Rhodamine-based Chemosensor for Hg^{2+} in Aqueous Solution with a Broad pH Range and Its Application in Live Cell Imaging

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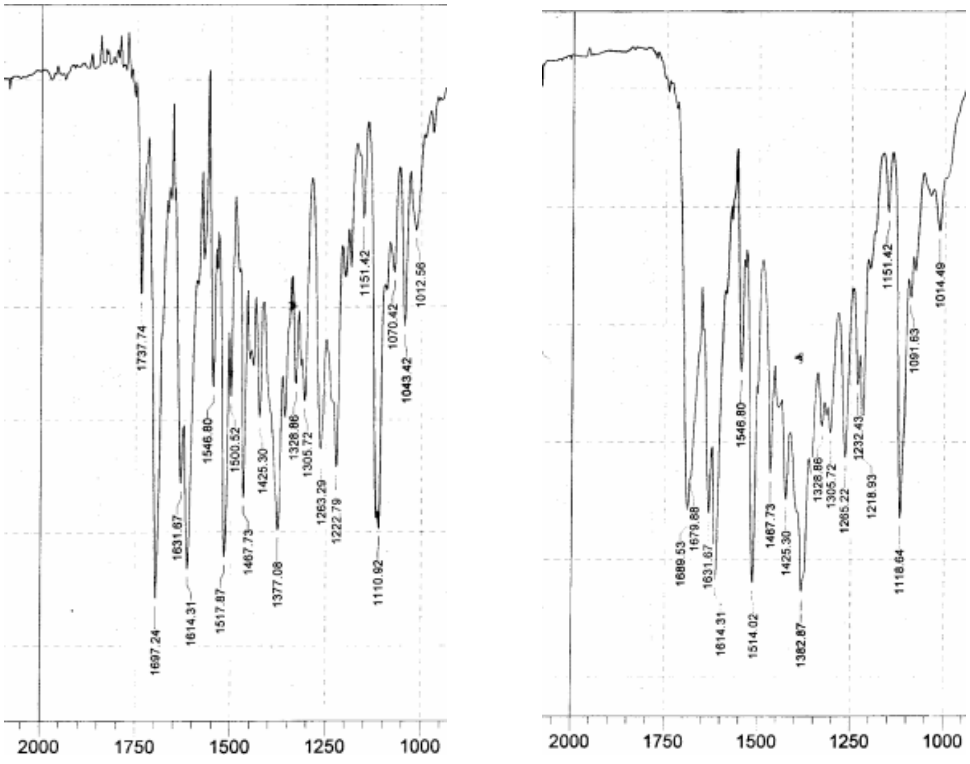
Electronic Supplementary Information (ESI†)

Contents

1. IR spectra of 1 and 1–Hg^{2+} complex in KBr disks



(a) (b)

Fig. S1 IR spectra of **1** (a) and **1**–Hg^{2+} (b) were taken in KBr disks, respectively.

2. ^{1}H NMR-titration experiments (**Fig. S2**).

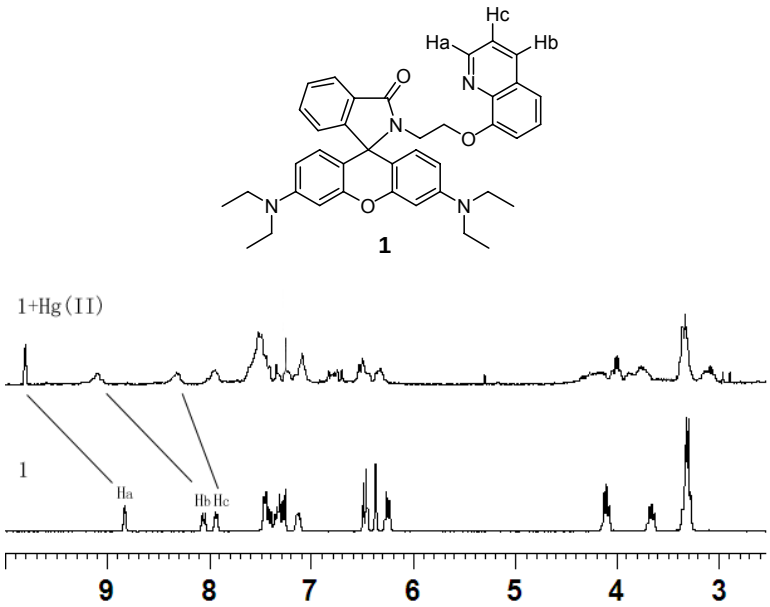


Fig. S2 Hg^{2+} ^{1}H NMR-titration of **1** (10.0 mM) with Hg^{2+} (5 equiv.) in $CDCl_3$.

3. Effects of water content on the fluorescence of **1**–Hg^{2+} system.

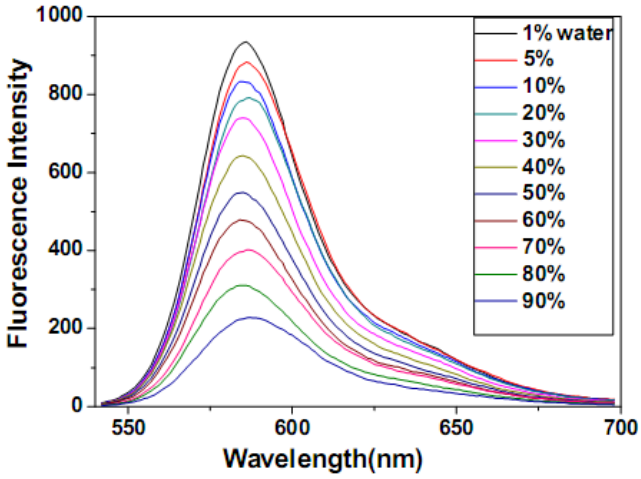


Fig. S3 Effects of water content on the fluorescence of **1**–Hg^{2+} system in aqueous acetonitrile solution. [**1**] = 20 μM, [Hg^{2+}] = 100μM.

4. Time-dependent change in fluorescence intensity of 1 after Hg^{2+} addition

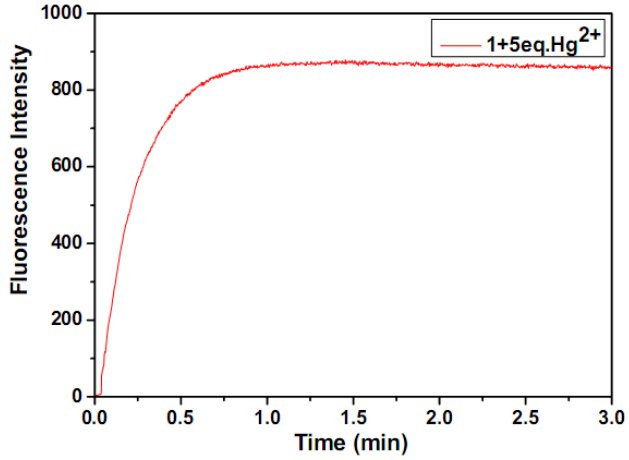


Fig. S4 Time course of the response of **1** (20 μM) in MeCN-water solution (95/5, v/v, pH=7.2) upon addition of 5 equiv. of $Hg(NO_3)_2$.

5. Determinatio of binding constant of the complex

The data obtained from fluorescence titration profile were fitted to be a 1:1 binding model according to following equation.

$$\Delta F = \frac{1}{2}\left\{\alpha\left([H]_0 + [G] + \frac{1}{K}\right) - \sqrt{\partial^2\left([H]_0 + [G] + \frac{1}{K}\right)^2 - 4[H]_0[G]\ \alpha^2}\right\}$$

The binding constant (K) is an important parameter, indicating the inclusion

capacity of the host-guest complex. The binding constants (K) can thus be obtained by a nonlinear least's quares analysis of ΔF versus [Hg^{2+}], fitting to the experimental data obtained from the absorption and fluorescence titrations .Where $[H]_0$ and $[G]_0$ are the initial concentrations of host sensor **1** and guest Hg^{2+}, respectively. ΔF denotes the change of the absorption and fluorescence intensity of sensor 1 with the addition of Hg^{2+}. α is a sensitive factor of the structure change of the complex 1-Hg^{2+} at the interactive course ($\alpha = (F_{max}-F_0)/[G]_0$).

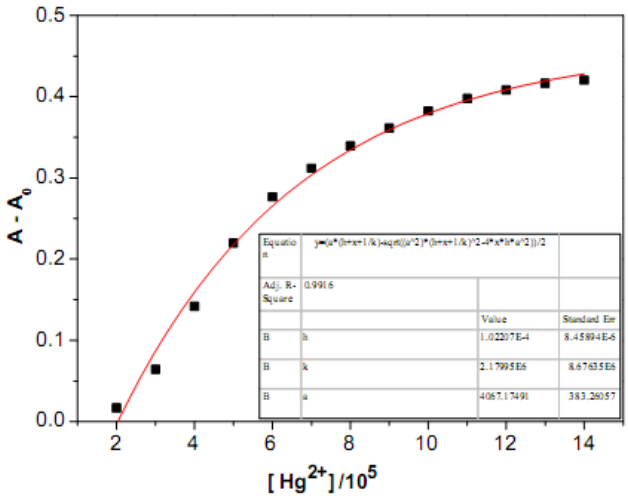


Fig. S5 UV/VIS titration profile of **1** (20μM) in MeCN-water solution (95:5, v/v, Ph=7.2), from which the association constant was determined, $K_a = 2.18 \times 10^6$ M^{-1} ($R^2 = 0.9916$).

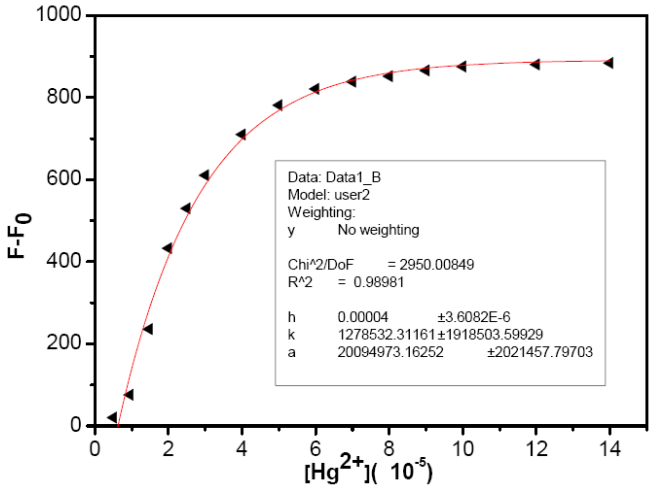


Fig. S6 Fluorescence titration profile (λ_{em} = 530 nm) of **1** (20μM) in MeCN-water solution (95:5, v/v, Ph=7.2), from which the association constant was determined, $K_a = 1.27 \times 10^6$ M^{-1} ($R^2 = 0.9898$).

6. Selectivity investigation by absorption spectra

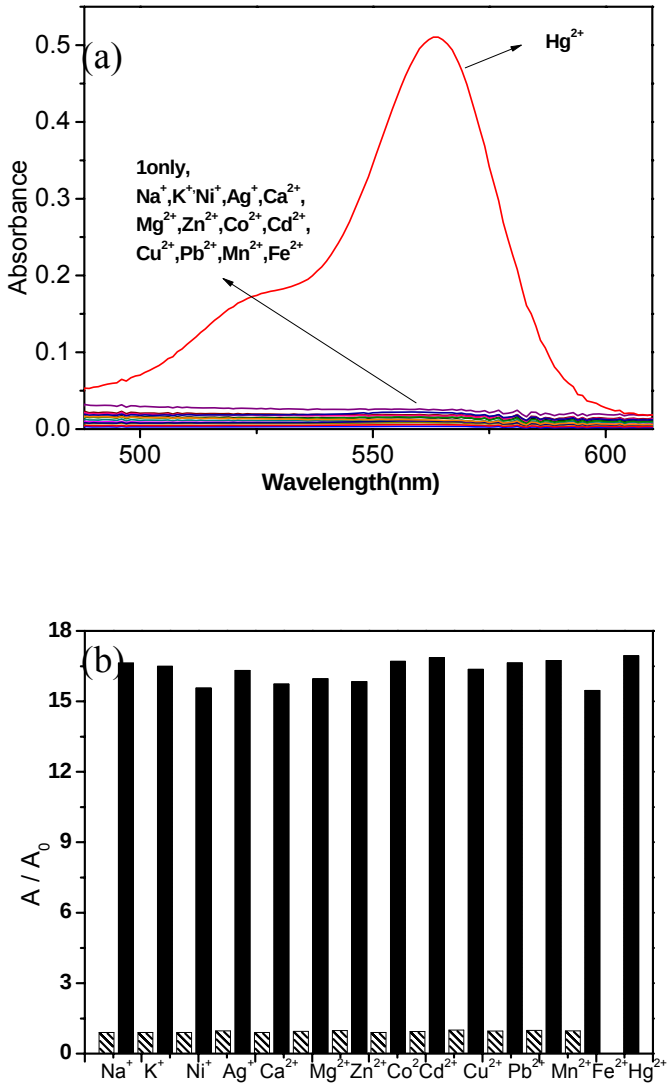


Fig. S7 (a) The absorption spectra of **1** (20 μM) upon addition of 100 μM of Hg^{2+} and various other metal ions in a MeCN-water solution (95/5, v/v, pH 7.2). (b) Absorption change of **1** (20 μM) to 100 μM of Hg^{2+} in a MeCN-water solution (95/5, v/v, pH 7.2) containing 100 μM of various metal ions.

7. Reversibility investigation by introduction of iodide anion.

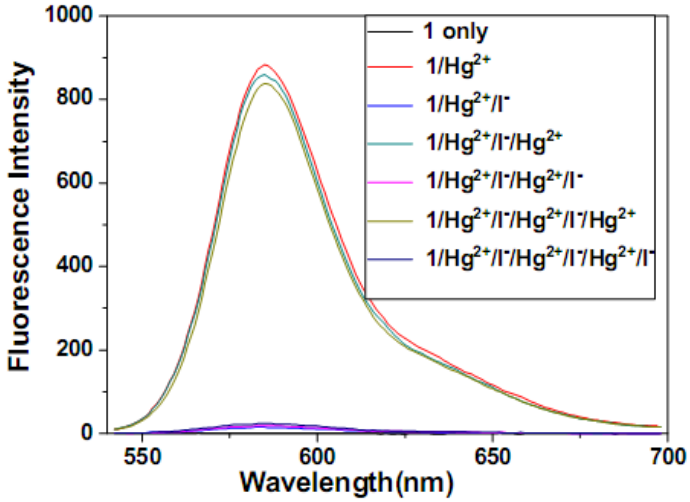


Fig. S8 Reversibility of Hg^{2+} coordination to probe **1** by I^-. Slash denotes the sequence of addition. [**1**] = 2.0 x 10^{-5} M, in aqueous acetonitrile solution (95/5, v/v, pH=7.2). [Hg^{2+}](1^{st}) = 1.0 × 10^{-4} M, [I^-] = 4.0 × 10^{-4} M, [Hg^{2+}] (2^{nd}) = 6.0 x 10^{-4} M, [I^-] = 2.4 × 10^{-3} M, [Hg^{2+}](3^{rd}) = 1.8 × 10^{-3} M, [I^-] = 7.2 × 10^{-2} M.

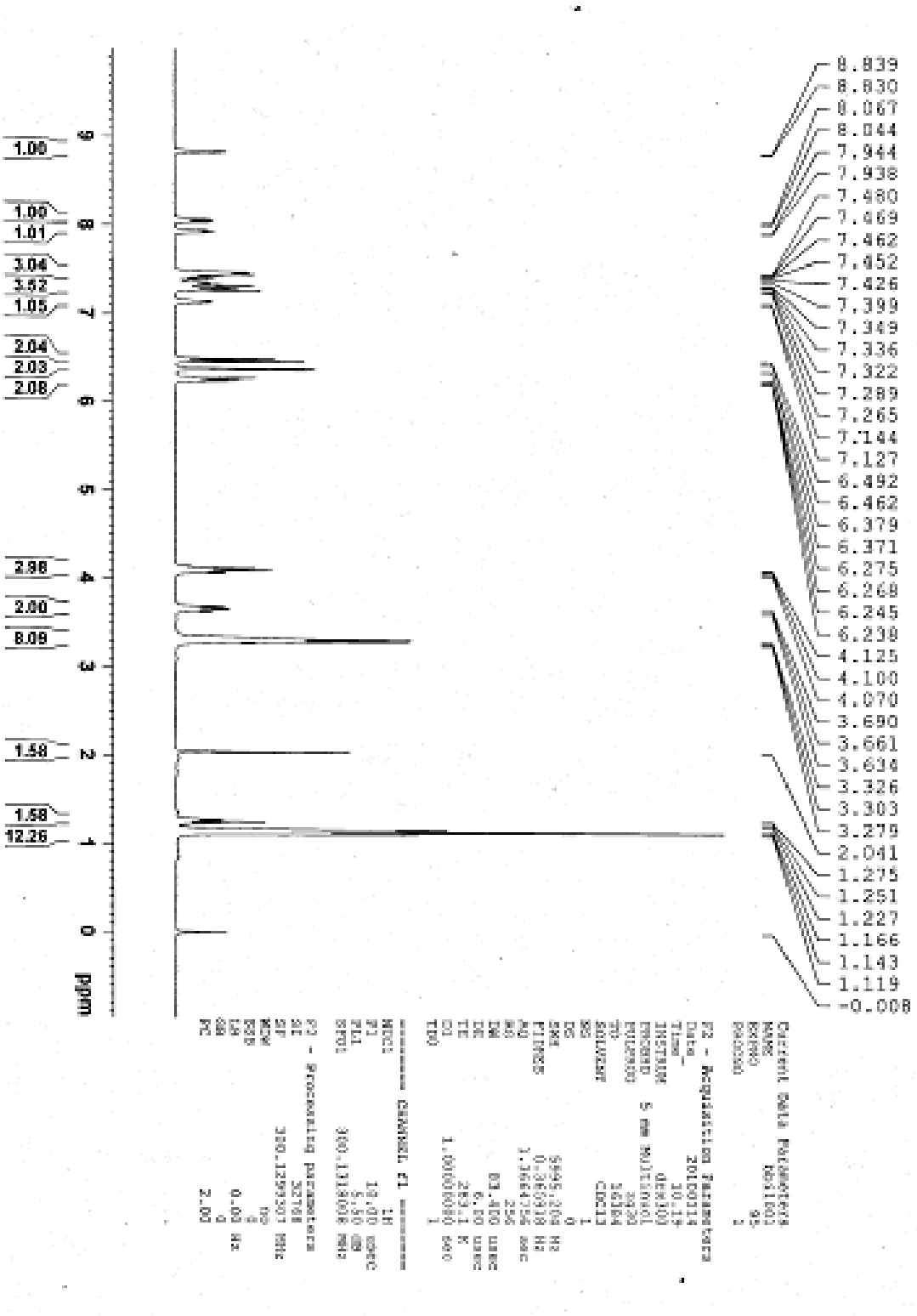


Fig. S9 ^{1}H NMR chart of **1** ($CDCl_3$, 300MHz)

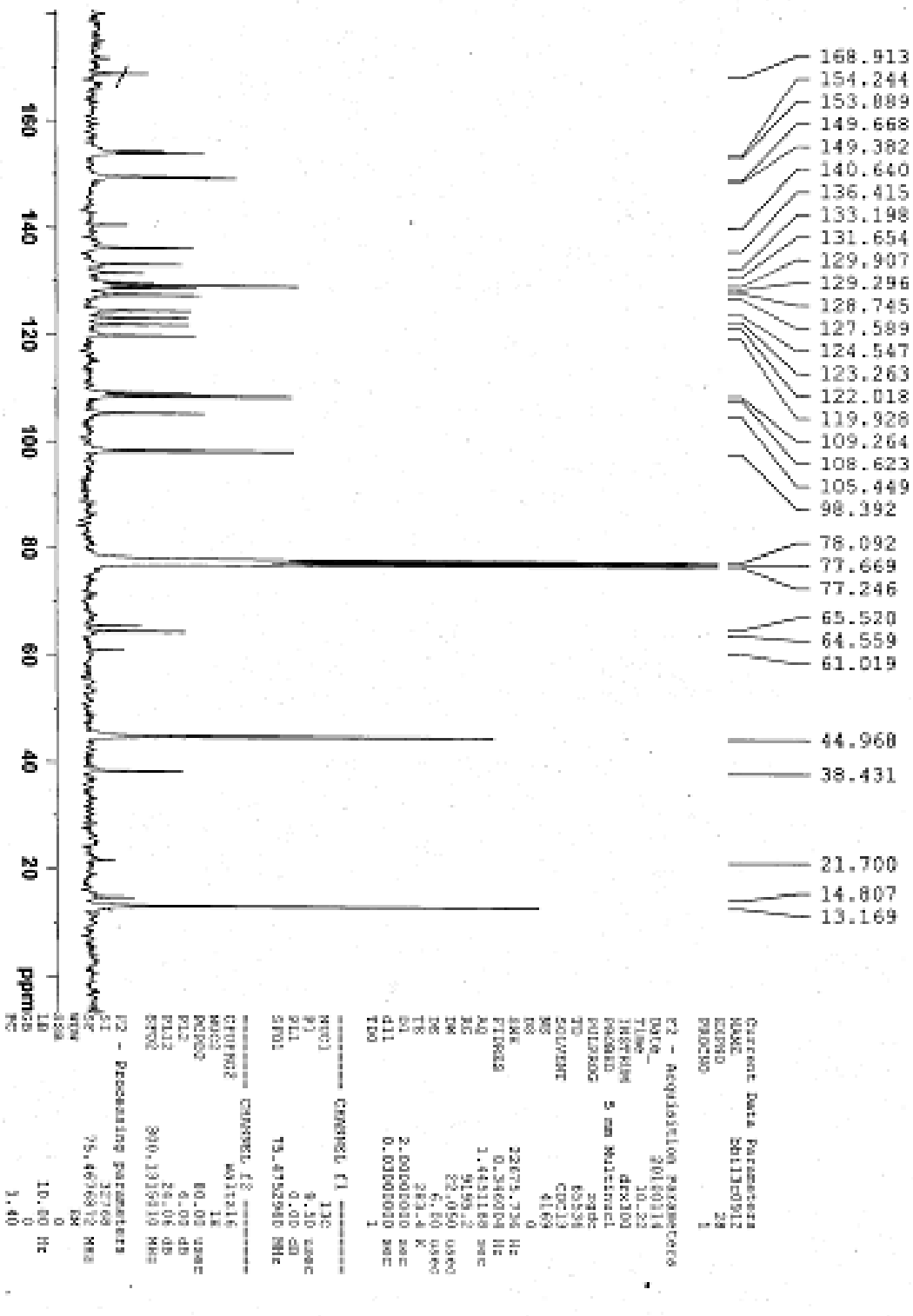


Fig. S10 ^{13}C NMR chart of **1** ($CDCl_3$, 75MHz)

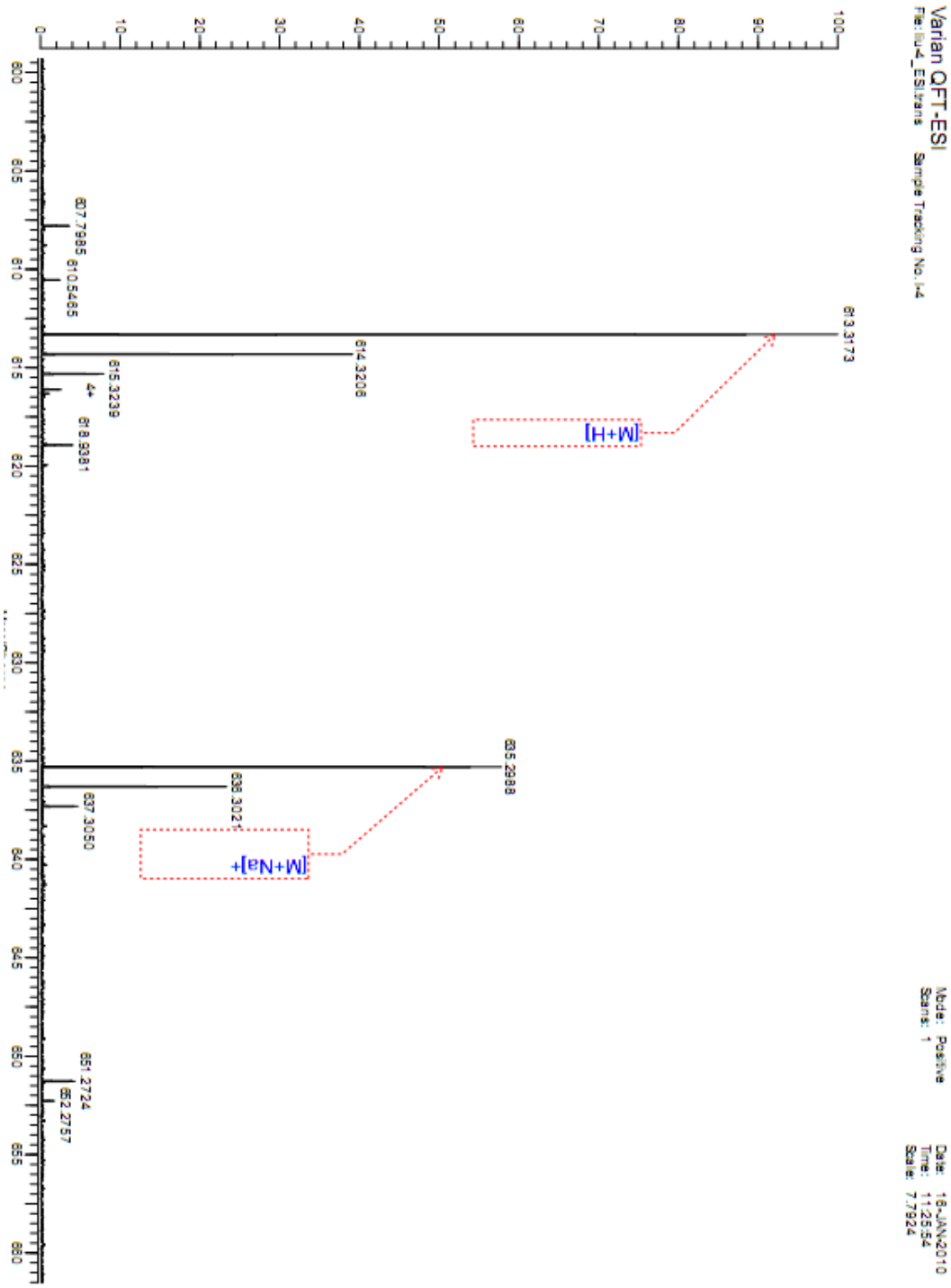


Fig. S11 EI-MS chart of **1**