

# **Copper-catalyzed three component system for arylsulenylation of imidazopyridines with elemental sulfur**

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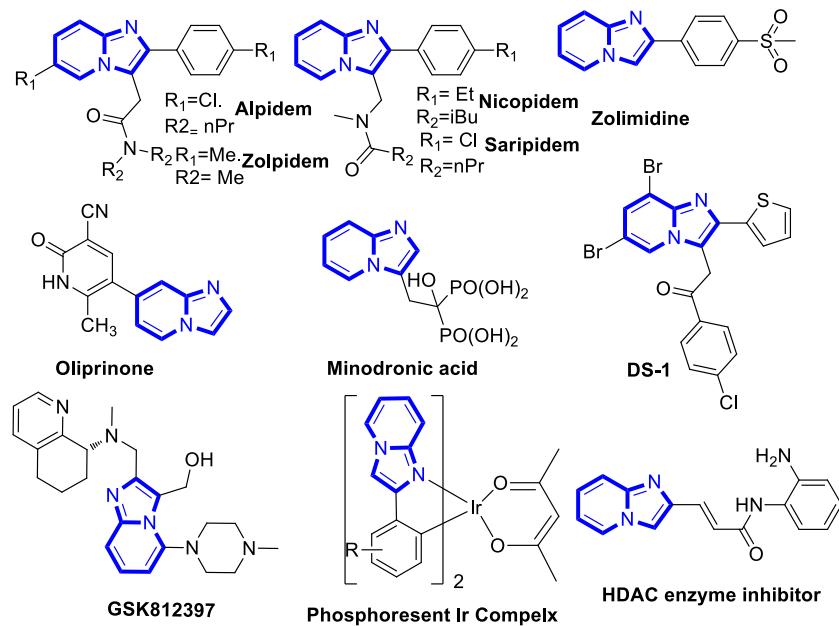
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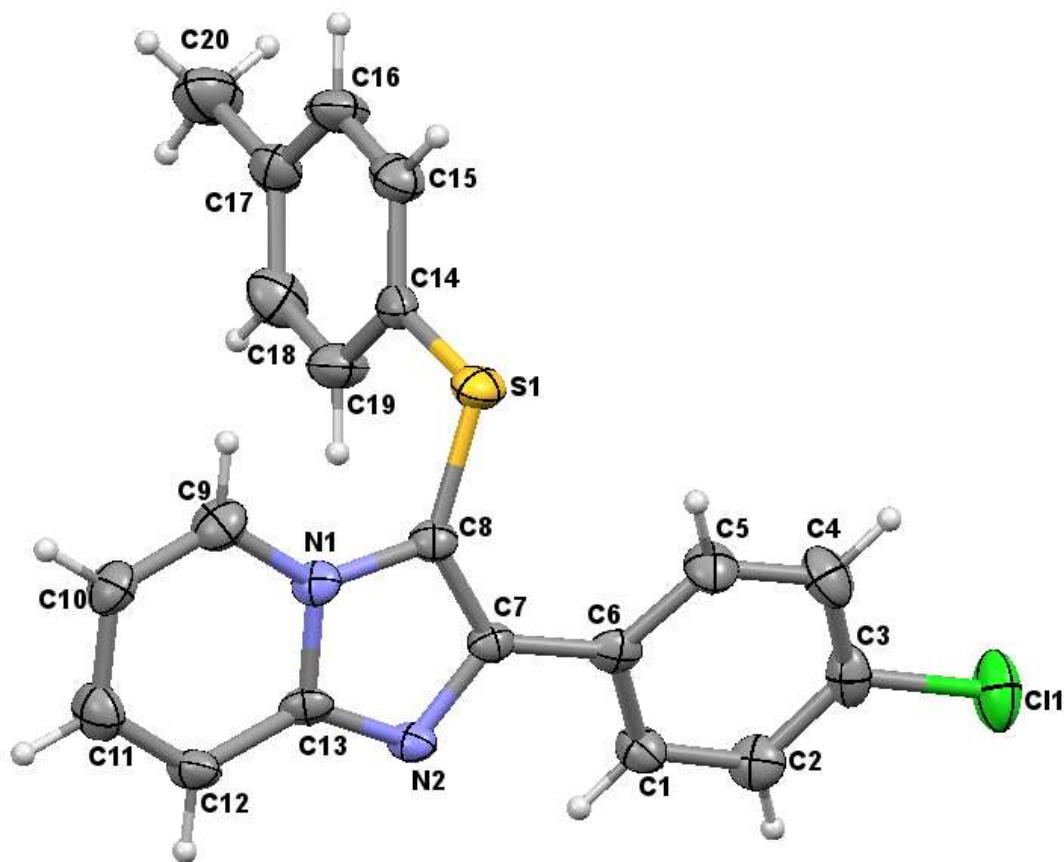
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## 1. Imidazo[1,2-a]pyridine-based molecules



**Figure S1.** Imidazo[1,2-a]pyridine-based molecules

2. Thermal ellipsoid plot for the crystal structure **4n**



Thermal ellipsoid plot for the compound **4n** with atom numbering scheme (40% probability factor for the thermal ellipsoids)

### **3. Crystal Data and Refinement Parameters**

Experimental : X-ray part

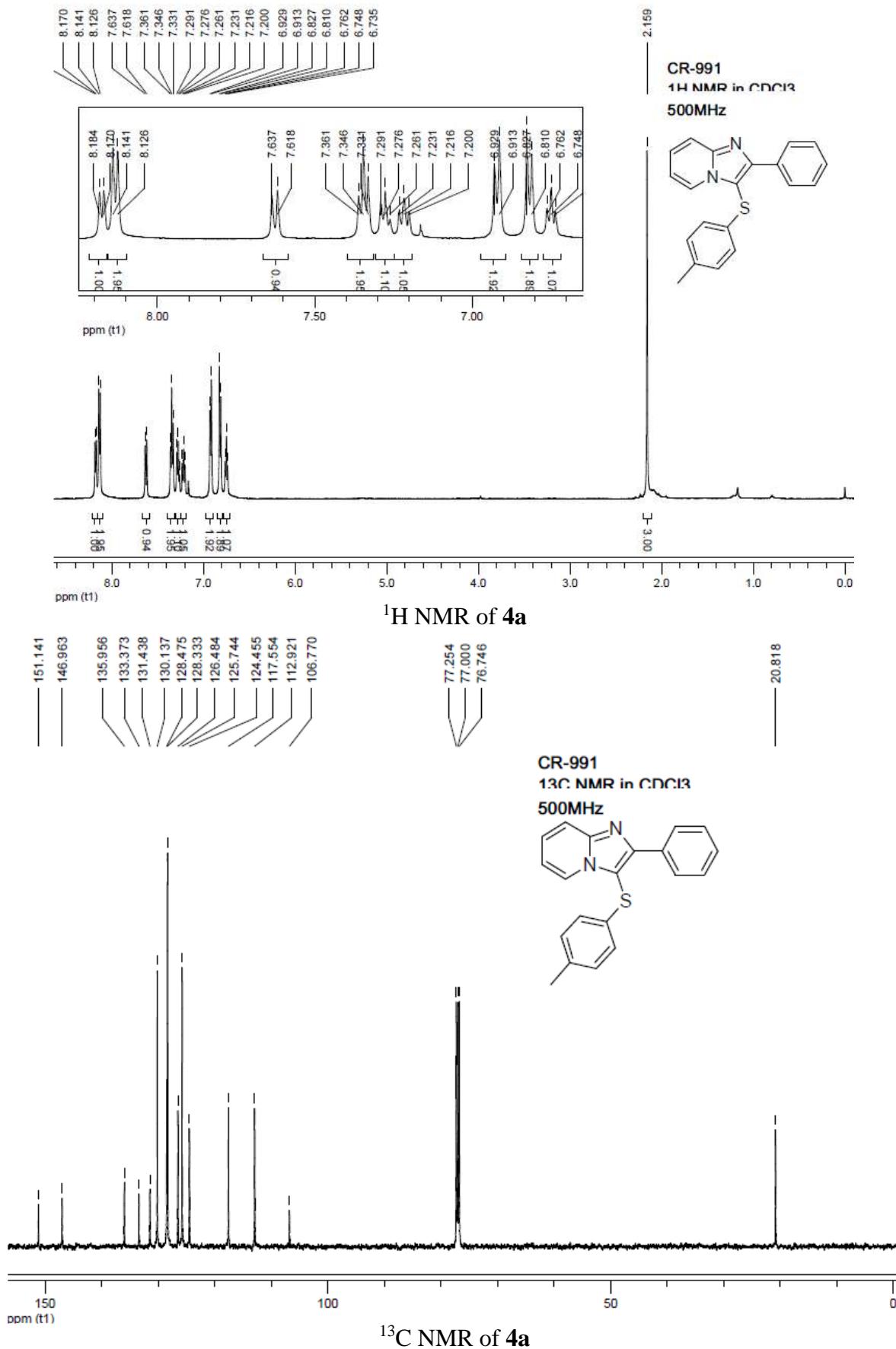
Crystal of suitable size was selected for the organic compound, immersed in partone oil and then mounted on the tip of a glass fiber using epoxy resin. Intensity data for all four crystals were collected at 100 K using graphite monochromatised MoK $\alpha$  ( $\lambda = 0.71073\text{\AA}$ ) radiation on diffractometer equipped with CCD area detector. The data integration and reduction were processed.<sup>1</sup> An empirical absorption correction was applied to the collected reflections.<sup>2</sup> The structures were solved by direct methods<sup>3</sup> and refined on  $F^2$  by the full-matrix least-squares technique<sup>4</sup> package. Graphics are generated.<sup>5,6</sup> Non-hydrogen atoms were refined anisotropically till convergence is reached and the hydrogen atoms of the organic compound is stereochemically fixed. Crystallographic parameters for the compound is given in Table S1.

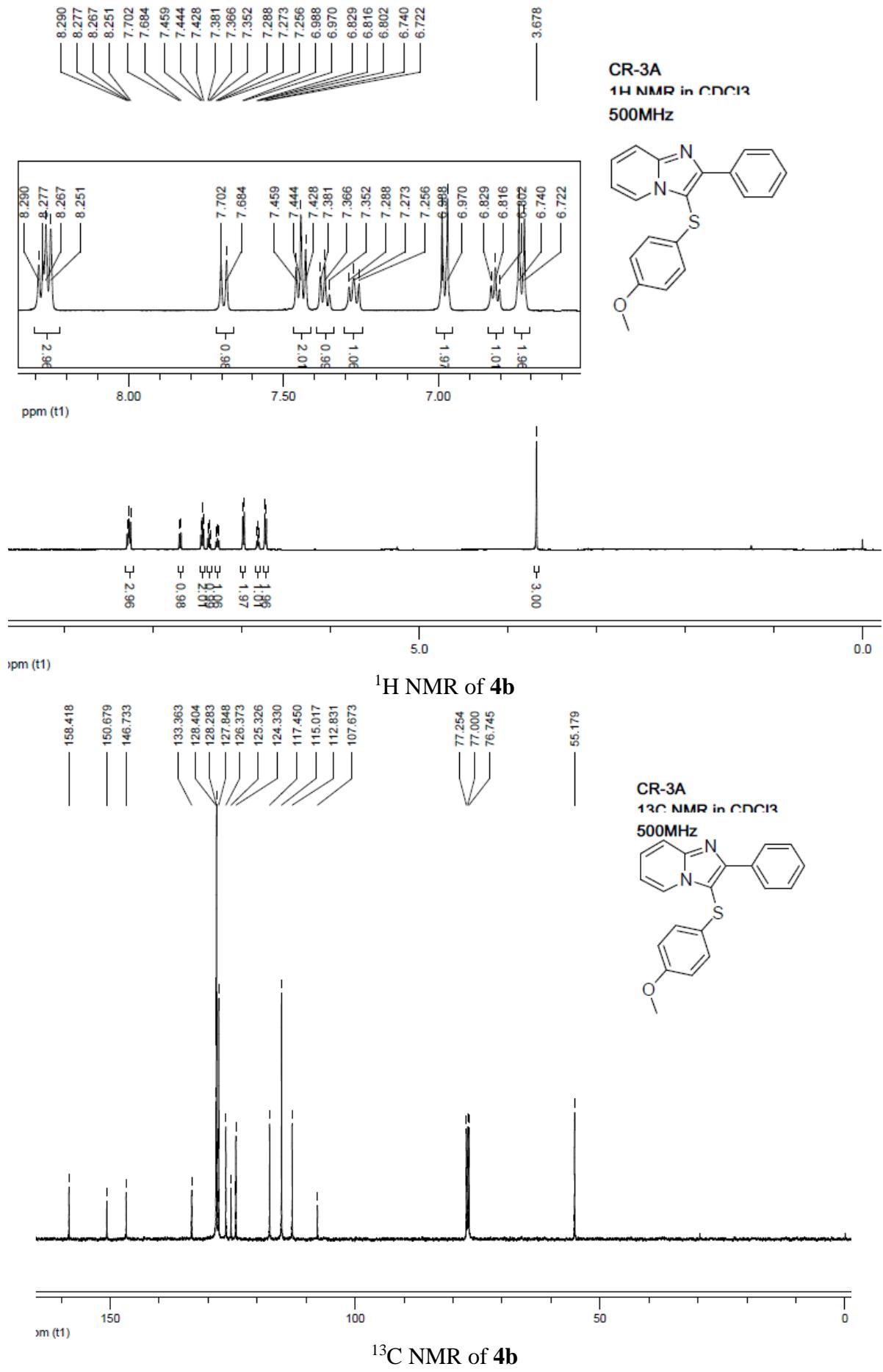
1. Sheldrick, G. M.; SAINT 5.1 ed.; Siemens Industrial Automation Inc.: Madison, WI, **1995**.
2. SADABS, Empirical Absorption Correction Program; University of Göttingen: Göttingen, Germany **1997**.
3. Sheldrick, G. M.; SHELXTL Reference Manual: Version 5.1; Bruker AXS: Madison, WI **1997**.
4. Sheldrick, G.M. SHELXL-97: Program for Crystal Structure Refinement; University of Göttingen: Göttingen, Germany (**1997**).
5. A.L.Spek, Acta Cryst. 2009, D65, 148-155
6. Mercury 1.3, Supplied with Cambridge Structural Database; CCDC: Cambridge, U.K., (**2003**).

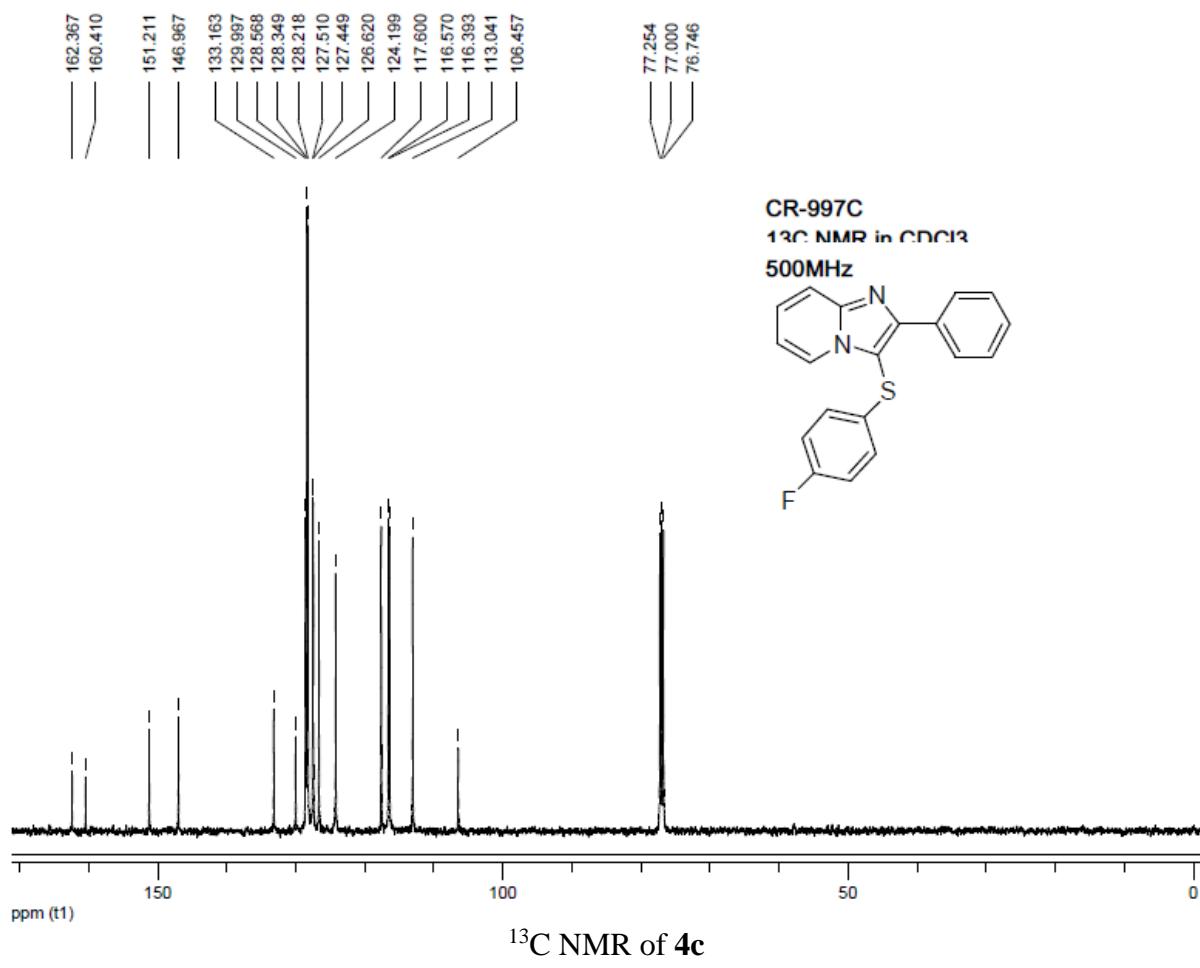
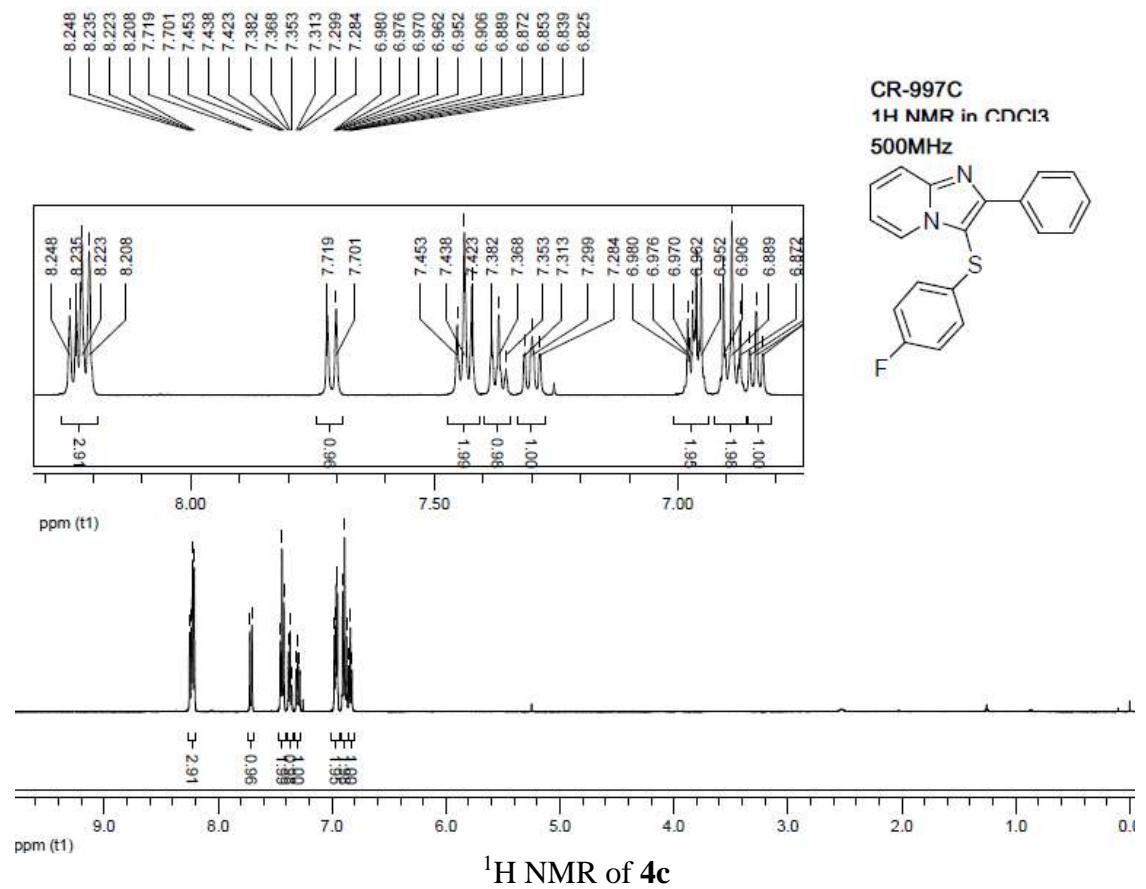
**Table S1.** Crystal Data and Refinement Parameters for Compounds **4n**

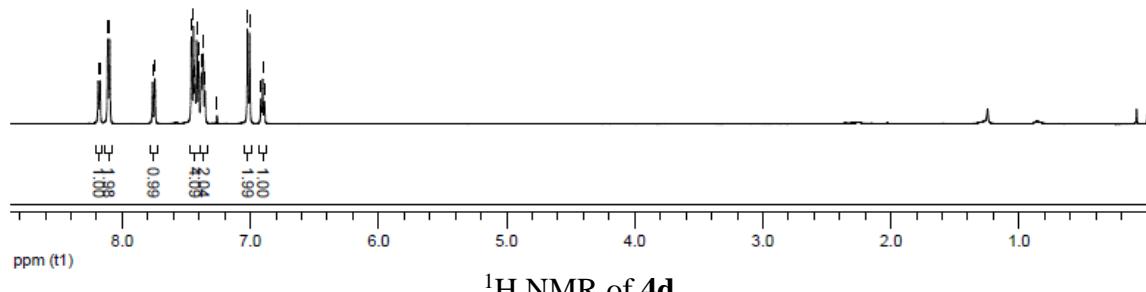
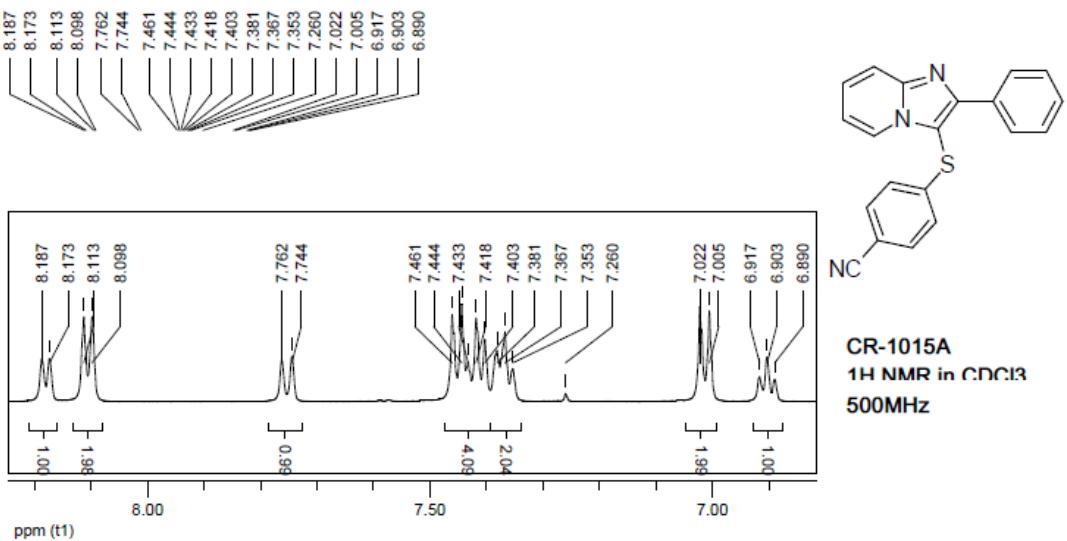
Identification code	<b>4n</b>
Chemical formula	C <sub>20</sub> H <sub>15</sub> N <sub>2</sub> Cl S
Formula weight	350.85
Crystal Colour	Colourless
Crystal Size (mm)	0.28x0.10x0.06
Temperature (K)	150(2)
Crystal System	Monoclinic
Space Group	P21/n
a(Å )	12.126(10)
b(Å )	5.863(5)
c(Å )	24.164(19)
α(°)	90
β(°)	103.359(13)
γ (°)	90
Z	4
V(Å <sup>3</sup> )	1672(2)
Density (Mg/m <sup>3</sup> )	1.394
μ (mm <sup>-1</sup> )	0.356
F(000)	728
Reflections Collected	7671
Independent Reflections	2925
R <sub>(int)</sub>	0.0599
Number of parameters	218
GOF on F <sup>2</sup>	1.179
FinalR1/wR2(I>2σ(I)	0.0890/0.1788
Weighted R1/wR2 (all data)	0.1208/0.1906
CCDC number	1484511

#### 4. Copies of $^1\text{H}$ and $^{13}\text{C}$ NMR spectra

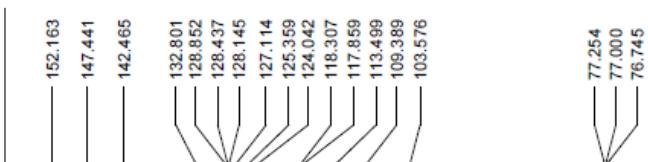




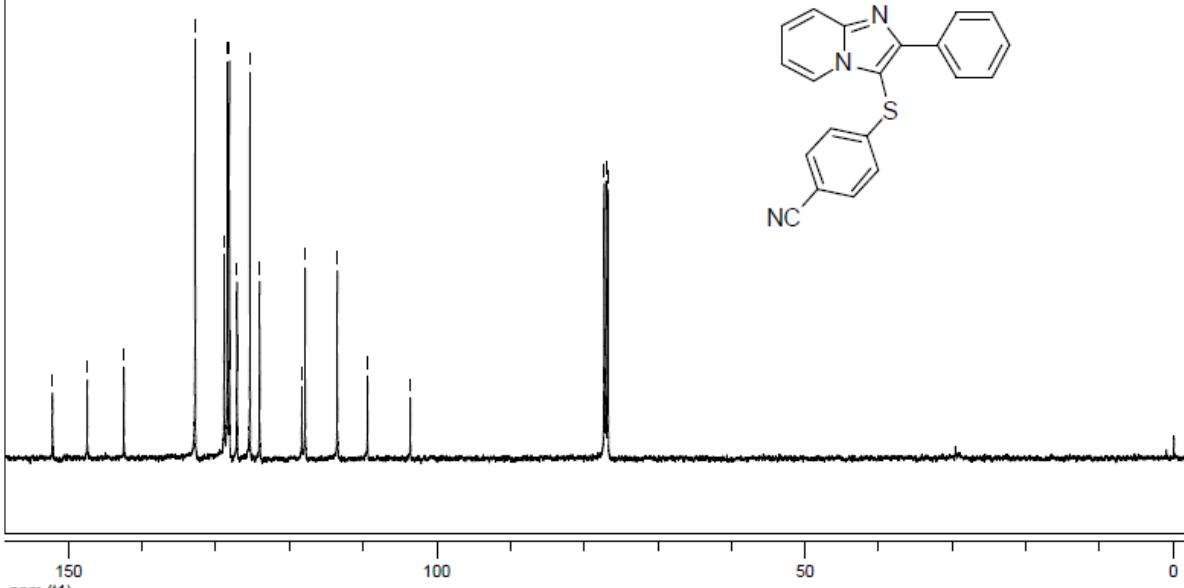
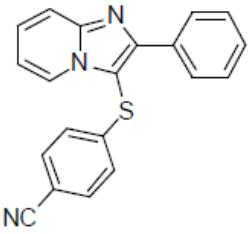




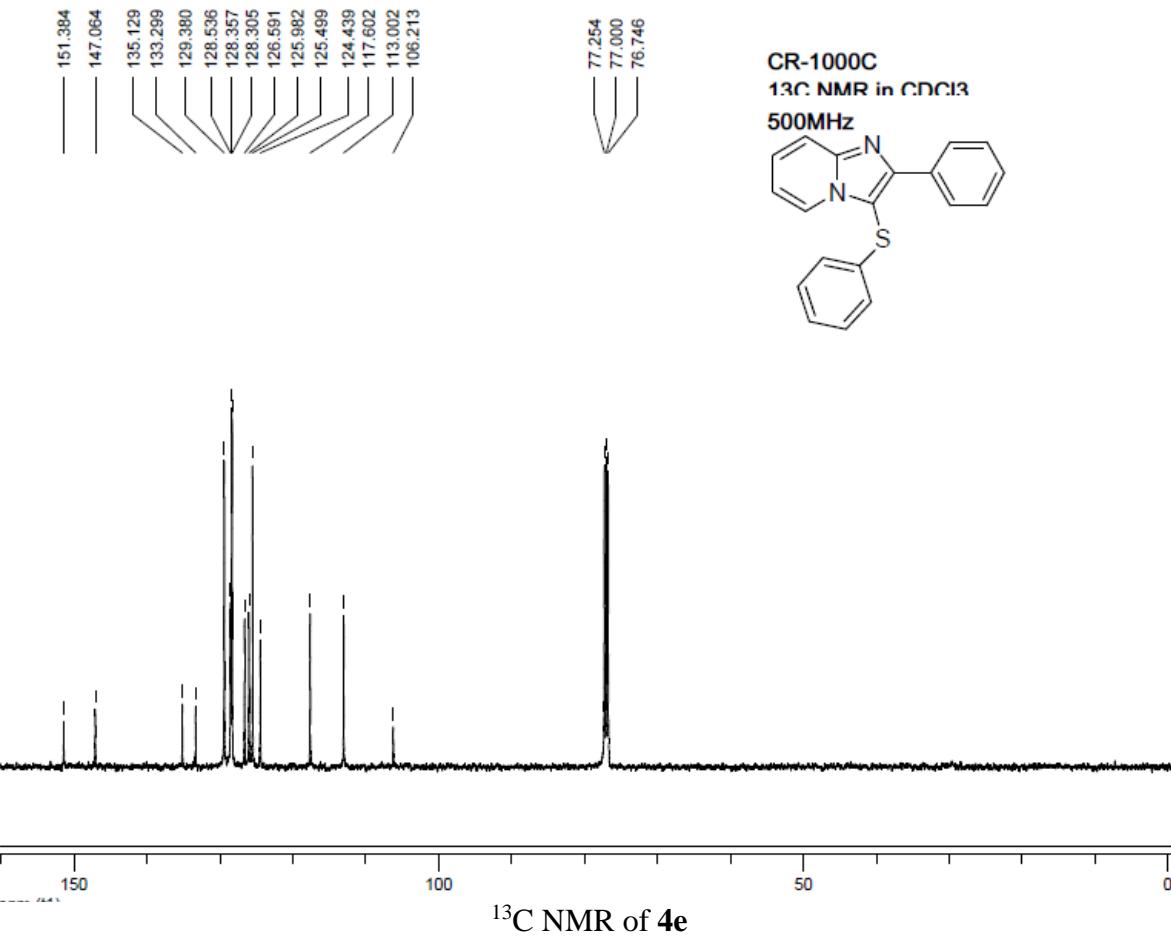
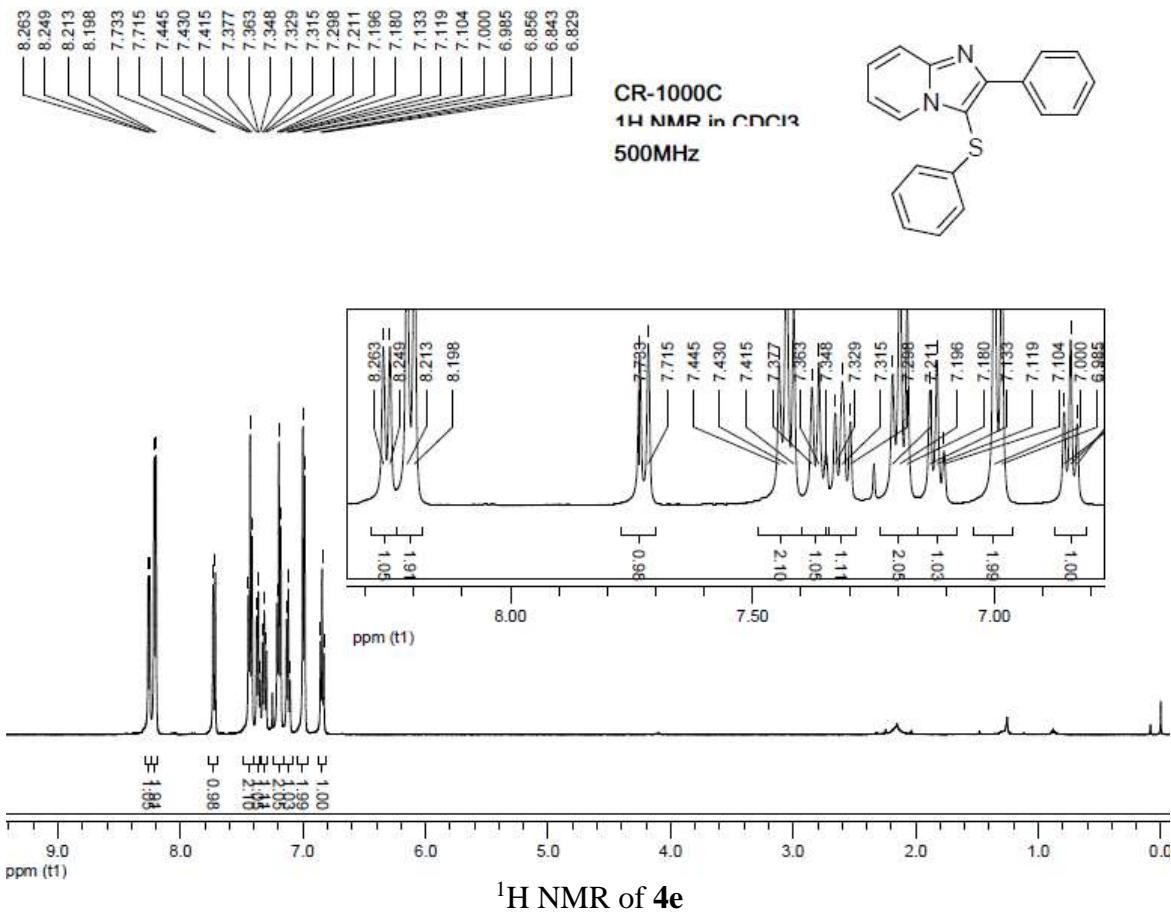
## <sup>1</sup>H NMR of 4d

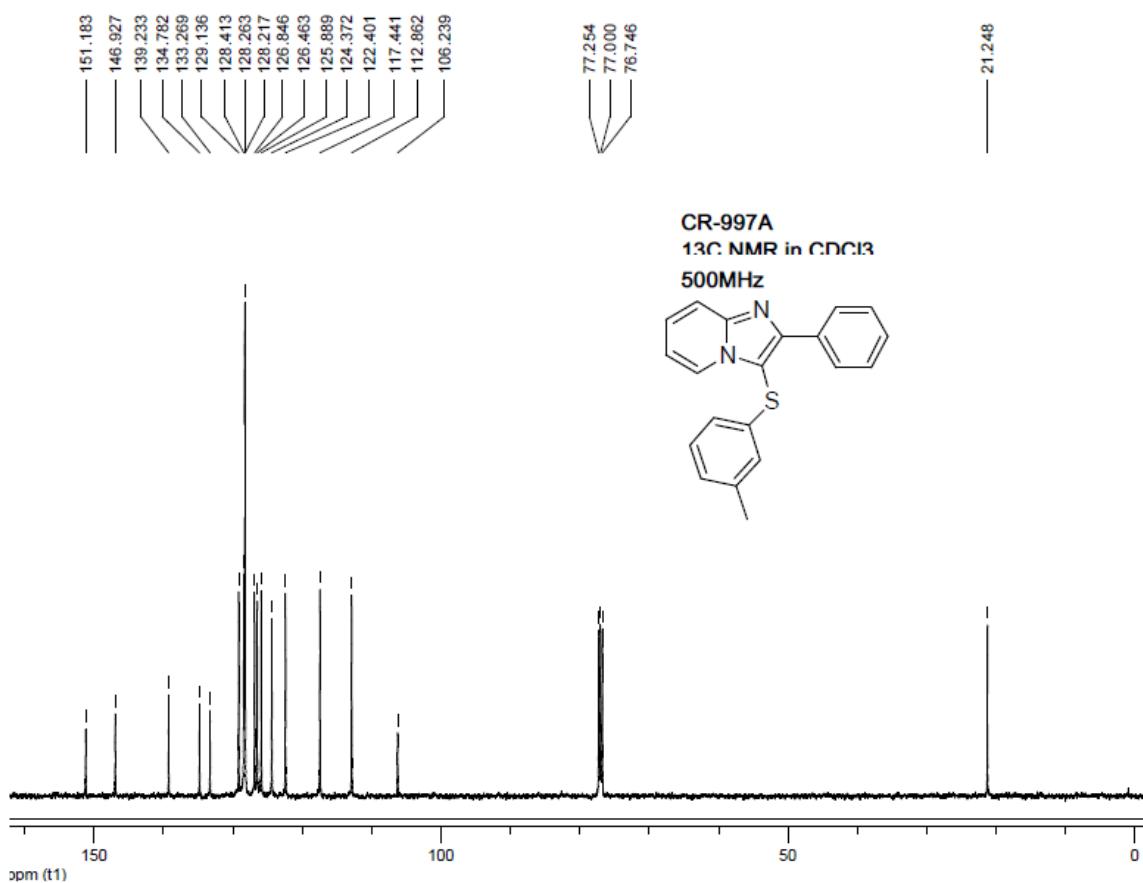
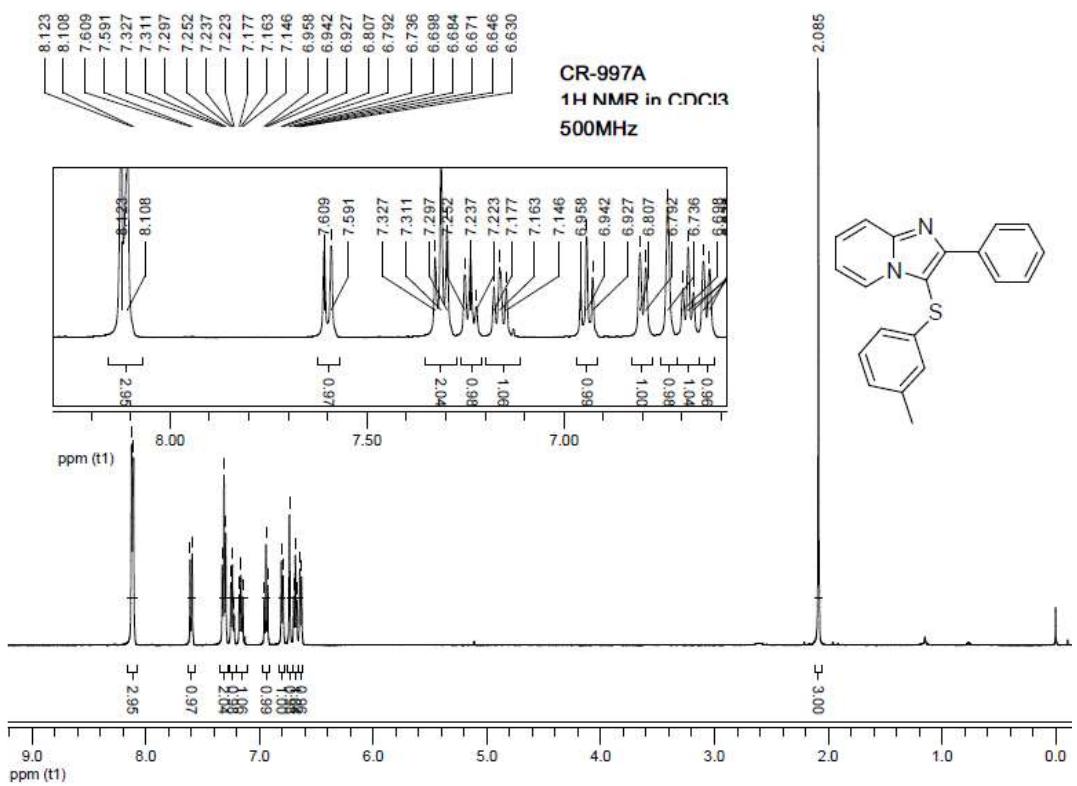


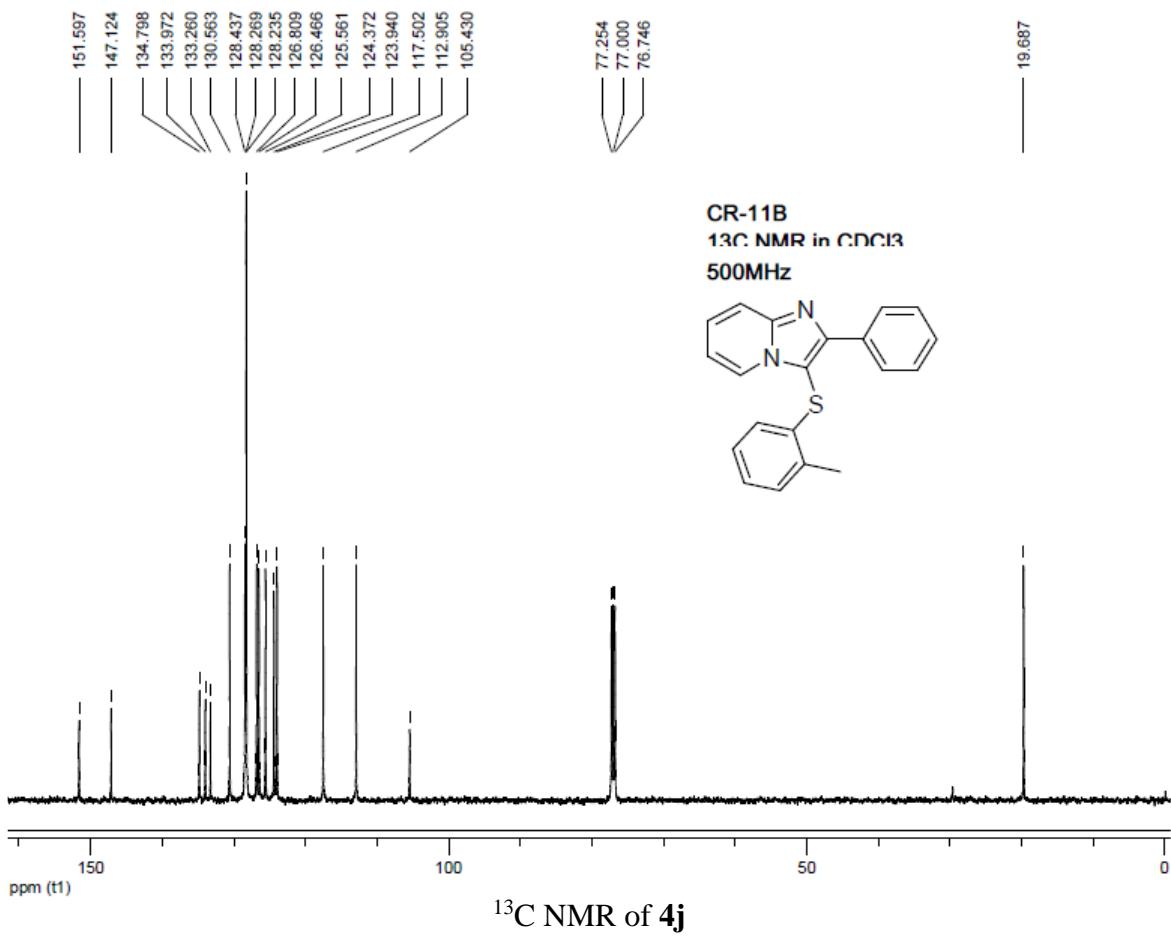
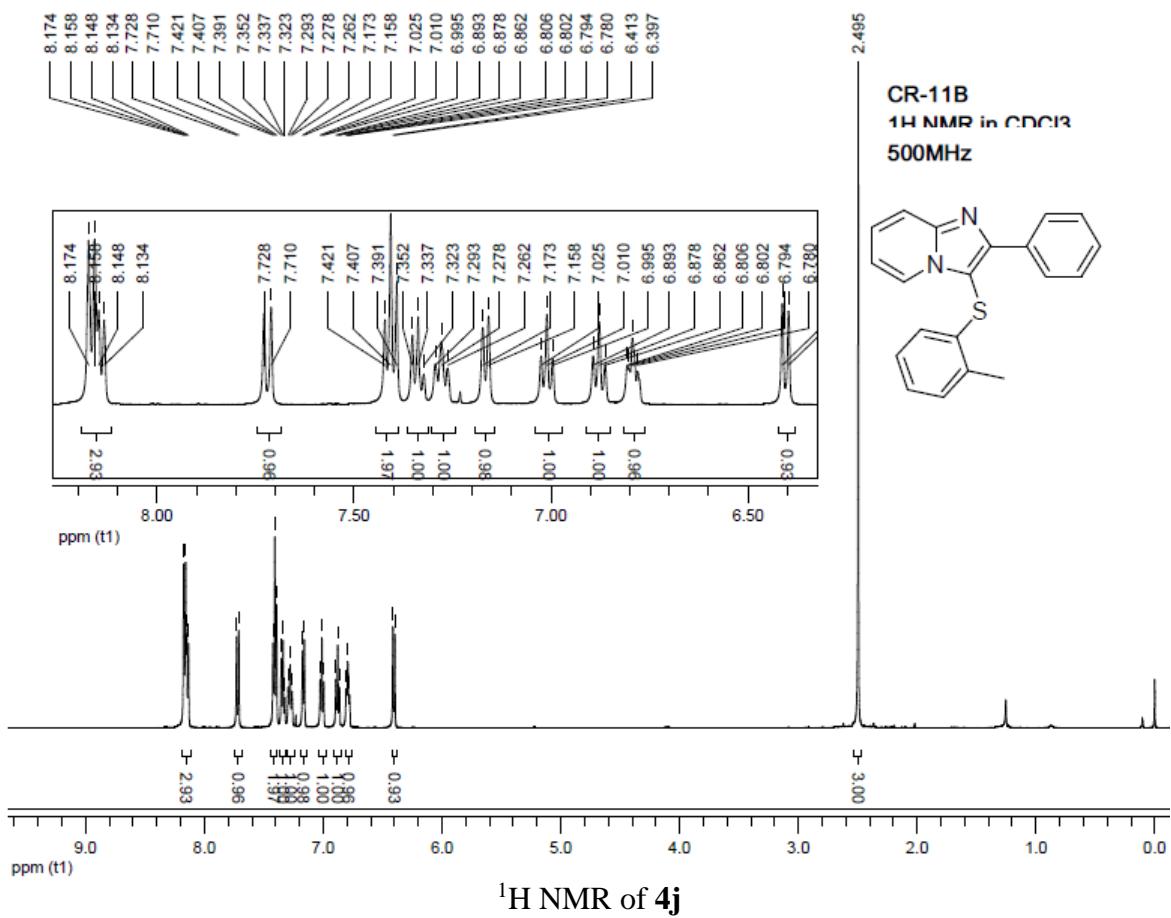
CR-1015A  
13C NMR in CDCl3  
500MHz

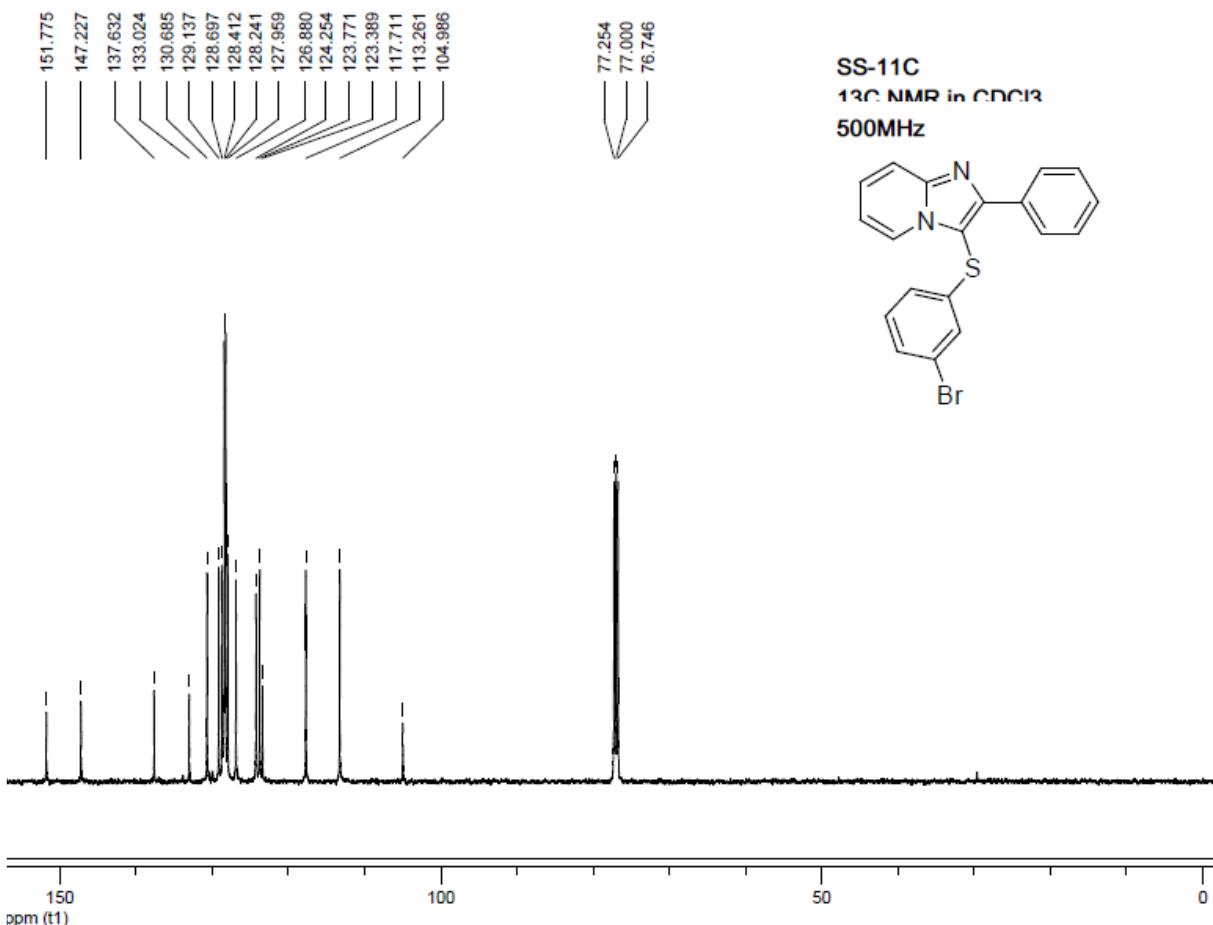
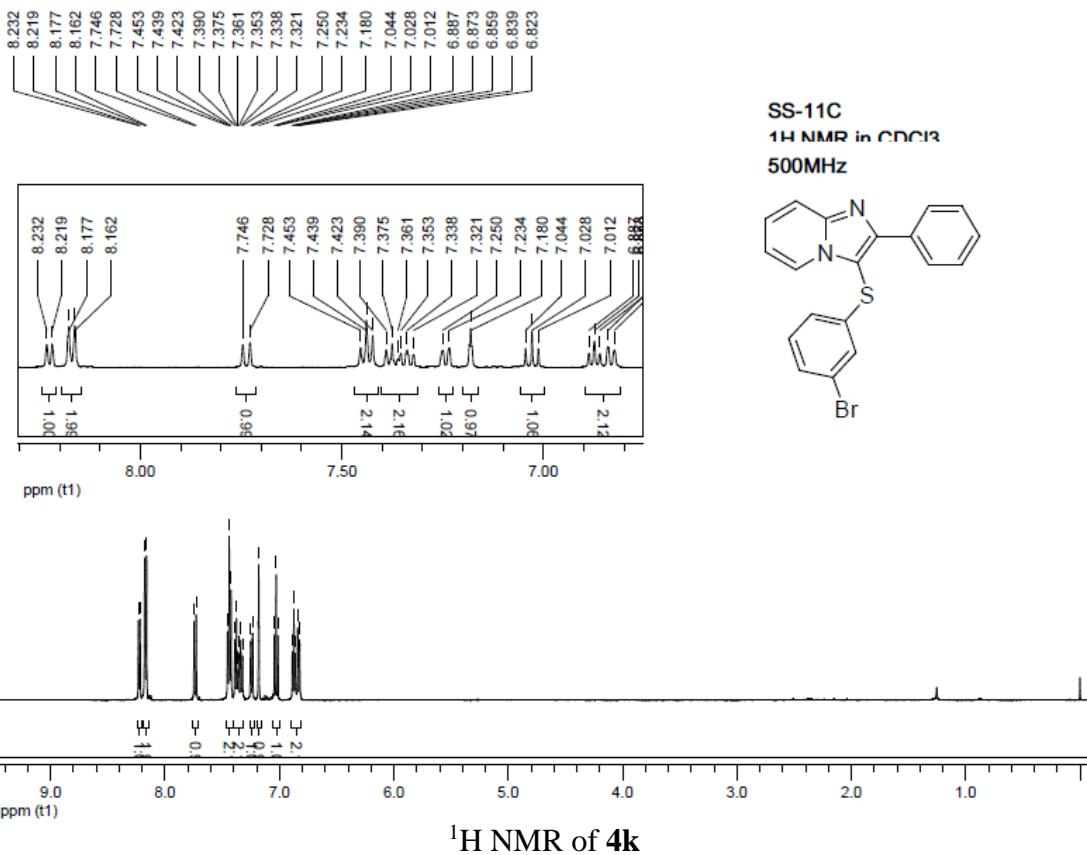


### <sup>13</sup>C NMR of **4d**

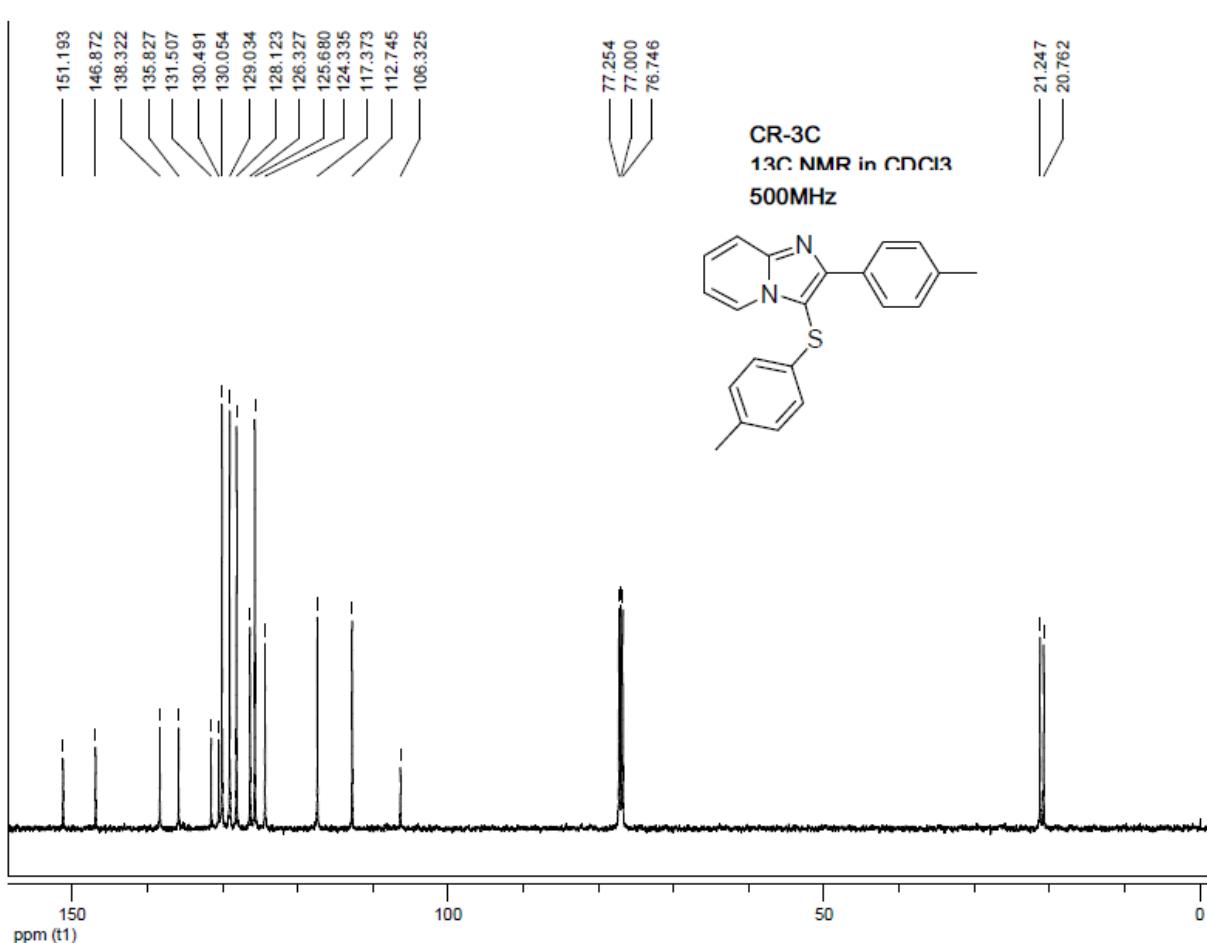
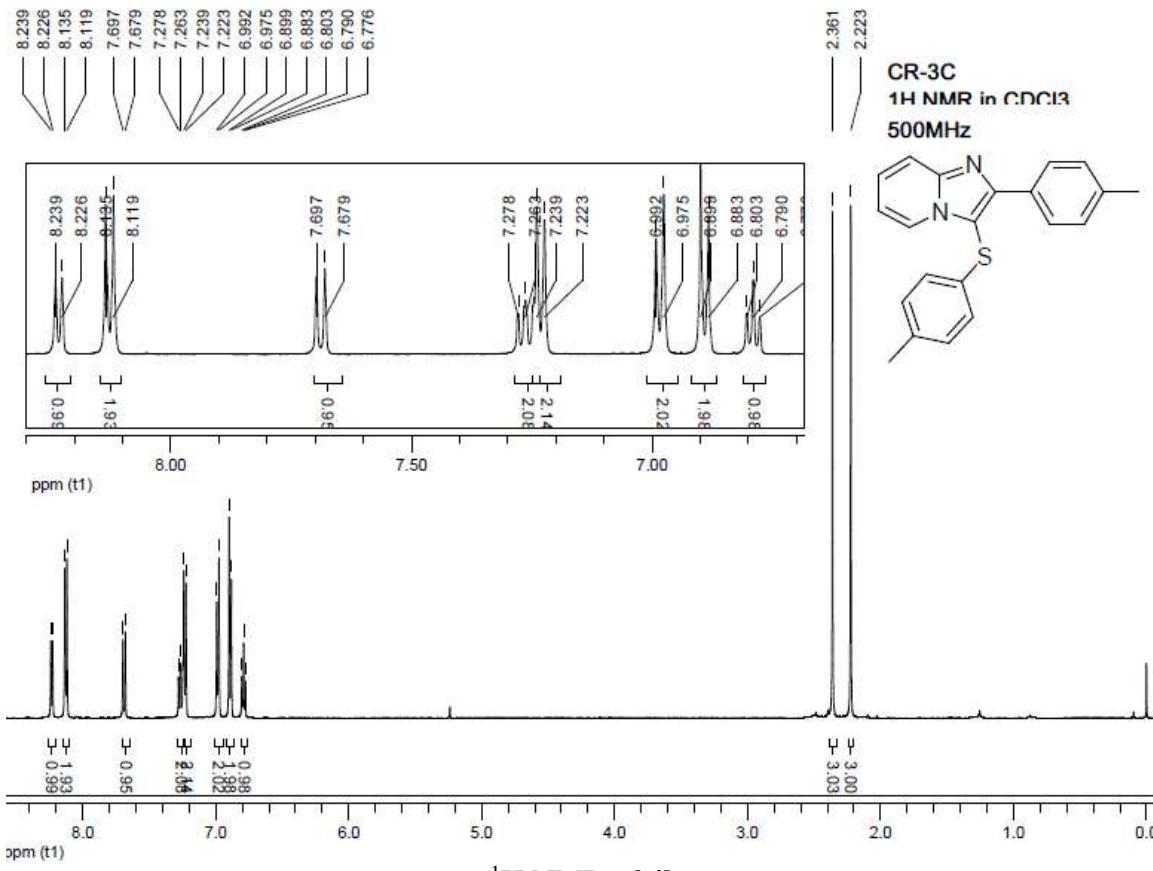




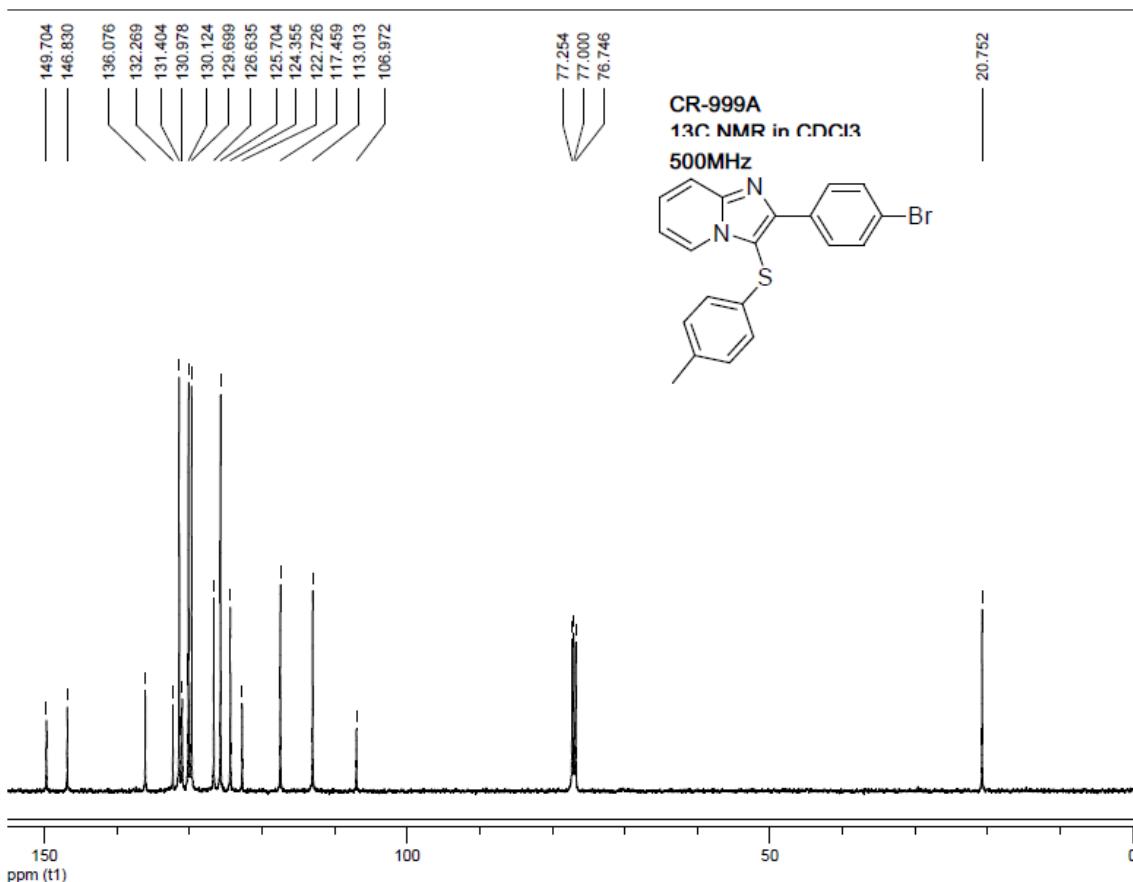
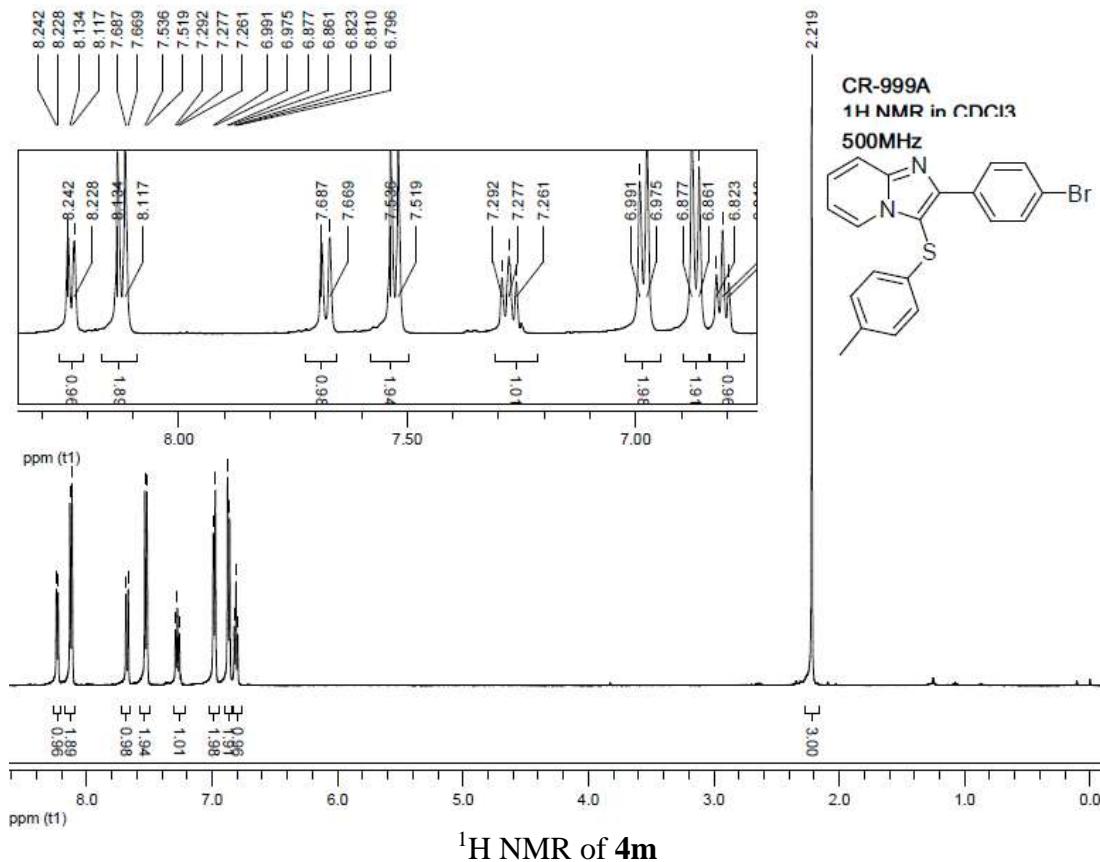


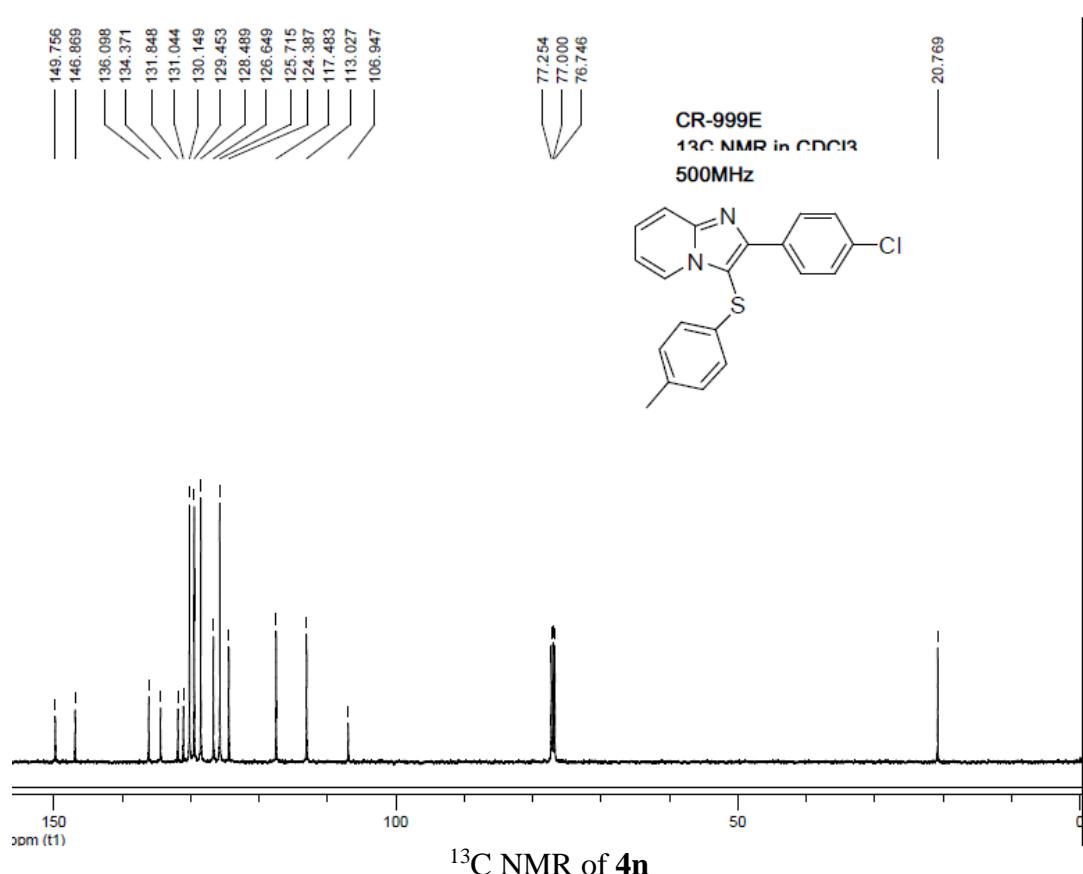
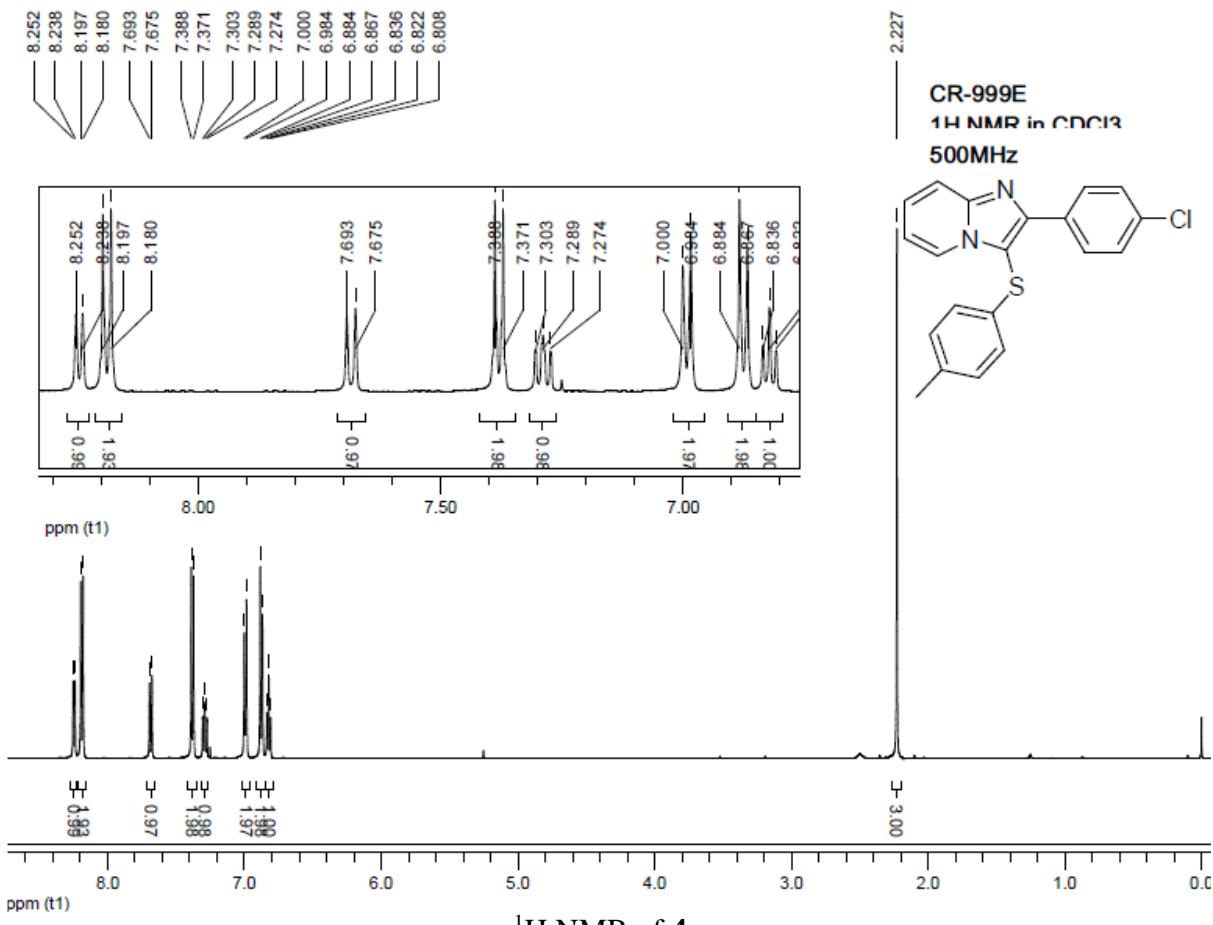


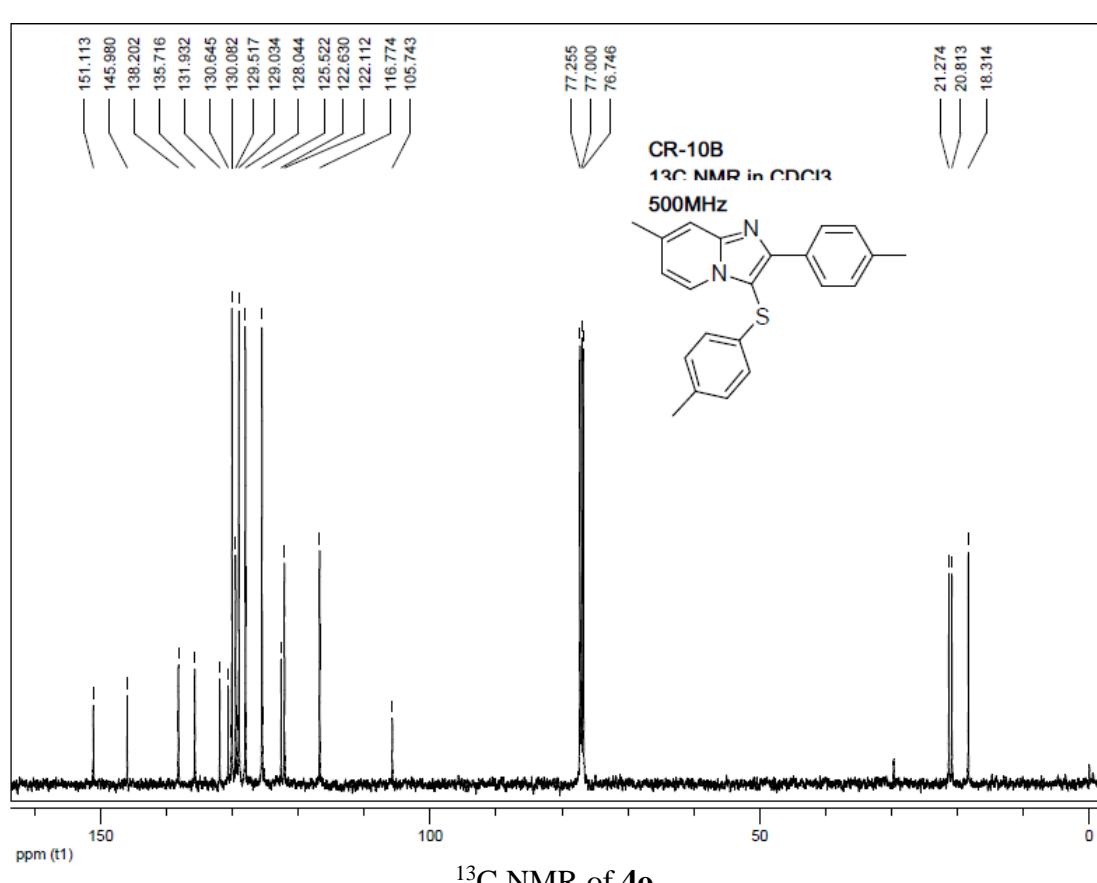
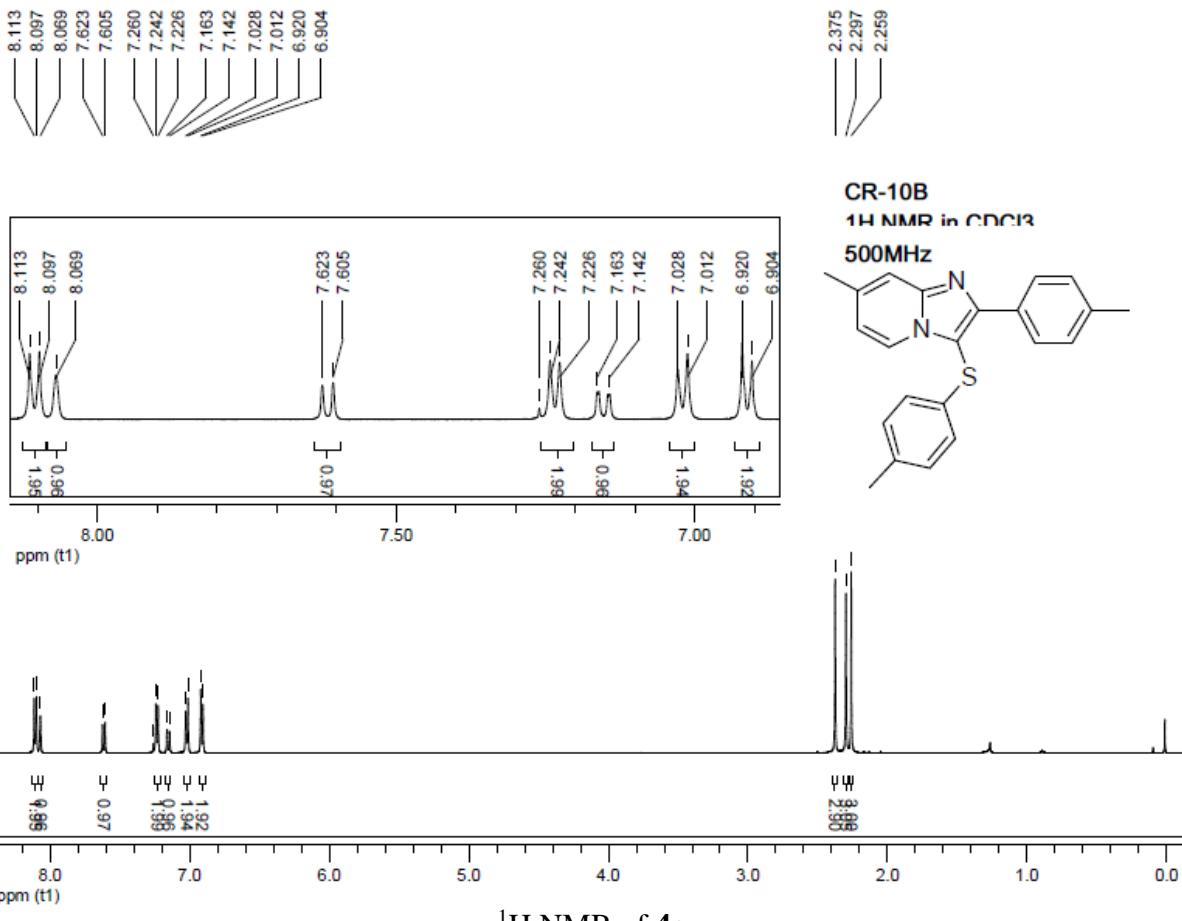
<sup>13</sup>C NMR of 4k

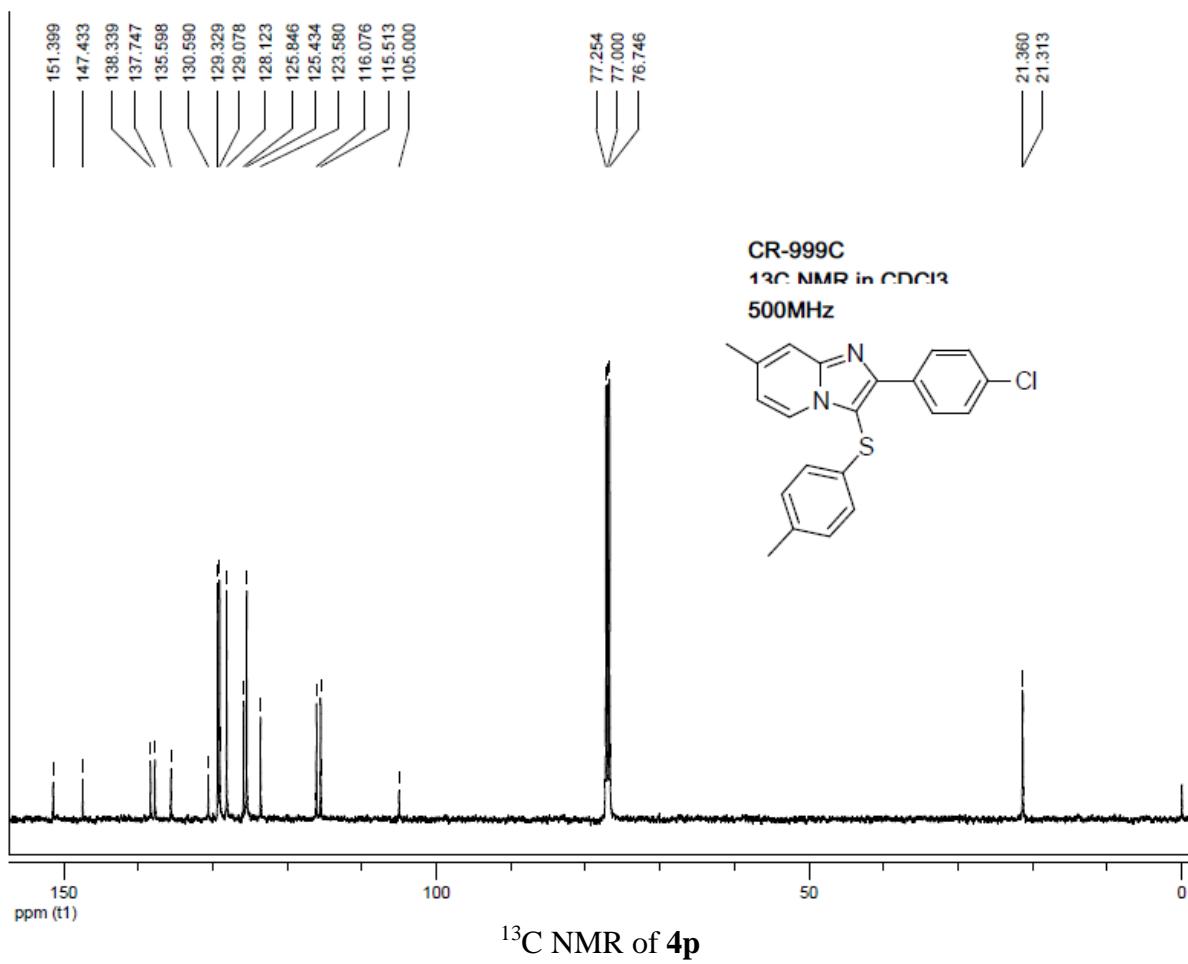
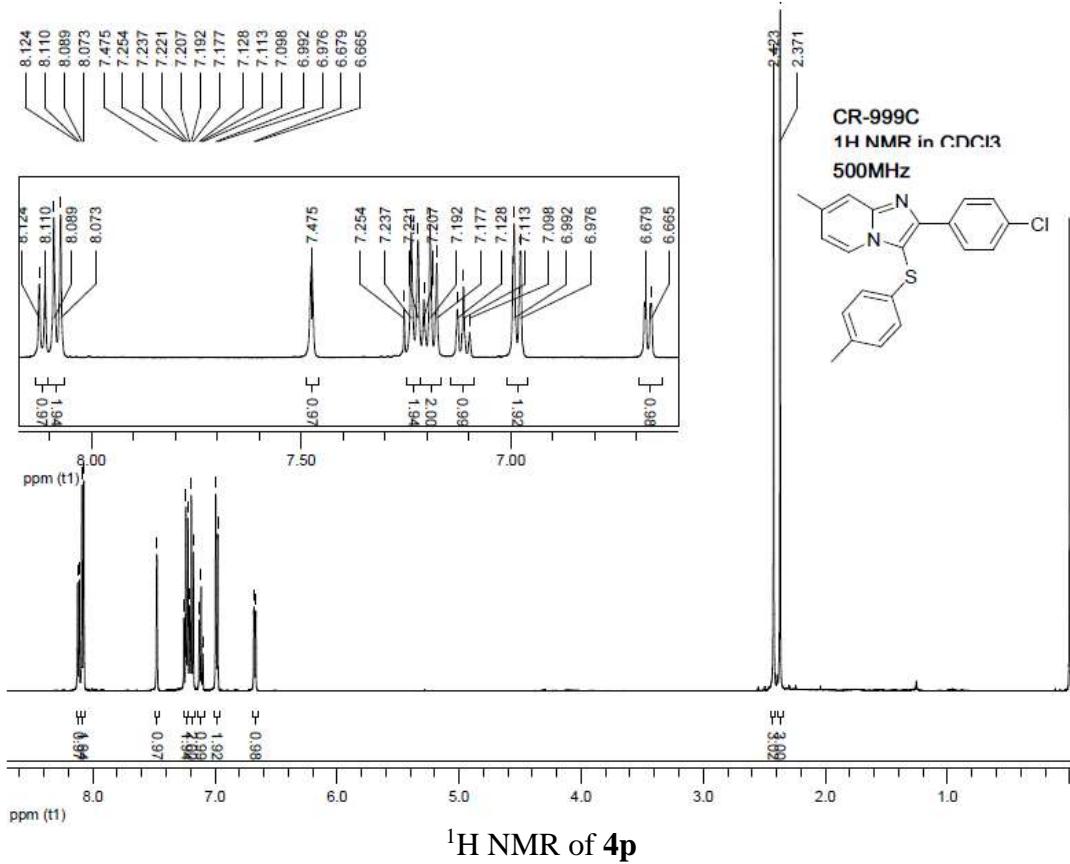


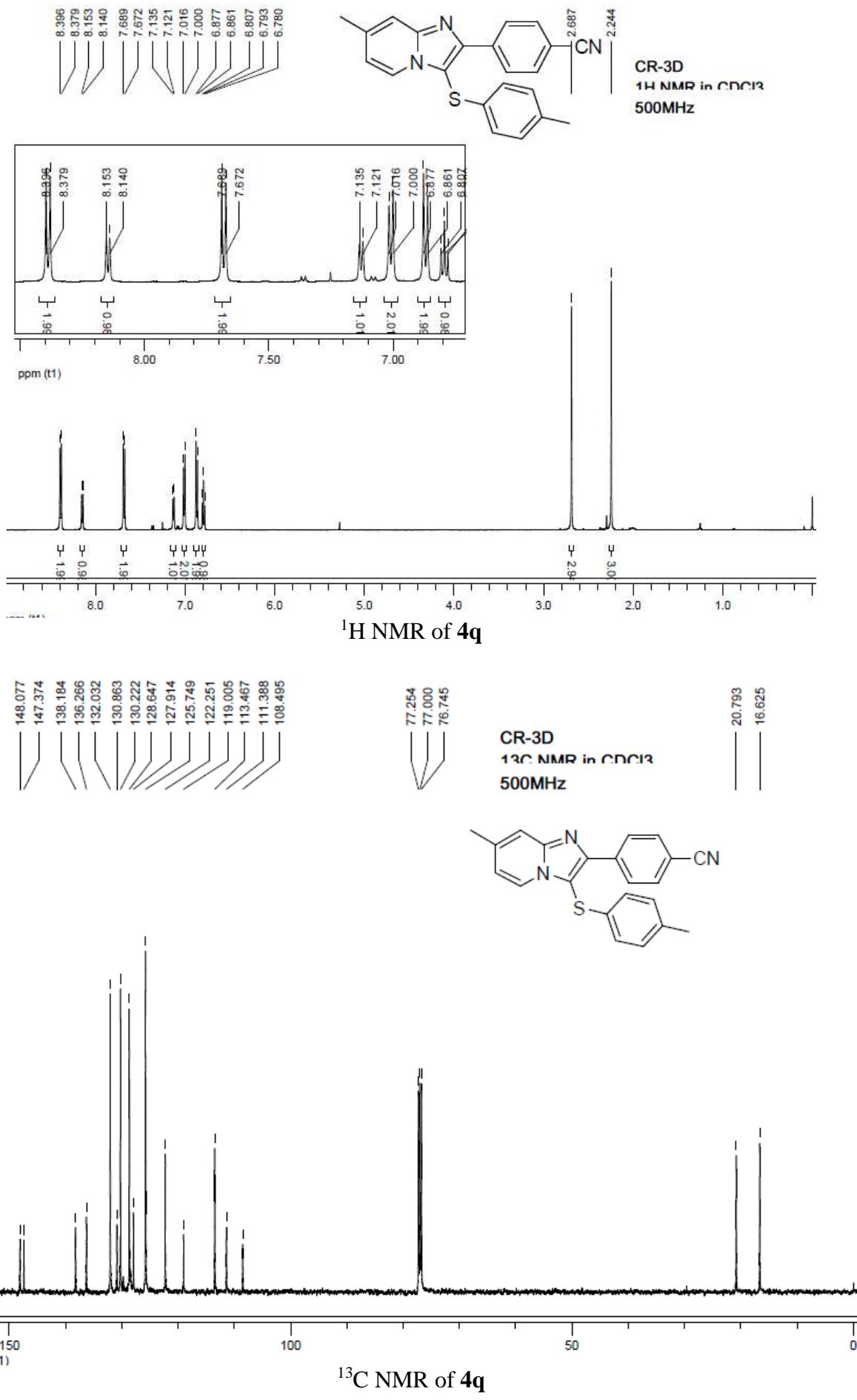
<sup>13</sup>C NMR of 4l

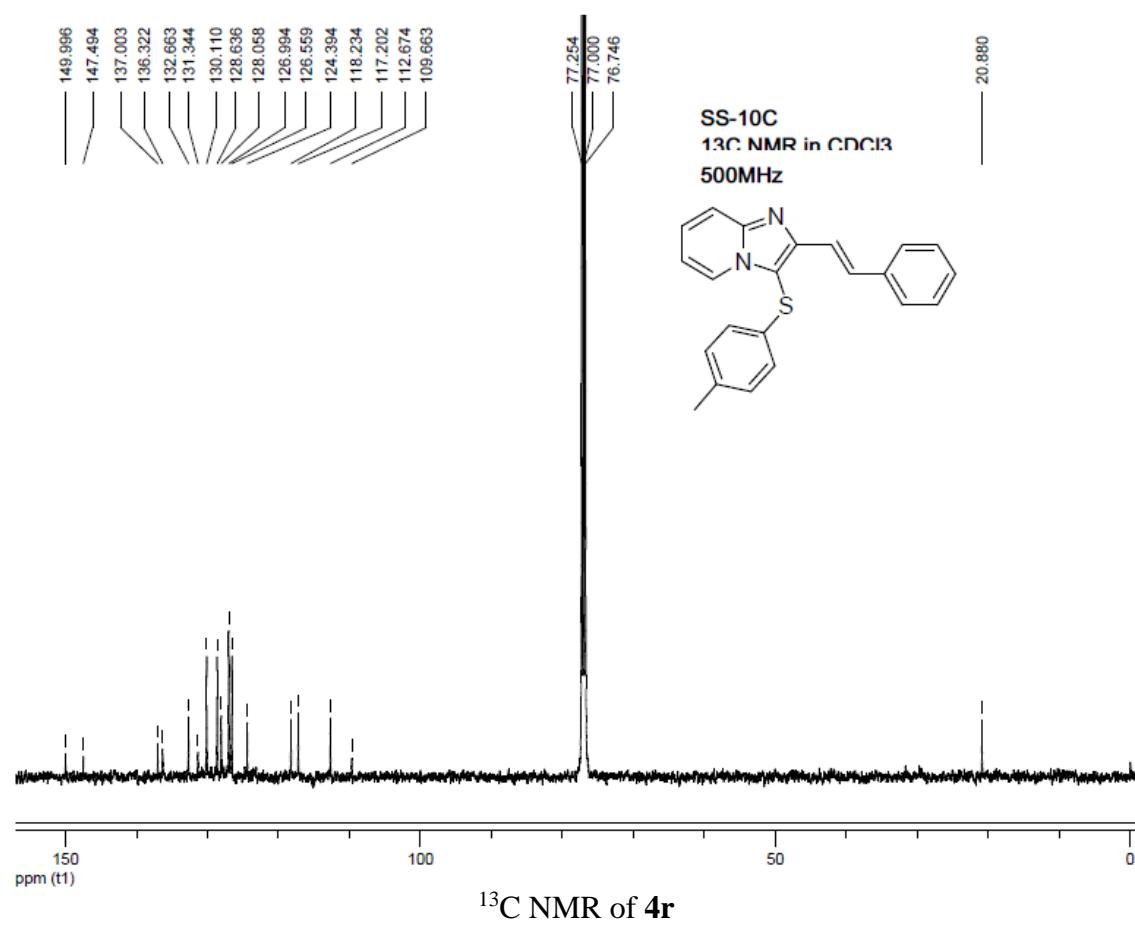
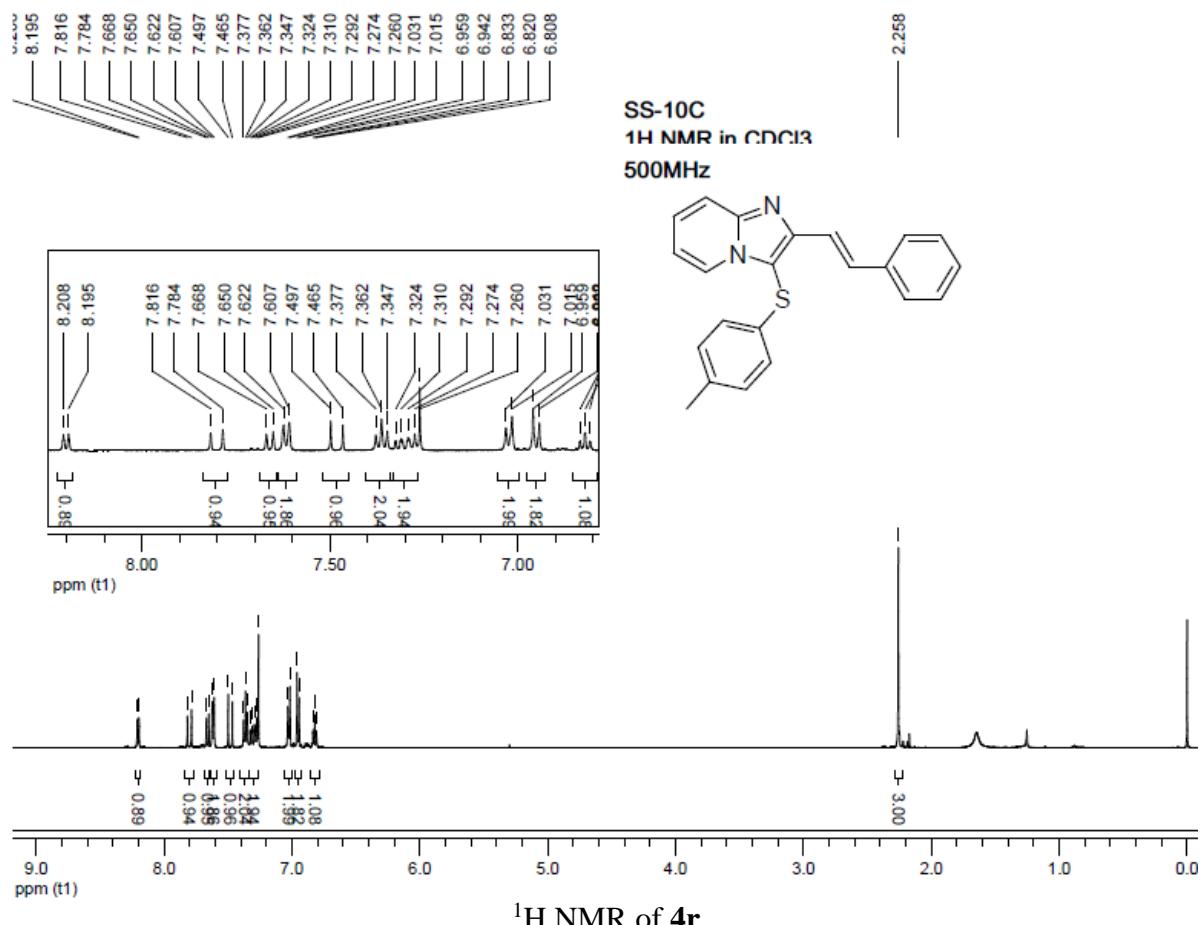


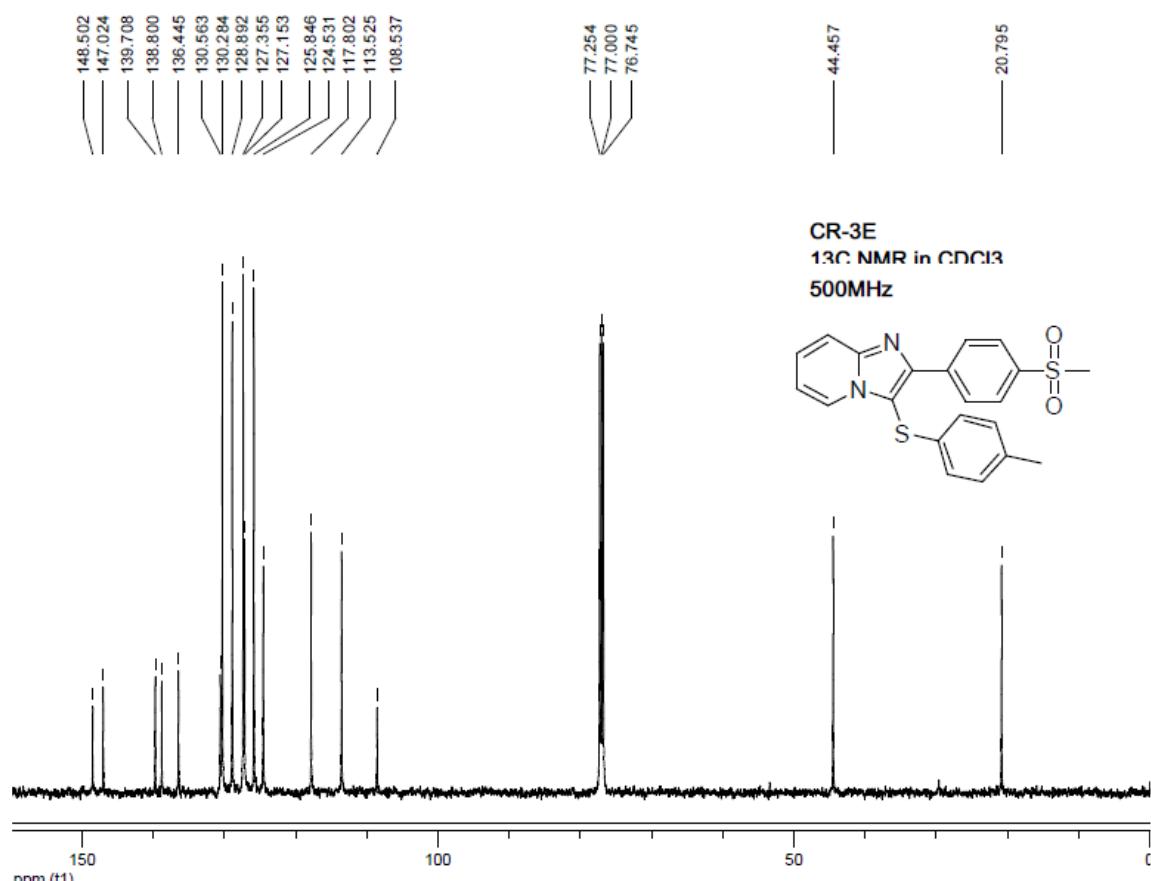
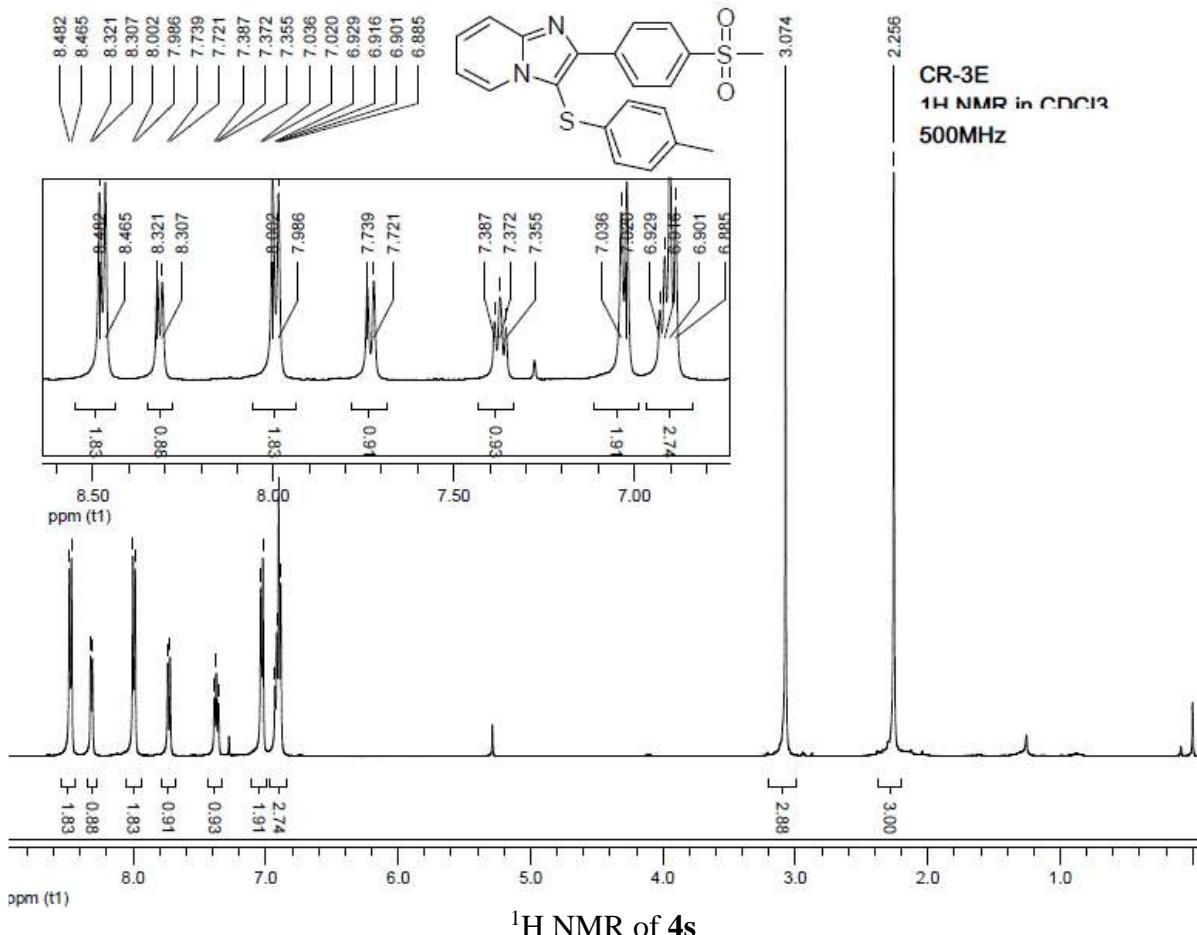


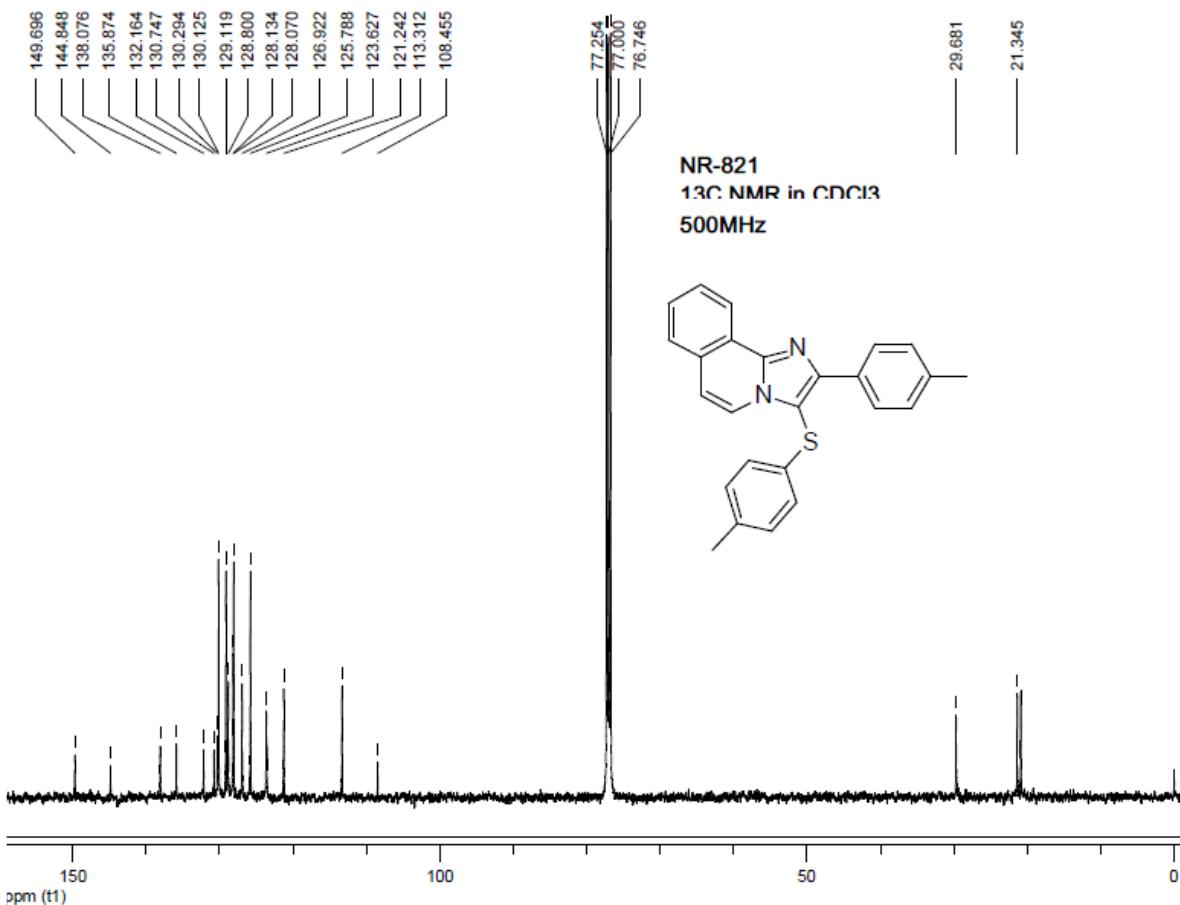
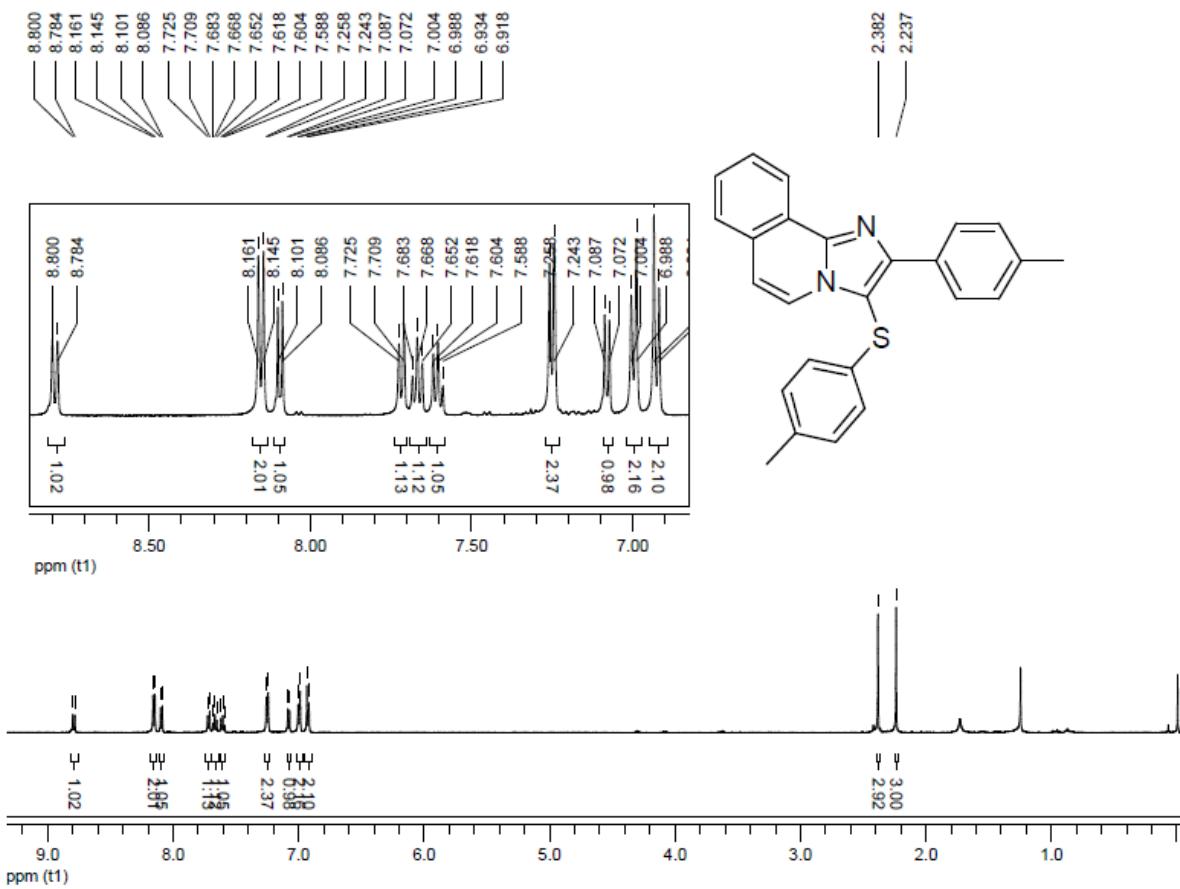


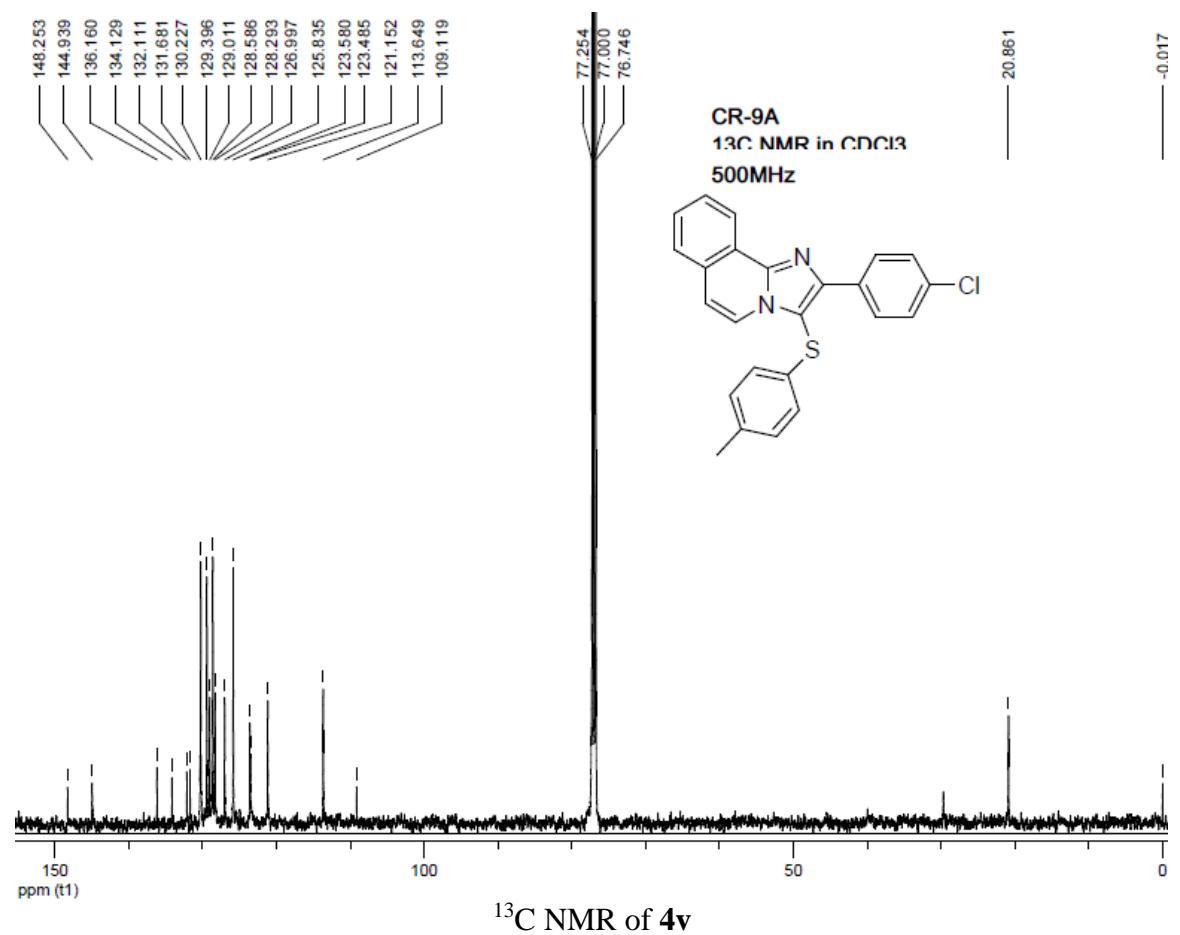
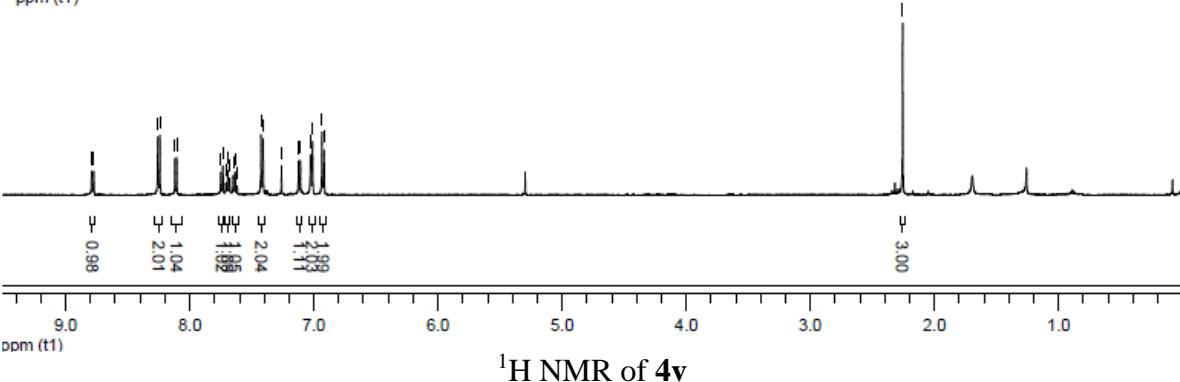
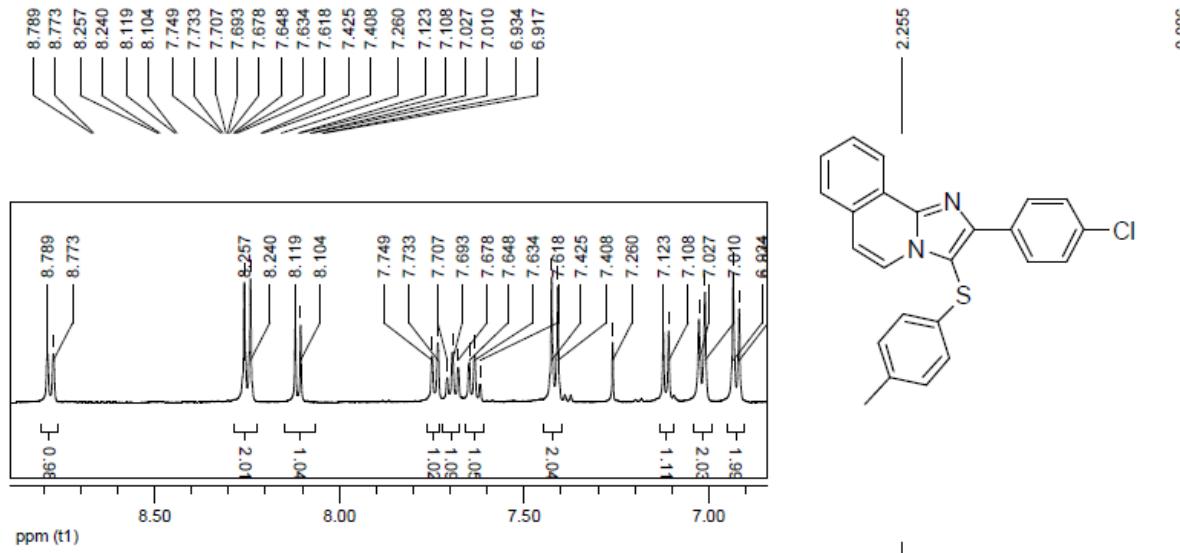


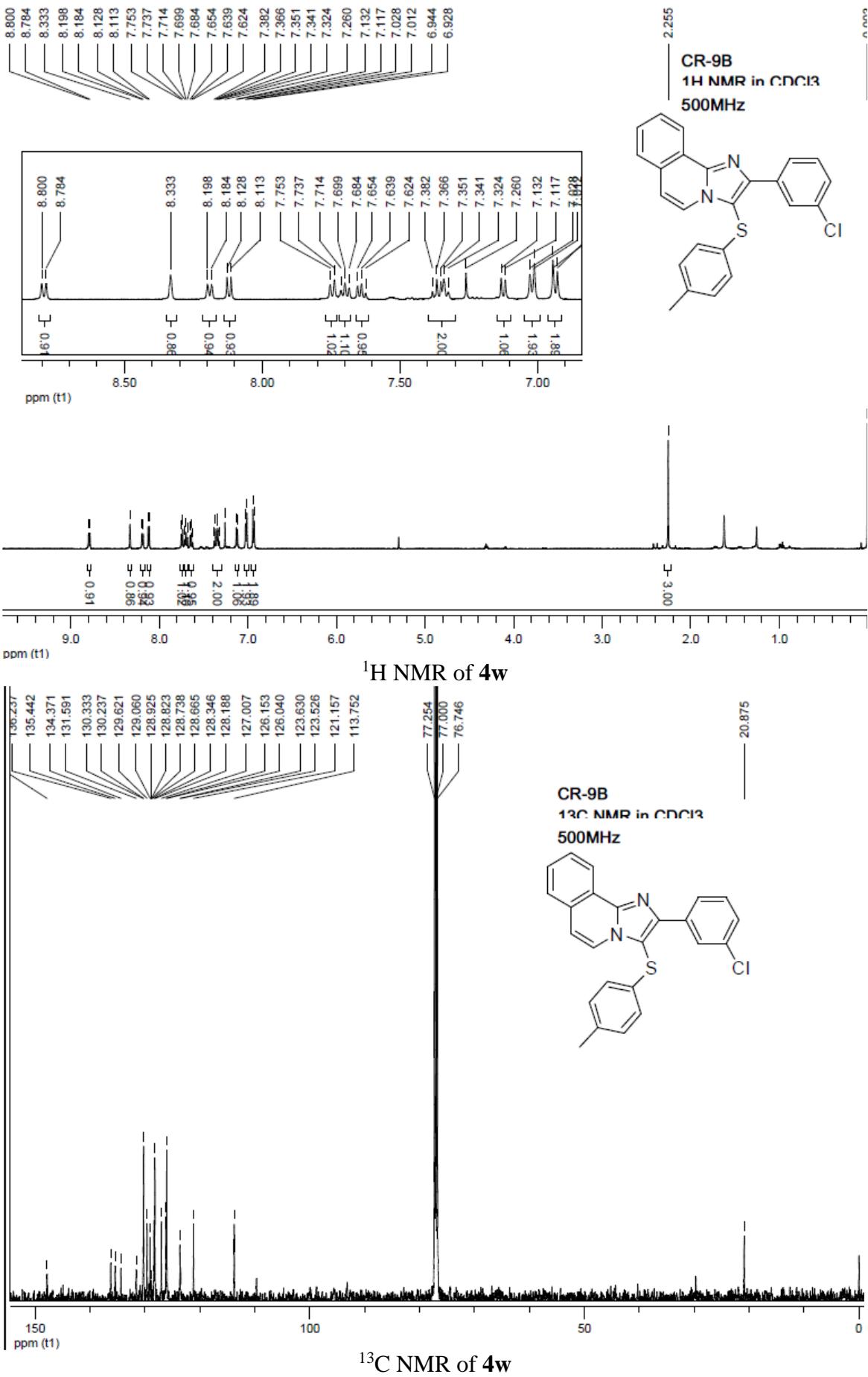


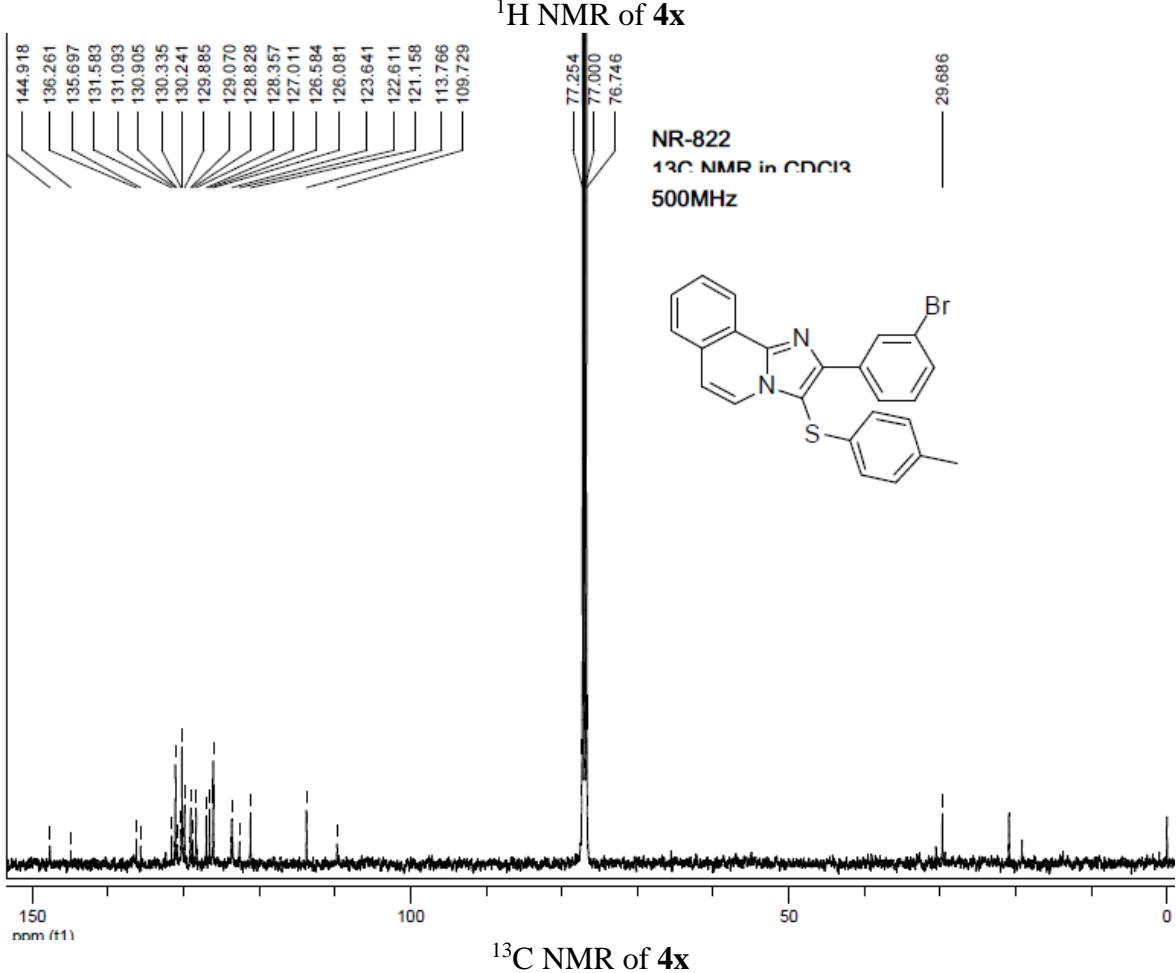
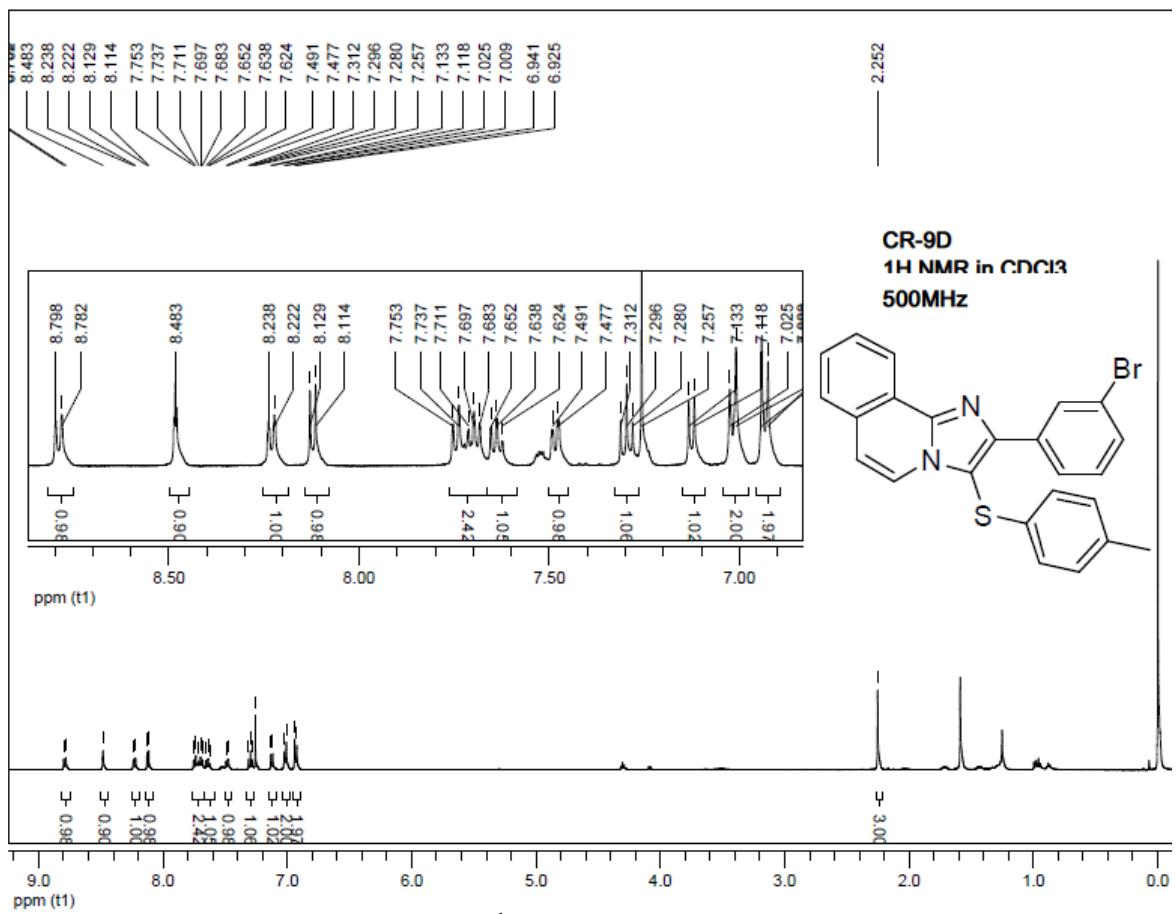


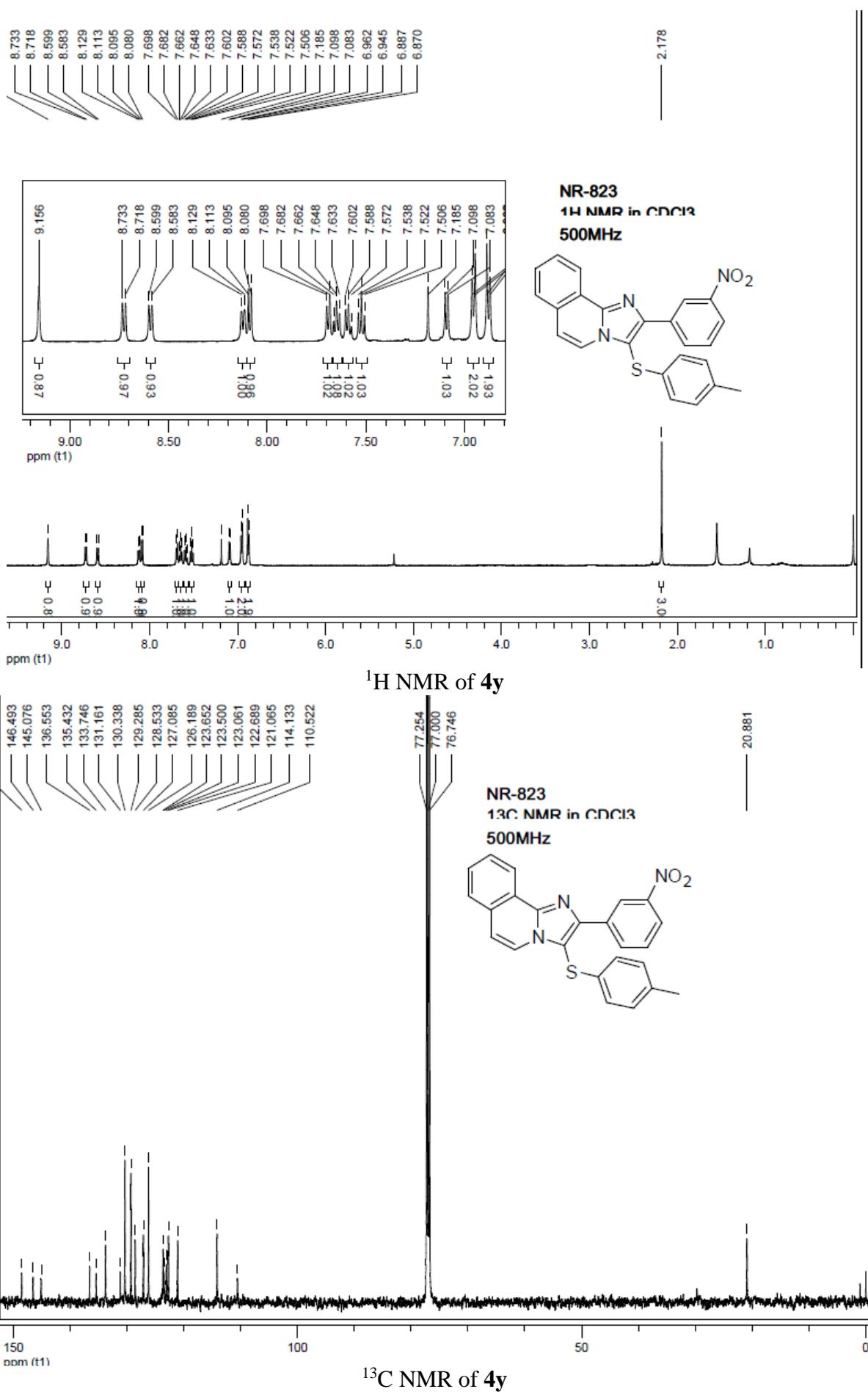


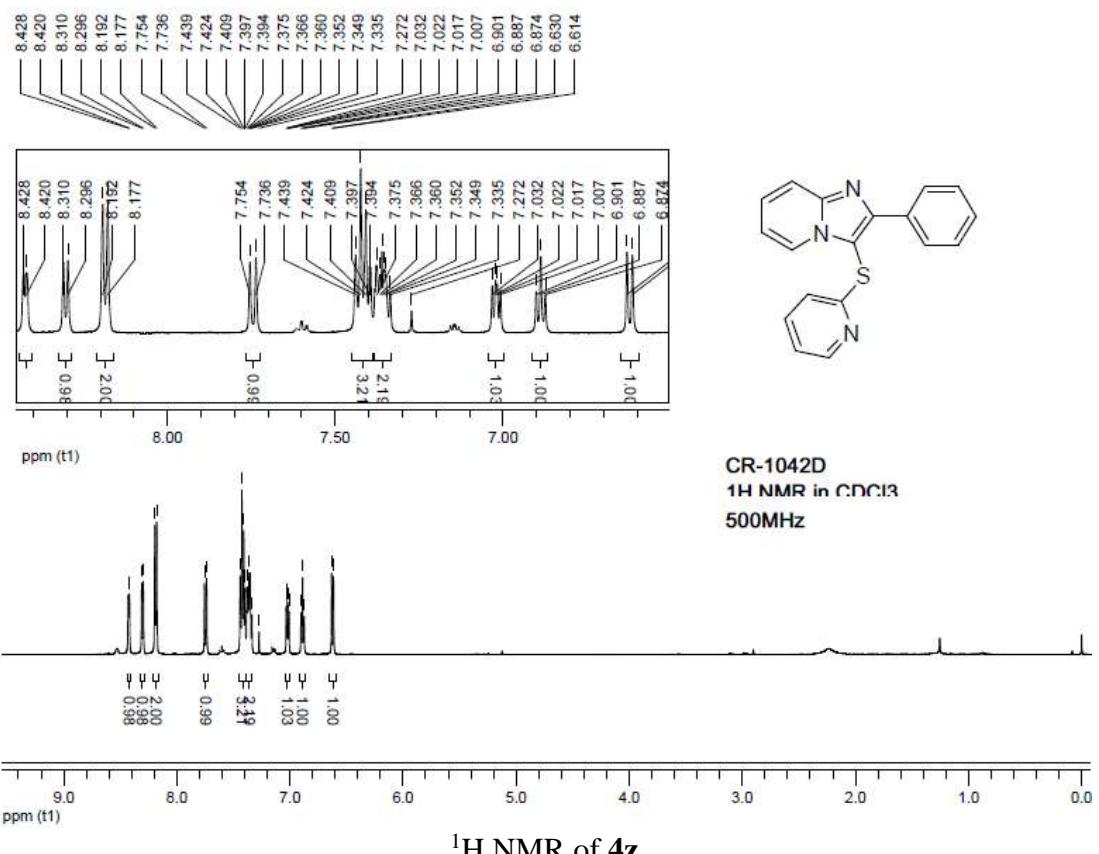




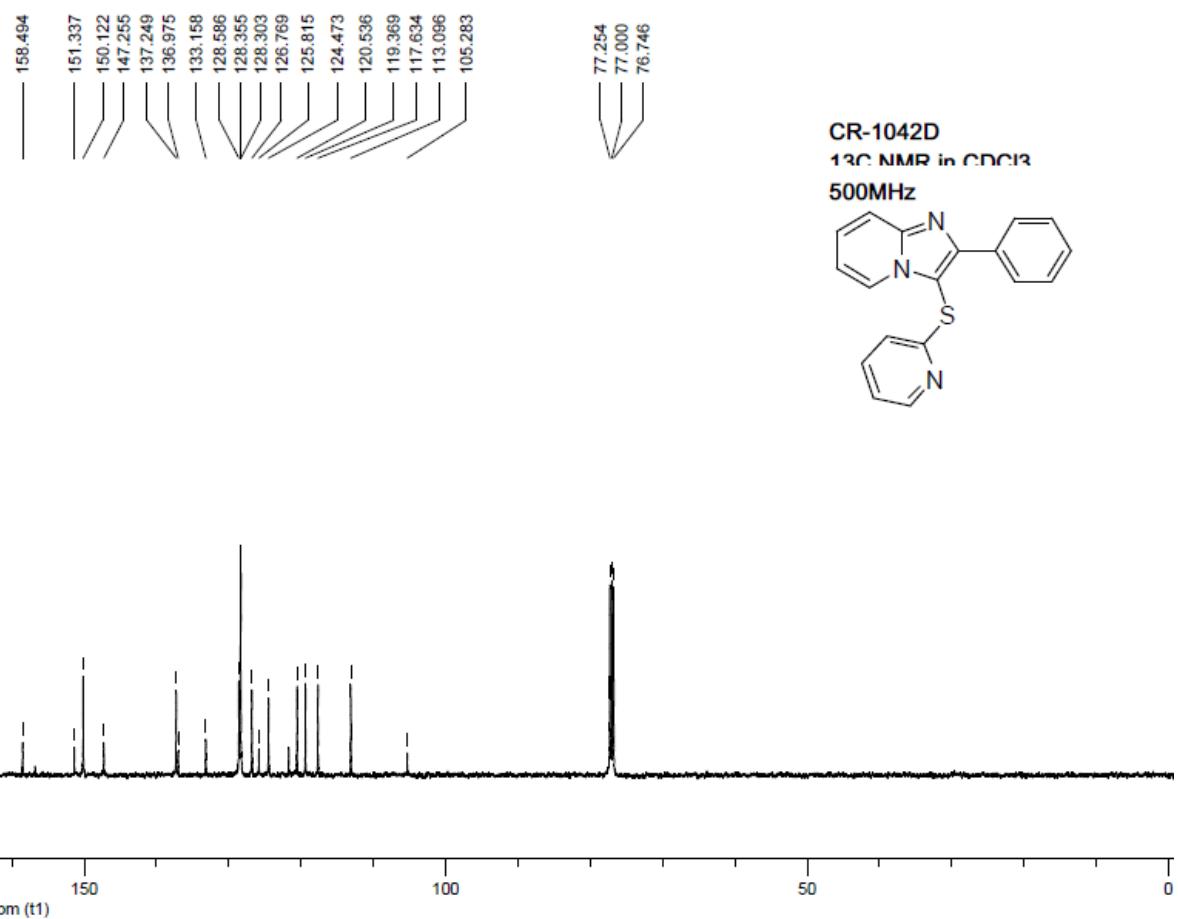




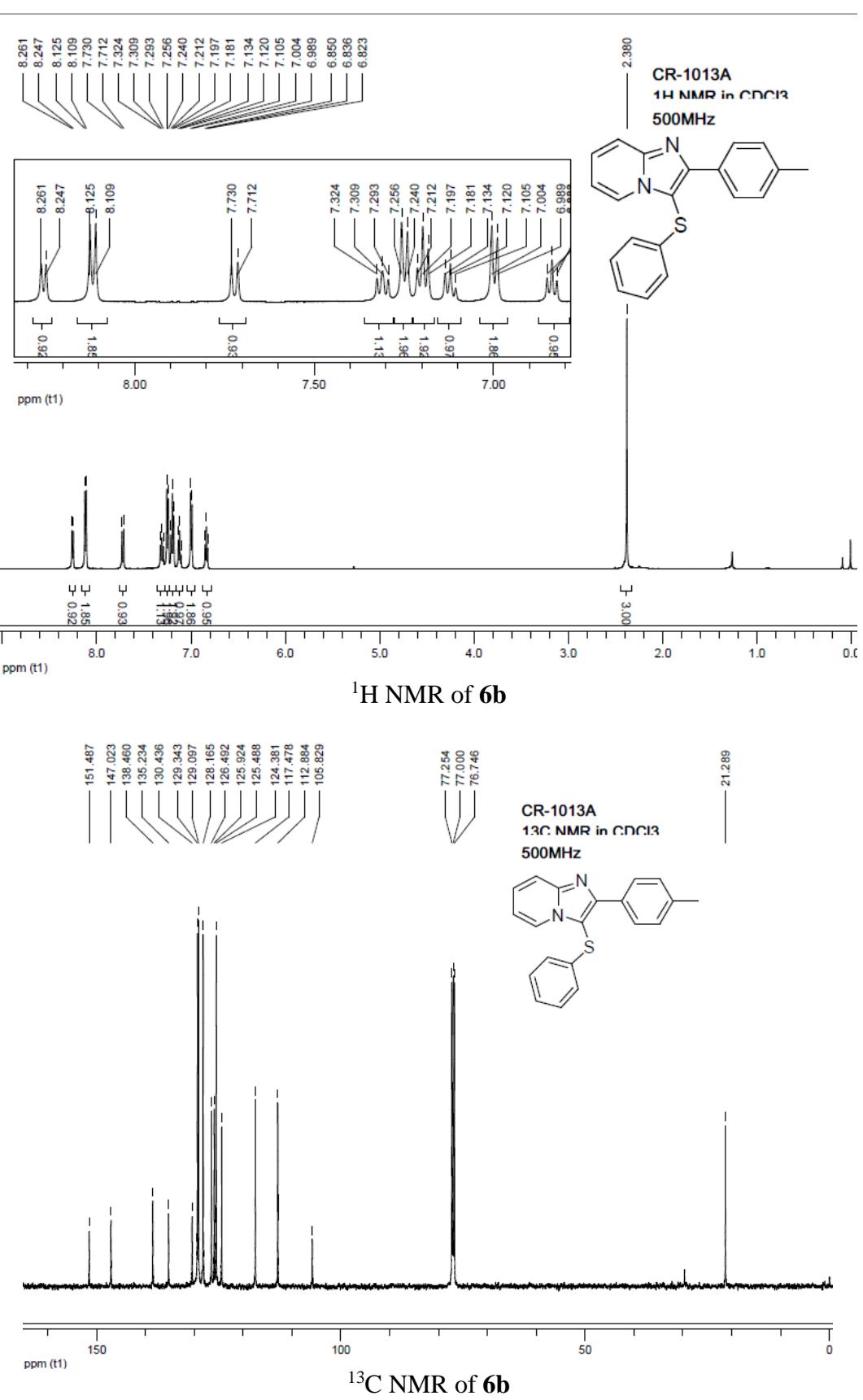


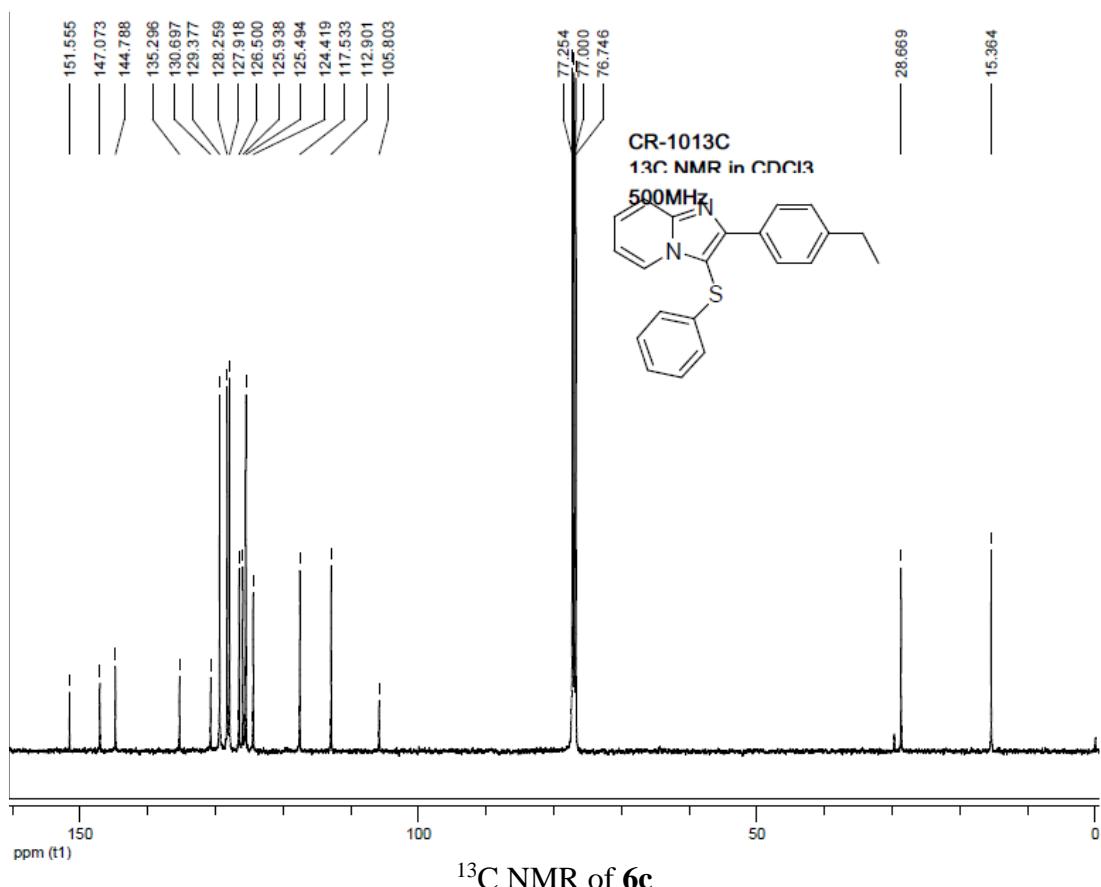
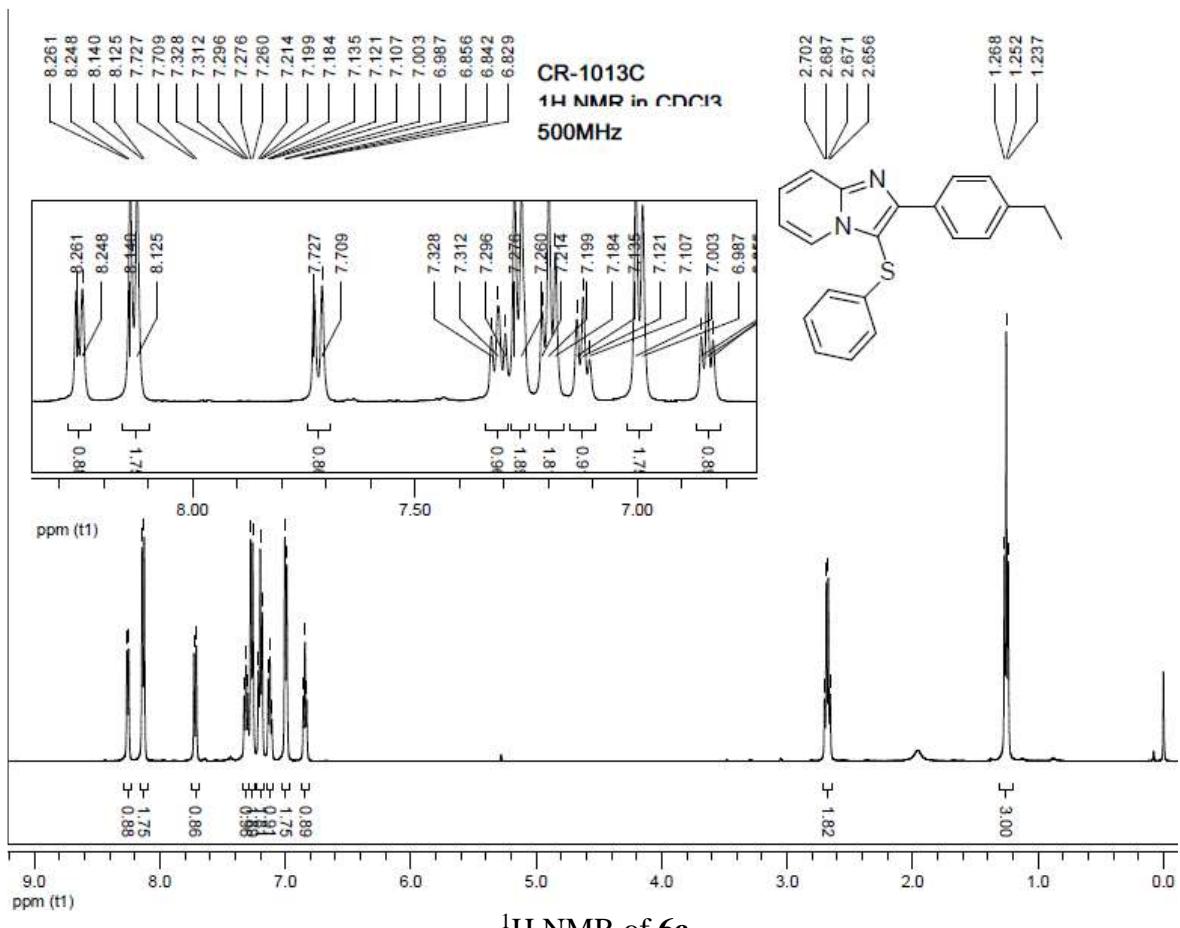


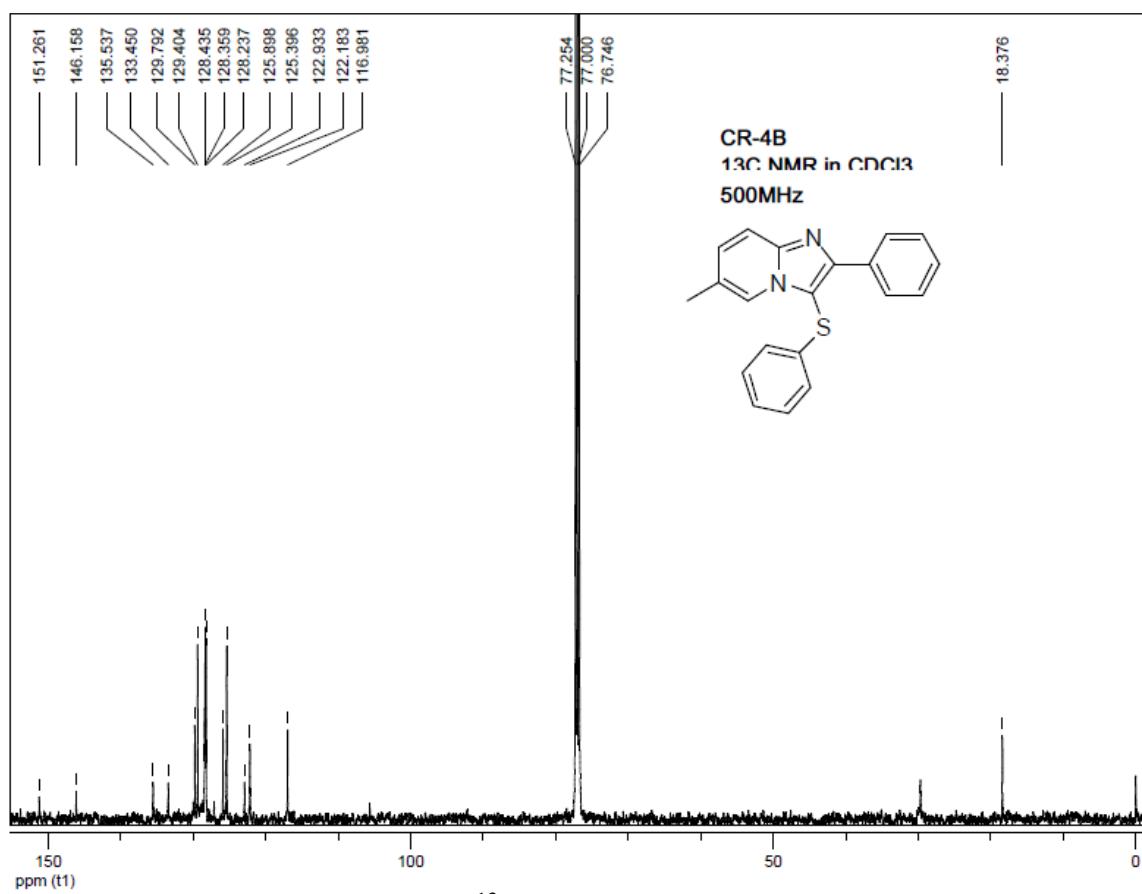
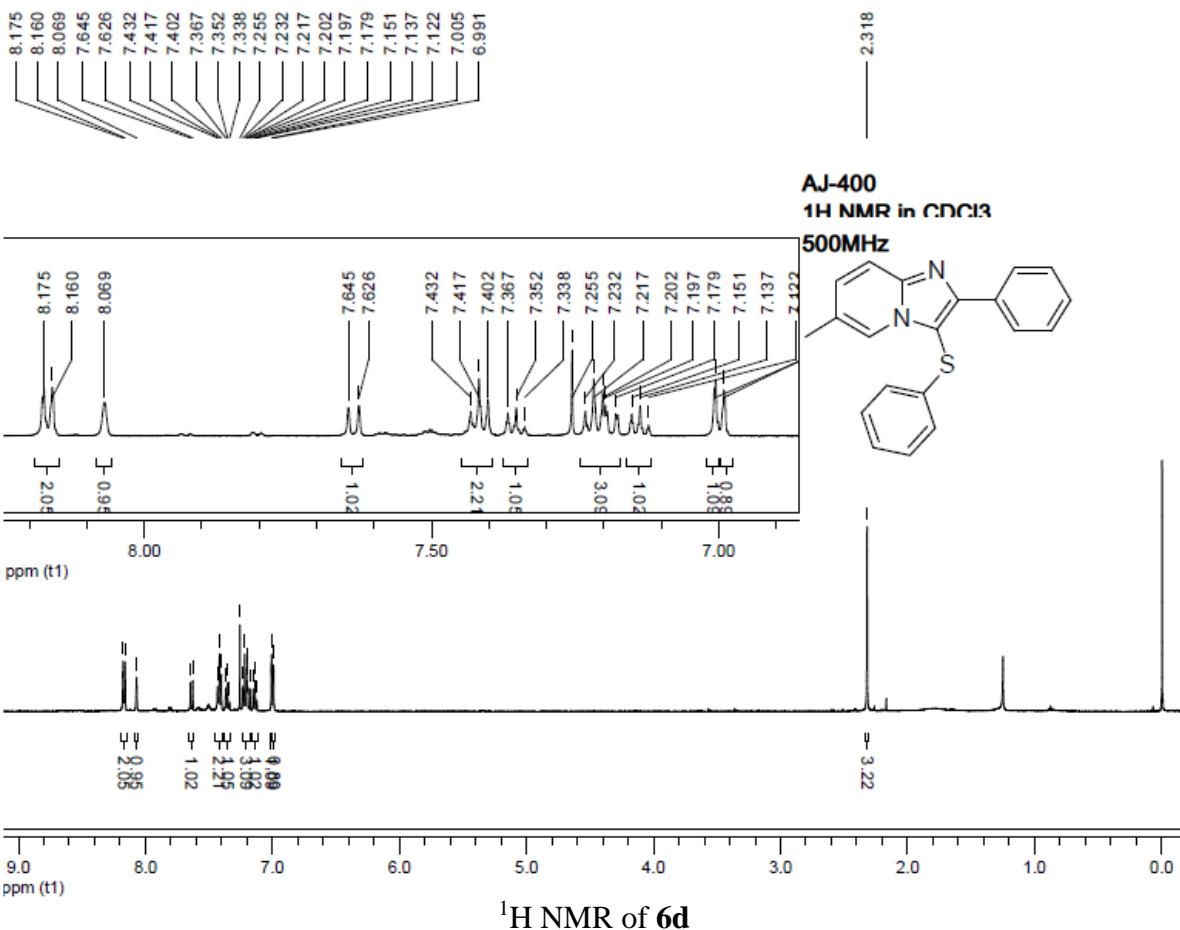
<sup>1</sup>H NMR of **4z**

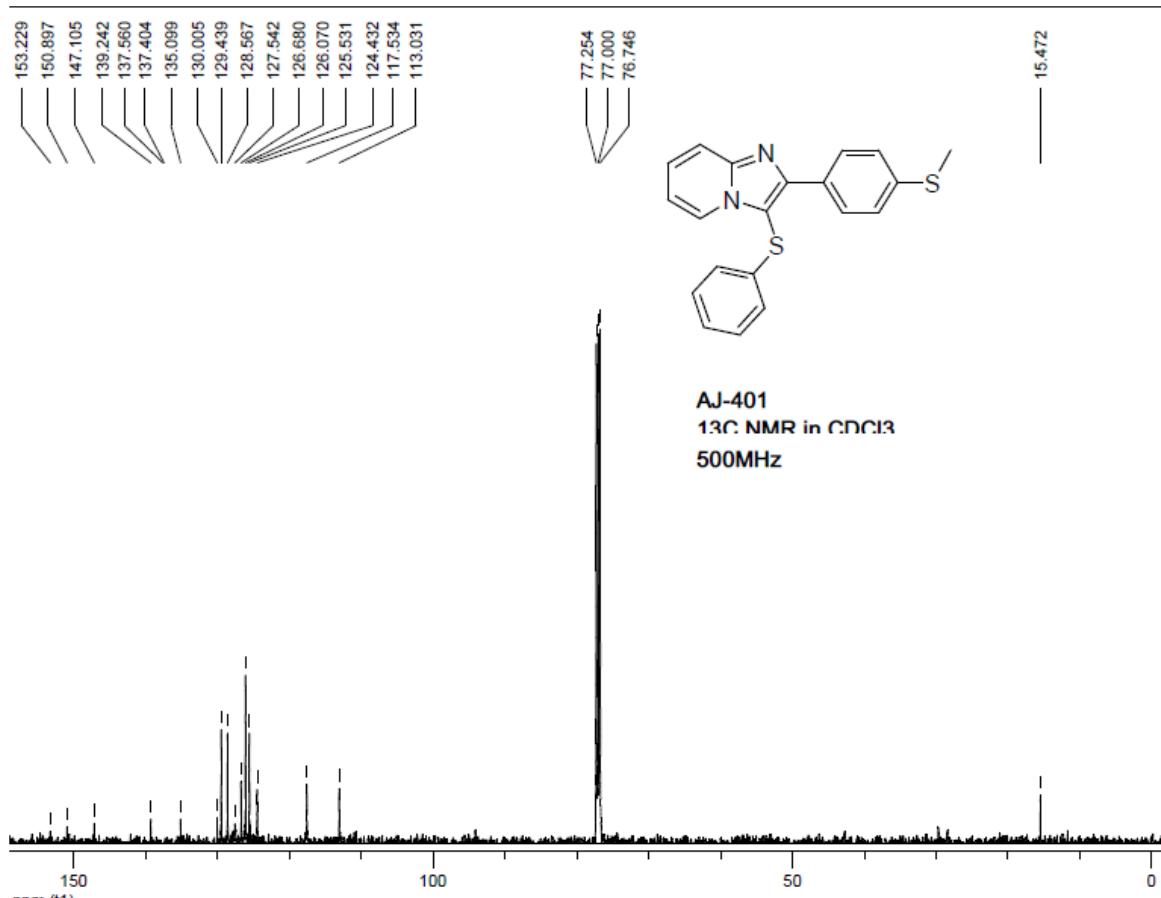
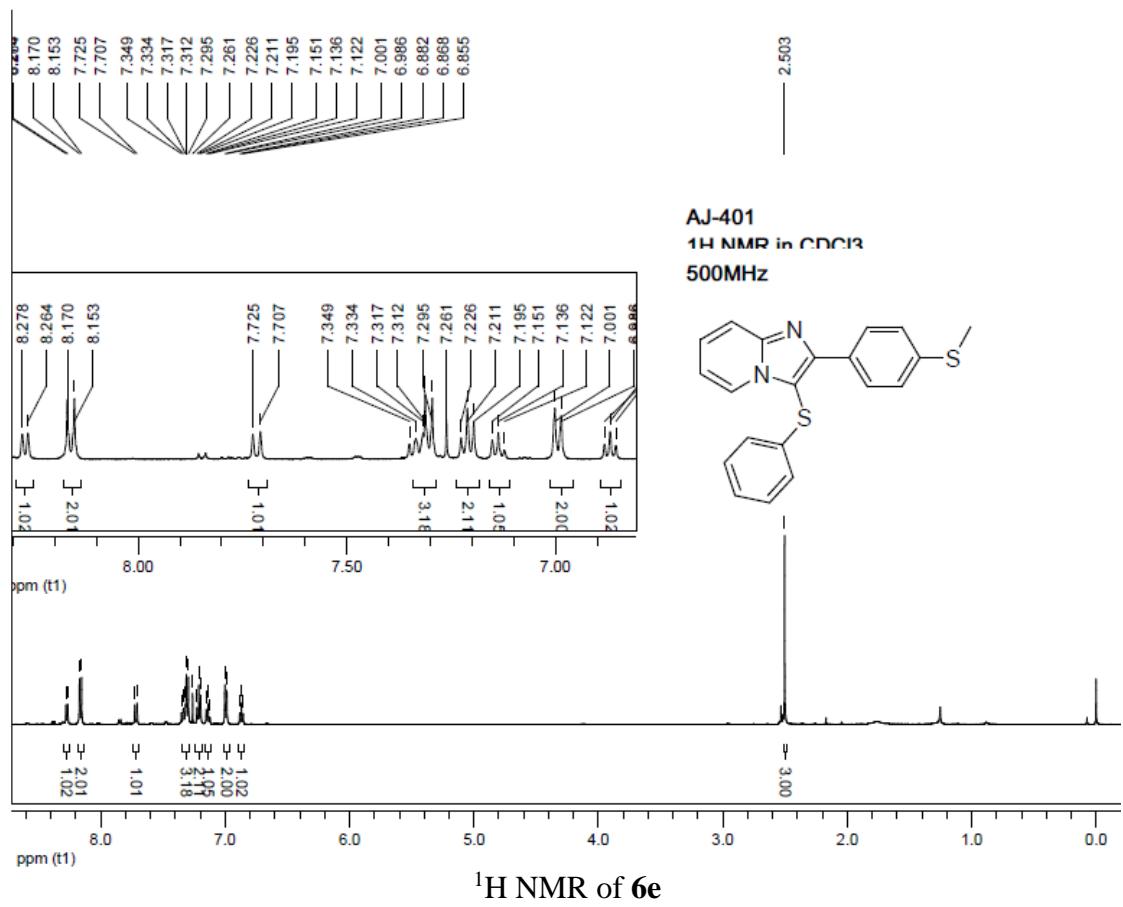


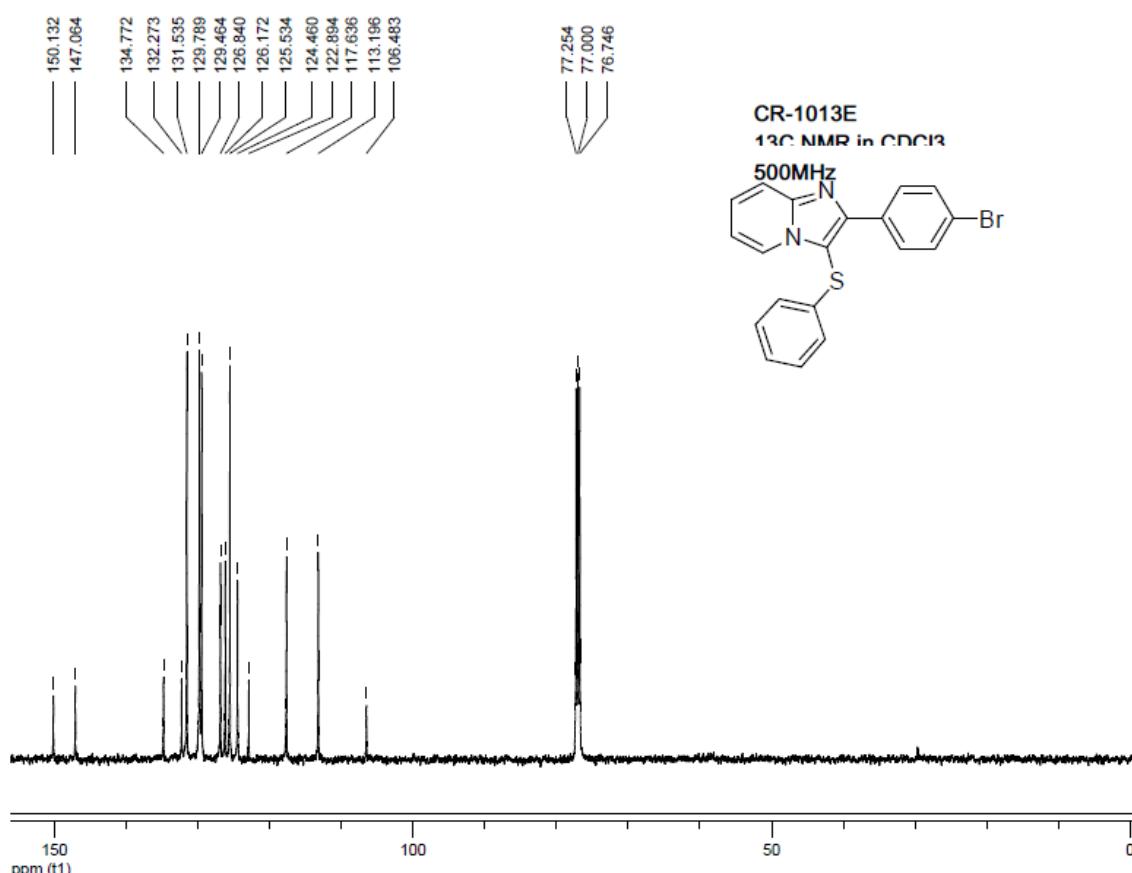
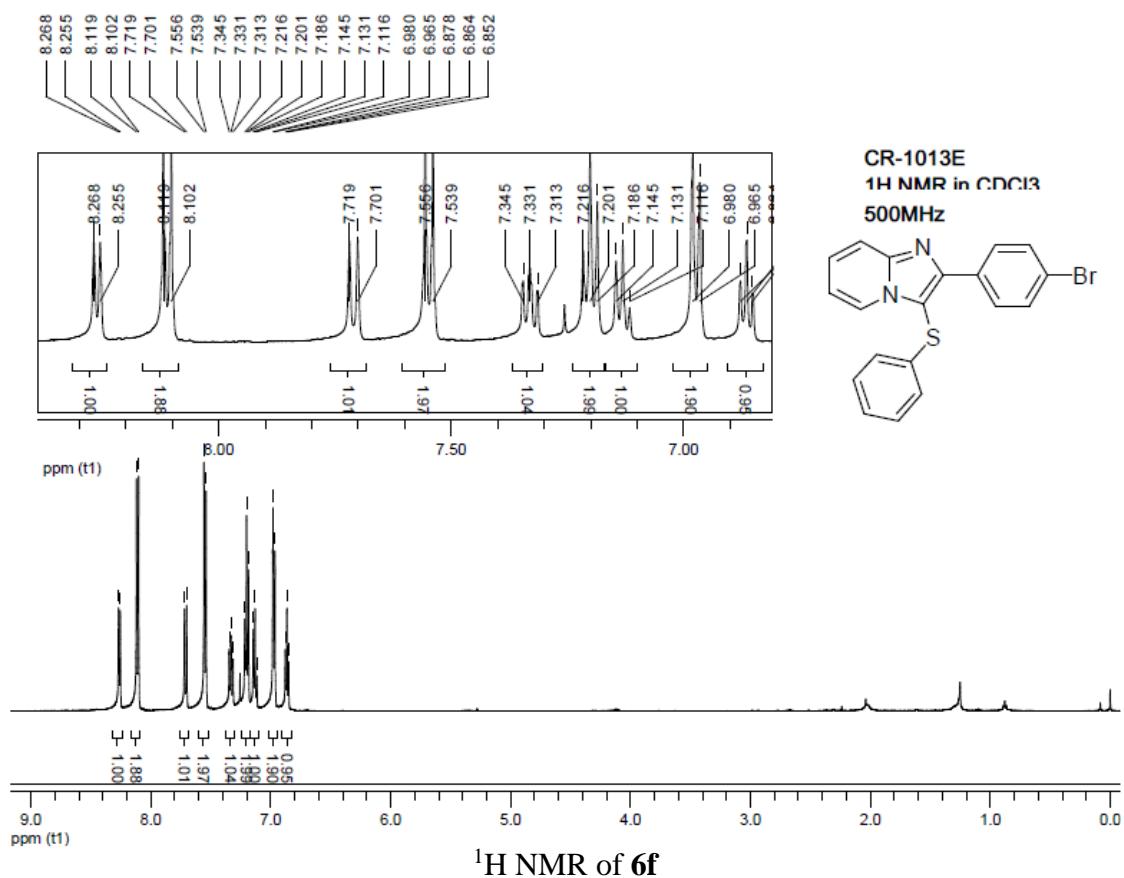
<sup>13</sup>C NMR of **4z**



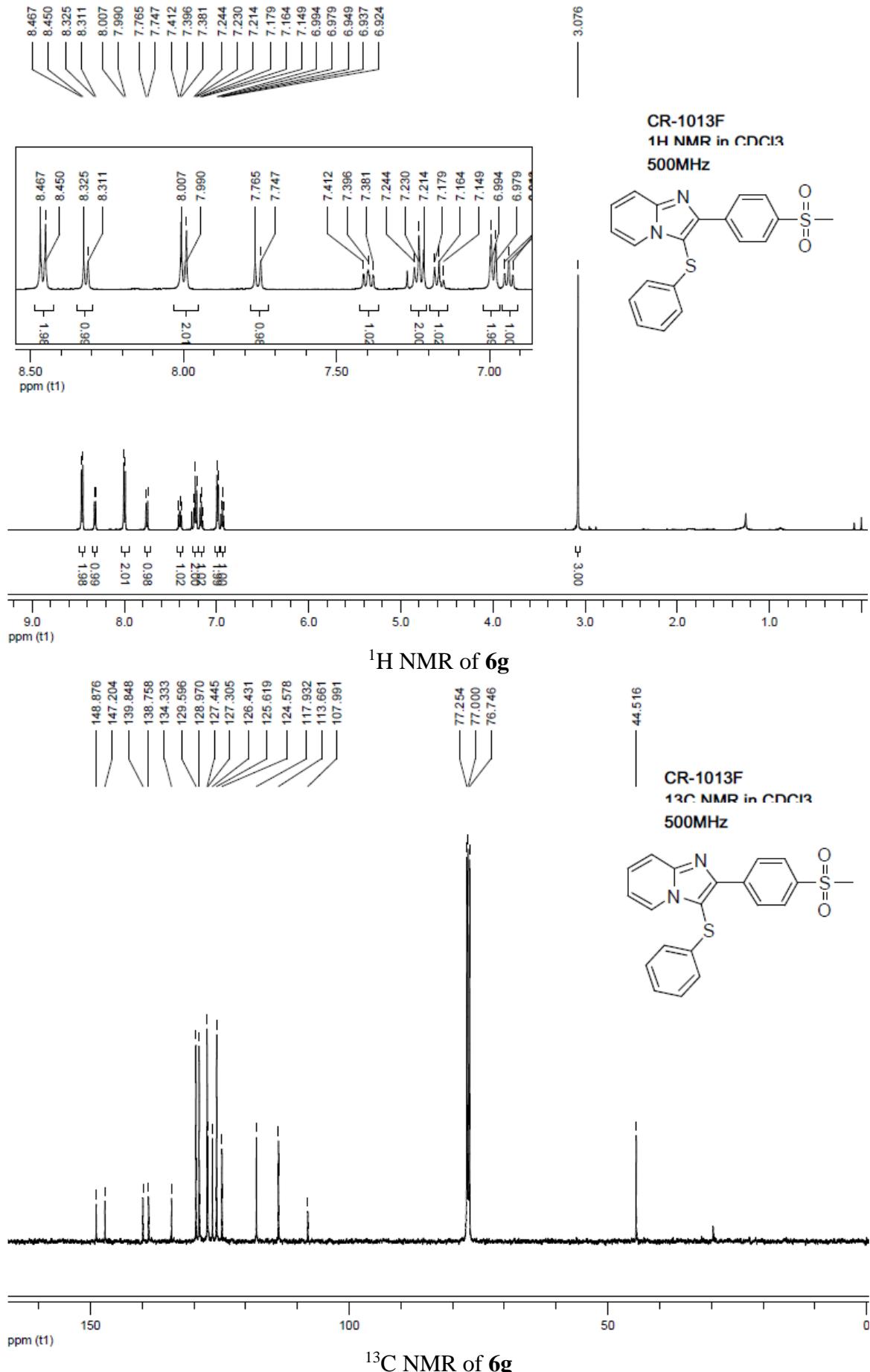


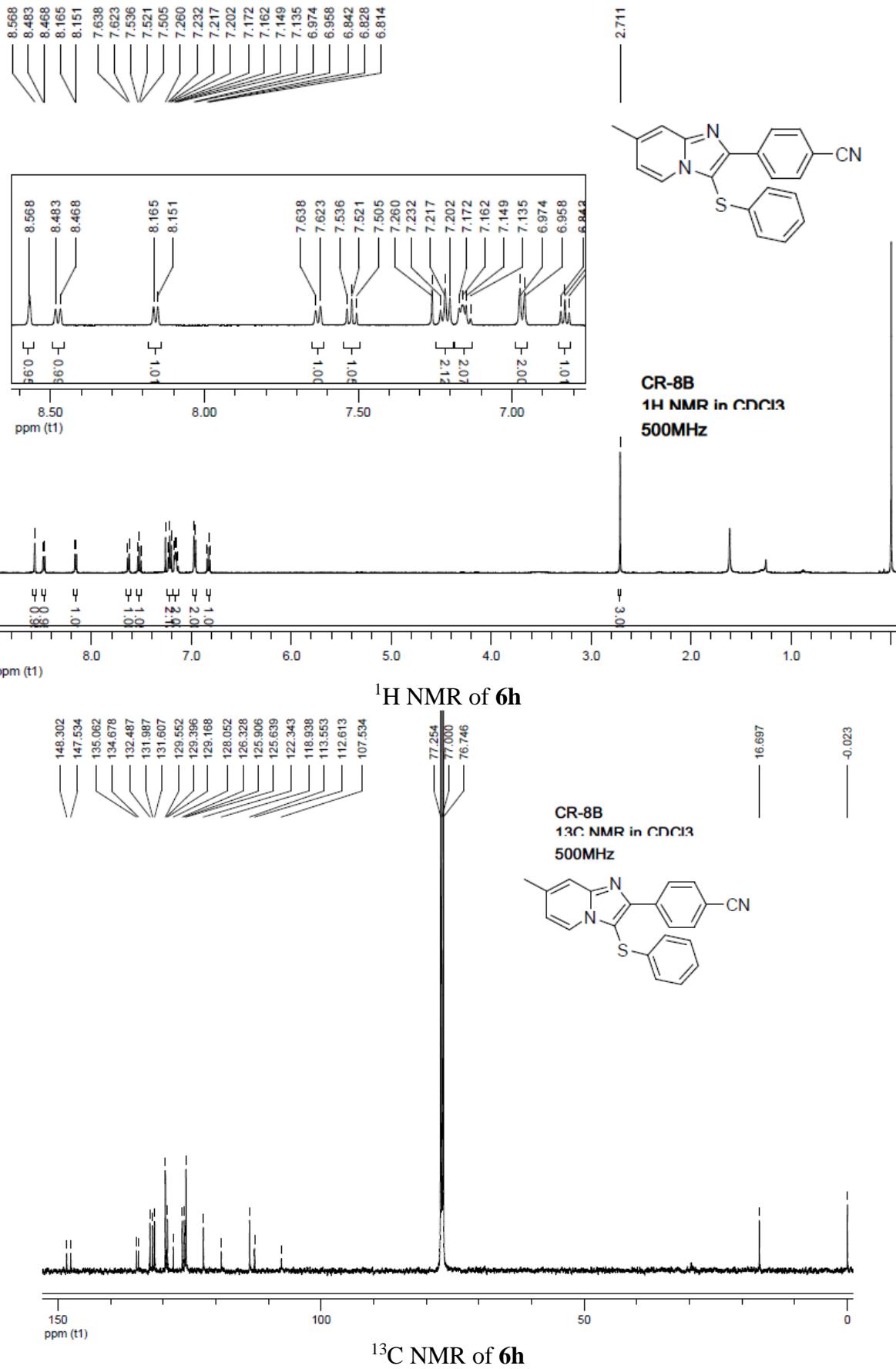


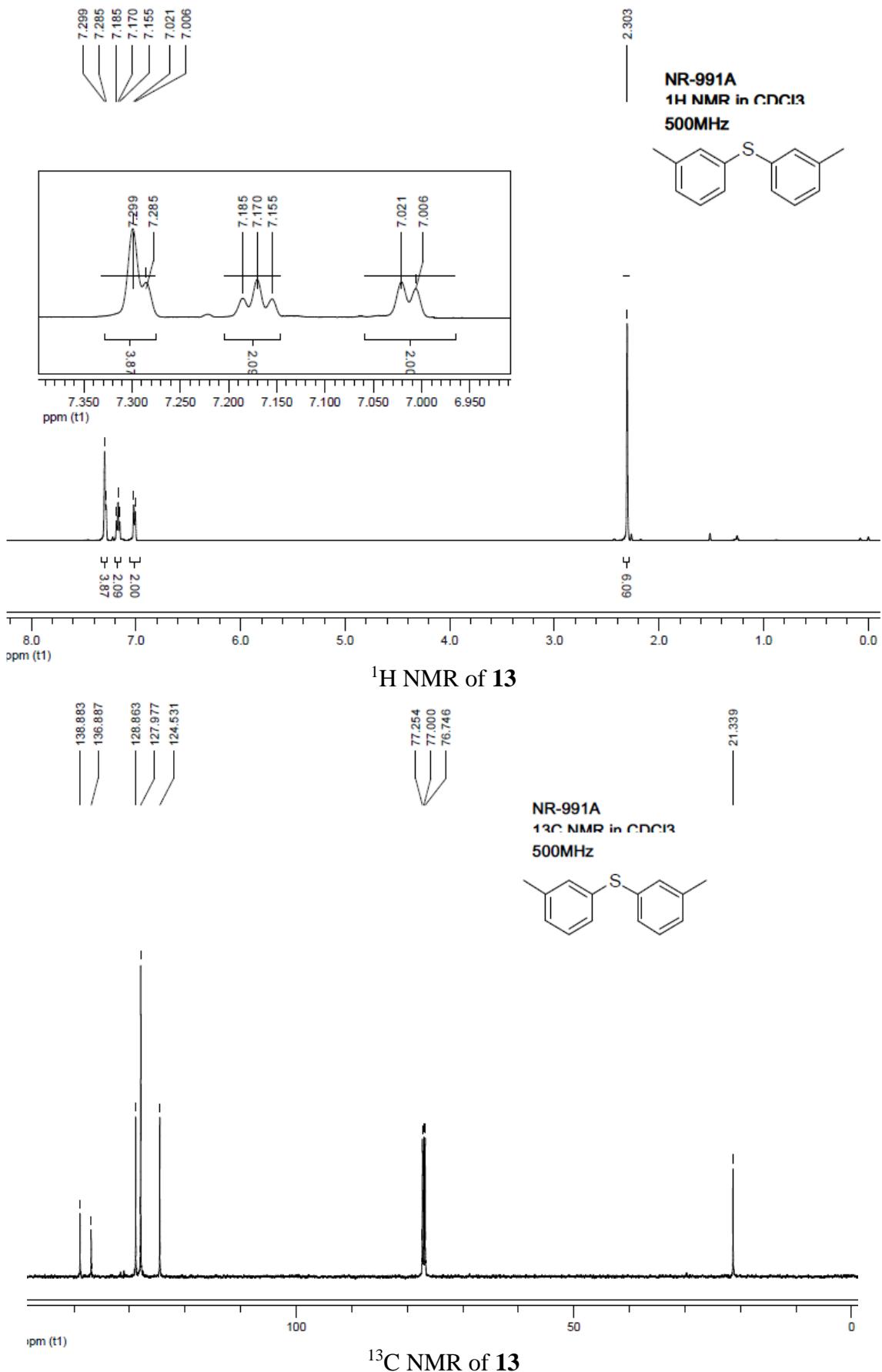




<sup>13</sup>C NMR of **6f**







## 5. Copies of HRMS spectra

Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

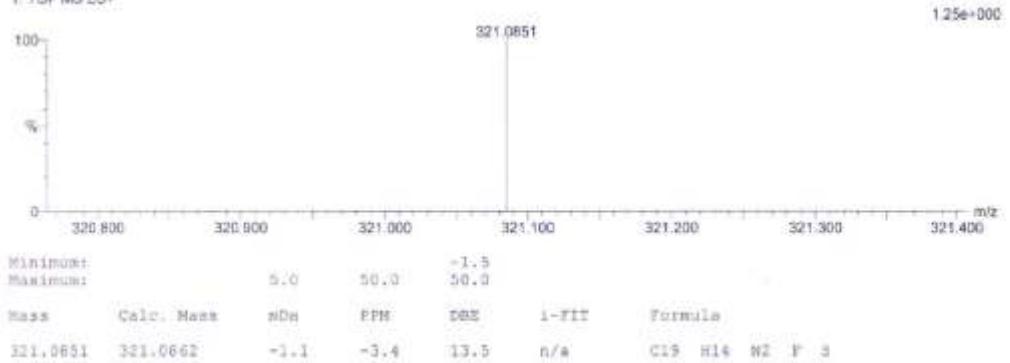
2D formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-19 H: 0-14 N: 0-2 F: 0-1 S: 0-1 Zn: 0-1

CR 95.0 24 (0.445)

I: TOF MS ES+



HRMS of 4c

Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

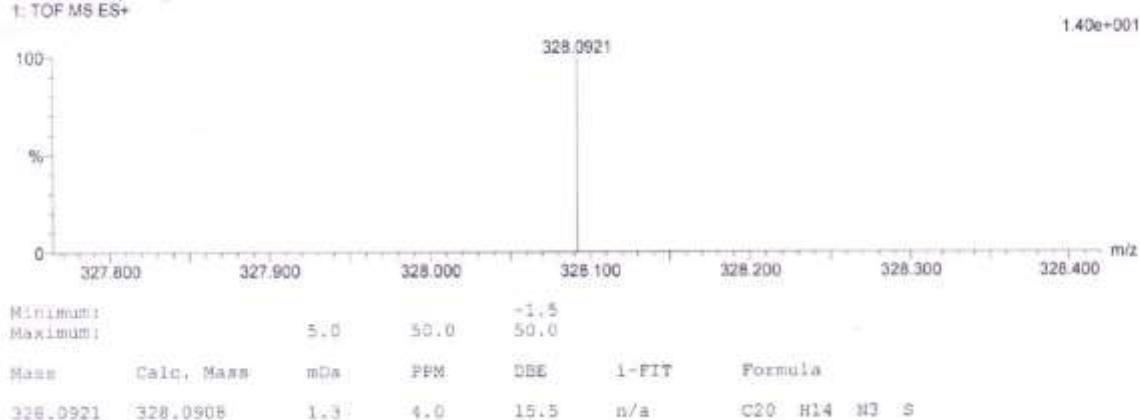
14 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-20 H: 0-14 N: 0-3 S: 0-1 Zn: 0-1

CR 15 A 1.45 (0.834)

I: TOF MS ES+



HRMS of 4d

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

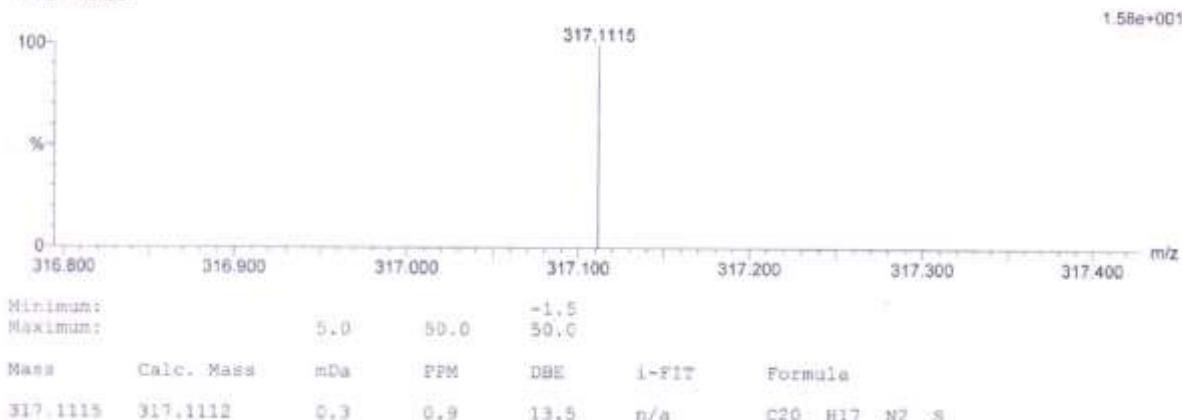
3 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-20 H: 0-17 N: 0-2 S: 0-1 Zn: 0-1

CR 99/ A 34 (0.631)

1: TOF MS ES+



### HRMS of 4i

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

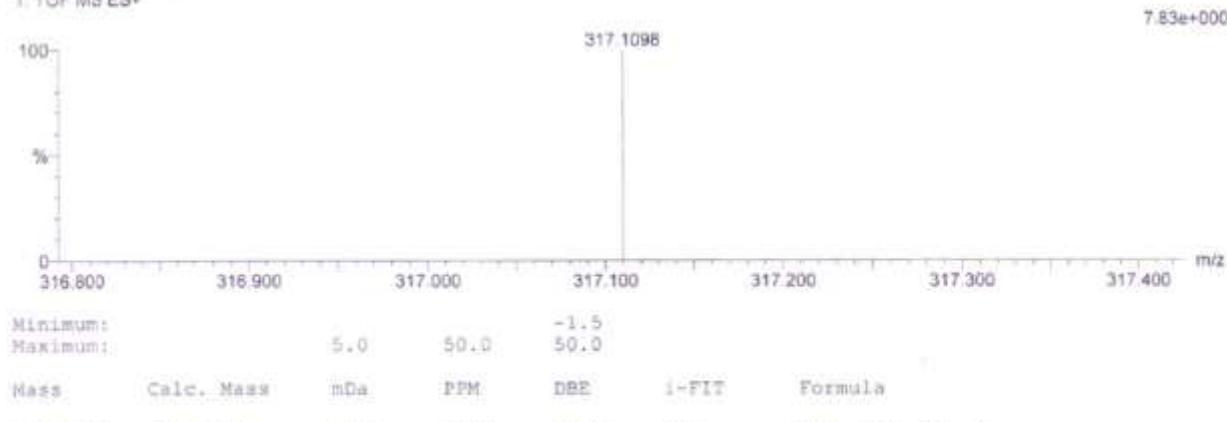
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Elements Used:

C: 0-20 H: 0-17 N: 0-2 S: 0-1

CR 11 B 1.53 (0.798)

1: TOF MS ES+



### HRMS of 4j

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

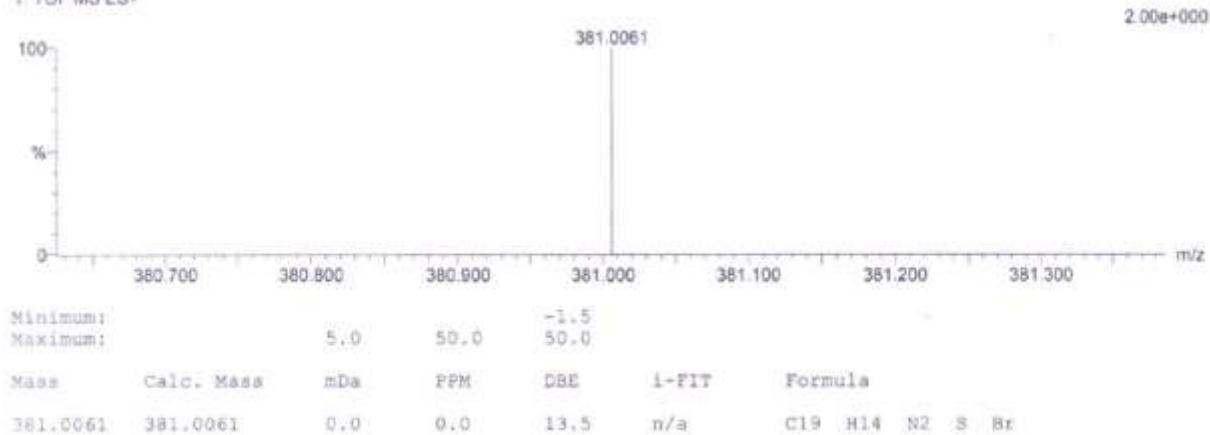
21 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-19 H: 0-14 N: 0-2 S: 0-1 Zn: 0-1 Br: 0-1

CR 11 C 47 (0.872)

1: TOF MS ES+



HRMS of 4k

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

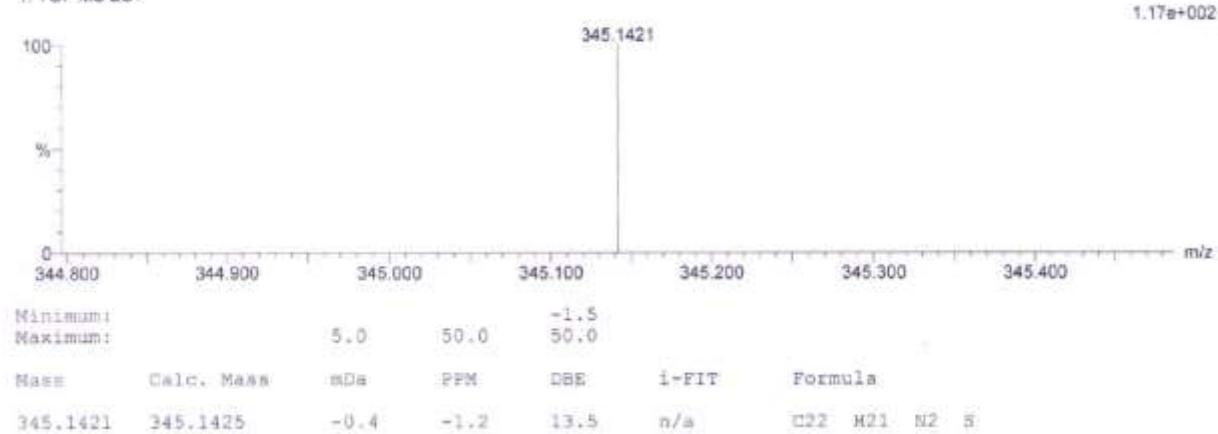
3 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-22 H: 0-21 N: 0-2 S: 0-1

CR 10B 22 (0.408)

1: TOF MS ES+



HRMS of 4o

**Single Mass Analysis**

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

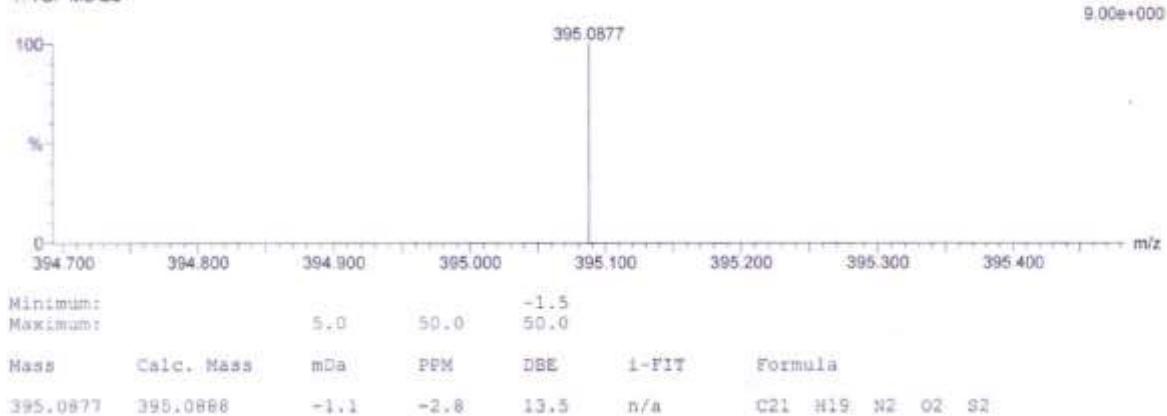
21 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-21 H: 0-19 N: 0-2 O: 0-2 S: 0-2

CR 3E 47 (0.872)

1. TOF MS ES+



HRMS of 4s

**Single Mass Analysis**

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

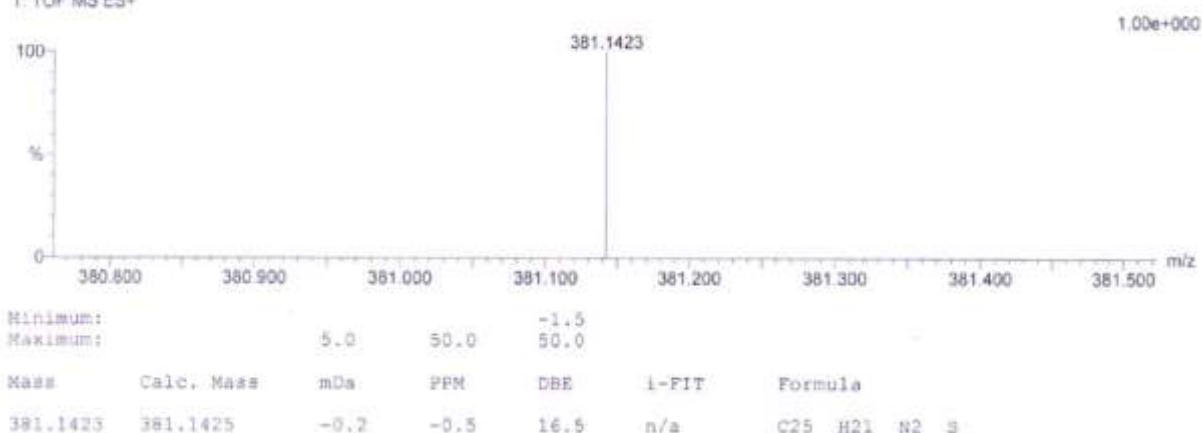
3 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-25 H: 0-21 N: 0-2 S: 0-1

CR 9C 28 (0.519)

1. TOF MS ES+



HRMS of 4u

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

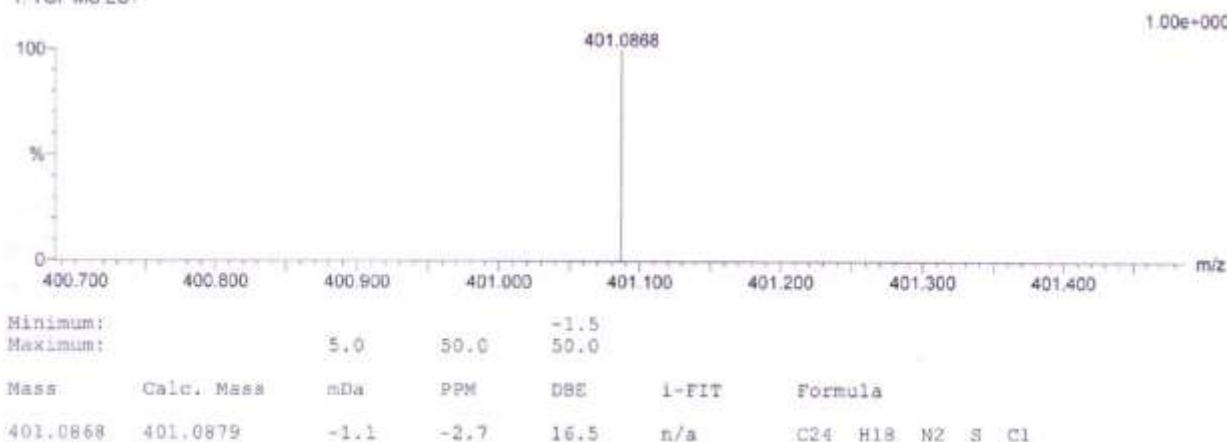
8 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used

C: 0-24 H: 0-18 N: 0-2 S: 0-1 Cl: 0-1

CR 9A 45 (0.835)

1: TOF MS ES+



HRMS of 4v

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

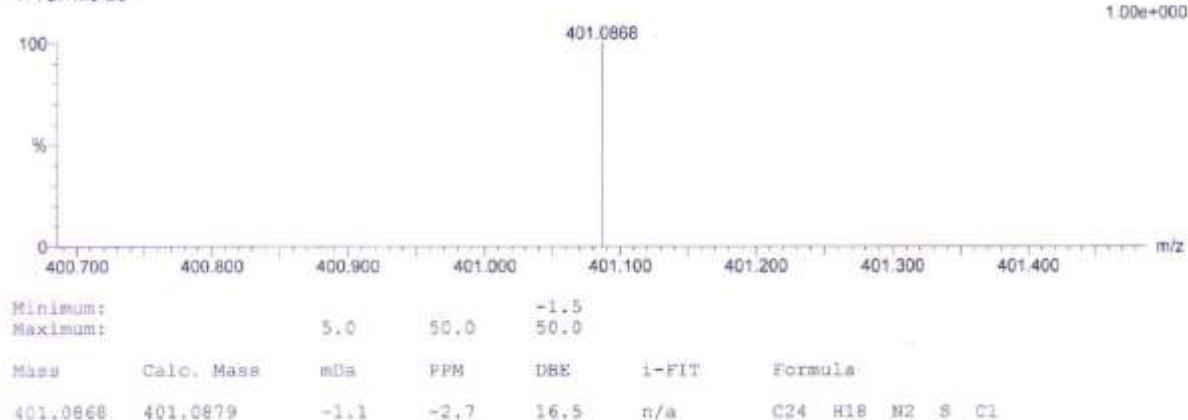
8 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used

C: 0-24 H: 0-18 N: 0-2 S: 0-1 Cl: 0-1

CR 9B 39 (0.724)

1: TOF MS ES+



HRMS of 4w

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

23 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-24 H: 0-18 N: 0-2 S: 0-1 Zn: 0-1 Br: 0-1

CR 9D 47 (0.872)  
1 TOF MS ES+



HRMS of 4x

## Elemental Composition Report

Page 1

### Single Mass Analysis

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

17 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

Elements Used:

C: 0-24 H: 0-18 N: 0-3 O: 0-2 S: 0-1

CR 9E 12 (0.223)

1 TOF MS ES+



HRMS of 4y

**Elemental Composition Report****Page 1****Single Mass Analysis**

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

5 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

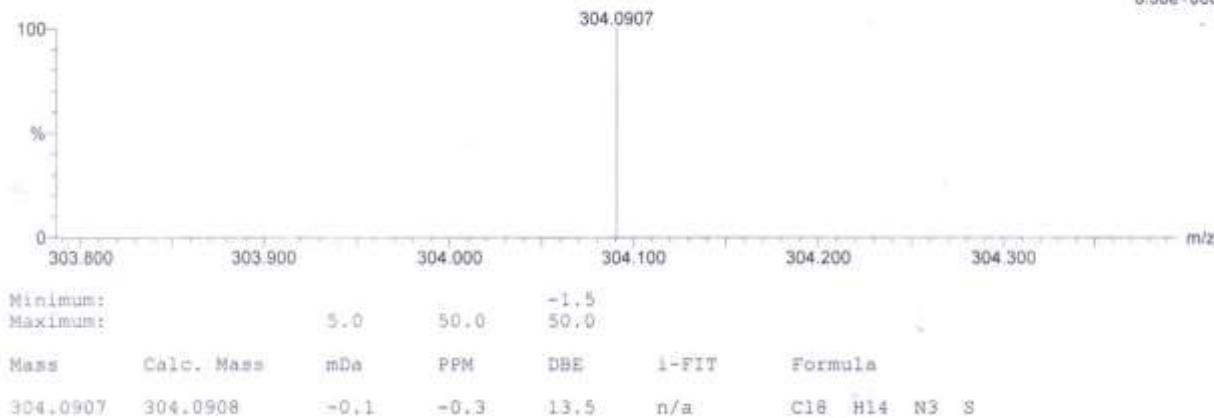
Elements Used:

C: 0-18 H: 0-14 N: 0-3 S: 0-1

CR-1042D 15 (0.278)

1: TOF MS ES+

8.56e+000

**HRMS of 4z****Elemental Composition Report****Page 1****Single Mass Analysis**

Tolerance = 50.0 PPM / DBE: min = -1.5, max = 50.0

Element prediction: Off

Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions

5 formula(e) evaluated with 1 results within limits (up to 50 closest results for each mass)

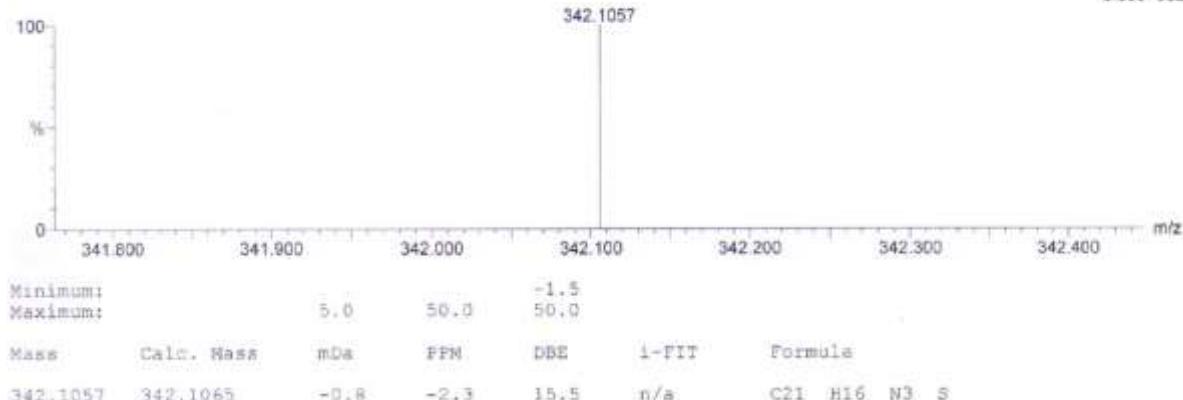
Elements Used:

C: 0-21 H: 0-16 N: 0-3 S: 0-1

CR 88.46 (0.053)

1: TOF MS ES+

8.56e+002

**HRMS of 6h**