

Supporting information for:

# Fluorescent azasteroids through ultrasound assisted cycloaddition reactions

Costel Moldoveanu <sup>1, \*</sup>, Ionel Mangalagiu <sup>1,2</sup> and Gheorghita Zbancioc <sup>1,\*</sup>

<sup>1</sup> Chemistry Department, Alexandru Ioan Cuza University of Iasi, 11 Carol 1st Bvd, Iasi -700506, Romania; ionelm@uaic.ro (I.M.)

<sup>2</sup> Integrated Centre of Environmental Science Studies in the North Eastern Region (CERNESIM), Alexandru Ioan Cuza University of Iasi, 11 Carol I, Iasi, 700506, Romania; ionelm@uaic.ro (I.M.)

\* Correspondence: costel.moldoveanu@uaic.ro (C.M.); gheorghita.zbancioc@uaic.ro (G.Z.) Tel.: +40-232-201278

## Contents

1. NMR spectra of the obtained compounds.....	2
2. IR spectra of the obtained compounds. ....	12
3. <sup>1</sup> H-NMR studies on compound 7a at room temperature.....	16
4. UV spectra of the obtained compounds.....	17
5. Emission spectra of the obtained compounds.....	24
6. Absorption vs emission spectra of the obtained compounds .....	31



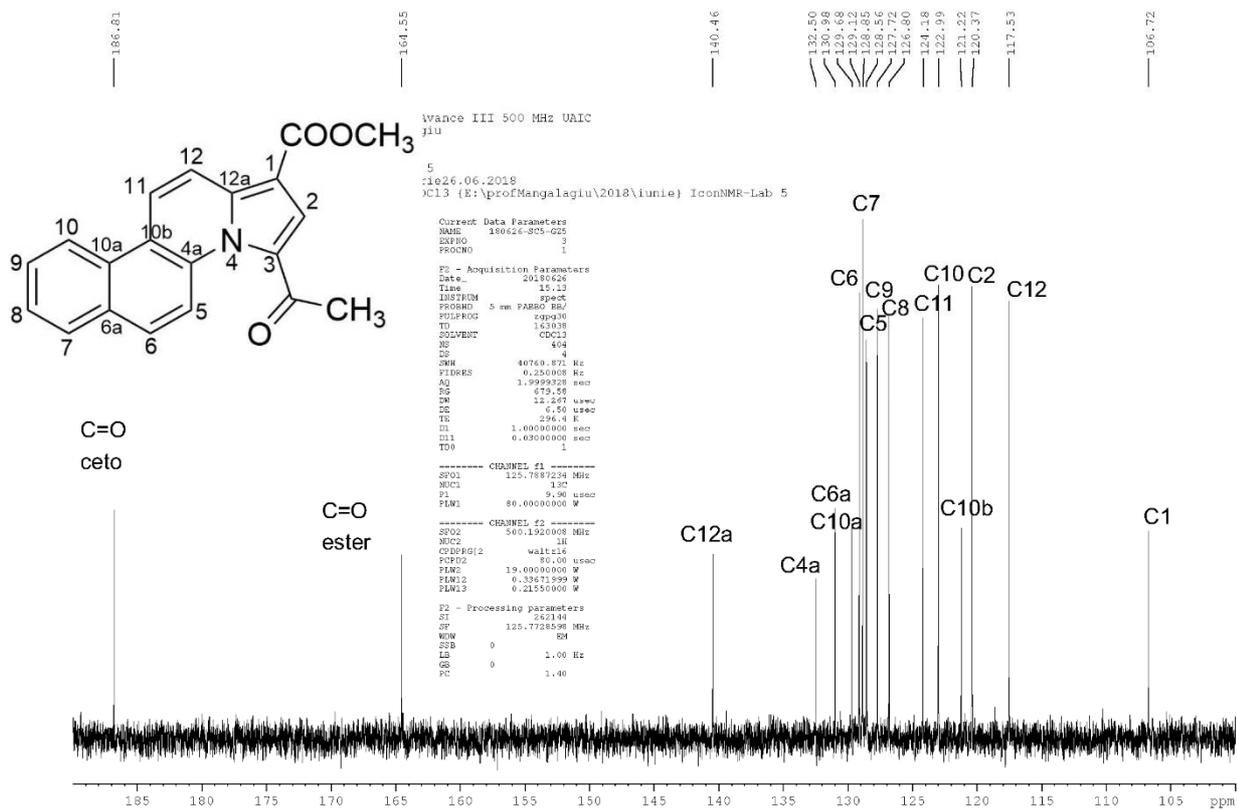


Figure S1c. Detail in the aromatic area of the  $^{13}\text{C}$  NMR spectrum of the compound 5a.

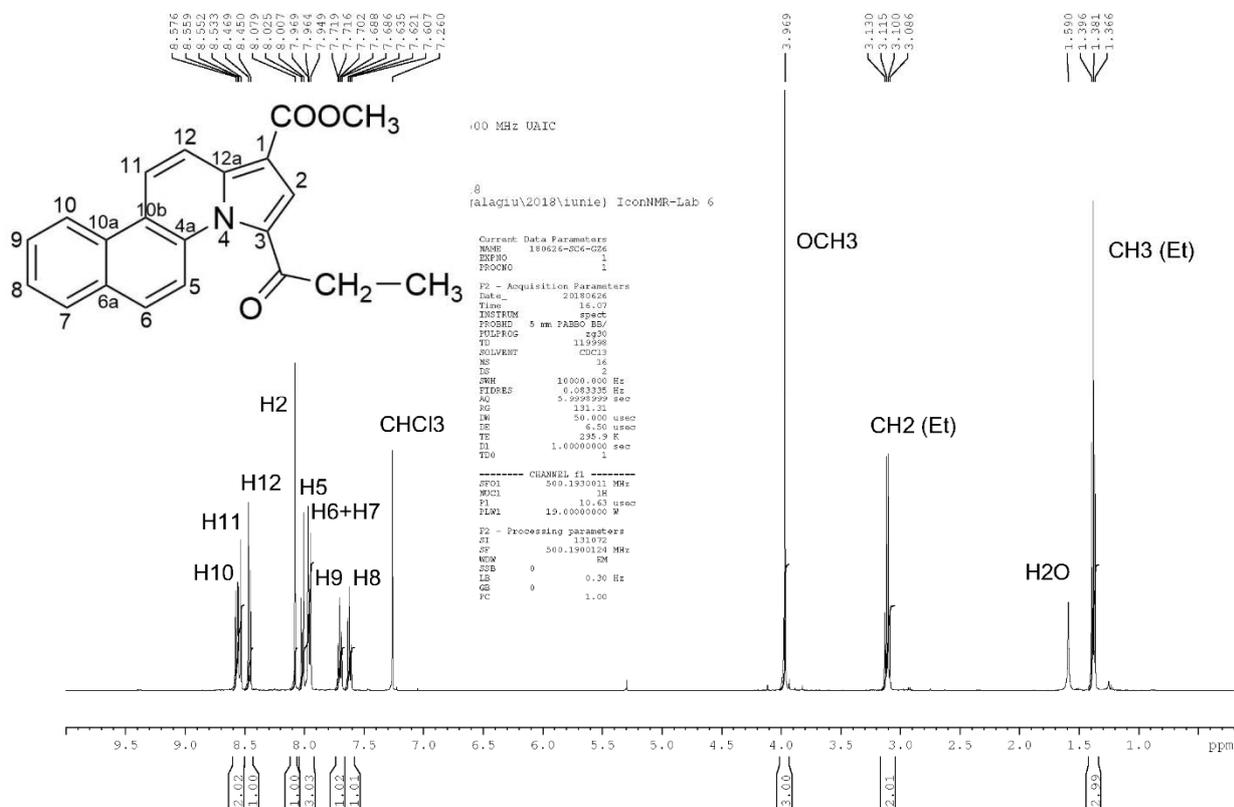


Figure S2a.  $^1\text{H}$  NMR spectrum of the compound 5b.





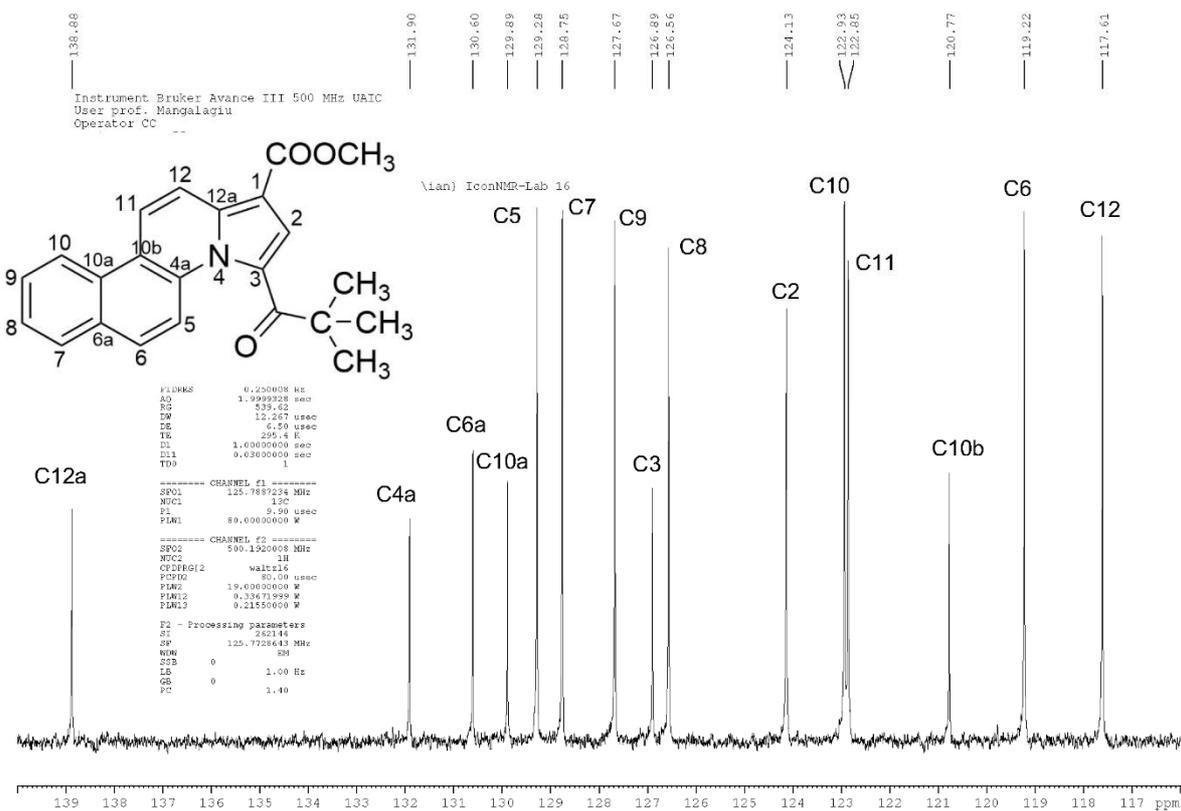


Figure S3c. Detail in the aromatic area of the <sup>13</sup>C NMR spectrum of the compound 5c.

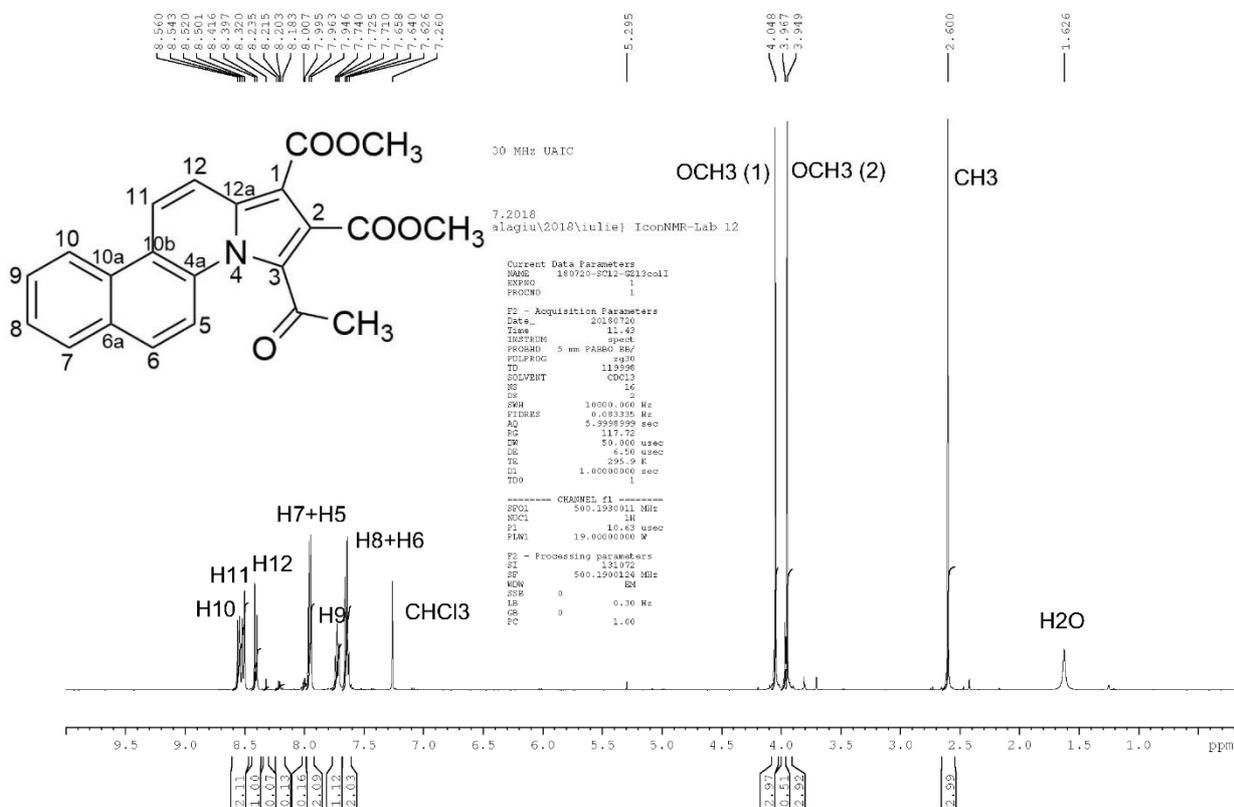


Figure S4a. <sup>1</sup>H NMR spectrum of the compound 7a.

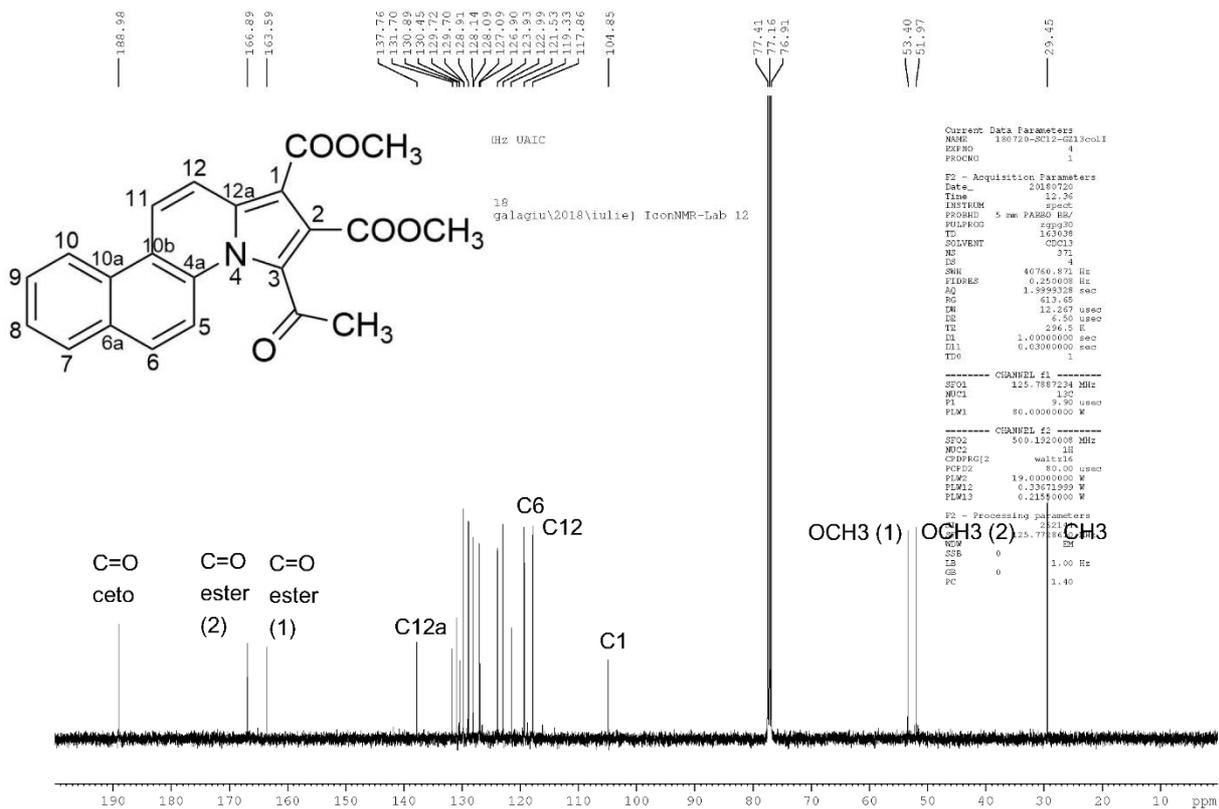


Figure S4b. <sup>13</sup>C NMR spectrum of the compound 7a.

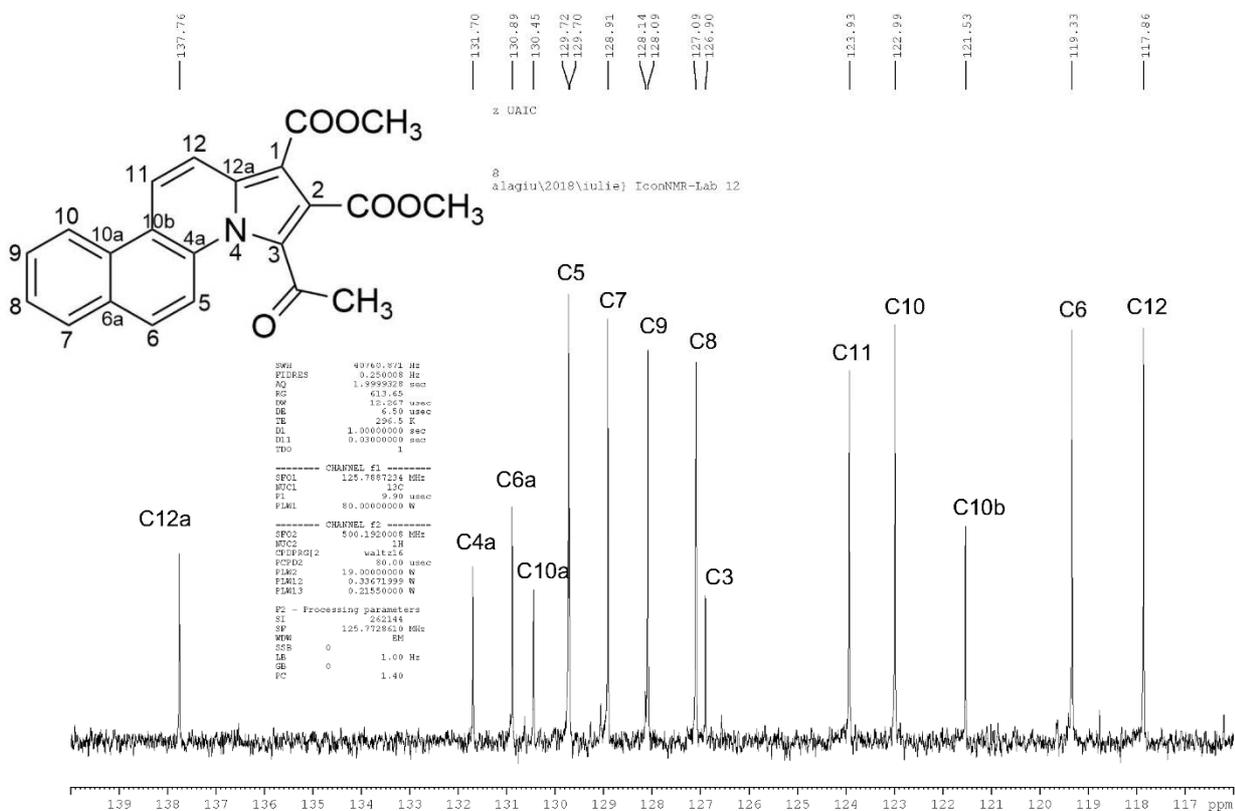


Figure S4c. Detail in the aromatic area of the <sup>13</sup>C NMR spectrum of the compound 7a.

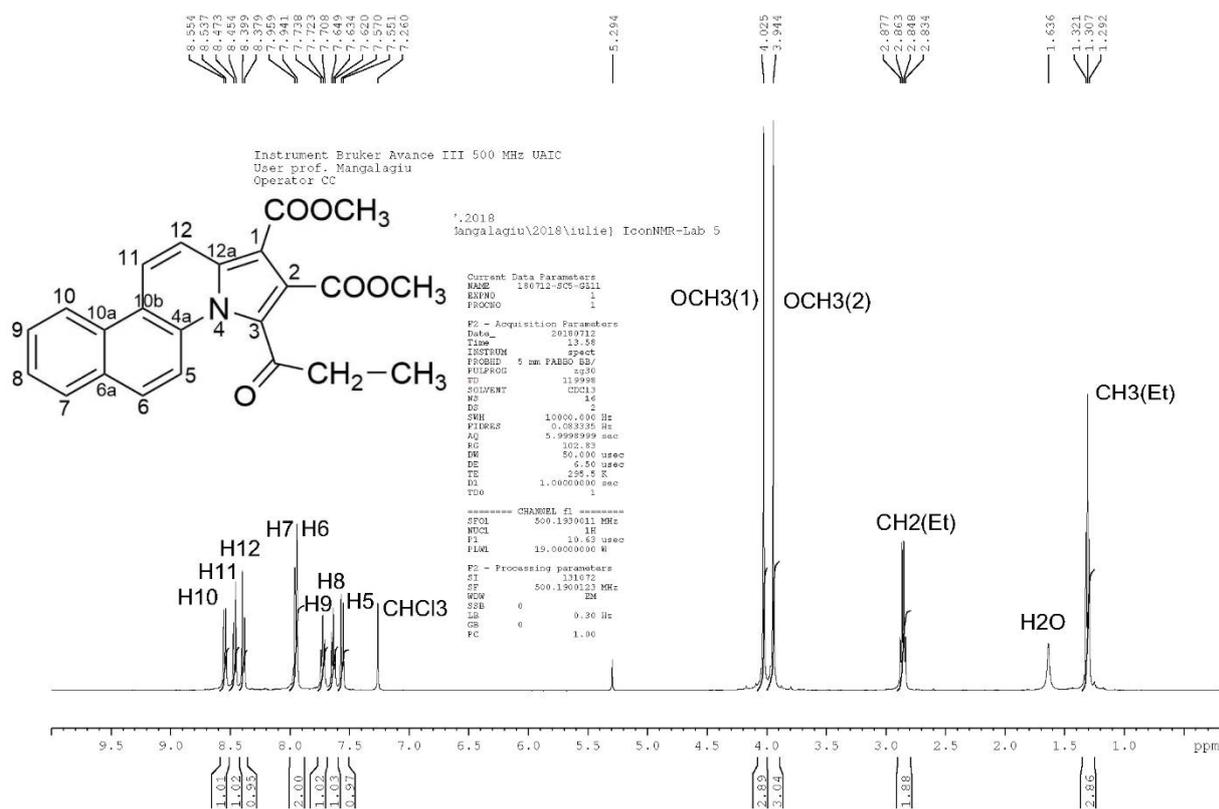


Figure S5a. <sup>1</sup>H NMR spectrum of the compound 7b.

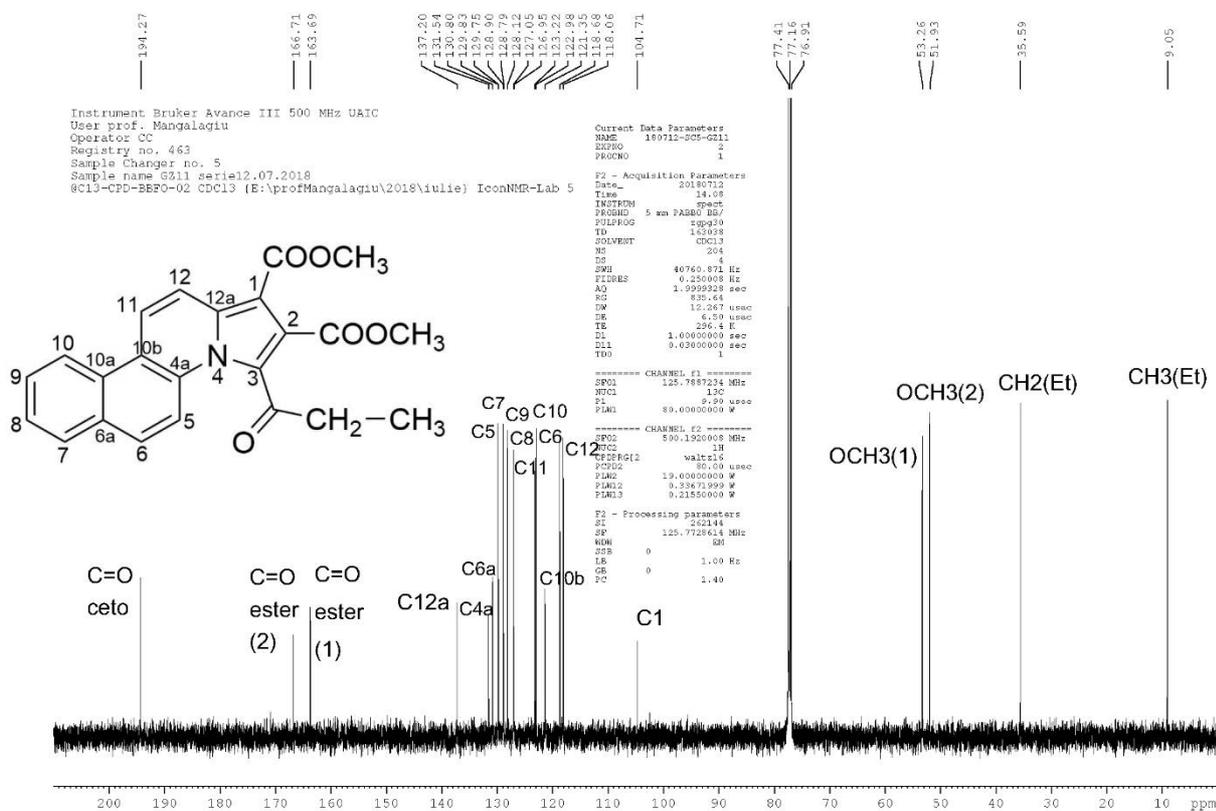


Figure S5b. <sup>13</sup>C NMR spectrum of the compound 7b.

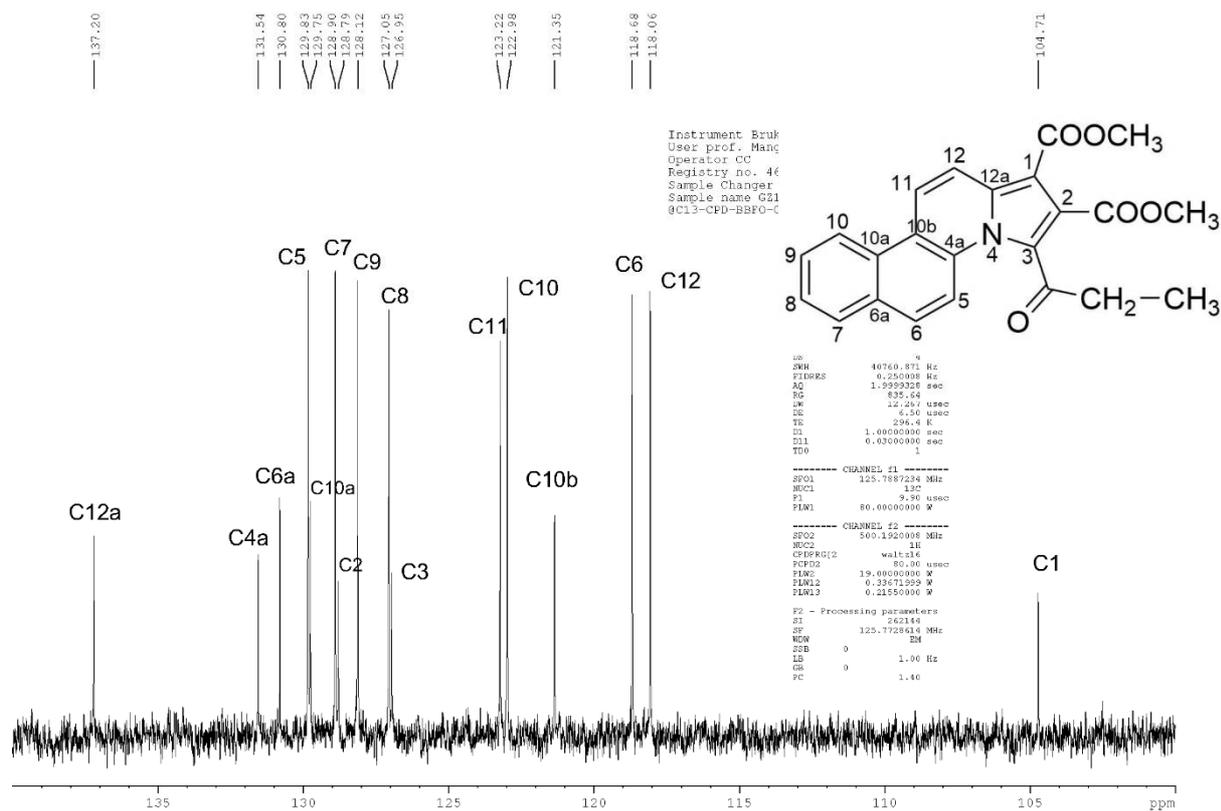


Figure S5c. Detail in the aromatic area of the  $^{13}\text{C}$  NMR spectrum of the compound **7b**.

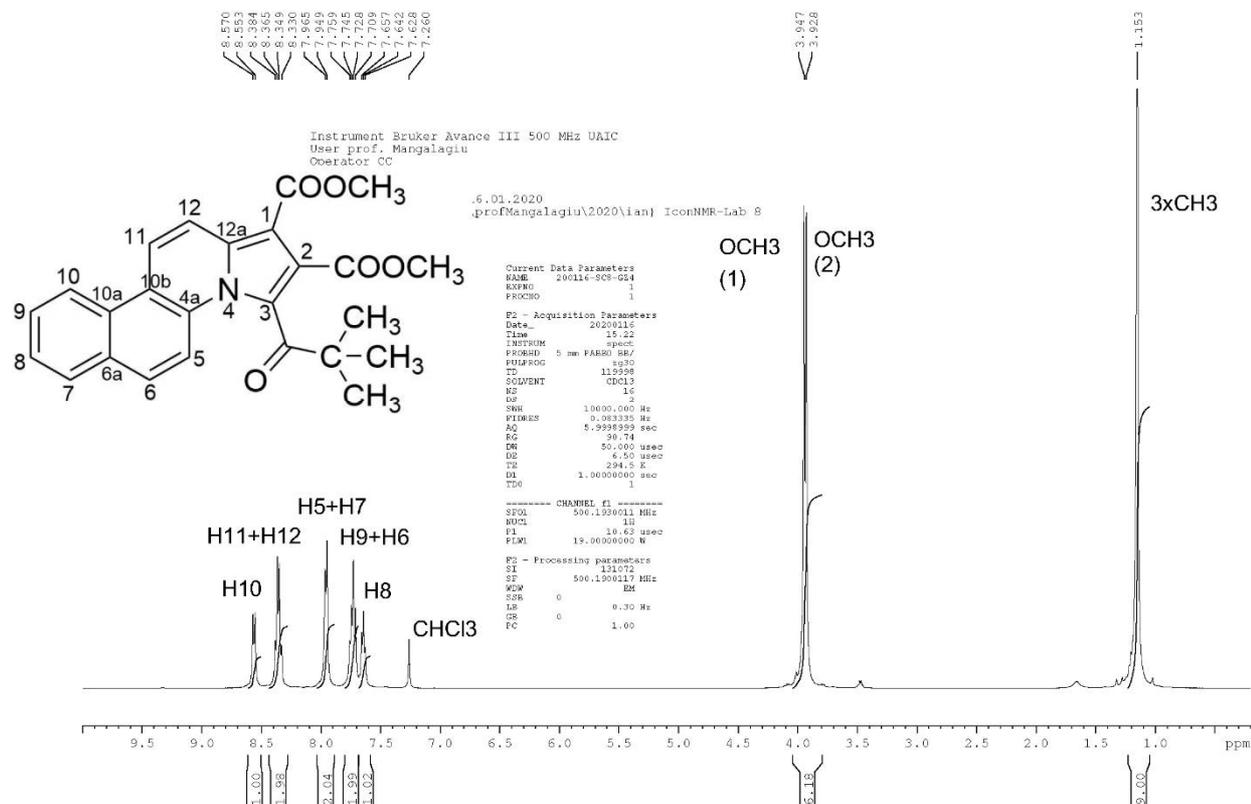


Figure S6a.  $^1\text{H}$  NMR spectrum of the compound **7c**.

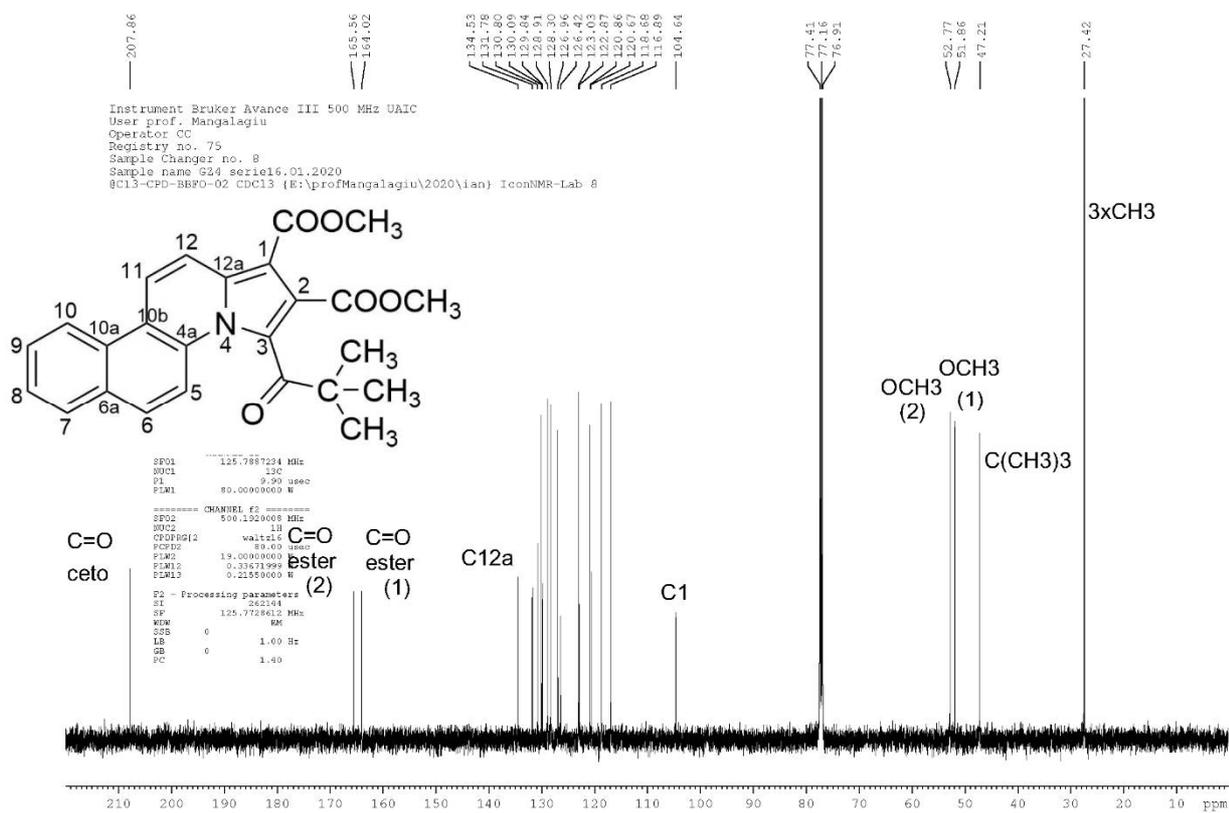


Figure S6b.  $^{13}\text{C}$  NMR spectrum of the compound 7c.

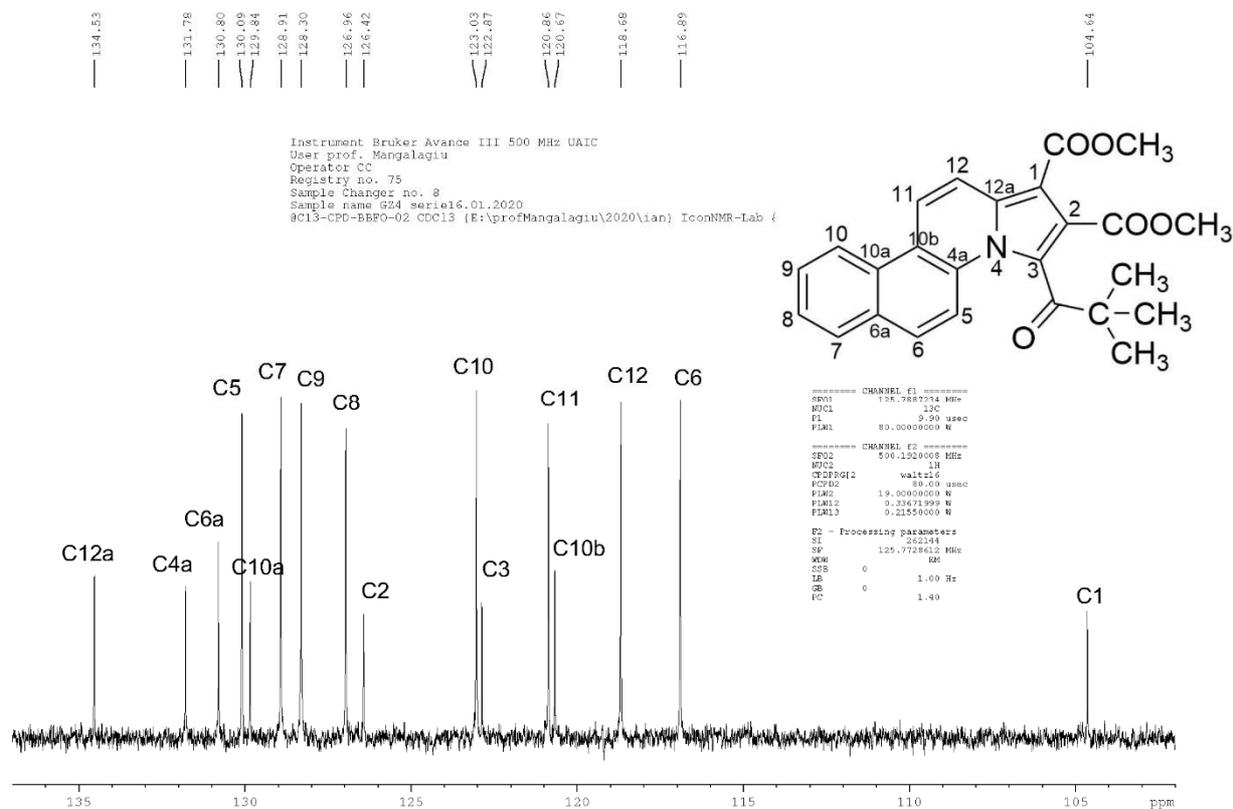


Figure S6c. Detail in the aromatic area of the  $^{13}\text{C}$  NMR spectrum of the compound 7c.

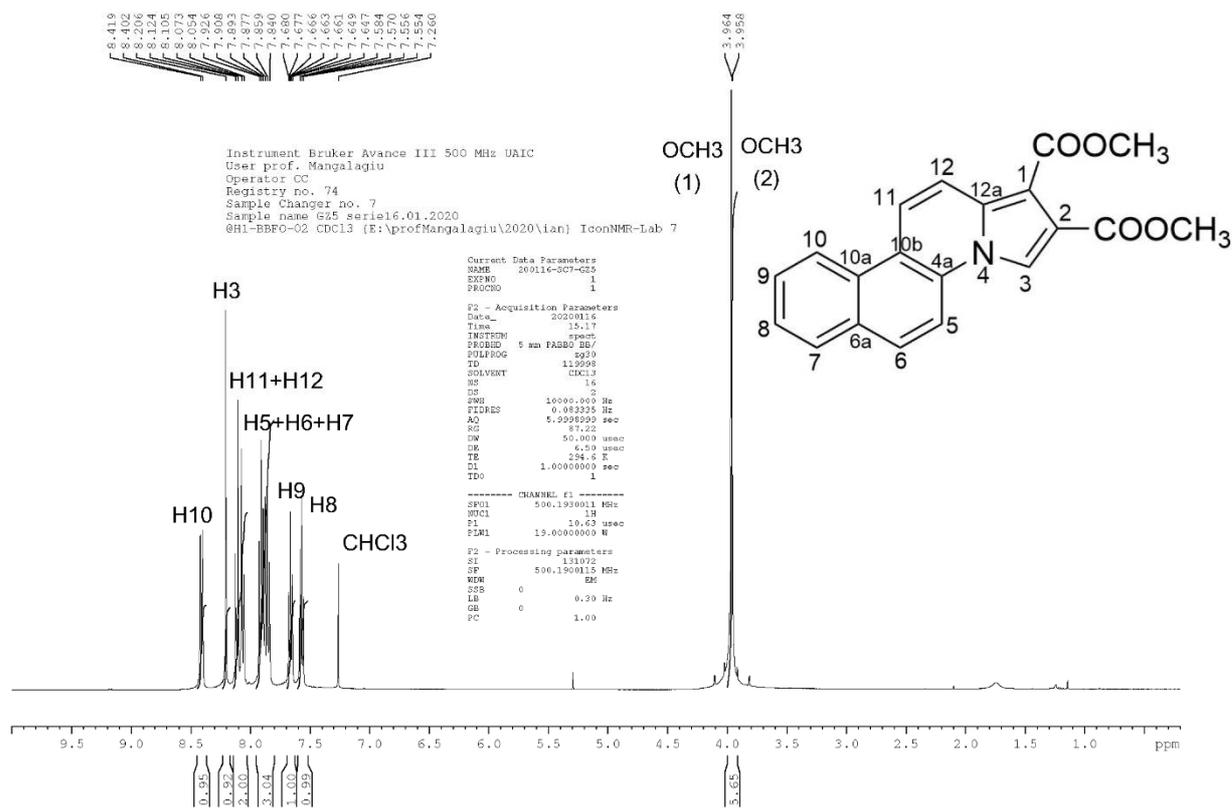


Figure S7a. <sup>1</sup>H NMR spectrum of the compound 8c.

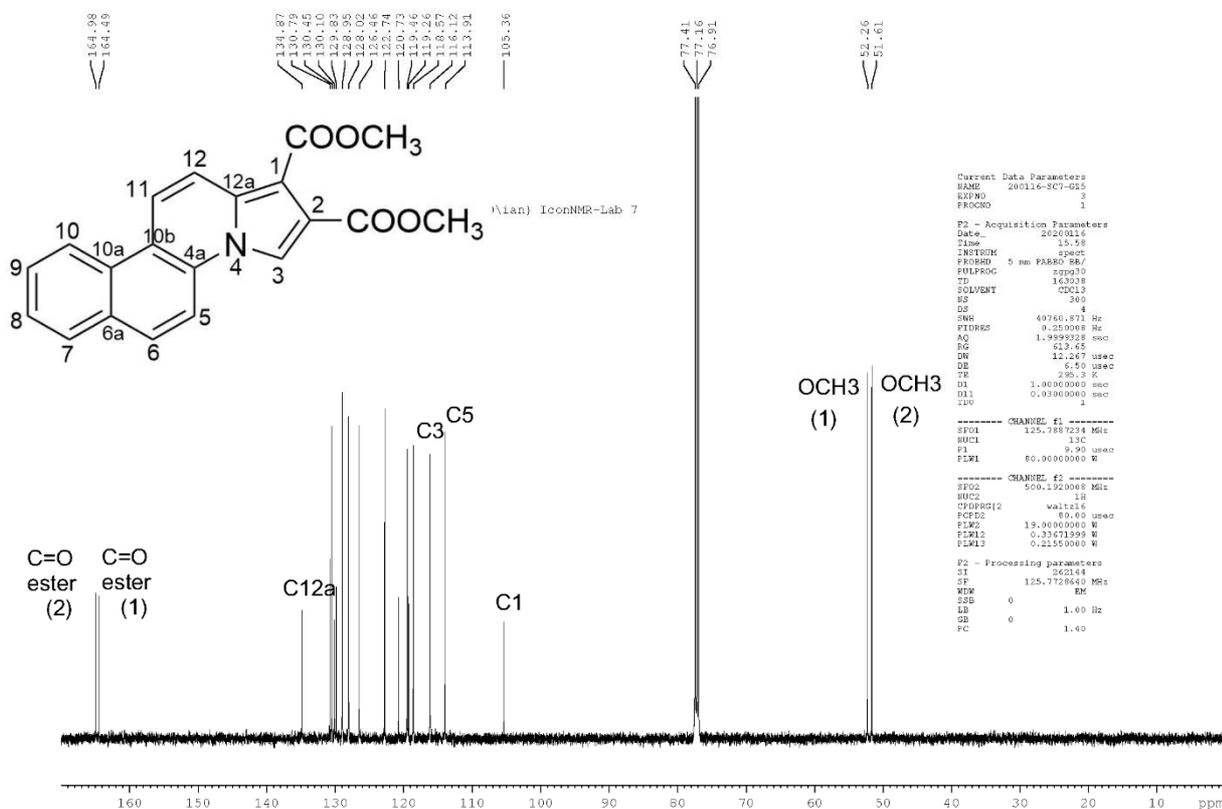


Figure S7b. <sup>13</sup>C NMR spectrum of the compound 8c.

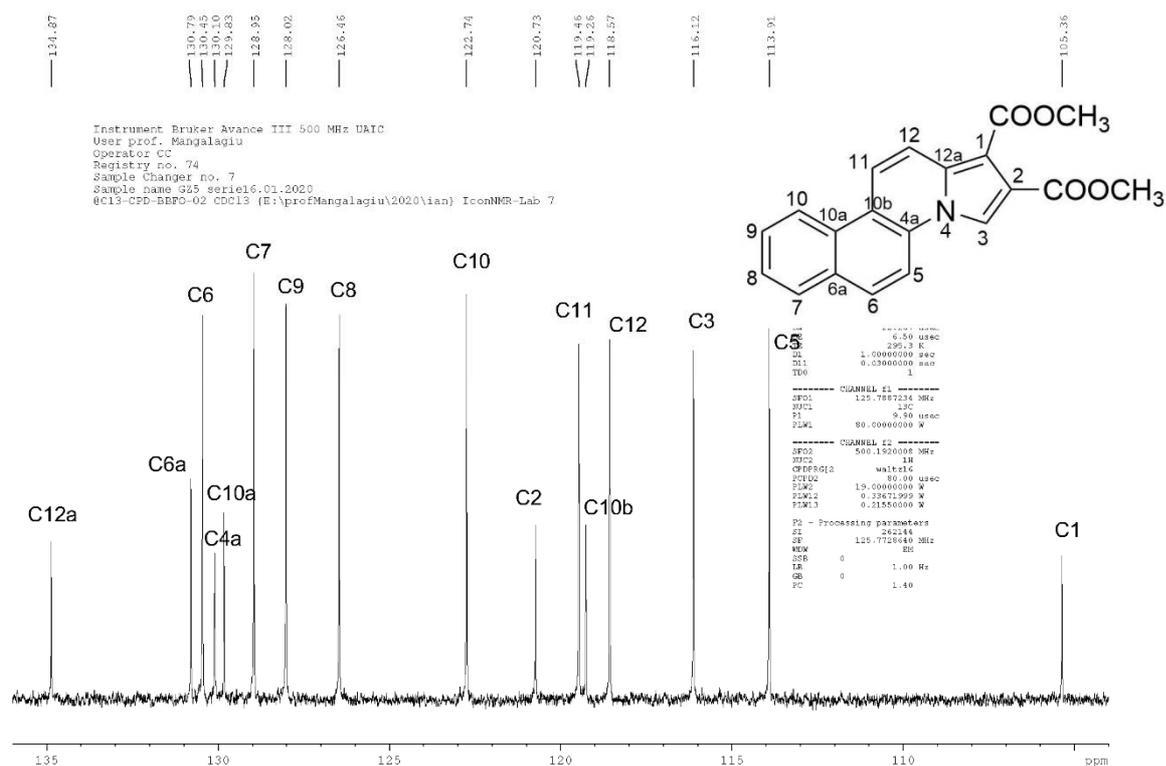
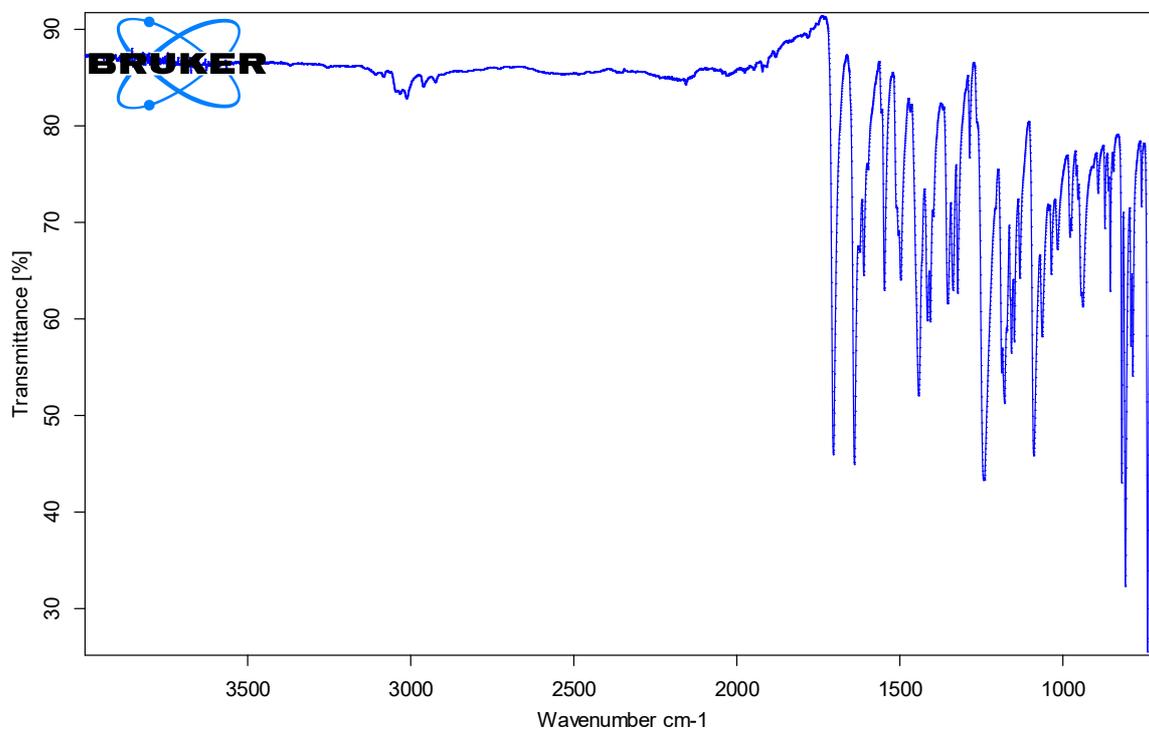


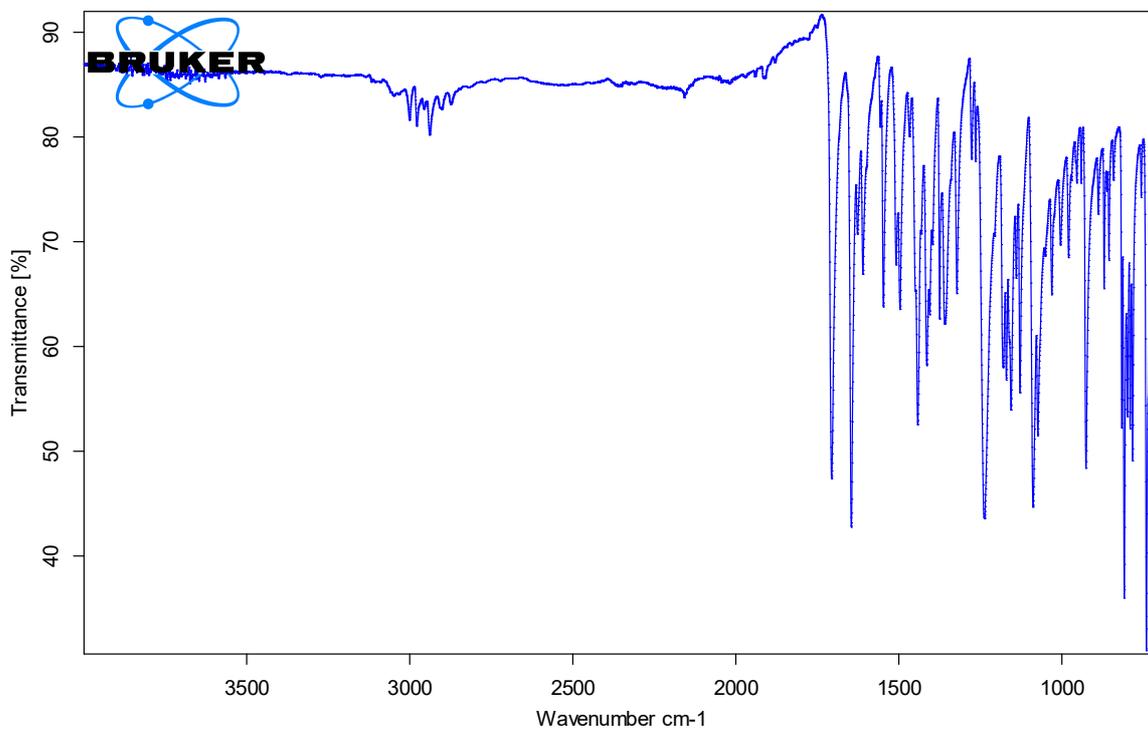
Figure S7c. Detail in the aromatic area of the  $^{13}\text{C}$  NMR spectrum of the compound 8c.

## 2. IR spectra of the obtained compounds.



C:\OPUS_7.0.129\WORK\2021-07-14\2021-07-14-5A.4	Sample description	Instrument type and / or accessory	14/07/2021
---	--------------------	------------------------------------	------------

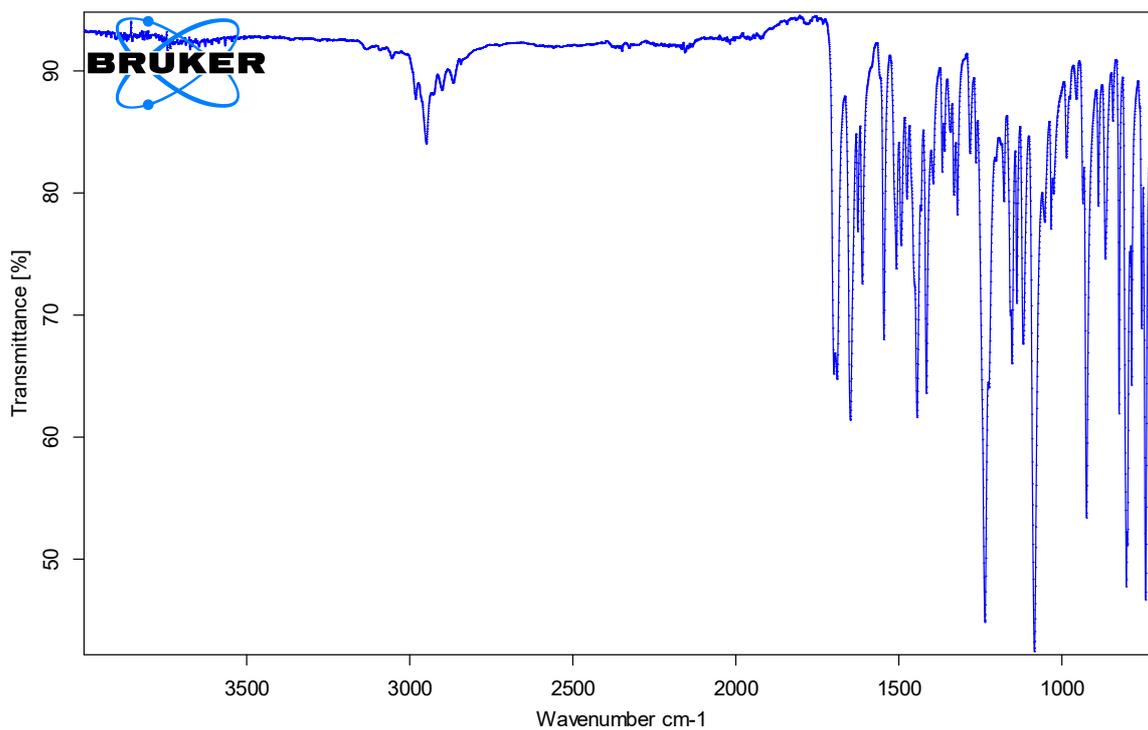
Figure S8. IR spectrum of the compound 5a.



C:\OPUS_7.0.129\WORK\2021-07-14\2021-07-14-5B.0	Sample description	Instrument type and / or accessory	14/07/2021
---	--------------------	------------------------------------	------------

Page 1/1

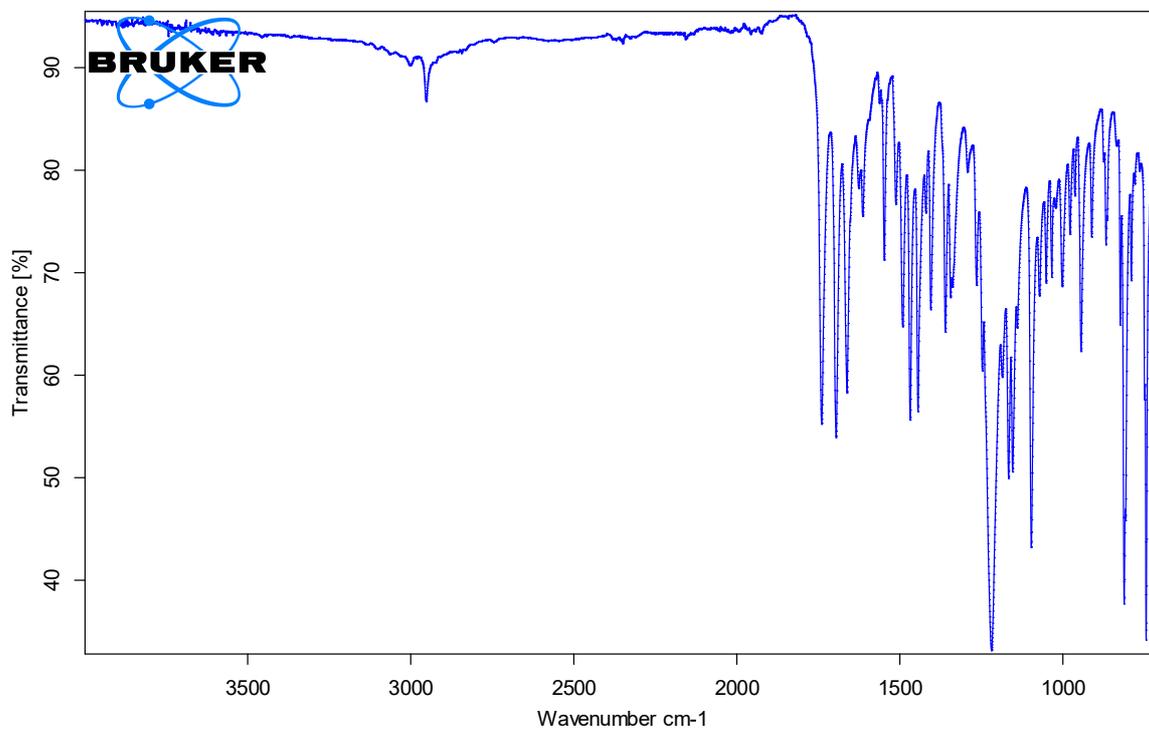
Figure S9. IR spectrum of the compound 5b.



C:\OPUS_7.0.129\WORK\2021-07-14\2021-07-14-5C.0	Sample description	Instrument type and / or accessory	14/07/2021
---	--------------------	------------------------------------	------------

Page 1/1

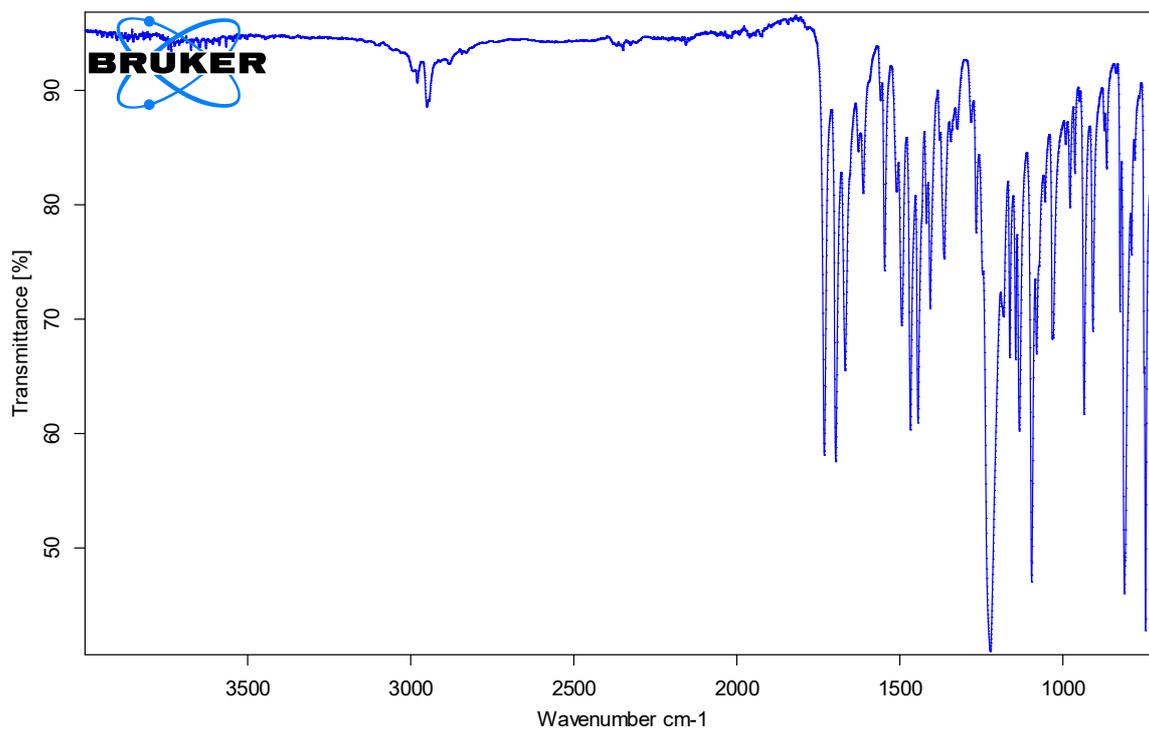
Figure S10. IR spectrum of the compound 5c.



C:\OPUS_7.0.129\WORK\2021-07-14\2021-07-14-7A.0	Sample description	Instrument type and / or accessory	14/07/2021
---	--------------------	------------------------------------	------------

Page 1/1

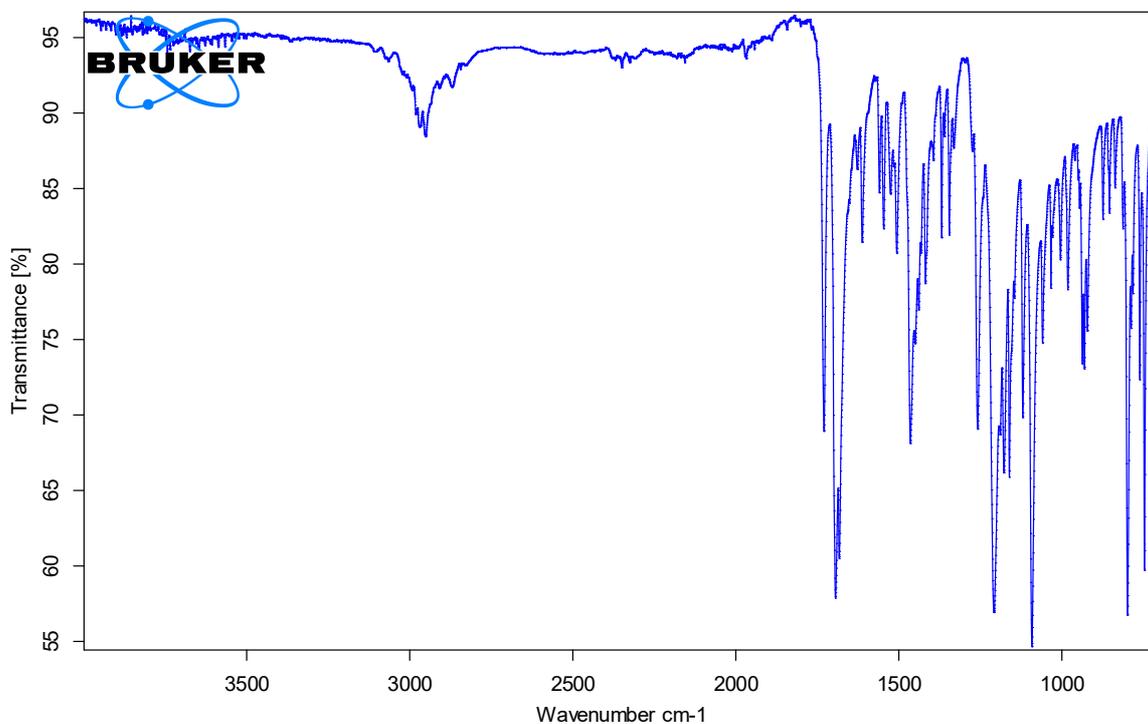
Figure S11. IR spectrum of the compound 7a.



C:\OPUS_7.0.129\WORK\2021-07-14\2021-07-14-7B.0	Sample description	Instrument type and / or accessory	14/07/2021
---	--------------------	------------------------------------	------------

Page 1/1

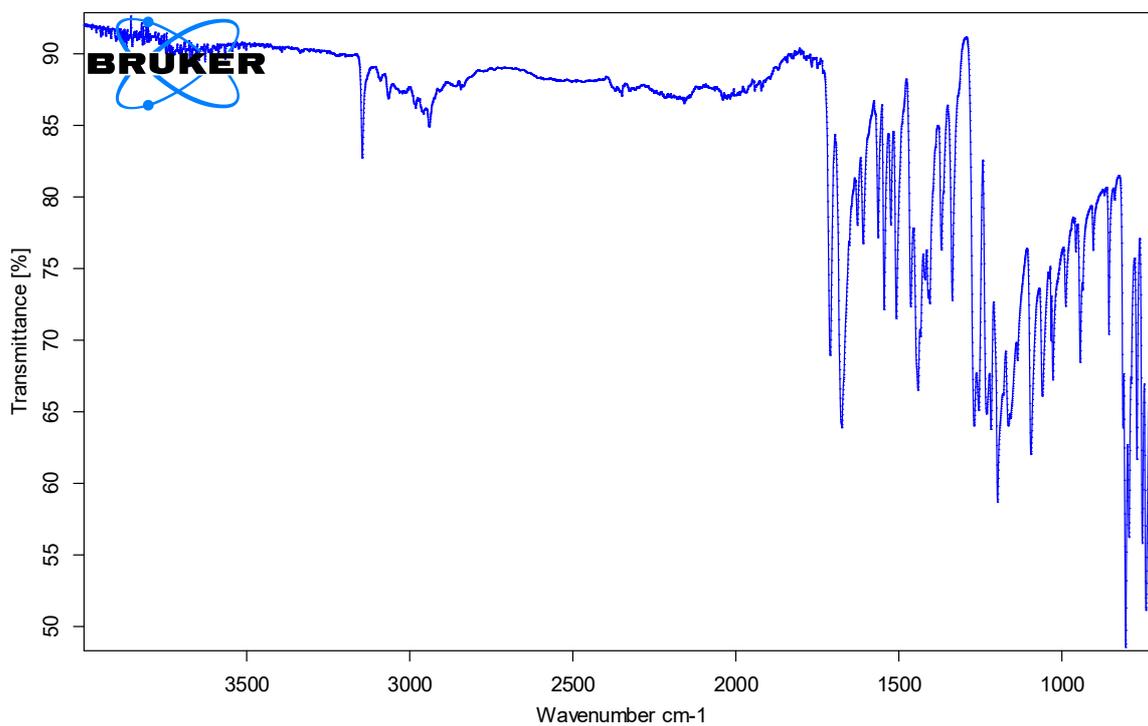
Figure S12. IR spectrum of the compound 7b.



C:\OPUS_7.0.129\WORK\2021-07-14\2021-07-14-7C.1	Sample description	Instrument type and / or accessory	14/07/2021
---	--------------------	------------------------------------	------------

Page 1/1

Figure S13. IR spectrum of the compound 7c.



C:\OPUS_7.0.129\WORK\2021-07-14\2021-07-14-8C.1	Sample description	Instrument type and / or accessory	14/07/2021
---	--------------------	------------------------------------	------------

Page 1/1

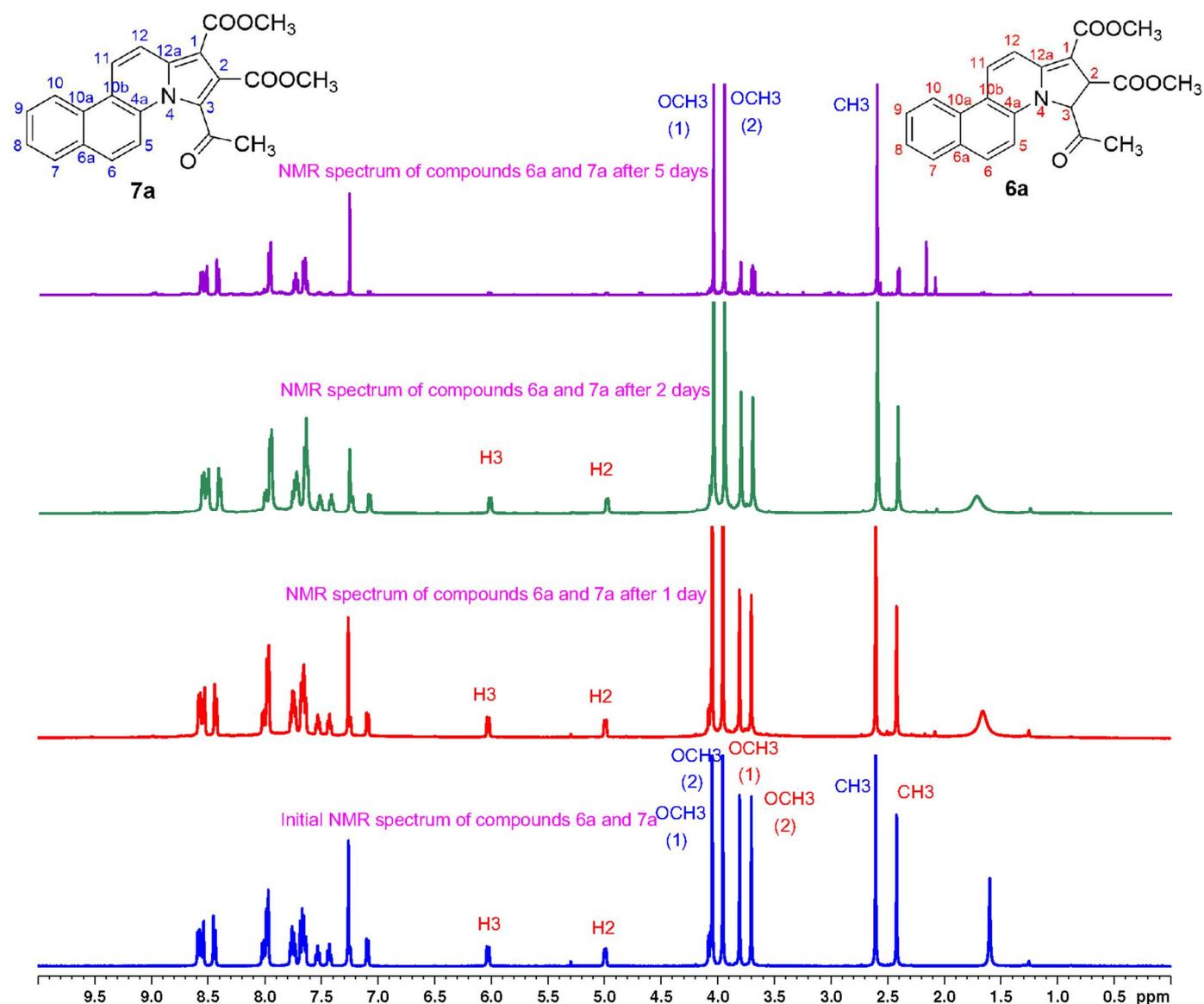
Figure S14. IR spectrum of the compound 8c.

### 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

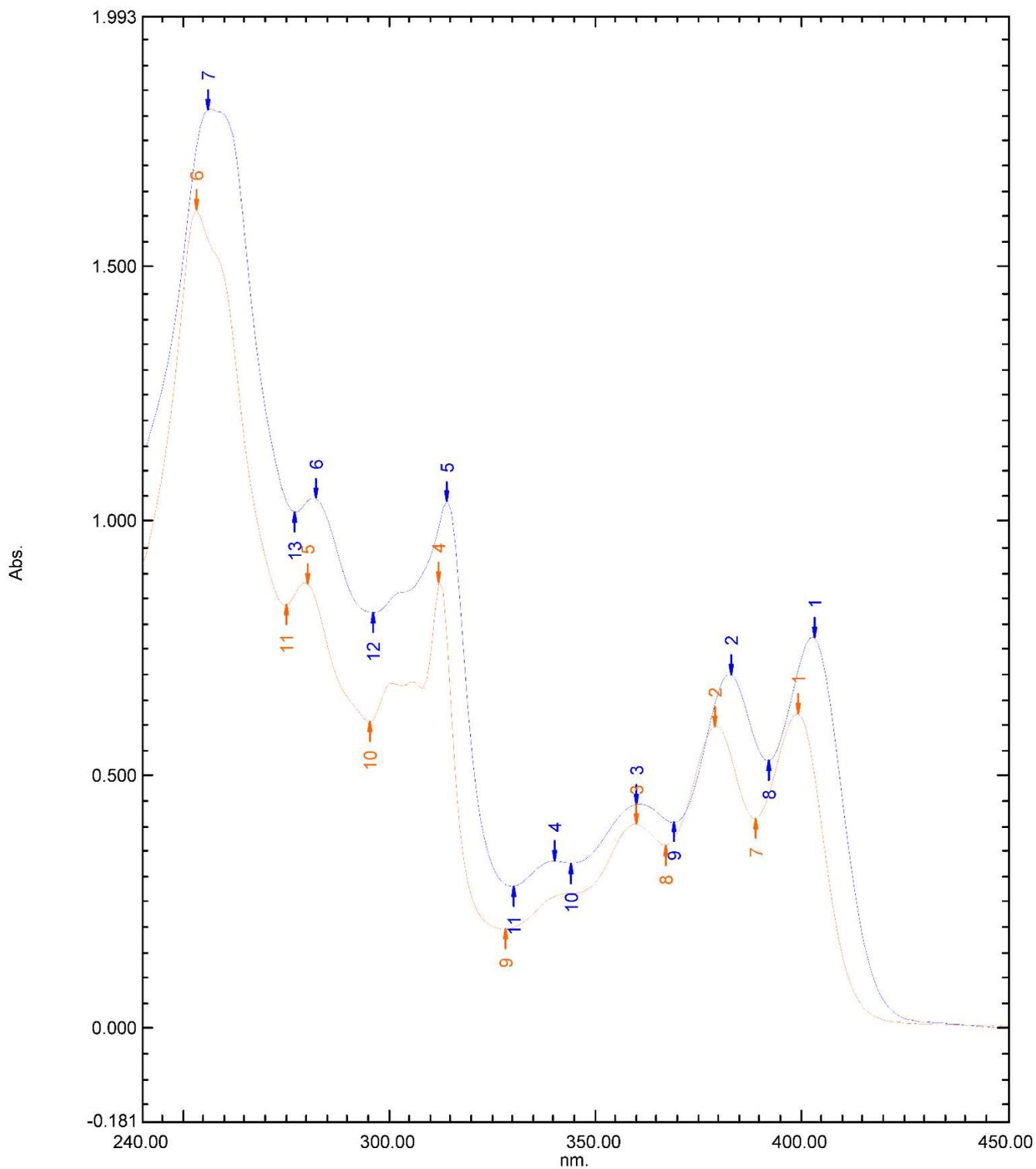


Figure S16. Overlaid UV-Vis spectra of the compound 5a in trichloromethane and cyclohexane.

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

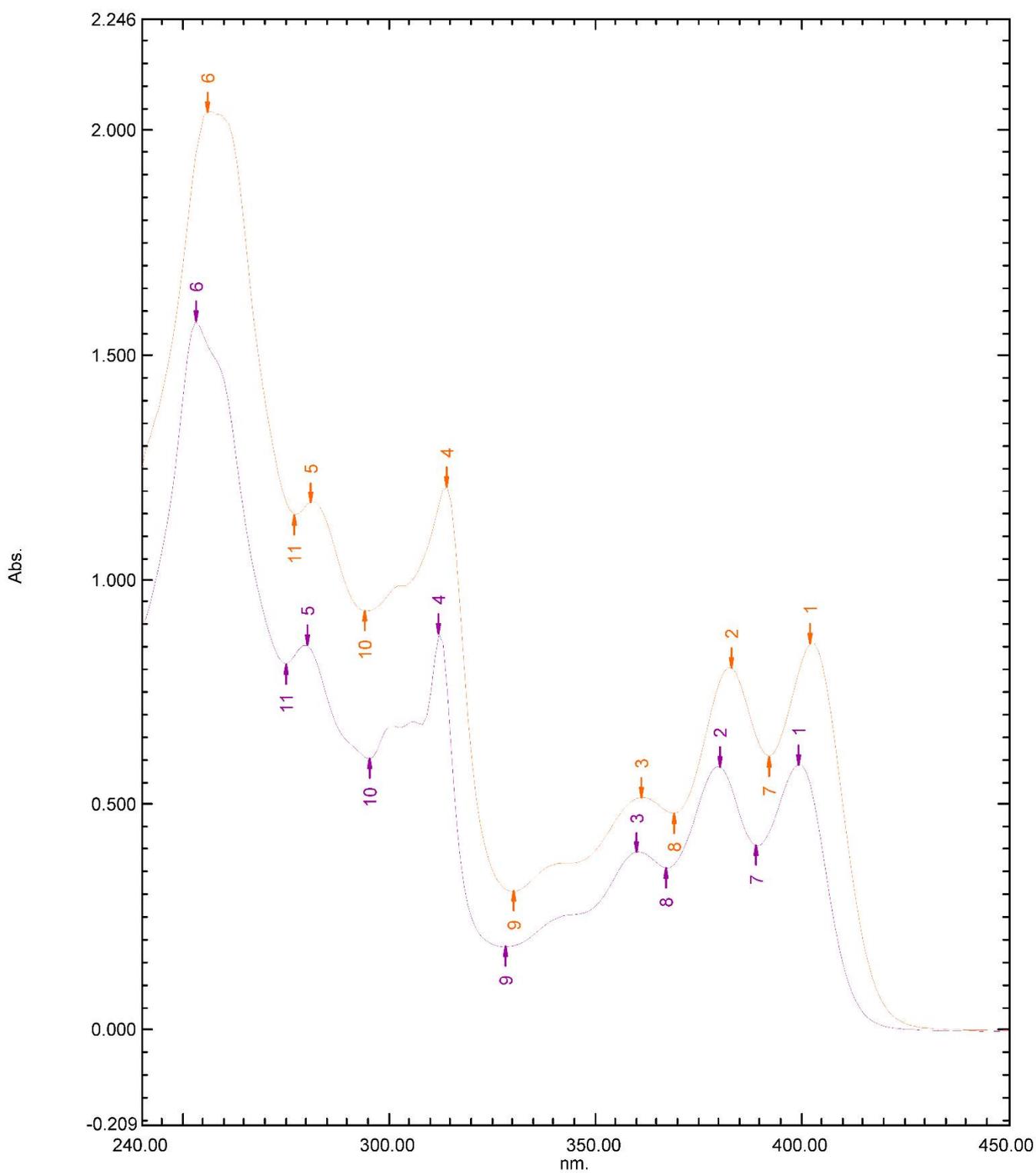


Figure S17. Overlaid UV-Vis spectra of the compound **5b** in trichloromethane and cyclohexane.

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

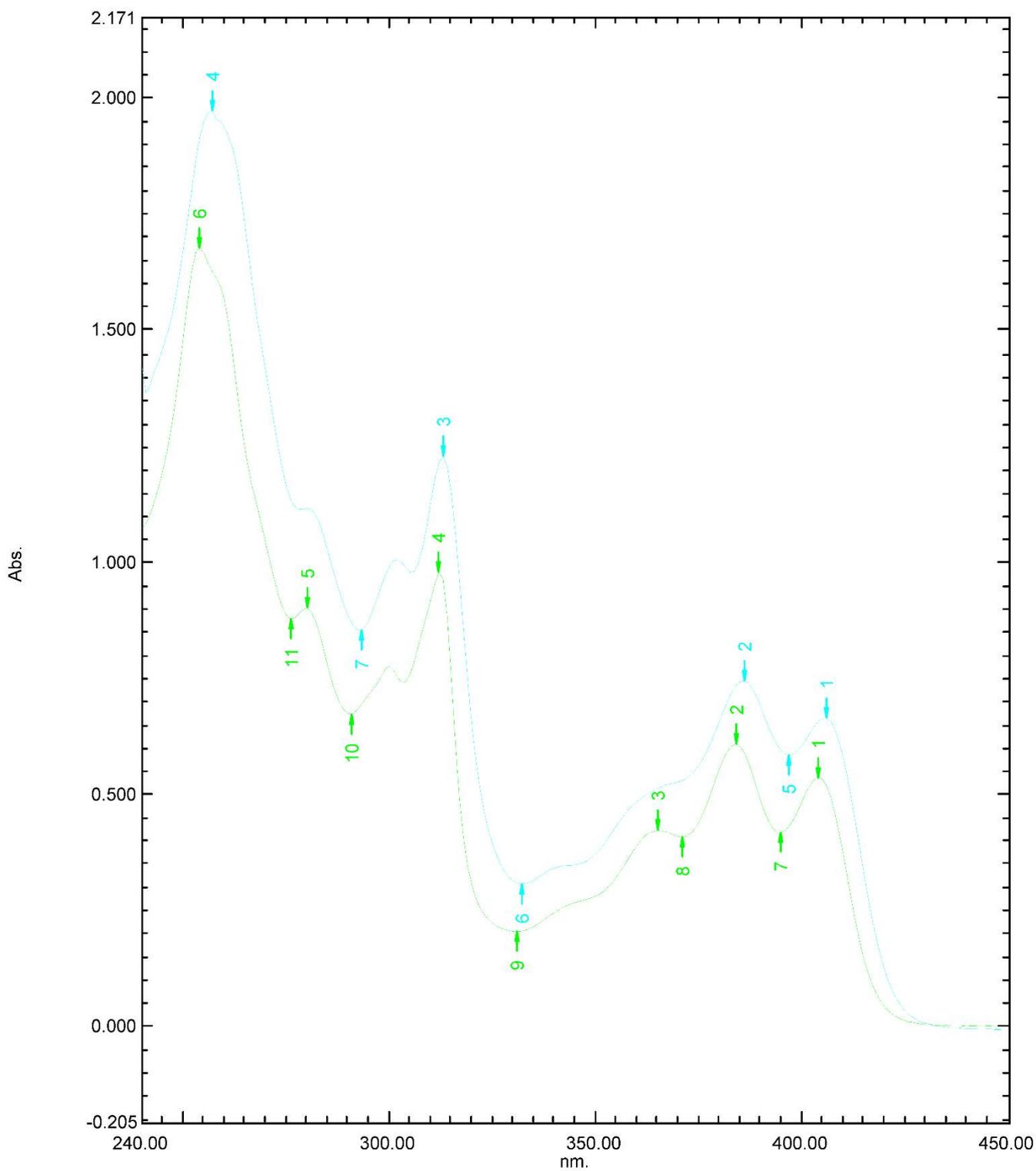


Figure S18. Overlaid UV-Vis spectra of the compound 5c in trichloromethane and cyclohexane.

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

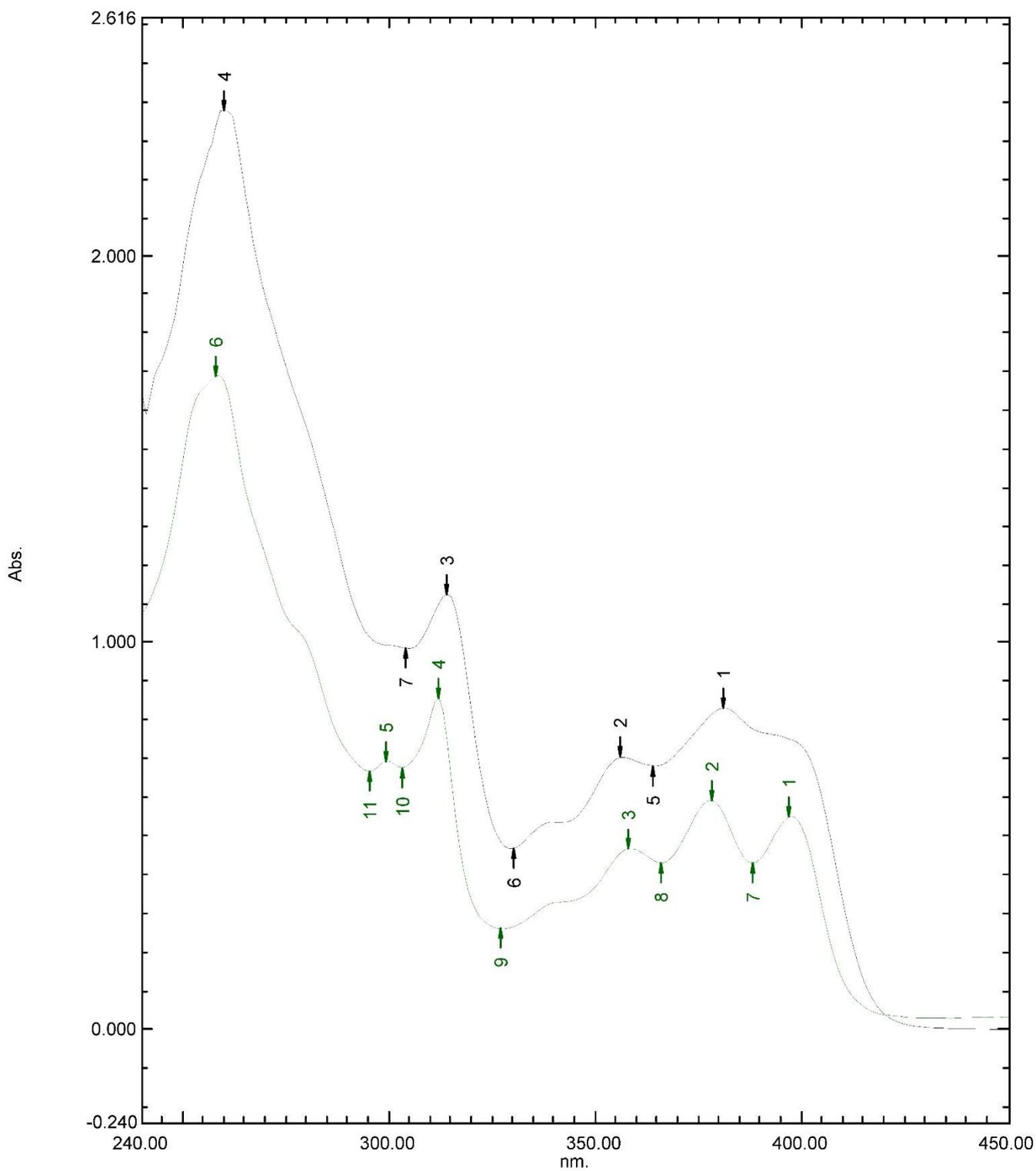


Figure S19. Overlaid UV-Vis spectra of the compound 7a in trichloromethane and cyclohexane.

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

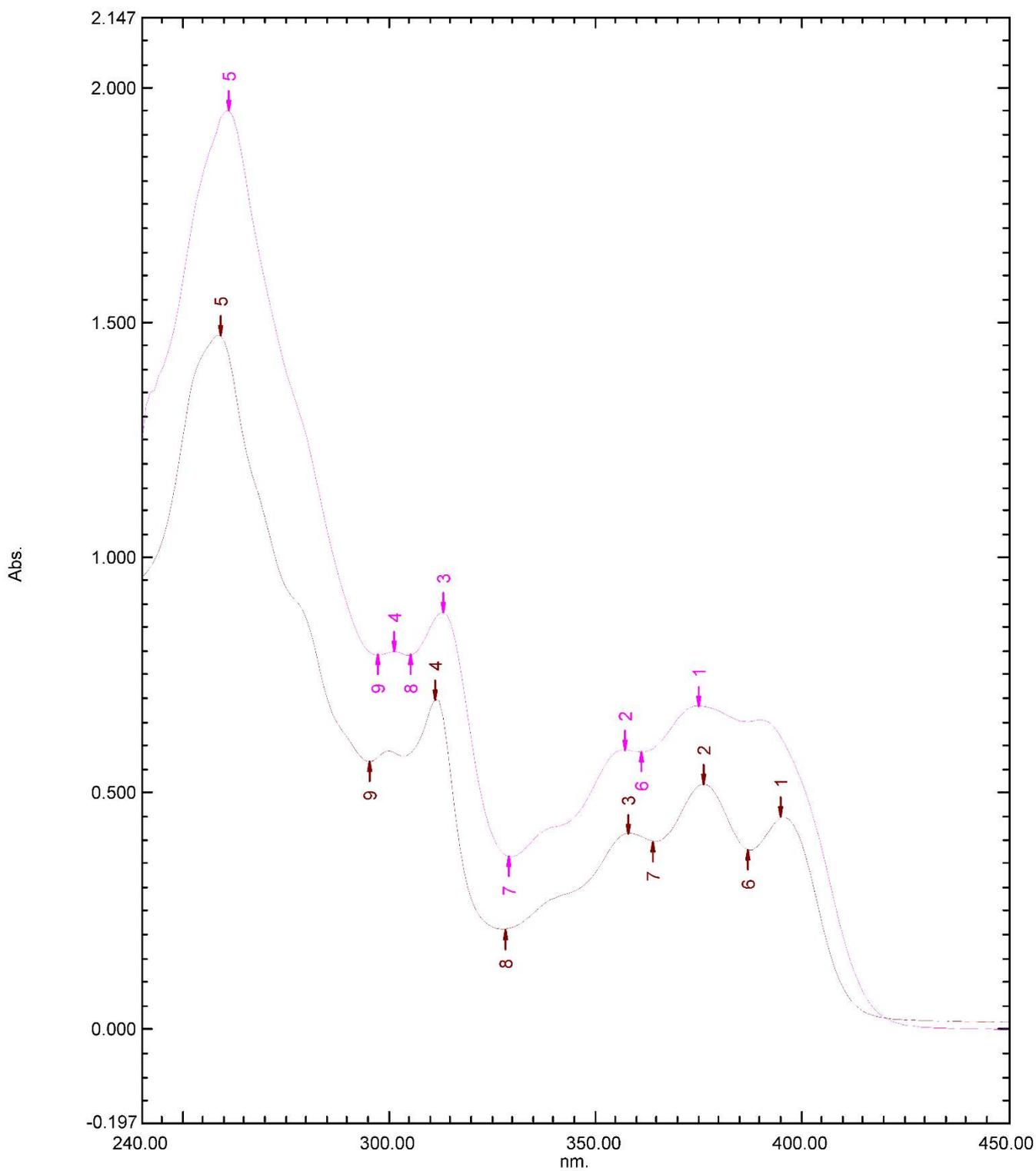


Figure S20. Overlaid UV-Vis spectra of the compound 7b in trichloromethane and cyclohexane.

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

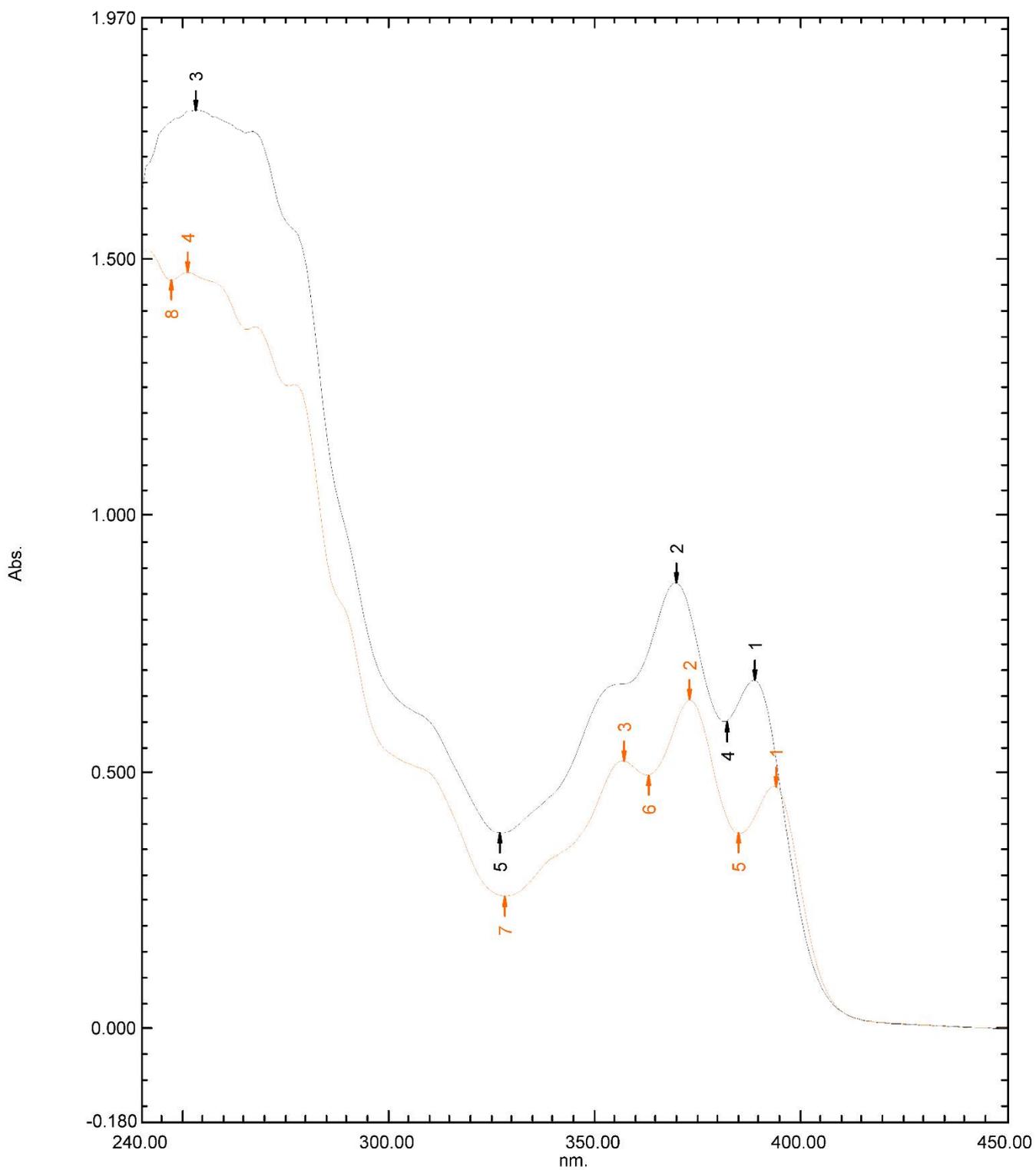


Figure S21. Overlaid UV-Vis spectra of the compound **7c** in trichloromethane and cyclohexane.

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

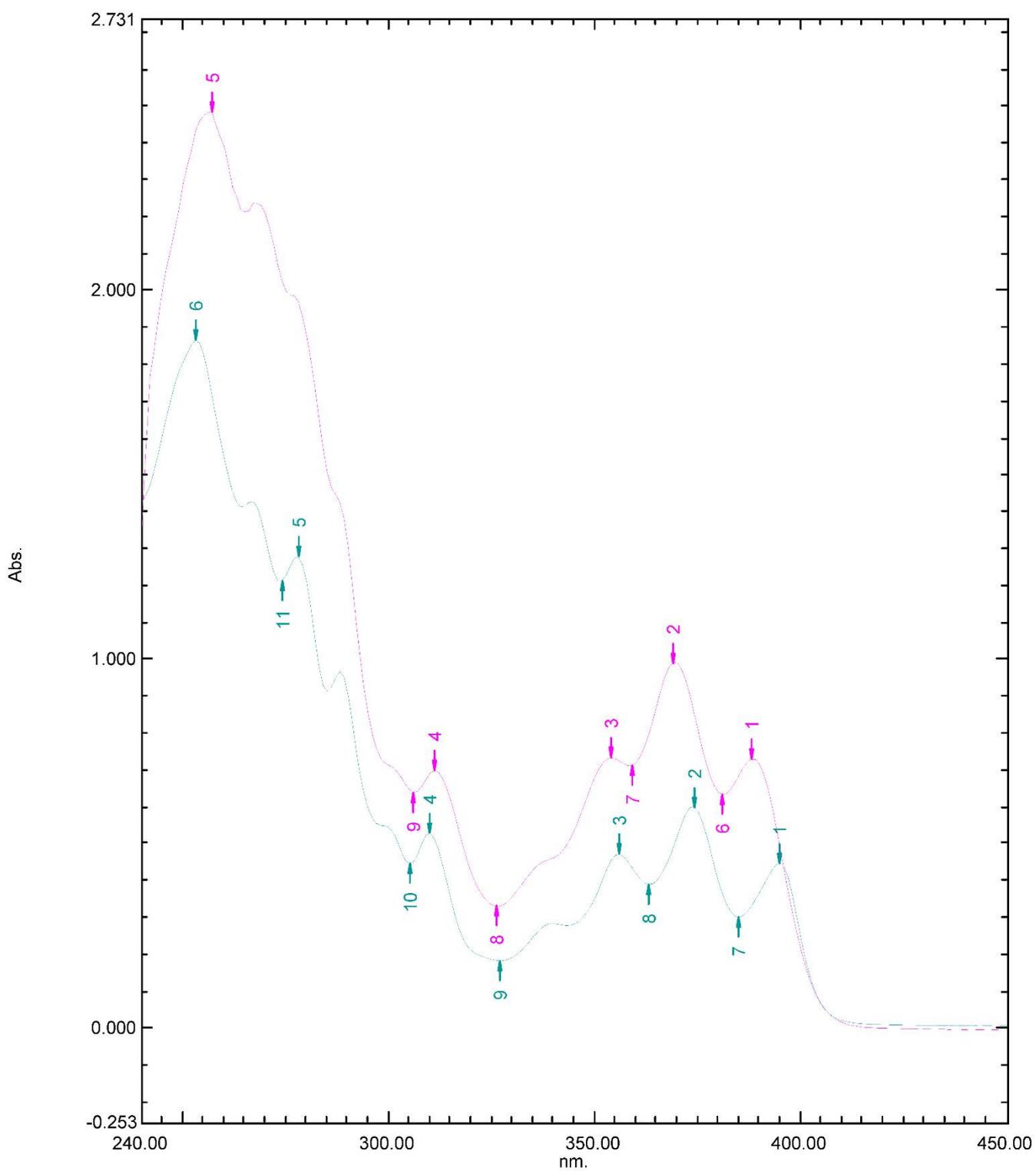


Figure S22. Overlaid UV-Vis spectra of the compound **8c** in trichloromethane and cyclohexane.

## 5. Emission spectra of the obtained compounds

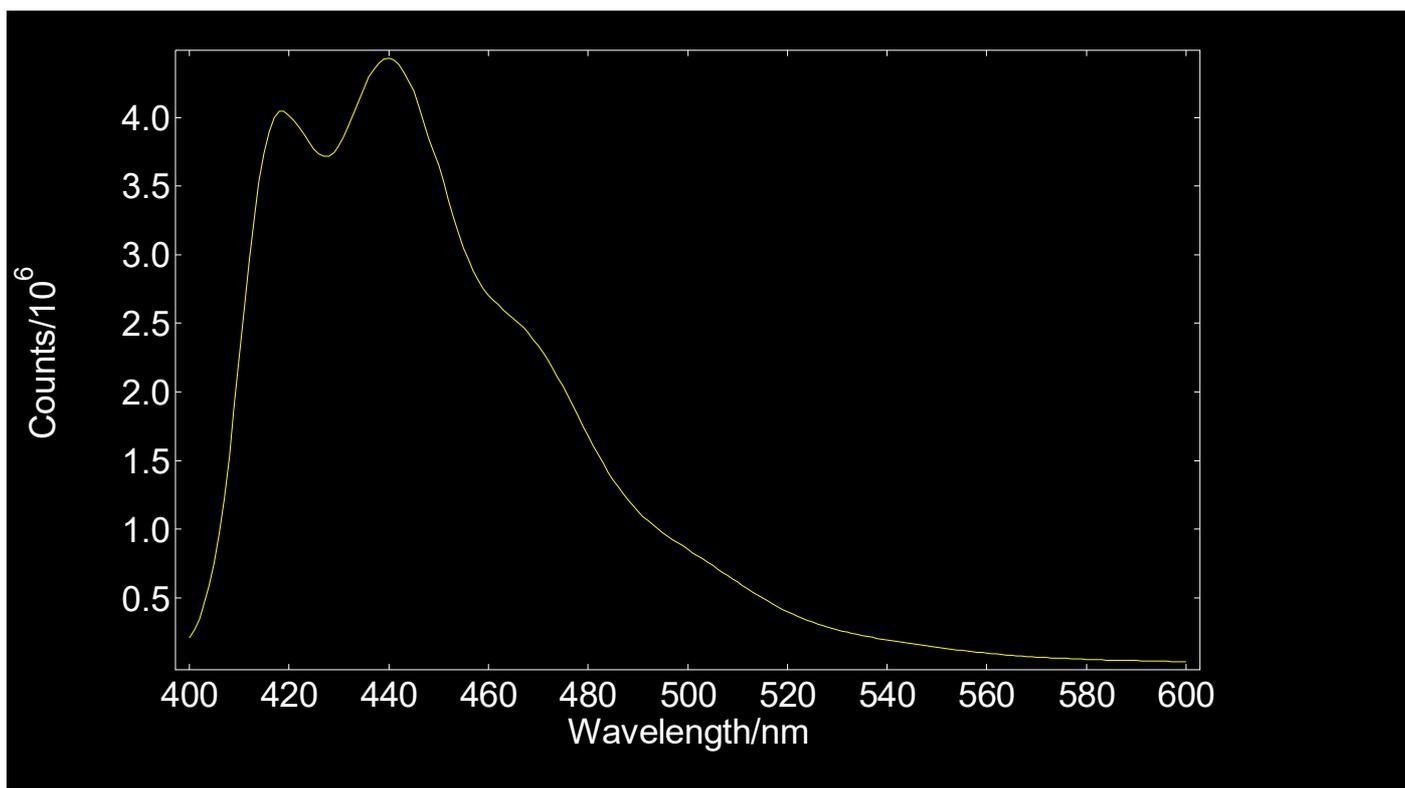


Figure S23. Emission spectrum of the compound 5a in trichloromethane.

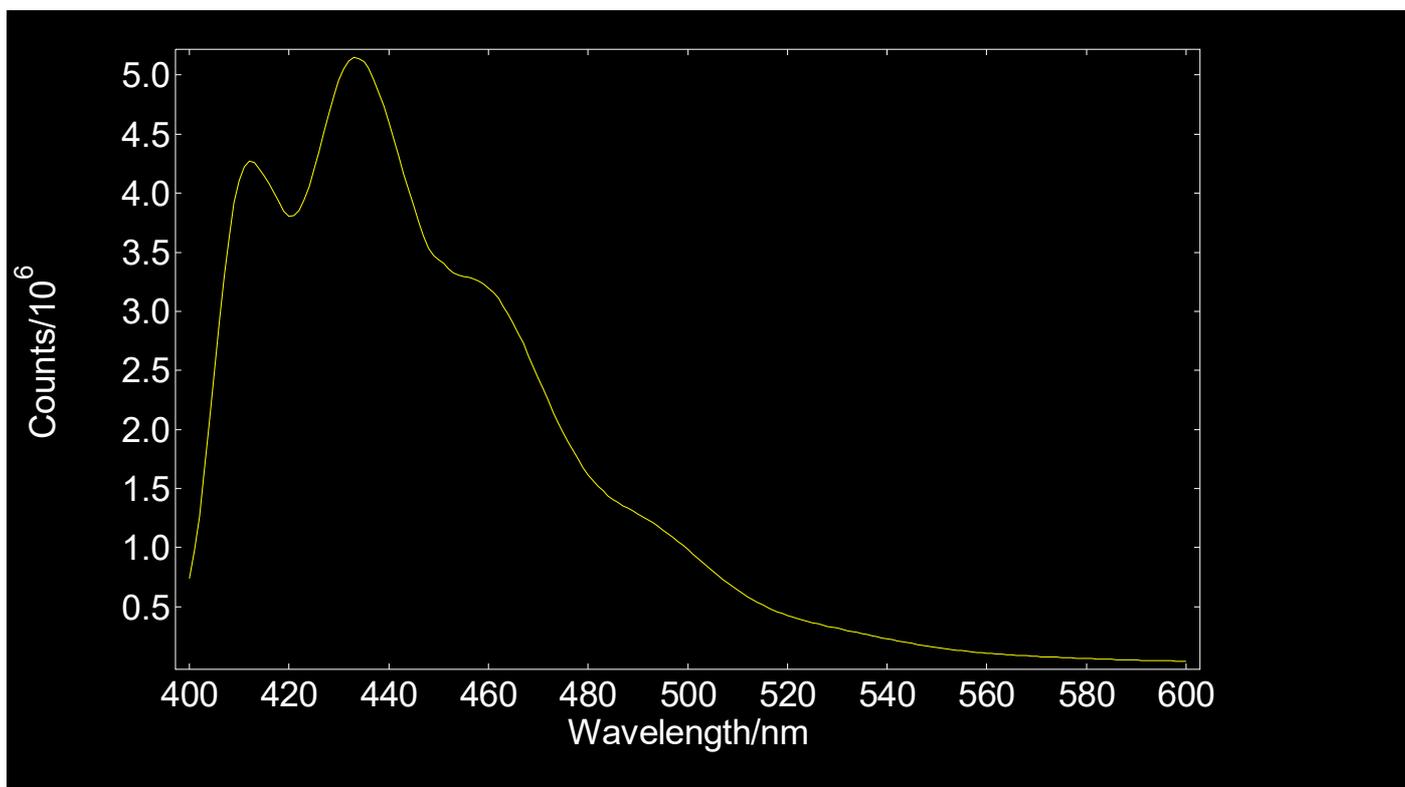


Figure S24. Emission spectrum of the compound 5a in cyclohexane.

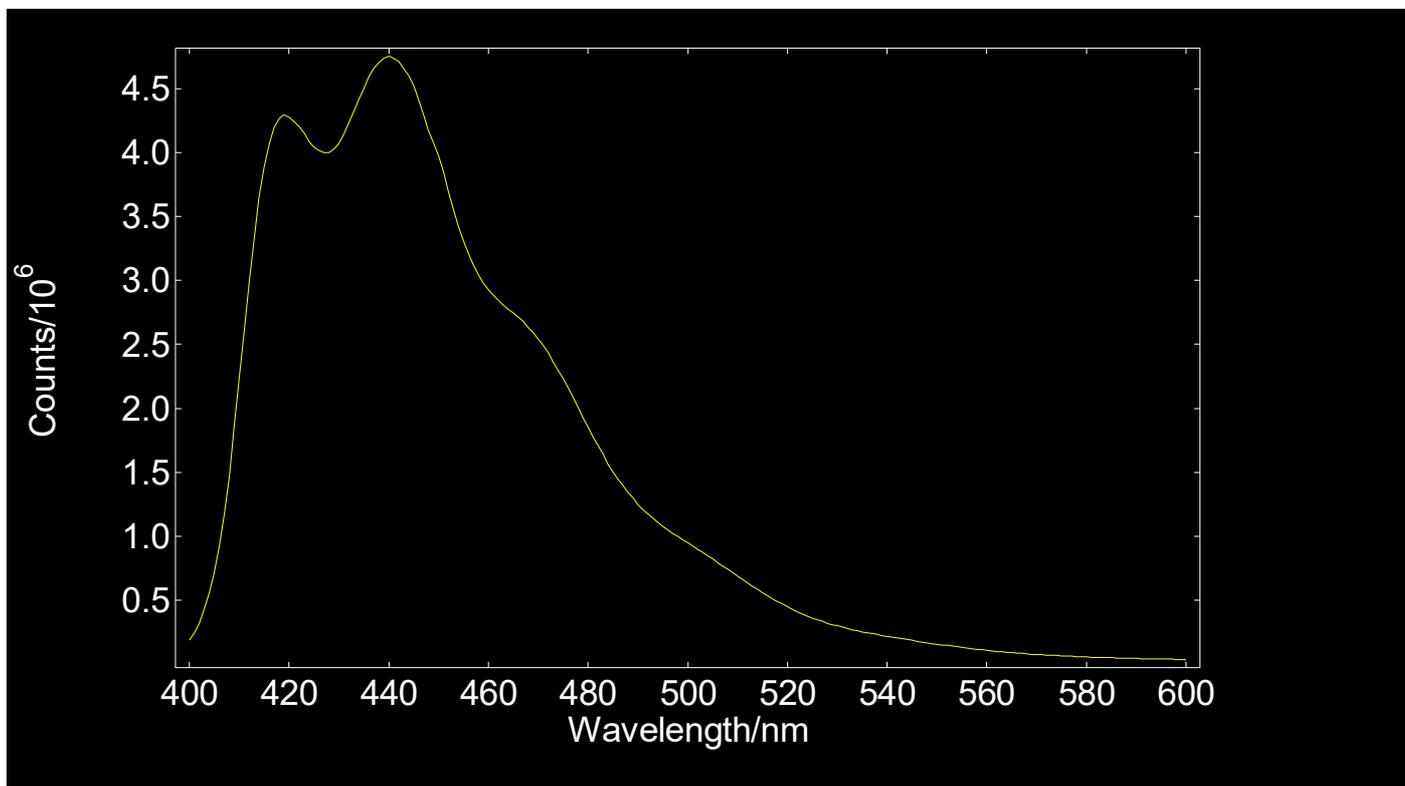


Figure S25. Overlaid UV-Vis spectra of the compound **5b** in trichloromethane and cyclohexane.

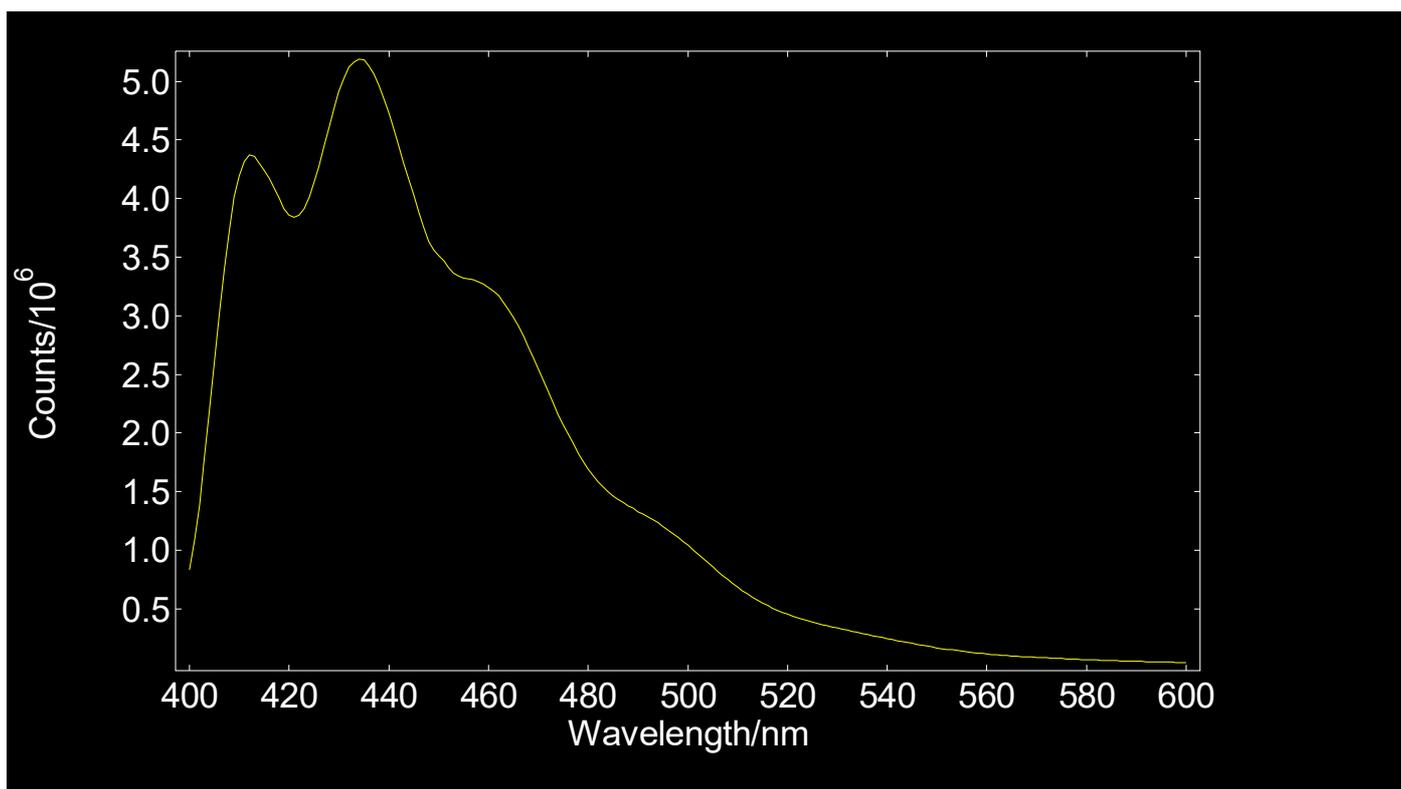


Figure S26. Emission spectrum of the compound **5b** in cyclohexane.

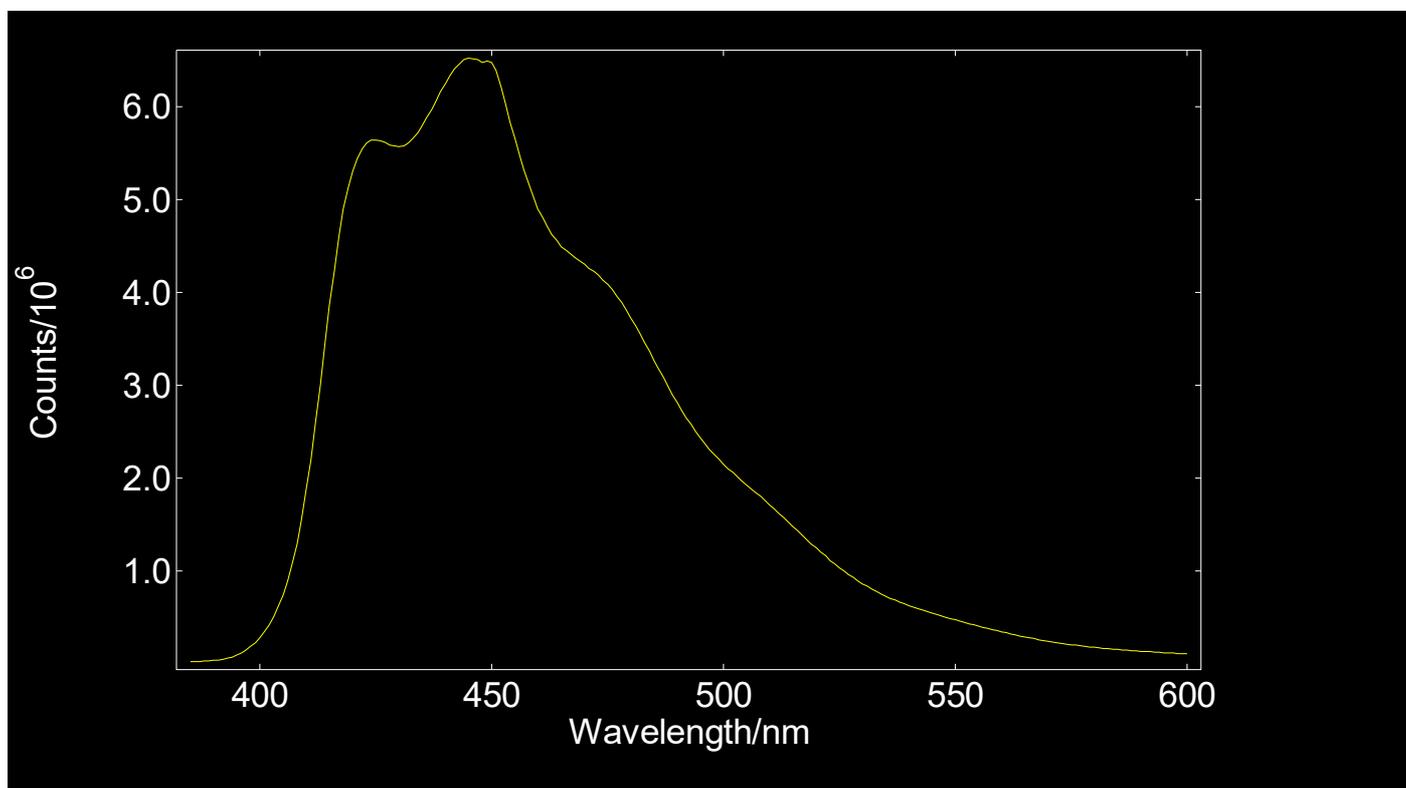


Figure S27. Emission spectrum of the compound **5c** in trichloromethane.

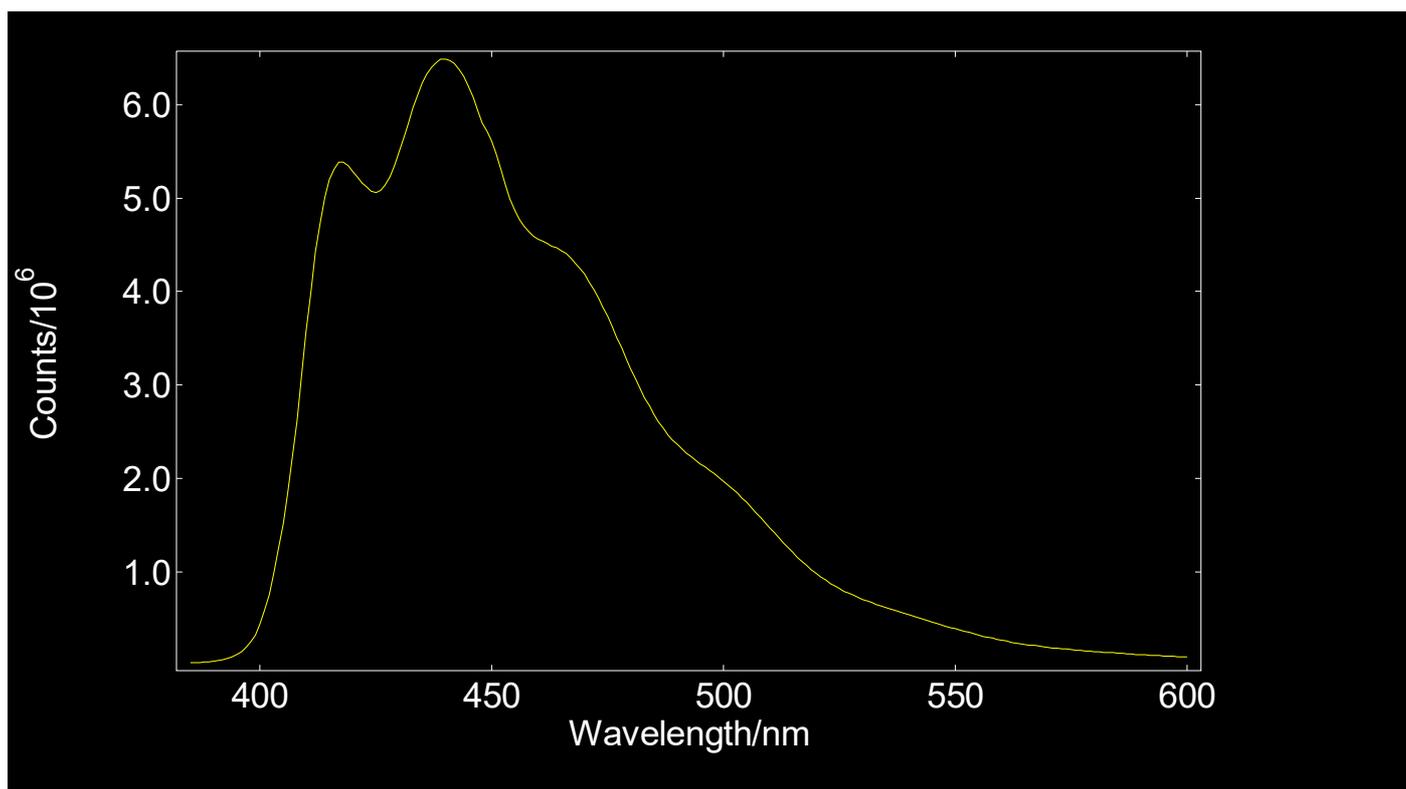


Figure S28. Emission spectrum of the compound **5c** in cyclohexane.

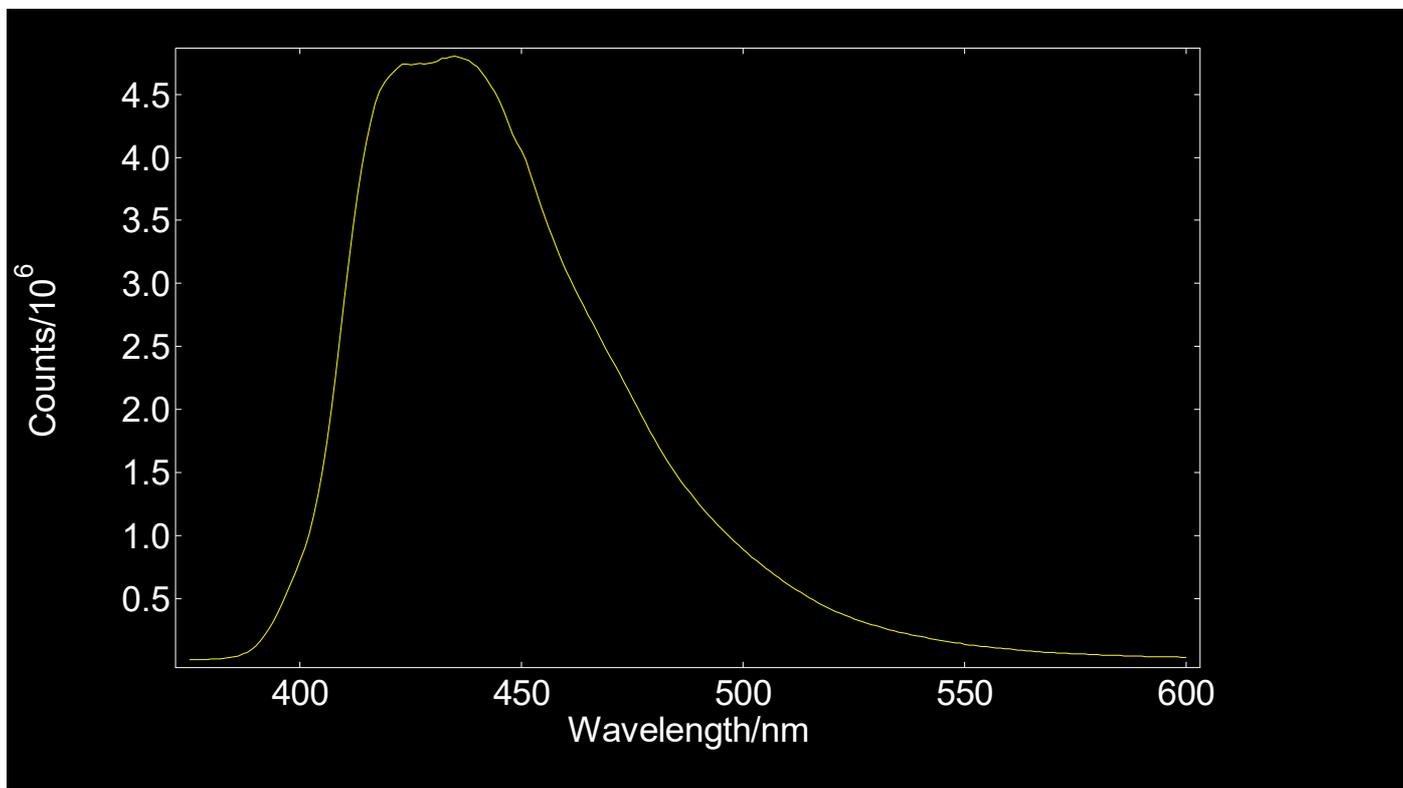


Figure S29. Emission spectrum of the compound 7a in trichloromethane.

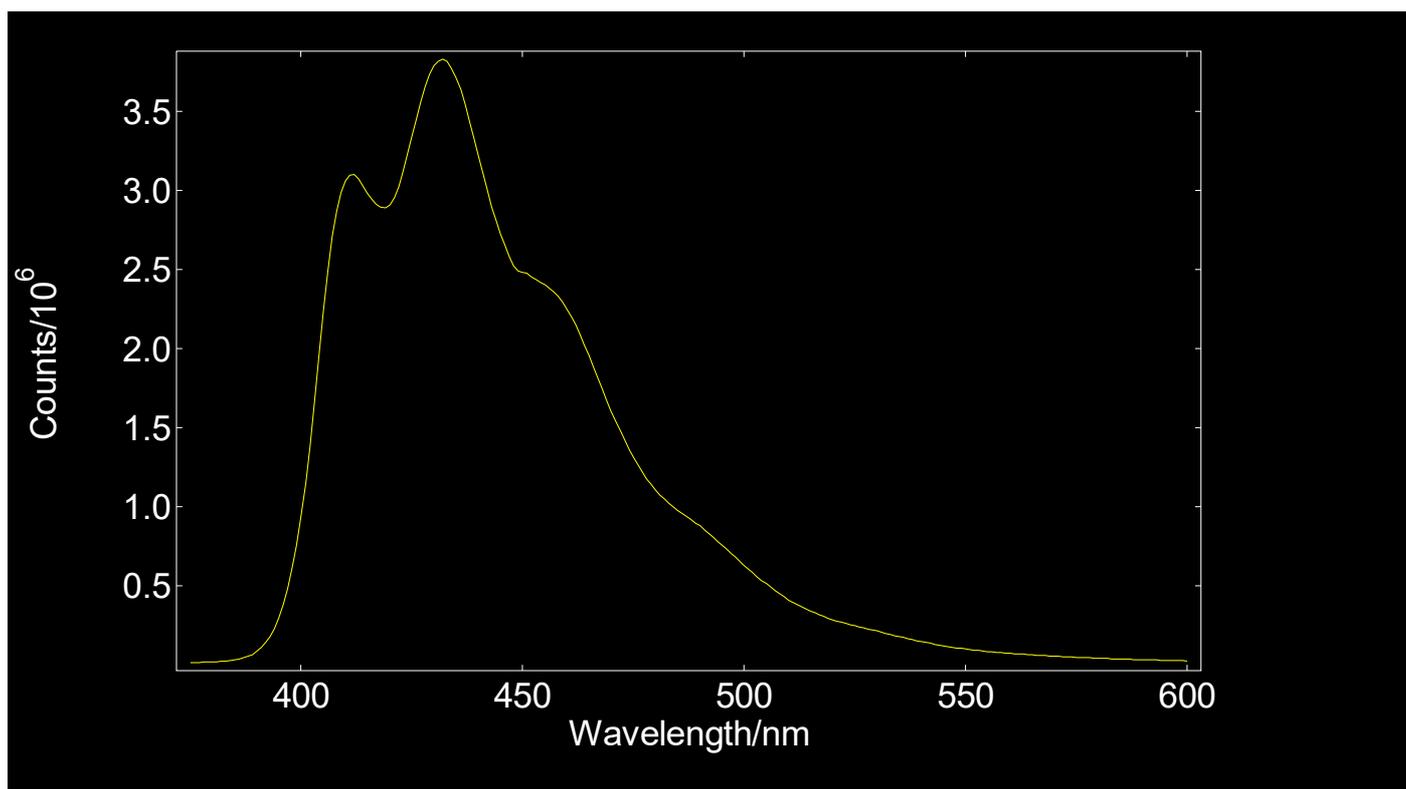


Figure S30. Emission spectrum of the compound 7a in cyclohexane.

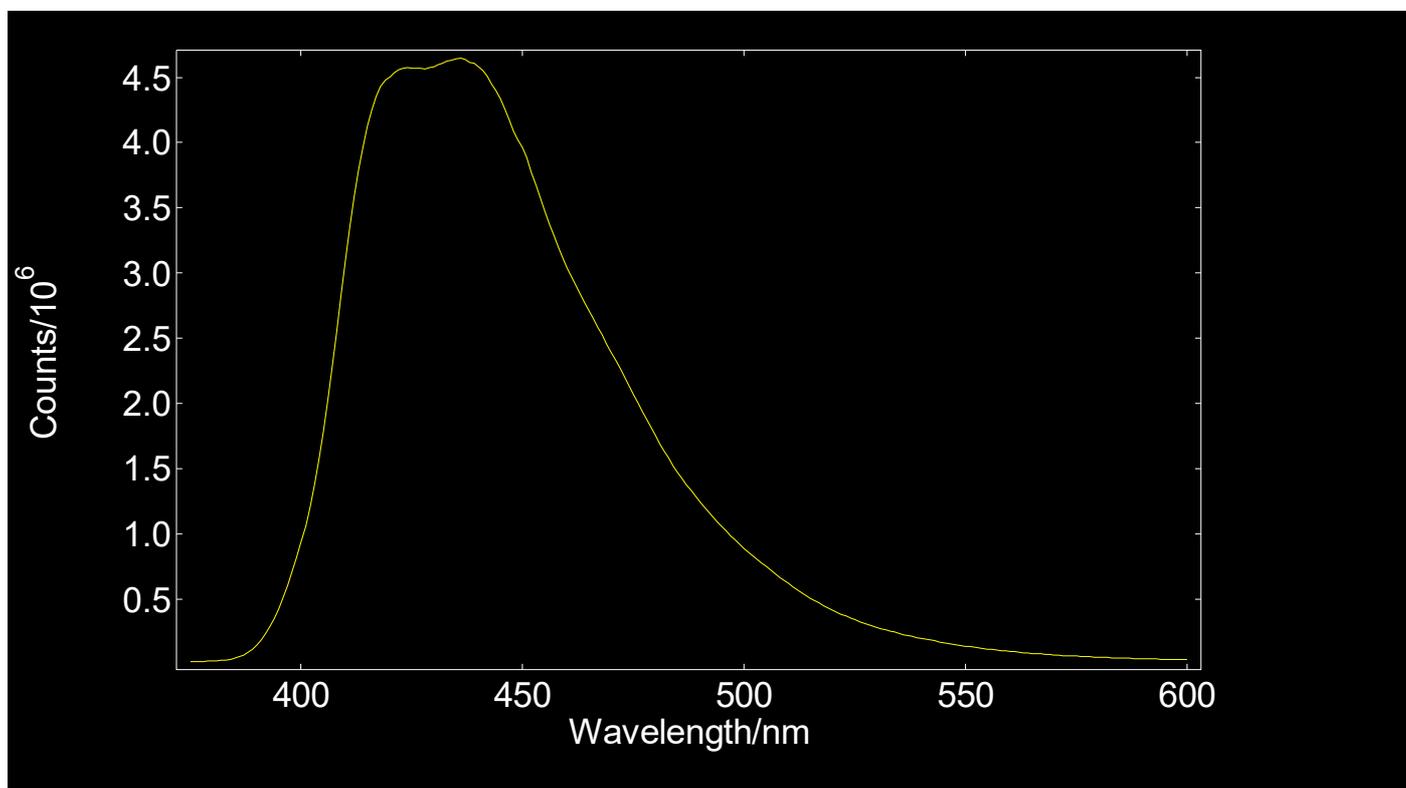


Figure S31. Emission spectrum of the compound **7b** in trichloromethane.

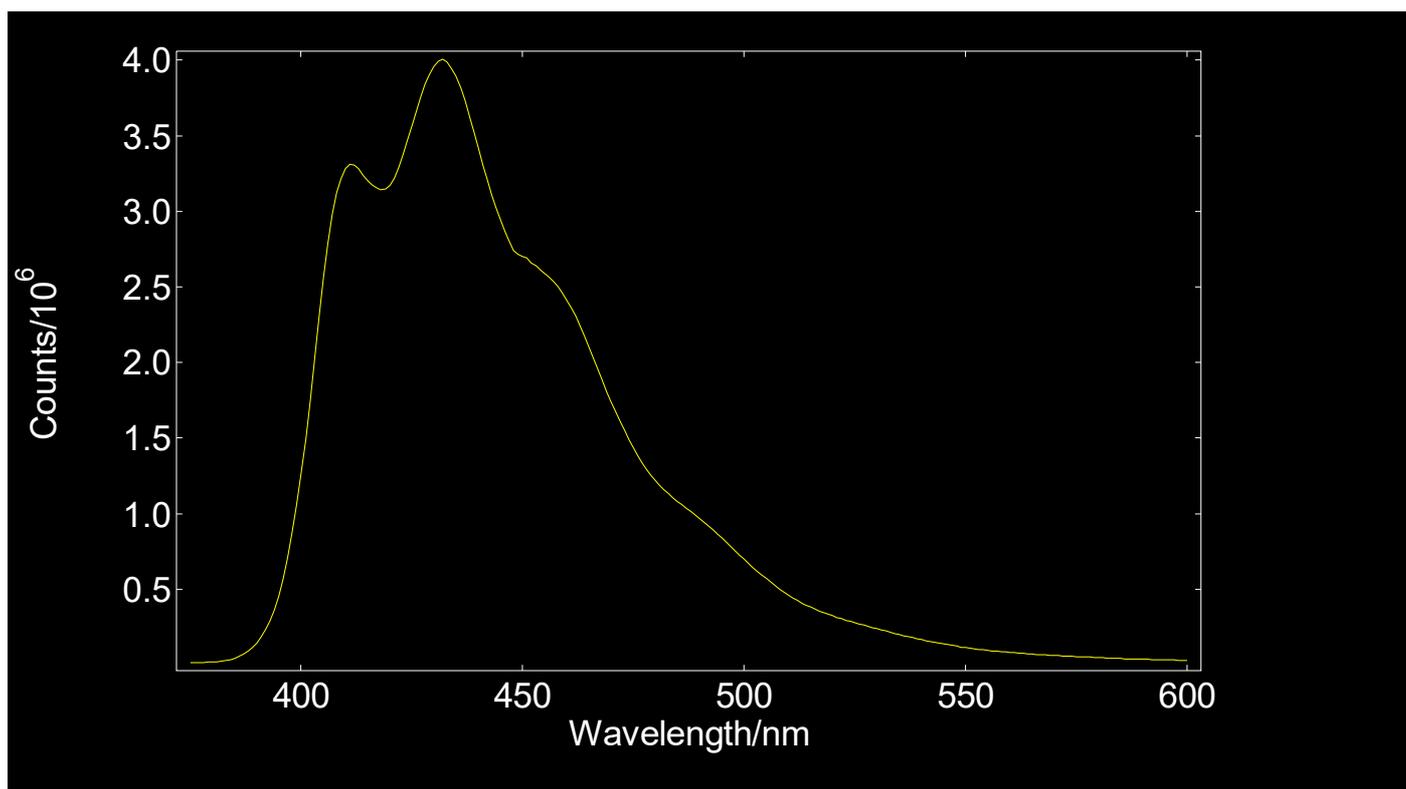


Figure S32. Emission spectrum of the compound **7b** in cyclohexane.

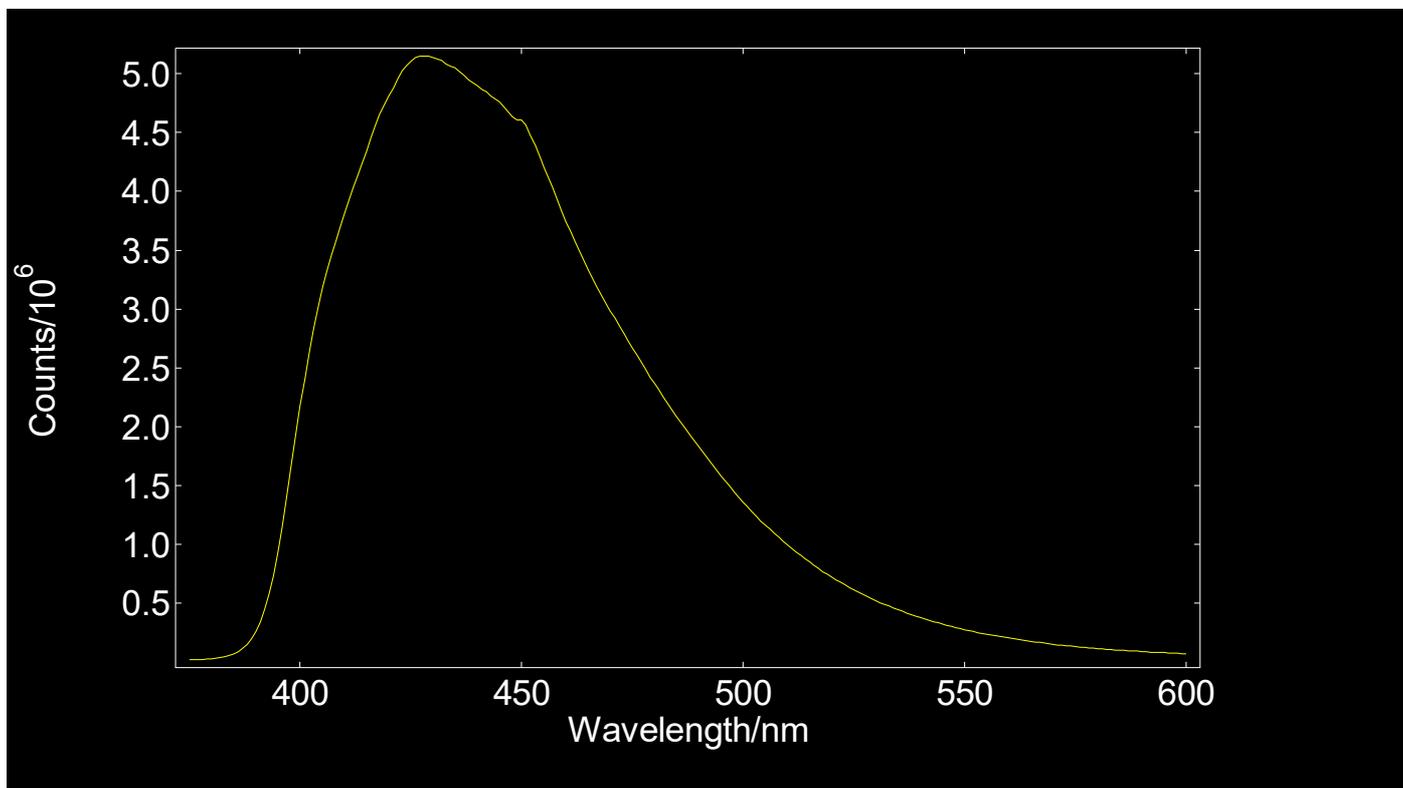


Figure S33. Emission spectrum of the compound 7c in trichloromethane.

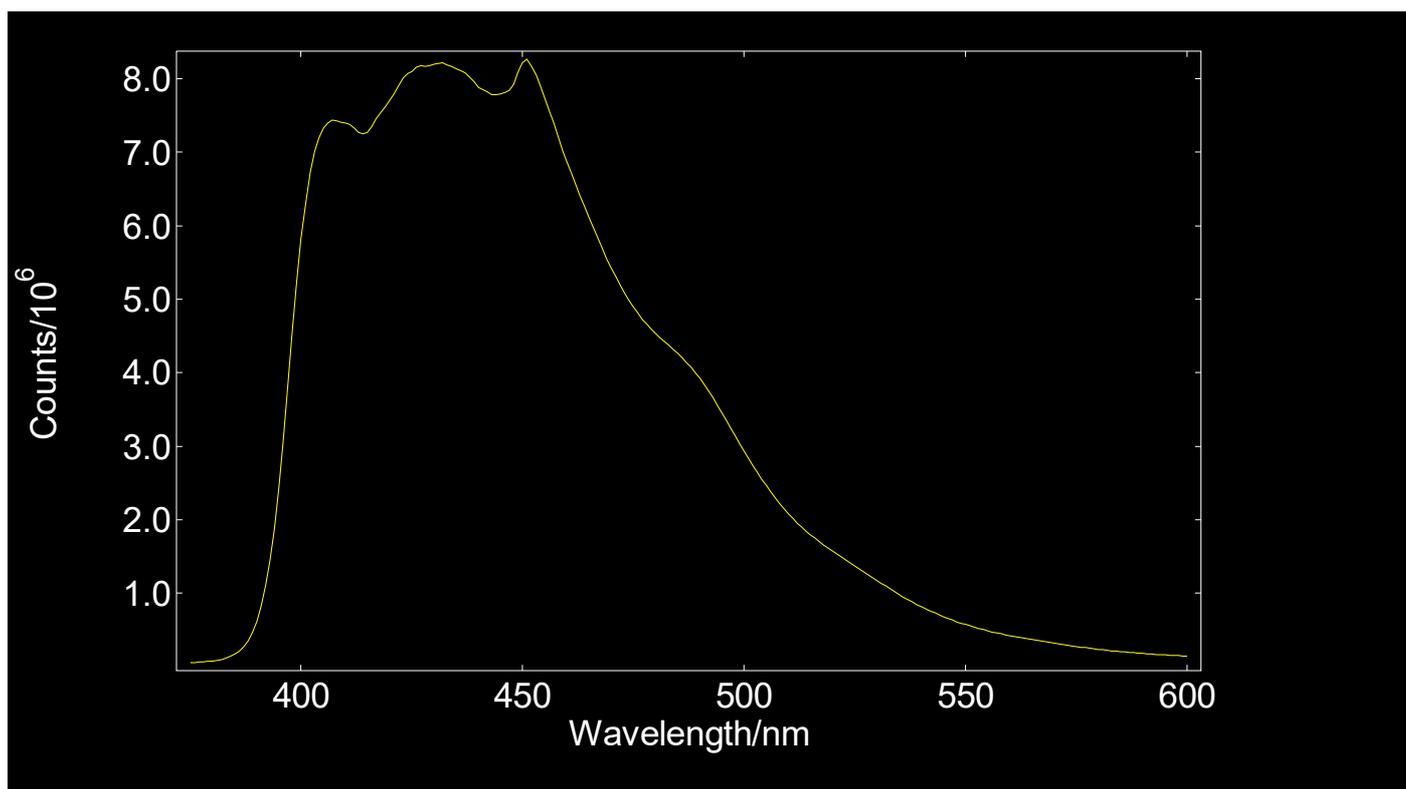


Figure S34. Emission spectrum of the compound 7c in cyclohexane.

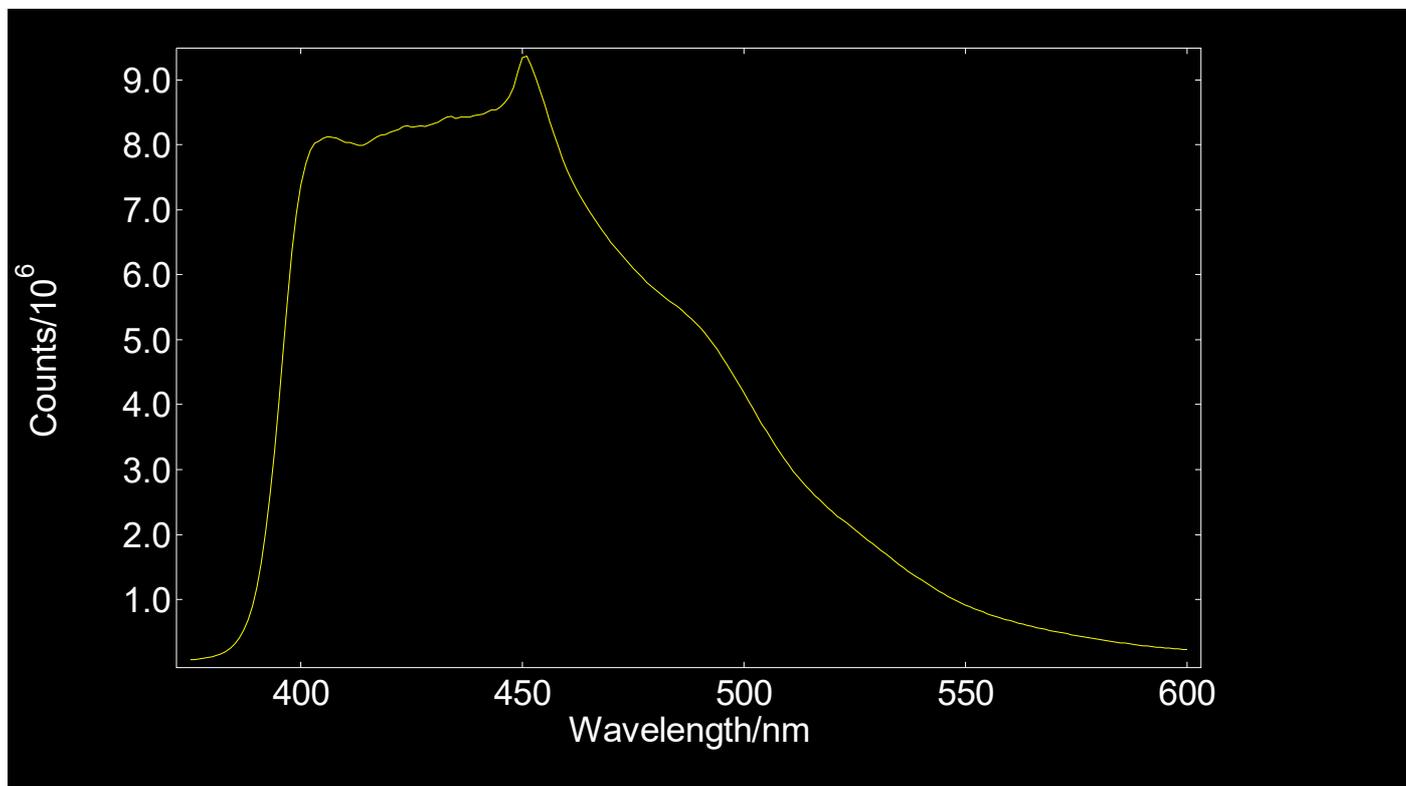


Figure S35. Emission spectrum of the compound **8c** in trichloromethane.

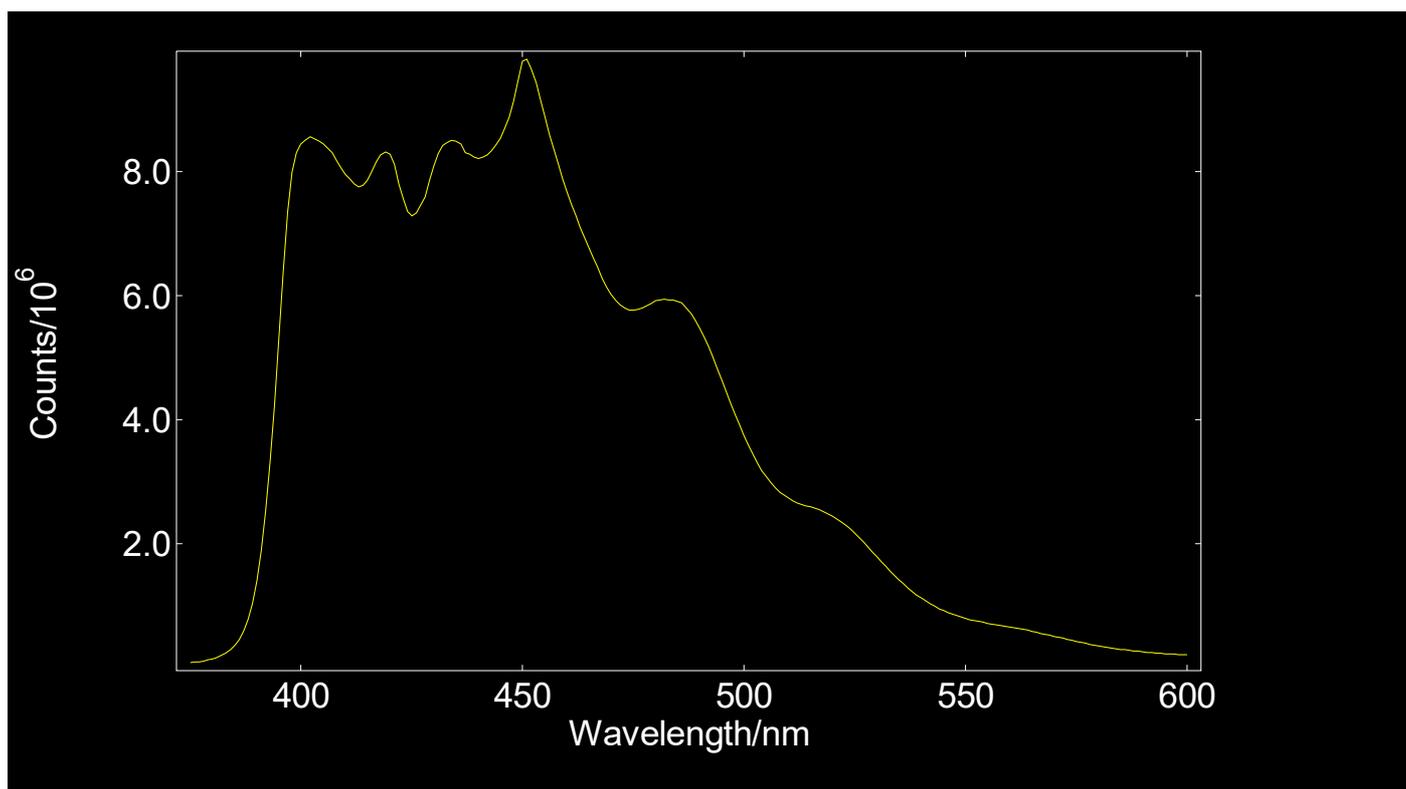
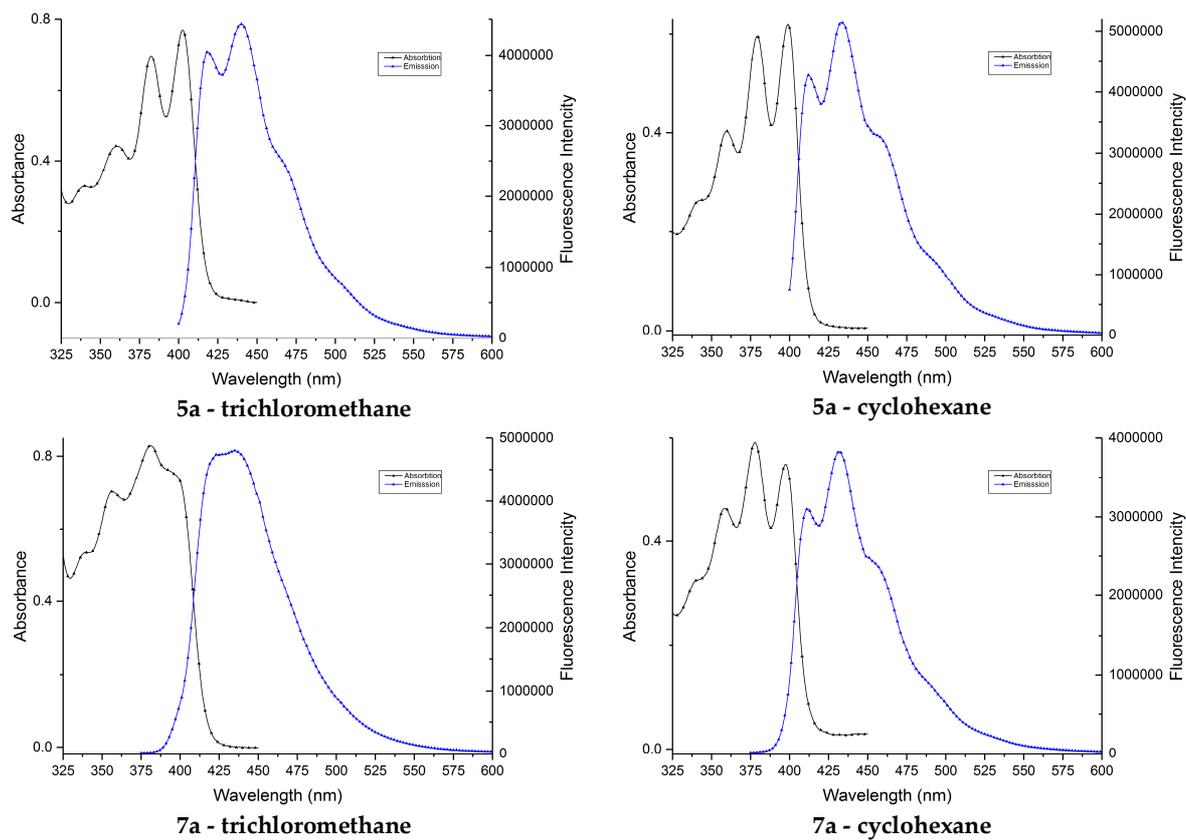
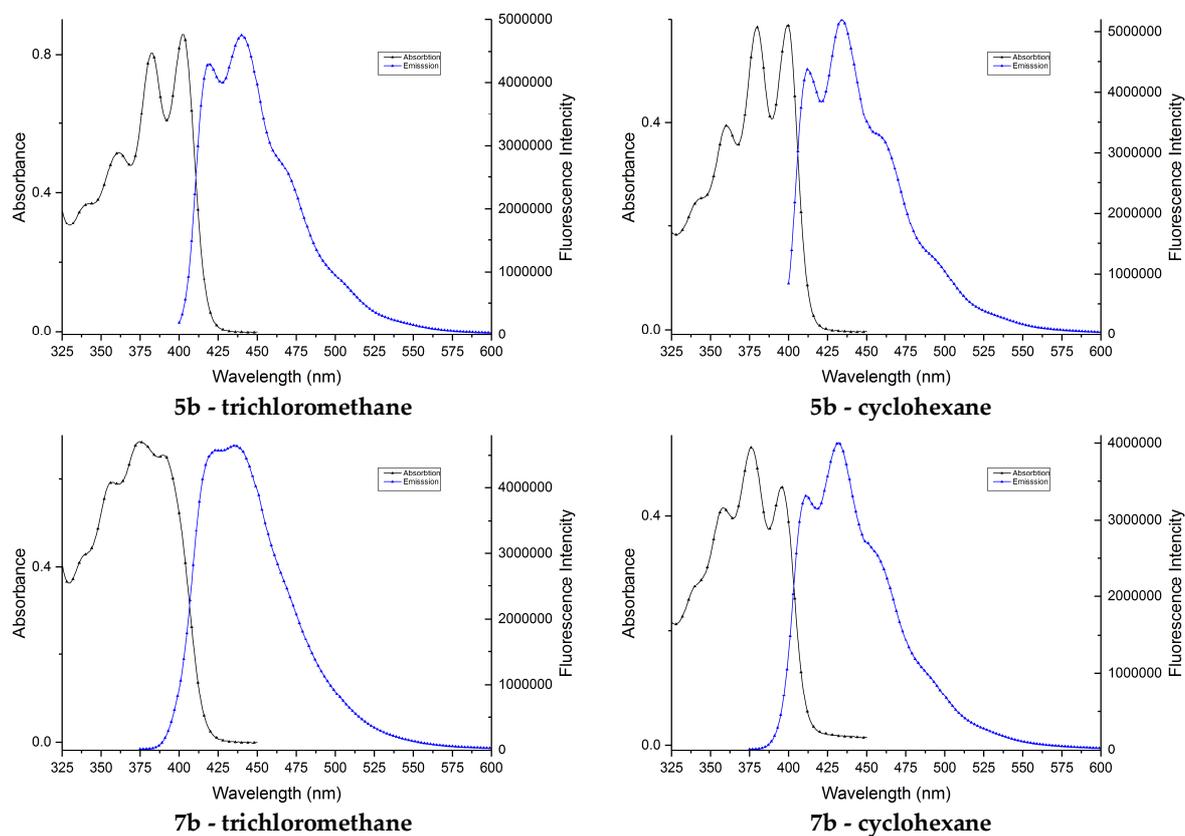


Figure S36. Emission spectrum of the compound **8c** in cyclohexane.

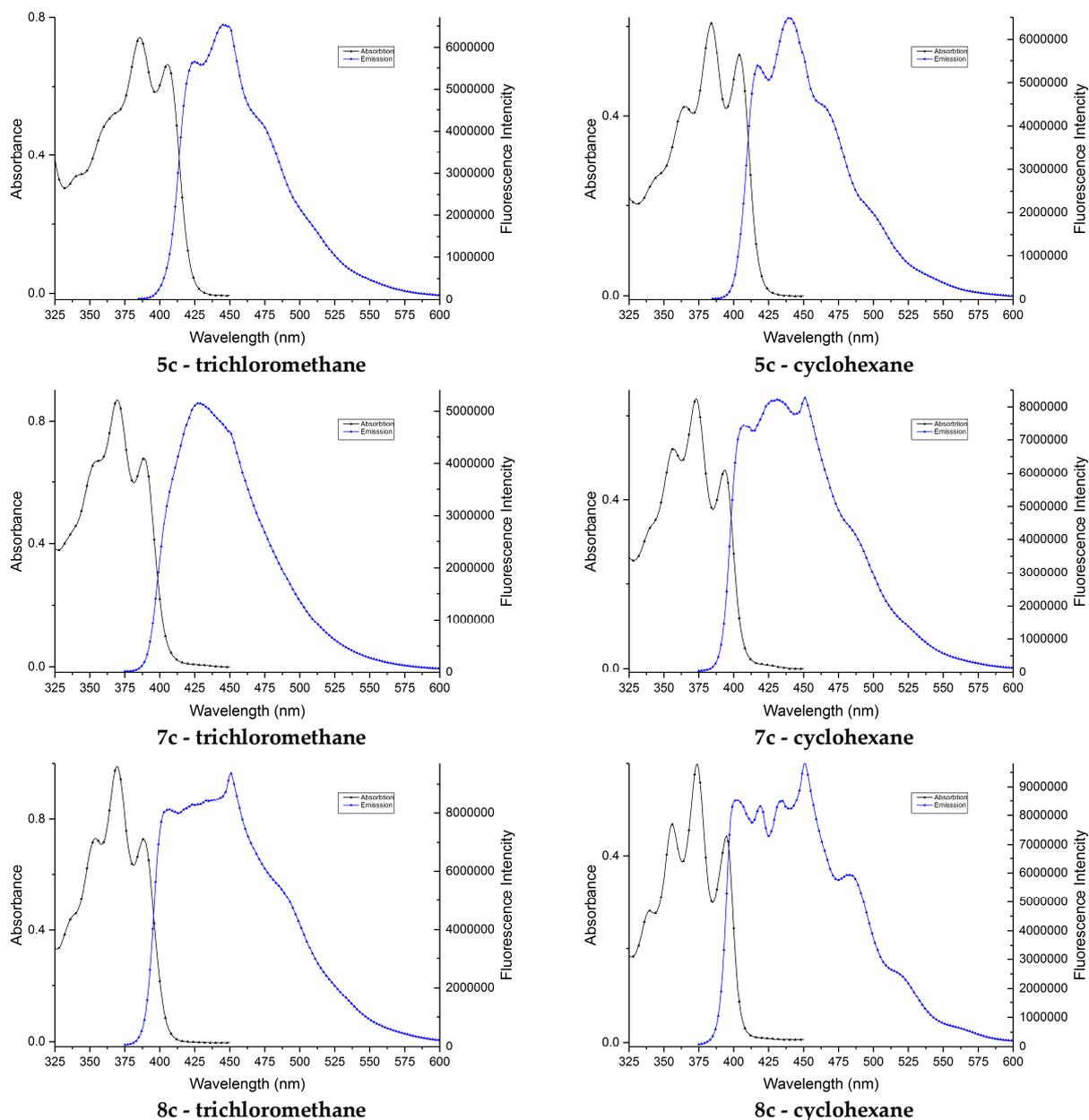
## 6. Absorption vs emission spectra of the obtained compounds



**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**.