Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

A comparison of chemiluminescent acridinium dimethylphenyl ester labels with different conjugation sites

Supplementary Material

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Table of contents

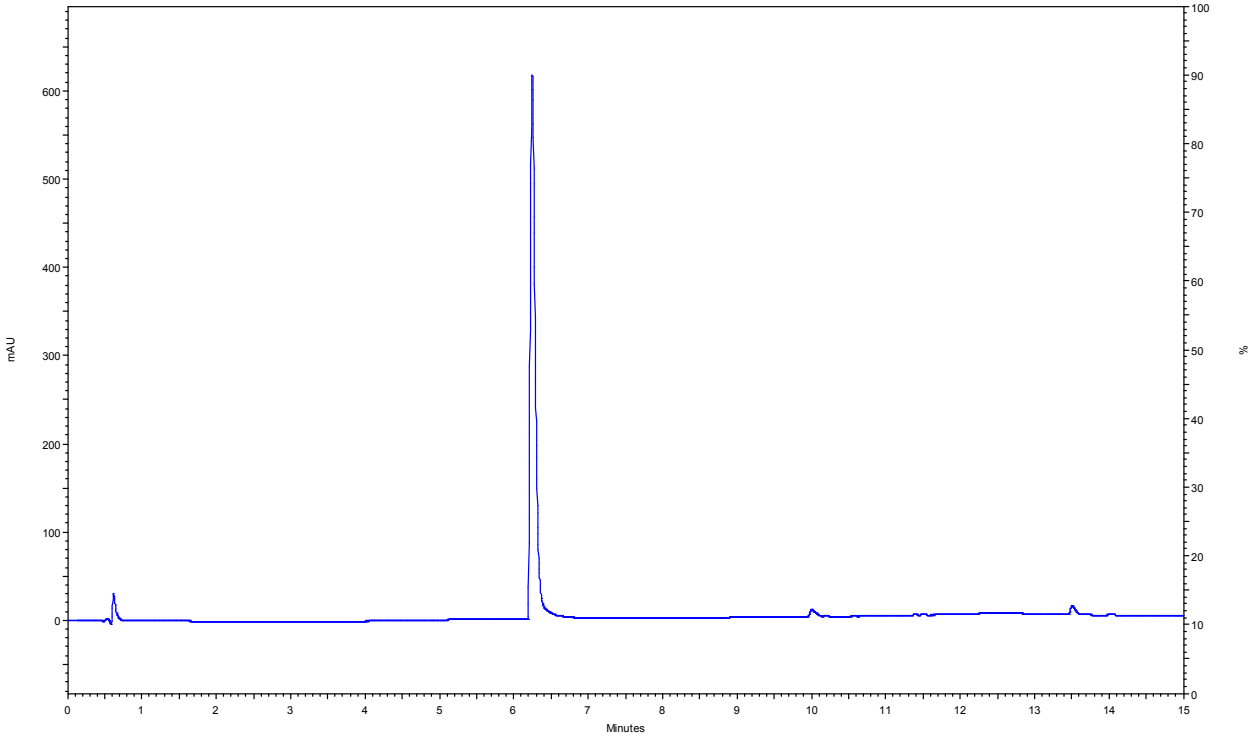
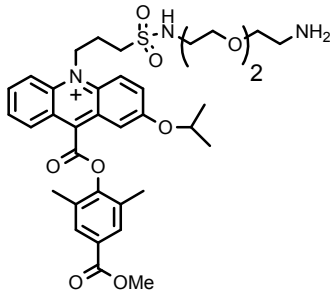


Figure S1A. HPLC trace of **2a**.



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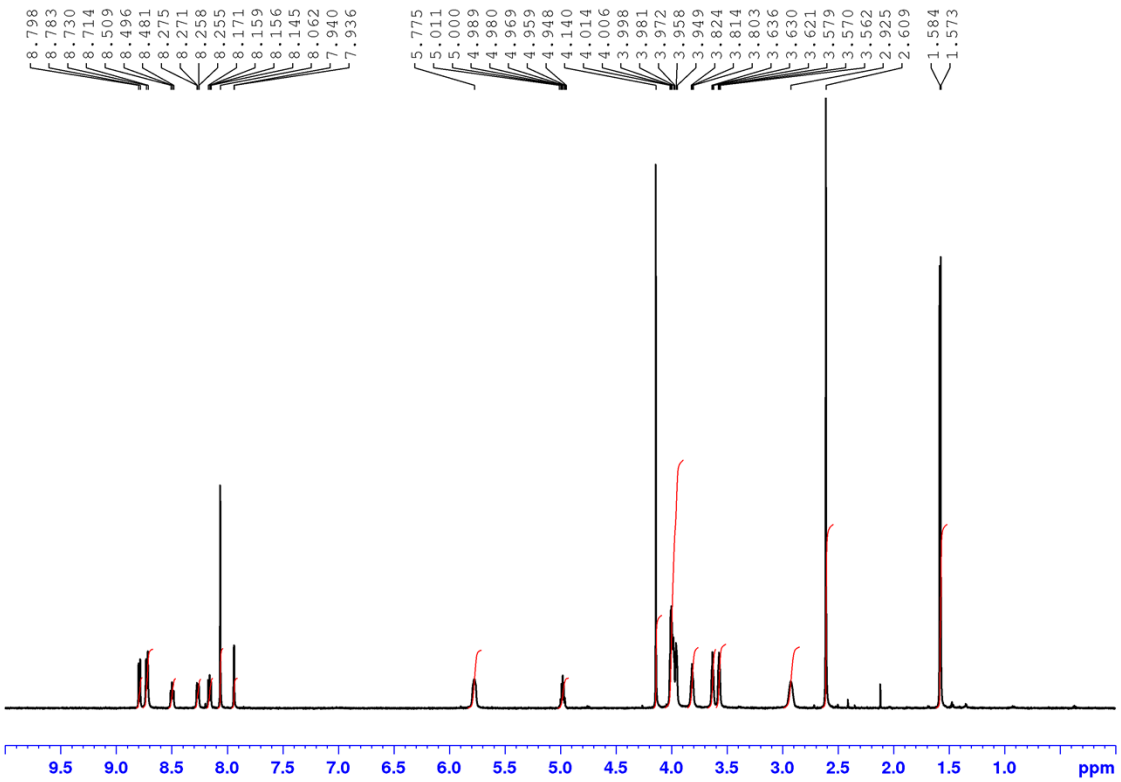
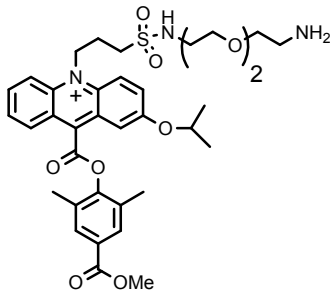


Figure S1B. ^{1}H-NMR spectrum of **2a.**



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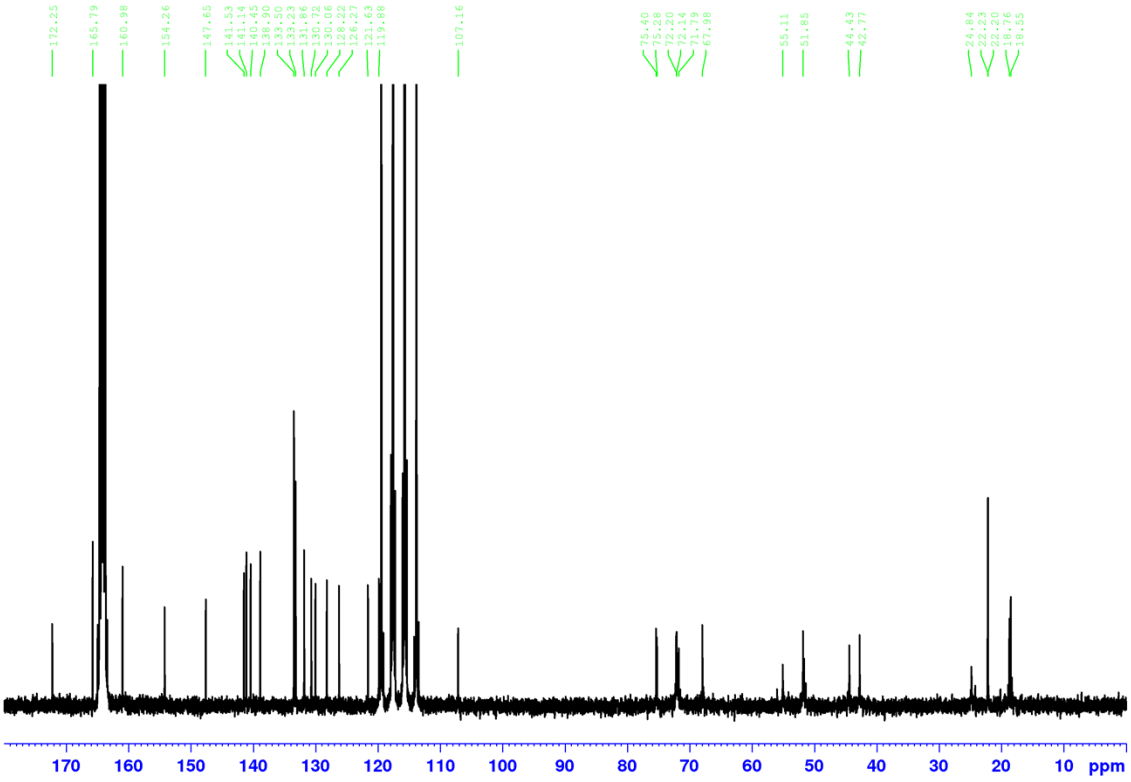
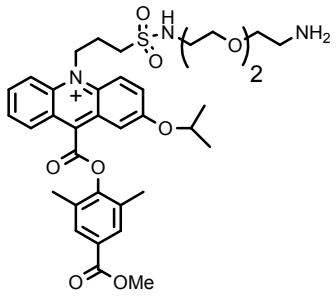


Figure S1C. ^{13}C-NMR spectrum of **2a**.



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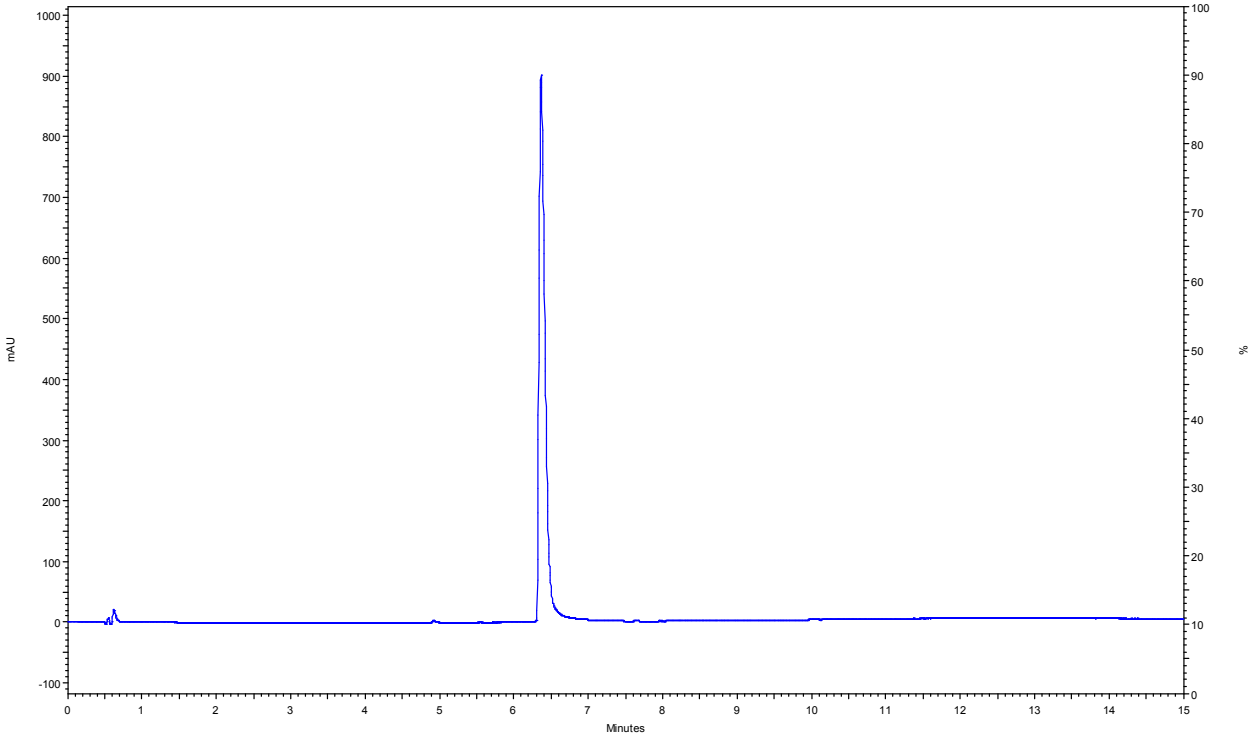

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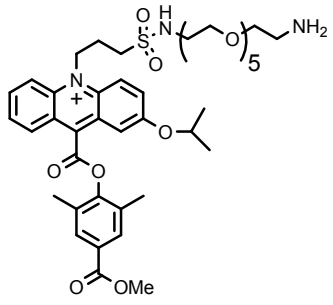

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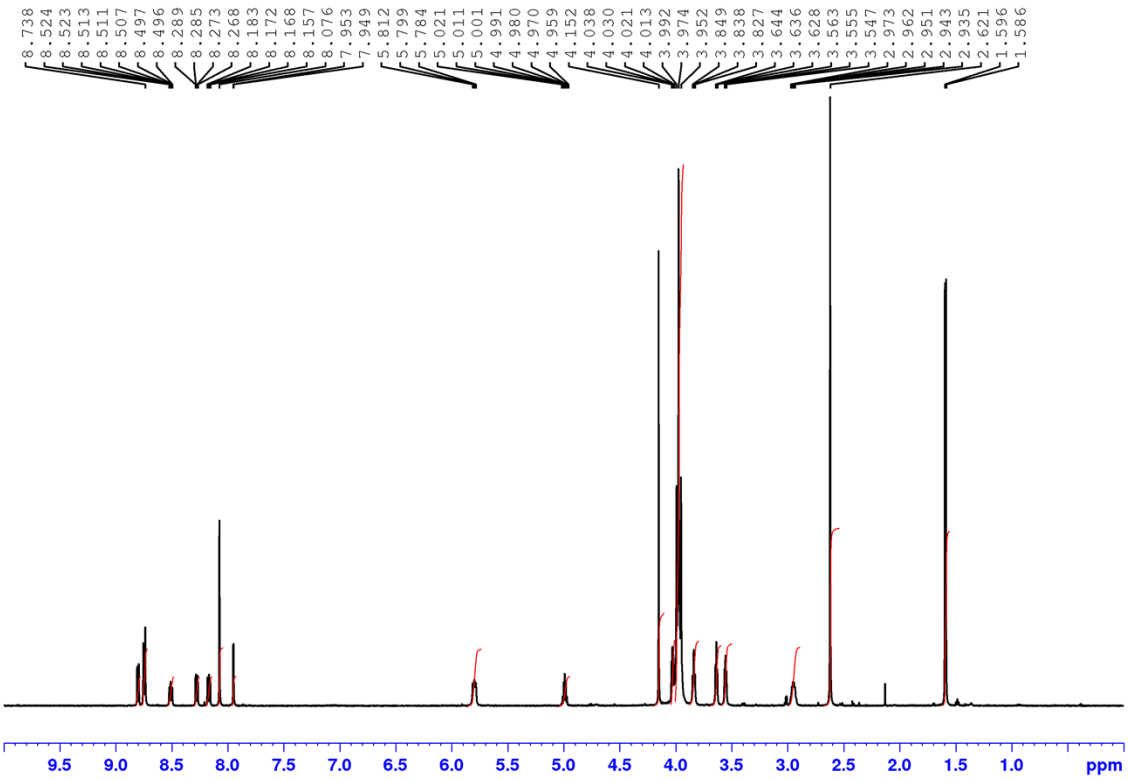

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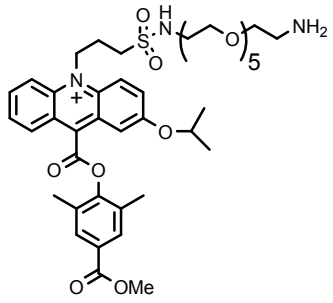

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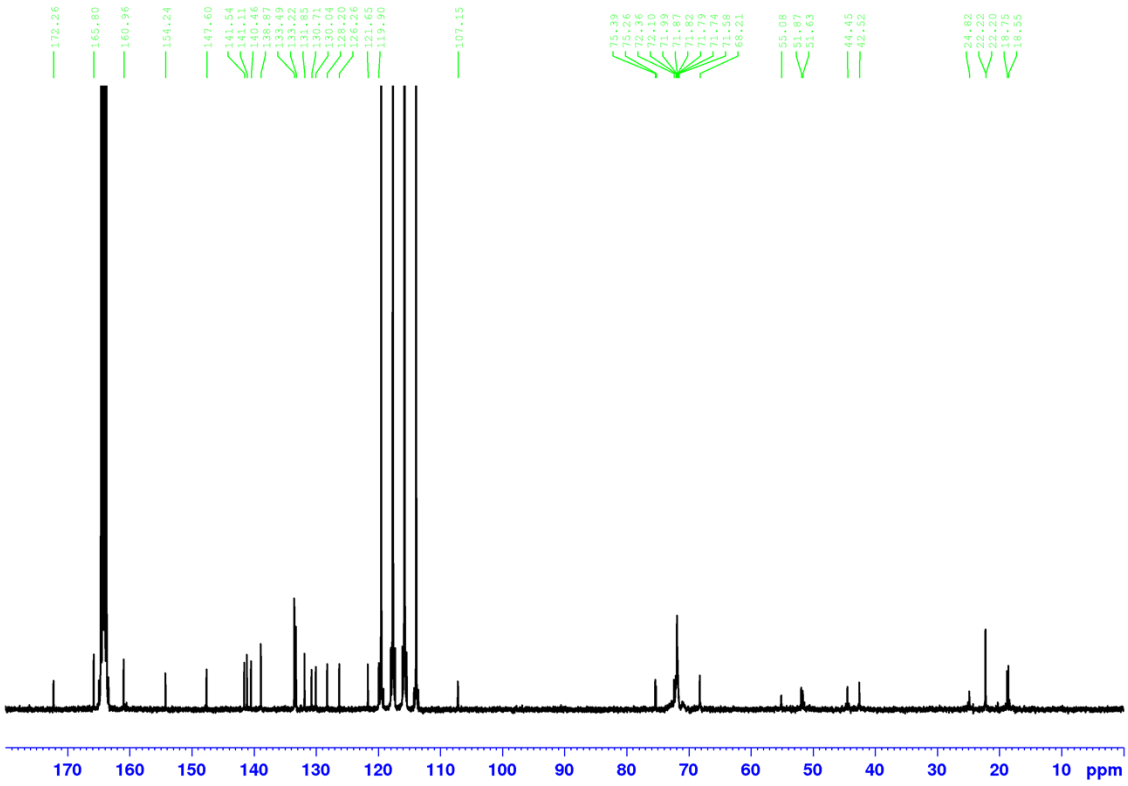

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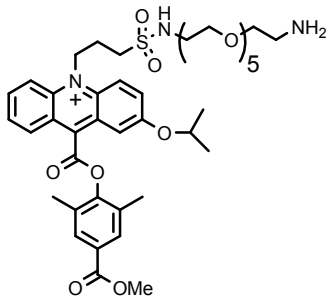

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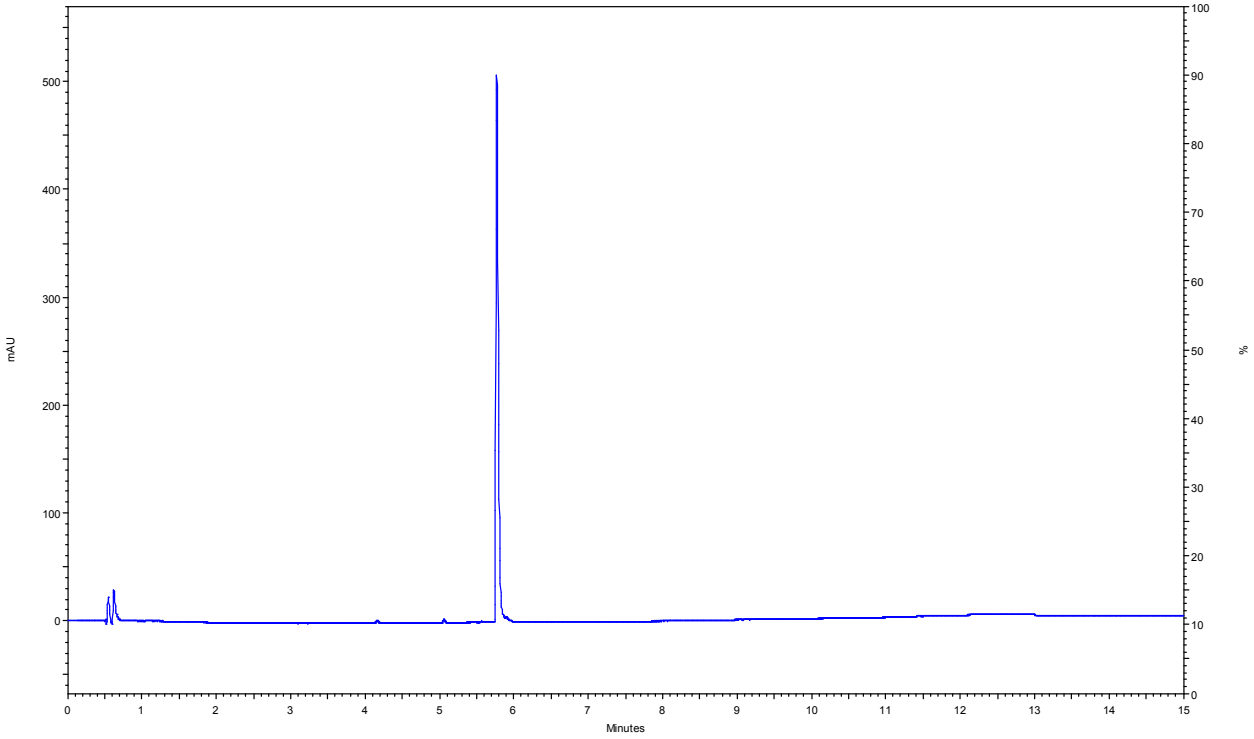

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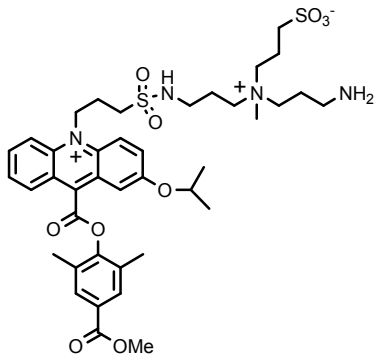

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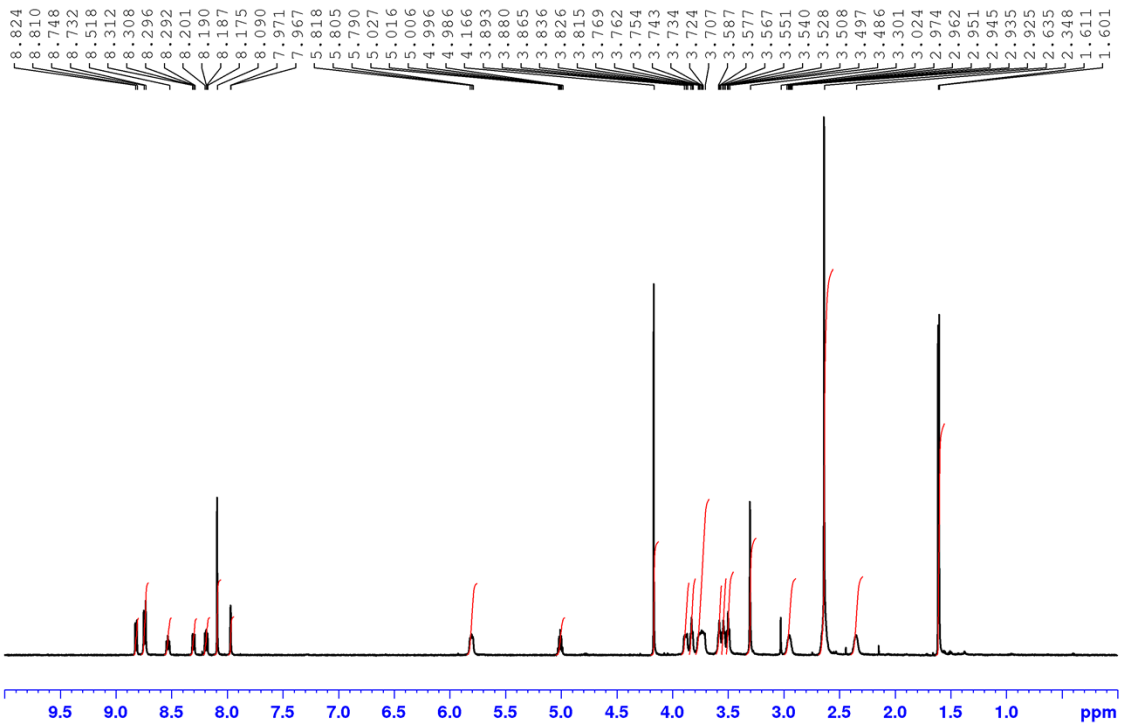

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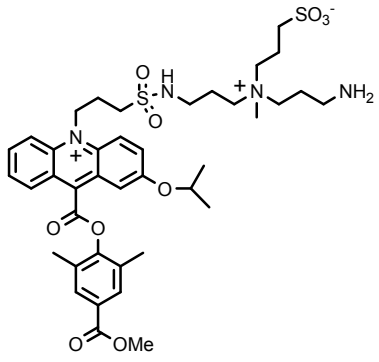

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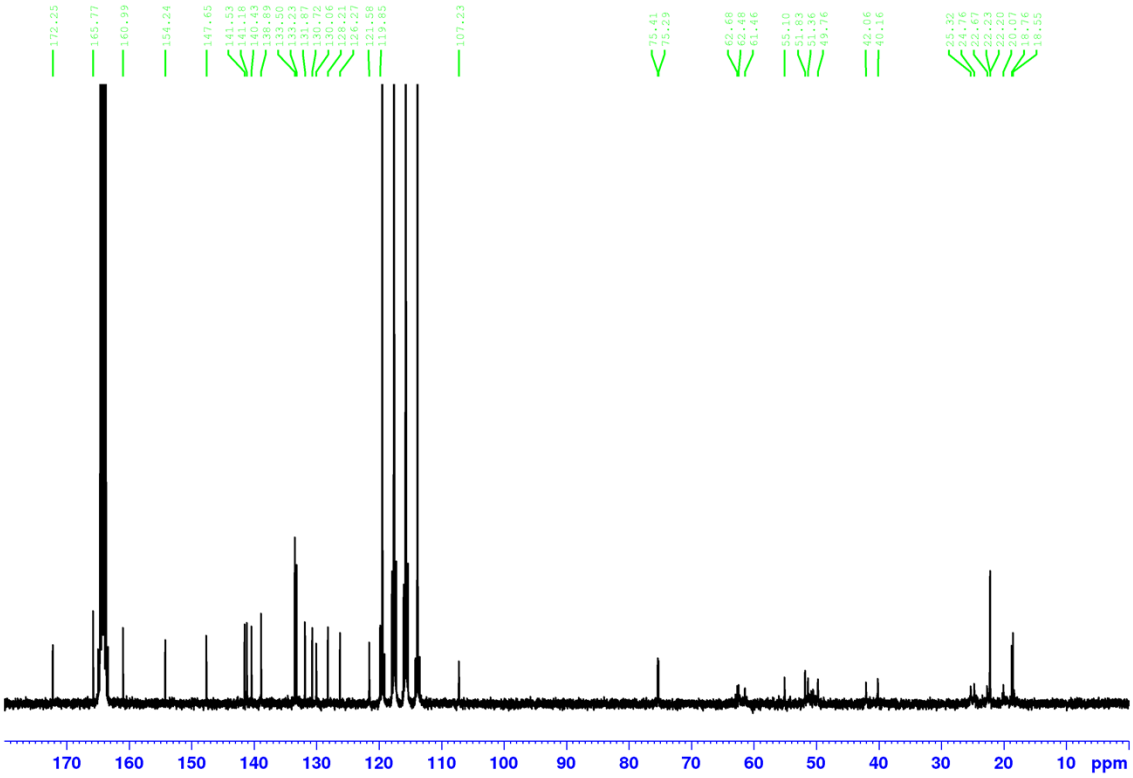
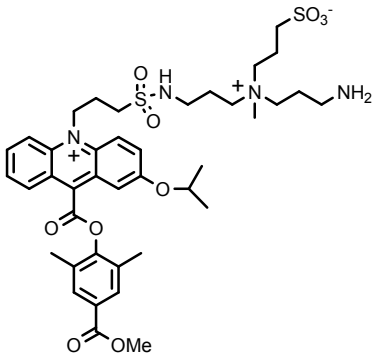


Figure S3C. ^{13}C-NMR of **2c**.



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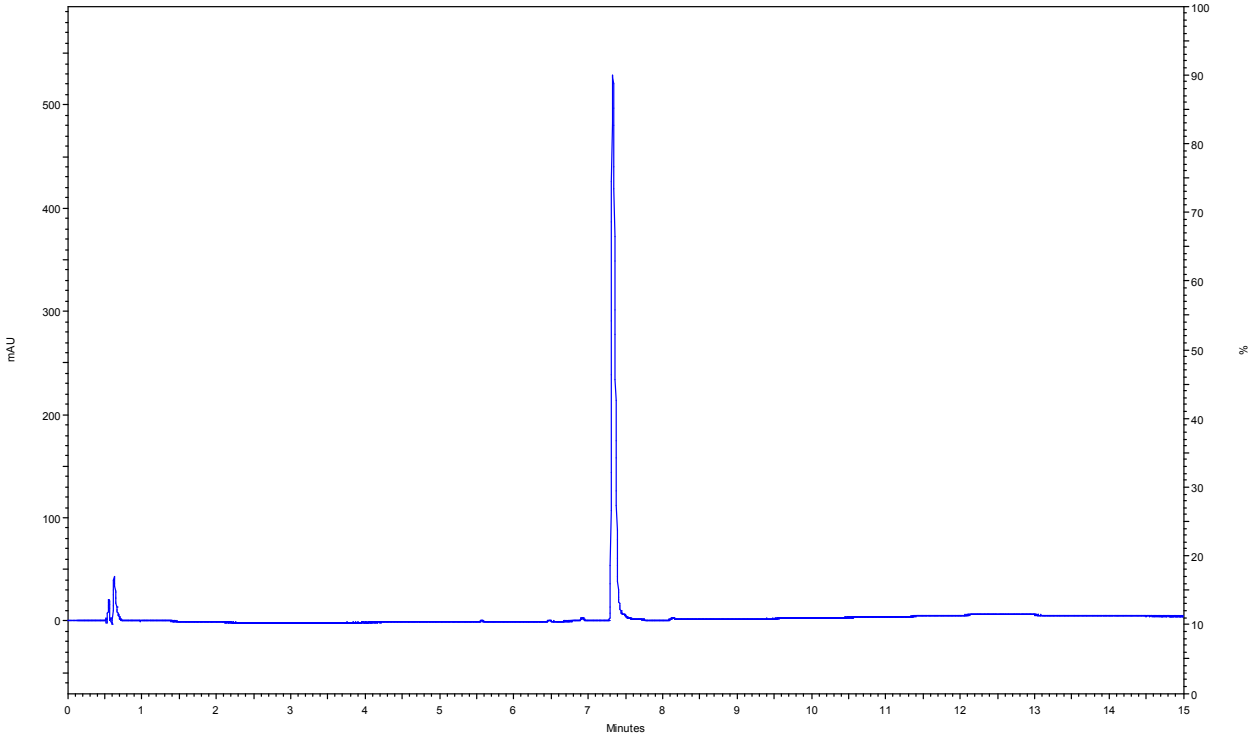

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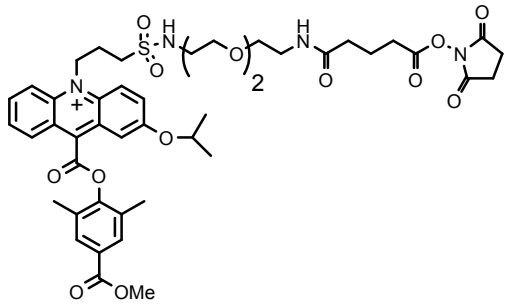

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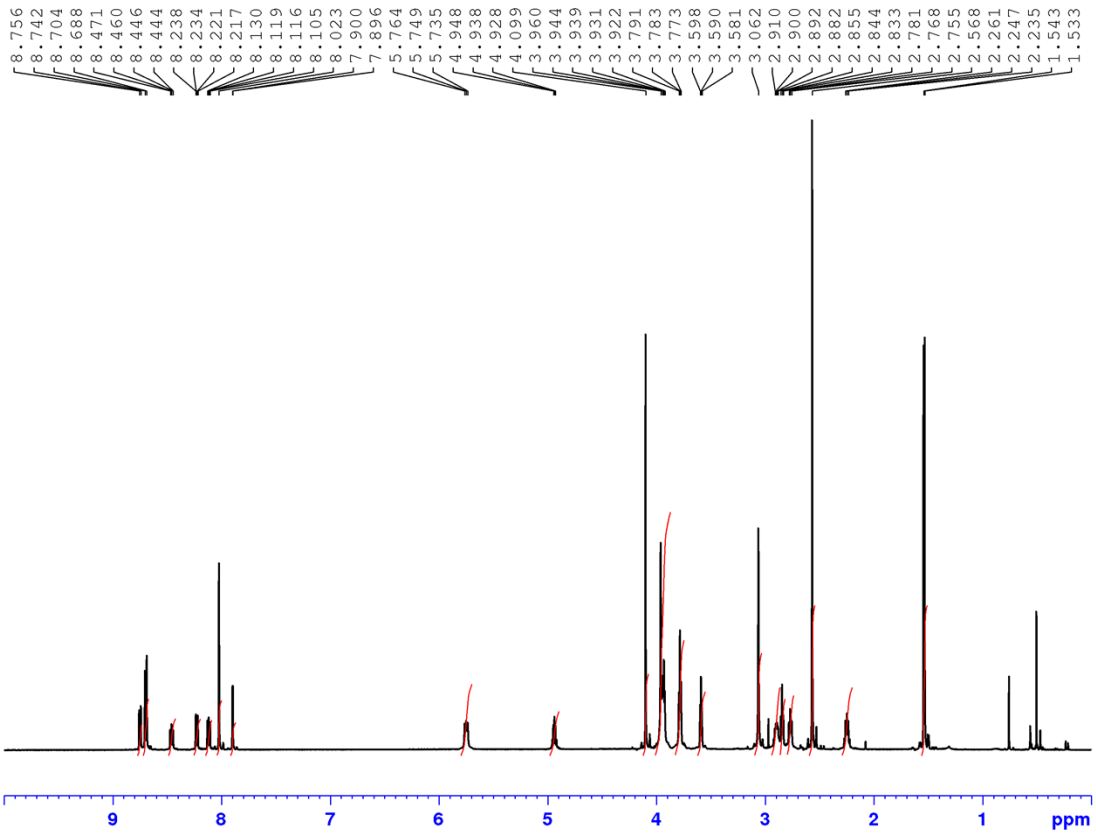

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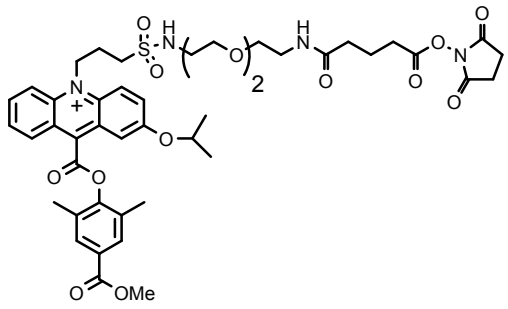

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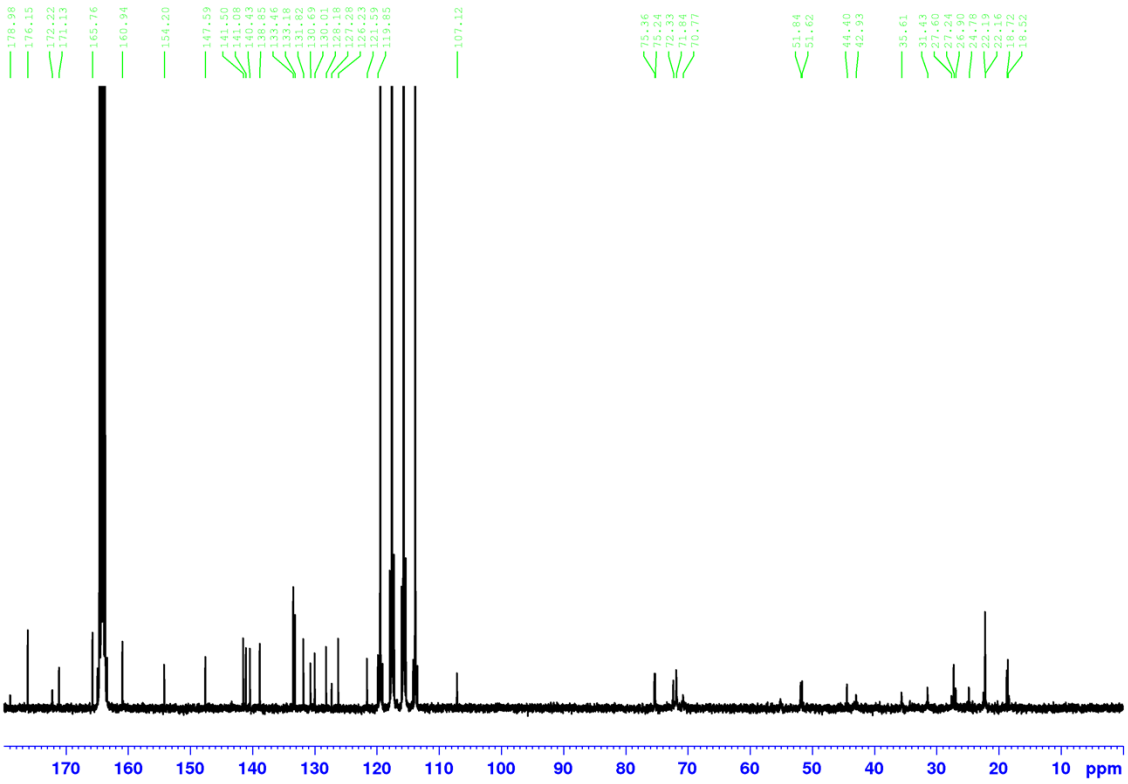

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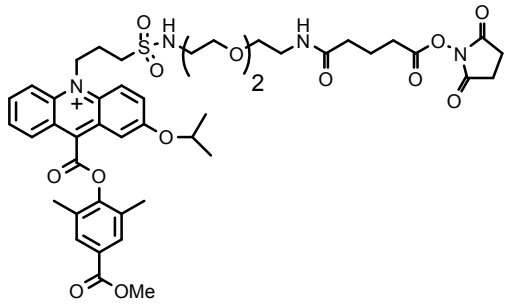

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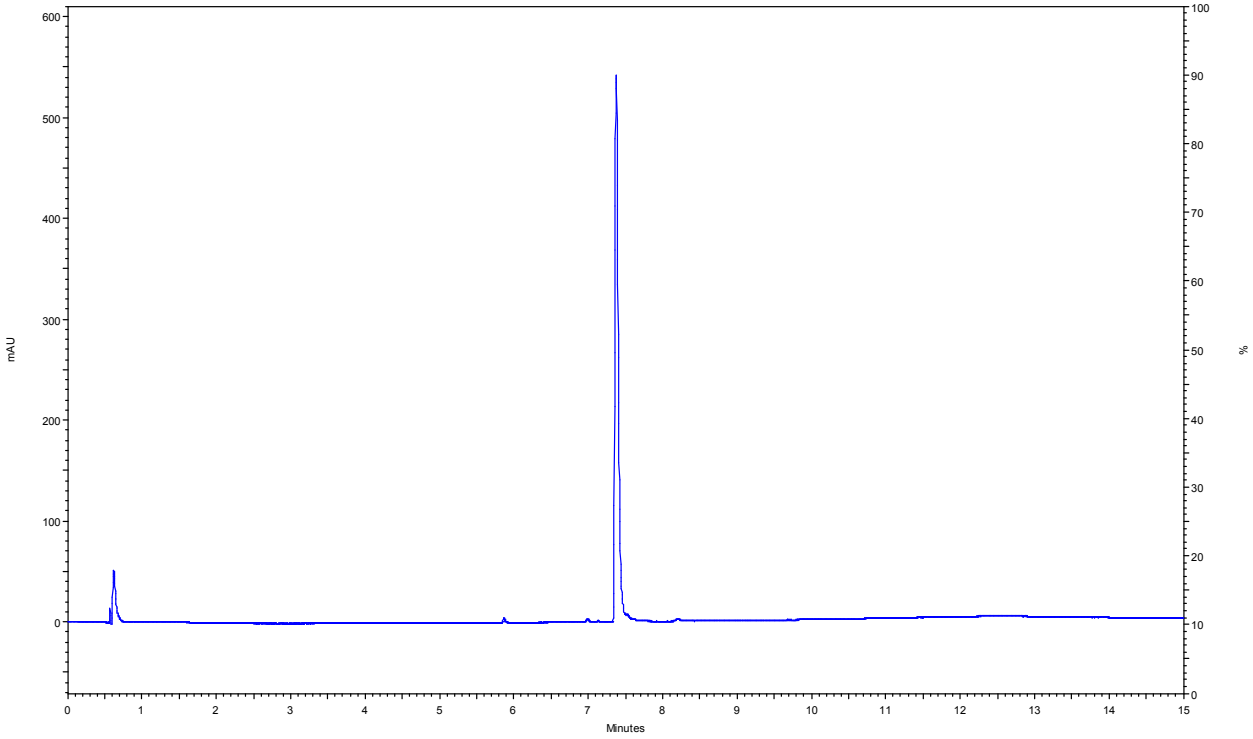

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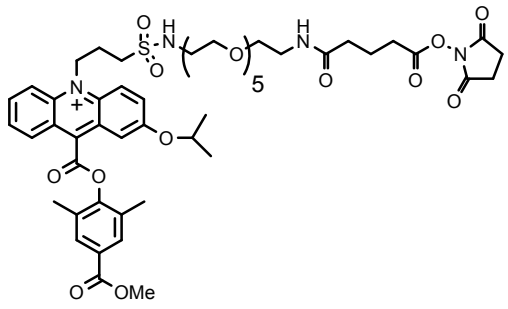

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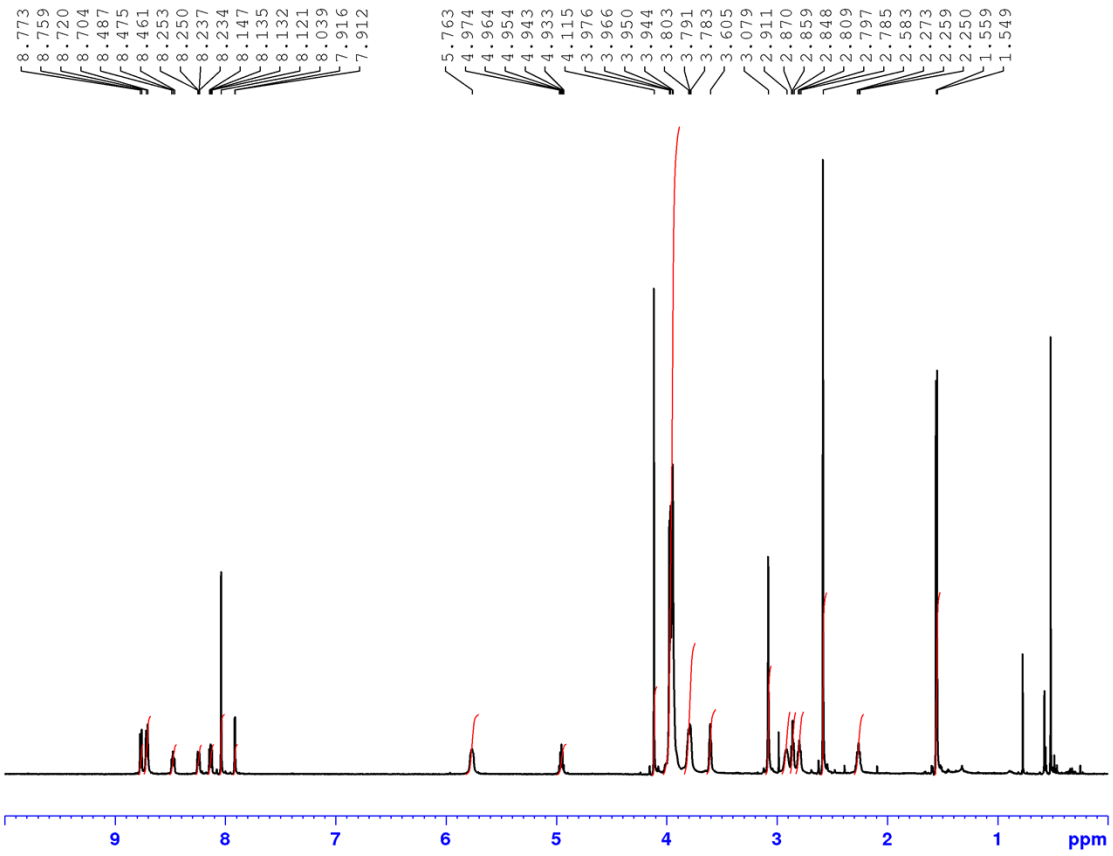
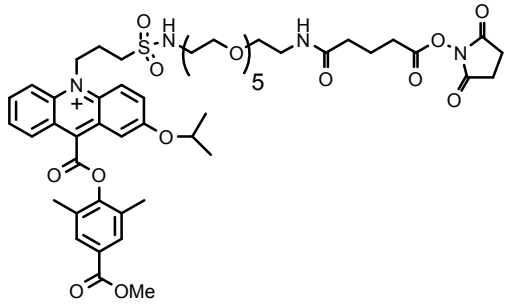


Figure S5B. ^{1}H-NMR spectrum of **3b**.



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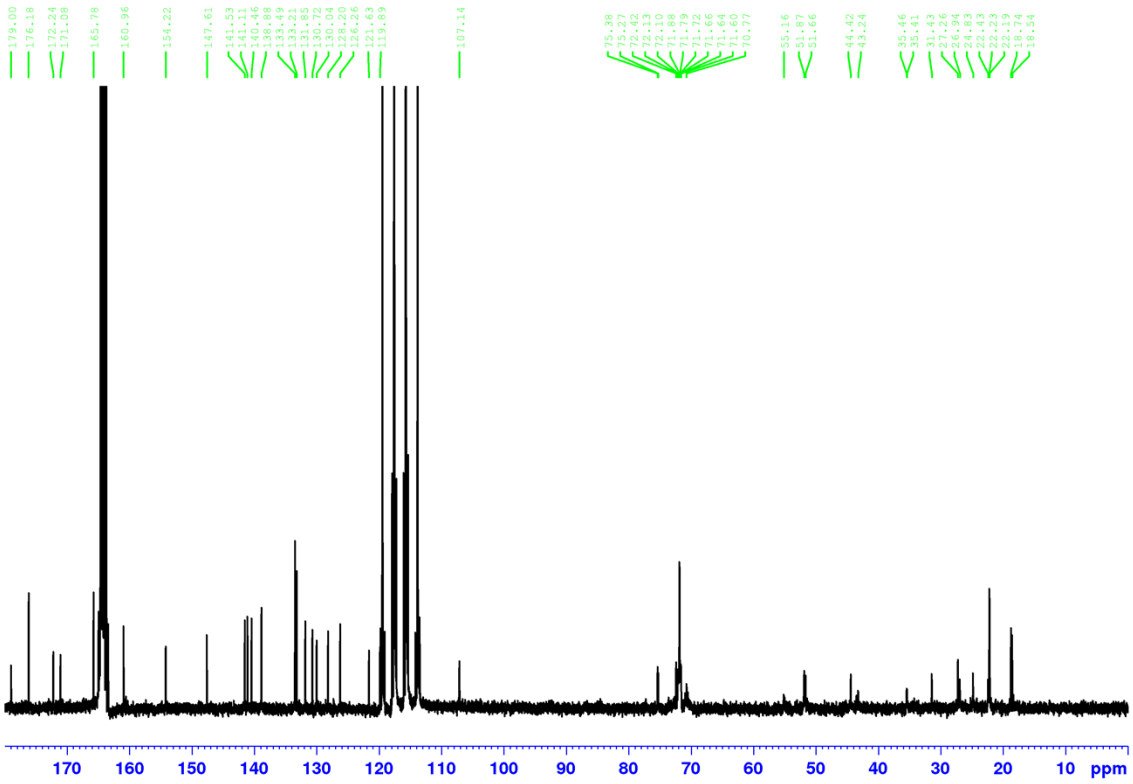
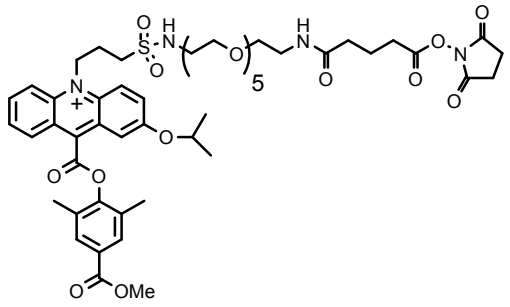


Figure S5C. ^{13}C-NMR spectrum of **3b**.



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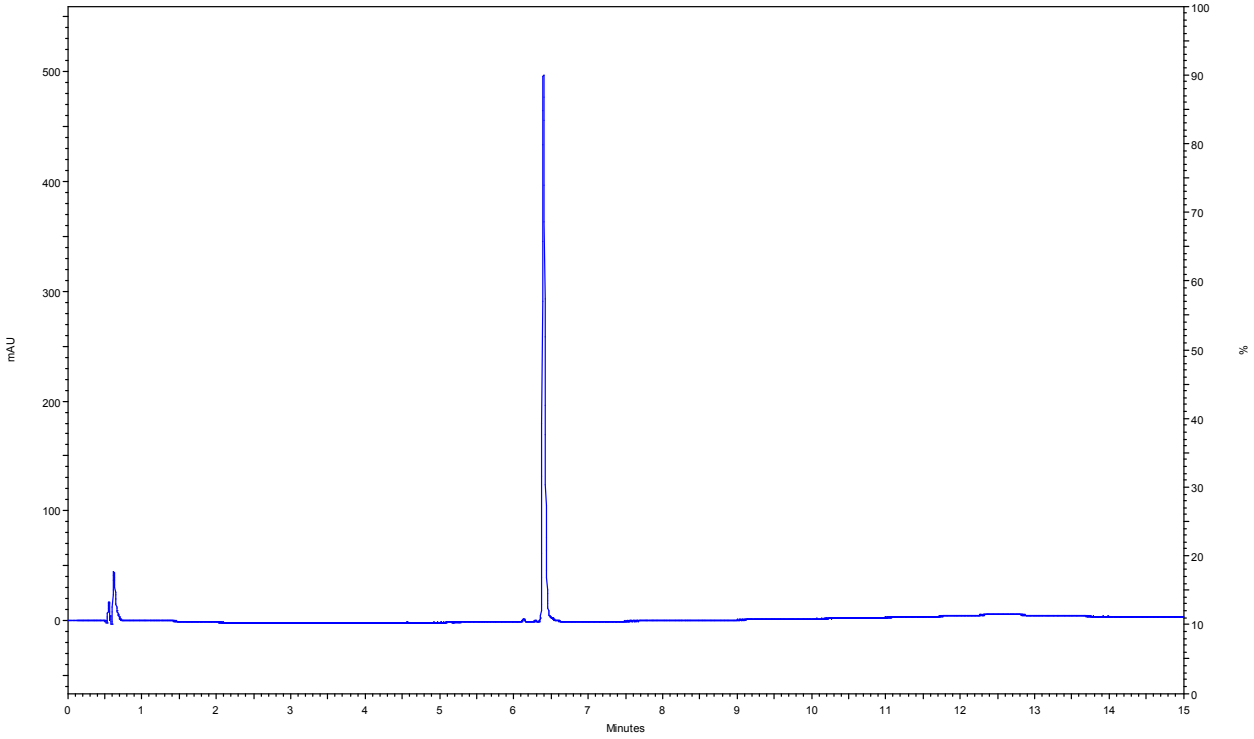

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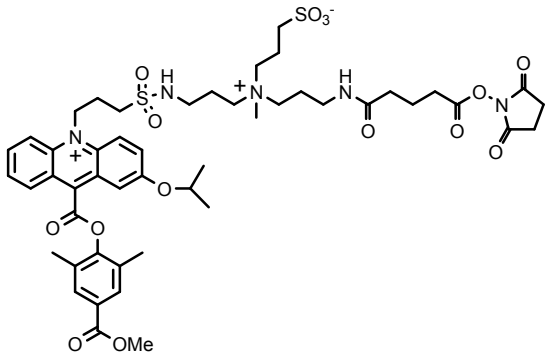

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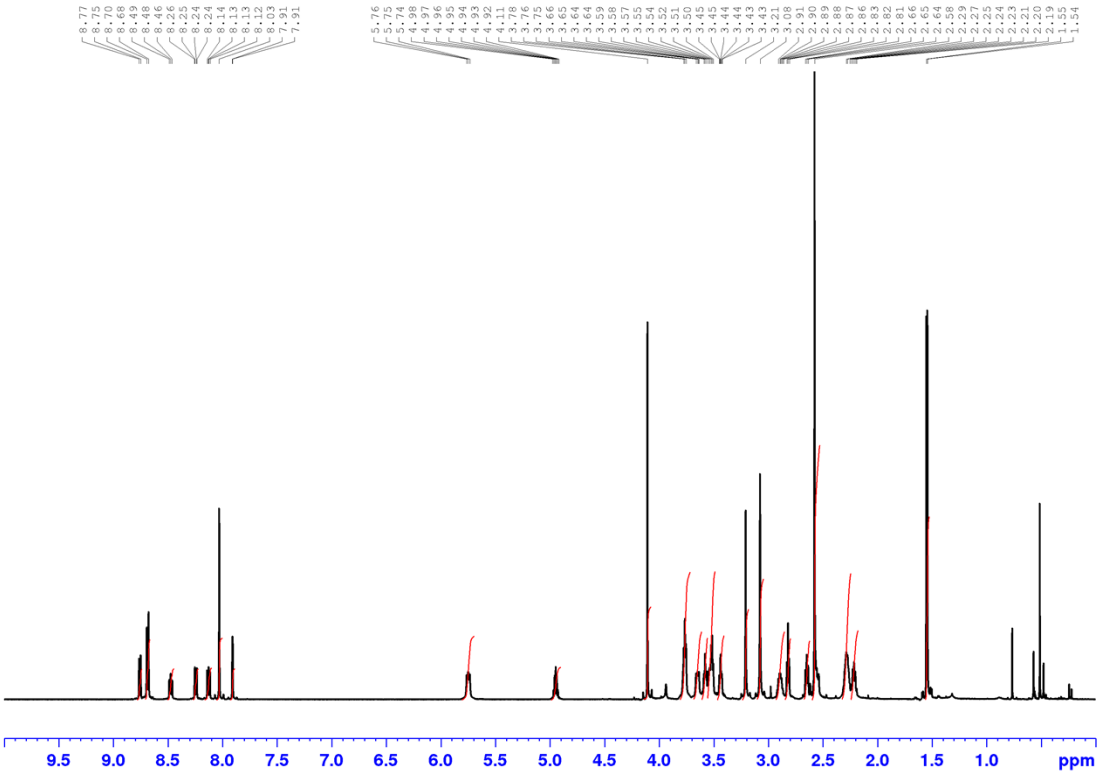
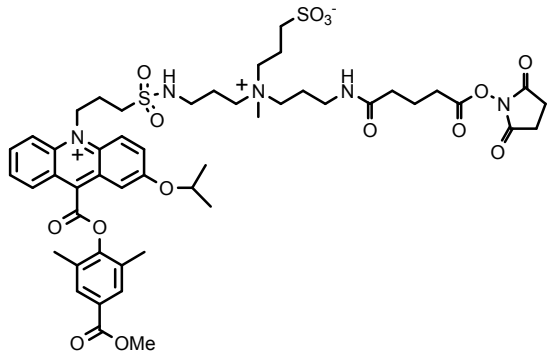


Figure S6B. ^{1}H-NMR spectrum of **3c**.



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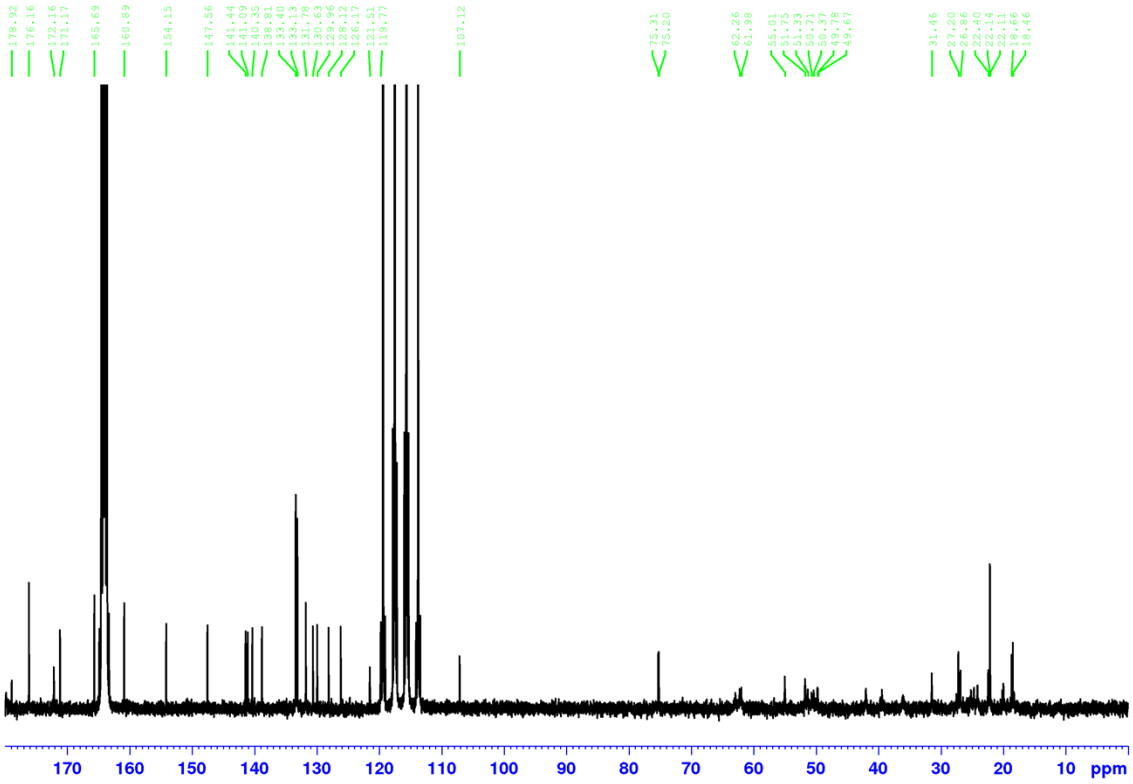
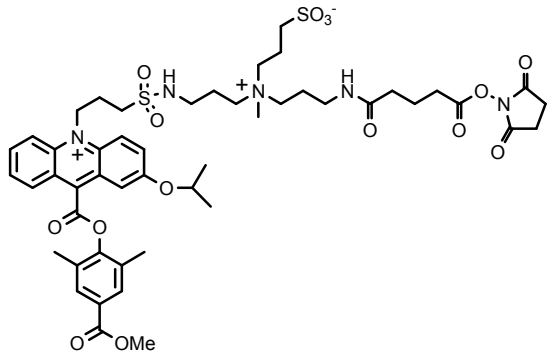


Figure S6C. ^{13}C-NMR spectrum of **3c**.



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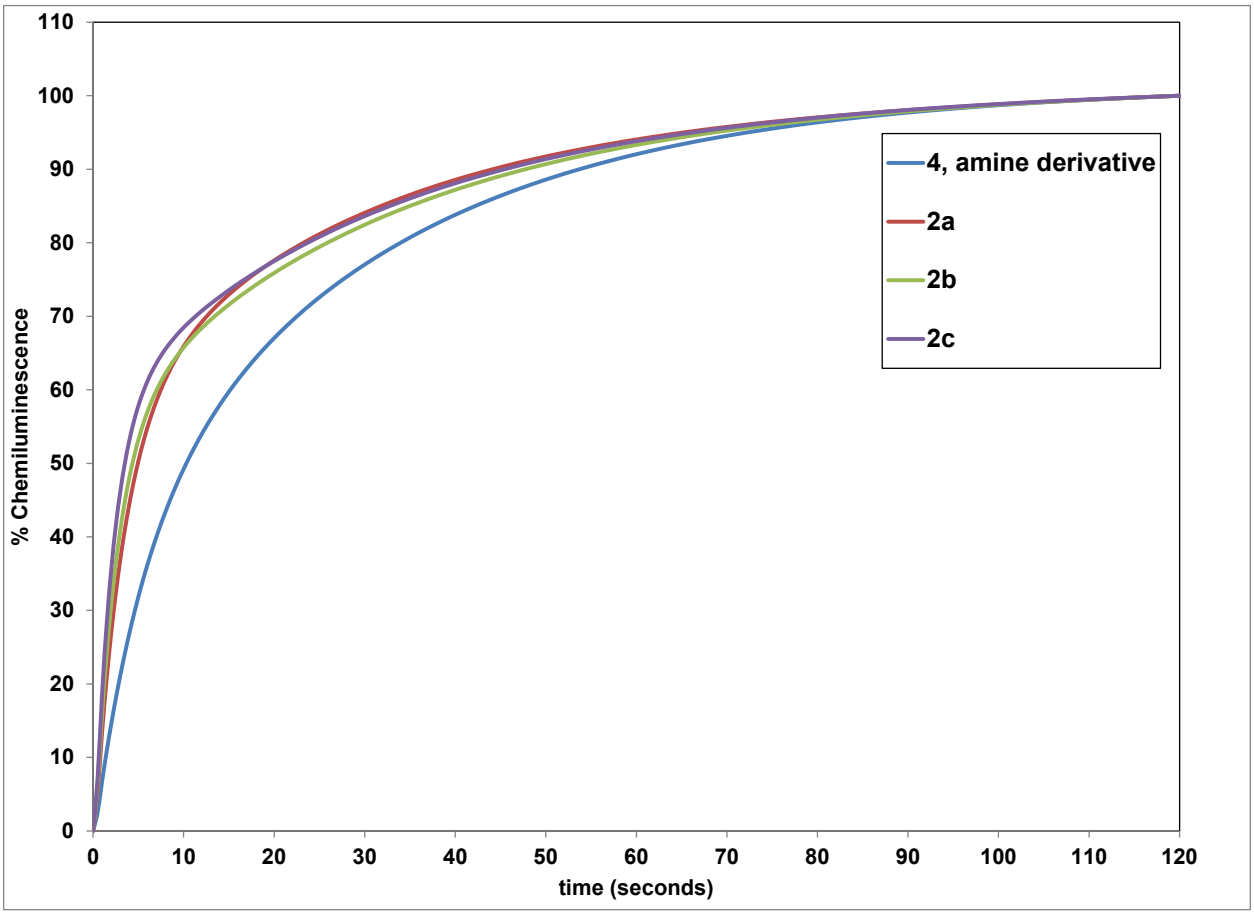

Figure S7. Chemiluminescence emission profiles of amine precursor of **4** and **2a**-**2c** in the absence of CTAC. Chemiluminescence was initiated by the sequential addition of 0.3 mL of 0.1 M nitric acid containing 0.5% hydrogen peroxide followed by 0.3 mL of 0.25 M sodium hydroxide.

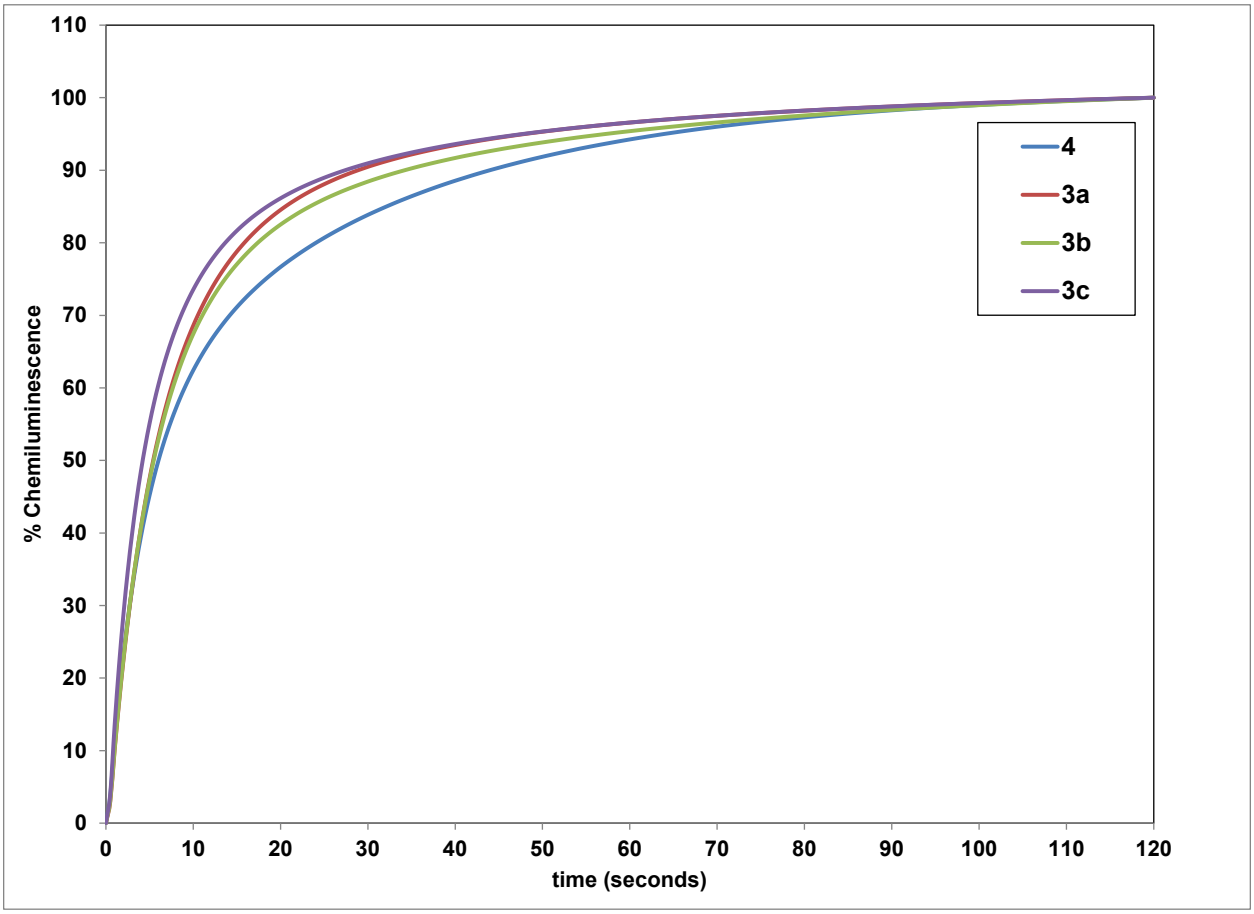

Figure S8. Chemiluminescence emission profiles of BSA conjugates of compound **4** and **3a**-**3c** in the absence of CTAC.

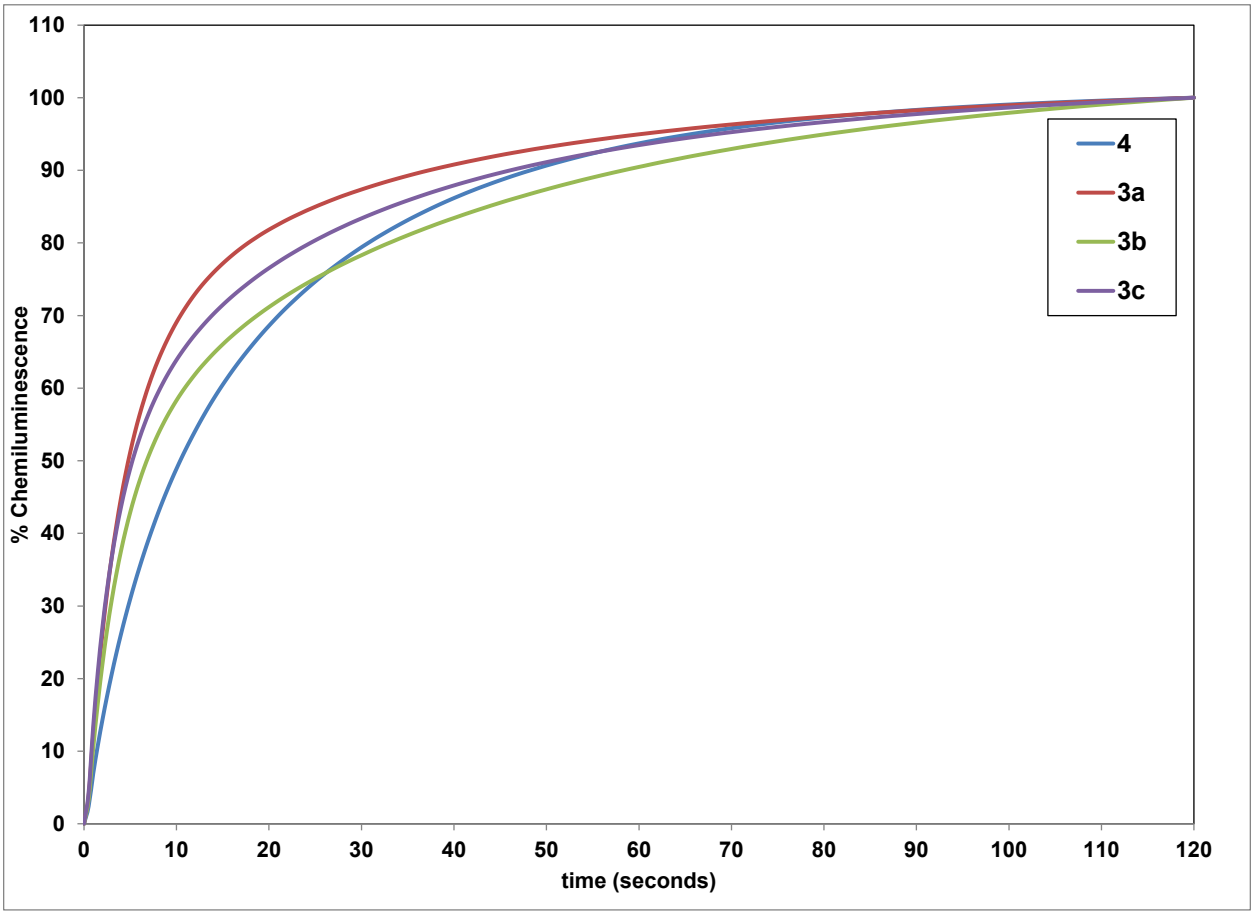

Figure S9. Chemiluminescence emission profiles of anti-TSH Mab conjugates of compound **4** and **3a**-**3c** in the absence of CTAC.

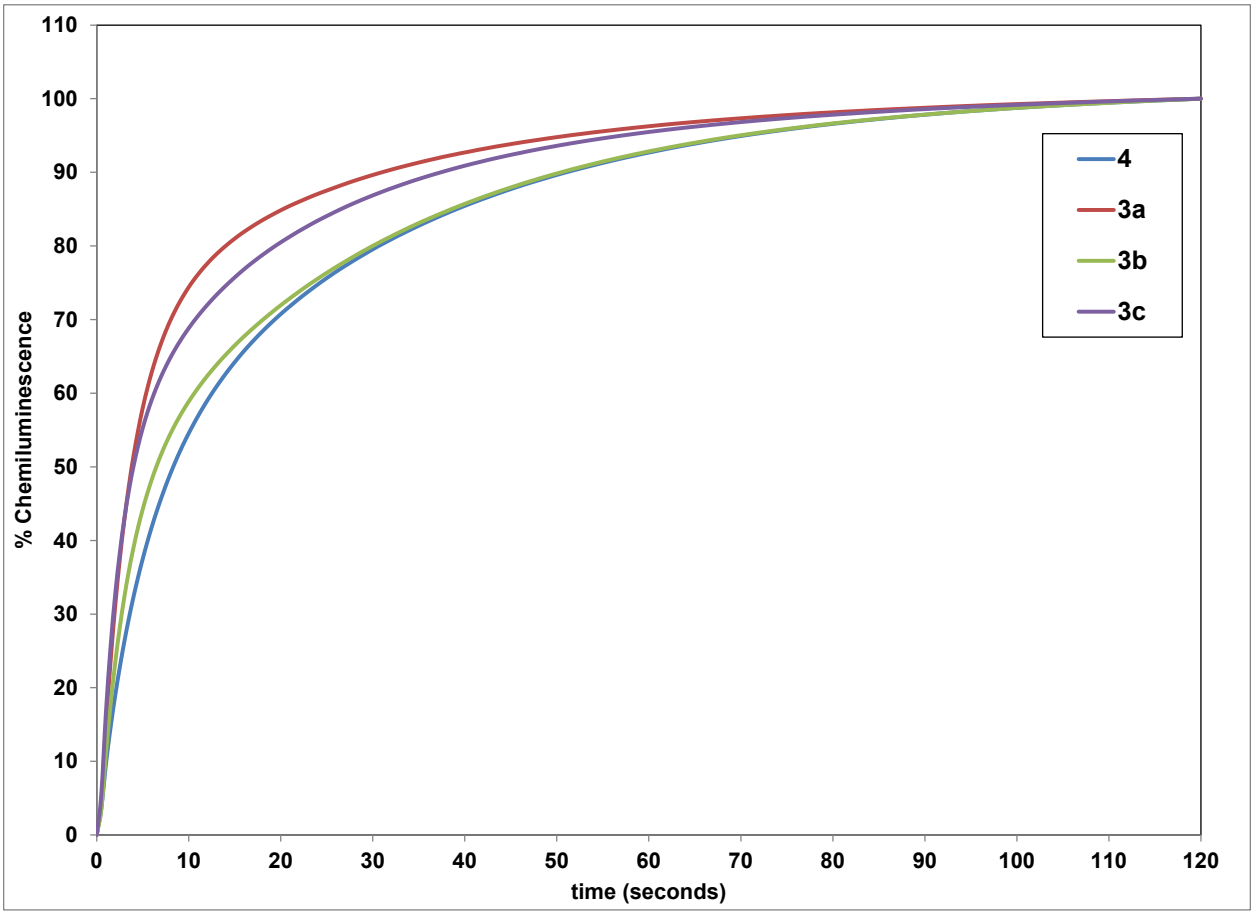

Figure S10. Chemiluminescence emission profiles of anti-HBsAg Mab conjugates of compound **4** and **3a**-**3c** in the absence of CTAC.

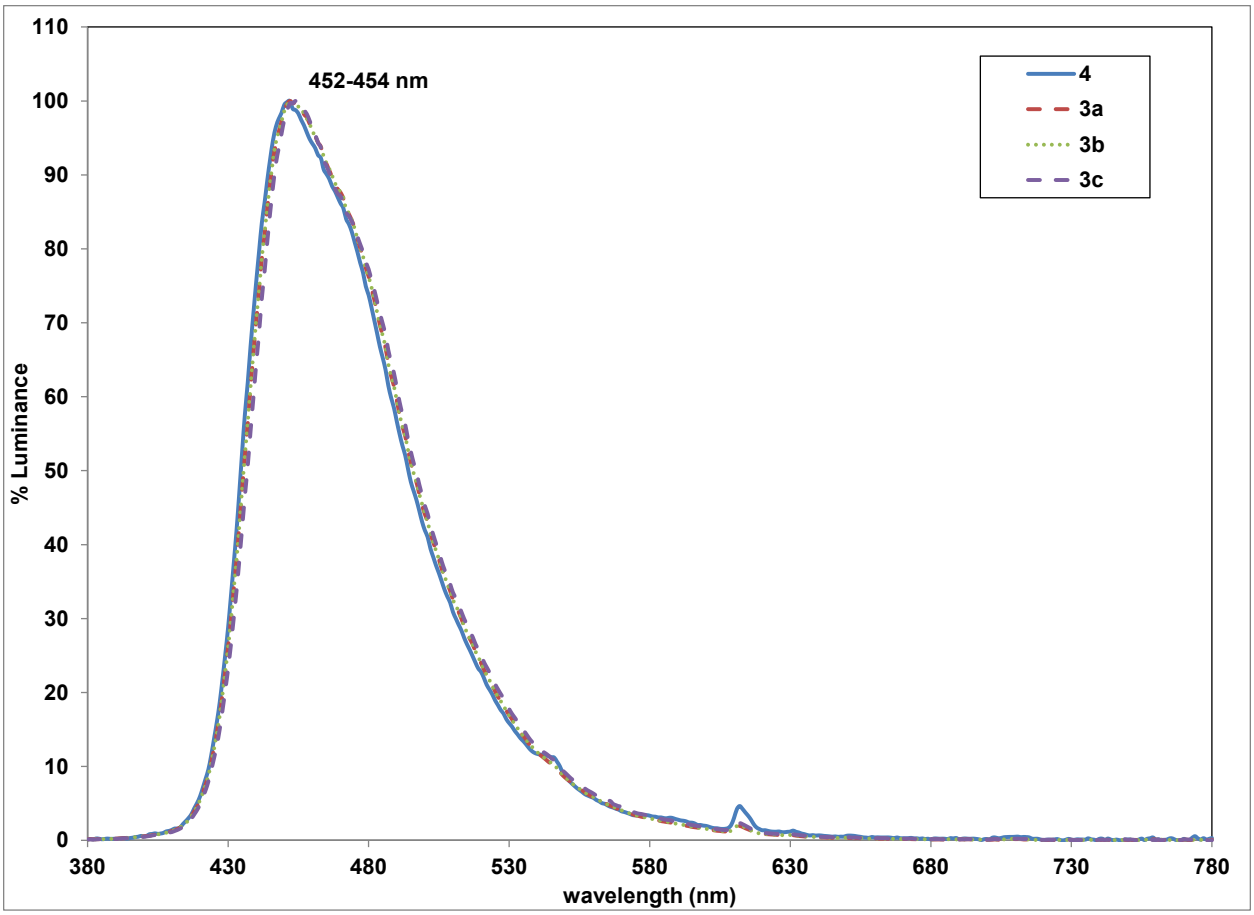

Figure S11. Emission spectra of anti-TSH antibody conjugates of **4, 3a**-**3c**. Similar to the BSA conjugates, all acridinium ester conjugates showed very similar emission spectra whether conjugation was performed at the phenol (**4**) or at the acridinium nitrogen (**3a**-**3c**).

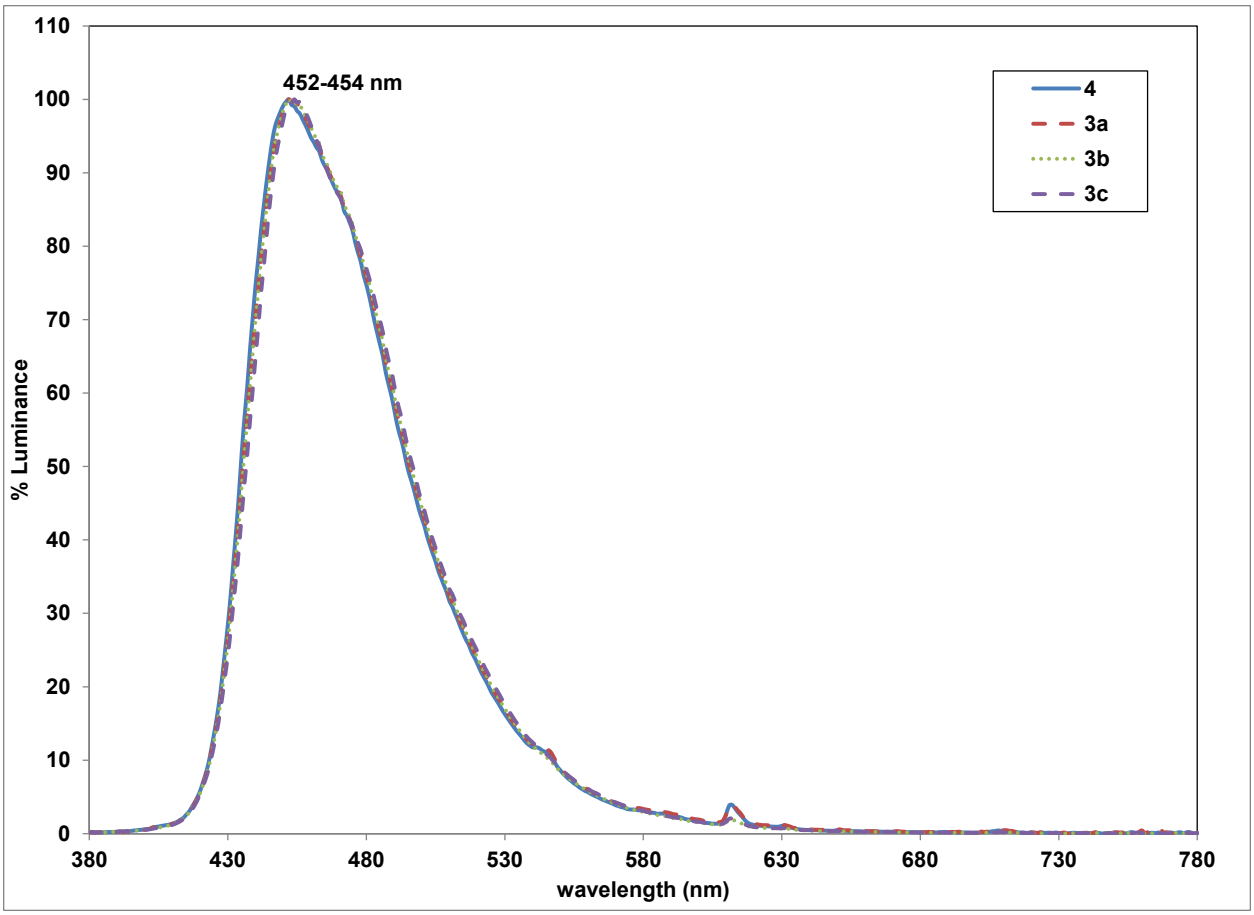

Figure S12. Emission spectra of anti-HBsAg antibody conjugates of **4, 3a**-**3c**. Similar to the BSA conjugates, all acridinium ester conjugates showed very similar emission spectra whether conjugation was performed at the phenol (**4**) or at the acridinium nitrogen (**3a**-**3c**).