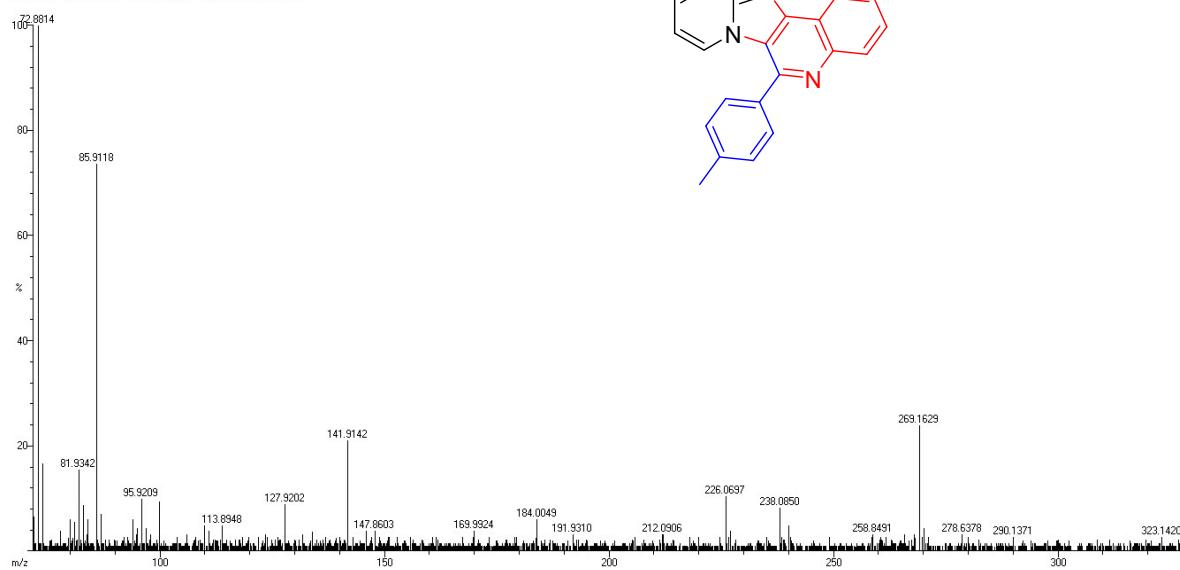


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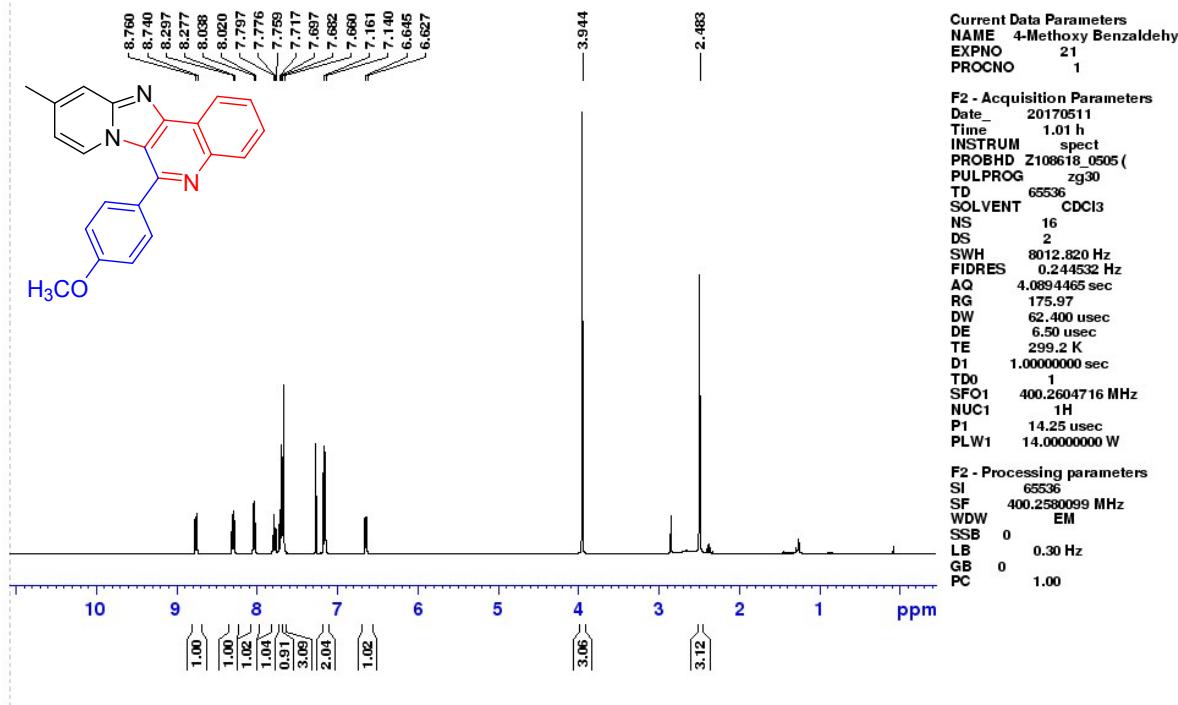
¹H-NMR and ¹³C-NMR of compound **6o** in CDCl₃.

P-19
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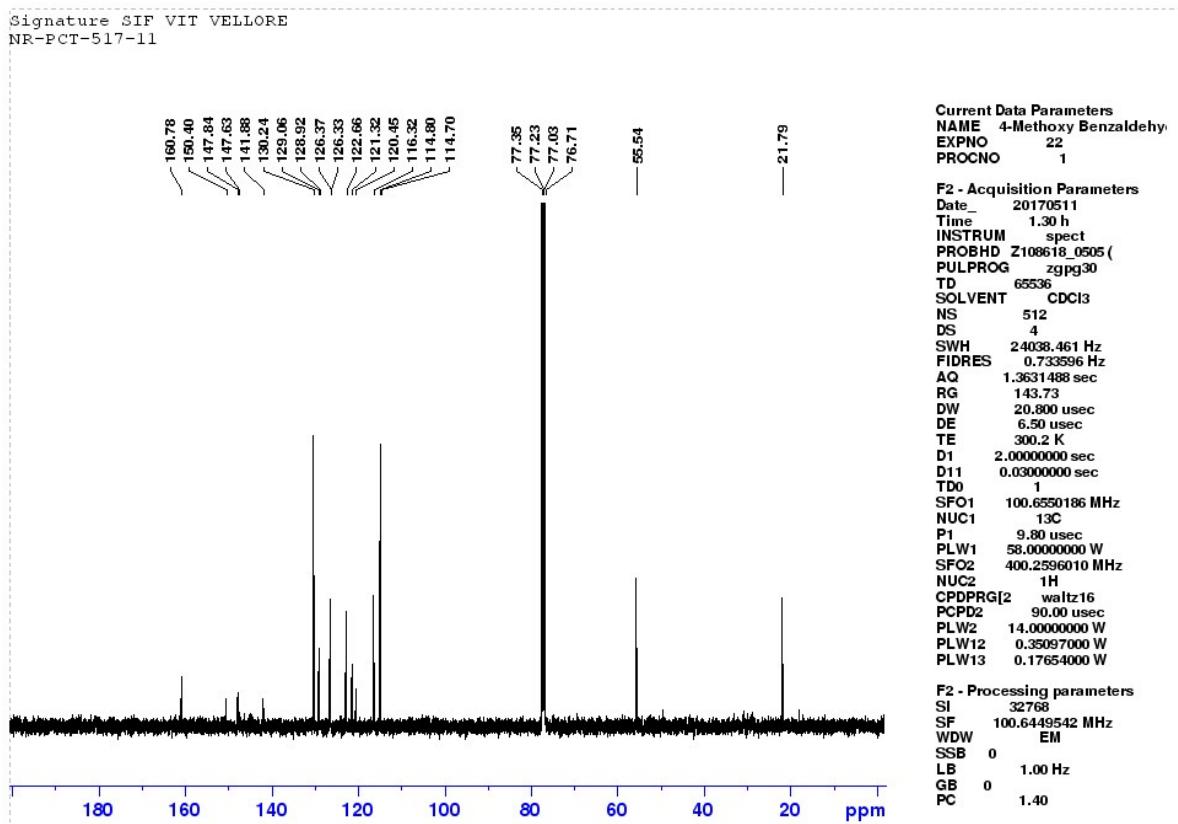


HRMS and IR of compound **6o**.

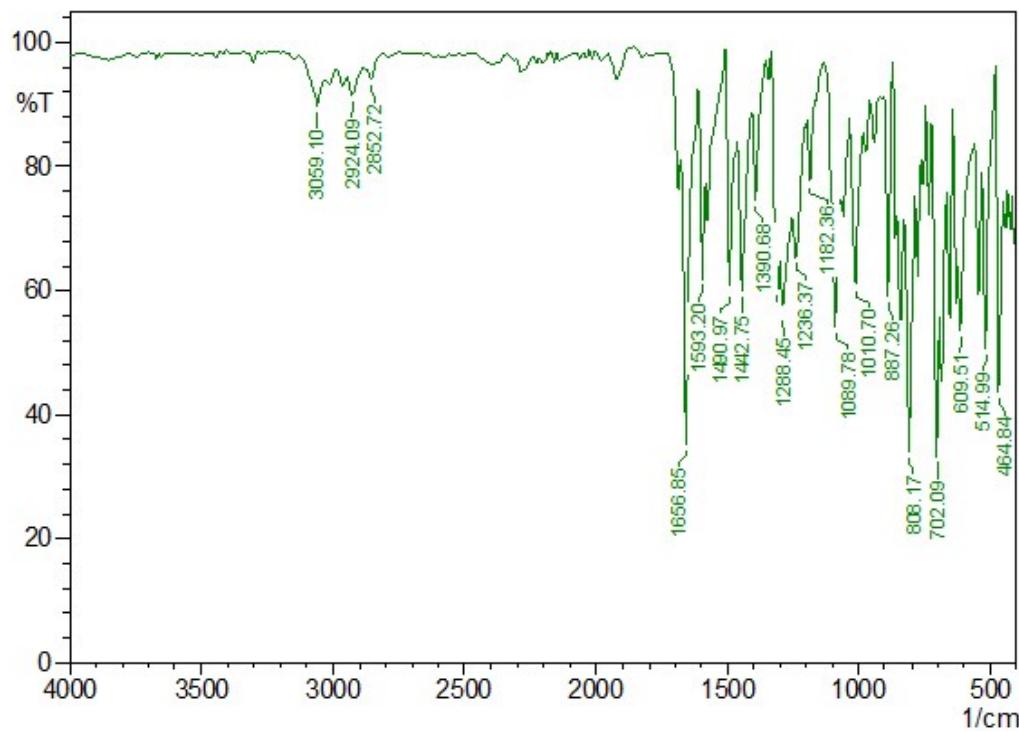
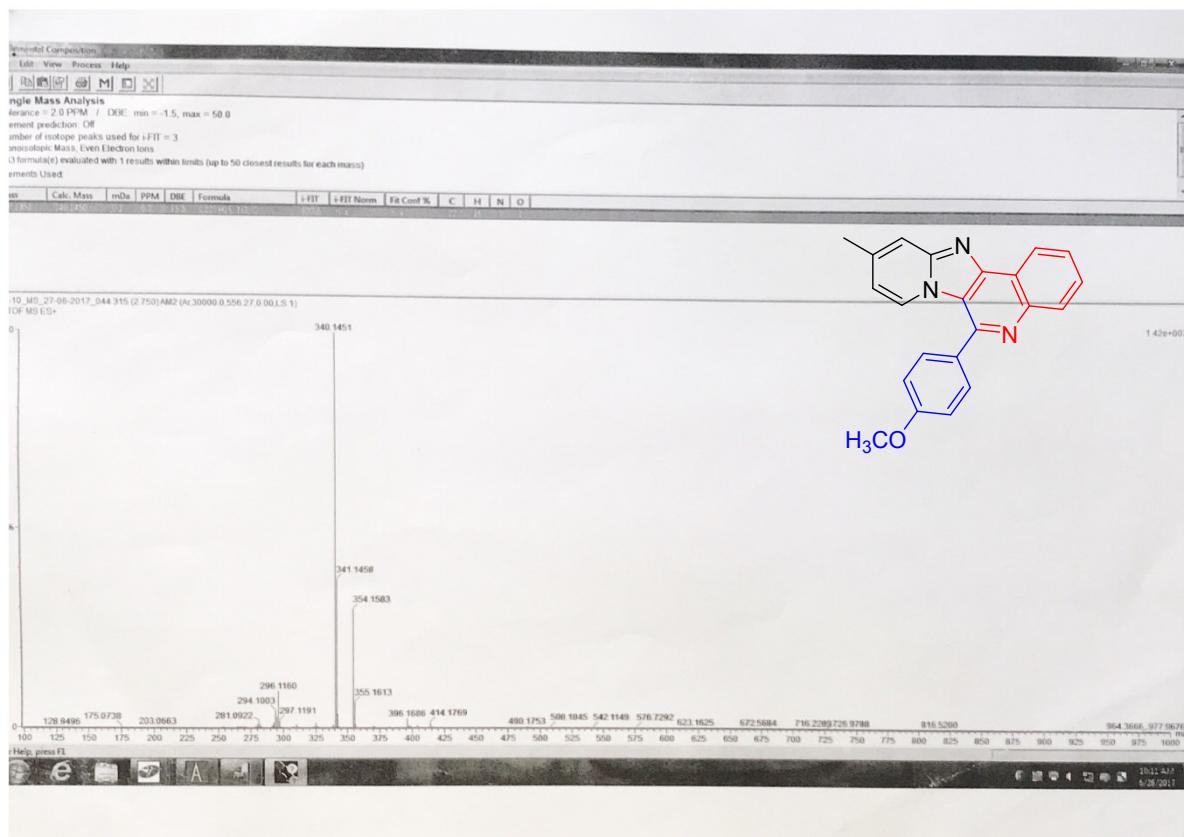
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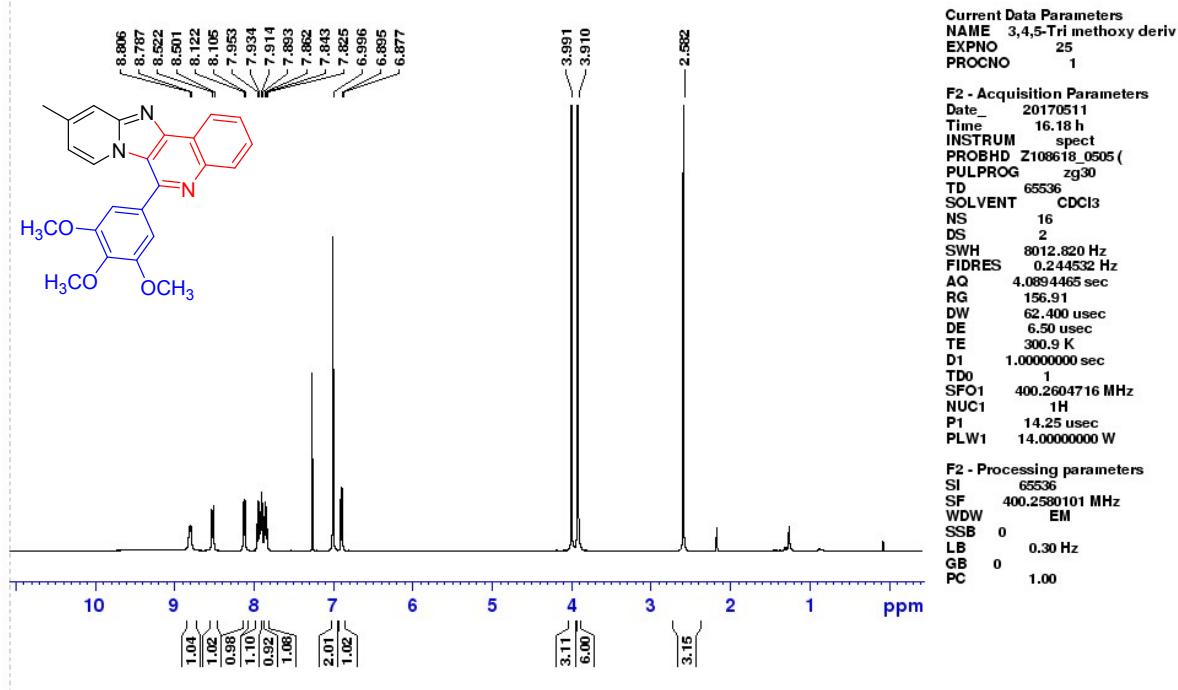


¹H-NMR and ¹³C-NMR of compound 6p in CDCl₃.

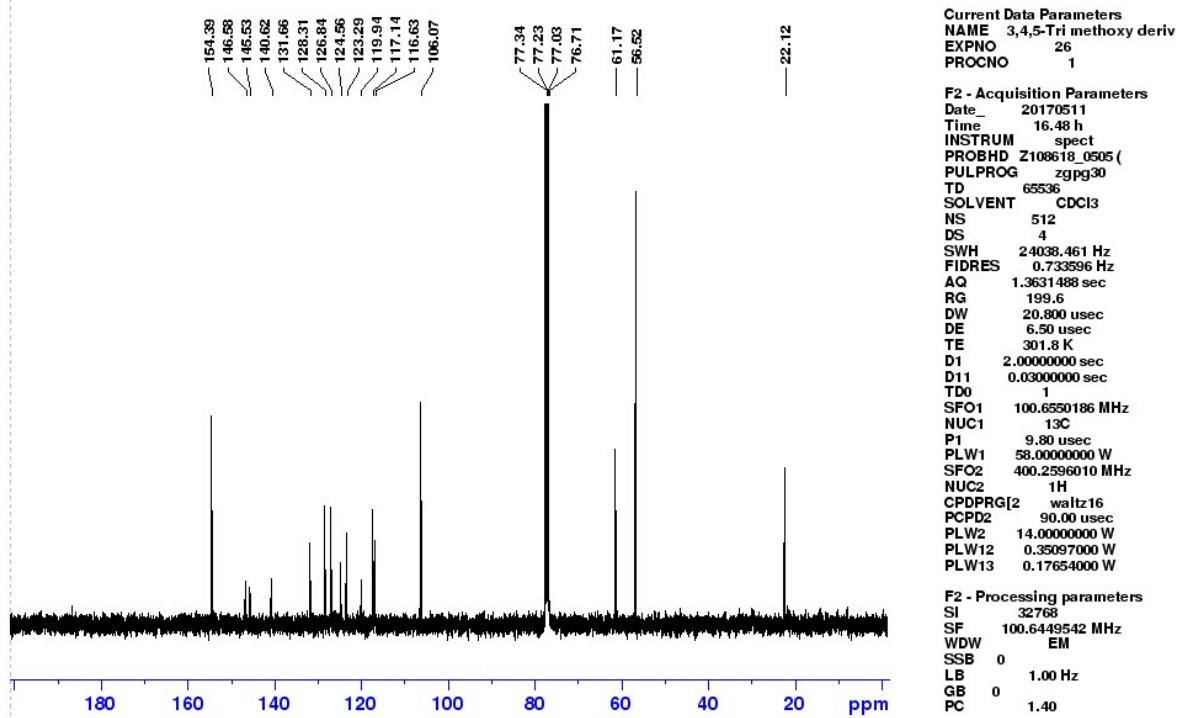


HRMS and IR of compound **6p**.

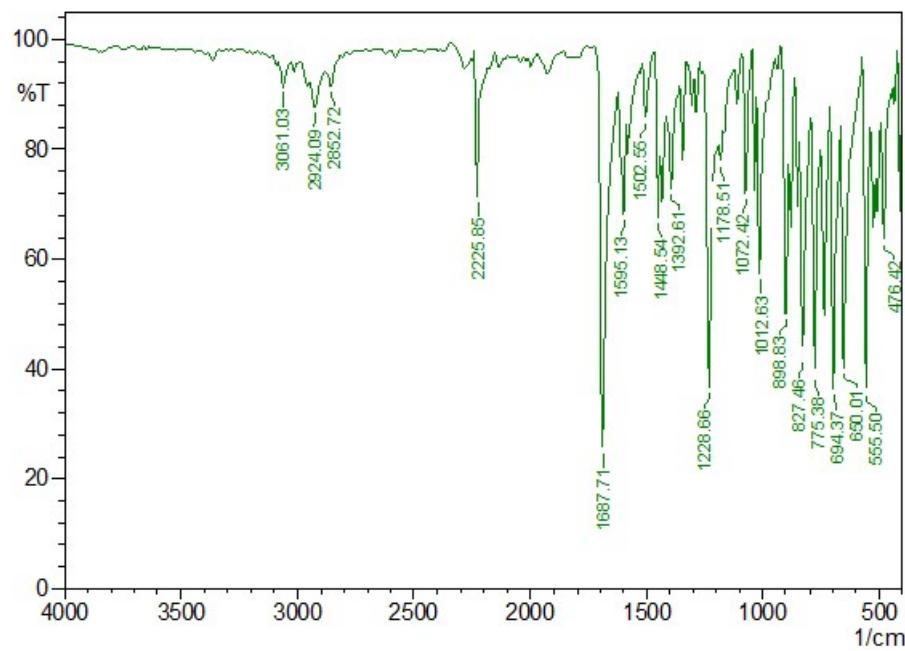
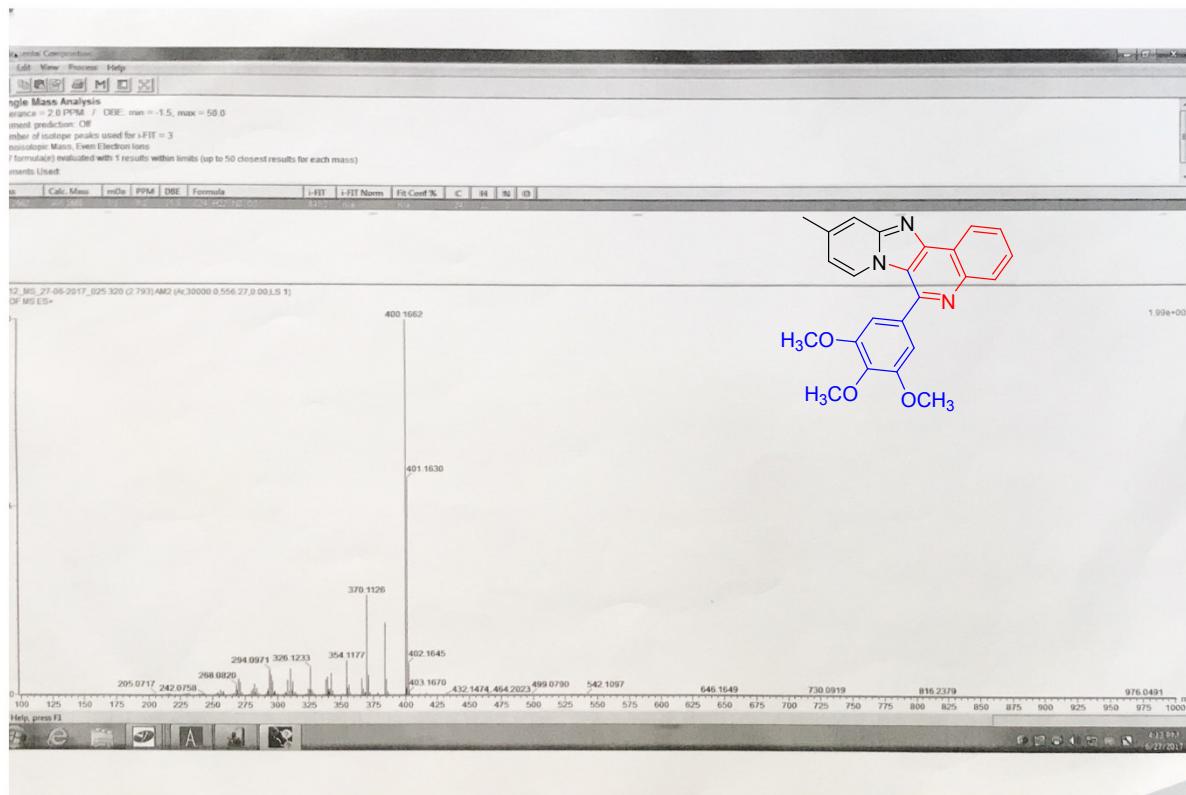
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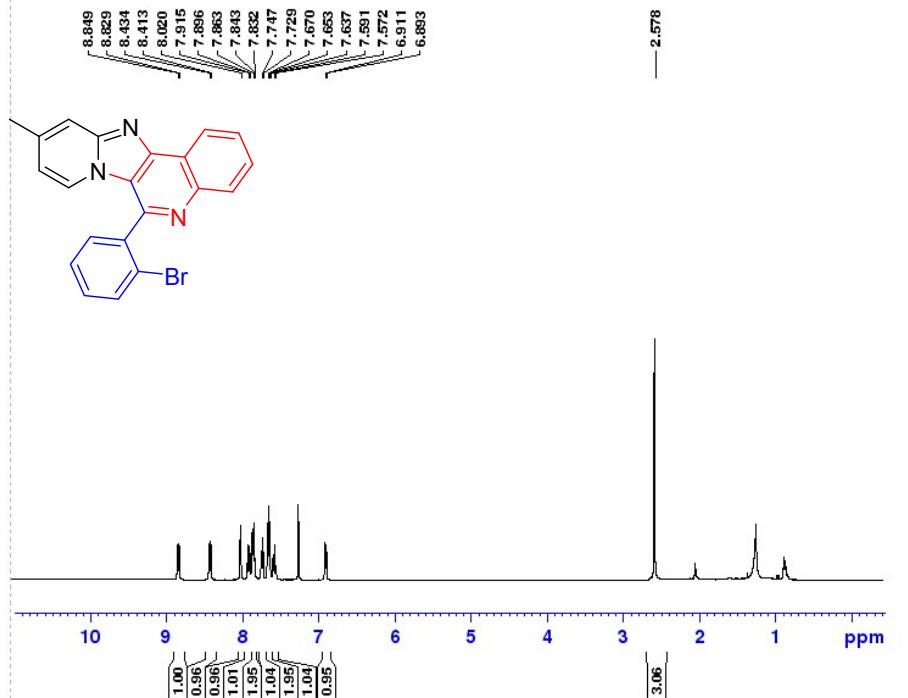


¹H-NMR and ¹³C-NMR of compound 6q in CDCl₃.



HRMS and IR of compound **6q**.

Signature SIF VIT VELLORE
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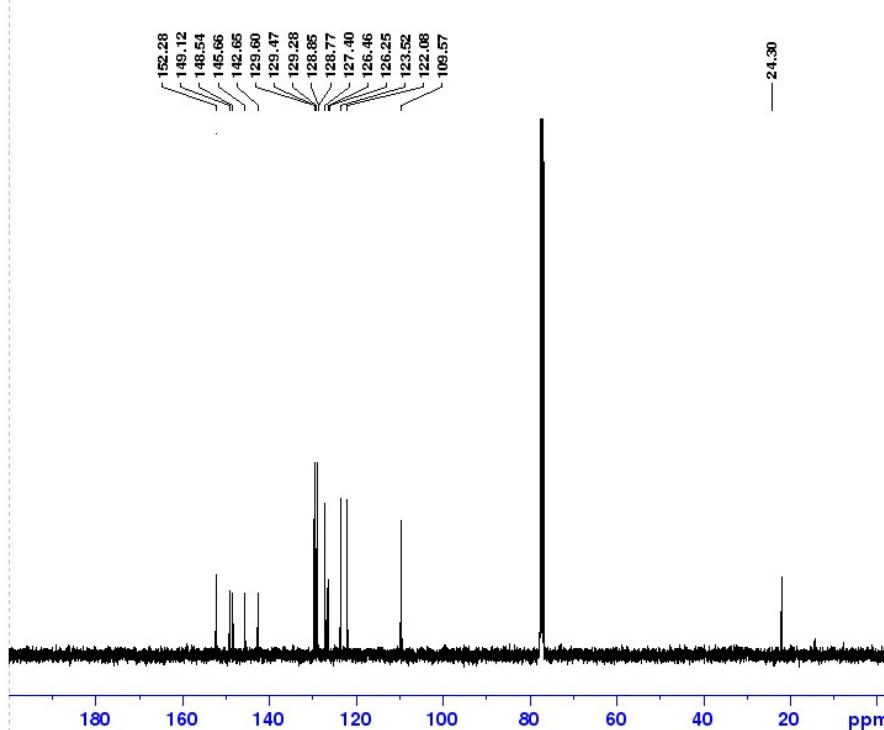


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EXPNO 20
PROCNO 1

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TD 65536
SOLVENT CDCl3
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DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 127.79
DW 62.400 usec
DE 6.50 usec
TE 297.7 K
D1 1.0000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 14.25 usec
PLW1 14.0000000 W

F2 - Processing parameters
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SF 400.2580097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Signature SIF VIT VELLORE

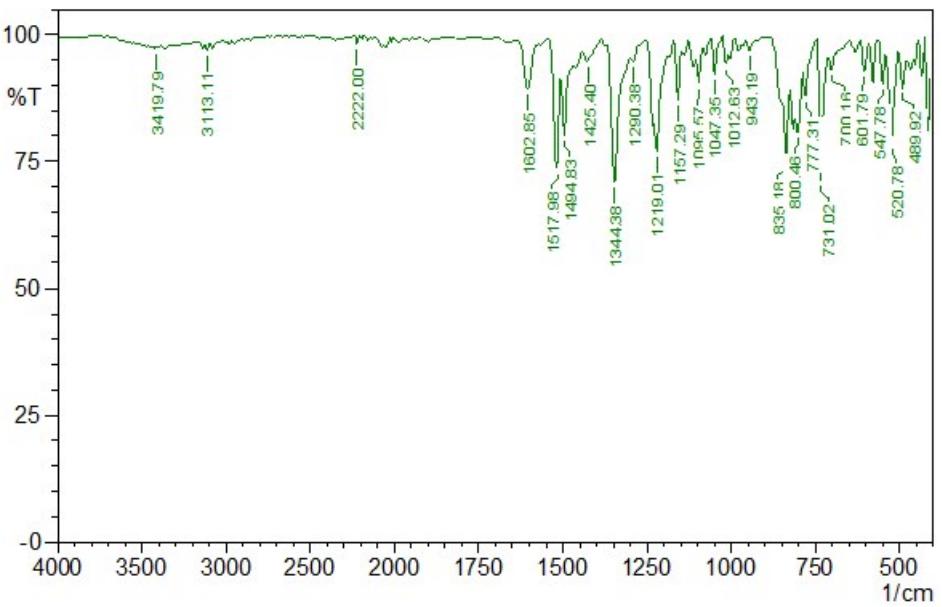
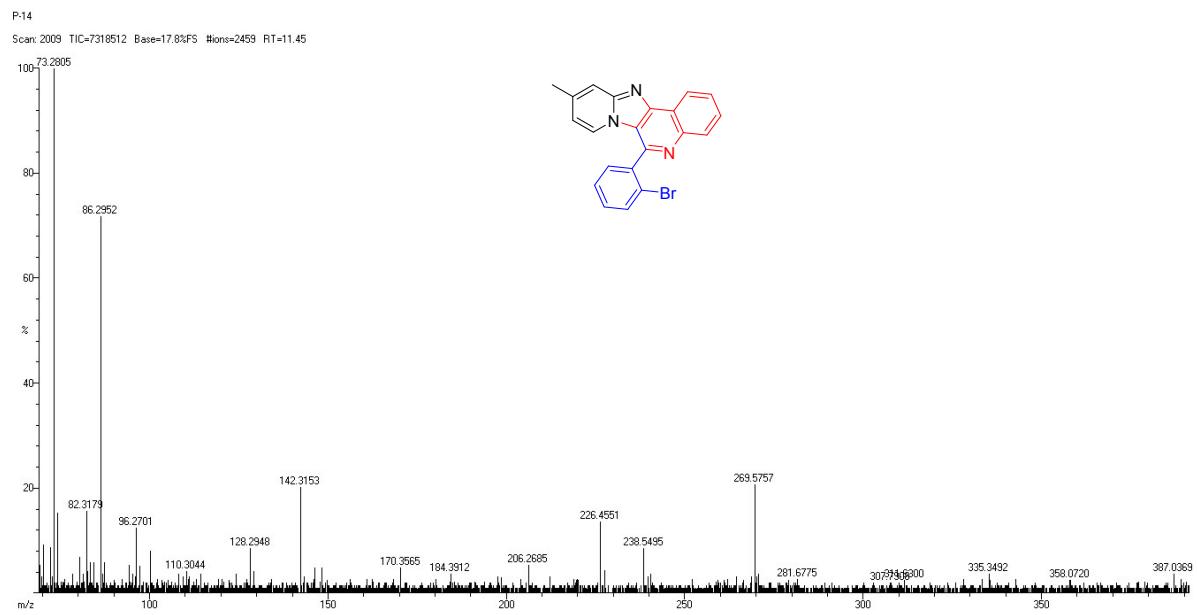


Current Data Parameters
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PROCNO 1

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SOLVENT CDCl3
NS 540
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 156.91
DW 20.800 usec
DE 6.50 usec
TE 299.9 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550186 MHz
NUC1 13C
P1 9.80 usec
PLW1 58.0000000 W
SFO2 400.2596010 MHz
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PLW12 0.35097000 W
PLW13 0.17654000 W

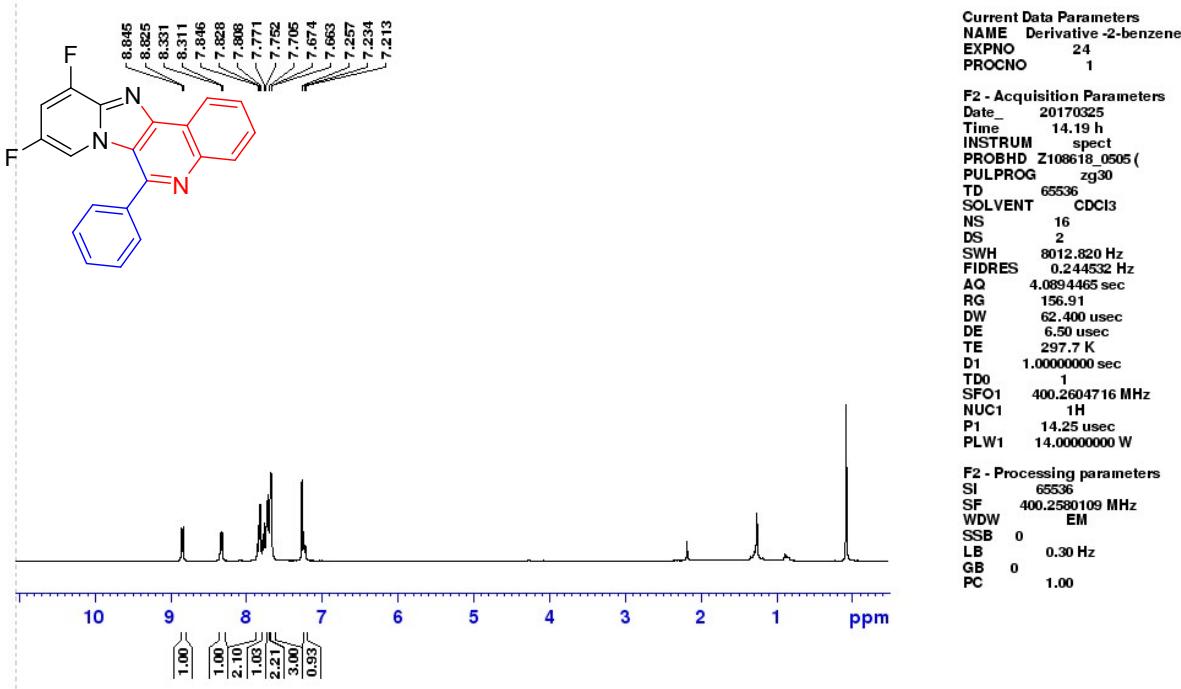
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¹H-NMR and ¹³C-NMR of compound 6r in CDCl₃

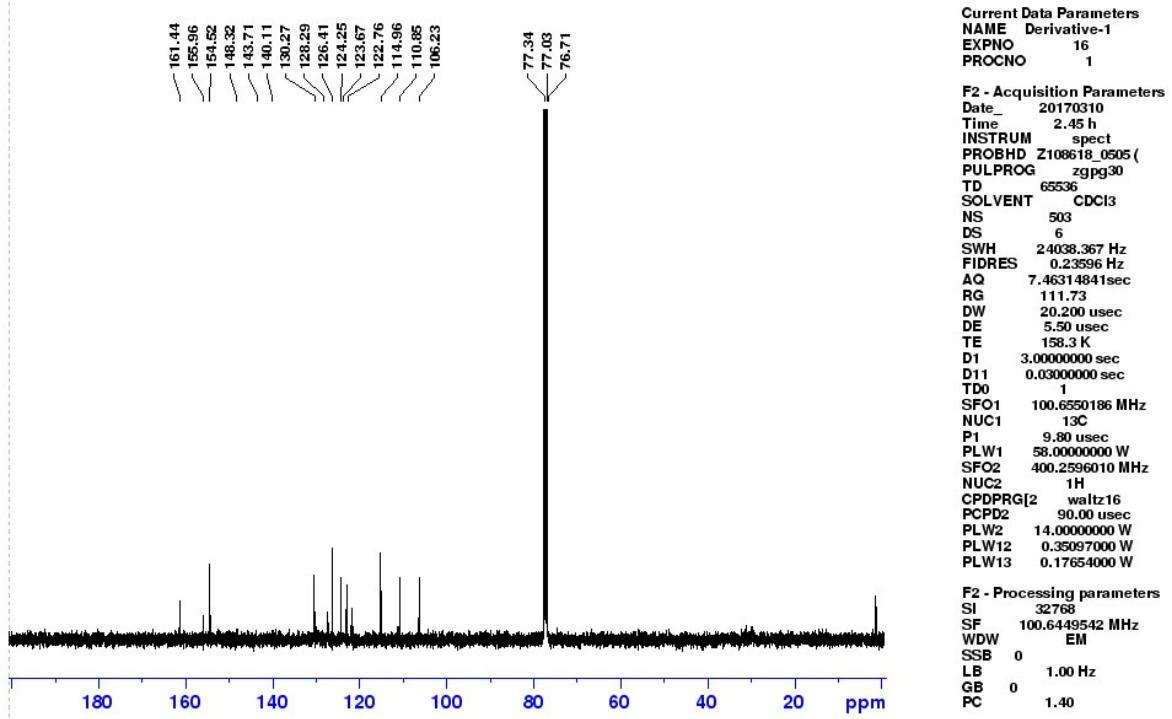


HRMS and IR of compound **6r**.

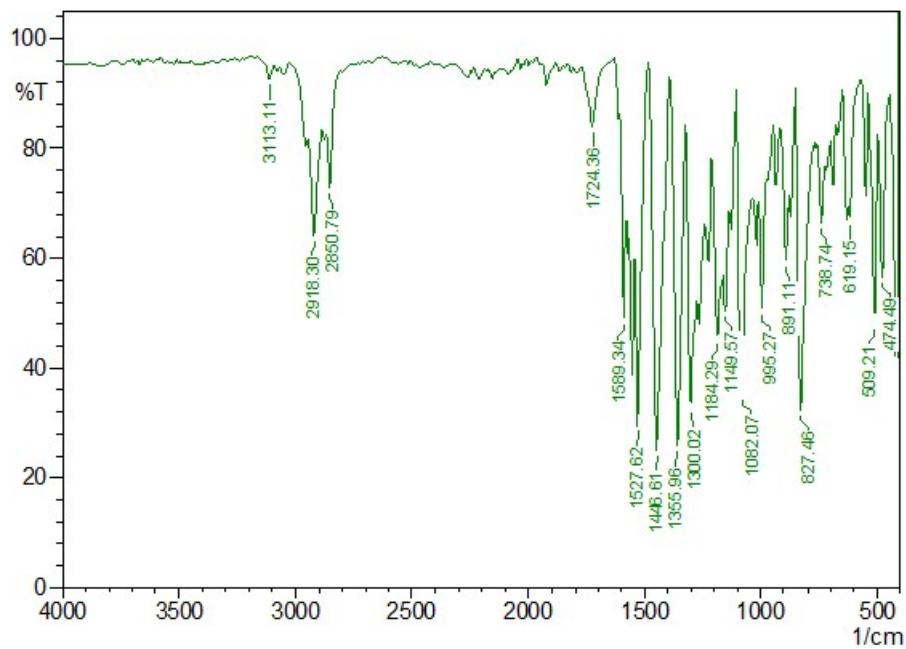
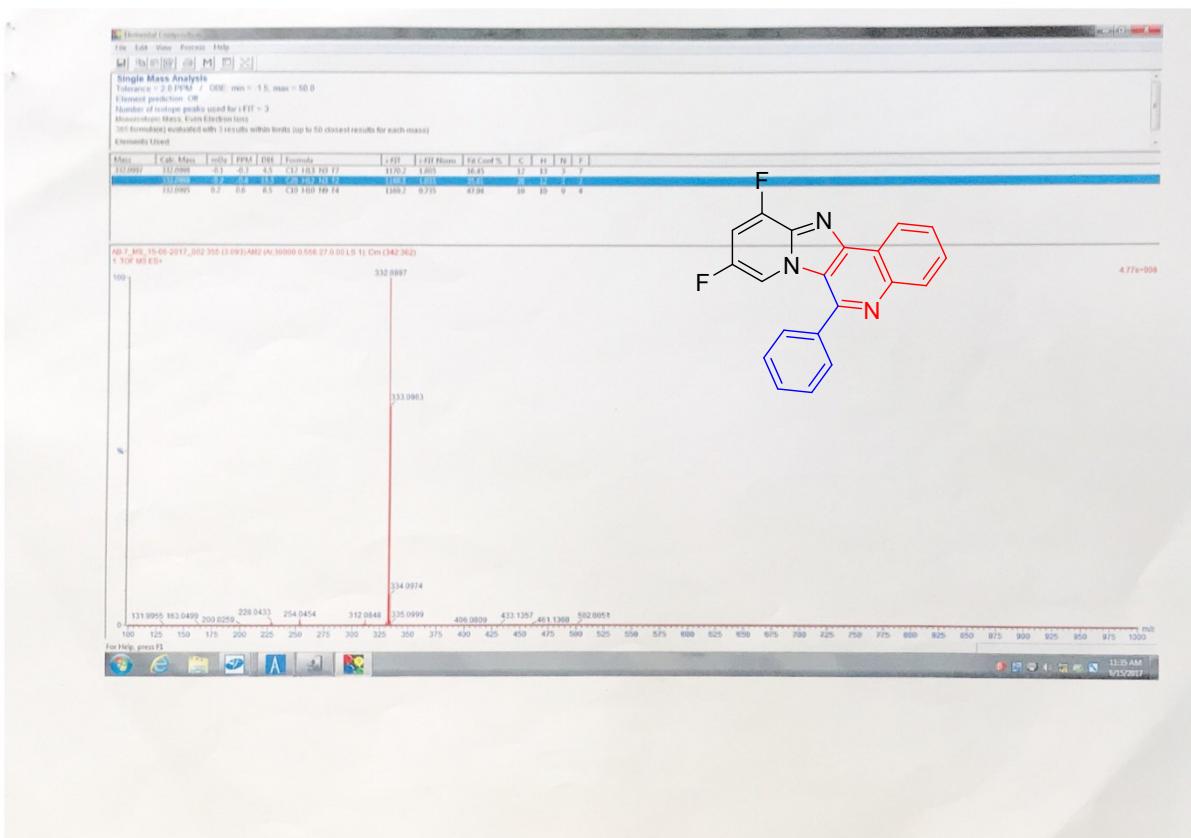
Signature SIF VIT VELLORE
NR-317-D2-PCT



Signature SIF VIT VELLORE

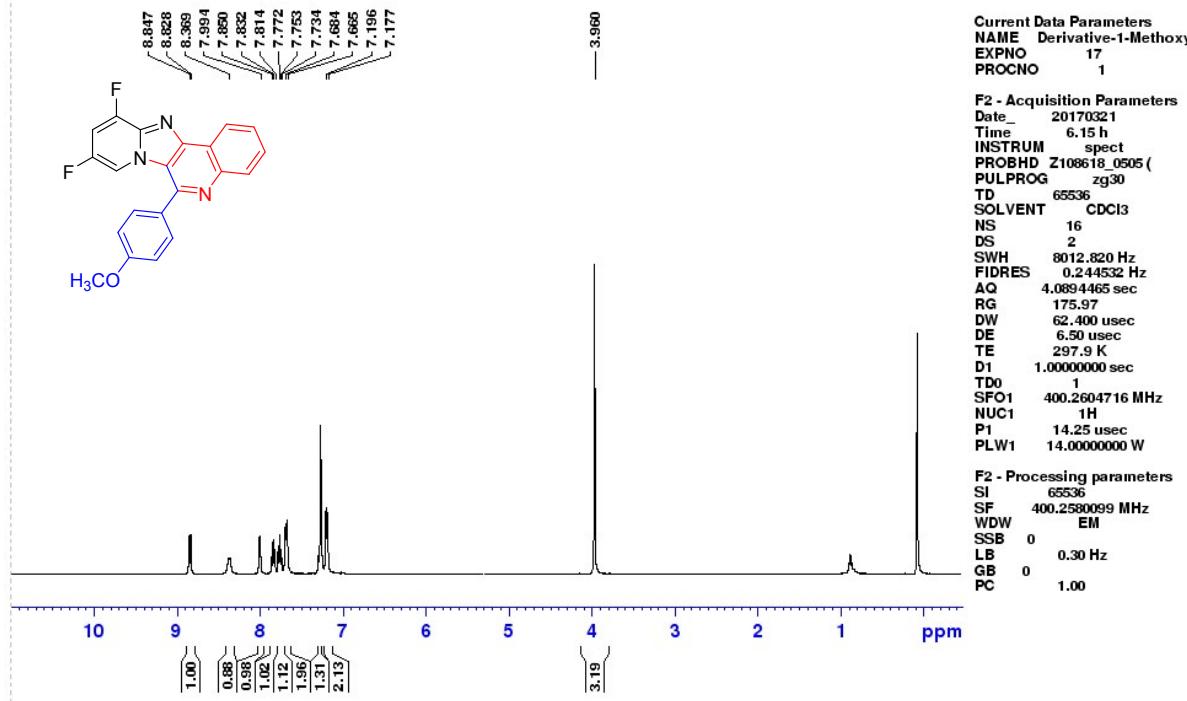


¹H-NMR and ¹³C-NMR of compound 6s in CDCl₃.

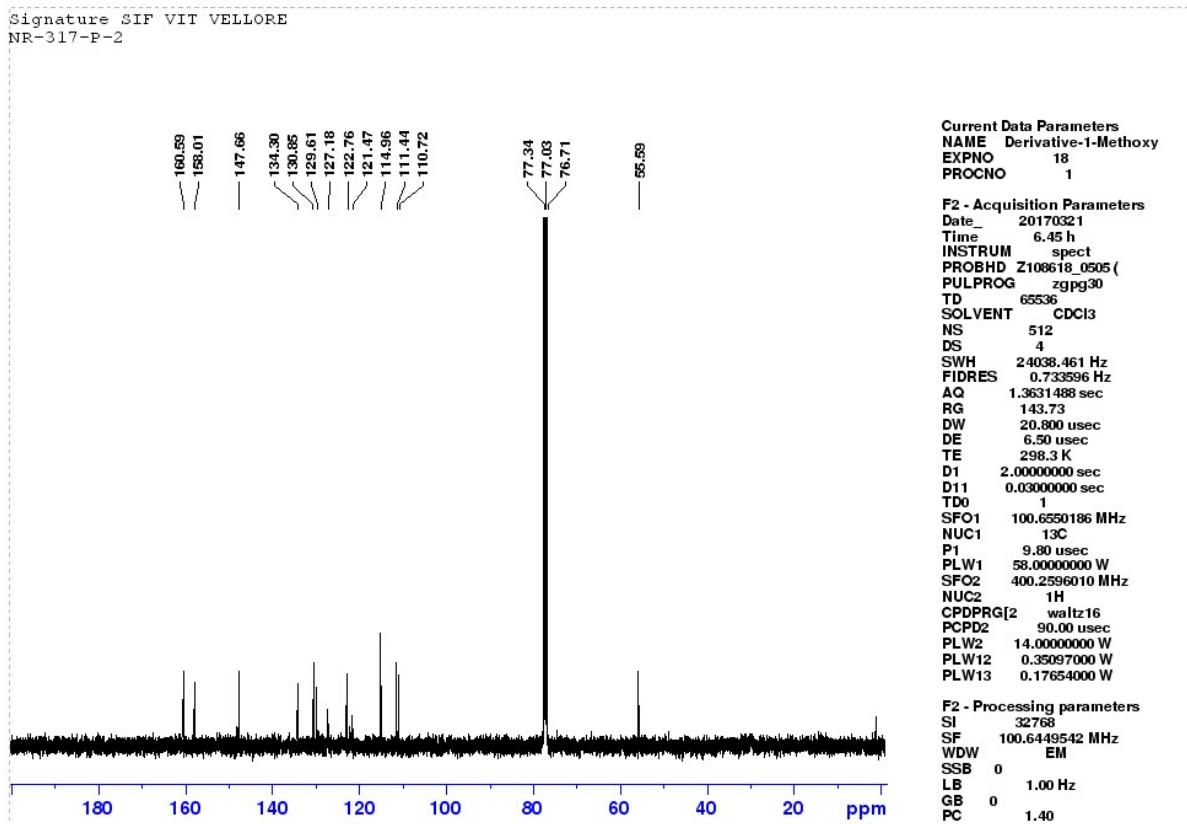


HRMS and IR of compound **6s**.

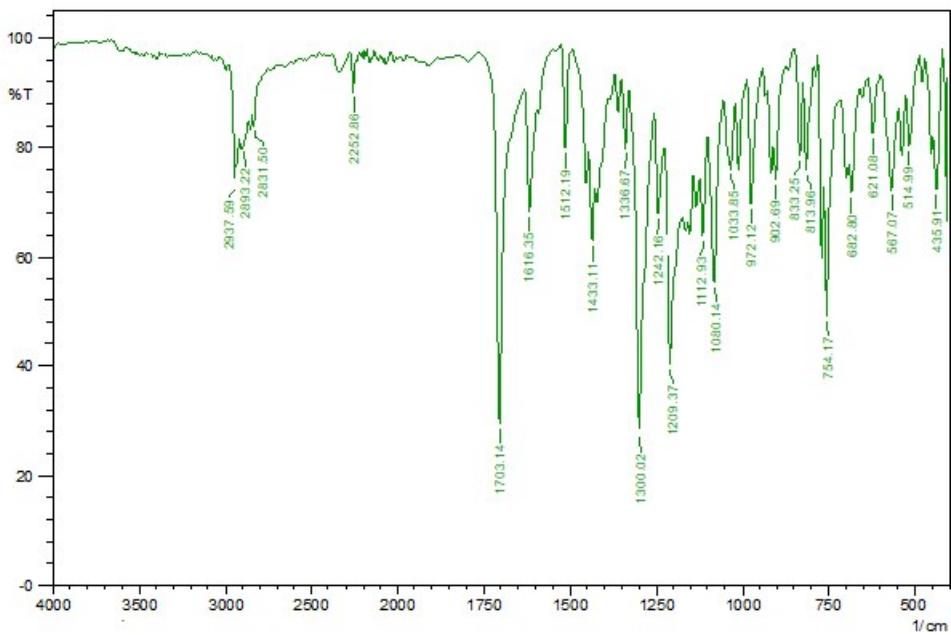
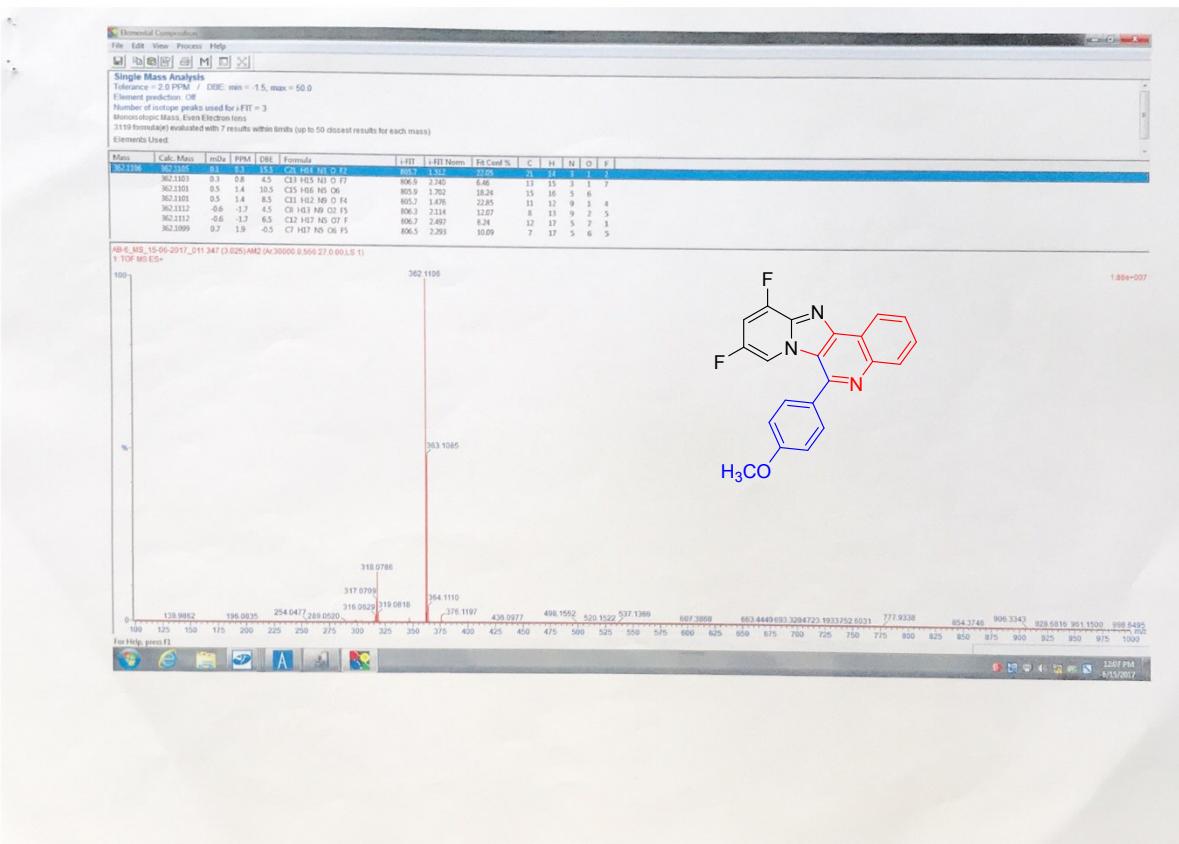
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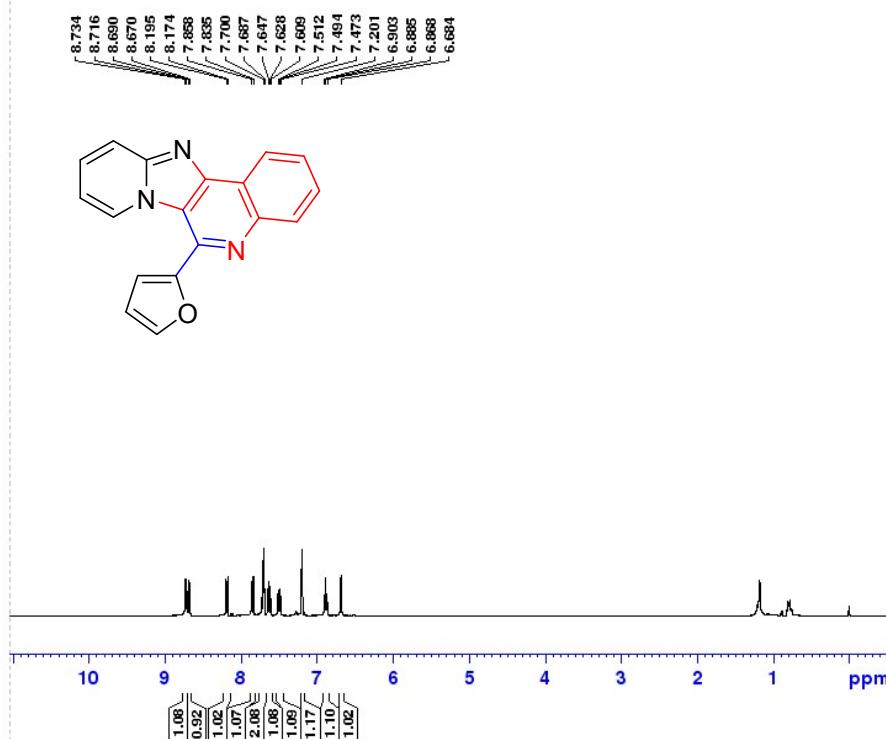


¹H-NMR and ¹³C-NMR of compound 6t in CDCl₃.

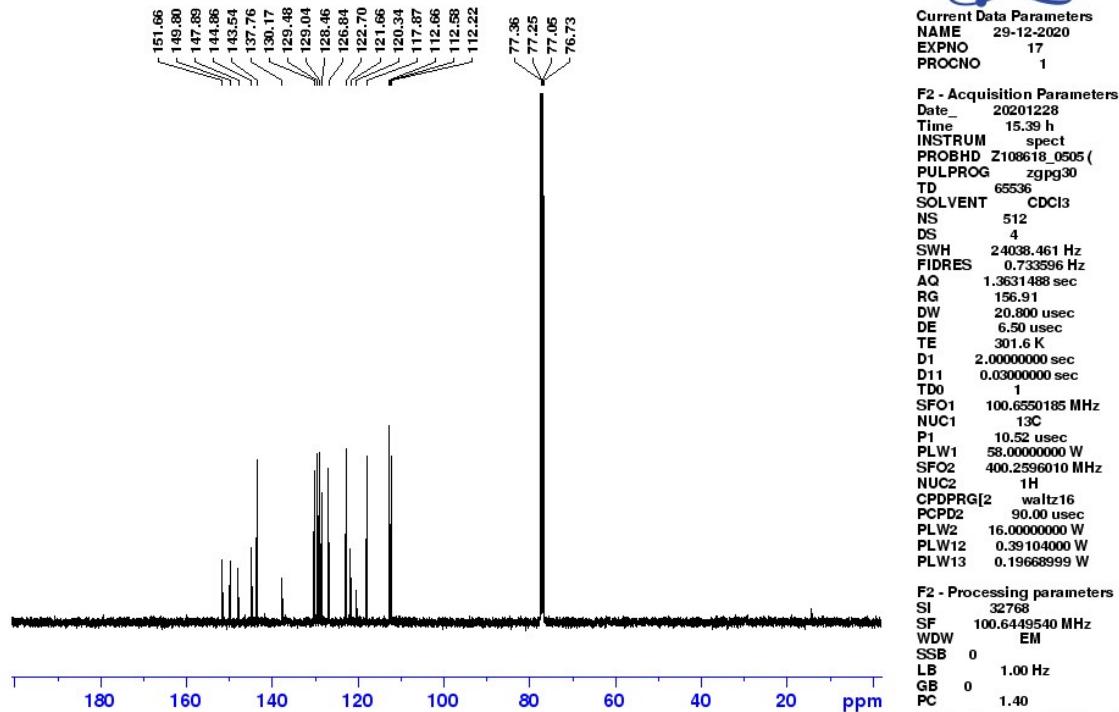


HRMS and IR of compound **6t**.

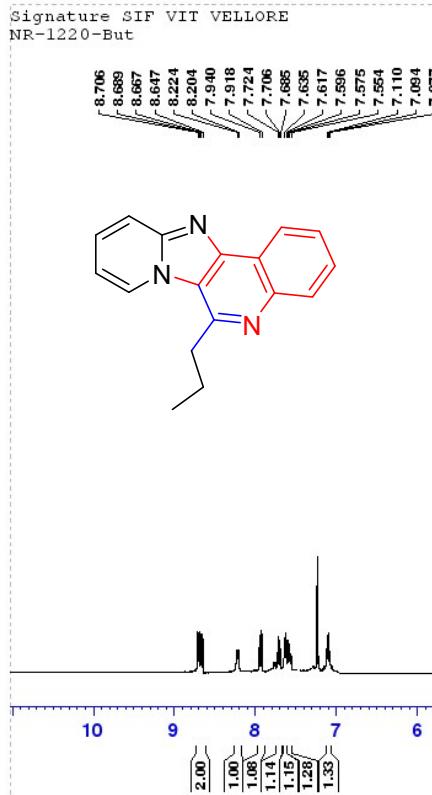
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NR-1220-FU



Signature SIF VIT VELLORE
NR-1220-FU



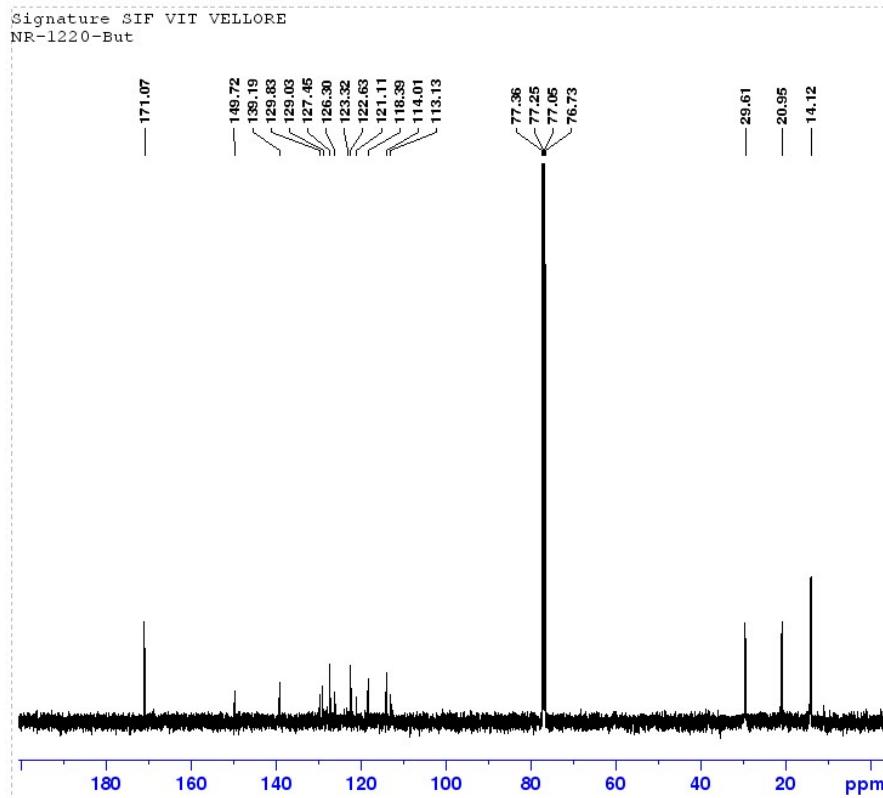
¹H-NMR and ¹³C-NMR of compound **6u** in CDCl₃.



Current Data Parameters
NAME New folder
EXPNO 18
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201230
Time 7.37 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.244532 Hz
AQ 4.0894465 sec
RG 35.49
DW 62.400 usec
DE 6.50 usec
TE 302.0 K
D1 1.0000000 sec
TD0 1
SFO1 400.2604716 MHz
NUC1 1H
P1 14.07 usec
PLW1 16.0000000 W

F2 - Processing parameters
SI 65536
SF 400.2580219 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0 1.00
PC 1.00



Current Data Parameters
NAME Butaraldehyde
EXPNO 19
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201230
Time 8.09 h
INSTRUM spect
PROBHD Z108618_0505 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 4
SWH 24038.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 112.69
DW 20.800 usec
DE 6.50 usec
TE 302.6 K
D1 2.0000000 sec
D11 0.03000000 sec
TD0 1
SFO1 100.6550185 MHz
NUC1 13C
P1 10.52 usec
PLW1 58.00000000 W
SFO2 400.2596010 MHz
NUC2 1H
CPDPG[2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.39104000 W
PLW13 0.19668999 W

F2 - Processing parameters
SI 32768
SF 100.6449540 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0 1.40
PC 1.40

¹H-NMR and ¹³C-NMR of compound 6v in CDCl₃.

