Supporting Information

Selectively lighting-up glyoxal in the living cell by an o-phenylenediamine fused hemicyanine

Zhiming Wang,[a,b] Chang Liu,[a,b*] Huirong Yao,[a,b] Song He,[a,b] Liancheng Zhao[c] and Xianshun Zeng[*a,b]

[a] Tianjin Key Laboratory for Photoelectric Materials and Devices, School of Materials Science & Engineering, Tianjin University of Technology, Tianjin 300384, China. Fax: (+86)22-60215226; Tel: (+86)22-60216748; E-mail: xshzeng@tjut.edu.cn.

[b] Key Laboratory of Display Materials and Photoelectric Devices, Ministry of Education, School of Materials Science & Engineering, Tianjin University of Technology, Tianjin, 300384, China.

[c] School of Materials Science and Engineering, Institute of Information Functional Materials& Devices, Harbin Institute of Technology, Harbin, 150001, China.

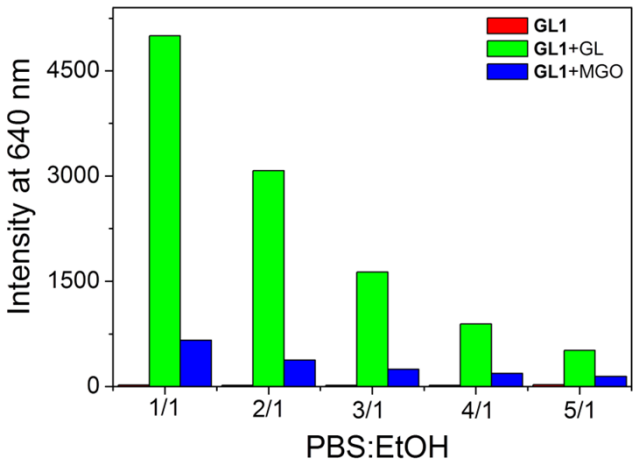

Figure S1. Fluorescence intensity of **GL1** (5 μM) upon the addition of 10 equiv. GL in different PBS with different contents of ethanol. λ_{ex} = 500 nm; slit = 10 nm, 10 nm.

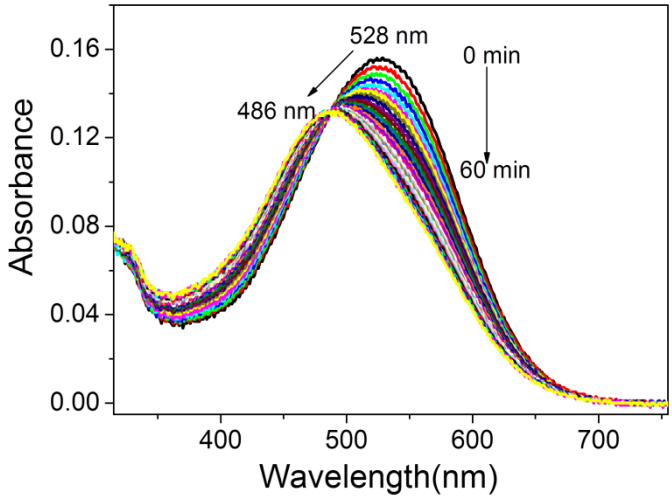

Figure S2. Time-dependent absorption spectra for the probe **GL1** (5 μM) upon addition of GL (50 mM).

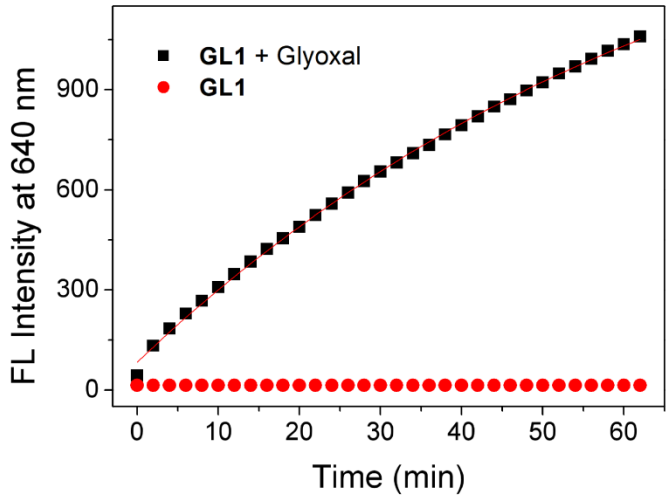

Figure S3. Plot of the fluorescence intensity at 640 nm against the reaction time (0-70 min) of **GL1** (5 μM) and GL (5 mM).

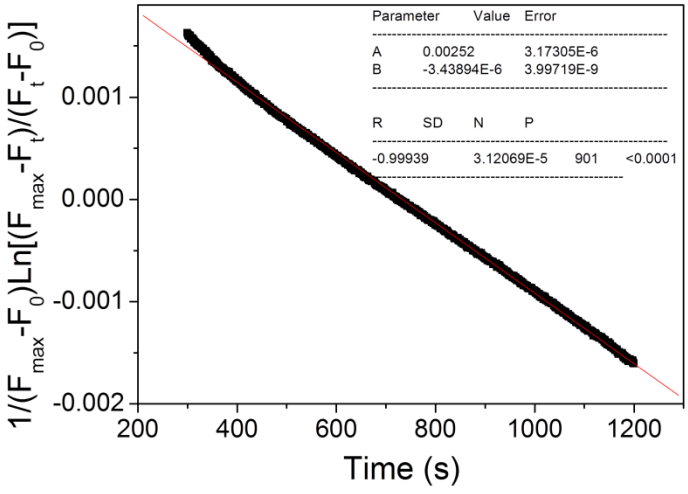

Figure S4. *Pseudo*-second-order kinetic plot of the reaction of **GL1** (5 μM) and GL (5 mM) in PBS (10 mM, pH 7.4, 25% EtOH).

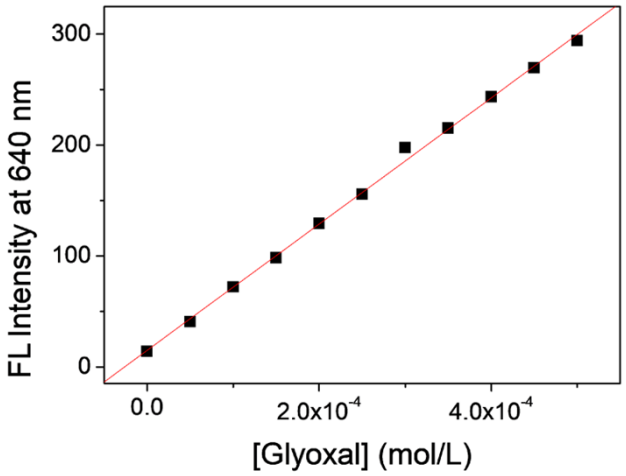

Figure S5. Fluorescence intensity at 640 nm of **GL1** against the GL concentrations, respectively. λ_{ex} = 500 nm; slit = 10 nm, 10 nm.

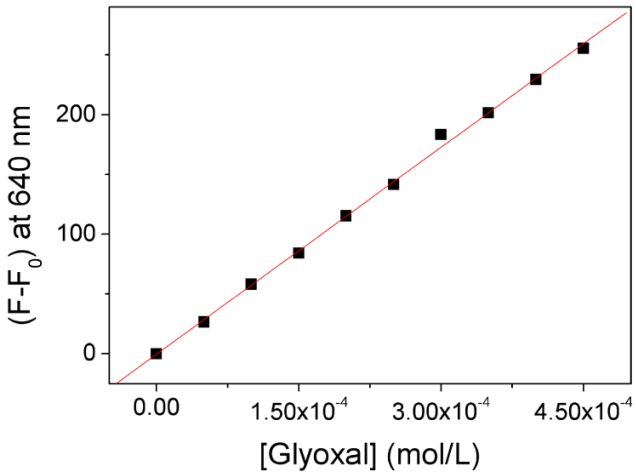

Figure S6. Emission at 640 nm of the **GL1** (5 μM) in different concentrations of GL. The detection limit can be calculated with the equation [S1], DL = 3σ/ *slope*, where "*slope*" is the calibration sensitivity of the fluorescence intensity change ($\Delta F = F - F_0$) versus [glyoxal], and "σ" is the standard deviation of the blank signal (F_0) obtained without GL. The detection limits for GL was found to be 2.1×10^{-8} mol/L under the testing conditions.

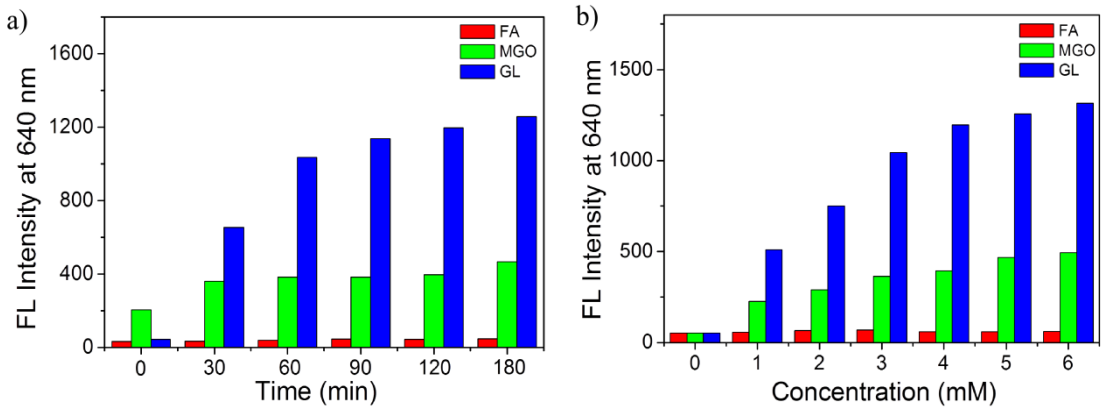

Figure S7. a) Relative fluorescence intensity at 640 nm for the probe **GL1** (5 μM) in the presence of FA (5 mM), MGO (5 mM) and GL (5 mM) in different times; b) Relative fluorescence intensity at 640 nm for the probe **GL1** (5 μM) in the presence of FA, MGO and GL in different concentrations (0 mM, 1 mM, 2 mM, 3 mM, 4 mM, 5 mM, 6 mM).

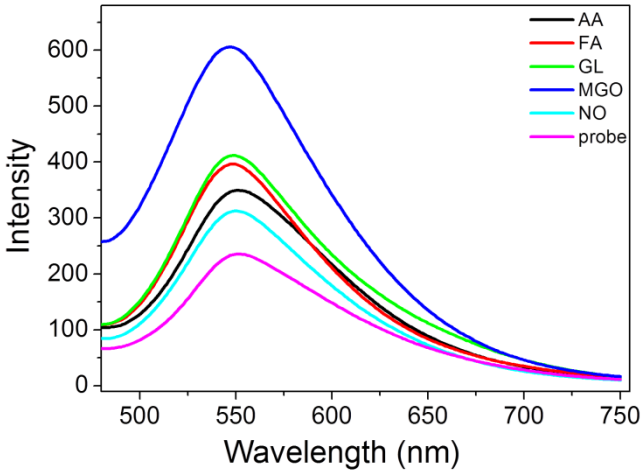

Figure S8. Fluorescence spectra of **GL0** (5 μM) toward relevant species (AA 5mM, FA 5 mM, MGO 5 mM, GL 5 mM and NO 5mM) in 10 mM PBS buffer (pH 7.4, containing 25% EtOH). λ_{ex} = 460 nm; slit = 10 nm, 10 nm.

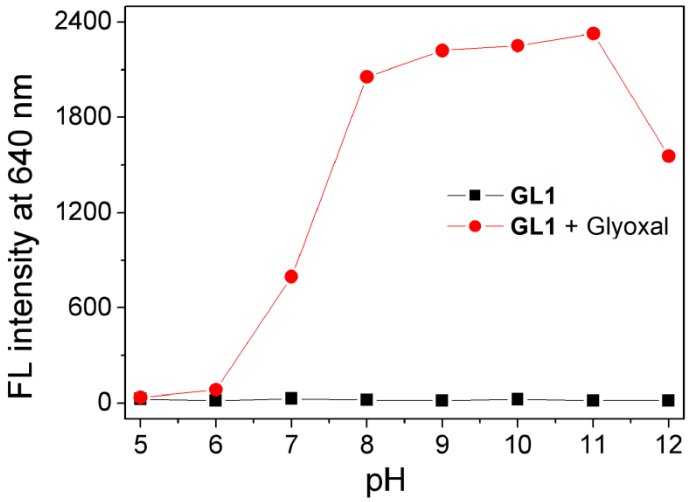

Figure S9. Fluorescence intensities of **GL1** (5 μM) at 640 nm in the presence and absence of GL (500 equiv.) at each pH.

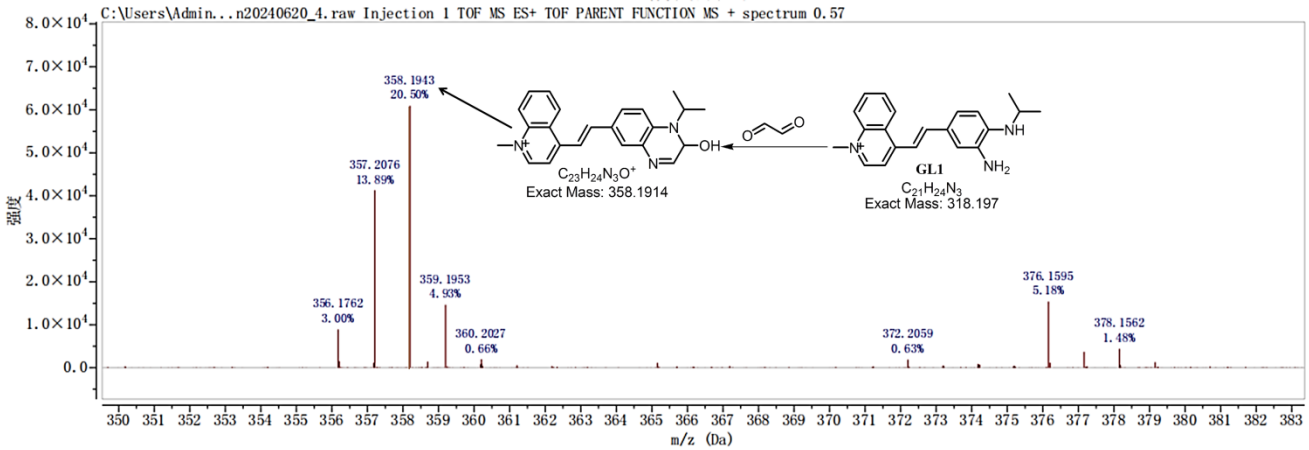

Figure S10. HRMS (LC/MS) spectrum of **GL1** in the presence of GL in PBS (10 mM, pH 7.4, 25% EtOH). The peak of 358.1943 m/z can be assigned to the reaction product of **GL1** with GL.

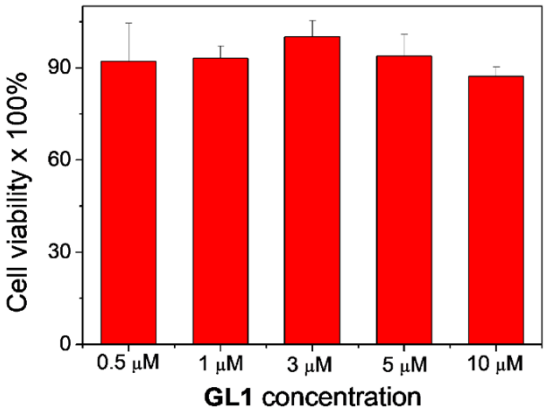

Figure S11. Effects of **GL1** at varied concentrations on the viability of HeLa cells after an incubation time of 24 h.

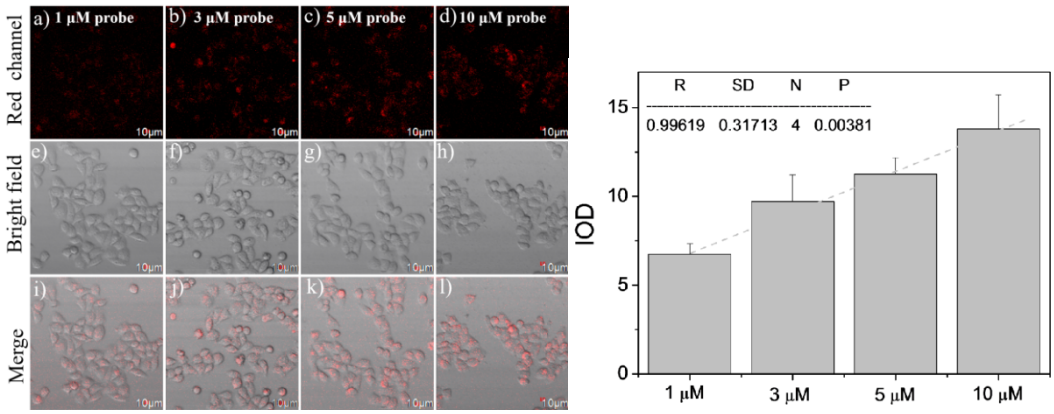

Figure S12. Confocal fluorescence images of HeLa cells incubated with different concentrations of **GL1**. λ_{ex} = 559 nm, λ_{em} = 590-680 nm; Scale bar: 10 μm.

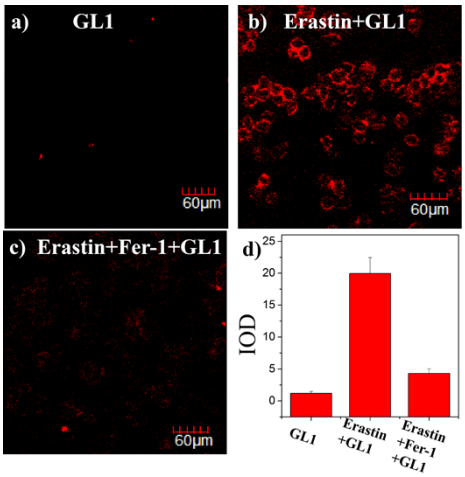

Figure S13. Fluorescence imaging of glyoxal in HeLa cells during ferroptosis. a) only **GL1** (1 μM) treated for 2 h; b) HeLa cells pre-incubated with erastin (20 μM) for 6 h and then incubated with **GL1** (1 μM) for another 2 h; c) HeLa cells were incubated with erastin (20 μM) in the presence of Fer-1 (40 μM) for 6 h, and then incubated with **GL1** (1 μM) for another 2 h; d) Mean fluorescence intensity in the red channel; the results are presented as means ± SE with replicates n = 3. Red channel: λ_{ex} = 559 nm, collected at 590-680 nm. Scale bar: 20 μm.

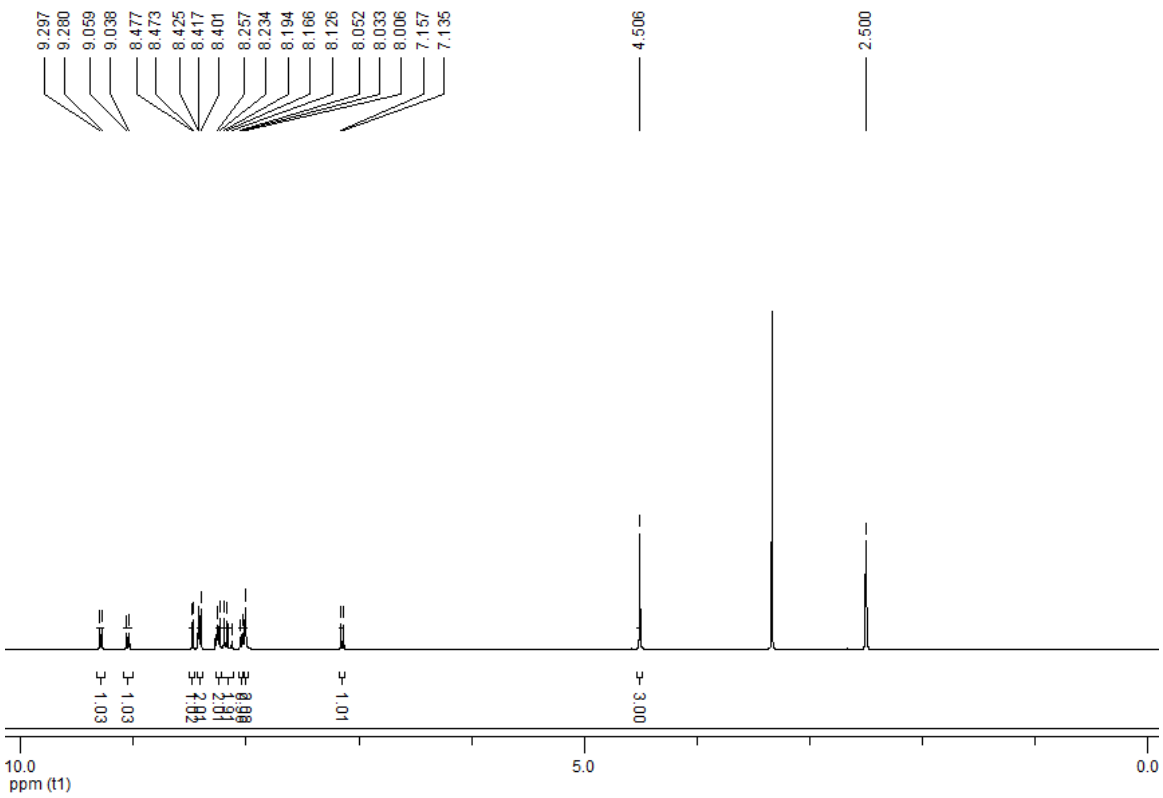

Figure S14. ^{1}H NMR spectrum of **1a** in DMSO-d_6.

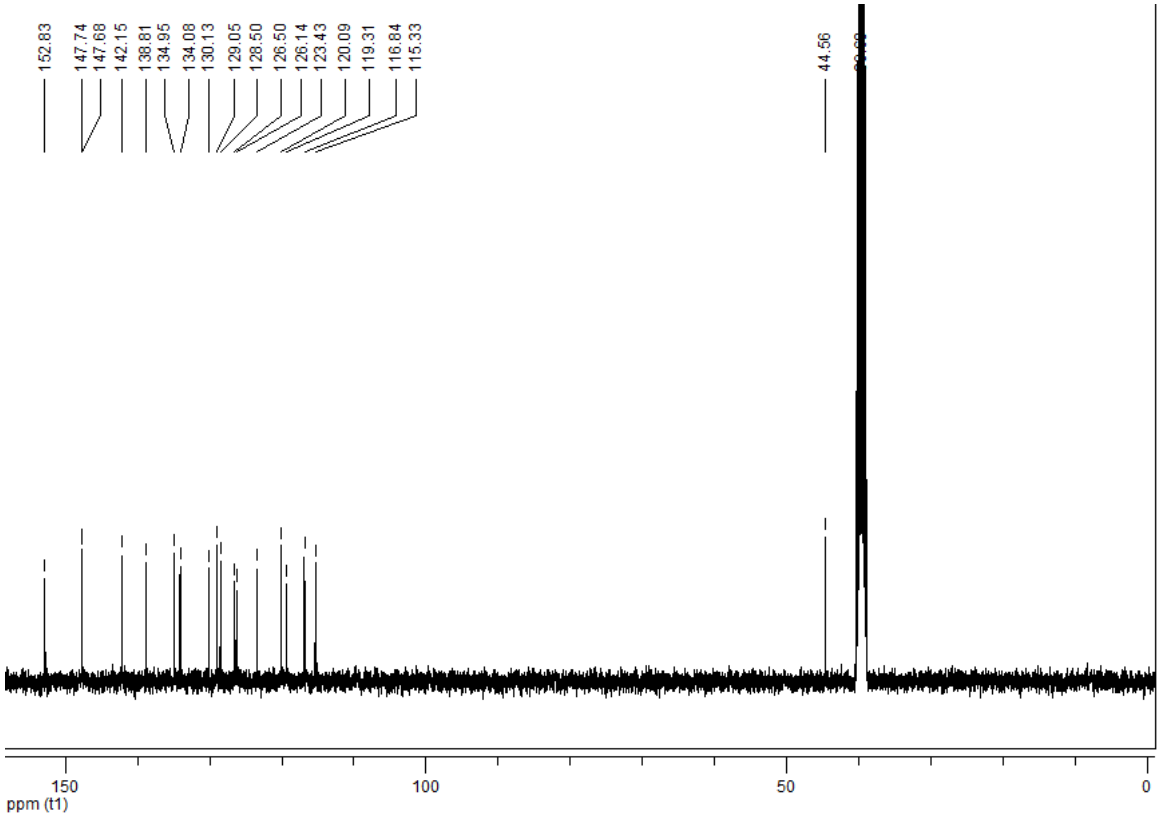

Figure S15. ^{13}C NMR spectrum of **1a** in DMSO-d_6.

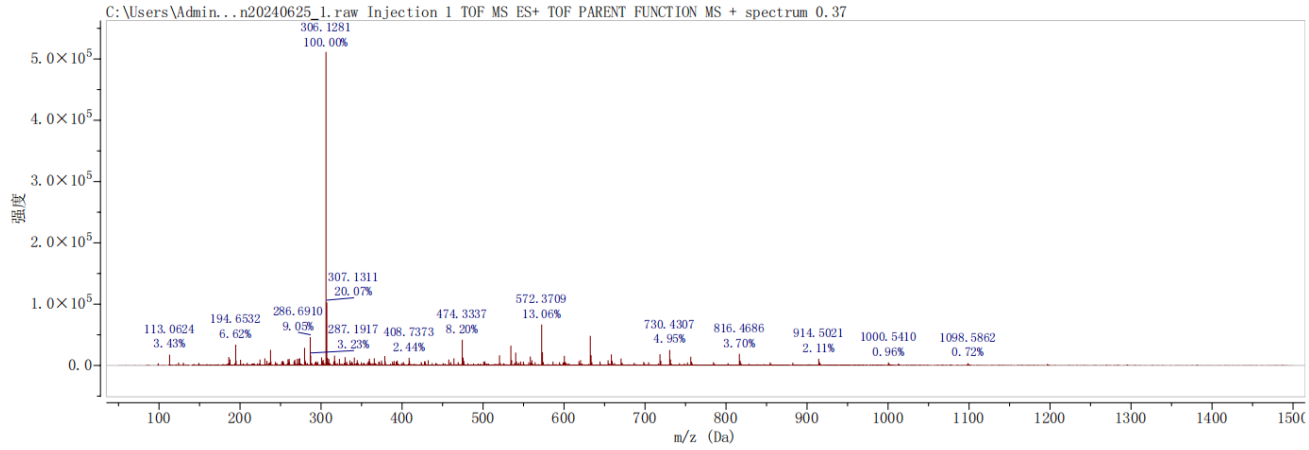

Figure S16. HRMS (LC/MS) spectra of **1a**. The peak at m/z = 306.1281 was assigned to the mass of **1a**.

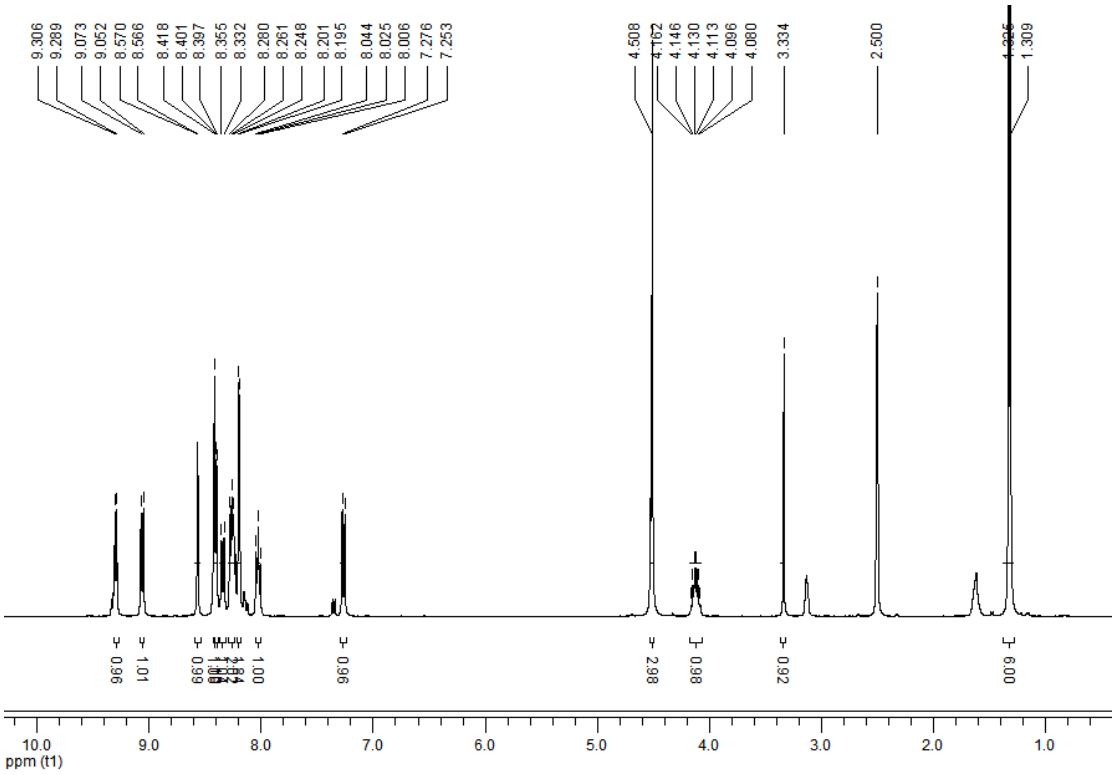

Figure S17. ^{1}H NMR spectrum of **1b** in DMSO-d_6.

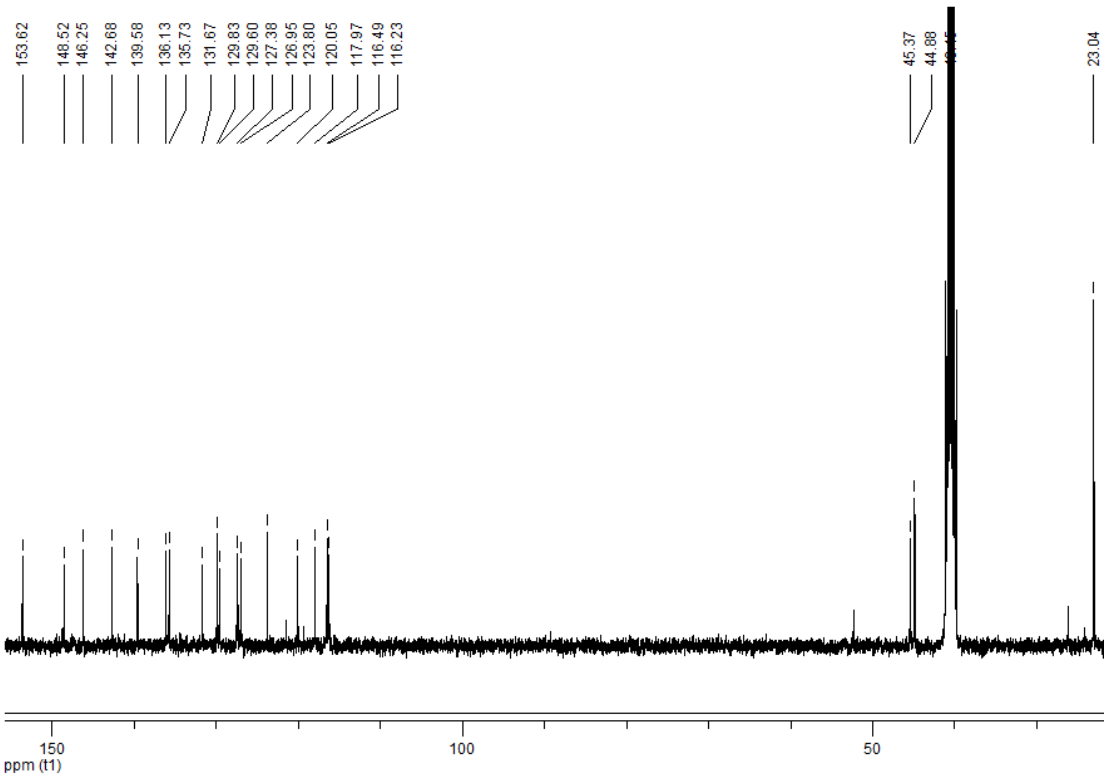

Figure S18. ^{13}C NMR spectrum of **1b** in DMSO-d_6.

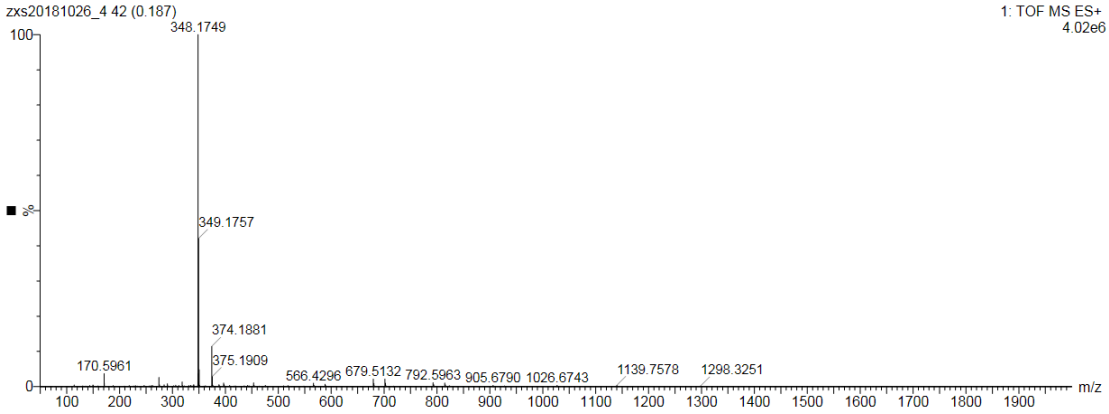

Figure S19. HRMS (LC/MS) spectra of **1b**. The peak at m/z = 348.1749 was assigned to the mass of **1b**.

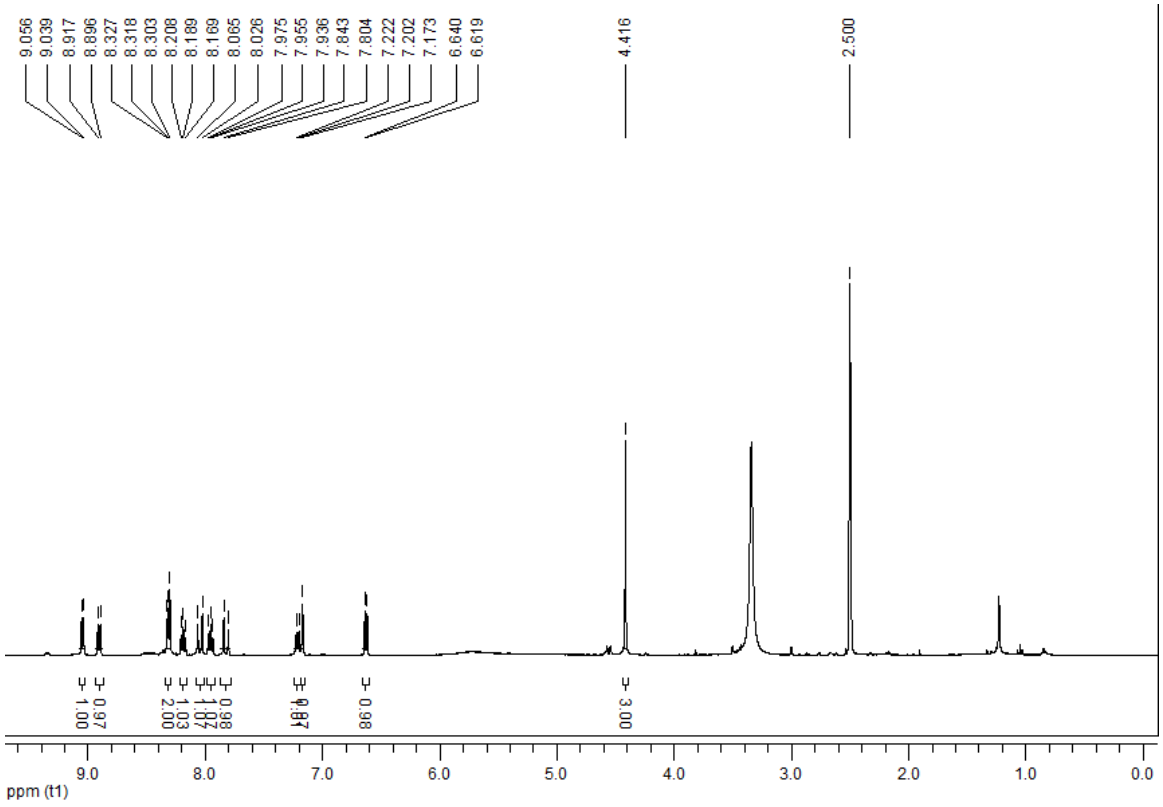

Figure S20. ^{1}H NMR spectrum of **GL0** in DMSO-d_6.

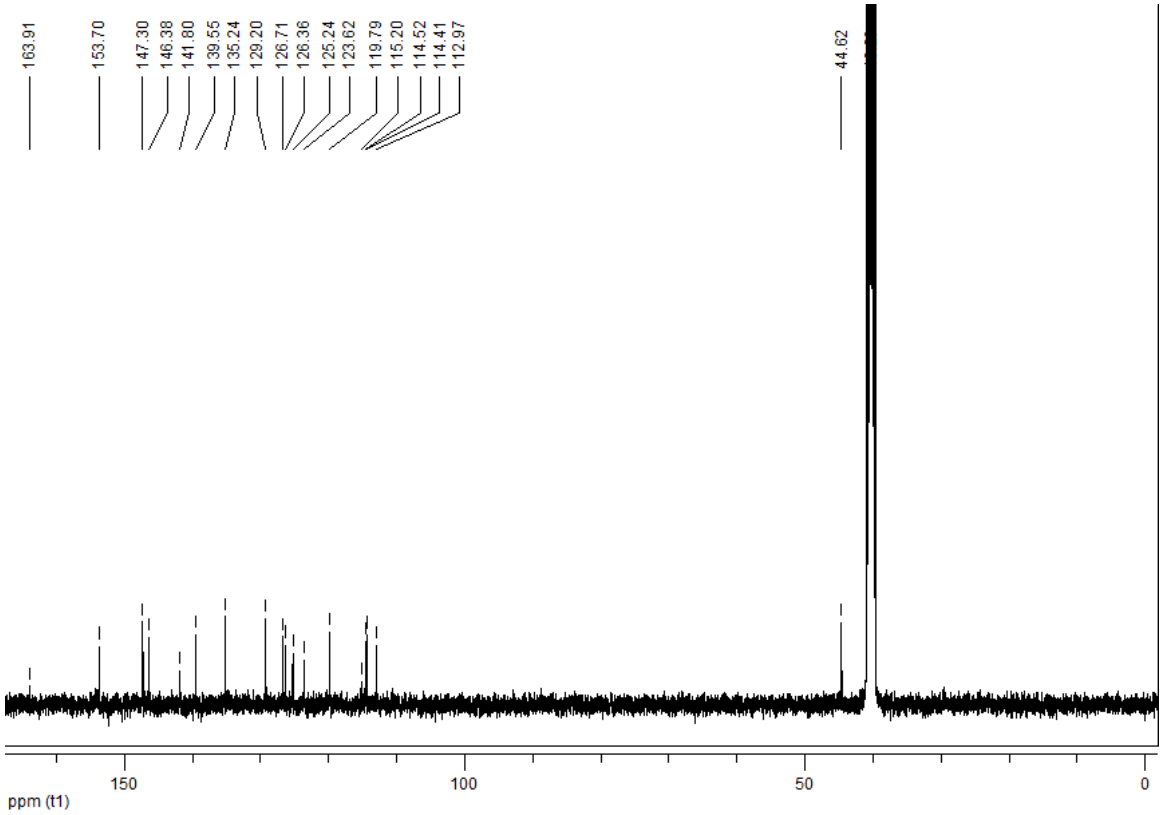

Figure S21. ^{13}C NMR spectrum of **GL0** in DMSO-d_6.

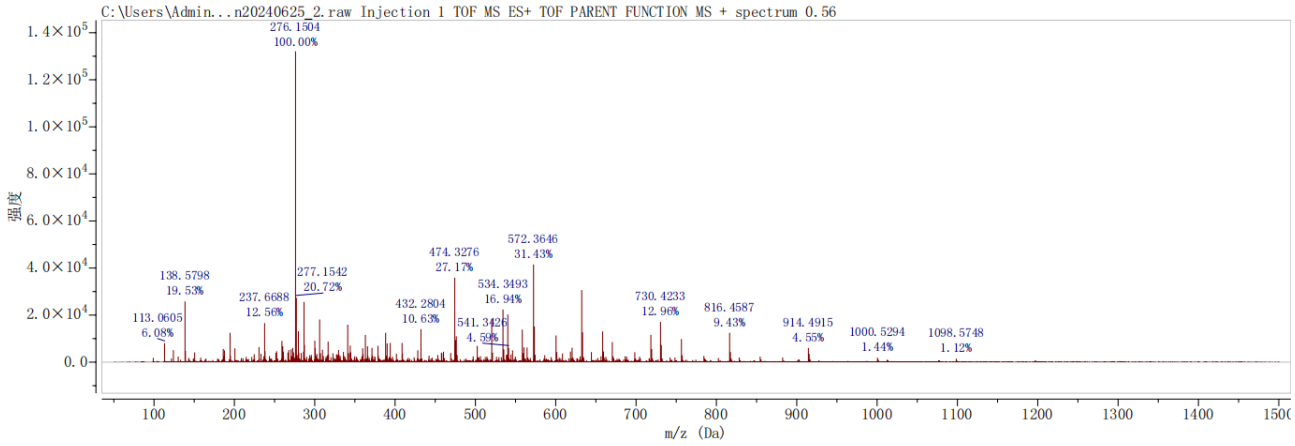

Figure S22. HRMS (LC/MS) spectra of **GL0**. The peak at m/z = 318.1986 was assigned to the mass of **GL0**.

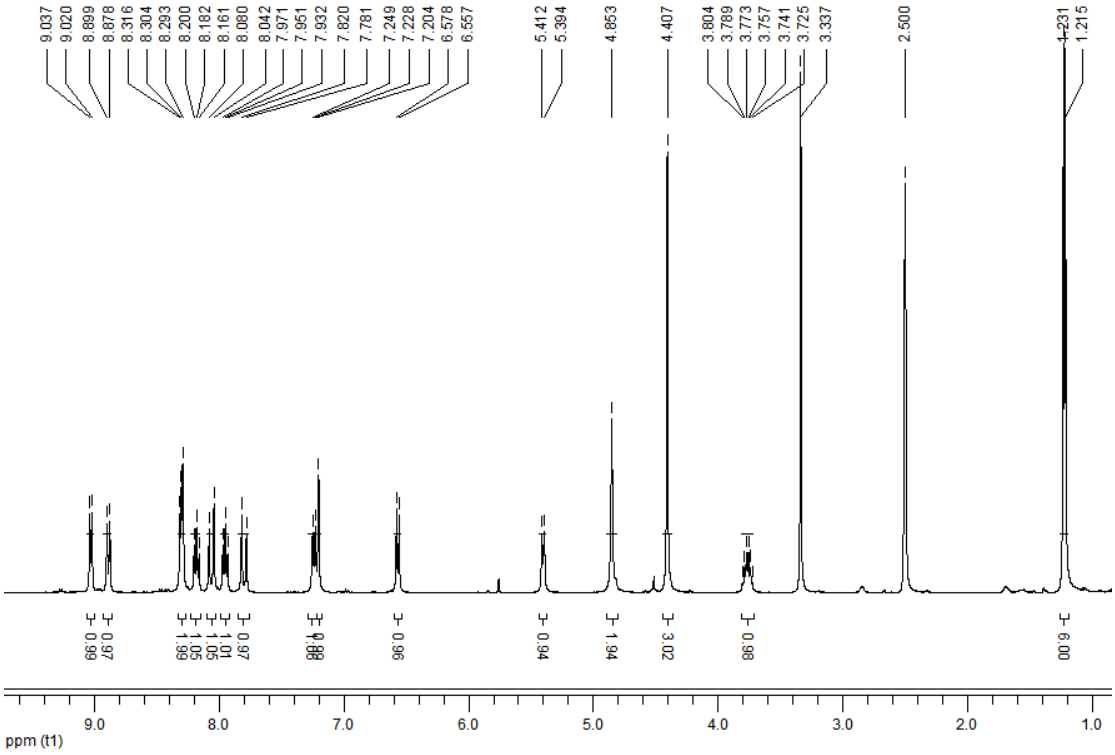

Figure S23. ^{1}H NMR spectrum of **GL1** in DMSO-d_6.

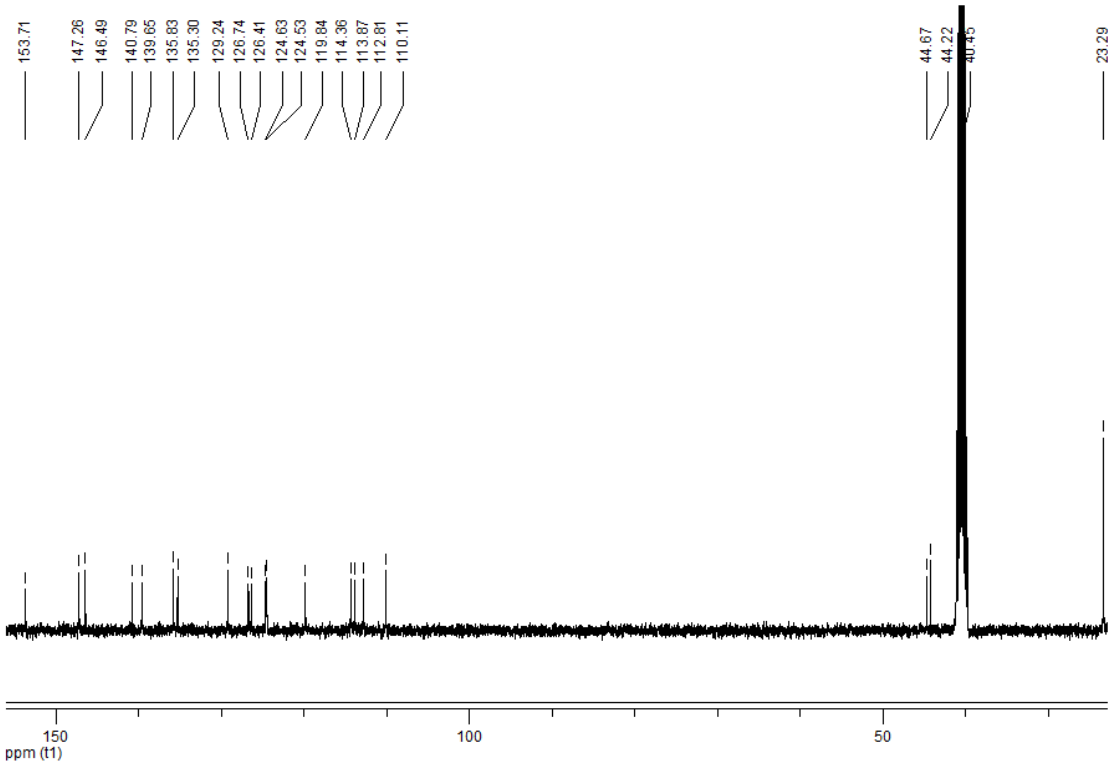

Figure S24. ^{13}C NMR spectrum of **GL1** in DMSO-d_6.

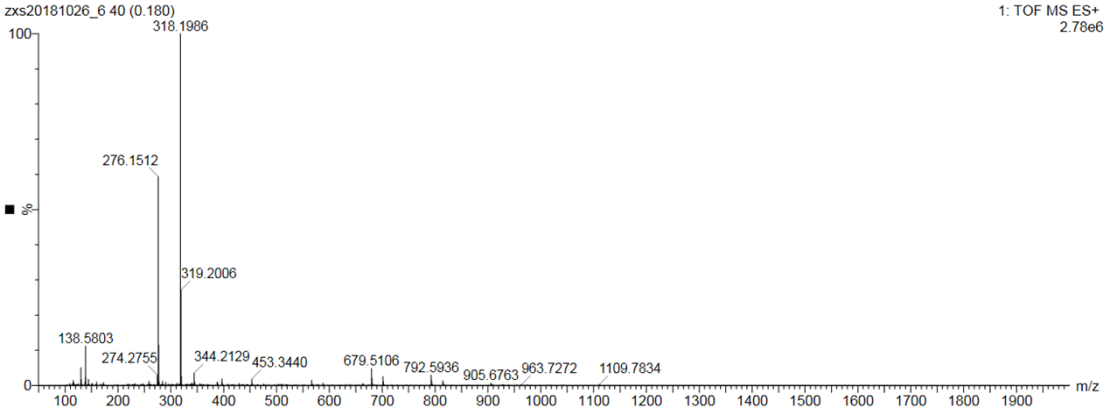

Figure S25. HRMS (LC/MS) spectra of **GL1**. The peak at m/z = 318.1986 was assigned to the mass of **GL1**.

References:

[S1] B. Zhang, X. Yang, R. Zhang, Y. Liu, X. Ren, M. Xian, Y. Ye and Y. Zhao. *Anal. Chem*., 2017, **89**, 10384.