

## Supplementary information

### Effect of Solubilizing Group on the Antibacterial Activity of Heptamethine Cyanine Photosensitizers

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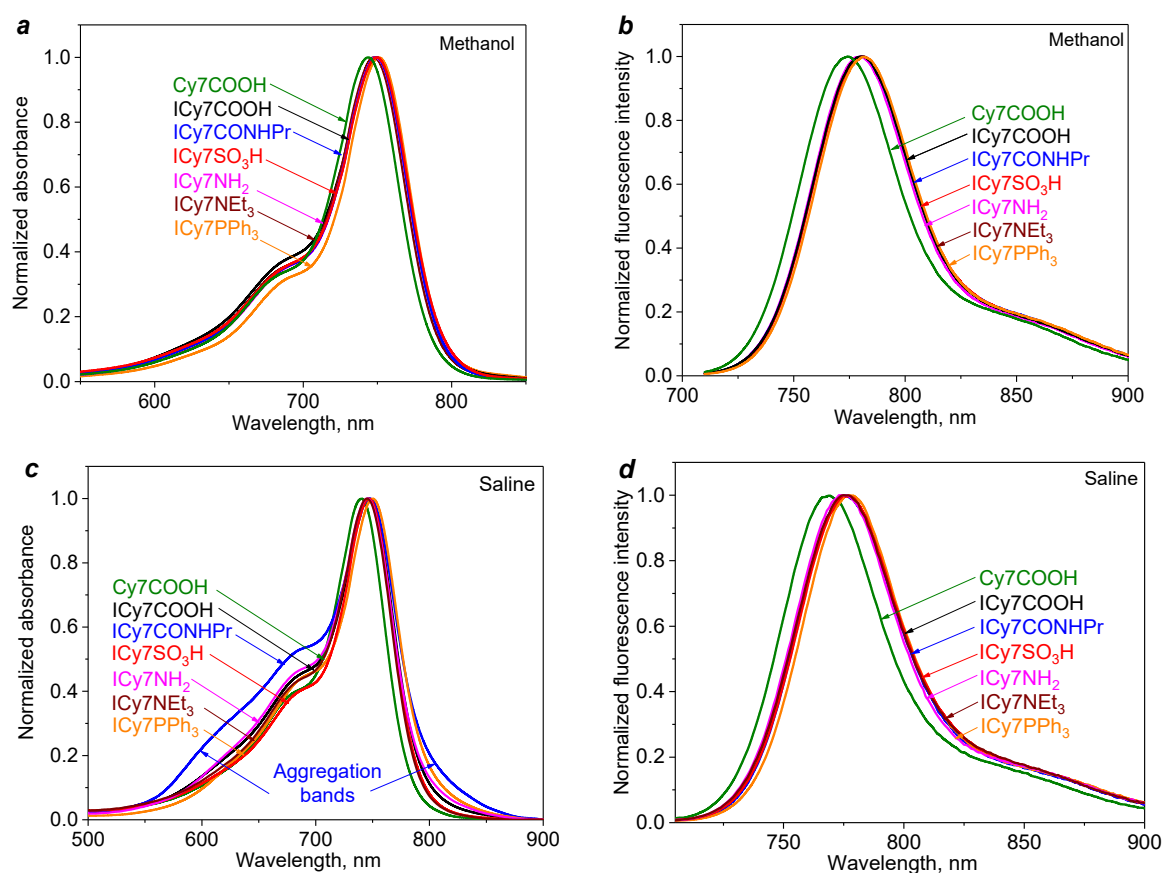
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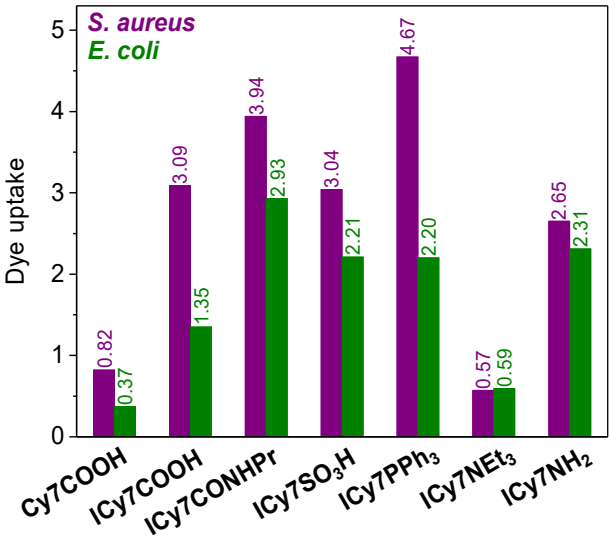
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#### 1. UV-Vis and fluorescence spectra

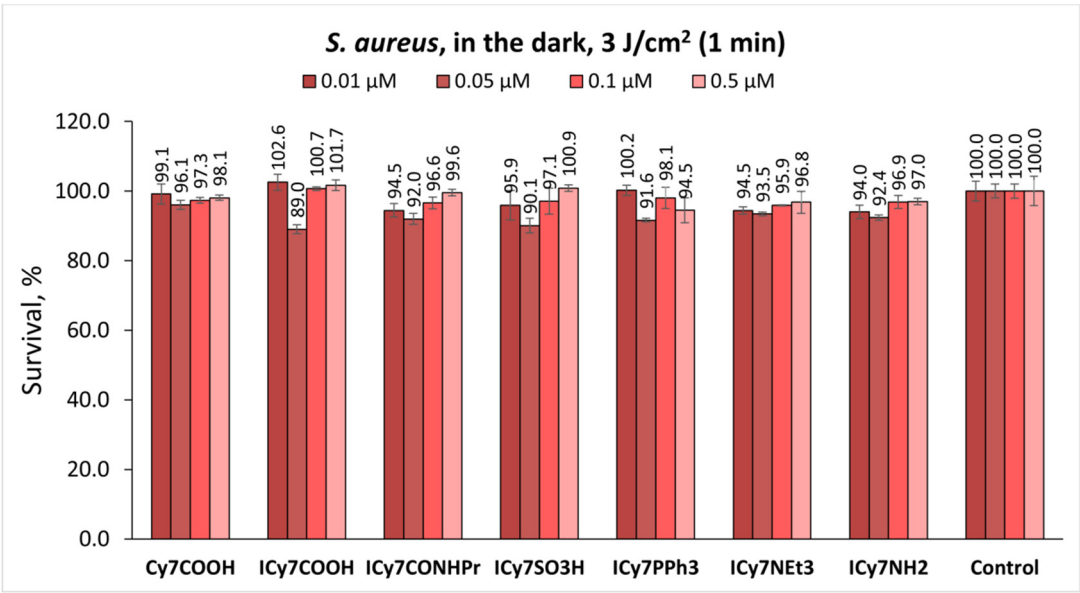


**Figure S1.** Absorption (*a, c*) and emission (*b, d*) spectra of cyanine dyes ( $c \sim 1 \mu\text{M}$ ) in methanol (*a, b*,  $\lambda^* 680 \text{ nm}$ ) and aqueous saline (*c, d*,  $\lambda^* 700 \text{ nm}$ ).

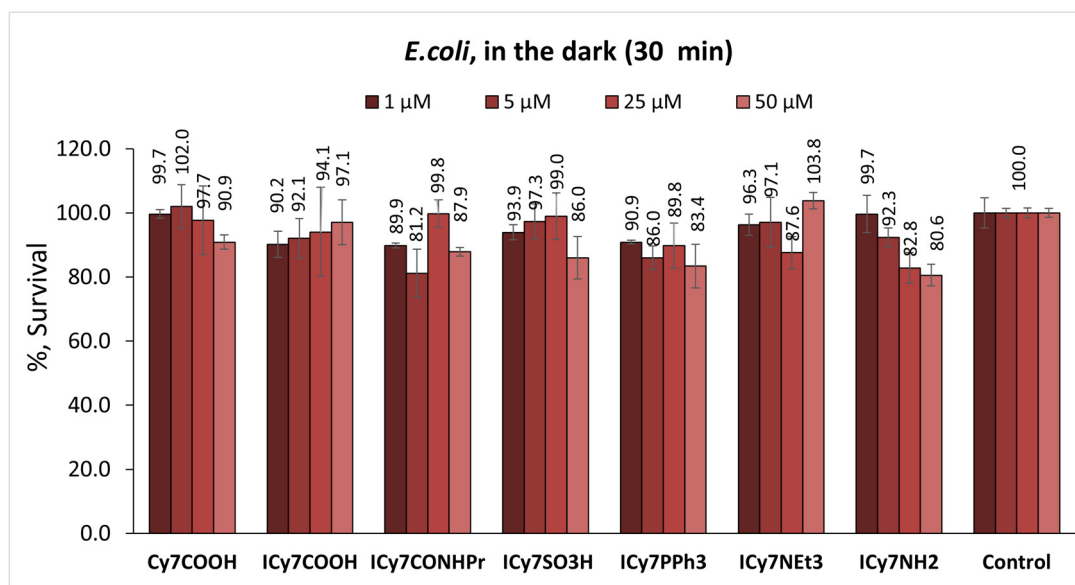
## 2. Data on dye uptake and photodynamic eradication in the dark



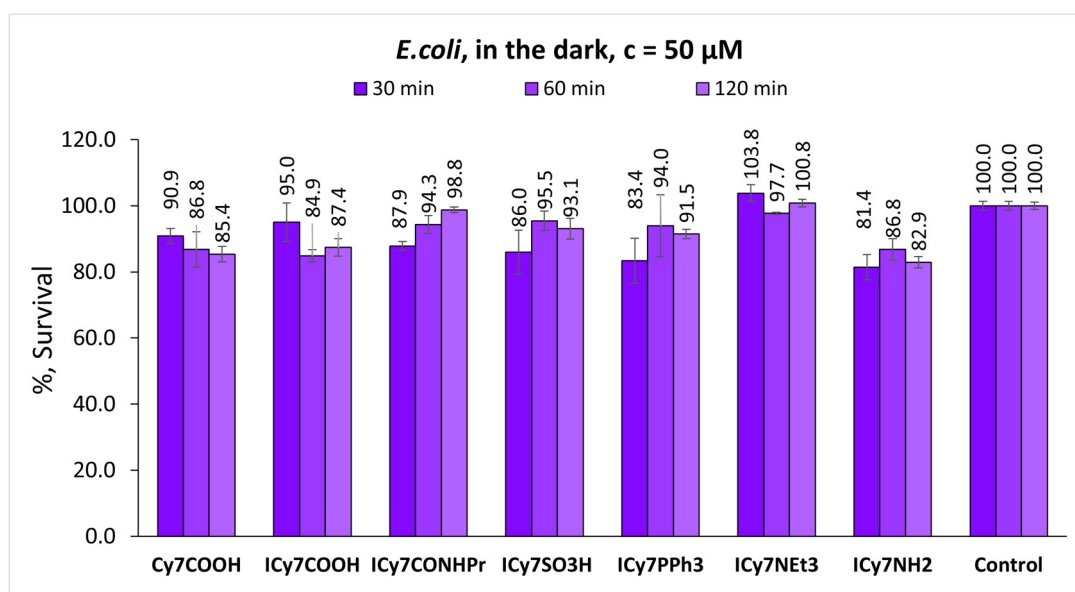
**Figure S2.** The uptake of dyes ( $c_{Dye} = 1 \mu M$ ) by *S. aureus* and *E. coli*.



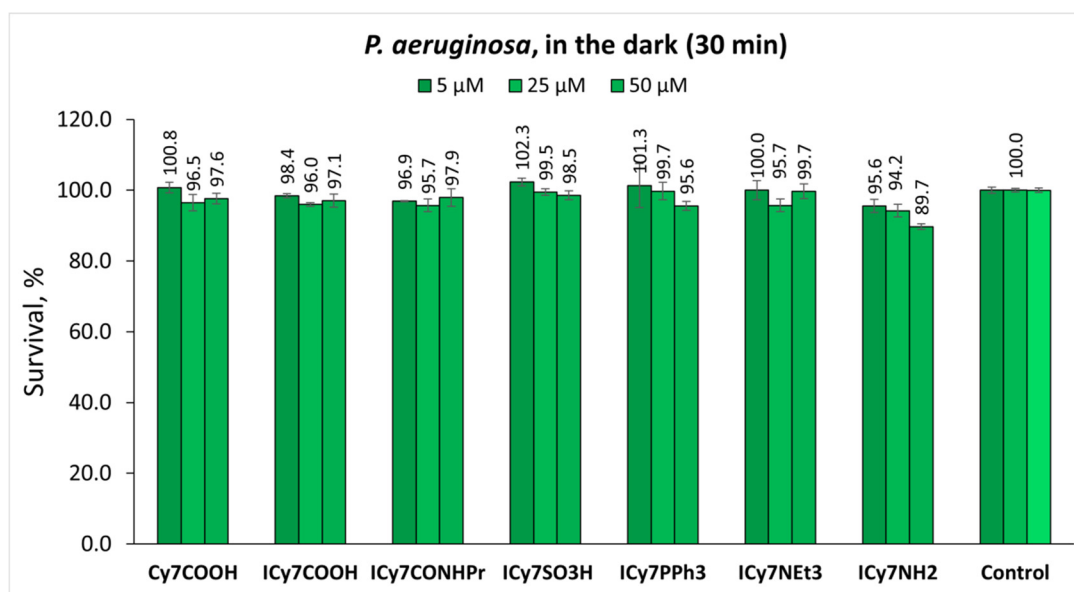
**Figure S3.** Survival of *S. aureus* in 0.7% DMSO in saline in the dark vs. the dye concentrations.



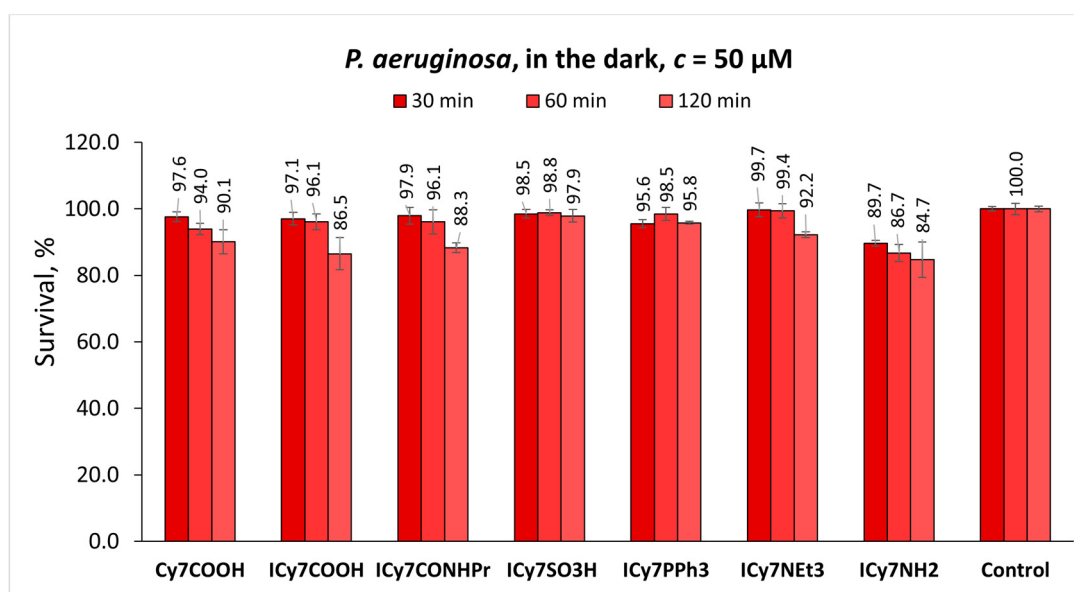
**Figure S4.** Survival of *E. coli* in 0.7% DMSO in saline in the dark vs. the dye concentrations.



**Figure S5.** Survival of *E. coli* at 50  $\mu\text{M}$  dye concentrations in 0.7% DMSO in saline for 30, 60 and 120 min in the dark.

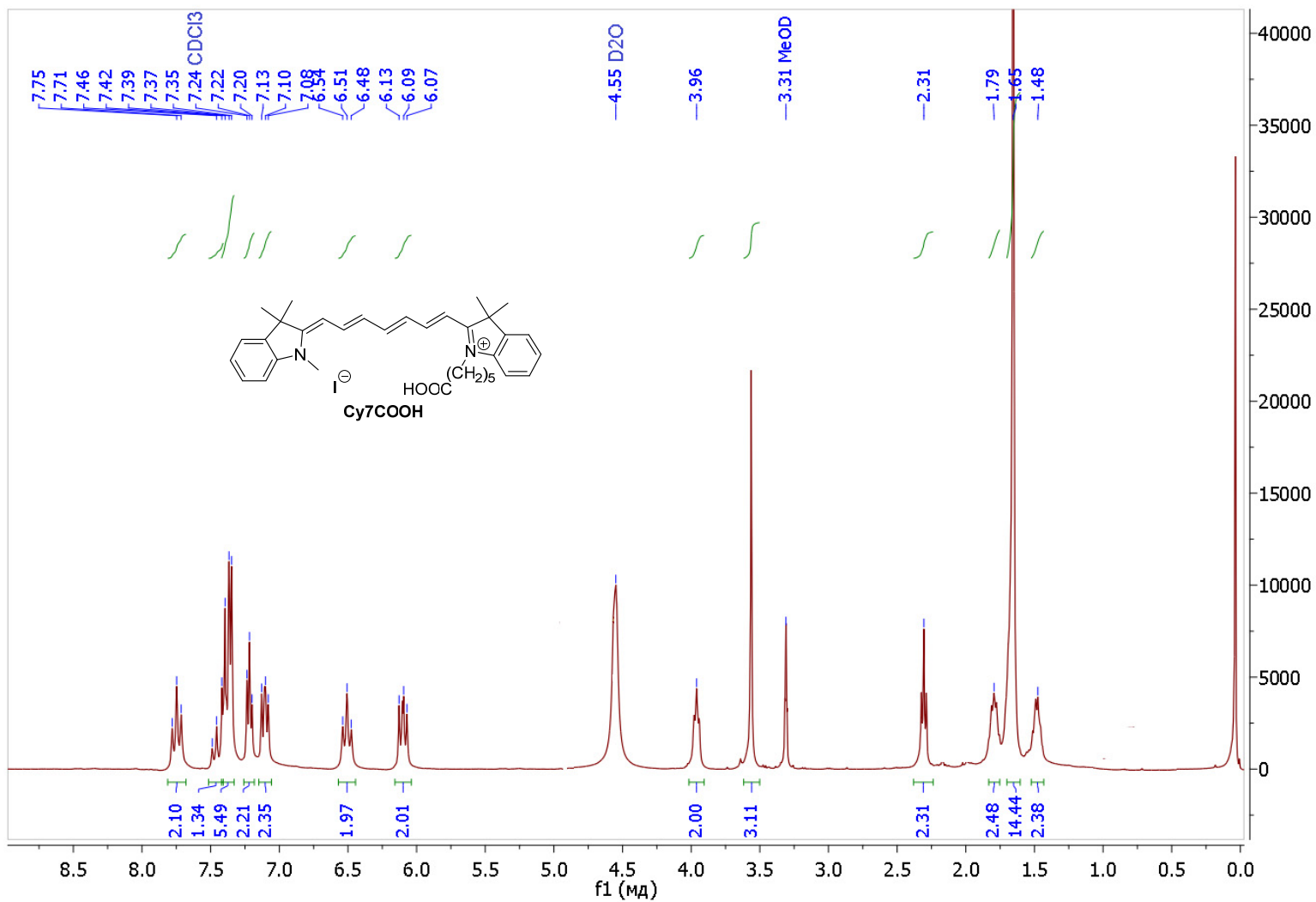


**Figure S6.** Survival of *P. aeruginosa* in 0.7% DMSO in saline in the dark vs. the dye concentrations.

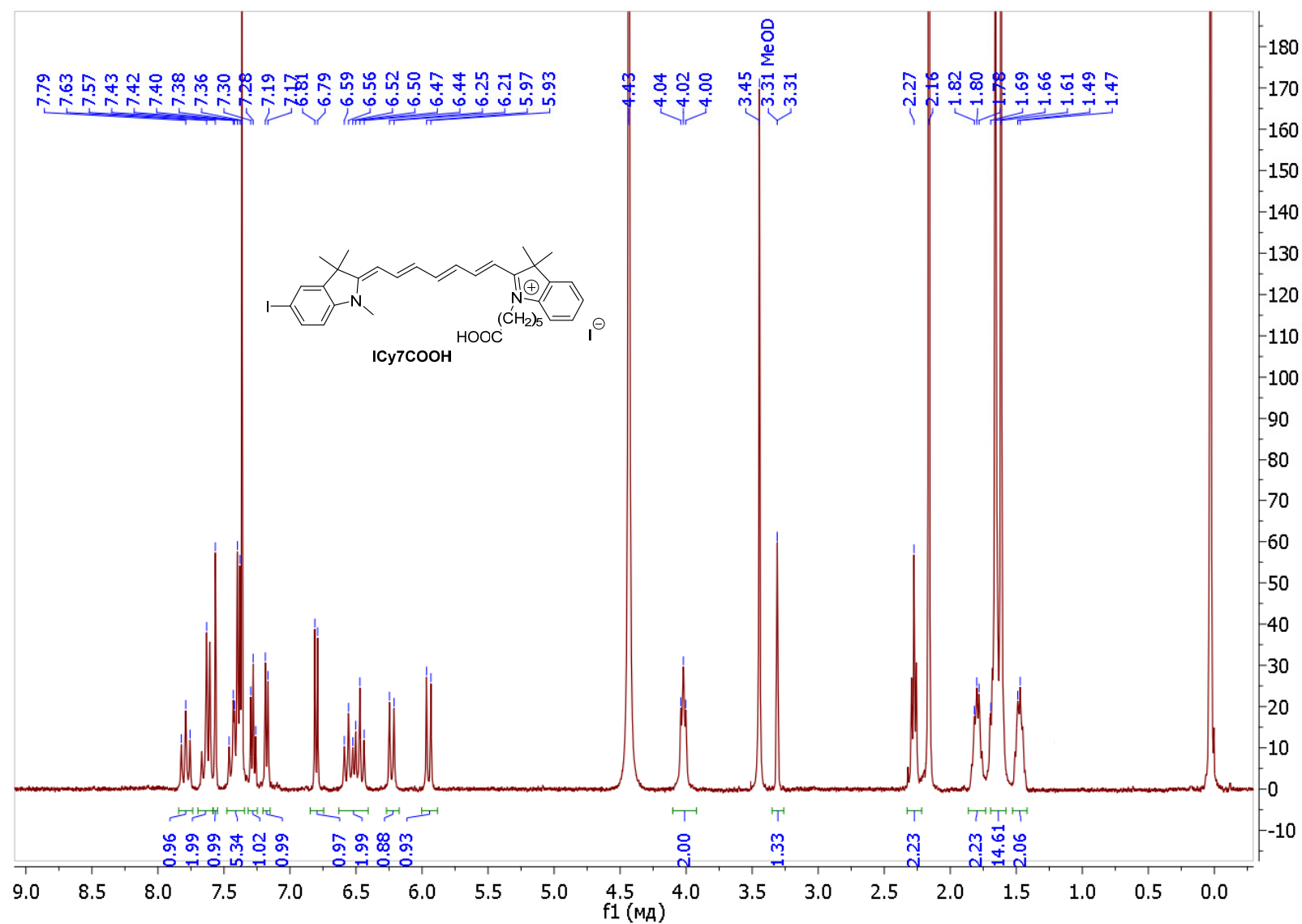


**Figure S7.** Survival of *P. aeruginosa* at 50  $\mu$ M dye concentrations in 0.7% DMSO in saline for 30, 60 and 120 min in the dark.

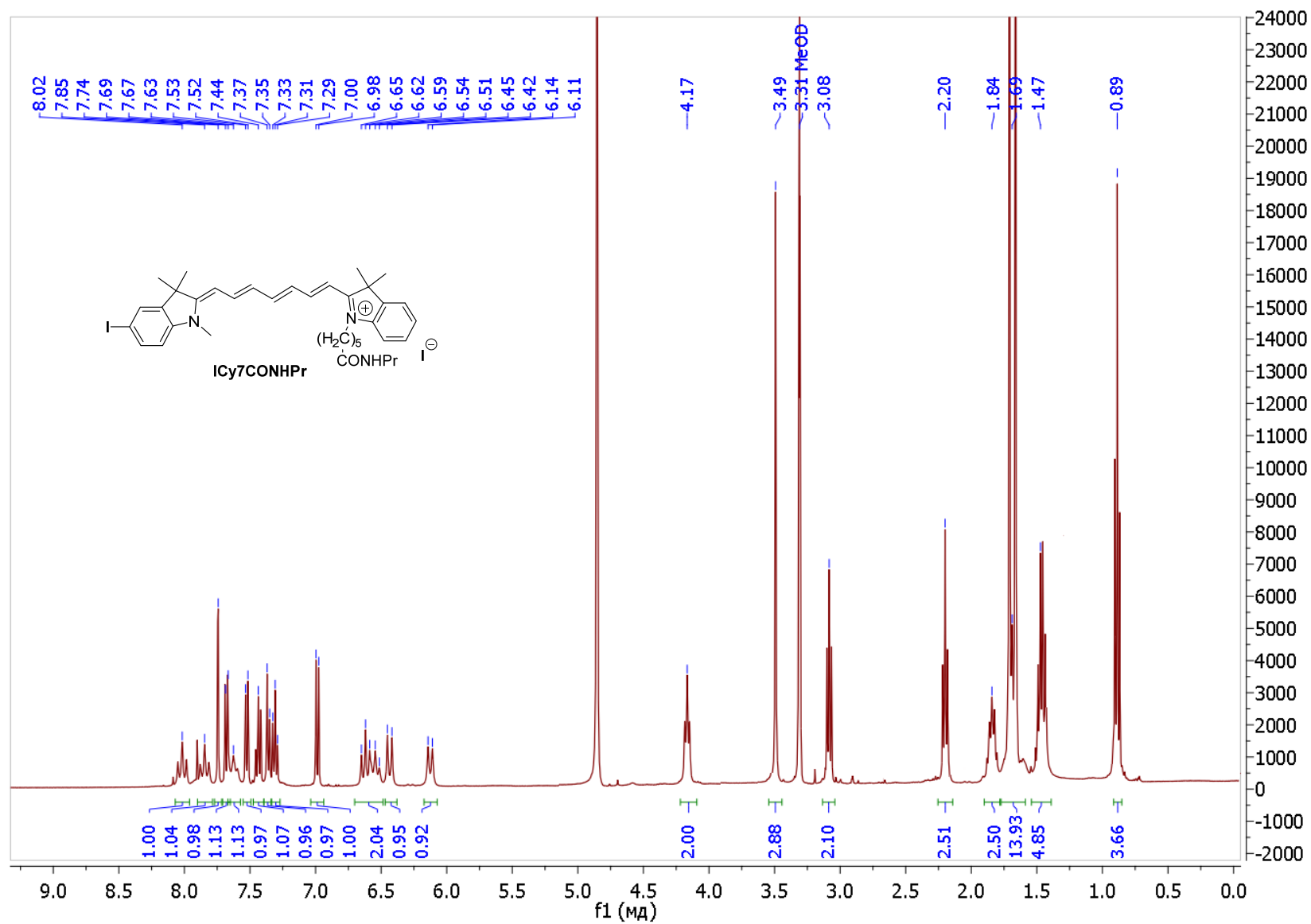
### 3. $^1\text{H}$ NMR spectra



**Figure S8.**  $^1\text{H}$  NMR spectrum of **Cy7COOH** (400 MHz,  $\text{CDCl}_3\text{-CD}_3\text{OD}$ ).



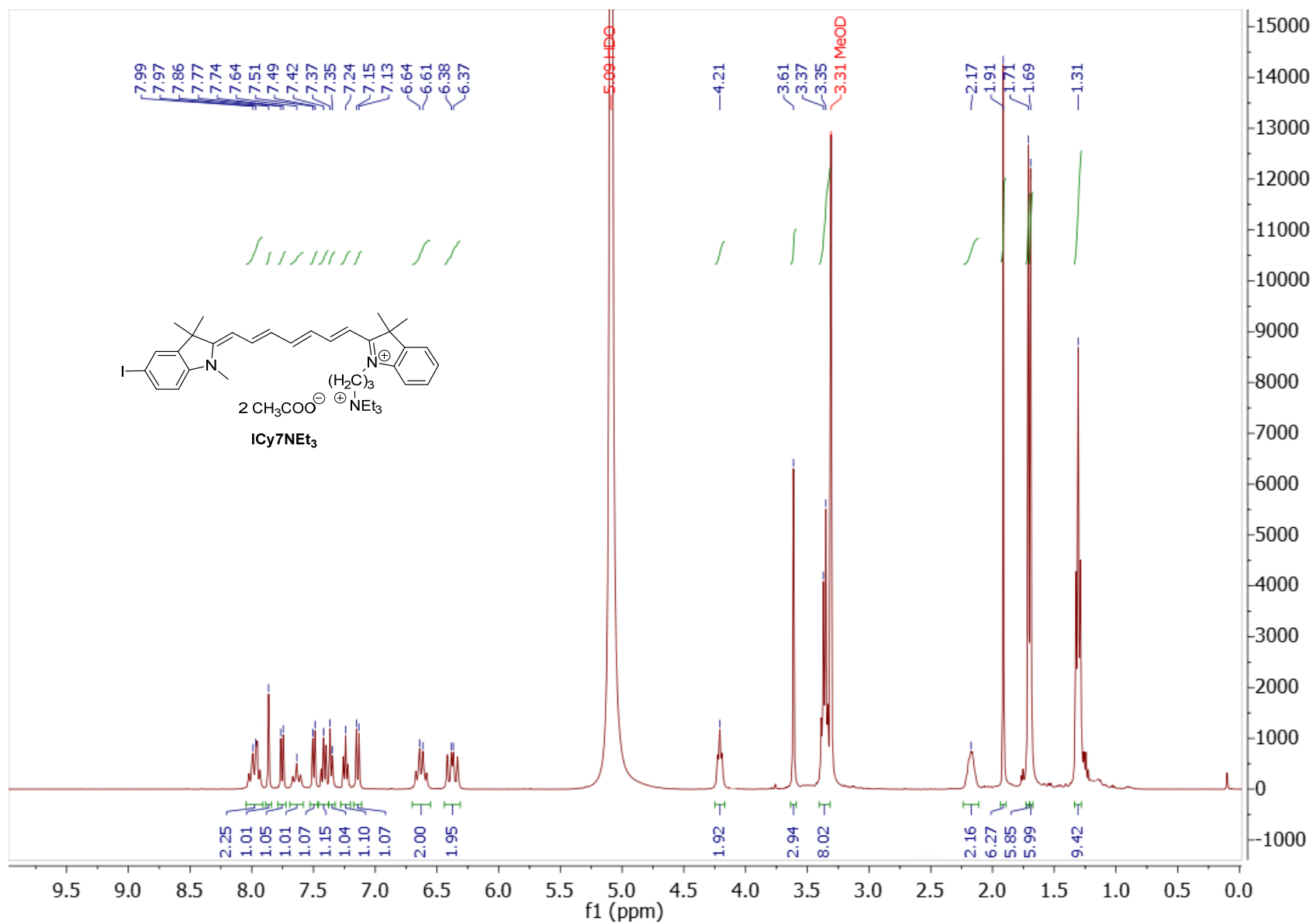
**Figure S9.**  $^1\text{H}$  NMR spectrum of ICy7COOH (400 MHz,  $\text{CDCl}_3\text{-CD}_3\text{OD}$ ).



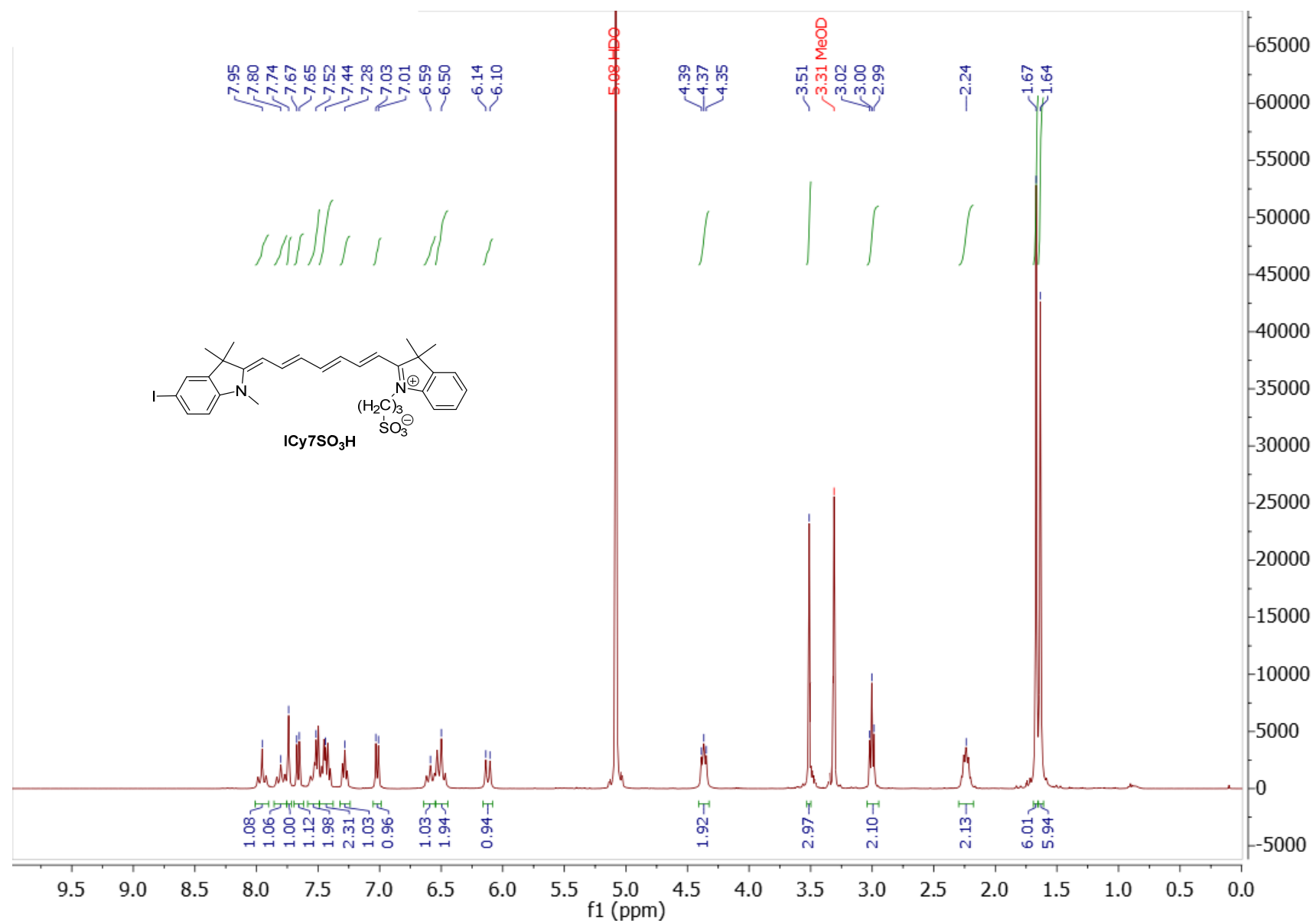
**Figure S10.** <sup>1</sup>H NMR spectrum of ICy7CONHPr (400 MHz, CD<sub>3</sub>OD).



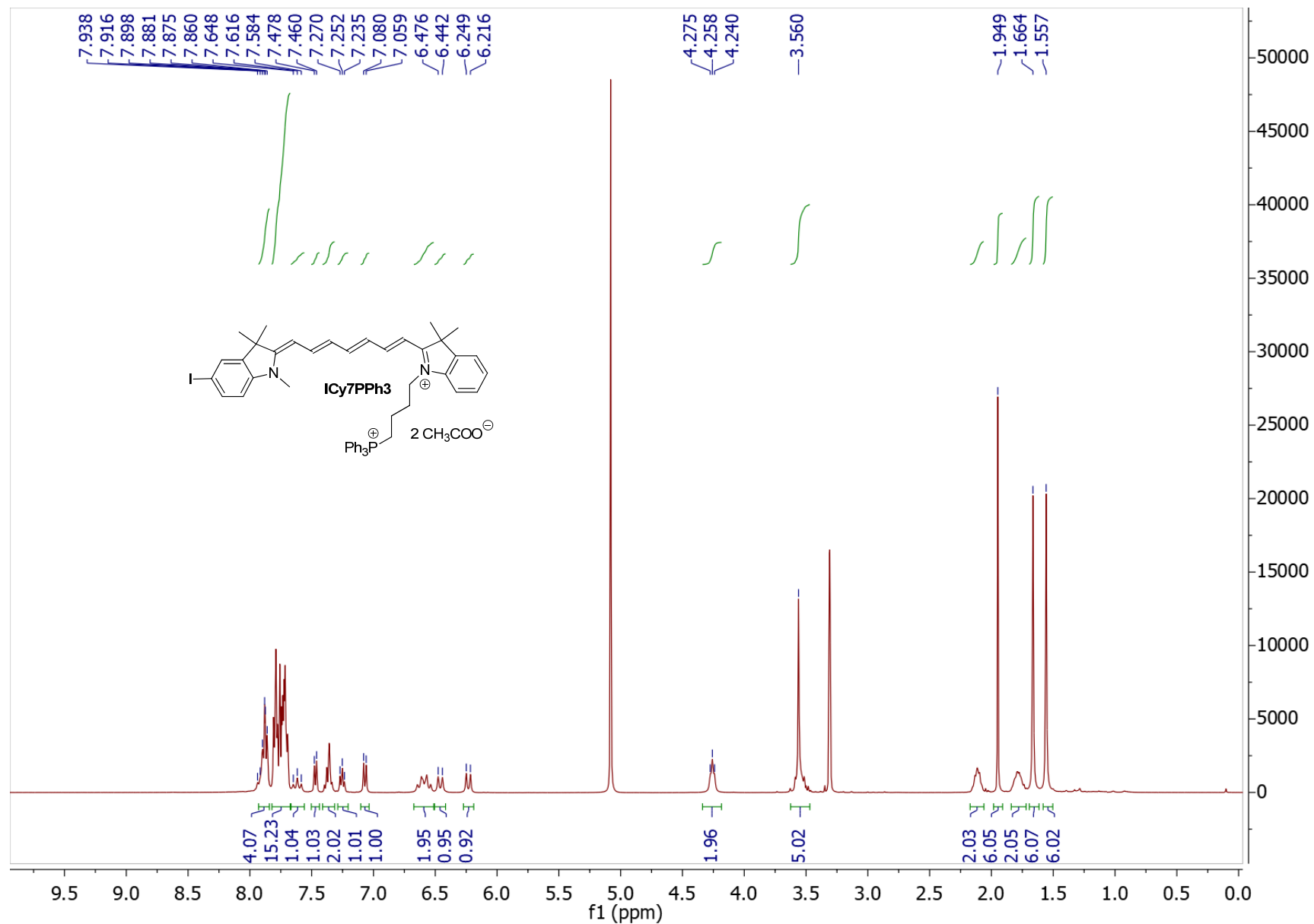




**Figure S12.** <sup>1</sup>H NMR spectrum of **ICy7NEt<sub>3</sub>** (400 MHz, CD<sub>3</sub>OD).

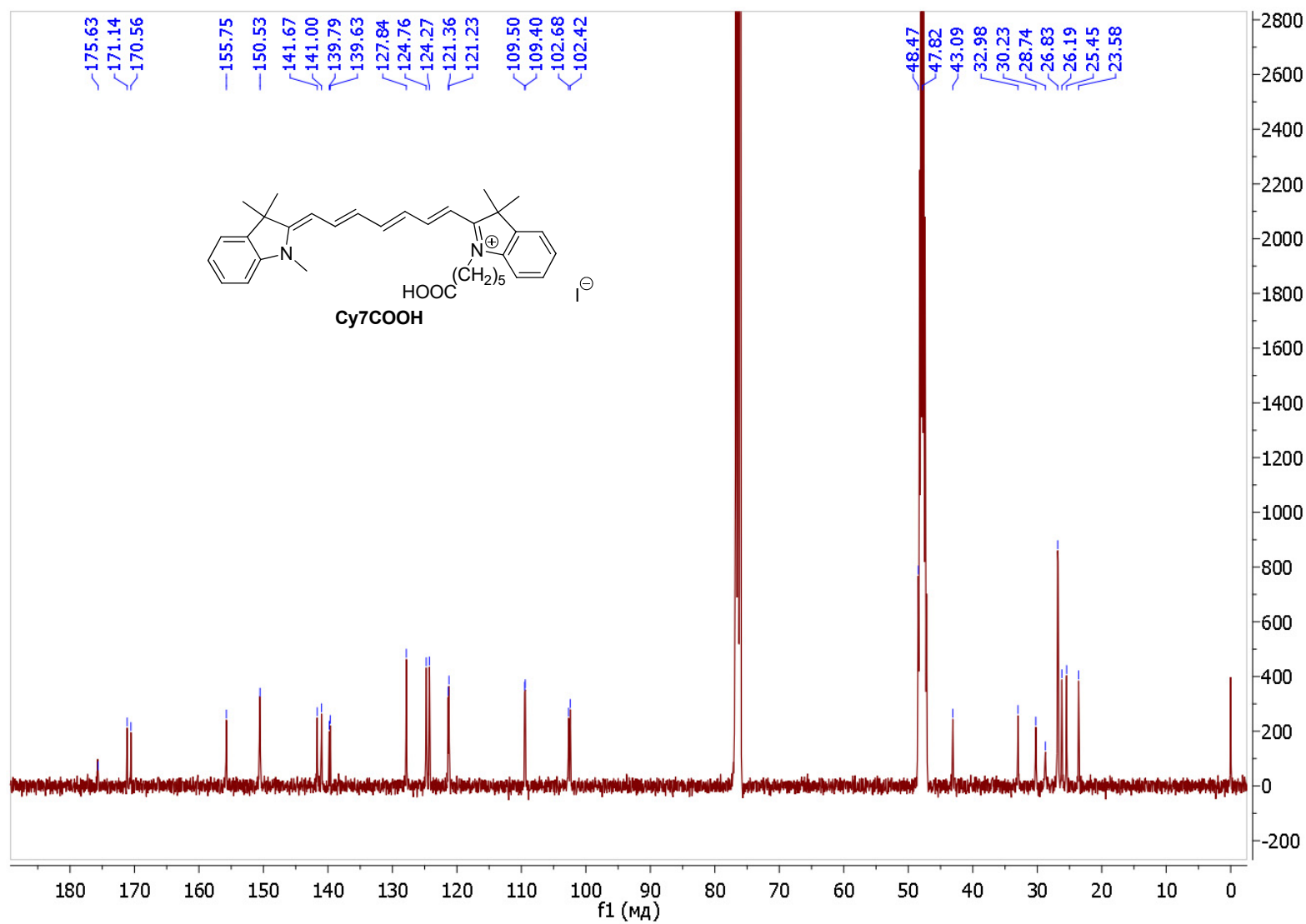


**Figure S13.**  $^1\text{H}$  NMR spectrum of **ICy7SO<sub>3</sub>H** (400 MHz,  $\text{CD}_3\text{OD}$ ).

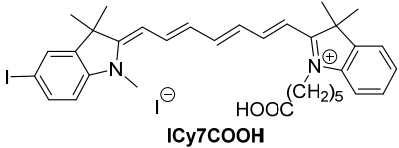


**Figure S14.** <sup>1</sup>H NMR spectrum of **ICy7PPh<sub>3</sub>** (400 MHz, CD<sub>3</sub>OD).

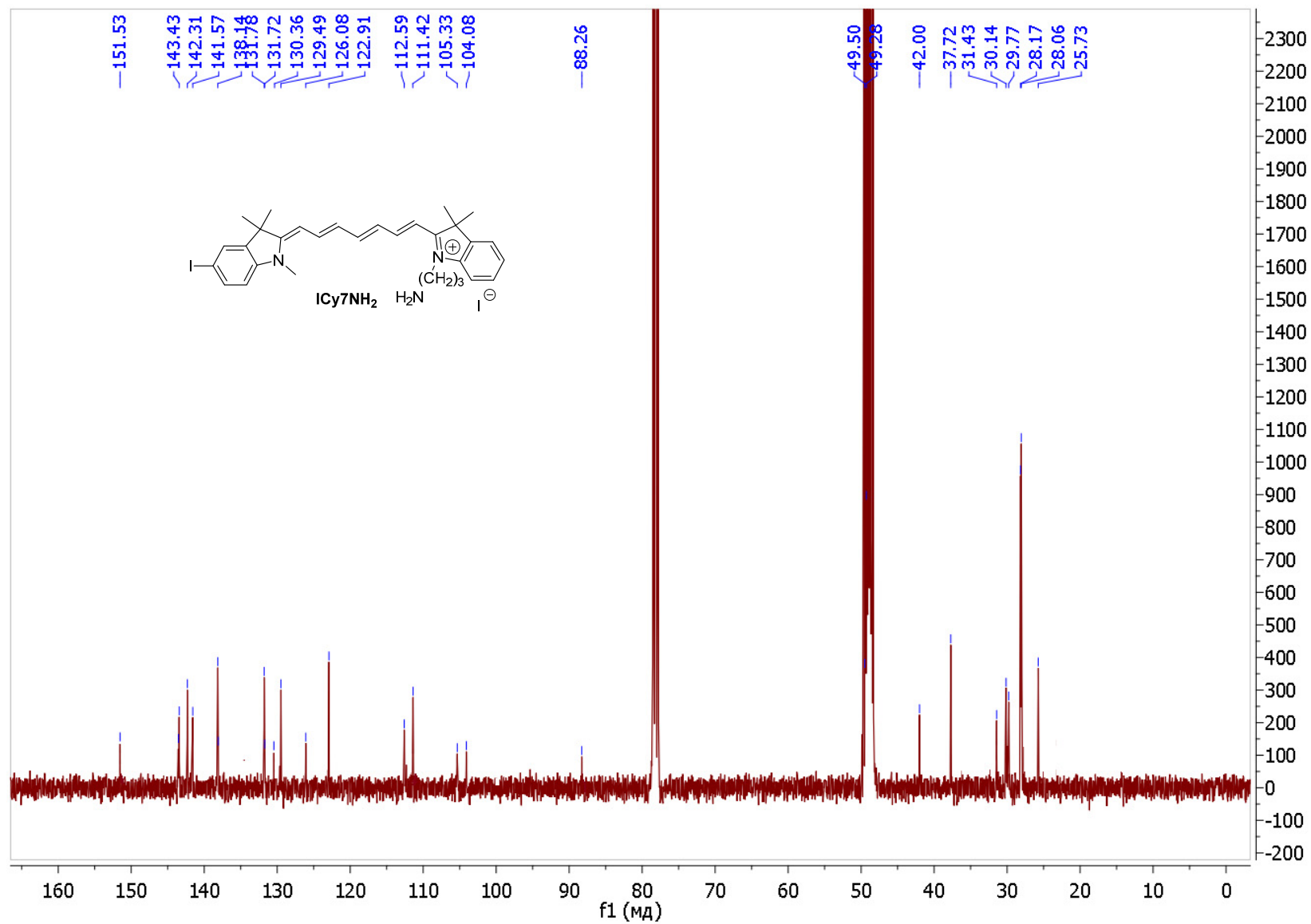
#### 4. $^{13}\text{C}$ NMR spectra



**Figure S15.**  $^{13}\text{C}$  NMR spectrum of **Cy7COOH** (100 MHz,  $\text{CDCl}_3\text{--CD}_3\text{OD}$ ).

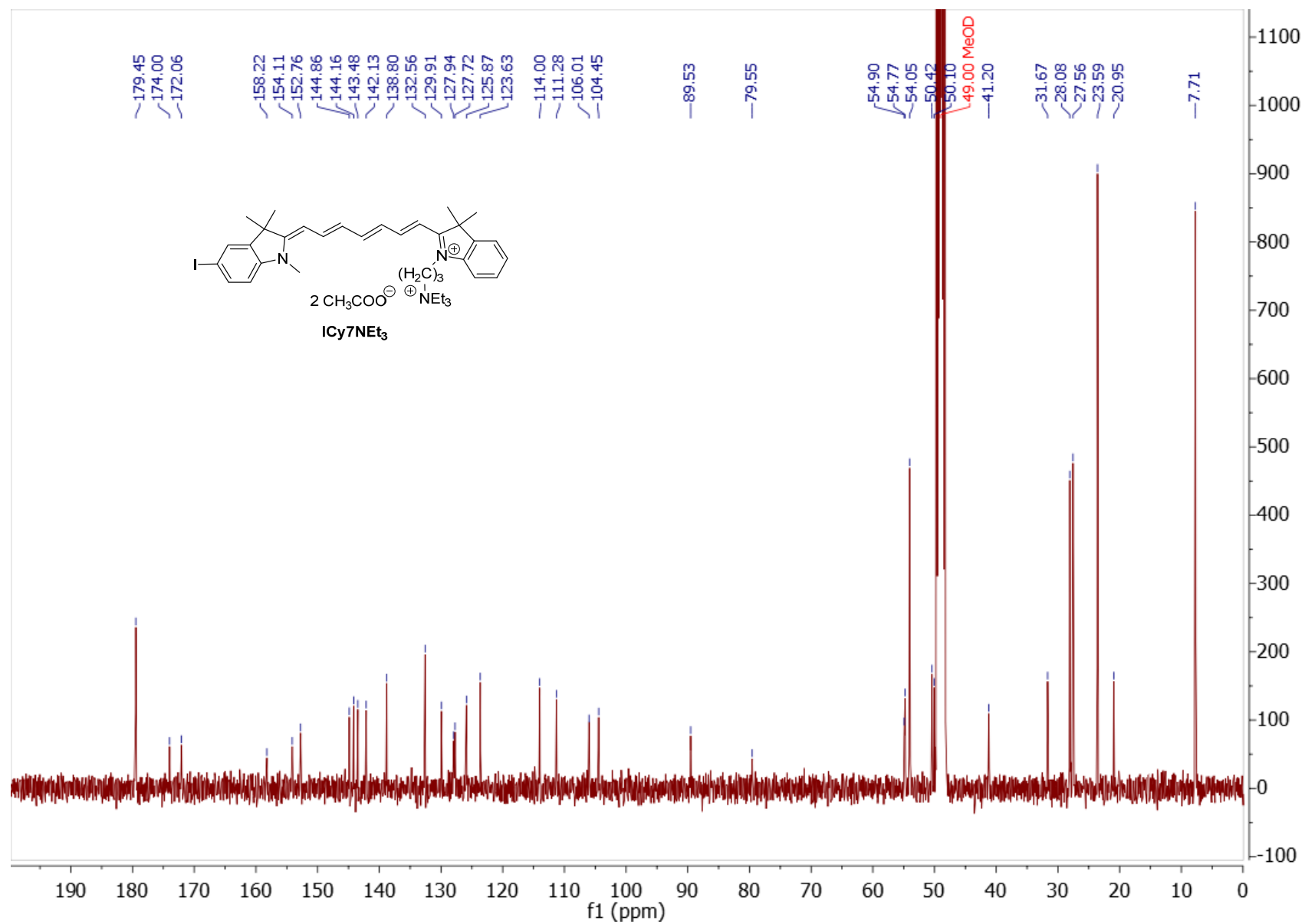




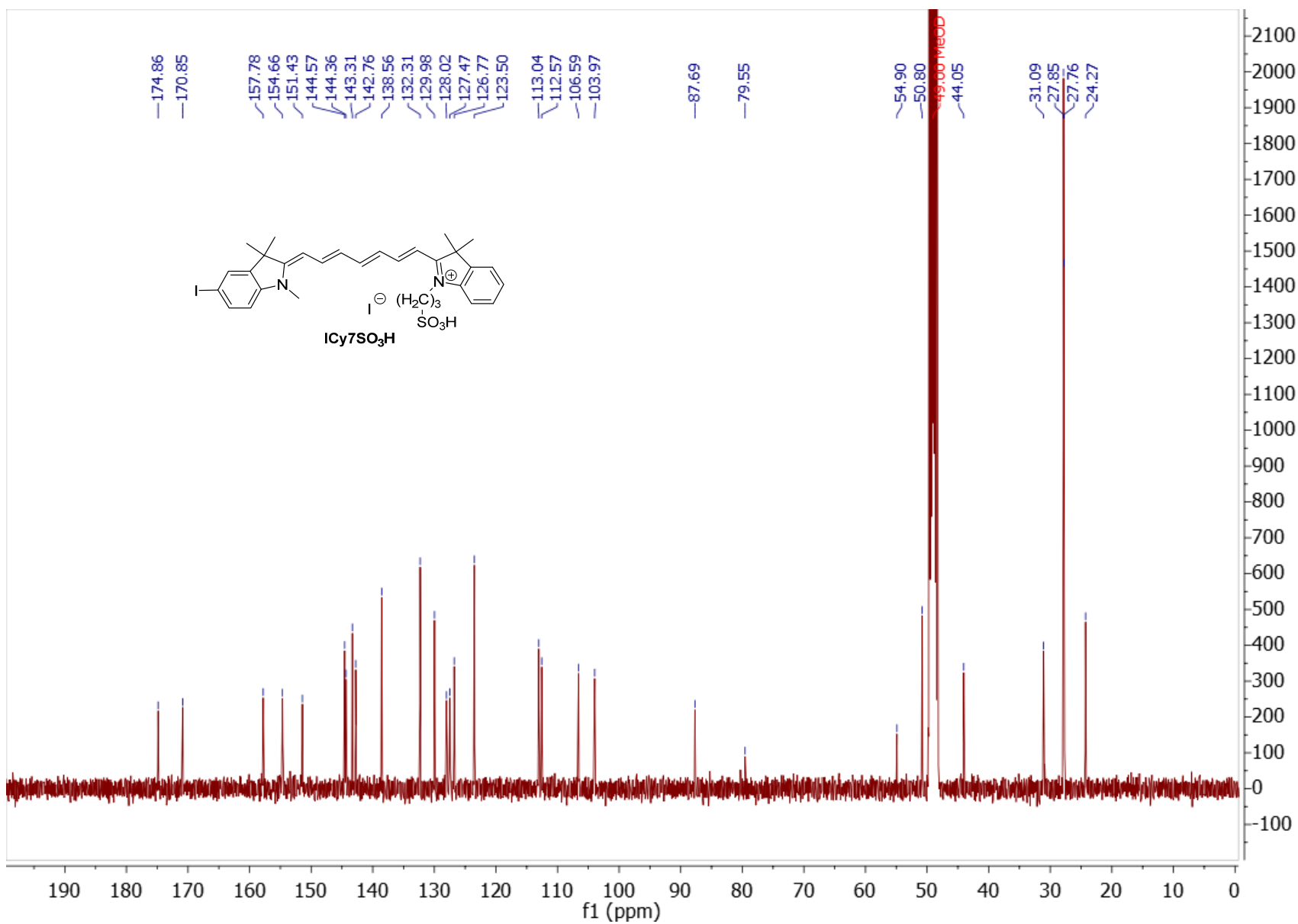


**Figure S18.** <sup>13</sup>C NMR spectrum of ICy7NH<sub>2</sub> (100 MHz, CD<sub>3</sub>OD).

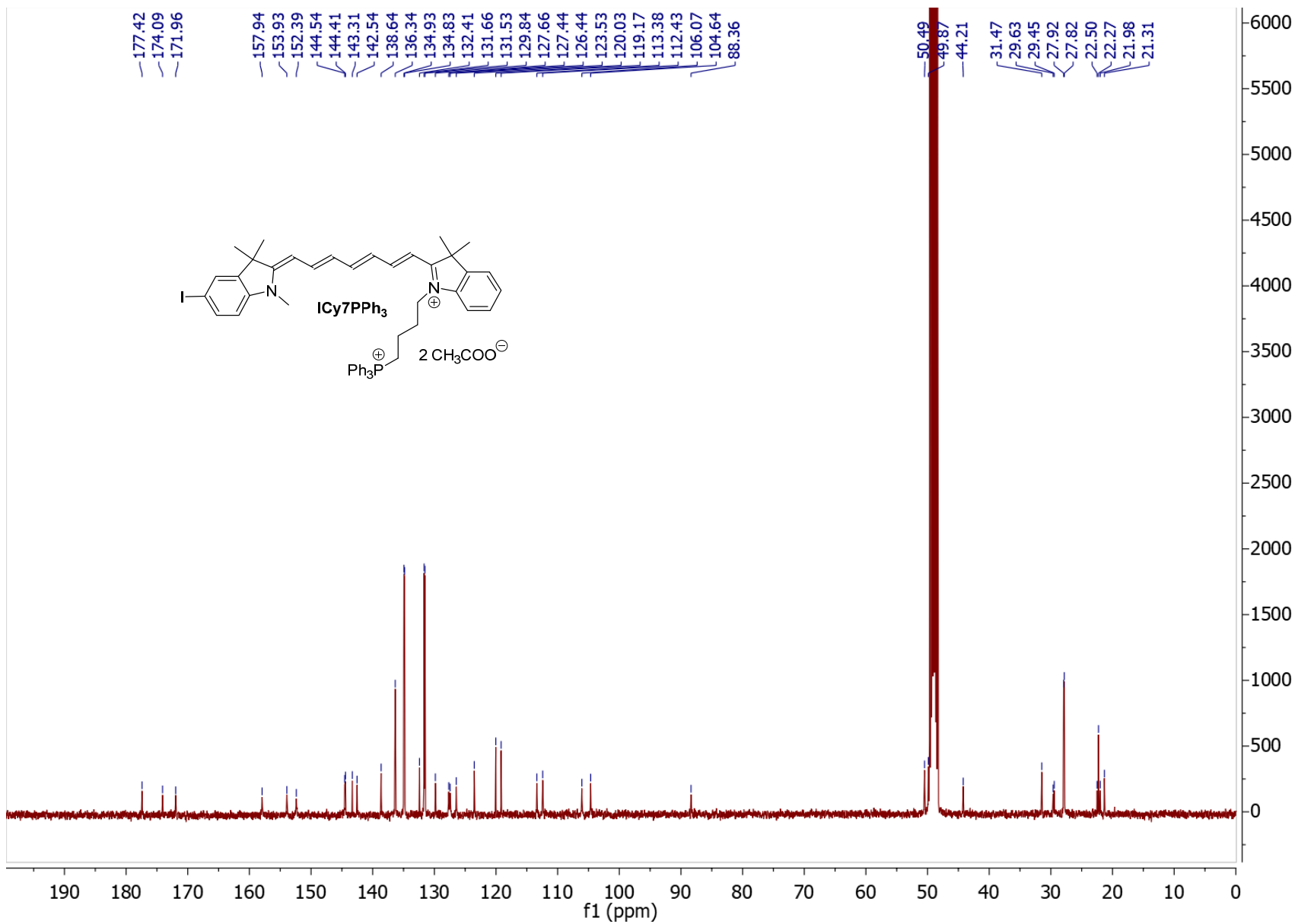




**Figure S19.** <sup>13</sup>C NMR spectrum of **ICy7NEt<sub>3</sub>** (100 MHz, CD<sub>3</sub>OD).

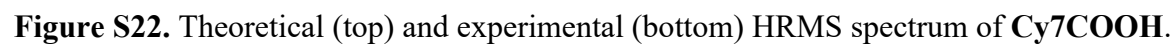


**Figure S20.** <sup>13</sup>C NMR spectrum of **ICy7SO<sub>3</sub>H** (100 MHz, CD<sub>3</sub>OD).



**Figure S21.** <sup>13</sup>C NMR spectrum of **ICy7PPh<sub>3</sub>** (100 MHz, CD<sub>3</sub>OD).

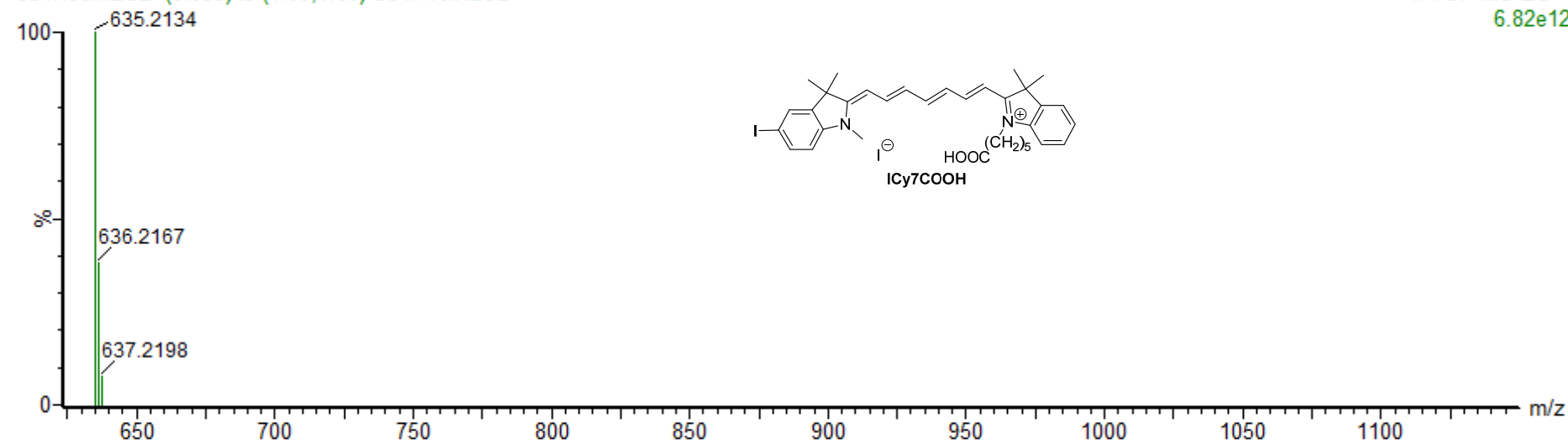
**Cy7COOH**



1ICy7

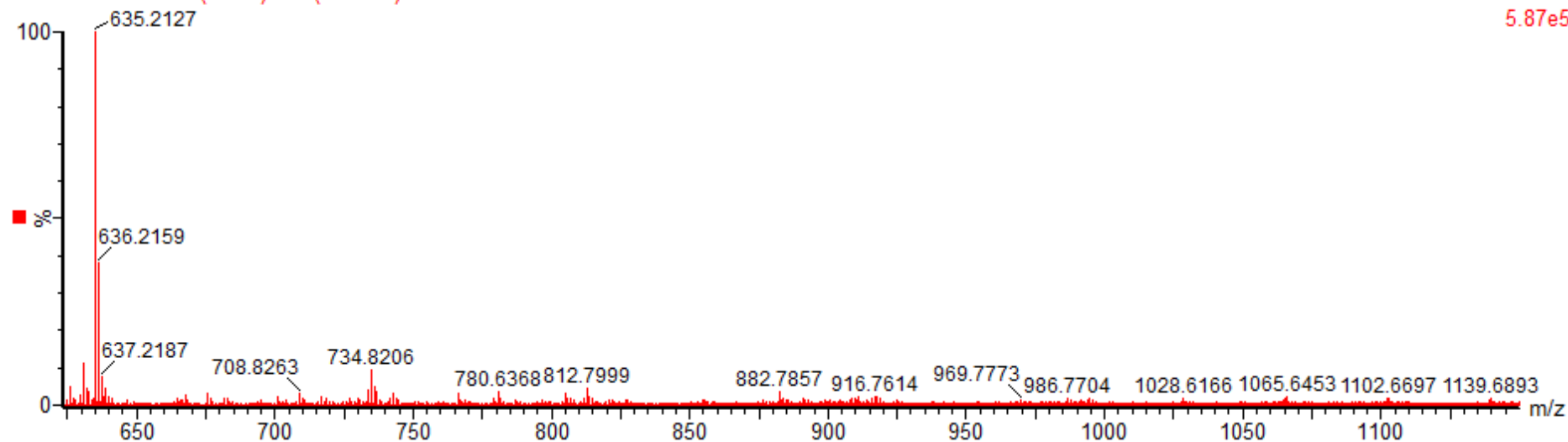
C<sub>34</sub>H<sub>39</sub>N<sub>2</sub>O<sub>2</sub> (0.053) Is (1.00,1.00) C<sub>34</sub>H<sub>40</sub>N<sub>2</sub>O<sub>2</sub>

1: TOF MS ES+  
6.82e12

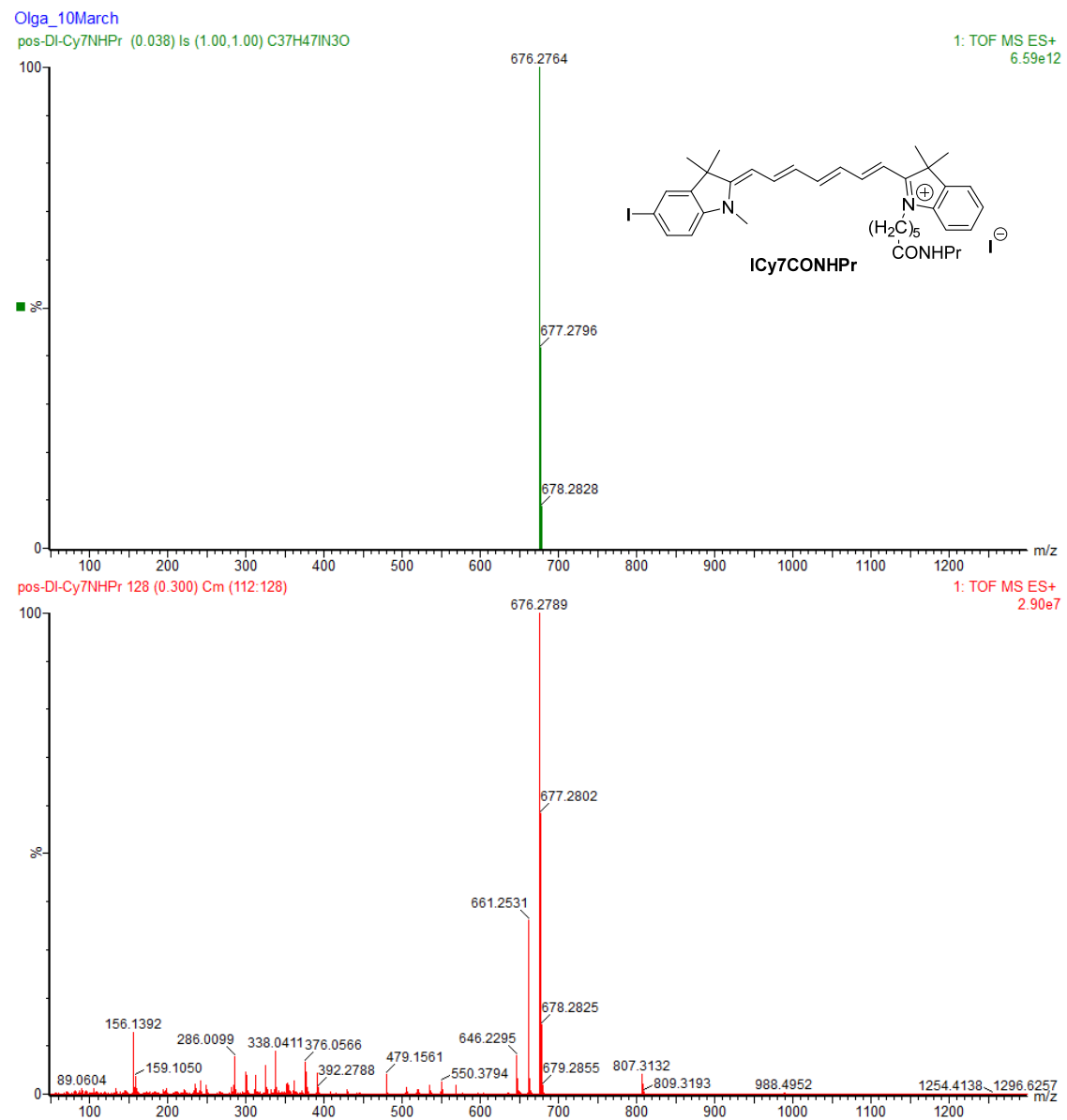


C<sub>34</sub>H<sub>39</sub>N<sub>2</sub>O<sub>2</sub> 127 (2.481) Cm (111:128)

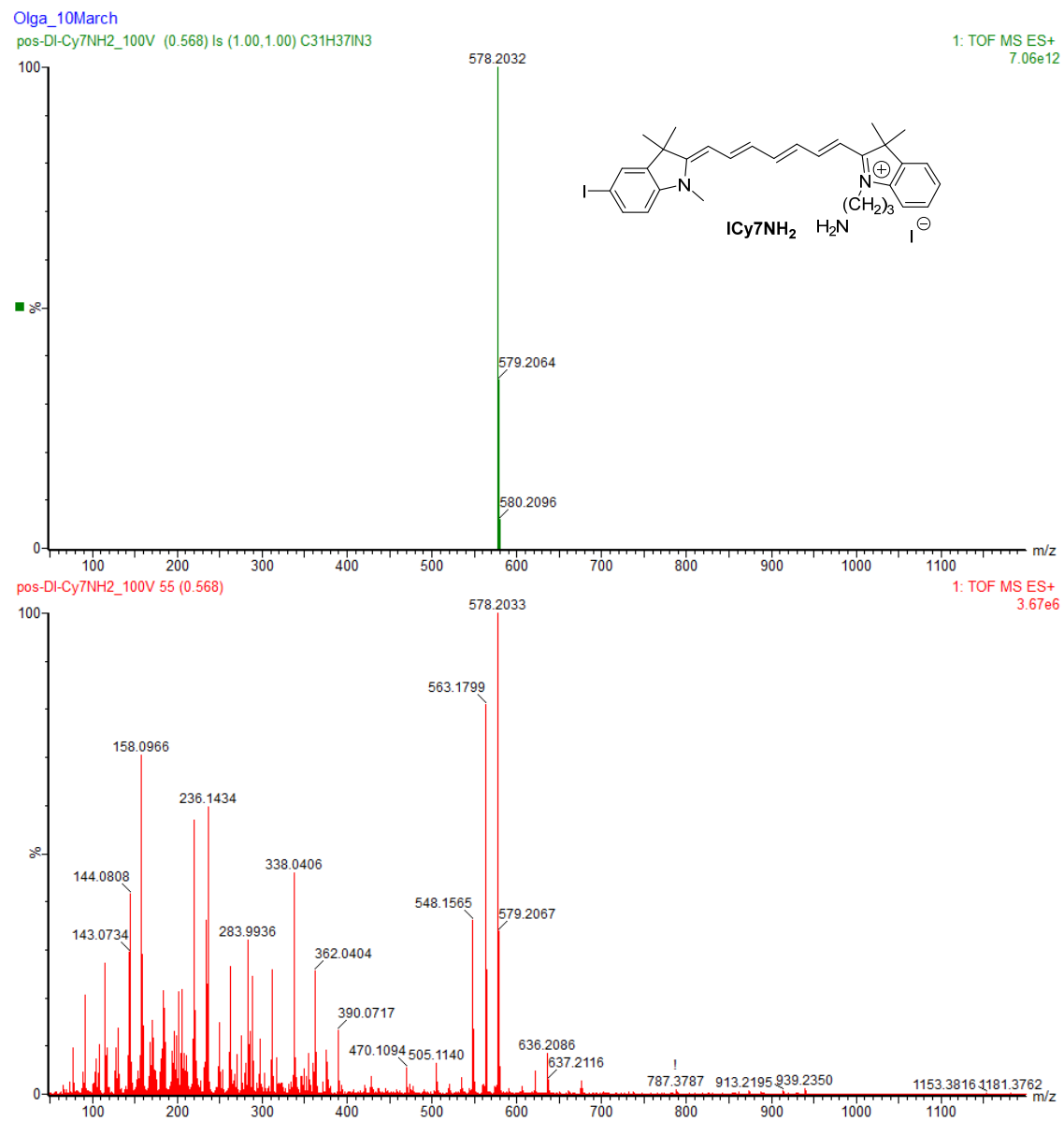
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5.87e5



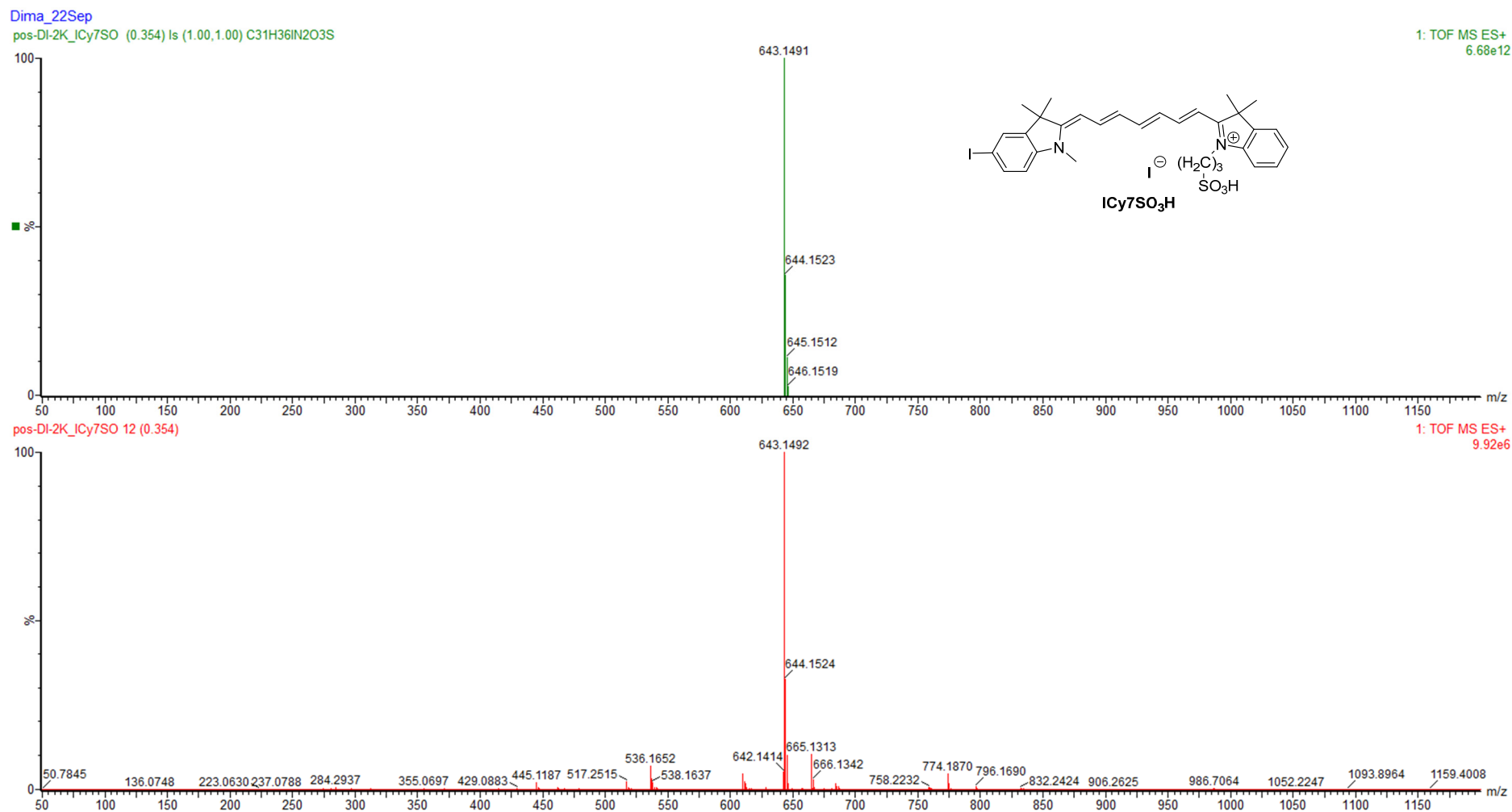
**Figure S23.** Theoretical (top) and experimental (bottom) HRMS spectrum of ICy7COOH.



**Figure S24.** Theoretical (top) and experimental (bottom) HRMS spectrum of ICy7CONHPr.

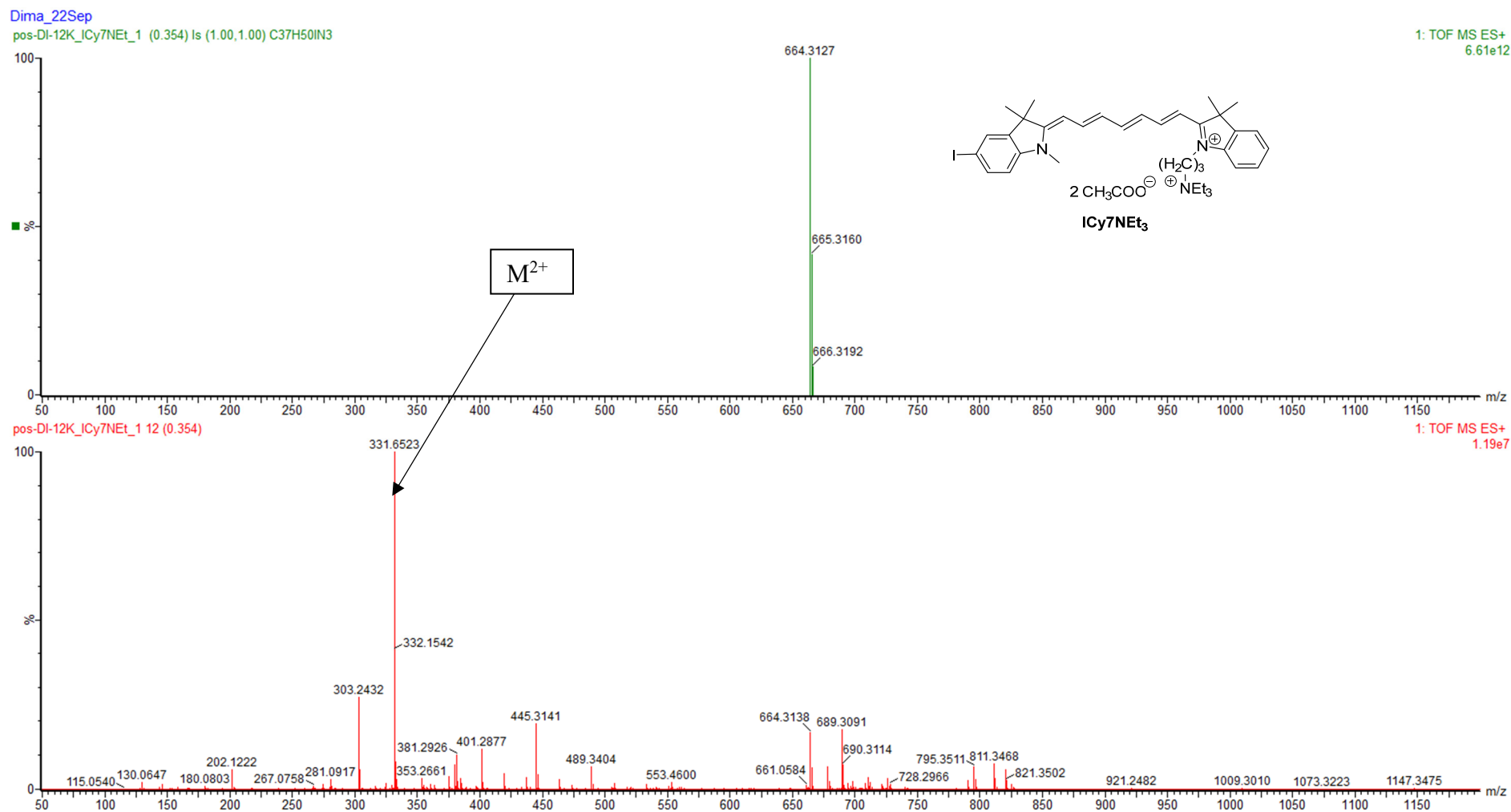


**Figure S25.** Theoretical (top) and experimental (bottom) HRMS spectrum of ICy7NH<sub>2</sub>.

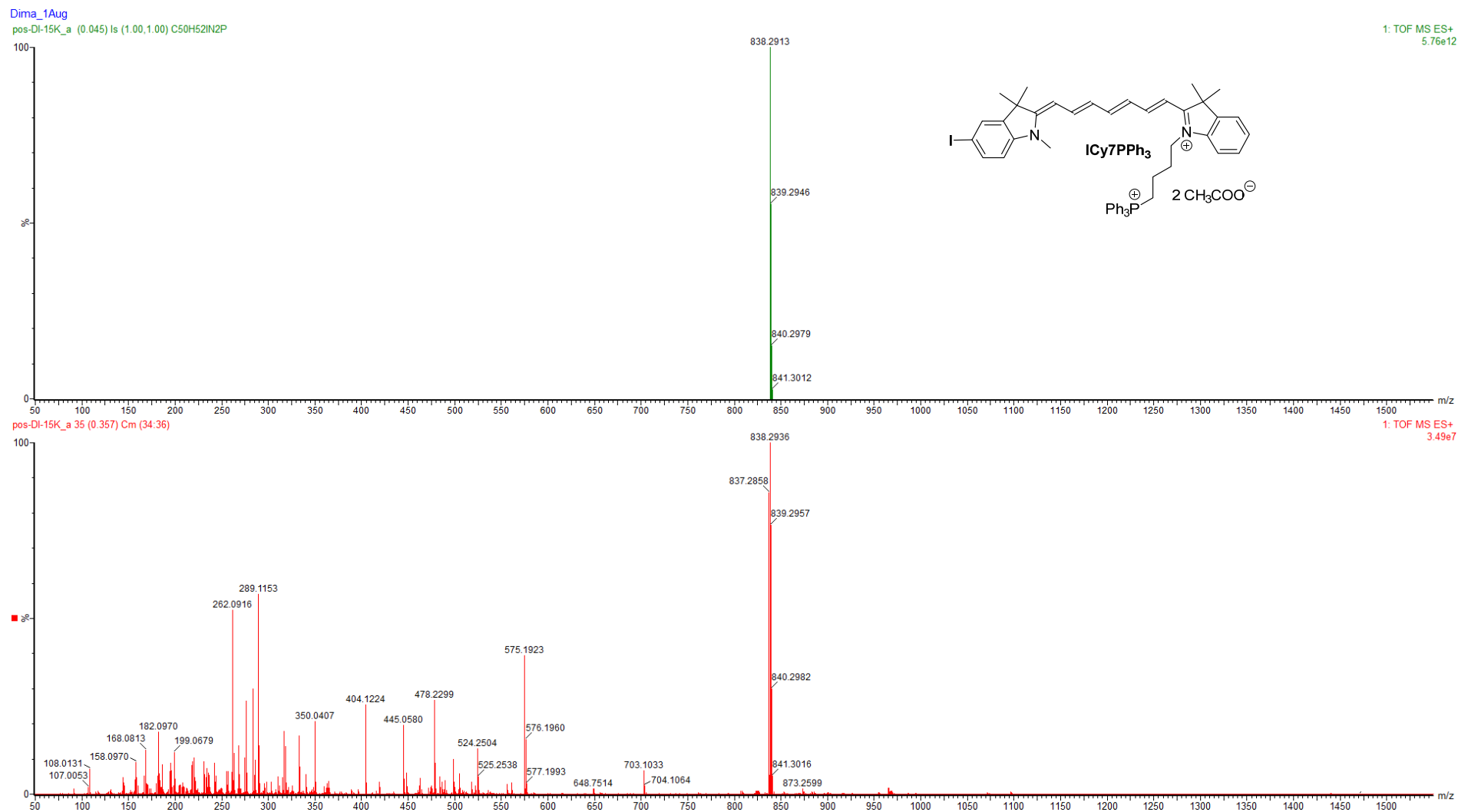


**Figure S26.** Theoretical (top) and experimental (bottom) HRMS spectrum of ICy7SO<sub>3</sub>H.



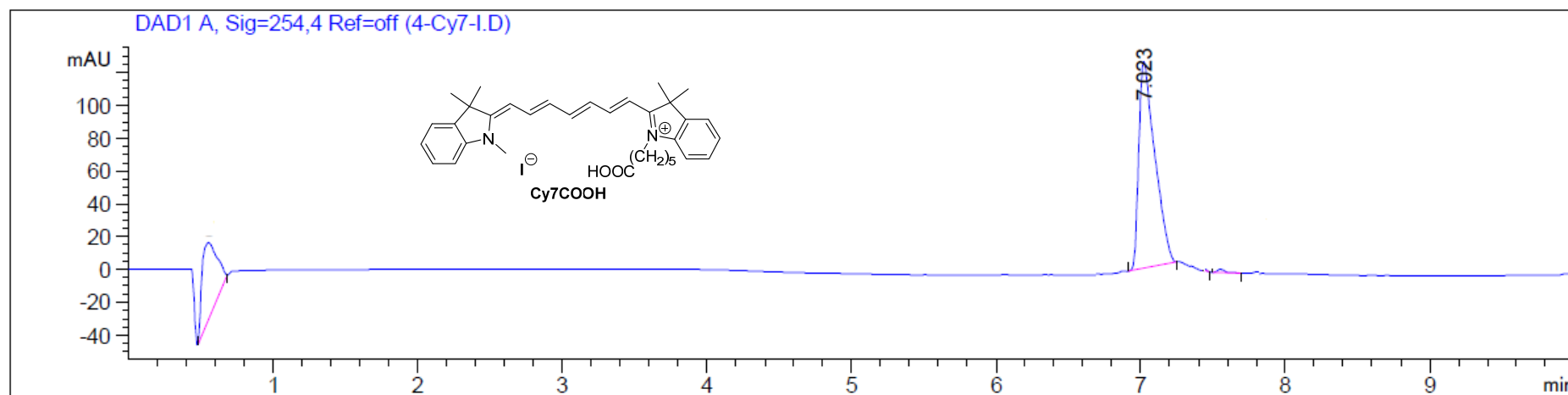


**Figure S27.** Theoretical (top) and experimental (bottom) HRMS spectrum of ICy7NEt<sub>3</sub>.

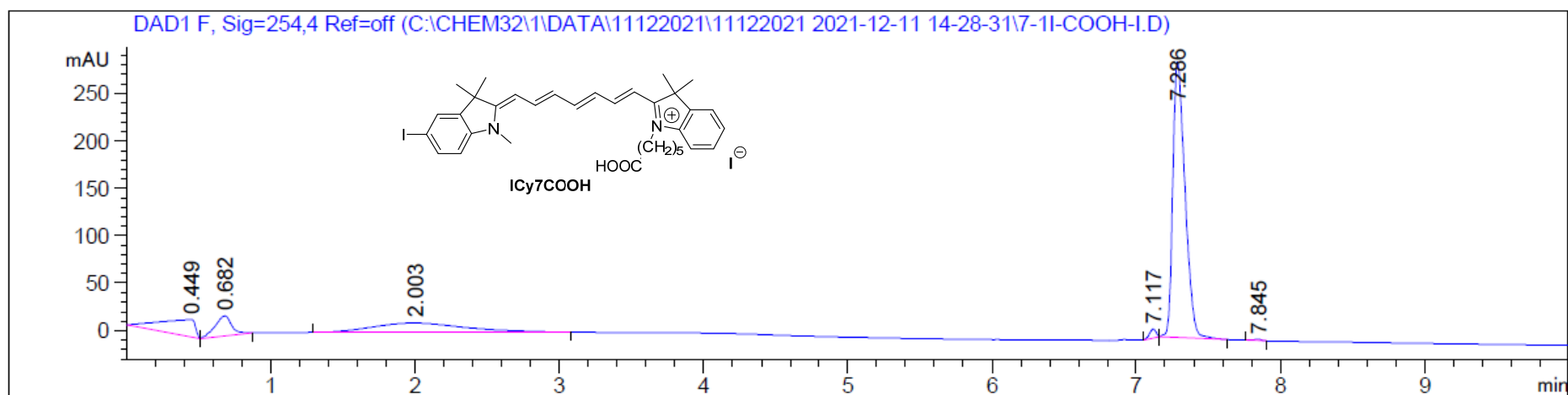


**Figure S28.** Theoretical (top) and experimental (bottom) HRMS spectrum of ICy7PPh<sub>3</sub>.

## 6. HPLC data



**Figure S29.** HPLC chromatogram of **Cy7COOH**.



**Figure S30.** HPLC chromatogram of ICy7COOH.

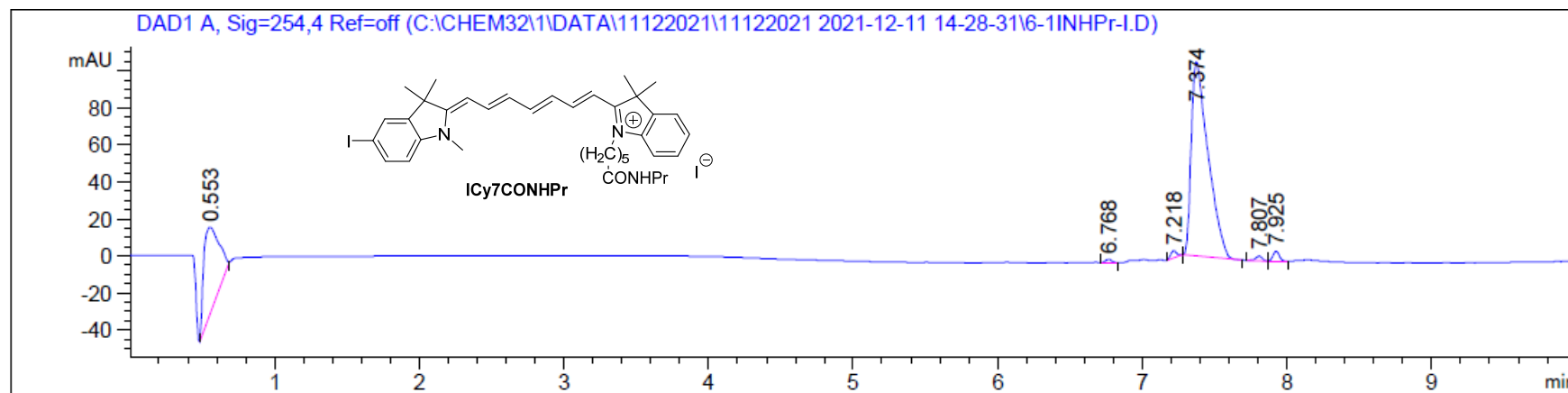


Figure S31. HPLC chromatogram of ICy7CONHPr.

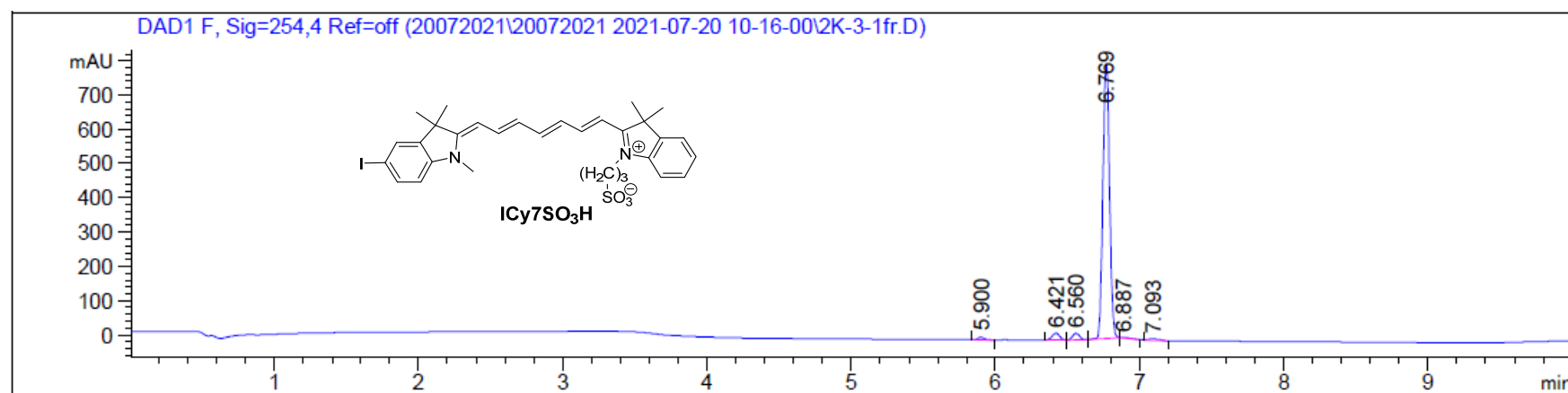
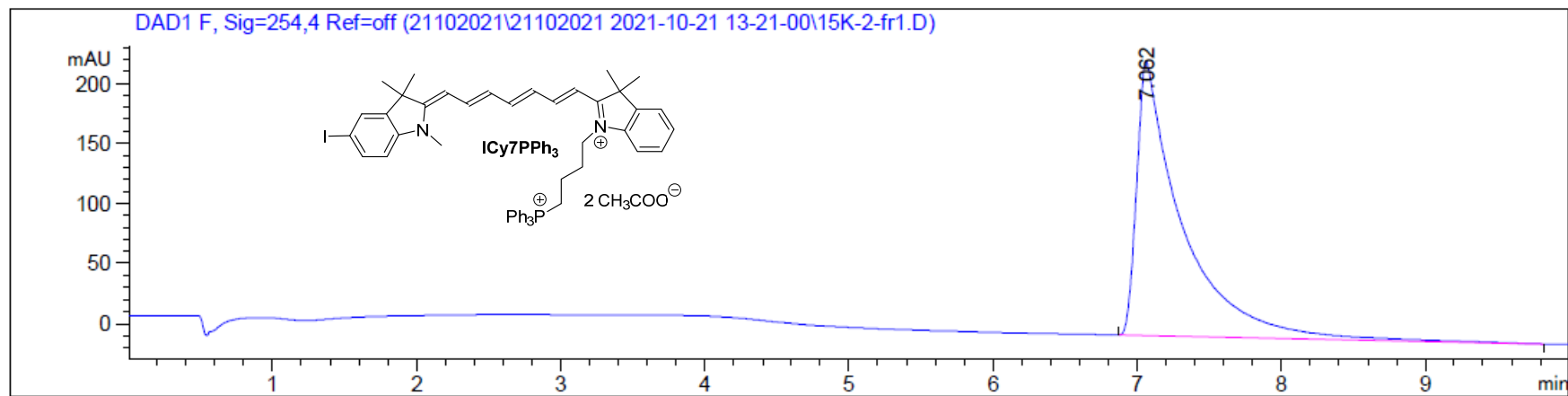
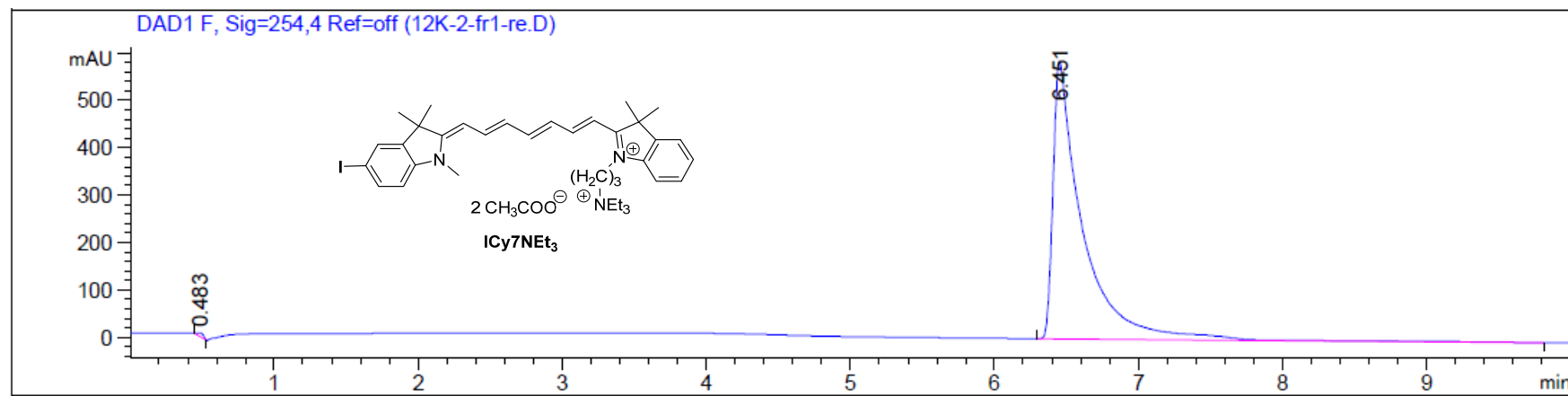


Figure S32. HPLC chromatogram of ICy7SO<sub>3</sub>H.



**Figure S33.** HPLC chromatogram of **ICy7PPh<sub>3</sub>**.



**Figure S34.** HPLC chromatogram of **ICy7NEt<sub>3</sub>**.

