

# Fluorescent azasteroids through ultrasound assisted cycloaddition reactions

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## 1. NMR spectra of the obtained compounds.

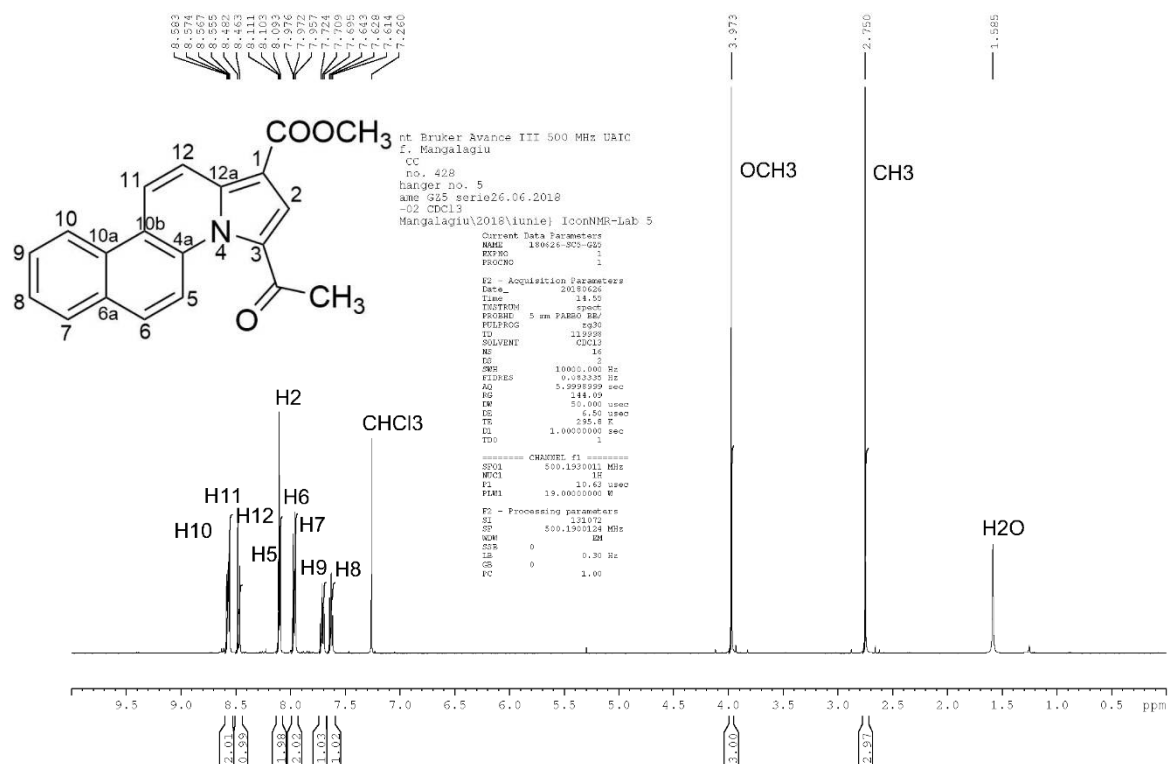


Figure S1a. <sup>1</sup>H NMR spectrum of the compound 5a.

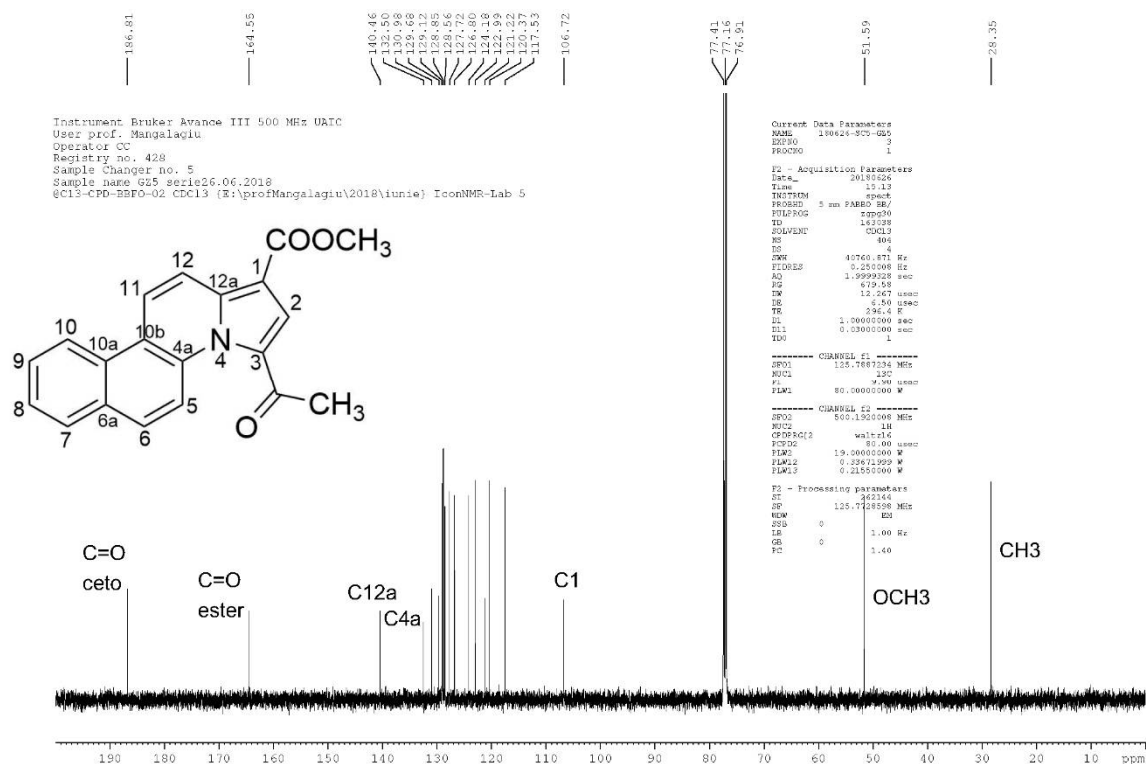


Figure S1b. <sup>13</sup>C NMR spectrum of the compound 5a.

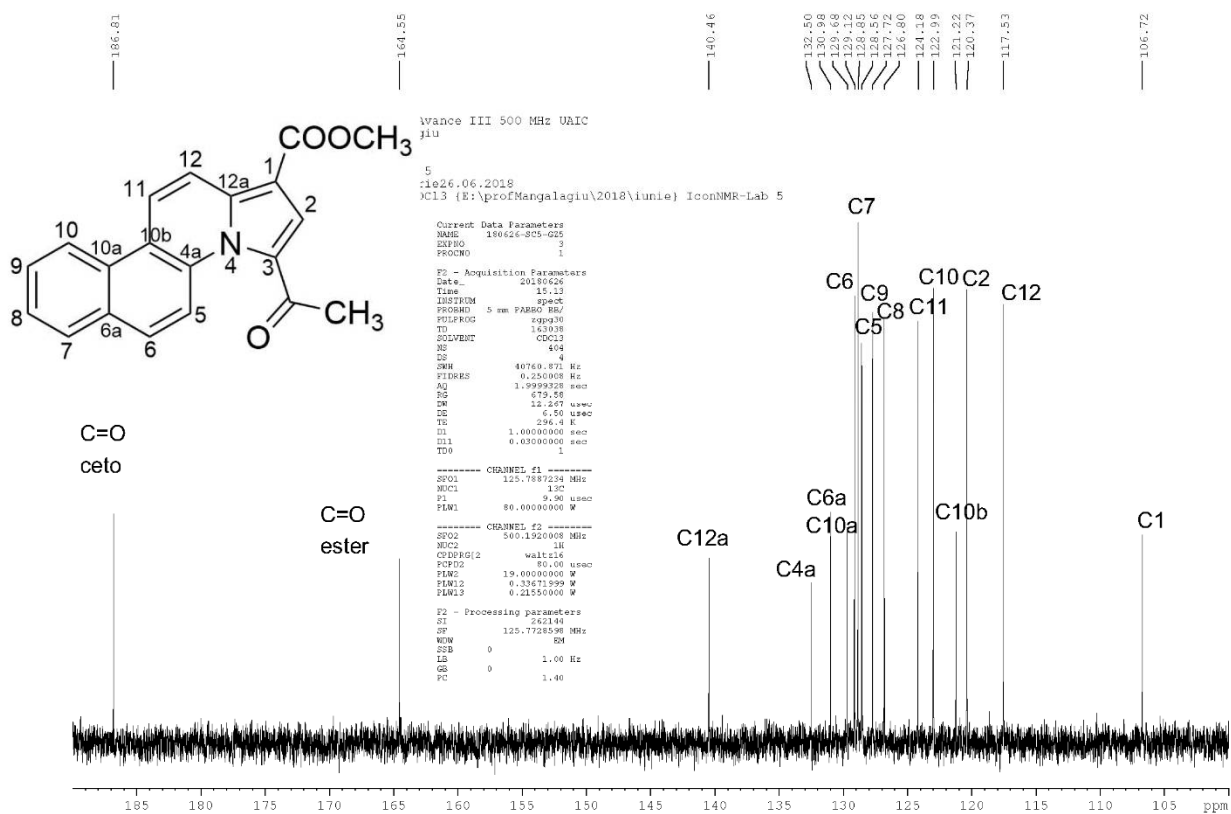


Figure S1c. Detail in the aromatic area of the  $^{13}\text{C}$  NMR spectrum of the compound 5a.

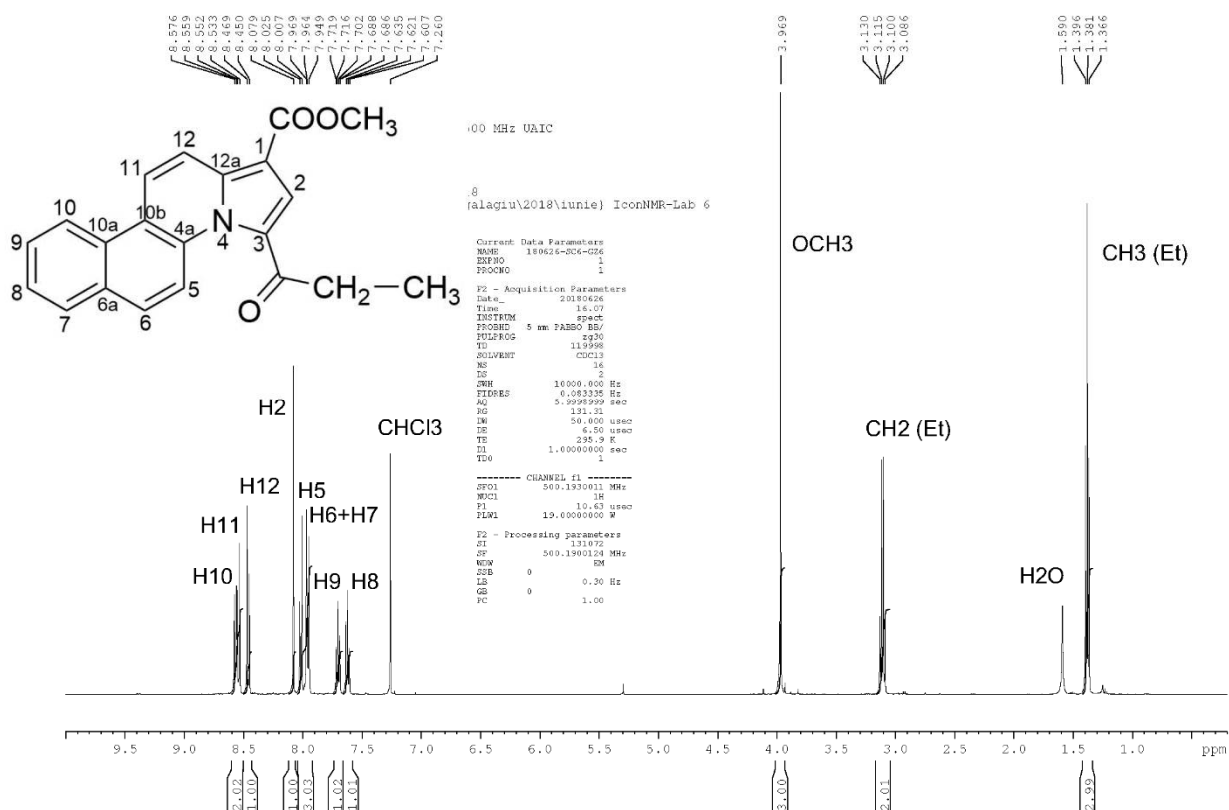


Figure S2a.  $^1\text{H}$  NMR spectrum of the compound 5b.

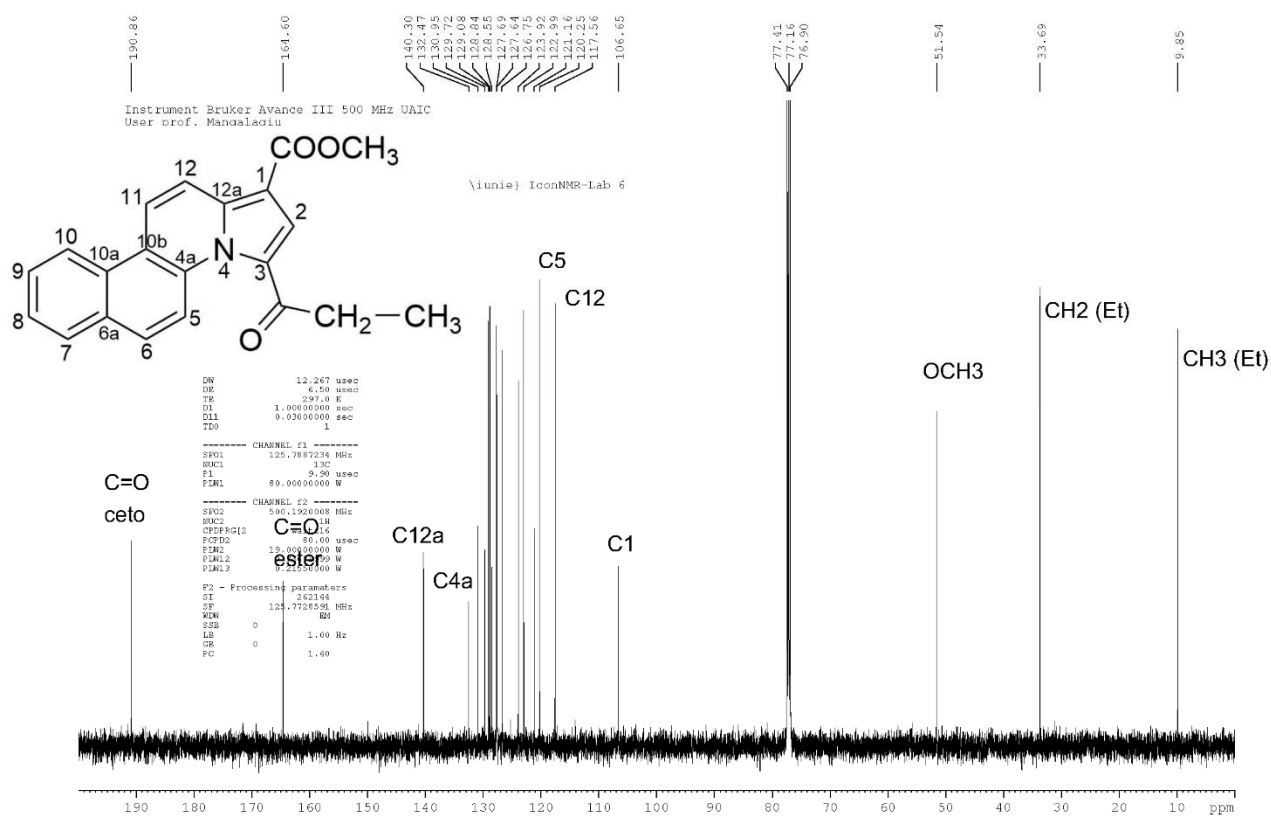


Figure S2b. <sup>13</sup>C NMR spectrum of the compound 5b.

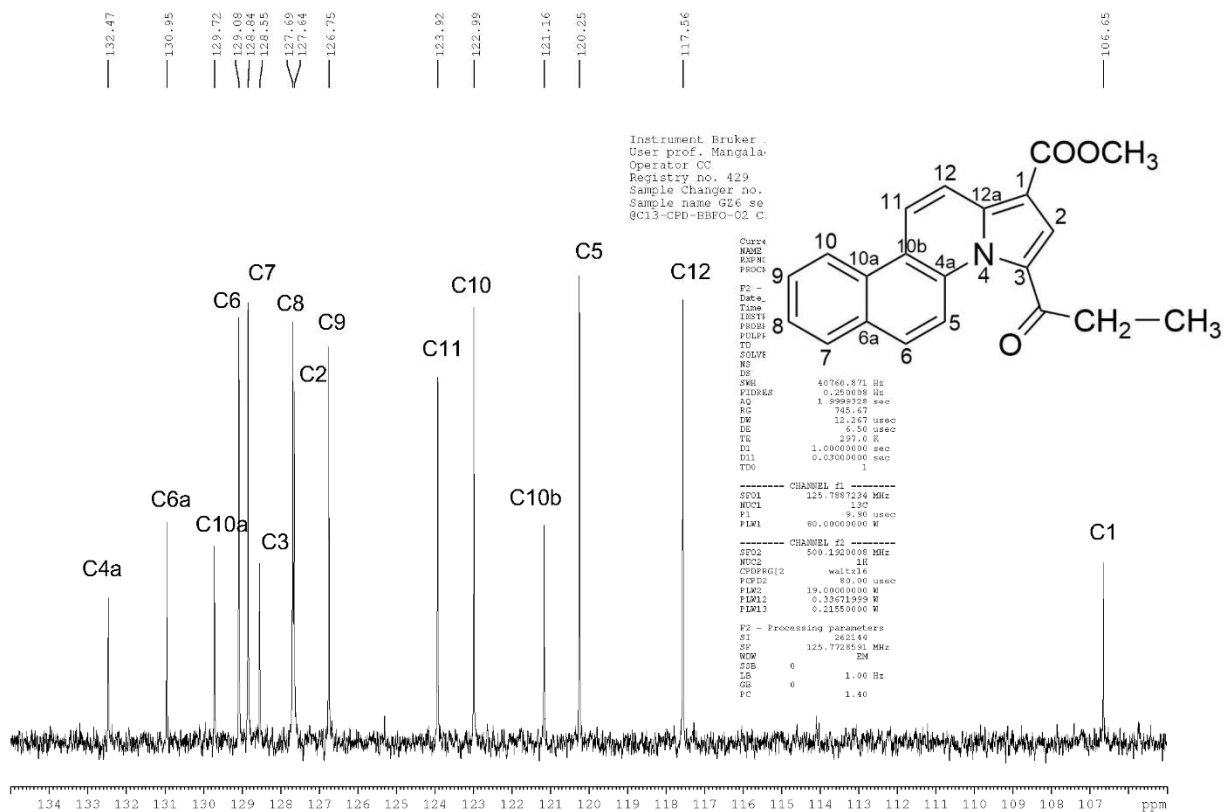


Figure S2c. Detail in the aromatic area of the <sup>13</sup>C NMR spectrum of the compound 5b.

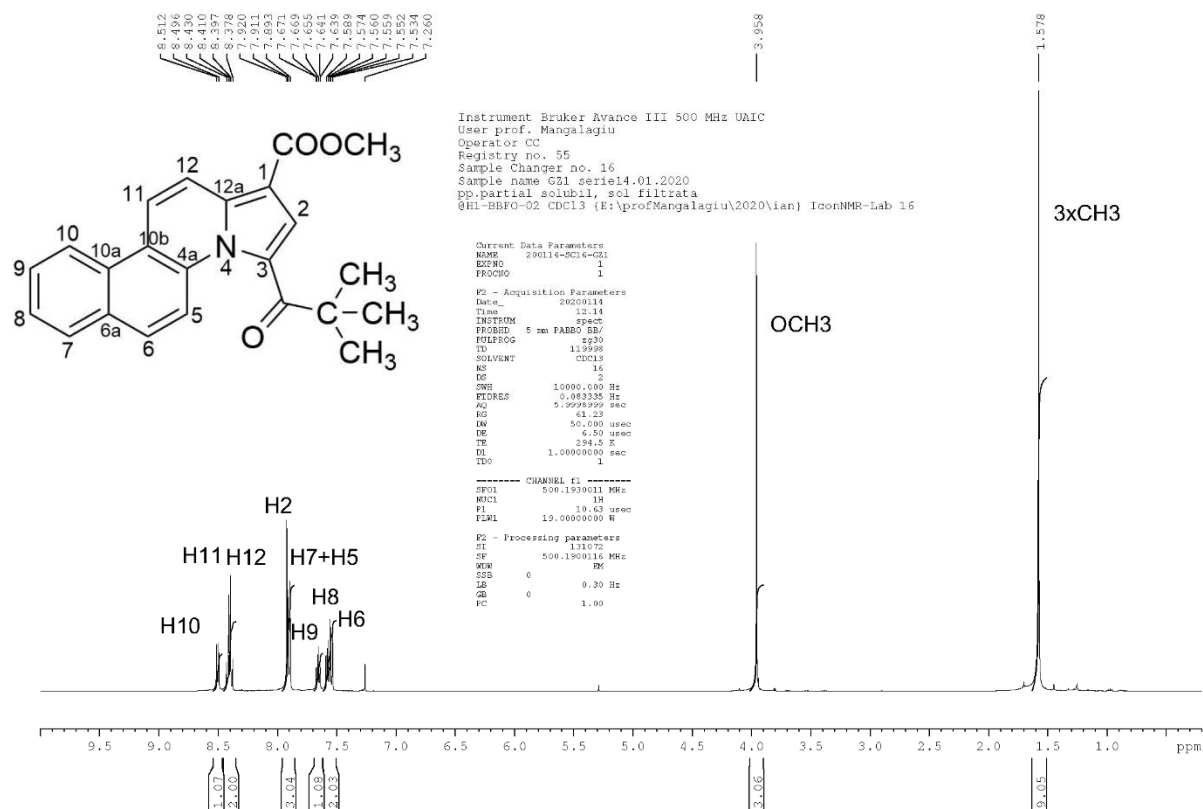


Figure S3a.  $^1\text{H}$  NMR spectrum of the compound 5c.

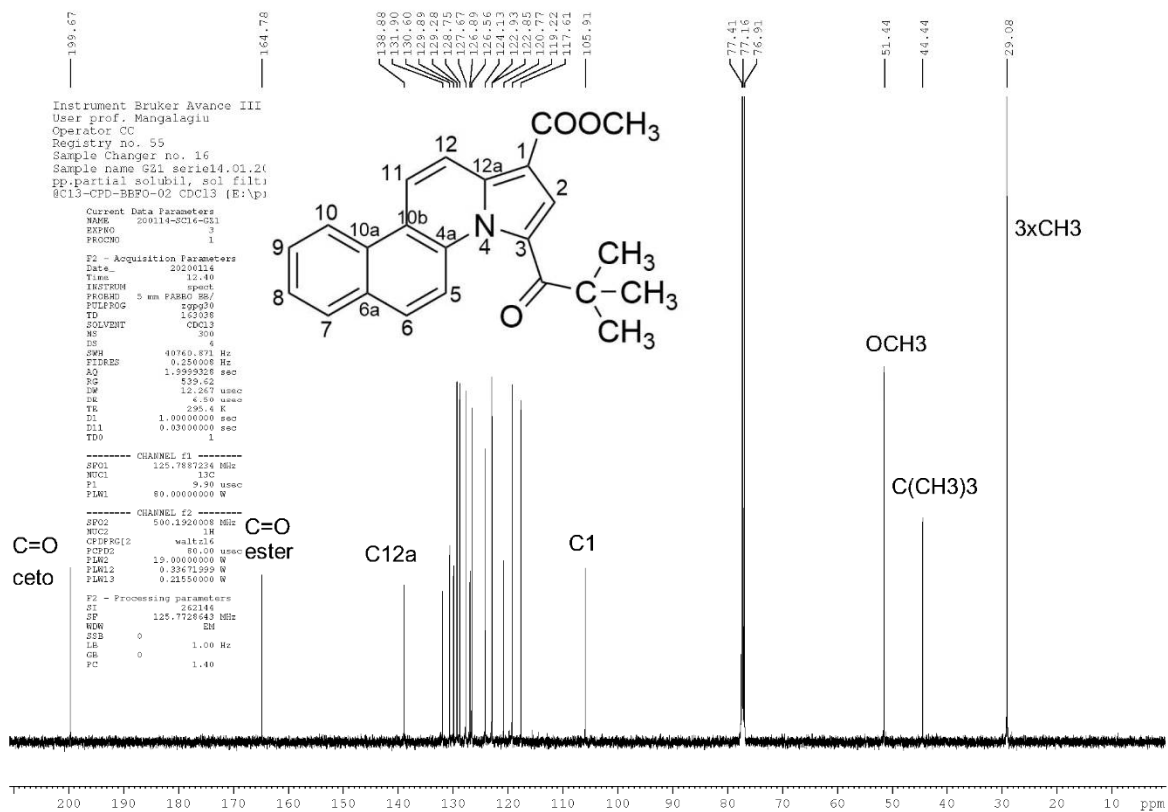


Figure S3b.  $^{13}\text{C}$  NMR spectrum of the compound 5c.

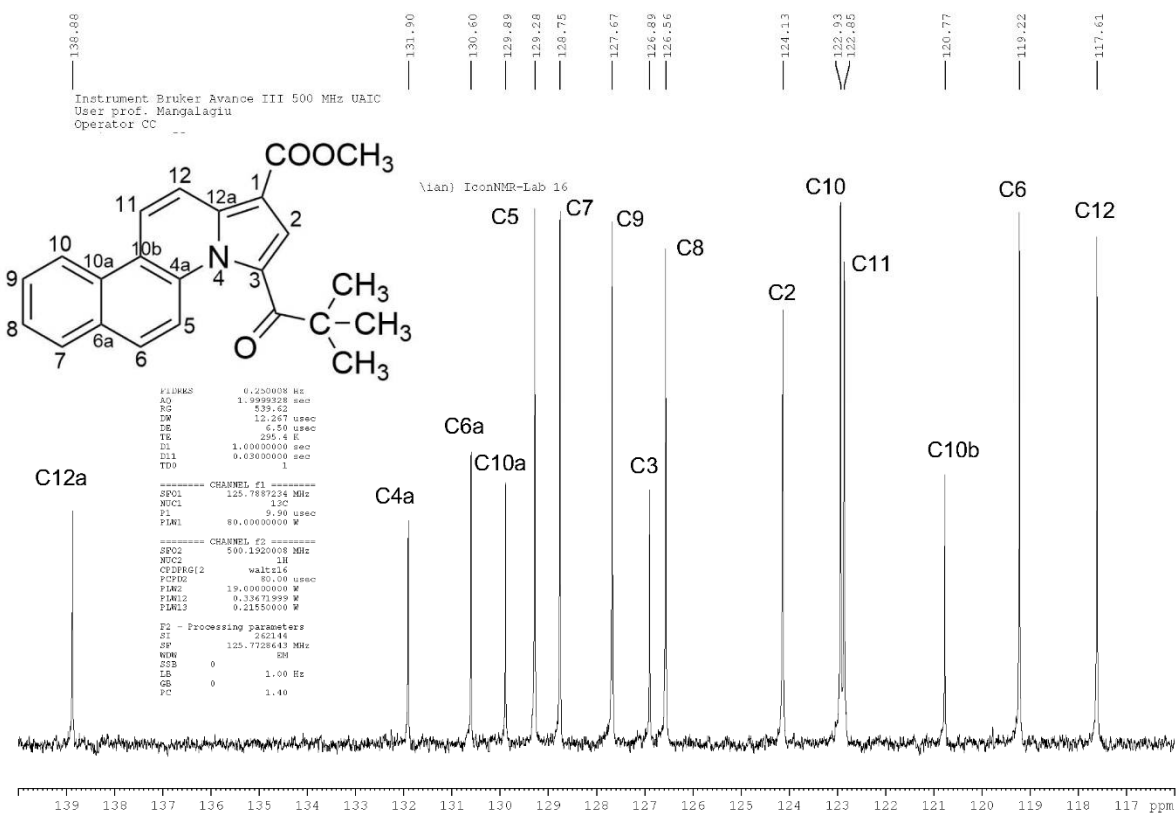


Figure S3c. Detail in the aromatic area of the  $^{13}\text{C}$  NMR spectrum of the compound 5c.

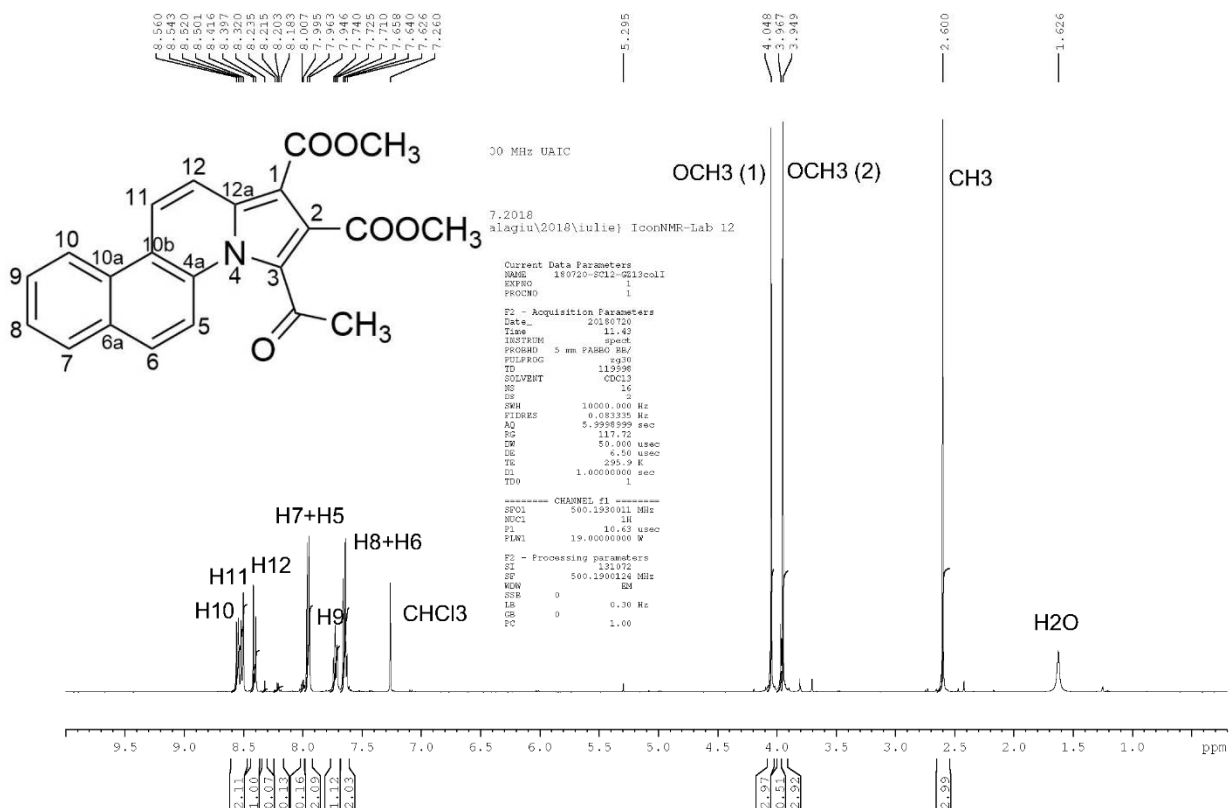


Figure S4a.  $^1\text{H}$  NMR spectrum of the compound 7a.

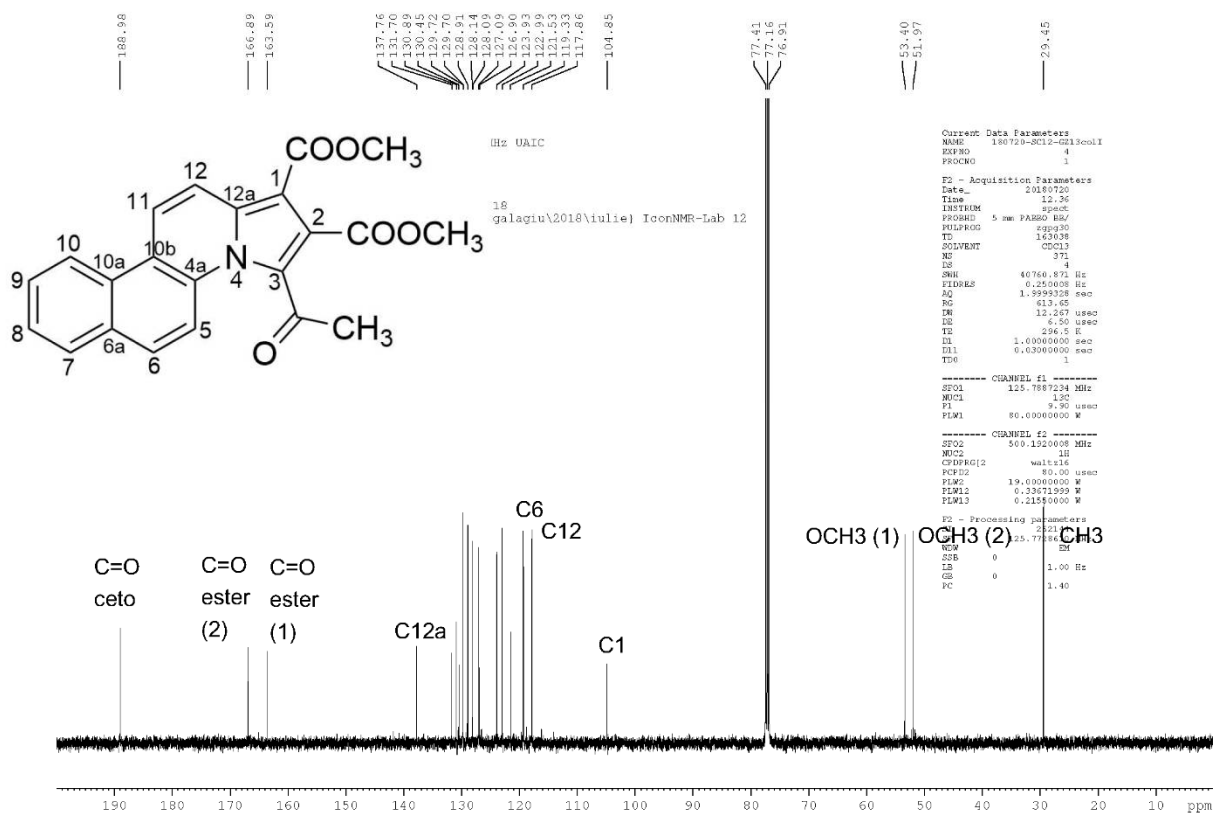


Figure S4b. <sup>13</sup>C NMR spectrum of the compound 7a.

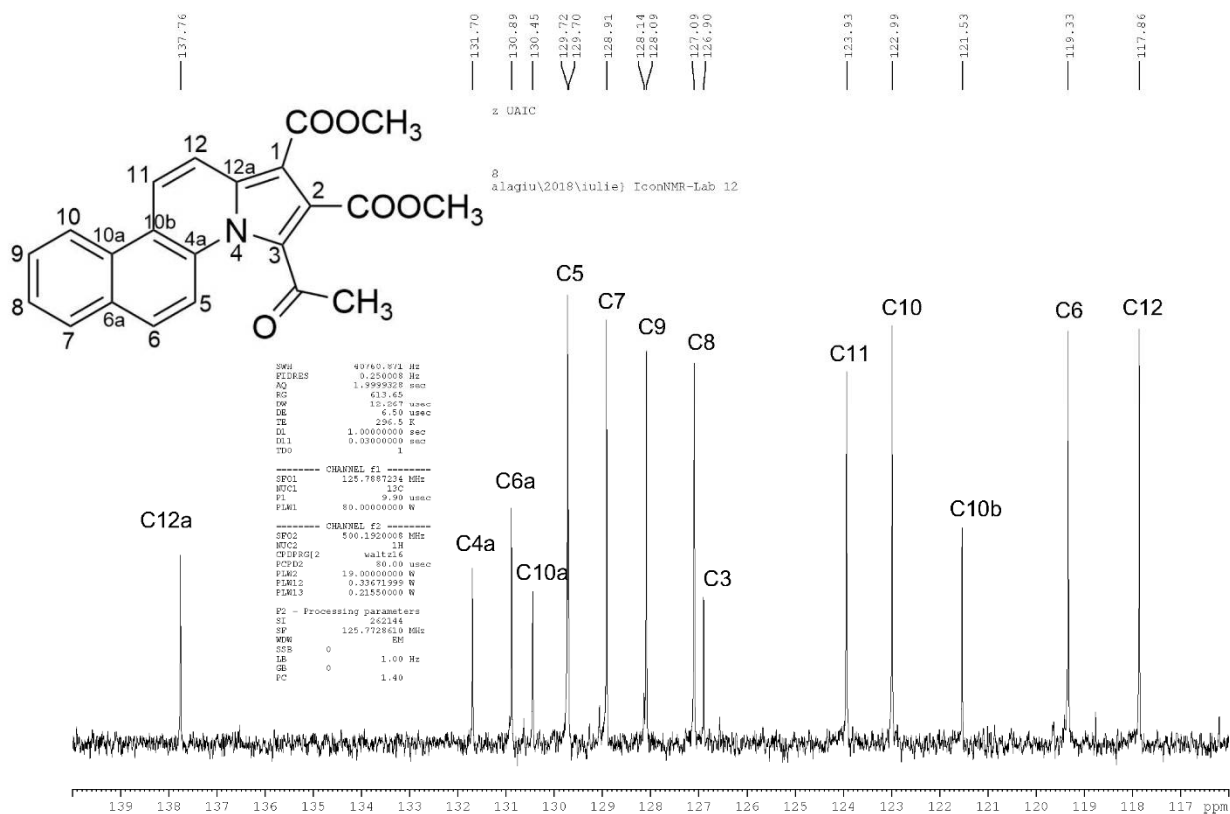


Figure S4c. Detail in the aromatic area of the <sup>13</sup>C NMR spectrum of the compound 7a.

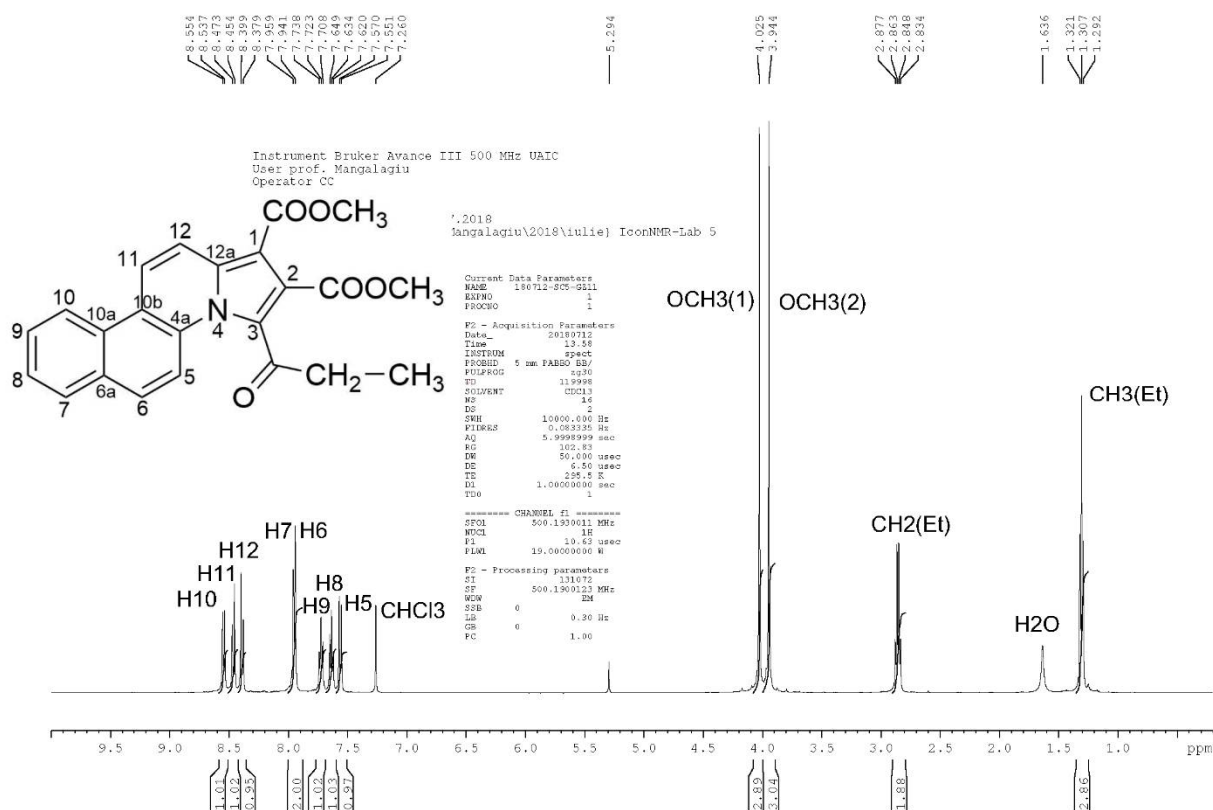


Figure S5a. <sup>1</sup>H NMR spectrum of the compound 7b.

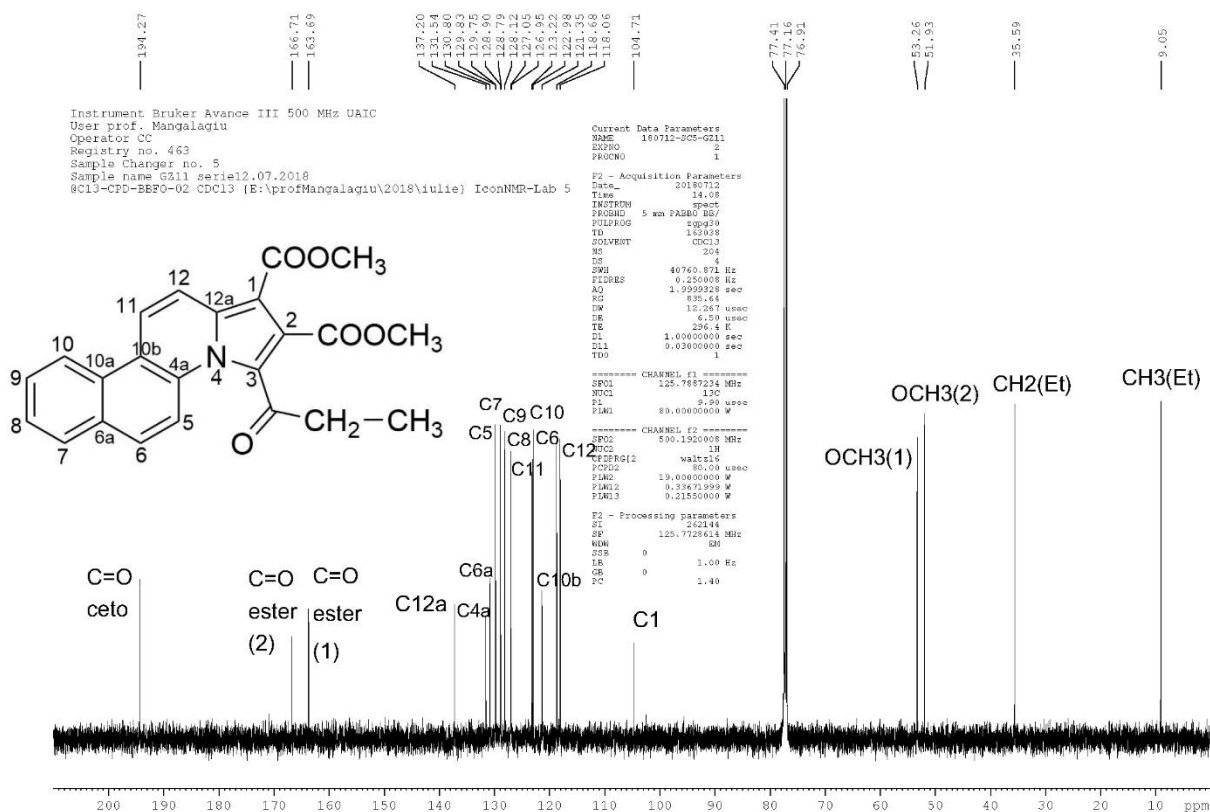


Figure S5b. <sup>13</sup>C NMR spectrum of the compound 7b.



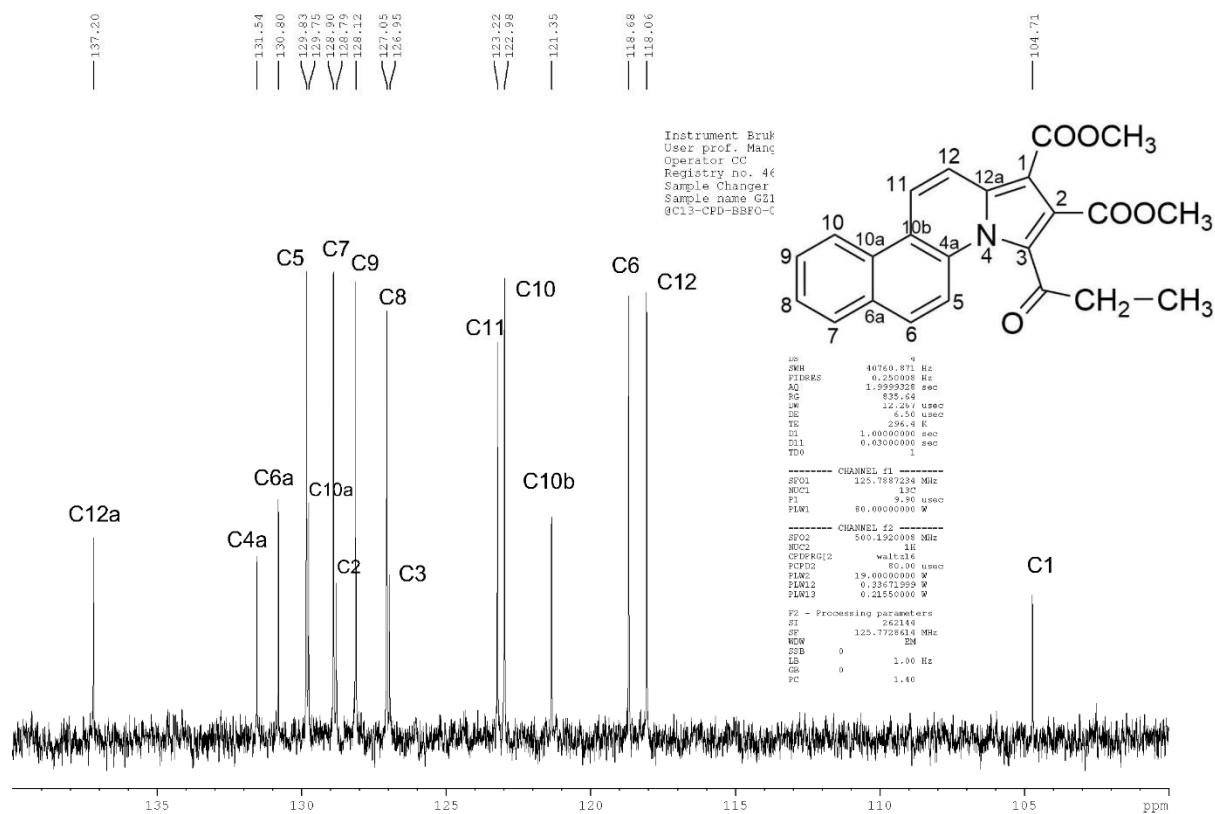


Figure S5c. Detail in the aromatic area of the  $^{13}\text{C}$  NMR spectrum of the compound 7b.

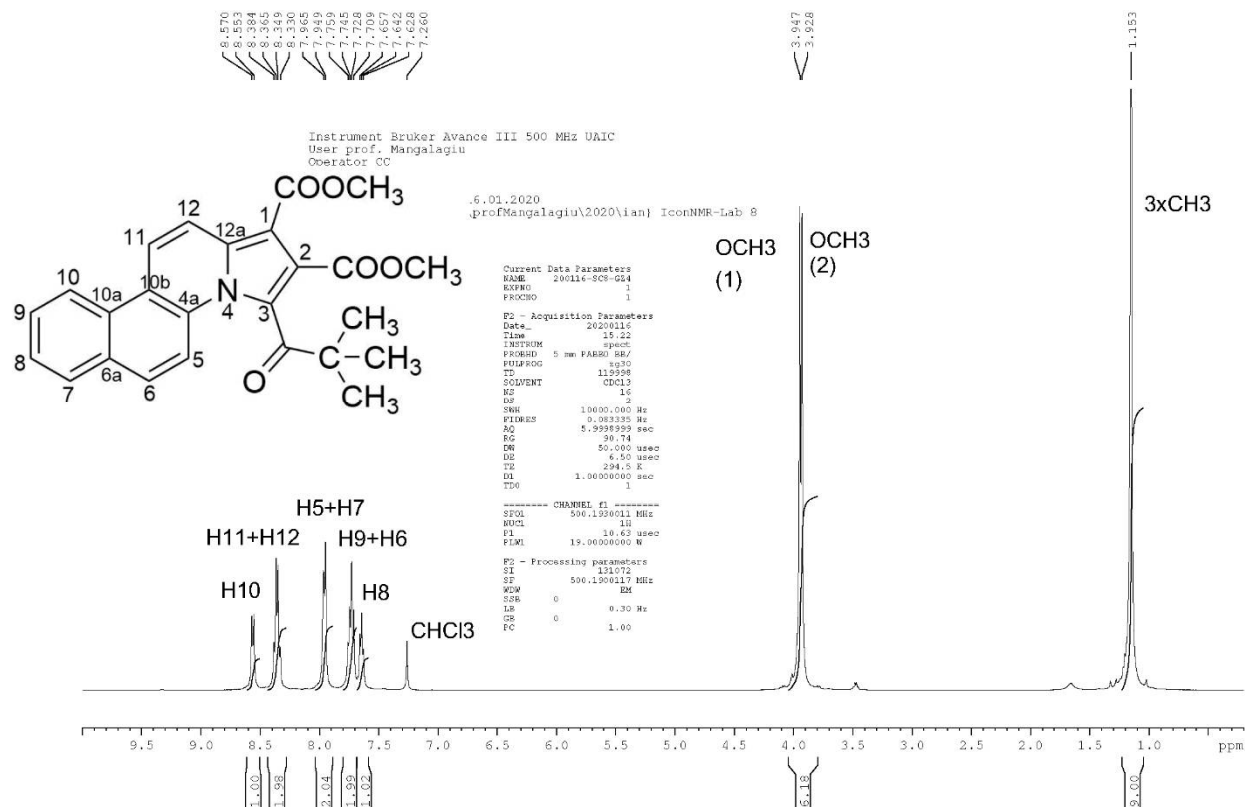


Figure S6a.  $^1\text{H}$  NMR spectrum of the compound 7c.

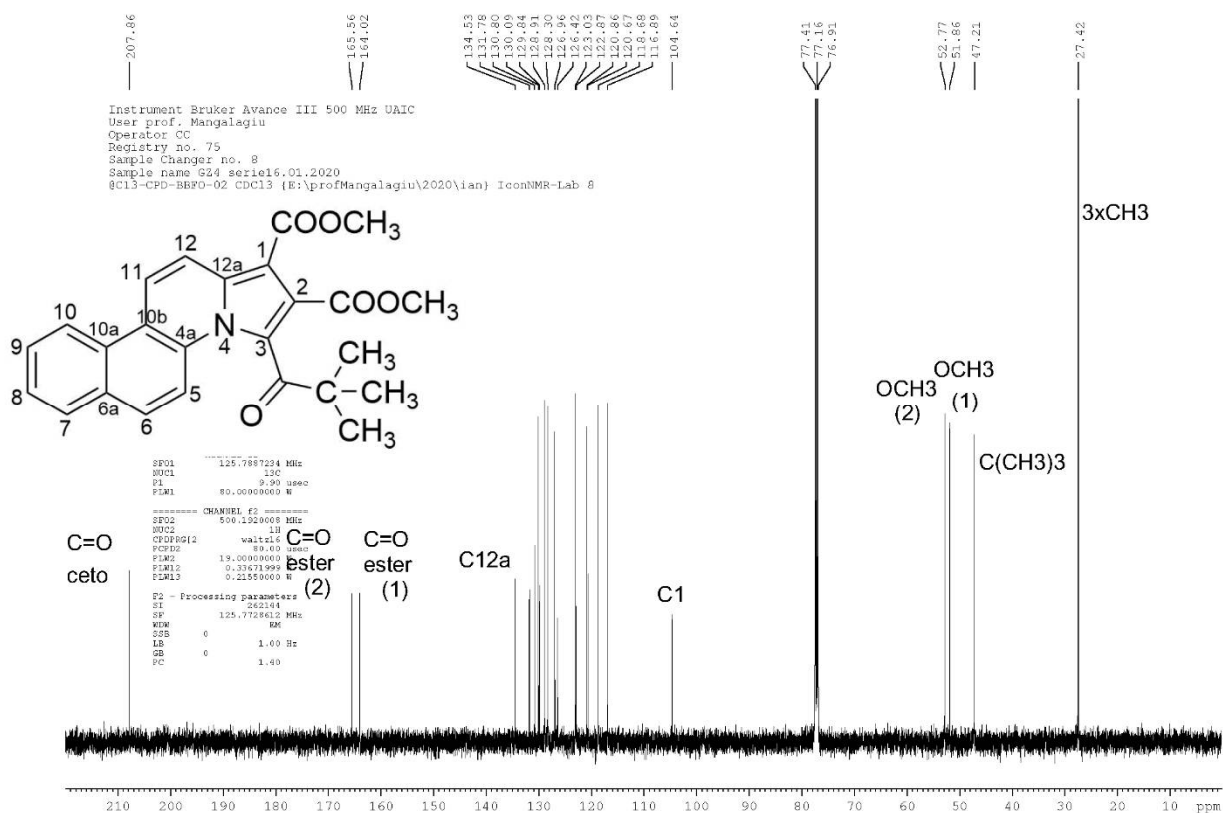


Figure S6b. <sup>13</sup>C NMR spectrum of the compound 7c.

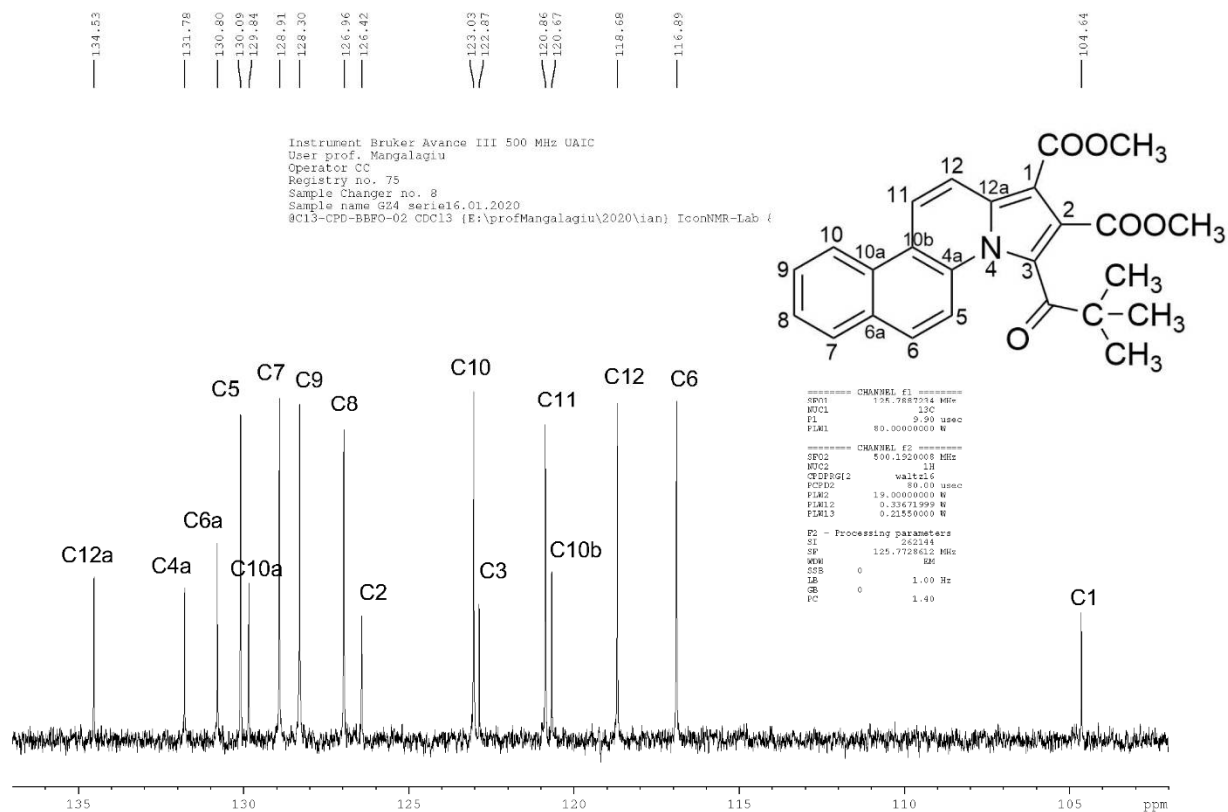


Figure S6c. Detail in the aromatic area of the <sup>13</sup>C NMR spectrum of the compound 7c.

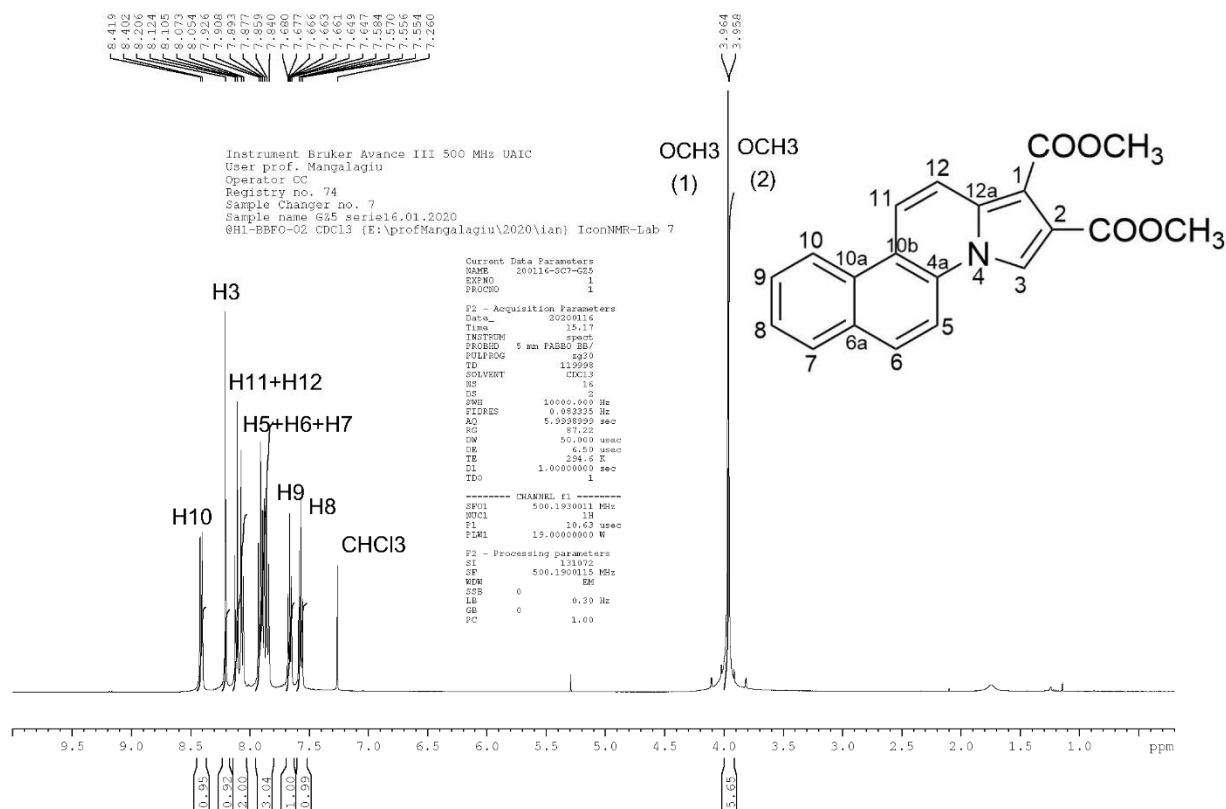


Figure S7a. <sup>1</sup>H NMR spectrum of the compound 8c.

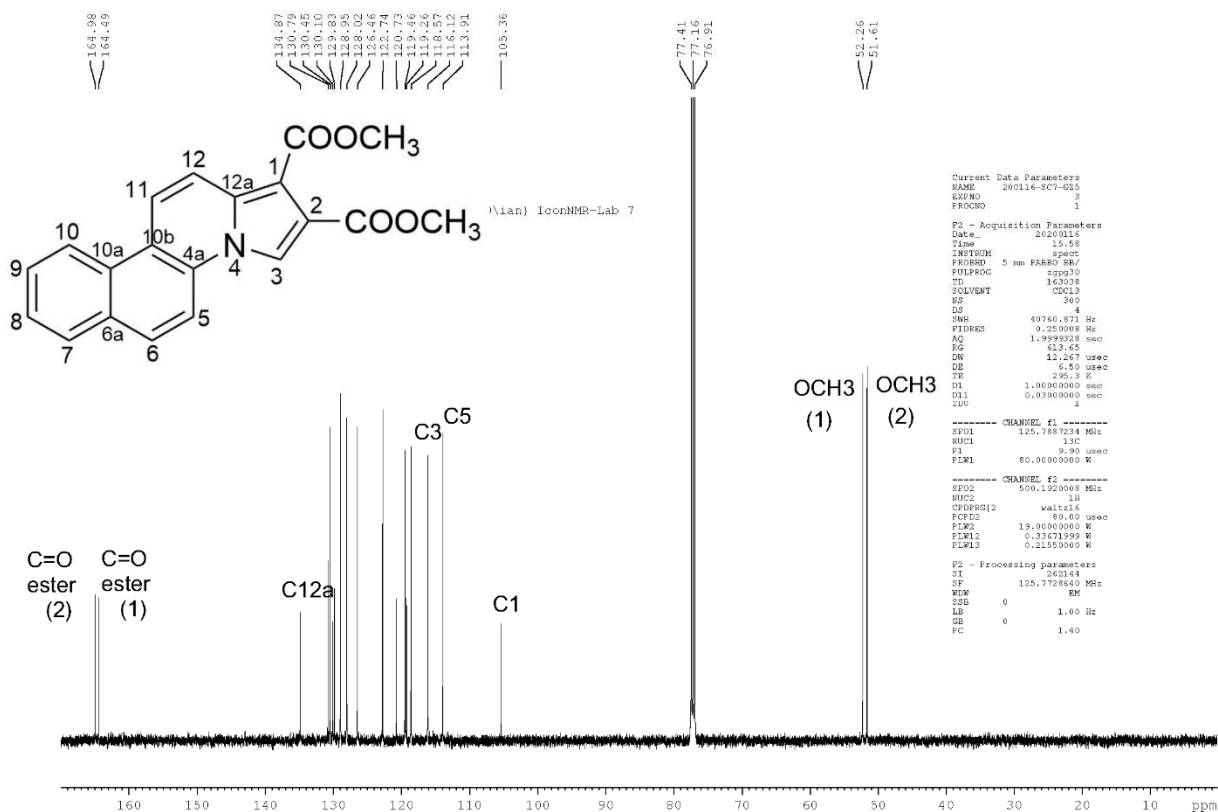
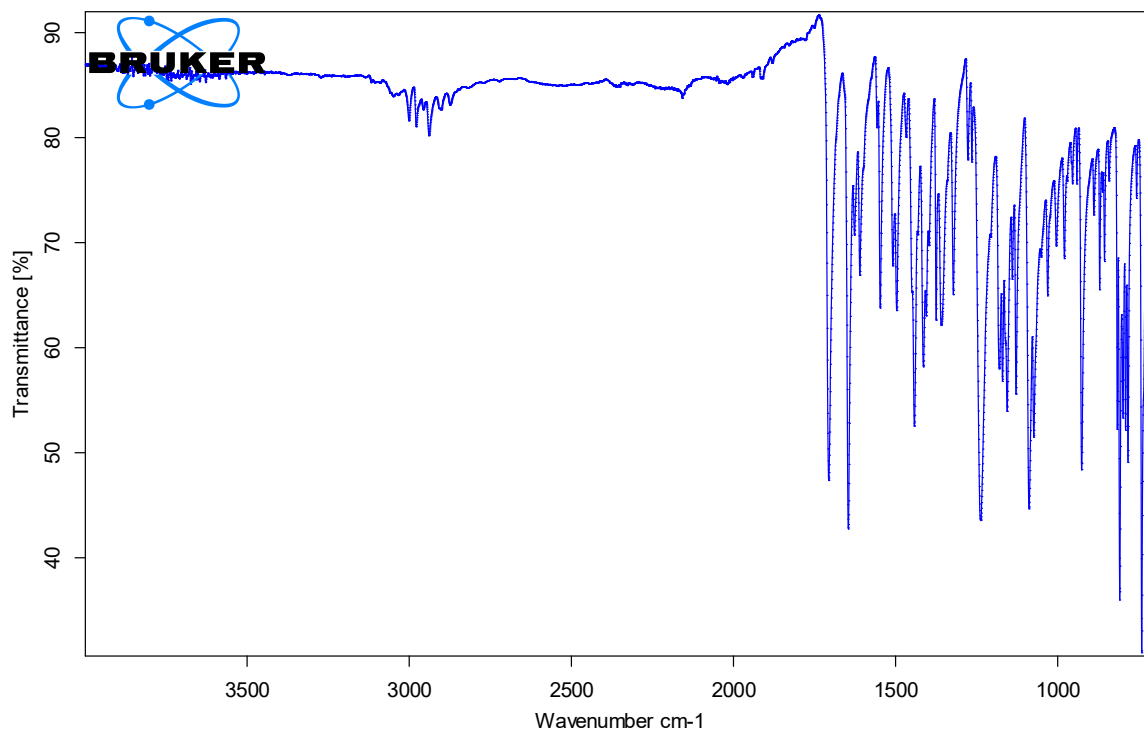


Figure S7b. <sup>13</sup>C NMR spectrum of the compound 8c.

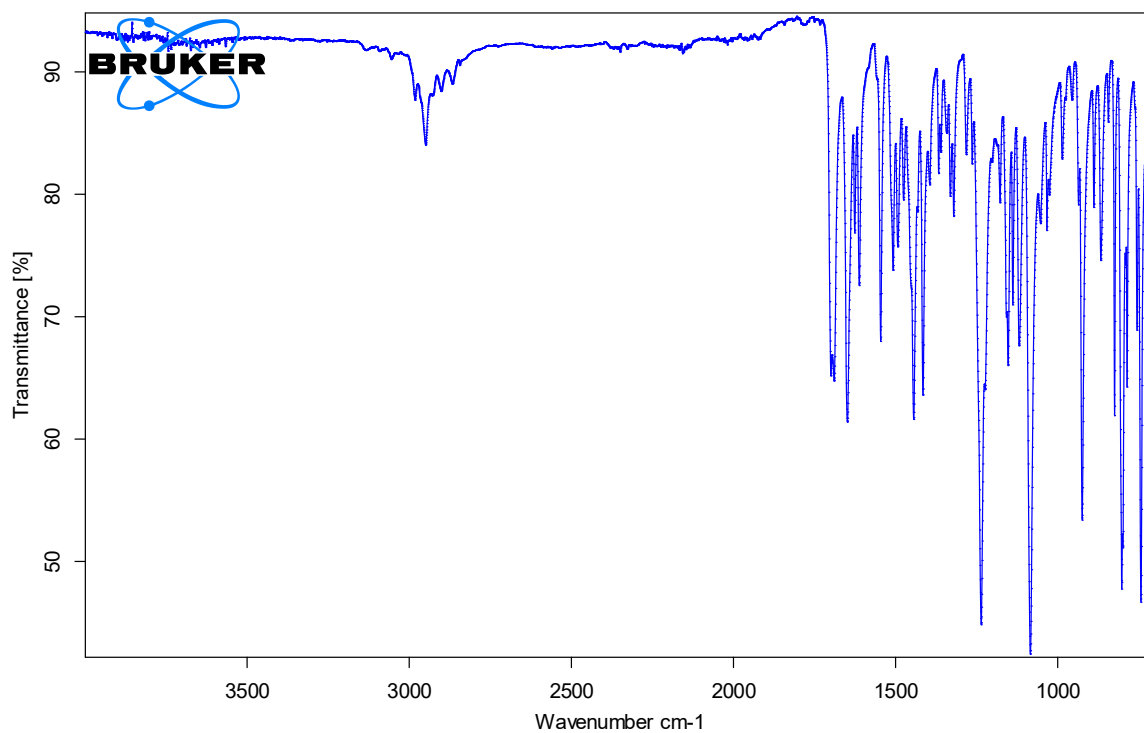




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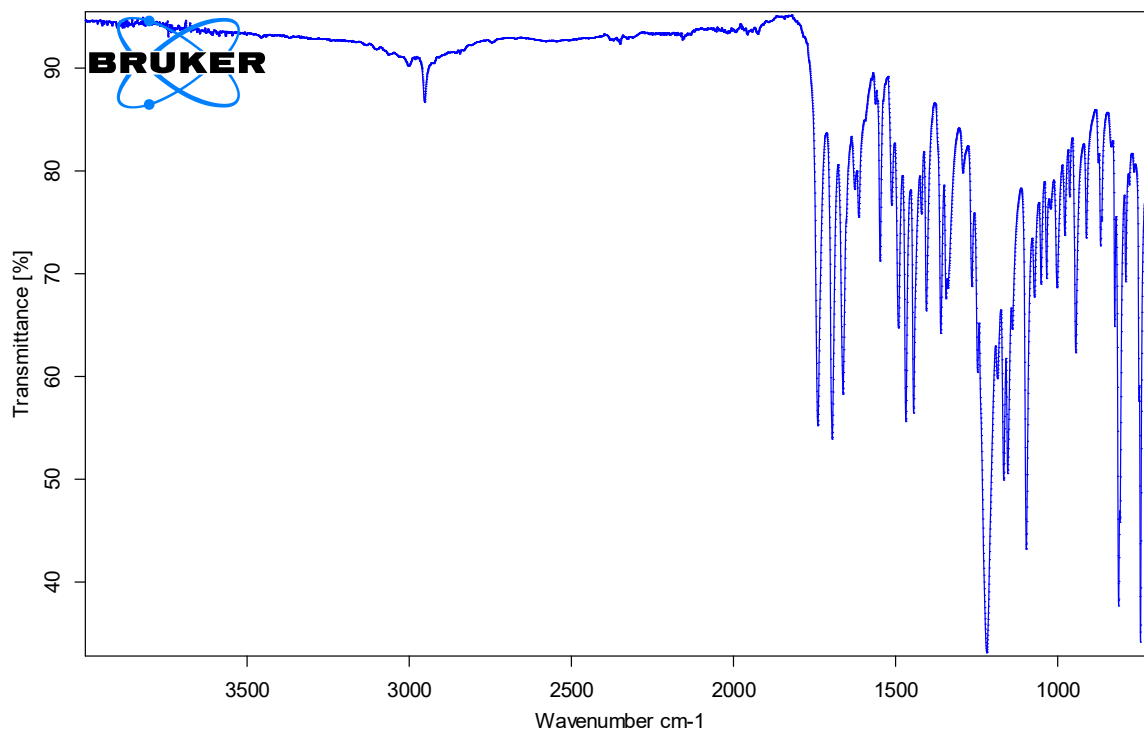
Figure S9. IR spectrum of the compound 5b.



C:\OPUS_7.0.129\WORK\2021-07-14\2021-07-14-5C.0	Sample description	Instrument type and / or accessory	14/07/2021
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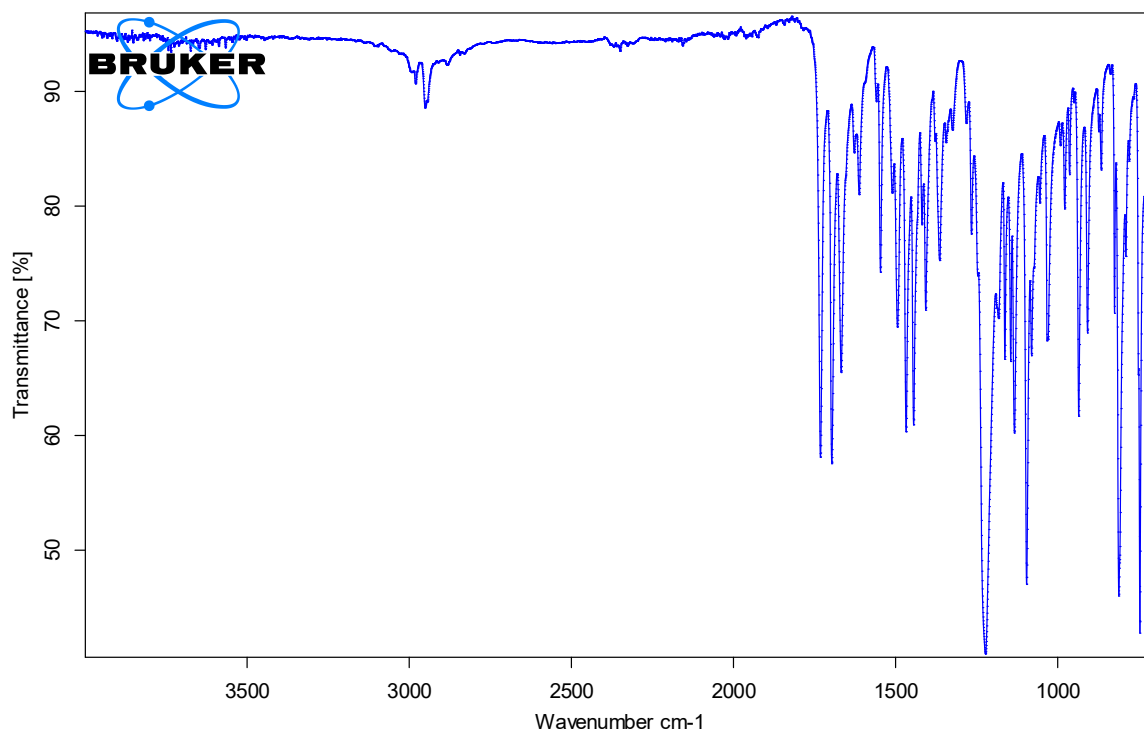
Figure S10. IR spectrum of the compound 5c.



C:\OPUS_7.0.129\WORK\2021-07-14\2021-07-14-7A.0	Sample description	Instrument type and / or accessory	14/07/2021
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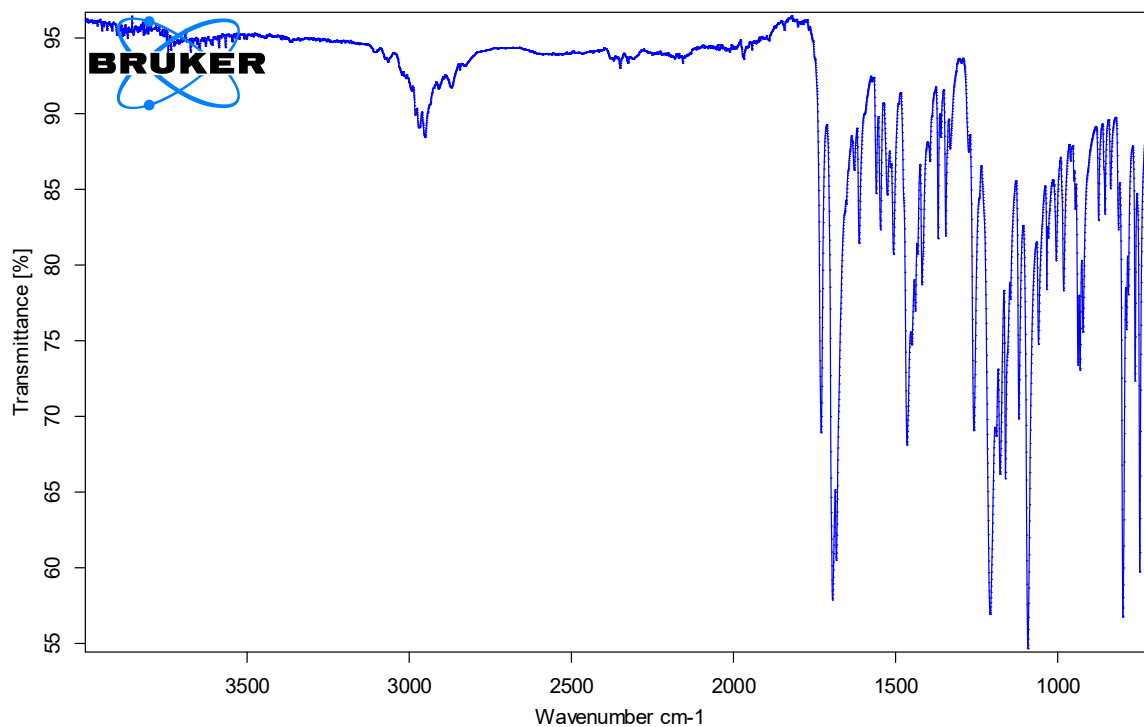
Figure S11. IR spectrum of the compound **7a**.



C:\OPUS_7.0.129\WORK\2021-07-14\2021-07-14-7B.0	Sample description	Instrument type and / or accessory	14/07/2021
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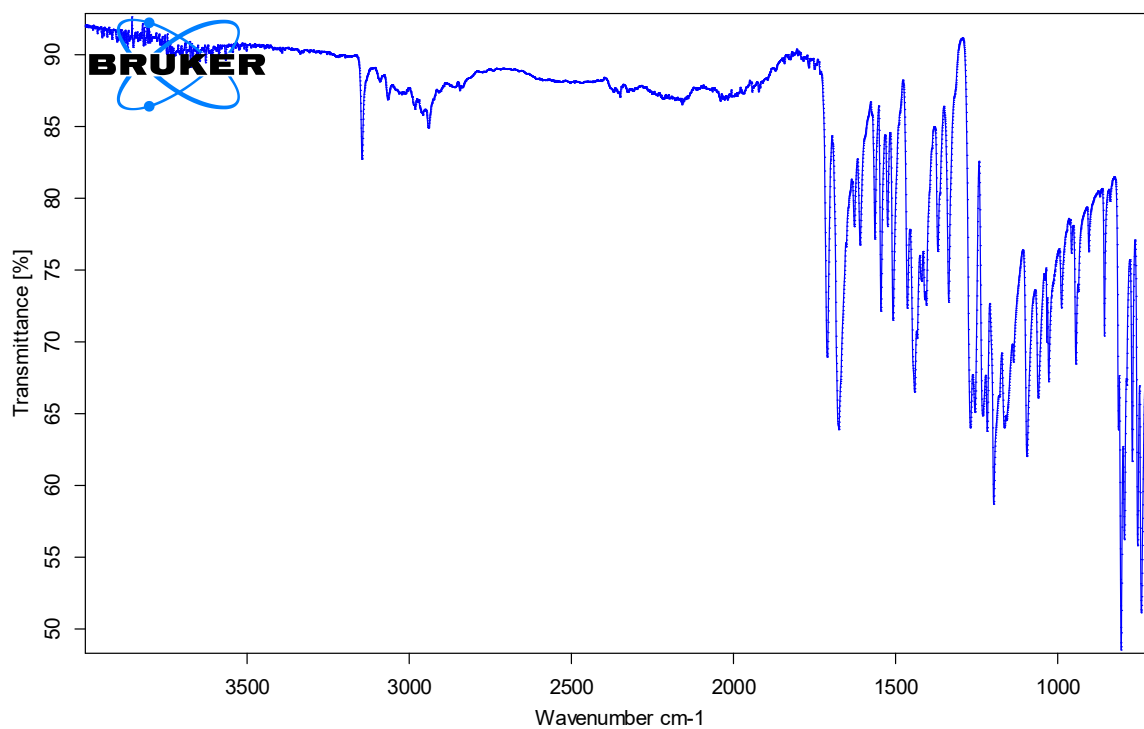
Figure S12. IR spectrum of the compound **7b**.



C:\OPUS_7.0.129\WORK\2021-07-14\2021-07-14-7C.1	Sample description	Instrument type and / or accessory	14/07/2021
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Figure S13. IR spectrum of the compound 7c.



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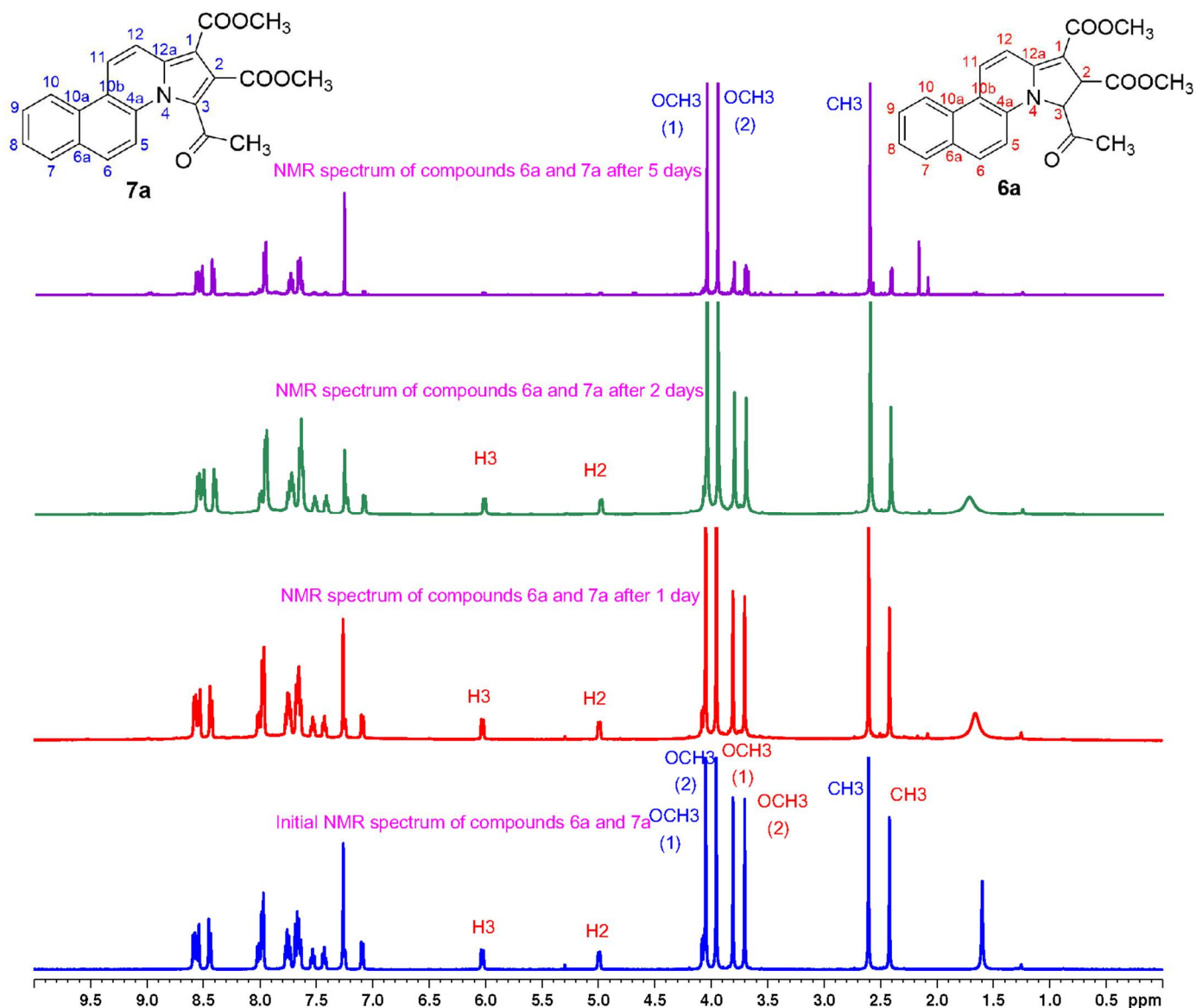
Figure S14. IR spectrum of the compound 8c.

### 3. $^1\text{H}$ -NMR studies on compound **7a** at room temperature.

#### *NMR sample preparation:*

10 mg of dimethyl 3-acetylbenzo[f]pyrrolo[1,2-a]quinoline-1,2-dicarboxylate (**7a**) were dissolved in 1 mL  $\text{CDCl}_3$  and inserted in a 5 mm diameter NMR tube and sealed with a polypropylene cap. A  $^1\text{H}$ -NMR spectrum was quickly recorded than the sample was stored at room temperature. After 1 day, 2 days and 5 days respectively a new  $^1\text{H}$ -NMR spectrum was recorded for the sample.

The  $^1\text{H}$ -NMR spectra are presented in the S15 Fig



**Figure S15.** Time evolution of the  $^1\text{H}$ -NMR spectrum of dimethyl 3-acetylbenzo[f]pyrrolo[1,2-a]quinoline-1,2-dicarboxylate (**7a**).



#### 4. UV spectra of the obtained compounds

5a CHCl<sub>3</sub>.spc - RawData  
5a CY.spc - RawData

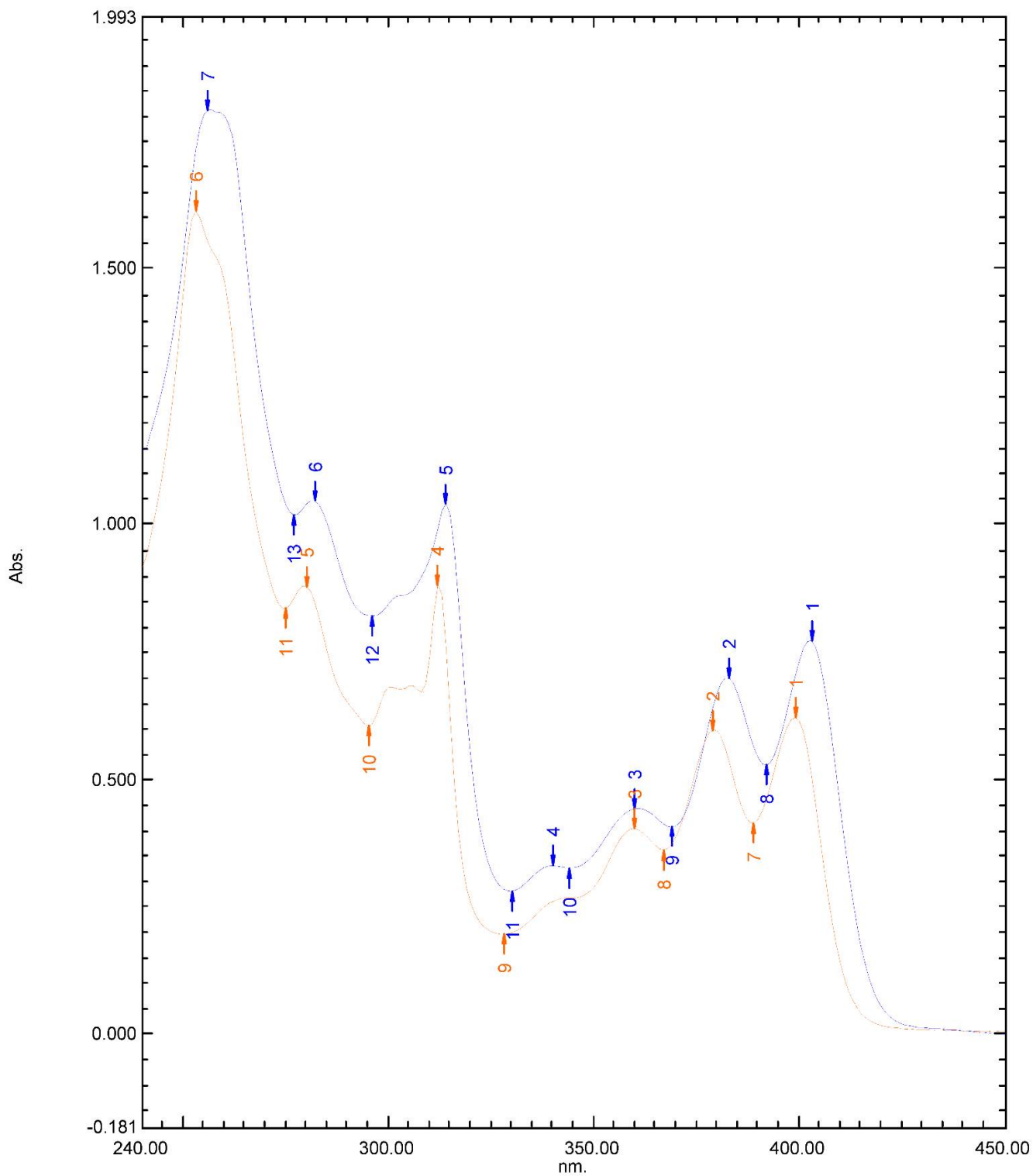
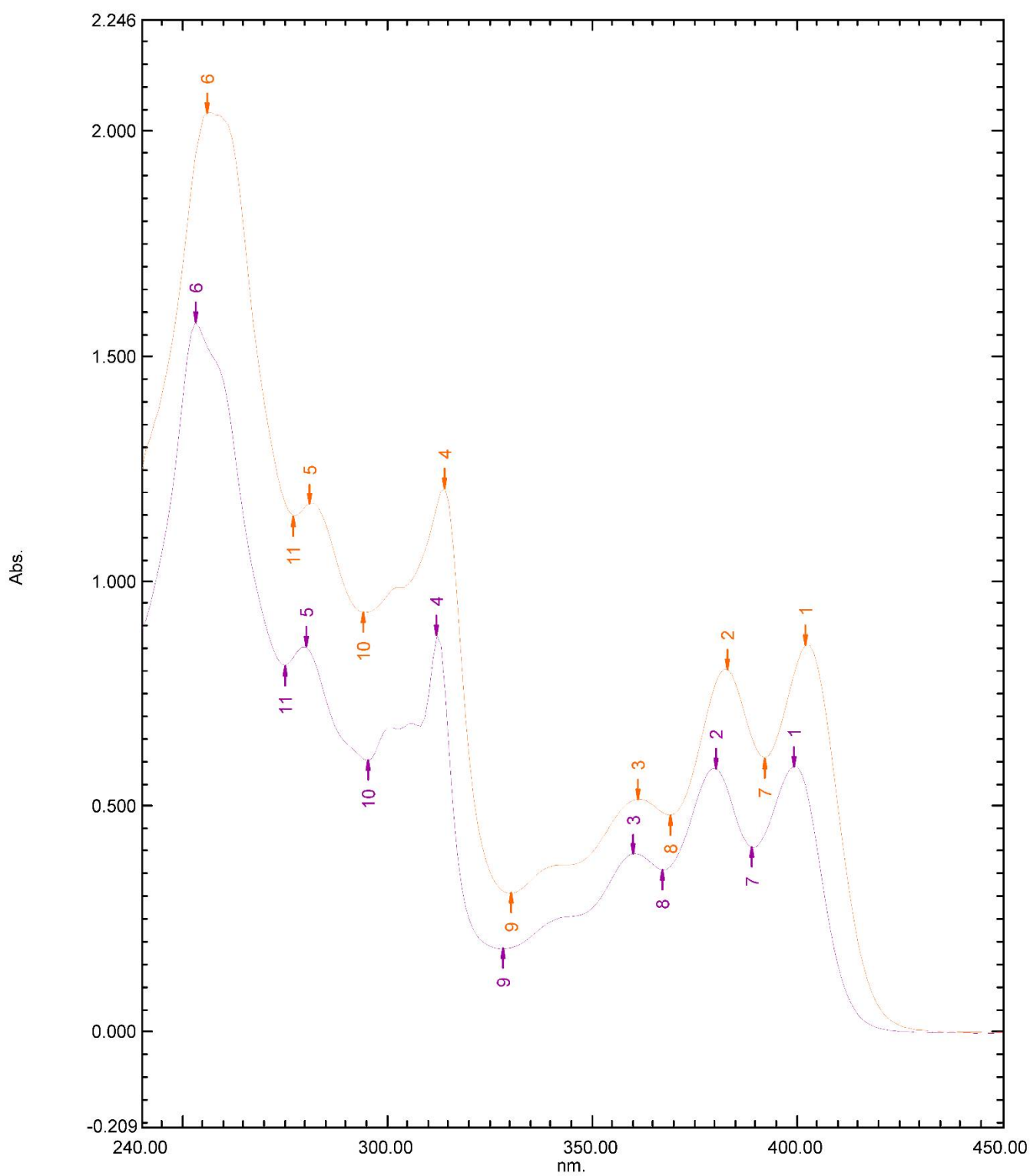


Figure S16. Overlaid UV-Vis spectra of the compound 5a in trichloromethane and cyclohexane.

5b CHCl3.spc - RawData  
5b CY.spc - RawData



**Figure S17.** Overlaid UV-Vis spectra of the compound **5b** in trichloromethane and cyclohexane.

5c CHCl3d.spc - RawData  
5c CY.spc - RawData

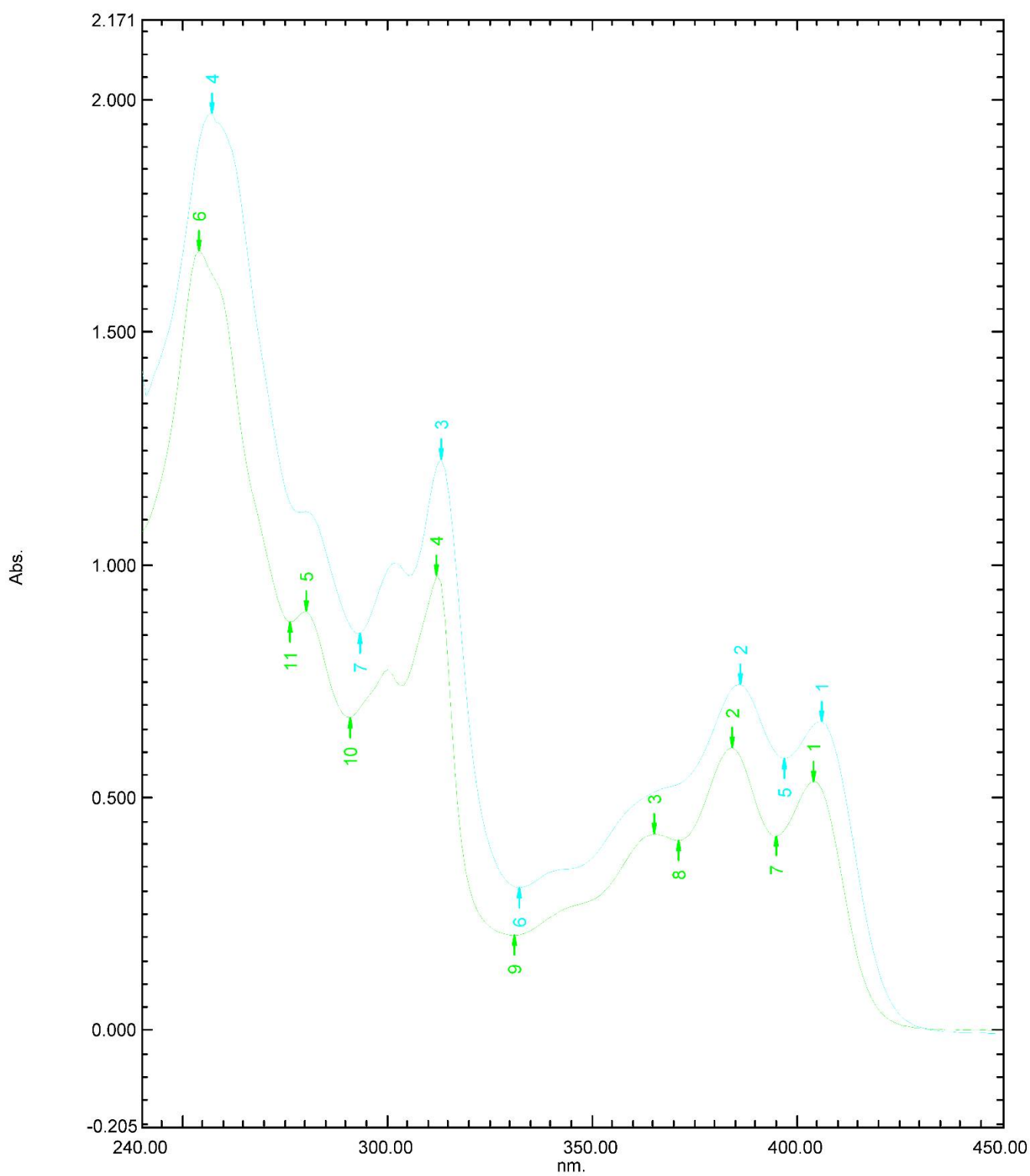


Figure S18. Overlaid UV-Vis spectra of the compound **5c** in trichloromethane and cyclohexane.

7a CHCl3.spc - RawData  
7a CY.spc - RawData

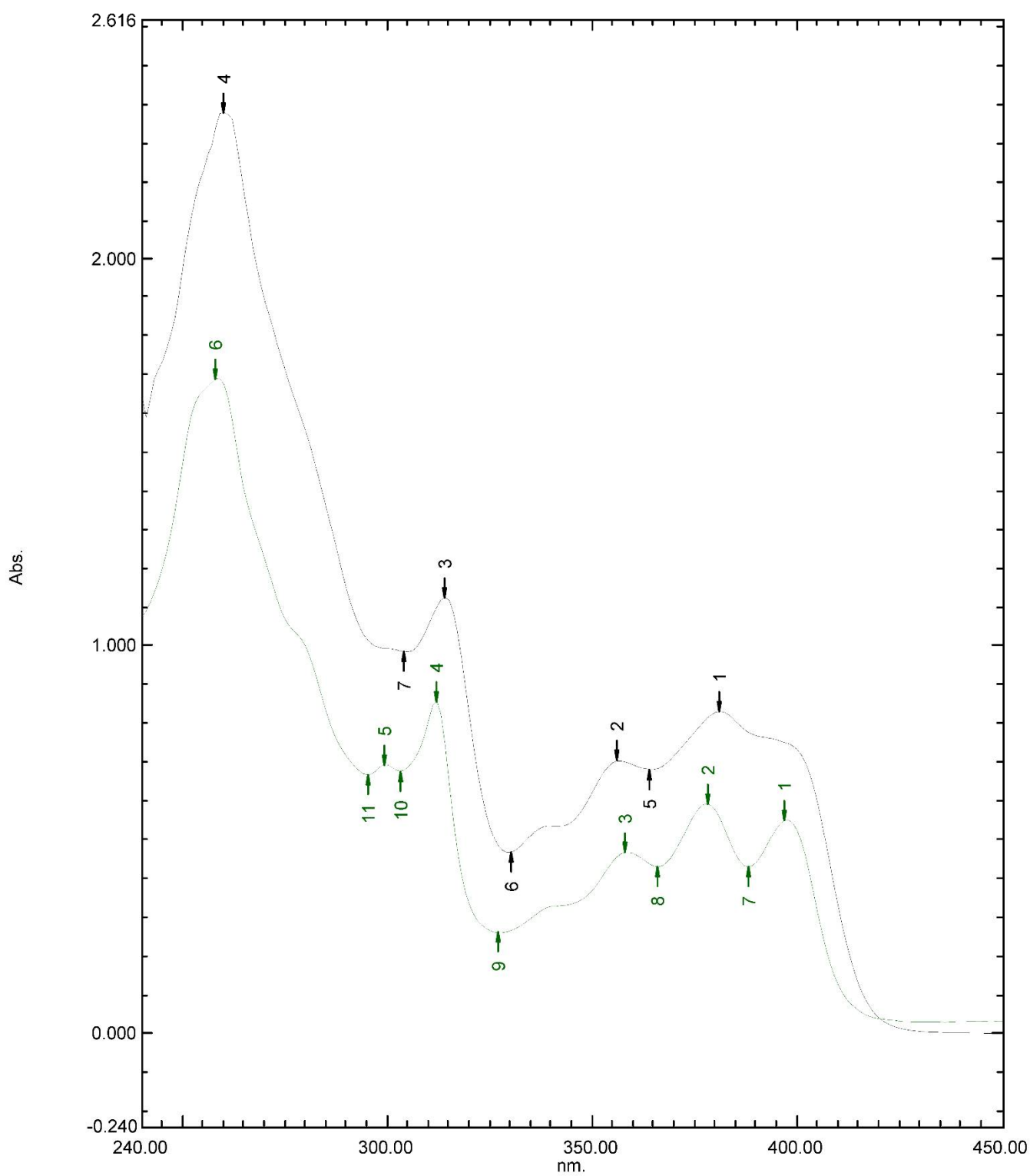
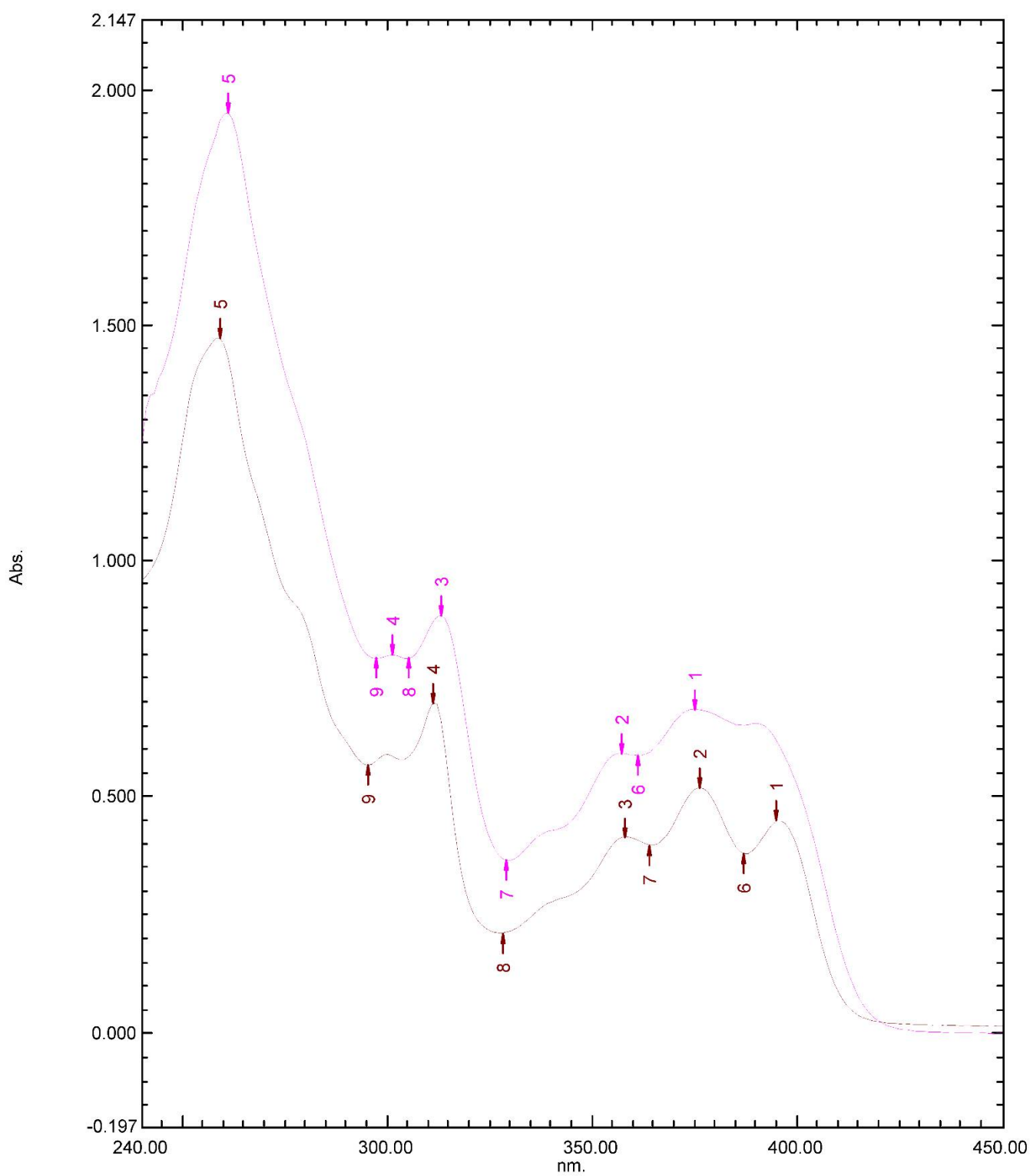


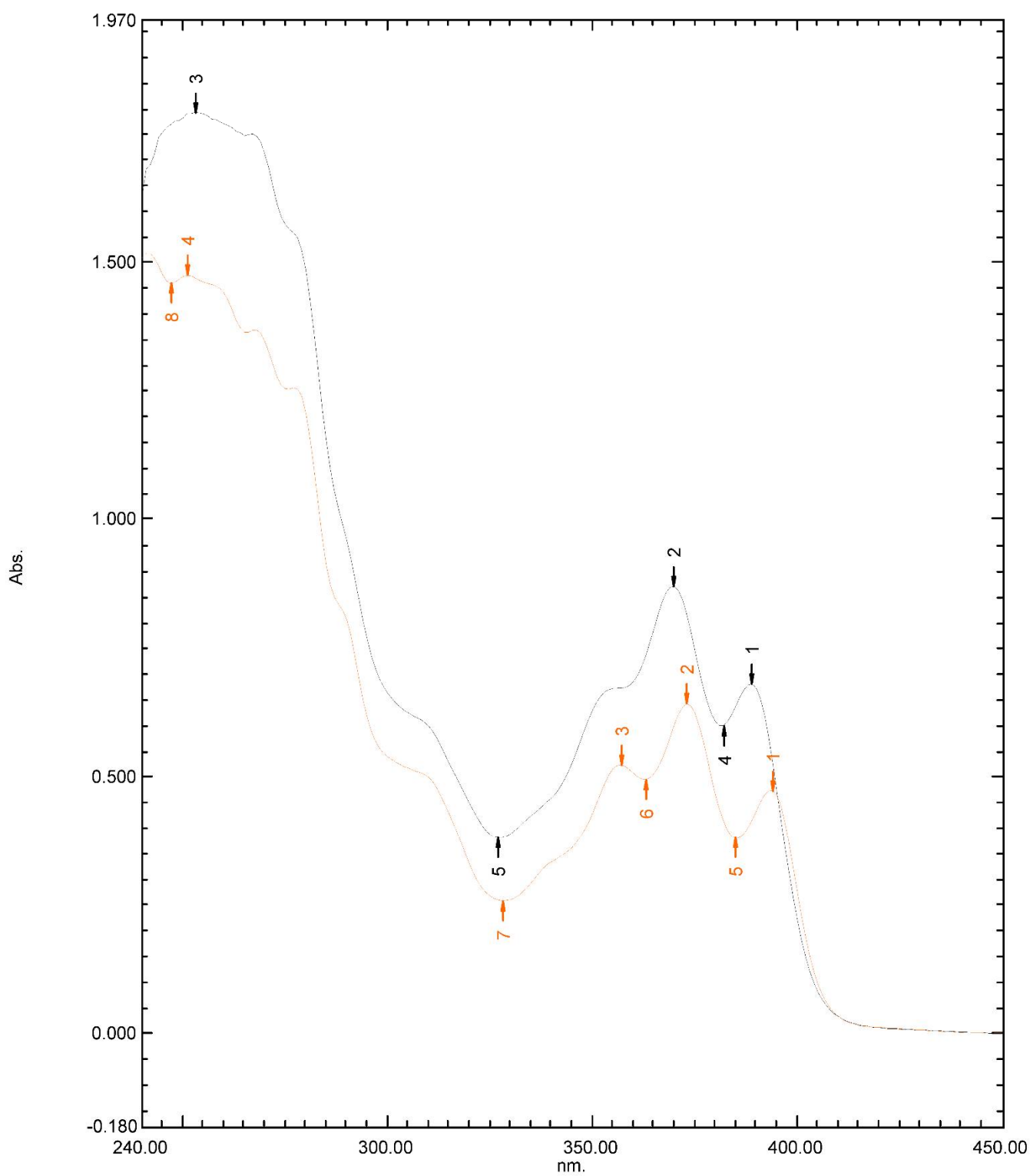
Figure S19. Overlaid UV-Vis spectra of the compound **7a** in trichloromethane and cyclohexane.

7b CHCl3.spc - RawData  
7b CY.spc - RawData



**Figure S20.** Overlaid UV-Vis spectra of the compound **7b** in trichloromethane and cyclohexane.

7c CHCl3.spc - RawData  
7c CY.spc - RawData



**Figure S21.** Overlaid UV-Vis spectra of the compound **7c** in trichloromethane and cyclohexane.

8c CHCl3.spc - RawData  
8c CY.spc - RawData

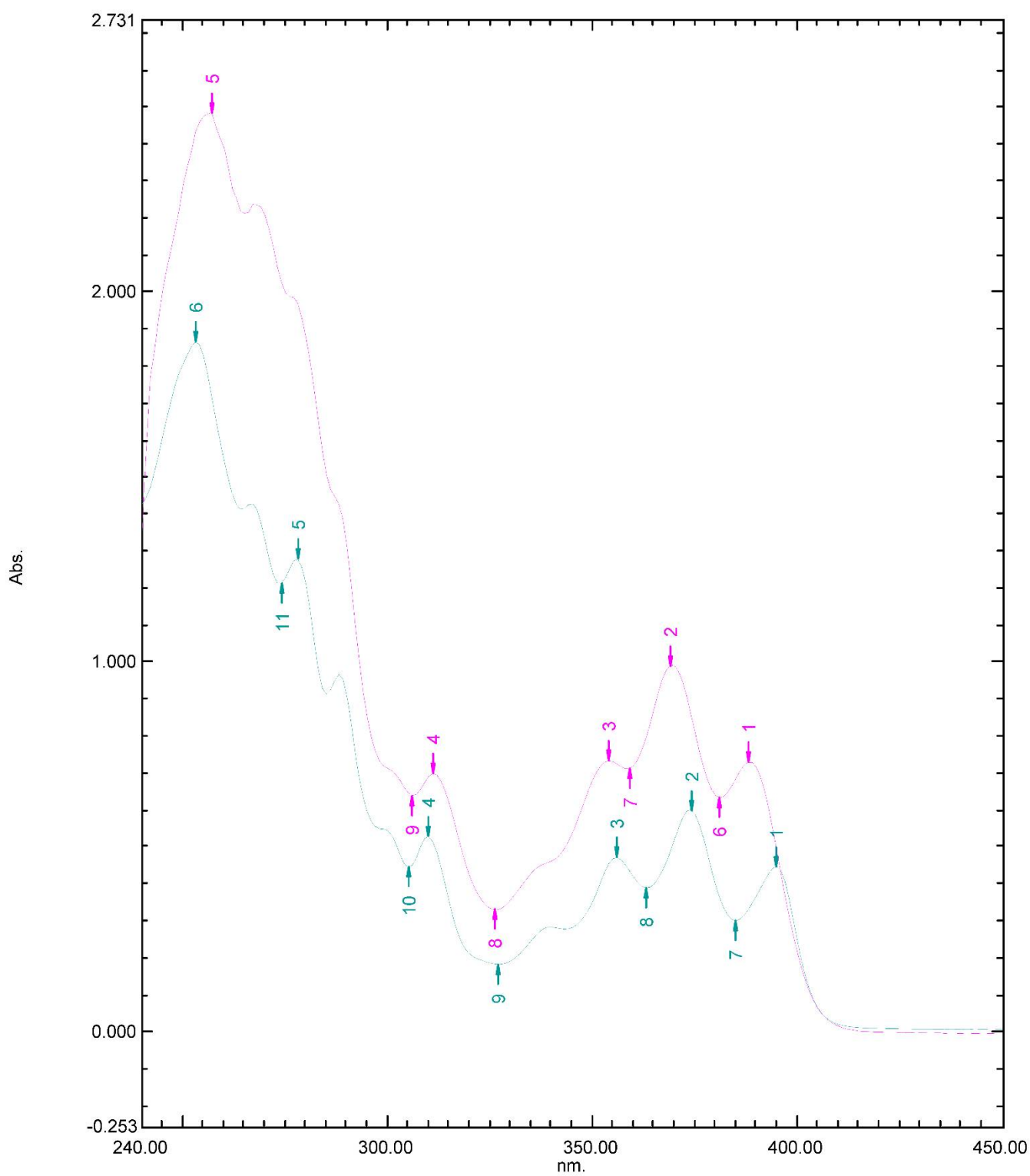


Figure S22. Overlaid UV-Vis spectra of the compound **8c** in trichloromethane and cyclohexane.

## 5. Emission spectra of the obtained compounds

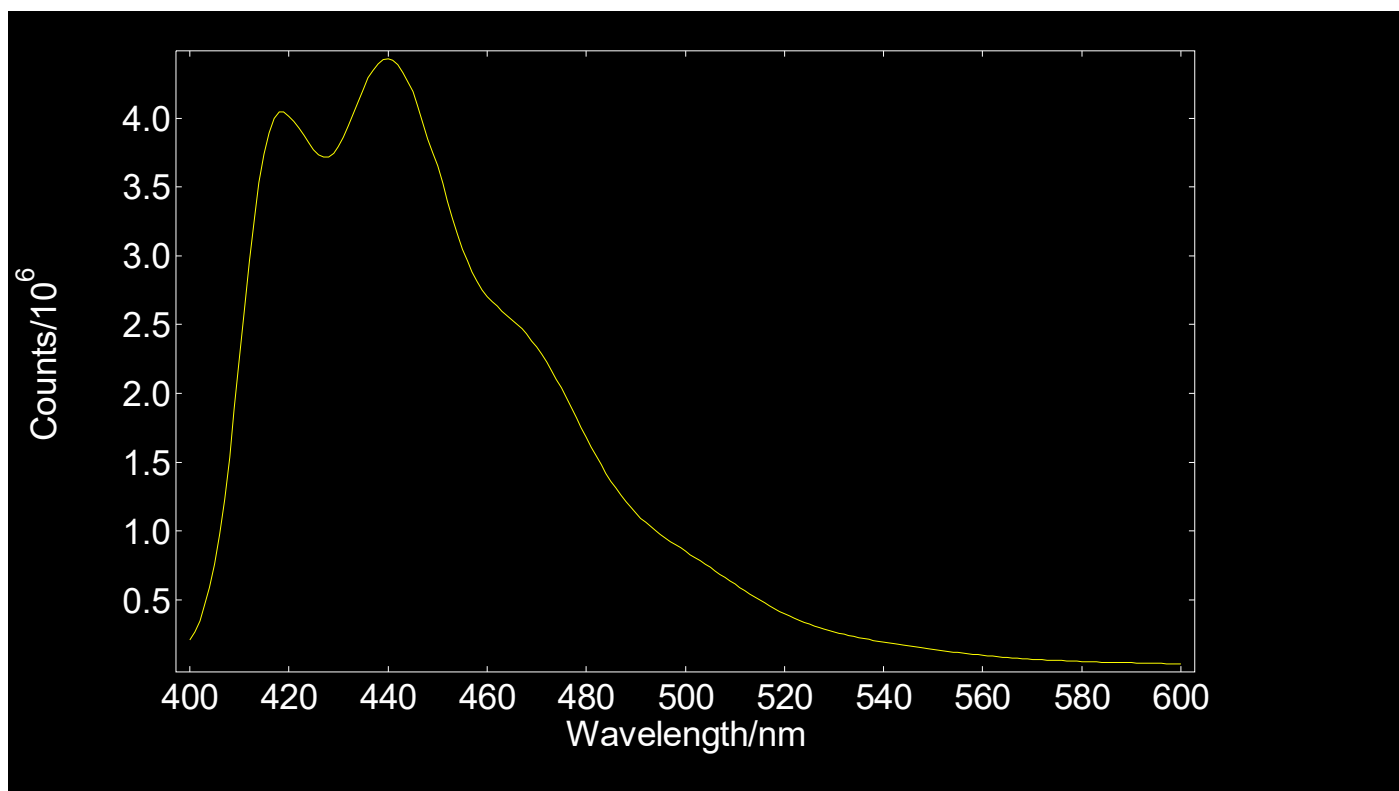


Figure S23. Emission spectrum of the compound **5a** in trichloromethane.

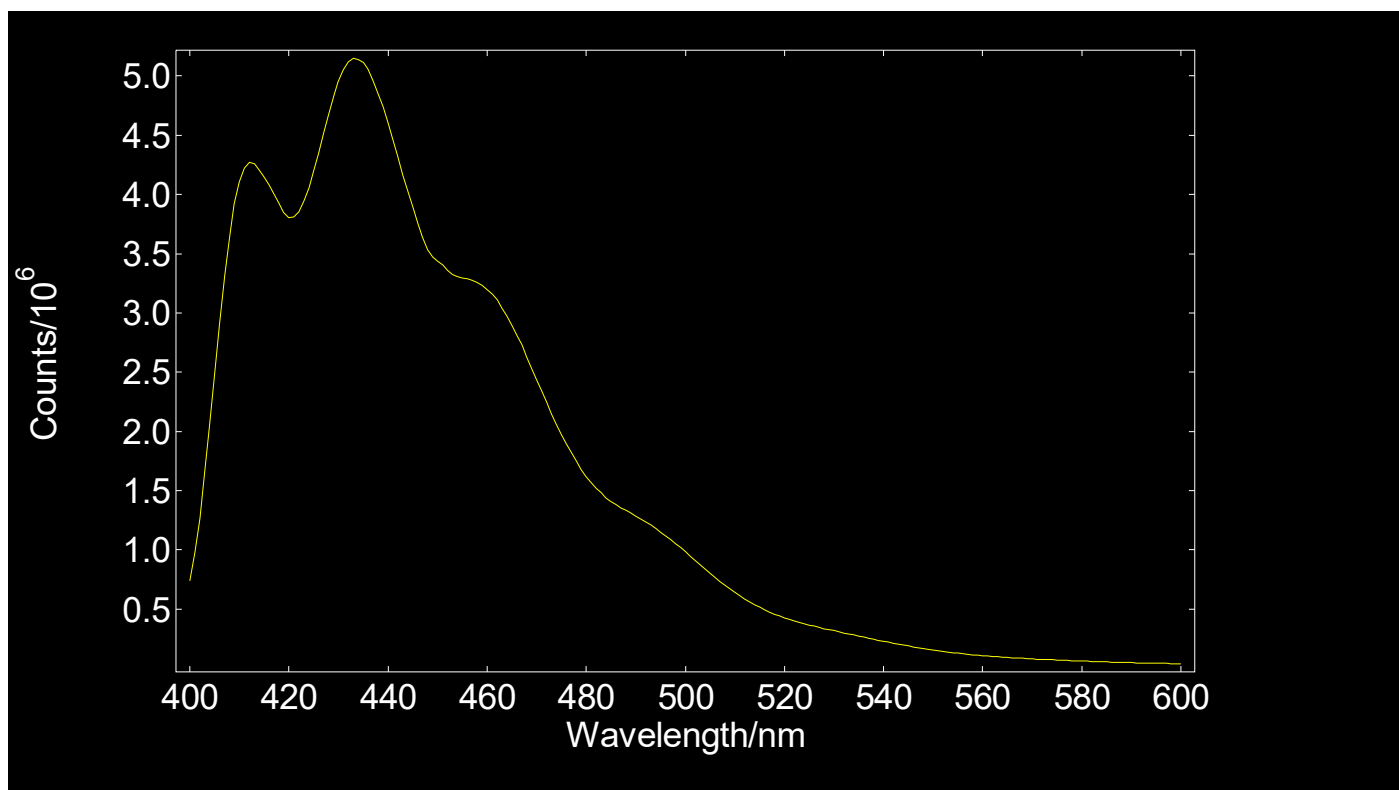


Figure S24. Emission spectrum of the compound **5a** in cyclohexane.



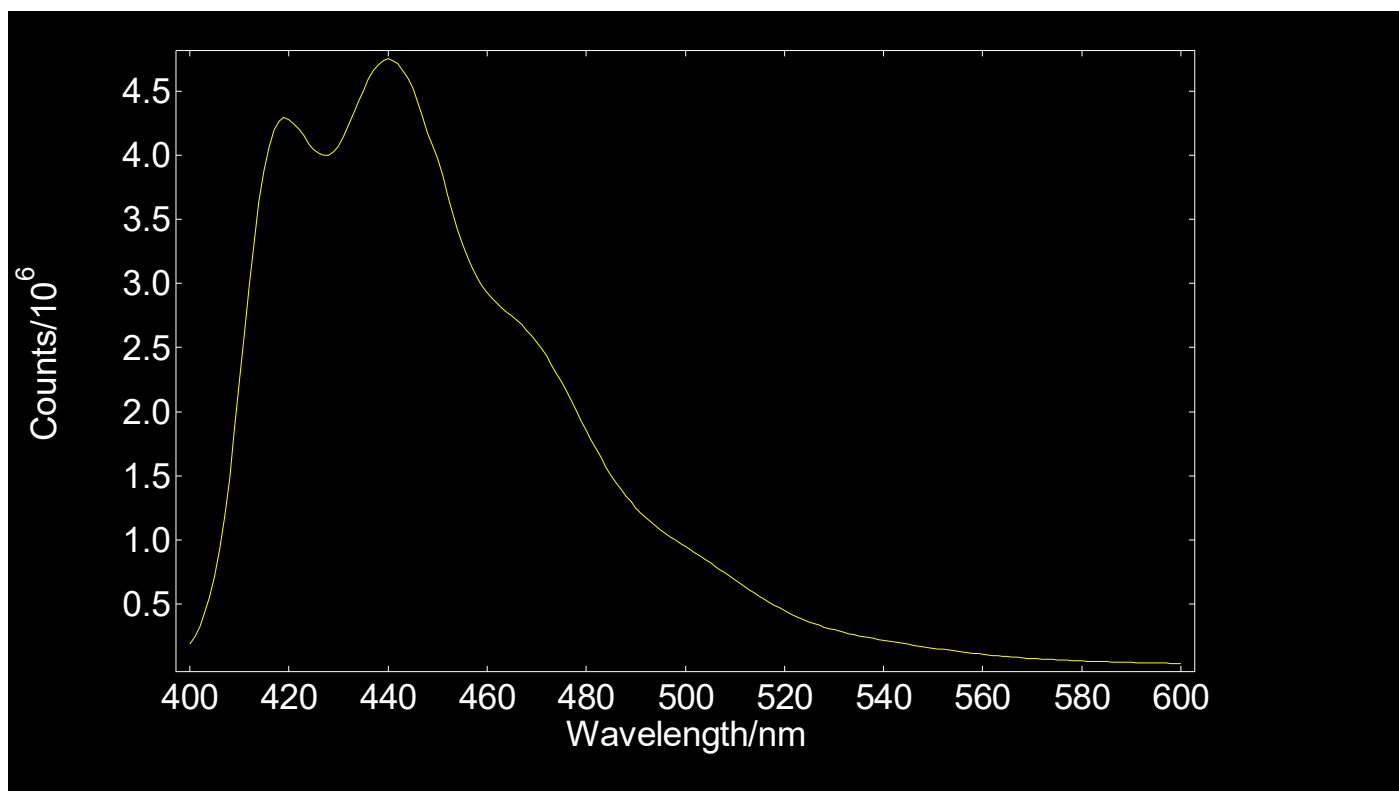


Figure S25. Overlaid UV-Vis spectra of the compound **5b** in trichloromethane and cyclohexane.

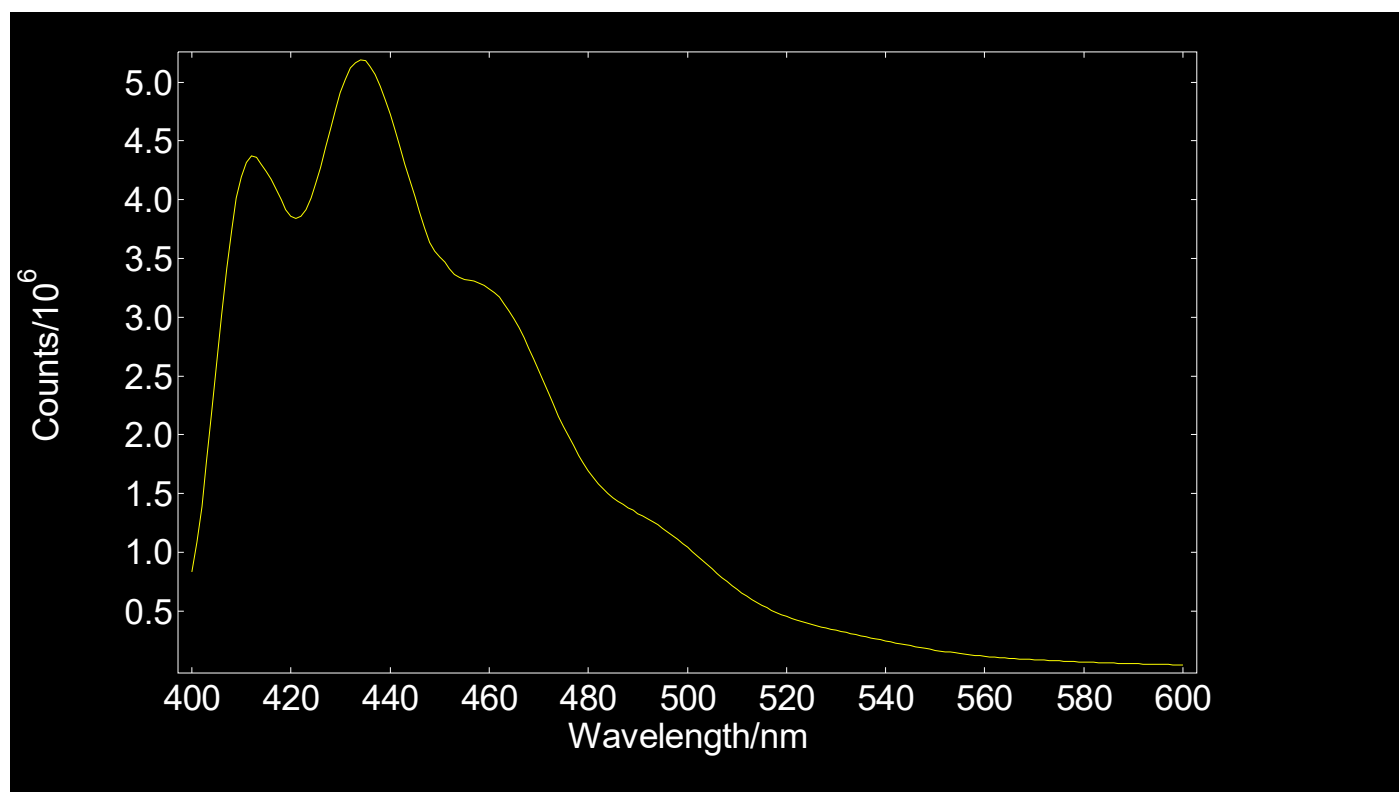
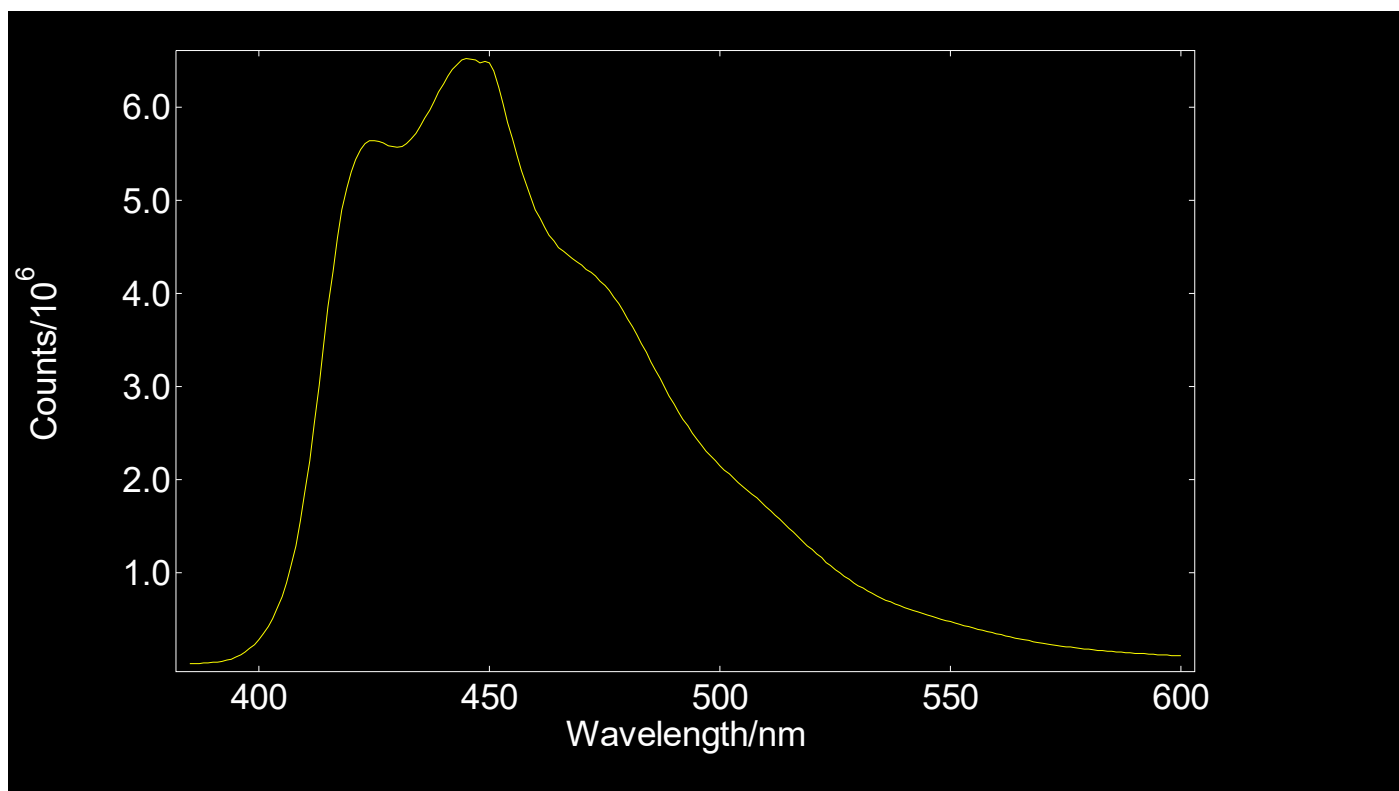
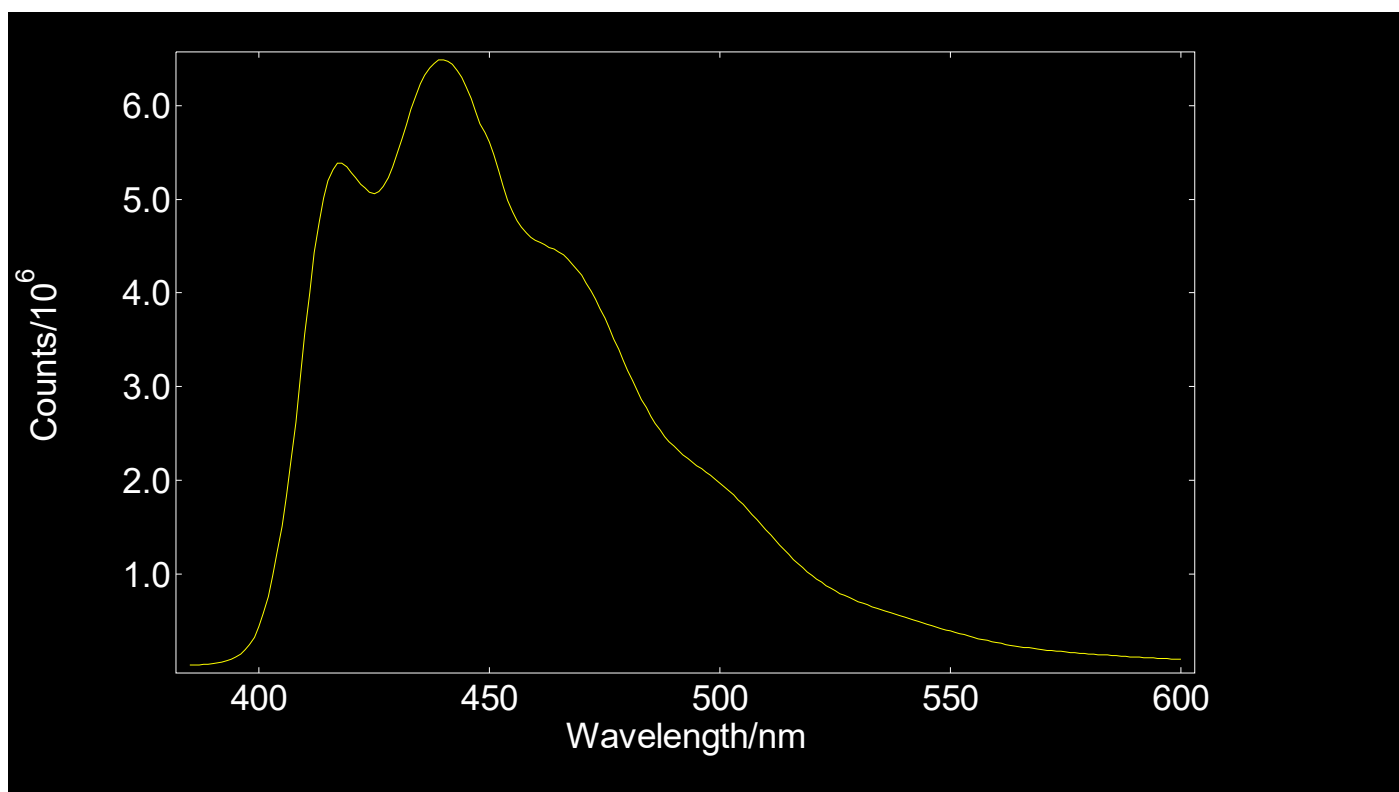


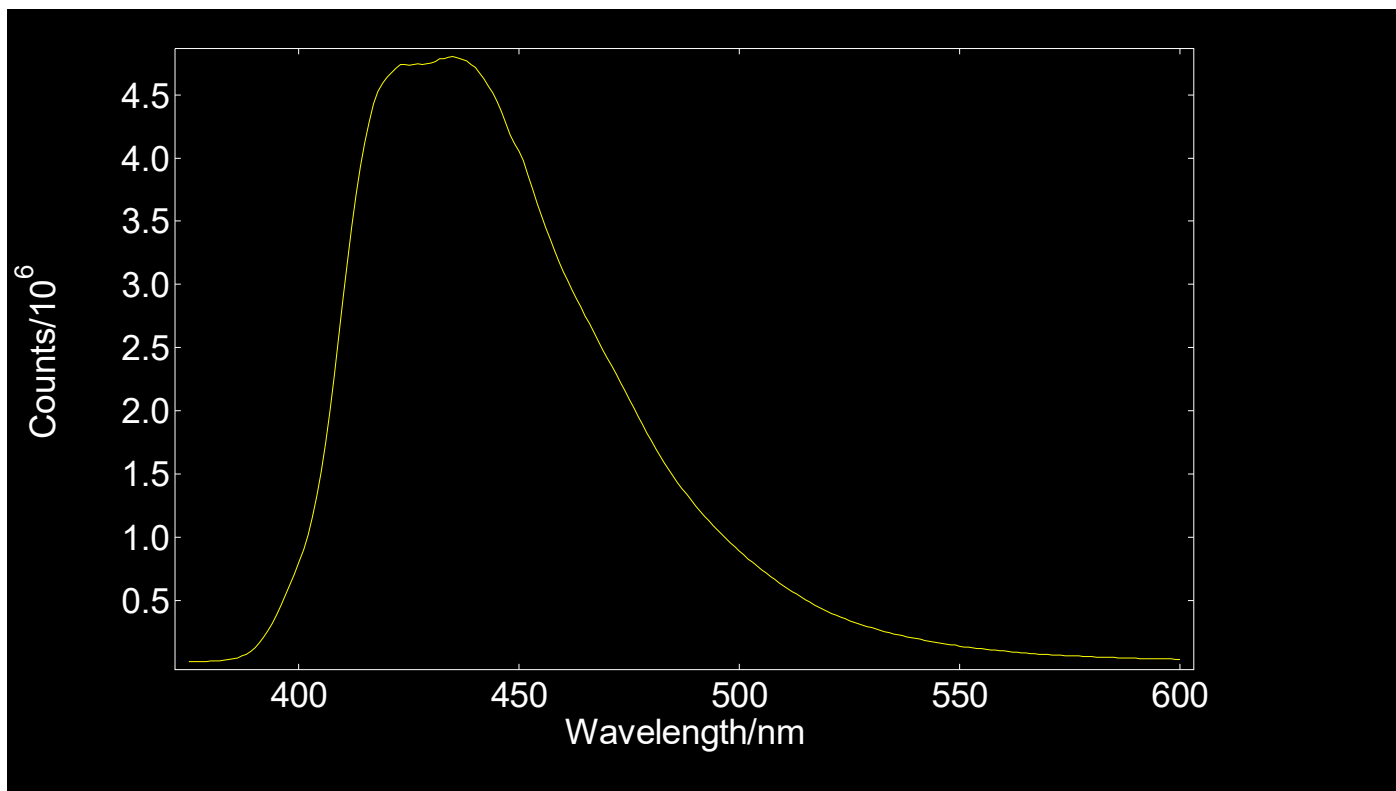
Figure S26. Emission spectrum of the compound **5b** in cyclohexane.



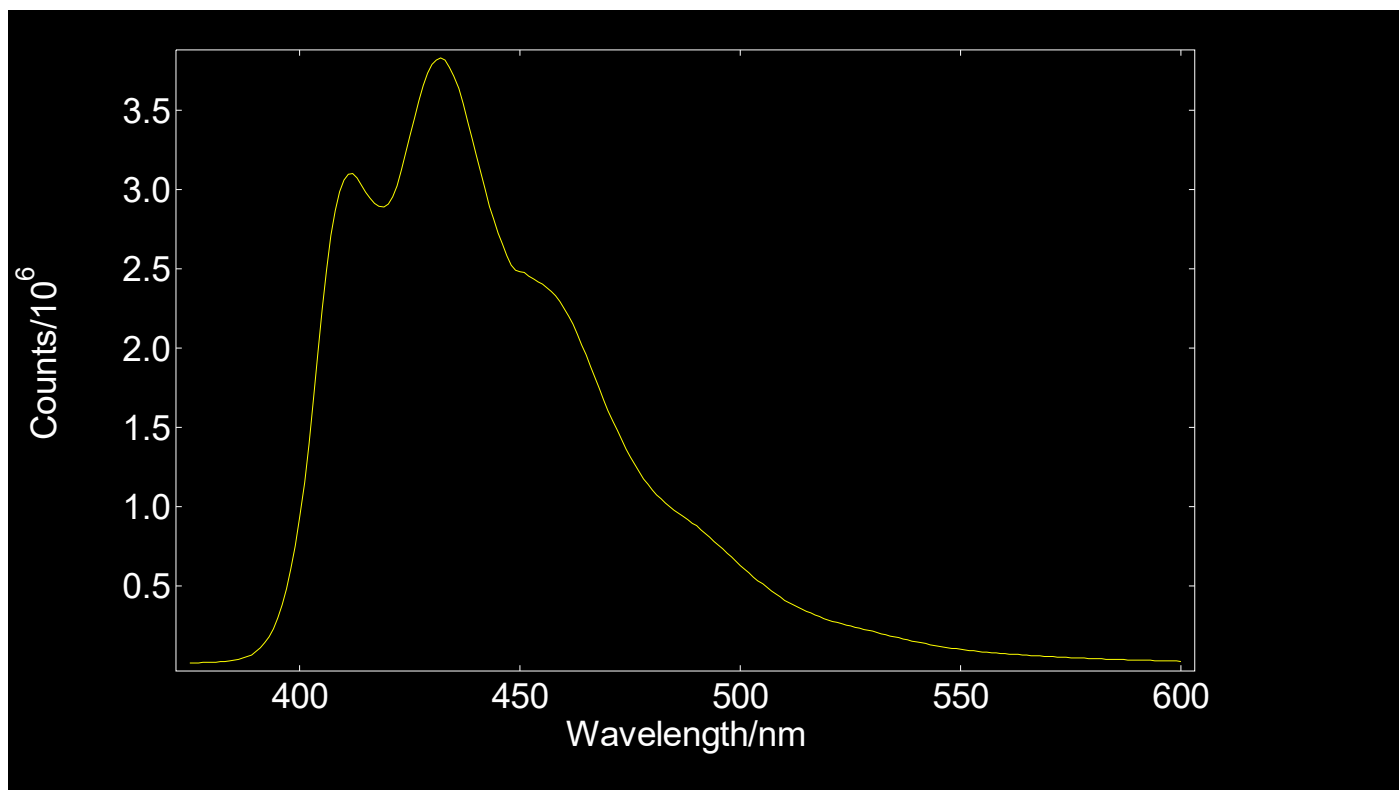
**Figure S27.** Emission spectrum of the compound **5c** in trichloromethane.



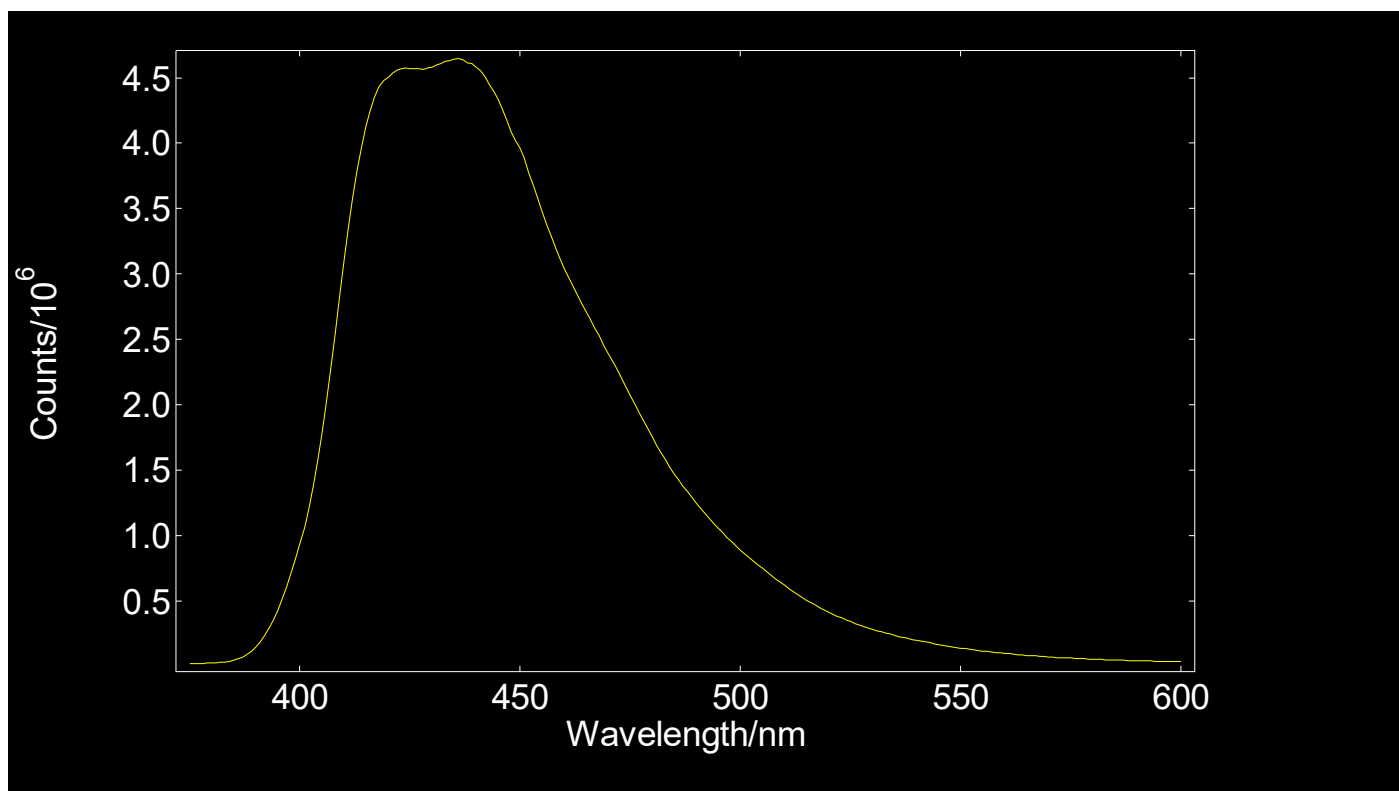
**Figure S28.** Emission spectrum of the compound **5c** in cyclohexane.



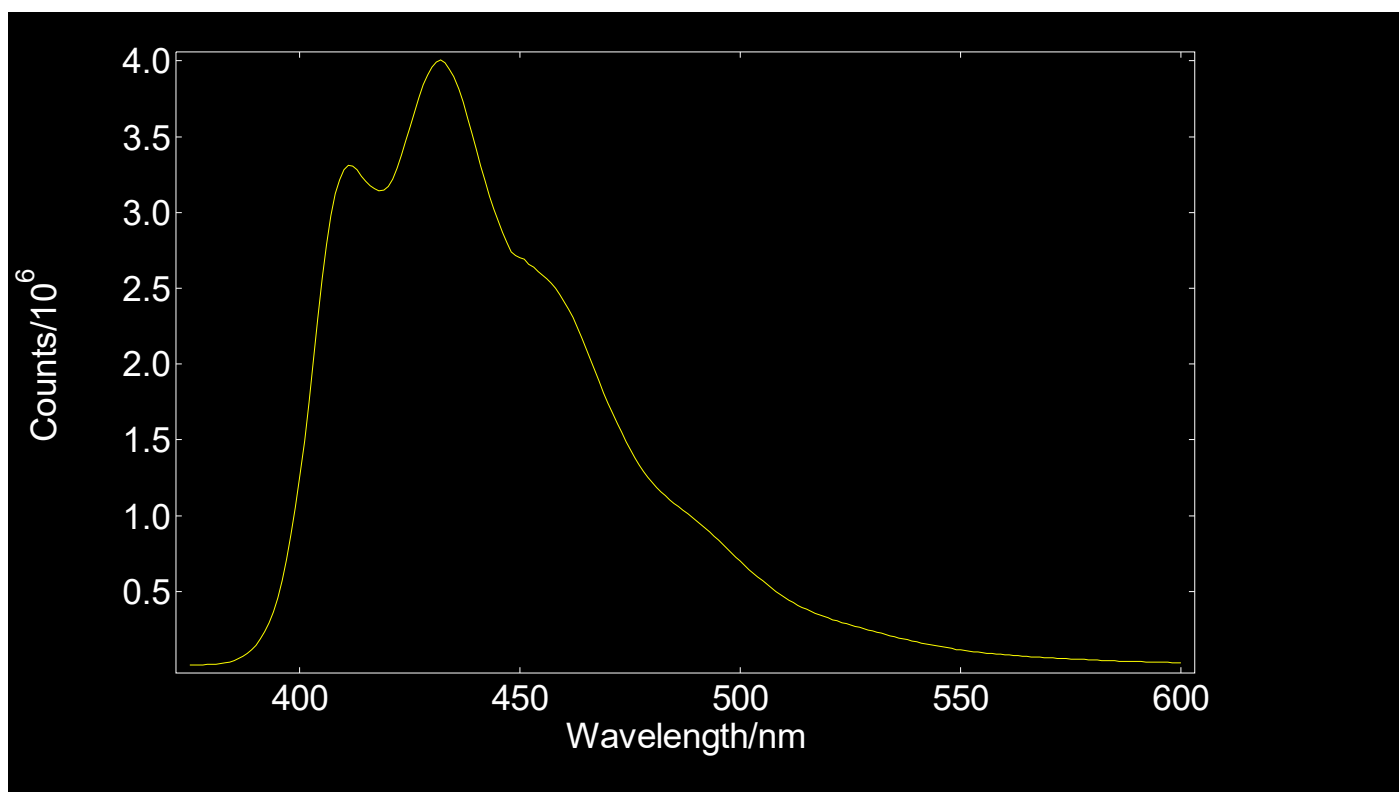
**Figure S29.** Emission spectrum of the compound **7a** in trichloromethane.



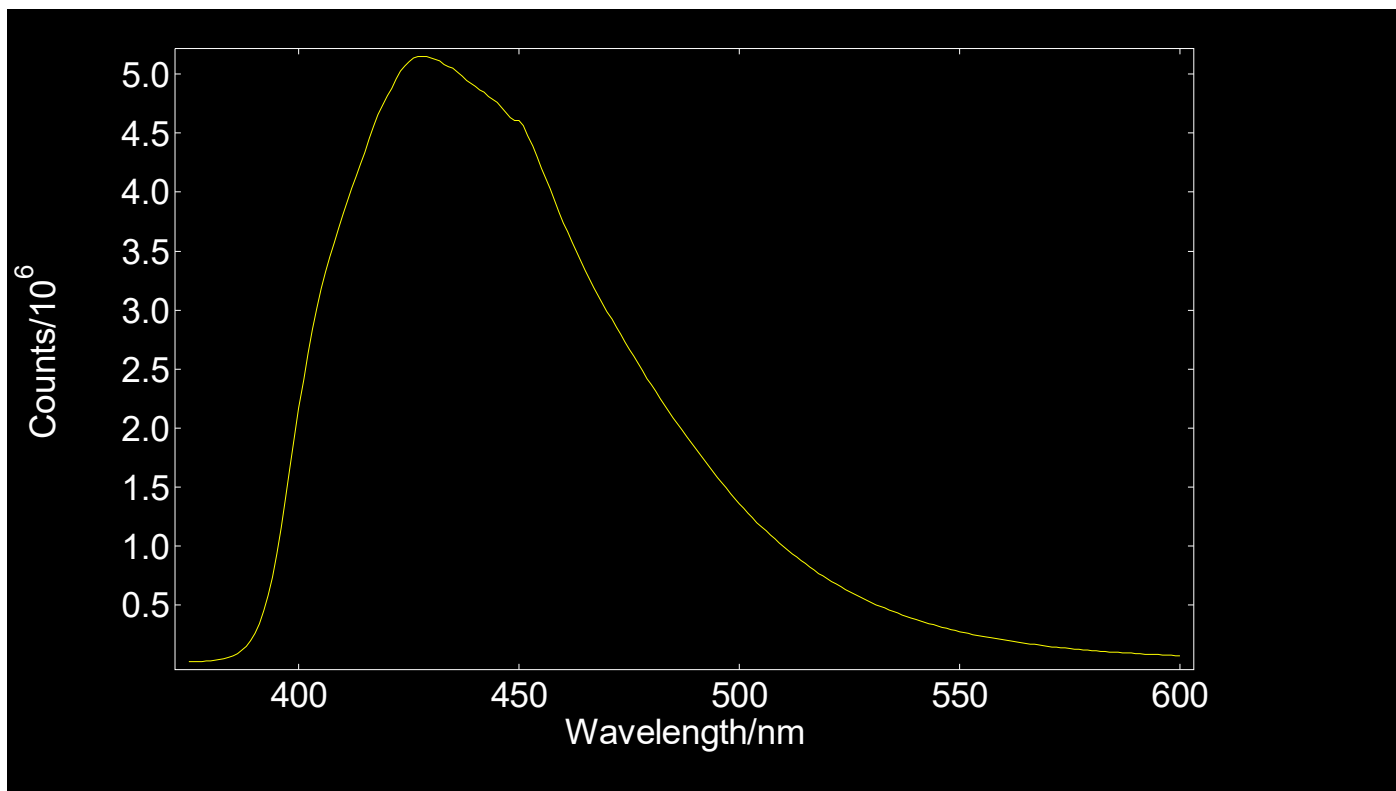
**Figure S30.** Emission spectrum of the compound **7a** in cyclohexane.



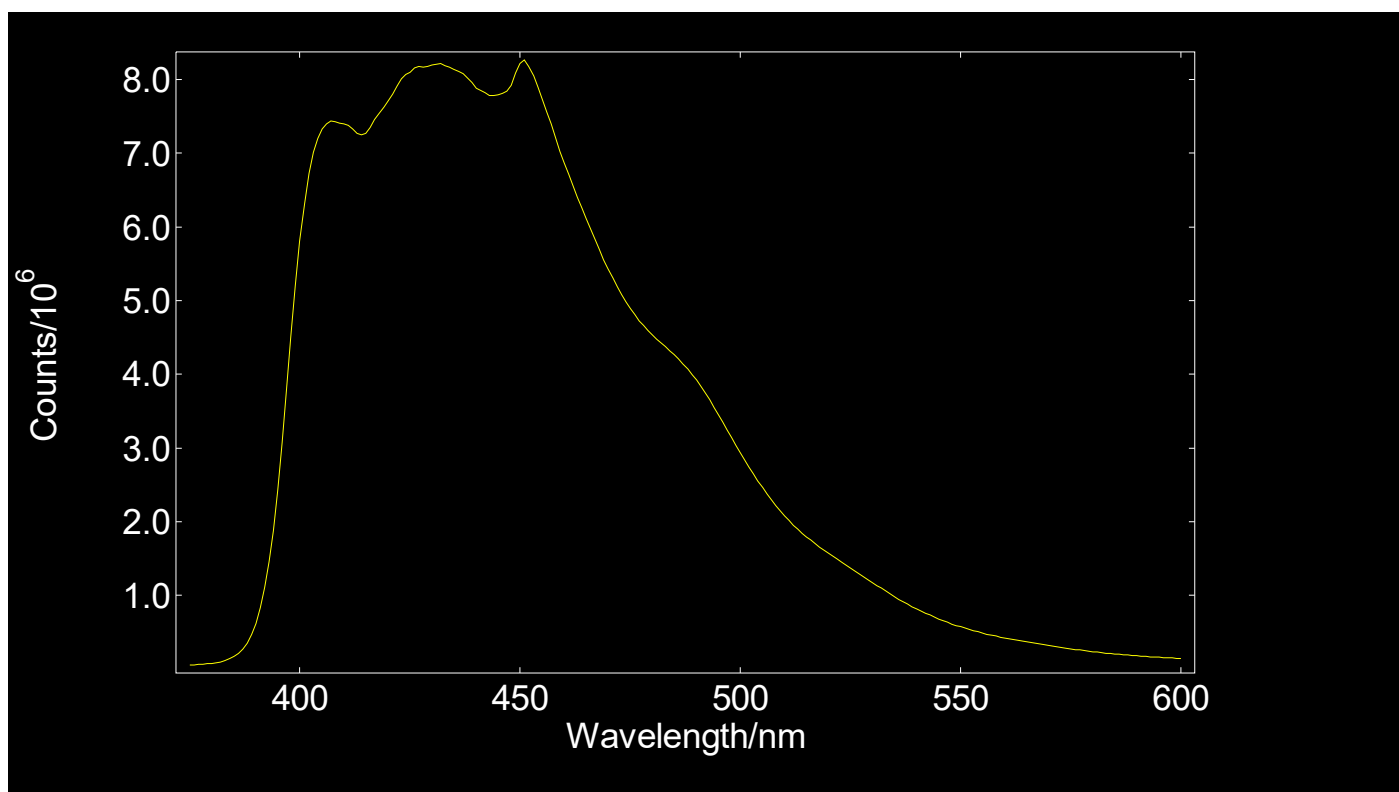
**Figure S31.** Emission spectrum of the compound **7b** in trichloromethane.



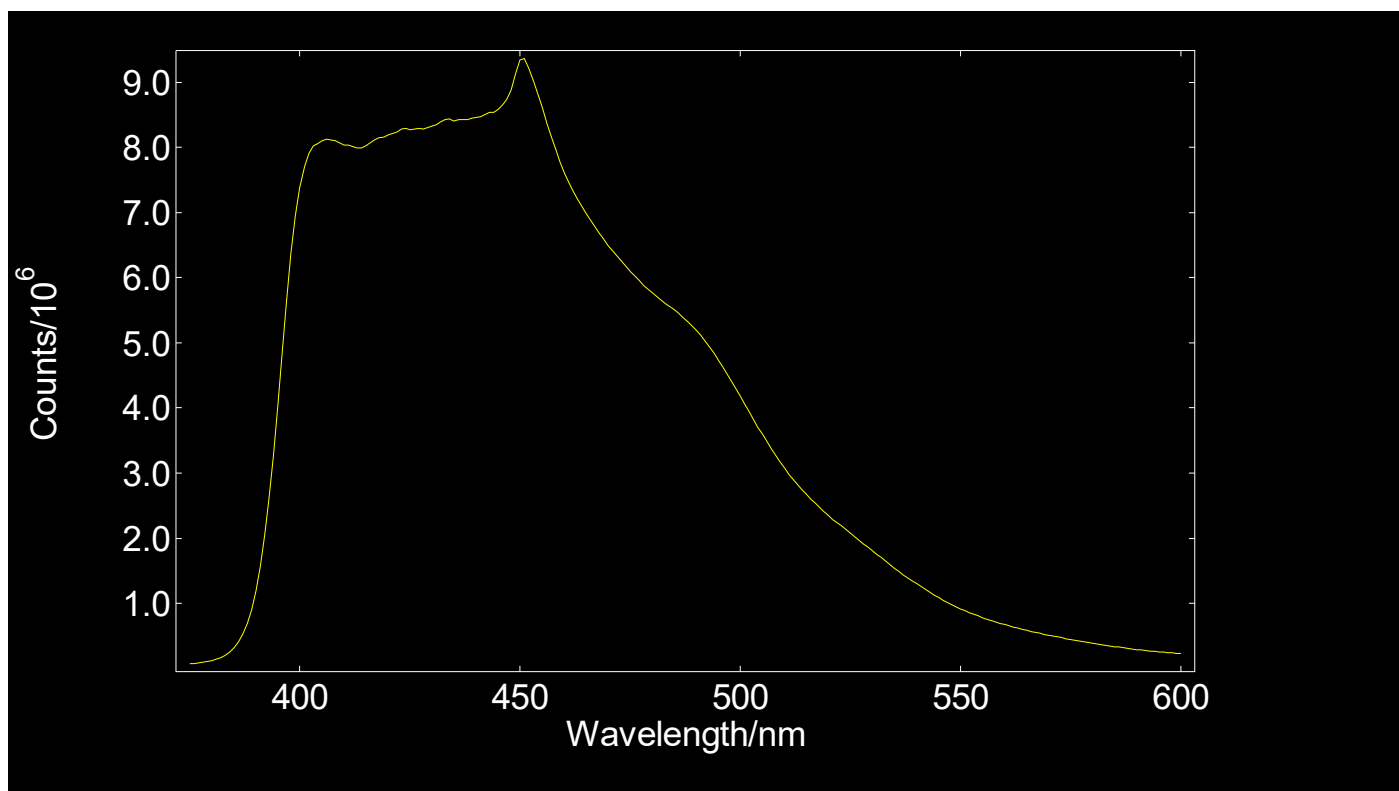
**Figure S32.** Emission spectrum of the compound **7b** in cyclohexane.



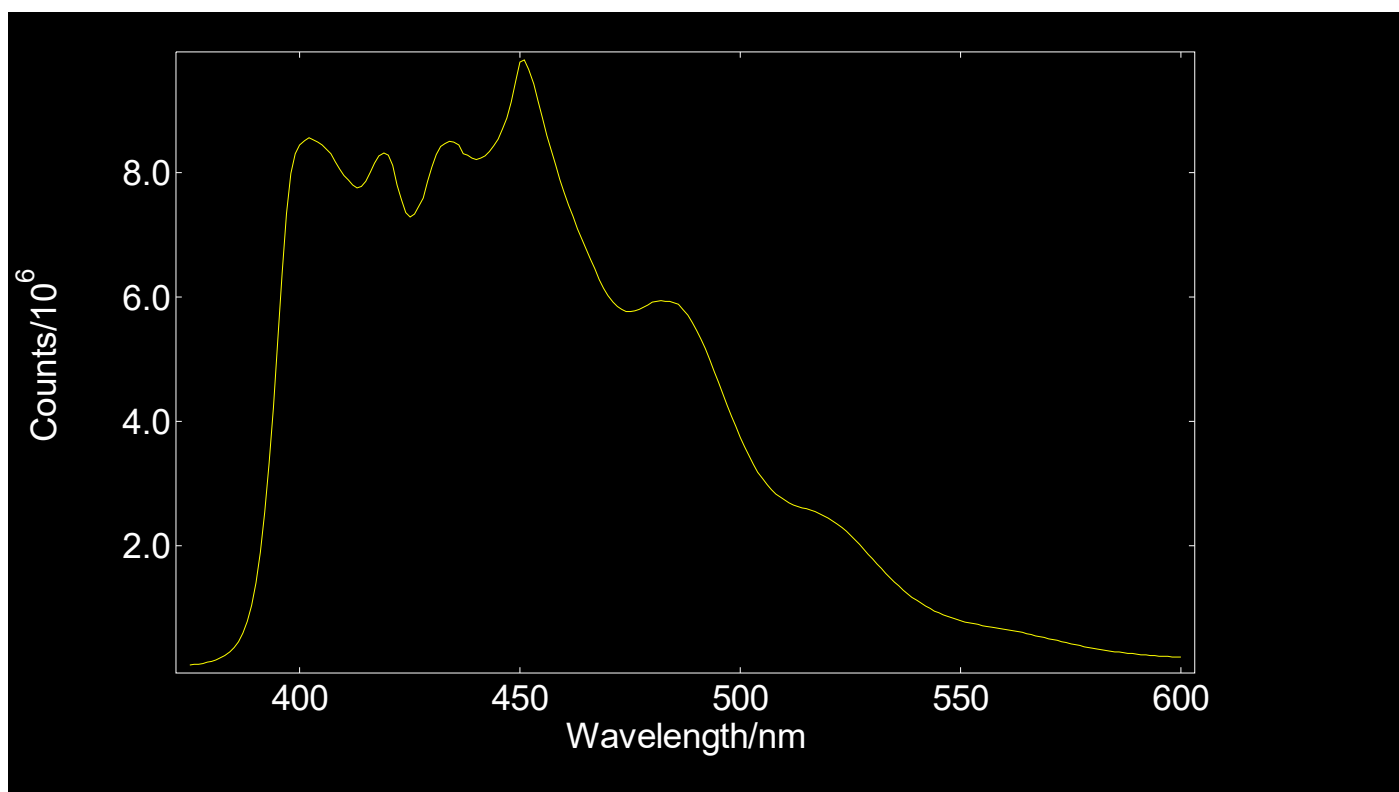
**Figure S33.** Emission spectrum of the compound **7c** in trichloromethane.



**Figure S34.** Emission spectrum of the compound **7c** in cyclohexane.

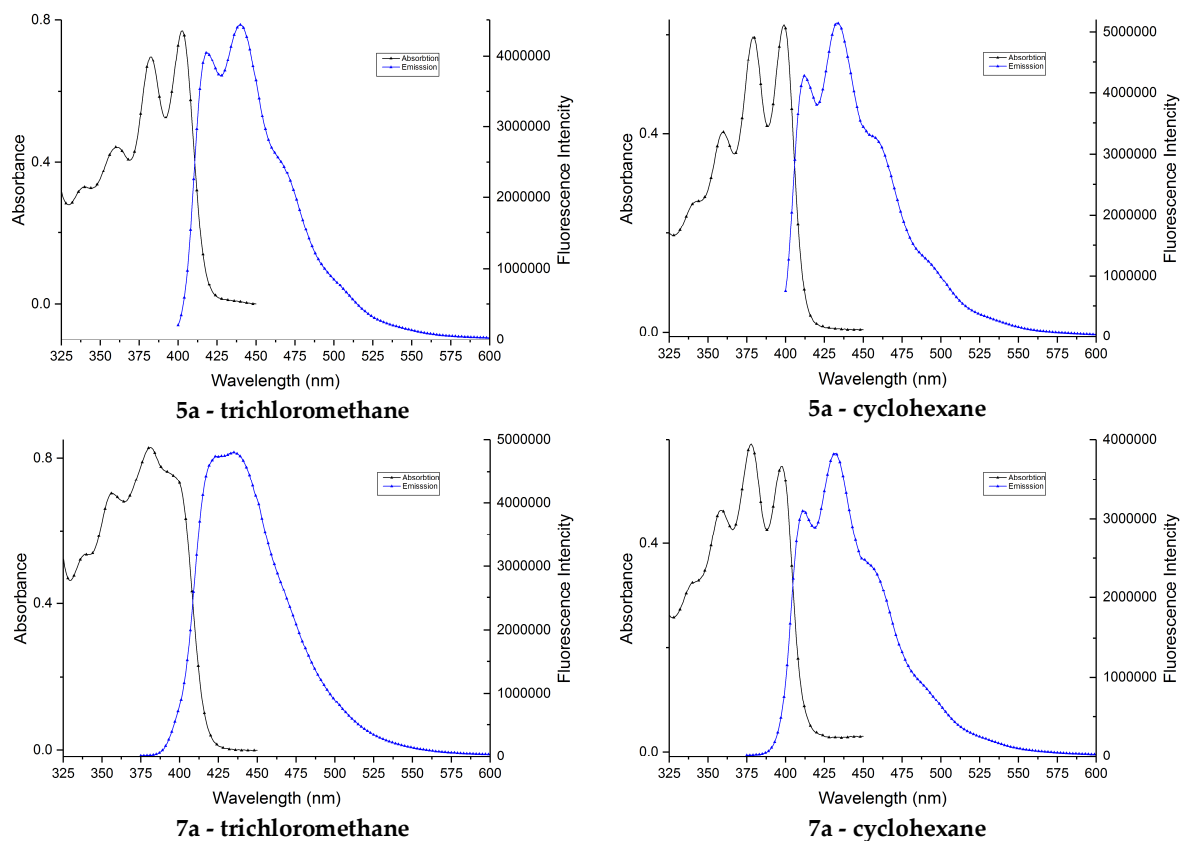


**Figure S35.** Emission spectrum of the compound **8c** in trichloromethane.

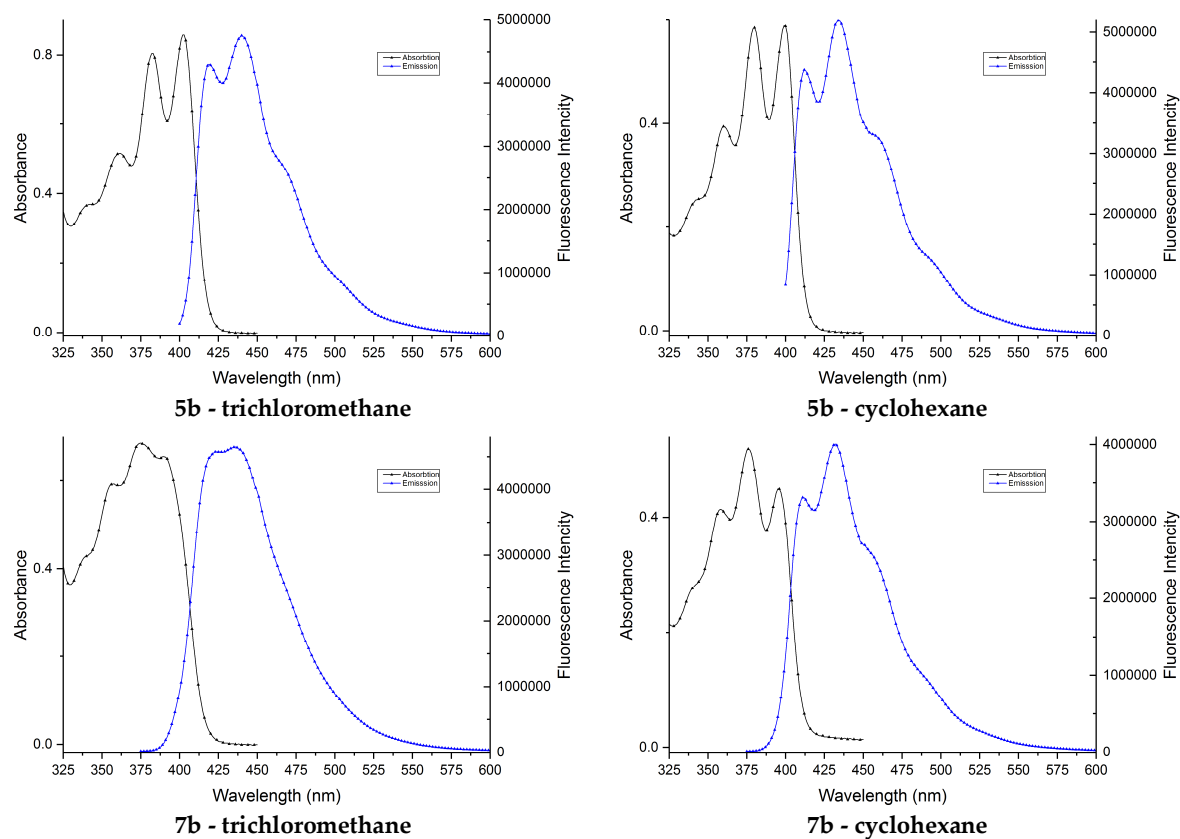


**Figure S36.** Emission spectrum of the compound **8c** in cyclohexane.

## 6. Absorption vs emission spectra of the obtained compounds

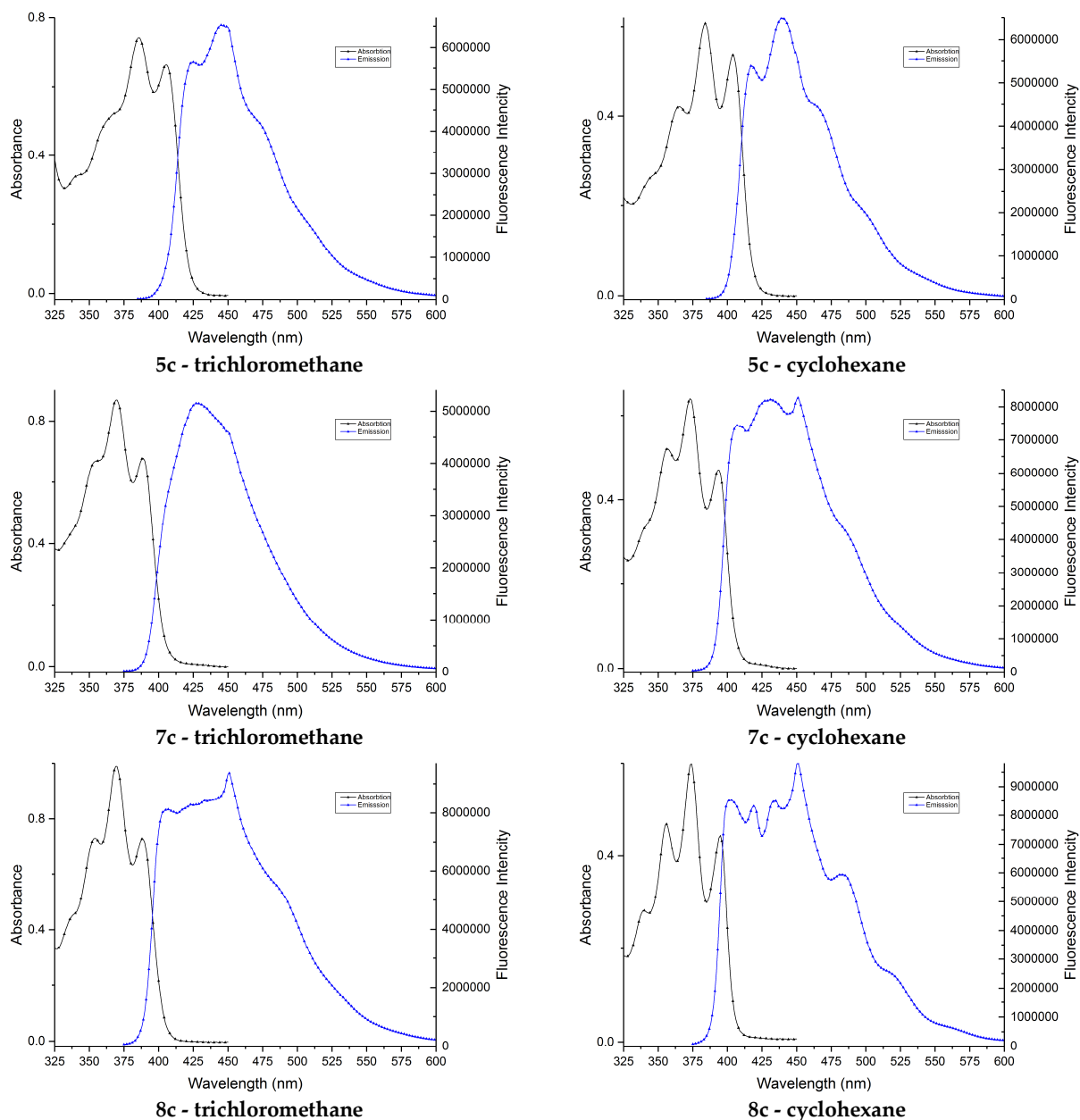


**Figure S37.** The absorption (black line) and emission (blue line) spectra of azasteroid derivatives **5a** and **7a** in trichloromethane (left column) and cyclohexane (right column). Excitation wavelength was: 396 nm for sample **5a** and 370 nm for samples **7b**.



**Figure S38.** The absorption (black line) and emission (blue line) spectra of azasteroid derivatives **5b** and **7b** in trichloromethane (left column) and cyclohexane (right column). Excitation wavelength was: 396 nm for sample **5a** and 370 nm for samples **7b**.





**Figure S39.** The absorption (black line) and emission (blue line) spectra of azasteroid derivatives **5c**, **7c** and **8c** in trichloromethane (left column) and cyclohexane (right column). Excitation wavelength was: 380 nm for sample **5c** and 365 nm for samples **7c** and **8c**.