

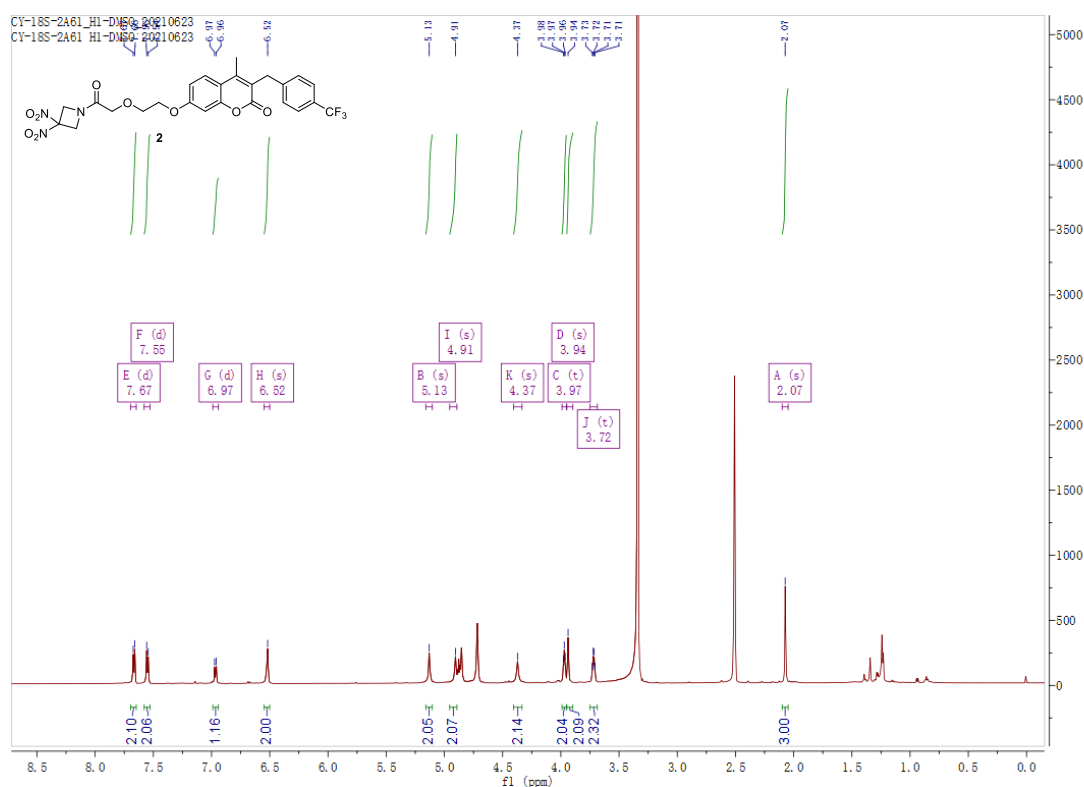
# Supplementary Information

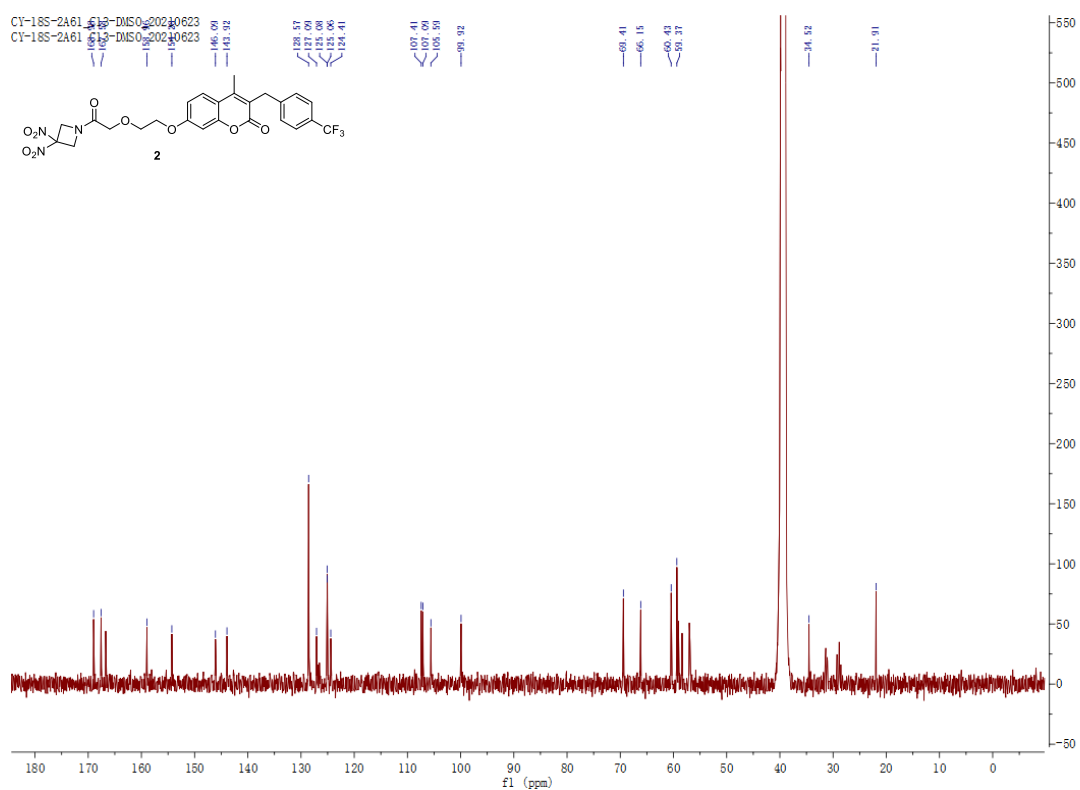
## Novel Nitric Oxide Donor Dinitroazetidine-Coumarin Hybrids as Potent Anti-Intrahepatic Cholangiocarcinoma Agents

Zhihui Yu <sup>1,†</sup>, Mengru Li <sup>2,†</sup>, Shiqi Guo <sup>1</sup>, Weijie Wang <sup>1</sup>, Feng Qu <sup>1</sup>, Yulei Ma <sup>2</sup>, Hongrui Liu <sup>2,\*</sup> and Ying Chen <sup>1,\*</sup>

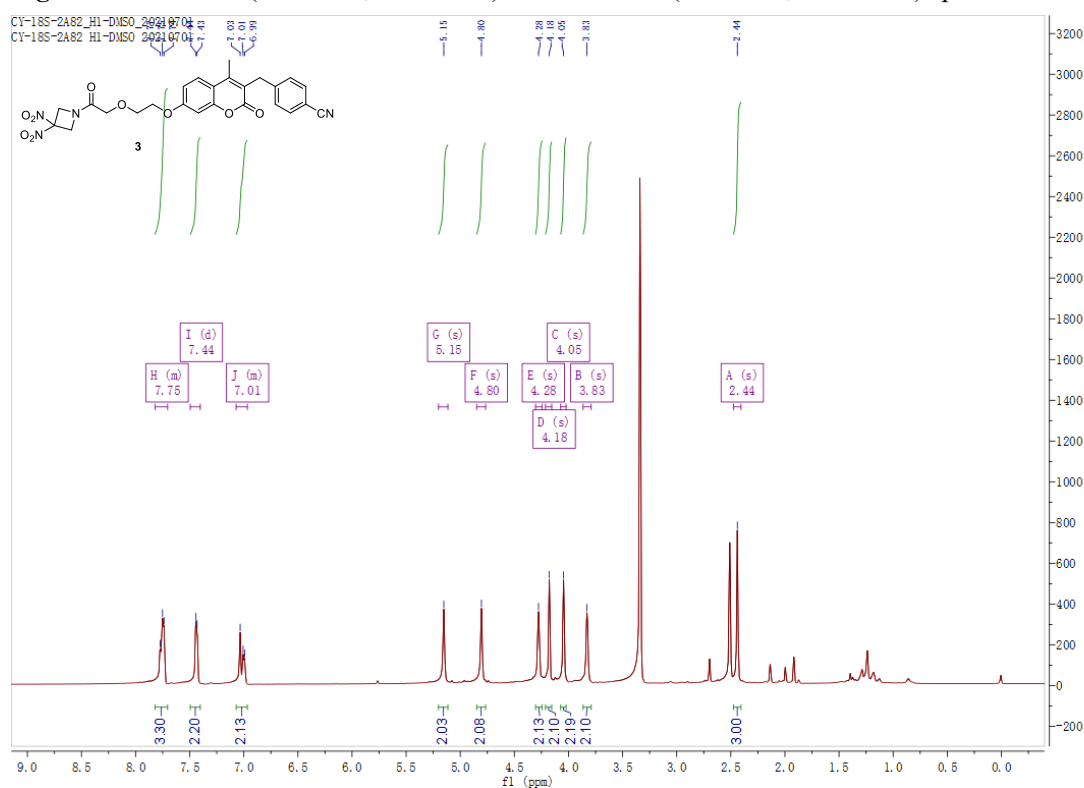
<sup>1</sup> Department of Medicinal Chemistry, School of Pharmacy, Fudan University, Shanghai 201203, China

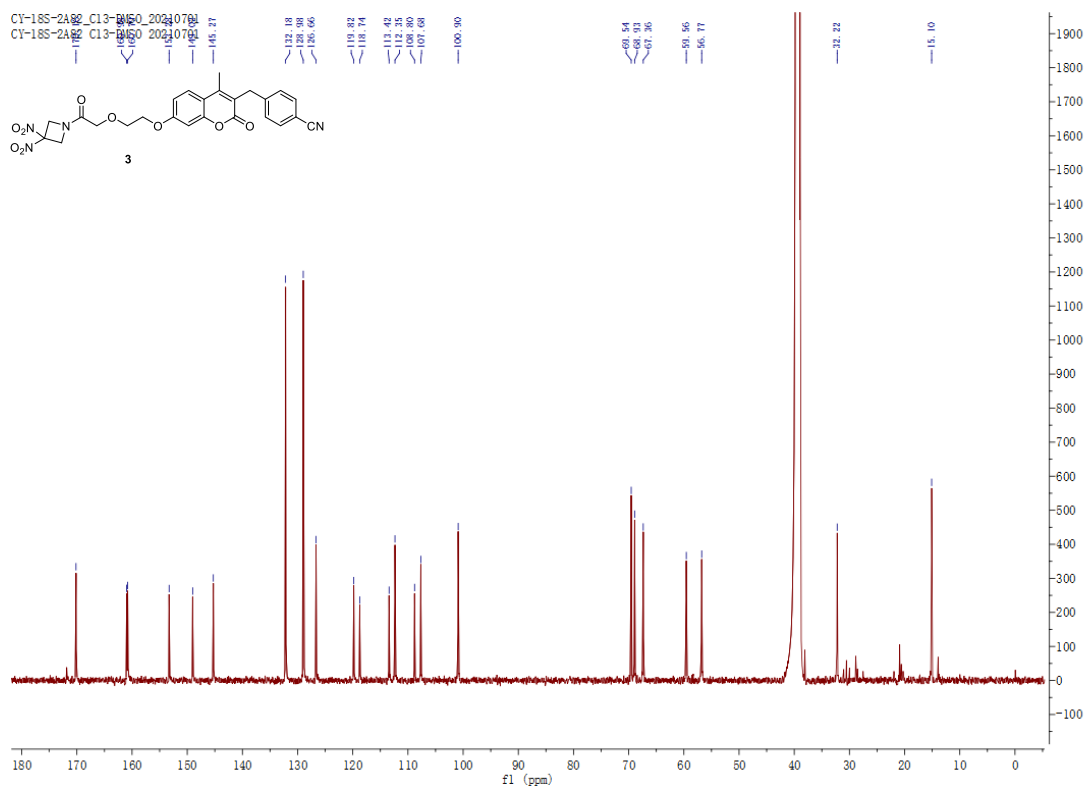
<sup>2</sup> Department of Pharmacology, School of Pharmacy, Fudan University, Shanghai 201203, China



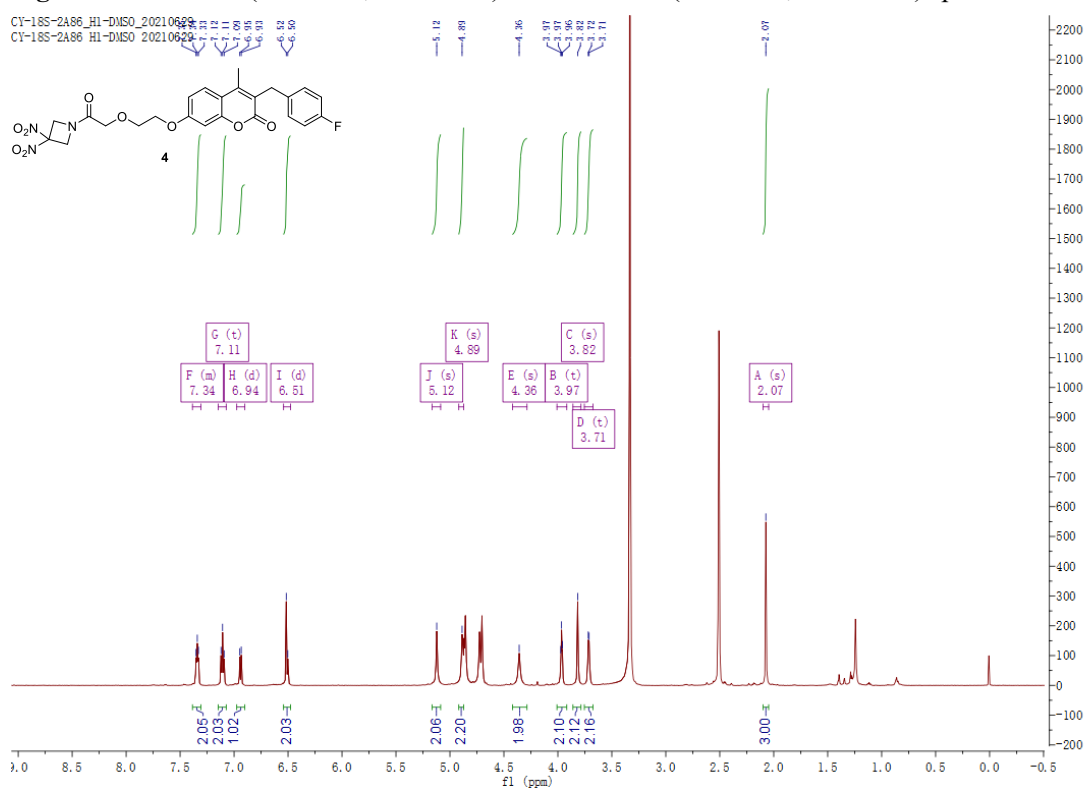


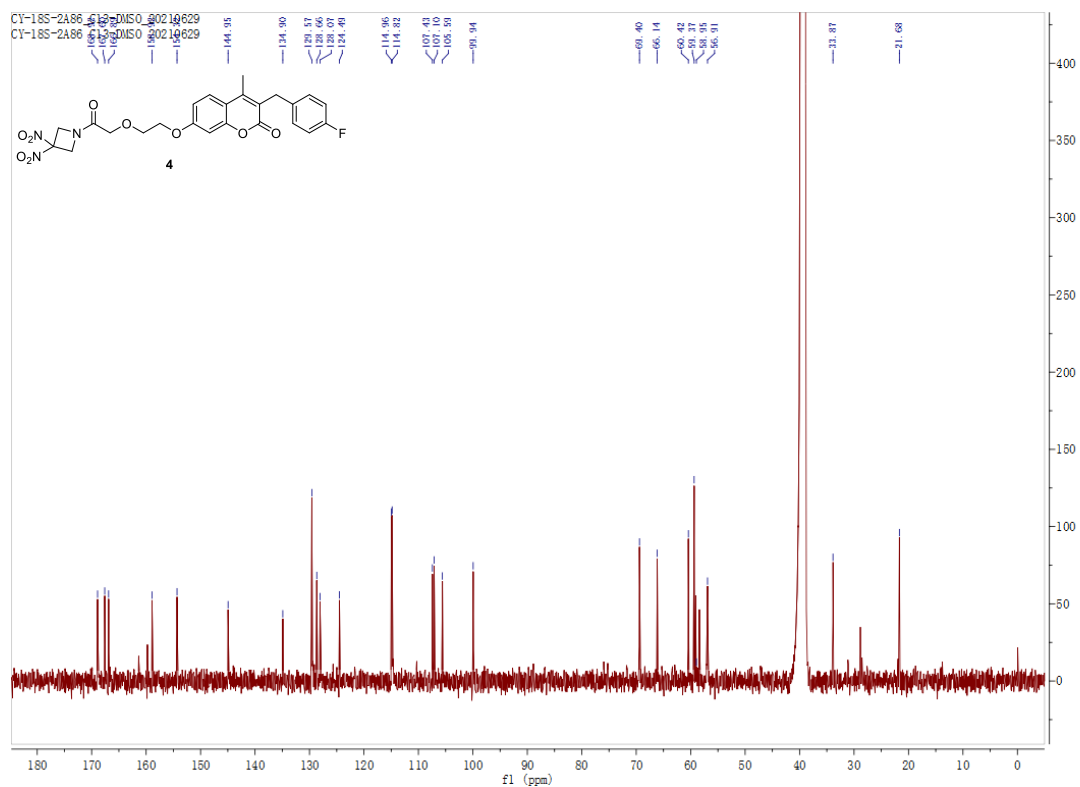
**Figure S1.** <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) and <sup>13</sup>C NMR (151 MHz, DMSO-*d*<sub>6</sub>) spectrum of **2**.



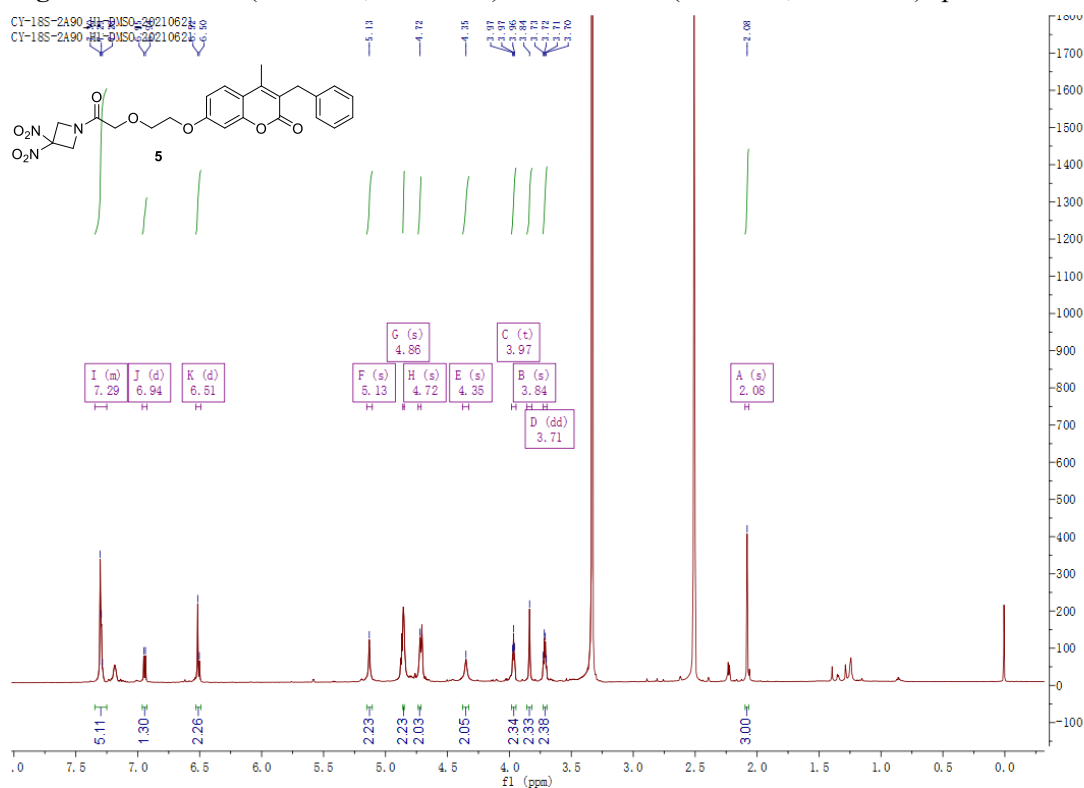


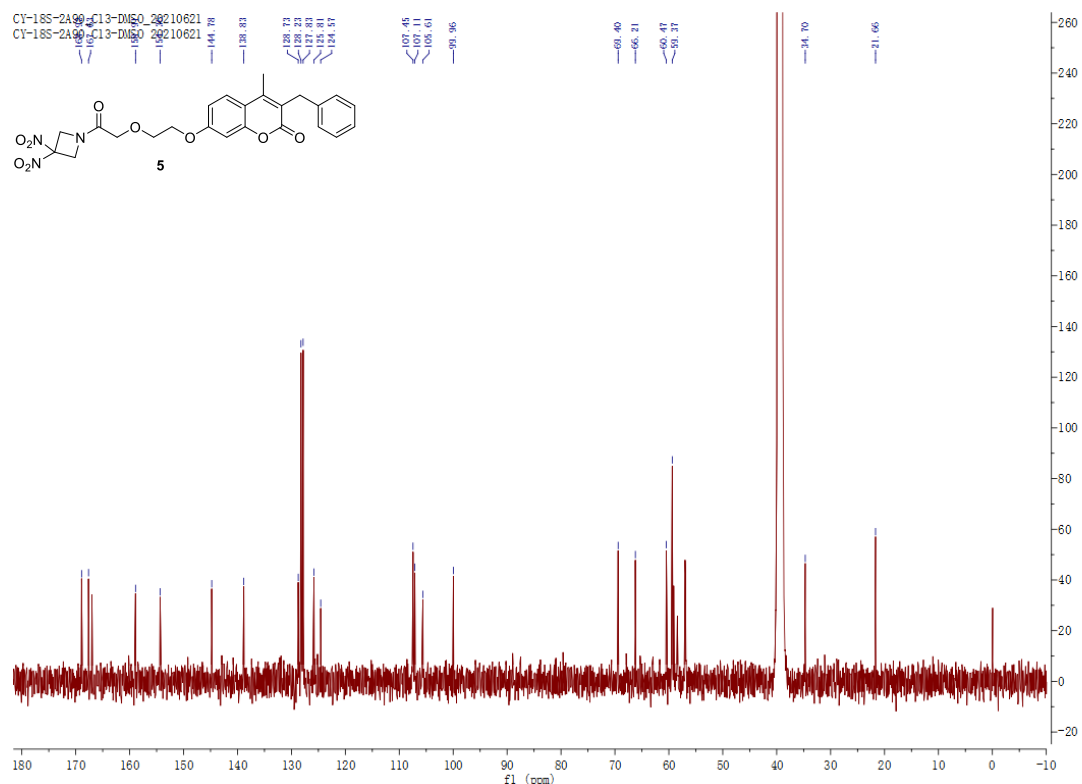
**Figure S2.**  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}d_6$ ) and  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO-}d_6$ ) spectrum of **3**.



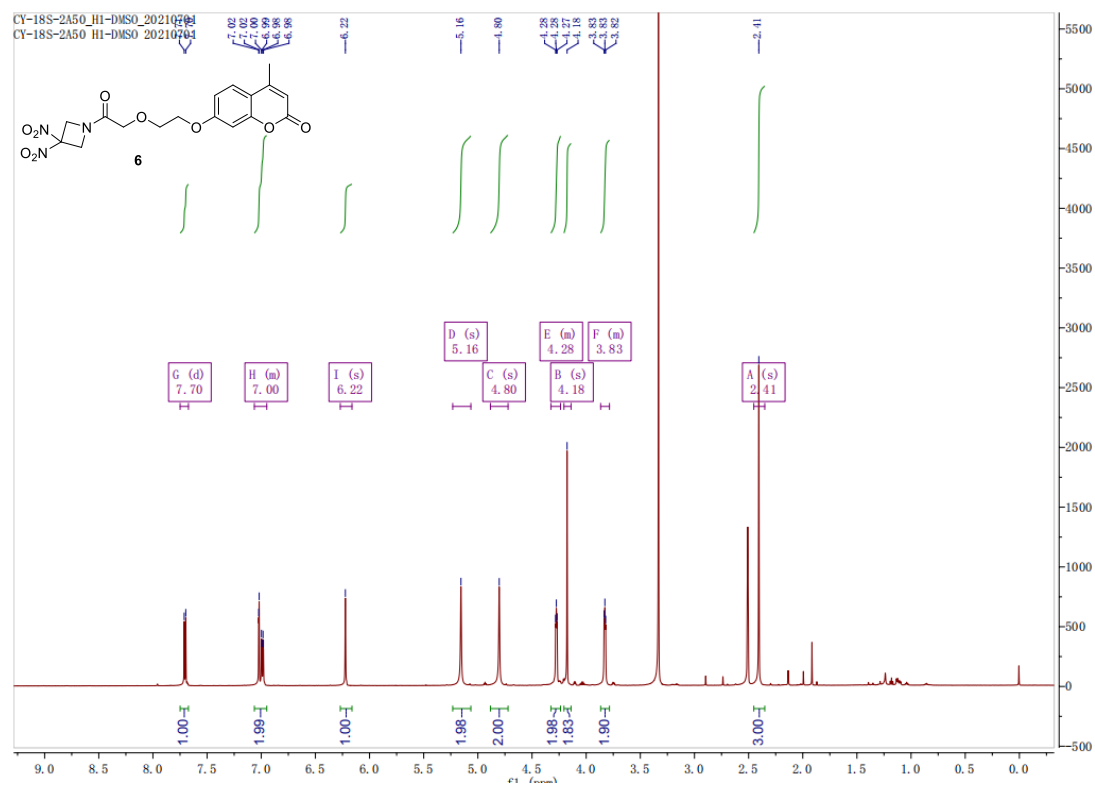


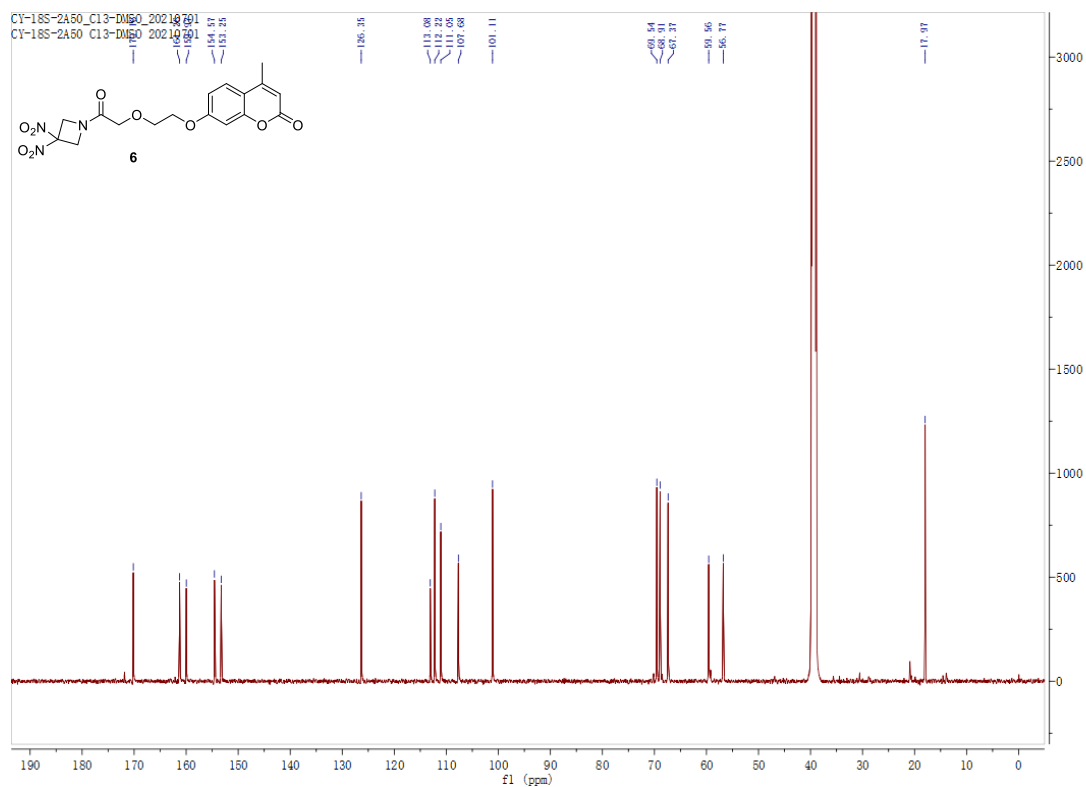
**Figure S3.**  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO}-d_6$ ) and  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **4**.



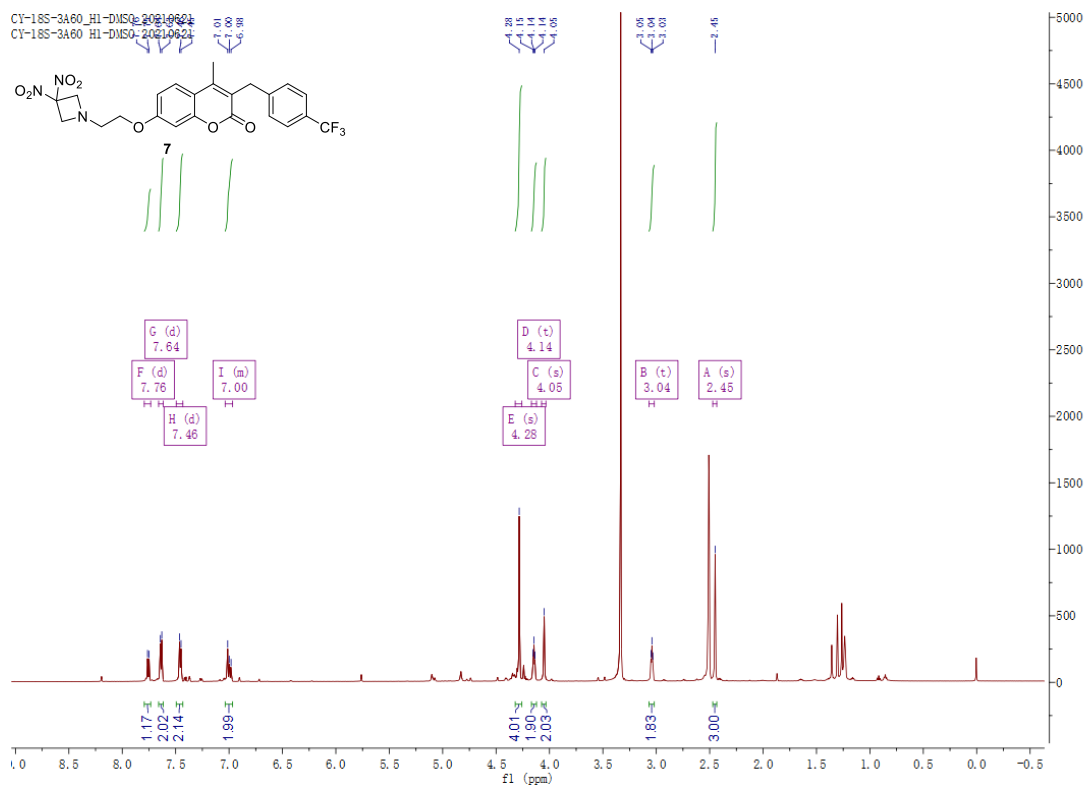


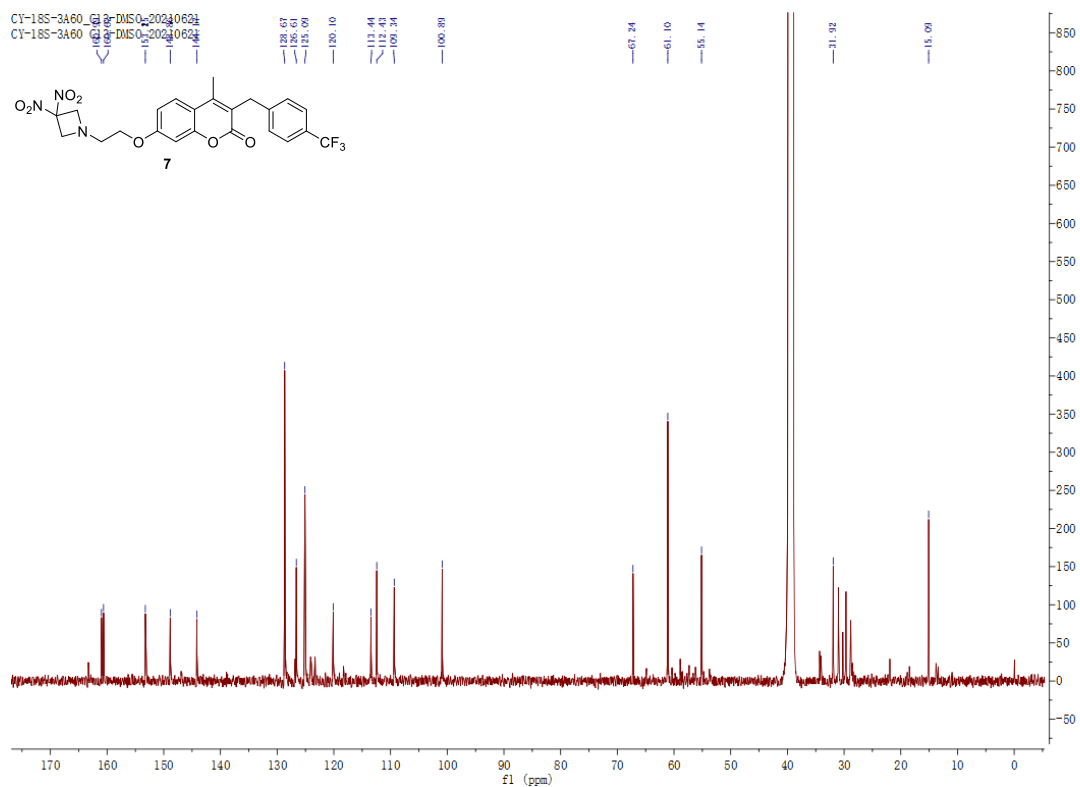
**Figure S4.** <sup>1</sup>H NMR (600 MHz, DMSO-d<sub>6</sub>) and <sup>13</sup>C NMR (151 MHz, DMSO-d<sub>6</sub>) spectrum of **5**.



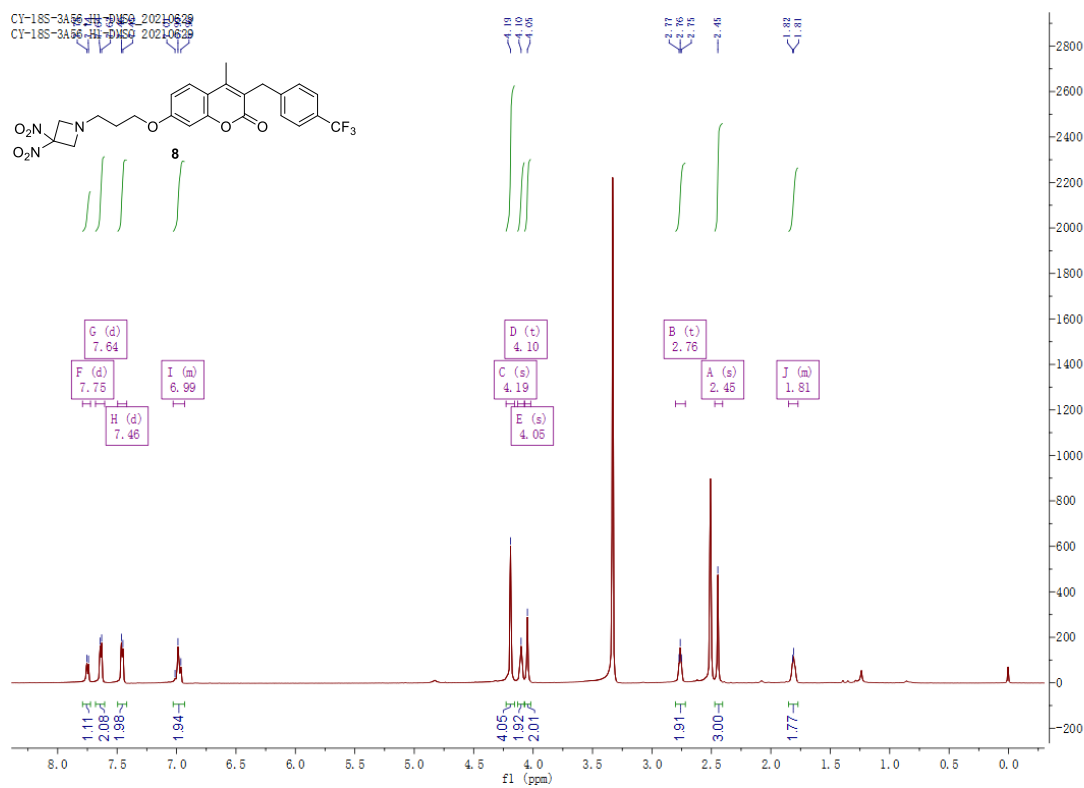


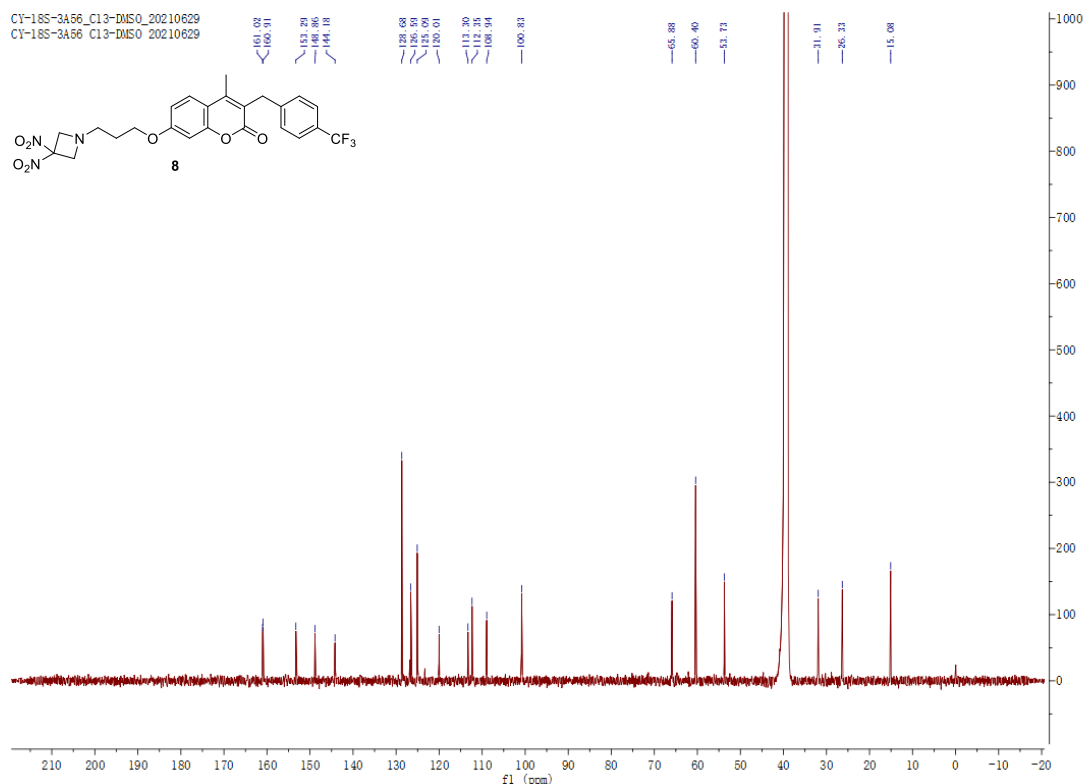
**Figure S5.**  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO-}d_6$ ) and  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO-}d_6$ ) spectrum of **6**.



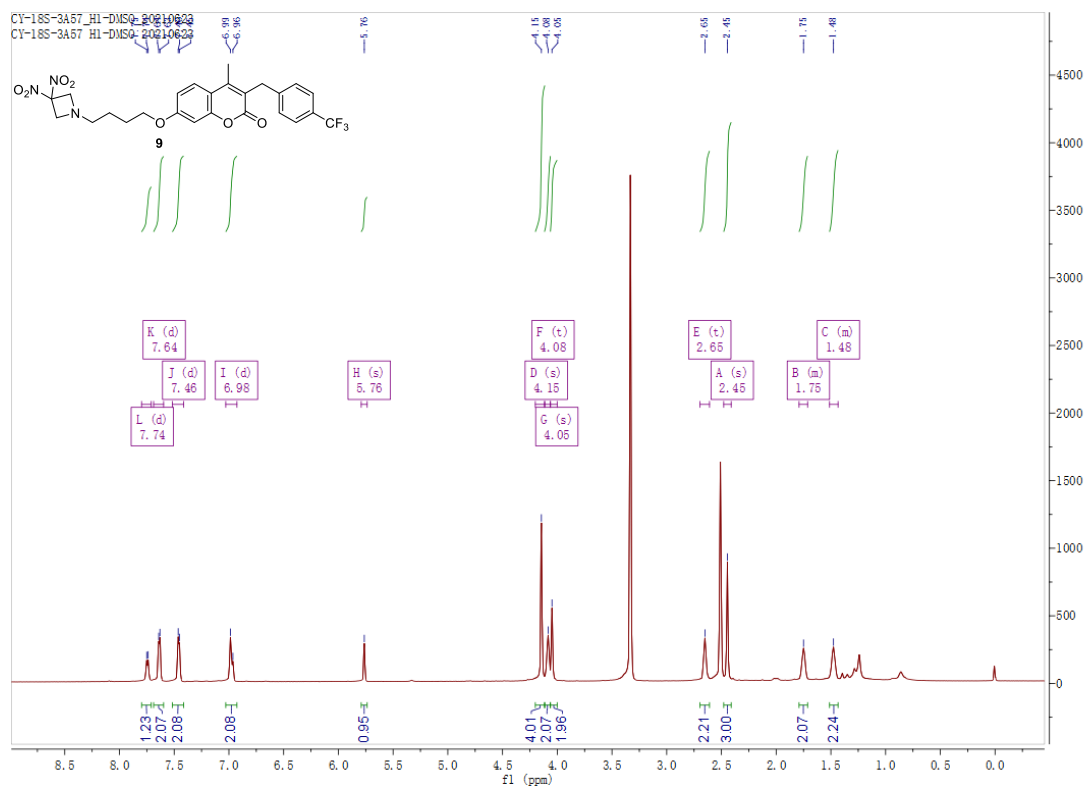


**Figure S6.** <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) and <sup>13</sup>C NMR (151 MHz, DMSO-*d*<sub>6</sub>) spectrum of **7**.

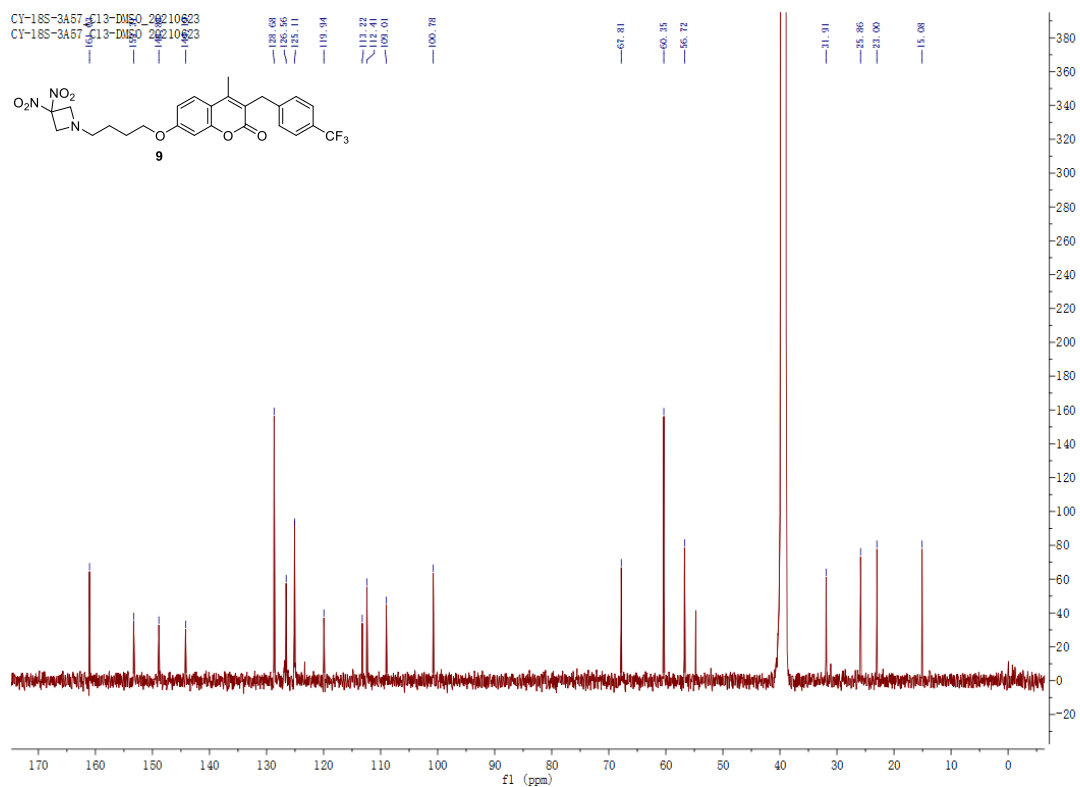




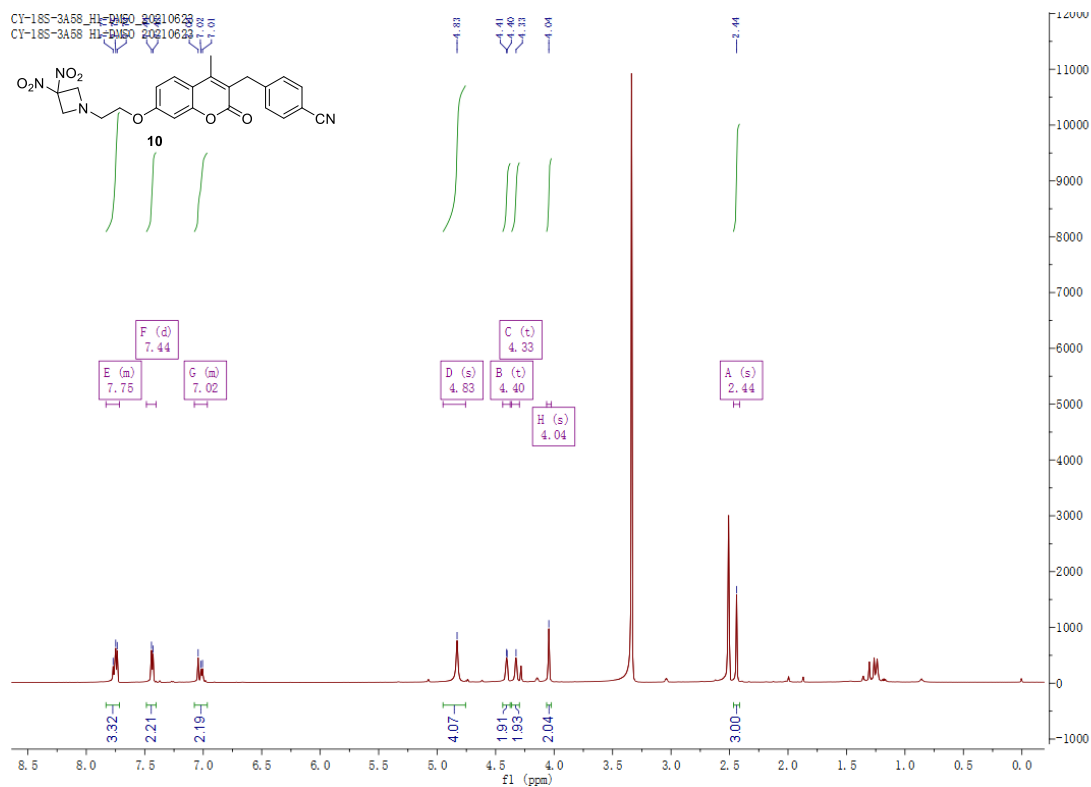
**Figure S7.**  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO}-d_6$ ) and  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **8**.

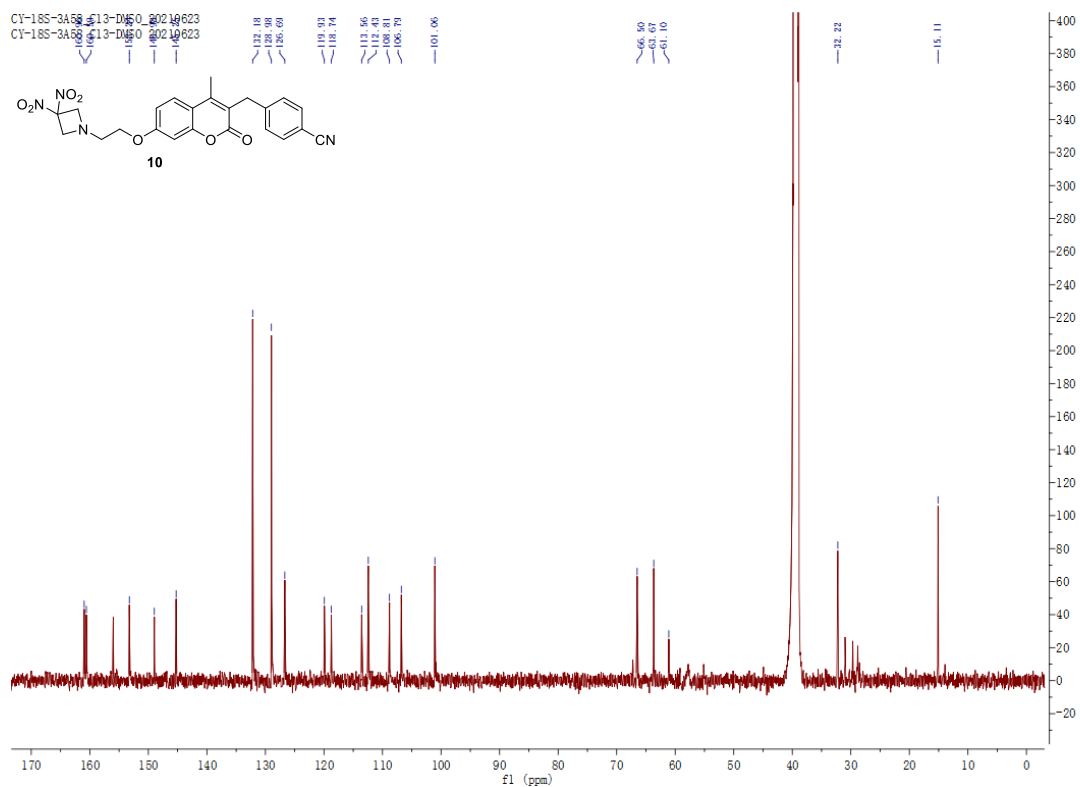




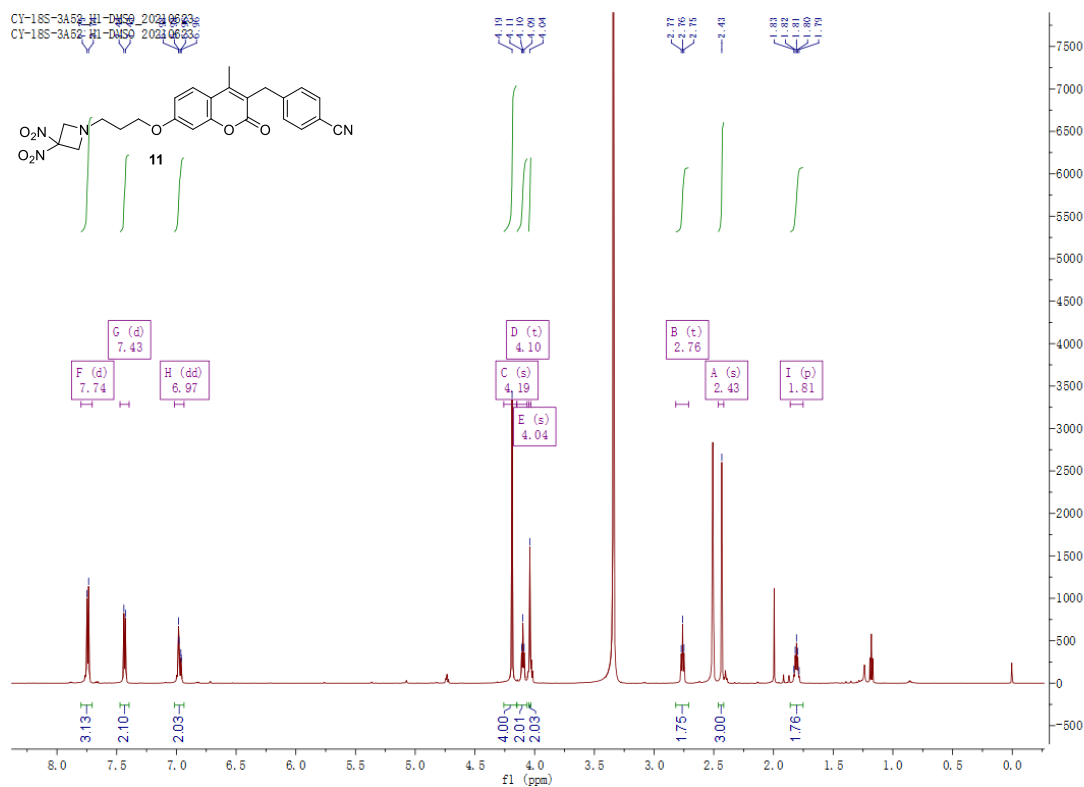


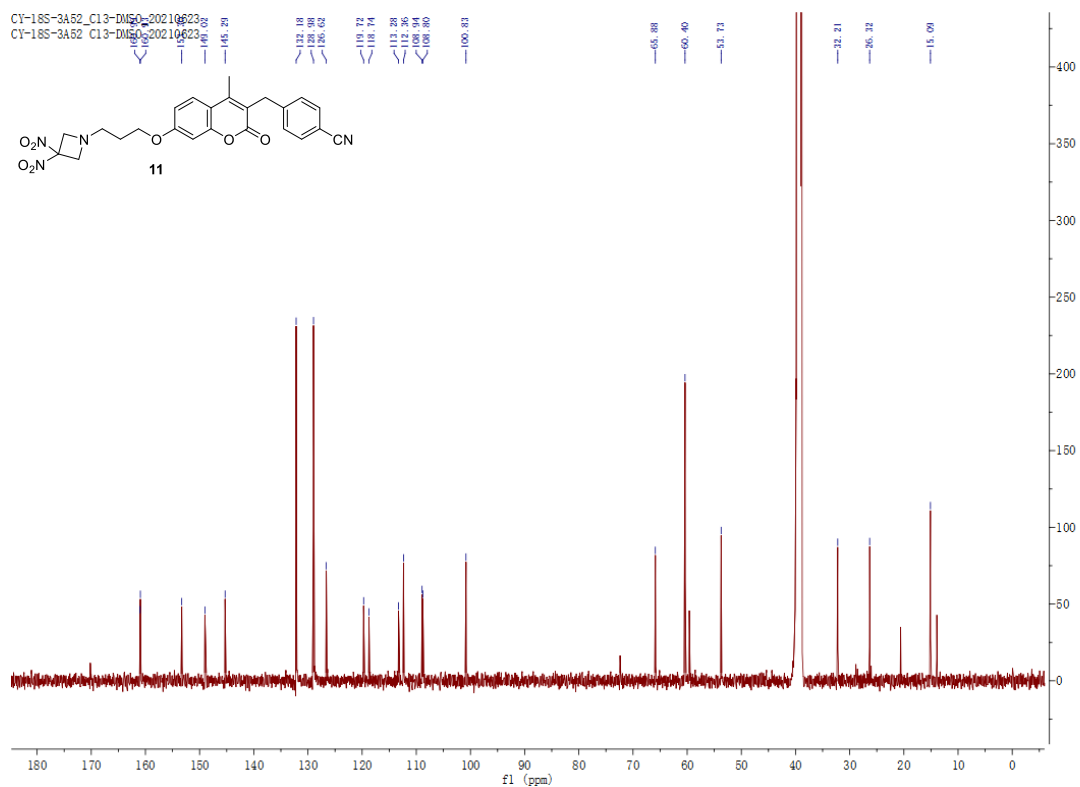
**Figure S8.**  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO}-d_6$ ) and  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **9**.



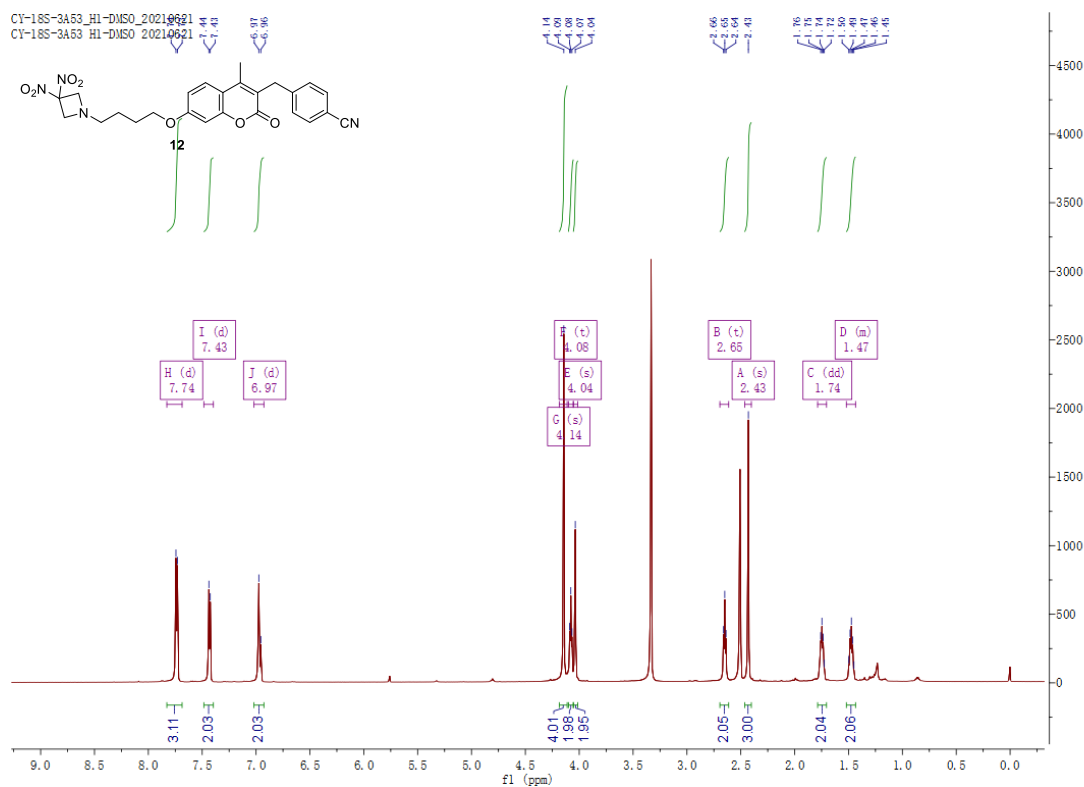


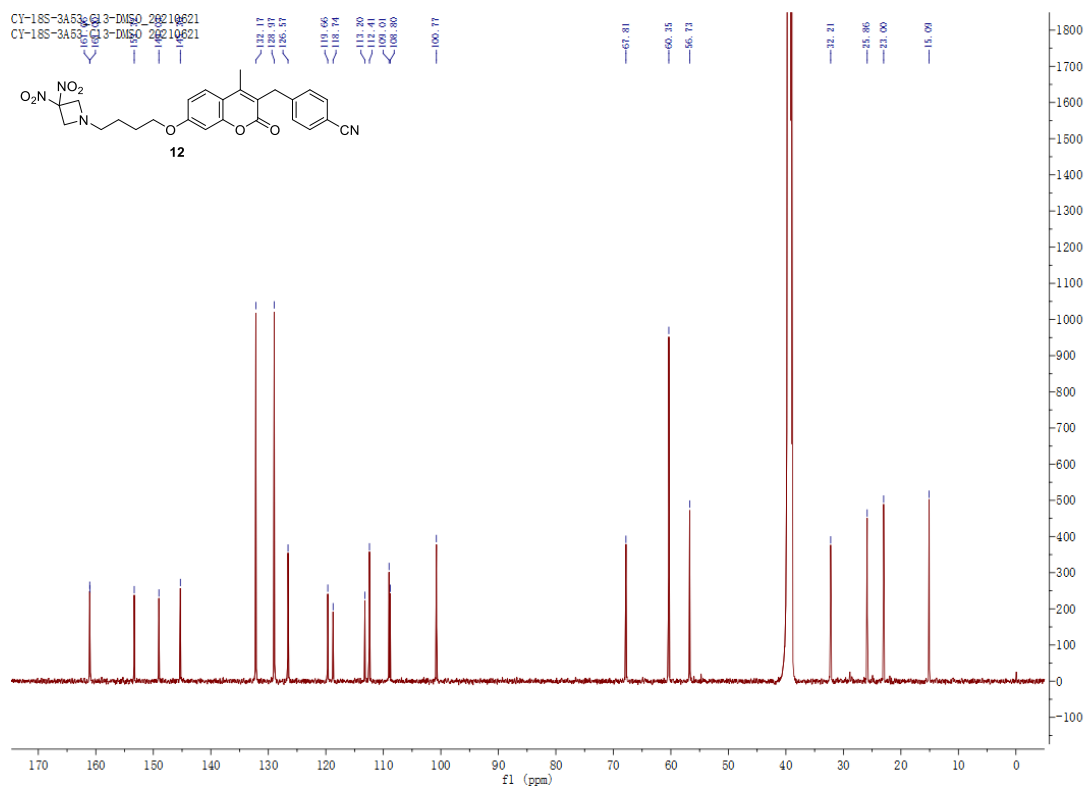
**Figure S9.**  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO}-d_6$ ) and  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **10**.



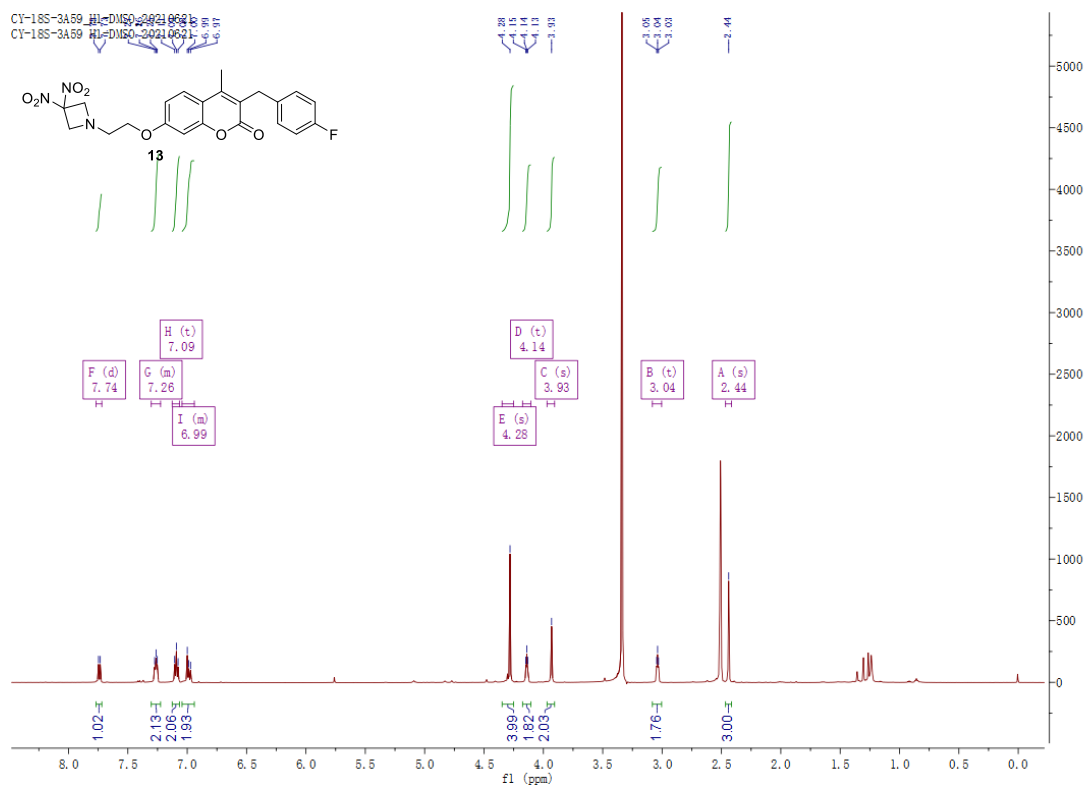


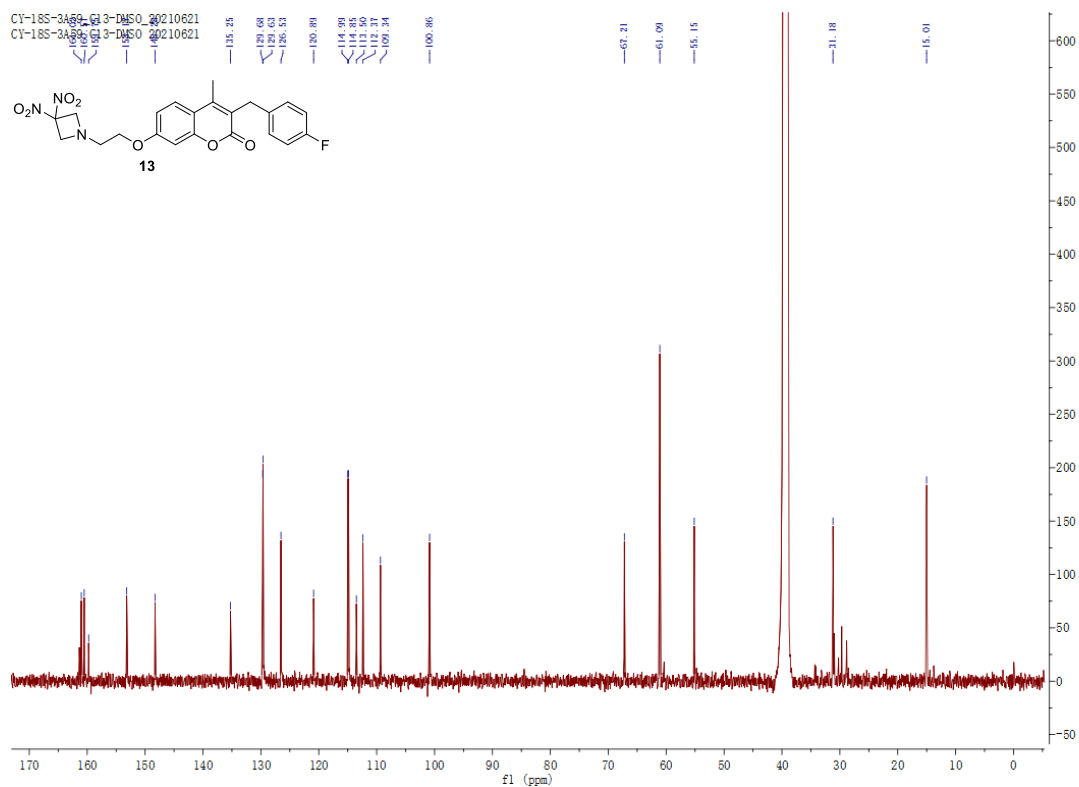
**Figure S10.**  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO}-d_6$ ) and  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **11**.



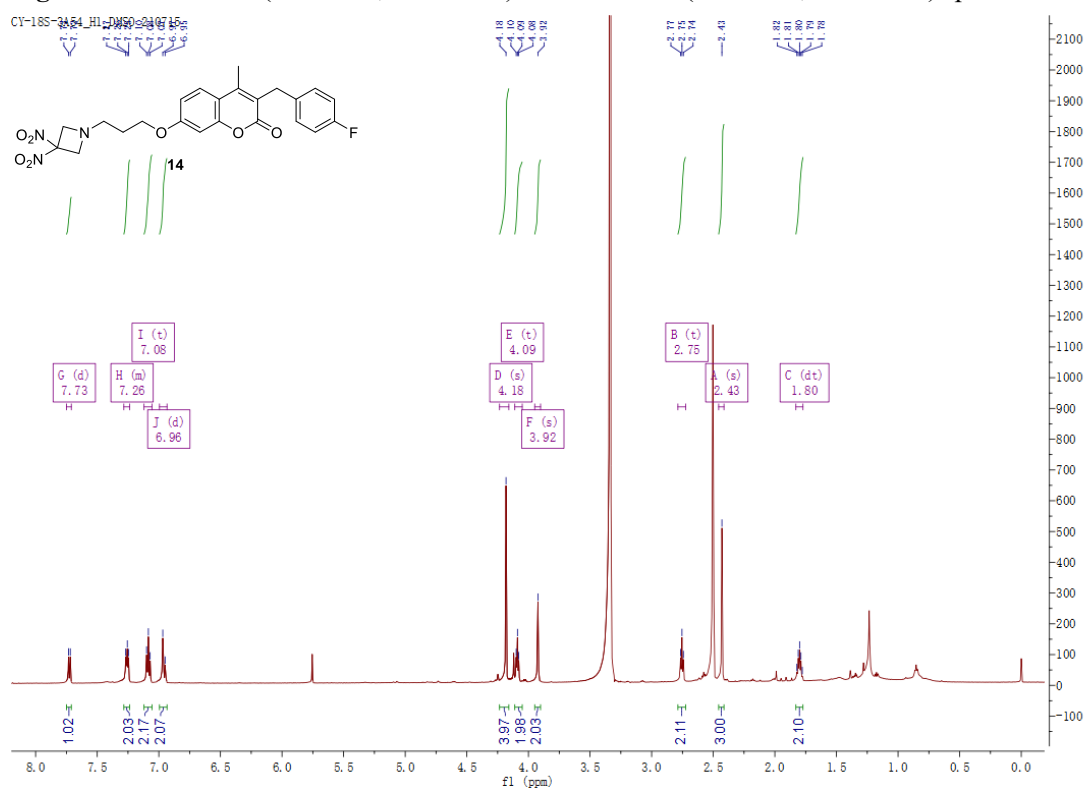


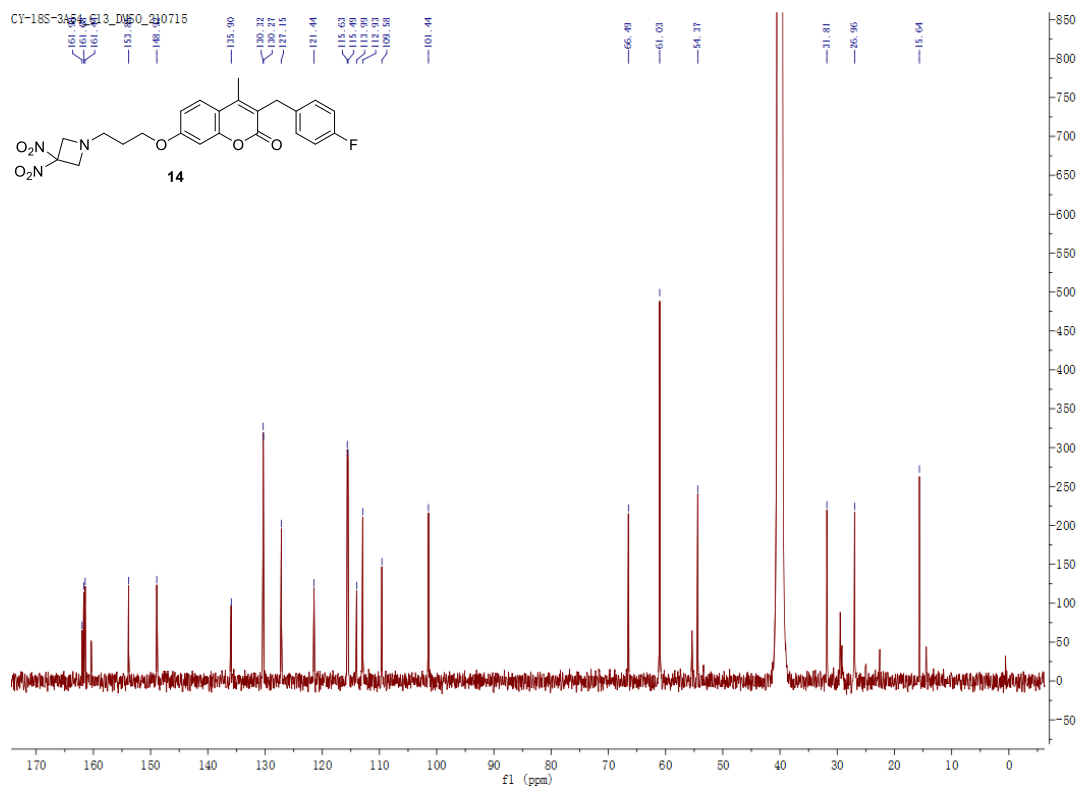
**Figure S11.**  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO}-d_6$ ) and  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **12**.



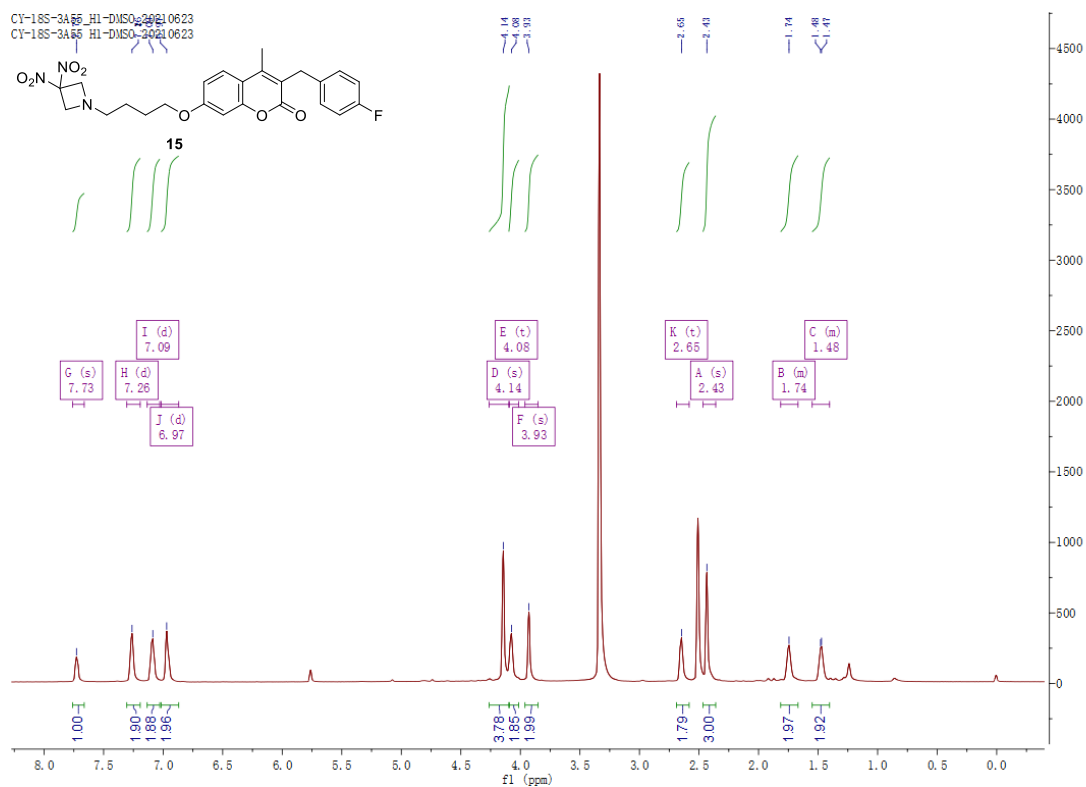


**Figure S12.**  $^1\text{H}$  NMR (600 MHz, DMSO- $d_6$ ) and  $^{13}\text{C}$  NMR (151 MHz, DMSO- $d_6$ ) spectrum of **13**.

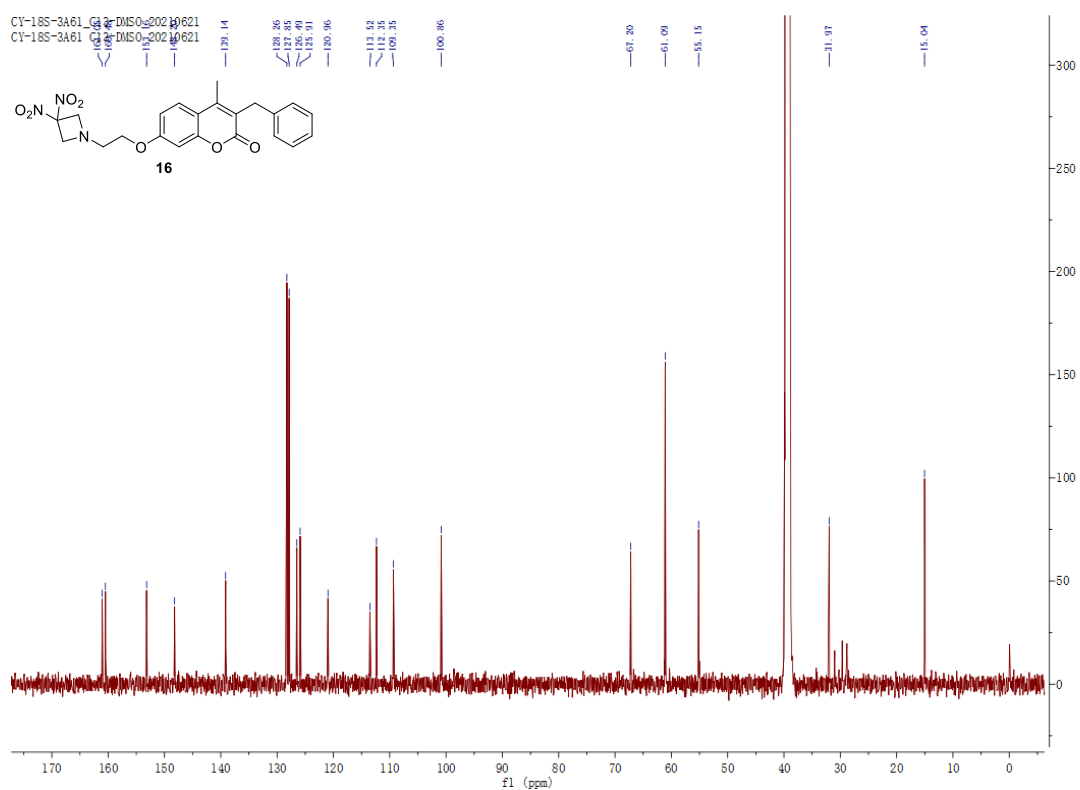




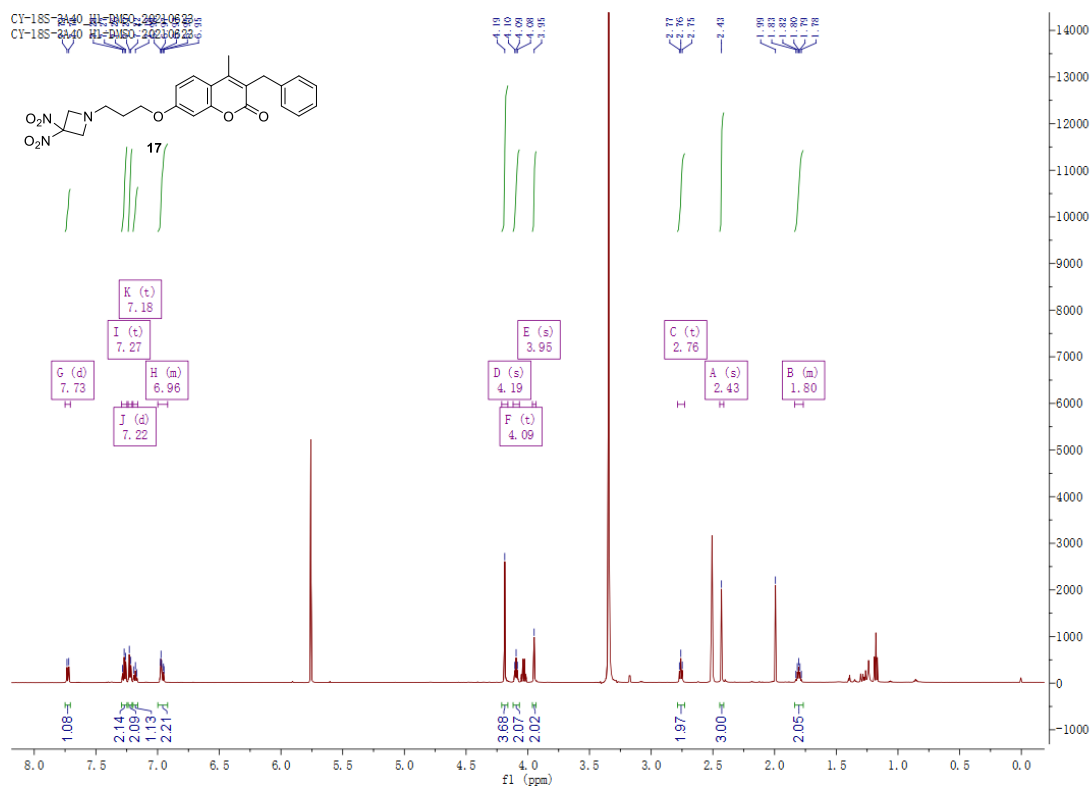
**Figure S13.** <sup>1</sup>H NMR (600 MHz, DMSO-*d*<sub>6</sub>) and <sup>13</sup>C NMR (151 MHz, DMSO-*d*<sub>6</sub>) spectrum of **14**.



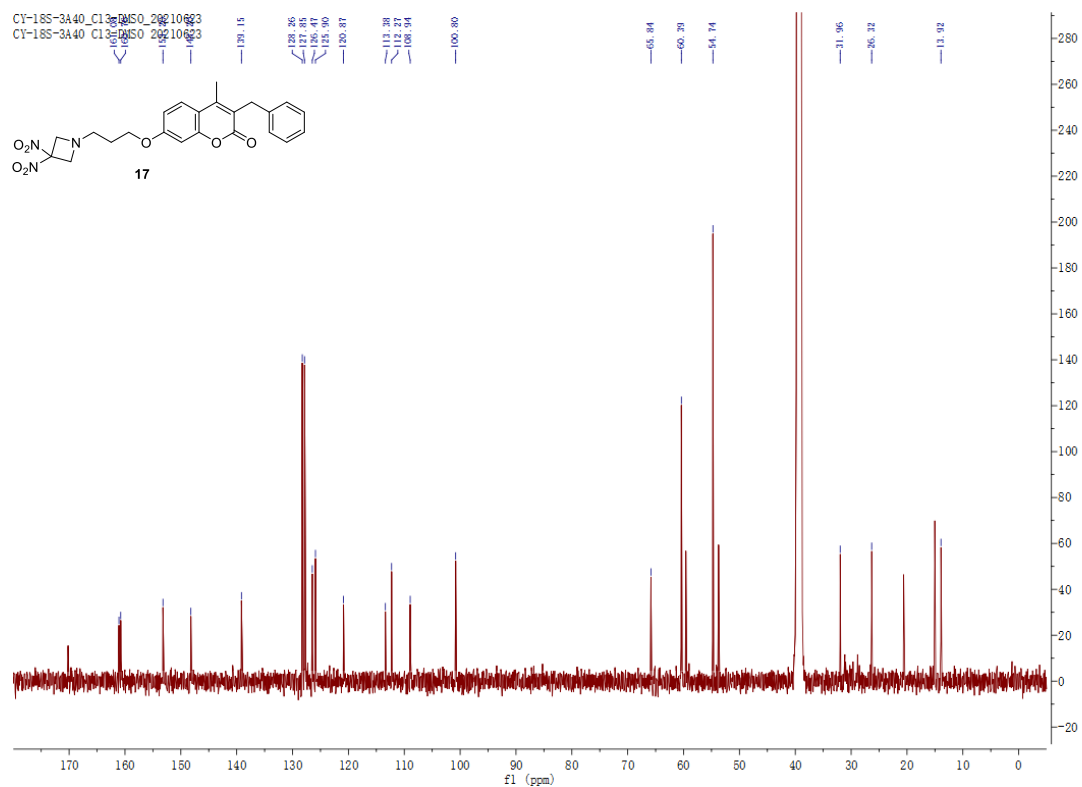




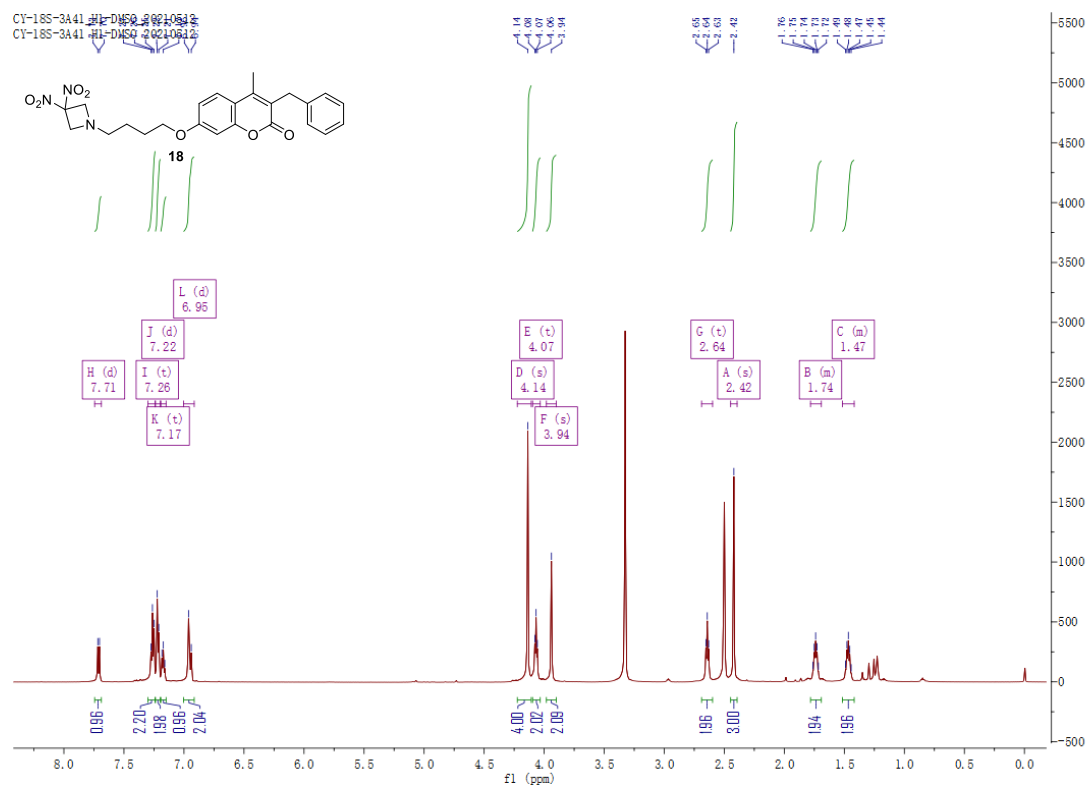
**Figure S15.**  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO}-d_6$ ) and  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **16**.

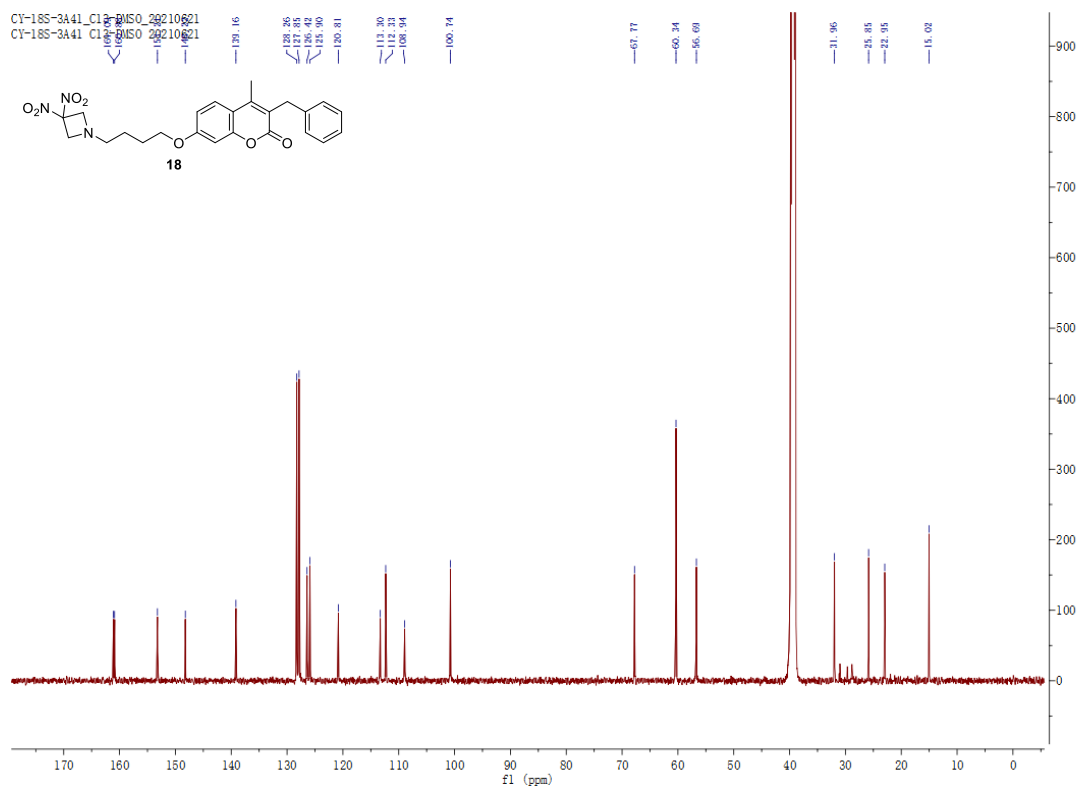




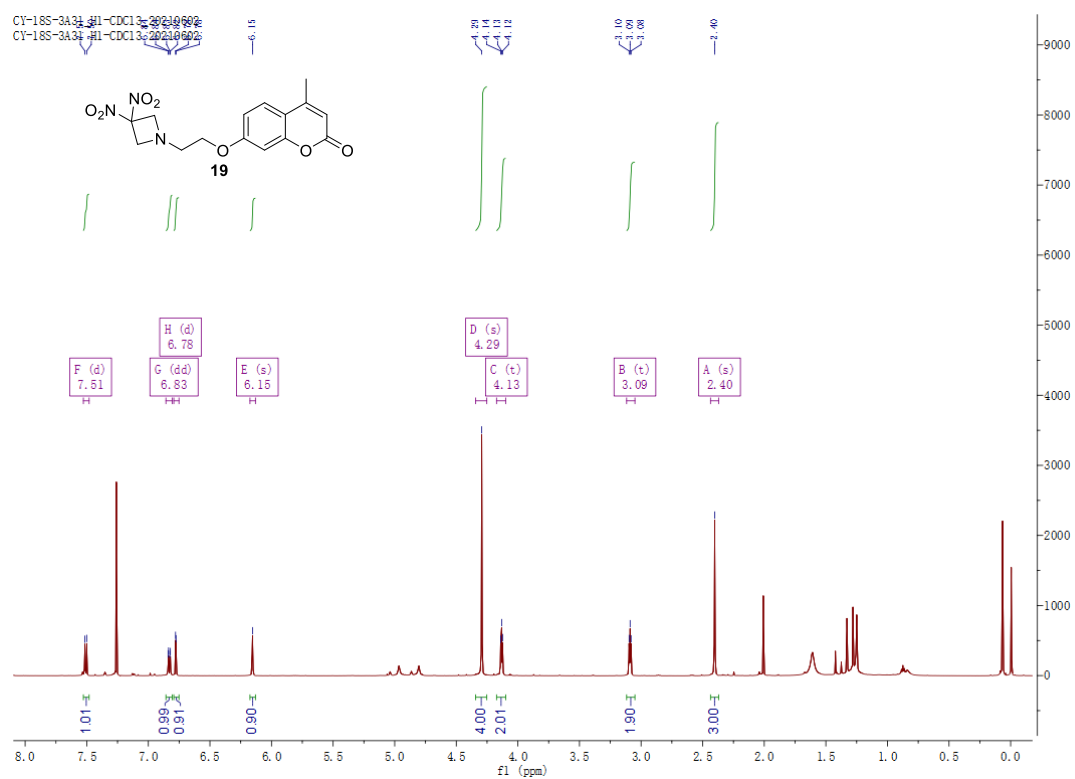


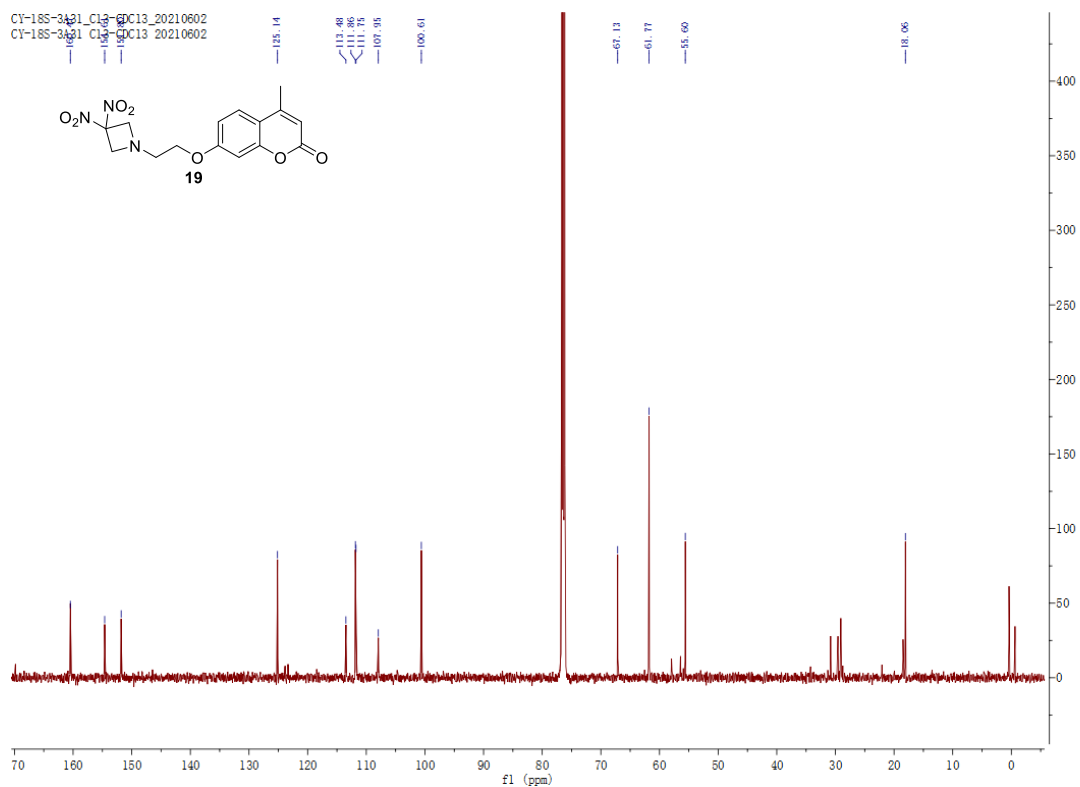
**Figure S16.**  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO}-d_6$ ) and  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **17**.





**Figure S17.**  $^1\text{H}$  NMR (600 MHz,  $\text{DMSO}-d_6$ ) and  $^{13}\text{C}$  NMR (151 MHz,  $\text{DMSO}-d_6$ ) spectrum of **18**.





**Figure S18.**  $^1\text{H}$  NMR (600 MHz,  $\text{CDCl}_3$ ) and  $^{13}\text{C}$  NMR (151 MHz,  $\text{CDCl}_3$ ) spectrum of **19**.

