

***N*-Phenacyldibromobenzimidazoles – synthesis optimization and evaluation of their cytotoxic activity**

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1. HPLC analysis - general remarks

HPLC analyses were performed on PE NELSON NCI900 chromatograph (Waltham, MA, USA) equipped with a UV-VIS (Perkin Elmer 785A detector, Waltham, MA, USA) and a reverse-phase column Hichrom HI-5C18-3959 (250 x 1.0 mm, 5 μ m). 10 μ l of sample was injected. A gradient method comprising water/ acetonitrile was applied as follows: 0-20 min 20/80 (1 ml/min), 20-25 min 20/80 – 0/100 (1 ml/min) 25-60 min 0/100 (1 ml/min). UV-VIS detector was set at a wavelength of 254 nm.

The calibration curve was prepared using seven concentrations of the model compound, 2-(5,6-dibromo-1*H*-benzimidazol-1-yl)-1-(2,4-dichlorophenyl)ethenone **4e** (1.520, 1.013, 0.676, 0.450, 0.300, 0.200, 0.133 mg/ml).

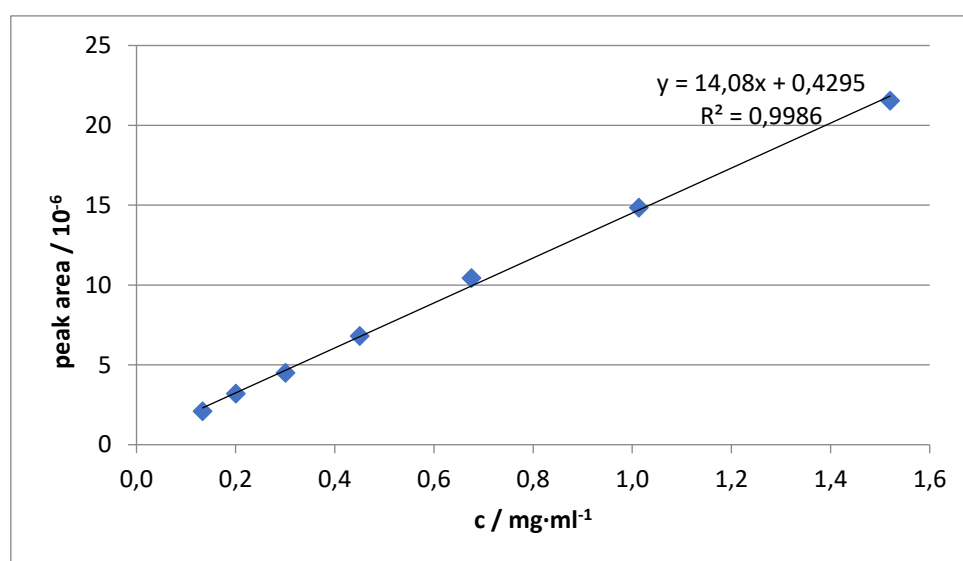


Figure S1. The calibration curve.

Procedure for optimization reactions (see Table 1 in the manuscript).

To the 5,6-dibromobenzimidazole **1** (0.1 mmol, 27.6 mg) in a solvent (5 ml, see Table 1) 2,4-dichlorophenacyl chloride **3e** (see Table 1) was added, followed by a base (see Table 1). The mixture was magnetically stirred (temperature and time given in Table 1). The solvent was evaporated, H₂O (10 ml) and CH₂Cl₂ (10 ml) were added, the phases were separated, the water phase was extracted with CH₂Cl₂ (2 x 10 ml), the combined organic phases were washed with H₂O (2 x 10 ml), dried with MgSO₄ and evaporated to dryness. The residue was dissolved in the volumetric flask (5 ml) in THF and diluted with MeCN (50 μ l of THF solution + 250 μ l of MeCN). The concentration of the product **4e** was determined by HPLC, injecting 10 μ l of a sample.

1. HPLC chromatograms of optimizations reactions presented in Table 1.

Table 1, Entry 1

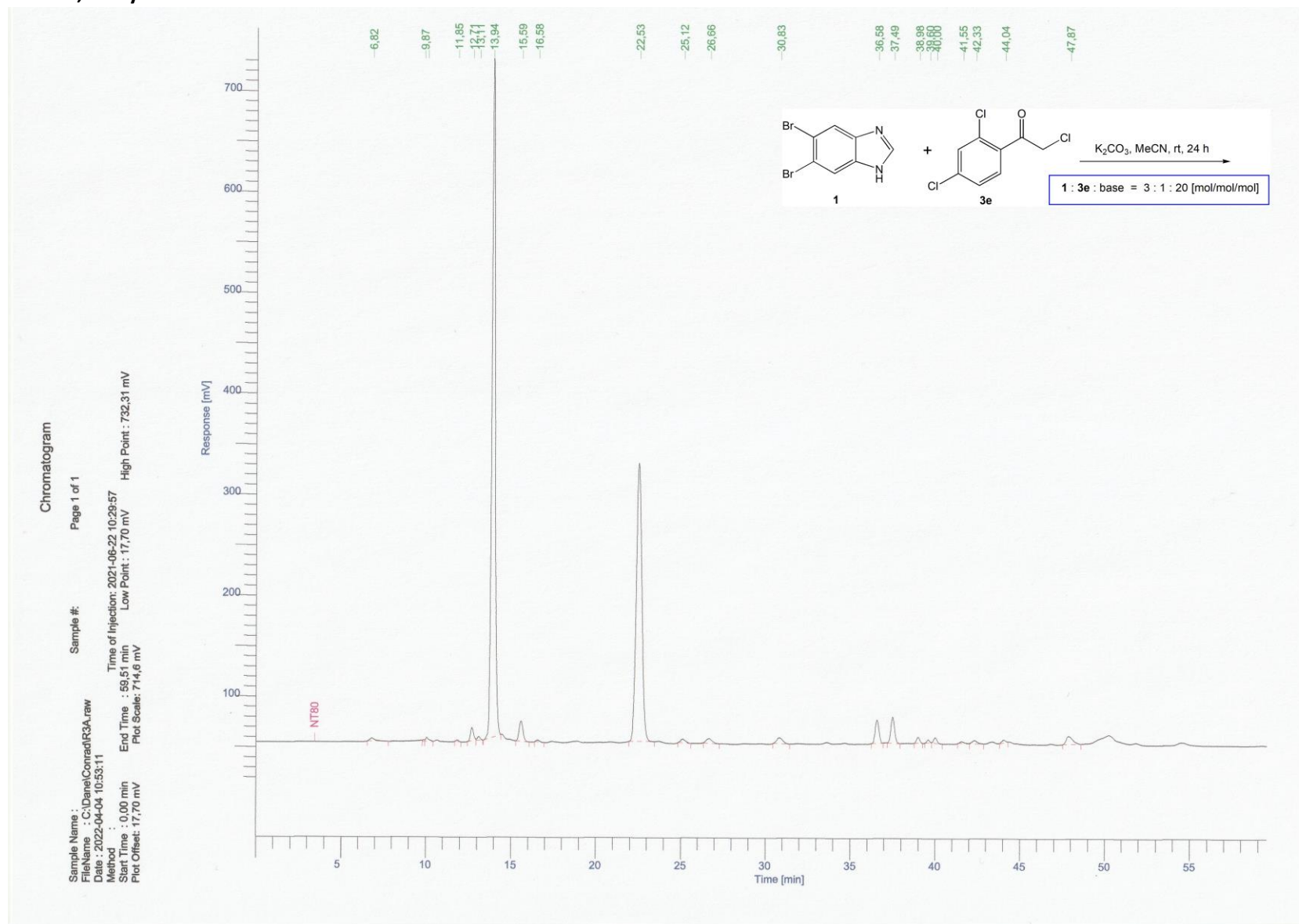


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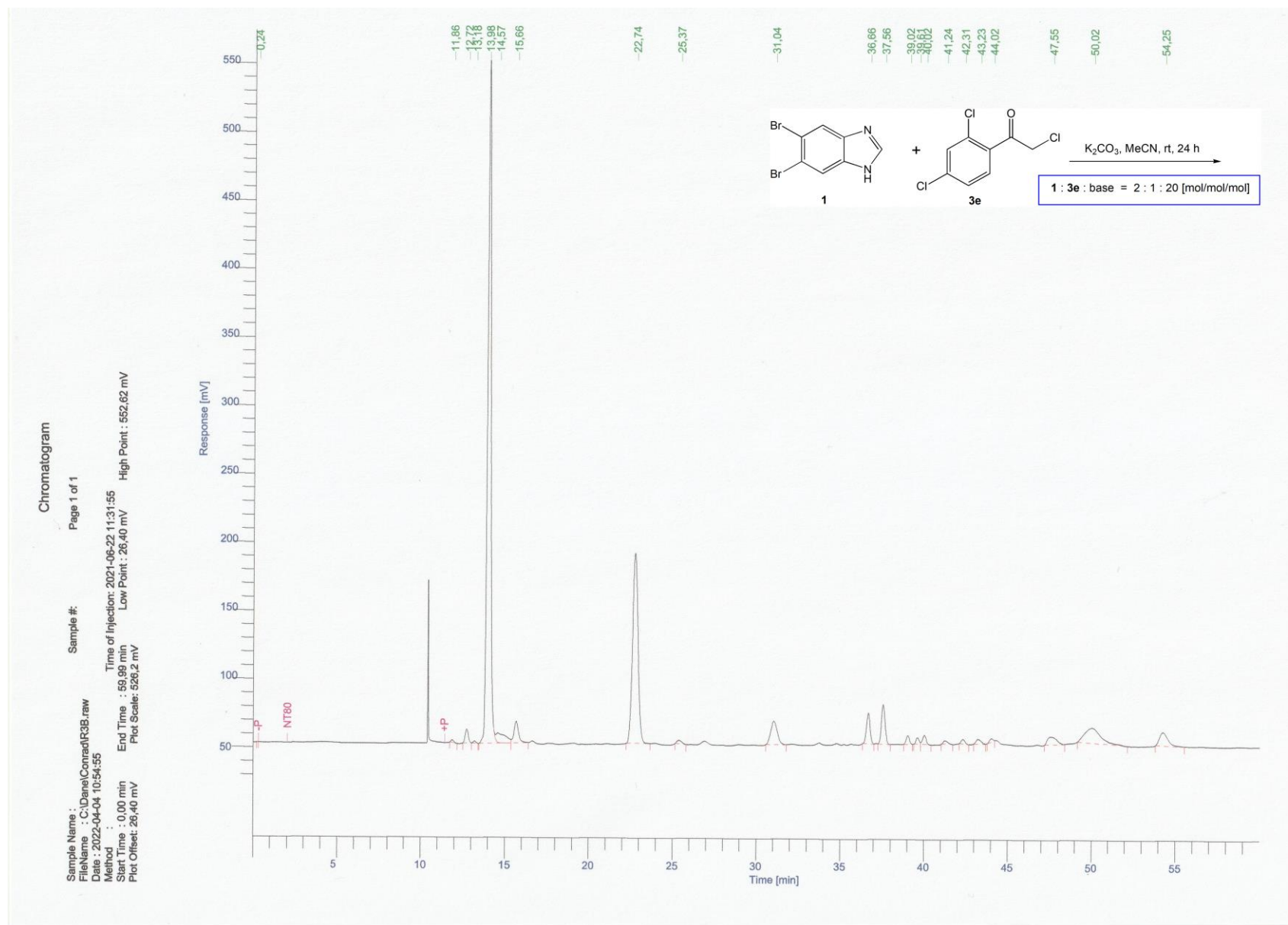


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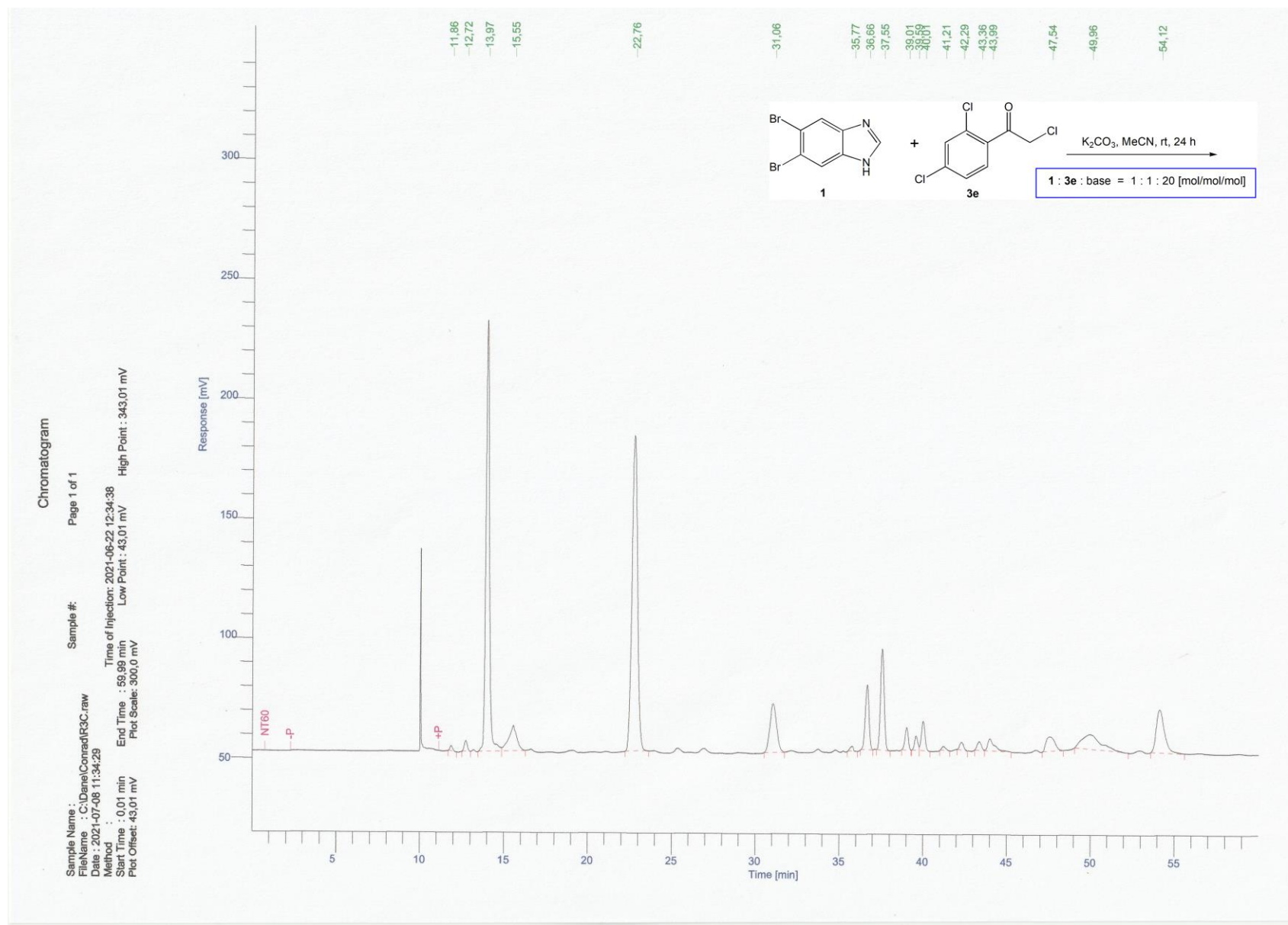


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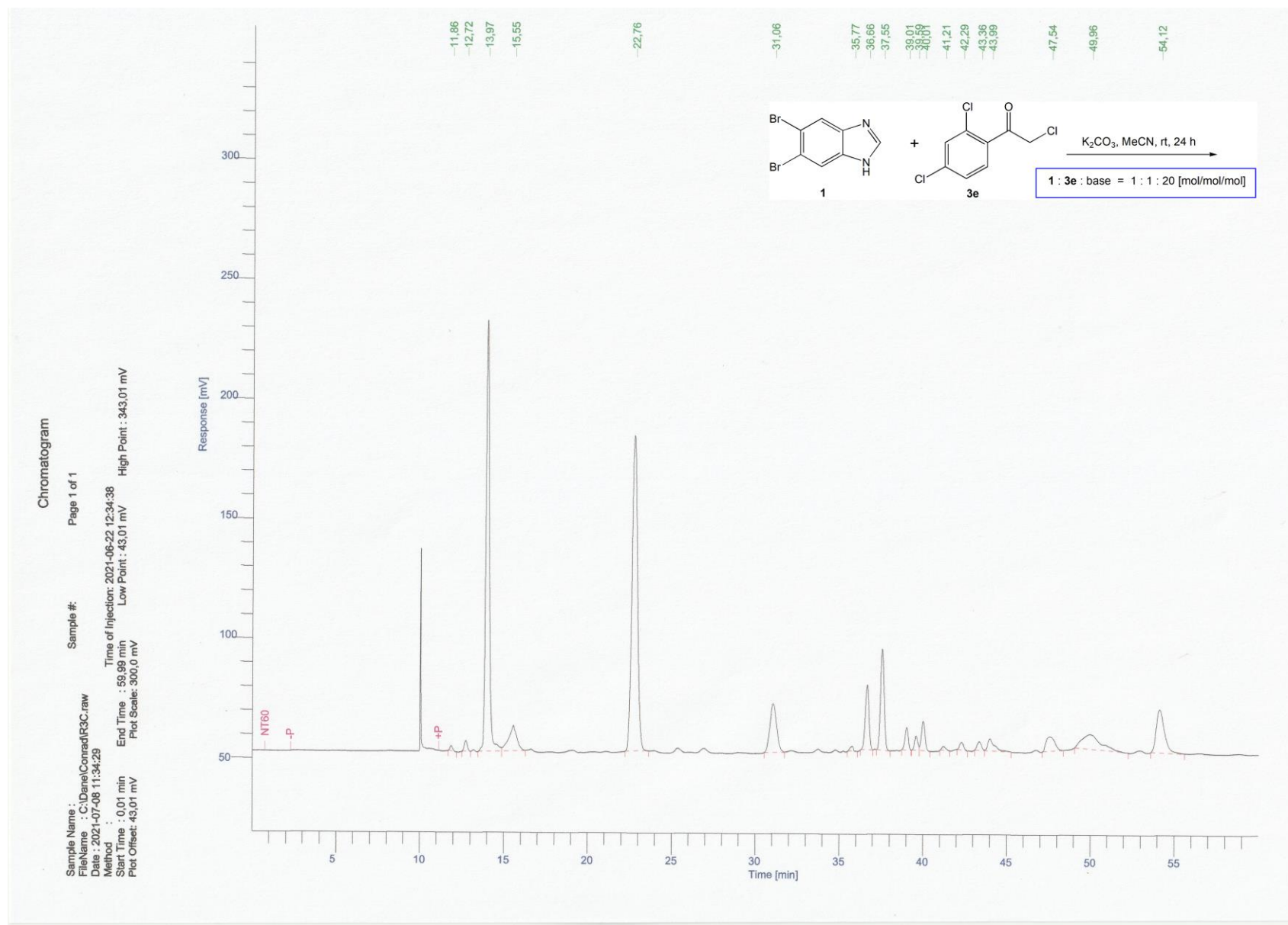


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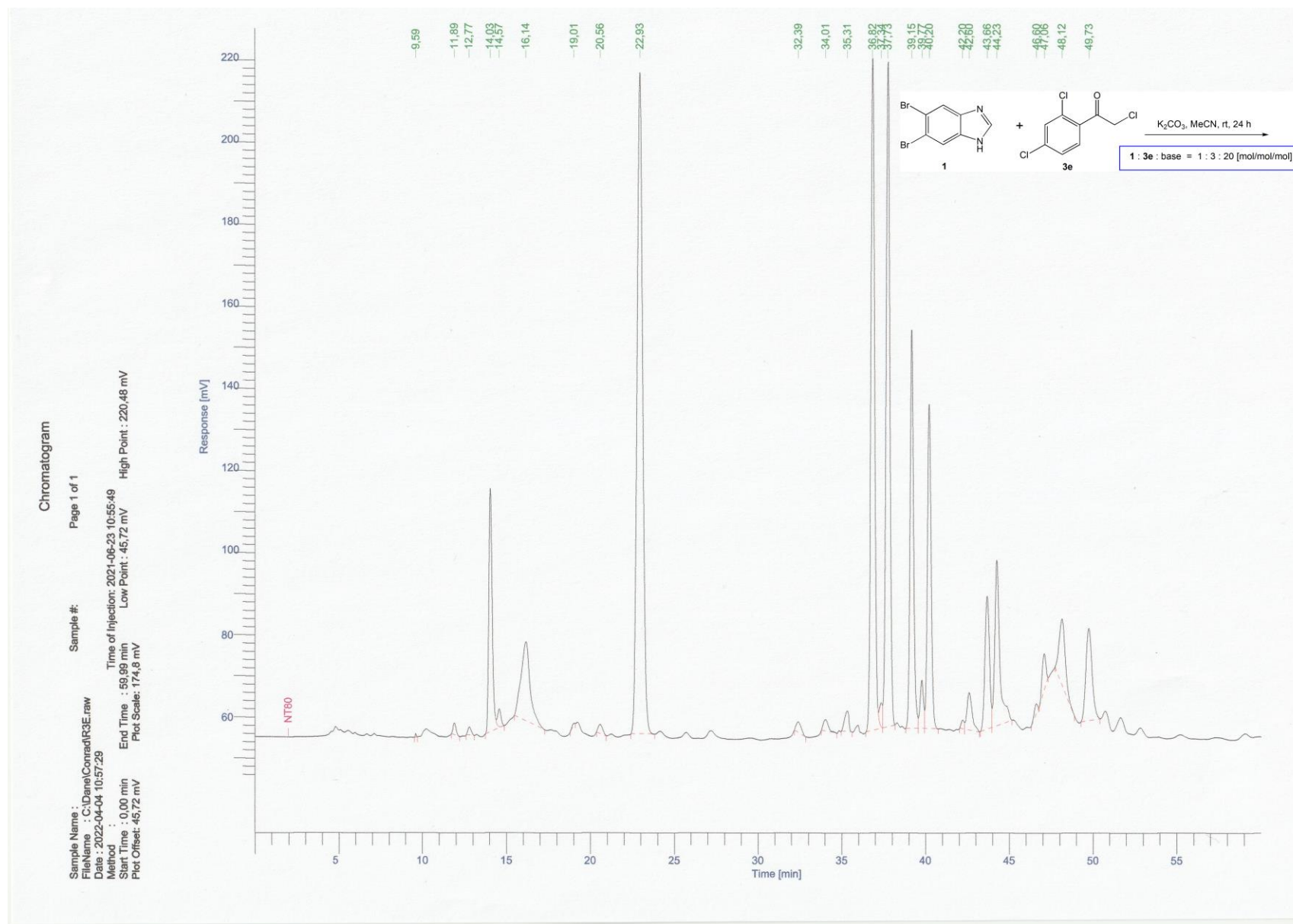


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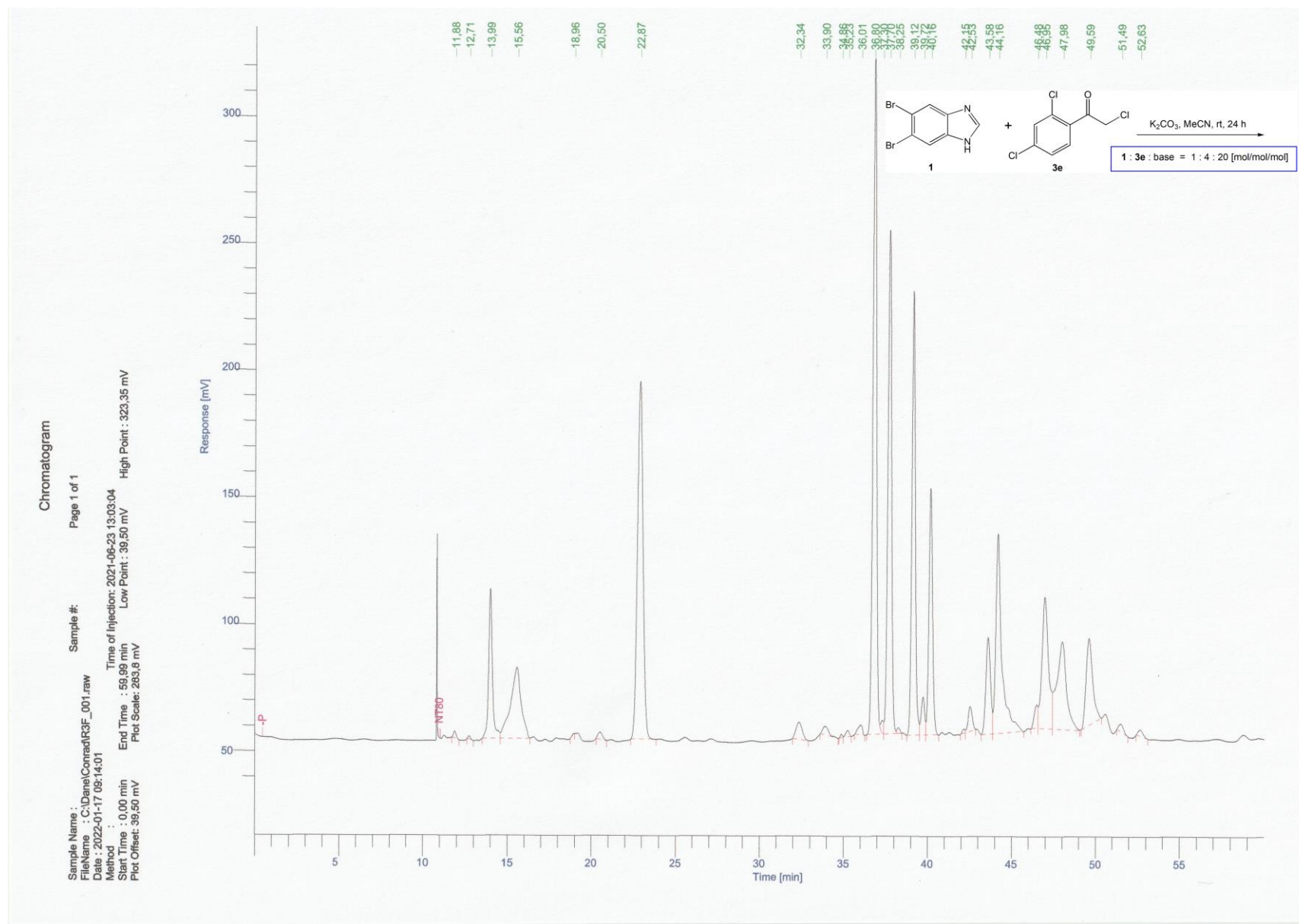


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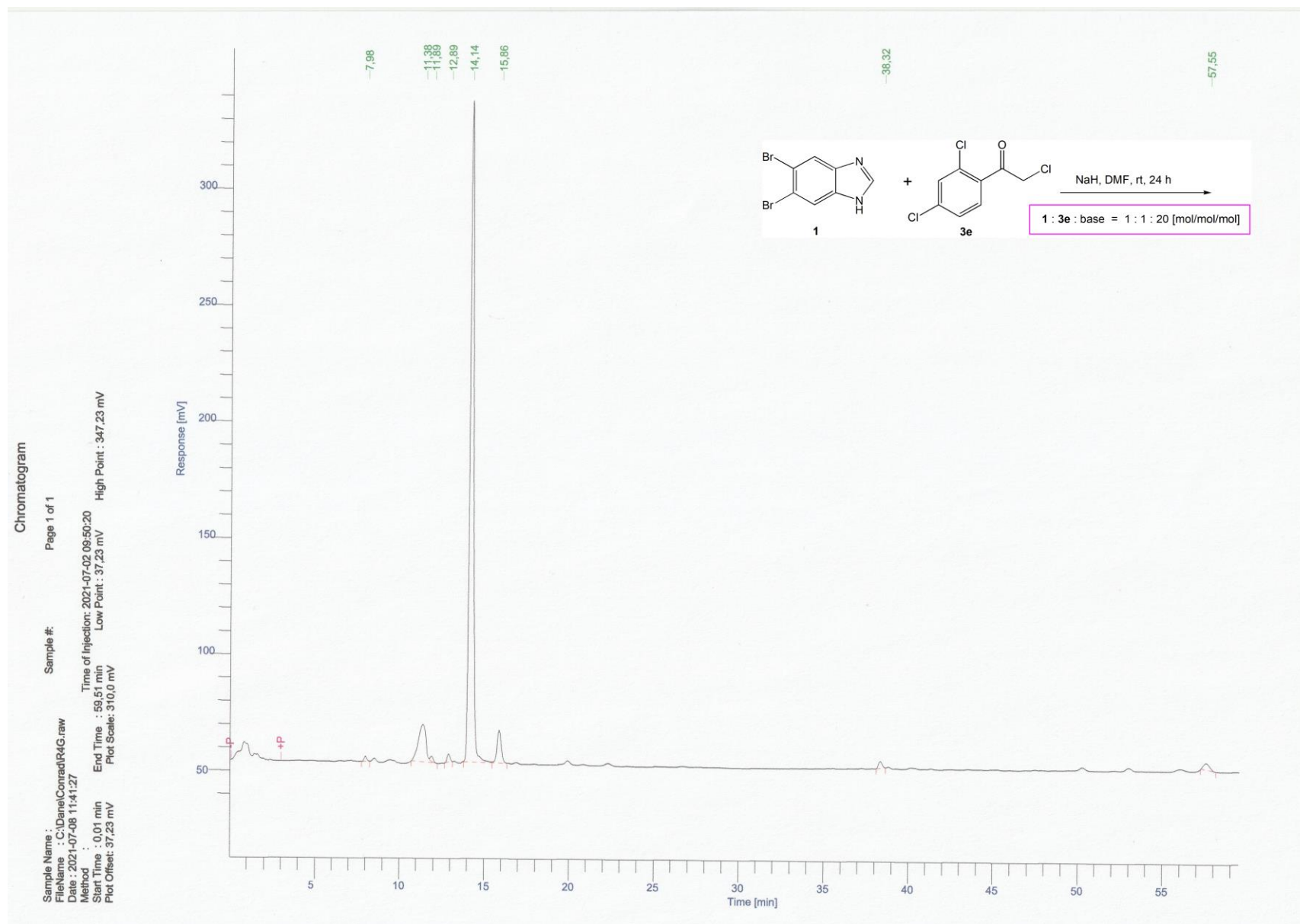


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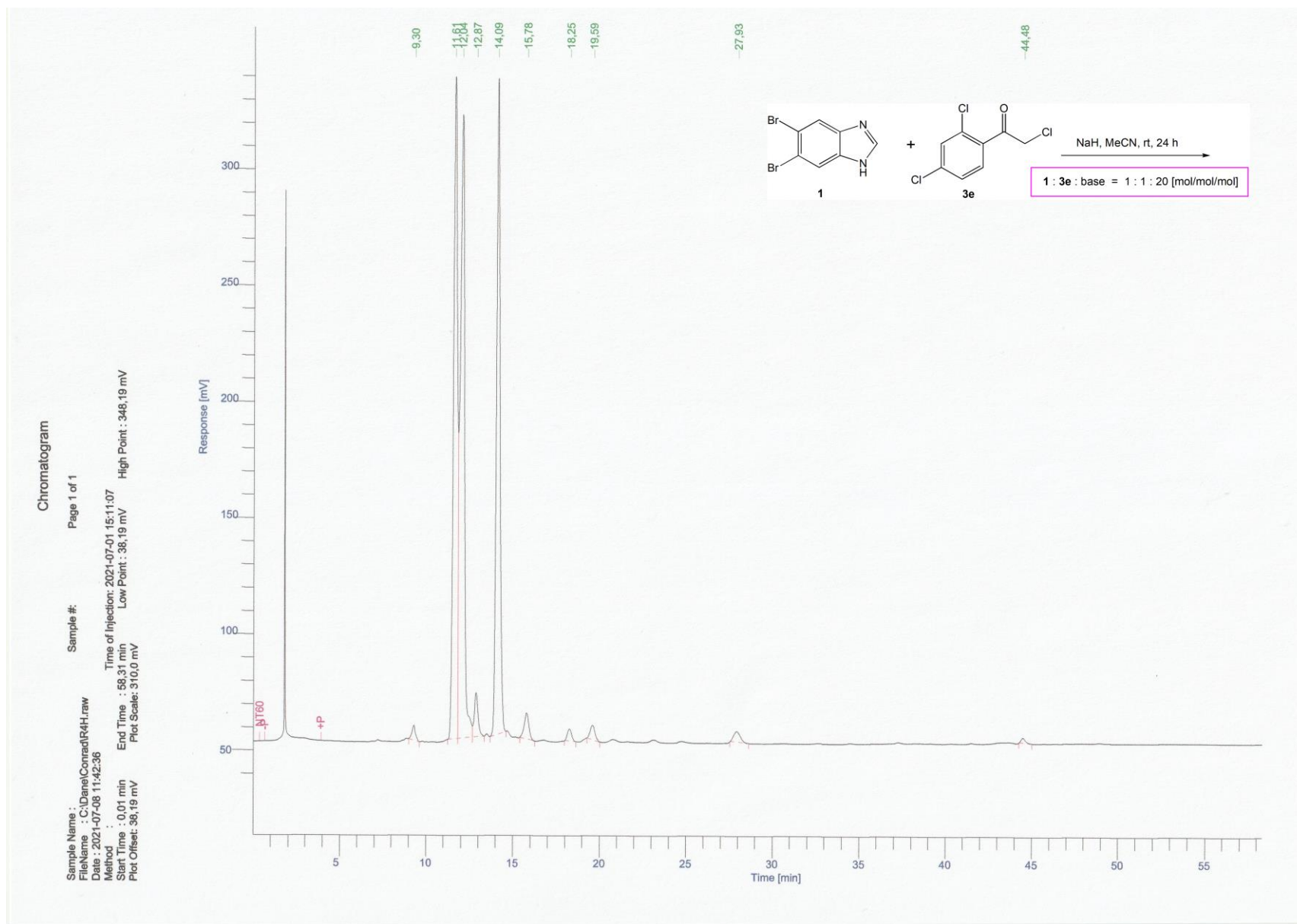


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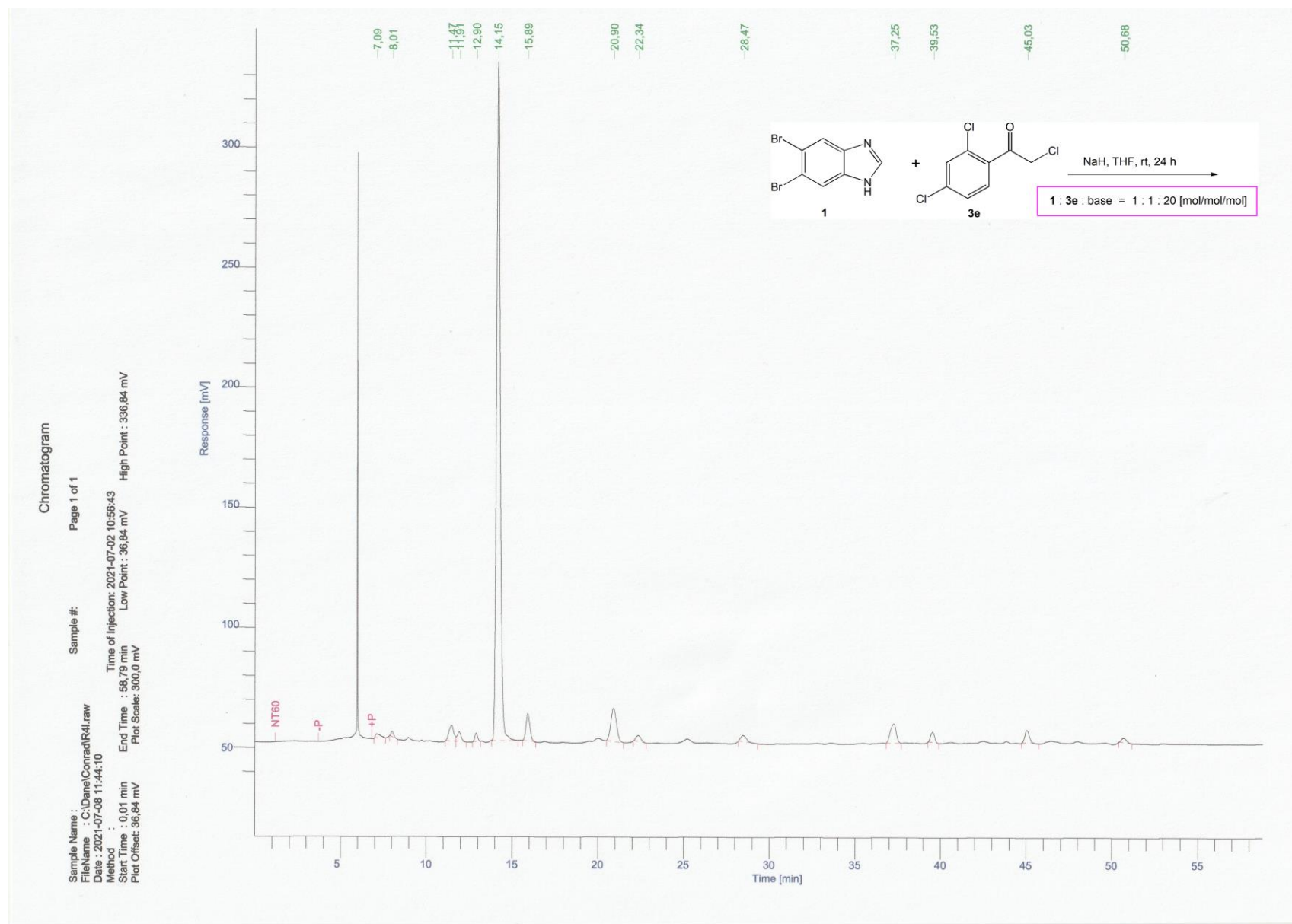


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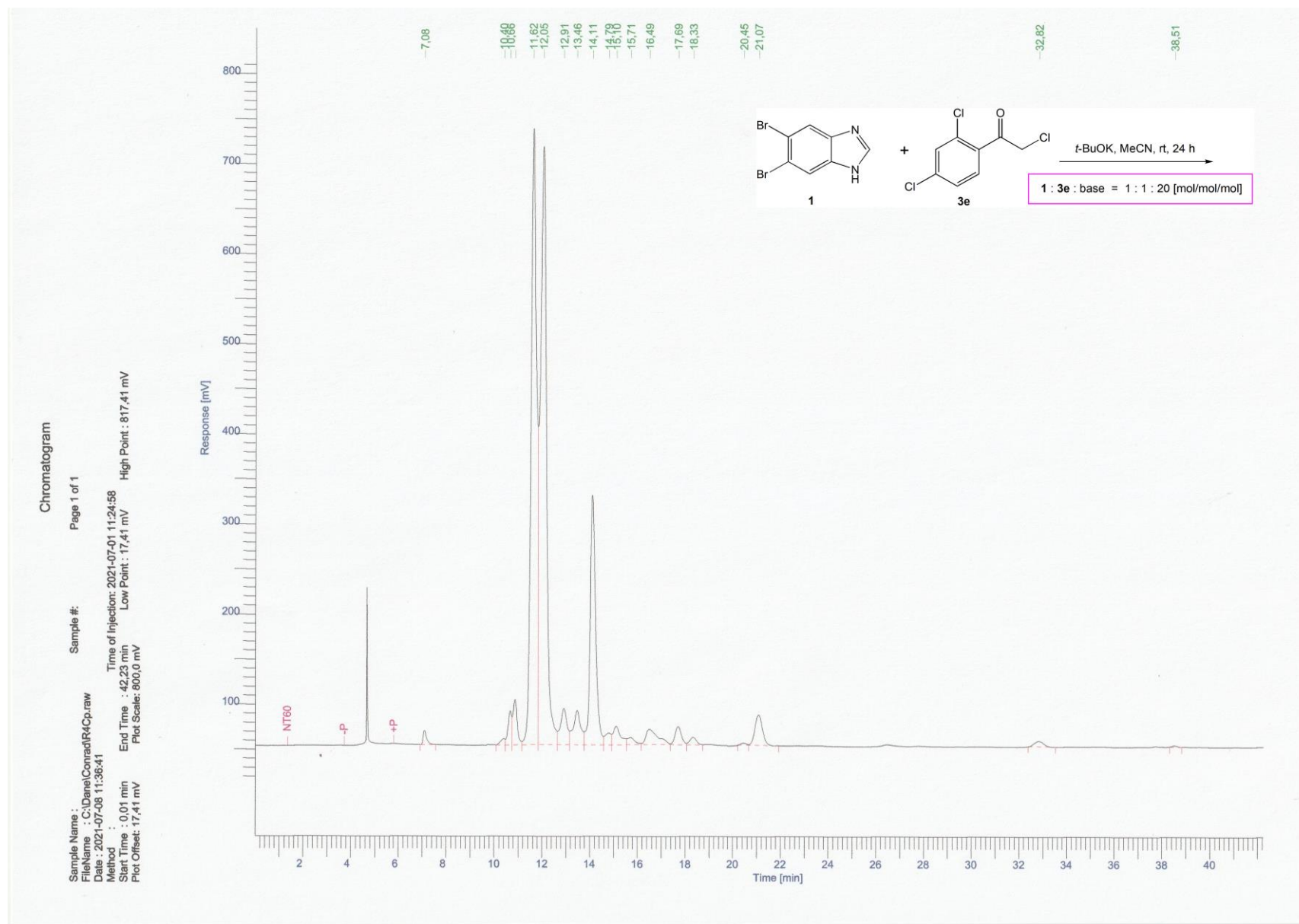


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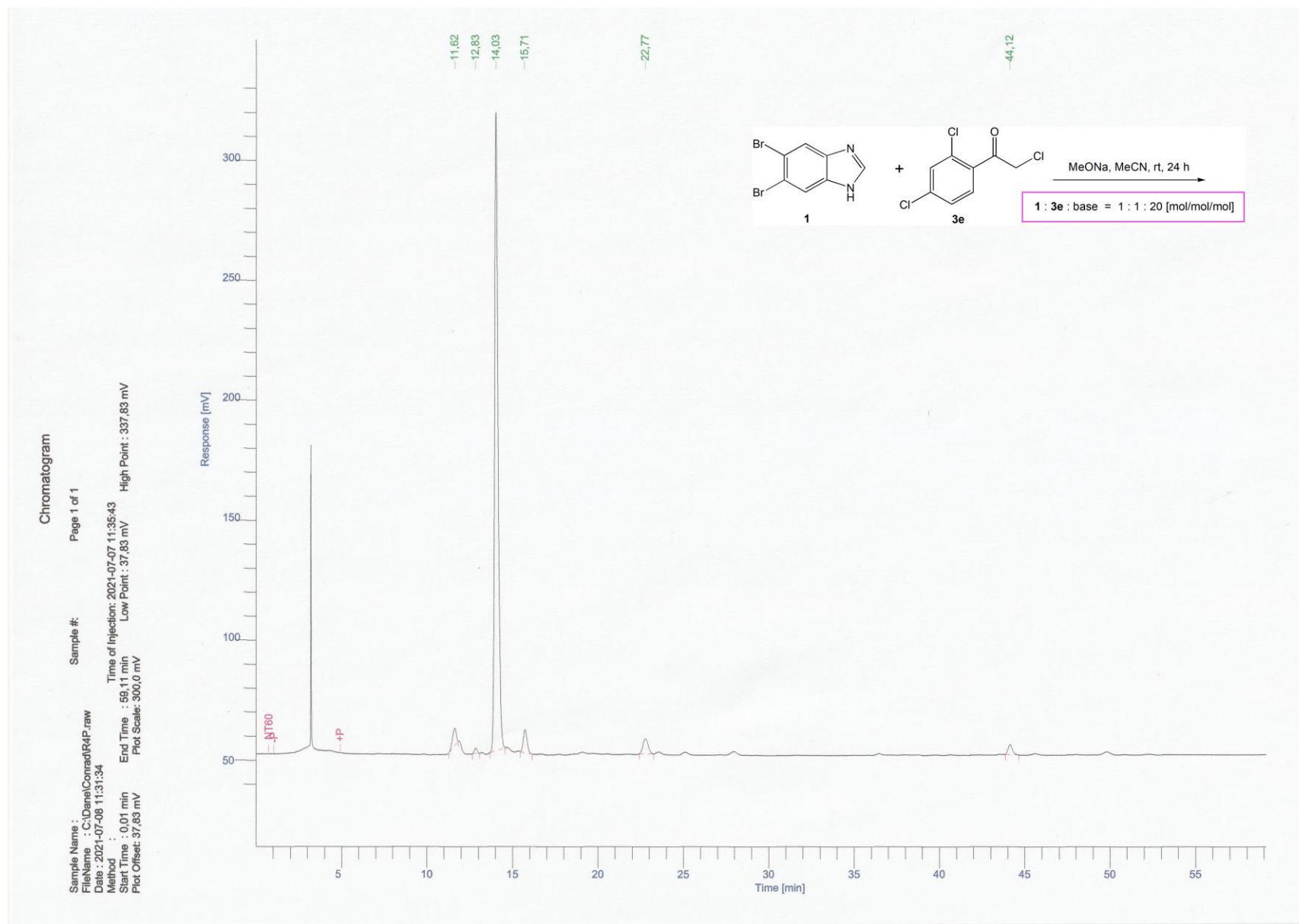


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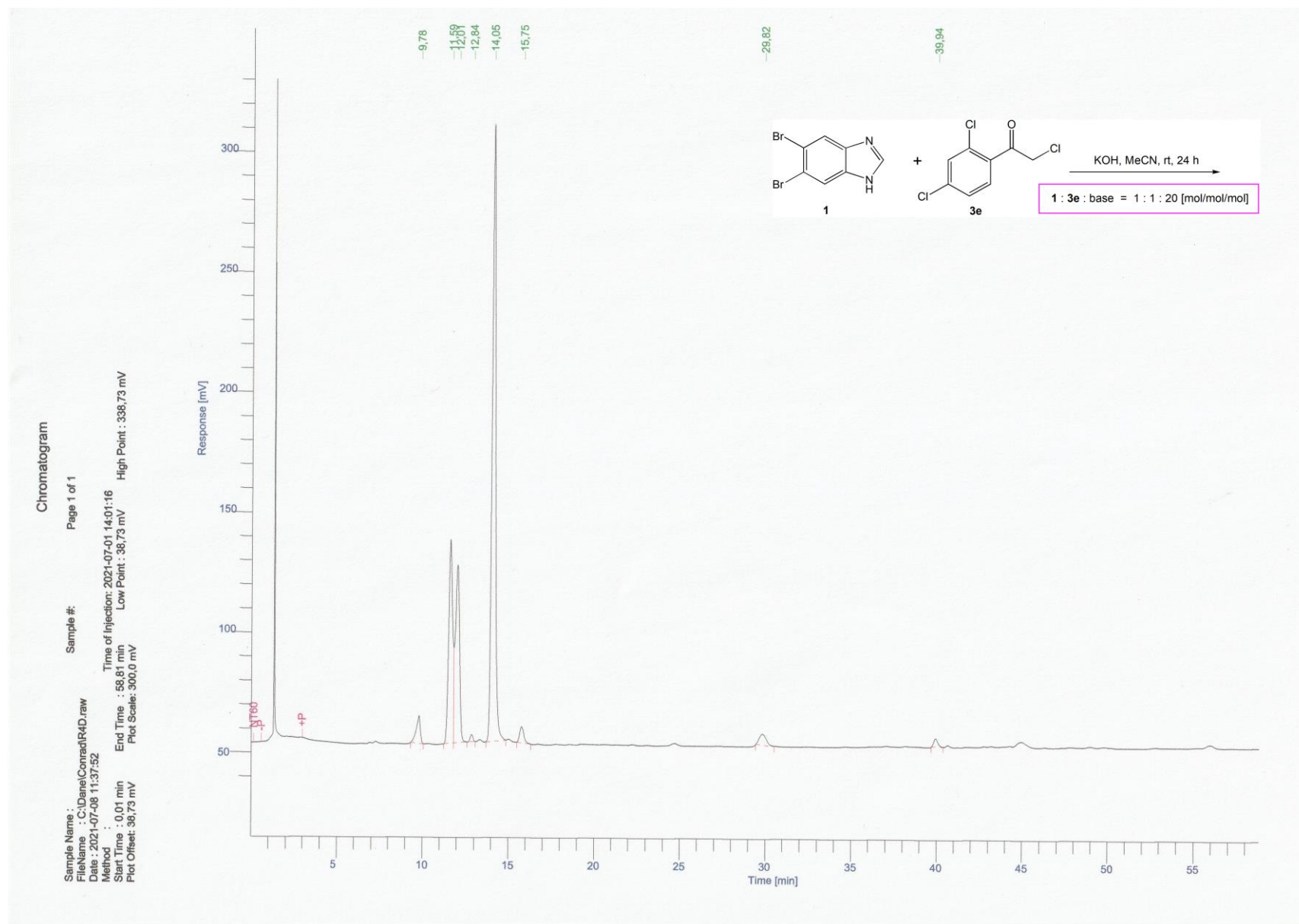


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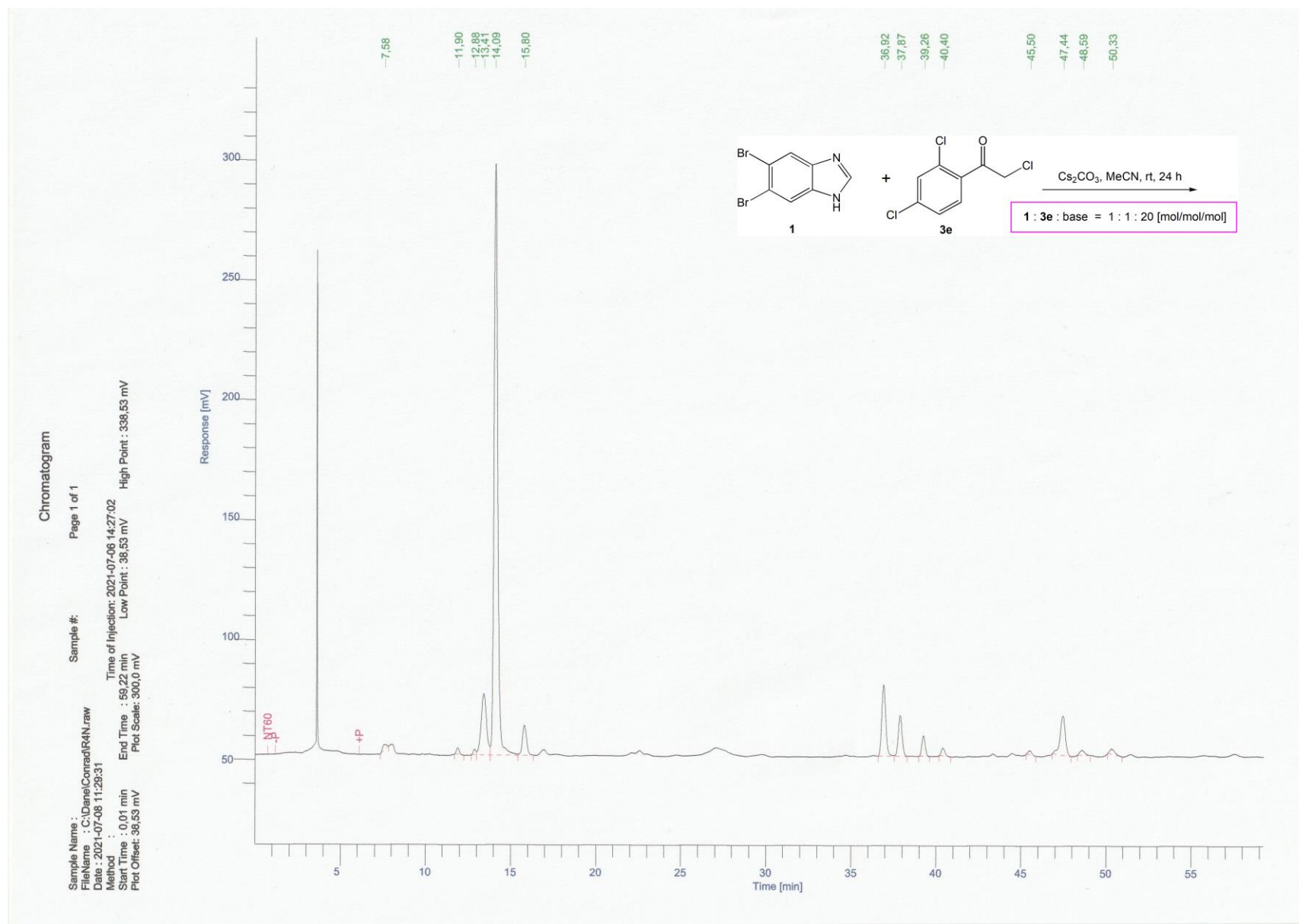


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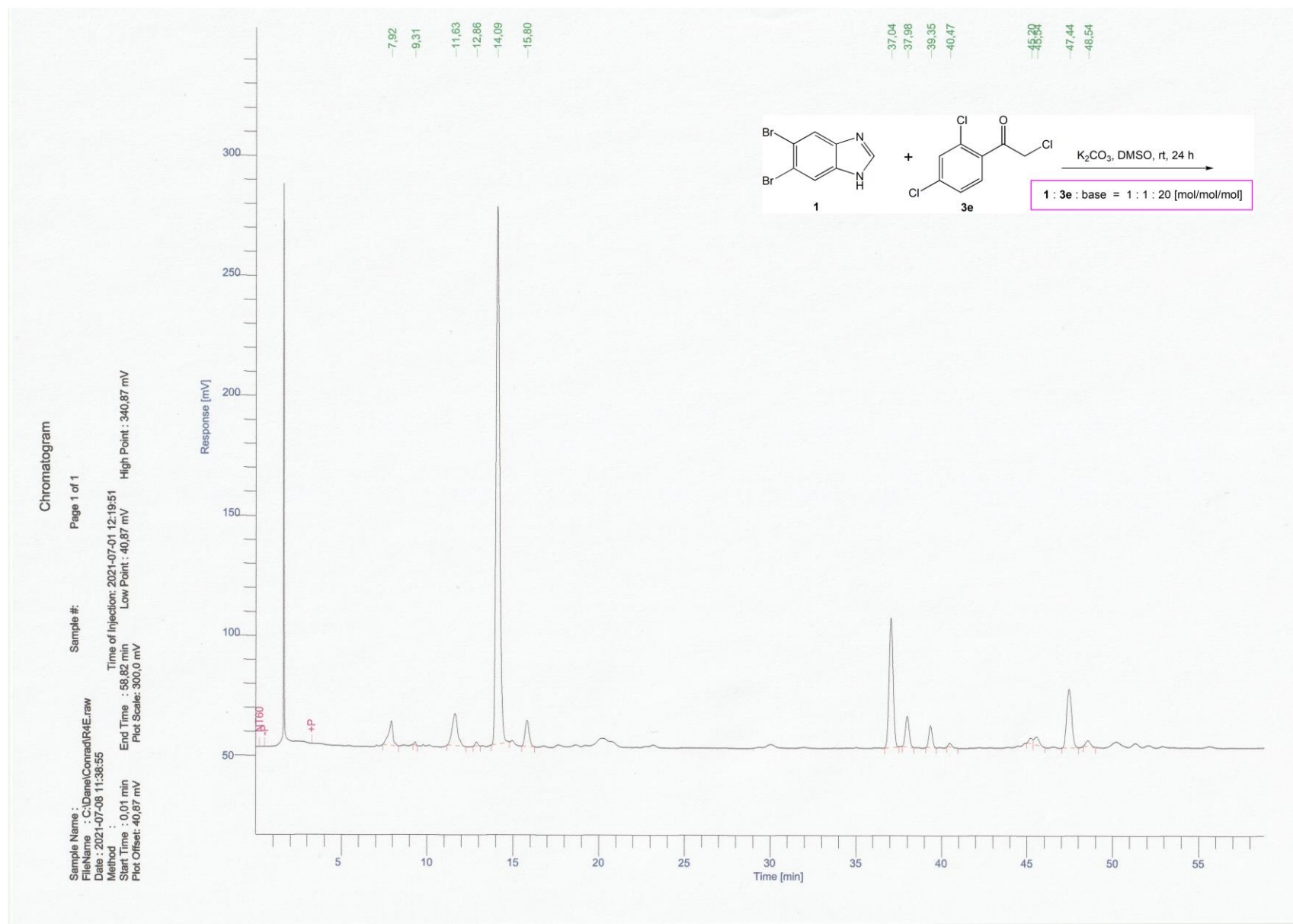


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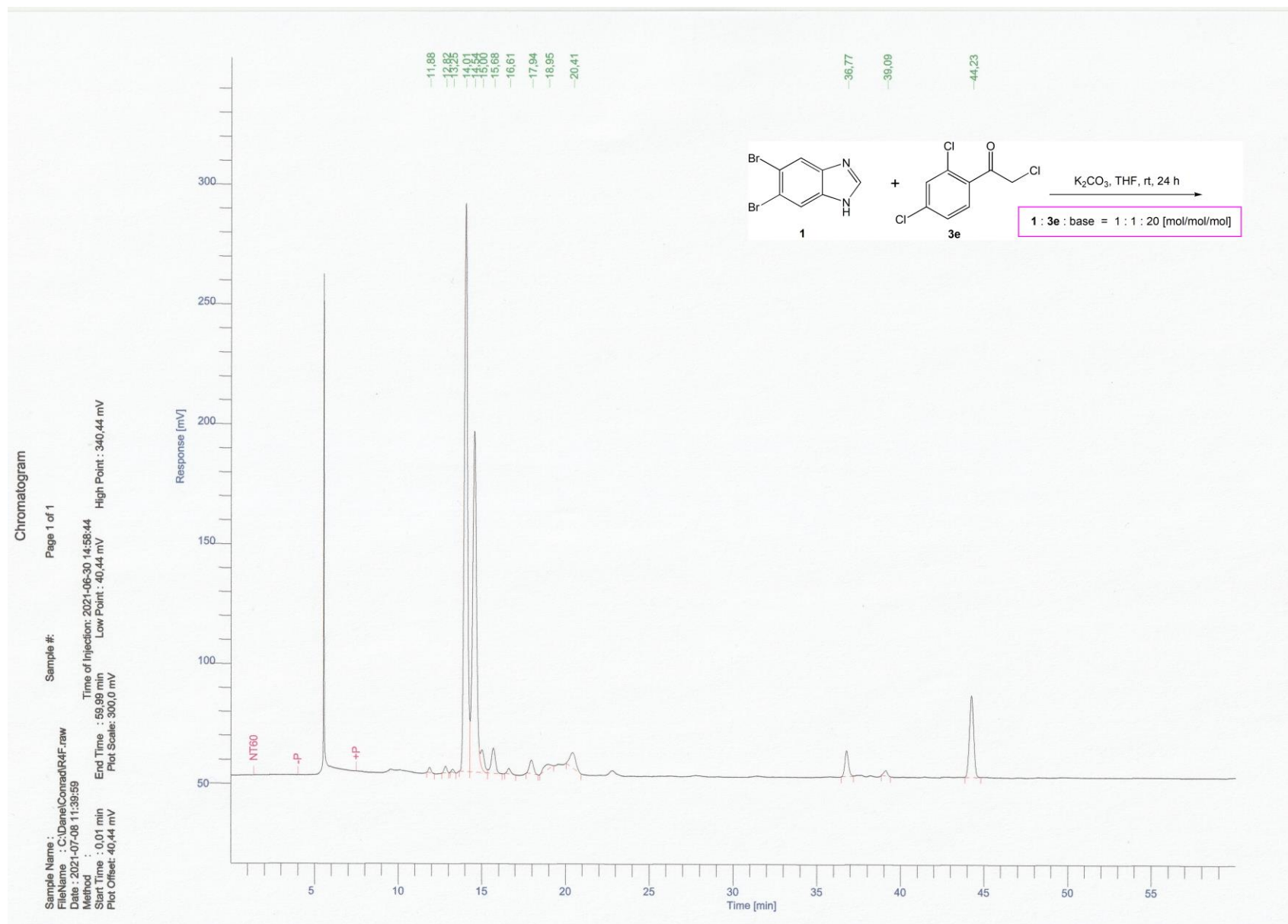


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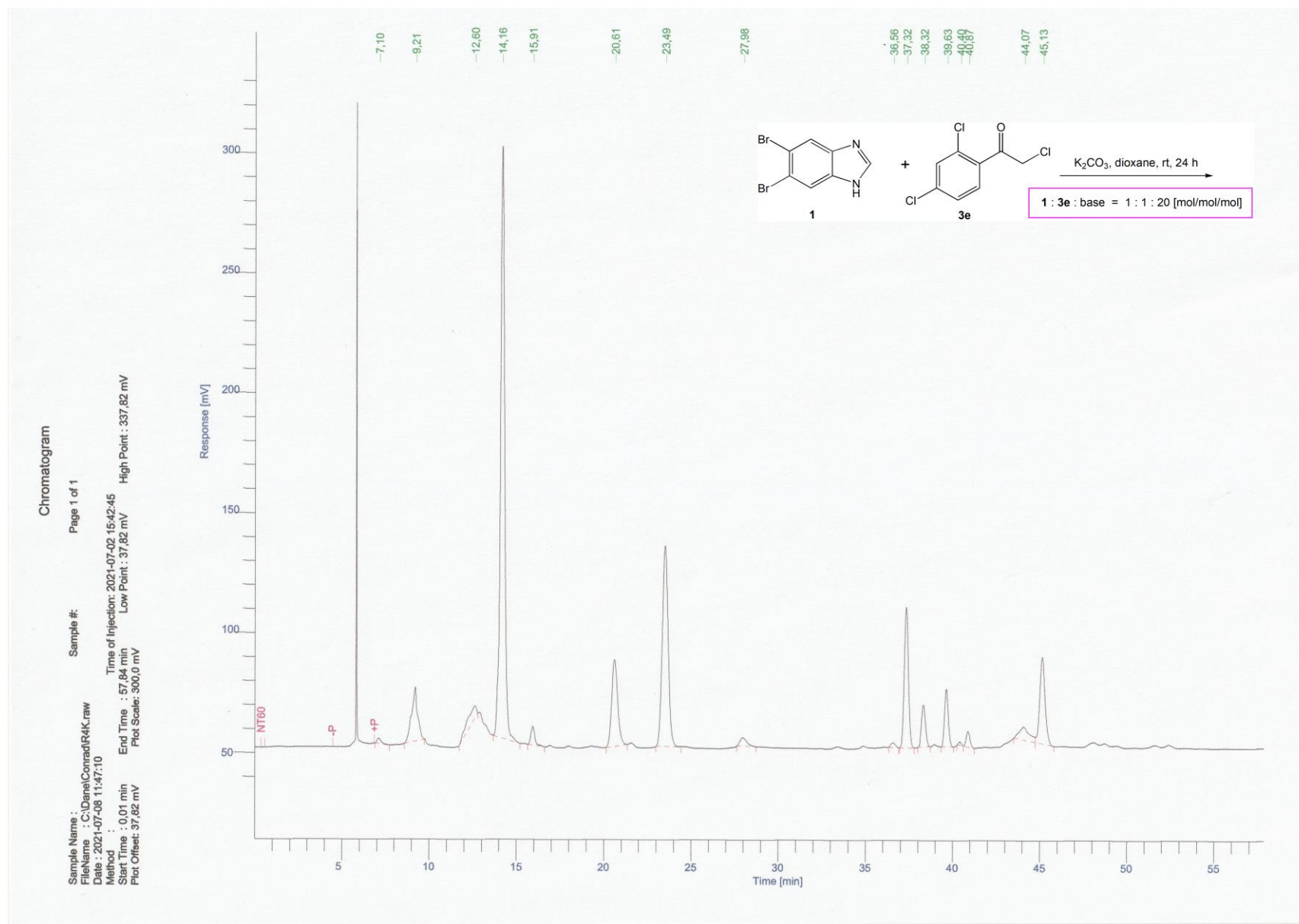


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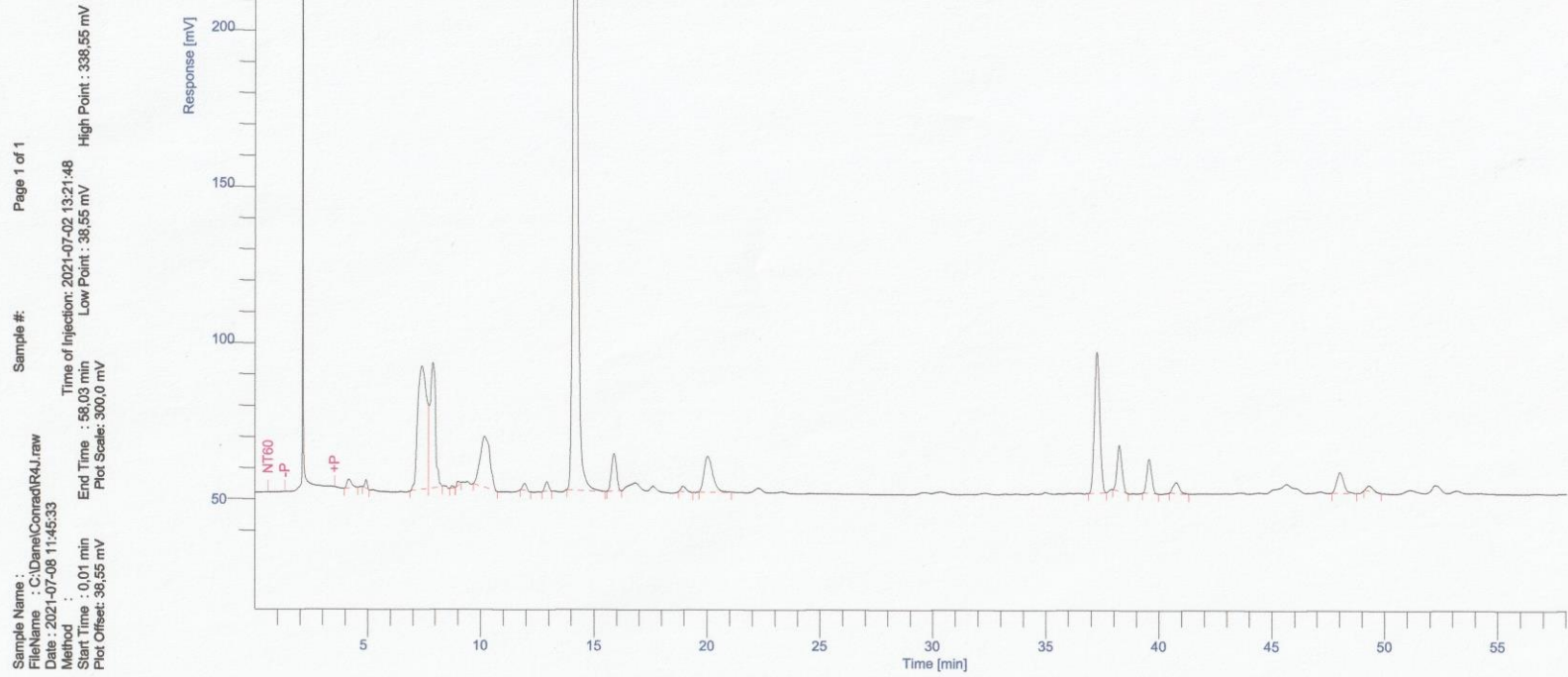


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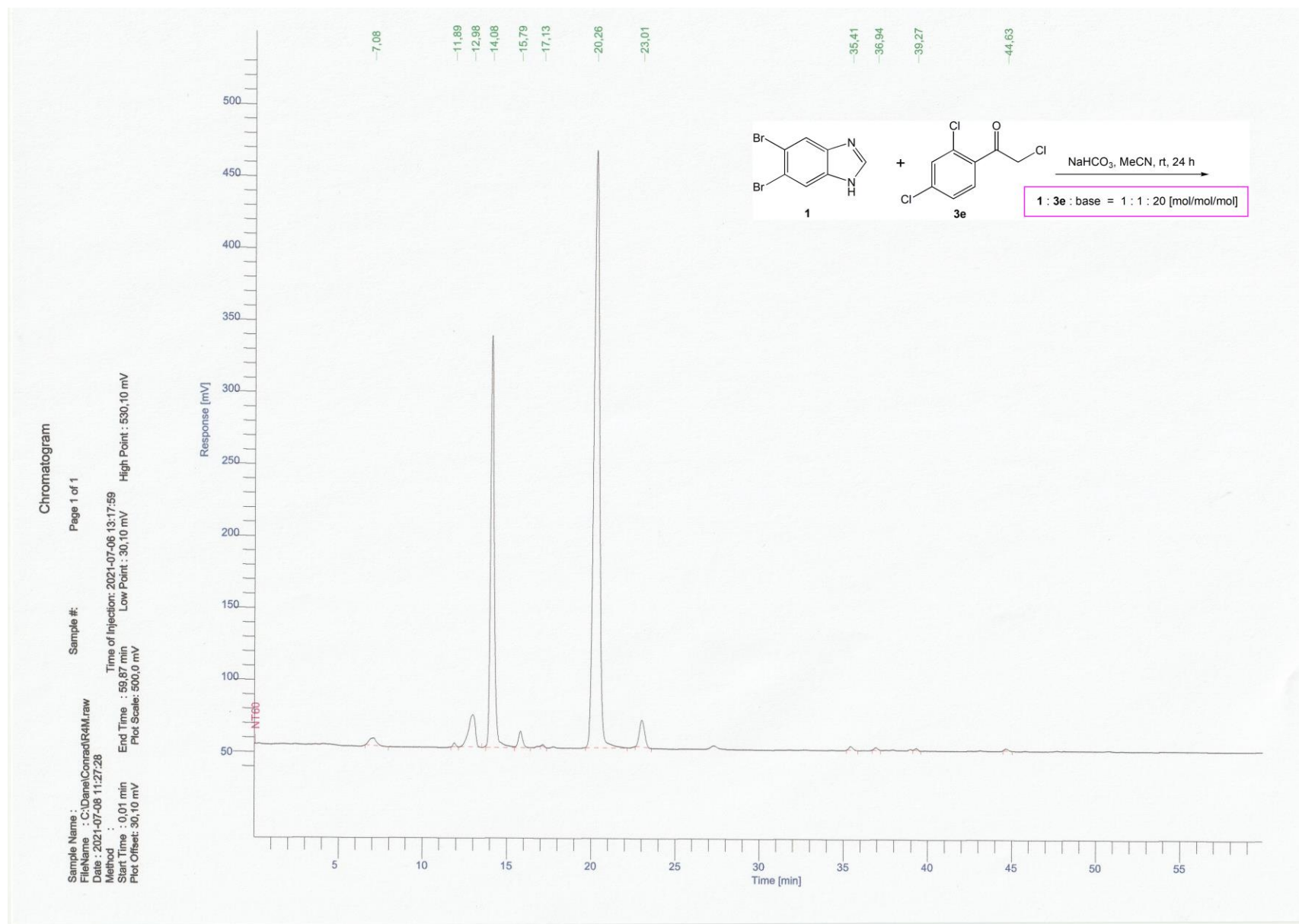


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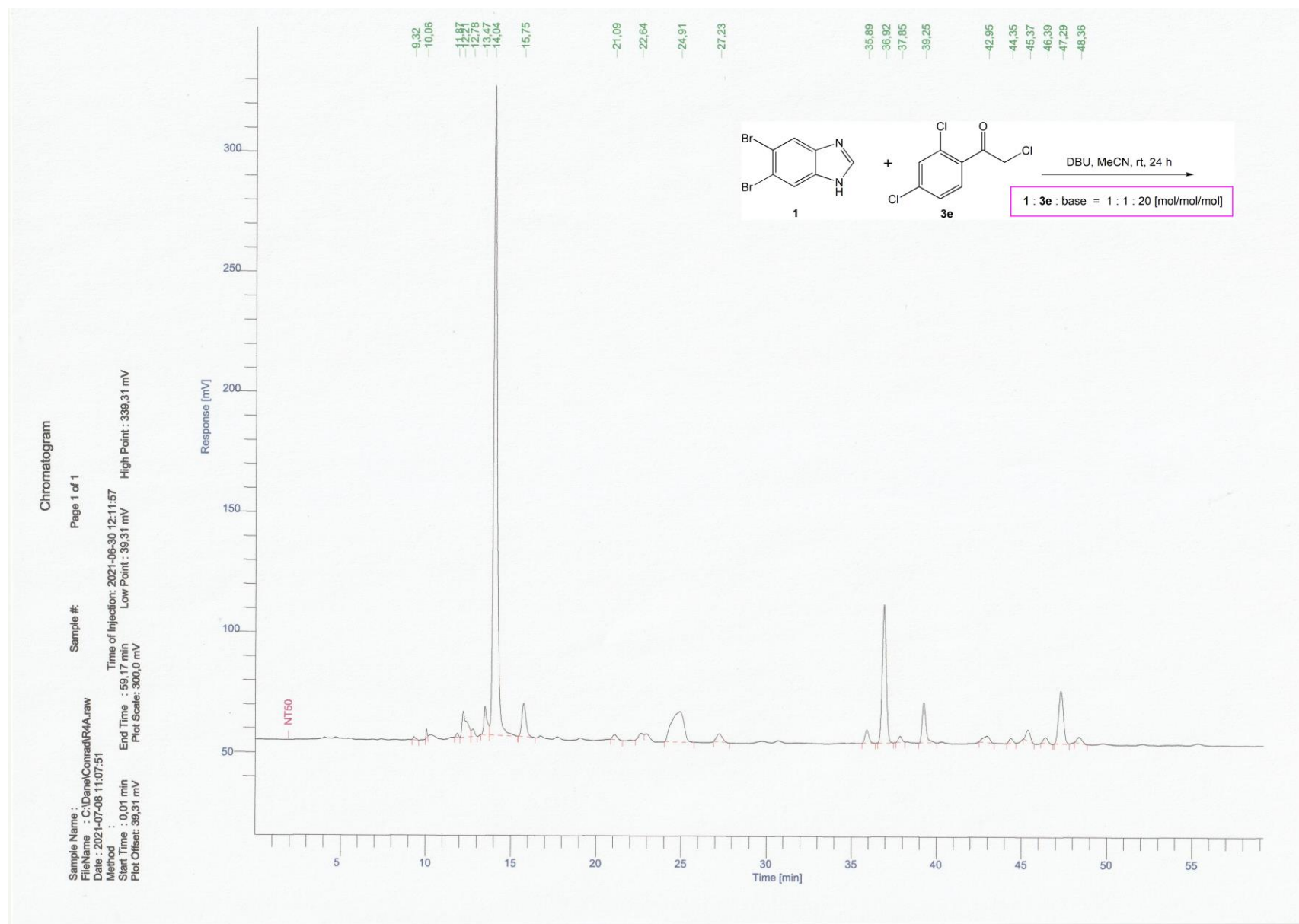


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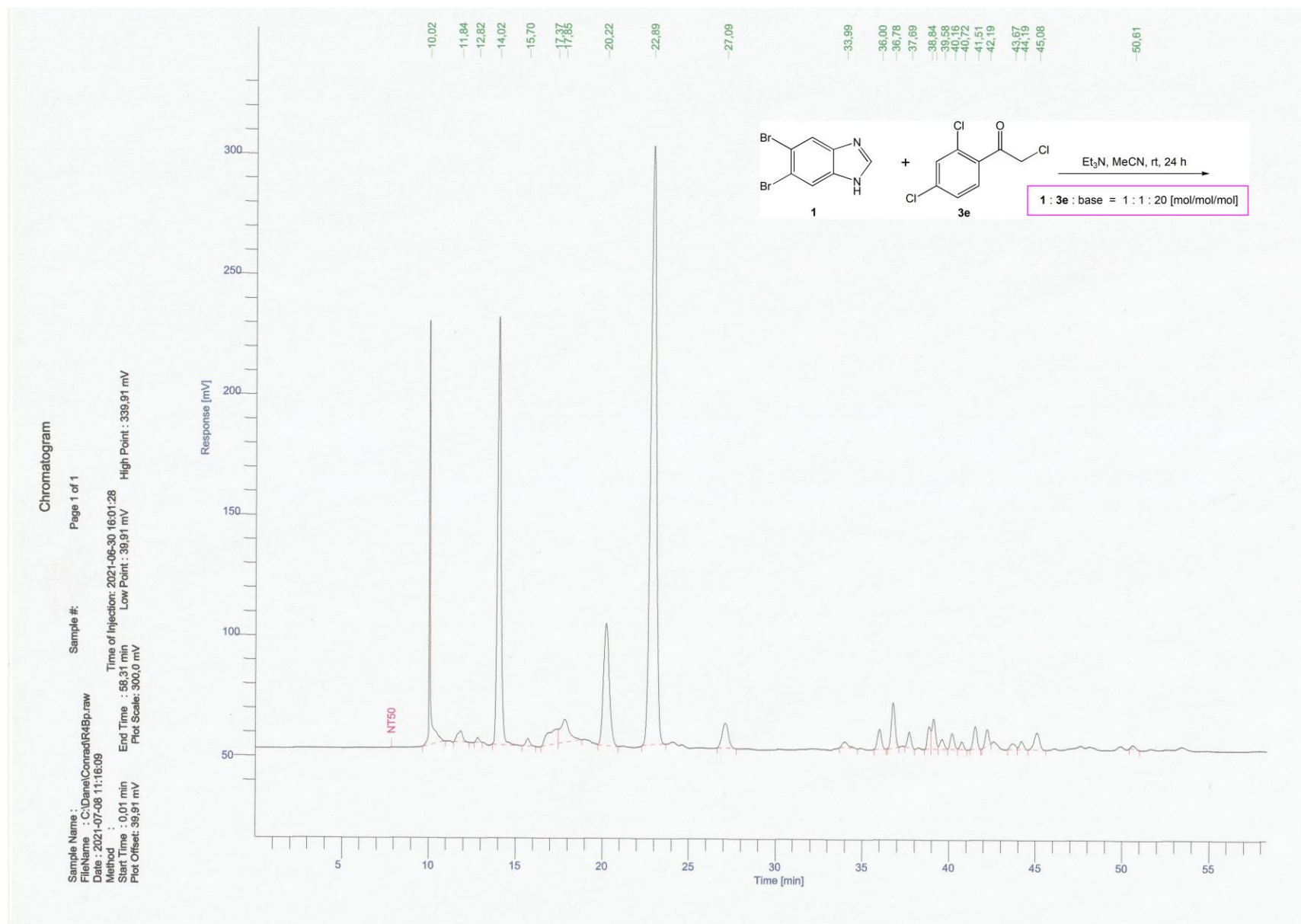


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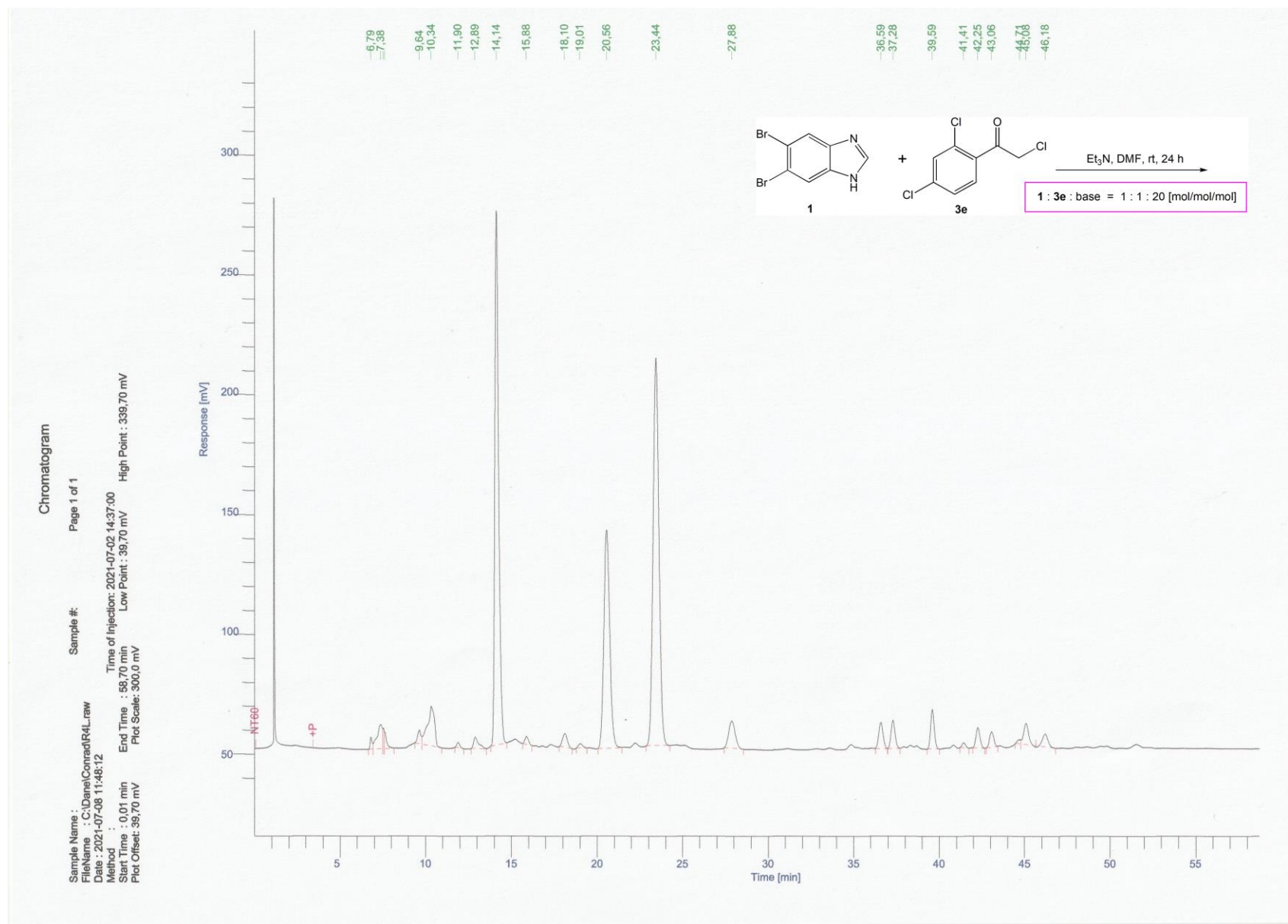


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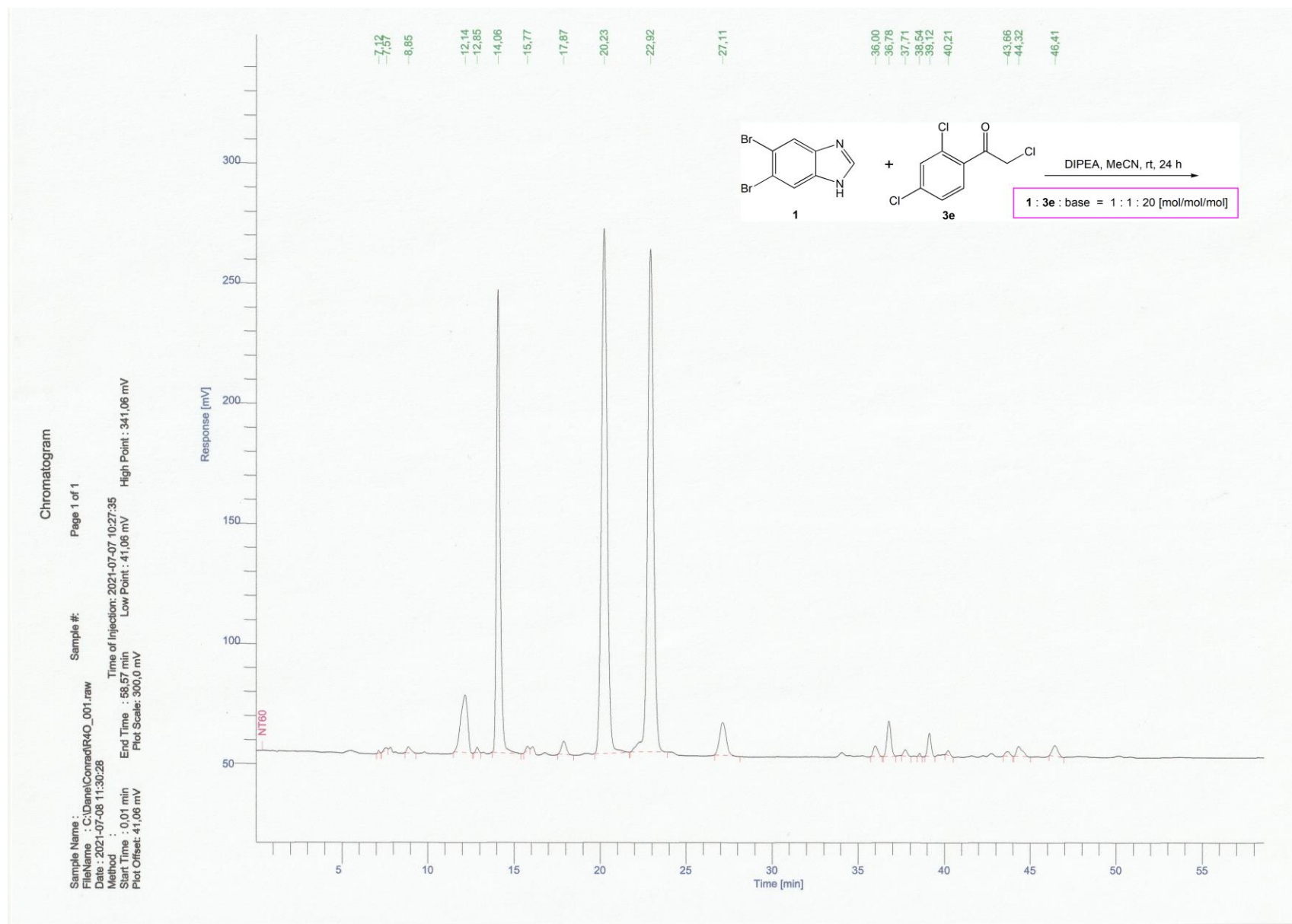


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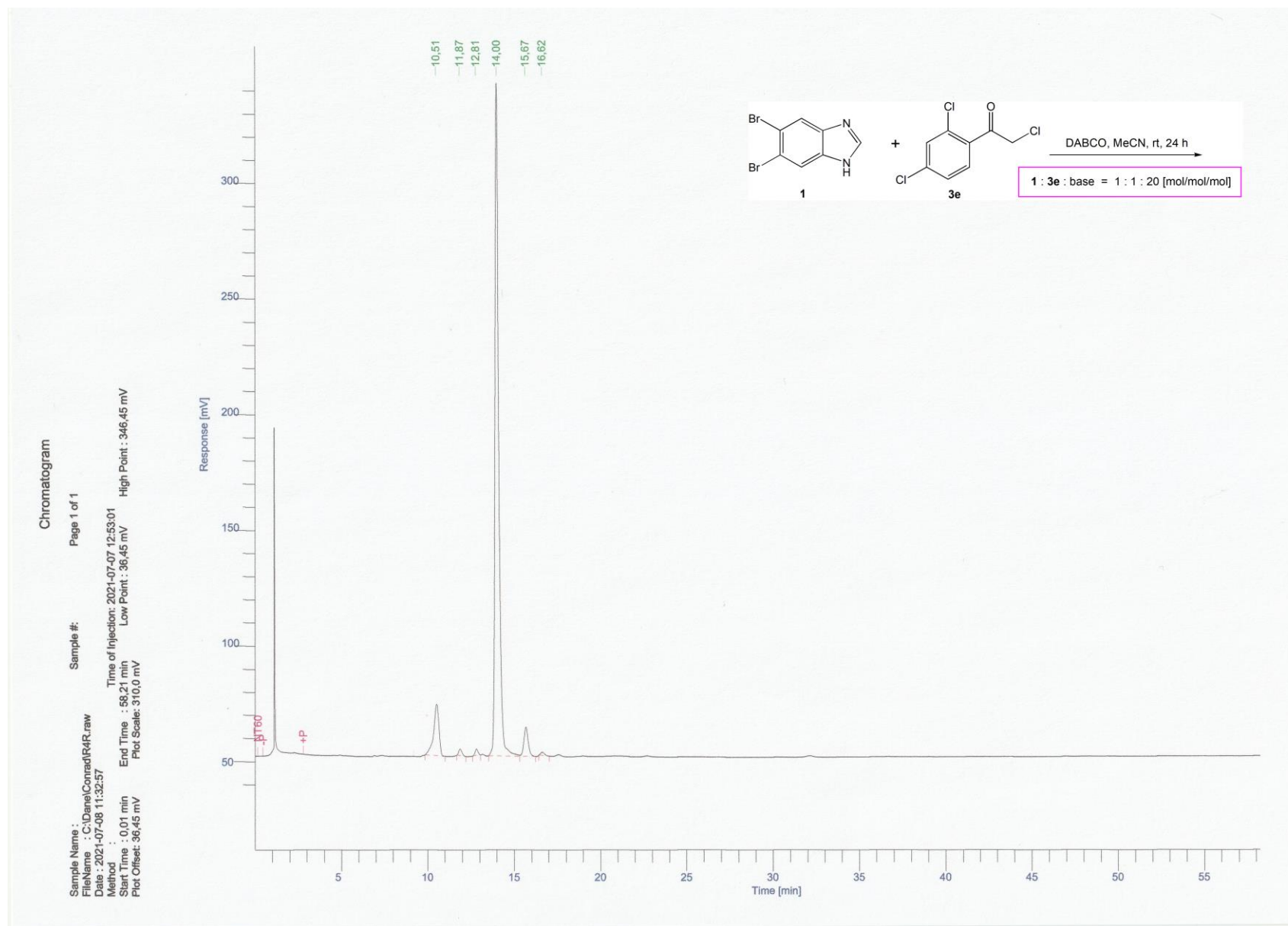


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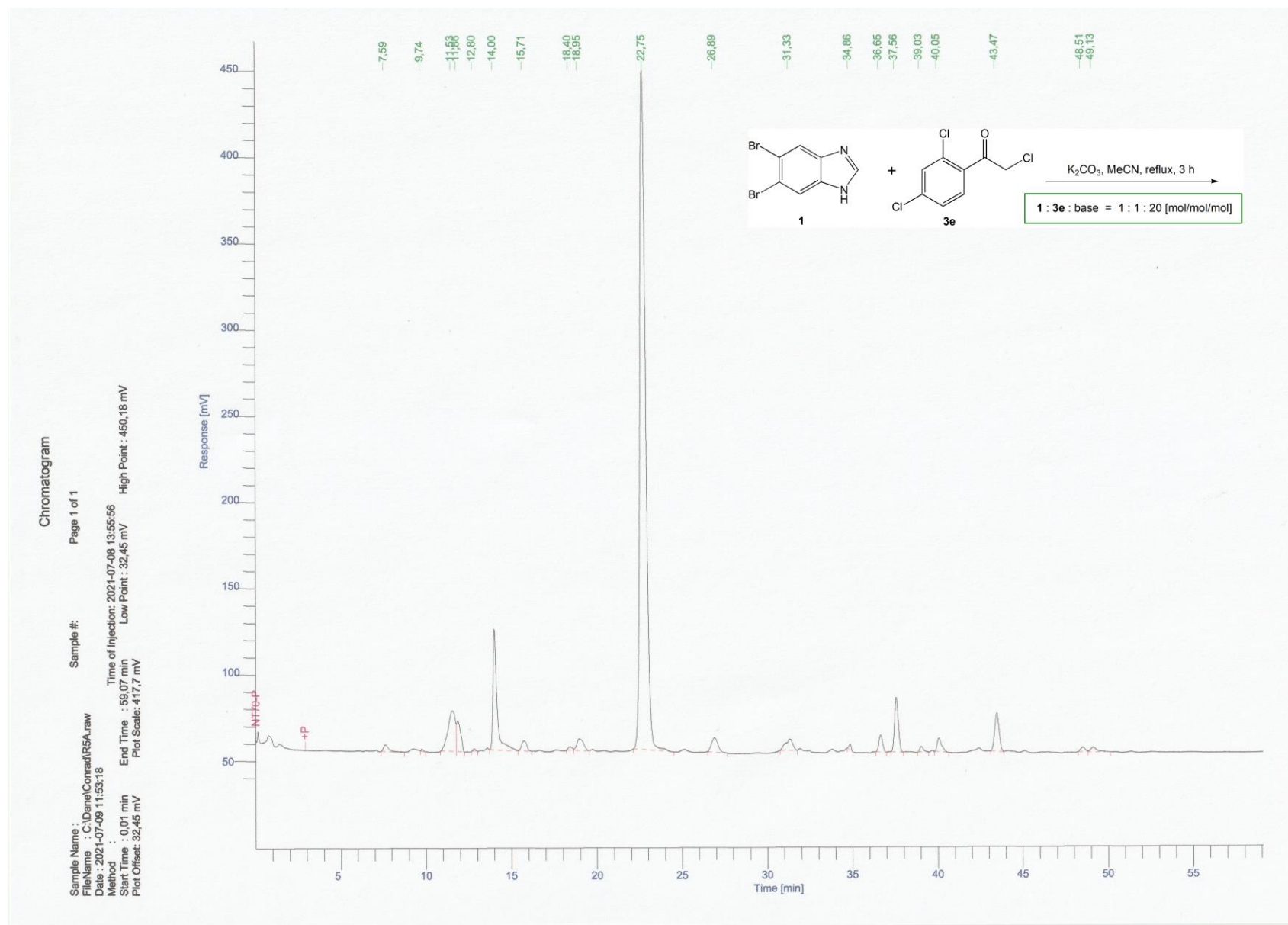


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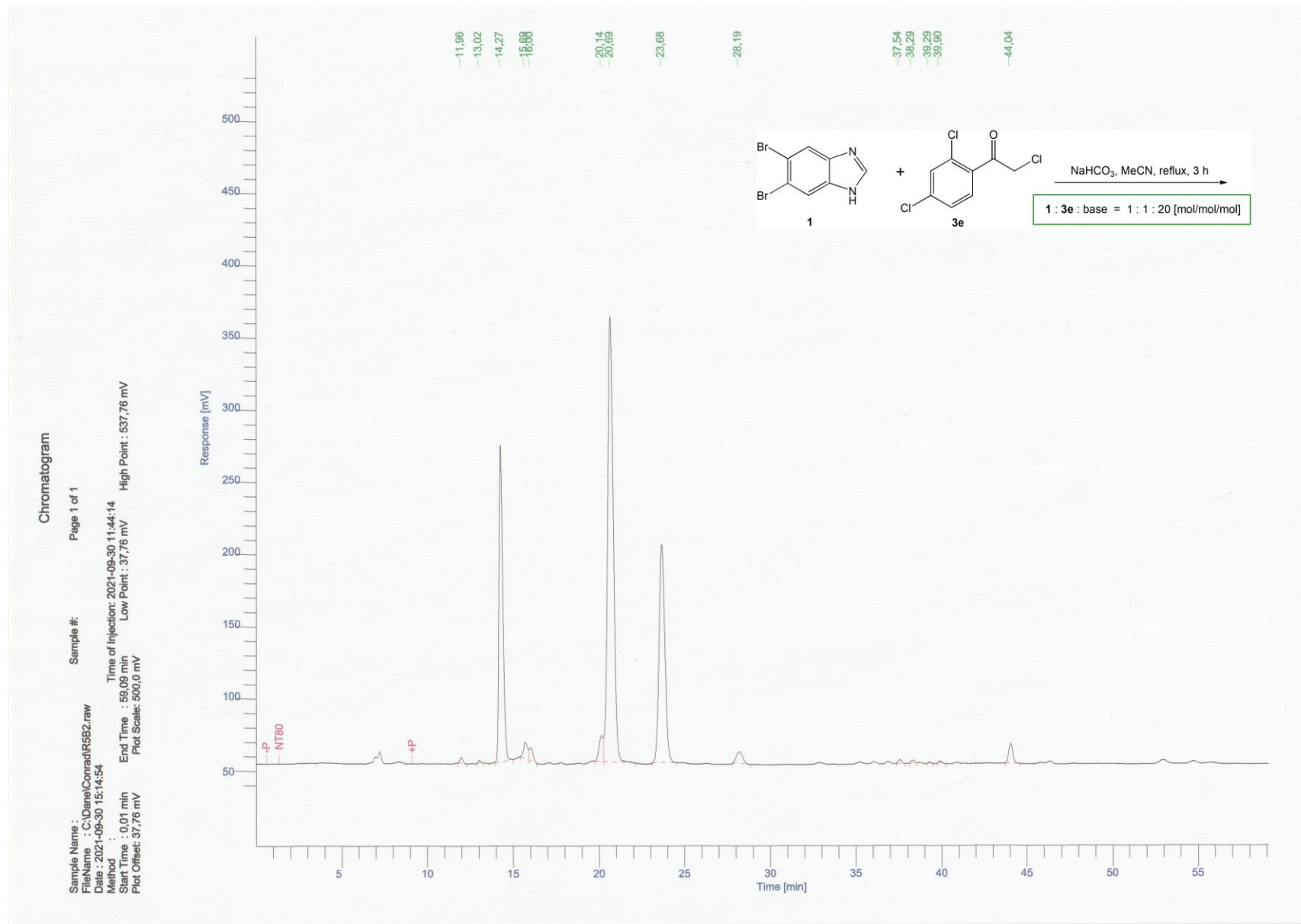


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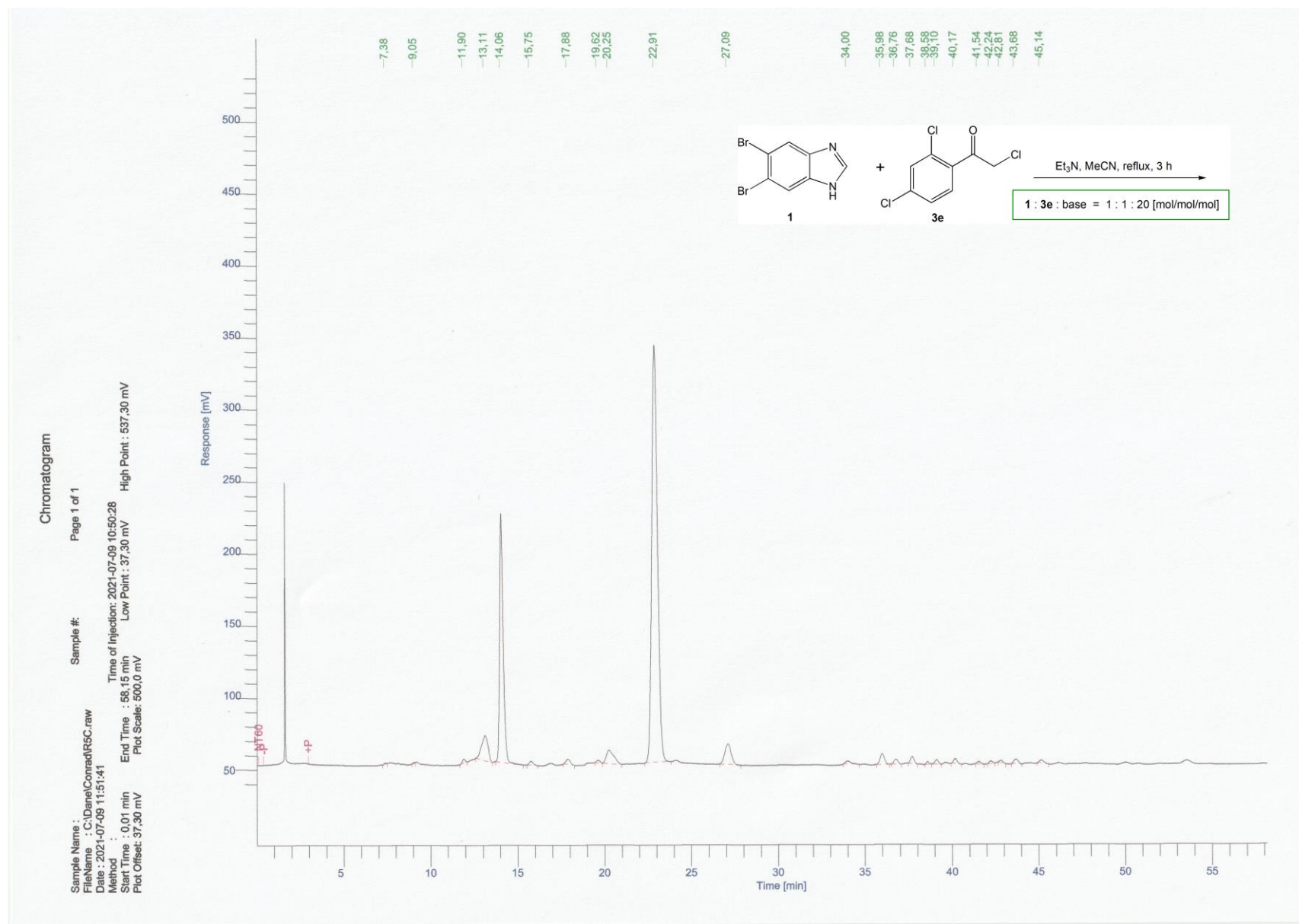


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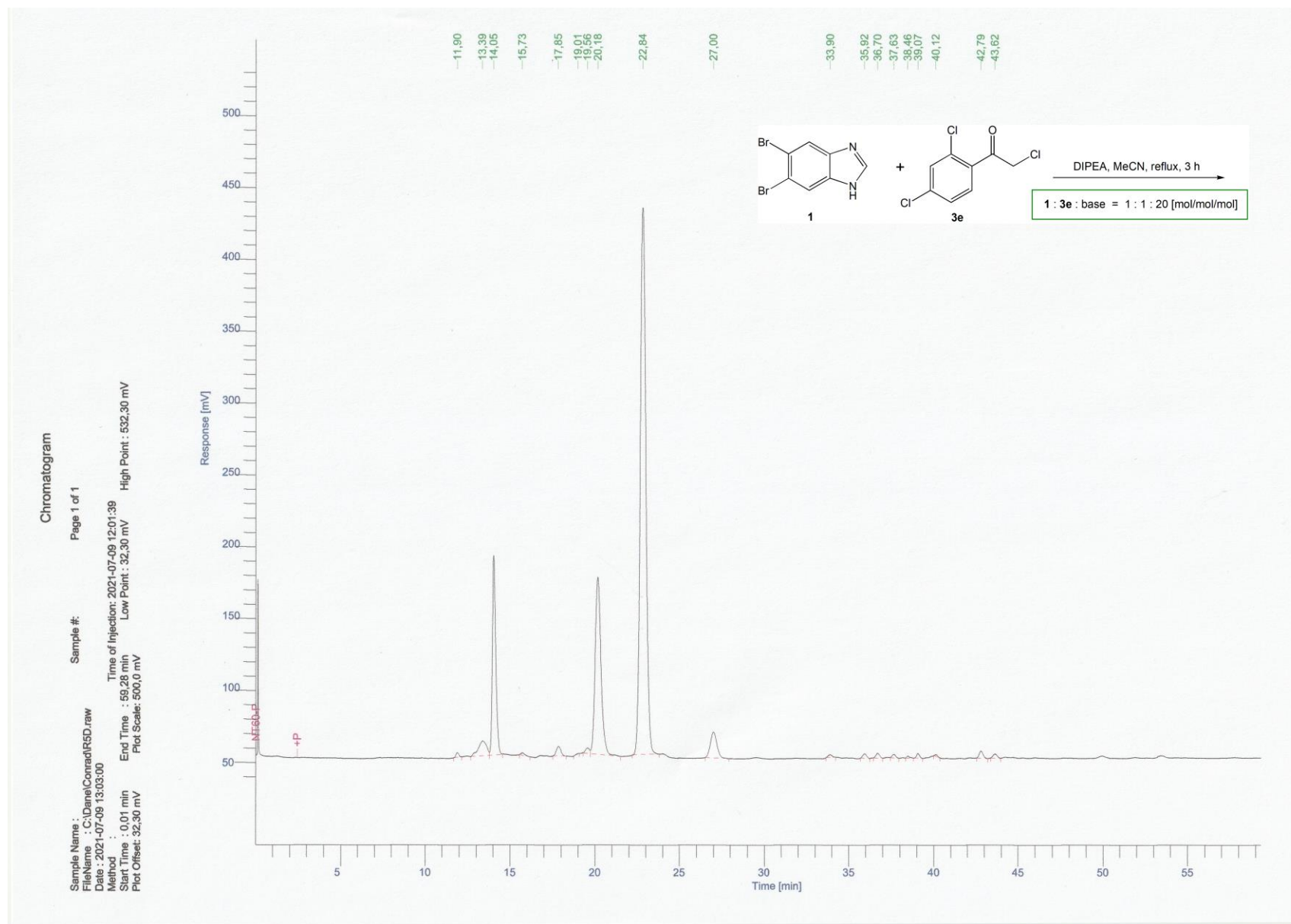


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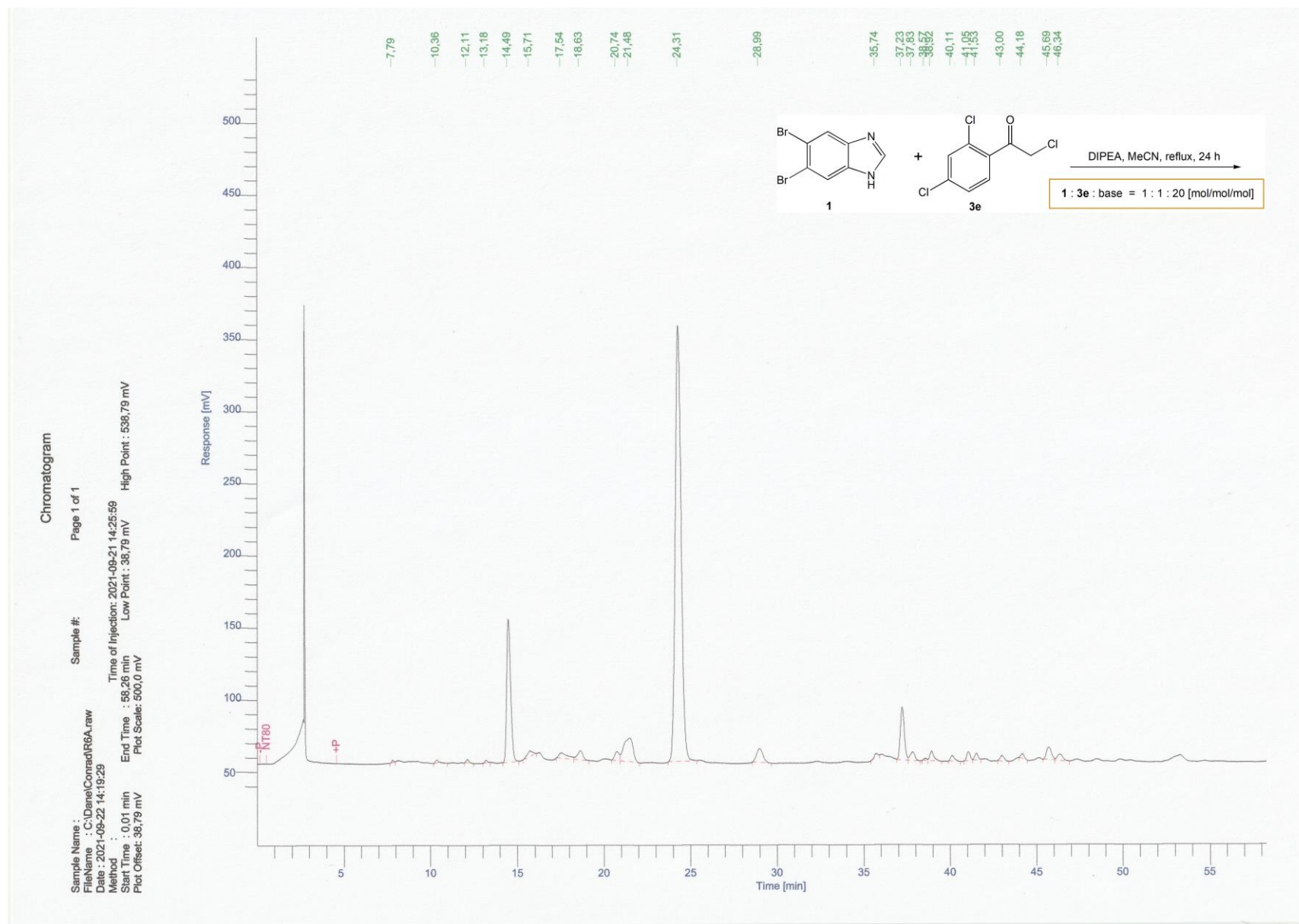


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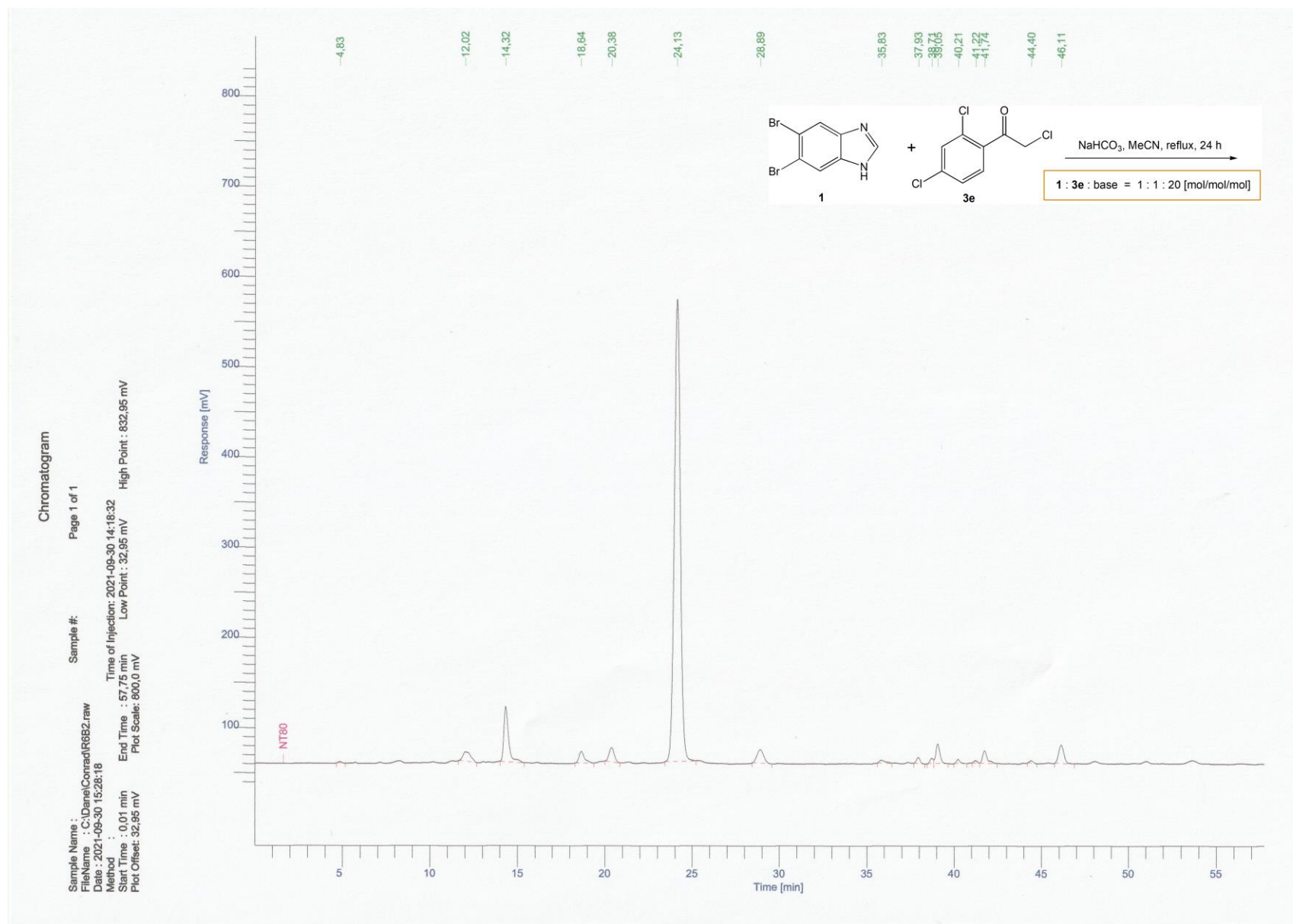


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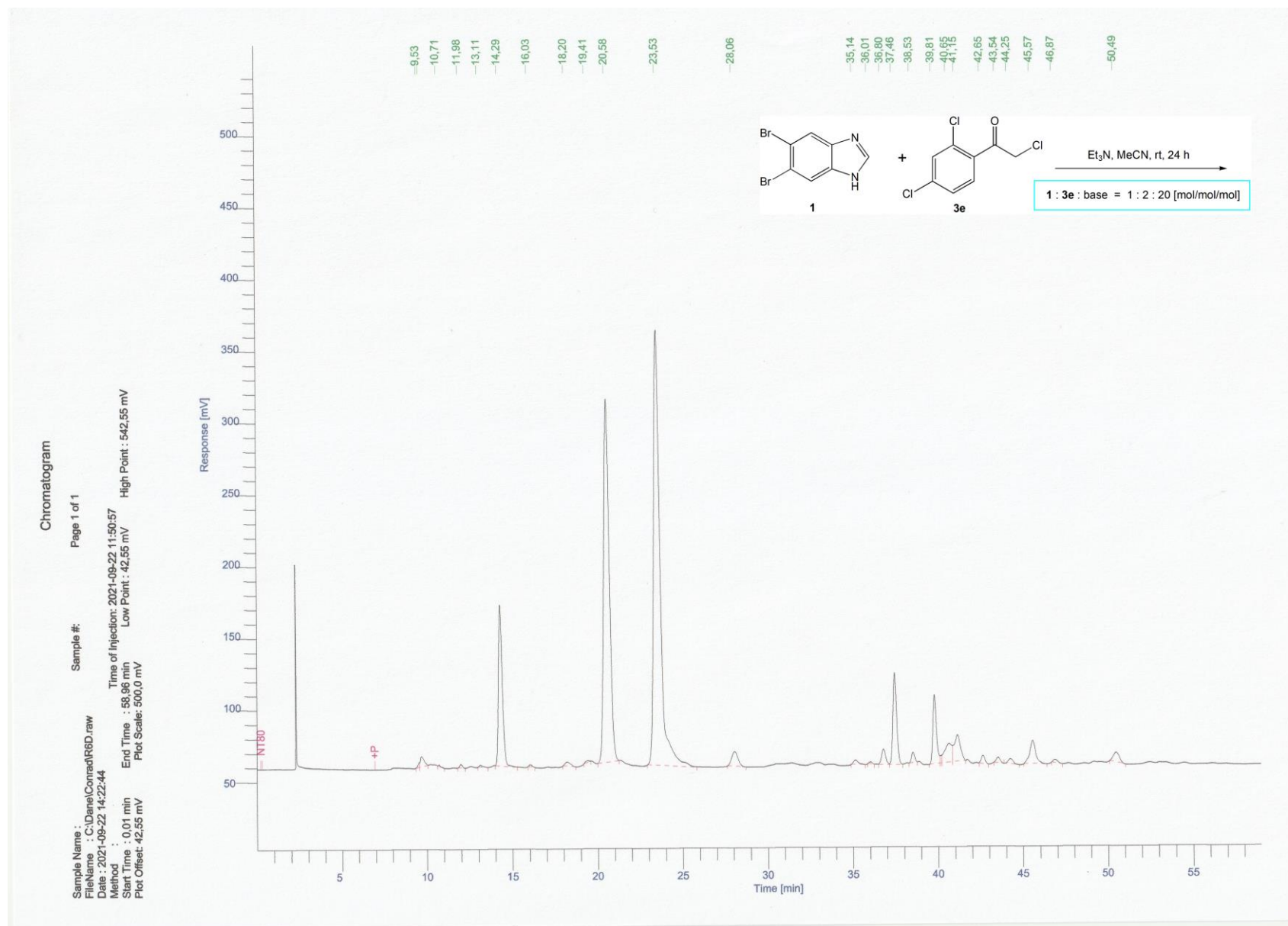


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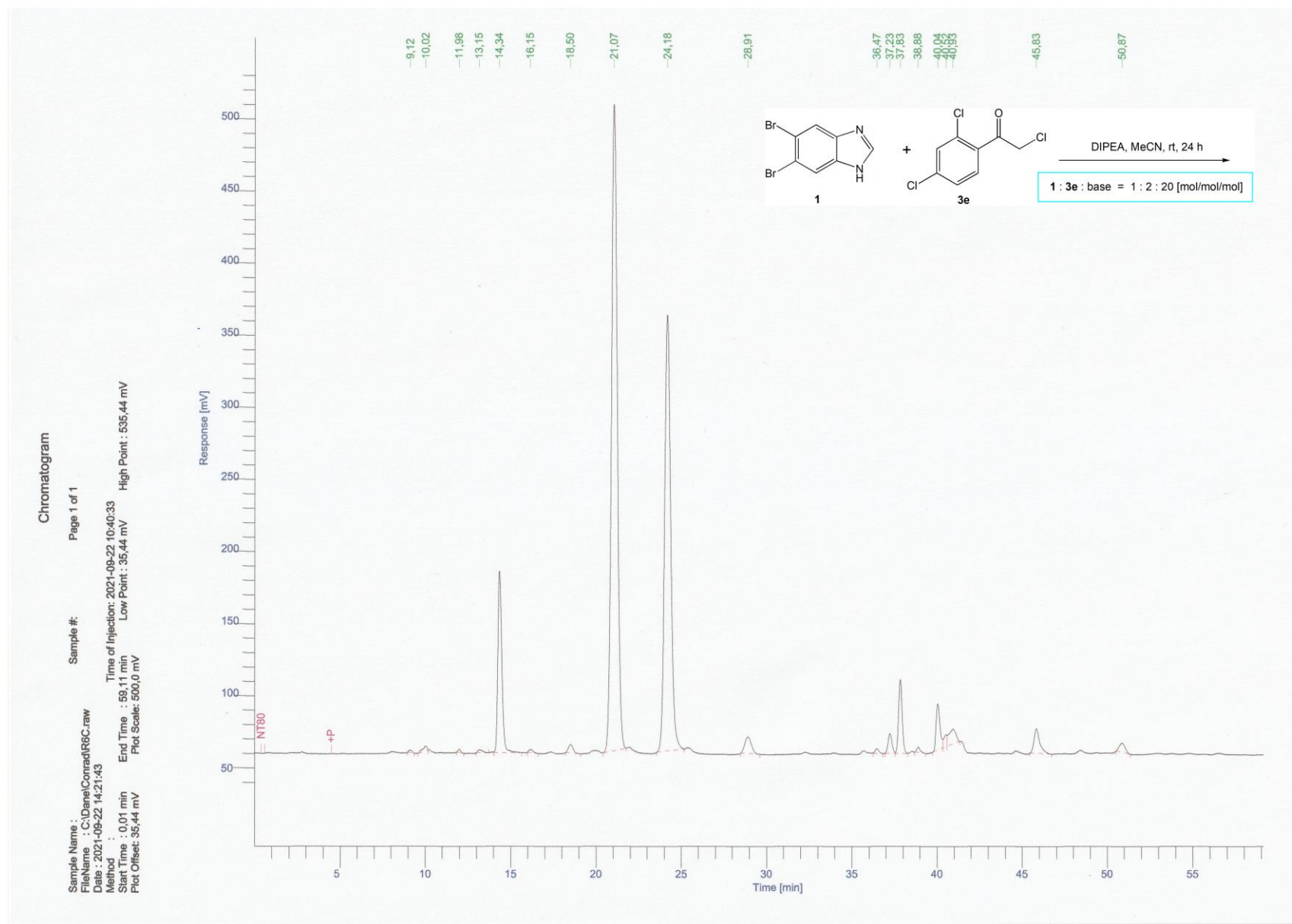


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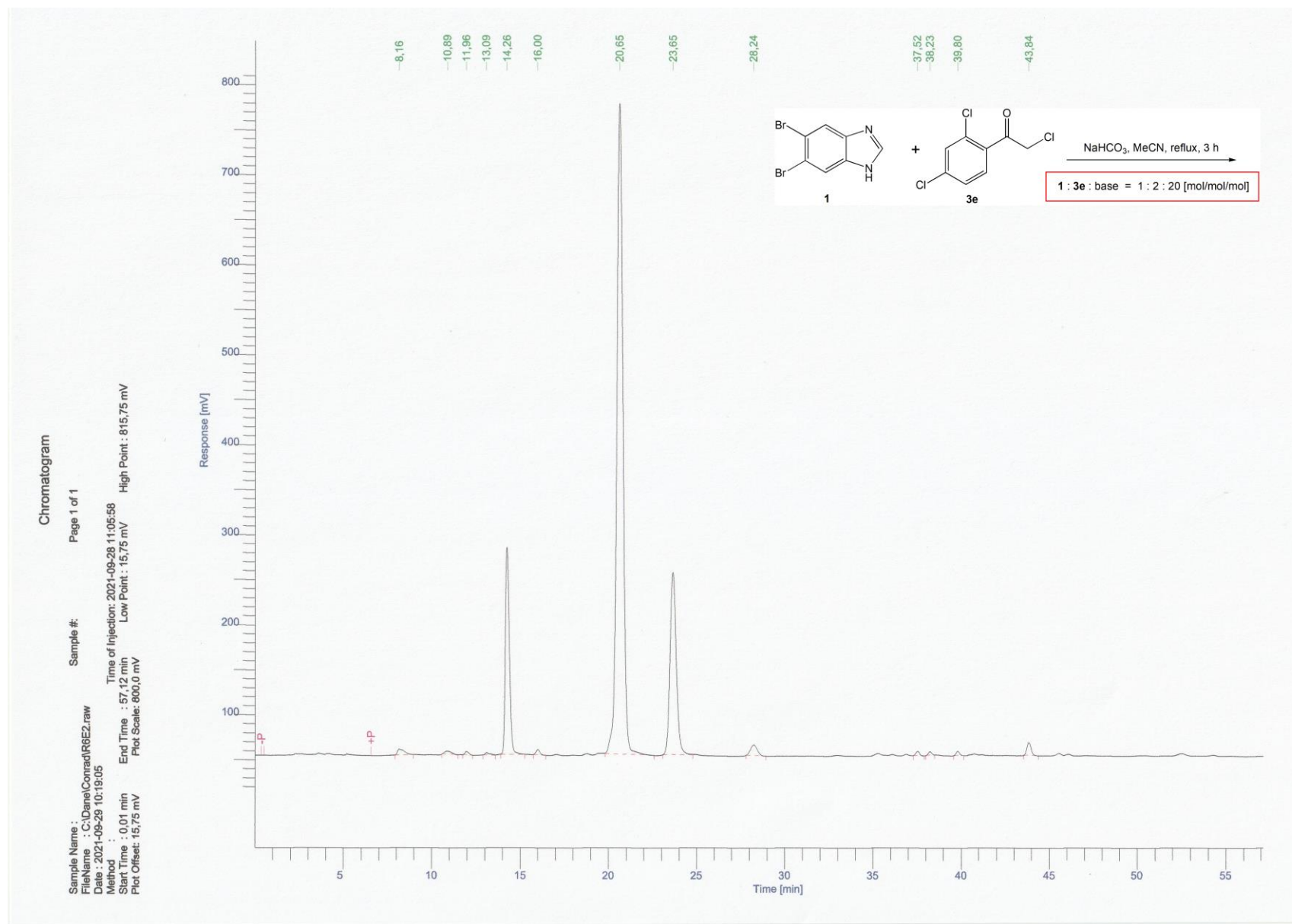


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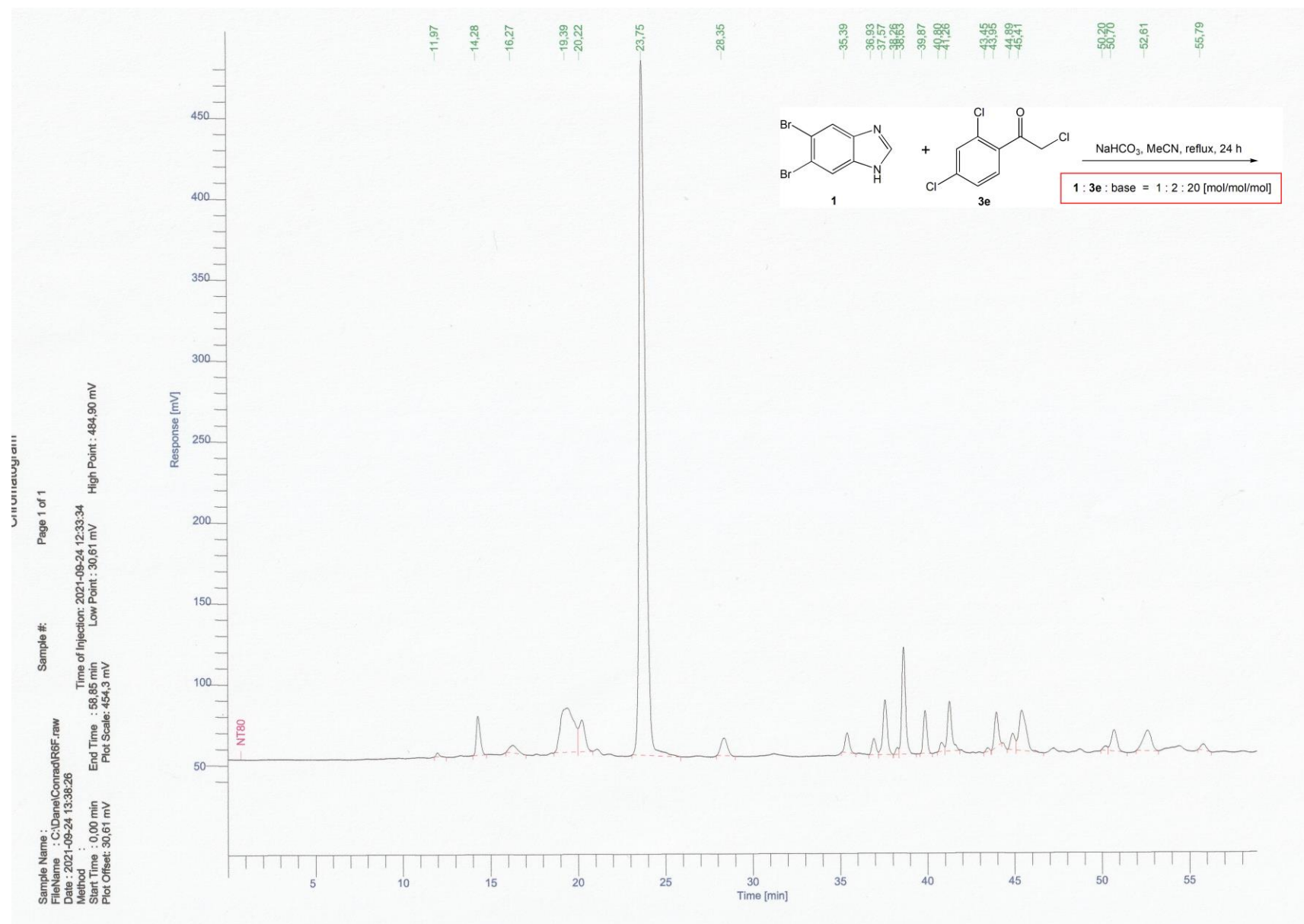


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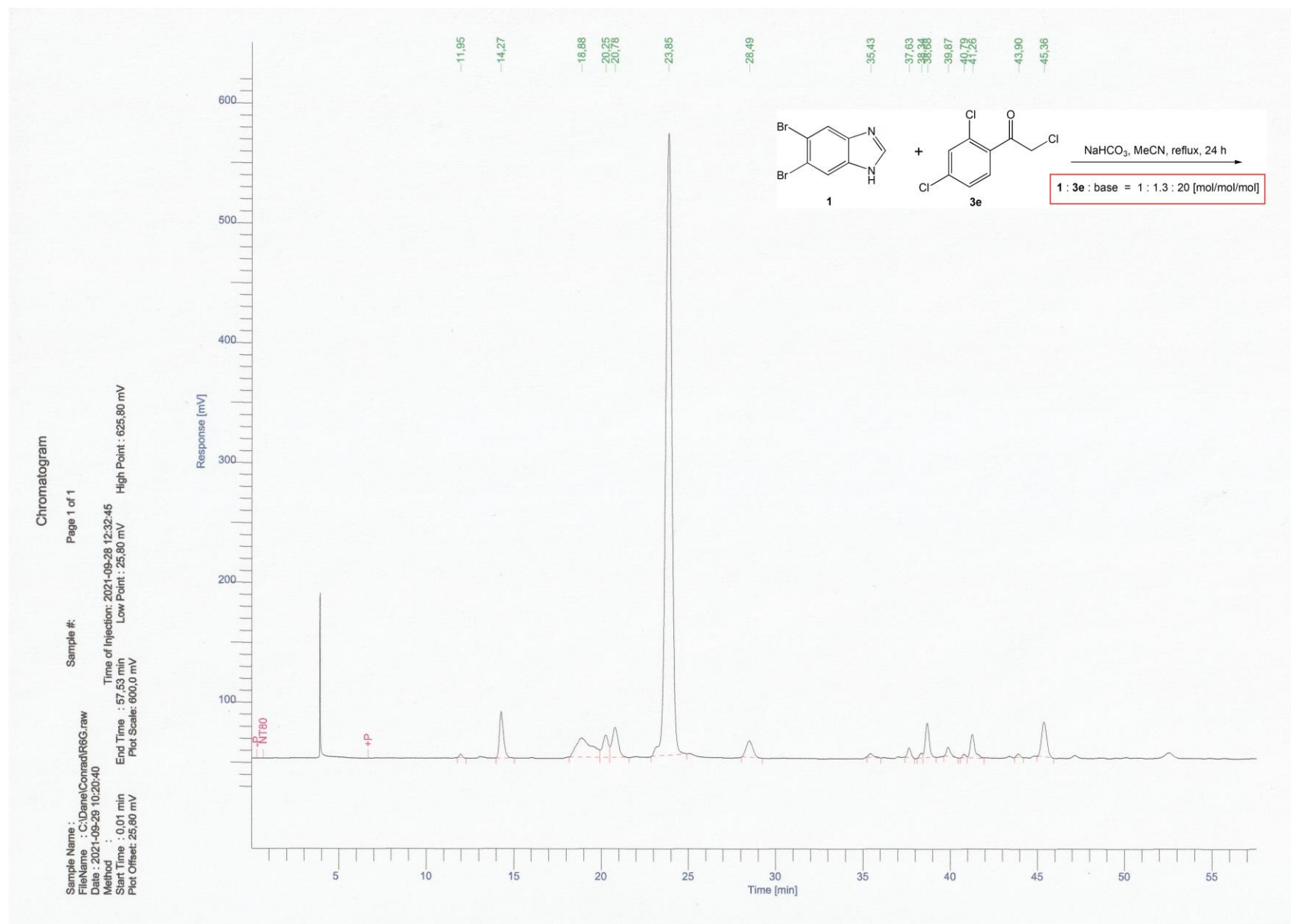


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