Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry
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Supporting Information

A Selective Colorimetric and Ratiometric Fluorescent Probe for Hydrogen Sulfide

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1. Quantum Yields.

Quantum yields were determined using fluorescein as a standard according to a published method.[1] The quantum yield was calculated according to the equation: ($\Phi_{sample} = \Phi_{standard}$ * (I_{sample} / $I_{standard}$) * (A_{sample} / $A_{standard}$)); where Φ is the quantum yield, $\Phi_{standard}$ = 0.85 in 0.1 M NaOH; I_{sample} and $I_{standard}$ are the integrated fluorescence intensities of the sample and the standard, A_{sample} and $A_{standard}$ are the optical densities, at the excitation wavelength, of the sample and the standard, respectively.

Quantum yield of Probe 1: Φ = 0.023. Quantum yield of Probe 3: Φ = 0.029

After the complete reaction with H_2S, the Quantum yield of Probe 1: Φ = 0.236 Quantum yield of Probe 3: Φ = 0.386

2. The isosbestic point of probe 1.

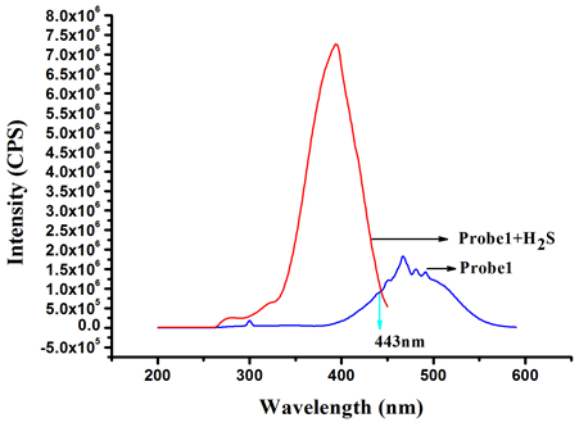
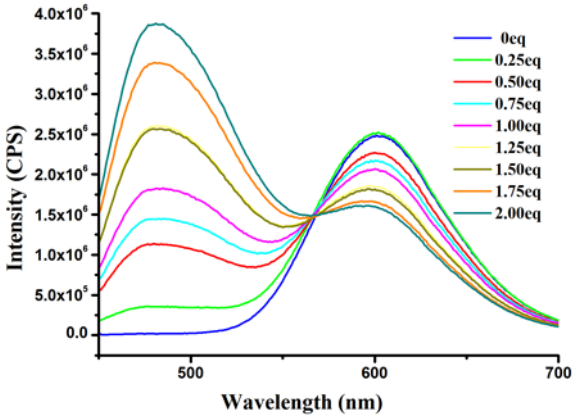


Fig. S1 The excitation spectrum of **Probe 1** and Probe + H_2S in DMF (Slit: 2 nm/3 nm).

3. Detection limit.

The detection limit was calculated based on the fluorescence titration.[2] Probe 1 was employed at 10 μM and the slit was adjusted to 2 nm/3 nm. To determine the S/N ratio, the emission intensity of Probe 1 without Na_2S was measured by 10 times and thestandard deviation of blank measurements was determined. Under the present conditions, a good linear relationship between the fluorescence intensity and the Na_2S concentration could be obtained in the 0 – 20 μM (R = 0.9915), as shown in Fig. S7. The detection limit is then calculated with the equation: detection limit = $3\sigma_{bi}/m$, where σ_{bi} is the standard deviation of blank measurements, m is the slope between intensity versus sample concentration. The detection limit was measured to be 2.5 μM at S/N = 3 (signal-to-noise ratio of 3:1).



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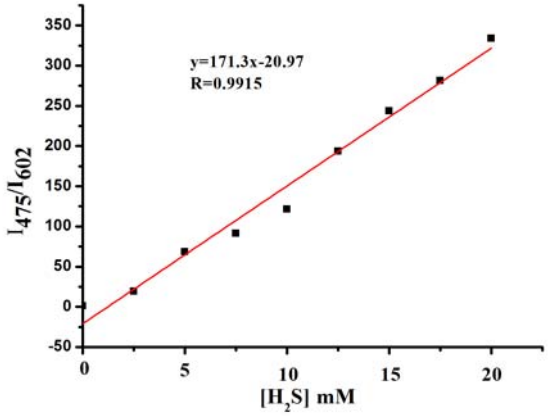
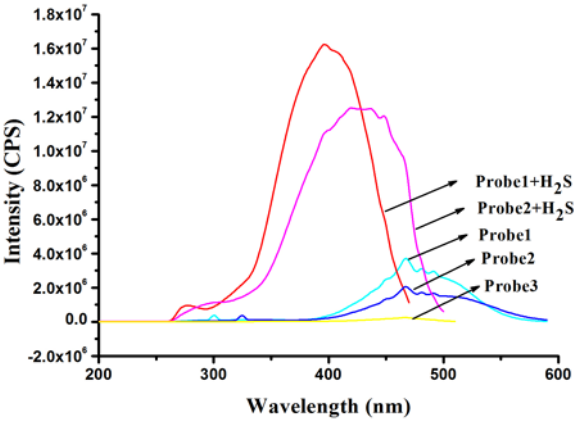


B

Fig. S2 (A) Fluorescence response of Probe 1 (10 μM) to H_2S (0, 2.5, 5.0, 7.5, 10.0, 12.5, 15.0, 17.5, 20.0 μM, 0-2 eq) (λ_{ex} = 443 nm. Slit: 2 nm/3 nm, λ_{scan} = 450 – 700 nm) in DMF. (B) Fluorescence intensity ratio at 475 nm and 602nm (I_{475}/I_{602}) of Probe 1 (10 μM) upon addition of H_2S (0–20 μM, 0-2 eq) (λ_{ex} = 443 nm. Slit: 2 nm/3 nm) in DMF.

4. The excitation spectrum of the probe 1, 2, 3 and their reaction product.



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5. The image of the probes in the absence and presence of H_2S under natural light (A) as well as UV light (B, λ = 254 nm).

A

B

Reference:

1. B. C. A. Parker, W. T. Rees, *Analyst*, 1960, **85**, 587.

2. B. P. Joshi, J. Park, W. I. Lee and K. Lee, *Talanta*., 2009, **78**, 903.

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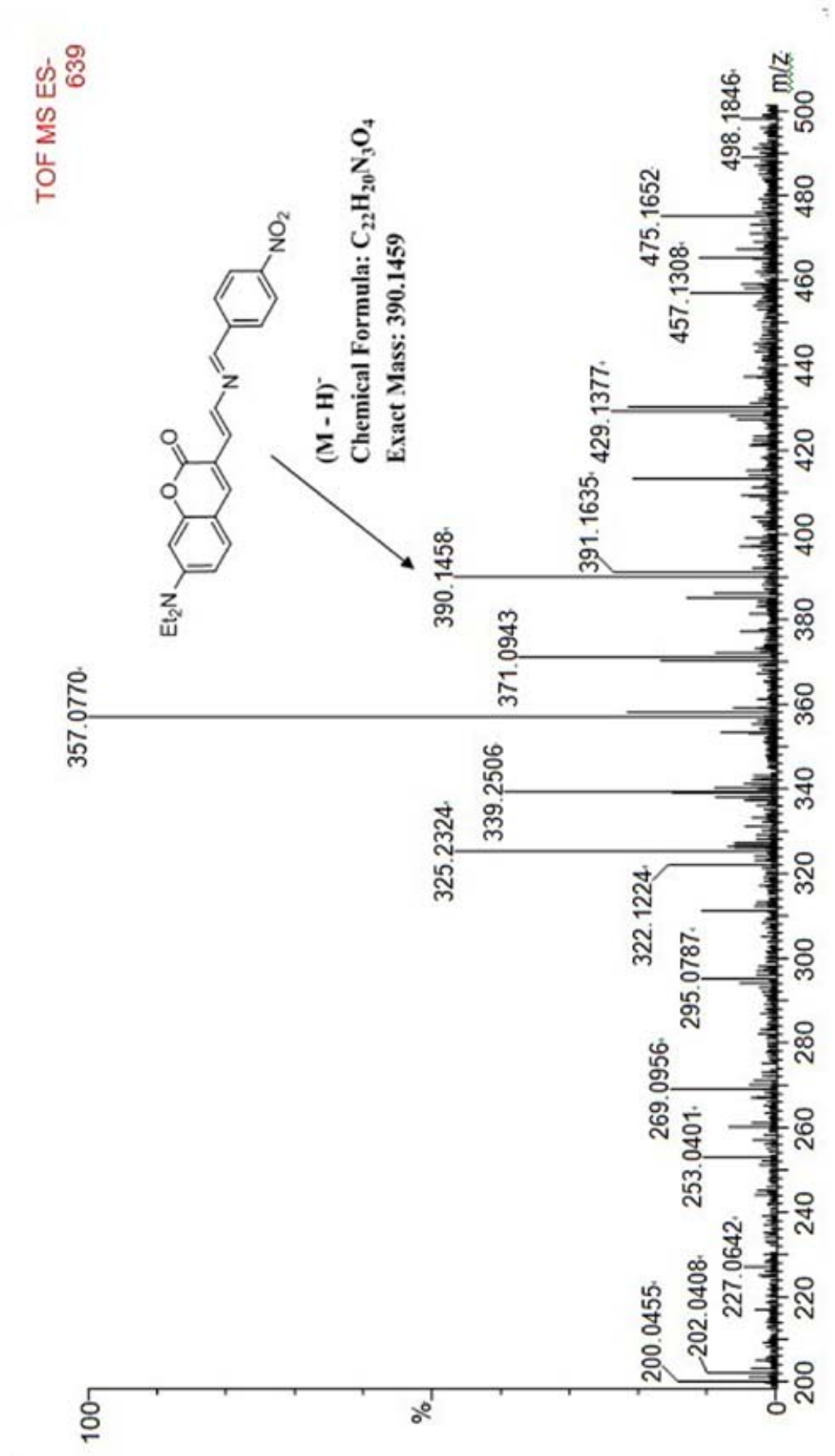
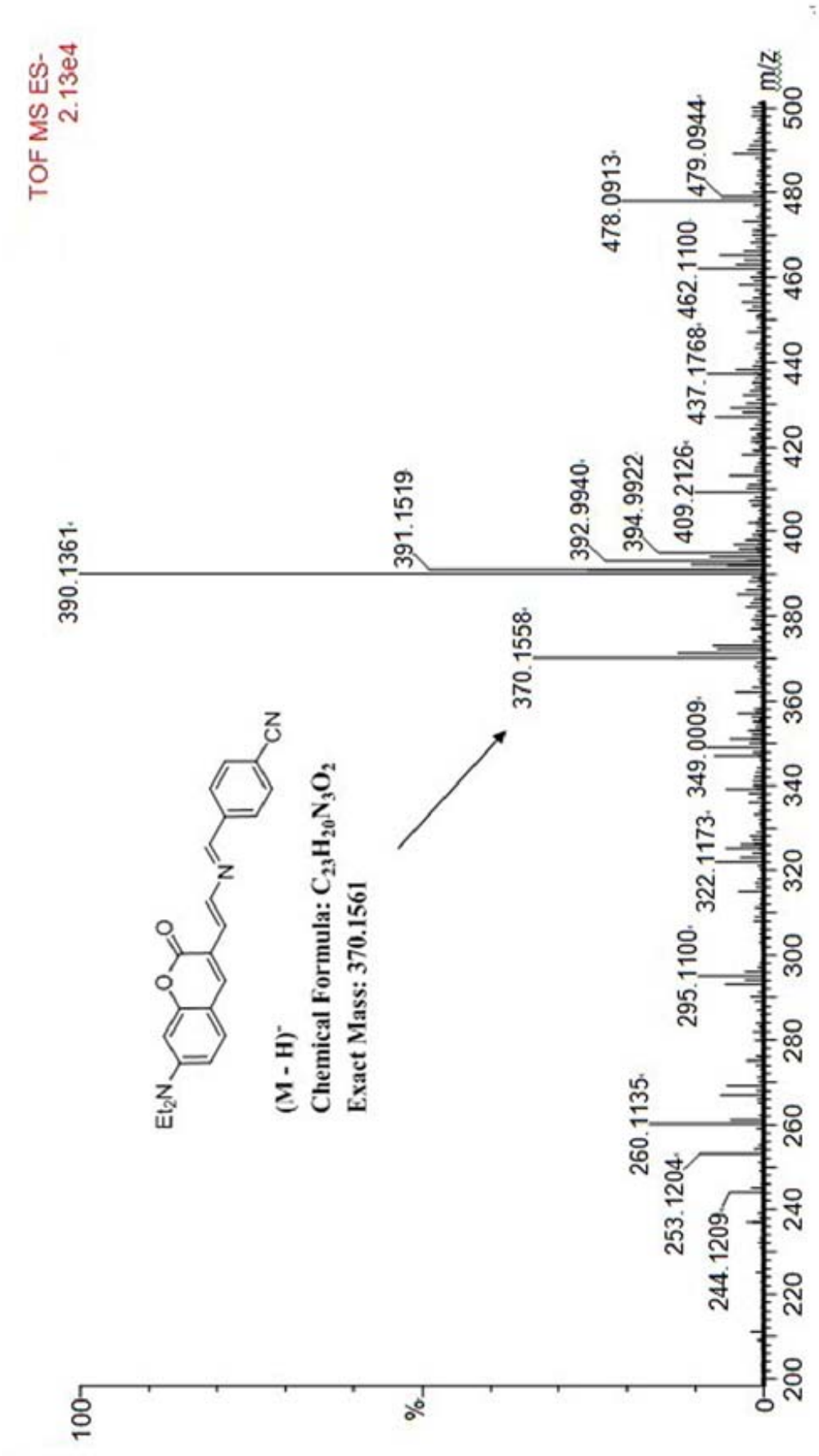
6. HRMS.

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O
O
N
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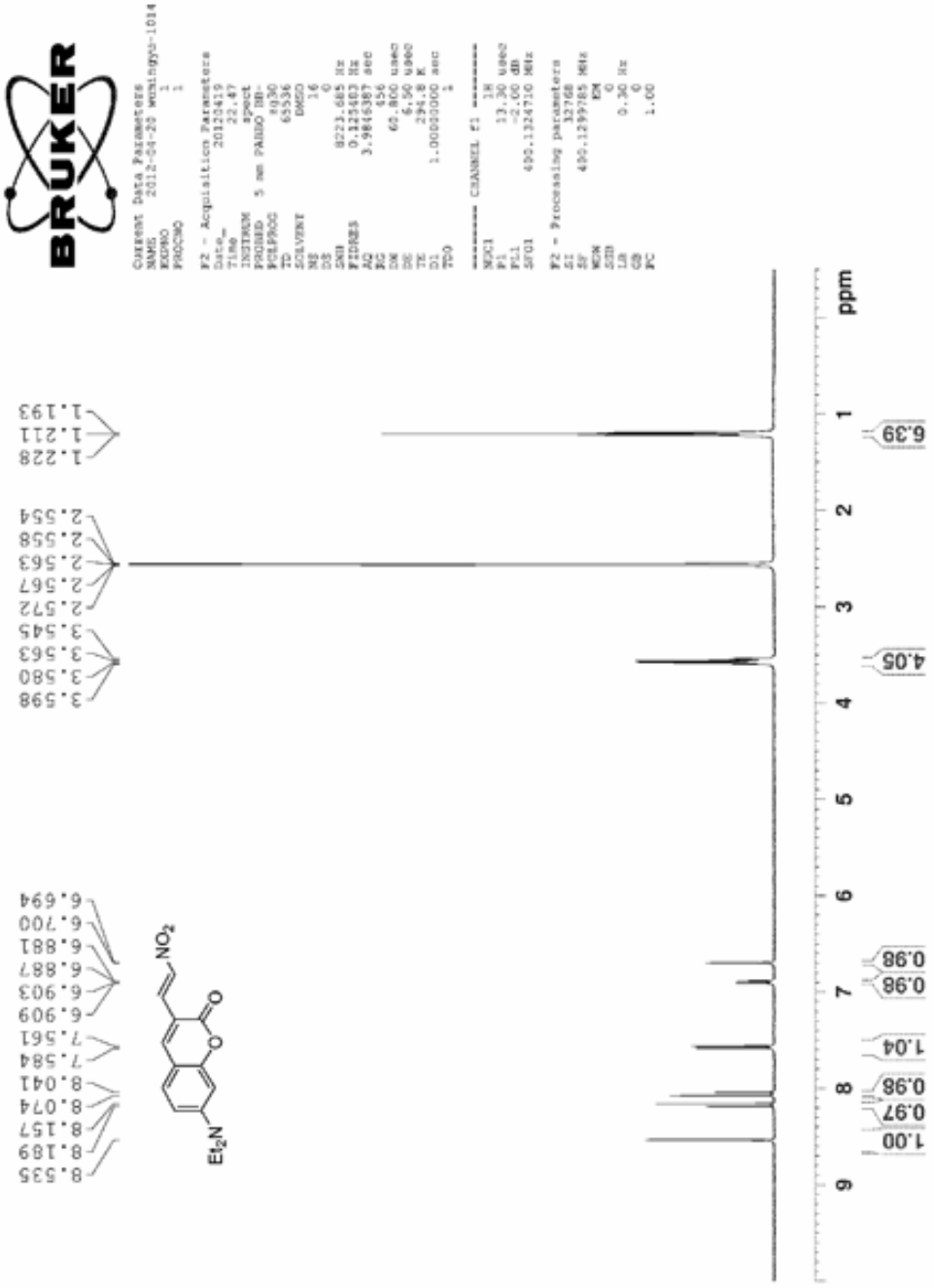
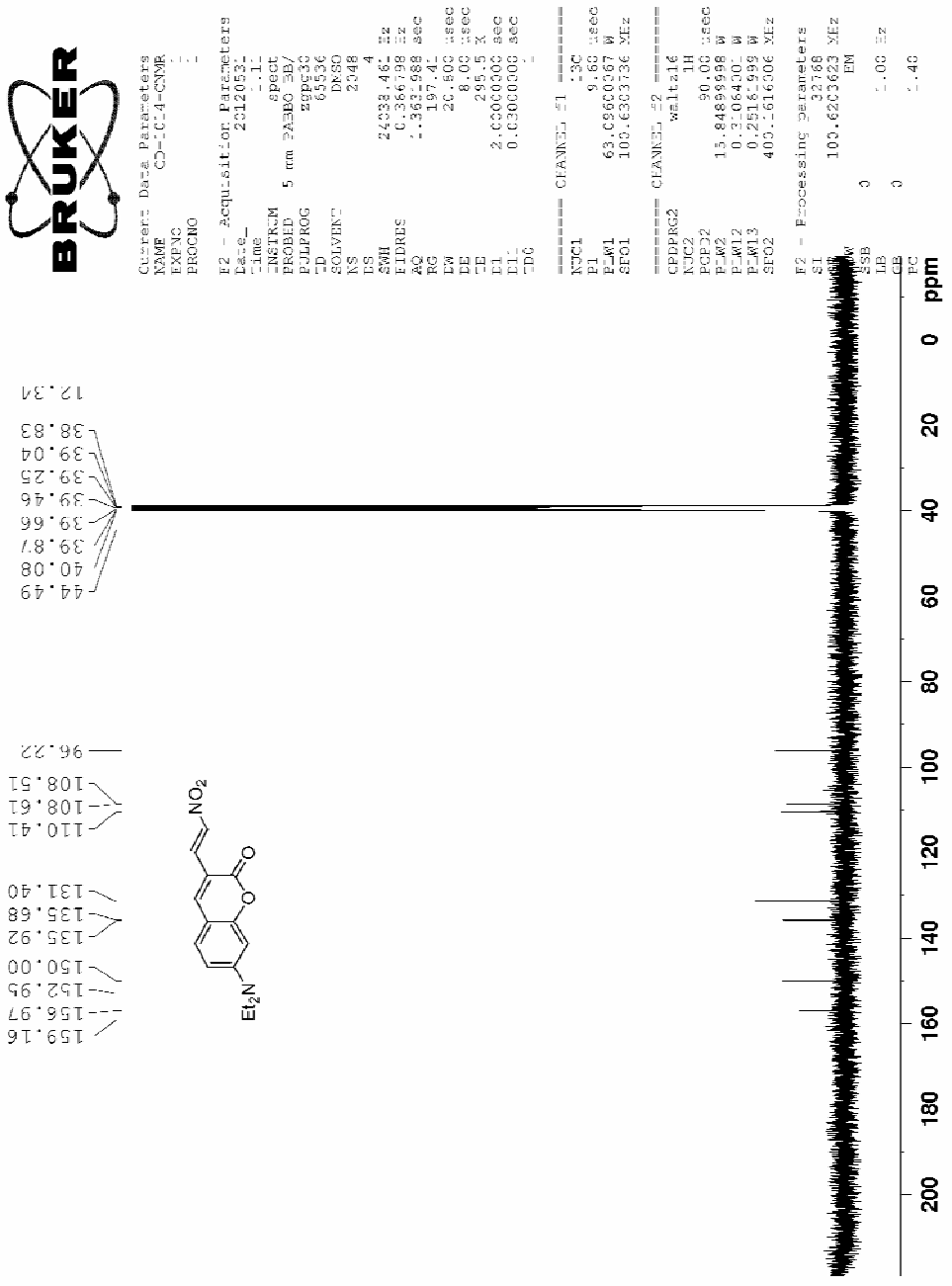
7. ^{1}H NMR and ^{13}C NMR spectrums.

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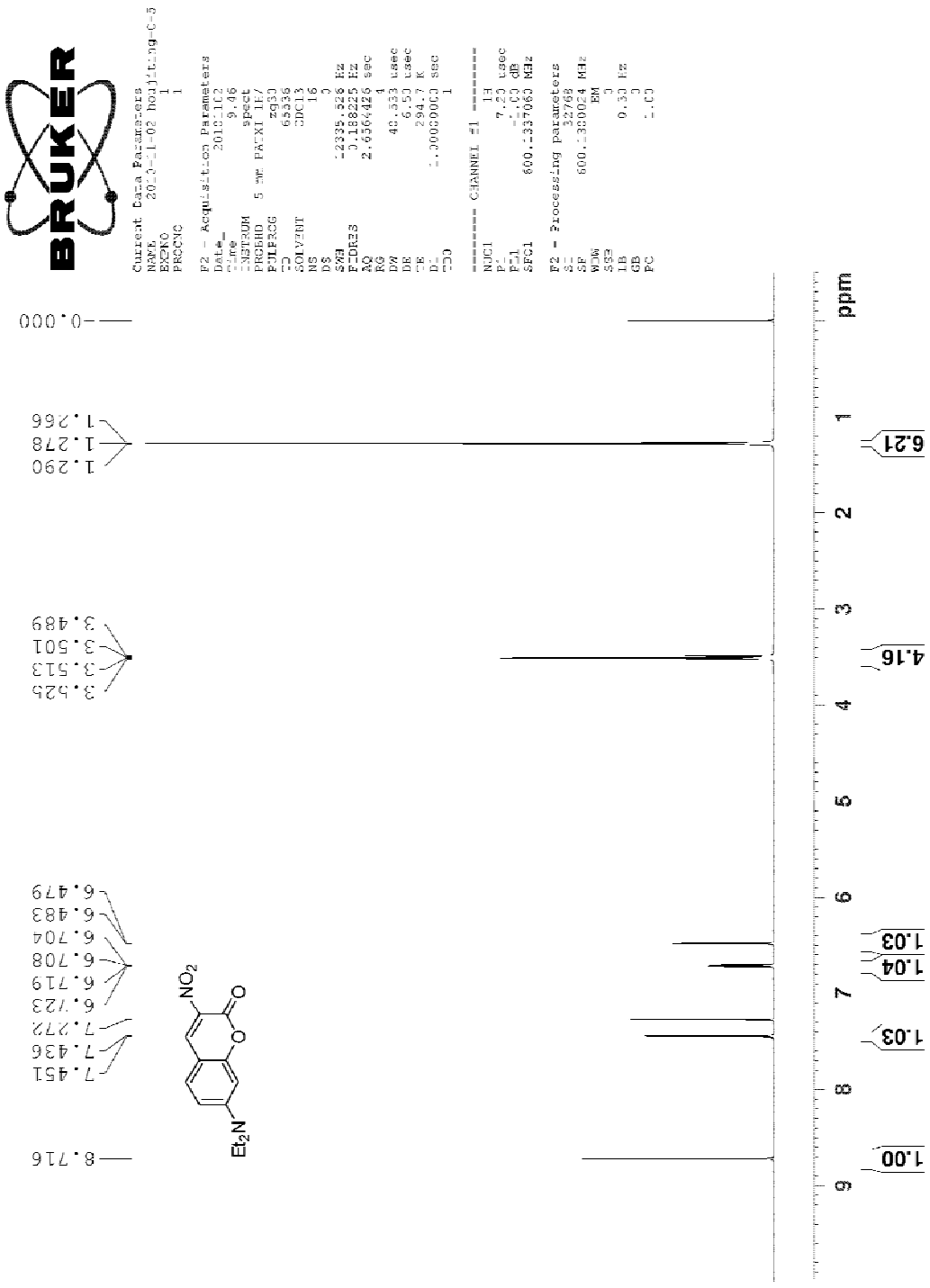
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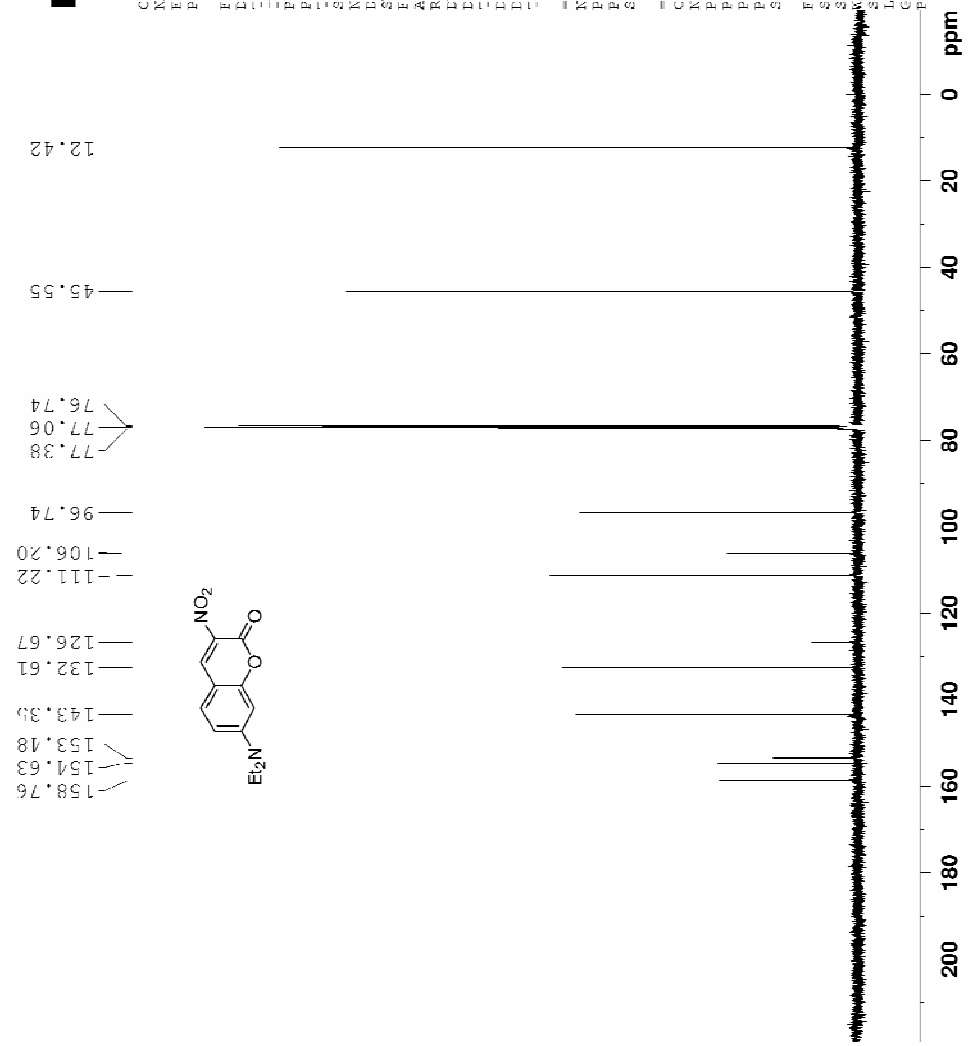
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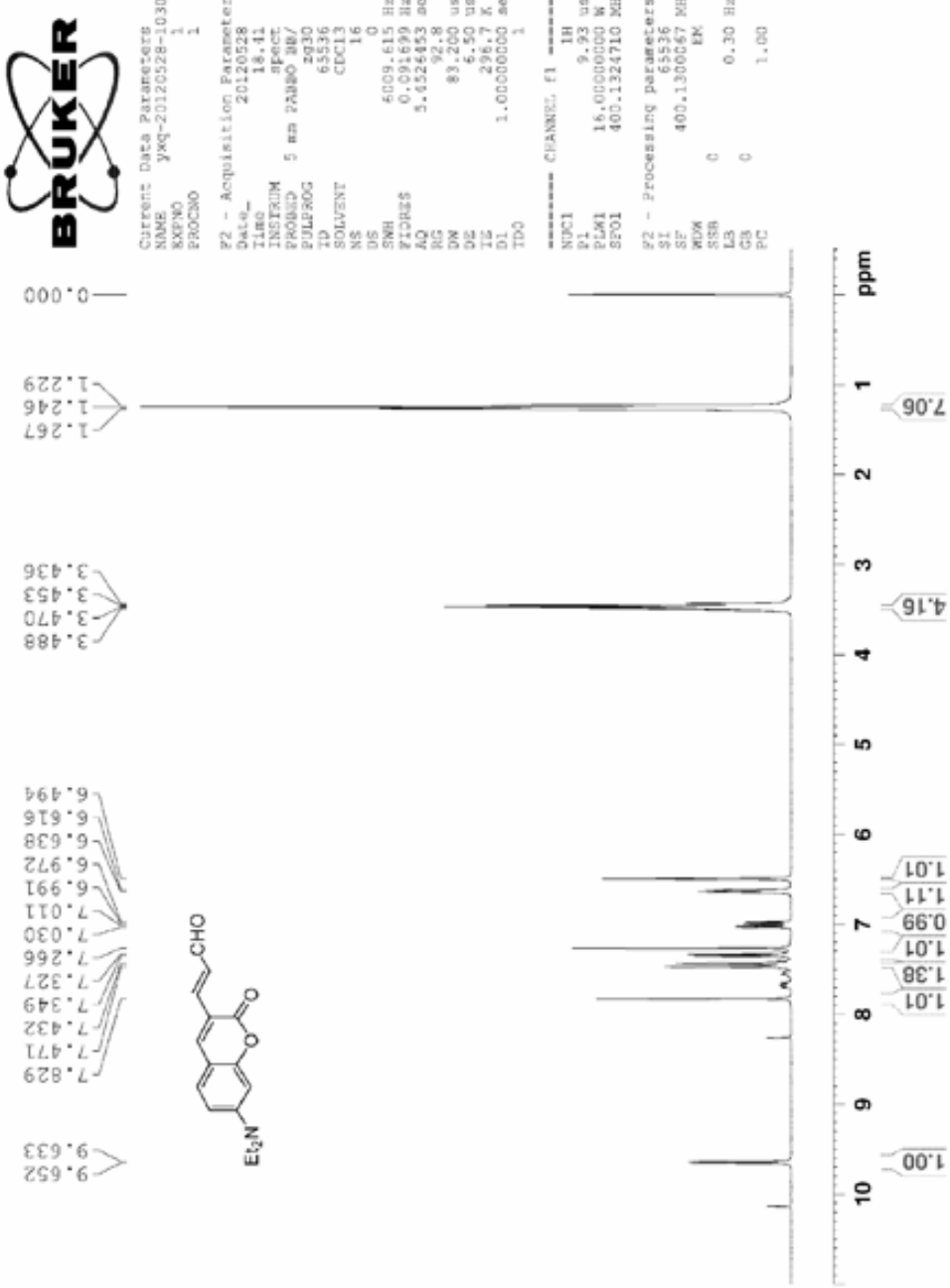
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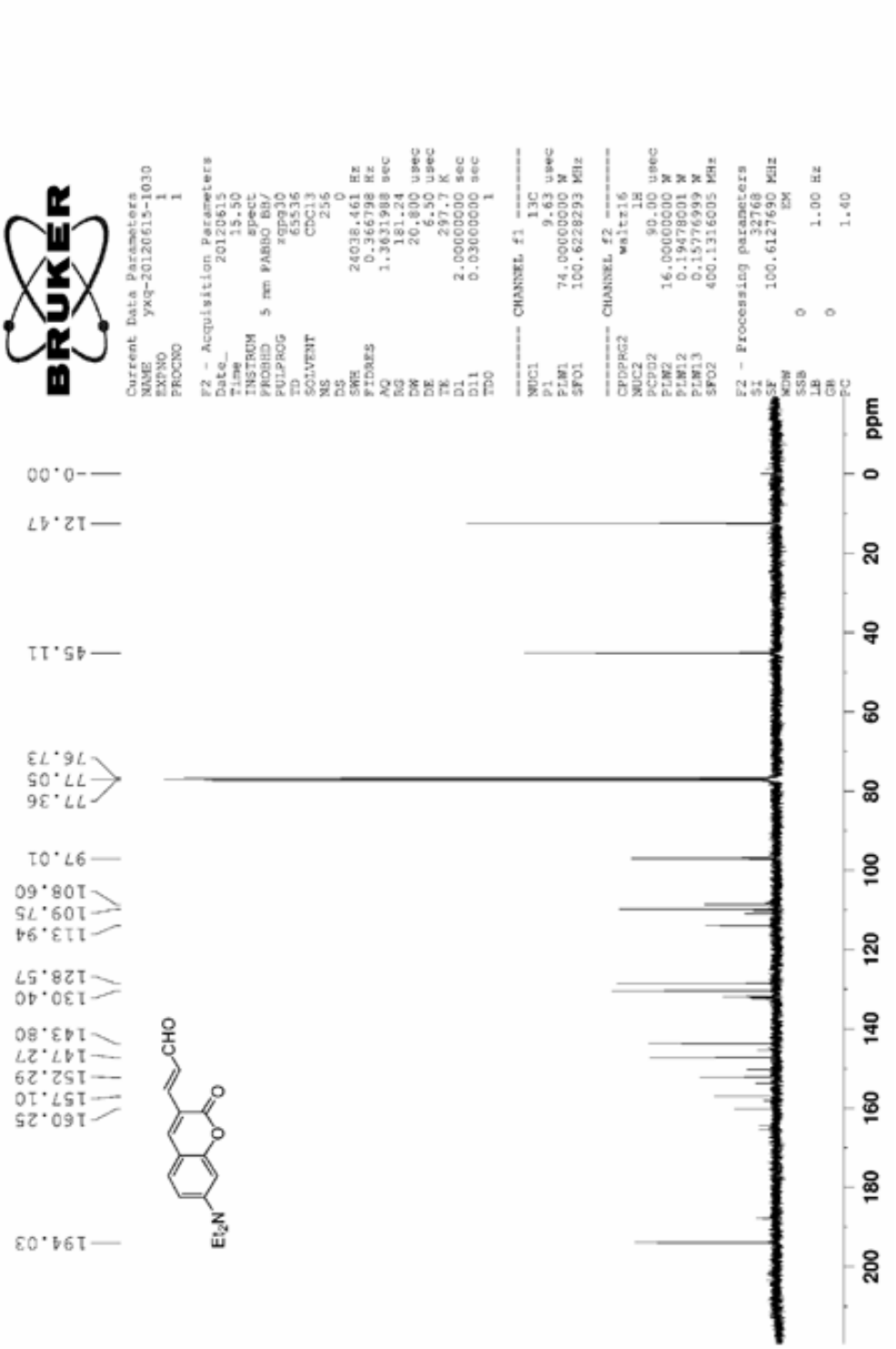

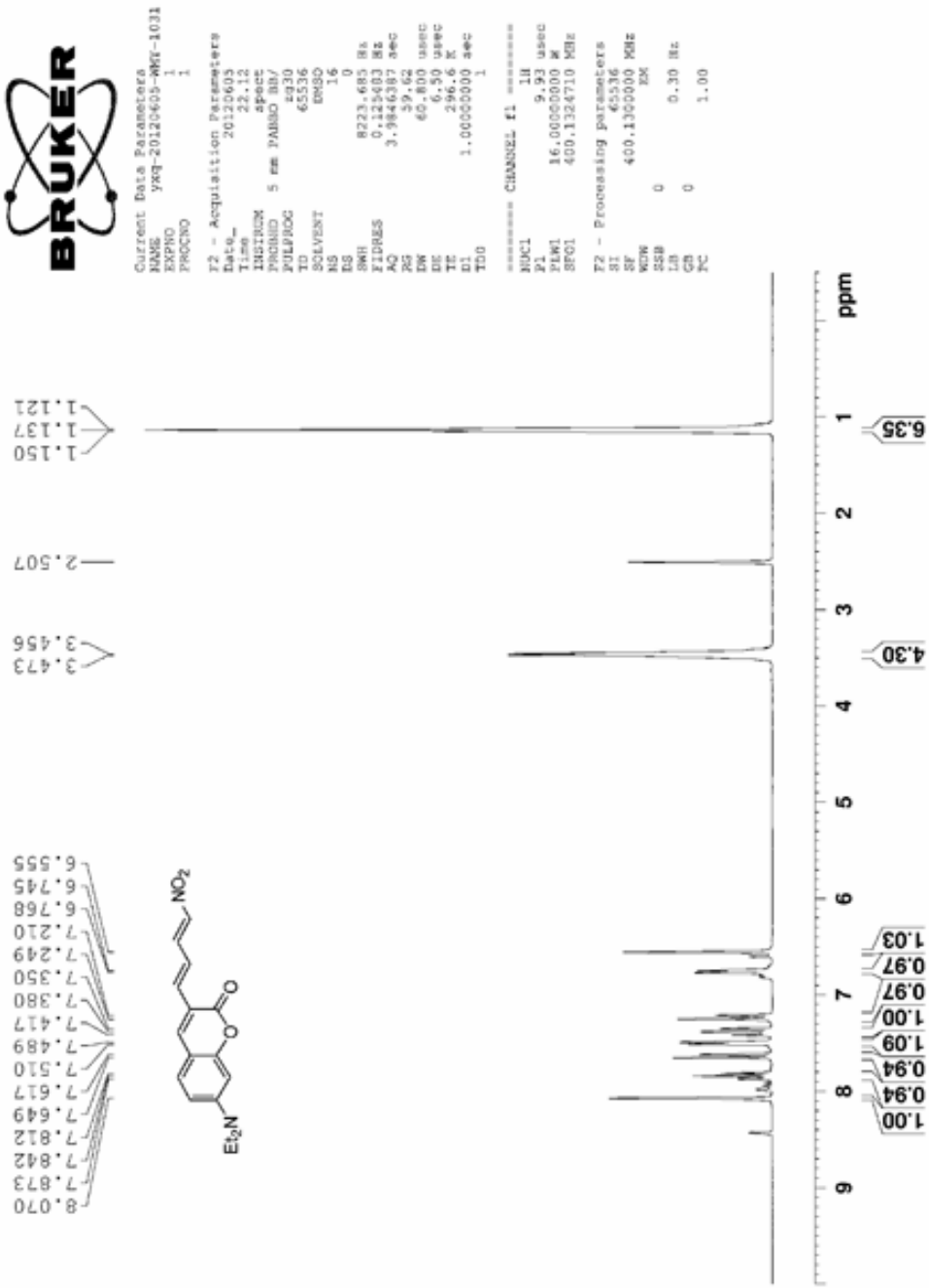
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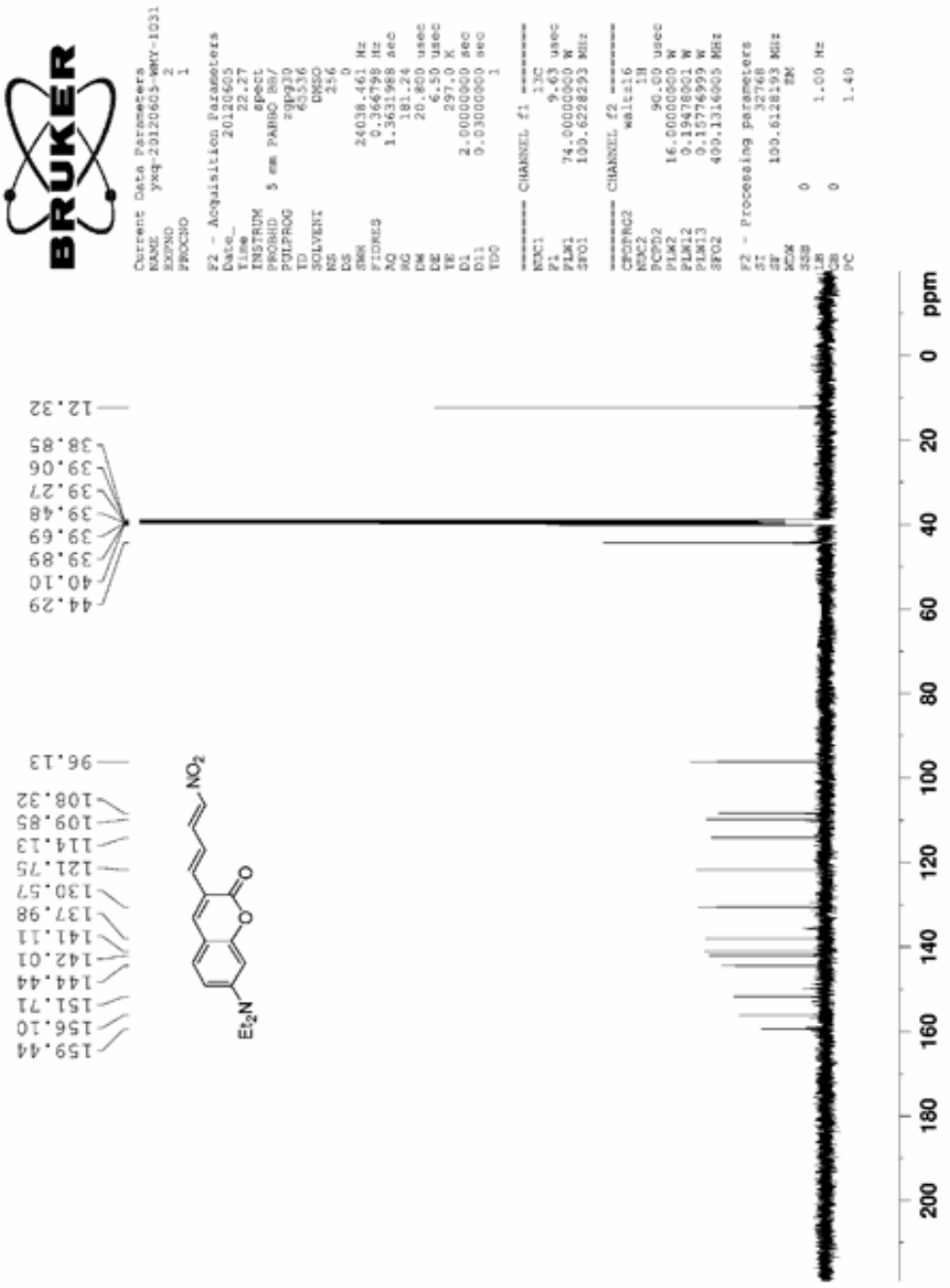
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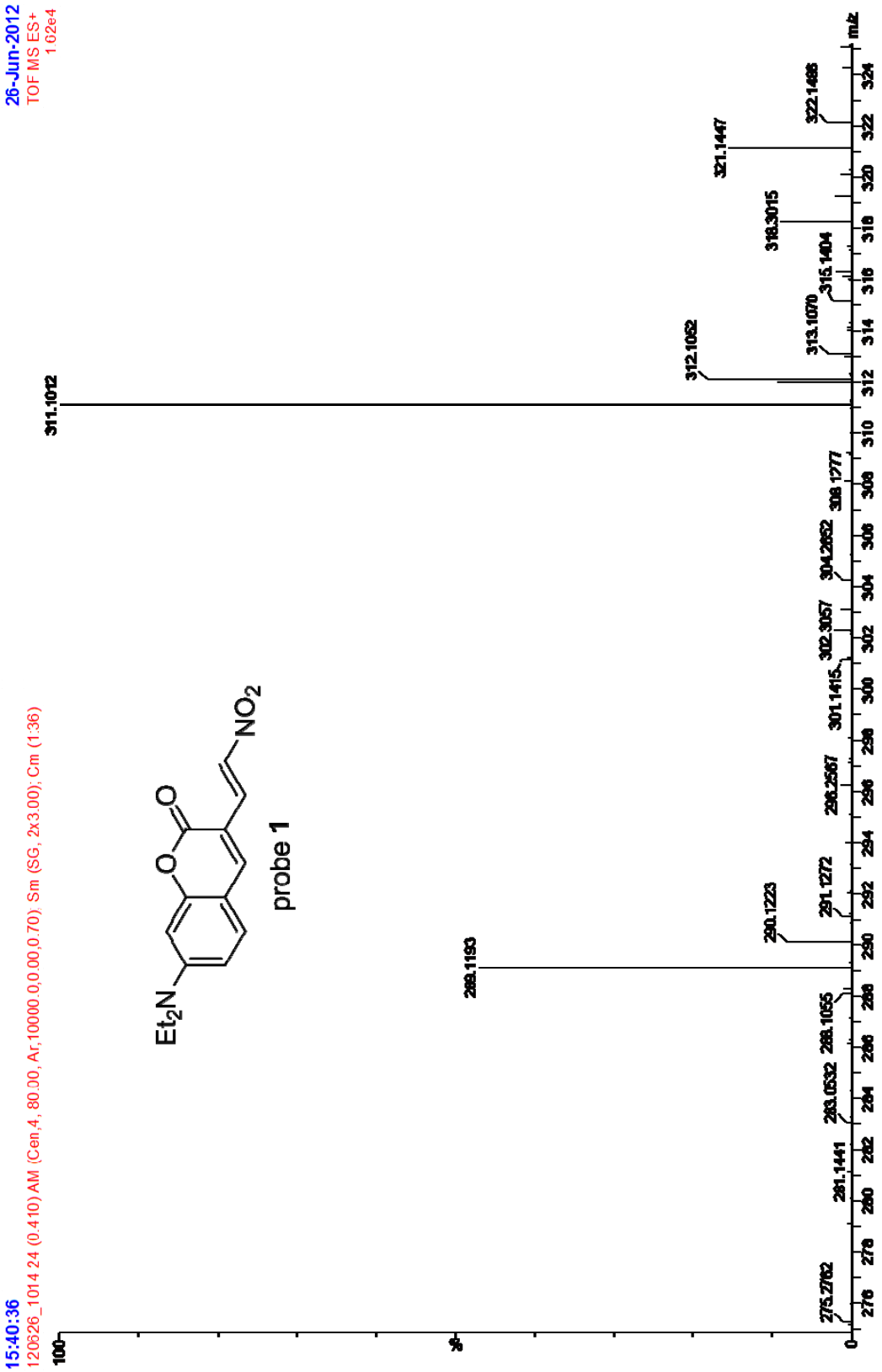
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