

## Improving Photostability of Azetidine Substituted Naphthalimide Dyes with Large Stokes Shifts for Imaging of Lipid Droplet in Live Cell

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## **Part A: Experimental Section**

### **1 General information on materials**

The chemical reagents were purchased from J&K Scientific Ltd or Beijing zhong sheng hua teng Technology Co., Ltd. and used as received. Solvents were either employed as purchased or dried according to procedures described in the literature. Deionized water was obtained from a Milli-Q water purification system (Millipore). Phosphate buffer saline (PBS) was purchased from Life Technologies Co., Ltd. All glassware was oven-dried prior to use when water- and/or air-sensitive reagents were used. The synthetic steps were performed under ambient atmosphere unless stated otherwise. The  $^1\text{H}$ -NMR spectra were recorded at 20°C on 400 MHz NMR spectrometer (Bruker). The  $^{13}\text{C}$ -NMR spectra were recorded at 20°C on 101 MHz NMR spectrometer (Bruker). Mass spectra were carried out using Thermo Finnigan TSQ Quantum Ultra AM EMR Mass Spectrometry or ApexUltra Fourier transform ion cyclotron resonance mass spectrometry (Bruker). UV/Vis spectra were recorded with a Shimadzu WV-2550 spectrophotometer. Fluorescence spectra were recorded on a Shimadzu RF-5301 fluorescence spectrophotometer. Fluorescence microscopy images of labelled cells were obtained with spectral confocal laser scanning microscopy (Olympus Fluoview FV-1000).

## 2 Supplementary Table and Figures

Table S1 photoluminescence quantum yields of the **MFGNI** dyes in different solvents.<sup>a</sup>

Comp , Φ (%)	Toluene	DCM	Ethyl Acetate	Dioxane	Methanol	DMSO	PBS
<b>LD-Blue</b>	79	85	87	96	90	47	46
<b>MFGNI-1</b>	68	65	62	83	56	48	43
<b>LD-Green</b>	62	61	39	93	47	43	41

<sup>a</sup> quinine sulfate dihydrate (QSH) in 1.0 M H<sub>2</sub>SO<sub>4</sub> (Φ = 55%) as the standard.

Photoluminescence quantum yields of **MFGNI** dyes were determined in different solvents, respectively, with quinine sulfate dihydrate as reference. The quantum yield was calculated using eq (1)

$$\Phi_u = [(A_s FA_u \eta^2) / (A_u FA_s \eta_0^2)] \Phi_s \quad (1)$$

where  $A_s$  and  $A_u$  are the absorbance of the reference and sample solution at the reference excitation wavelength,  $FA_s$  and  $FA_u$  are the corresponding integrated fluorescence intensities, and  $\eta$  and  $\eta_0$  are the solvent refractive indexes of sample and reference, respectively. Absorbance of sample and reference at their respective excitation wavelengths was controlled to be lower than 0.1.

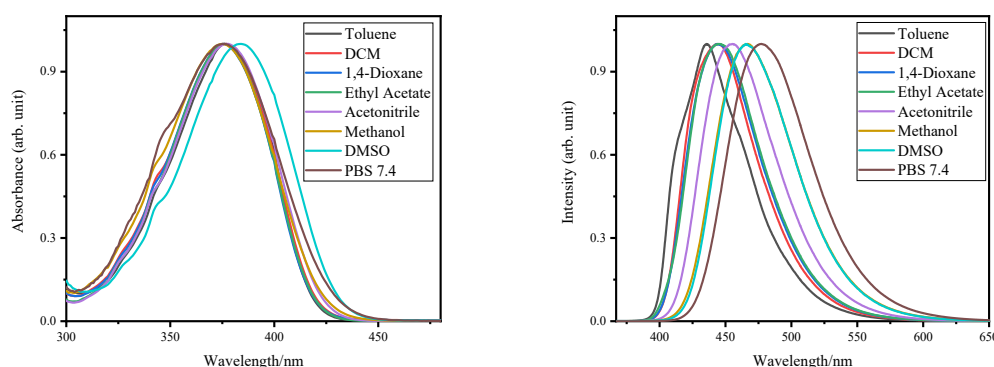


Figure S1 Normalized absorption and fluorescence spectra of **LD-Blue** in different polarity solvents.

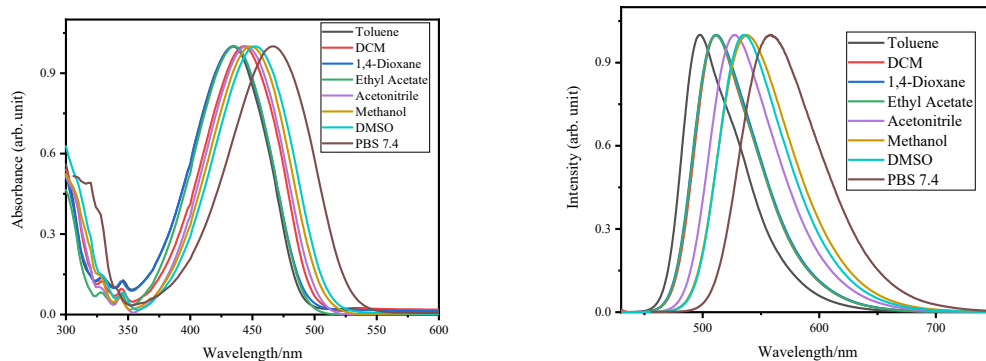


Figure S2 Normalized absorption and fluorescence spectra of **MFGNI-1** in different polarity solvents.

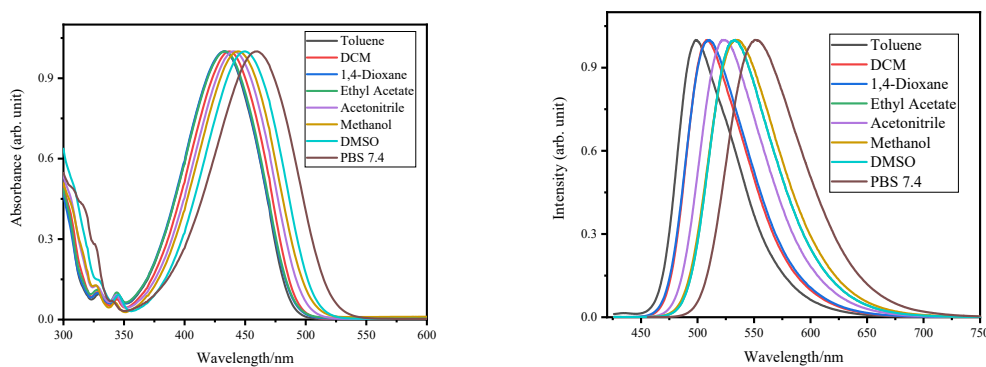


Figure S3 Normalized absorption and fluorescence spectra of **LD-Green** in different polarity solvents.

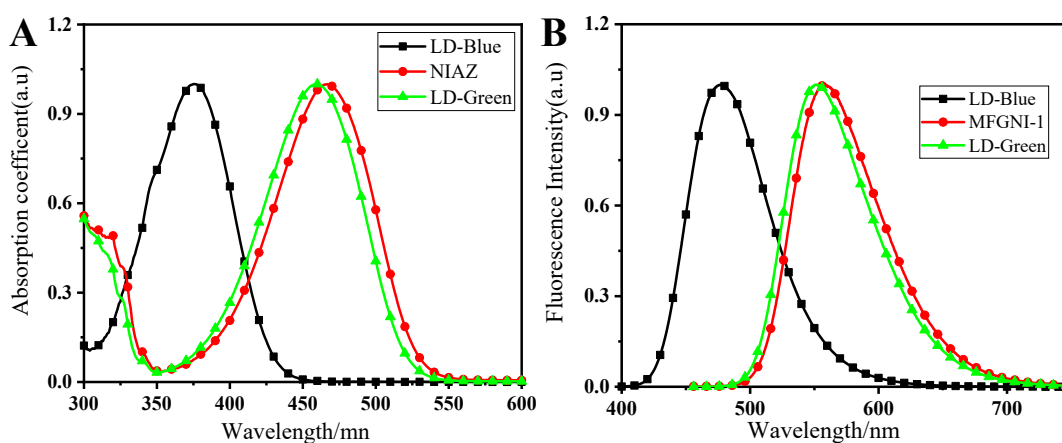


Figure S4 Absorption and fluorescence spectra of MFGNI dyes in PBS (pH=7.4).

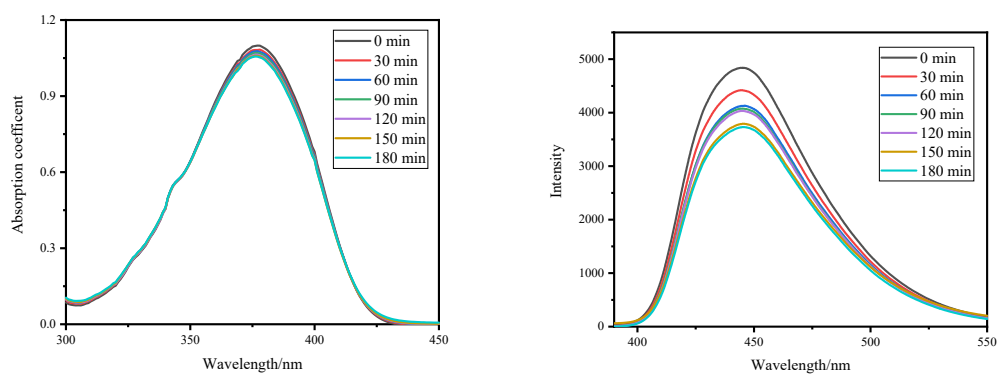


Figure S5 Absorption and fluorescence spectra of **LD-Blue** in dichloromethane solution under continuous irradiation with a 250 W Xe lamp.

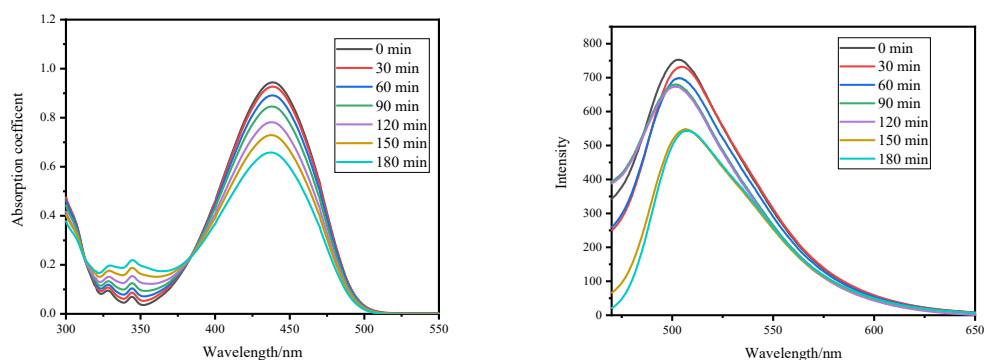


Figure S6 Absorption and fluorescence spectra of **LD-Green** in dichloromethane solution under continuous irradiation with a 250 W Xe lamp.

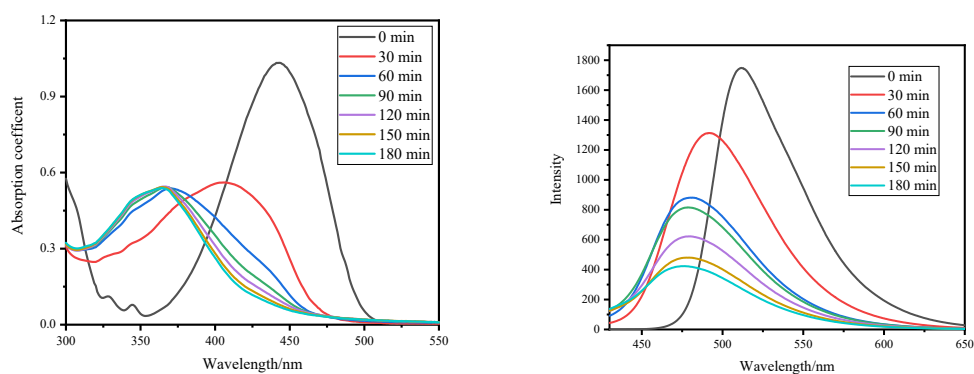


Figure S7 Absorption and fluorescence spectra of **MFGNI-1** in dichloromethane solution under continuous irradiation with a 250 W Xe lamp.

## Part B: $^1\text{H}$ -NMR spectrum, $^{13}\text{C}$ -NMR spectrum and Mass spectrum

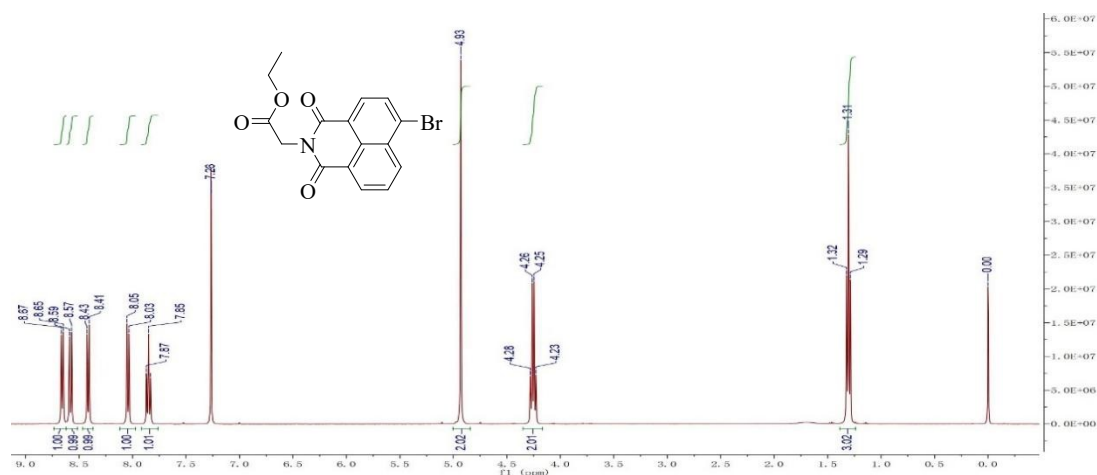


Figure S8  $^1\text{H}$  NMR (400 MHz) spectra of 4-bromo-N-ethylglycinate-1,8-naphthalimide in  $\text{CDCl}_3$

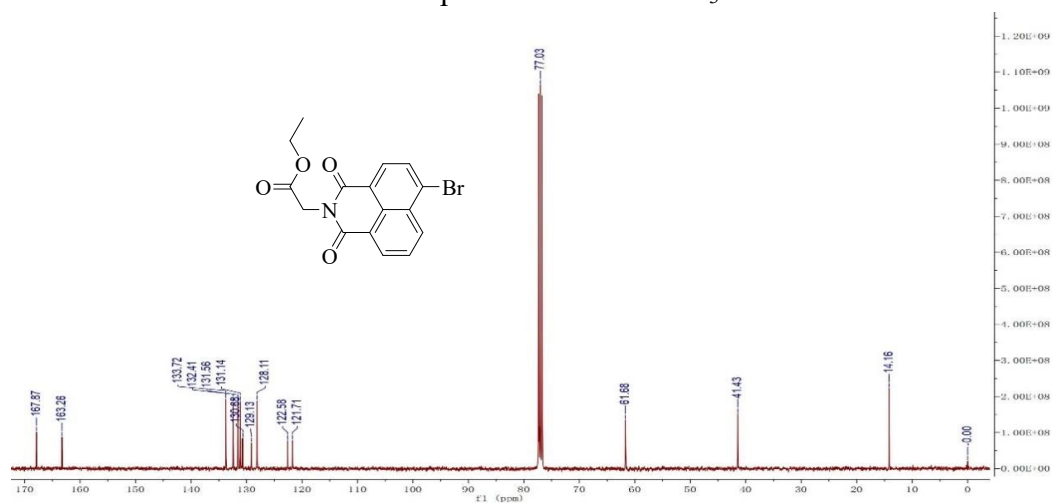


Figure S9  $^{13}\text{C}$  NMR (100 MHz) spectra of 4-bromo-N-ethylglycinate-1,8-naphthalimide in  $\text{CDCl}_3$

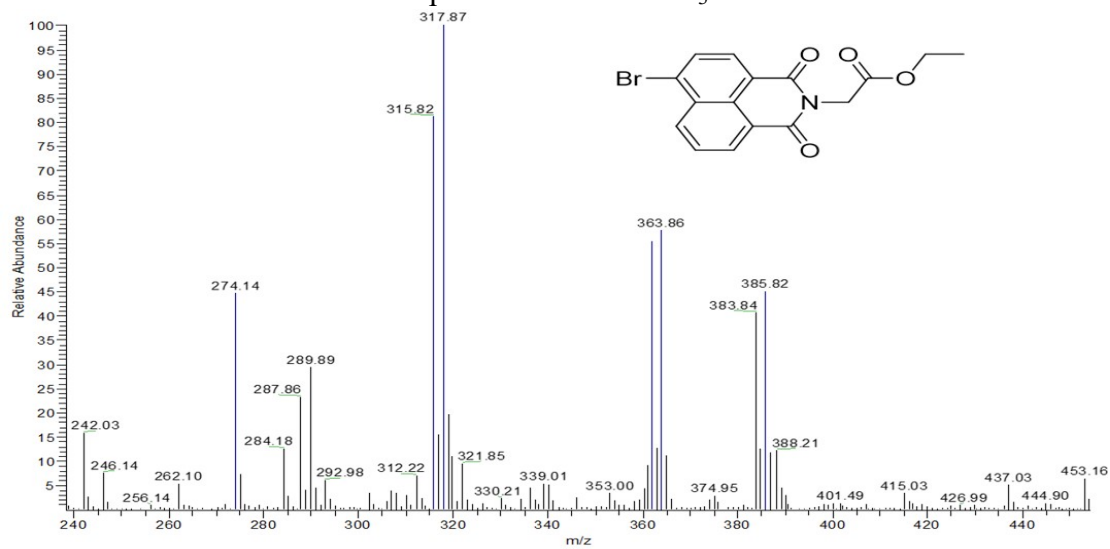


Figure S10 MS spectrum of 4-bromo-N-ethylglycinate-1,8-naphthalimide

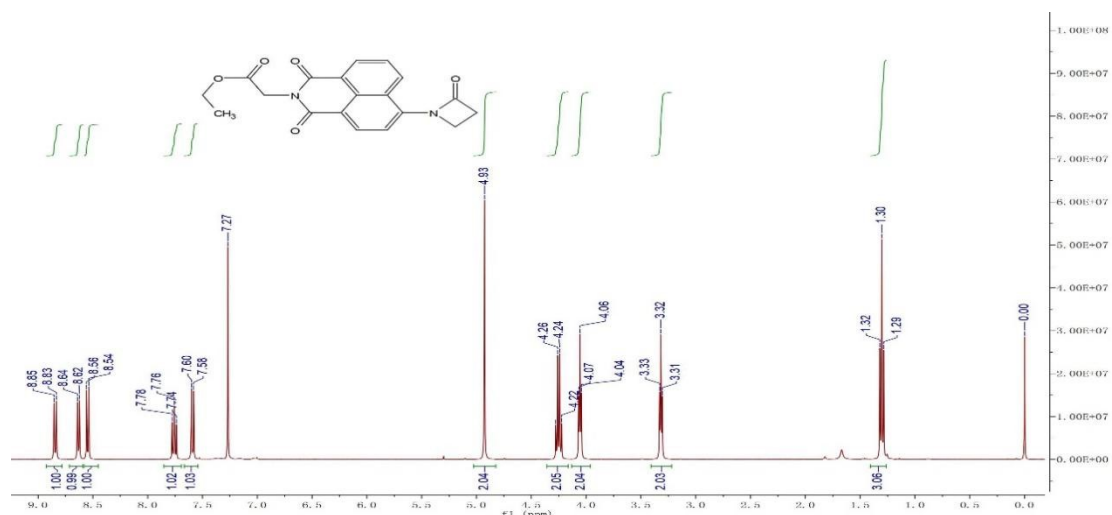


Figure S11  $^1\text{H}$  NMR (400 MHz) spectra of LD-Blue in  $\text{CDCl}_3$

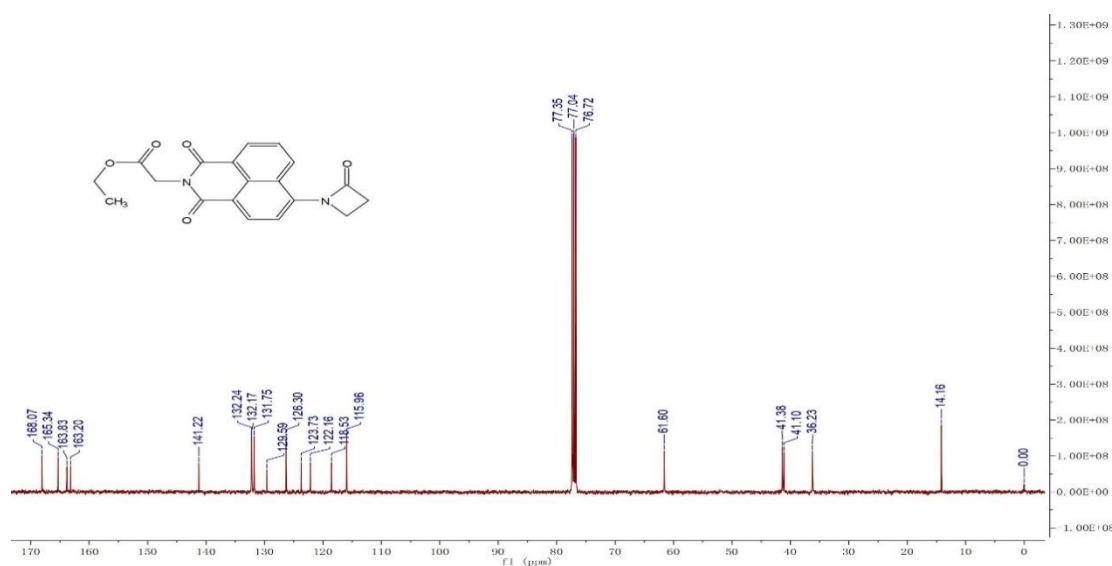


Figure S12  $^{13}\text{C}$  NMR (100 MHz) spectra of LD-Blue in  $\text{CDCl}_3$

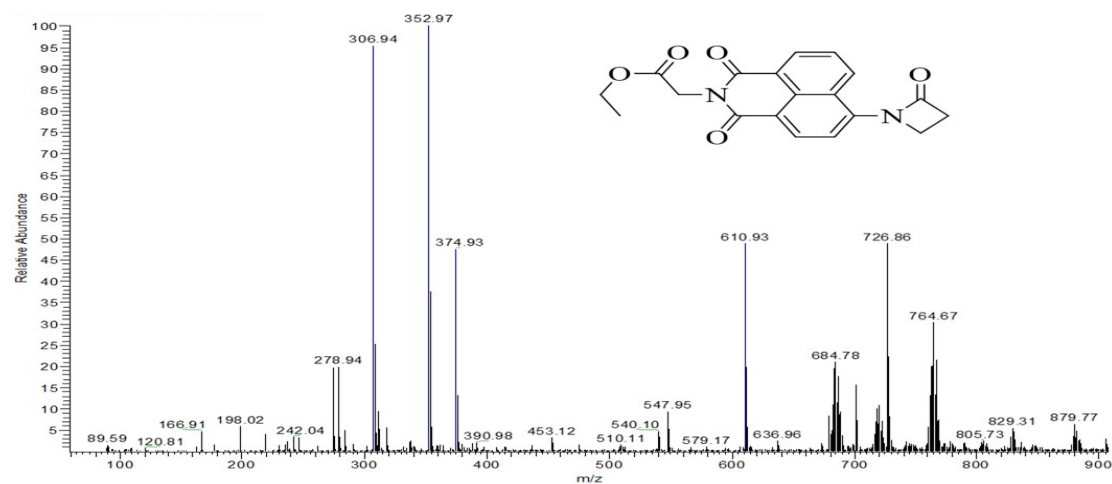


Figure S13 MS spectrum of LD-Blue



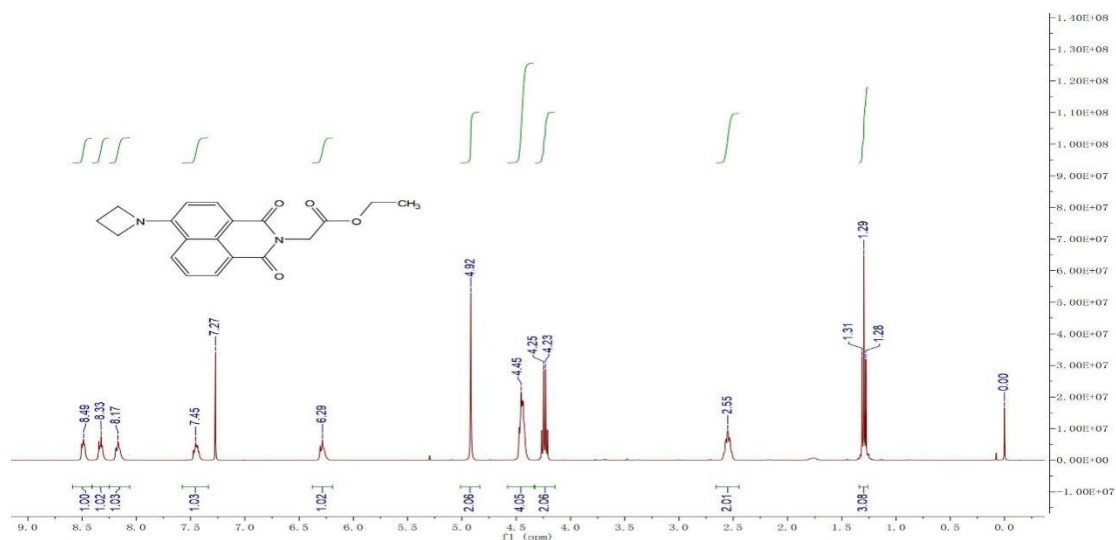


Figure S14  $^1\text{H}$  NMR (400 MHz) spectra of MFGNI-1 in  $\text{CDCl}_3$

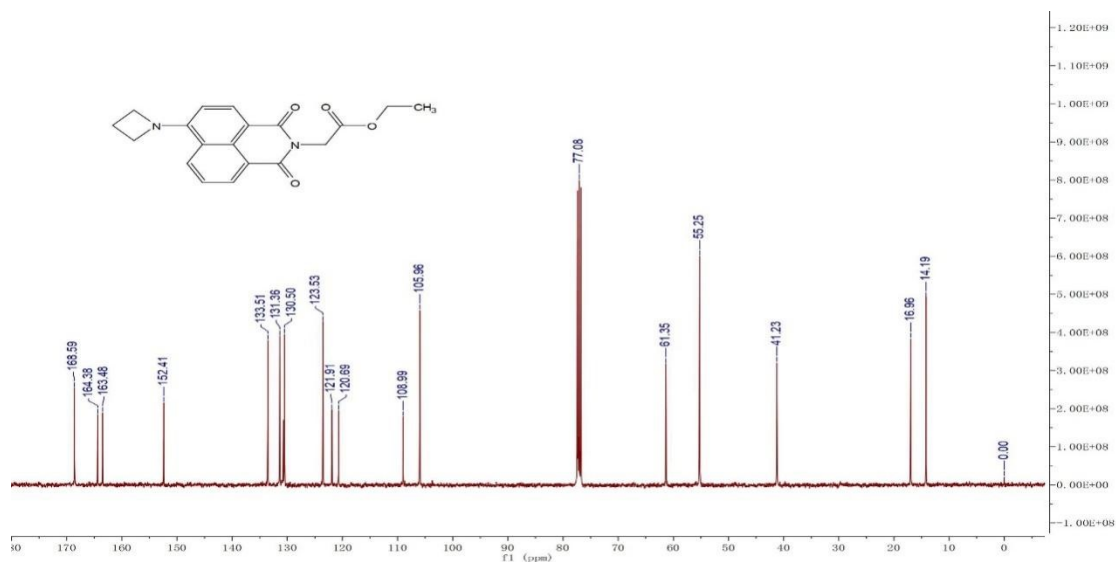


Figure S15  $^{13}\text{C}$  NMR (100 MHz) spectra of MFGNI-1 in  $\text{CDCl}_3$

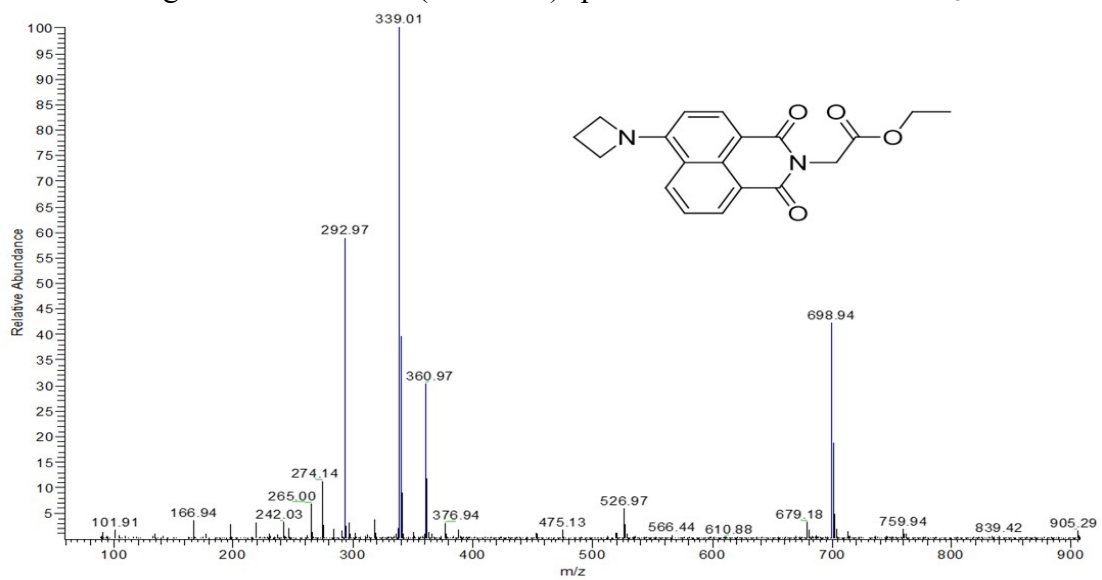


Figure S16 MS spectrum of MFGNI-1

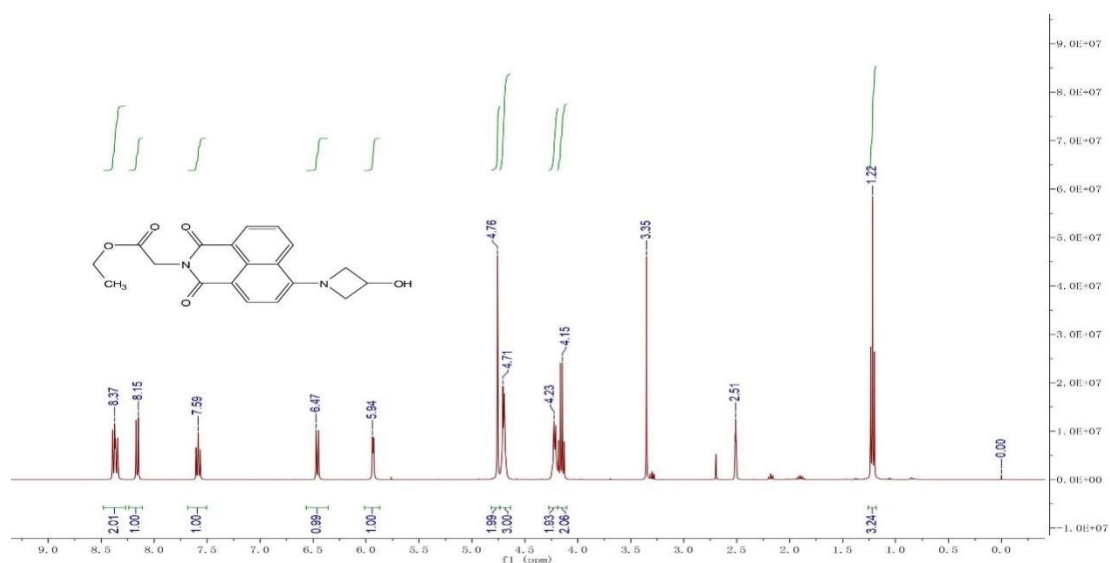


Figure S17  $^1\text{H}$  NMR (400 MHz) spectra of LD-Green in  $\text{CDCl}_3$

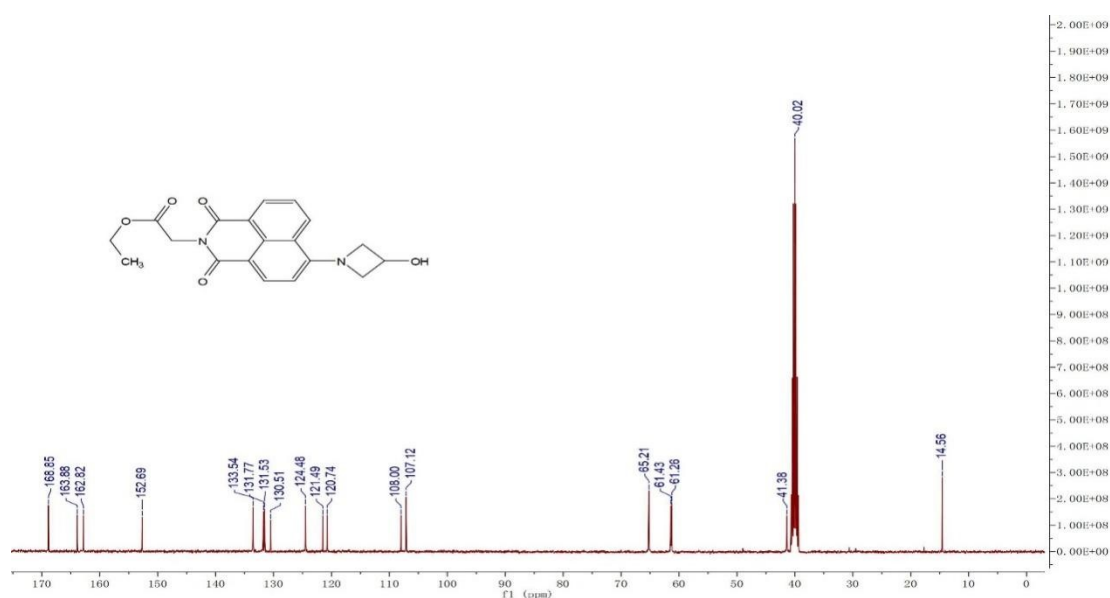


Figure S18  $^{13}\text{C}$  NMR (100 MHz) spectra of LD-Green in  $\text{CDCl}_3$

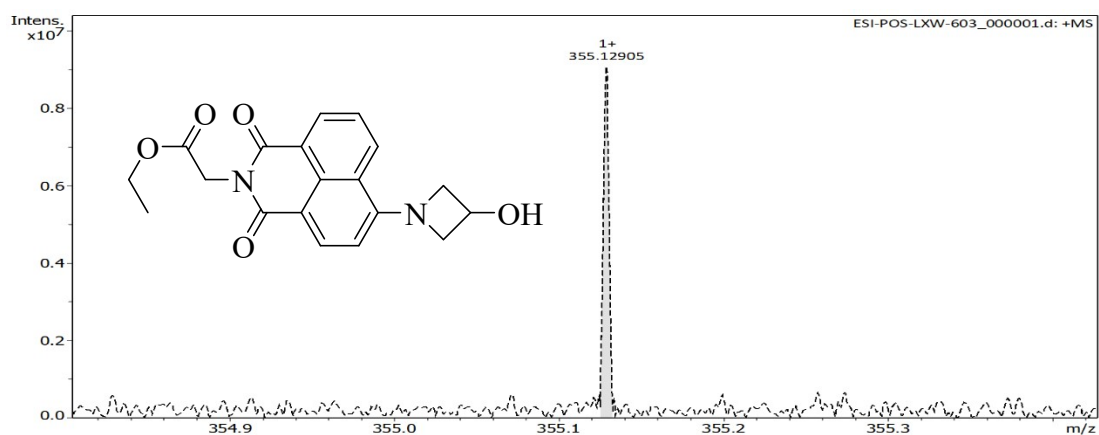


Figure S19 MS spectrum of LD-Green