

## **Supplementary Material**

for

# **Glutathione-responsive disassembly of disulfide dicyanine for tumor imaging with reduction in background signal intensity**

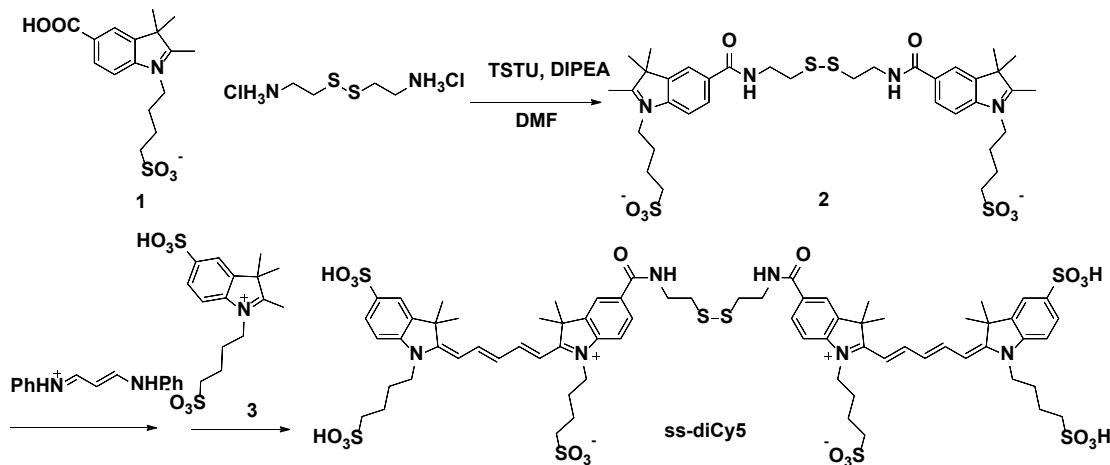
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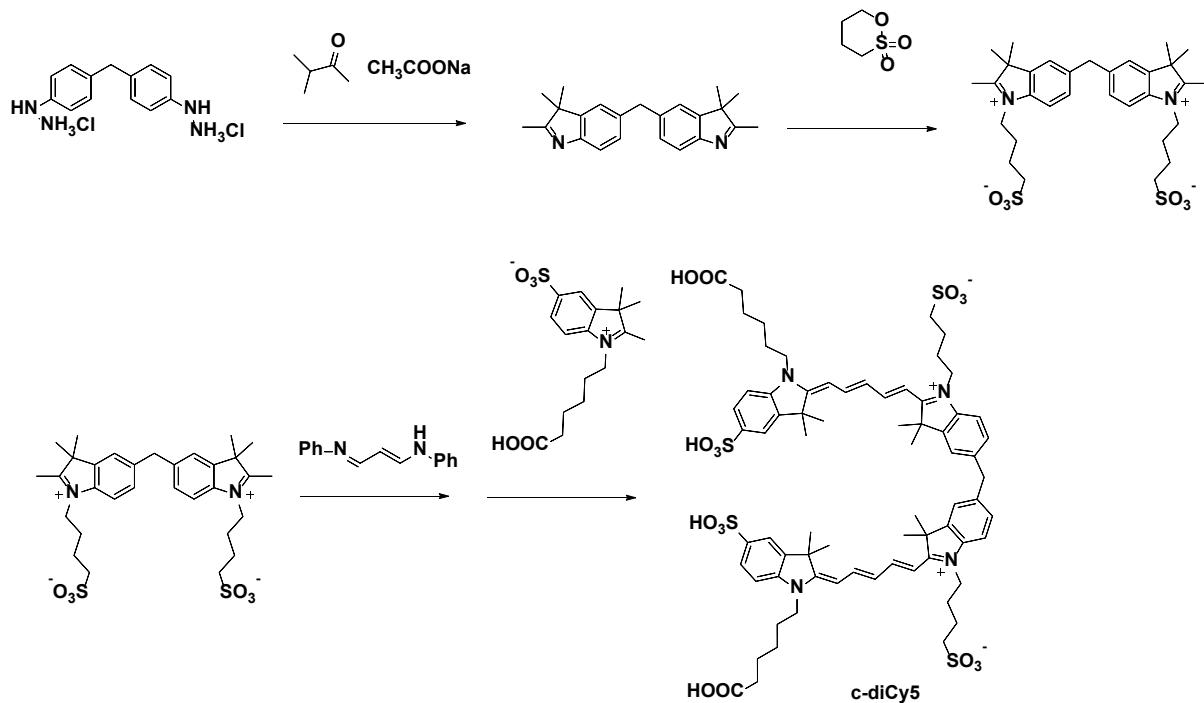
2 College of Life Science and Bioengineering, Beijing University of Technology, Beijing 100124,  
China  
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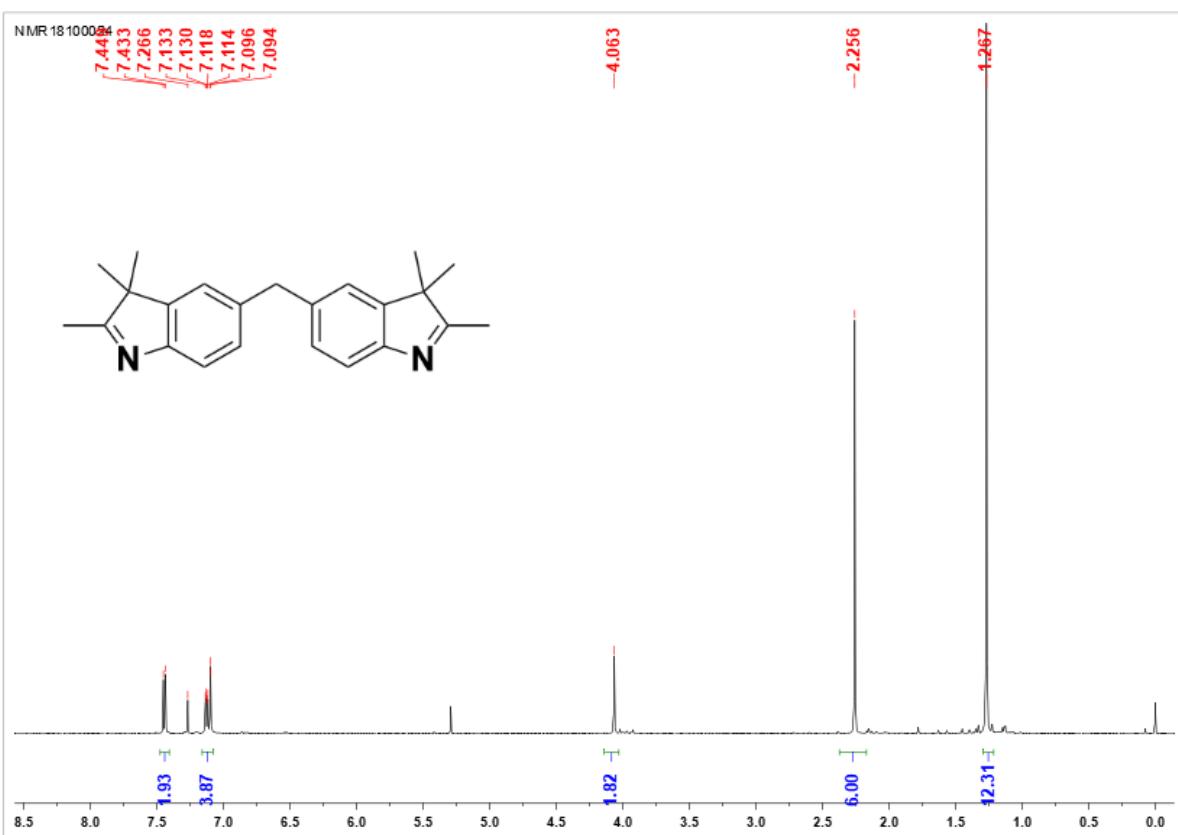
\* These authors contributed equally to this work.



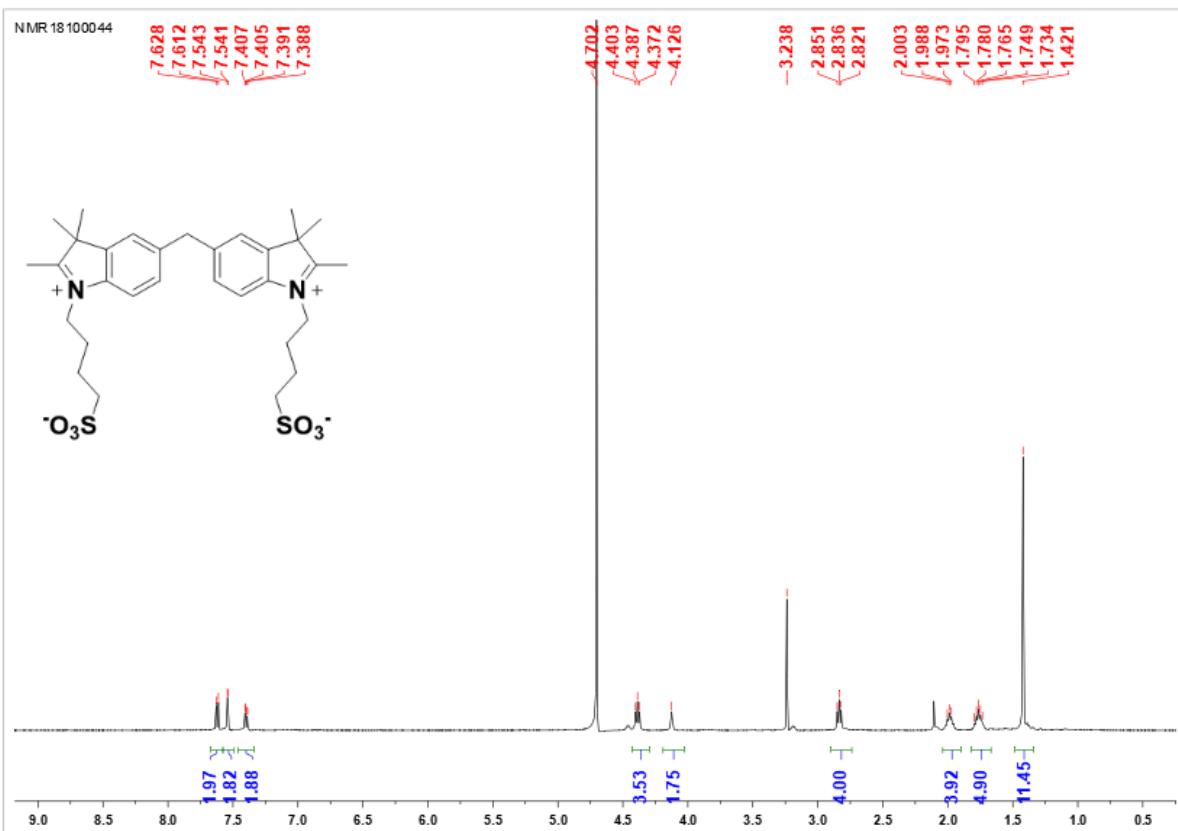
**Figure S1:** The synthesis route of ss-diCy5



**Figure S2:** The synthesis route of c-diCy5

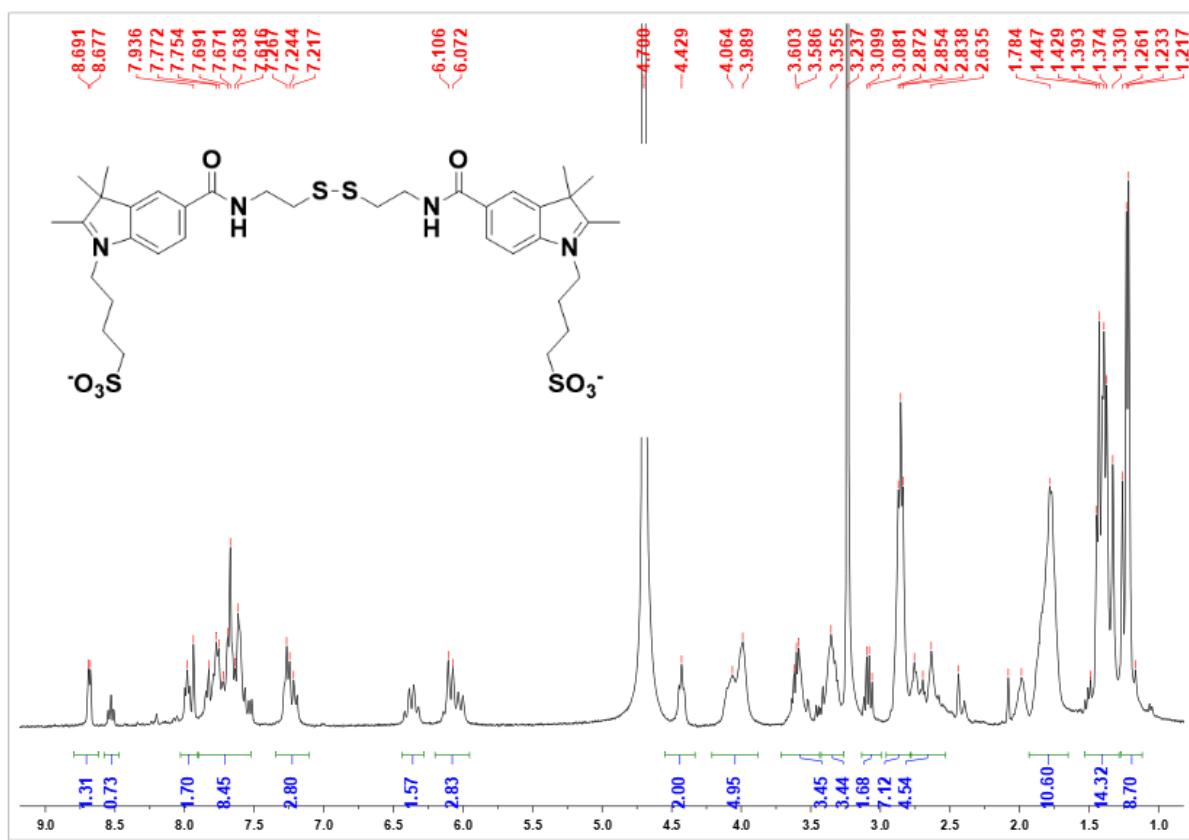


**Figure S3:**  $^1\text{H}$  NMR spectra of diindole intermediates.

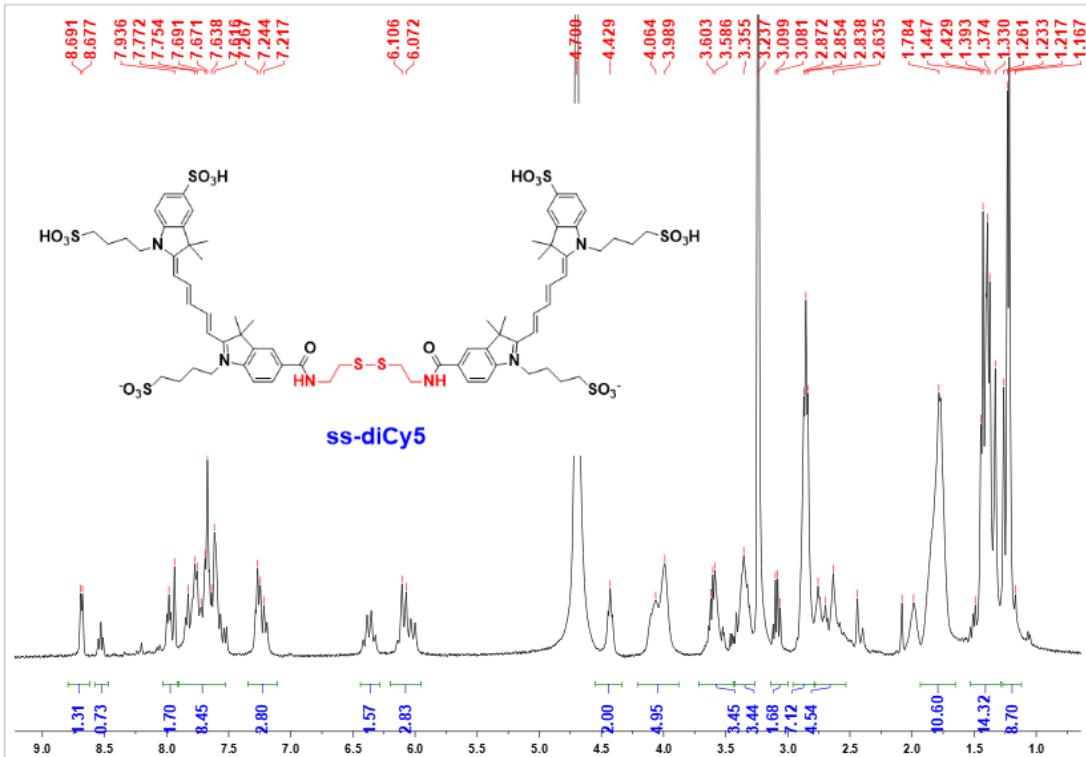


**Figure S4:**  $^1\text{H}$  NMR spectra of Methylene diindole quaternary ammonium salt

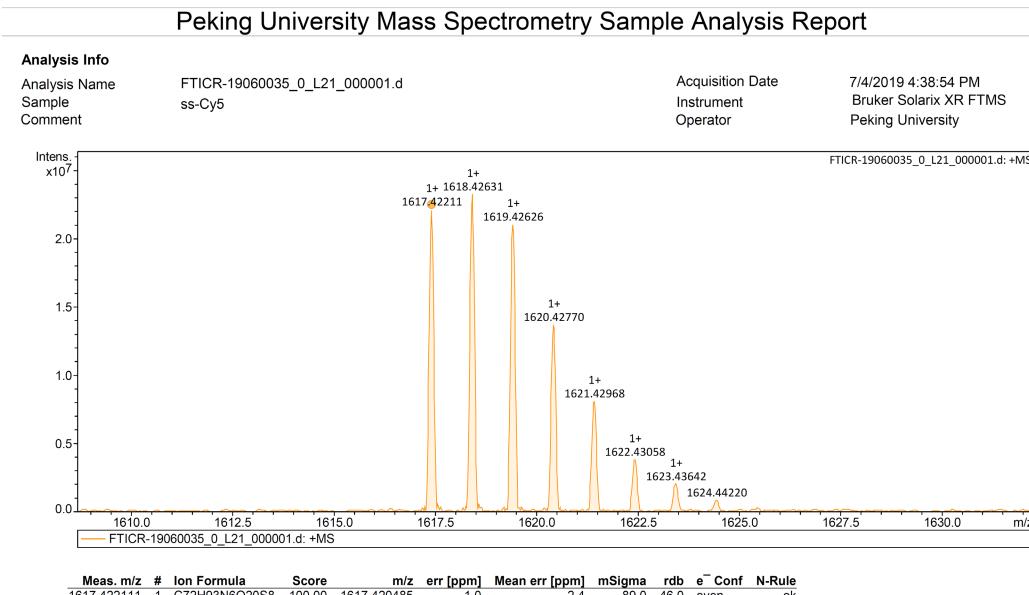
**Figure S5:** HRMS spectra of c-diCy5



**Figure S6:** <sup>1</sup>H NMR spectra of disulfide diindole quaternary ammonium salt

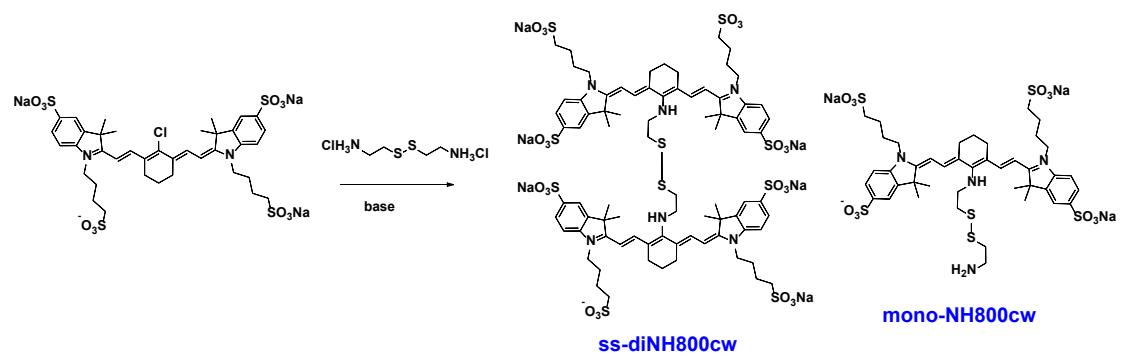


**Figure S7:**  $^1\text{H}$  NMR spectra of ss-diCy5

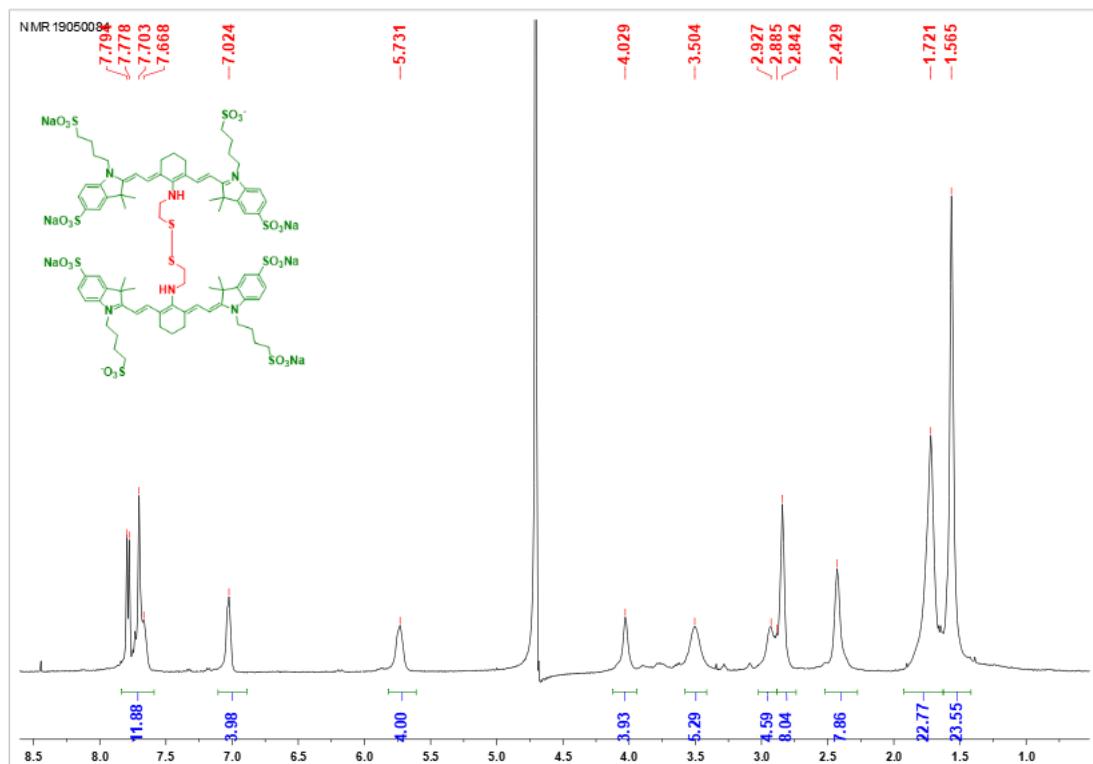


**Figure S8:** HRMS spectra of ss-diCy5

## Synthesis of ss-diNH800cw



**Figure S9:** Synthetic route of ss-diNH800CW



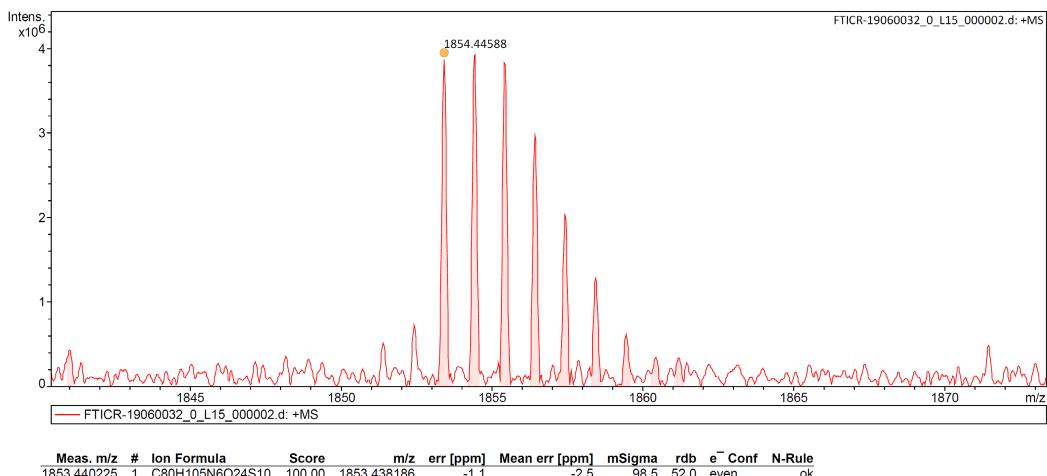
**Figure S10:** <sup>1</sup>H NMR spectra of ss-diNH800CW

## Peking University Mass Spectrometry Sample Analysis Report

### Analysis Info

Analysis Name: FTICR-19060032\_0\_L15\_000002.d  
 Sample: ss-diNH800CW  
 Comment:

Acquisition Date: 7/4/2019 4:12:03 PM  
 Instrument Operator: Bruker Solarix XR FTMS  
 Peking University



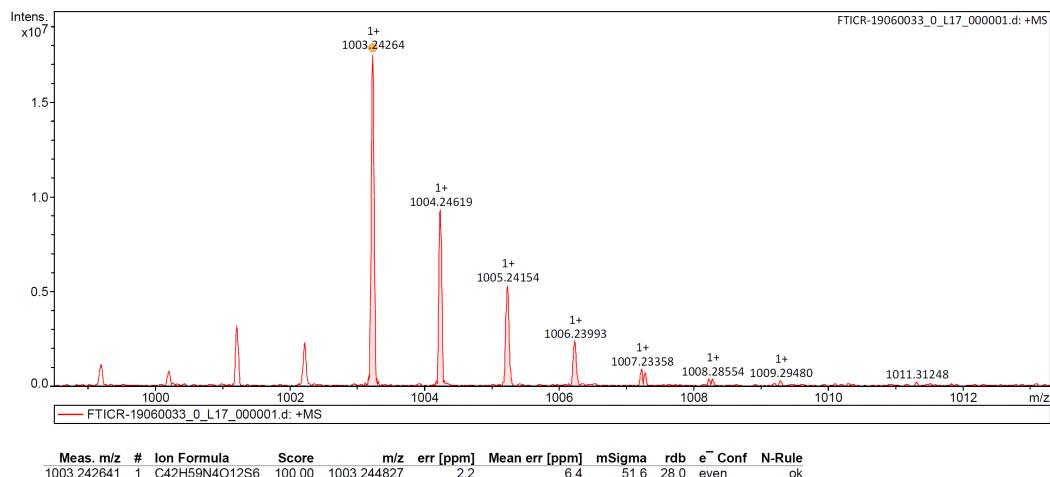
**Figure S11:** HRMS spectra of ss- diNH800CW

## Peking University Mass Spectrometry Sample Analysis Report

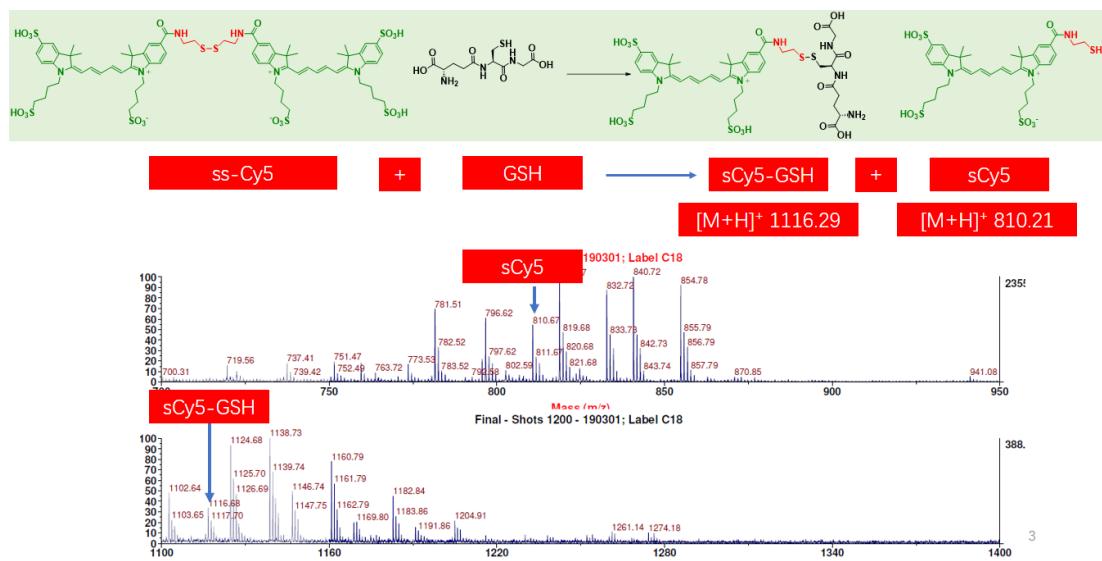
### Analysis Info

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 Comment:

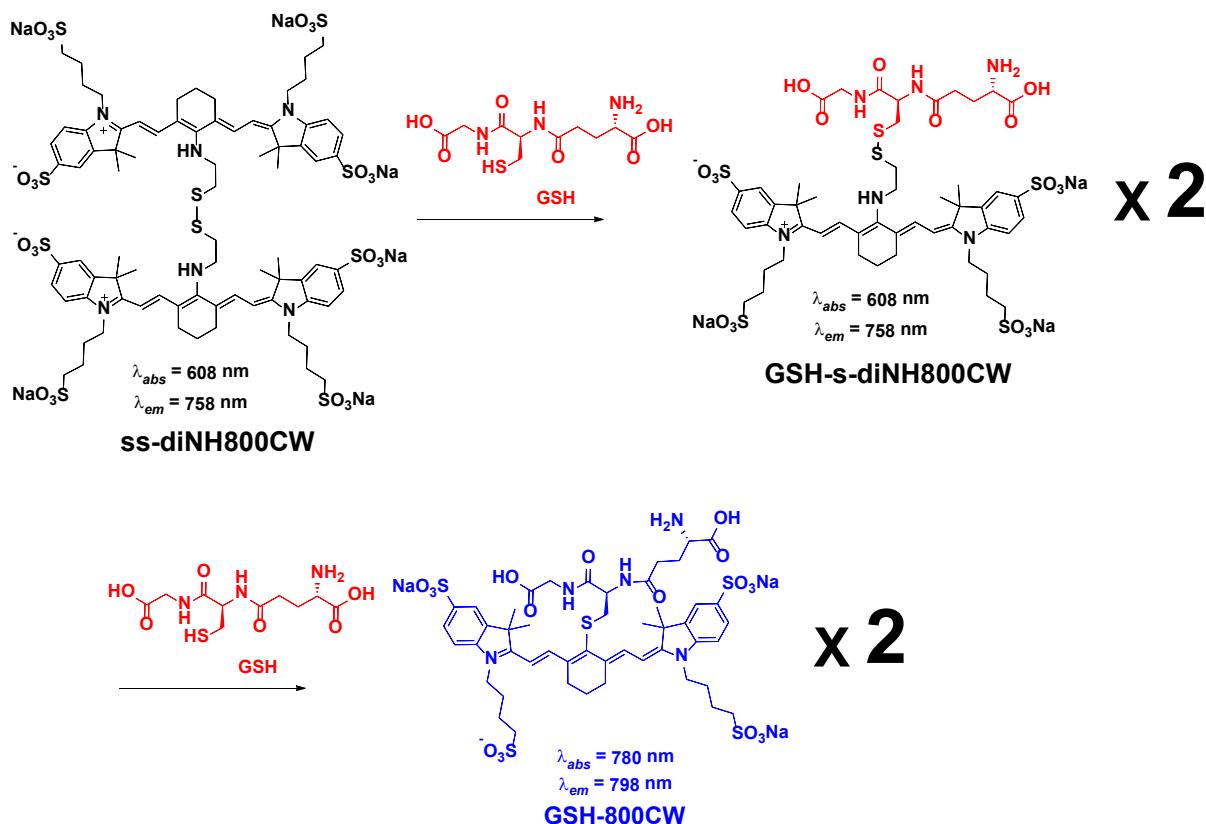
Acquisition Date: 7/4/2019 4:17:20 PM  
 Instrument Operator: Bruker Solarix XR FTMS  
 Peking University



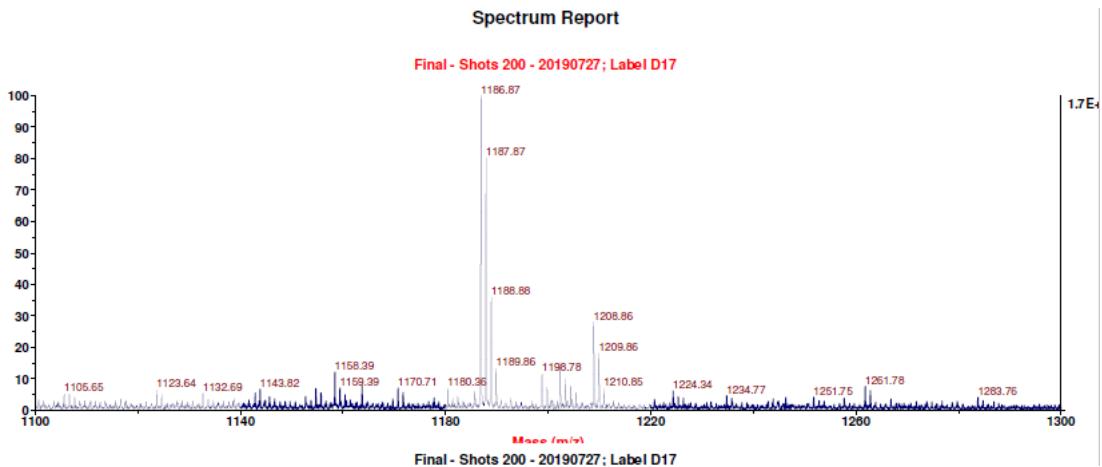
**Figure S12:** HRMS spectra of mono-NH800CW



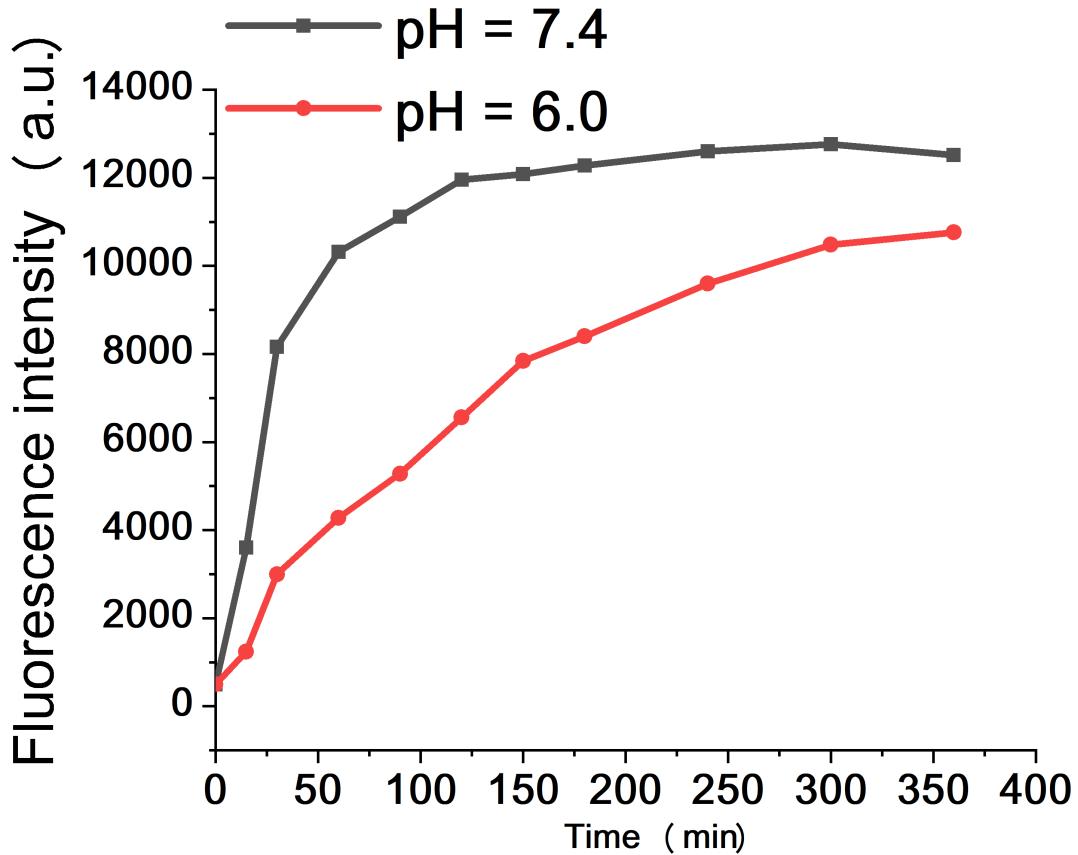
**Figure S13:** MALDI-TOF spectra of ss-diCy5 in GSH solution



**Figure S14:** The proposed reactions in ss- diNH800CW GSH solution



**Figure S15:** MALDI-TOF spectra of ss- diNH800CW in [the](#) GSH solution



**Figure S16:** The fluorescence intensity enhancement of ss-diNH800CW(5  $\mu$ M) at [the](#) pH of 6.0 and 7.4 in the presence of GSH (1.5 mM) in PBS solution (25 °C).  $\lambda_{ex}$  = 650 nm.