Electronic Supplementary Material (ESI) for Dalton Transactions
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Supporting Information

A rhodamine-based "turn-on" fluorescent probe for Fe^{3+} in aqueous solution

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1. Job's plot of **RD1** and Fe^{3+}

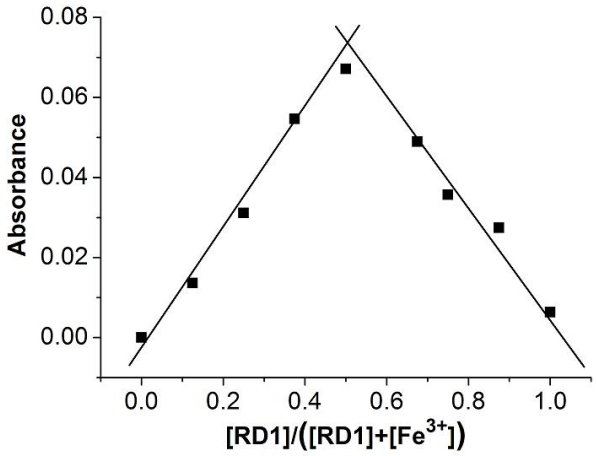

Fig. S1 Job's plot of **RD1** and Fe^{3+}. The total concentrations of **RD1** and Fe^{3+} are 10 μM. The experiments were measured at room temperature in methanol/water (1/99) buffer (20 mM HEPES, 50mM, $NaNO_3$).

2. The reversibility experiment

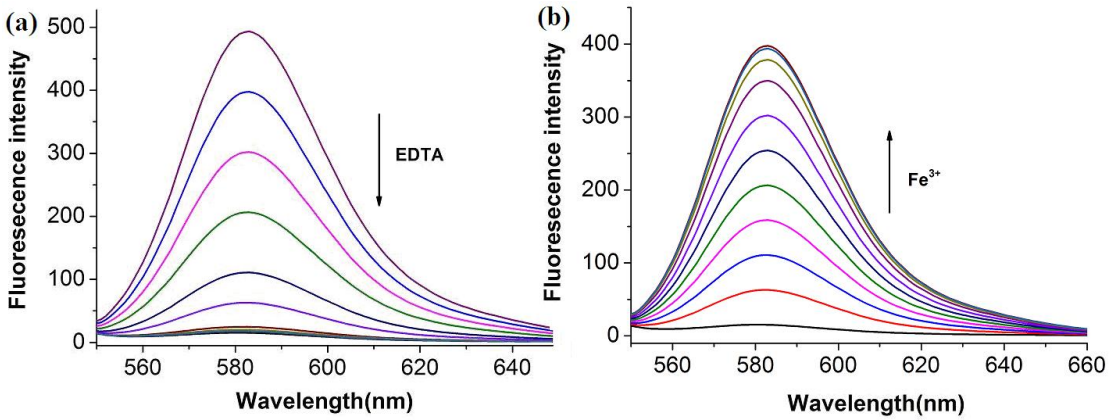

Figure S2. (a) The fluorescent spectra titration of **RD1** (10 μM)/Fe^{3+} (20 μM) upon adding of EDTA (0–2.0 equiv.) in methanol/water (1/99) buffer (pH 7.0, 20 mM HEPES 50mM $NaNO_3$, λ_{ex}= 530 nm). (b) Fluorescence emission spectra of above mixed solution with the excitation at 530 nm, upon the titration of Fe^{3+} (0–2.0 equiv.).

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3. Fluorescence of 10 μM **RD1** at various pH values

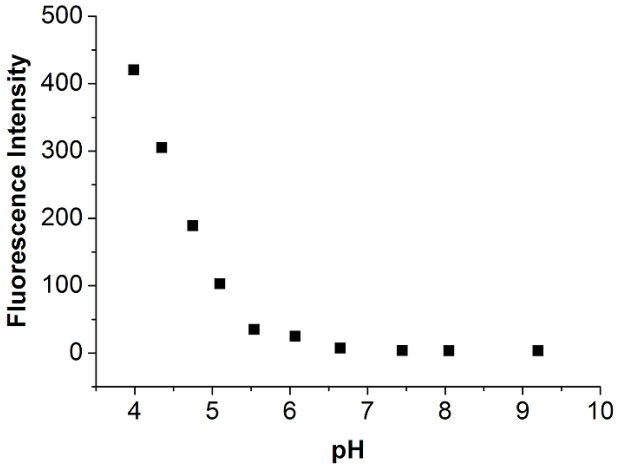

Fig. S3 Fluorescence of 10 μM **RD1** at various pH values in methanol/water (1/99) buffer (20 mM HEPES, 50 mM $NaNO_3$, λ_{ex} = 530 nm, λ_{em}= 586 nm).

4. Cytotoxicity assays in Cells

To test the cytotoxic effect of the probe in cells for over a 24 h period, MTT (5-dimethylthiazol-2-yl-2,5-diphenyltetrazolium bromide) assay was performed as previously reported.[45] 7402 cells were passed and plated to ca. 70% confluence in 96-well plates 24h before treatment. Prior to **RD1** treatment, DMEM (Dulbecco's Modified Eagle Medium) with 10% FCS (Fetal Calf Serum) was removed and replaced with fresh DMEM, and aliquots of **RD1** stock solutions (5 mM DMSO) were added to obtain final concentrations of 10, 30 and 50 μM respectively. The treated cells were incubated for 24 h at 37 °C under 5% CO_2. Subsequently, cells were treated with 5 mg/mL MTT (40 μL /well) and incubated for an additional 4 h (37 °C, 5% CO_2). Then the cells were dissolved in DMSO (150 μL/well), and the absorbance at 570 nm was recorded. The cell viability (%) was calculated according to the following equation: Cell viability% = OD570(sample)/OD570(control)×100, where OD570(sample) represents the optical density of the wells treated with various concentration of **RD1** and OD570(control) represents that of the wells treated with DMEM containing 10% FCS. The percent of cell survival values is relative to untreated control cells.

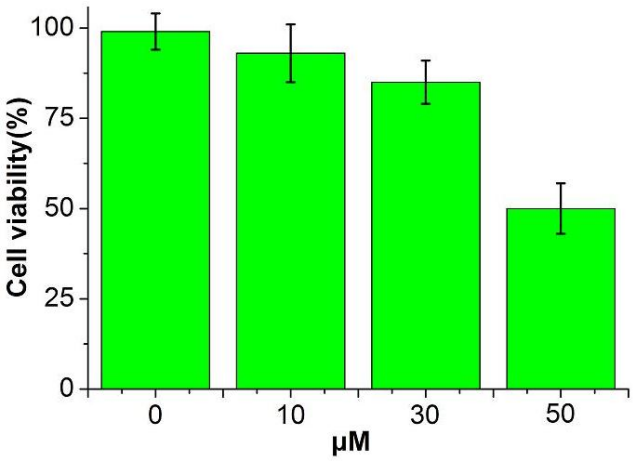

Fig. S4 Cytotoxicity data of **RD1** (7402 cells incubated for 24 h).

5. Fluorescence quantum yield

Fluorescence quantum yield was determined using optically matching solutions of Rhodamine B ($\Phi_f = 0.31$ in water) as standards at an excitation wavelength of 514 nm and the quantum yield is calculated using equation (1).

$$\phi_u = \frac{\phi_s (F_u A_s)}{F_s A_U} \left(\frac{\eta_u}{\eta_s}\right)^2 \quad (1)$$

Where Φ_u and Φ_s are the fluorescence quantum yields of the sample and standard, F_u and F_s are the integrated emission intensities of the corrected spectra for the sample and standard, A_u and A_s are the absorbance of the sample and standard at the same excitation wavelength, and η_s and η_u are the indices of refraction of the sample and standard solutions, respectively.

6. Association constant

The association constant(K_a) for the formation of the respective complexes was evaluated using the modified Benesi−Hildebrand (B−H) plot (eq. 2).

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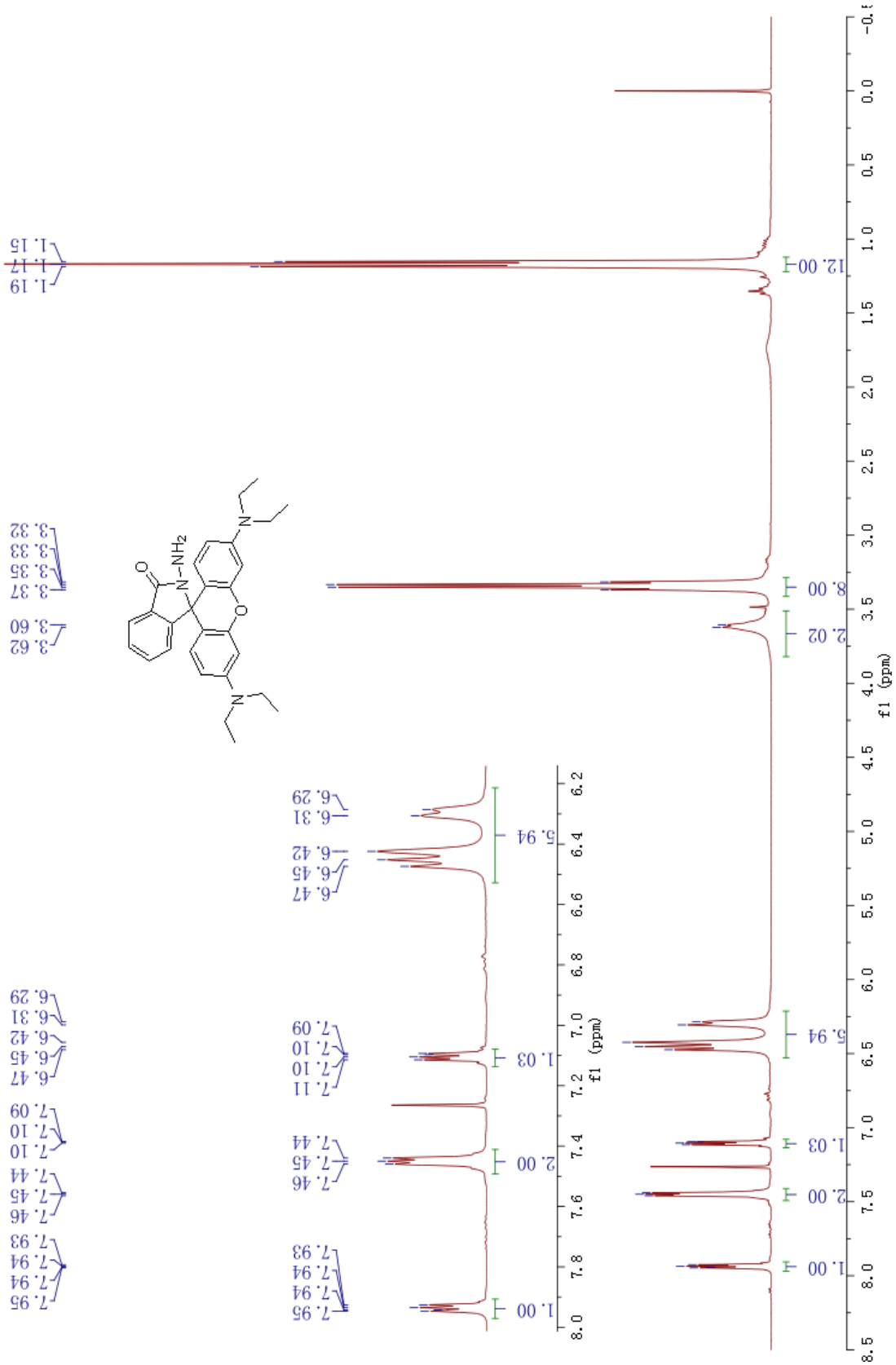
$$\frac{1}{F - F_0} = \frac{1}{K_a (F_{\max} - F_0)[Fe]^{3+}} + \frac{1}{F_{\max} - F_0} \quad (2)$$

where F_0, F_{max}, and F represent the emission intensity of free RD1, RD1 in the presence of excess amount and RD1 in the presence of a certain concentration of Fe^{3+} at 586 nm (λ_{ex} = 530 nm).

7. NMR spectra



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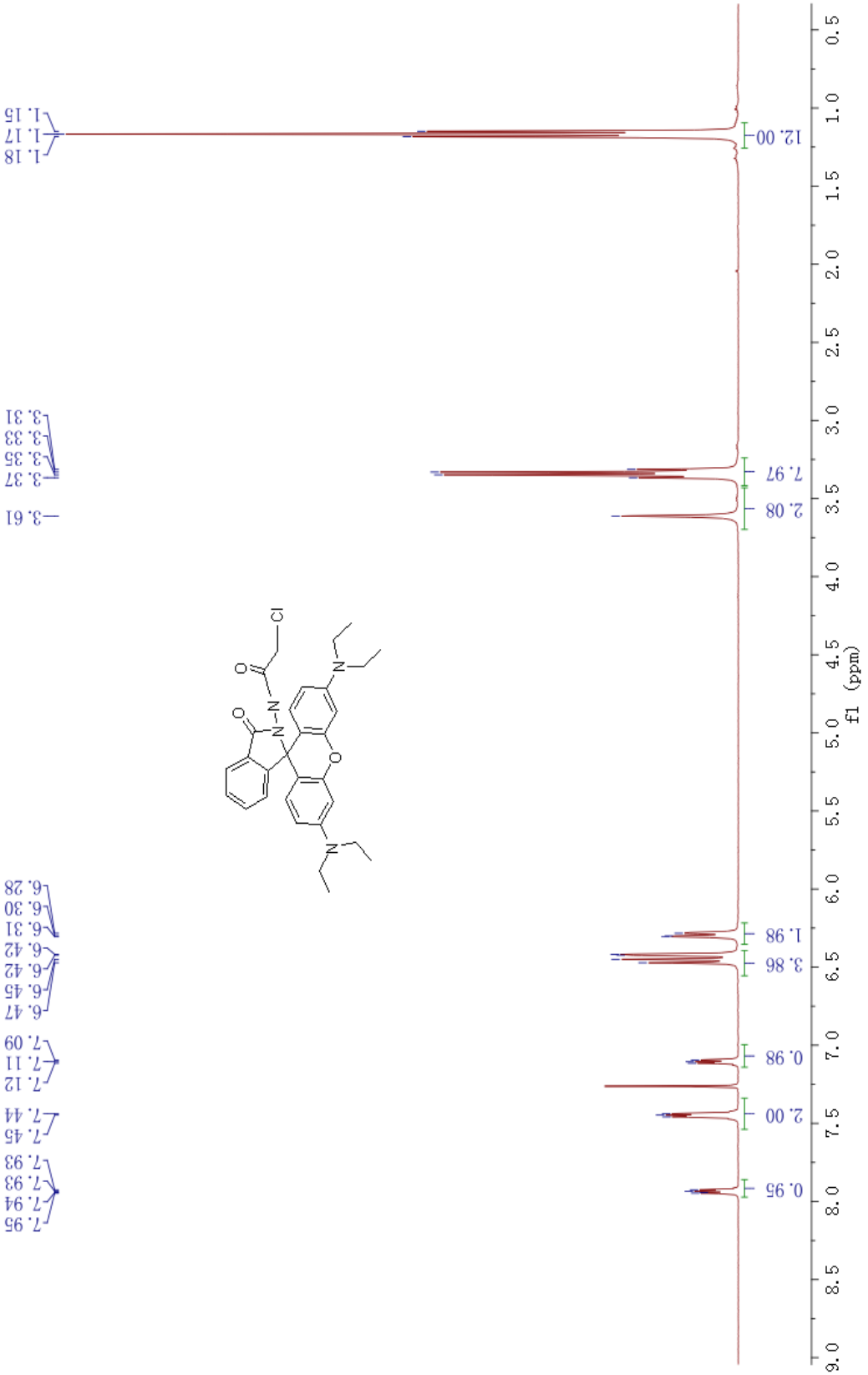

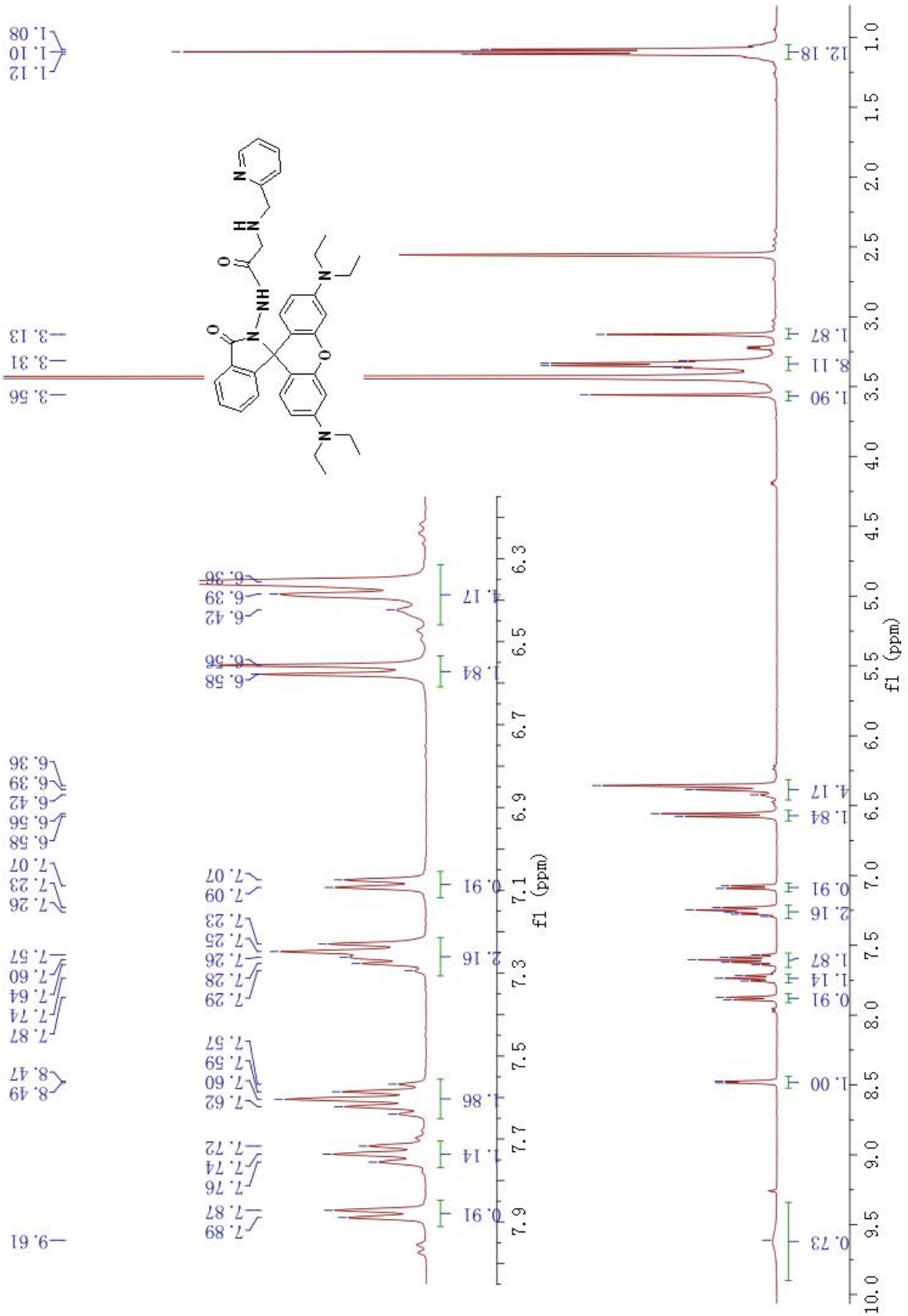
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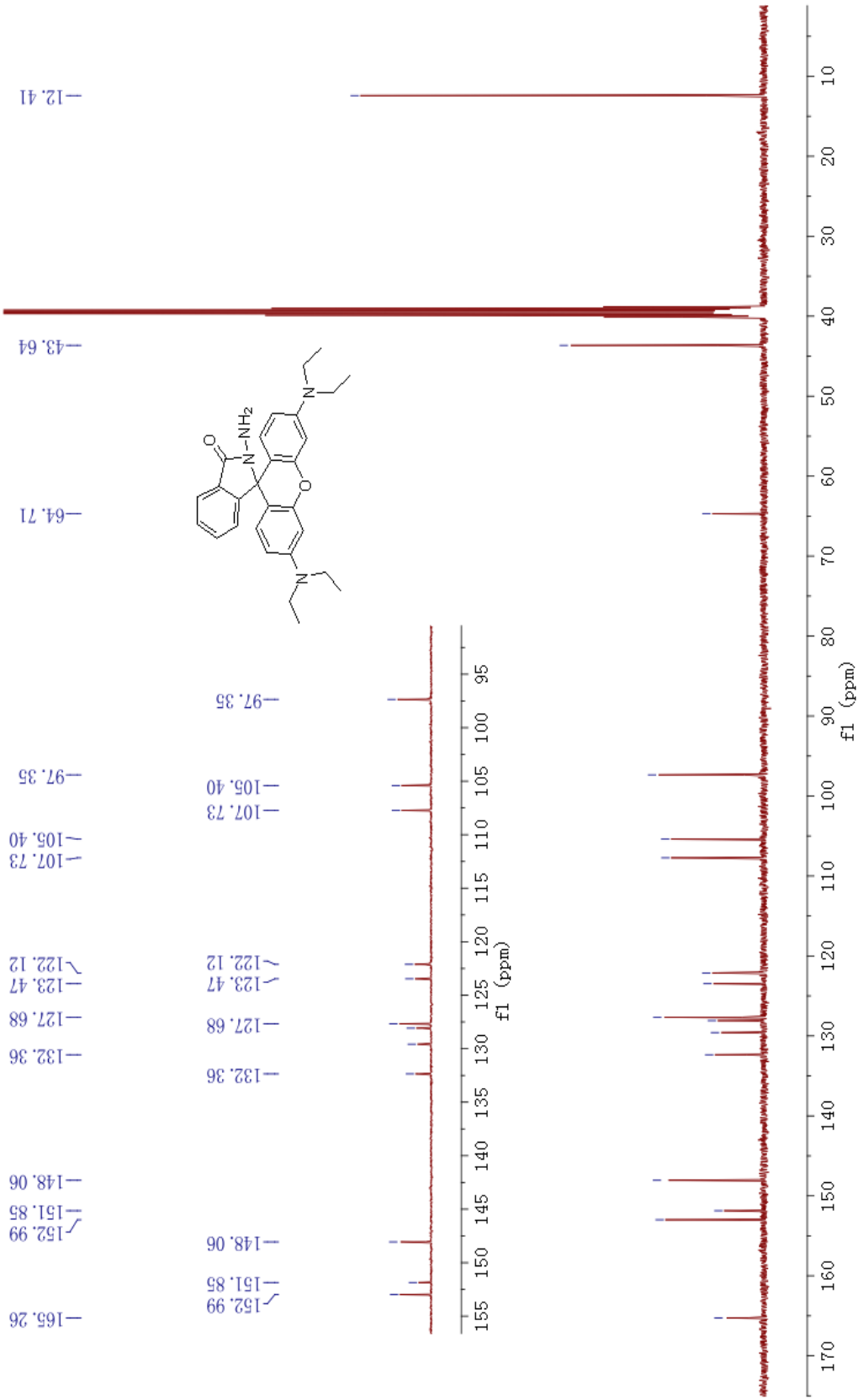
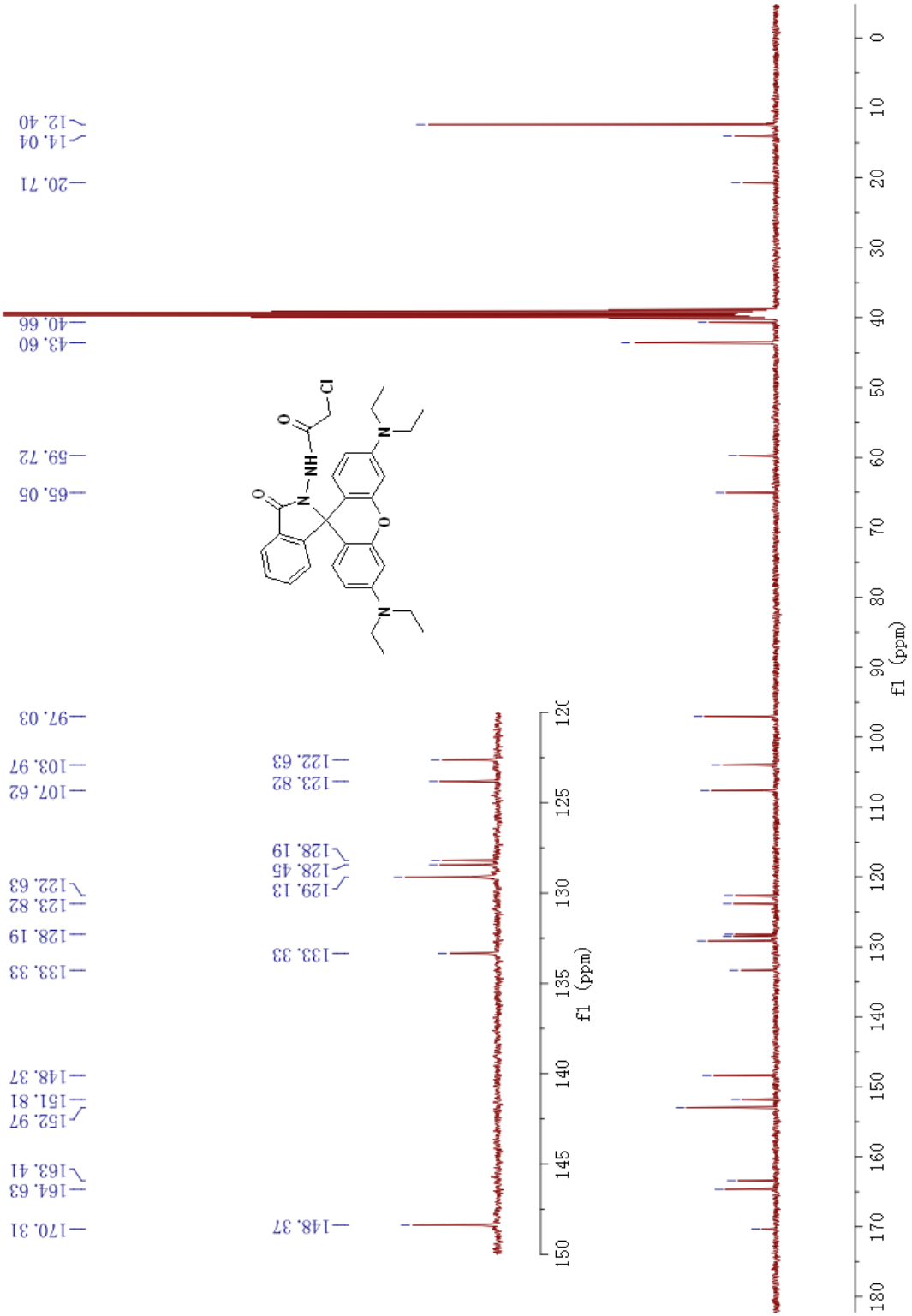

12.41
43.64
64.71
97.35
105.40
107.73
122.12
123.47
127.68
132.36
148.06
151.85
152.99
165.26
f1 (ppm)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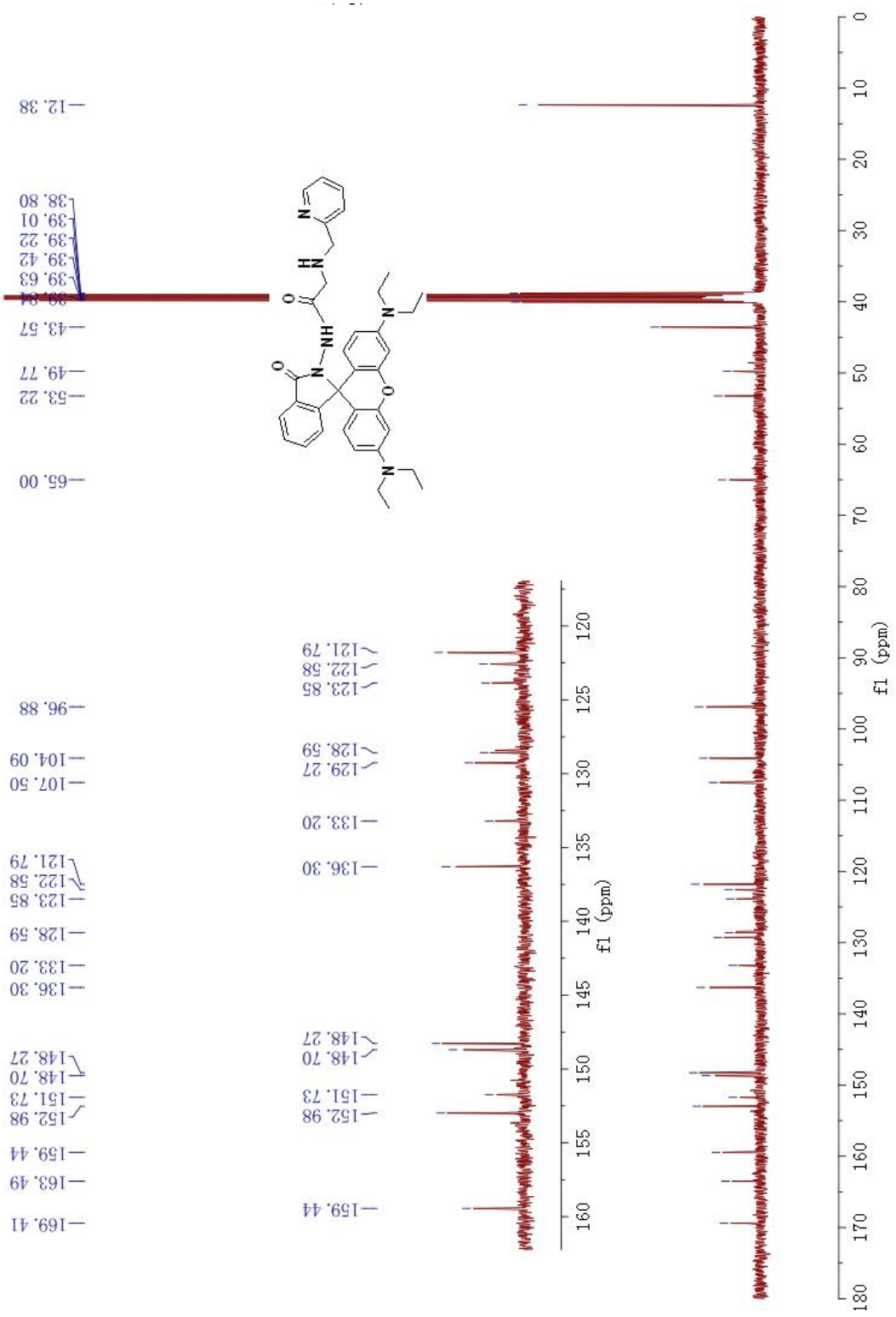
14.04
20.71
40.66
43.60
59.72
65.05
97.03
103.97
107.62
122.63
123.82
128.19
128.45
129.13
133.33
148.37
151.81
152.97
163.41
164.63
170.31
f1 (ppm)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38.80
39.01
39.22
39.42
39.63
39.84
43.57
49.77
53.22
65.00
96.88
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107.50
121.79
122.58
123.85
128.59
133.20
136.30
148.27
148.70
151.73
152.98
159.44
163.49
169.41
f1 (ppm)