Supplementary Information

Construction of NIR and Ratiometric Fluorescent Probe for Hg^{2+} Based on a Rhodamine-Inspired Dye Platform

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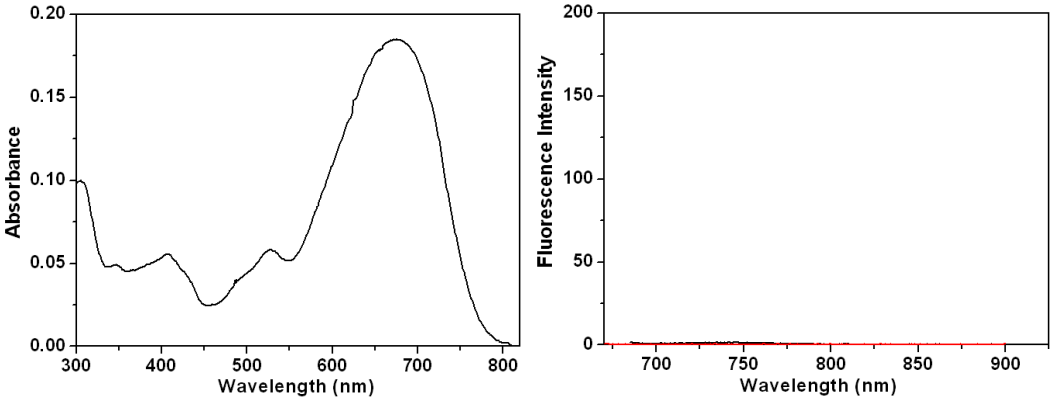

Figure S1. Absorption (left) and fluorescence (right) spectra of **1** in CH_2Cl_2. λ_{ex} = 675 nm.

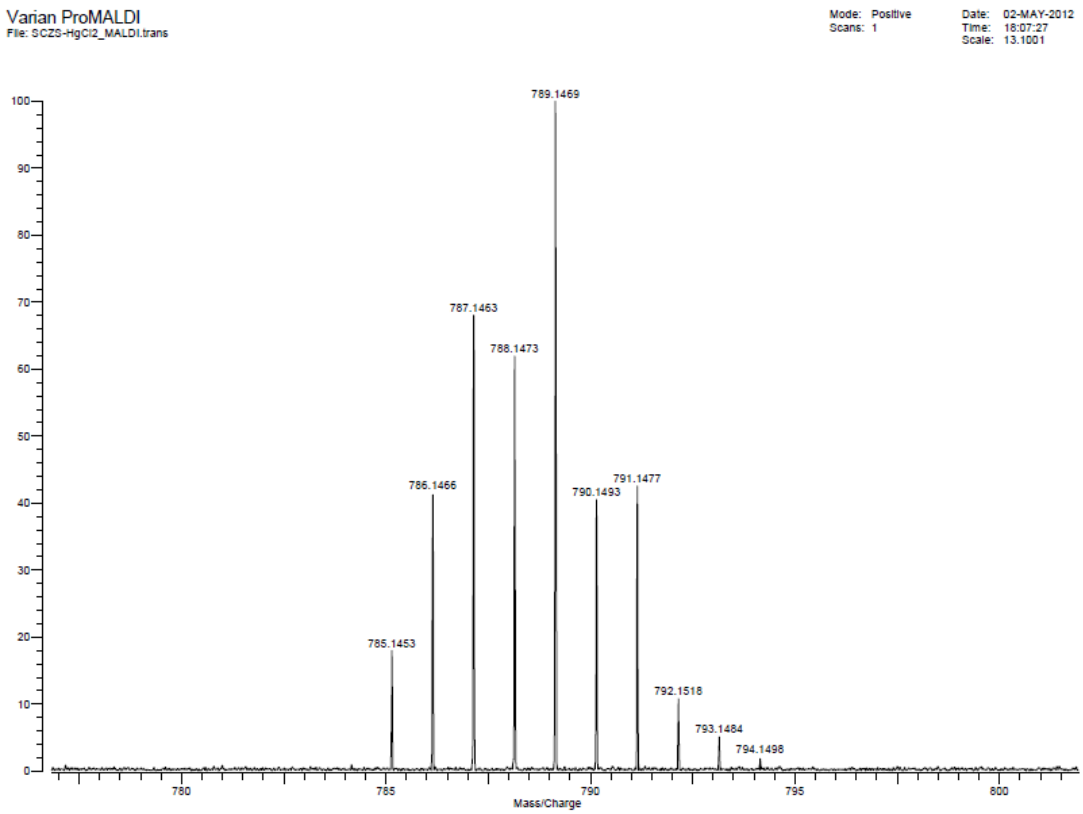

Figure S2. HRMS chart of **R1**-HgCl complex.

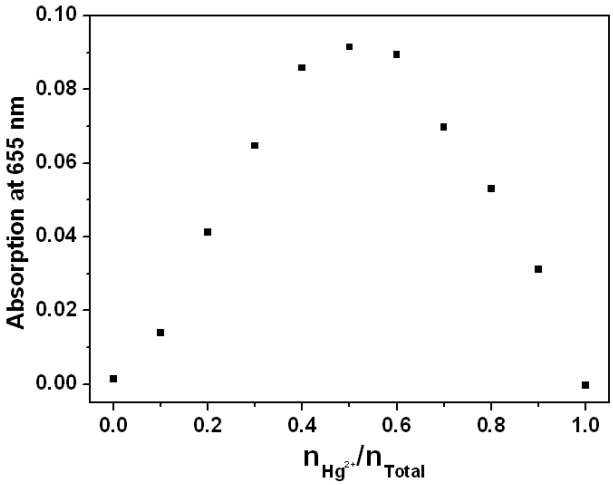

Figure S3. Job's plots of the complexation between **R1** and Hg^{2+} in Tris-HCl/CH_3CN (10 mM, pH = 7.4, 1:1, v/v). Total concentration of **R1** + Hg^{2+} was kept constant at 10 μM.

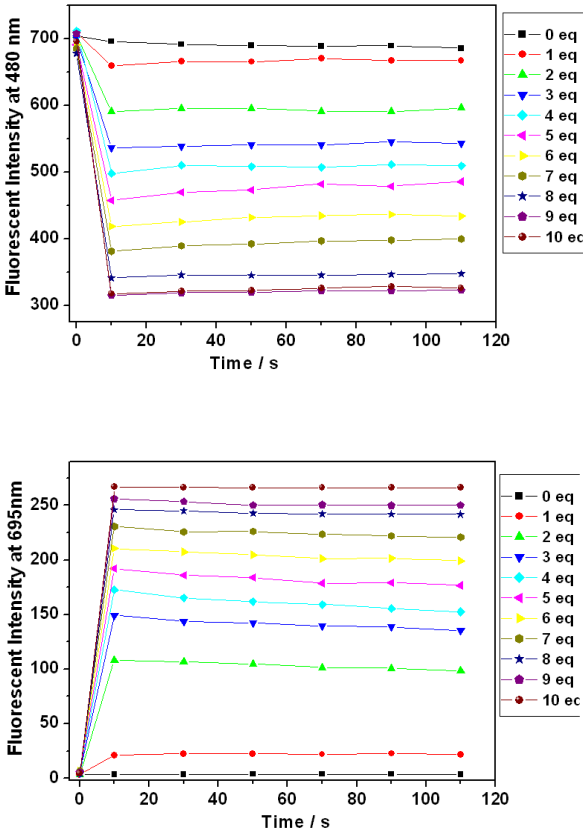

Figure S4. Time-dependent fluorescence spectra of **R1** in the presence of Hg^{2+} in Tris-HCl/CH_3CN (10 mM, pH = 7.4, 1:1, v/v).

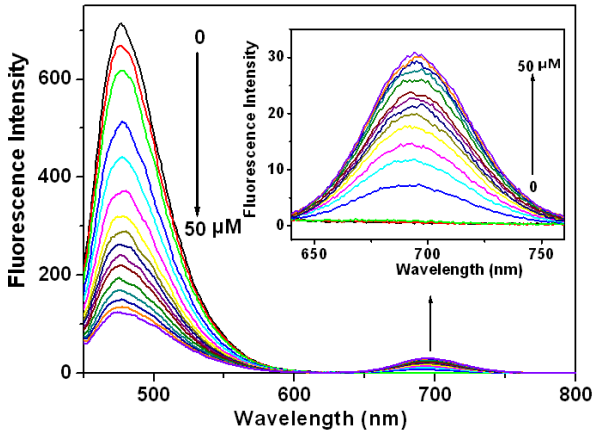

Figure S5. Emission spectra of **R1** (5 μM) upon addition of increasing concentrations of Hg^{2+} (0–20 equiv.) in Tris-HCl/CH_3CN (10 mM, pH = 7.4, 1:1, v/v) excited at 430 nm.

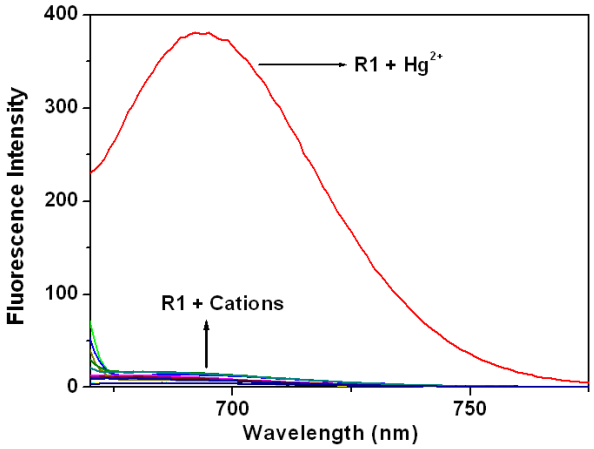

Figure S6. The fluorescence spectra of **R1** (5 μM) in NIR region upon addition of 10 equiv. various species, including Na^+, K^+, Mg^{2+}, Ca^{2+}, Cu^{2+}, Zn^{2+}, Fe^{2+}, Fe^{3+}, Ni^{2+}, Cr^{3+}, Al^{3+}, Cd^{2+}, Mn^{2+}, Pb^{2+}, Ag^+, Co^{2+}, and Hg^{2+}, in Tris-HCl/CH_3CN (10 mM, pH = 7.4, 1:1, v/v).

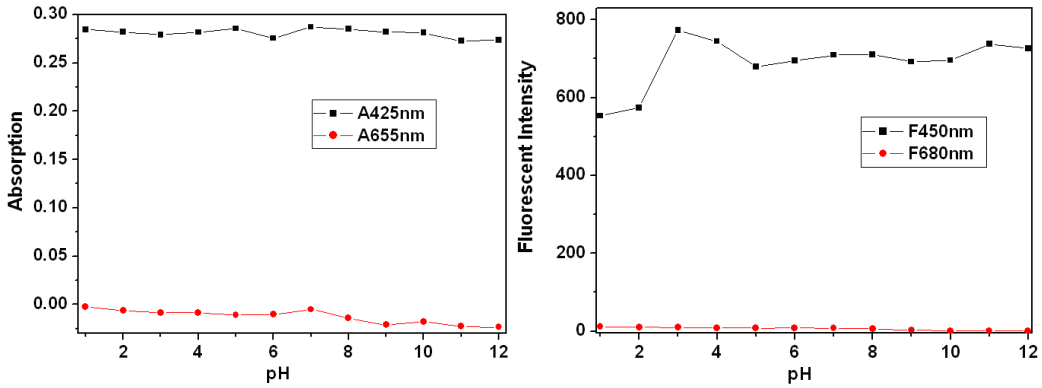

Figure S7. The absorption (left) and fluorescent (right) intensity of **R1** (5 μM) in CH_3CN –water (1:1, v/v) at varied pH values. Using a digital pH meter equipped with a glass electrode, the pH was monitored and adjusted to acidic or basic conditions using small aliquots of a 2M HCl or 2M NaOH solution, respectively.

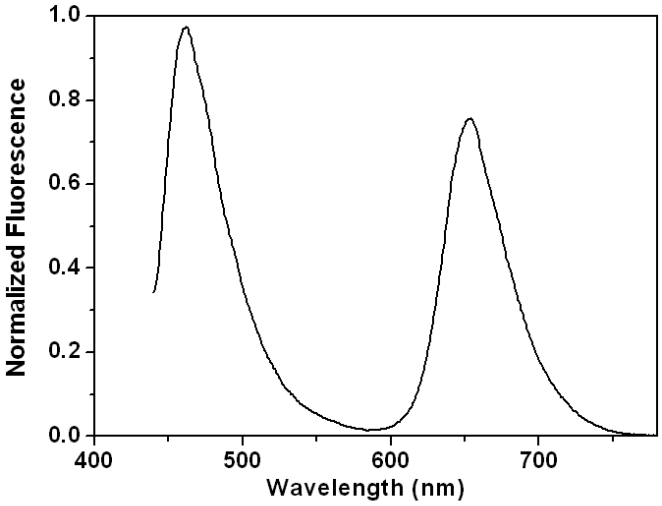

Figure S8. Normalized emission spectrum of **2** in CH_2Cl_2. excited at 430 nm. Note that except for the NIR emission, the visible emission at 465 nm was also observed. This is probably due to the slight deconjugation between the diethylamino-coumarin moiety and the benzopyrylium moiety in **2**, which leads to the emission of the diethylamino-coumarin dye at 465 nm (see, *Org. Lett.*, 2011, **13**, 3730–3733.).

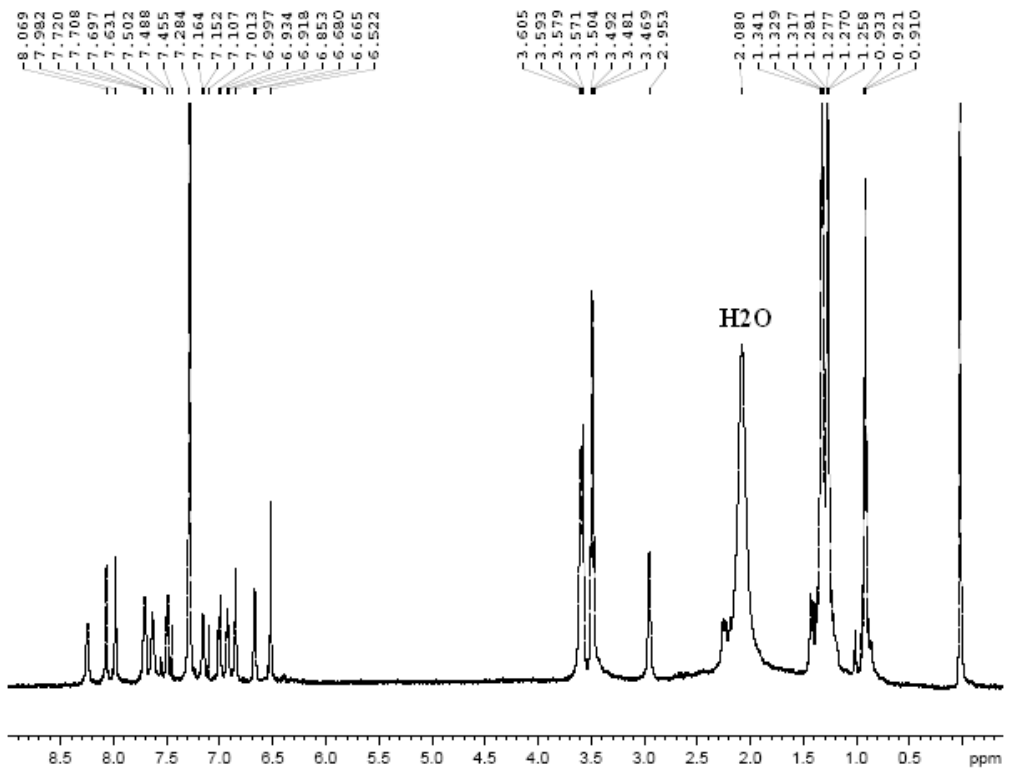

Figure S9. ^{1}H NMR chart of **1** ($CDCl_3$) (600 MHz).

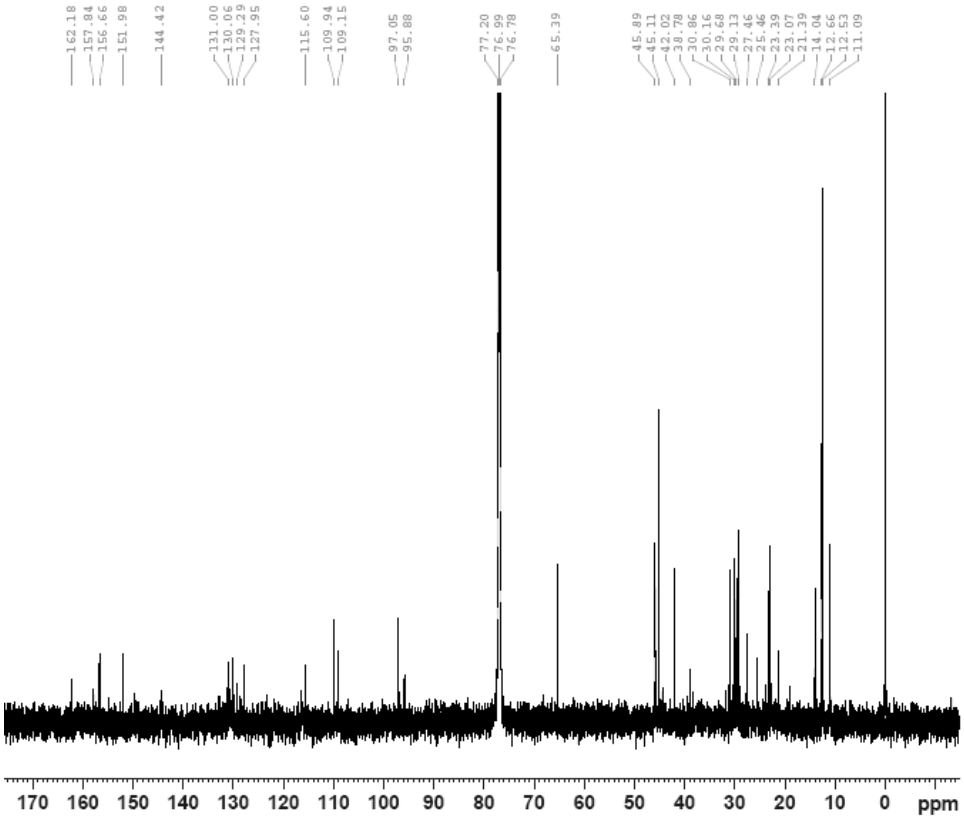

Figure S10. ^{13}C NMR chart of **1** ($CDCl_3$) (150 MHz)**.**

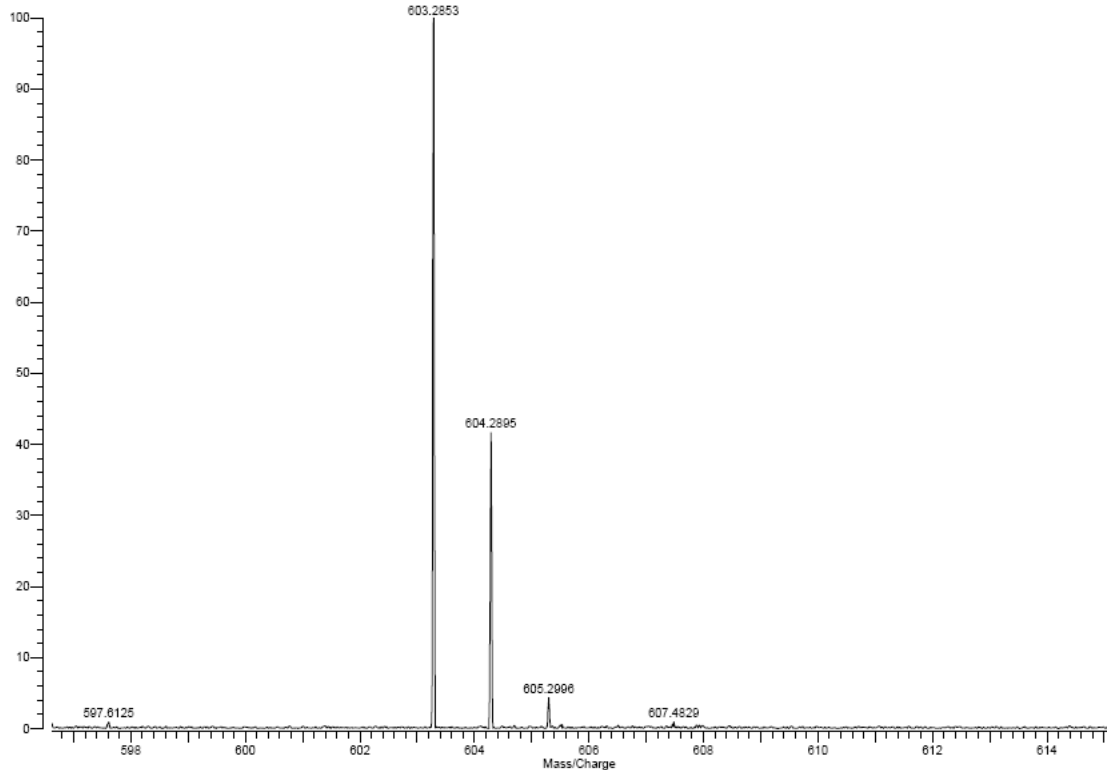

Figure S11. HRMS chart of **1**.

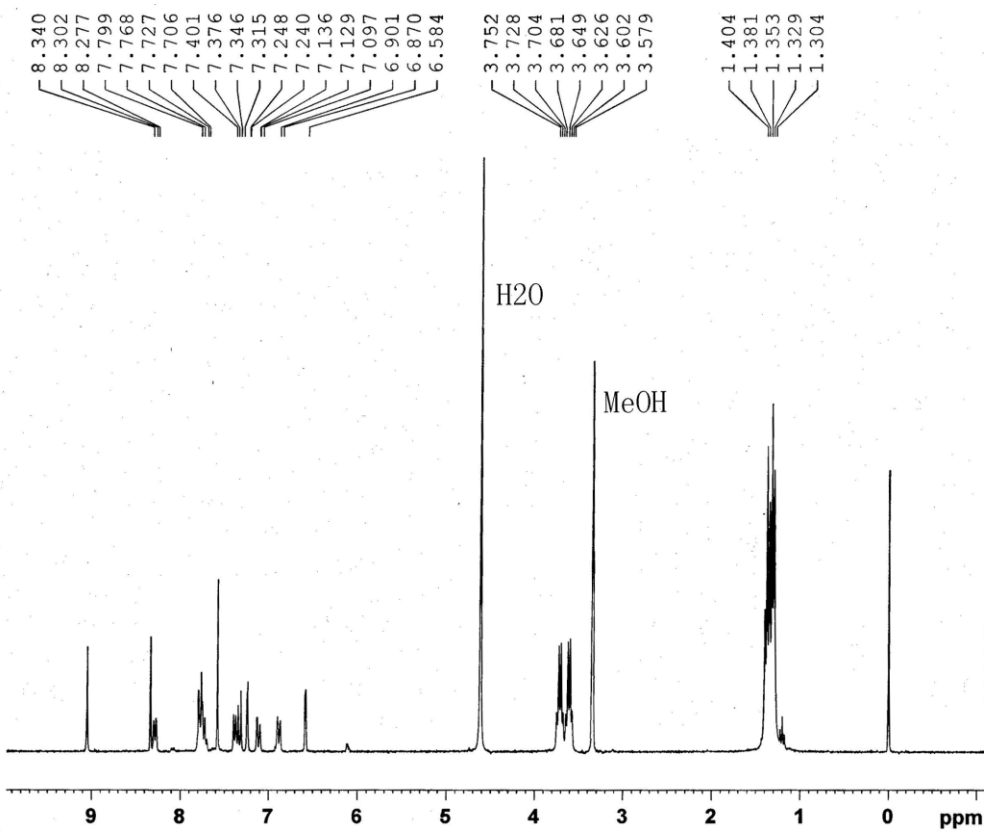

Figure S12. ^{1}H NMR chart of **2** ($CDCl_3$/CD_3OD, 1:1) (300 MHz).

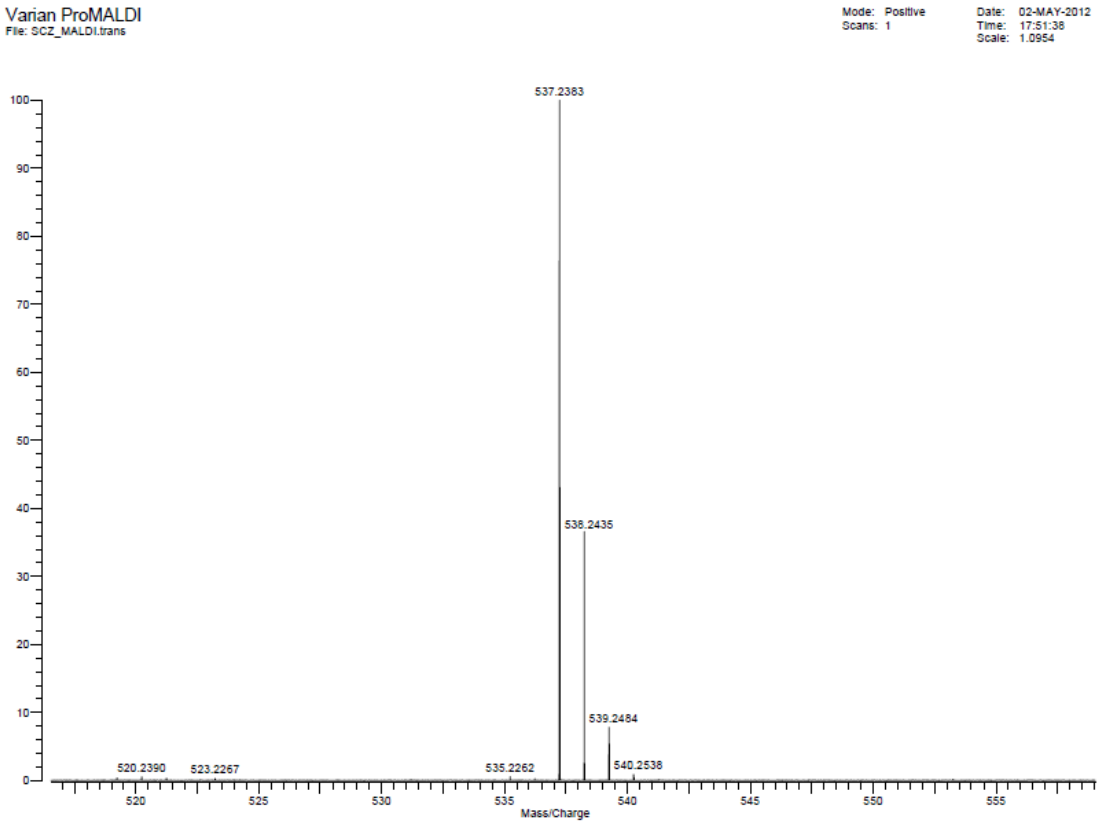

Figure S13. HRMS chart of **2**.

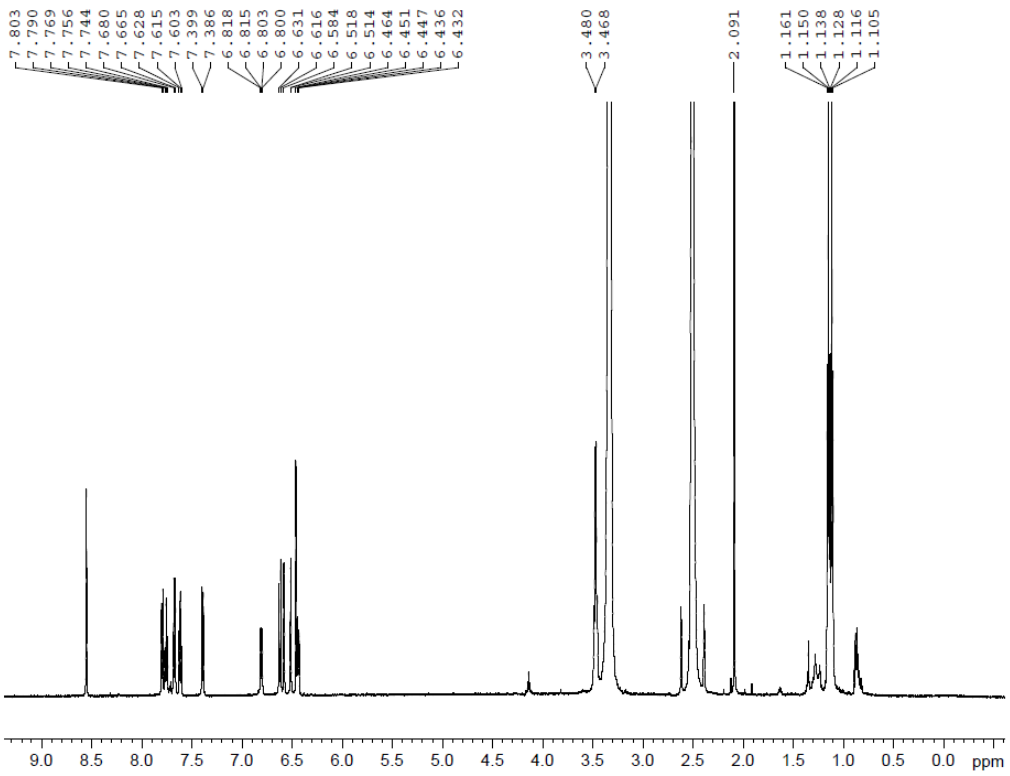

Figure S14. ^{1}H NMR chart of **R1** (DMSO-d_6) (600 MHz)**.**

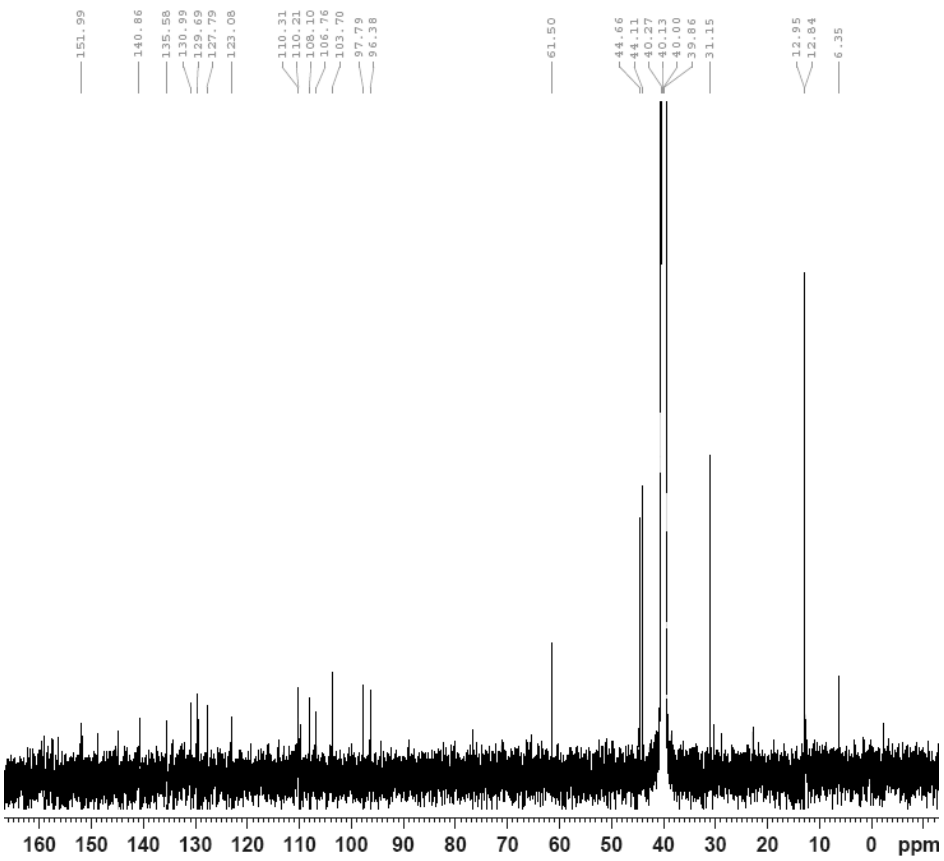

Figure S15. ^{13}C NMR chart of **R1** (DMSO-d_6) (150 MHz)**.**

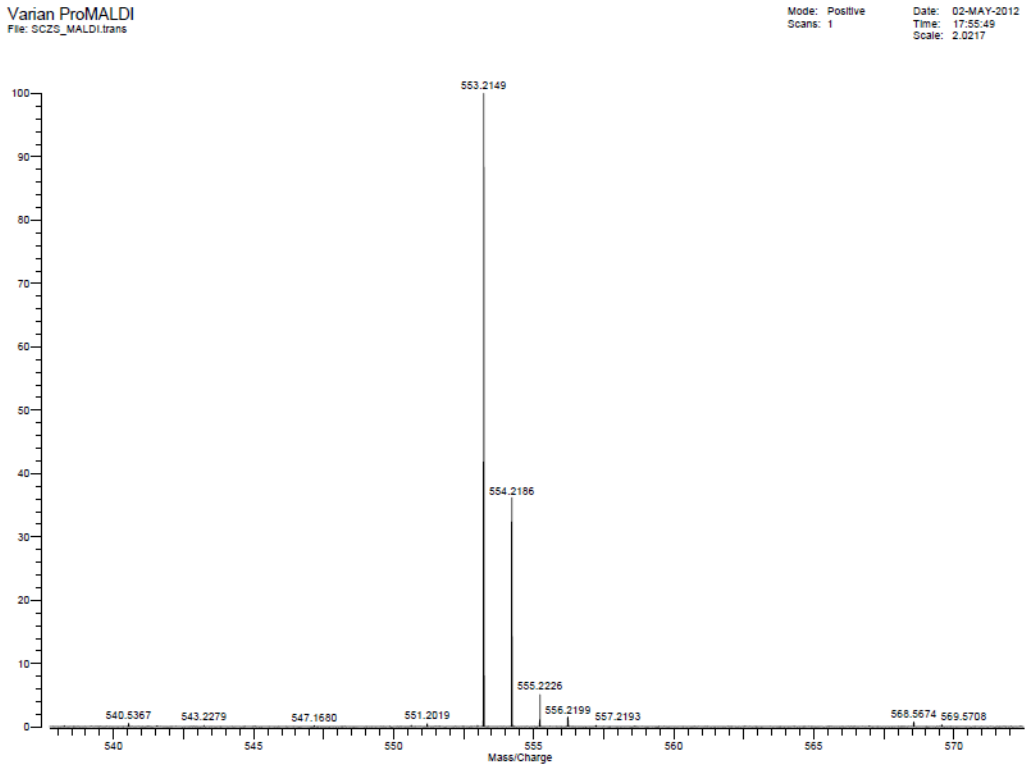

Figure S16. HRMS chart of **R1**.