

# Linear and Star-shaped Pyrazine-containing Acene Dicarboximides with High Electron-affinity

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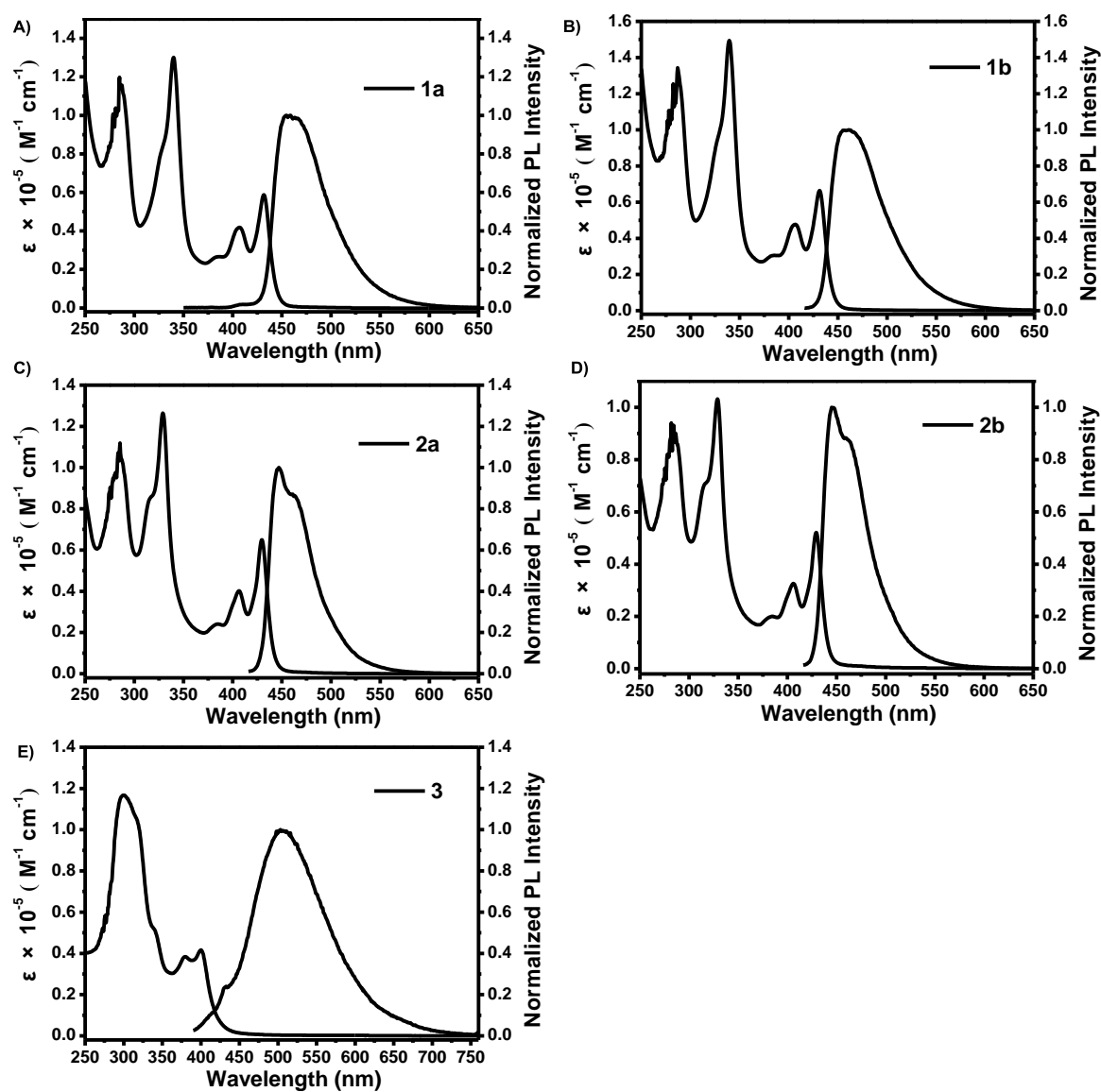
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## Table of Contents

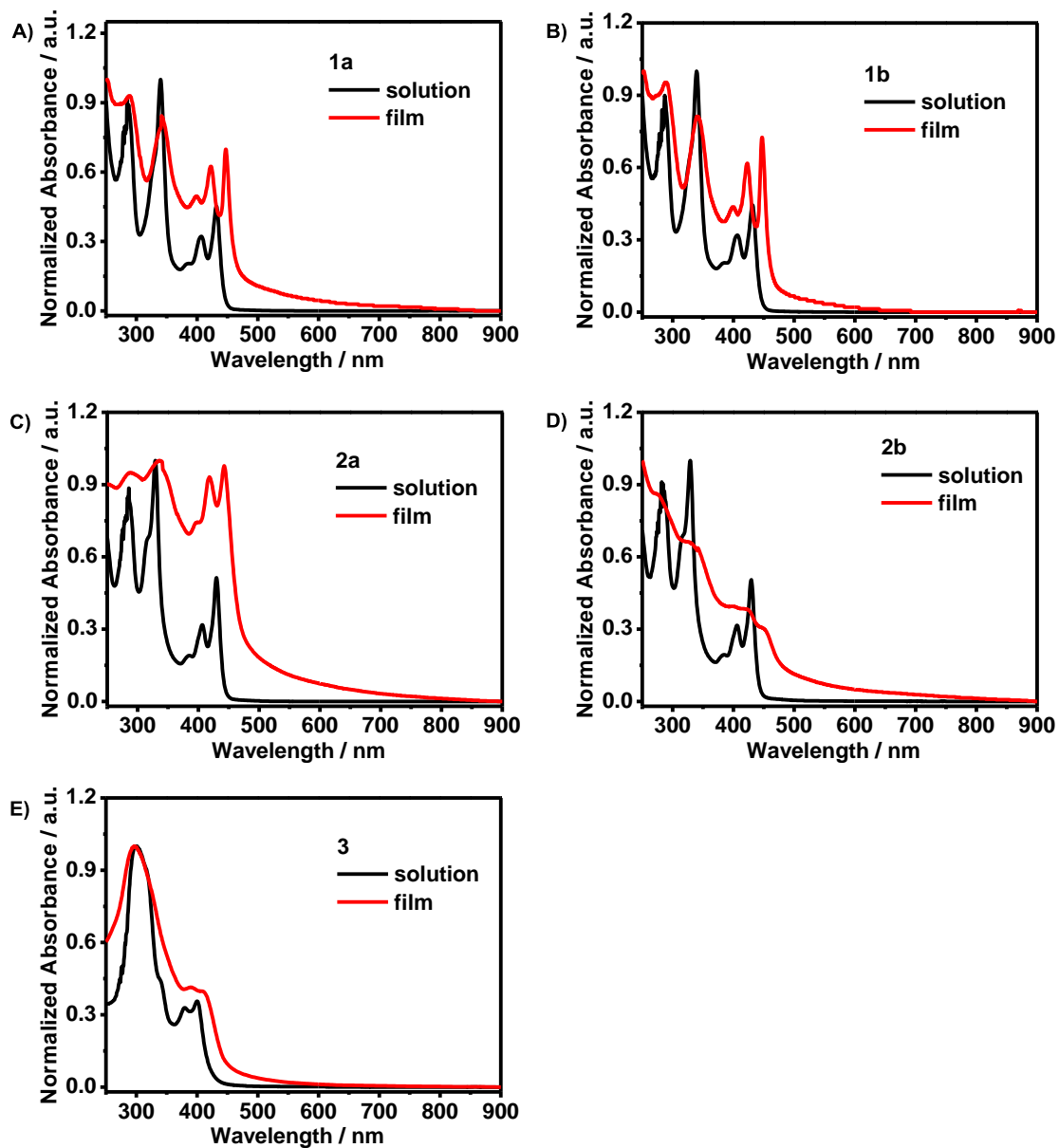
1. Absorption and emission spectra for <b>1a-b</b> , <b>2a-b</b> , and <b>3</b> .....	S2
2. Absorption spectra of <b>1a-b</b> , <b>2a-b</b> , and <b>3</b> in solution and in thin film .....	S3
3. CV curves and DPV curves for <b>1a-b</b> , <b>2a-b</b> , and <b>3</b> .....	S5
4. Thermogravimetric analysis (TGA) curves for <b>1a-b</b> , <b>2a-b</b> , and <b>3</b> .....	S6
5. Additional differential scanning calorimetry (DSC) curves for <b>1a-b</b> and <b>2b</b> .....	S7
6. Additional polarizing optical microscopy (POM) images for <b>1a-b</b> , and <b>2b</b> .....	S8
7. X-ray diffraction (XRD) data for <b>1a-b</b> , <b>2a-b</b> , and <b>3</b> .....	S9
8. Additional space-charge limited-current measurements for <b>1b</b> and <b>2b</b> .....	S11
9. <sup>1</sup> H NMR and <sup>13</sup> C NMR spectra.....	S12
10. MALDI-TOF mass spectra for <b>1a-b</b> , <b>2a-b</b> and <b>3</b> .....	S46
11. References .....	S51

## 1. Absorption and emission spectra of 1a-b, 2a-b, and 3



**Fig. S1.** Absorption spectra and normalized emission spectra of compounds **1a-b**, **2a-b** and **3** in THF. The emission spectra of **1a-b**, **2a-b** and **3** were recorded under the excitation wavelength of 340, 406, 406, 406 and 380 nm, respectively.

## 2. Absorption spectra of 1a-b, 2a-b, and 3 in solution and in thin film



**Fig. S2.** Normalized absorption spectra in THF solution and solid film (spin-coated from  $\text{CHCl}_3$  solution) for compounds **1a-b**, **2a-b**, and **3**

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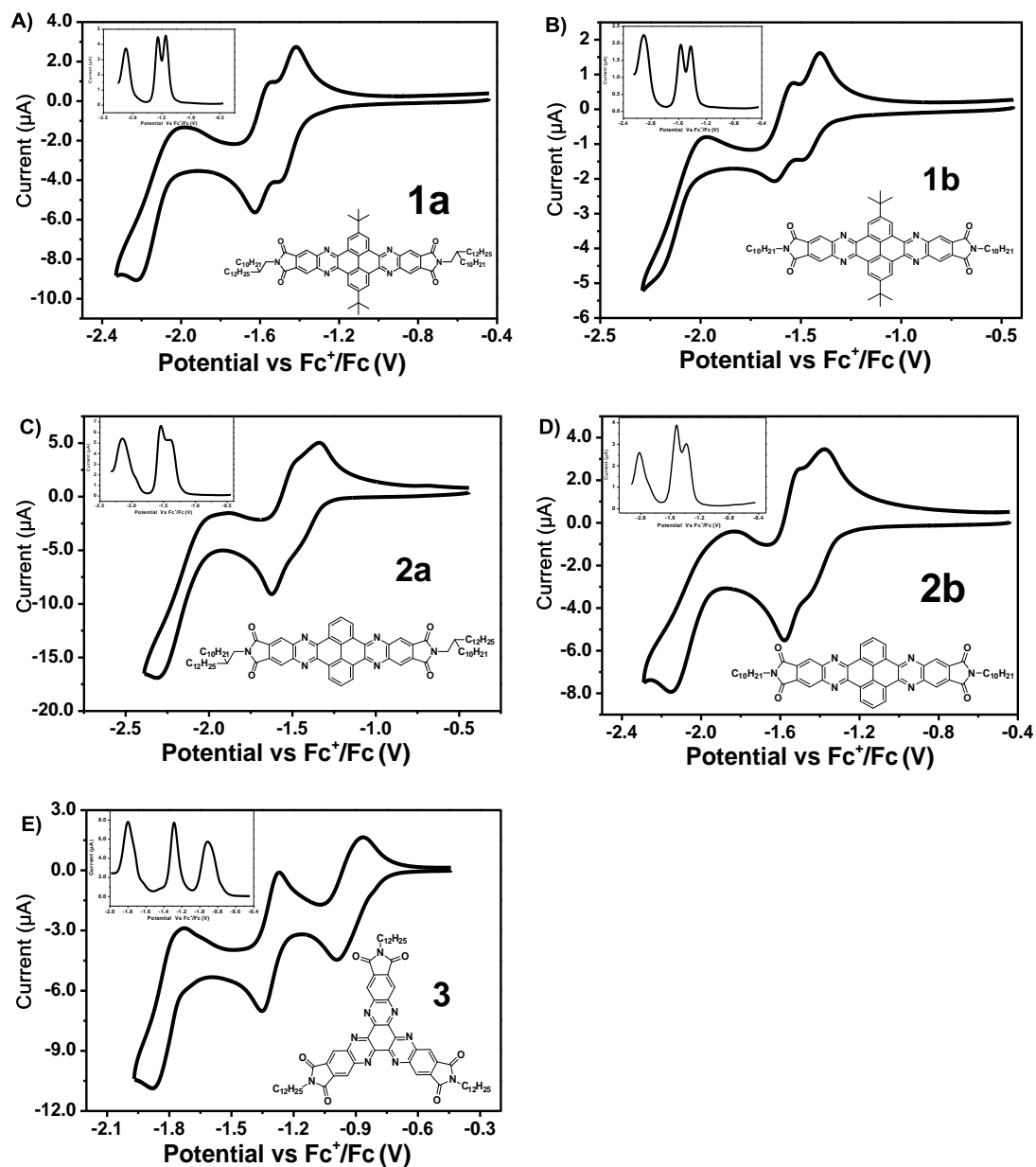
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**Table S1.** UV and PL data for compounds **1a-b**, **2a-b**, and **3**

	Solution			Film
	$\lambda_{\text{abs}} / \text{nm}$	$\epsilon_{\text{max}} / \text{M}^{-1} \text{cm}^{-1}$	$\lambda_{\text{PL}} / \text{nm}$	$\lambda_{\text{abs}} / \text{nm}$
<b>1a</b>	431	5800	457	447
<b>1b</b>	431	6500	457	447
<b>2a</b>	429	6400	447	442
<b>2b</b>	429	5200	447	443
<b>3</b>	399	4100	504	411

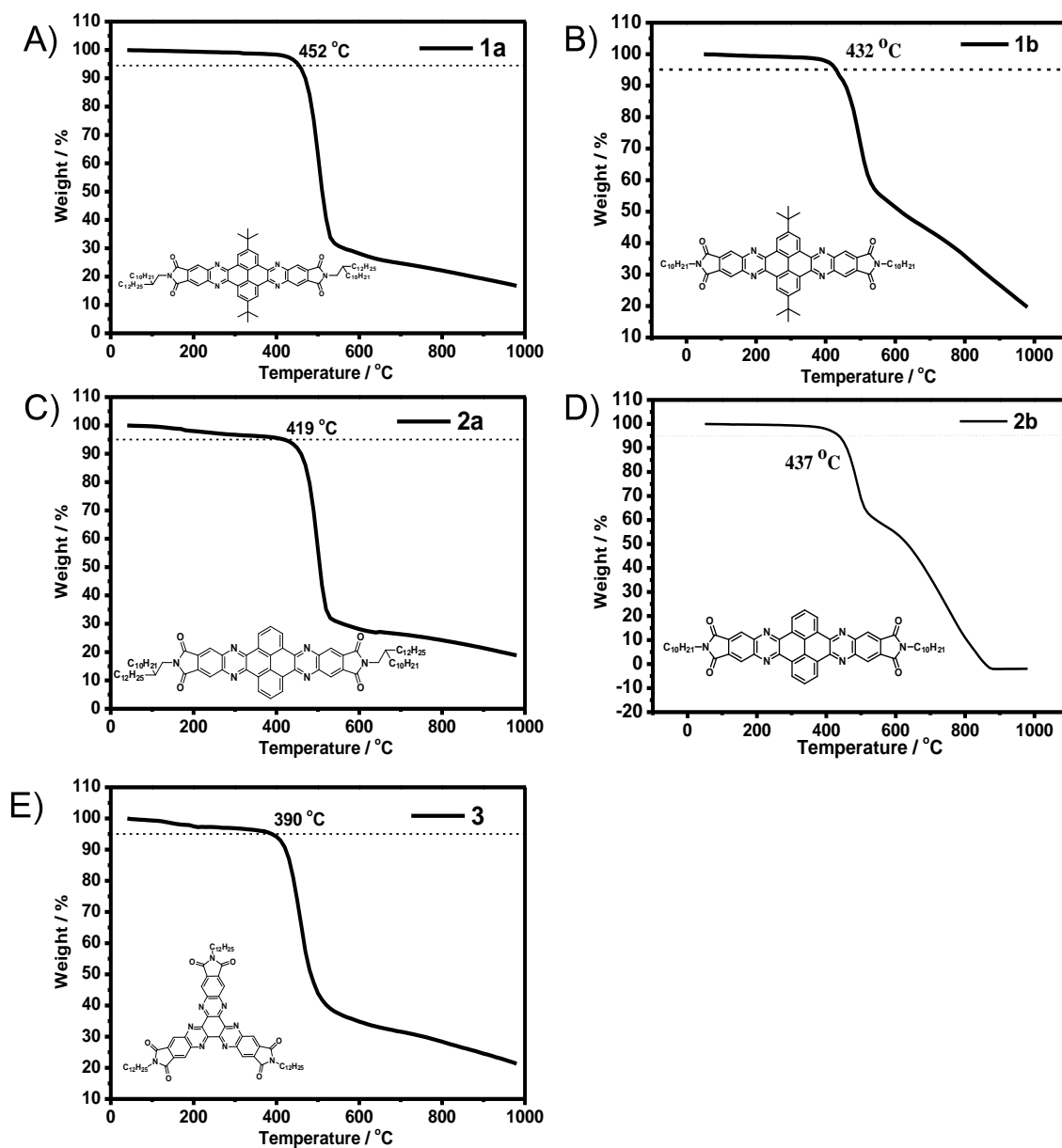
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3. CV curves and DPV curves of 1a-b, 2a-b, and 3



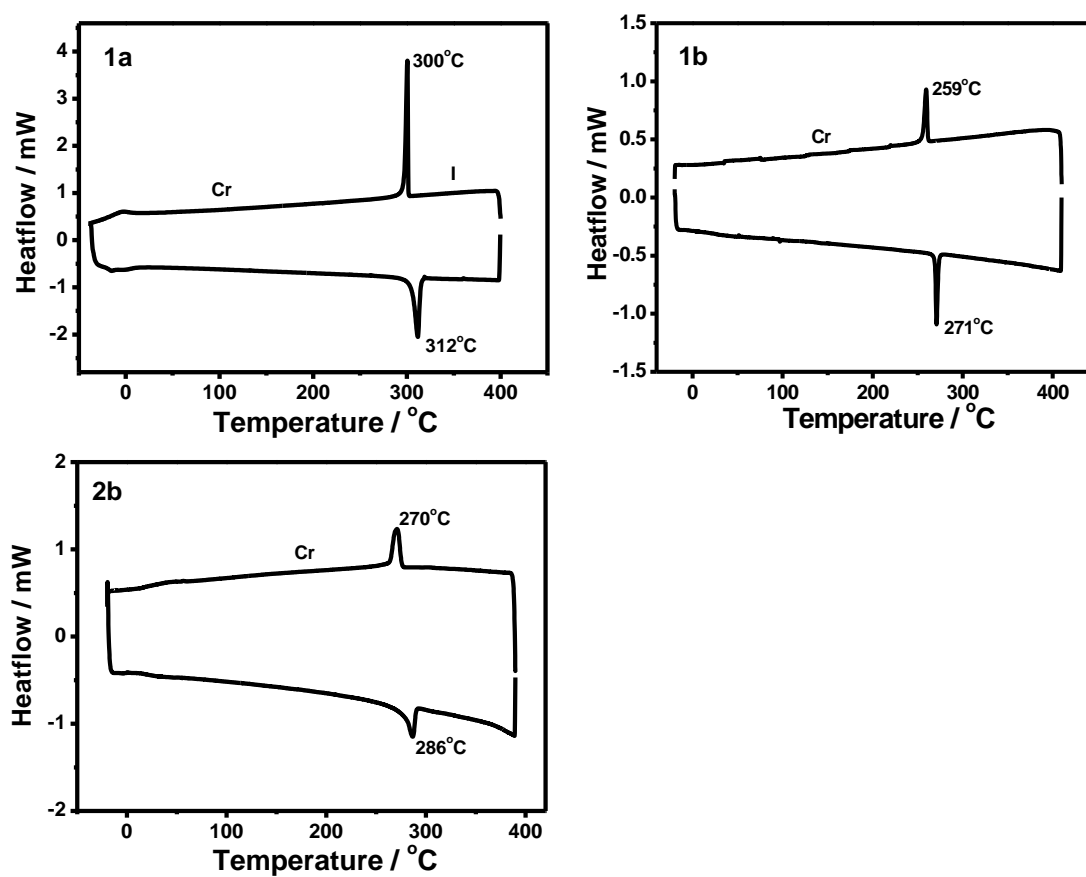
**Fig. S3.** CV curves and DPV curves (inset) for compounds **1a-b**, **2a-b**, and **3** in DCM with 0.1 M Bu<sub>4</sub>NPF<sub>6</sub> as supporting electrolyte, a gold electrode with a diameter of 2 mm, a Pt wire, and an Ag/AgCl electrode were used as the working electrode, the counter electrode, and the reference electrode, respectively, with a scan rate at 100 mV/s.

#### 4. Thermogravimetric analysis (TGA) curves for 1a-b, 2a-b, and 3.



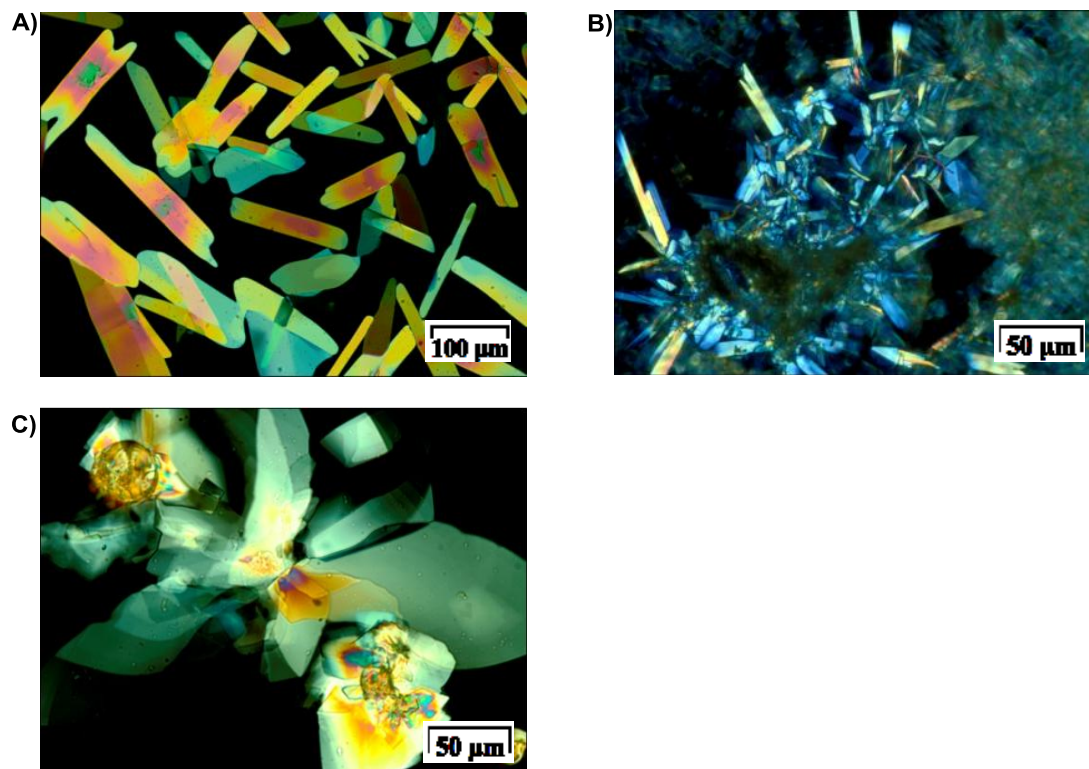
**Fig. S4.** Thermogravimetric analysis (TGA) curves for compounds **1a-b**, **2a-b**, and **3** with a heating rate of 10 °C/min under nitrogen.

5. Additional differential scanning calorimetry (DSC) curves for 1a-b and 2b.



**Fig. S5.** DSC curves for compounds **1a-b** and **2b** with a heating/cooling scan rate of 10 °C/min under nitrogen (Cr = crystalline phase, I = isotropic phase).

**6. Additional polarizing optical microscopy (POM) images of 1a-b and 2b**



**Fig. S6.** POM images for **1a**, **1b** and **2b**. A) **1a**, at 250 °C upon slow cooling; B) **1b**, at 260 °C upon slow cooling; C) **2b**, at 315 °C upon slow cooling.



### 7. X-ray diffraction (XRD) data of 1a-b, 2a-b, and 3

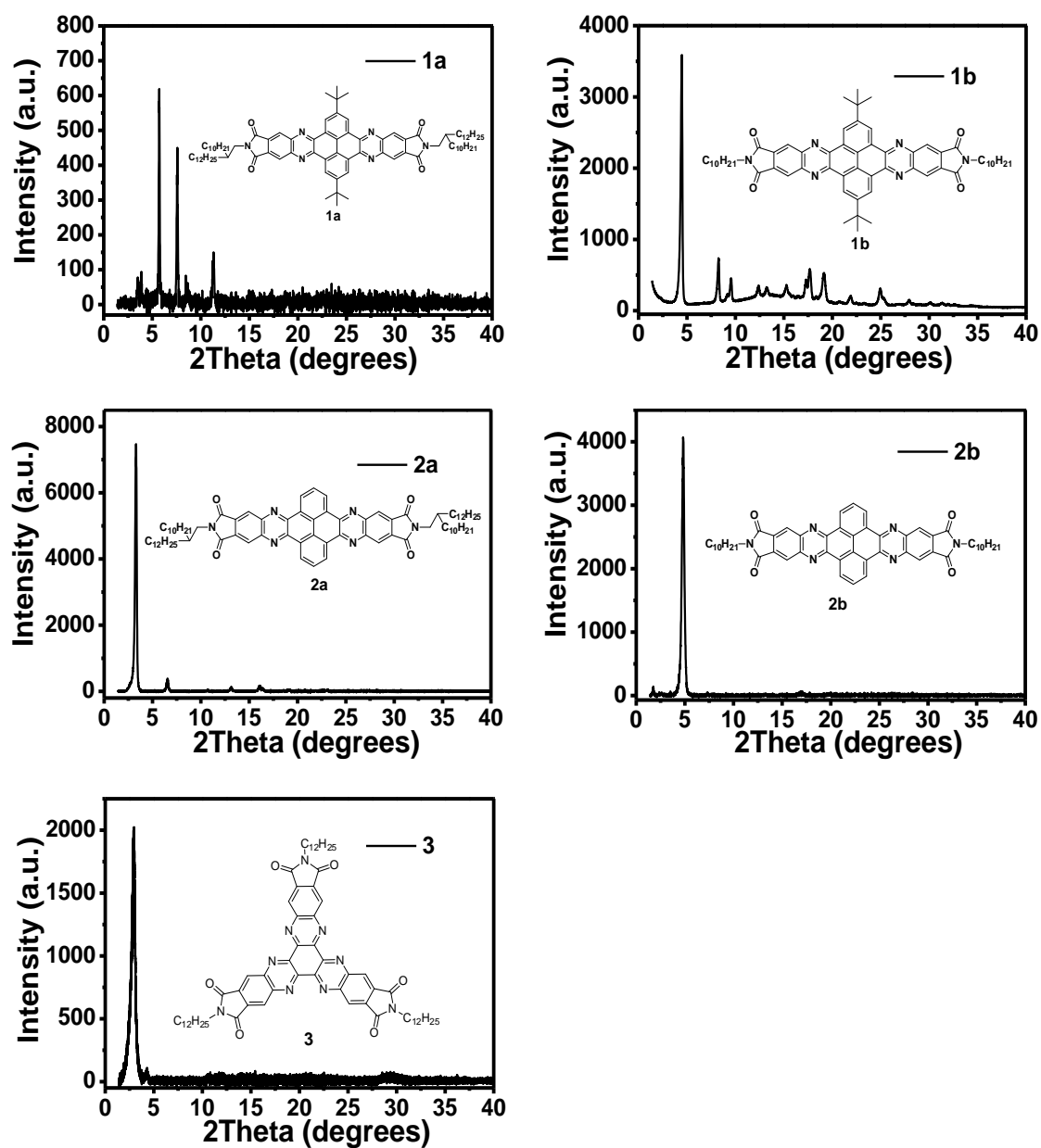
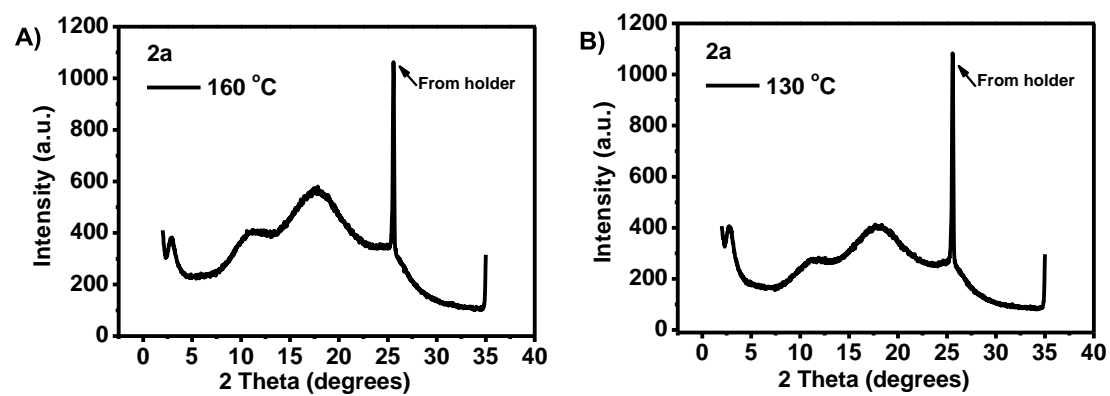


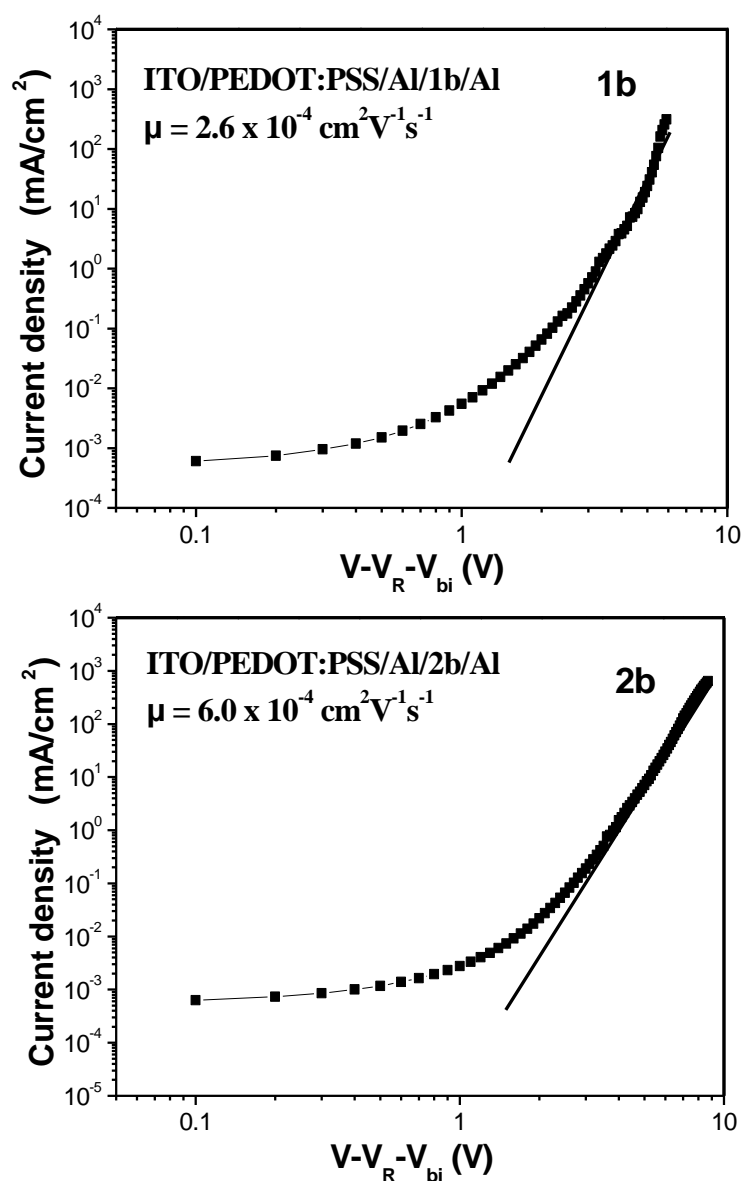
Fig. S7. Powder XRD patterns for 1a-b, 2a-b, and 3 at room temperature

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**Fig. S8.** Variable-Temperature Powder XRD (VT-XRD) patterns for **2a** at 160 °C and 130 °C.

8. Additional space-charge limited-current measurements for 1b and 2b.

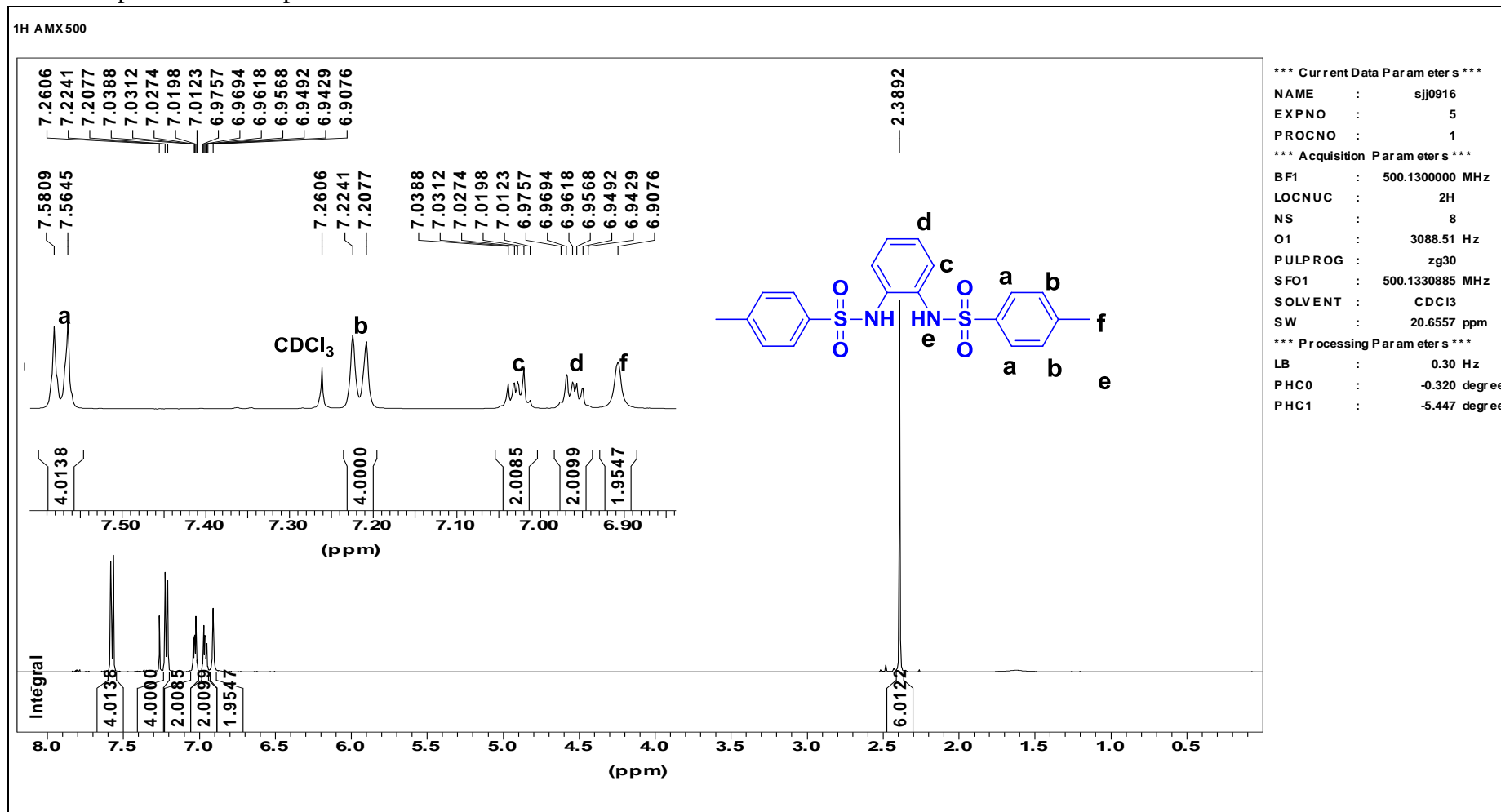


**Fig. S9.** Double logarithmic plot of the current density ( $J$ ) versus applied voltage ( $V$ ) curves for **1b** and **2b**.

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### 9. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra

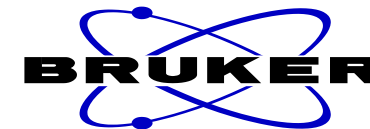
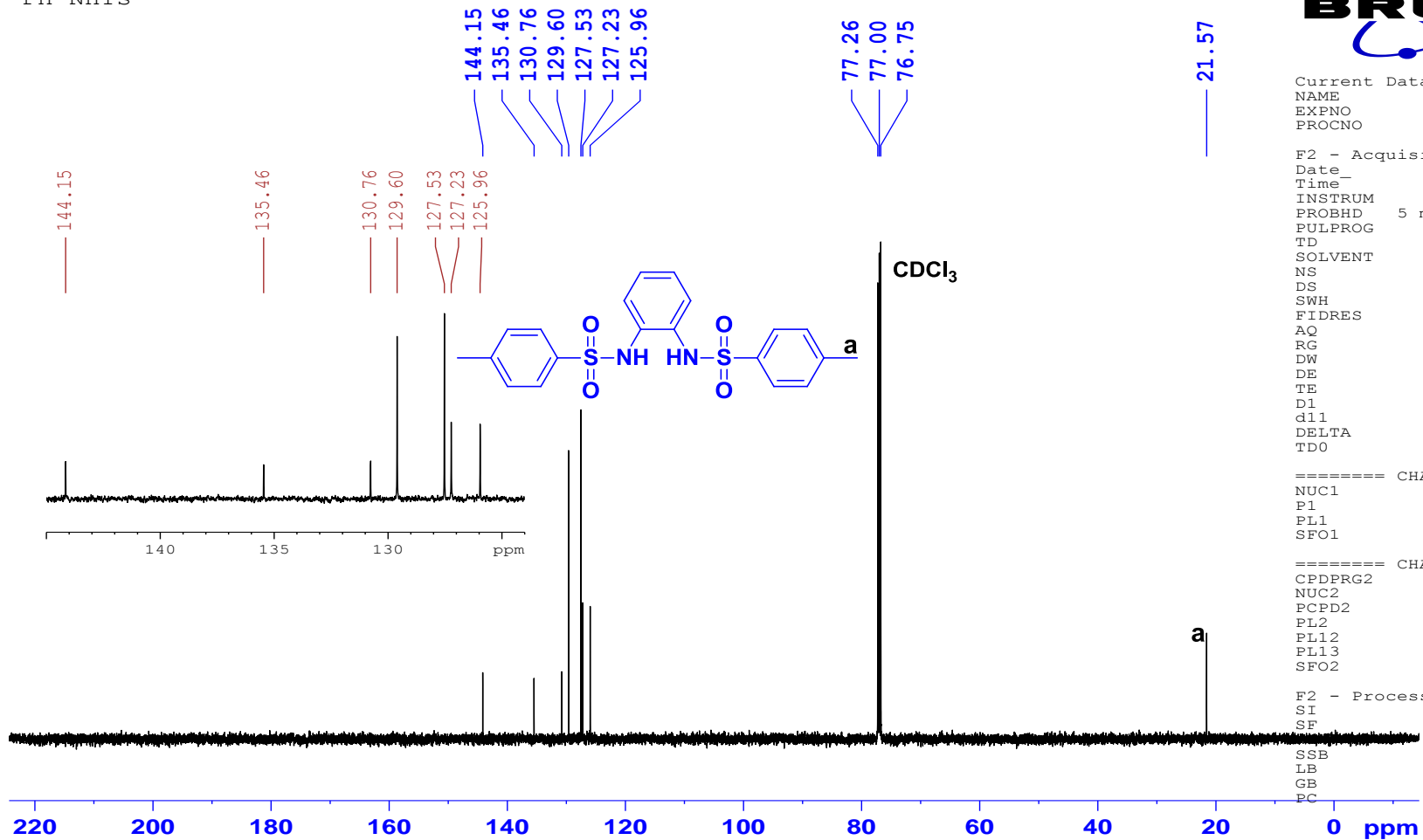
#### <sup>1</sup>H NMR spectrum of compound 5



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<sup>13</sup>C NMR spectrum of compound 5

<sup>13</sup>C AMX500  
Ph-NHTs



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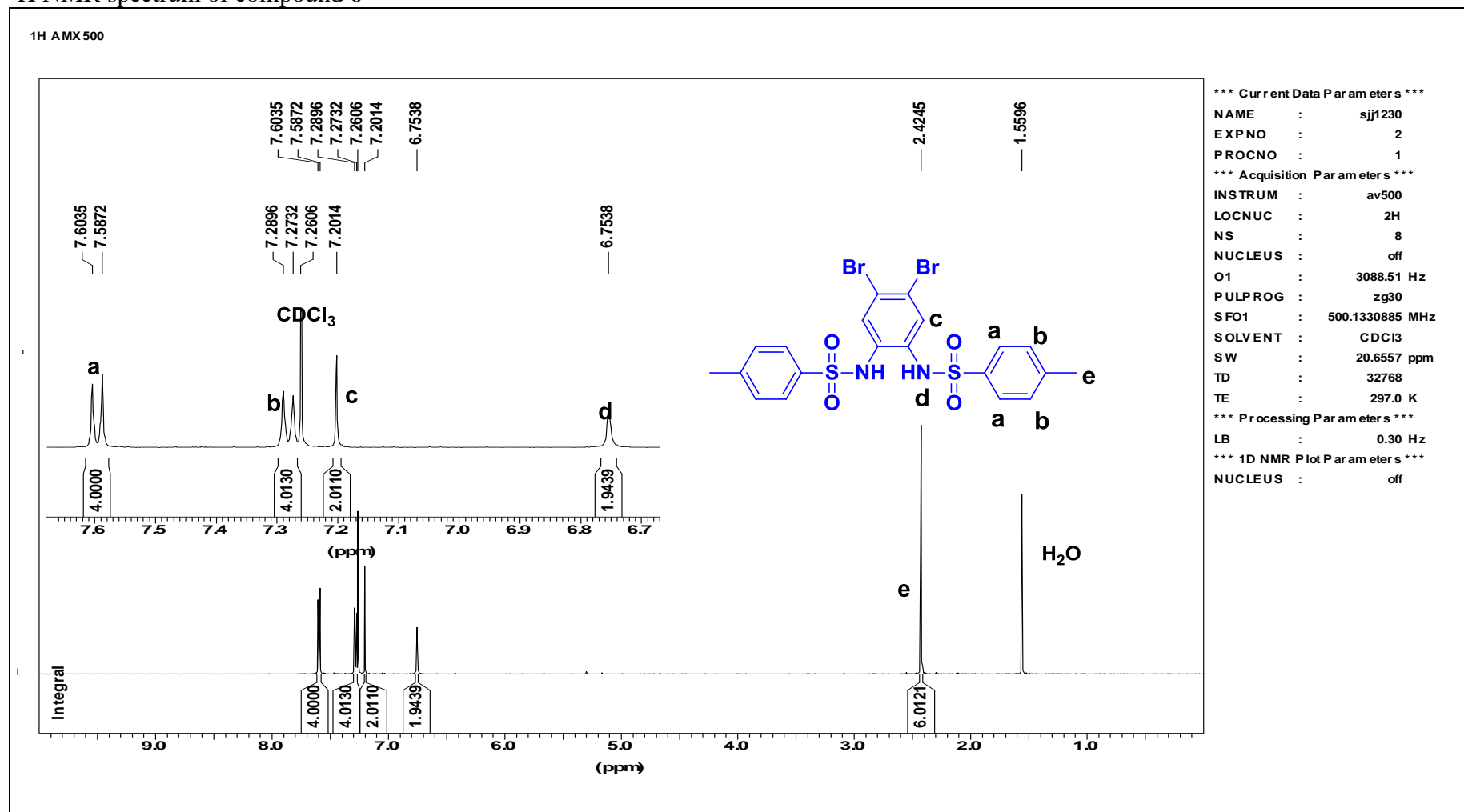
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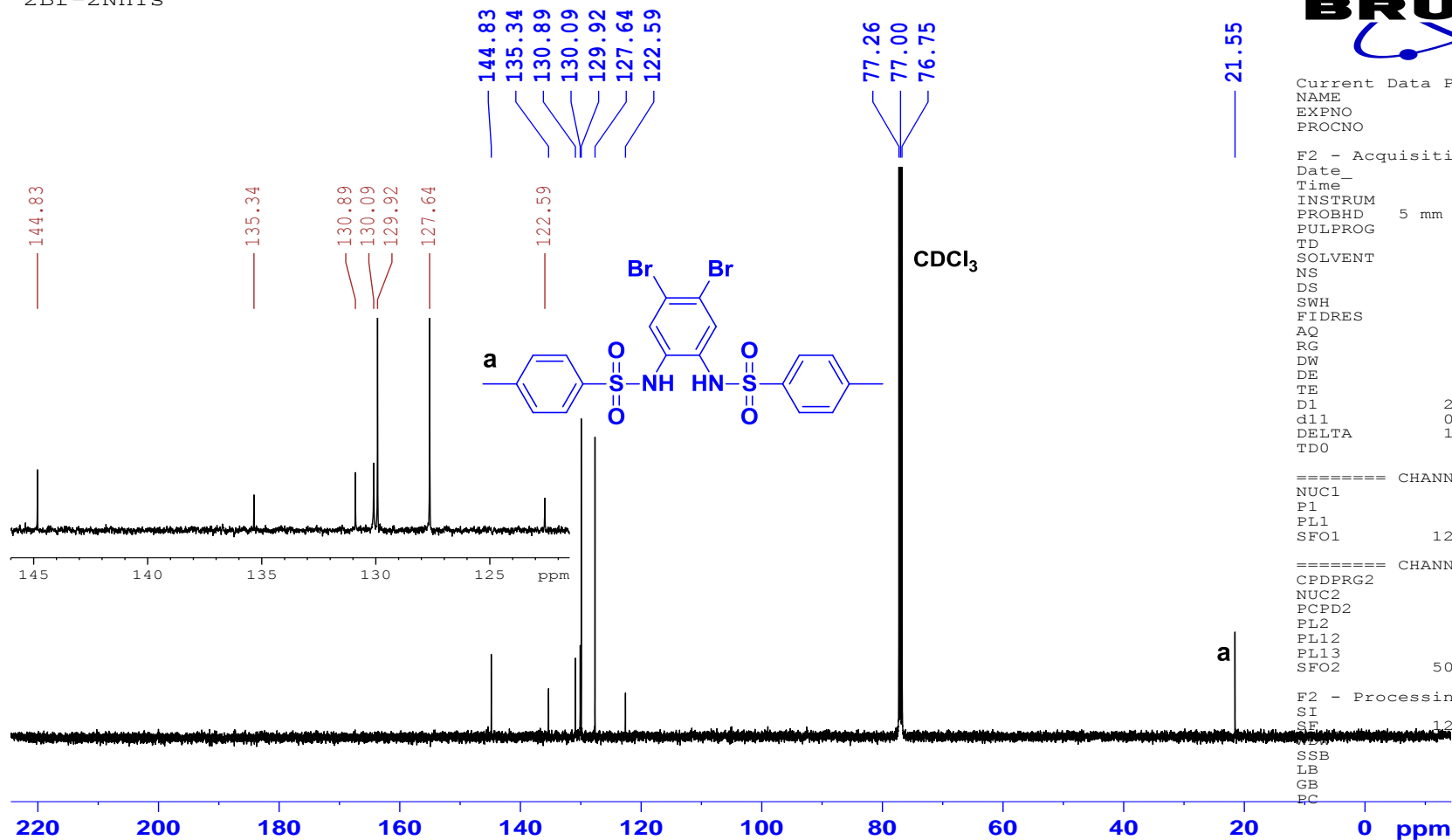
<sup>1</sup>H NMR spectrum of compound 6



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$^{13}\text{C}$  NMR spectrum of compound **6**

$^{13}\text{C}$  AMX500  
2Br-2NHTs



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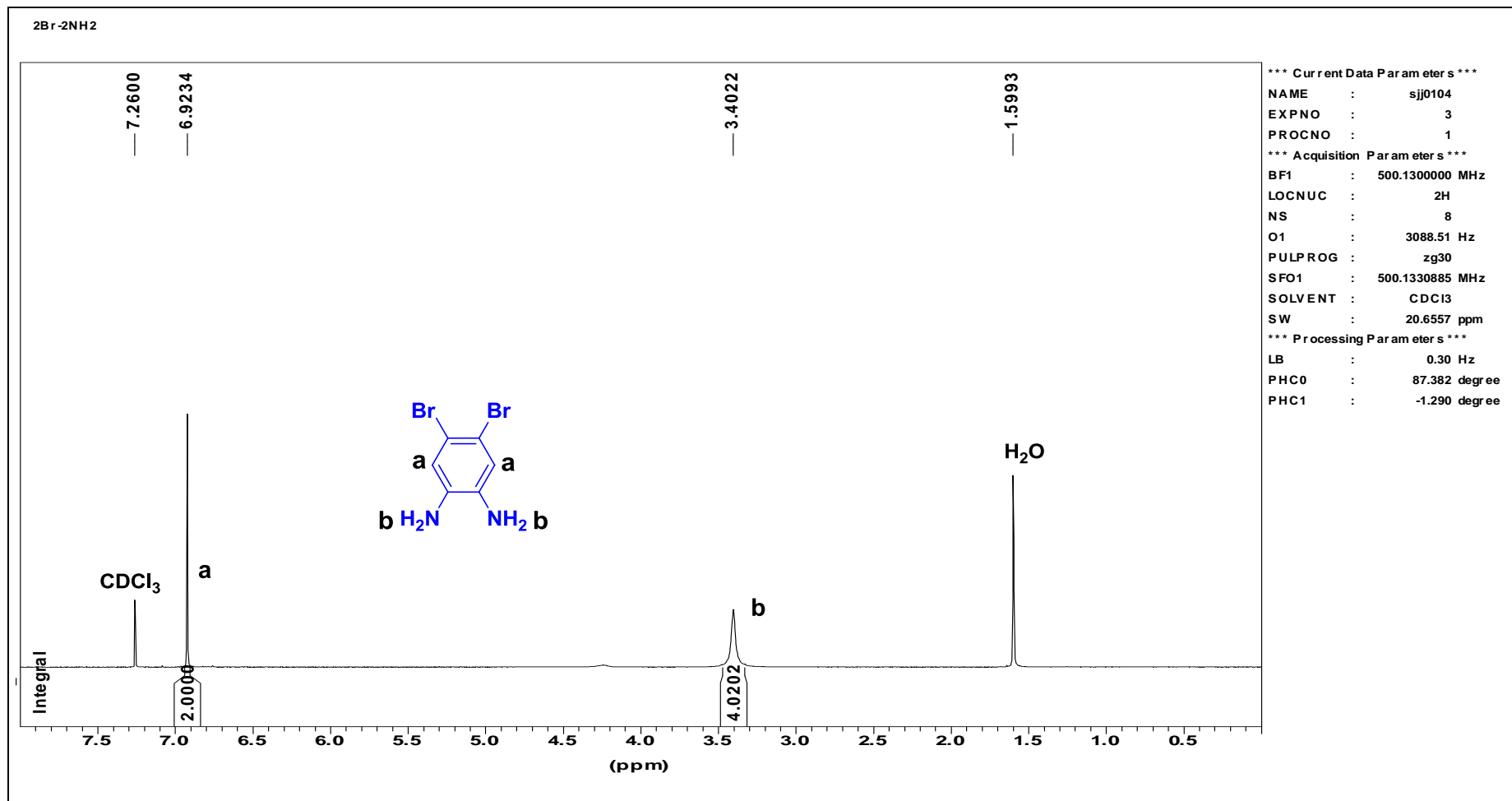
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<sup>1</sup>H NMR spectrum of compound 7





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$^{13}\text{C}$  NMR spectrum of compound 7

$^{13}\text{C}$  AMX500  
2Br-2NH<sub>2</sub>



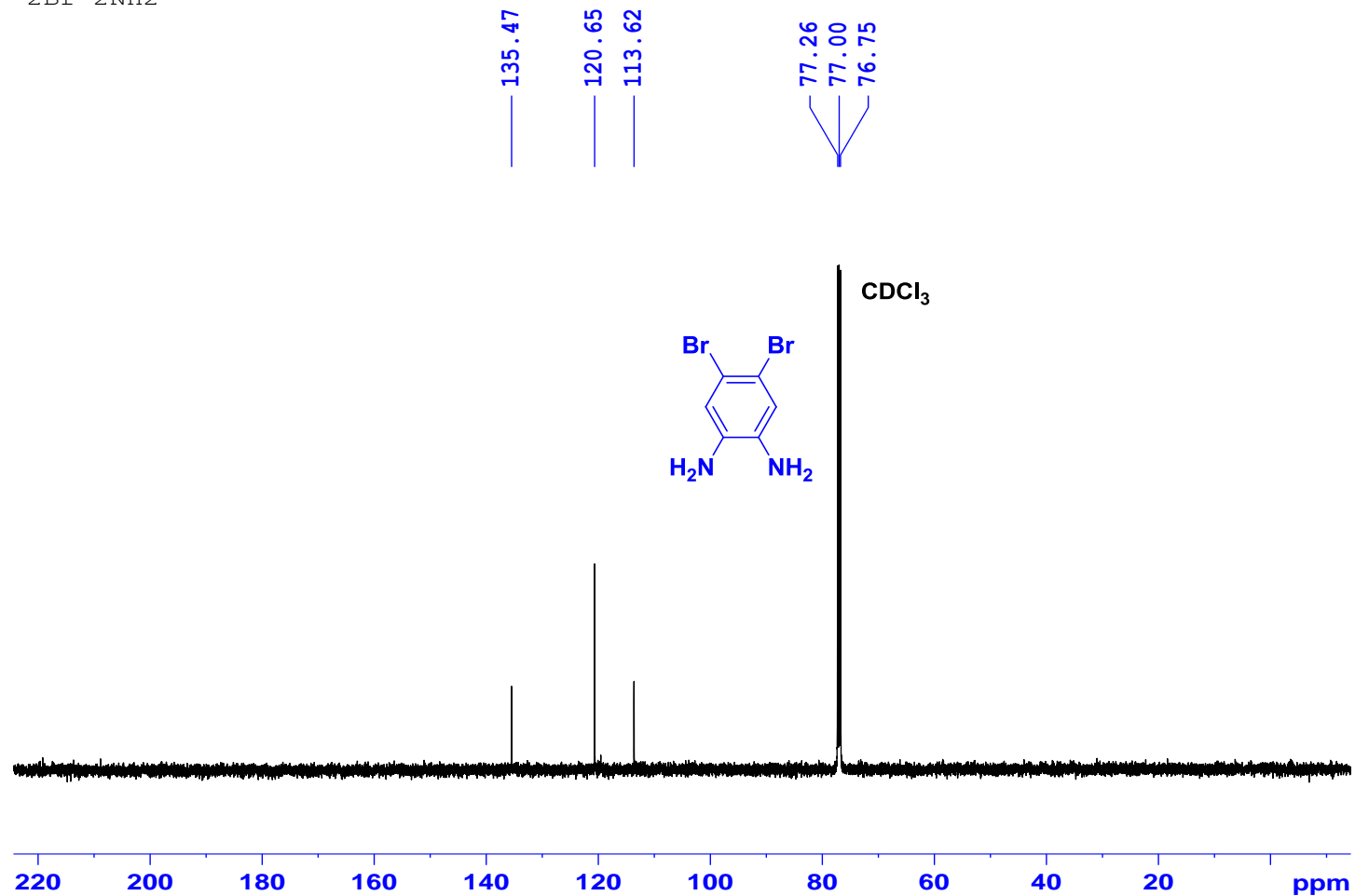
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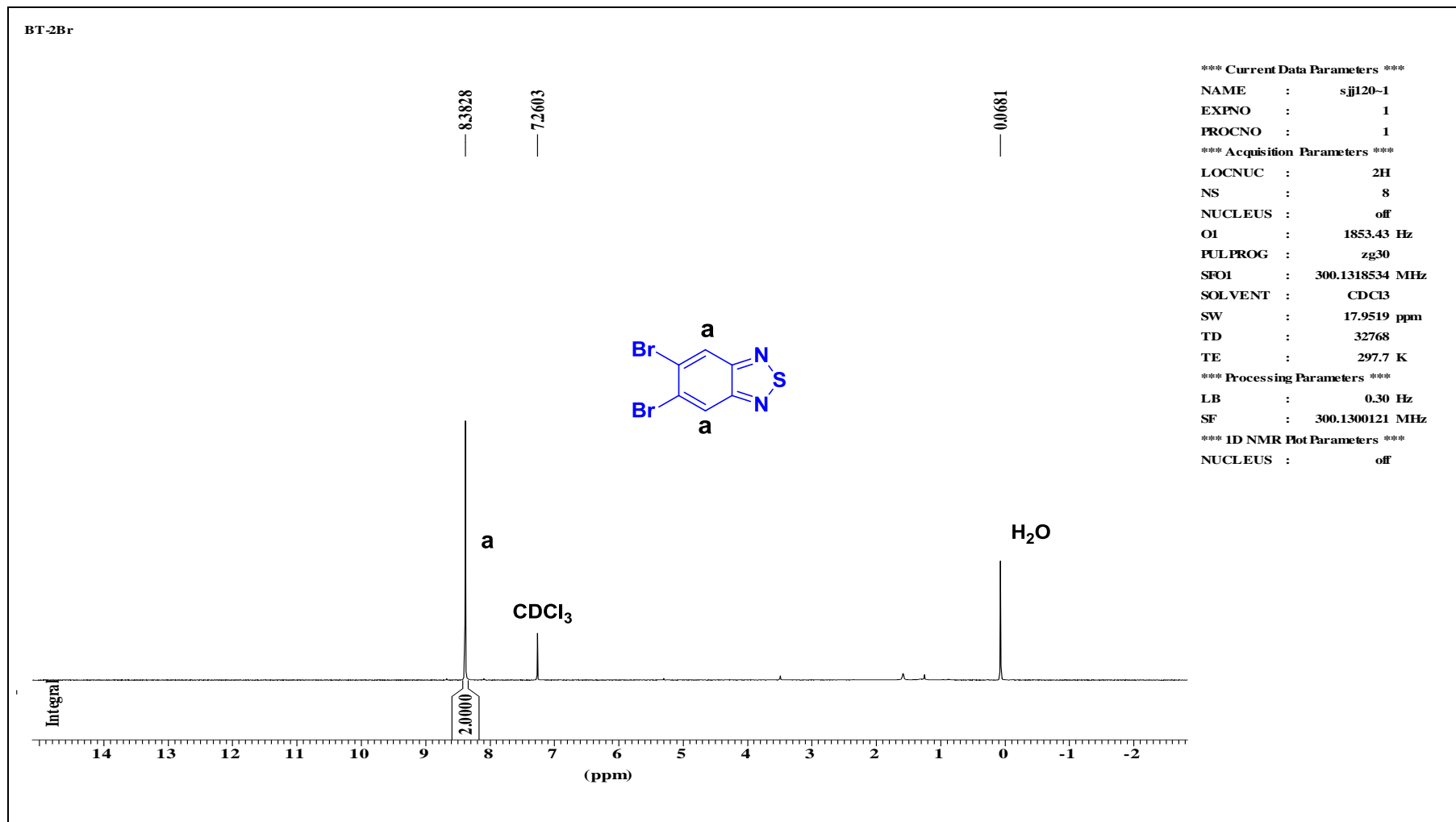
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<sup>1</sup>H NMR spectrum of compound **8**



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<sup>13</sup>C NMR spectrum of compound **8**

<sup>13</sup>C AMX500  
2Br-BT



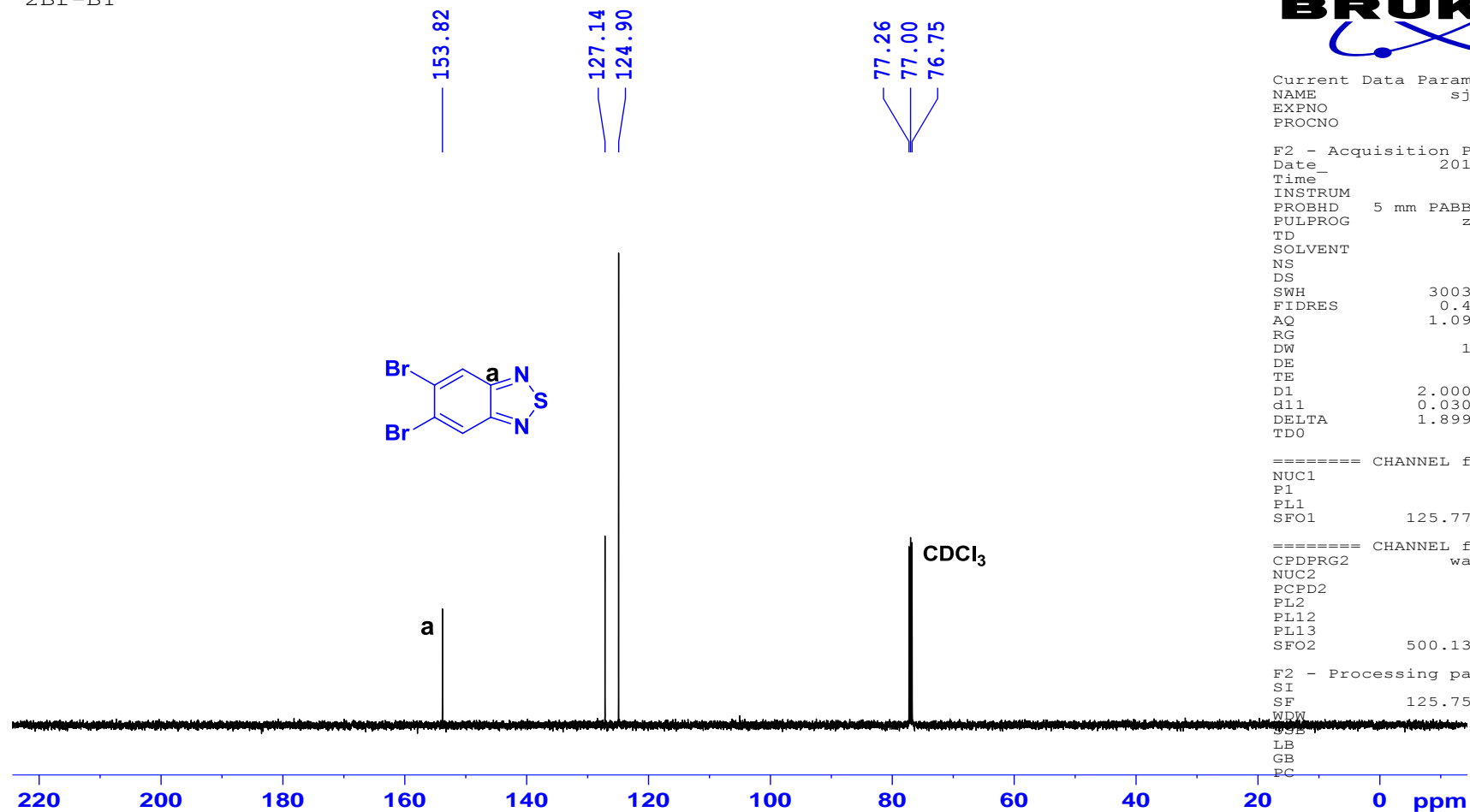
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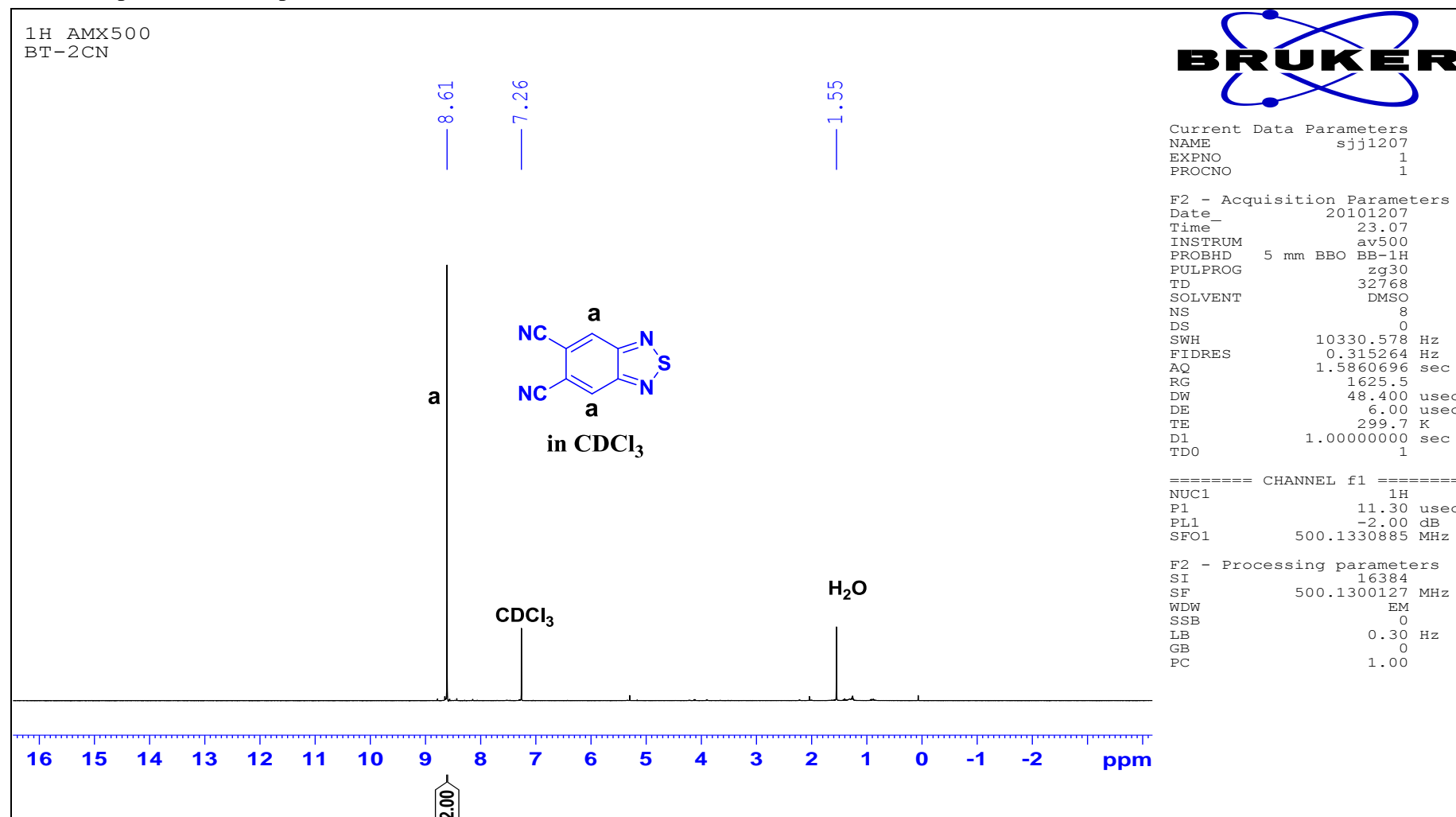
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<sup>1</sup>H NMR spectrum of compound **9**



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$^{13}\text{C}$  NMR spectrum of compound **9**

$^{13}\text{C}$  AMX500



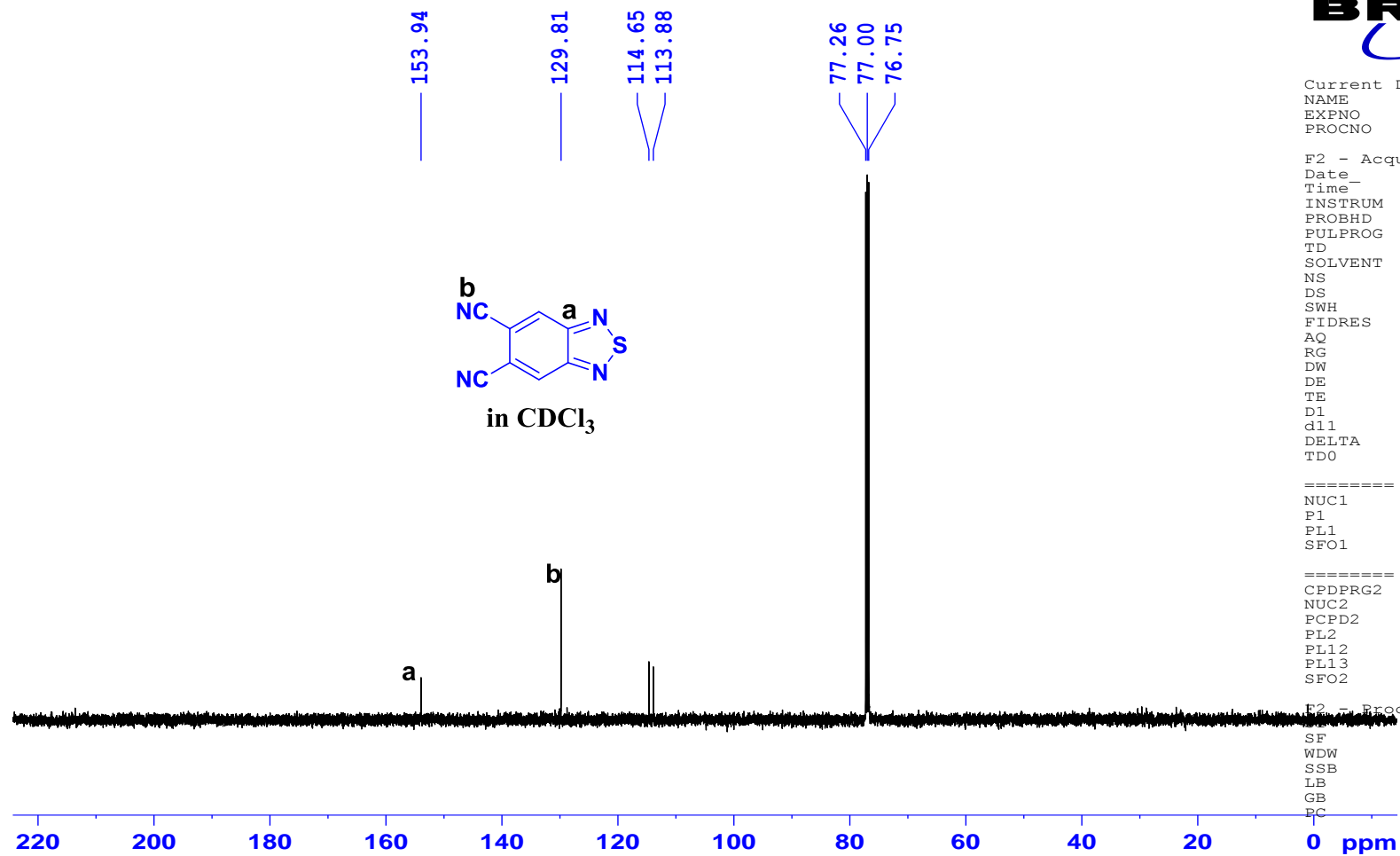
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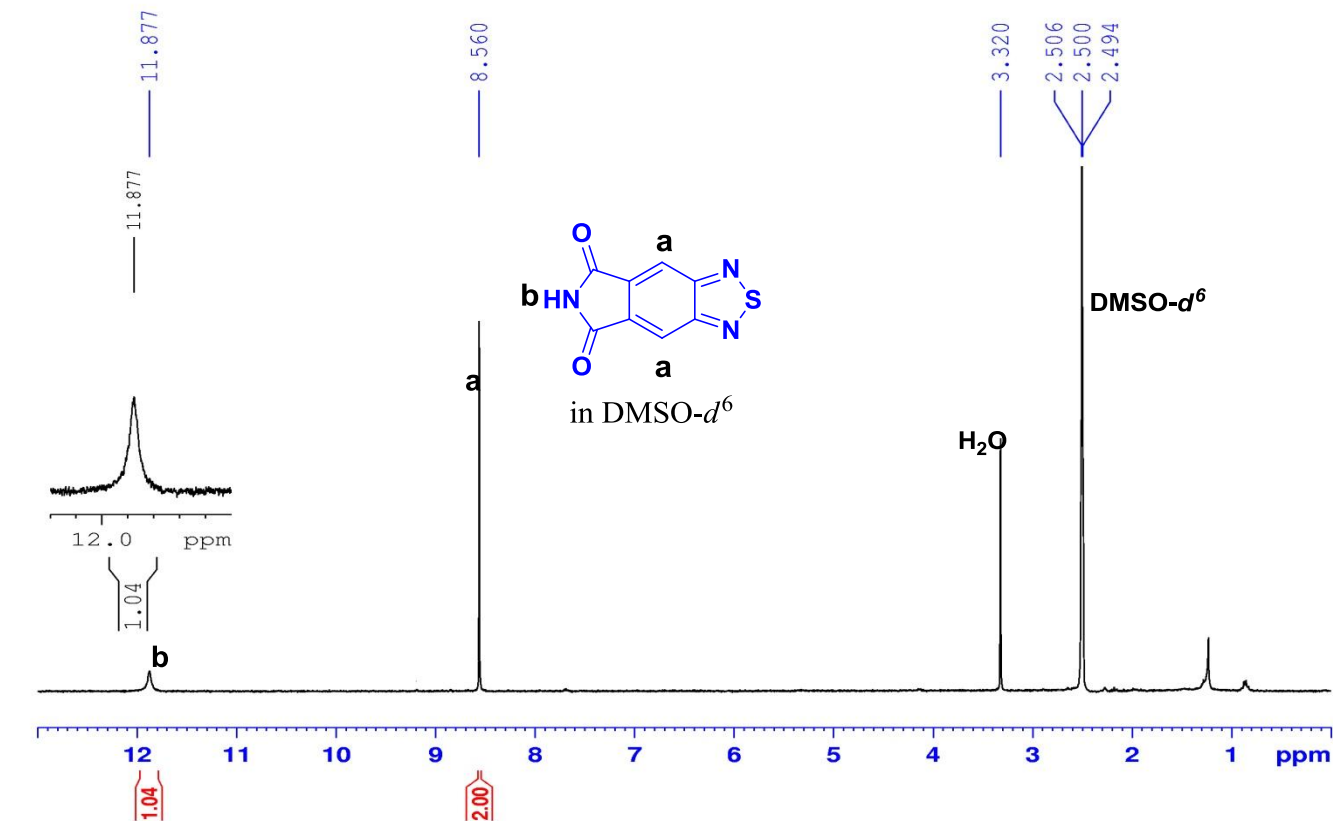
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<sup>1</sup>H NMR spectrum of compound **10**

<sup>1</sup>H normal range AC300  
BT-imide



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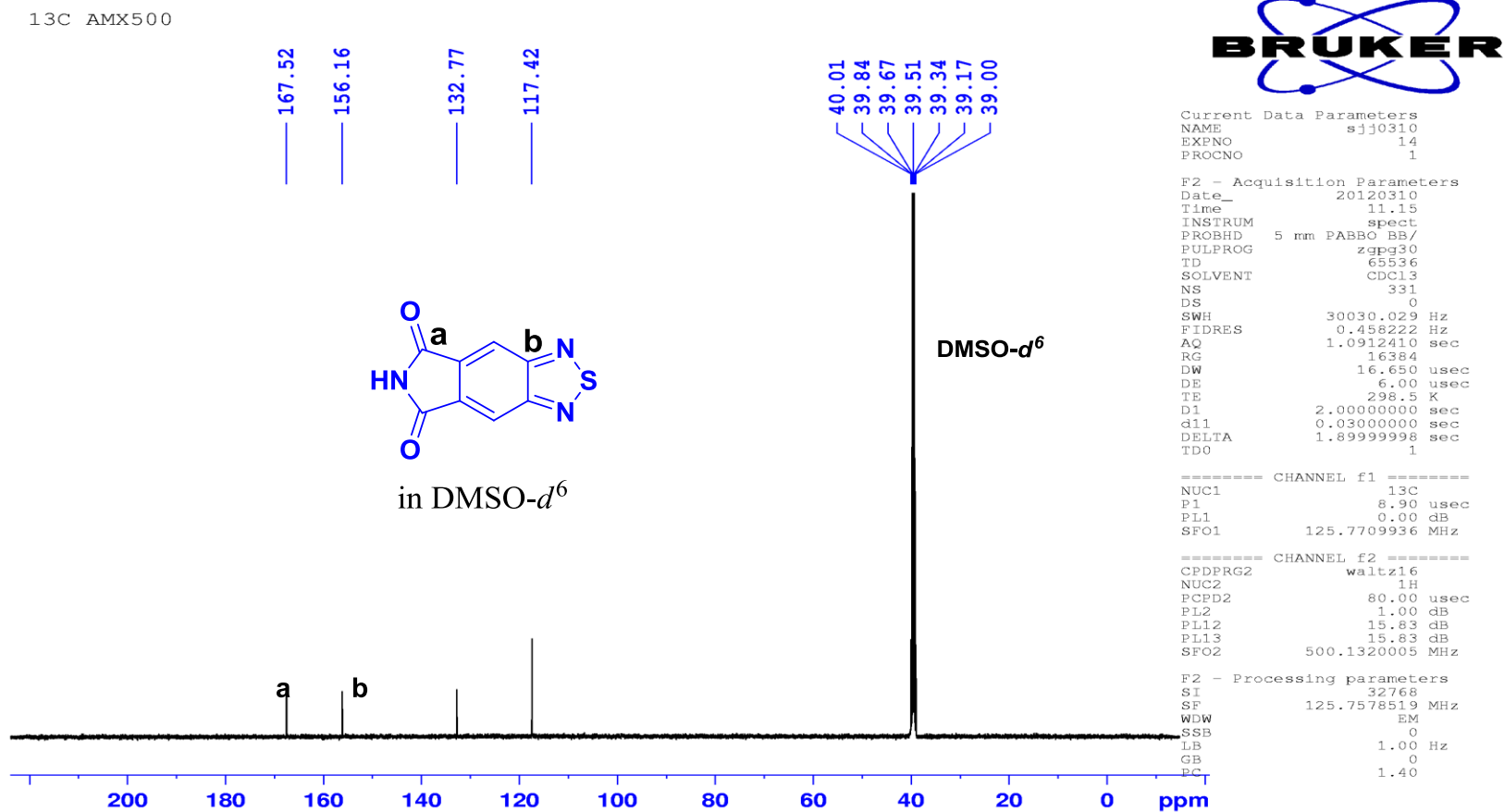
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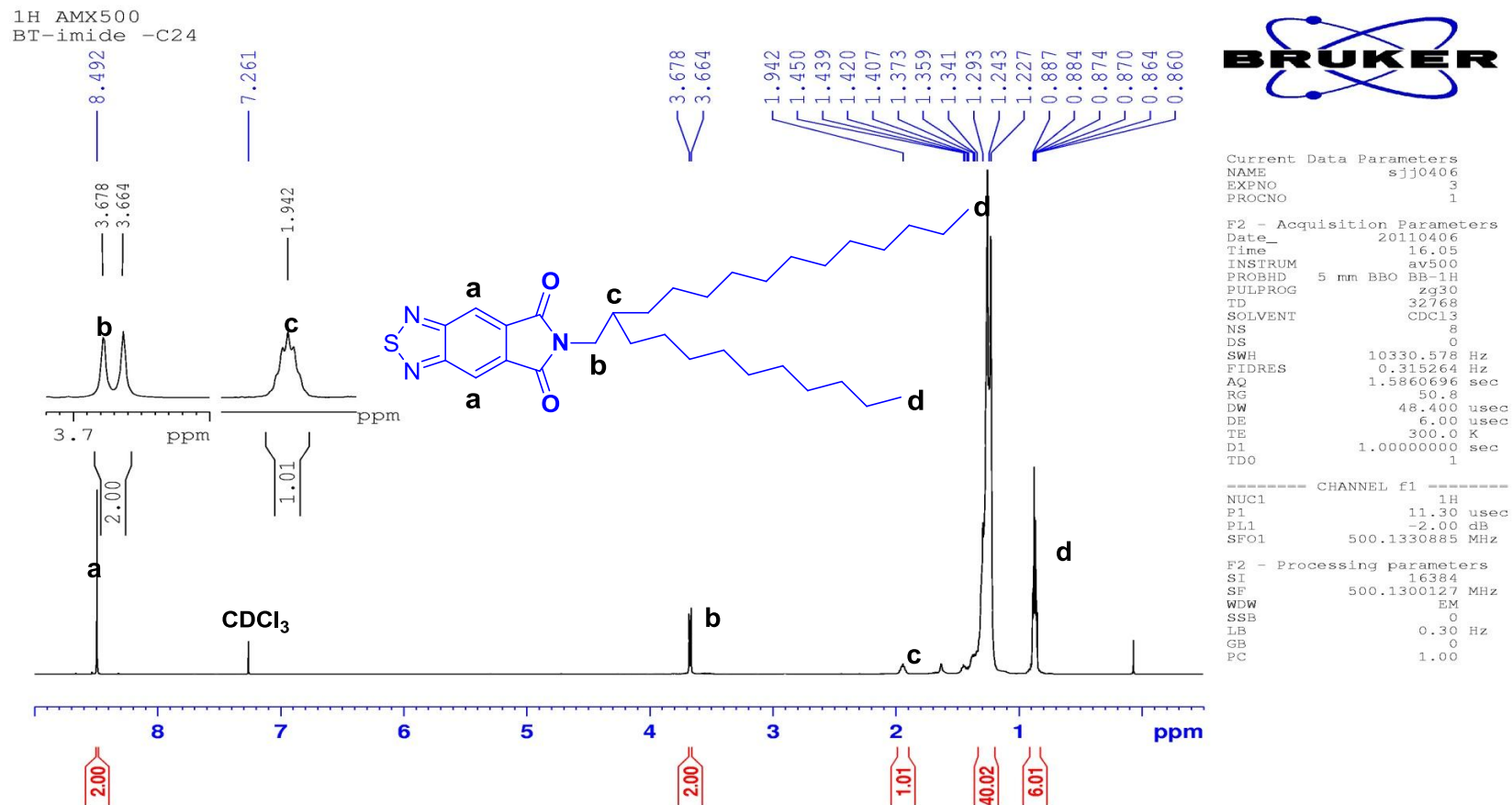
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$^{13}\text{C}$  NMR spectrum of compound **10**



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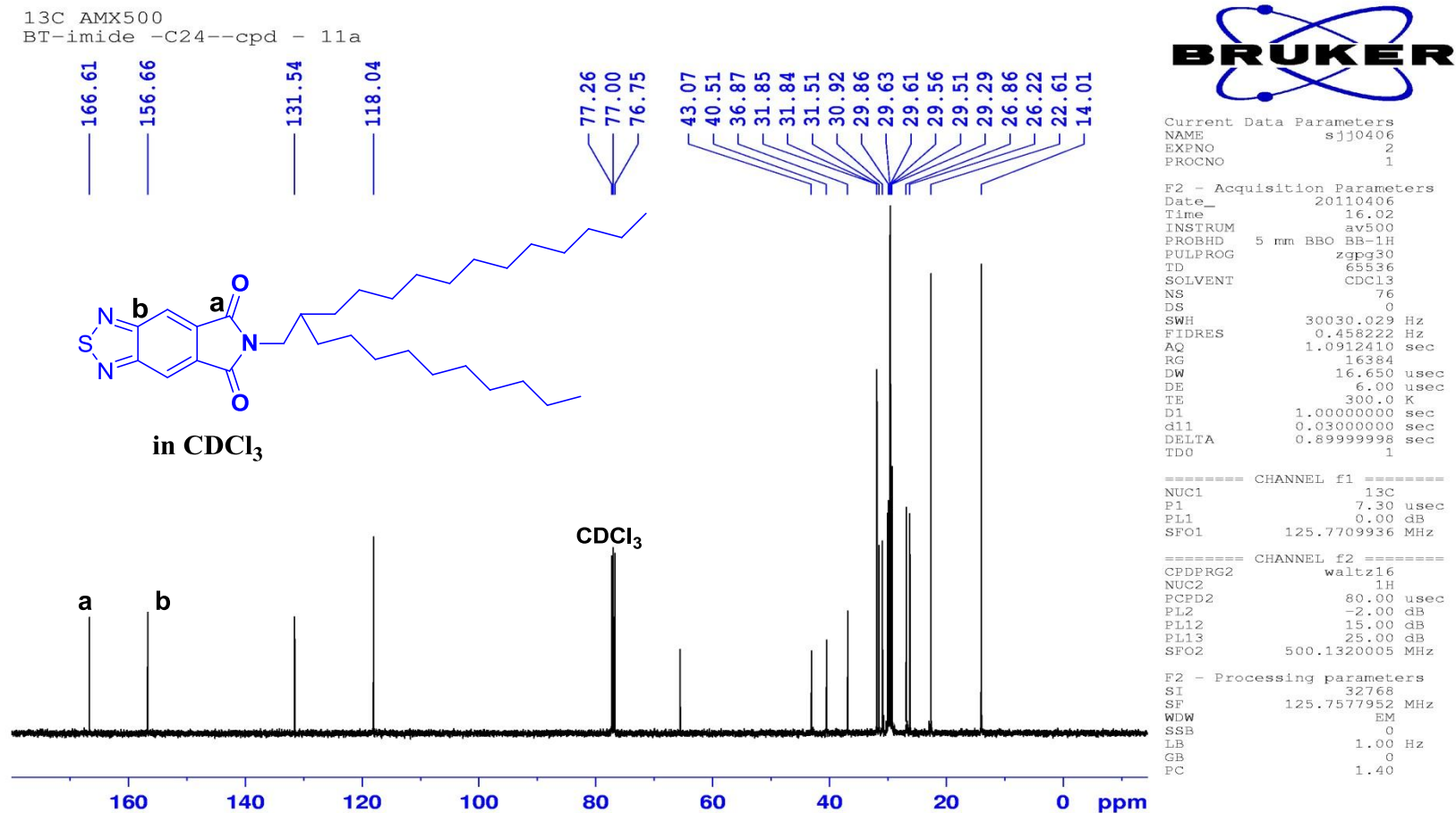
<sup>1</sup>H NMR spectrum of compound **11a**





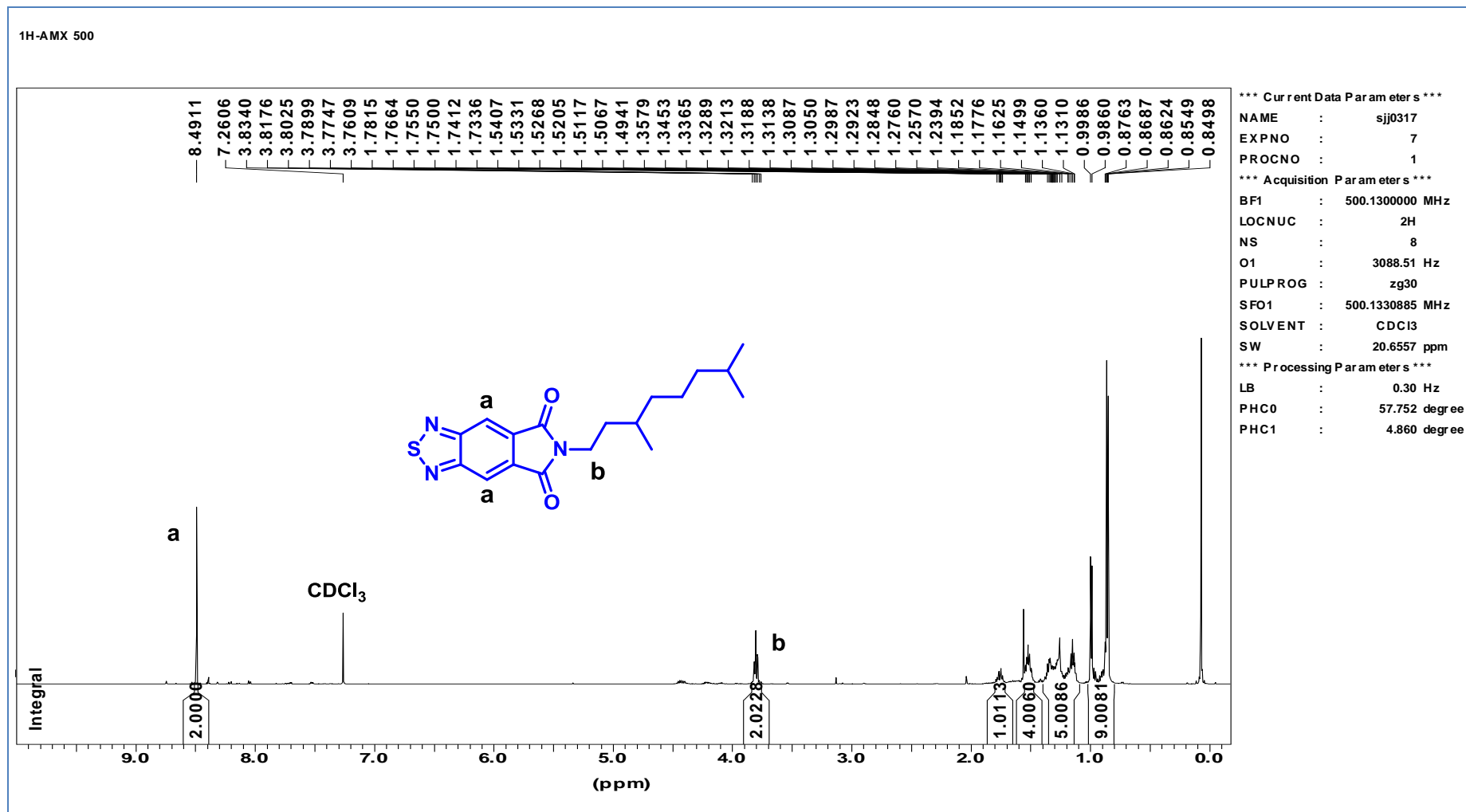
Electronic Supplementary Information (ESI) for Organic & Biomolecular Chemistry

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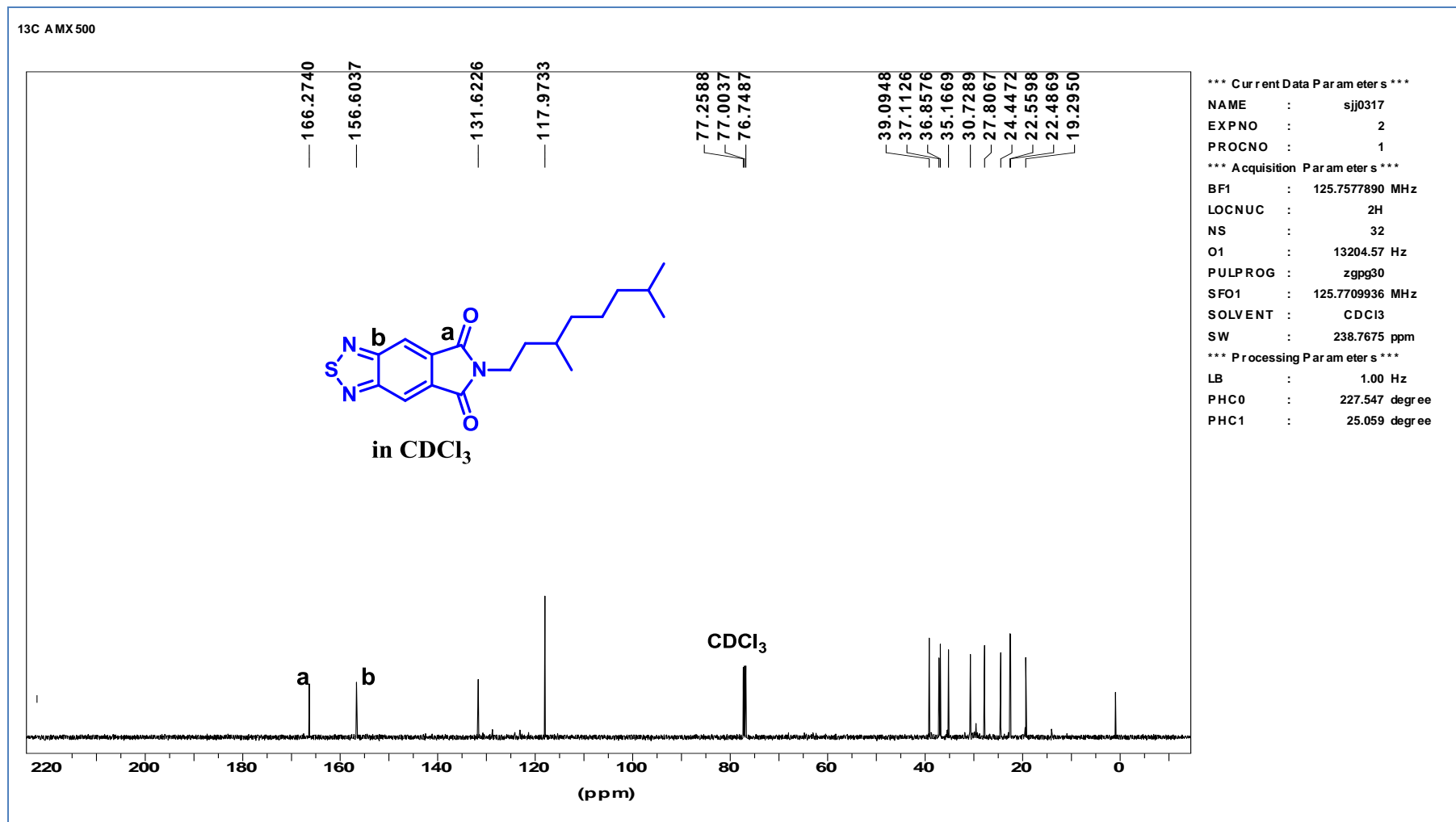
Electronic Supplementary Information (ESI) for Organic & Biomolecular Chemistry

<sup>1</sup>H NMR spectrum of compound **11b**



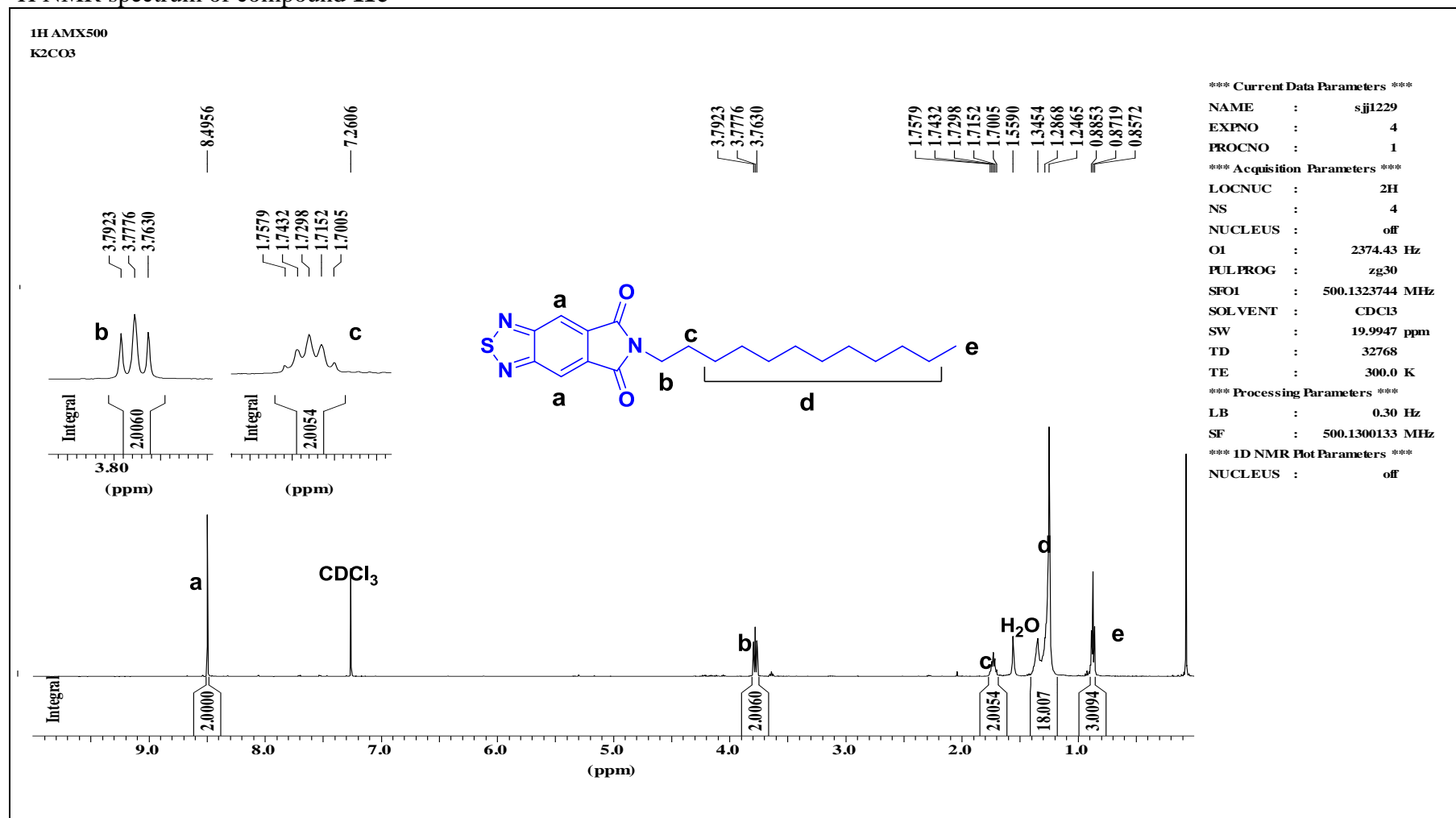
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<sup>13</sup>C NMR spectrum of compound **11b**



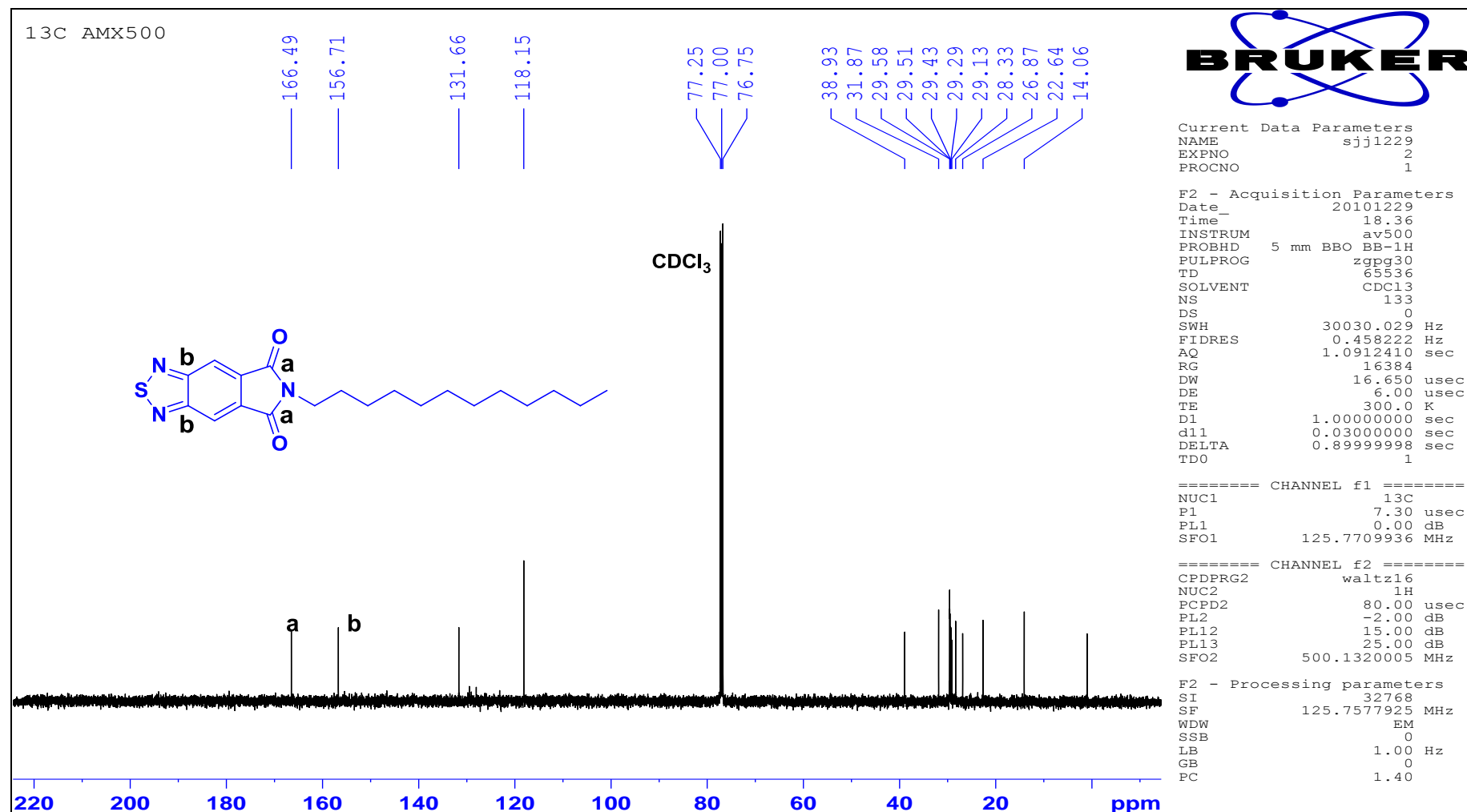
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<sup>1</sup>H NMR spectrum of compound **11c**



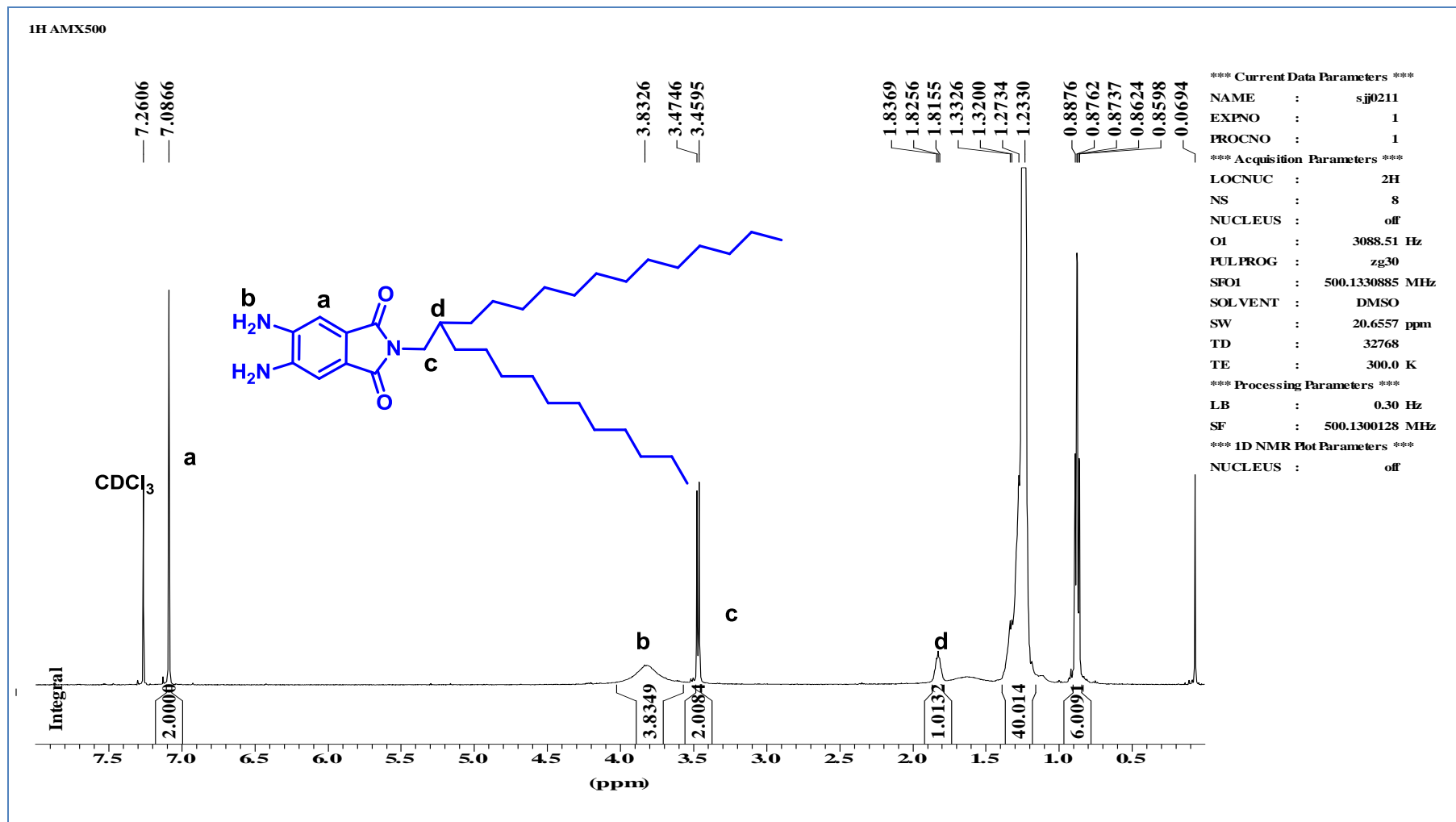
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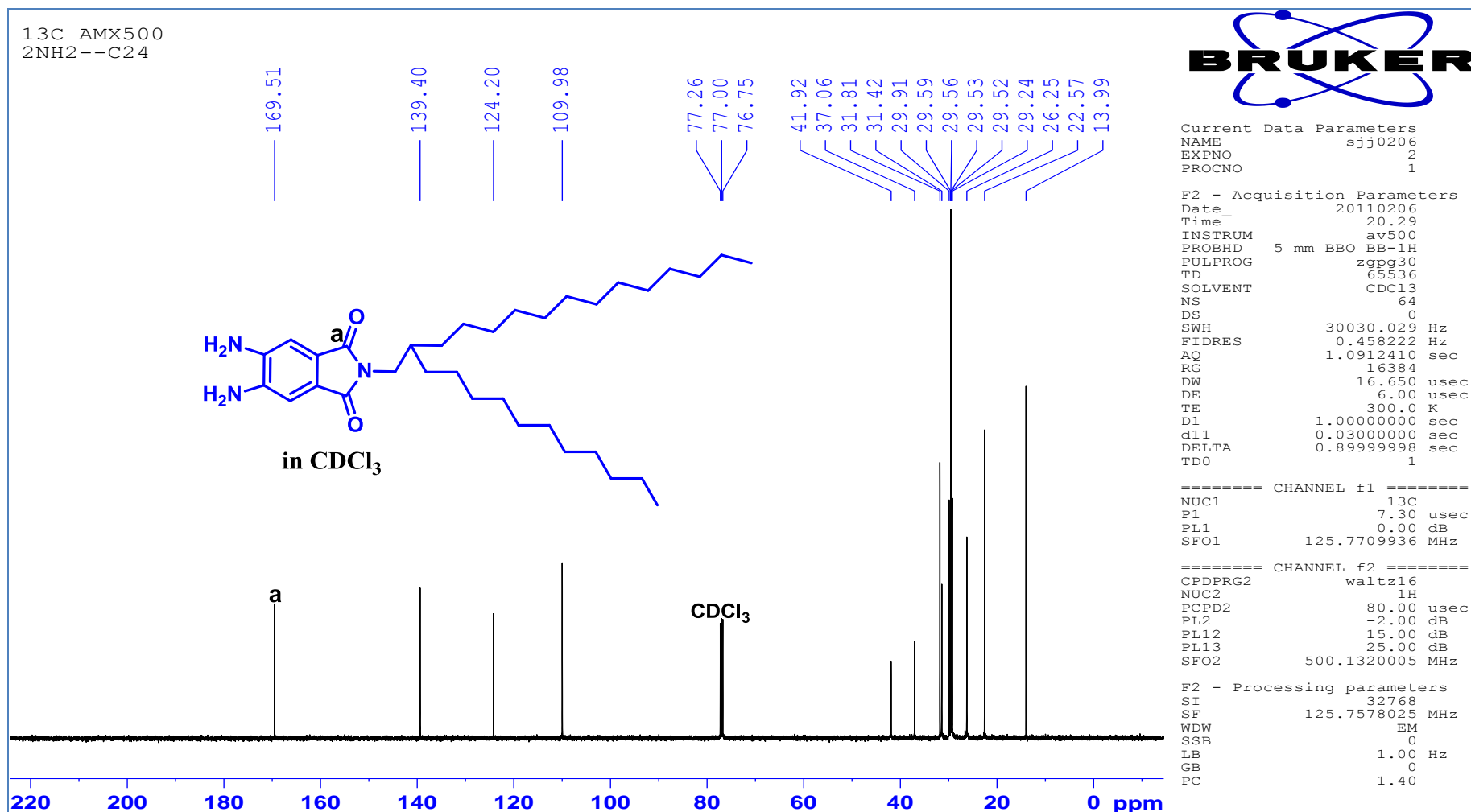
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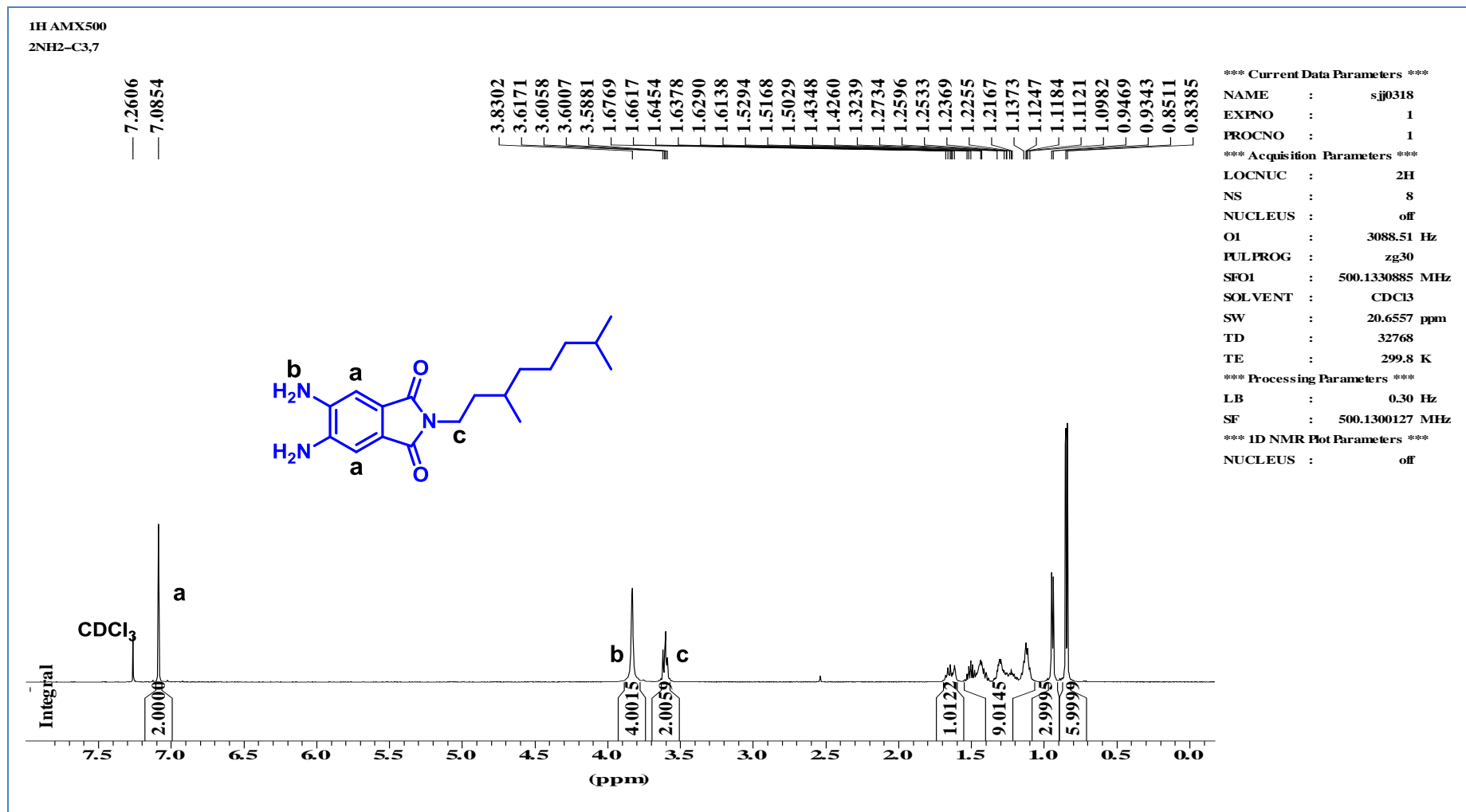
Electronic Supplementary Information (ESI) for Organic & Biomolecular Chemistry

<sup>13</sup>C NMR spectrum of compound **12a**



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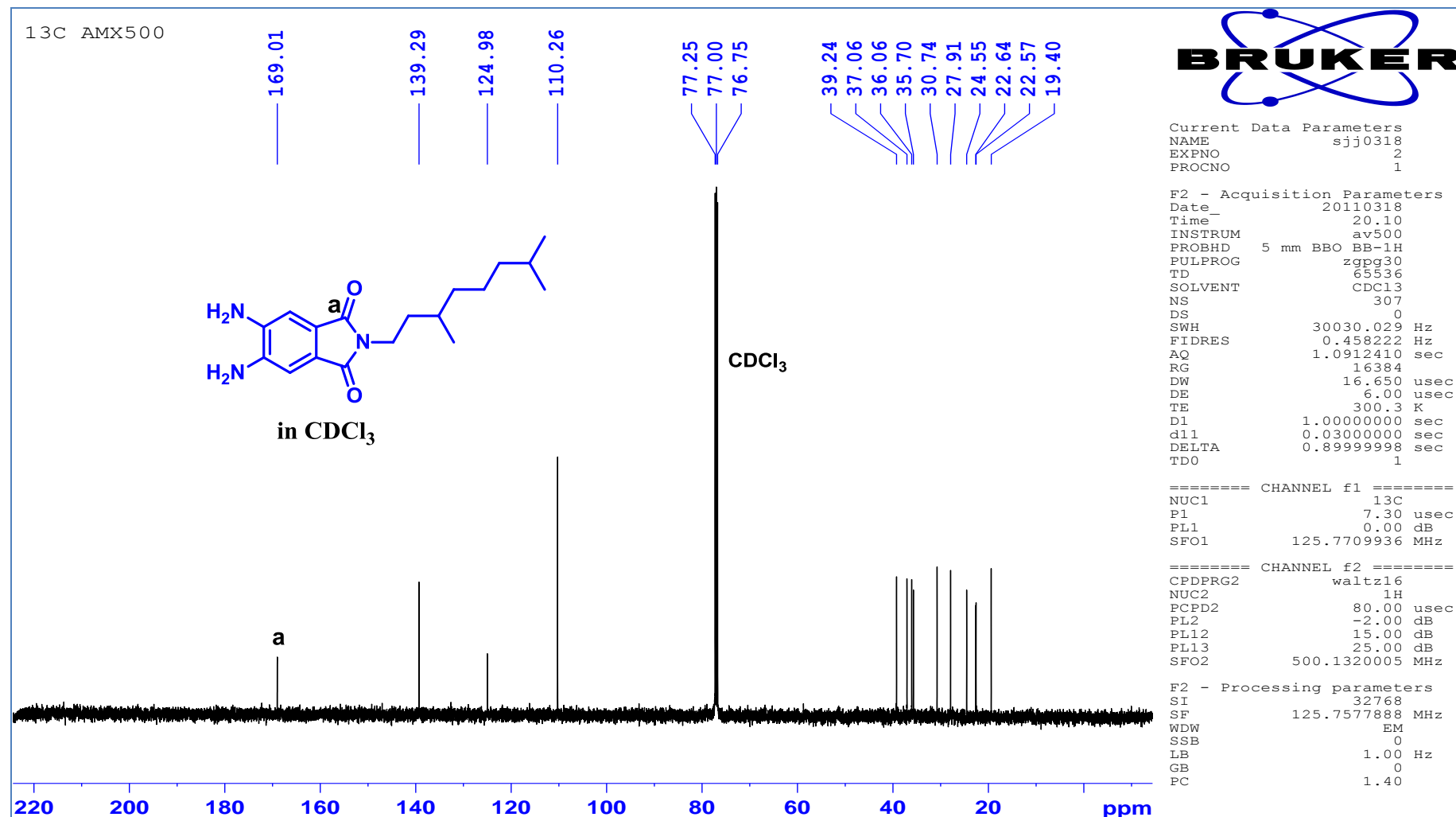
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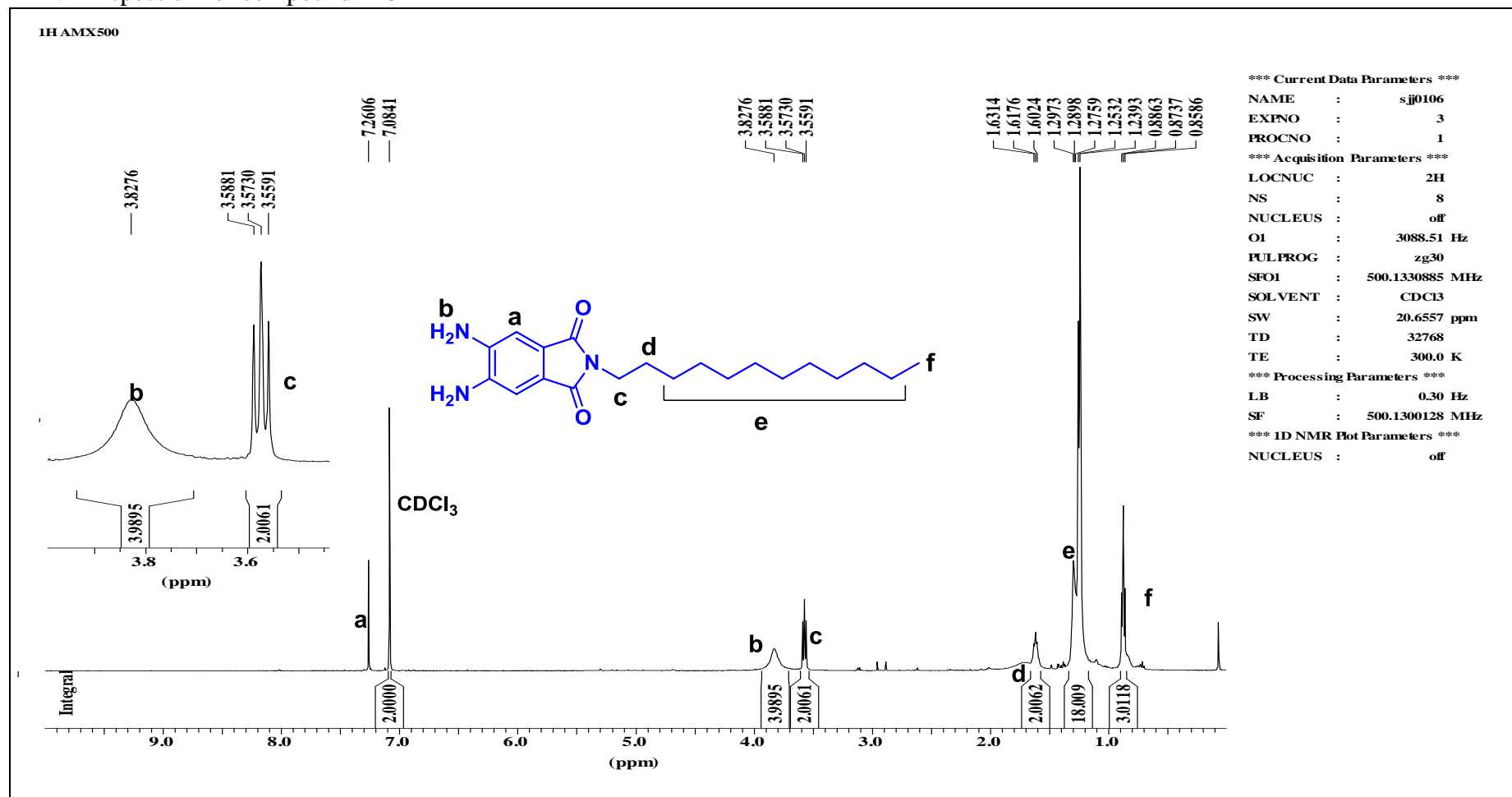
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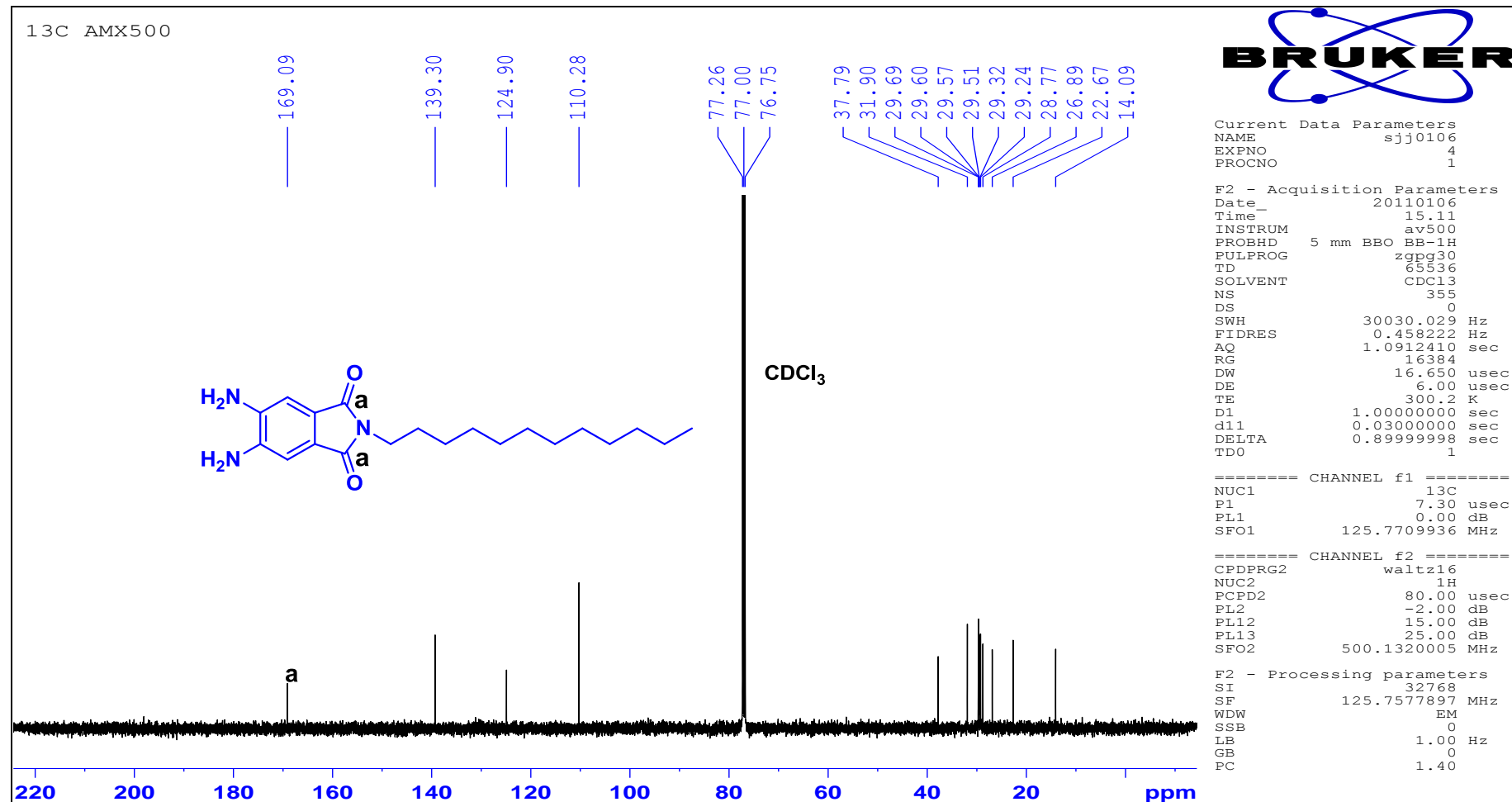
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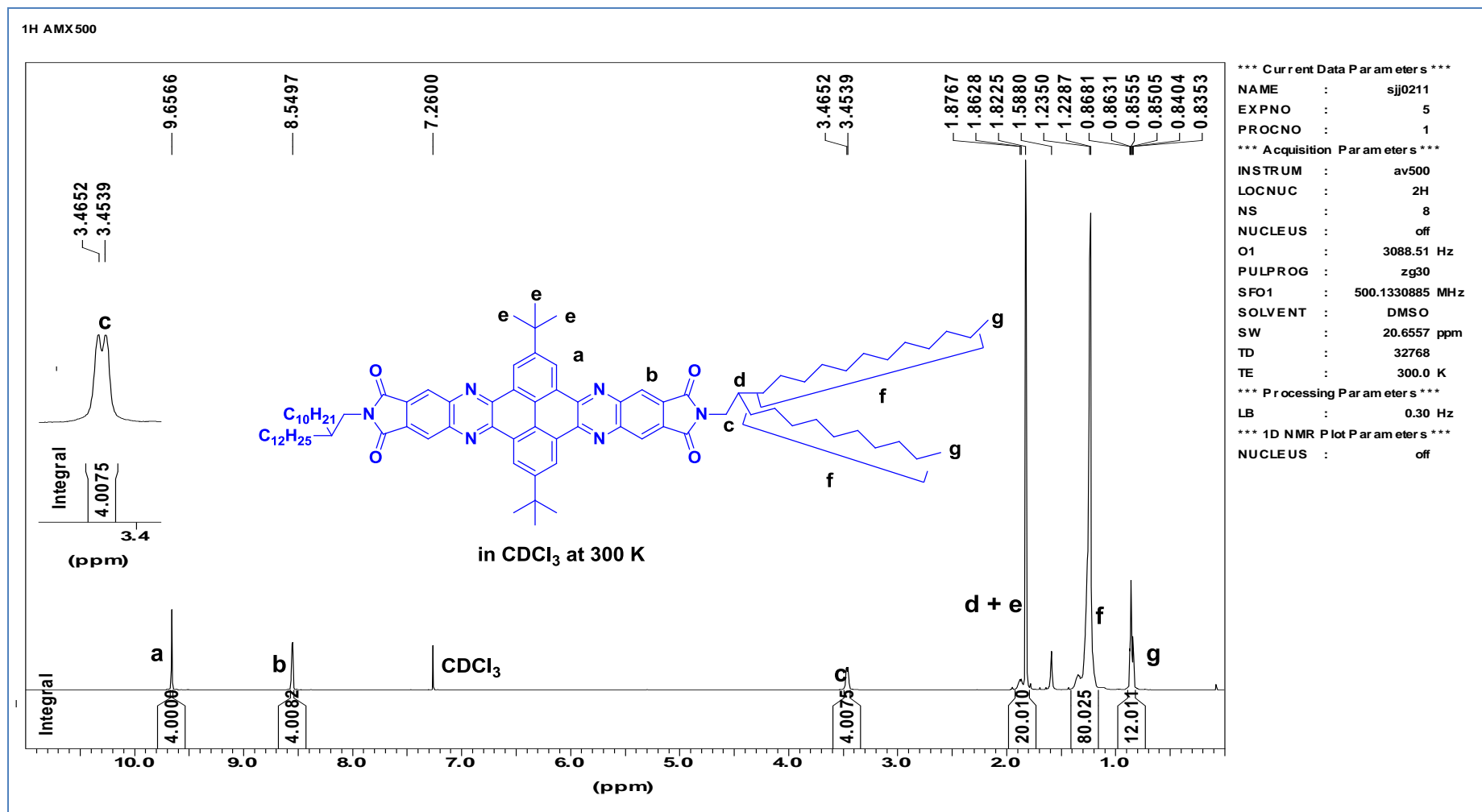
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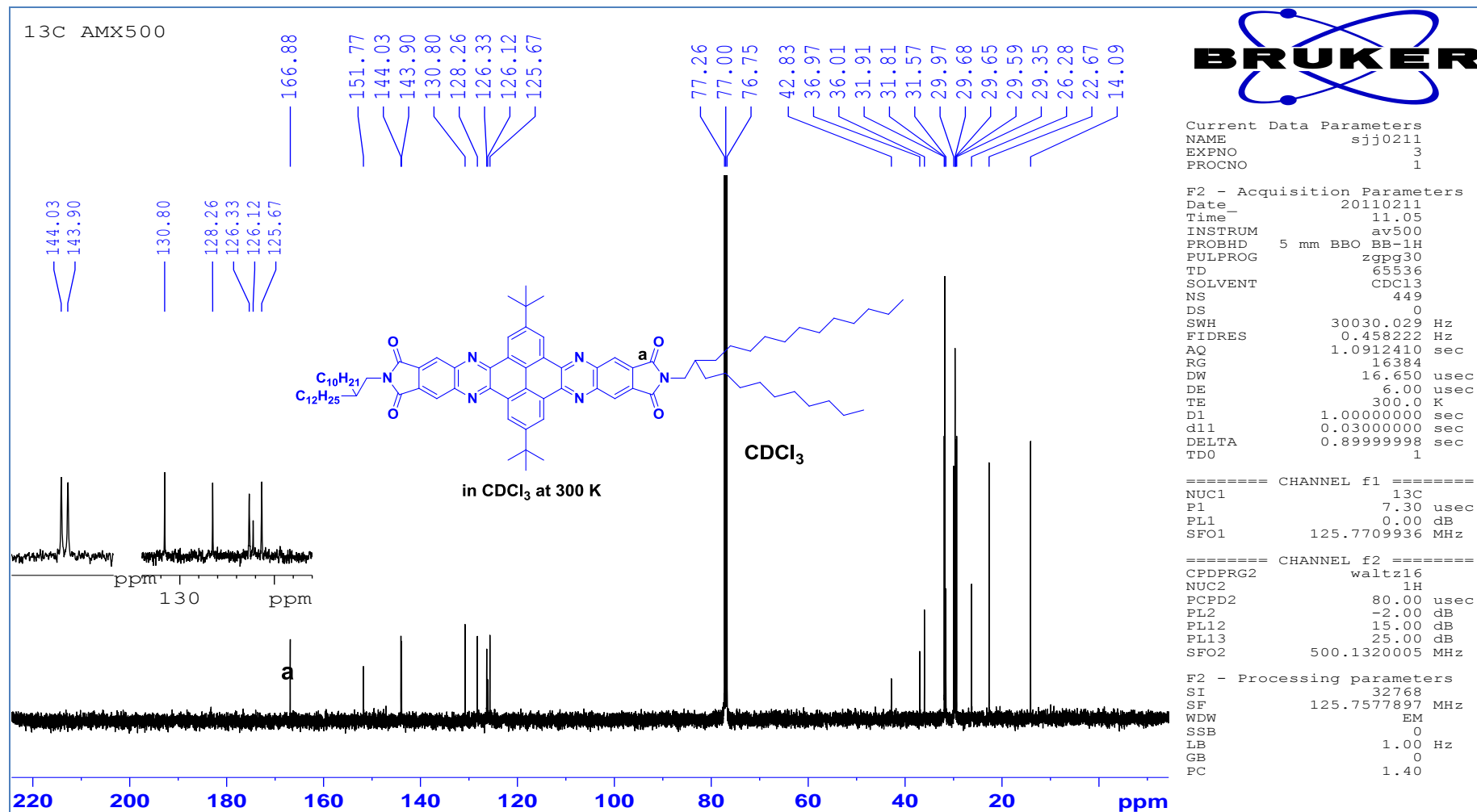
Electronic Supplementary Information (ESI) for Organic & Biomolecular Chemistry

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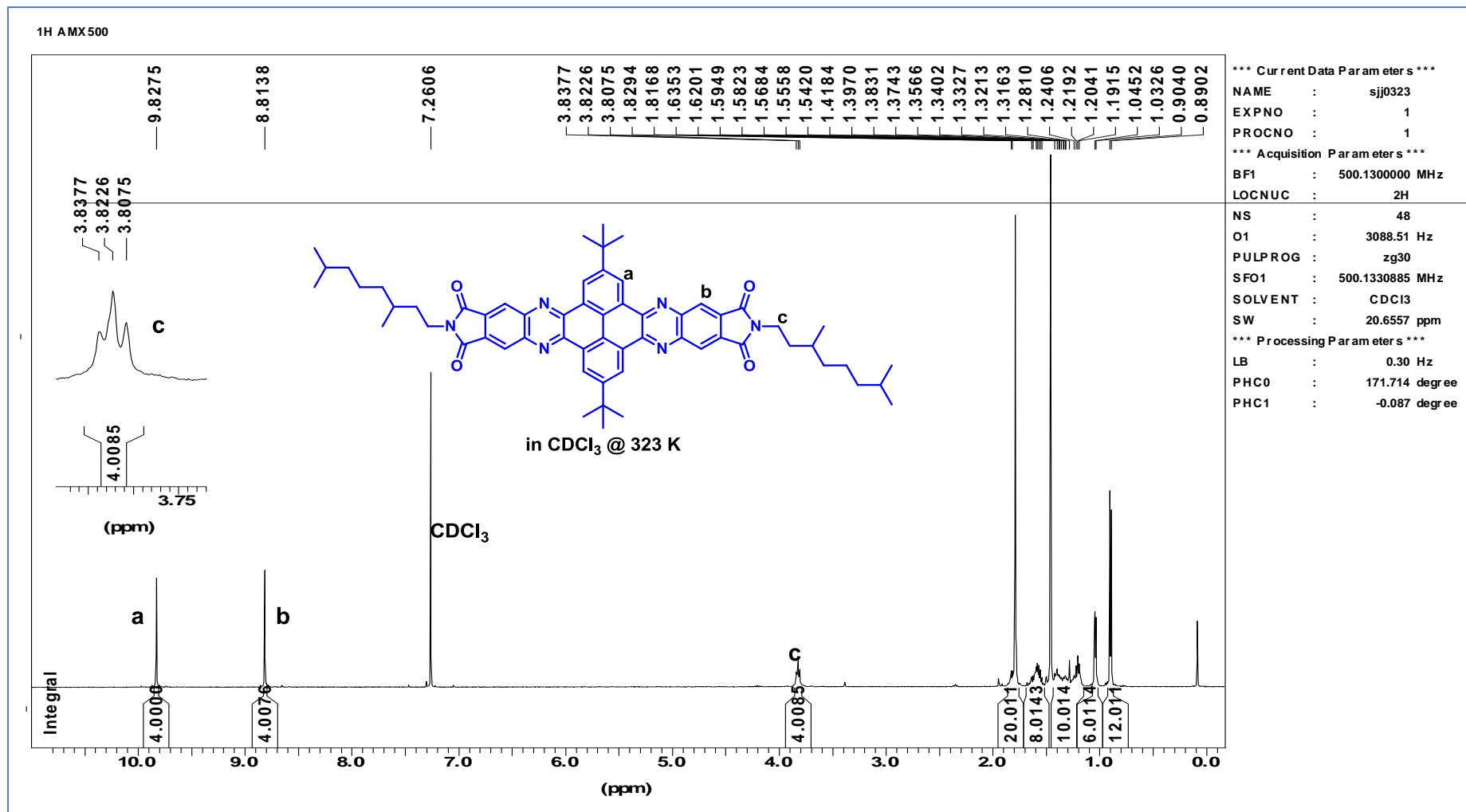
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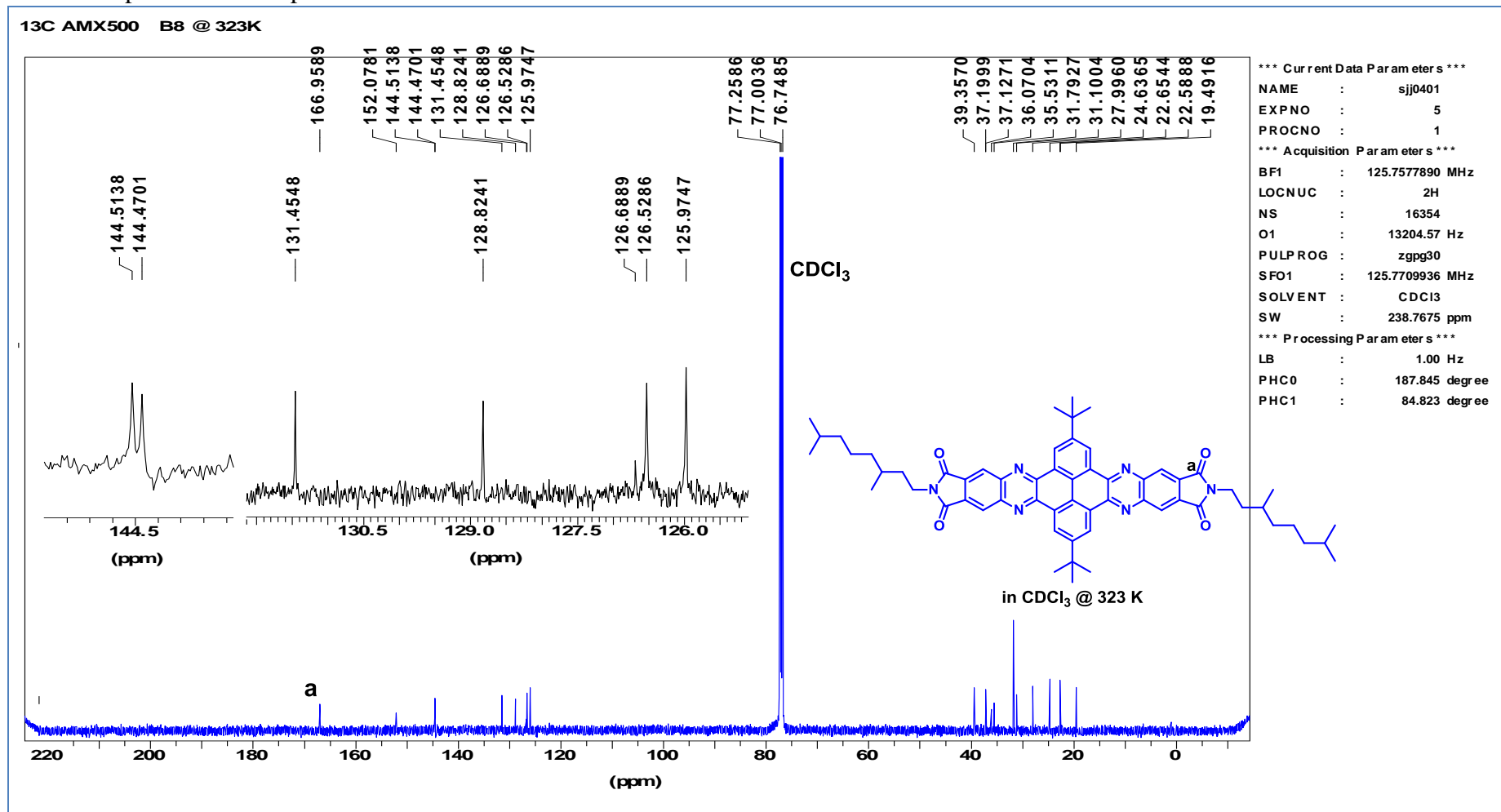
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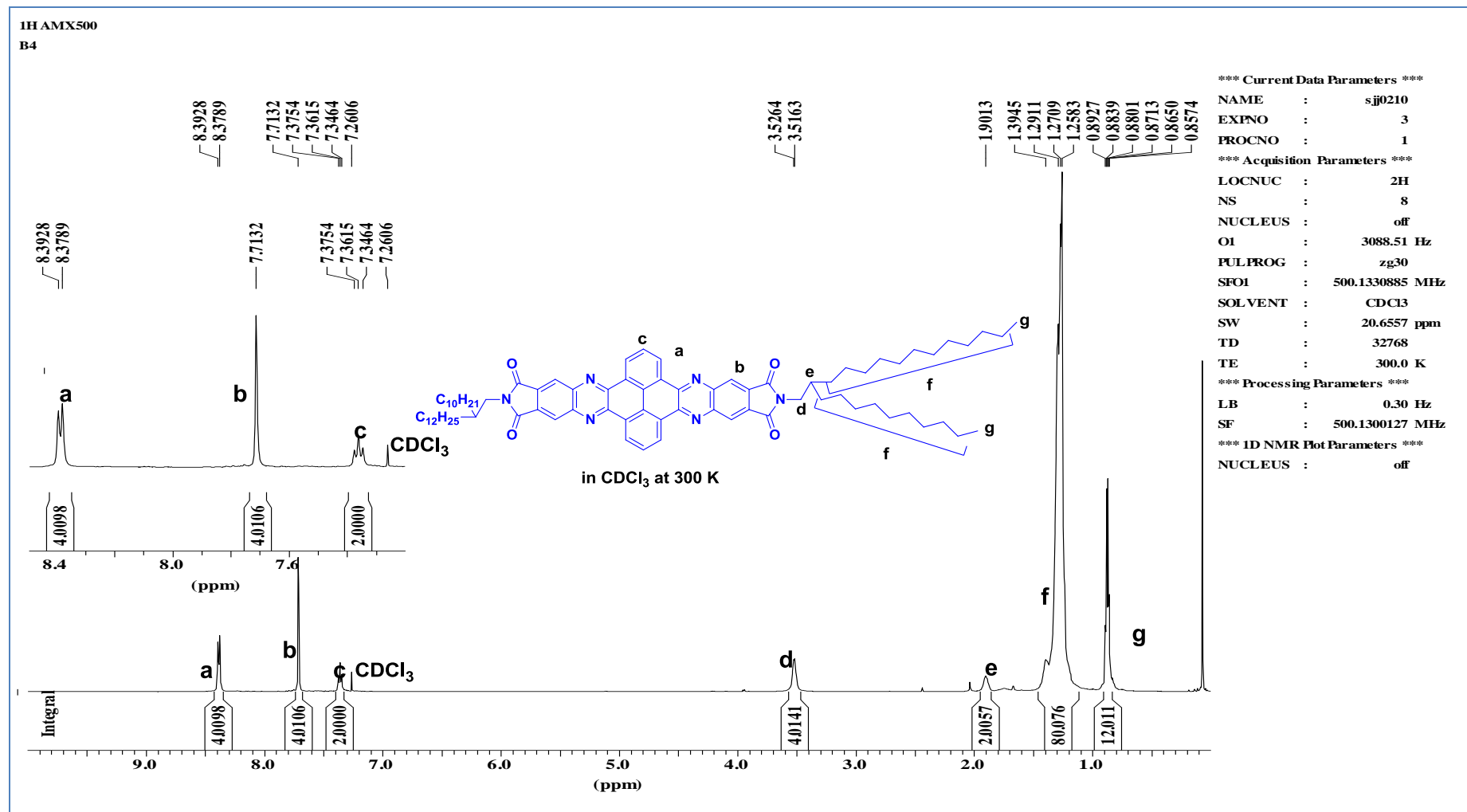
Electronic Supplementary Information (ESI) for Organic & Biomolecular Chemistry

<sup>13</sup>C NMR spectrum of compound **1b**



Electronic Supplementary Information (ESI) for Organic & Biomolecular Chemistry

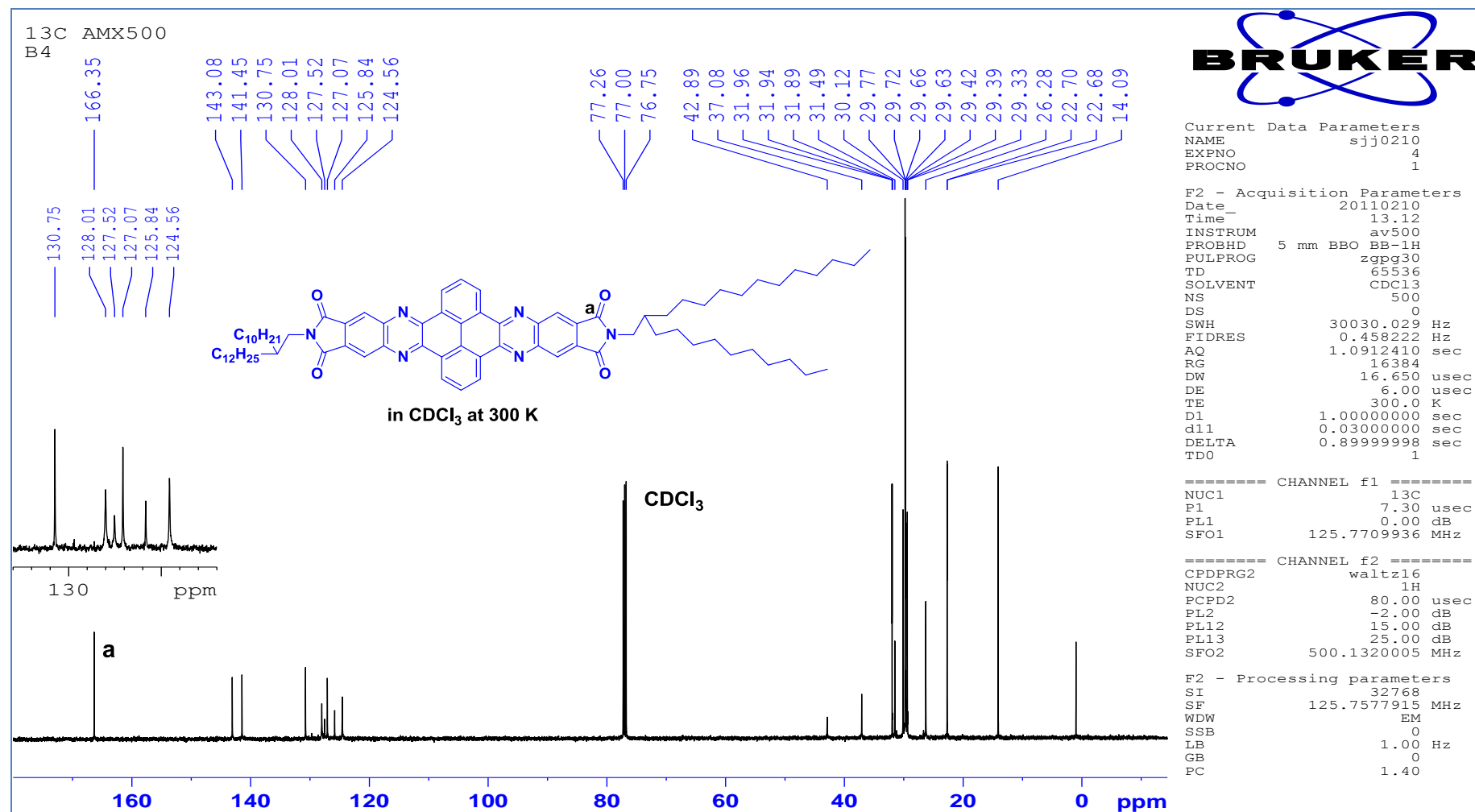
<sup>1</sup>H NMR spectrum of compound 2a





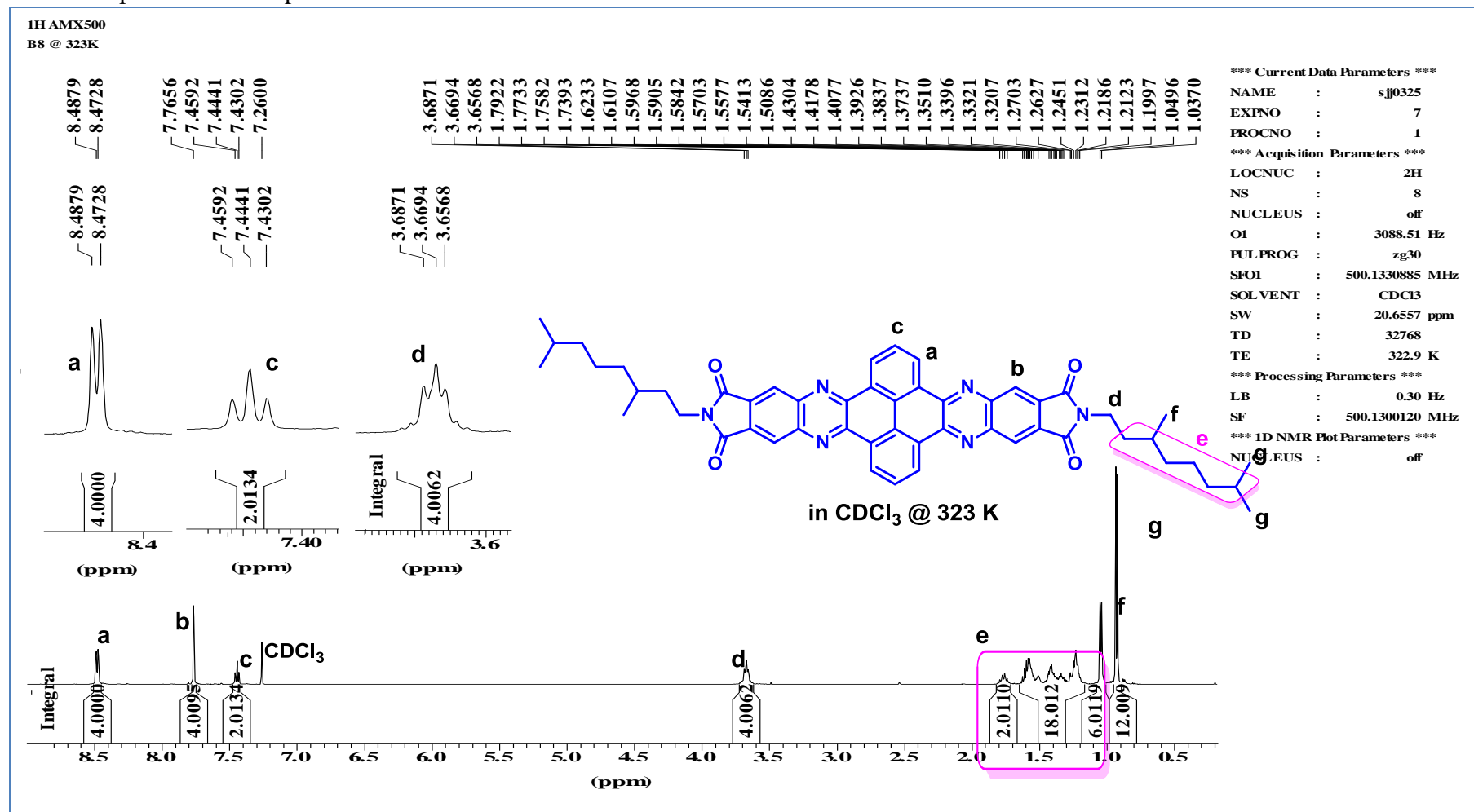
Electronic Supplementary Information (ESI) for Organic & Biomolecular Chemistry

$^{13}\text{C}$  NMR spectrum of compound **2a**



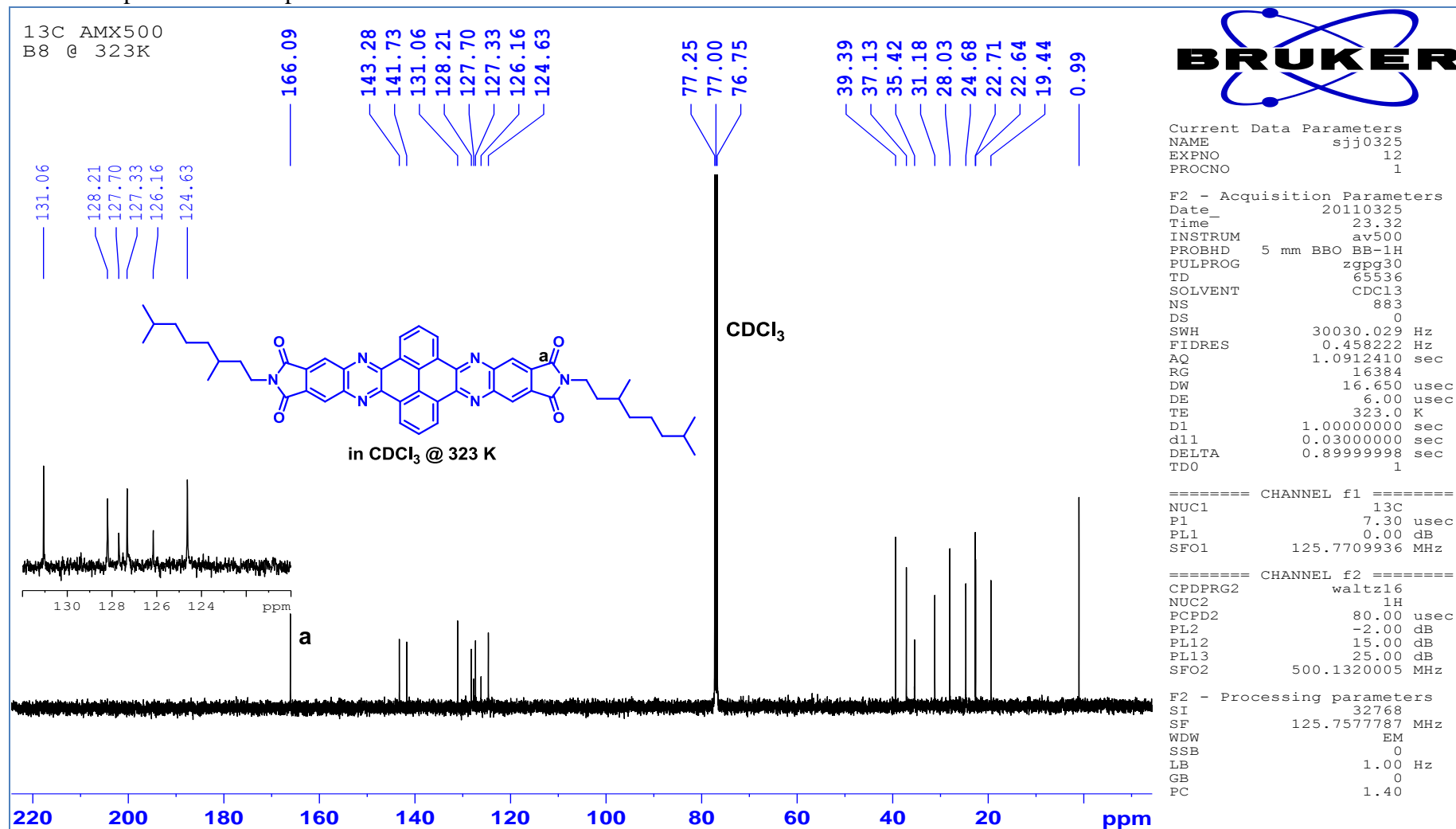
Electronic Supplementary Information (ESI) for Organic & Biomolecular Chemistry

<sup>1</sup>H NMR spectrum of compound **2b**



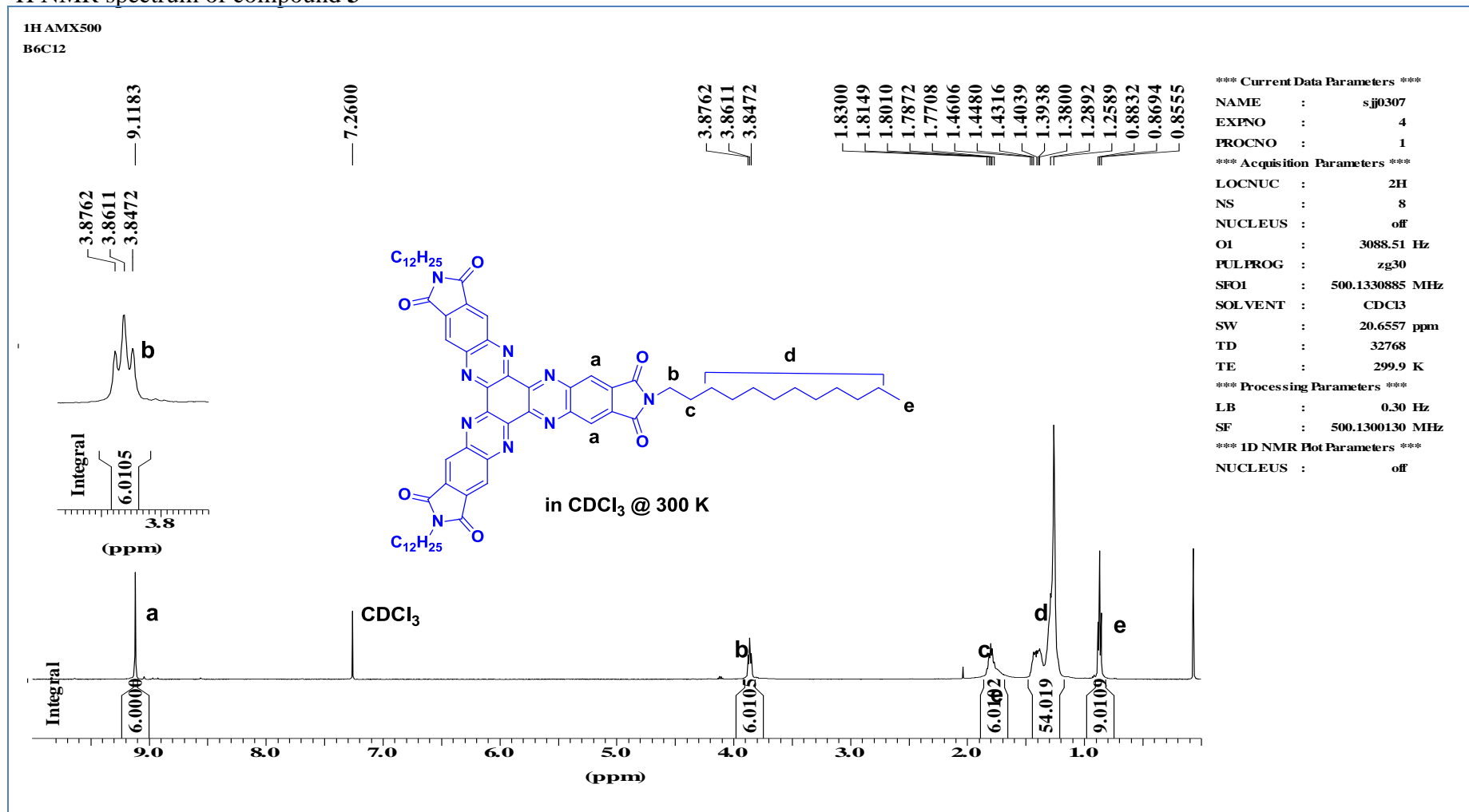
Electronic Supplementary Information (ESI) for Organic & Biomolecular Chemistry

<sup>13</sup>C NMR spectrum of compound **2b**



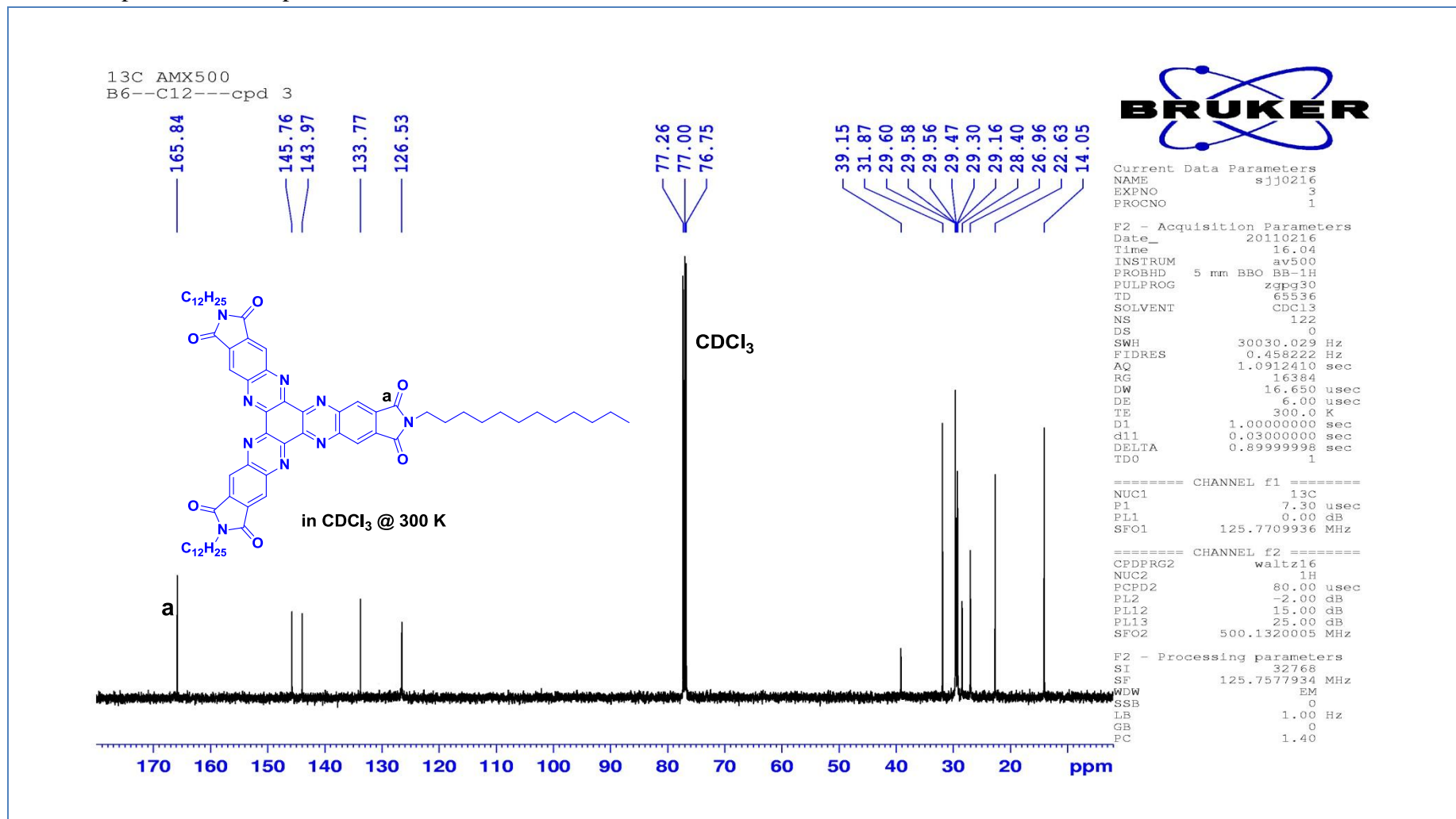
Electronic Supplementary Information (ESI) for Organic & Biomolecular Chemistry

<sup>1</sup>H NMR spectrum of compound 3



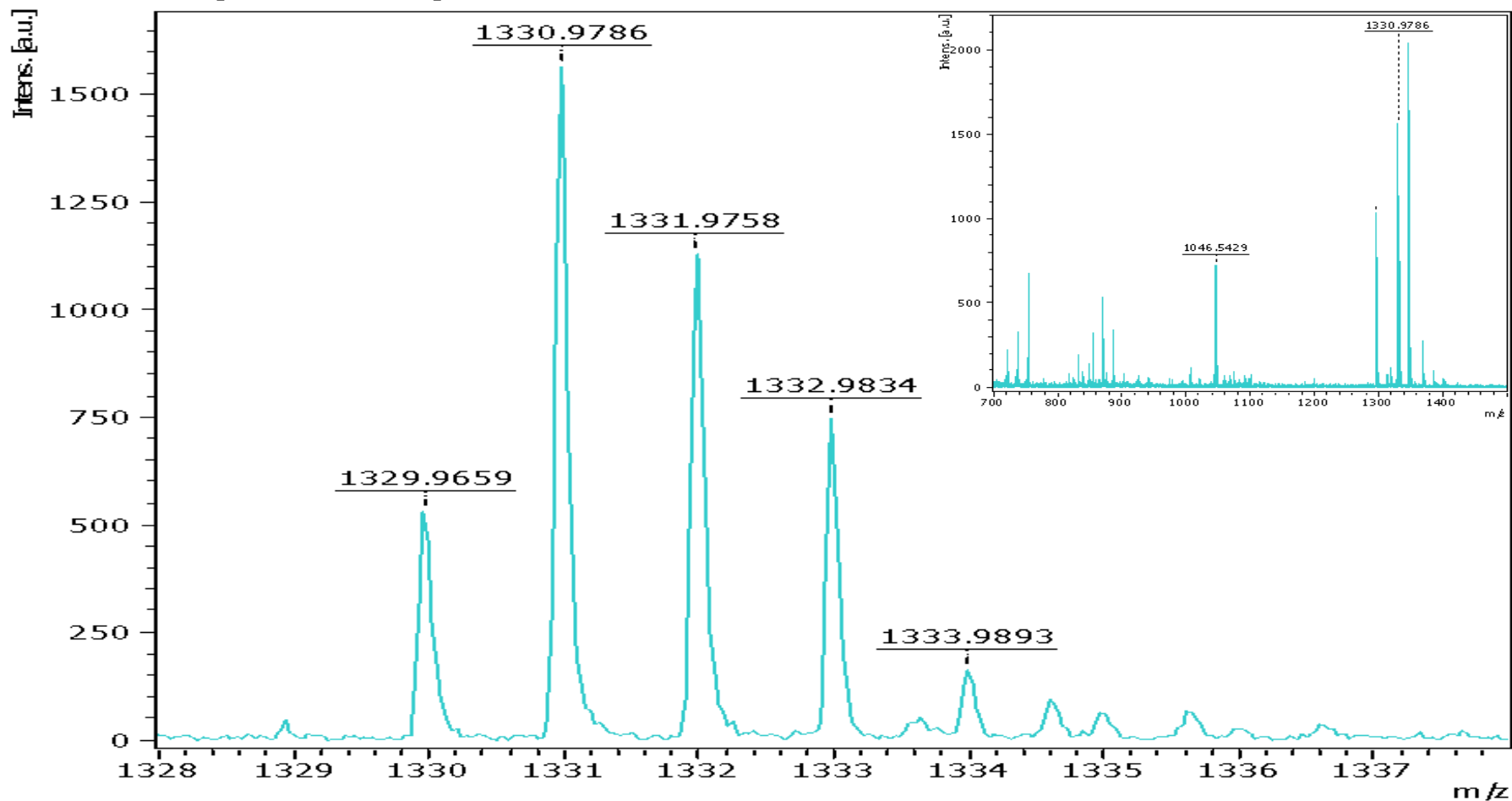
Electronic Supplementary Information (ESI) for Organic & Biomolecular Chemistry

$^{13}\text{C}$  NMR spectrum of compound 3



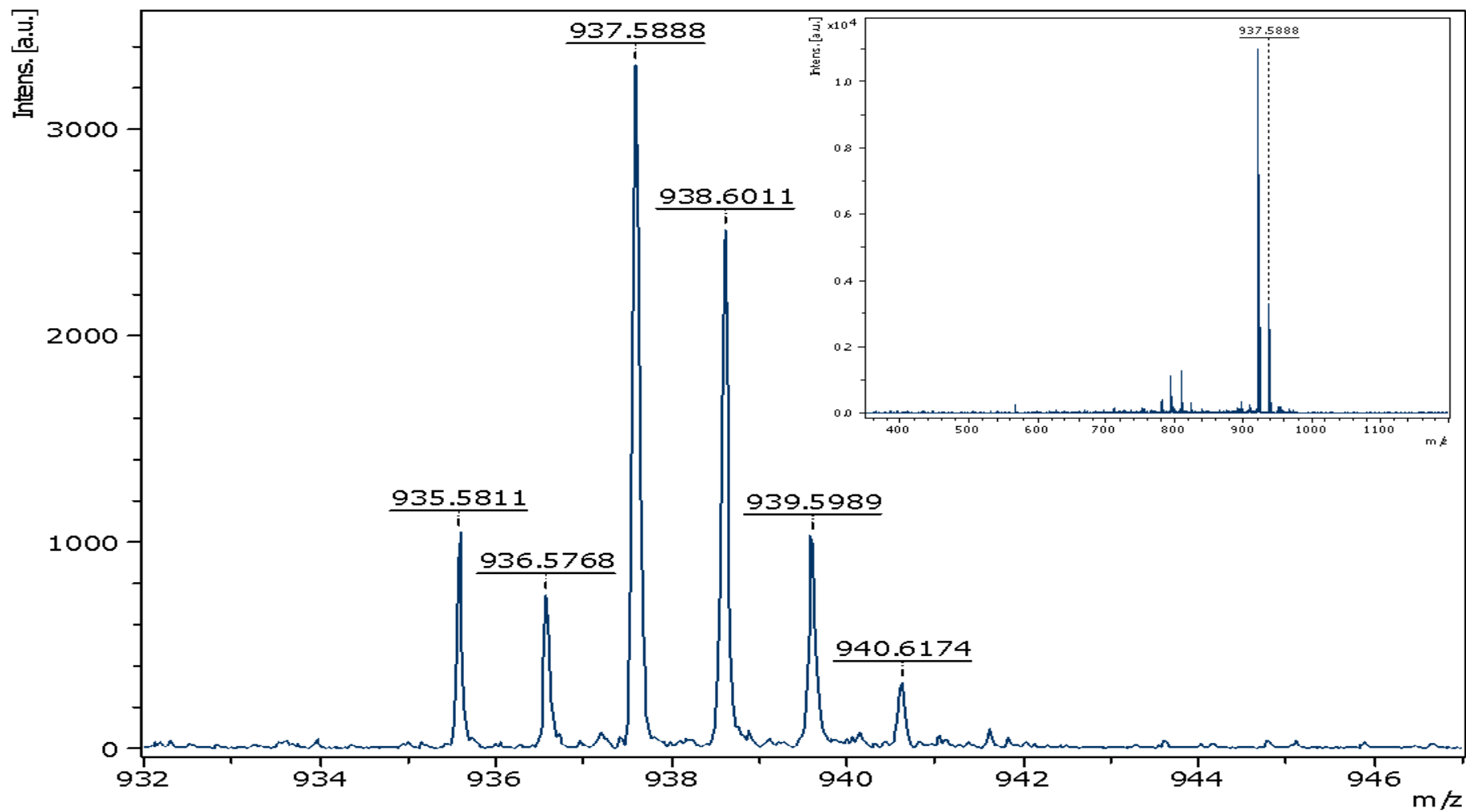
## 10. MALDI-TOF mass spectra for 1a-b, 2a-b and 3.

### MALDI-TOF MS spectrum for 1a (Pepmix as internal standard)



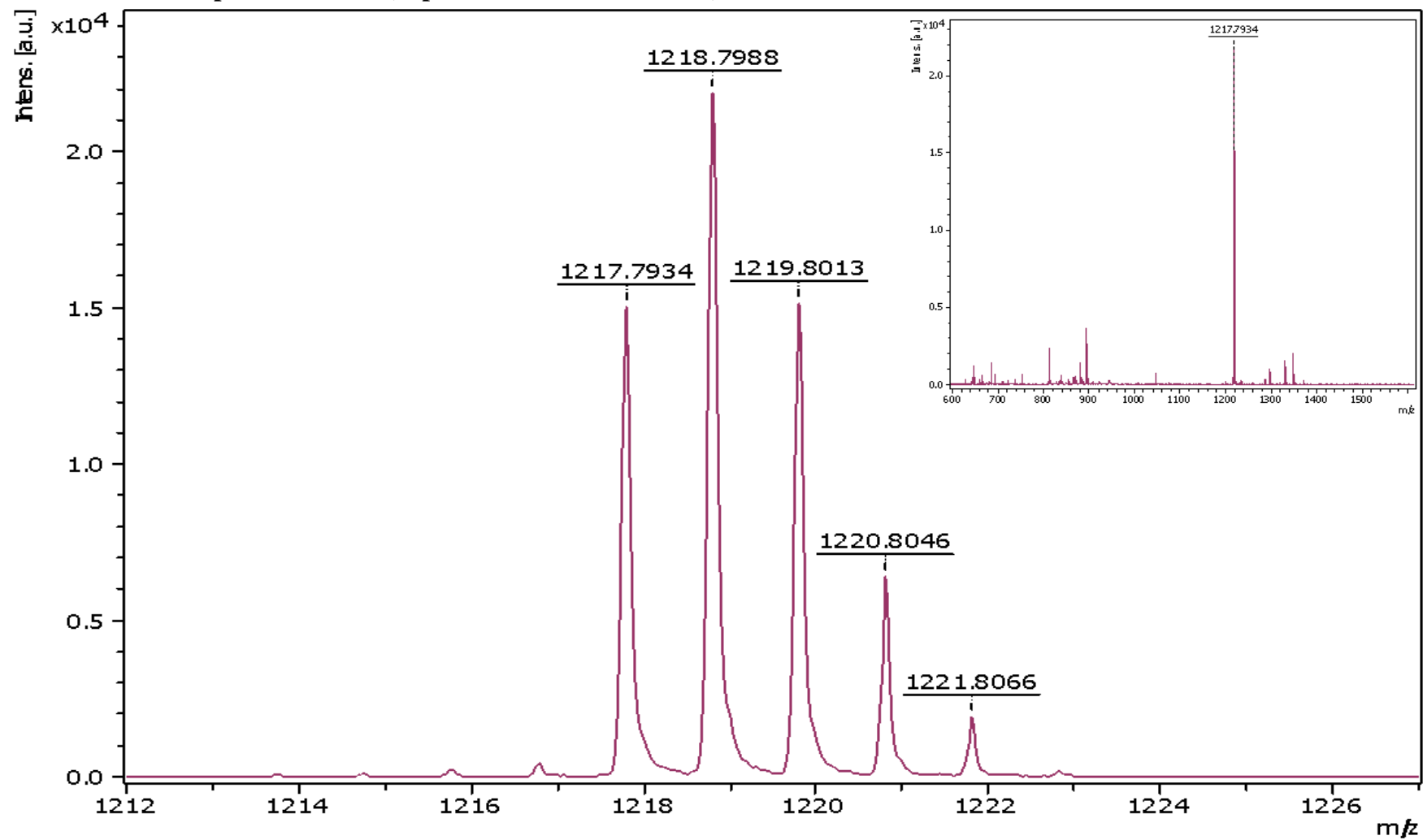
Electronic Supplementary Information (ESI) for Organic & Biomolecular Chemistry

MALDI-TOF MS spectrum for 1b (Pepmix as external standard)



Electronic Supplementary Information (ESI) for Organic & Biomolecular Chemistry

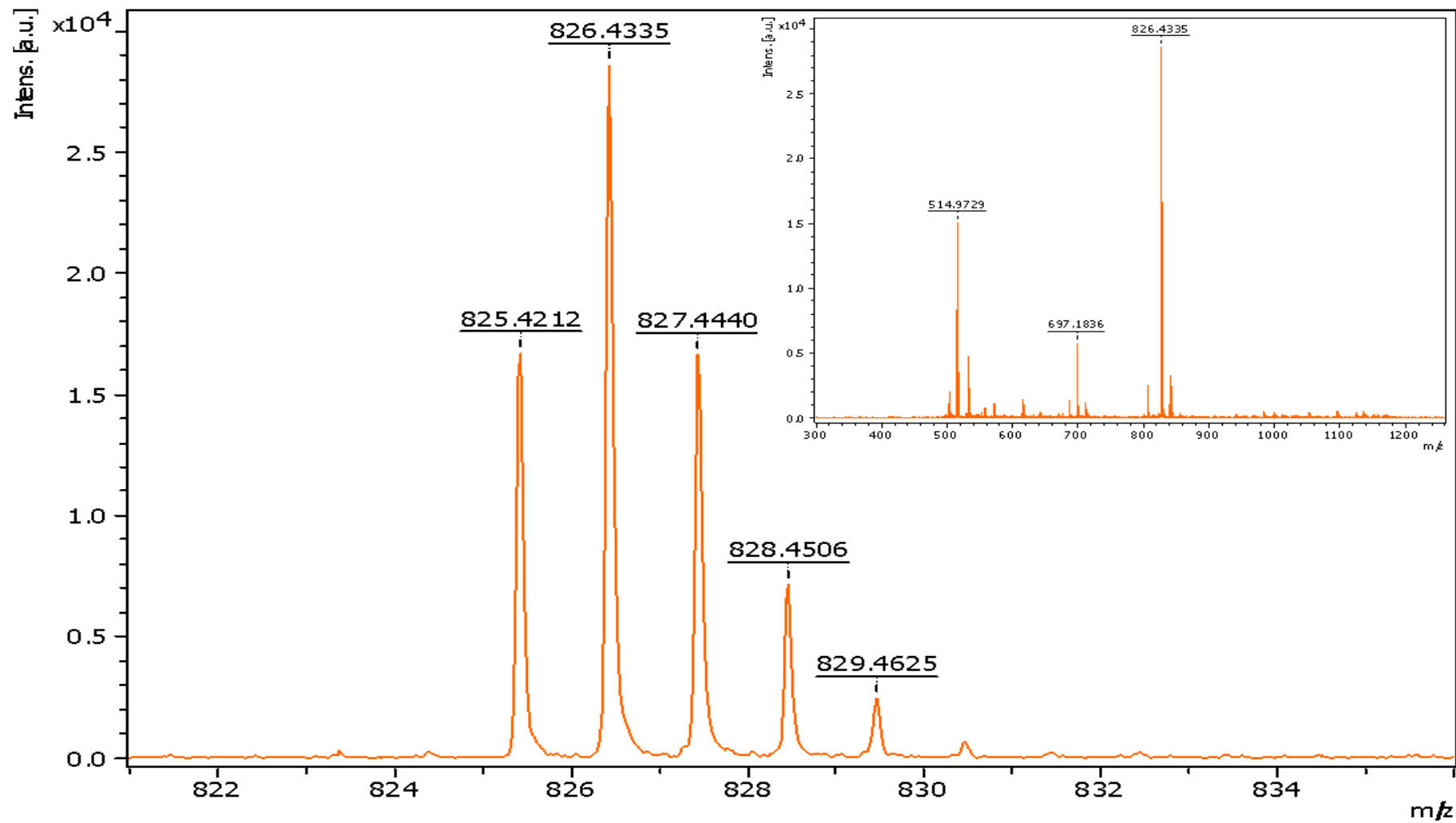
MALDI-TOF MS spectrum for 2a (Pepmix as external standard)





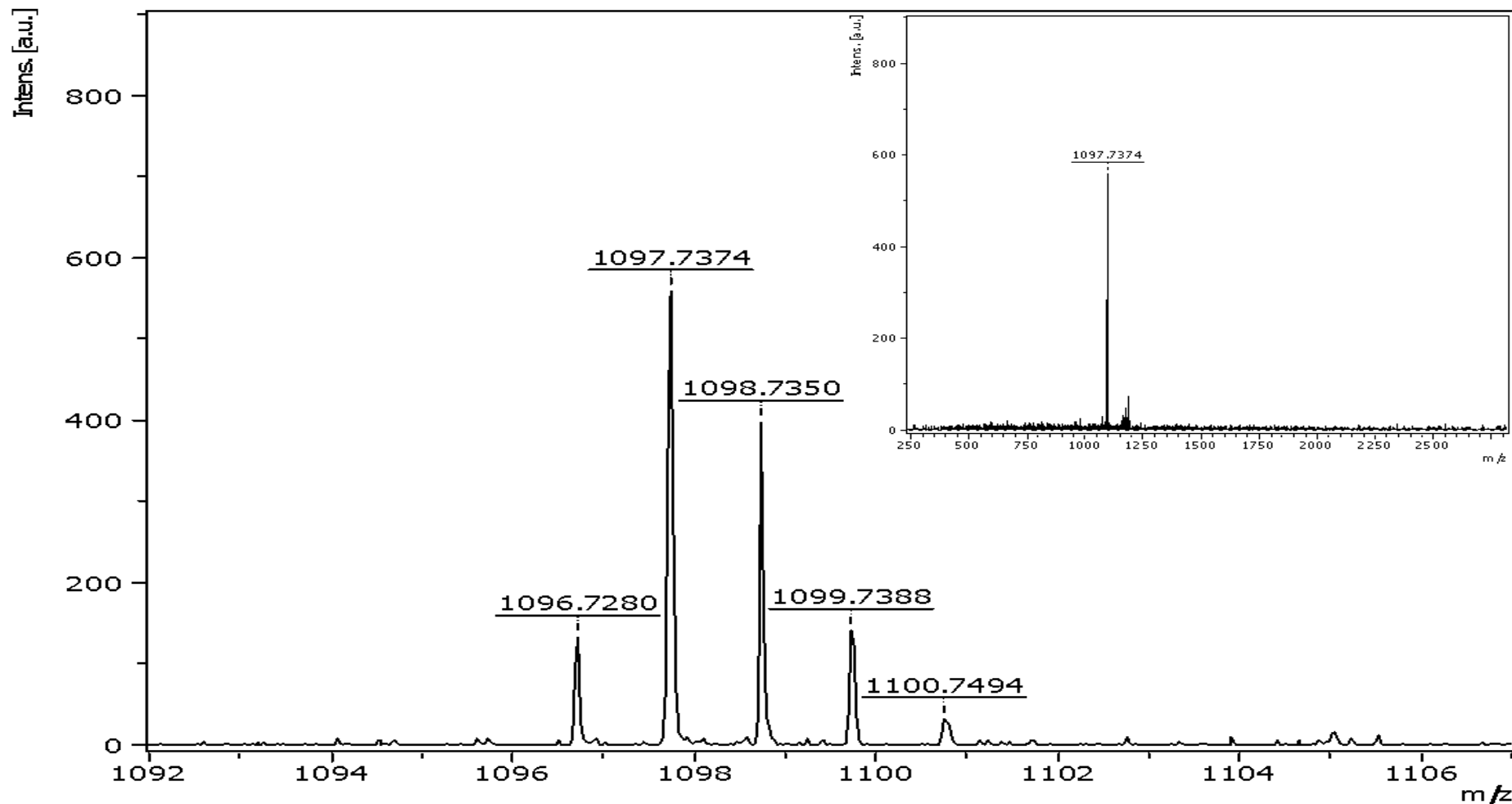
Electronic Supplementary Information (ESI) for Organic & Biomolecular Chemistry

MALDI-TOF MS spectrum for 2b (Pepmix as external standard)



*Electronic Supplementary Information (ESI) for Organic & Biomolecular Chemistry*

**MALDI-TOF MS spectrum for 3 (Pepmix as external standard)**



*Electronic Supplementary Information (ESI) for Organic & Biomolecular Chemistry*

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**11. Reference**

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- 2) (a) Arp, F. O.; Fu, G. C. *J. Am. Chem. Soc.*, **2005**, 127, 10482. (b) Qu, H; Luo, J; Zhang, X; Chi, C. *J. Polym. Sci. Part A: Polym Chem.*, **2010**, 48, 186.
- 3) Qu, H; Cui, W; Li, J; Shao, J; Chi, C. *Org. Lett.*, **2011**, 13, 924.