

# SUPPORTING MATERIALS

## **Site-Specific Labeling Of Proteins With Near-IR Heptamethine Cyanine Dyes**

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## A. Characterization Spectra of Compound 1a

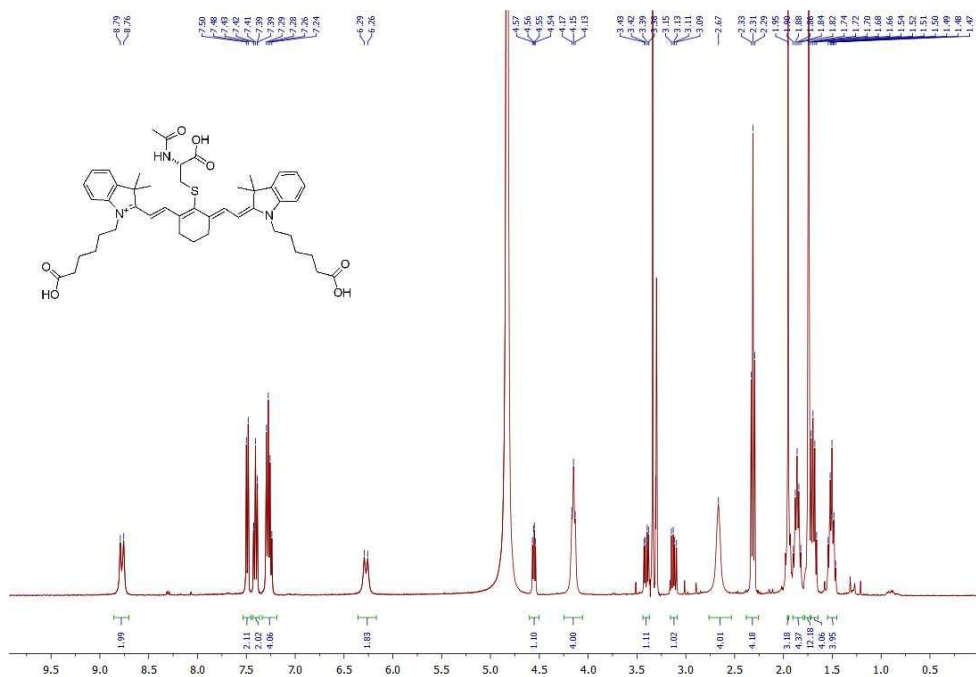


Figure S1. <sup>1</sup>H NMR of compound 1a in Methanol-d<sub>4</sub>

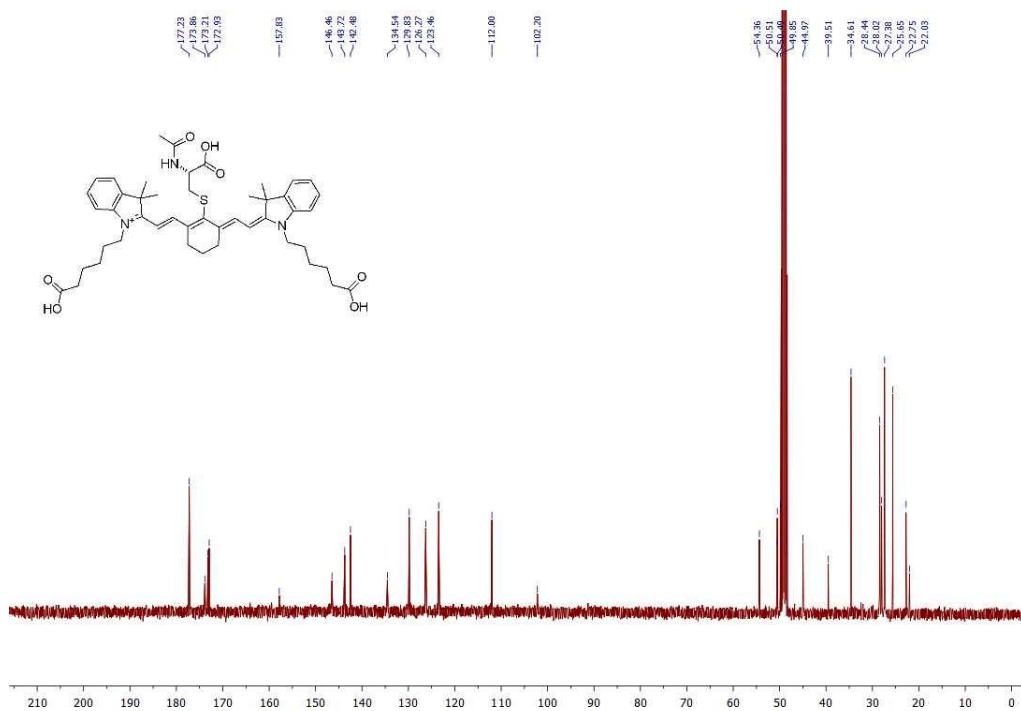
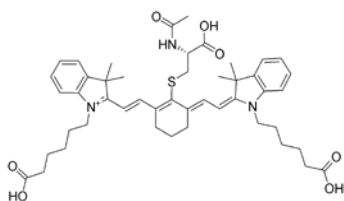


Figure S2. <sup>13</sup>C NMR of compound 1a in Methanol-d<sub>4</sub>



Chemical Formula:  $C_{47}H_{60}N_3O_7S^+$   
Exact Mass: 810.4146

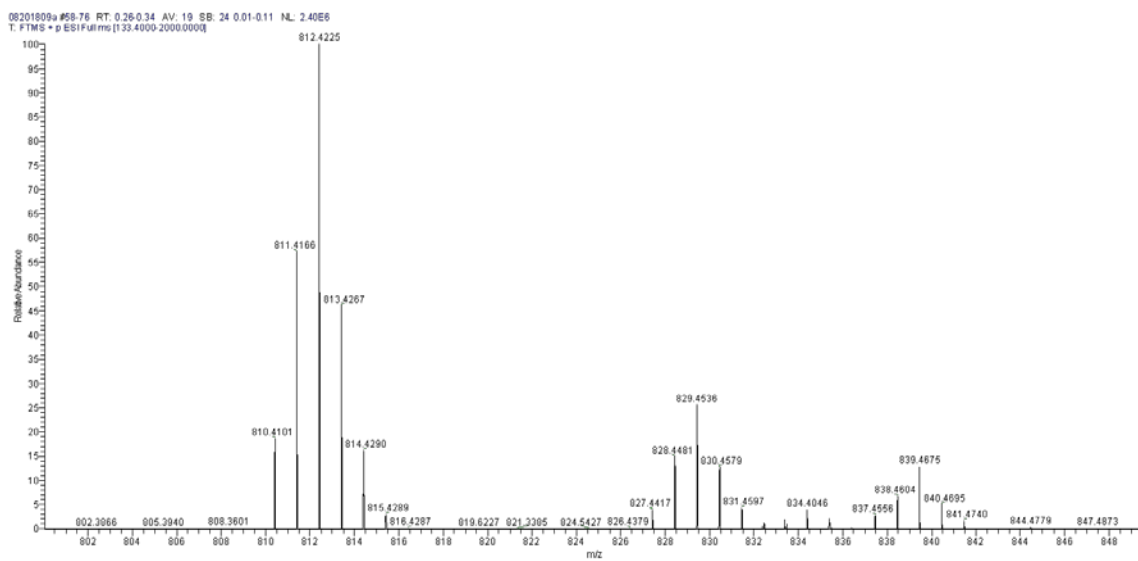


Figure S3. HRMS of compound 1a

## B. Characterization Spectra of Compound 1b

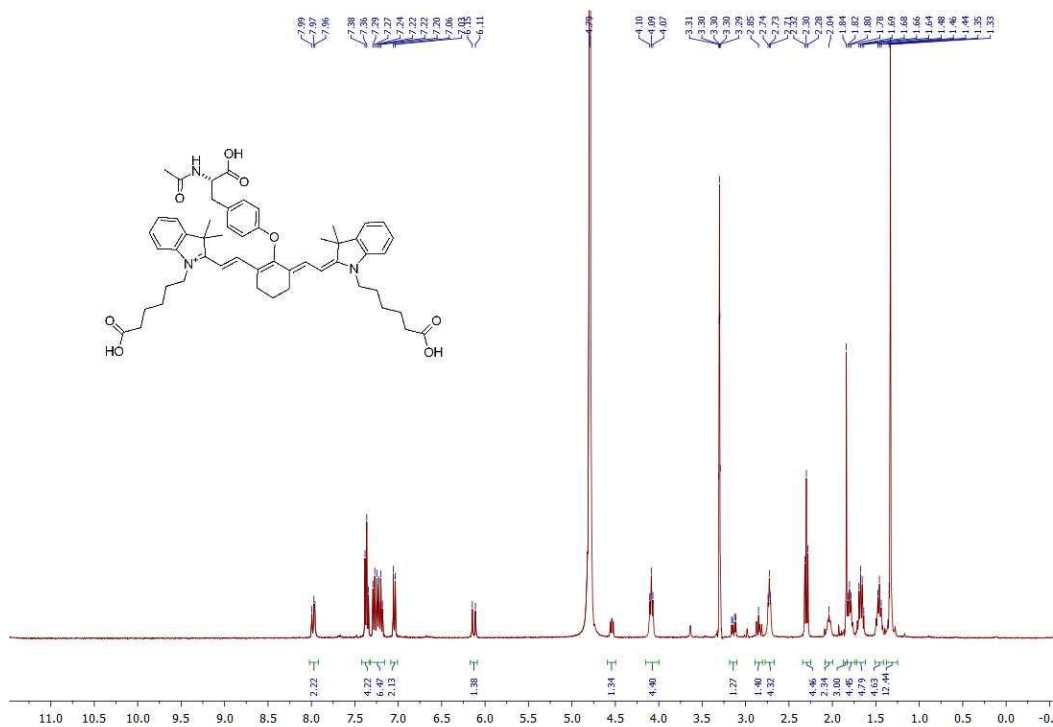


Figure S4. <sup>1</sup>H NMR of compound 1b in Methanol-d<sub>4</sub>

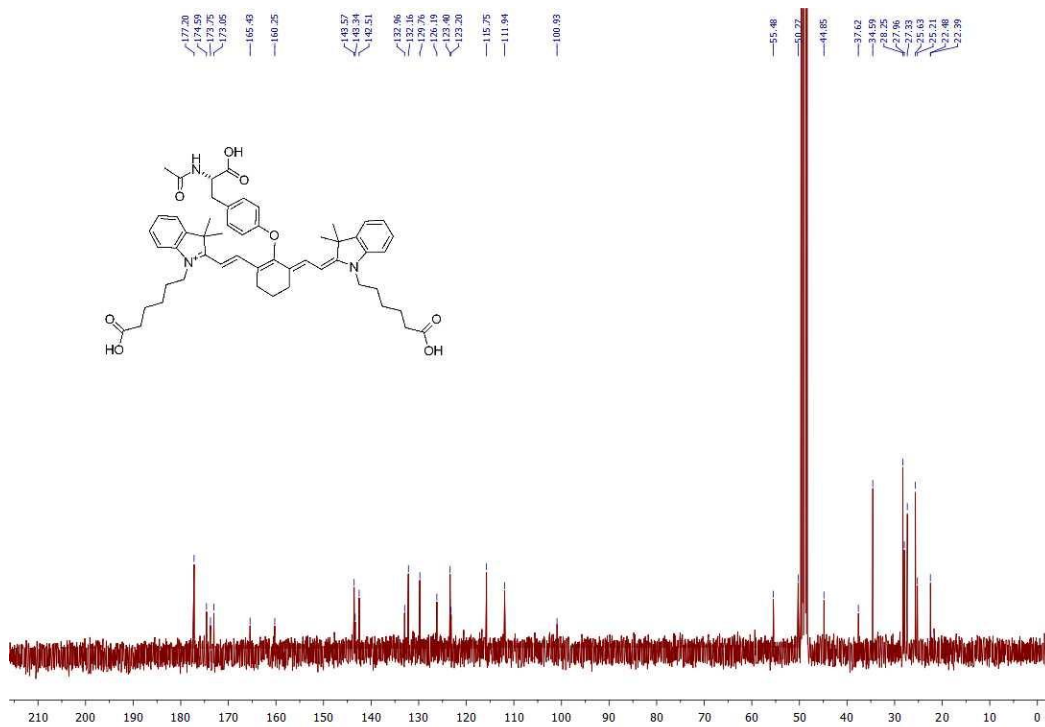
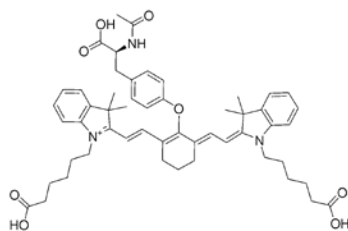


Figure S5. <sup>13</sup>C NMR of compound 1b in Methanol-d<sub>4</sub>



Chemical Formula:  $C_{53}H_{64}N_3O_8^+$   
Exact Mass: 870.4688

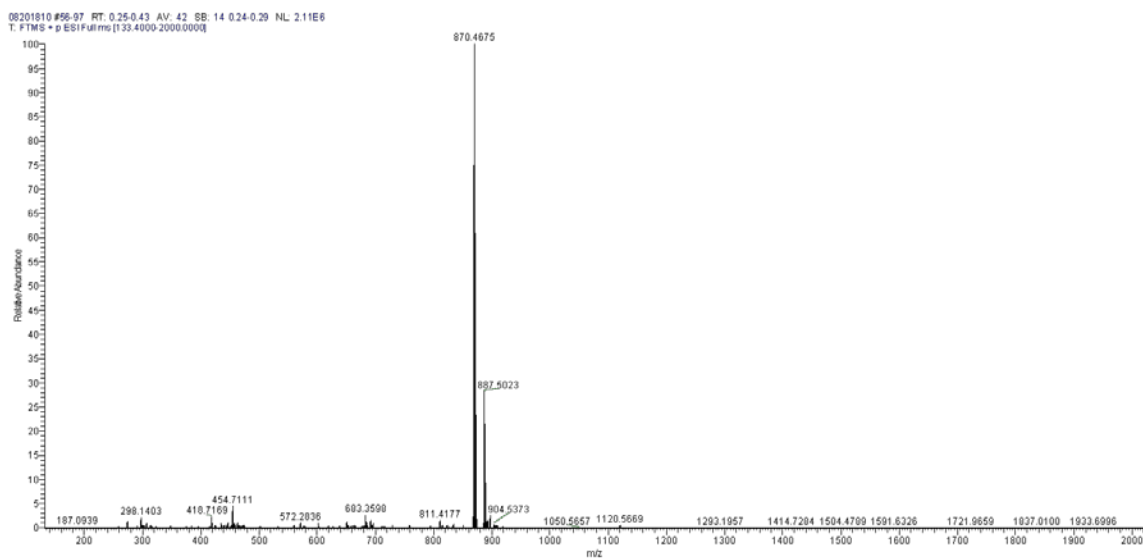


Figure S6.  $^1H$  NMR of compound 1b

### C. Characterization Spectra of Compound 1c

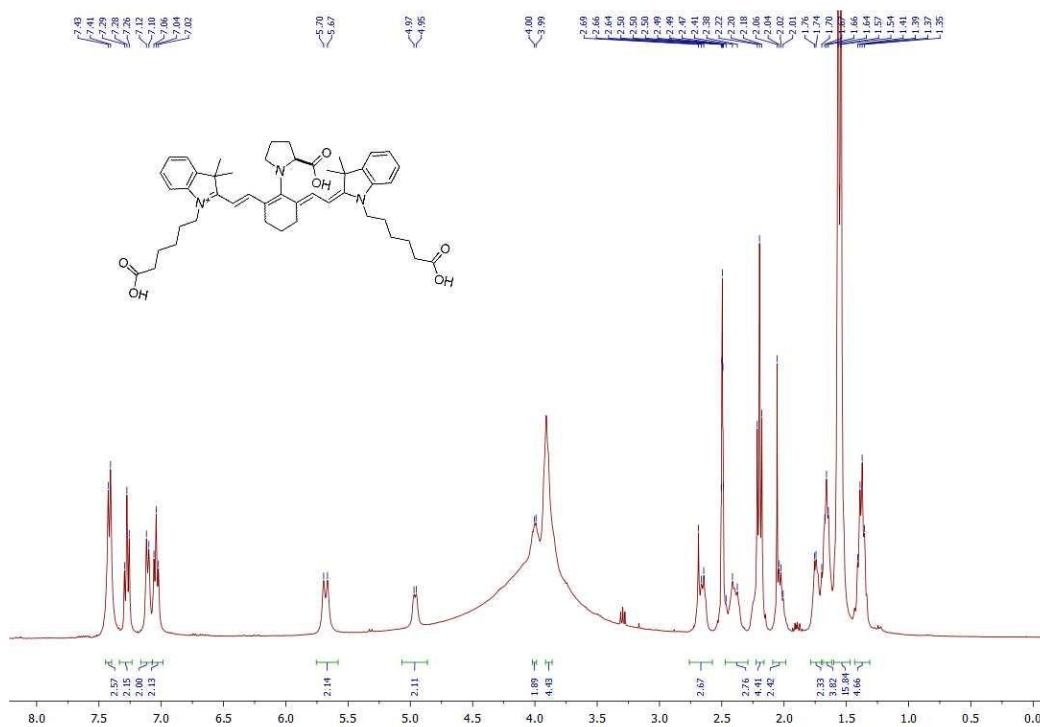


Figure S7. <sup>1</sup>H NMR of compound 1c in Methanol-d<sub>4</sub>

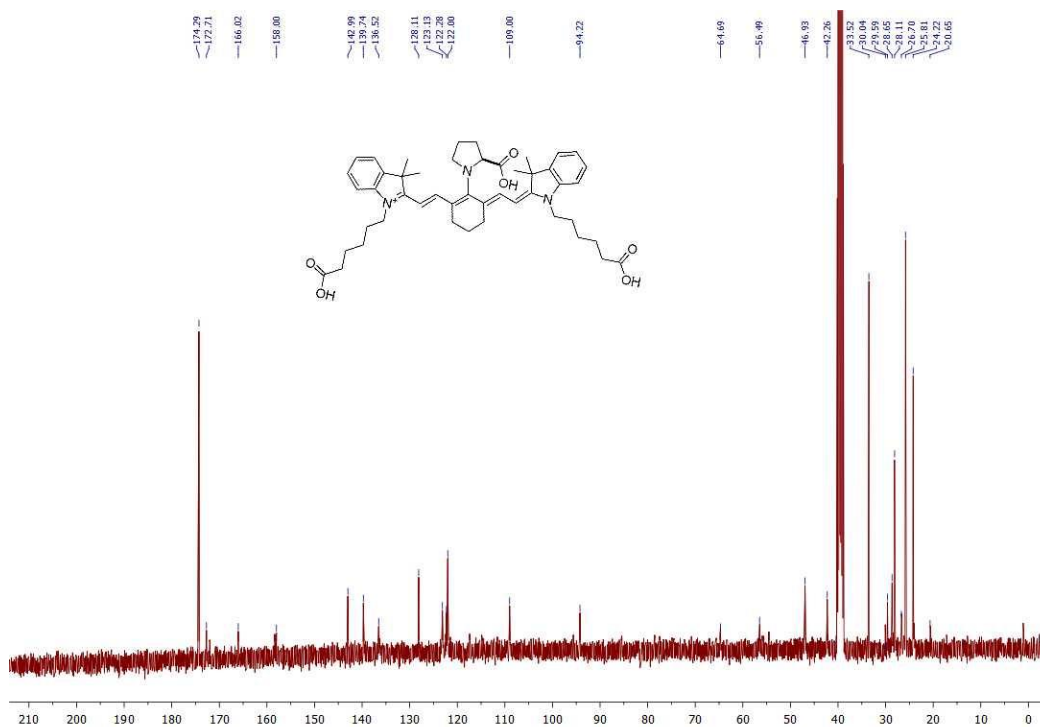
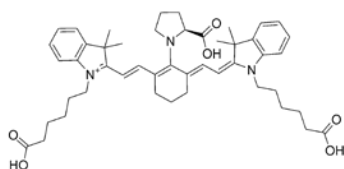


Figure S8. <sup>13</sup>C NMR of compound 1c in Methanol-d<sub>4</sub>



Chemical Formula:  $C_{47}H_{60}N_3O_6^+$   
Exact Mass: 762.4477

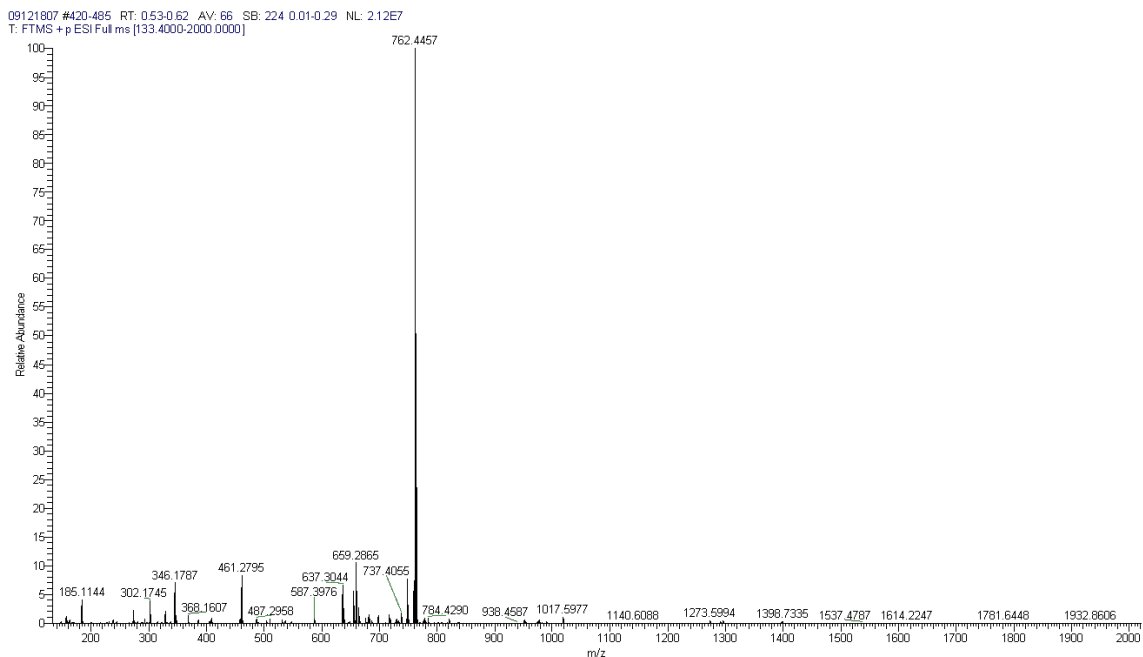


Figure S9. HRMS of compound 1c



## D. Characterization Spectra of Compound 1d

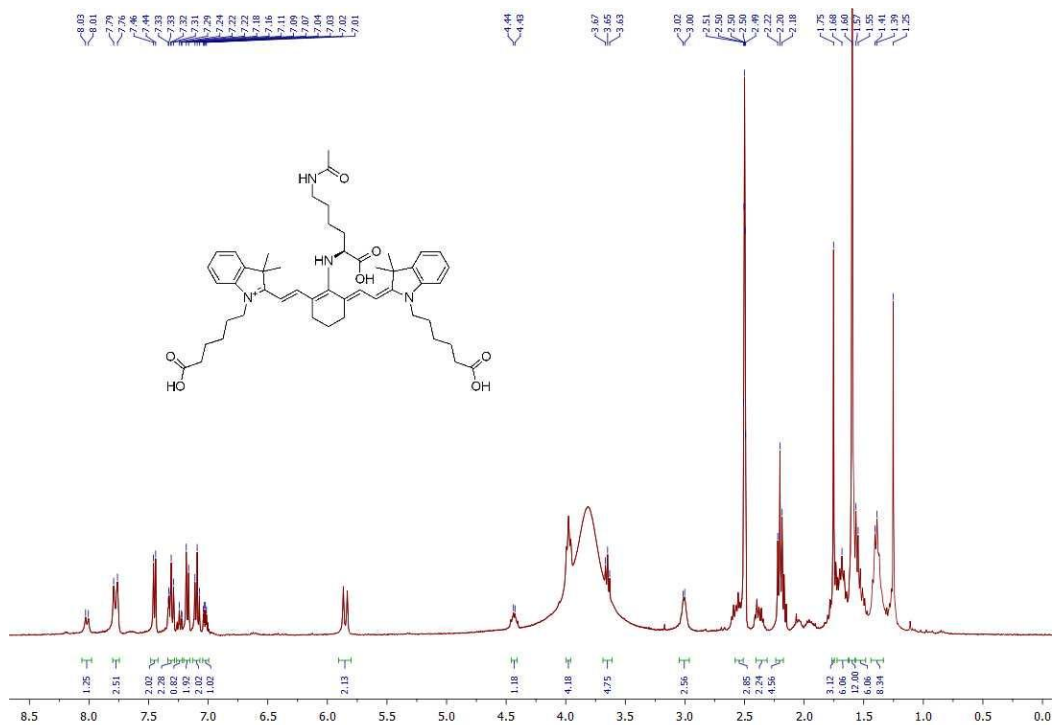


Figure S10. <sup>1</sup>H NMR of compound 1d in Methanol-d<sub>4</sub>

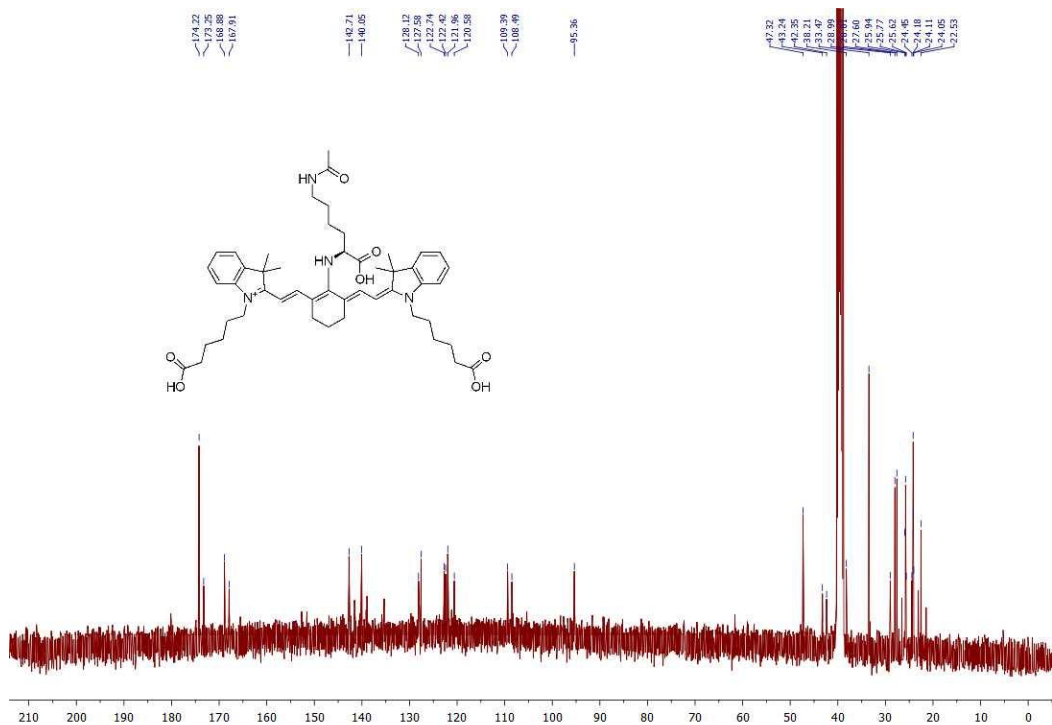
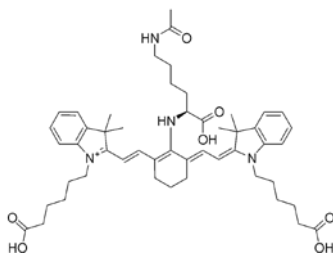


Figure S11. <sup>13</sup>C NMR of compound 1d in Methanol-d<sub>4</sub>



Chemical Formula:  $C_{50}H_{67}N_4O_7^+$   
Exact Mass: 835.5004

09171809.s #1593-1817 RT: 2.01-2.30 AV: 225 SB: 394 0.02-0.52 NL: 5.40E7  
T: FTMS +p ESI Full ms [100.0000-1000.0000]

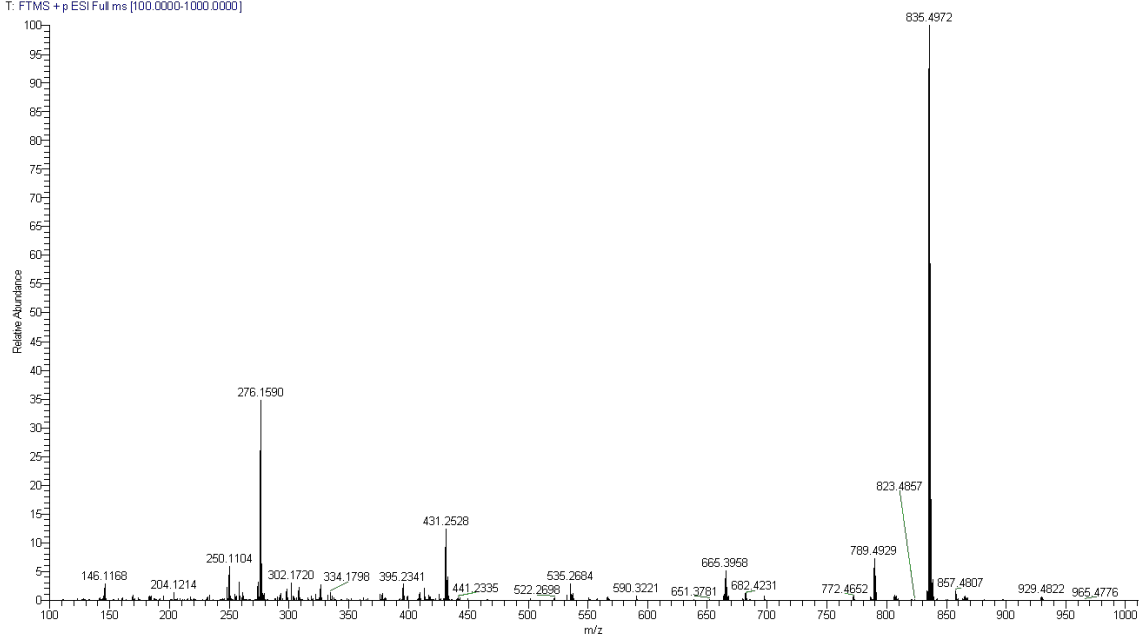
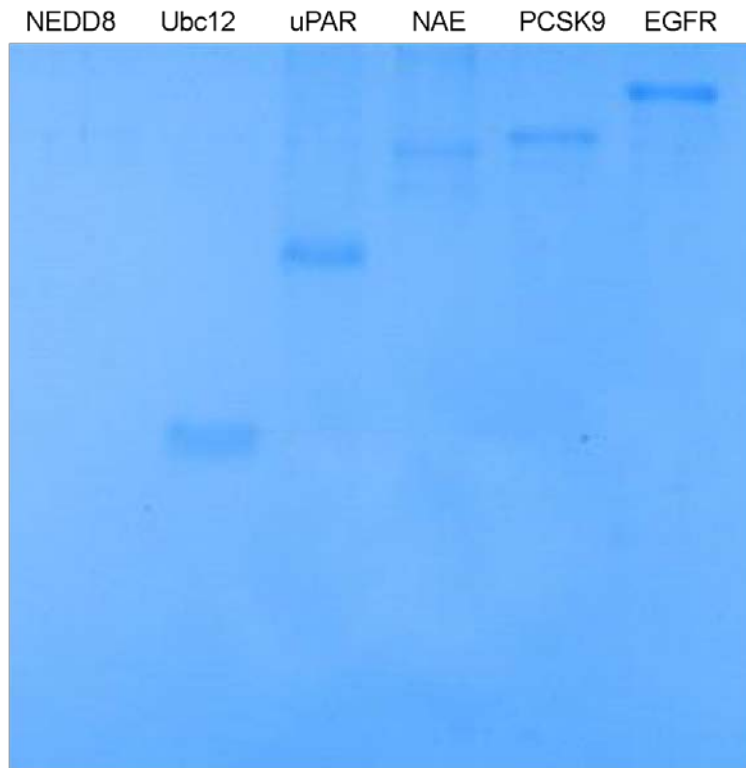


Figure S12. HRMS of compound 1d

## E. Coomassie Blue Staining of Diverse Proteins Gel



**Figure S13.** CBB-G250 staining of SDS-PAGE gel referred to Figure 6.