Supplementary Material (ESI) for Chemical Communications

Conformational Control the Regioselective Synthesis of N-2-Substituted-1,2,3-Triazoles

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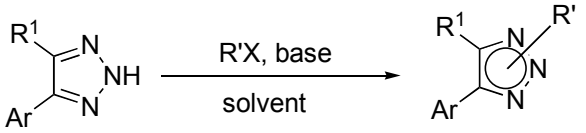
I. General Methods and Materials: Unless otherwise noted, all commercial reagents and solvents were obtained from the commercial provider and used without further purification. Air and/or moisture-sensitive reactions were carried out under an atmosphere of nitrogen using oven/flame-dried glassware and standard syringe/septa techniques. ^{1}H-NMR and ^{13}C-NMR spectra were recorded on Joel 270 MHz spectrometers. Chemical shifts were reported relative to internal tetramethysilane (δ 0.00 ppm) or $CDCl_3$ (δ 7.26 ppm) or CD_3OD (δ 3.31 ppm) for ^{1}H and $CDCl_3$ (δ 77.0 ppm) or CD_3OD (δ 49.1 ppm) for ^{13}C. Flash column chromatography was performed on 230-430 mesh silica gel. Analytical thin layer chromatography was performed with precoated glass baked plates (250μ) and visualized by fluorescence and by charring after treatment with potassium permanganate stain.

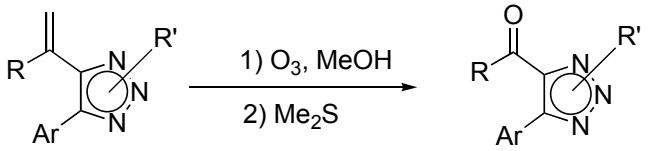
The NH-triazole starting materials were prepared according to literature procedure. (Sengupta, S.; Duan, H.; Lu, W.; Petersen, J. L.; Shi, X. *Org. Lett.* **2008**, *10*, 1493-1496.

General Procedure for synthesis of N-substituted-triazole :



To a mixture of NH-triazole **1** (1.0 equiv) and base (1.5 equiv) in acetone (0.2 M of **1**) was added R'X (1.5 equiv or indicated in Table 2). The resulting reaction mixture was stirred at room temperature (heated to 45 ℃ or reflux in the cases of dicloroethane as electrophile) and monitored by TLC. After the reaction completed, the resulting solution was diluted with acetone followed by filtration. The filtrate was condensed under vacuum and the product was purified by flash silica gel chromatography gave the N-substituted-1,2,3-triazole.

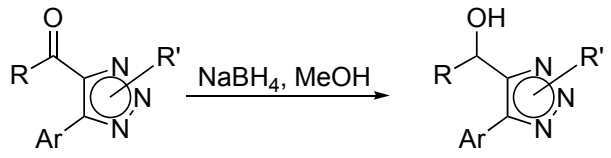
General Procedure for transformation 3 to 4:



3 **4**

The vinyl-substituted triazole **3** was dissolved in methanol (20 mL) in a 50 mL two-neck flask equipped with a gas dispersing tube. A stream of ozone was bubbled through the solution at 0 ℃. Ozone treatment was terminated when the starting material was disappeared. To the solution was then added Me_2S after which the solvent was removed under reduced pressure and the residue was purified by flash silica gel chromatography to give 5-carbonyl substituted triazole **4**.

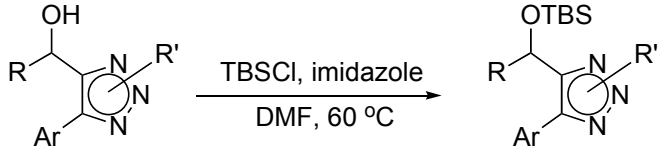
General Procedure for transformation 4 to 5:



4 **5**

To a solution of **4** in methanol (0.2 M) was added $NaBH_4$ at room temperature (when R'=H, heat up to refluxing) and monitored by TLC. After removing the solvent, the residue was diluted with ethyl acetate and wash with water. The water phase was extracted with ethyl acetate three times. The combined organic phases were then washed with brine and dried over anhydrous sodium sulfate. The solvent was removed under reduced pressure and product was purified by flash silica gel chromatography gave **5**.

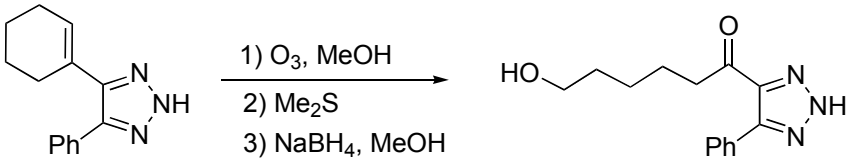
General Procedure for transformation 5 to 6:



5 **6**

To a solution of hydroxyl triazole **5** (1.0 equiv) and imidizole (1.2 equiv) in DMF (0.2 M) was added TBSCl (1.2 equiv). The resulting solution was heated at 60 ℃ for 5 hr. After cooled to room temperature, the reaction mixture was poured into water and extracted with ethyl acetate three times. The combined organic layers were then washed with brine and dried over anhydrous sodium sulfate. The solvent was removed under reduced pressure and product was purified by flash column chromatography to give TBS protected triazole **6**.

Procedure for synthesis of 6-hydroxy-1-(5-phenyl-2H-1,2,3-triazol-4-yl)hexan-1-one (4b):

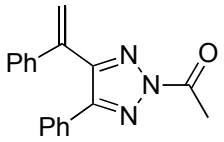


1f **4b**

The triazole **1f** (550 mg, 2 mmol) was dissolved in methanol (20 mL) in a 50 mL two-neck flask equipped with a gas dispersing tube. A stream of ozone was bubbled through the solution at 0 ℃. Ozone treatment was terminated when the starting material was disappeared monitored by TLC. The remaining solution was then treated with Me_2S (3 mL) followed by the removal of solvents under vacuum. The resulting crude product was dissolved in methanol (20 mL) at 0 ℃. To this solution was added $NaBH_4$ (152 mg, 4 mmol), and the reaction was monitored by TLC. After the completion of the reduction, the solvent was removed in vaco and the residue was diluted

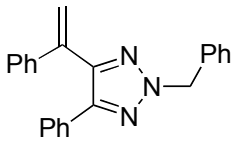
with ethyl acetate (50 mL) and washed with water. The aqueous solution was extracted with ethyl acetate (3 x 50 mL). The combined organic solutions were then washed with brine and dried over anhydrous sodium sulfate. The solvent was removed under reduced pressure and product was purified by flash column chromatography (hexane-EtOAc, v/v = 2/1) gave **4b** (360 mg, 1.4 mmol; yield: 70%) as colorless oil. ^{1}H NMR (270 MHz, CD_3OD): δ 7.67-7.90 (m, 2H), 7.28-7.50 (m, 3H), 3.56 (t, J = 6.4 Hz, 2H), 3.12 (t, J = 7.2 Hz, 2H), 1.64-1.81 (m, 2H), 1.35-1.64 (m, 4H); ^{13}C NMR (67.5 MHz, CD_3OD): δ 197.2, 142.5, 130.7, 130.3, 129.4, 129.1, 129.0, 62.9, 41.5, 33.5, 26.7, 25.1; HRMS Calculated for $C_{14}H_{18}N_3O_2$ $[M+H]^+$: 260.13935, Found: 260.13925.

II. Compounds Characterization:



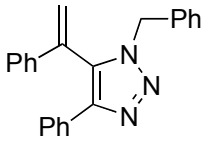
2a

1-(4-phenyl-5-(1-phenylvinyl)-2H-1,2,3-triazol-2-yl)ethanone (**2a**): **2a** was purified by flash chromatography (hexane-EtOAc, v/v = 5/1) as white solid (yield: 98%), m.p. 95-97 ℃ ; ^{1}H NMR (270 MHz, $CDCl_3$): δ 7.60-7.70 (m, 2H), 7.16-7.40 (m, 8H), 5.97 (s, 1H), 5.66 (s, 1H), 2.87 (s, 3H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 166.2, 149.6, 149.2, 138.2, 137.5, 129.4, 128.5, 128.3, 128.0, 126.6, 120.2, 22.2; HRMS Calculated for $C_{18}H_{15}N_3O$ $[M+H]^+$: 290.12879; the molecular signal did not find in MS, the major peak is $[M+2H-CH_3CO]^+$, calculated: 248.11877 Found: 248.11811.



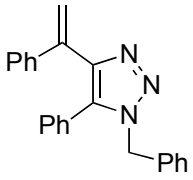
N-2-**3a**

2-benzyl-4-phenyl-5-(1-phenylvinyl)-2H-1,2,3-triazole (N-2-**3a)**: N-2-**3a** was purified by flash chromatography (hexane-EtOAc, v/v = 10/1) as colorless oil (yield: 50%). ^{1}H NMR (270 MHz, $CDCl_3$): δ 7.81-7.92 (m, 2H), 7.27-7.62 (m, 13H), 6.02 (s, 1H), 5.77 (s, 2H), 5.74 (s,1H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 146.0, 144.9, 139.6, 139.0, 135.6, 130.8, 129.0, 128.6, 128.6, 128.3, 127.8, 127.1, 118.9, 59.0; HRMS Calculated for $C_{23}H_{20}N_3$ $[M+H]^+$: 338.16517, Found: 338.16512.



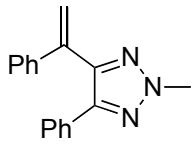
N-1-**3a**

1-benzyl-4-phenyl-5-(1-phenylvinyl)-1H-1,2,3-triazole (N-1-**3a**): N-1-**3a** was purified by flash chromatography (hexane-EtOAc, v/v = 10/1) as white solid (yield: 28%), m.p. 145-146 ℃ ; ^{1}H NMR (270 MHz, $CDCl_3$): δ 7.77-7.85 (m, 2H), 7.04-7.35 (m, 13H), 6.05 (s, 1H), 5.29 (s, 2H), 5.27 (s, 1H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 145.2, 136.7, 135.9, 135.0, 132.9, 130.7, 128.9, 128.50, 128.45, 128.1, 127.74, 127.69, 126.5, 126.0, 121.2, 52.1; HRMS Calculated for $C_{23}H_{20}N_3$ $[M+H]^+$: 338.16517, Found: 338.16496.



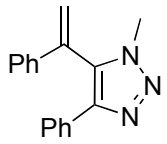
N-3-**3a**

1-benzyl-5-phenyl-4-(1-phenylvinyl)-1H-1,2,3-triazole (N-3-**3a**): N-3-**3a** was purified by flash chromatography (hexane-EtOAc, v/v = 10/1) as white solid (yield: 13%), m.p. 119-120 ℃ ; ^{1}H NMR (270 MHz, $CDCl_3$): δ 6.94-7.34 (m, 15H), 5.54 (d, *J* = 1.2 Hz, 1H), 5.51 (d, *J* = 1.2 Hz, 1H), 5.44 (s 2H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 145.1, 139.2, 139.1, 135.3, 129.6, 129.0, 128.6, 128.4, 128.0, 127.8, 127.5, 127.4, 127.3, 127.1, 117.5, 51.9. HRMS Calculated for $C_{23}H_{20}N_3$ $[M+H]^+$: 338.16517, Found: 338.16498.



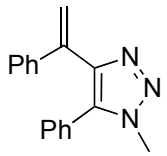
N-2-**3b**

2-methyl-4-phenyl-5-(1-phenylvinyl)-2H-1,2,3-triazole (N-2-**3b**): N-2-**3b** was purified by flash chromatography (hexane-EtOAc, v/v = 10/1) as colorless oil (yield: 60%). ^{1}H NMR (270 MHz, $CDCl_3$): δ 7.54-7.64 (m, 2H), 7.31-7.39 (m, 2H), 7.16-7.28 (m, 6H), 5.83 (s, 1H), 5.53 (s, 1H), 4.22 (s, 3H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 145.2, 144.2, 139.2, 138.7, 130.3, 128.2, 128.0, 127.8, 127.3, 126.7, 118.4, 41.7; HRMS Calculated for $C_{17}H_{16}N_3$ $[M+H]^+$: 262.13387, Found: 262.13381.



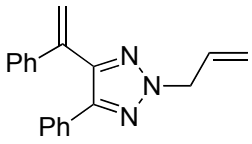
N-1-**3b**

1-methyl-4-phenyl-5-(1-phenylvinyl)-1H-1,2,3-triazole (N-1-**3b**): N-1-**3b** was purified by flash chromatography (hexane-EtOAc, v/v = 10/1) as white solid (yield: 28%), m.p. 99-101 ℃ ; ^{1}H NMR (270 MHz, $CDCl_3$): δ 7.78-7.88 (m, 2H), 7.20-7.40 (m, 8H), 6.16 (s, 1H), 5.47 (s, 1H), 3.79 (s, 3H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 144.9, 136.6, 136.0, 133.2, 130.7, 129.0, 128.4, 127.7, 126.4, 125.8, 120.7, 35.0; HRMS Calculated for $C_{17}H_{16}N_3$ $[M+H]^+$: 262.13387, Found: 262.13382.



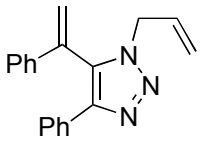
N-3-**3b**

1-methyl-5-phenyl-4-(1-phenylvinyl)-1H-1,2,3-triazole (N-3-**3b**): N-3-**3b** was purified by flash chromatography (hexane-EtOAc, v/v = 10/1) as colorless oil (yield: 8%). ^{1}H NMR (270 MHz, $CDCl_3$): δ 7.12-7.35 (m, 10H), 5.55 (dd, *J* = 5.7, 1.2 Hz, 2H), 3.99 (s, 3H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 145.0, 139.2, 135.4, 129.4, 129.0, 128.6, 127.9, 127.6, 127.4, 127.1, 117.6, 35.5; HRMS Calculated for $C_{17}H_{16}N_3$ $[M+H]^+$: 262.13387, Found: 262.13382.



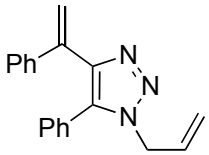
N-2-**3c**

2-allyl-4-phenyl-5-(1-phenylvinyl)-2H-1,2,3-triazole (N-2-**3c**): N-2-**3c** was purified by flash chromatography (hexane-EtOAc, v/v = 10/1) as colorless oil (yield: 55%). ^{1}H NMR (270 MHz, $CDCl_3$): δ 7.52-7.62 (m, 2H), 7.16-7.40 (m, 8H), 6.08-6.24 (m, 1H), 5.85 (d, *J* = 1.0 Hz, 1H), 5.53 (d, *J* = 1.0 Hz, 1H), 5.29-5.40 (m, 2H), 5.05-5.12 (m, 2H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 145.0, 144.1, 139.0, 138.4, 131.3, 130.1, 127.94, 127.88, 127.69, 127.57, 127.1, 126.4, 118.9, 118.2, 57.0; HRMS Calculated for $C_{19}H_{18}N_3$ $[M+H]^+$: 288.14952, Found: 288.14940.



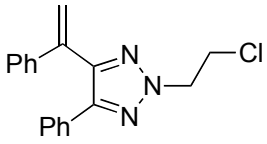
N-1-**3c**

1-allyl-4-phenyl-5-(1-phenylvinyl)-1H-1,2,3-triazole (N-1-**3c**): N-1-**3c** was purified by flash chromatography (hexane-EtOAc, v/v = 10/1) as white solid (yield: 24%), m.p. 60-61 ℃ ; ^{1}H NMR (270 MHz, $CDCl_3$): δ 7.78-7.86 (m, 2H), 7.19-7.36 (m, 8H), 6.13 (s, 1H), 5.78-5.94 (m, 1H), 5.46 (s, 1H), 4.97-5.18 (m, 2H), 4.65-4.75(m, 2H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 144.8 136.8, 135.9, 132.8, 131.4, 130.7, 128.9, 128.4, 127.7, 126.4, 126.0, 121.0, 119.0, 50.7; HRMS Calculated for $C_{19}H_{18}N_3$ $[M+H]^+$: 288.14952, Found: 288.14942



N-3-**3c**

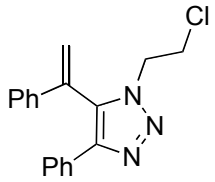
1-allyl-5-phenyl-4-(1-phenylvinyl)-1H-1,2,3-triazole (N-3-**3c)**: N-3-**3c** was purified by flash chromatography (hexane-EtOAc, v/v = 10/1) as colorless oil (yield: 5%). ^{1}H NMR (270 MHz, $CDCl_3$): δ 7.10-7.36 (m, 10H), 5.89-6.04 (m, 1H), 5.53 (s, 2H), 5.18-5.25 (m, 1H), 4.95- 5.06 (m, 1H), 4.82- 4.91 (m, 2H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 144.9, 139.2, 135.3, 132.0, 129.4, 129.0, 128.5, 127.8, 127.7, 127.3, 127.1, 118.7, 117.6, 50.6; HRMS Calculated for $C_{19}H_{18}N_3$ $[M+H]^+$: 288.14952, Found: 288.14941.



N-2-**3d**

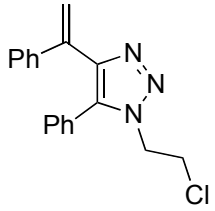
2-(2-chloroethyl)-4-phenyl-5-(1-phenylvinyl)-2H-1,2,3-triazole (N-2-**3d)**: N-2-**3d** was purified by flash chromatography (hexane-EtOAc, v/v = 10/1) as colorless oil (yield: 60%); ^{1}H NMR (270 MHz, $CDCl_3$): δ 7.57-7.66 (m, 2H), 7.33-7.40 (m, 2H), 7.20-7.32 (m, 6H), 5.88 (d, *J* = 0.9 Hz, 1H), 5.56 (d, *J* = 0.9 Hz, 1H), 4.78 (t, *J* = 6.4 Hz, 2H), 4.05 (t, *J* = 6.4 Hz, 2H); ^{13}C NMR

(67.5 MHz, $CDCl_3$): δ 145.8, 144.8, 139.1, 138.6, 130.1, 128.3, 128.2, 128.1, 127.5, 126.7, 118.7, 55.8, 41.4; HRMS Calculated for $C_{18}H_{17}ClN_3$ $[M+H]^+$: 310.11055, Found: 310.11059.



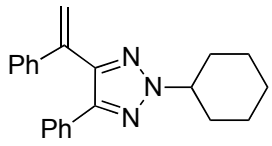
N-1-**3d**

1-(2-chloroethyl)-4-phenyl-5-(1-phenylvinyl)-1H-1,2,3-triazole (N-1-**3d**): N-1-**3d** was purified by flash chromatography (hexane-EtOAc, v/v = 10/1) as colorless oil (yield: 23%); ^{1}H NMR (270 MHz, $CDCl_3$): δ 7.78-7.86 (m, 2H), 7.10-7.39 (m, 8H), 6.20 (s, 1H), 5.52 (s, 1H), 4.38 (t, *J* = 6.8 Hz, 2H), 3.82 (t, *J* = 6.8 Hz, 2H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 144.7, 136.5, 135.6, 133.2, 130.4, 129.2, 129.1, 128.4, 127.8, 126.4, 125.9, 121.4, 49.2, 41.2. HRMS Calculated for $C_{18}H_{17}ClN_3$ $[M+H]^+$: 310.11055, Found: 310.11038.



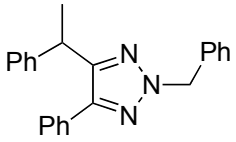
N-3-**3d**

1-(2-chloroethyl)-5-phenyl-4-(1-phenylvinyl)-1H-1,2,3-triazole (N-3-**3d**): N-3-**3d** was purified by flash chromatography (hexane-EtOAc, v/v = 10/1) as colorless oil (yield: 8%); ^{1}H NMR (270 MHz, $CDCl_3$): δ 7.19-7.38(m, 10H), 5.53 (dd, *J* = 5.7, 1.2 Hz, 2H), 4.53 (t, *J* = 6.4 Hz, 2H), 3.90(t, *J* = 6.4 Hz, 2H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 144.9, 139.2, 139.0, 135.9, 129.7, 129.3, 128.8, 127.9, 127.7, 127.4, 126.8, 117.8, 49.1, 41.7. HRMS Calculated for $C_{18}H_{17}ClN_3$ $[M+H]^+$: 310.11055, Found: 310.11038.



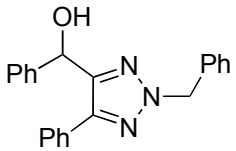
N-2-**3e**

2-cyclohexyl-4-phenyl-5-(1-phenylvinyl)-2H-1,2,3-triazole (N-2-**3e**): N-2-**3e** was purified by flash chromatography (hexane-EtOAc, v/v = 10/1) as colorless oil (yield: 90%); ^{1}H NMR (270 MHz, $CDCl_3$): δ 7.53-7.68 (m, 2H), 7.15-7.43 (m, 8H), 5.84 (d, *J* = 0.8 Hz, 1H), 5.52 (d, *J* = 0.8 Hz, 1H), 4.42-4.58 (m, 1H), 2.17-2.35 (m, 2H), 1.83-2.09 (m, 4H), 1.66-1.79 (m, 1H), 1.16-1.55 (m, 3H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 144.4, 143.4, 139.6, 138.9, 130.8, 128.2, 127.9, 127.7, 127.4, 126.8, 125.2, 118.3, 64.3, 32.7, 25.1. HRMS Calculated for $C_{22}H_{24}N_3$ $[M+H]^+$: 330.19647, Found: 330.19648.



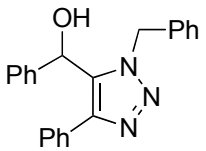
N-2-**3f** (**7g**)

2-benzyl-4-phenyl-5-(1-phenylethyl)-2H-1,2,3-triazole (N-2-**3f** (**7g**)): **7g** was purified by flash chromatography (hexane-EtOAc, v/v = 10/1) as colorless oil (yield: 85%). ^{1}H NMR (270 MHz, $CDCl_3$): δ 7.48-55 (m, 2H), 7.18-7.44 (m, 13H), 5.68 (s, 2H), 4.40 (q, *J* = 7.2 Hz, 1H), 1.74 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 148.1, 145.2, 145.0, 135.7, 130.9, 128.6, 128.5, 128.4, 127.9, 127.7, 127.4, 126.2, 58.4, 36.7, 23.1; HRMS Calculated for $C_{23}H_{22}N_3$ $[M+H]^+$:340.18082 , Found:340.18062 .



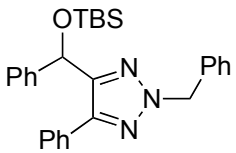
N-2-**5a** (**7i**)

(2-benzyl-5-phenyl-2H-1,2,3-triazol-4-yl)(phenyl)methanol (N-2-**5a** (**7i**)): **7i** was purified by flash chromatography (hexane-EtOAc, v/v = 5/1) as white solid (yield: 63%), m.p. 98-100 ℃; ^{1}H NMR (270 MHz, $CDCl_3$): δ 7.50-7.60 (m, 2H), 7.22-7.42 (m, 13H), 6.07 (m, 1H), 5.60 (m, 2H), 2.90 (br, 1H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 146.7, 145.6, 141.8, 135.3, 130.3, 128.9, 128.7, 128.6, 128.5, 128.4, 128.15, 128.09, 128.0, 127.0, 68.9, 58.9; HRMS Calculated for $C_{22}H_{20}N_3O$ $[M+H]^+$: 342.14009, Found: 342.14937.



N-1-**5a**

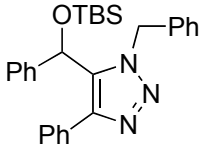
(3-benzyl-5-phenyl-3H-1,2,3-triazol-4-yl)(phenyl)methanol (N-1-**5a**): N-1-**5a** was purified by flash chromatography (hexane-EtOAc, v/v = 4/1) as white solid (yield: 26%), m.p. 168-170 ℃ ; ^{1}H NMR (270 MHz, $CDCl_3$): δ 7.56-7.66 (m, 2H), 7.14-7.46 (m, 11H), 6.99-7.10 (m, 2H), 6.31 (d, *J* = 5.0 Hz, 1H), 5,45 (d, *J* = 15.1 Hz, 1H), 5.23 (d, *J* = 15.1 Hz, 1H), 2.76-2.81(m, 1H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 146.5, 139.4, 135.1, 133.9, 130.7, 128.74, 128.66, 128.4, 128.2, 128.13, 128.08, 127.9, 125.8, 65.5, 53.0 HRMS Calculated for $C_{22}H_{20}N_3O$ $[M+H]^+$: 342.14009, Found: 342.13989.



N-2-**6a** (**7l**)

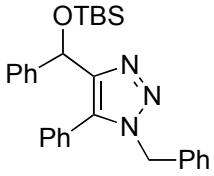
7l was purified by flash chromatography (hexane-EtOAc, v/v = 10/1) as colorless oil (yield: 62%). ^{1}H NMR (270 MHz, $CDCl_3$): δ 7.20-7.70 (m, 2H), 7.10-7.37 (m, 13H), 6.26 (s, 1H), 5.62 (s, 2H), 0.83 (s, 9H), 0.03 (s, 3H), -0.21 (s, 3H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 147.6, 145.7,

142.1, 135.5, 130.4, 128.7, 128.4, 128.1, 127.9, 127.7, 126.9, 125.8, 69.1, 58.5, 25.7, 18.2, -5.0, -5.2; HRMS Calculated for $C_{28}H_{34}N_3OSi$ $[M+H]^+$: 456.24657, Found: 456.24625.



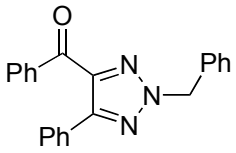
N-1-**6a**

N-1-**6a** was purified by flash chromatography (hexane-EtOAc, v/v = 10/1) as colorless oil (yield: 12%). ^{1}H NMR (270 MHz, $CDCl_3$): δ 7.04-7.38 (m, 11H), 6.80-7.00 (m, 4H), 6.12 (s, 1H), 5.35 (d, J = 20.0 Hz, 1H), 5.28 (d, J = 20.0 Hz, 1H), 0.79 (s, 9H), -0.03 (s, 3H), -0.14 (s, 3H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 148.4, 142.9, 135.3, 134.8, 130.0, 129.0, 128.4, 128.0, 127.8, 127.6, 127.1, 126.8, 126.5, 125.6, 69.7, 51.6, 25.6, 18.0, -4.9, -5.3; HRMS Calculated for $C_{28}H_{34}N_3OSi$ $[M+H]^+$: 456.24657, Found: 456.24625.



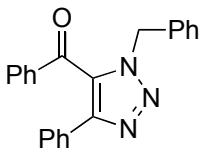
N-3-**6a**

N-3-**6a** was purified by flash chromatography (hexane-EtOAc, v/v = 10/1) as colorless oil (yield: 18%). ^{1}H NMR (270 MHz, $CDCl_3$): δ 7.64-7.71 (m, 2H), 7.34-7.48 (m, 3H), 7.18-7.28 (s, 5H), 7.58-7.18 (m, 3H), 6.87 (dd, J = 7.2 Hz, 1.5 Hz, 2H), 6.32 (s, 1H), 5.37 (s, 2H), 0.81 (s, 9H), -0.15 (s, 3H), -0.36 (s, 3H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 145.9, 140.6, 134.7, 134.4, 130.9, 128.8, 128.6, 128.3, 128.2, 128.0, 127.9, 127.6, 127.6, 125.4, 65.7, 52.5, 25.7, 18.11, -5.3, -5.7; HRMS Calculated for $C_{28}H_{34}N_3OSi$ $[M+H]^+$: 456.24657, Found: 456.24606.



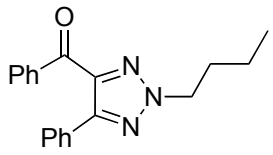
N-2-**4a** (**7a**)

(2-benzyl-5-phenyl-2H-1,2,3-triazol-4-yl)(phenyl)methanone (N-2-**4a** (**7a**)): **7a** was purified by flash chromatography (hexane-EtOAc, v/v = 5/1) as white solid (yield: 82%), m.p. 104-105 ℃ ; ^{1}H NMR (270 MHz, $CDCl_3$): δ 8.00-8.08 (m, 2H), 7.78-7.86 (m, 2H), 7.48-7.58 (m, 1H), 7.26-7.46 (m, 10H), 5.64 (s, 2H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 187.7, 149.9, 142.1, 137.1, 134.4, 133.2, 130.3, 129.5, 129.0, 128.7, 128.6, 128.5, 128.2, 128.0, 59.1; HRMS Calculated for $C_{22}H_{18}N_3O$ $[M+H]^+$: 340.14444, Found: 340.14426.



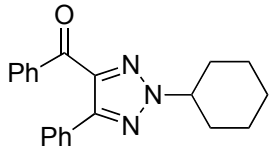
N-1-**4a**

(3-benzyl-5-phenyl-3H-1,2,3-triazol-4-yl)(phenyl)methanone (N-1-**4a**): was purified by flash chromatography (hexane-EtOAc, v/v = 5/1) as colorless oil (yield: 8%). ^{1}H NMR (270 MHz, $CDCl_3$): δ 7.32-7.54 (m, 5H), 7.09-7.26 (m, 10H), 5.74 (s, 2H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 187.5, 148.5, 135.5, 134.5, 134.0, 130.2, 129.4, 128.6, 128.3, 128.2, 128.0, 53.3; HRMS Calculated for $C_{22}H_{18}N_3O$ $[M+H]^+$: 340.14444, Found: 340.14441.



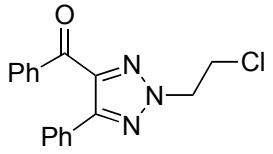
7b

(2-butyl-5-phenyl-2H-1,2,3-triazol-4-yl)(phenyl)methanone (**7b**): **7b** was purified by flash chromatography (hexane-EtOAc, v/v = 5/1) as colorless oil (yield: 90%). ^{1}H NMR (270 MHz, $CDCl_3$): δ 8.02-8.10 (m, 2H), 7.78-7.88 (m, 2H), 7.30-7.58 (m, 6H), 4.49 (t, J = 7.2 Hz, 2H), 1.94-2.07 (m, 2H), 1.31-1.46 (m, 2H), 0.95 (t, J = 7.4 Hz, 3H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 187.7, 149.3, 141.5, 137.2, 133.1, 130.2, 129.6, 128.8, 128.5, 128.1, 55.1, 31.4, 19.5, 13.4; HRMS Calculated for $C_{19}H_{20}N_3O$ $[M+H]^+$: 306.16009, Found: 306.15992.



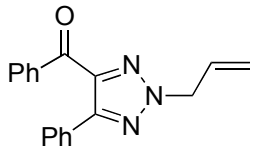
7c

(2-cyclohexyl-5-phenyl-2H-1,2,3-triazol-4-yl)(phenyl)methanone (**7c**): **7c** was purified by flash chromatography (hexane-EtOAc, v/v = 5/1) as colorless oil (yield: 90%). ^{1}H NMR (270 MHz, $CDCl_3$): δ 8.04-8.15 (m, 2H), 7.79-7.88 (m 2H), 7.55-7.64 (m, 1H), 7.34-7.53 (m, 5H), 4.50-4.66 (m, 1H), 2.20-2.37 (m, 2H), 1.85-2.10 (m, 4H), 1.67-1.82 (m, 1H), 1.18-1.58 (m, 3H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 188.1, 149.2, 141.4, 137.5, 133.2, 130.6, 130.5, 130.1, 129.0, 128.8, 128.4, 65.0, 32.7, 25.2, 25.1; HRMS Calculated for $C_{21}H_{22}N_3O$ $[M+H]^+$:332.17574, Found: 332.17556.



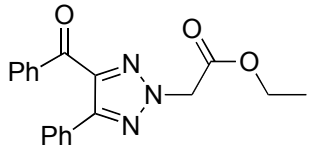
7d

(2-(2-chloroethyl)-5-phenyl-2H-1,2,3-triazol-4-yl)(phenyl)methanone (**7d**): **7d** was purified by flash chromatography (hexane-EtOAc, v/v = 5/1) as white solid (yield: 95%), m.p. 127-128 ℃; ^{1}H NMR (270 MHz, $CDCl_3$): δ 8.02-8.10 (m, 2H), 7.76-7.87 (m, 2H), 7.52-7.62 (m, 1H), 7.33-7.50 (m, 5H), 4.79 (t, J = 6.2 Hz, 2H), 4.04 (t, J = 6.2 Hz, 2H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 187.6, 149.9, 142.2, 137.0, 133.3, 130.3, 129.3, 129.1, 128.6, 128.3, 56.3, 41.3; HRMS Calculated for $C_{17}H_{15}ClN_3O$ $[M+H]^+$:312.08981 , Found:312.08982 .



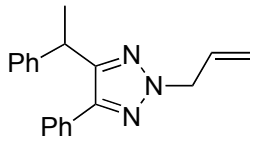
7e

(2-allyl-5-phenyl-2H-1,2,3-triazol-4-yl)(phenyl)methanone (**7e**): **7e** was purified by flash chromatography (hexane-EtOAc, v/v = 5/1) as colorless oil (yield: 74%). ^{1}H NMR (270 MHz, $CDCl_3$): δ 8.07-8.15 (m, 2H), 7.83-7.92 (m, 2H), 7.54-7.62 (m, 1H), 7.34-7.52 (m, 5H), 6.08-6.25 (m, 1H), 5.29-5.42 (m, 2H), 5.04-5.17 (m, 2H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 187.5, 141.8, 137.0, 133.1, 130.7, 130.2, 129.4, 128.8, 128.5, 128.1, 119.8, 57.6; HRMS Calculated for $C_{18}H_{16}N_3O$ $[M+H]^+$: 290.12879, Found: 290.12868.



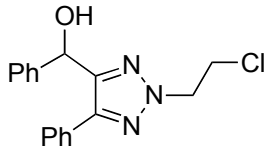
7f

ethyl 2-(4-phenylcarbonyl-5-phenyl-2H-1,2,3-triazol-2-yl)acetate (**7f**): **7f** was purified by flash chromatography (hexane-EtOAc, v/v = 10/1) as colorless oil (yield: 84%); ^{1}H NMR (270 MHz, $CDCl_3$): δ 8.04-8.12 (m, 2H), 7.80-7.88 (m, 2H), 7.55-7.63 (m, 1H), 7.38-7.52 (m, 5H), 5.31 (s, 2H), 4.28 (q, *J* = 7.2 Hz, 2H), 1.30 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 187.6, 166.0, 150.2, 142.7, 137.0, 133.4, 130.3,129.2, 128.6, 128.3, 62.3, 55.9, 14.0(d); HRMS Calculated for $C_{19}H_{18}N_3O_3$ $[M+H]^+$: 336.13427, Found: 336.13432.



7h

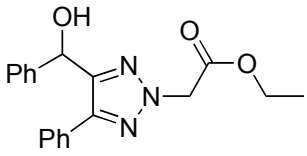
2-allyl-4-phenyl-5-(1-phenylethyl)-2H-1,2,3-triazole (**7h**): **7h** was purified by flash chromatography (hexane-EtOAc, v/v = 10/1) as colorless oil (yield: 76%). ^{1}H NMR (270 MHz, $CDCl_3$): δ 7.20-7.51 (m, 10H), 6.06-6.24 (m, 1H), 5.22-5.38 (m, 2H), 5.02-5.14 (m, 2H), 4.35 (q, *J* = 7.2 Hz, 1H), 1.68 (d, *J* = 7.2 Hz, 3H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 148.0, 145.0, 132.0, 130.9, 128.5, 128.4, 127.9, 127.4, 126.2, 118.7, 57.2, 36.6, 23.0; HRMS Calculated for $C_{19}H_{20}N_3$ $[M+H]^+$: 290.16517 , Found: 290.16505.



7j

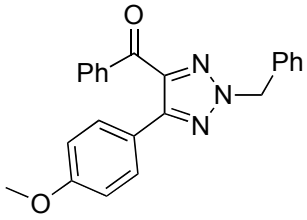
(2-(2-chloroethyl)-5-phenyl-2H-1,2,3-triazol-4-yl)(phenyl)methanol (7j): 7j was purified by flash chromatography (hexane-EtOAc, v/v = 4/1) as colorless oil (yield: 90%). ^{1}H NMR (270 MHz, $CDCl_3$): δ 7.53-7.64 (m, 2H), 7.24-7.45 (m, 8H), 6.08 (s, 1H), 4.71 (t, *J* = 6.4 Hz, 2H), 3.99 (t, *J* = 6.4 Hz, 2H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 146.7, 145.6, 141.5, 129.9, 128.5,

128.0, 126.9, 68.7, 55.8, 41.4; HRMS Calculated for $C_{17}H_{17}ClN_3O$ $[M+H]^+$: 314.10547, Found: 314.10547.



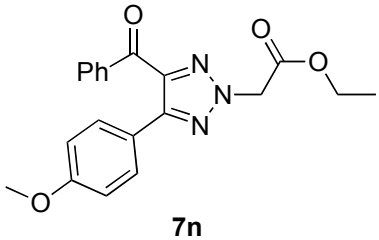
7k

Ethyl 2-(4-(hydroxy(phenyl)methyl)-5-phenyl-2H-1,2,3-triazol-2-yl)acetate (7k): 7k was purified by flash chromatography (hexane-EtOAc, v/v = 3/1) as colorless oil (yield: 73%); ^{1}H NMR (270 MHz, $CDCl_3$): δ 7.54-7.63 (m, 2H), 7.24-7.44 (m, 8H), 6.00 (s, 1H), 5.11 (s, 2H), 4.11 (q, *J* = 6.9 Hz, 2H), 3.12 (br, 1H), 1.16 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 166.7, 147.4, 146.1, 141.4, 129.8, 128.5, 128.4, 128.0, 127.9, 126.9, 68.6, 62.0, 55.5, 14.0; HRMS Calculated for $C_{19}H_{20}N_3O_3$ $[M+H]^+$: 338.14992, Found: 338.14994.



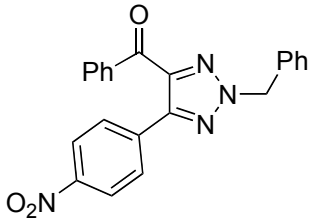
7m

(2-benzyl-5-(4-methoxyphenyl)-2H-1,2,3-triazol-4-yl)(phenyl)methanone (7m): 7m was purified by flash chromatography (hexane-EtOAc, v/v = 8/1) as colorless oil (yield: 80%); ^{1}H NMR (270 MHz, $CDCl_3$): δ 8.05-8.13 (m, 2H), 7.84 (d, *J* = 8.9 Hz, 2H), 7.56-7.64 (m, 1H), 7.32-7.55 (m, 7H), 6.95 (d, *J* = 8.9 Hz, 2H), 5.68 (s, 2H), 3.83 (s, 3H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 187.8, 160.2, 149.9, 141.7, 137.3, 134.5, 133.1, 130.4, 130.1, 128.5, 128.5, 128.2, 128.1, 122.0, 113.7, 59.1, 55.2 ; HRMS Calculated for $C_{23}H_{20}N_3O_2$ $[M+H]^+$: 247.29145, Found: 247.29164.



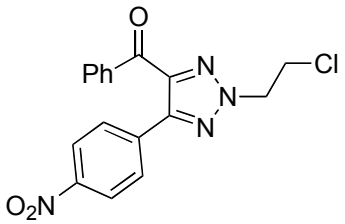
7n

Ethyl-2-(4-phenylcarbonyl-5-(4-methoxyphenyl)-2H-1,2,3-triazol-2-yl)acetate (7n): 7n was purified by flash chromatography (hexane-EtOAc, v/v = 10/1) as colorless oil (yield: 65%); ^{1}H NMR (270 MHz, $CDCl_3$): δ 8.07 (d, *J* = 7.2 Hz, 2H), 7.81 (d, *J* = 8.9 Hz, 2H), 7.59 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 7.2 Hz, 2H), 6.94 (d, *J* = 8.9 Hz, 2H), 5.29 (s, 2H), 4.28 (q, *J* = 7.2 Hz, 2H), 3.83 (s, 3H), 1.30 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 187.8, 166.1, 160.3, 150.1, 142.4, 137.2, 133.3, 130.3, 130.1, 128.2, 121.7, 113.7, 62.4, 55.2, 14.1; HRMS Calculated for $C_{20}H_{20}N_3O_4$ $[M+H]^+$: 366.14483, Found: 366.14461.



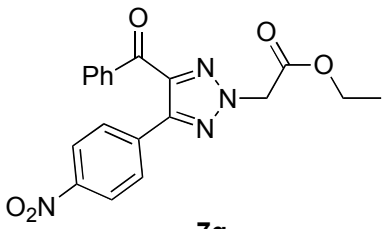
7o

(2-benzyl-5-(4-nitrophenyl)-2H-1,2,3-triazol-4-yl)(phenyl)methanone (7o): 7o was purified by flash chromatography (hexane-EtOAc, v/v = 8/1) as colorless oil (yield: 87%); ^{1}H NMR (270 MHz, $CDCl_3$): δ 8.21-8.30 (m, 2H), 8.02-8.13 (m, 4H), 7.59-7.68 (m, 1H), 7.35-7.56 (m, 7H), 5.71 (s, 2H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 187.4, 147.9, 142.7, 136.8, 136.0, 133.9, 133.7, 130.5, 129.6, 129.0, 128.9, 128.4, 128.3, 123.5, 59.5; HRMS Calculated for $C_{22}H_{17}N_4O_3$ $[M+H]^+$: 385.12952, Found: 385.12937.



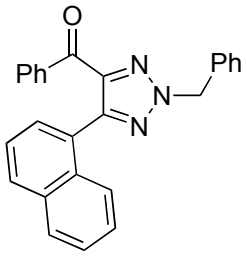
7p

(2-(2-chloroethyl)-5-(4-nitrophenyl)-2H-1,2,3-triazol-4-yl)(phenyl)methanone (7p): 7p was purified by flash chromatography (hexane-EtOAc, v/v = 5/1) as colorless oil (yield: 90%); ^{1}H NMR (270 MHz, $CDCl_3$): δ 8.27 (d, J = 8.6 Hz, 2H), 8.00-8.14 (m, 4H), 7.64 (t, J = 7.4 Hz, 1H), 7.51 (t, J = 7.7 Hz, 2H), 4.88 (t, J = 6.0 Hz, 2H), 4.12 (t, J = 6.0 Hz, 2H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 187.3, 147.9(d), 142.8, 136.7, 135.8, 133.8, 130.5, 129.6, 128.5, 123.5, 56.7, 41.3 ; HRMS Calculated for $C_{17}H_{14}ClN_4O_3$ $[M+H]^+$: 357.07490, Found: 357.07494.



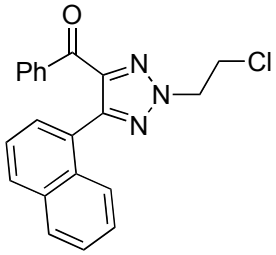
7q

Ethyl 2-(4-phenylcarbonyl-5-(4-nitrophenyl)-2H-1,2,3-triazol-2-yl)acetate (7q): 7q was purified by flash chromatography (hexane-EtOAc, v/v = 10/1) as colorless oil (yield: 92%); ^{1}H NMR (270 MHz, $CDCl_3$): δ 8.25 (d, J = 8.6 Hz, 2H), 8.02-8.13 (m, 4H), 7.63 (t, J = 7.2 Hz, 1H), 7.50 (t, J = 7.2 Hz, 2H), 5.35 (s, 2H), 4.31 (q, J = 7.2 Hz, 2H), 1.33 (t, J = 7.2 Hz, 3H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 187.3, 165.8, 148.1, 148.0, 143.3, 136.7, 135.6, 133.8, 130.5, 129.7, 128.4, 123.4, 62.6, 56.1, 14.0; HRMS Calculated for $C_{19}H_{17}N_4O_5$ $[M+H]^+$: 381.11935, Found: 381.11941.



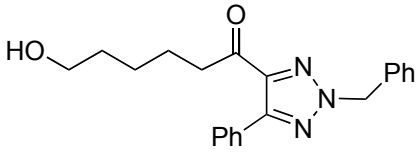
7r

(2-benzyl-5-(naphthalen-1-yl)-2H-1,2,3-triazol-4-yl)(phenyl)methanone (**7r**): was purified by flash chromatography (hexane-EtOAc, v/v = 5/1) as colorless oil (yield: 62%). ^{1}H NMR (270 MHz, $CDCl_3$): δ 8.07-8.18 (m, 2H), 7.76-7.98 (m, 3H), 7.36-7.67 (m, 12H), 5.81 (s, 2H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 186.5, 149.2, 144.0, 136.8, 134.4, 133.5, 133.1, 131.5, 130.2, 129.5, 128.9, 128.6, 128.5, 128.4, 128.2, 128.1, 127.3, 126.5, 125.8, 125.0, 124.9, 59.4; HRMS Calculated for $C_{26}H_{20}N_3O$ $[M+H]^+$: 390.16009, Found: 390.16023.



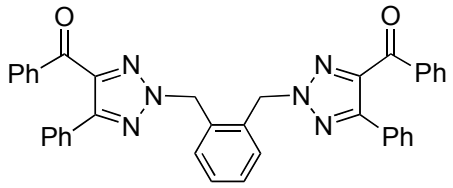
7s

(2-(2-chloroethyl)-5-(naphthalen-1-yl)-2H-1,2,3-triazol-4-yl)(phenyl)methanone (**7s**): **7s** was purified by flash chromatography (hexane-EtOAc, v/v = 5/1) as white solid (yield: 81%), m.p. 117-118 ℃; ^{1}H NMR (270 MHz, $CDCl_3$): δ 8.04-8.13 (m, 2H), 7.78-8.00 (m, 3H), 7.35-7.64 (m, 7H), 4.91 (t, *J* = 6.2 Hz, 2H), 4.13 (t, *J* = 6.2 Hz, 2H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 186.4, 149.3, 144.1, 136.7, 133.5, 133.2, 131.5, 130.2, 129.6, 128.5, 128.4, 128.2, 127.1, 126.6, 125.9, 124.9, 56.5, 41.5; HRMS Calculated for $C_{21}H_{17}ClN_3O$ $[M+H]^+$: 362.10547, Found: 362.10528 .



7t

1-(2-benzyl-5-phenyl-2H-1,2,3-triazol-4-yl)-6-hydroxyhexan-1-one (7t): was purified by flash chromatography (hexane-EtOAc, v/v = 2/1) as colorless oil (yield: 83%); ^{1}H NMR (270 MHz, $CDCl_3$): δ 7.86-7.92 (m, 2H), 7.32-7.48 (m, 8H), 5.64 (s, 2H), 3.64 (t, *J* = 6.4 Hz, 2H), 3.09 (t, *J* = 7.4 Hz, 2H), 1.68-1.82 (m, 2H), 1.38-1.68 (m, 4H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 195.2, 149.0, 142.5, 134.3, 129.6, 129.2, 129.1, 128.9, 128.6, 128.1, 62.7, 59.2, 40.5, 32.5, 25.3, 23.5; HRMS Calculated for $C_{21}H_{24}N_3O_2$ $[M+H]^+$: 350.18630, Found: 350.18639.



7u

Bis-triazole-benzyl-box (keto-triazole-benzyl) (7u) was purified by flash chromatography (hexane-EtOAc, v/v = 5/1) as white solid (yield: 85%), m.p. 160-161 ℃; ^{1}H NMR (270 MHz, $CDCl_3$): δ 7.98-8.13 (m, 4H), 7.72-7.88 (m, 4H), 7.28-7.64 (m, 16H), 6.05 (s, 4H); ^{13}C NMR (67.5 MHz, $CDCl_3$): δ 187.7, 150.0, 142.2, 137.1, 133.4, 133.3, 130.7, 130.4, 129.6, 129.4, 129.1, 128.6, 128.32, 128.26, 56.4; HRMS Calculated for $C_{38}H_{29}N_6O_2$ $[M+H]^+$: 601.23465, Found: 601.23452.

III. ORTEP Drawing of the Crystal Structures

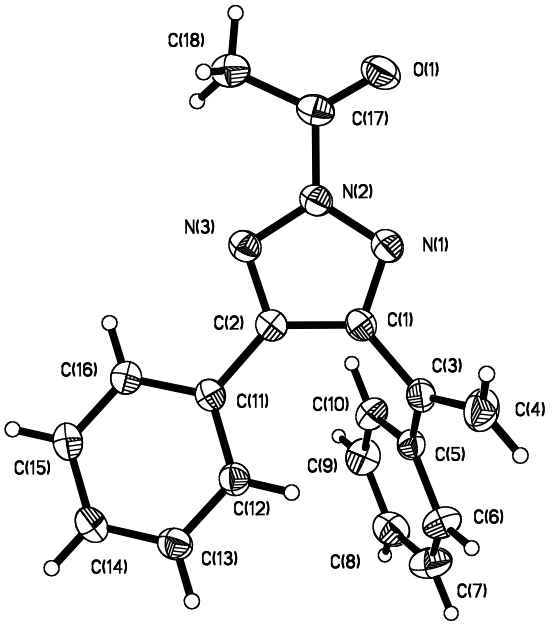


Figure S-1. Perspective view of the molecular structure of **2a** with the atom labeling scheme. The thermal ellipsoids are scaled to enclose 30% probability.

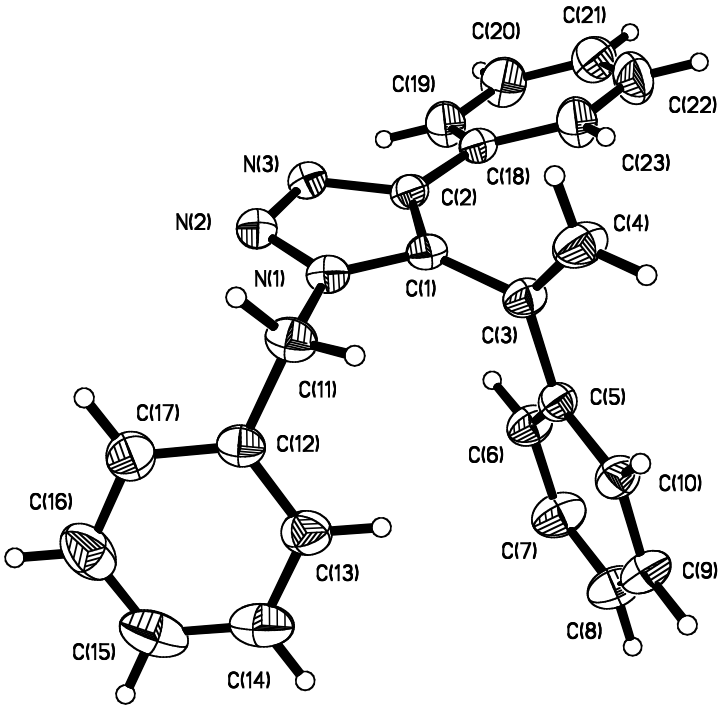


Figure S-2: Perspective view of the molecular structure of N-1-**3a** with the atom labeling scheme. The thermal ellipsoids are scaled to enclose 30% probability.

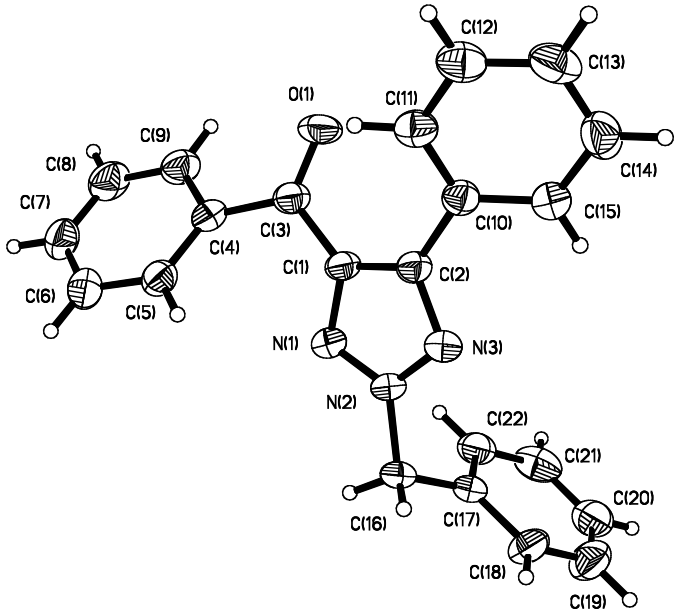


Figure S-3. Perspective view of the molecular structure of N-2-**4a** (**7a**) with the atom labeling scheme. The thermal ellipsoids are scaled to enclose 30% probability.

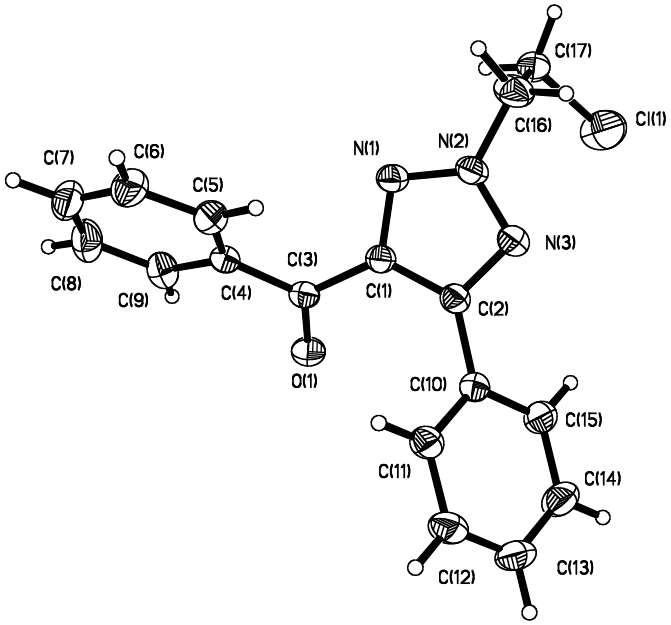


Figure S-4. Perspective view of the molecular structure of **7d** with the atom labeling scheme. The positions of atoms C(16), C(17), and Cl(1) exhibit a 2:1 conformational disorder within the lattice. The thermal ellipsoids are scaled to enclose 30% probability.

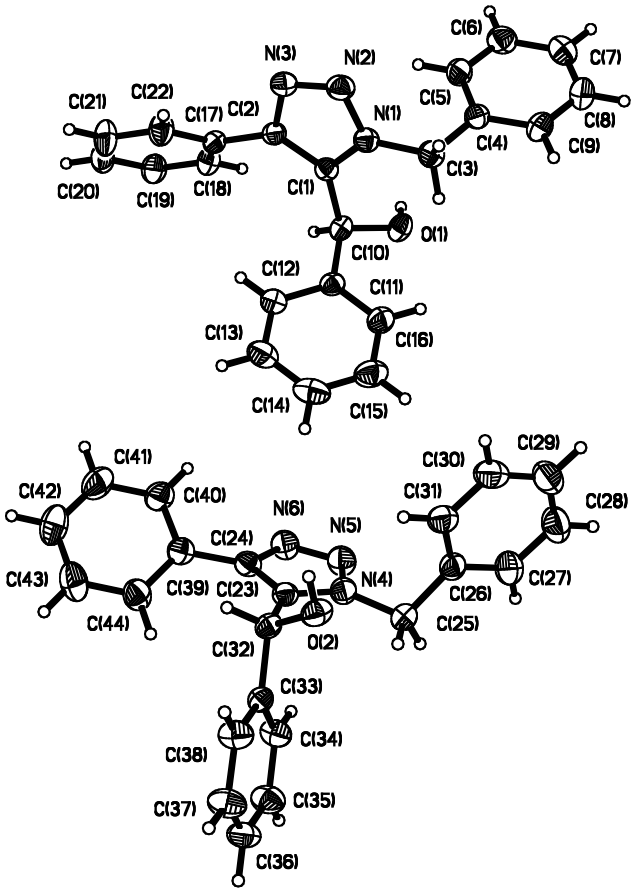
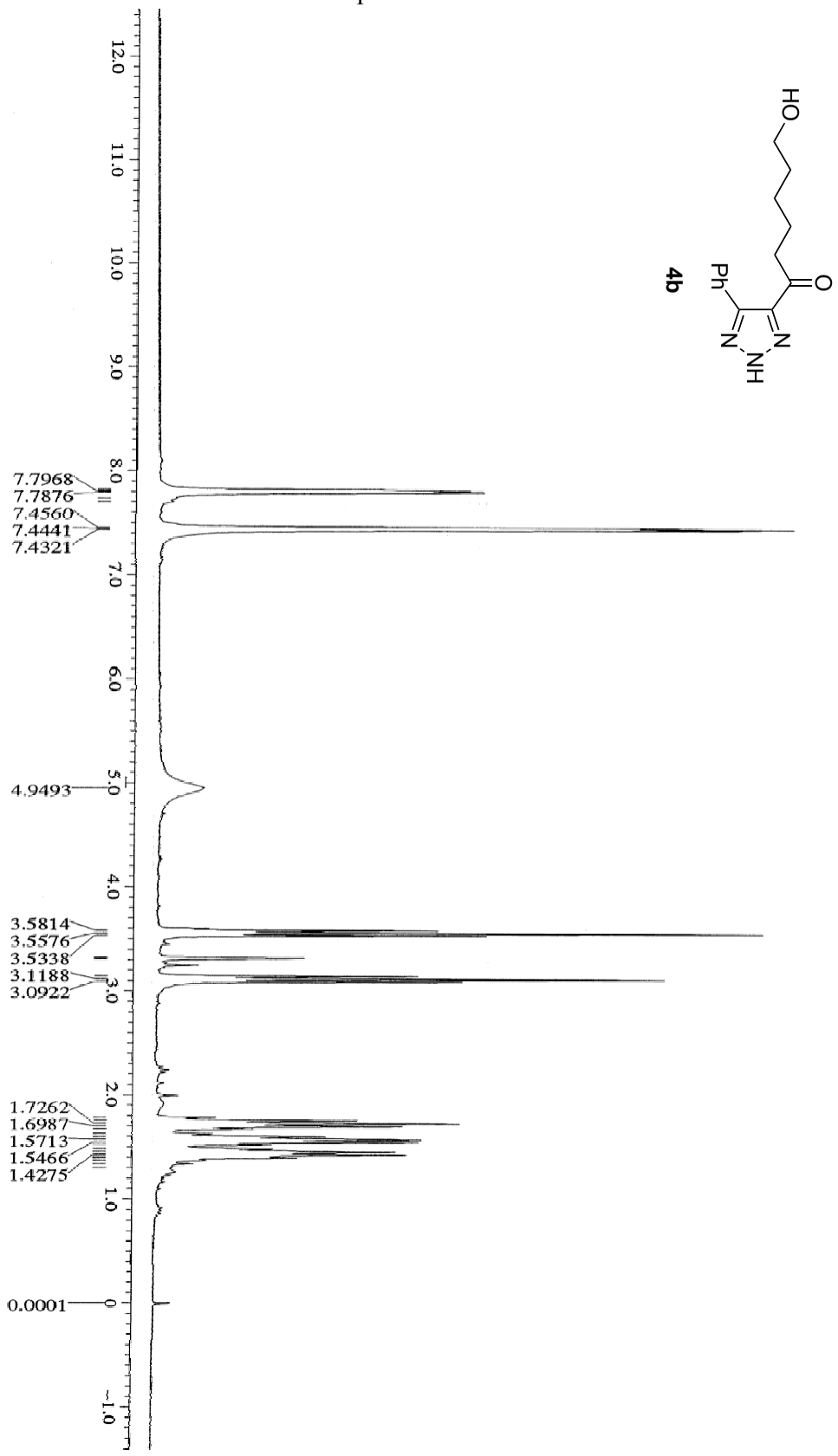
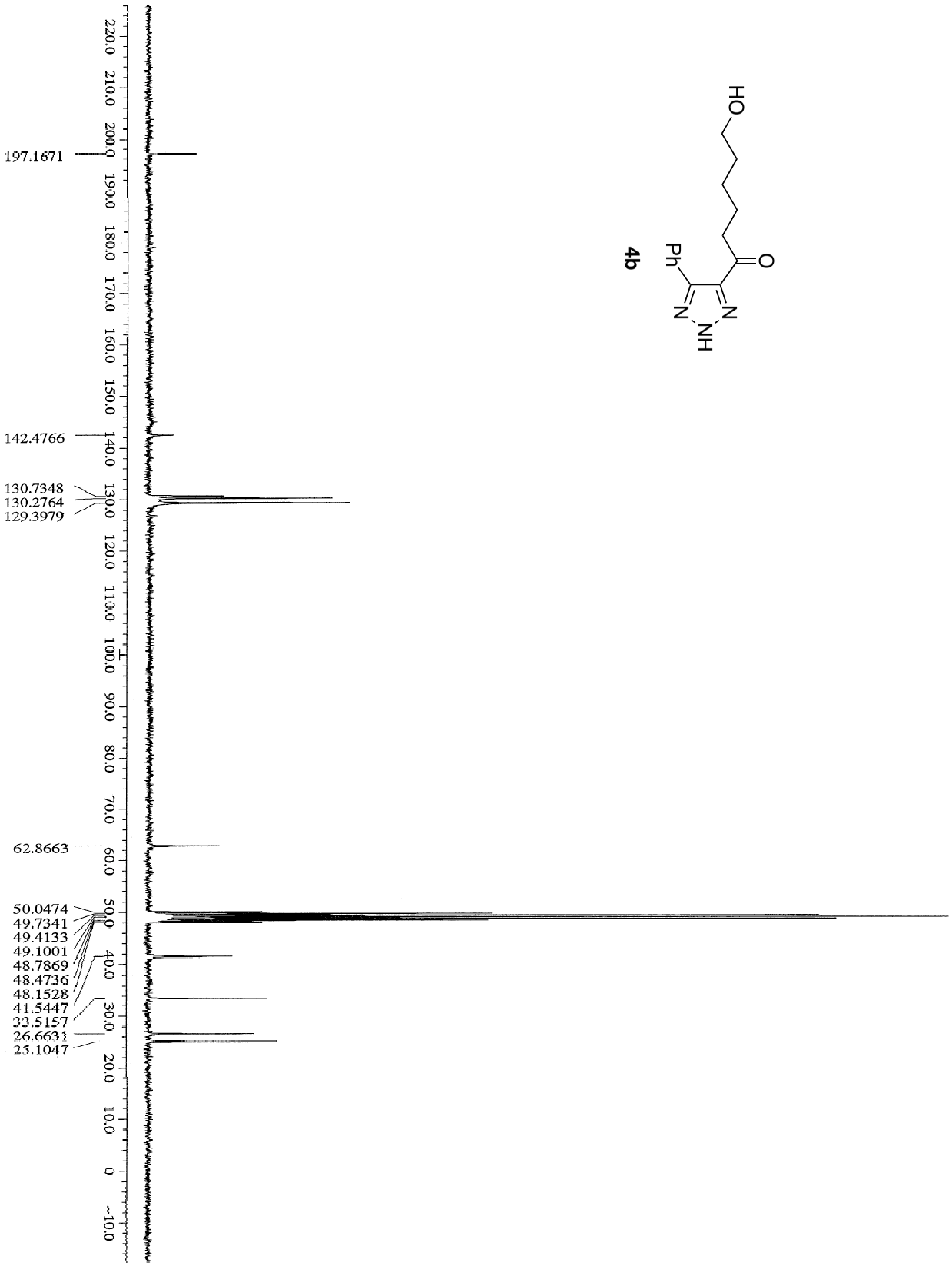


Figure S-5. Perspective view of the molecular structures of the two independent molecules of N-1-**5a** with the atom labeling scheme. The thermal ellipsoids are scaled to enclose 30% probability

IV. ^{1}H-NMR and ^{13}C-NMR Spectra

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48.1528
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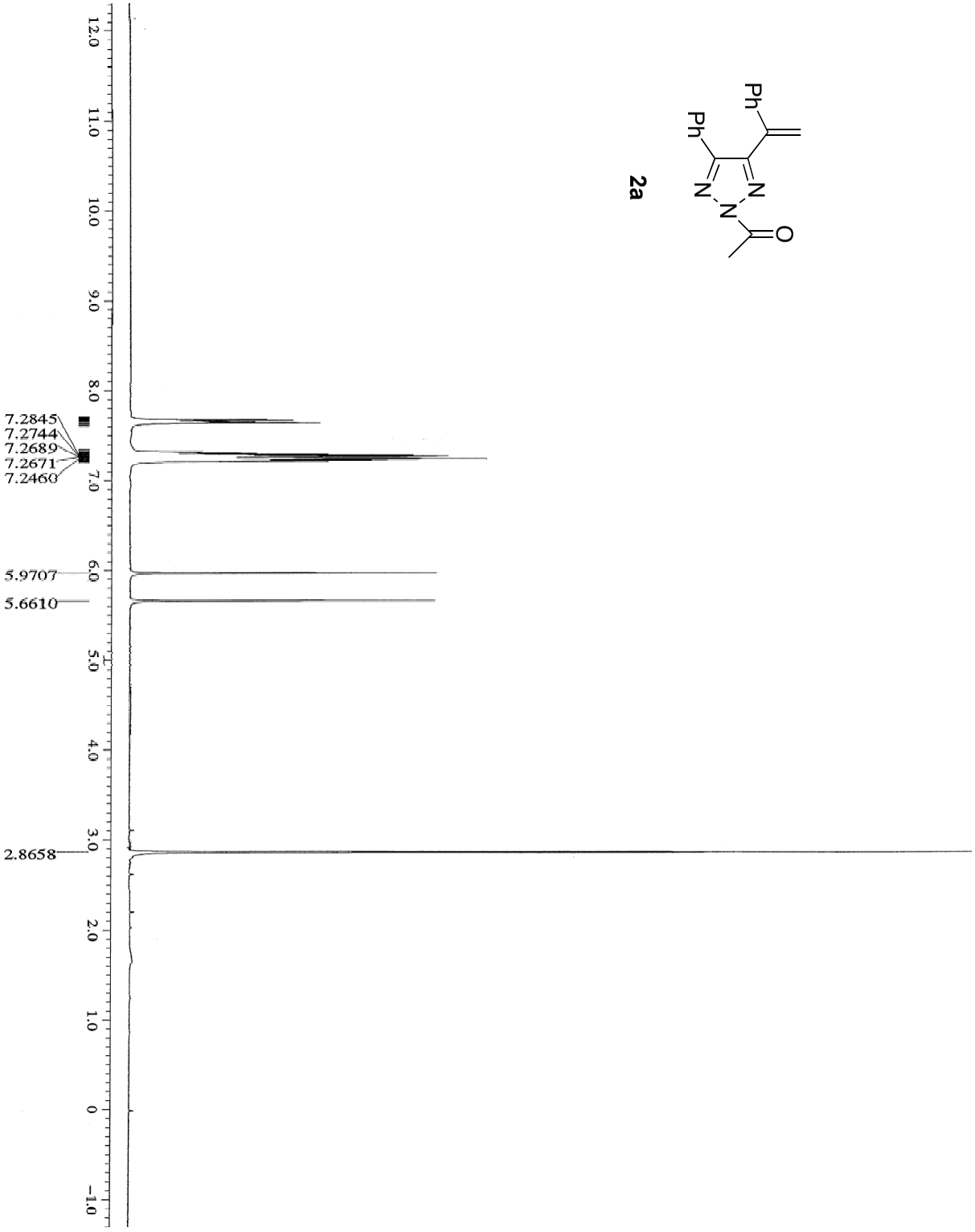
O
Ph
N
NH
N

4b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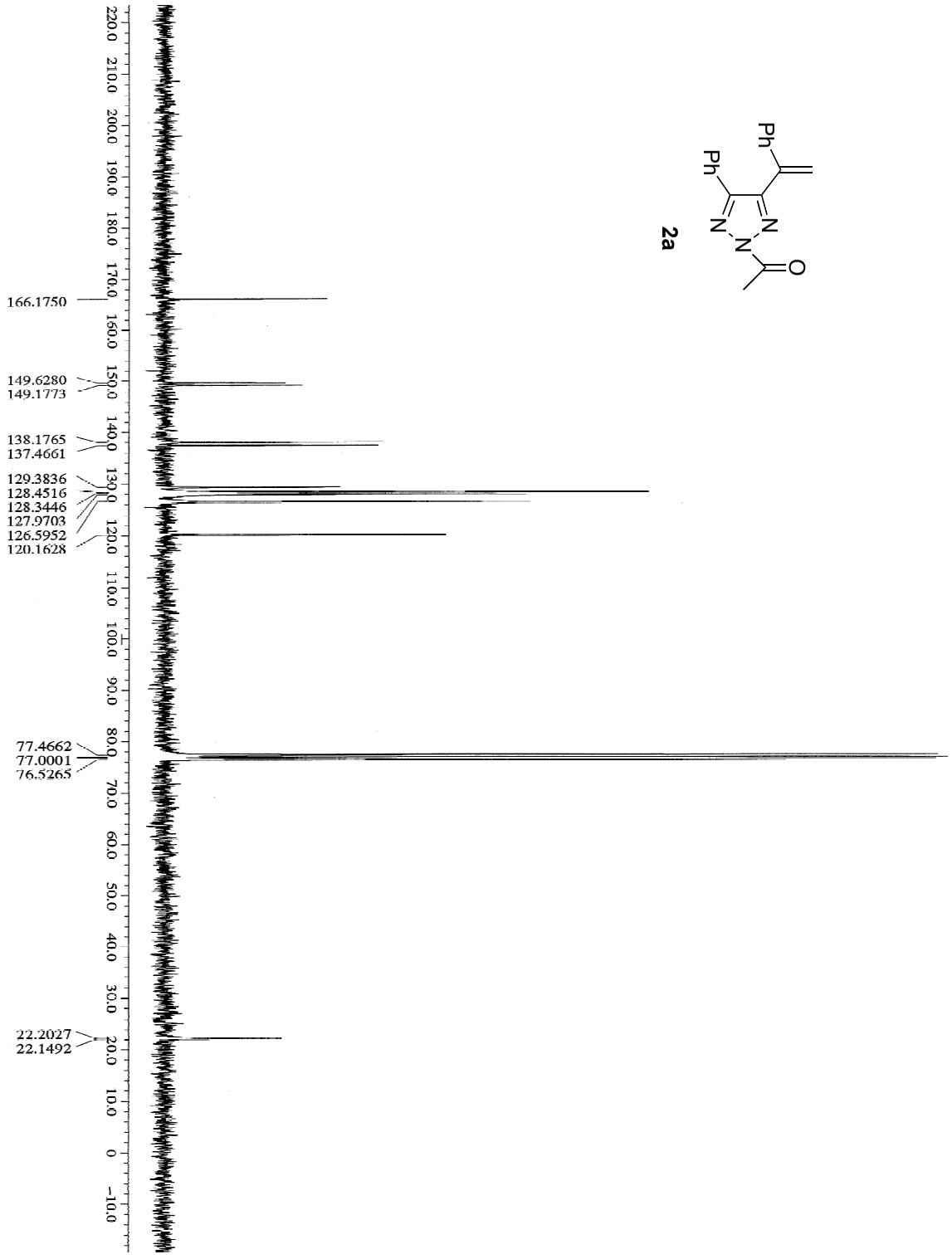
N
N
O

2a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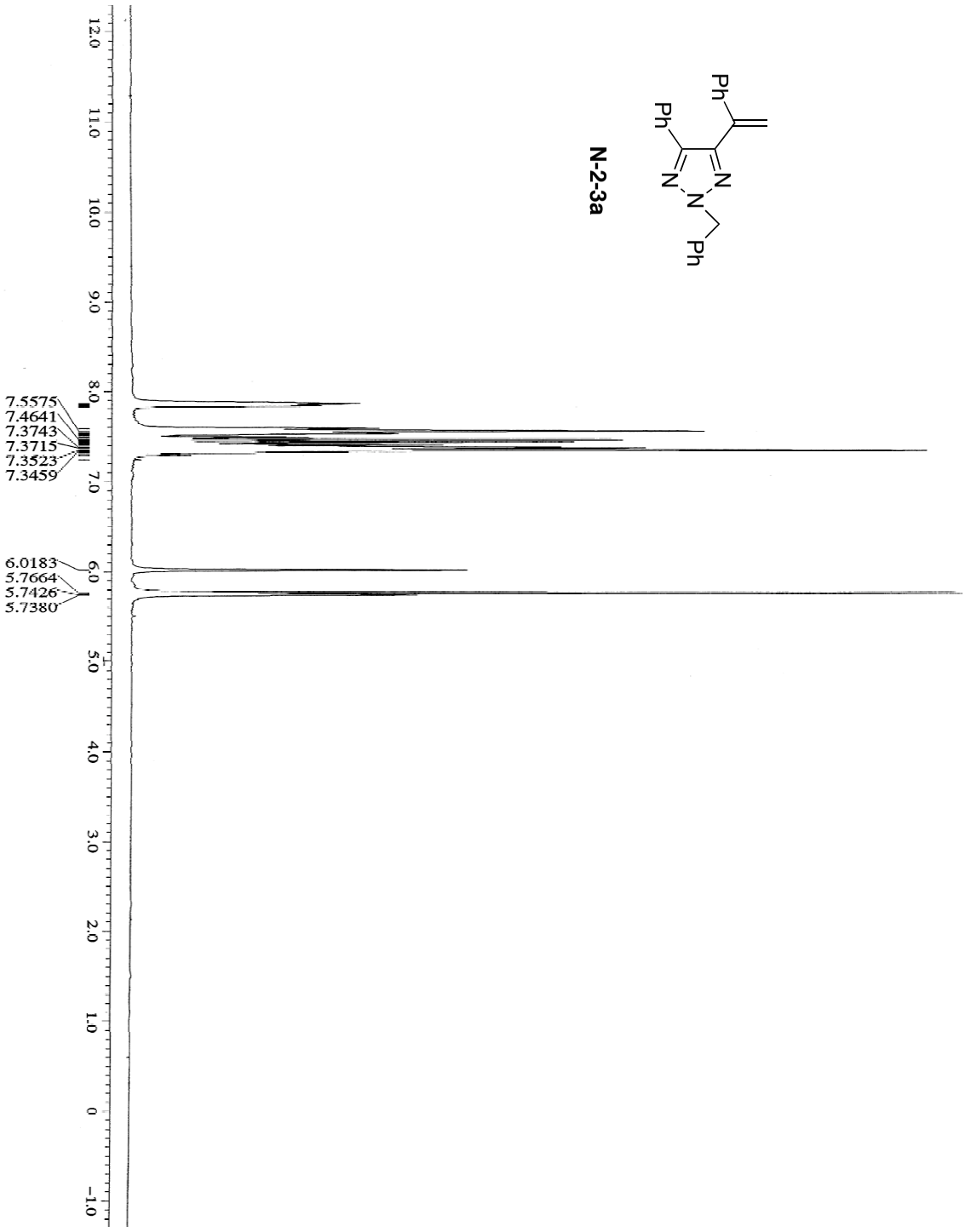
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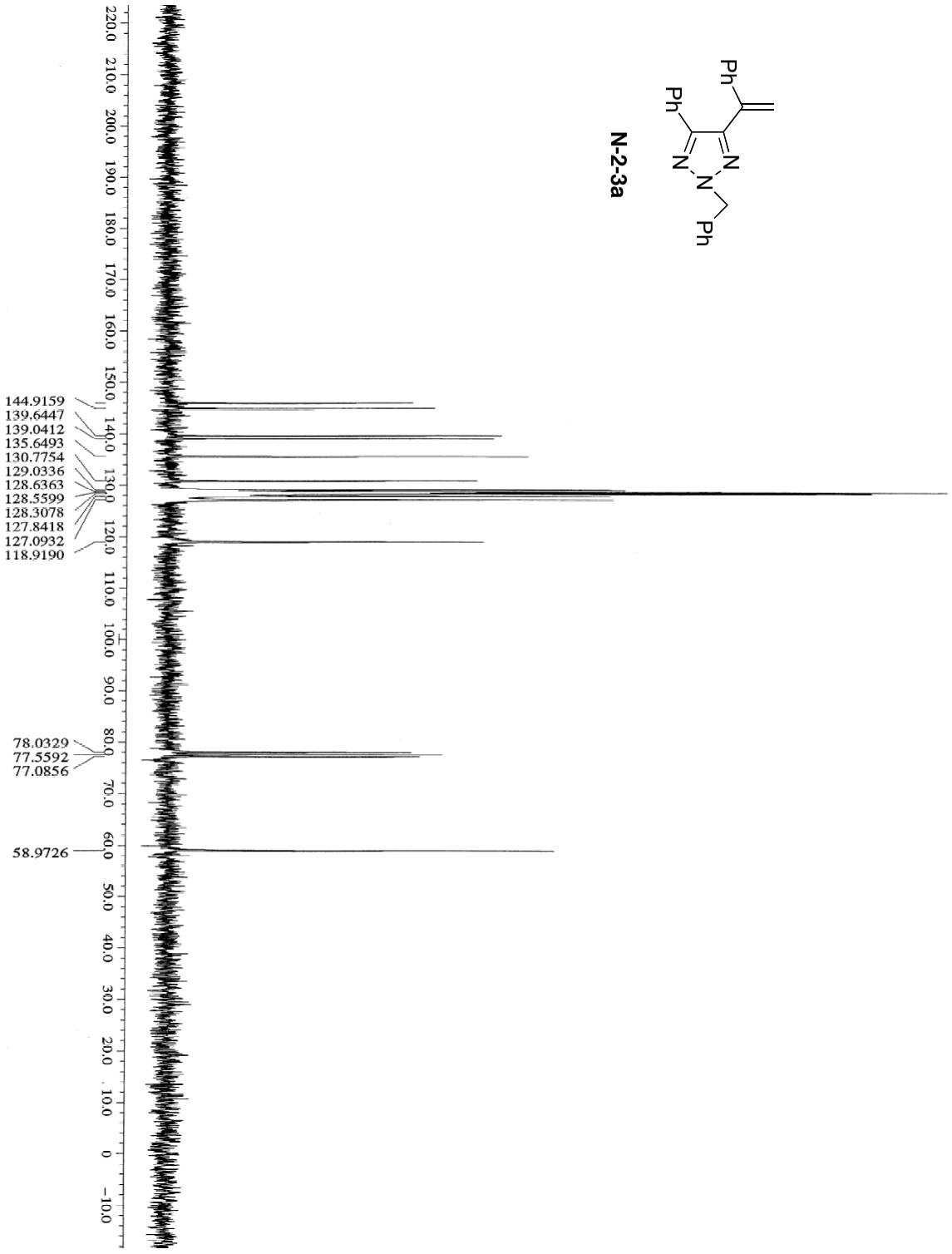
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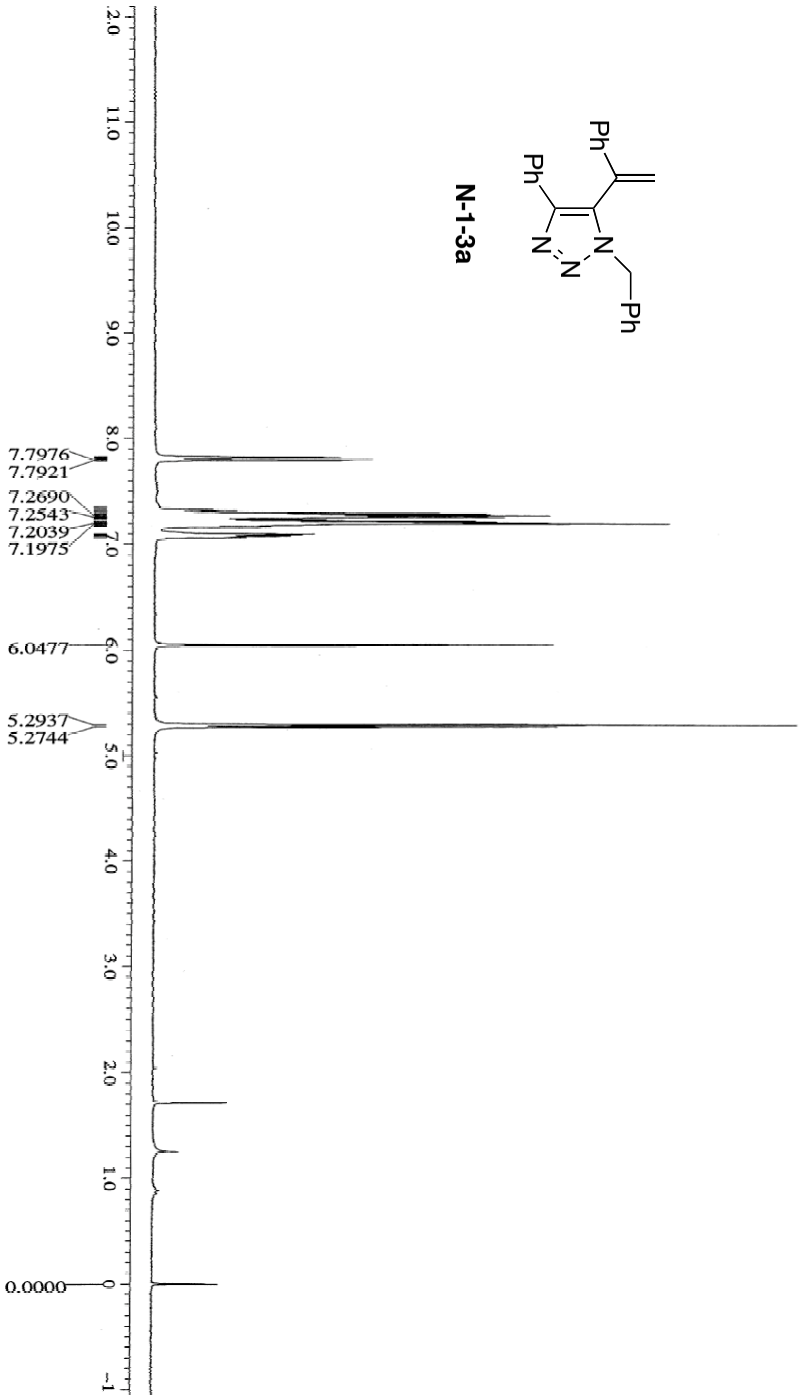
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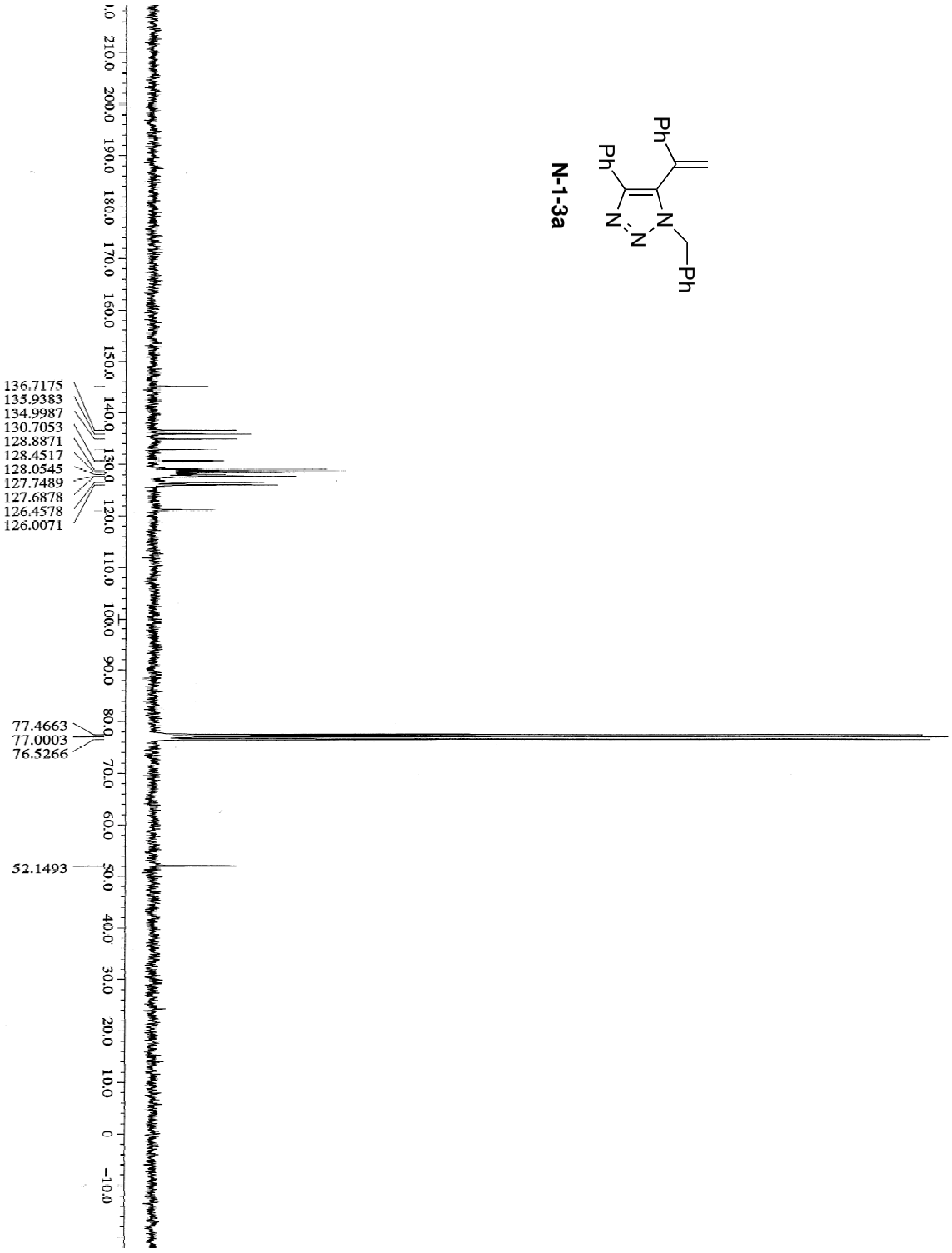
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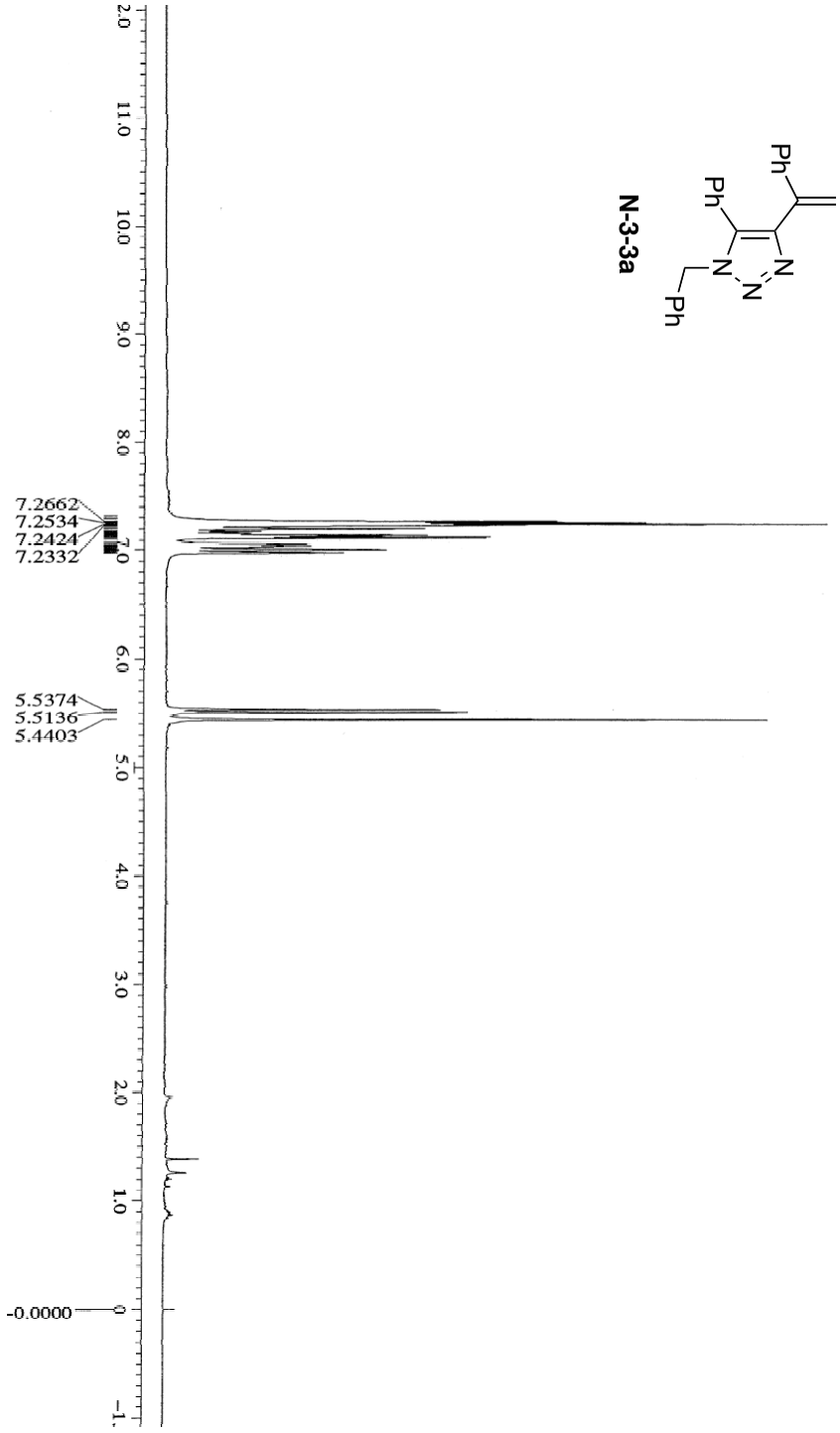
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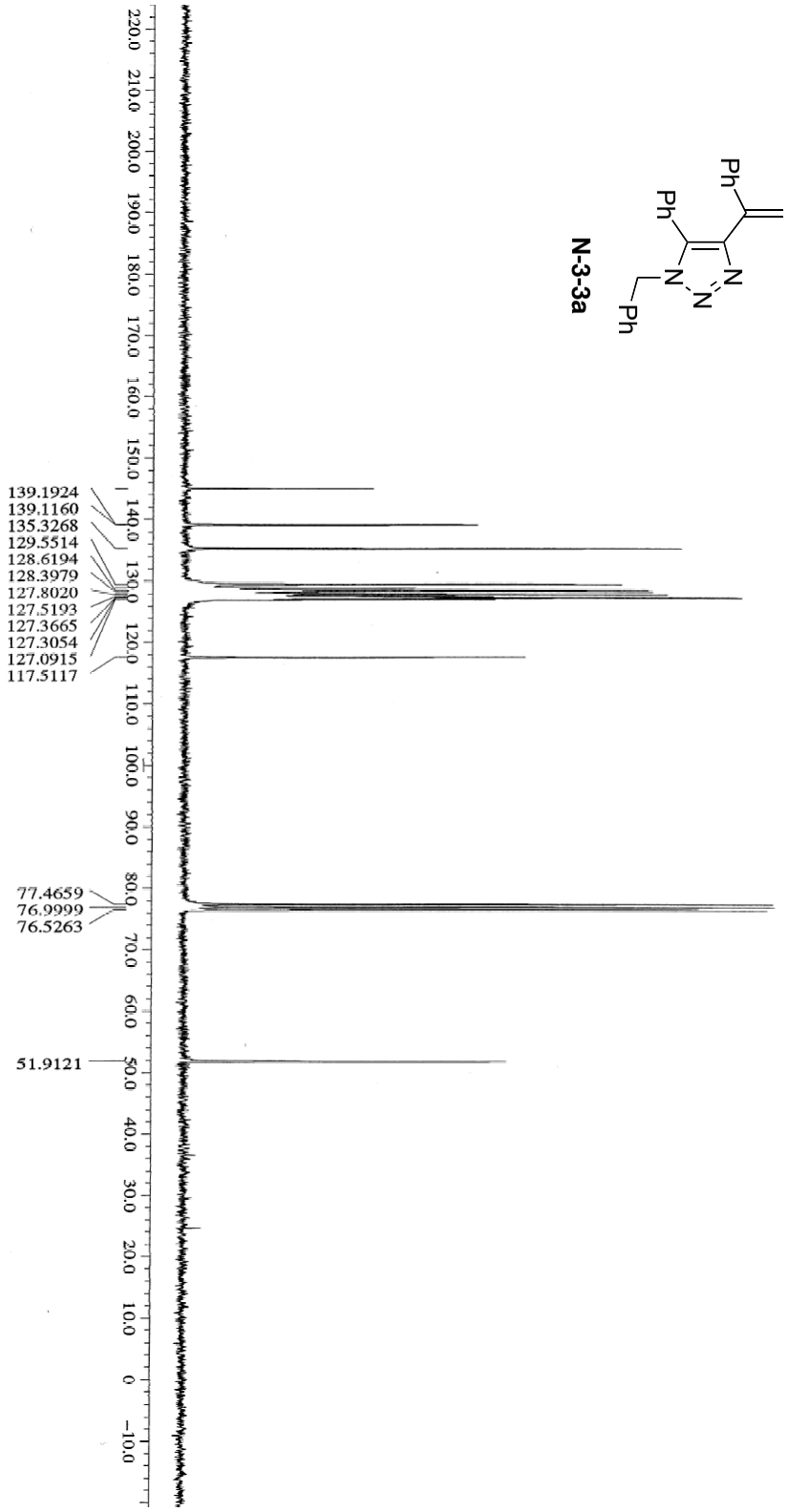
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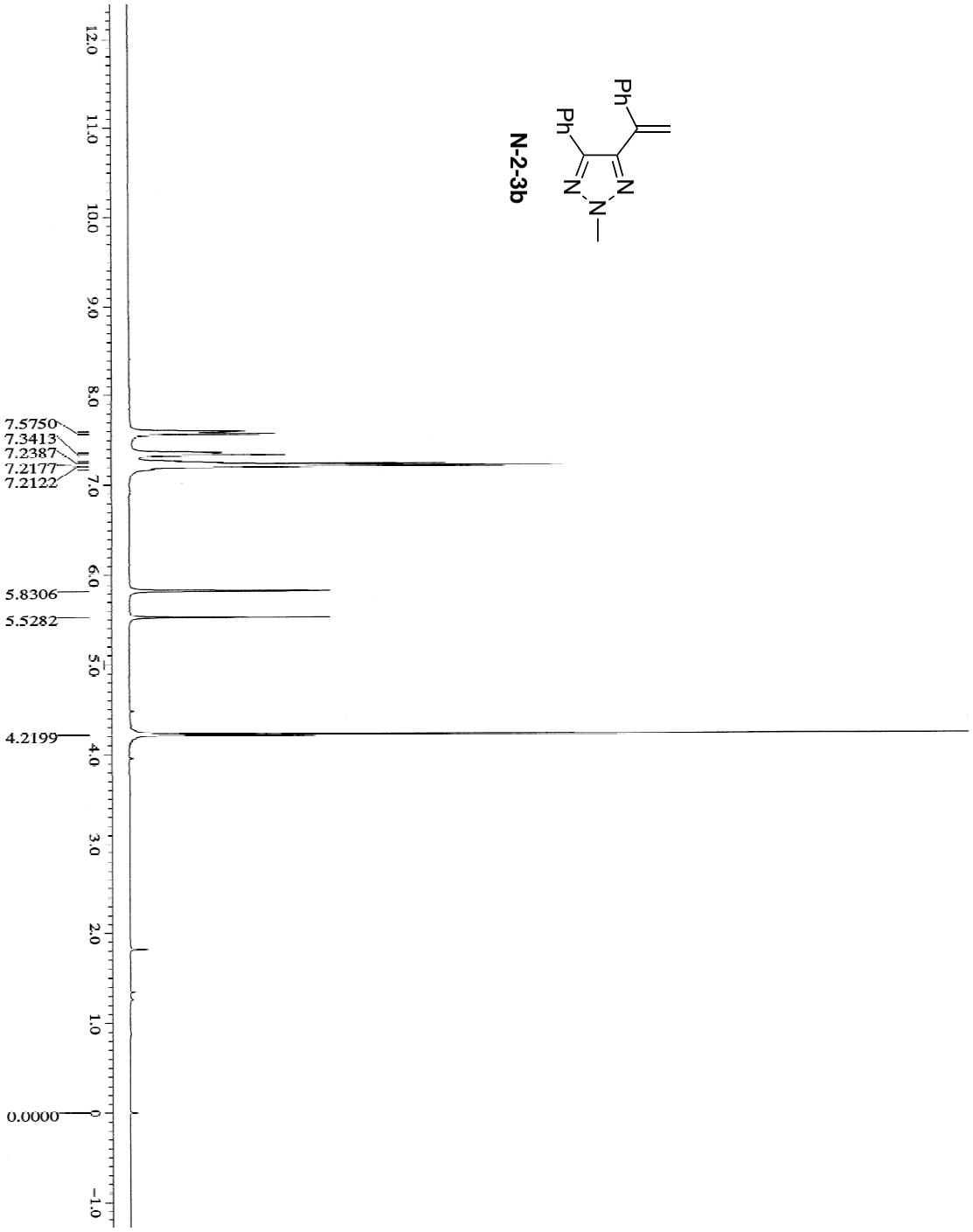
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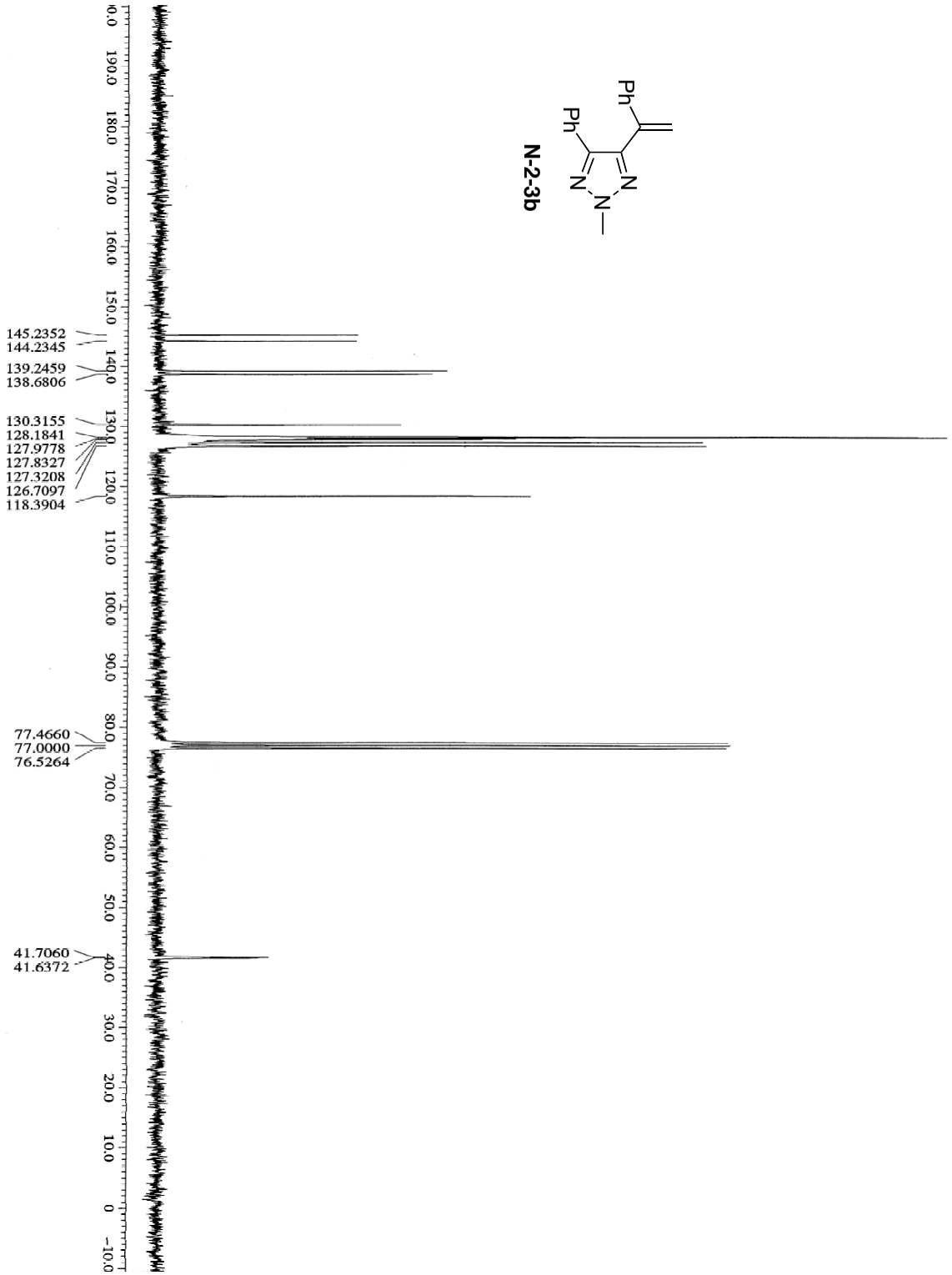
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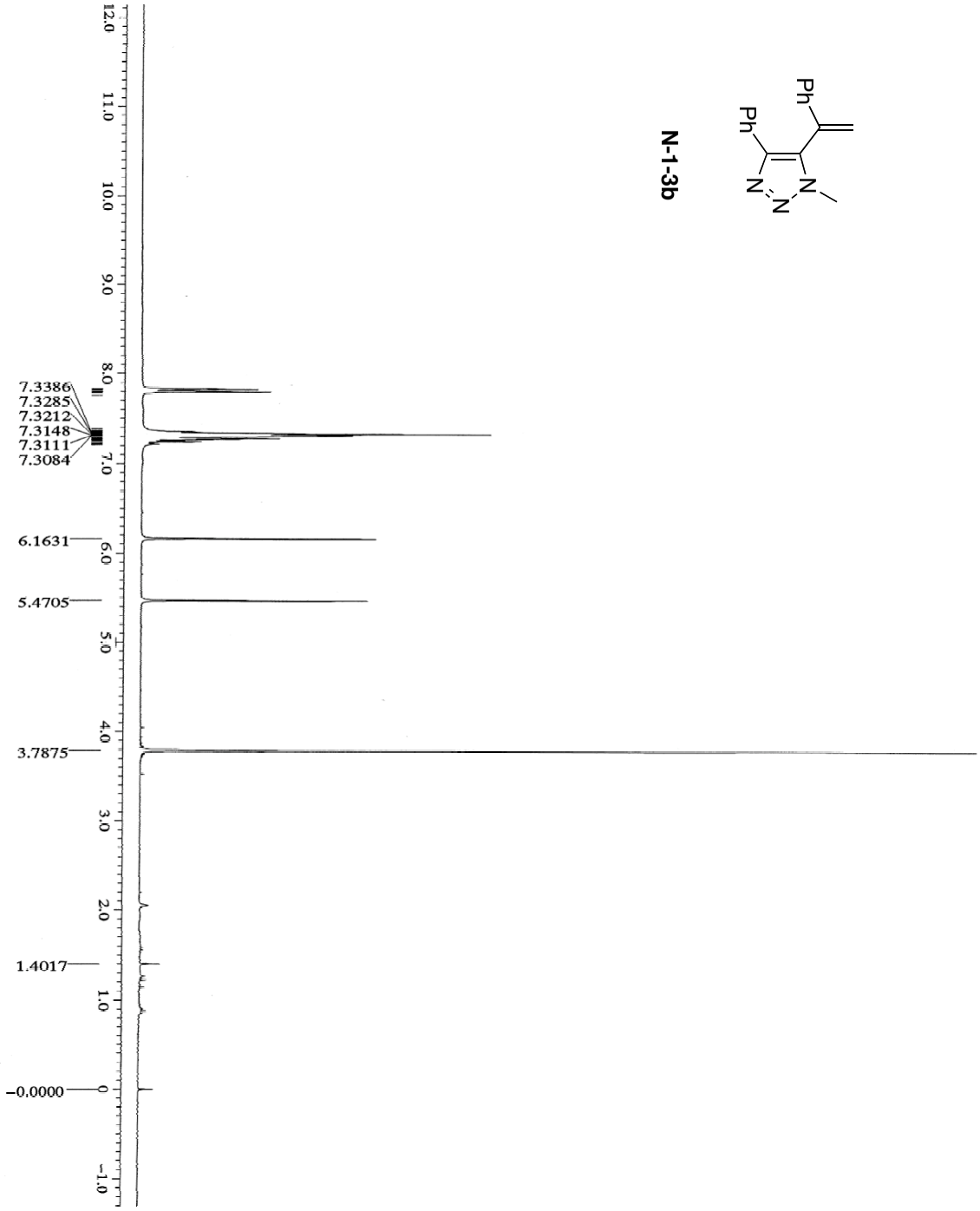
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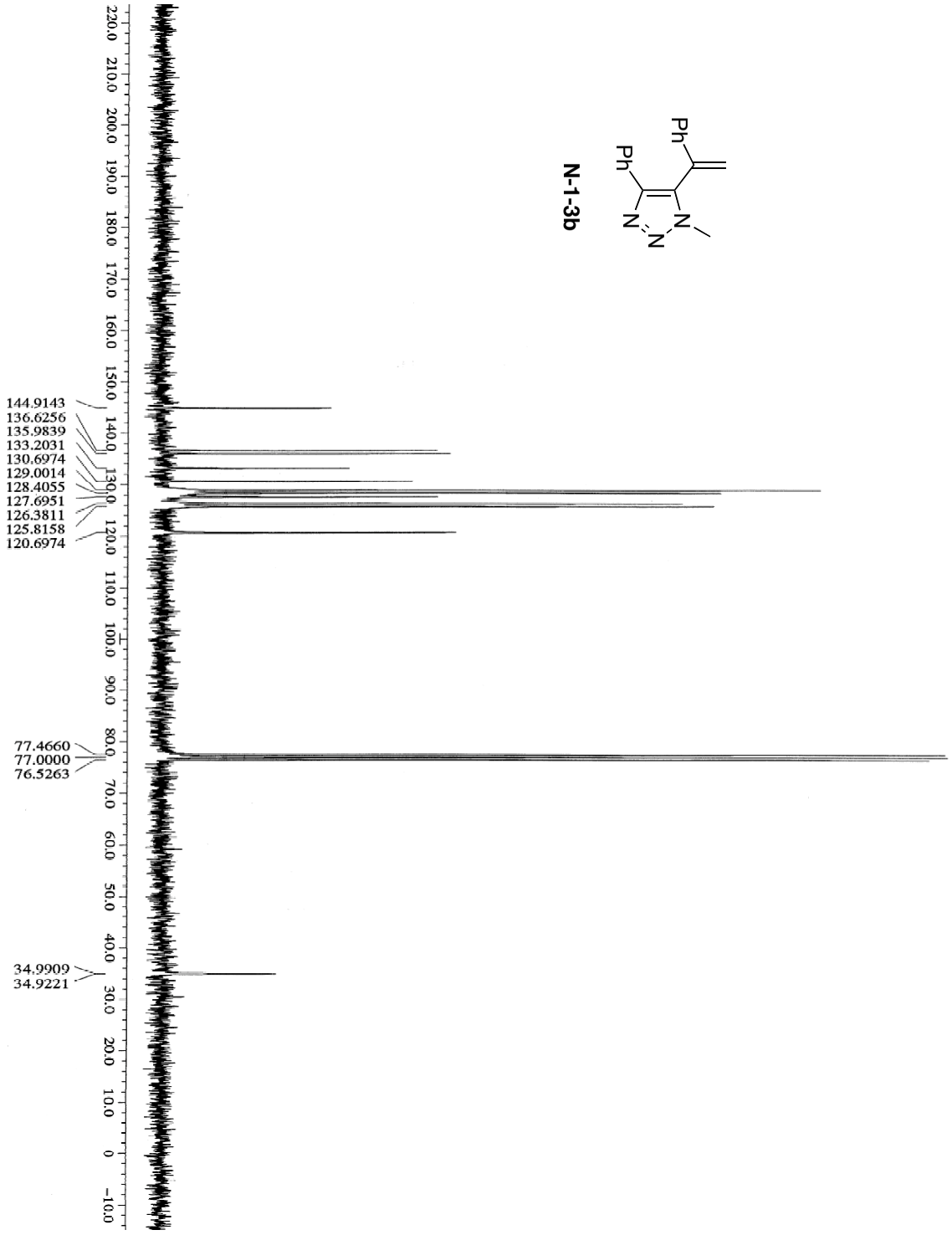
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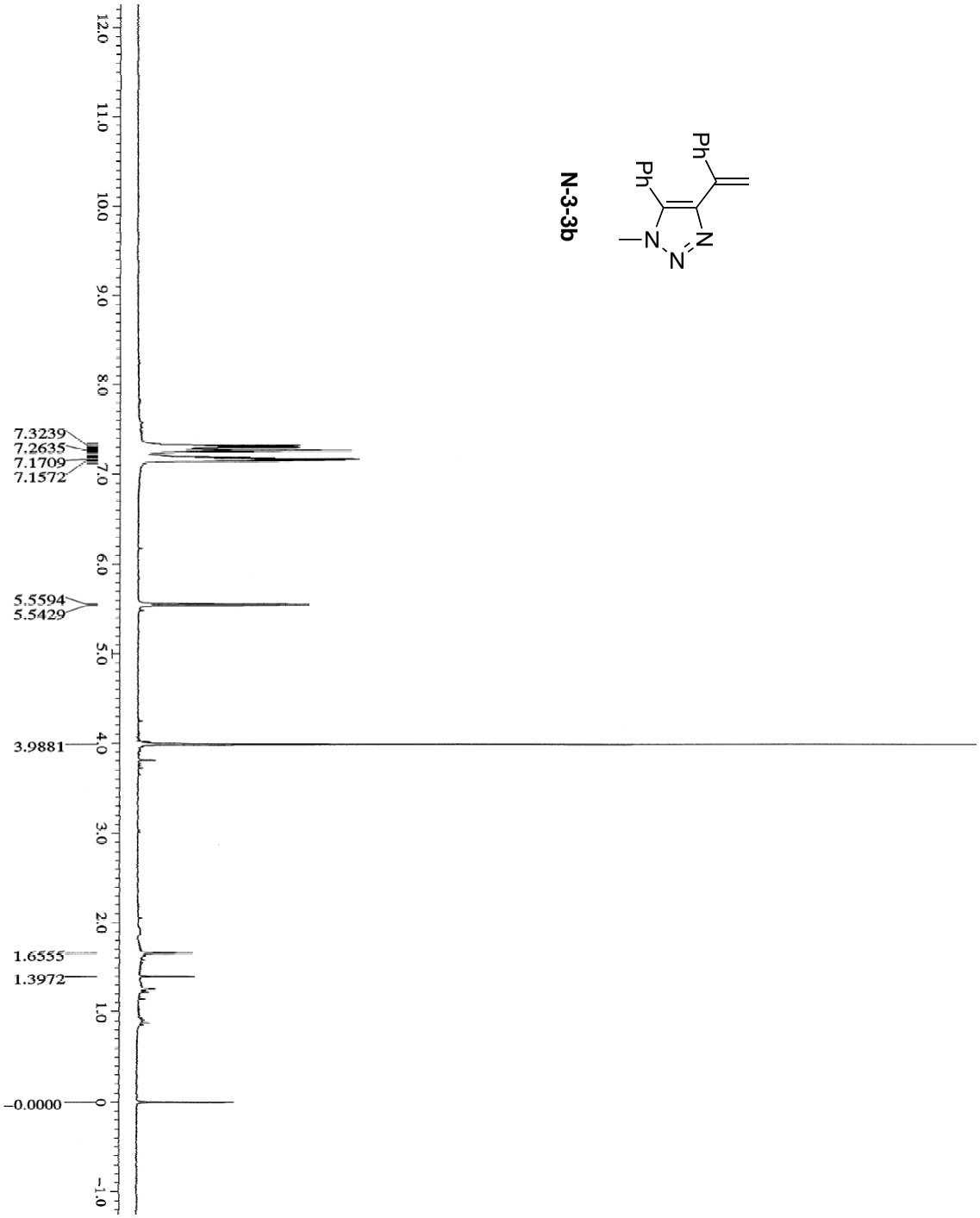
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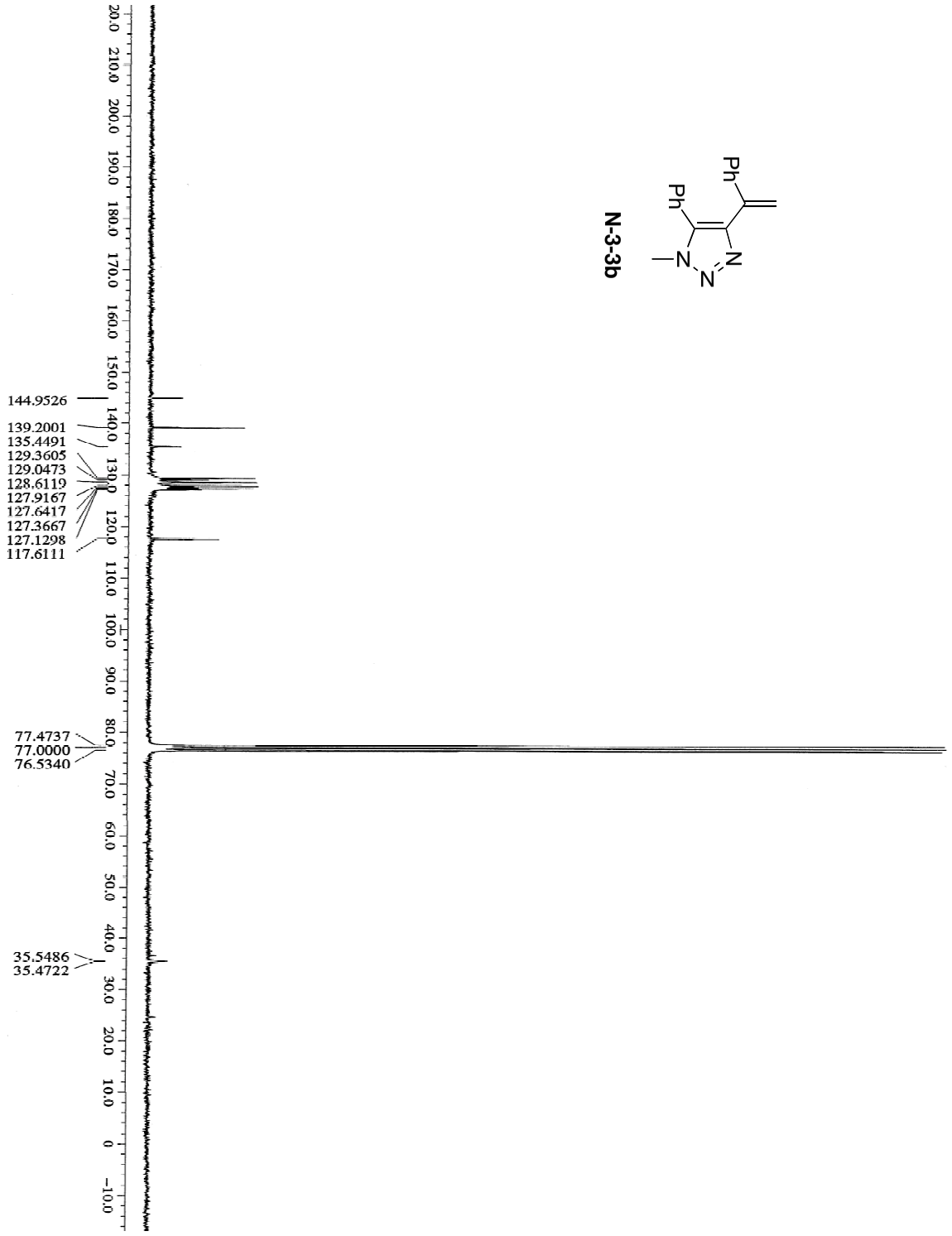
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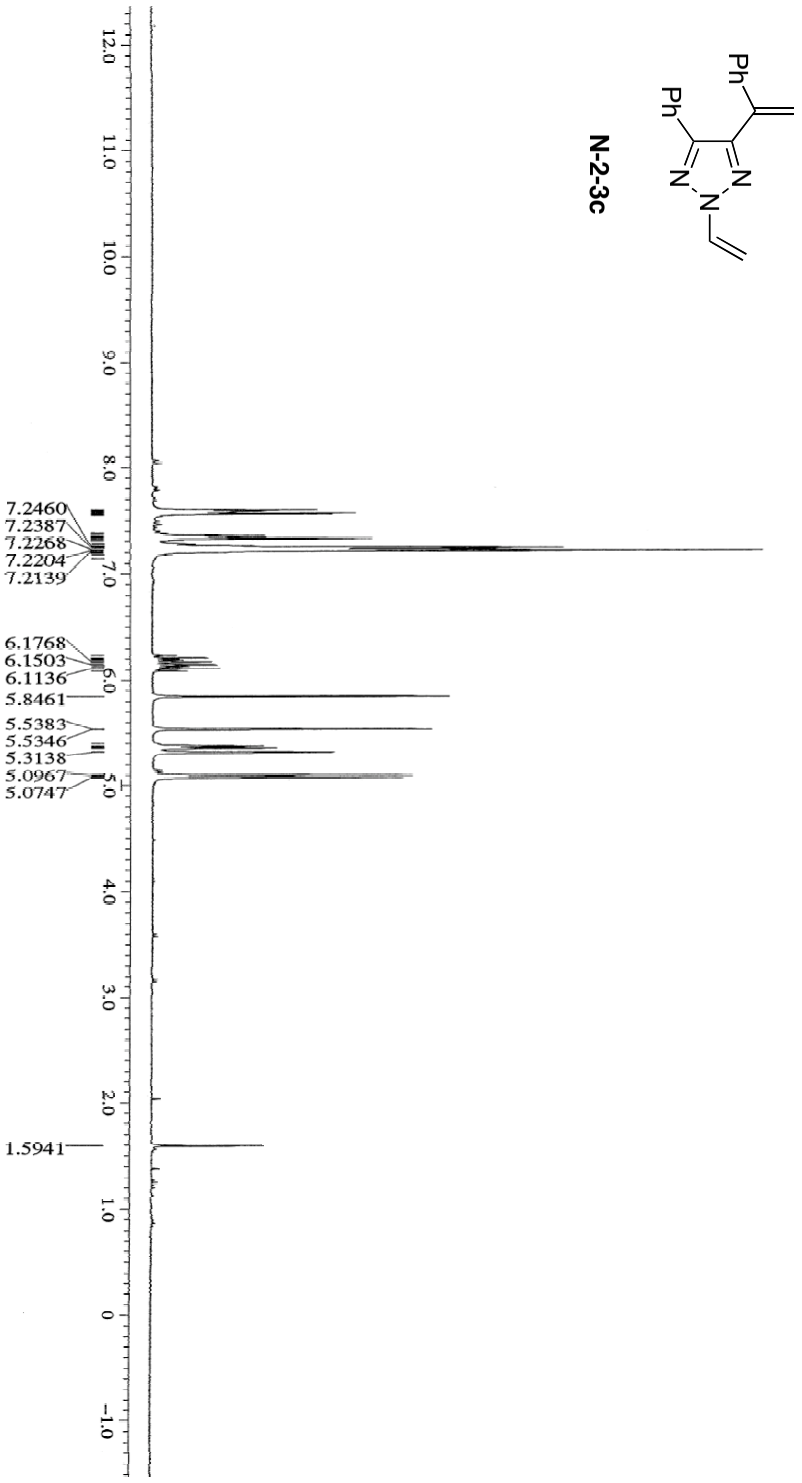
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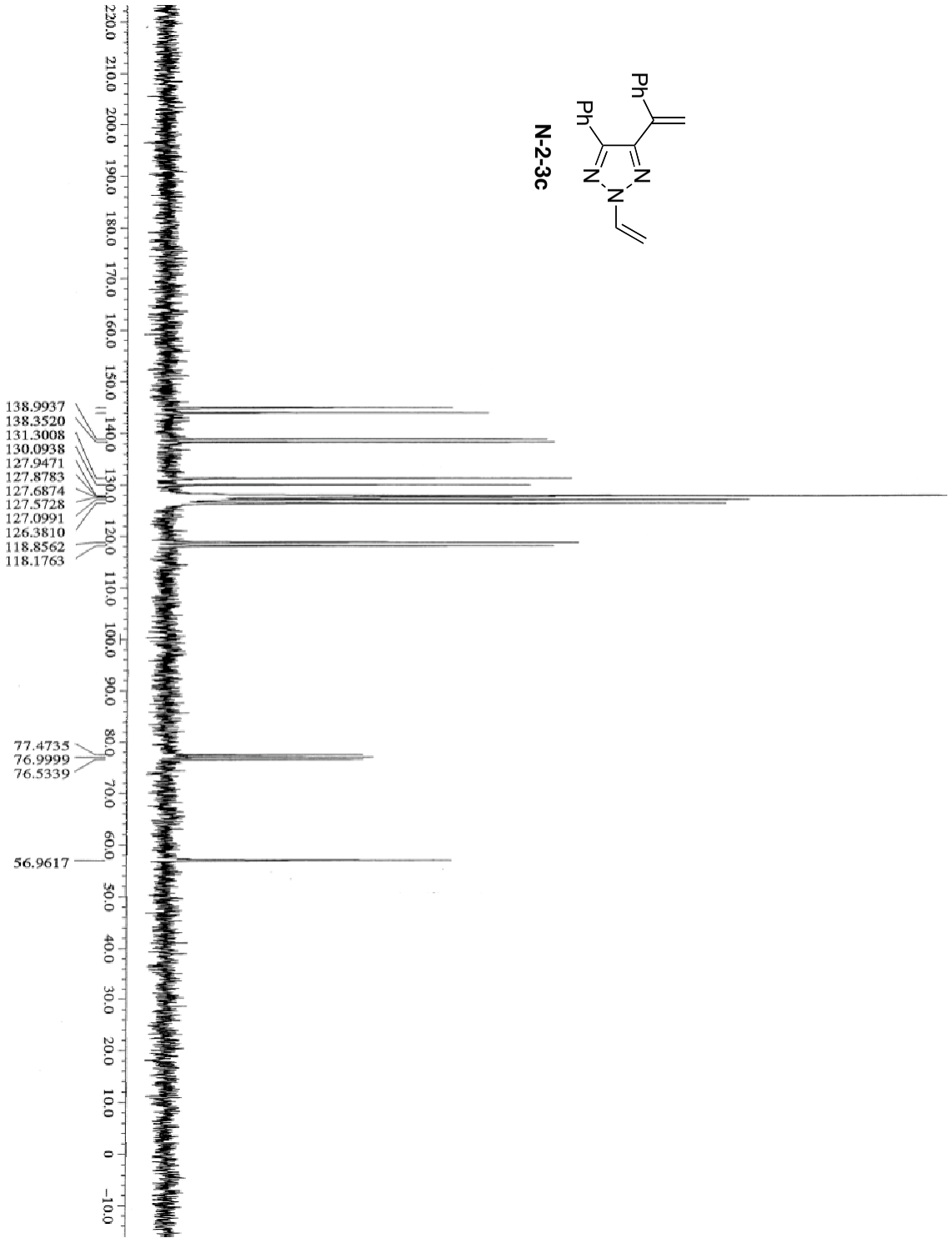
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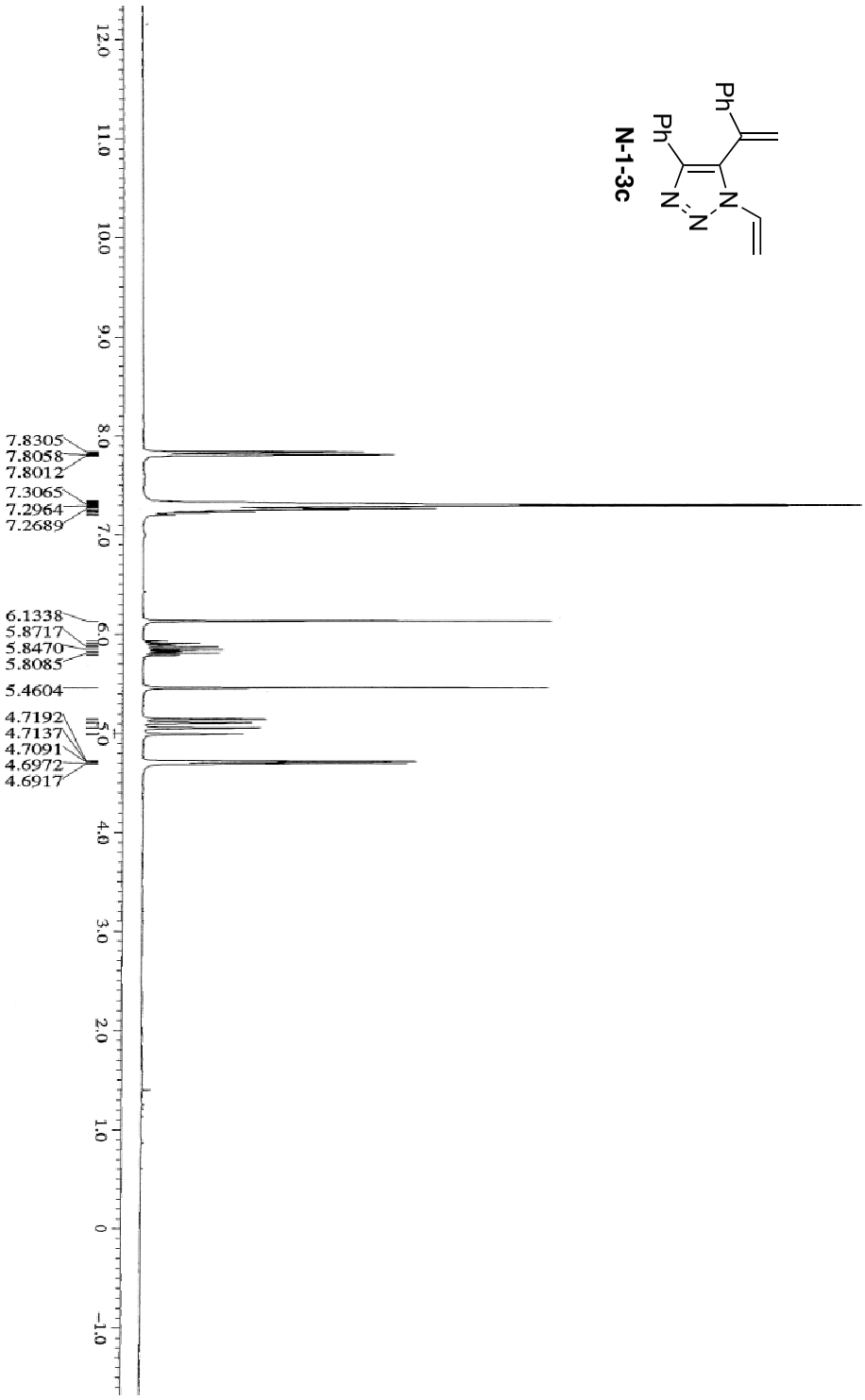
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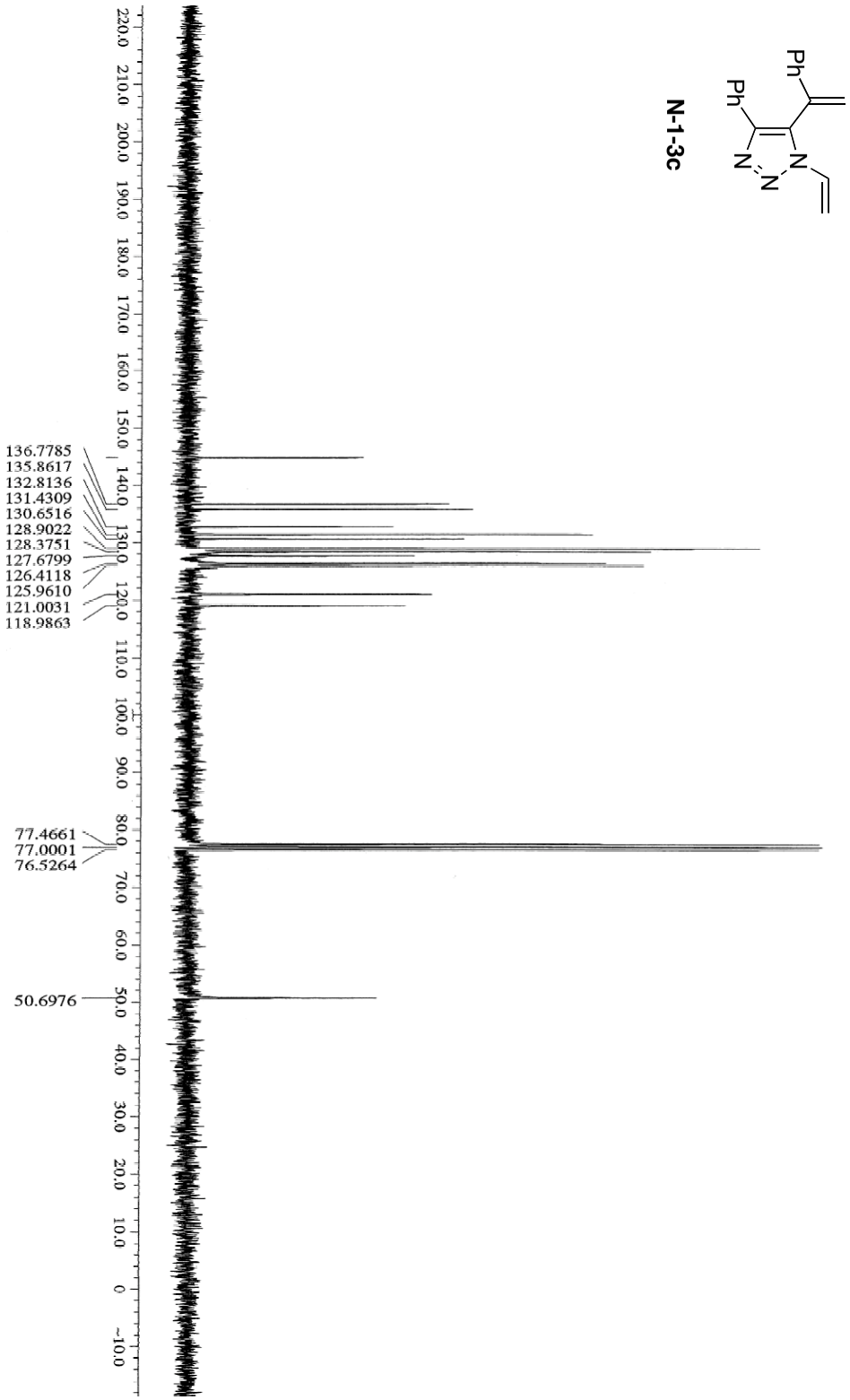
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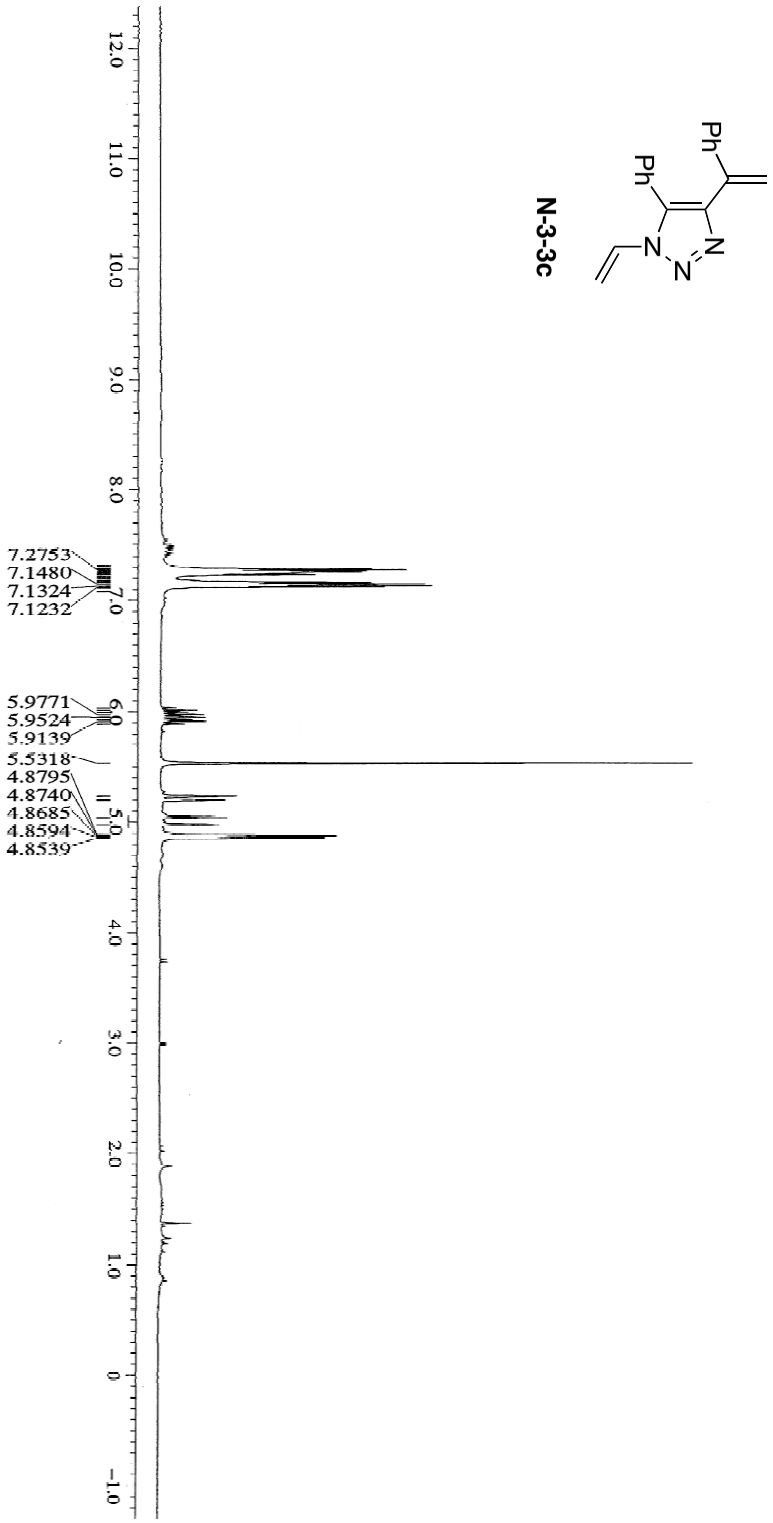
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N-3-3c

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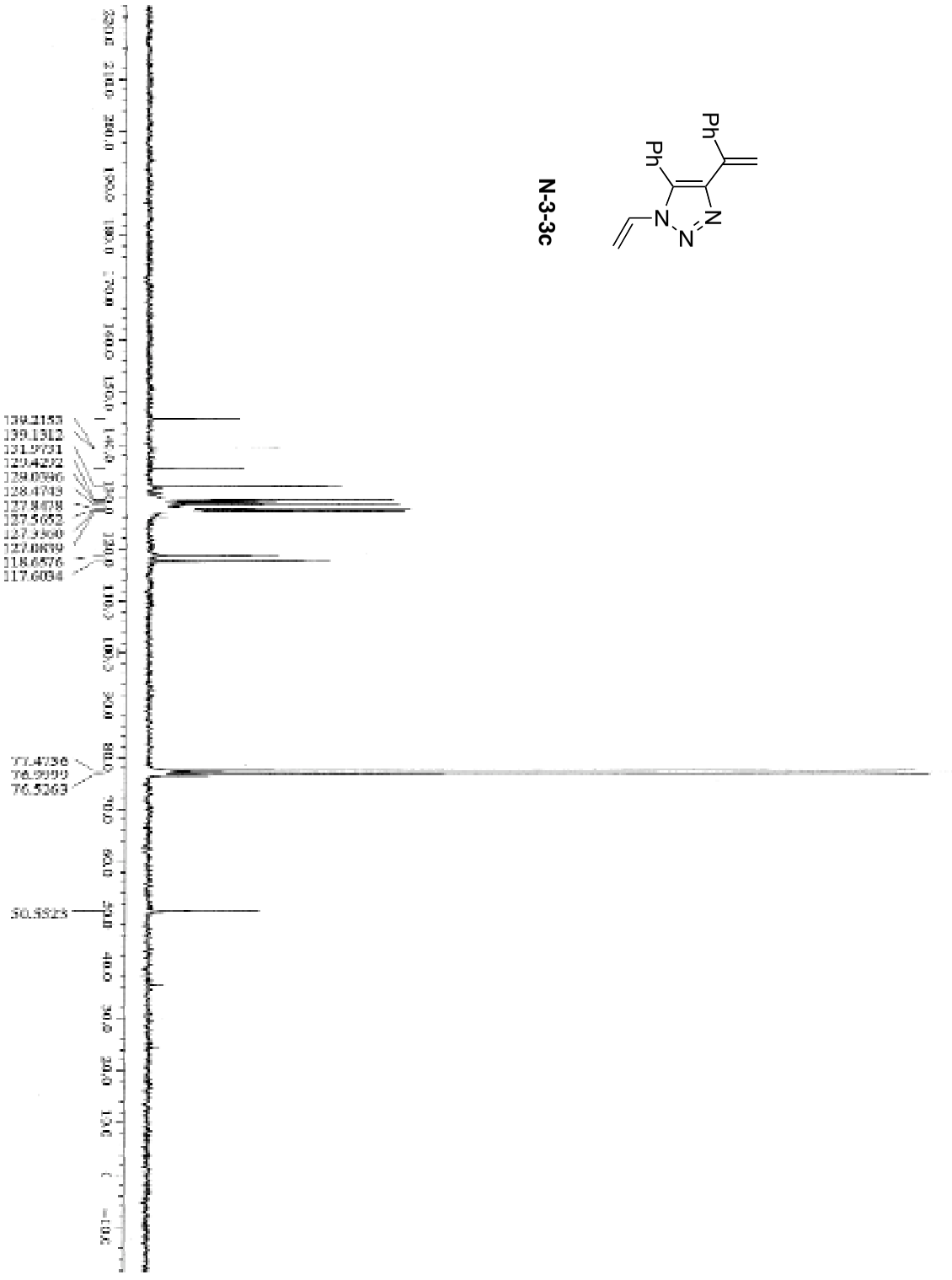
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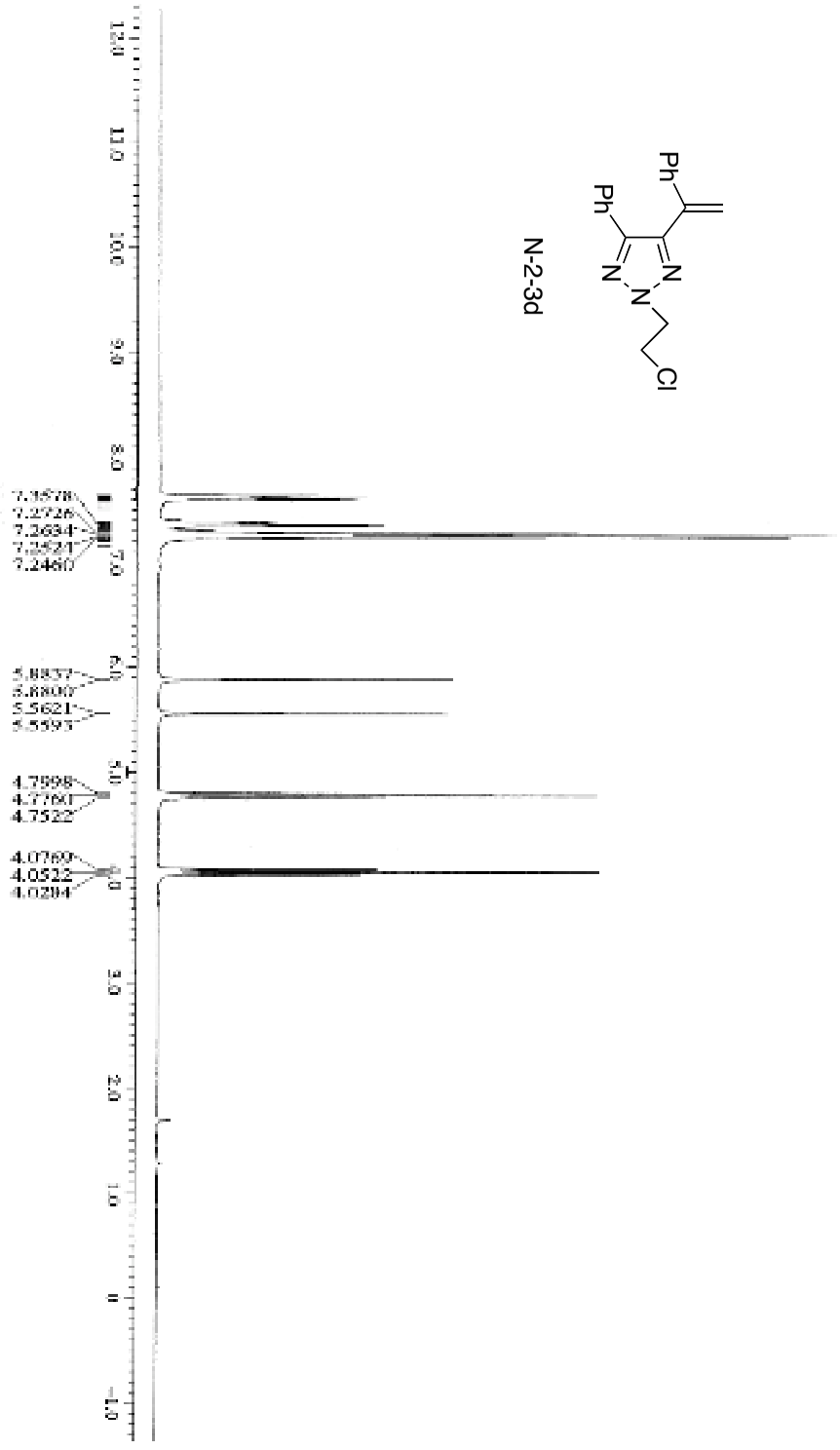
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Ph
N
N
N
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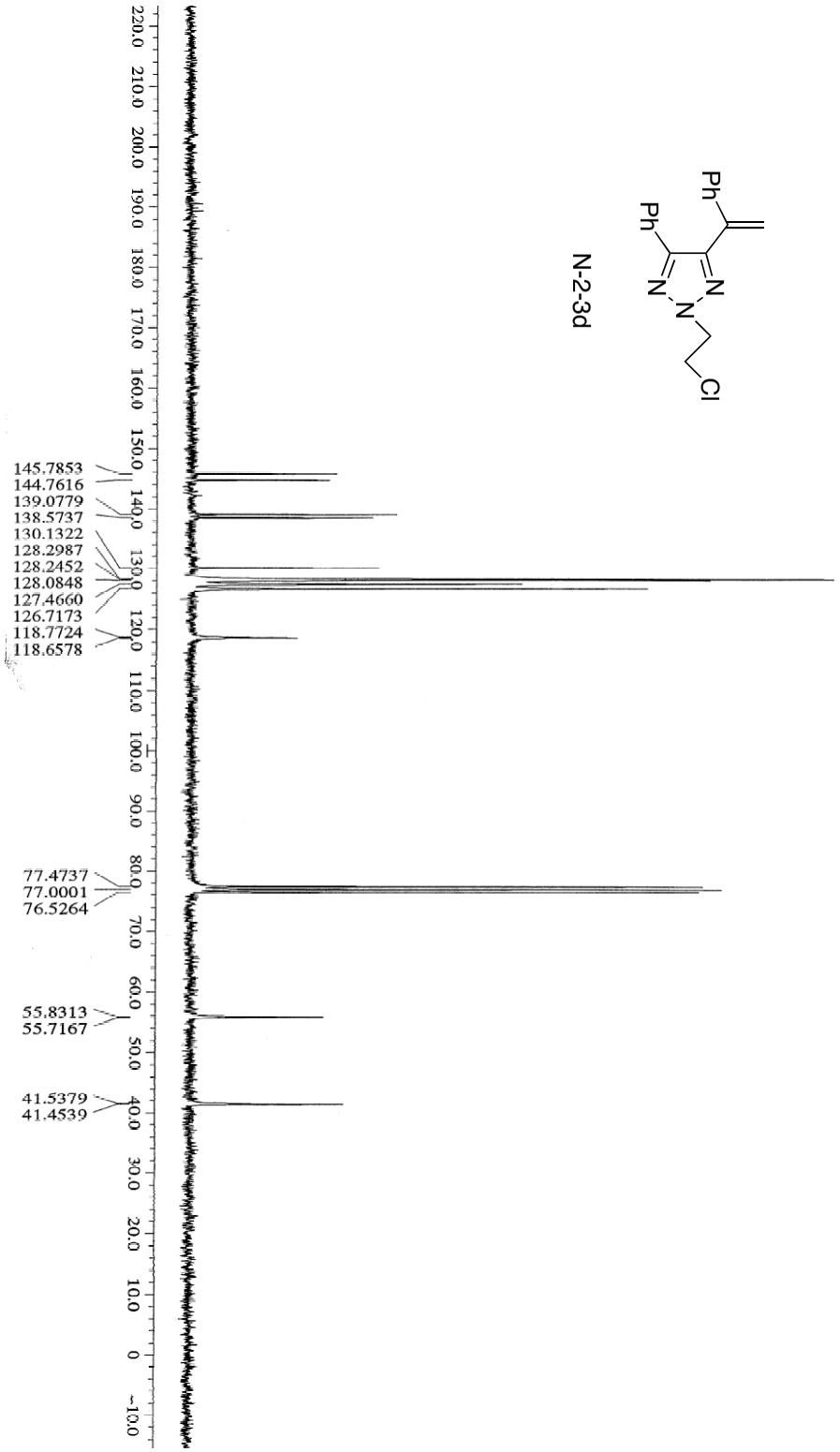
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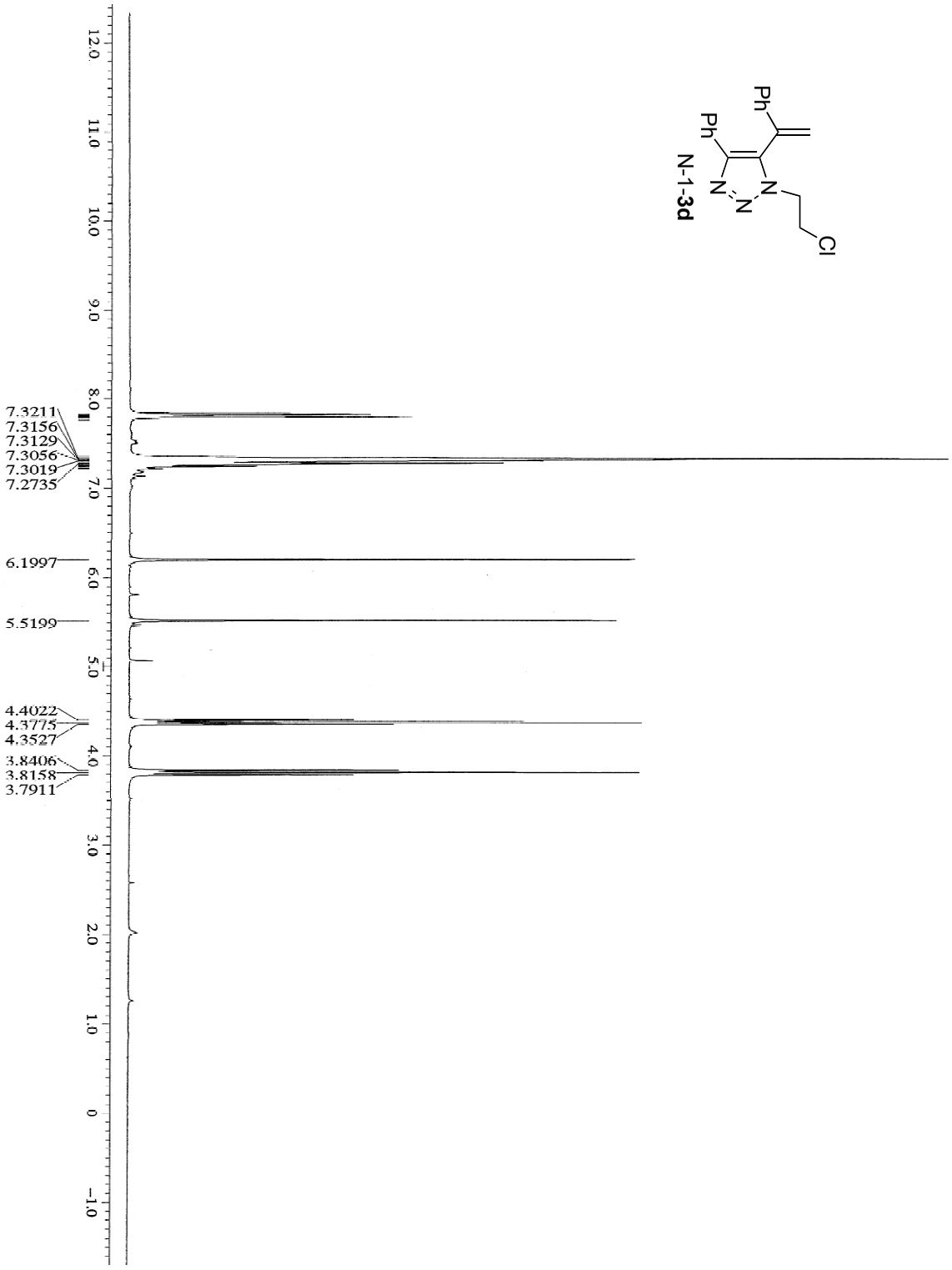
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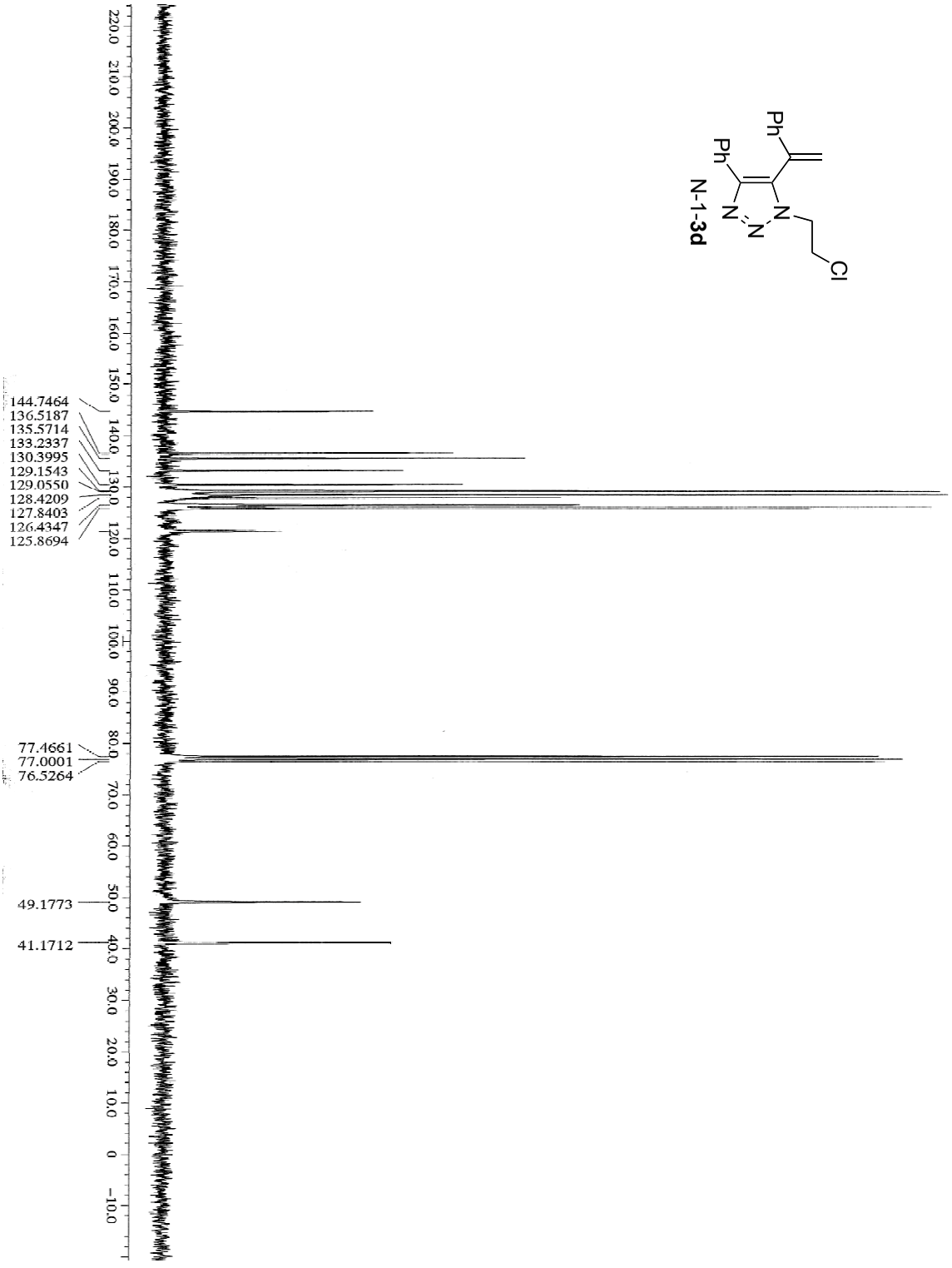
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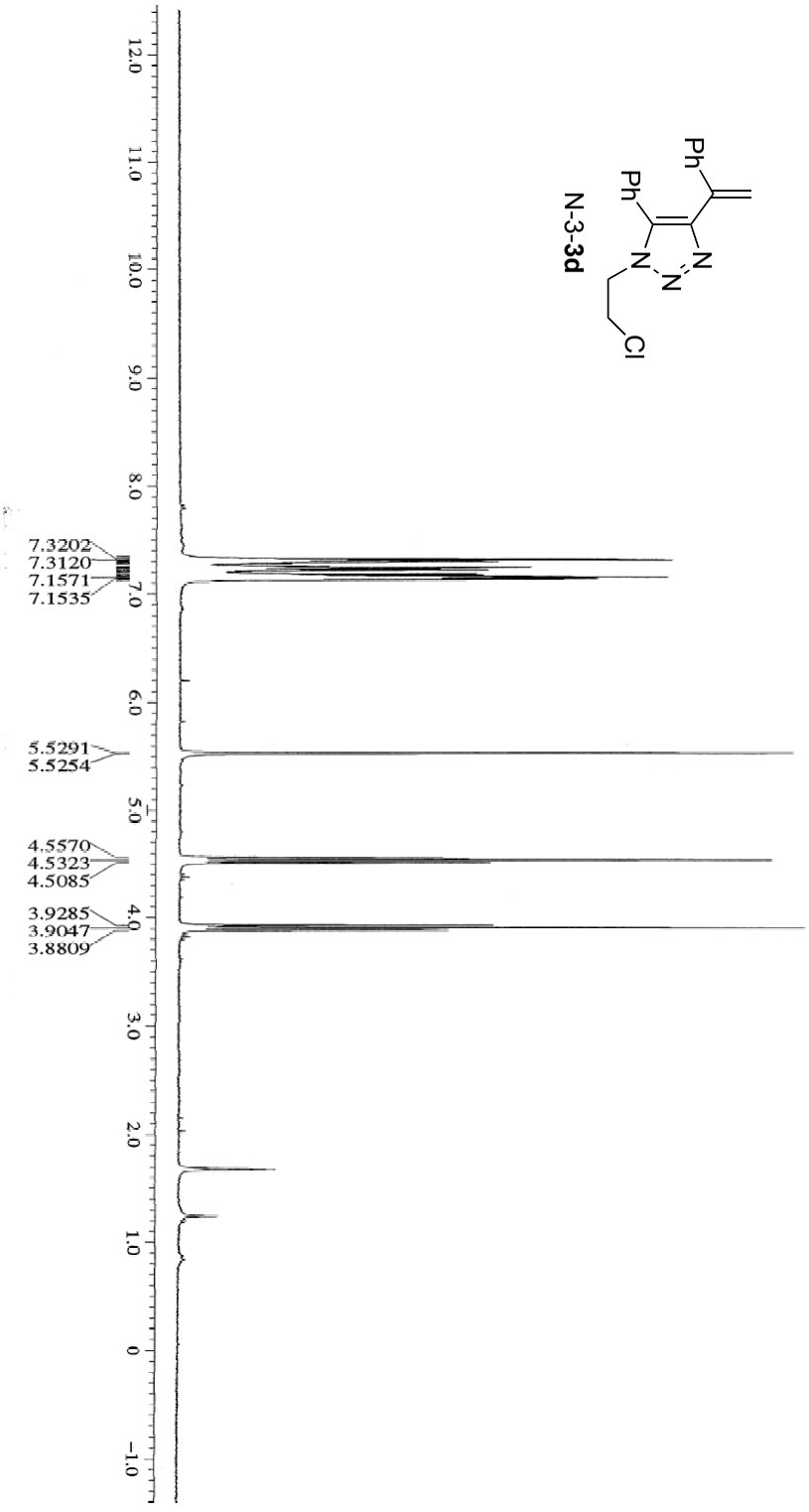
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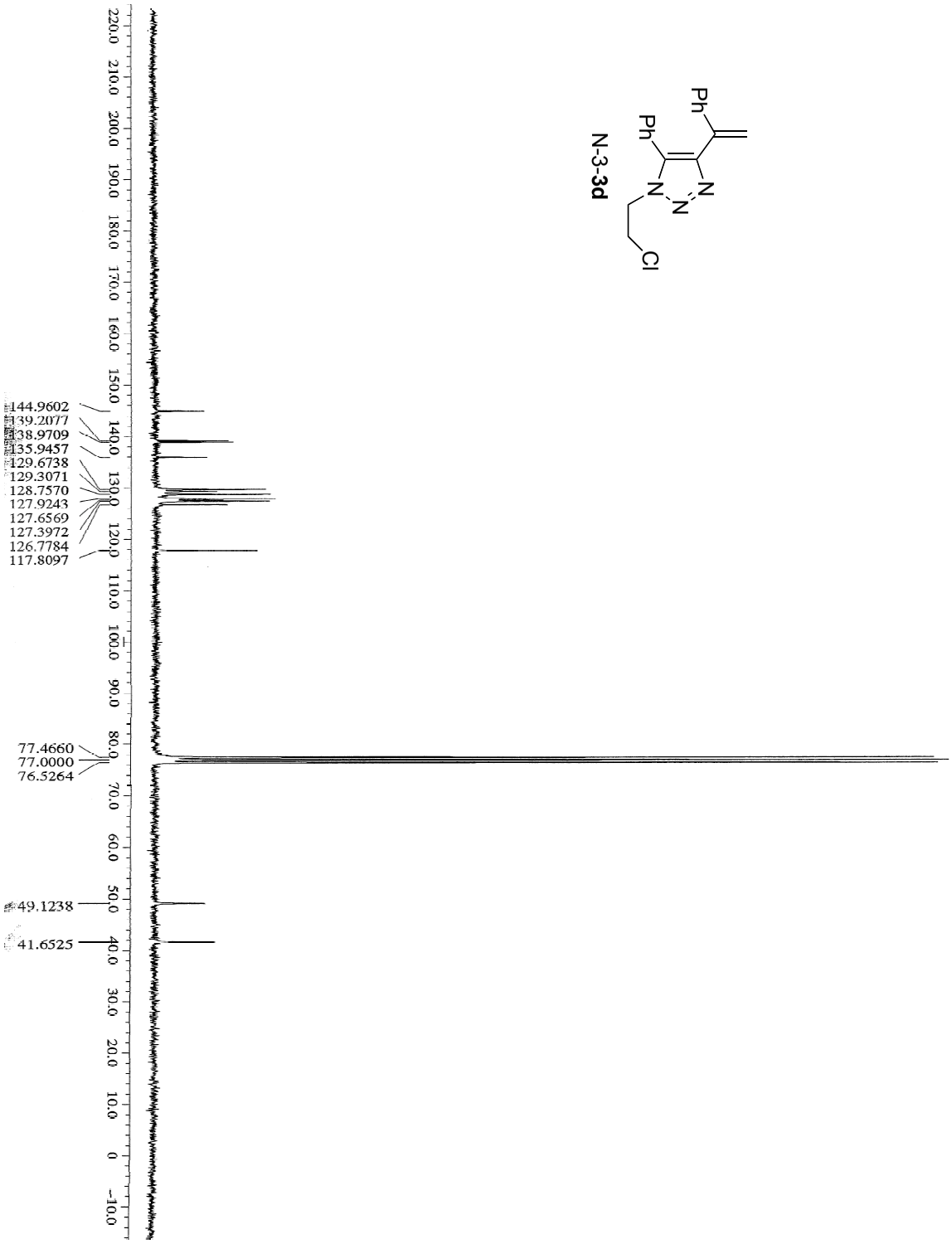
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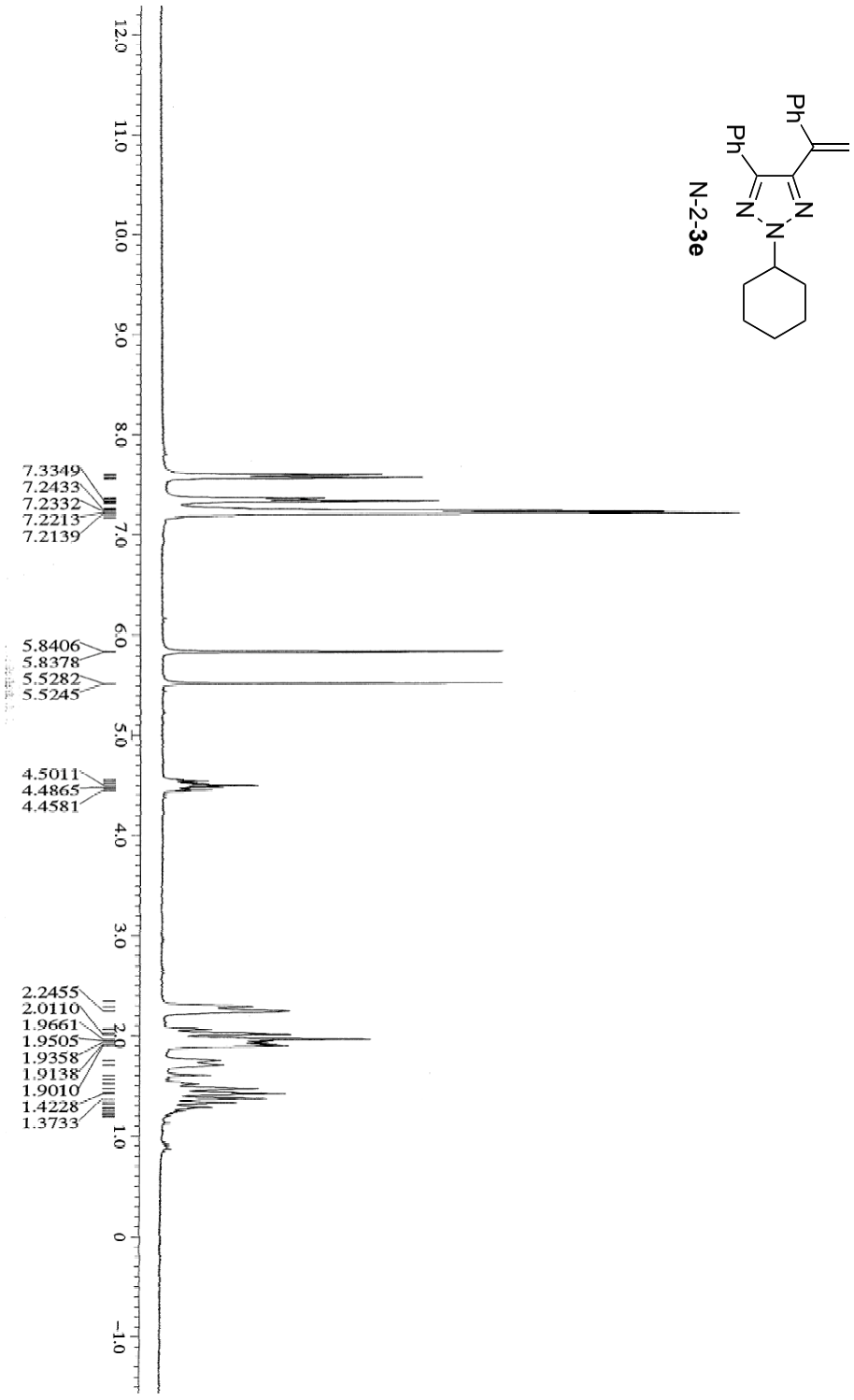
Ph
Ph
N
N
N
Cl

N-3-**3d**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Ph
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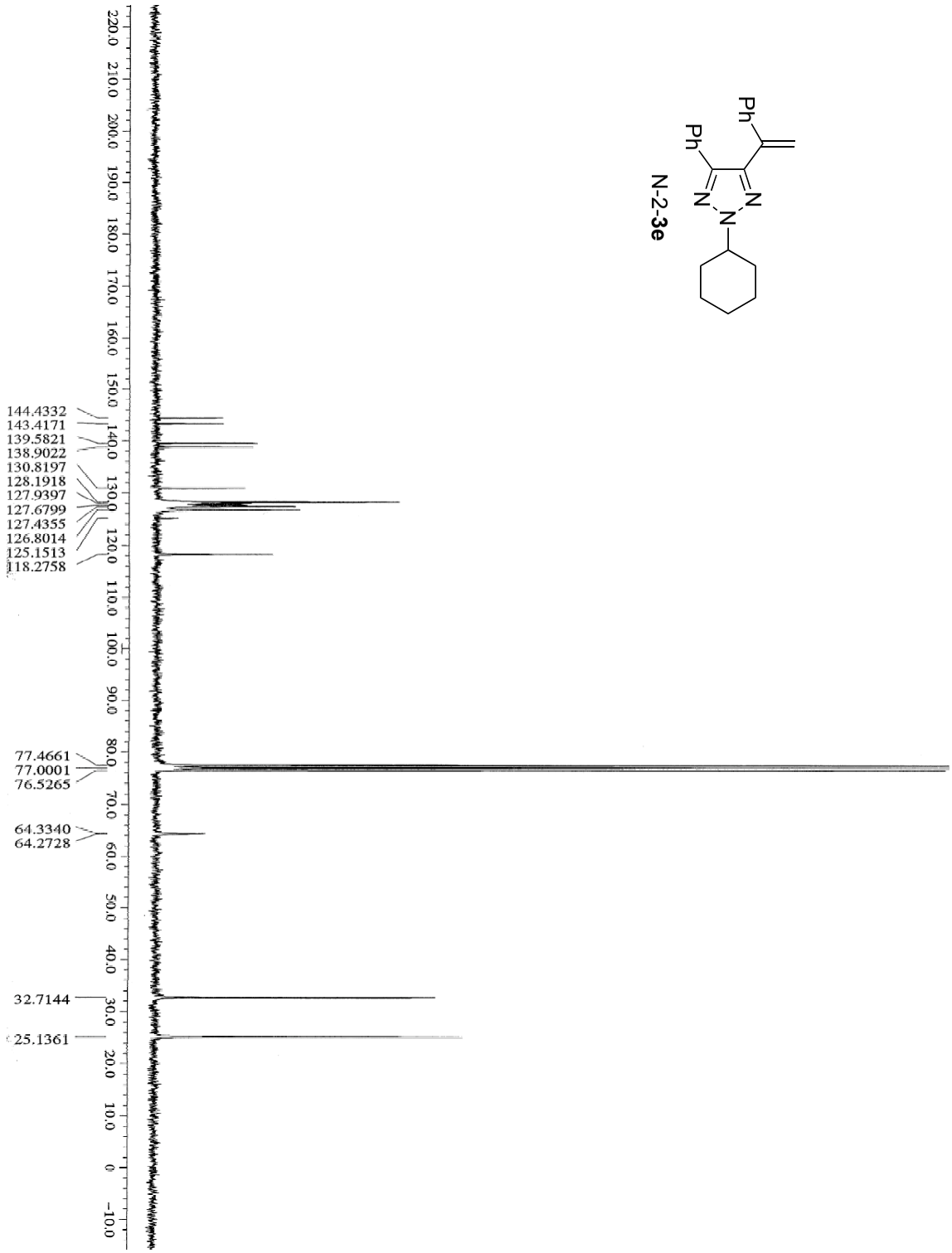
N
N
N-2-3e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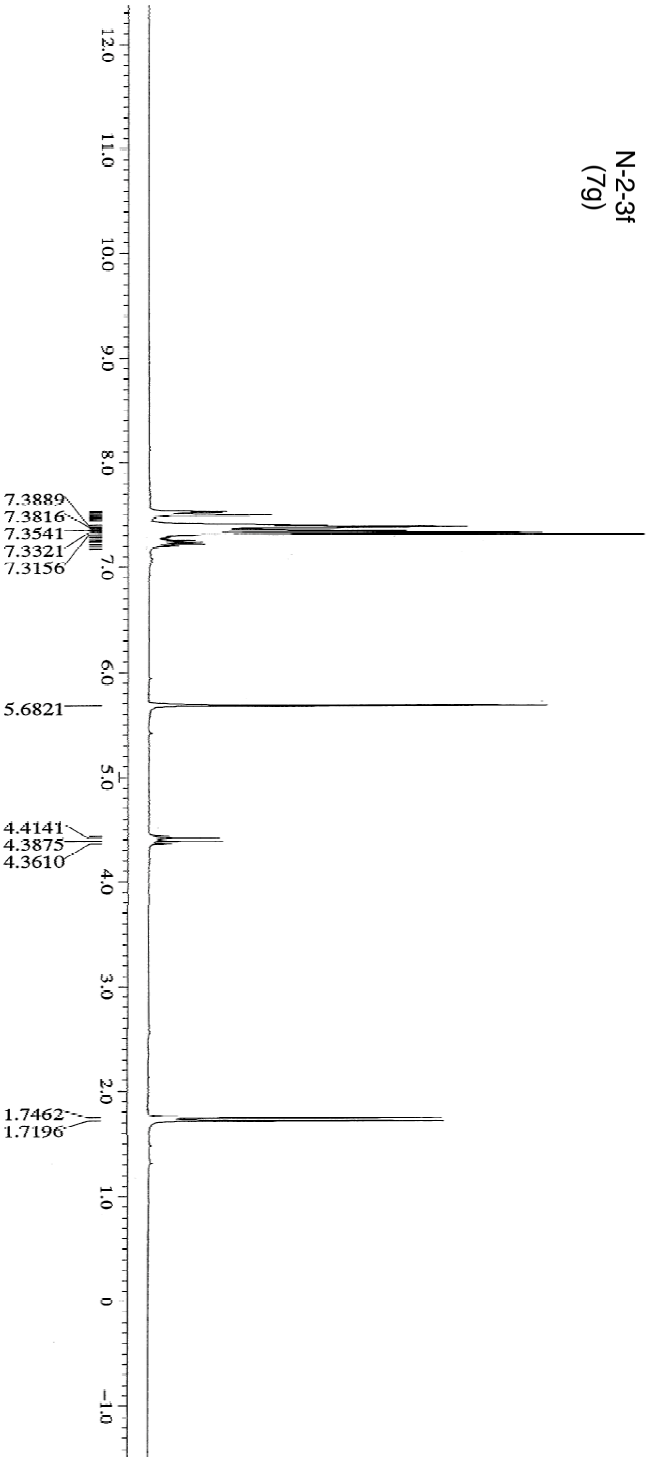
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(7g)
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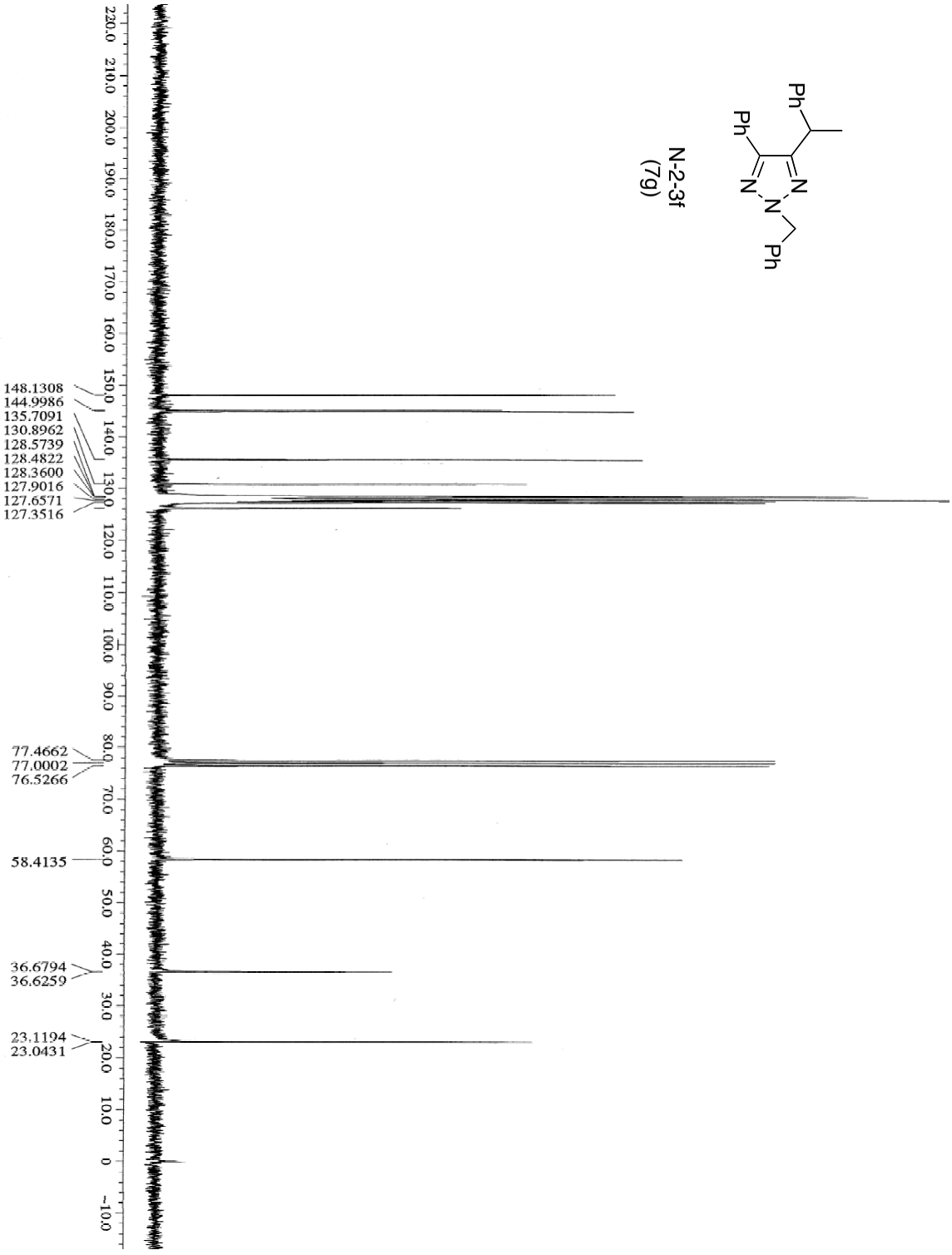
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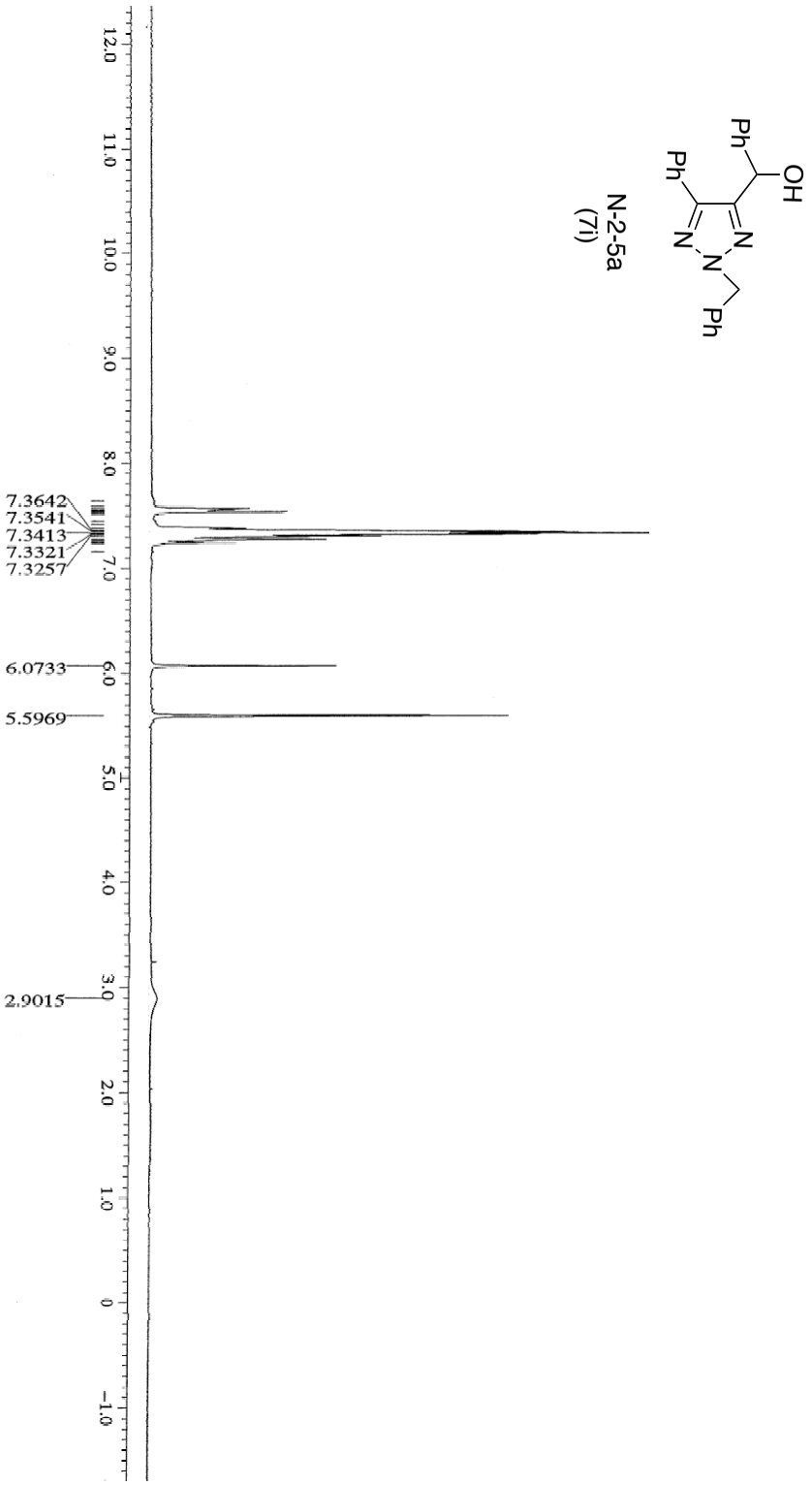
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N
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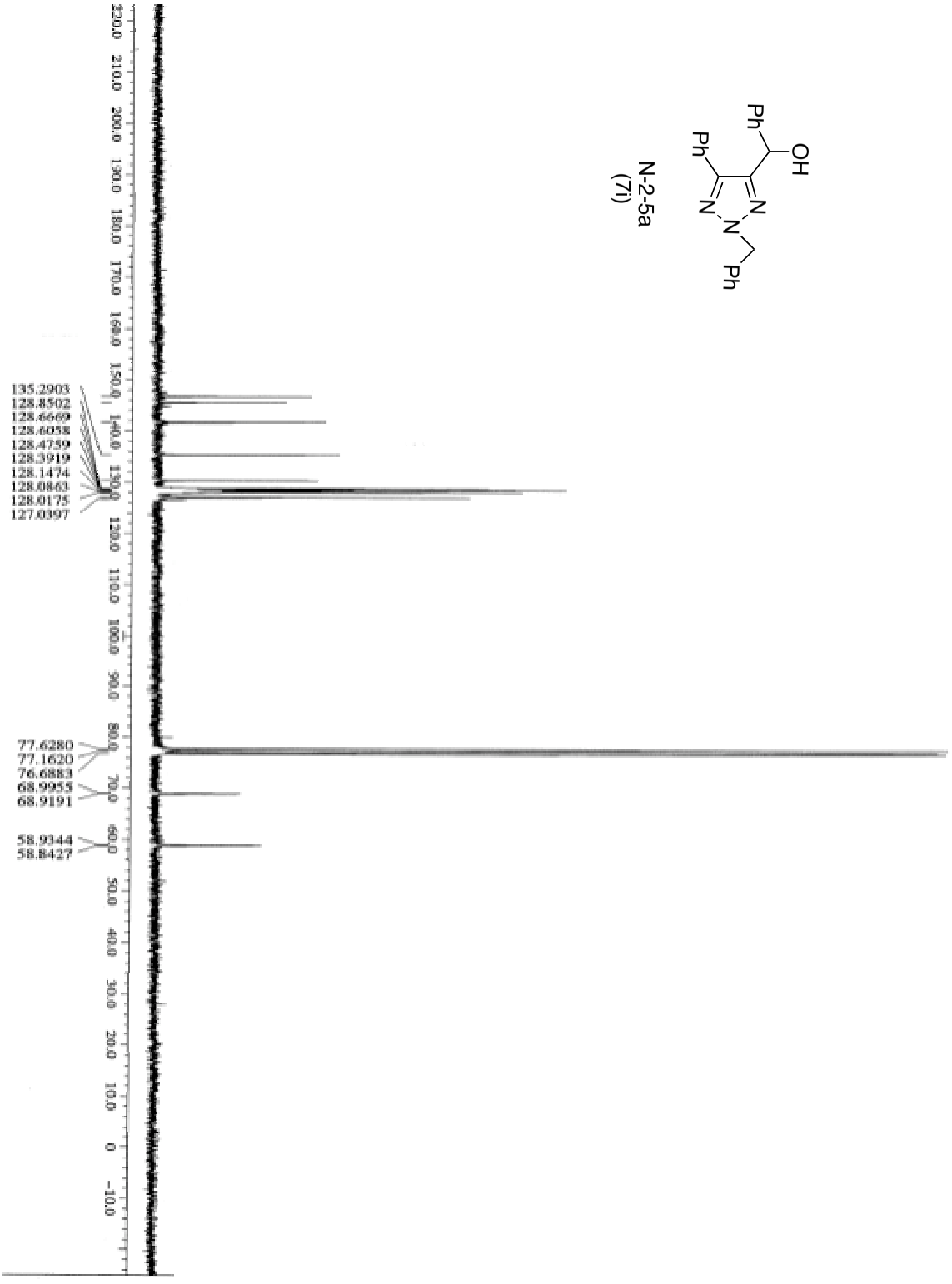
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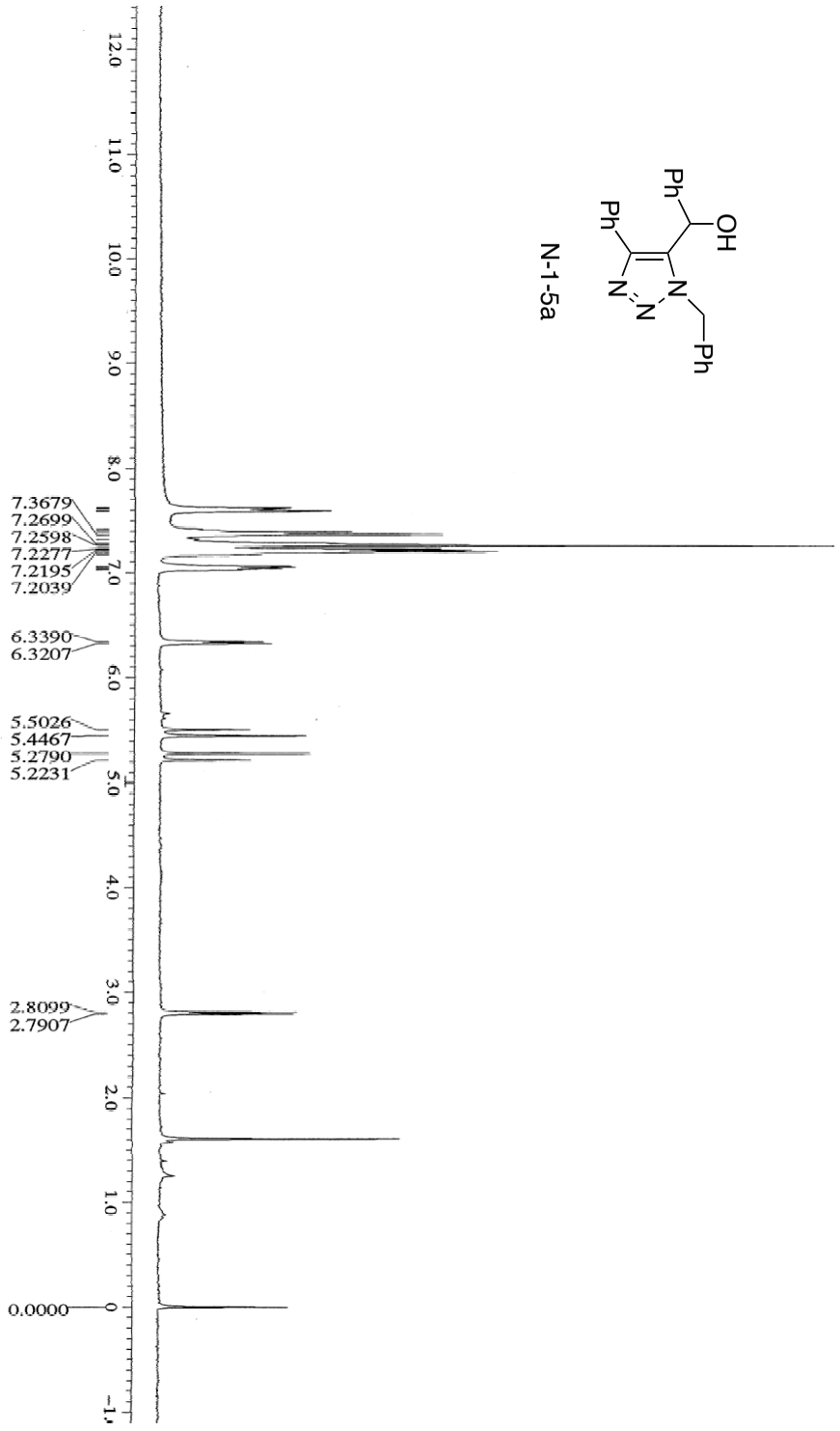
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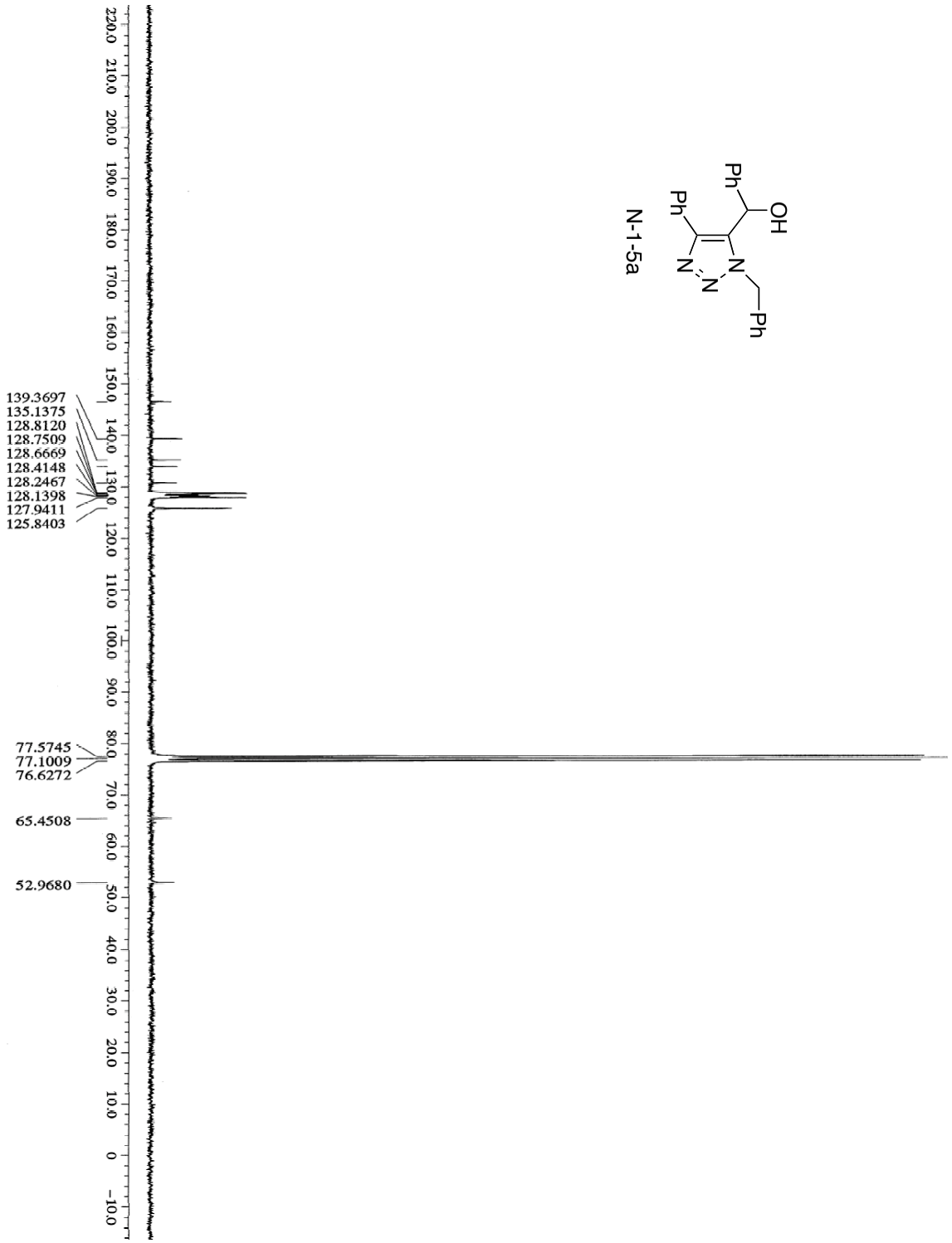
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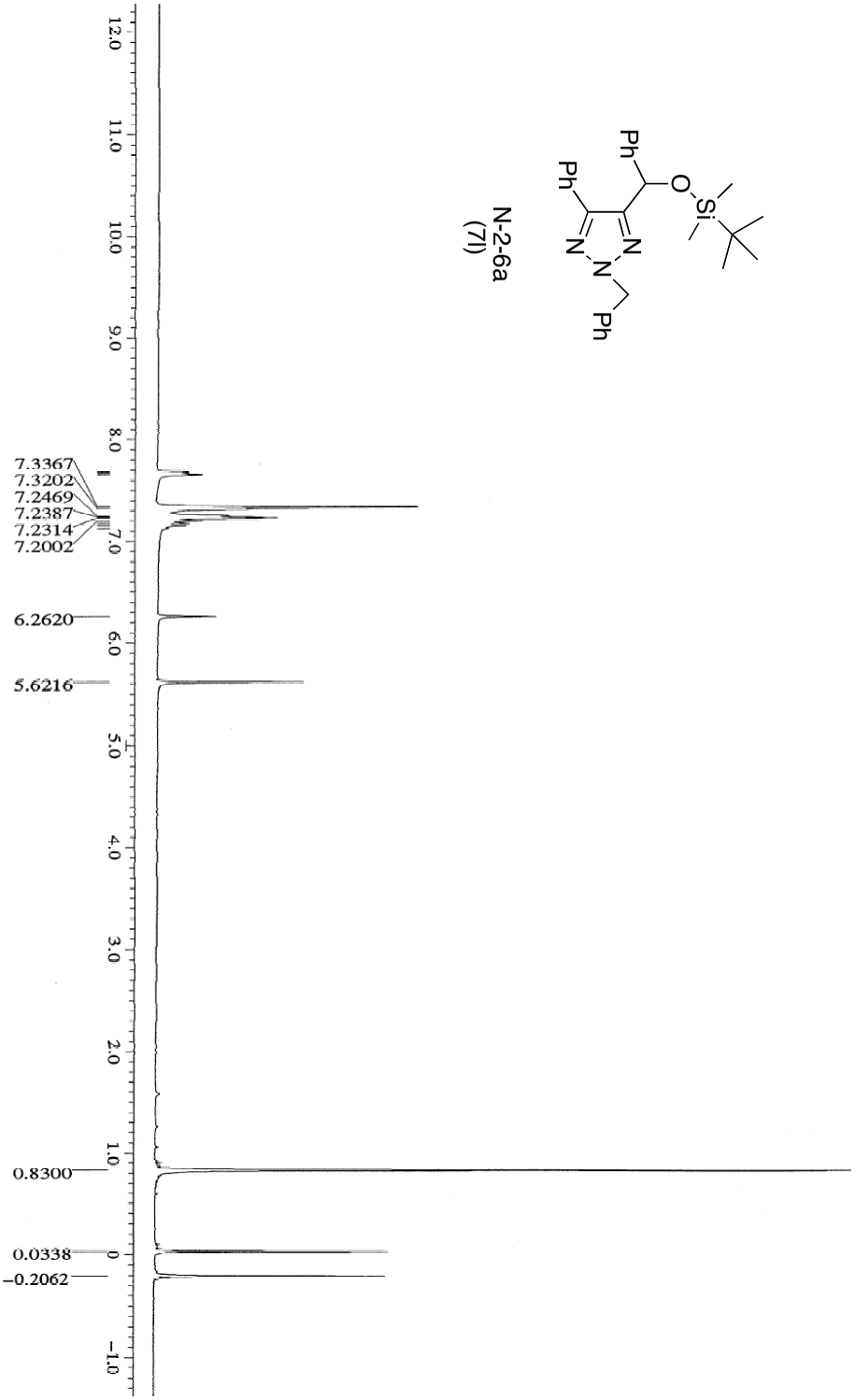
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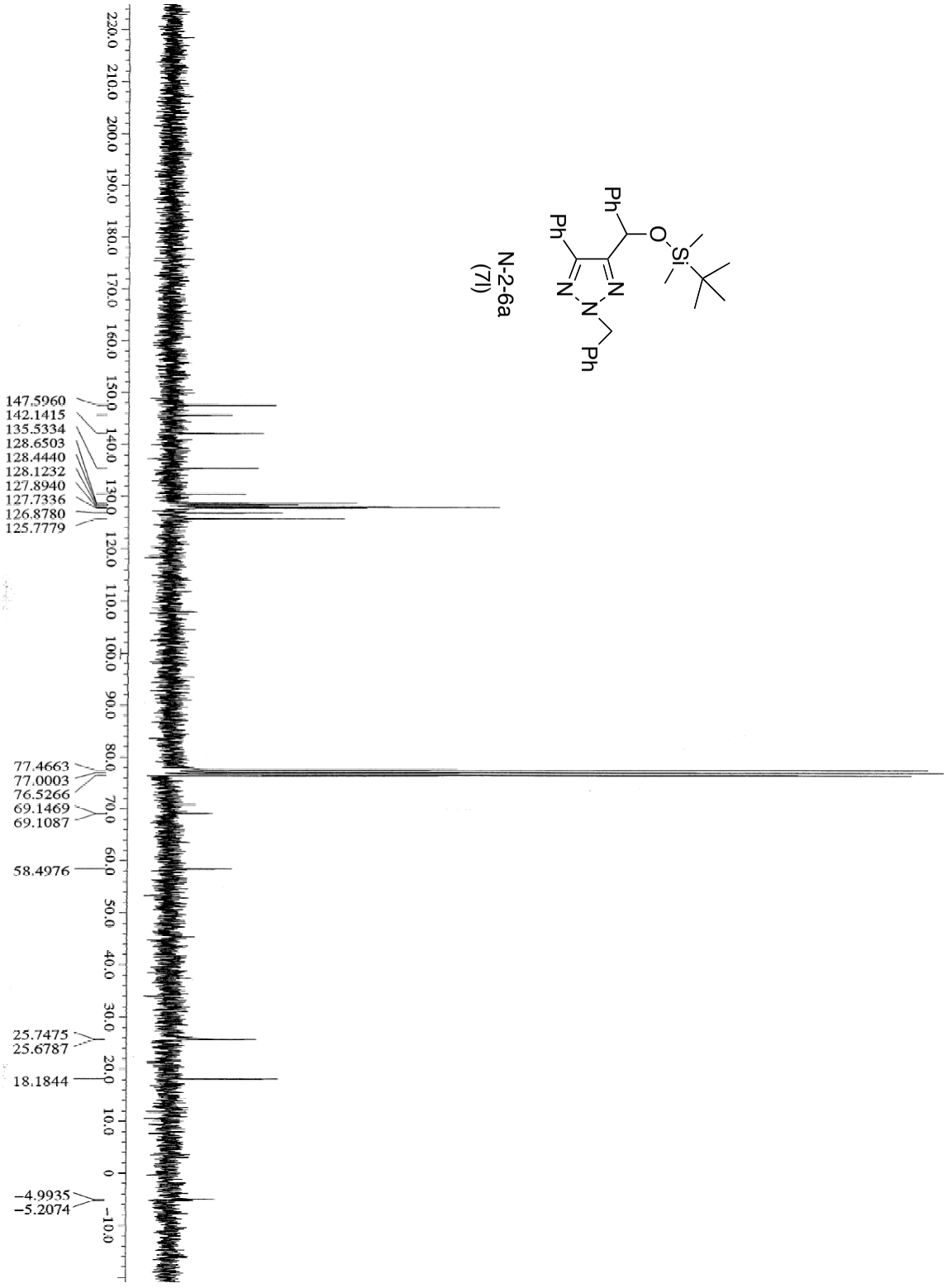
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(7l)
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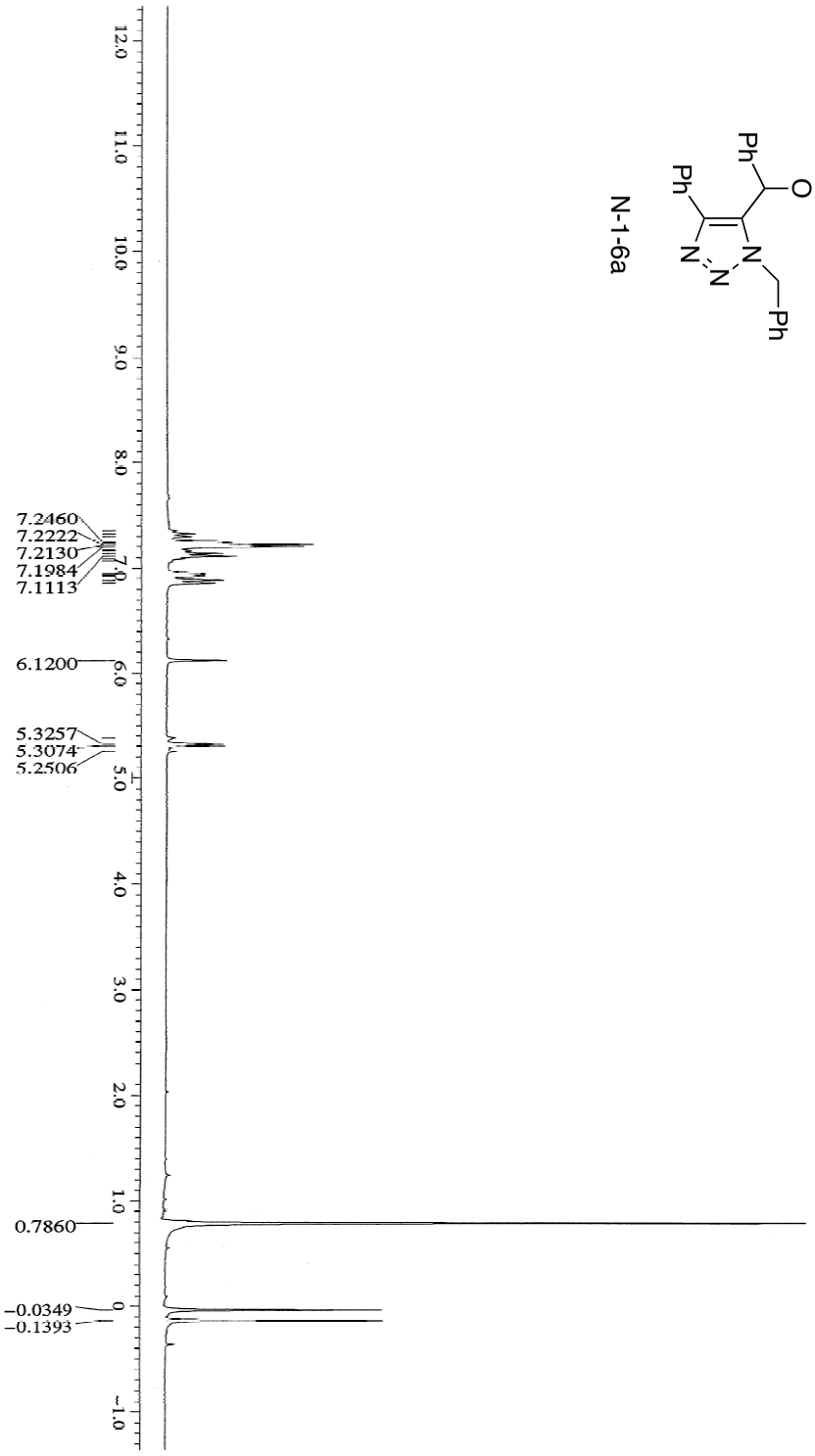
Ph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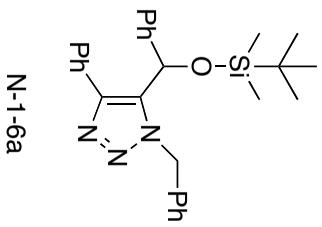
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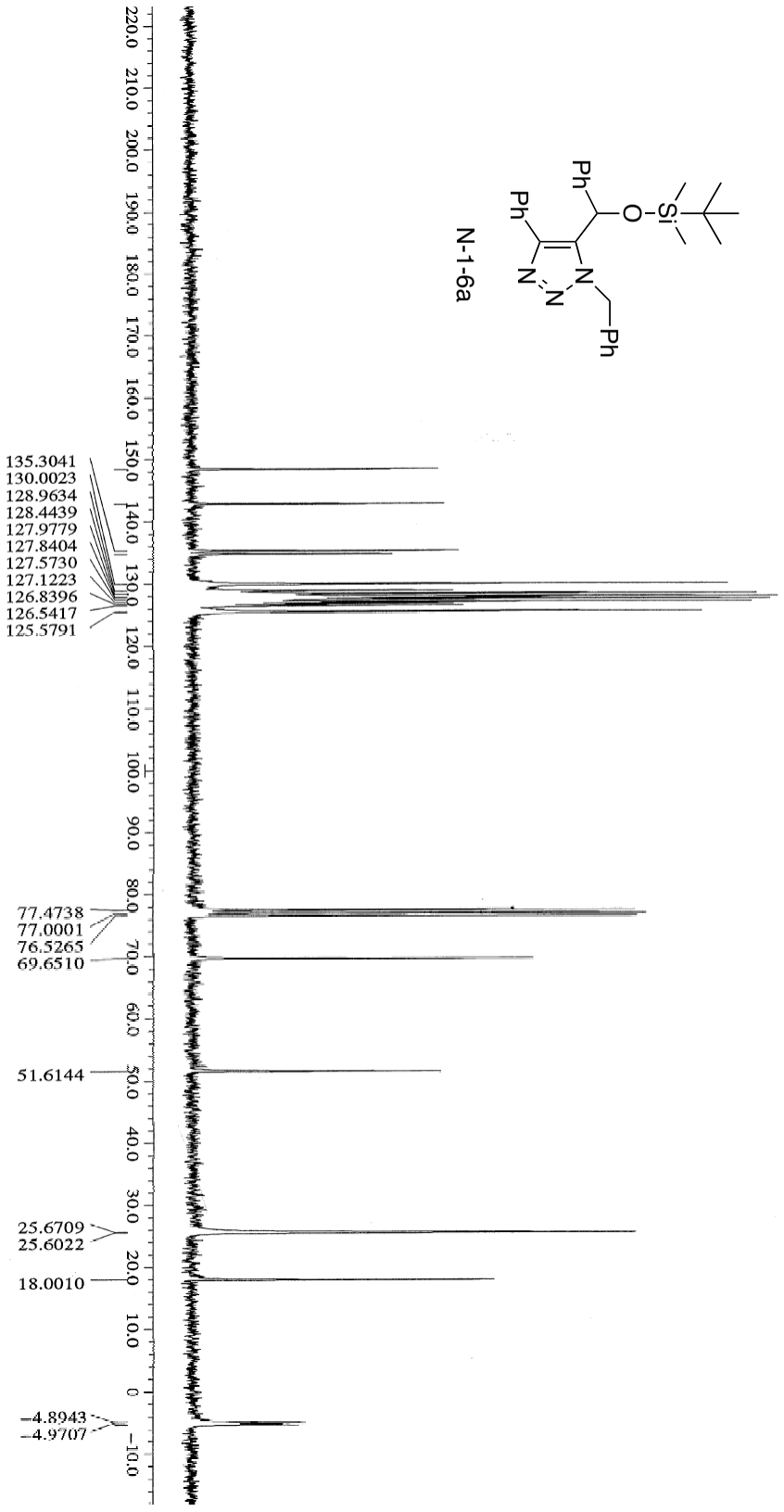
N-1-6a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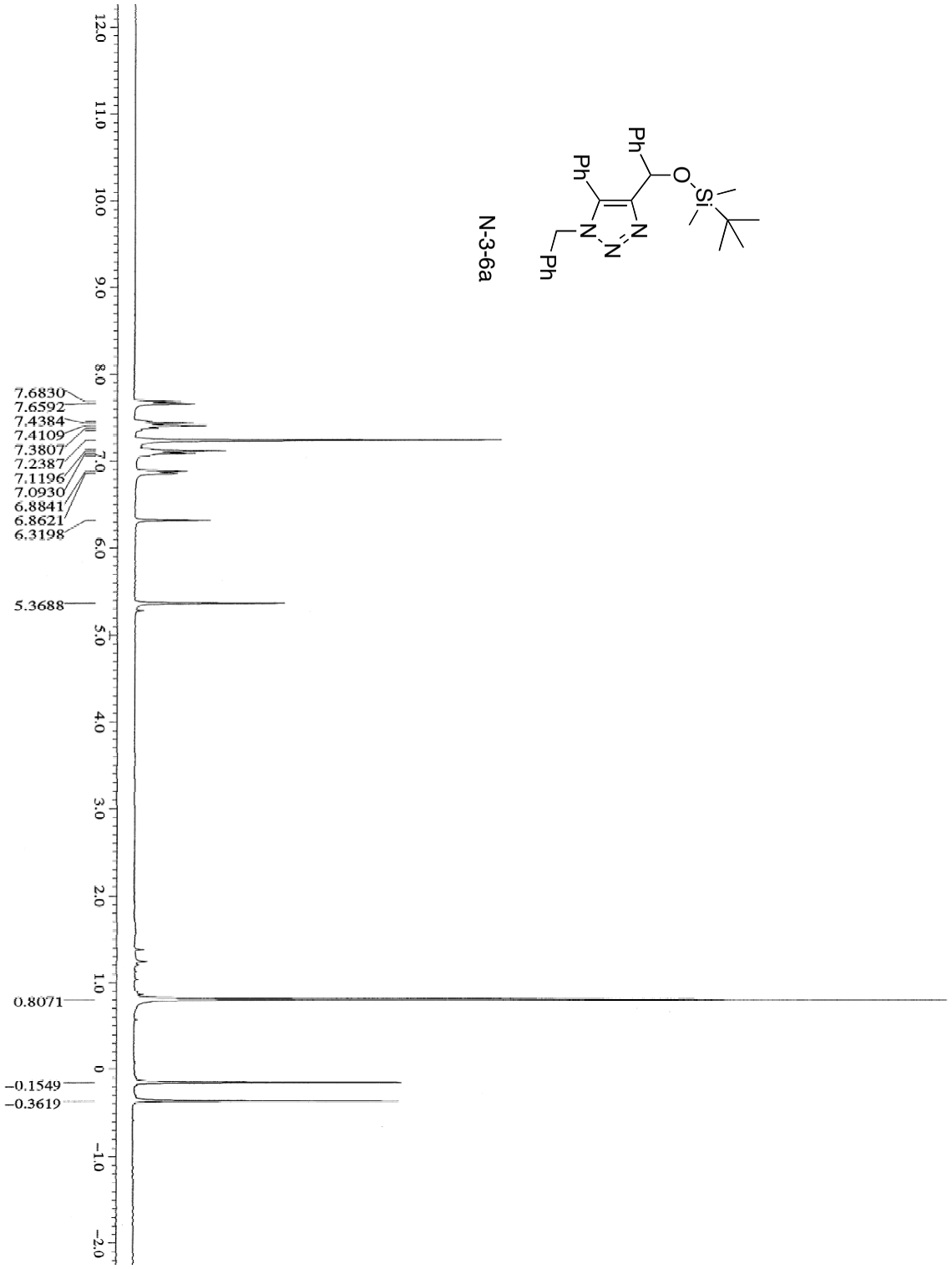
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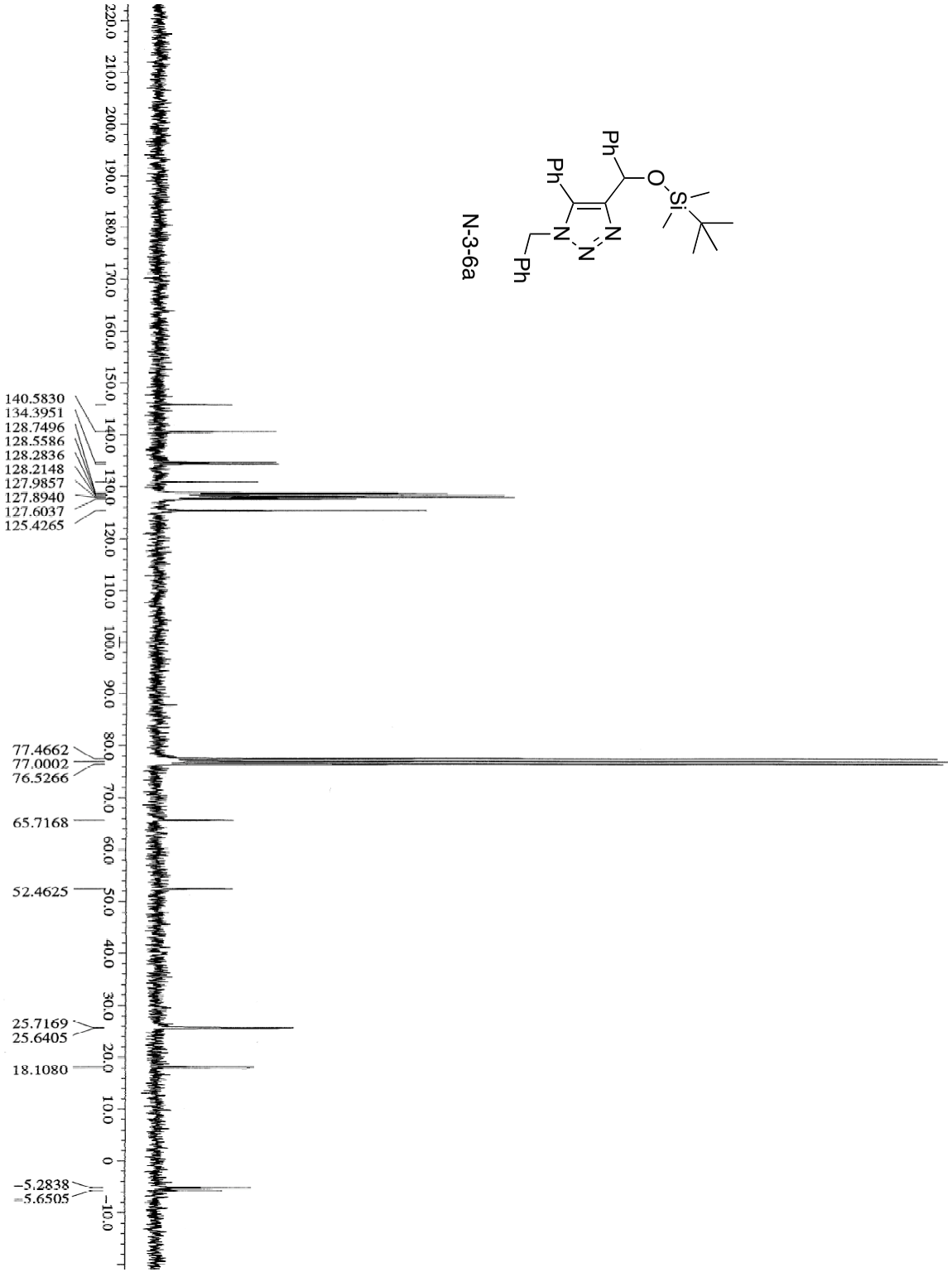
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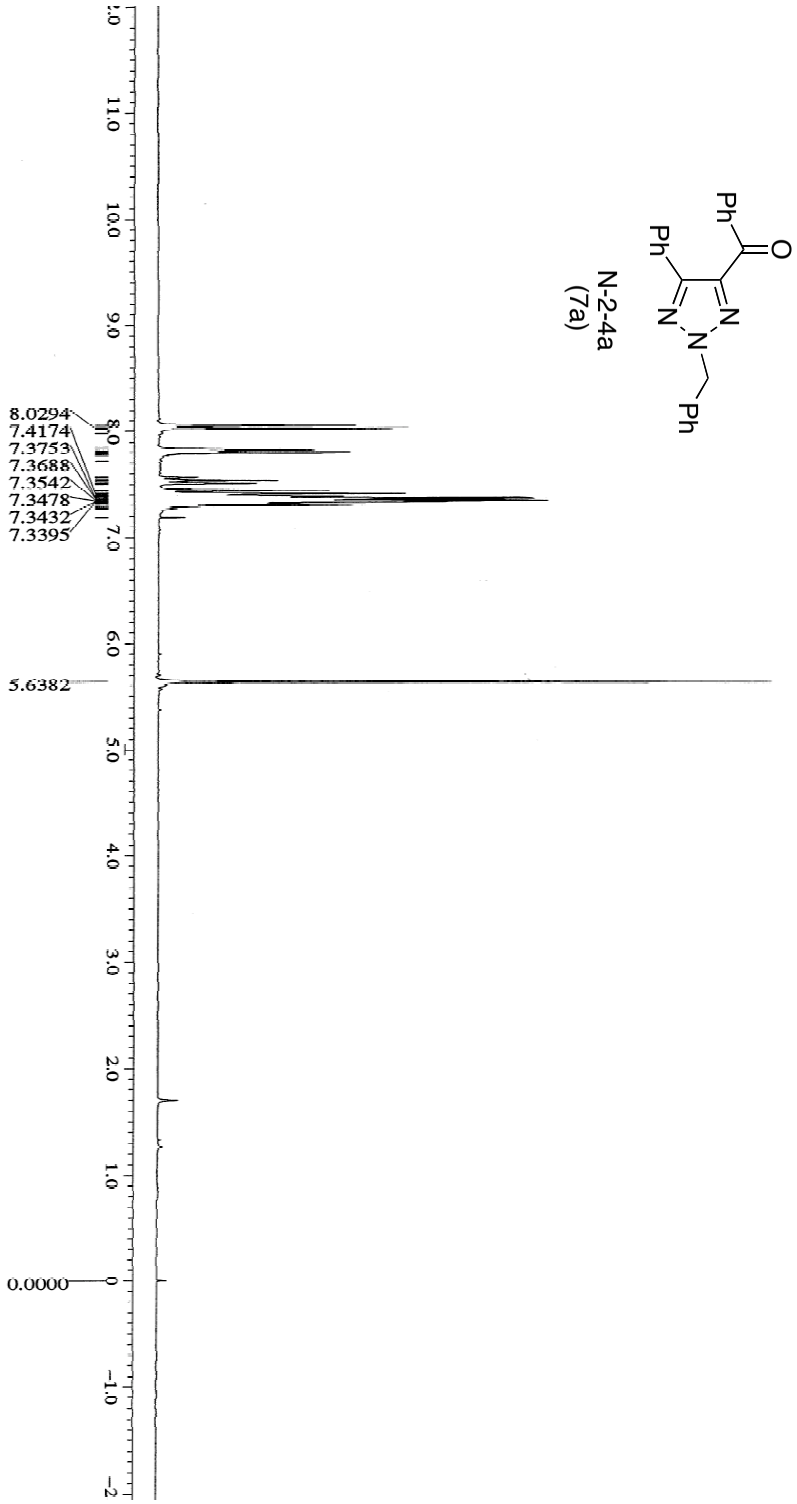
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(7a)
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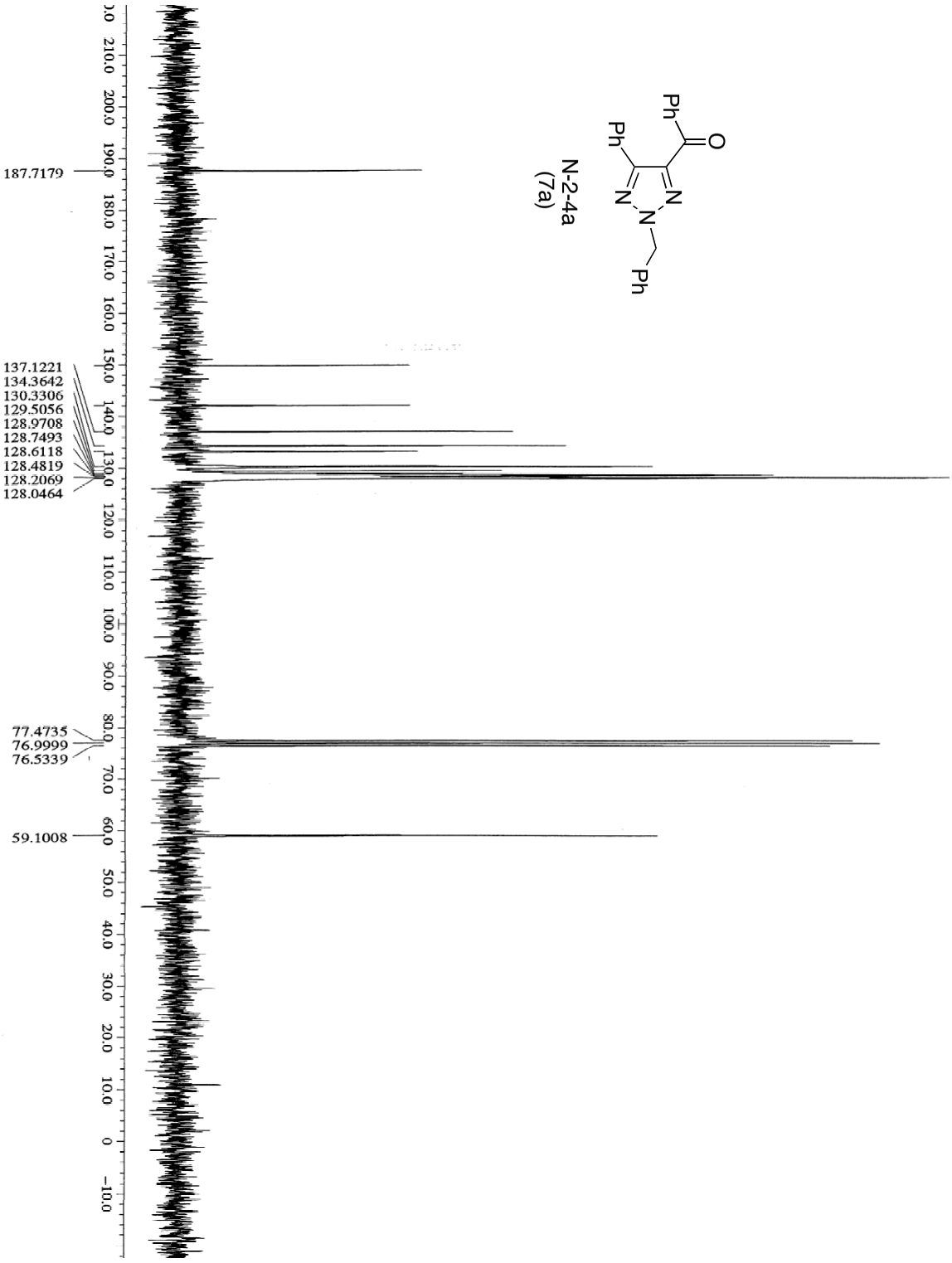
Ph
N
N
N
Ph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(7a)
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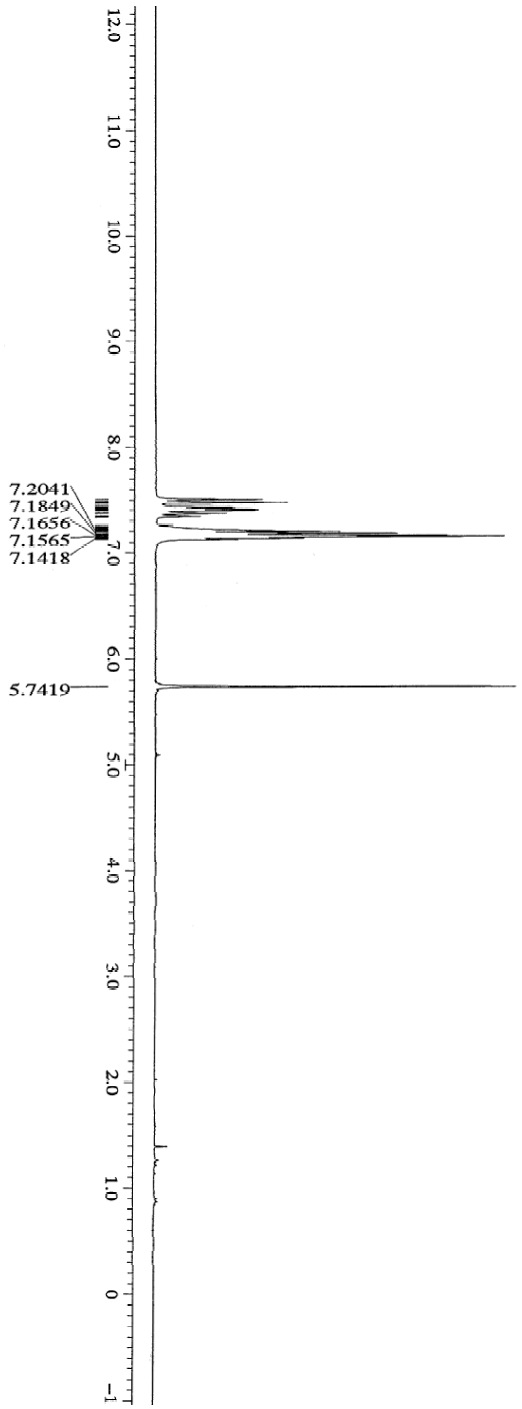
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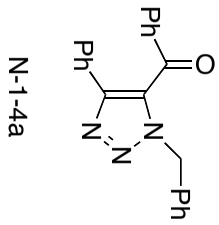
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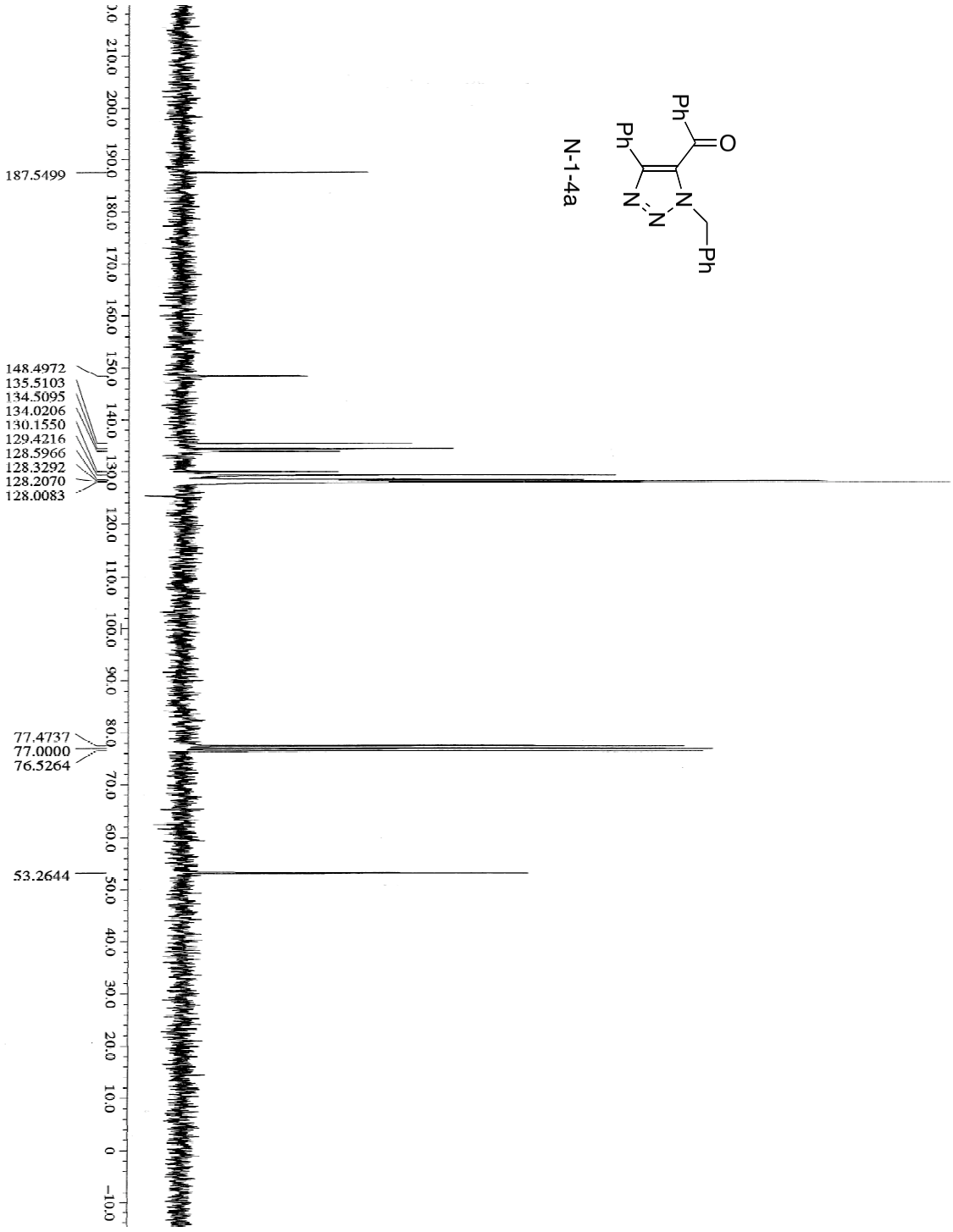
N-1-4a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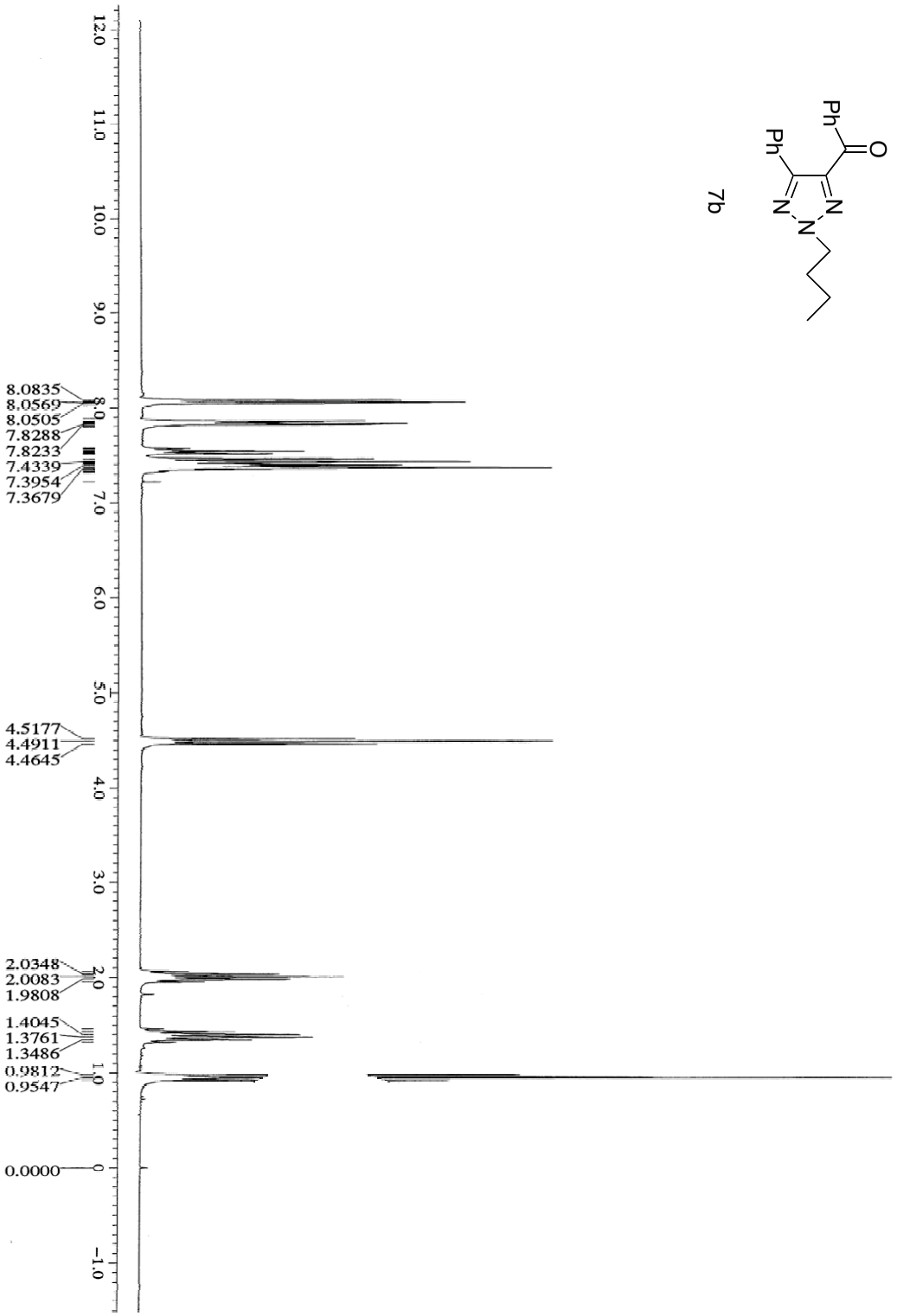
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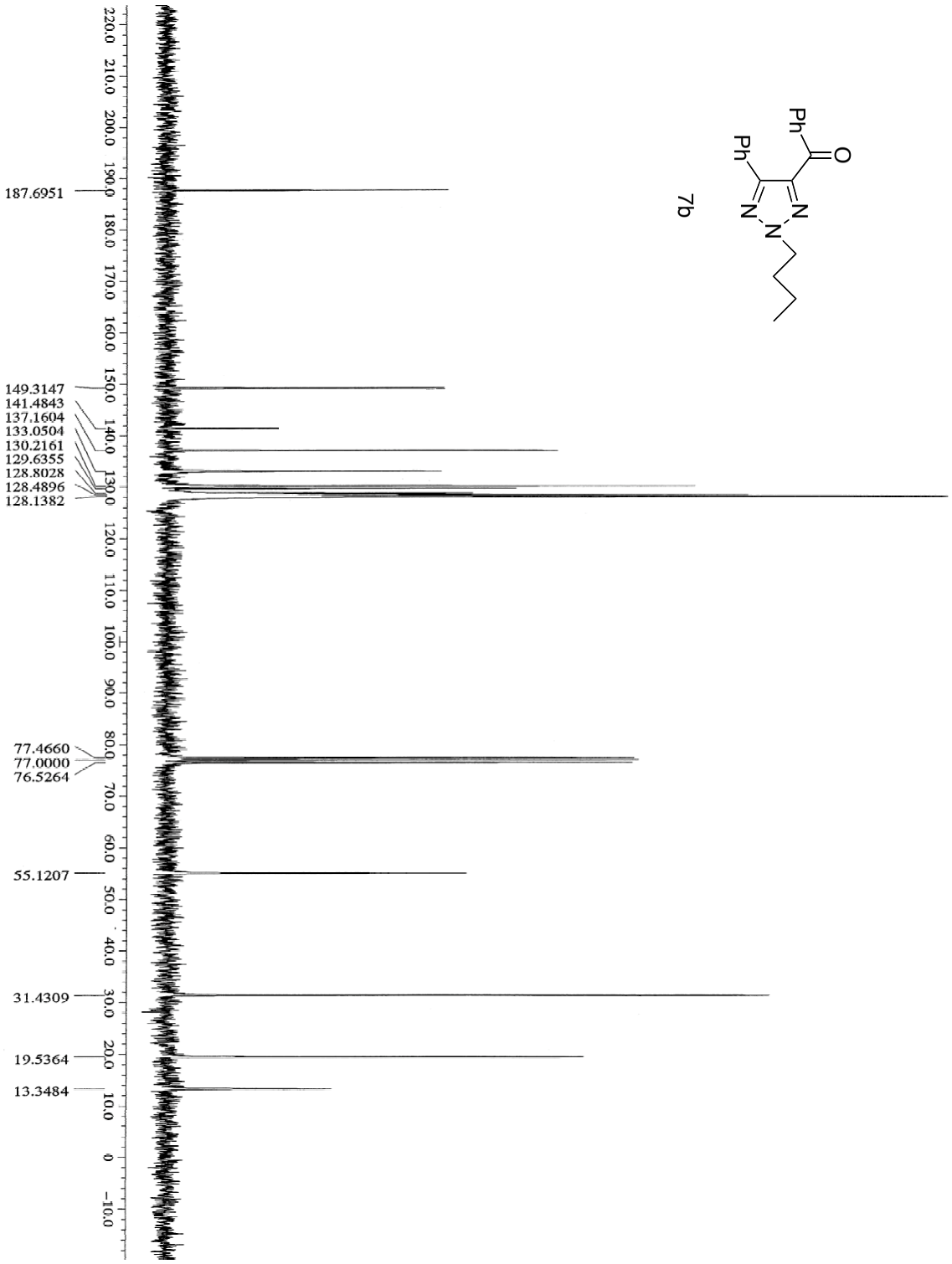
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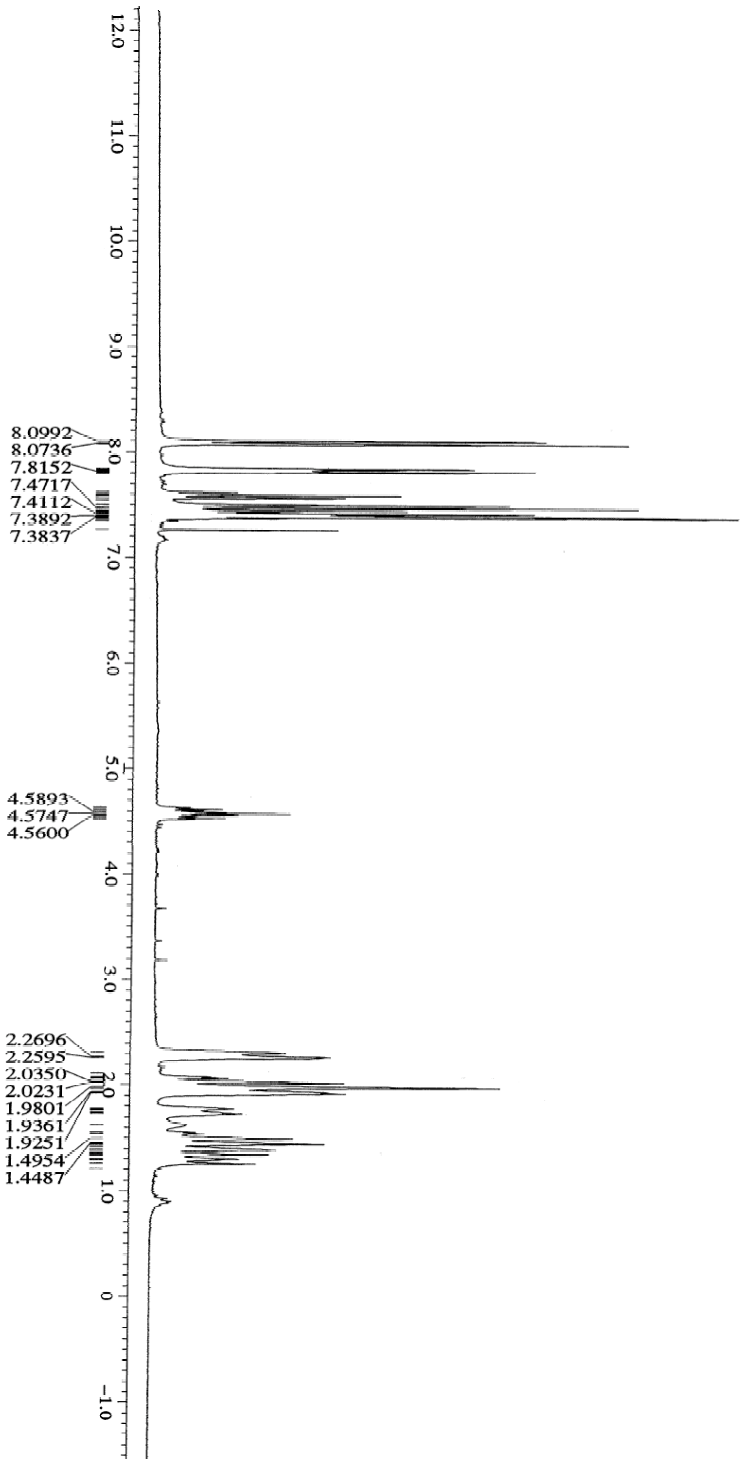
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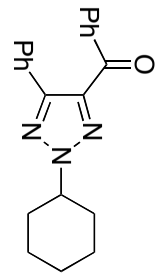
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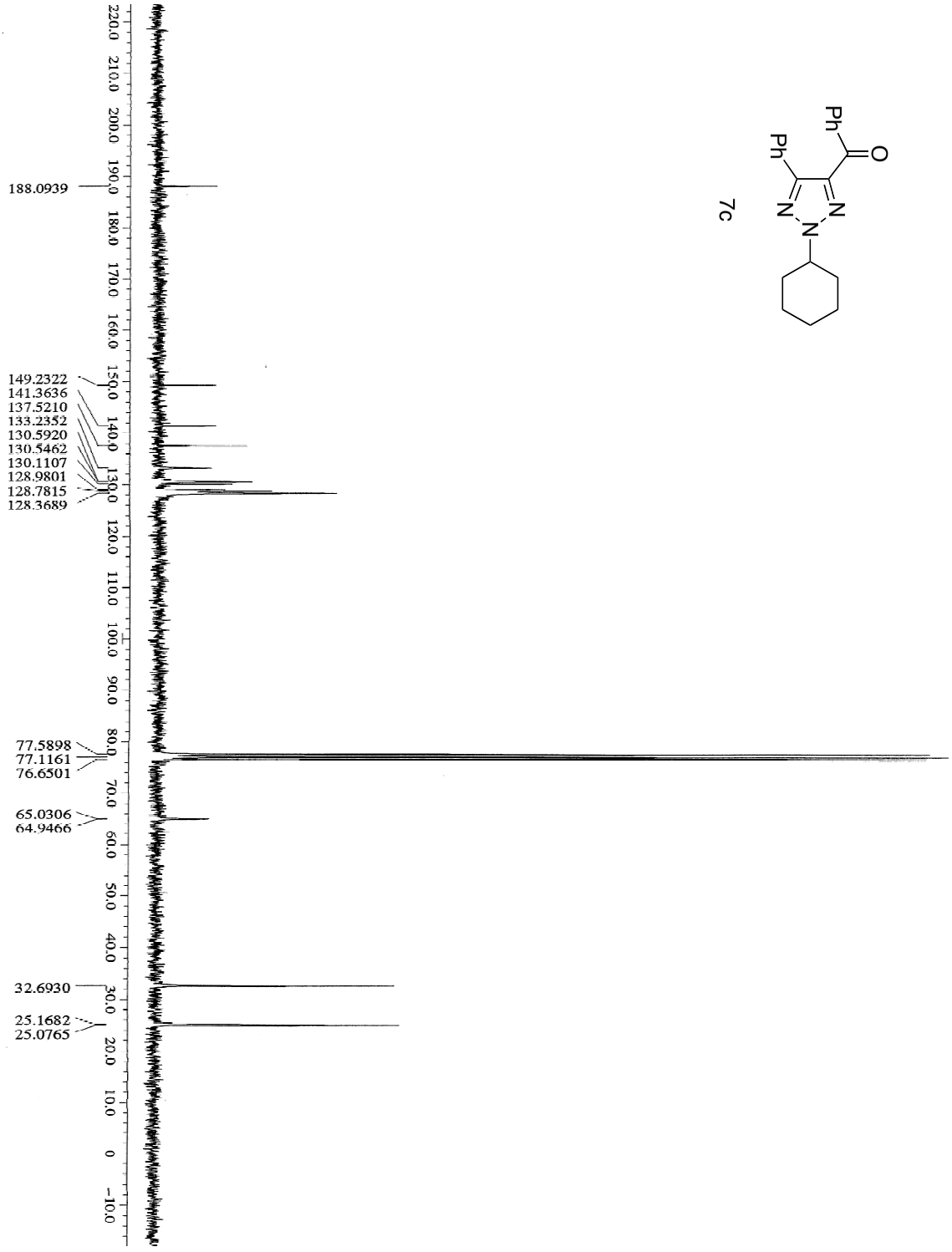
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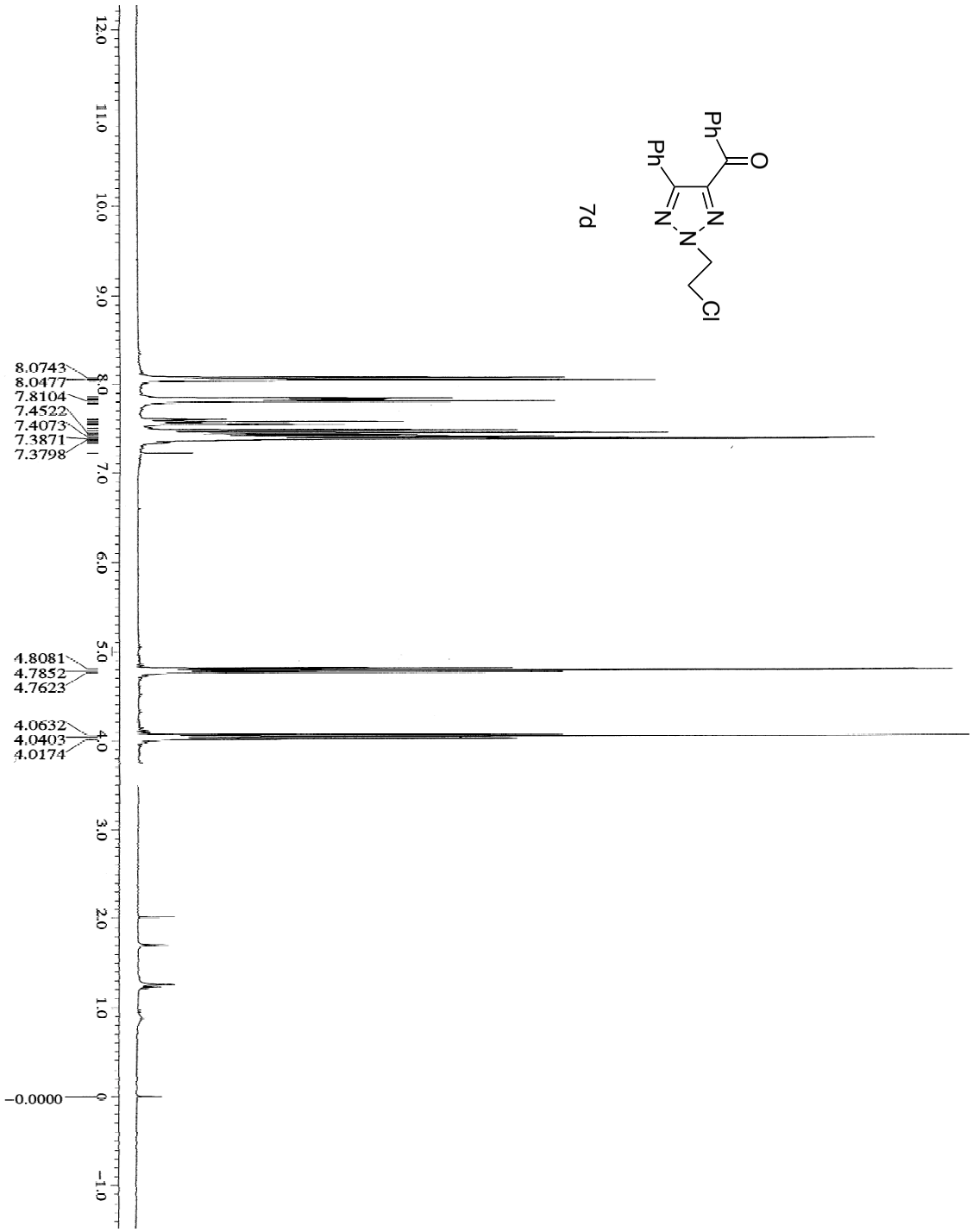
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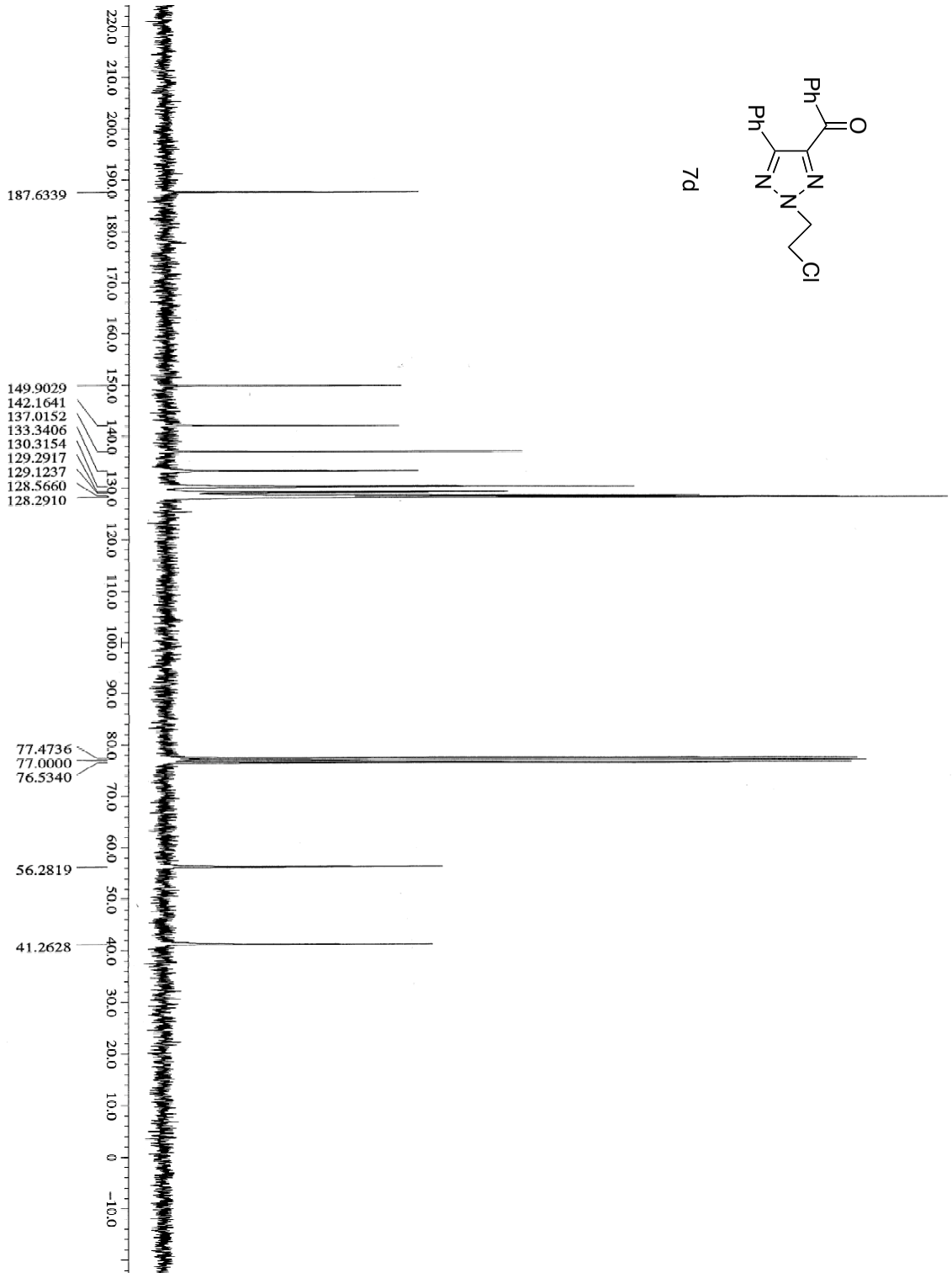
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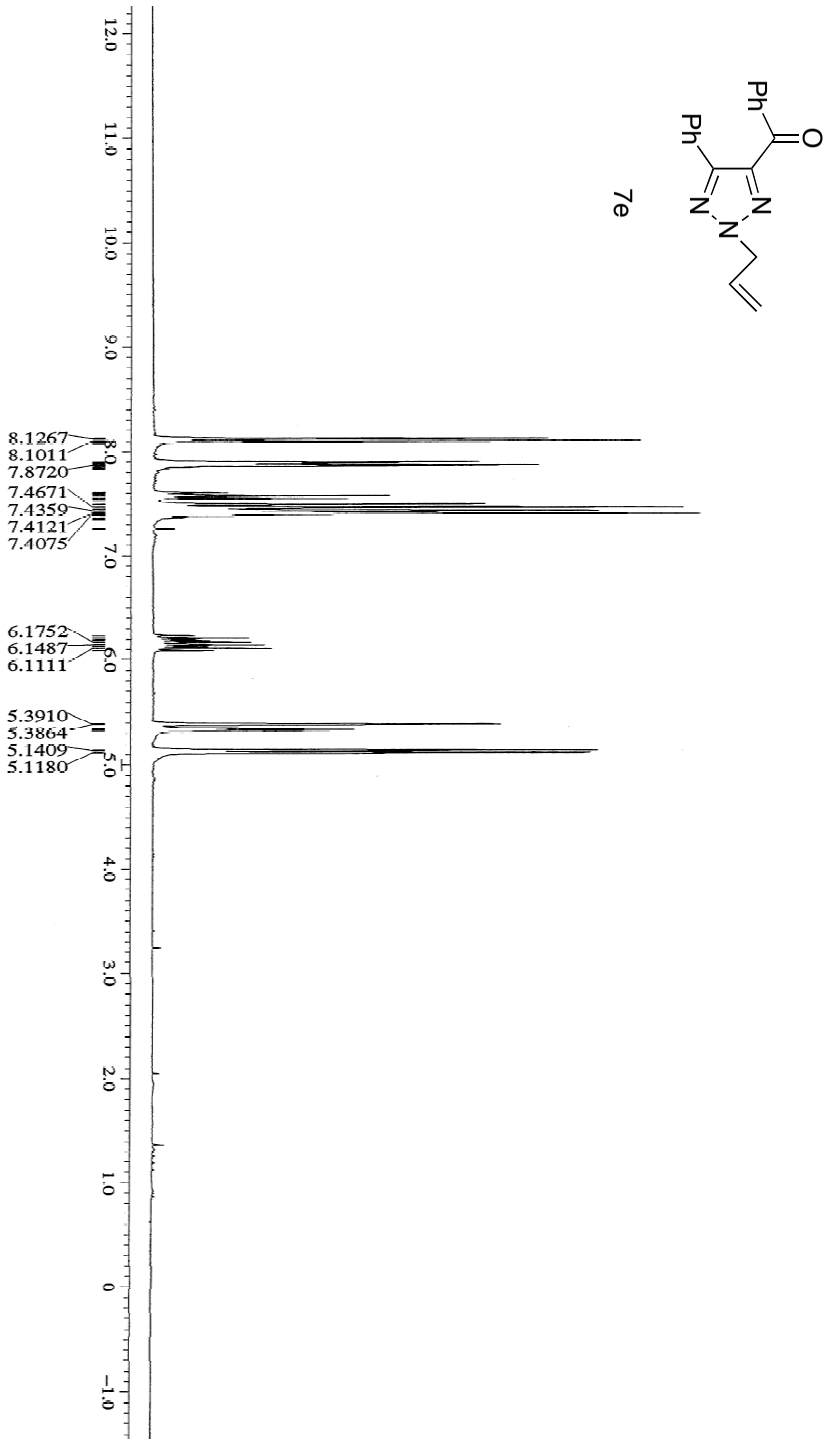
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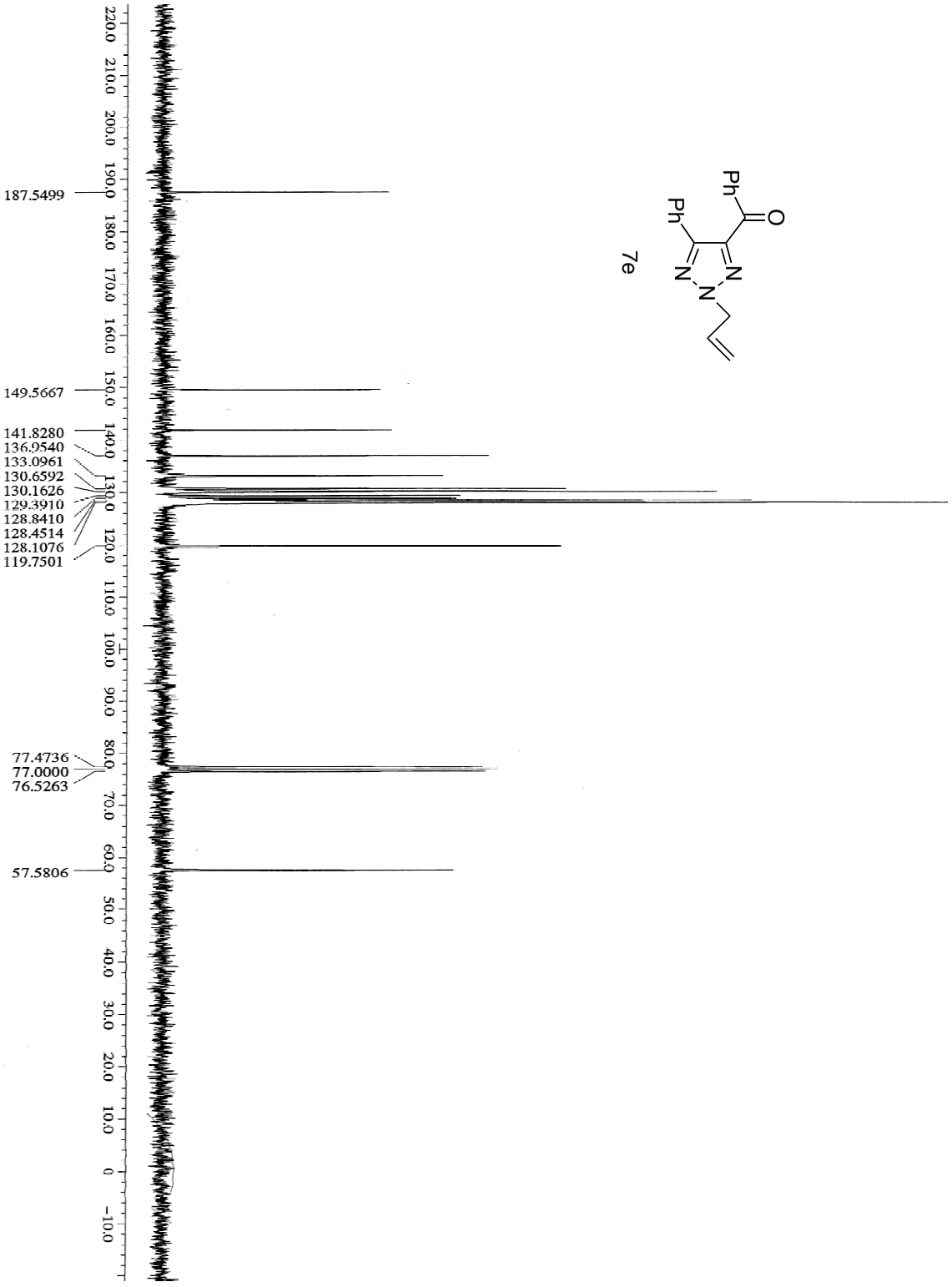
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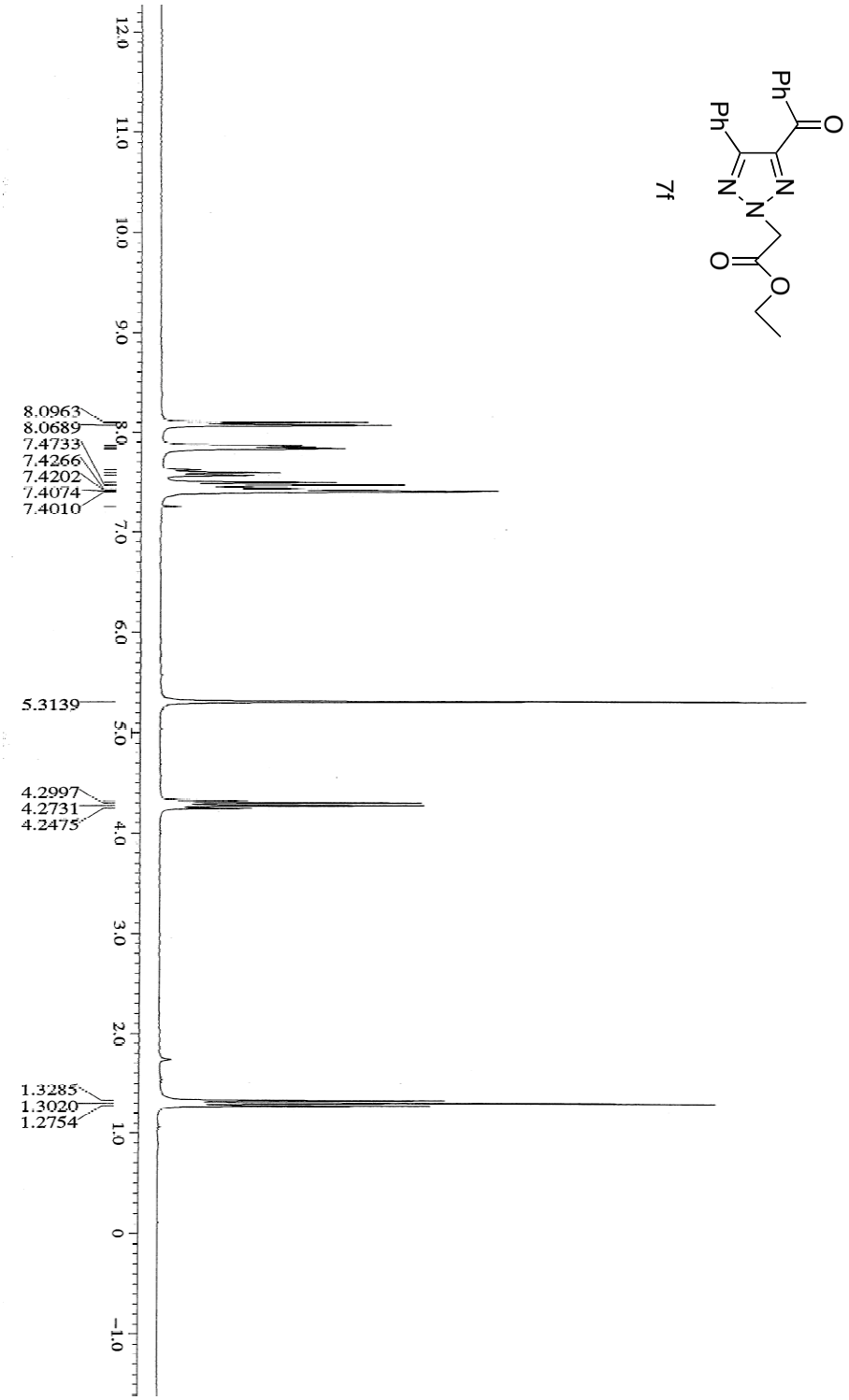
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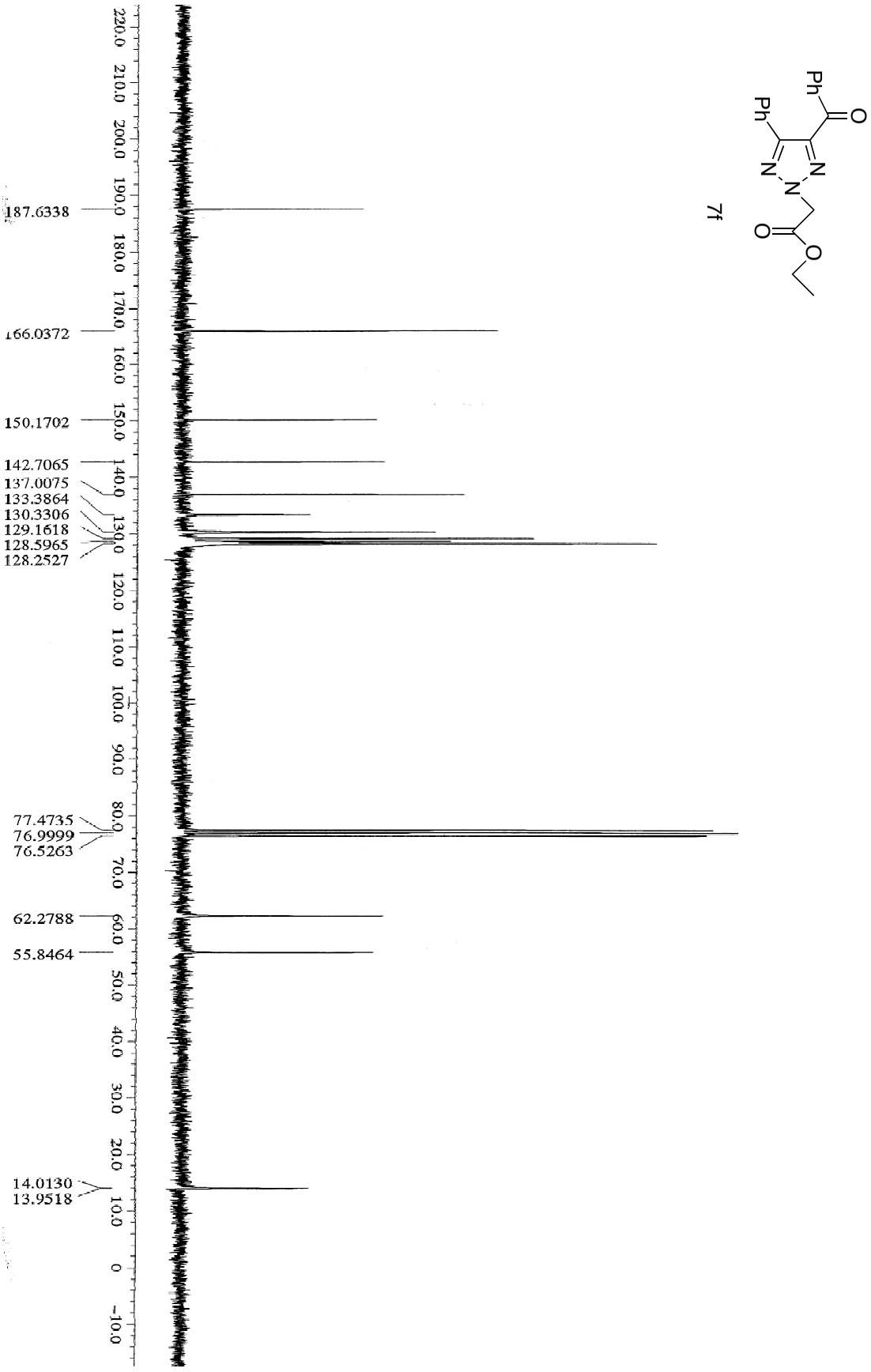
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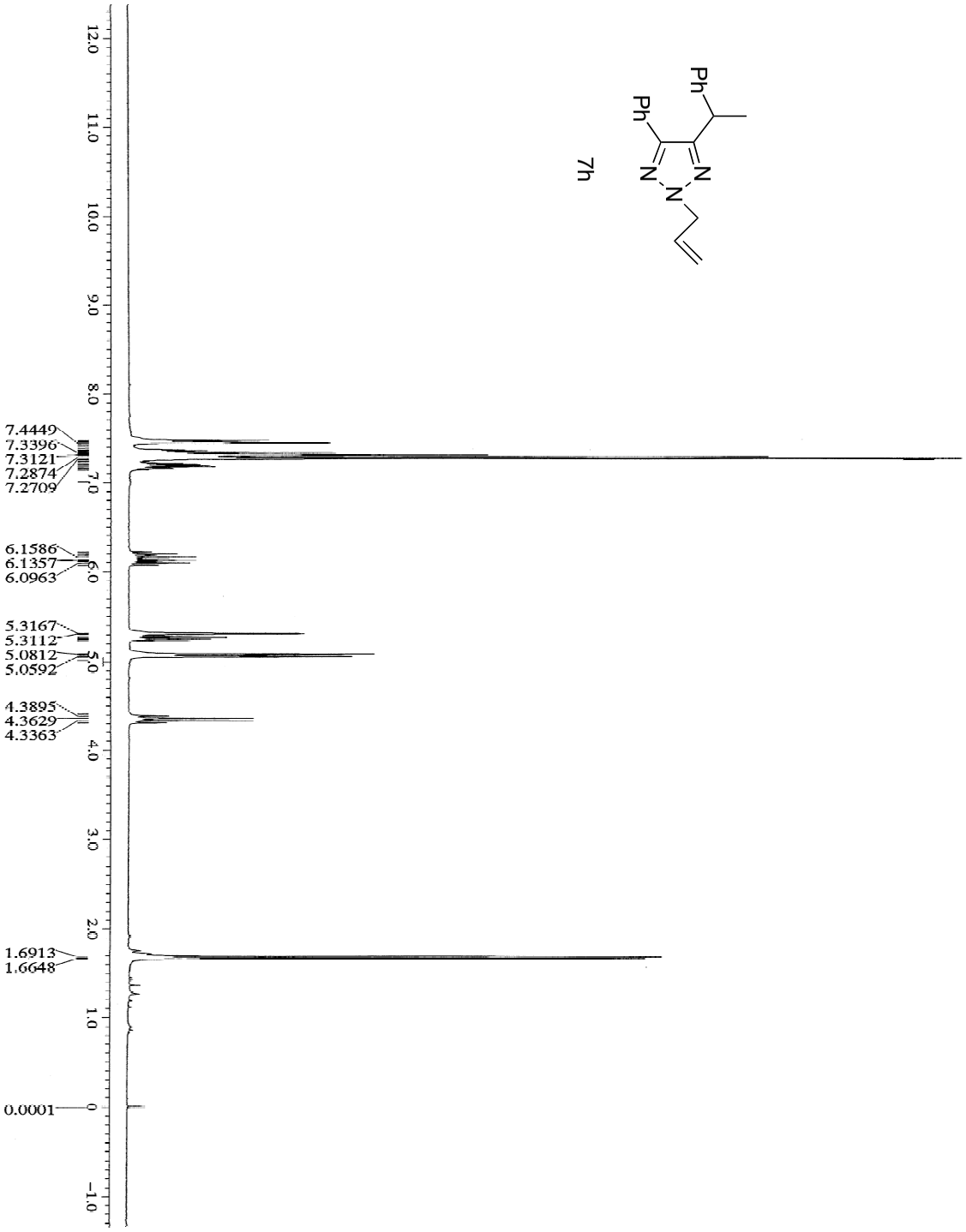
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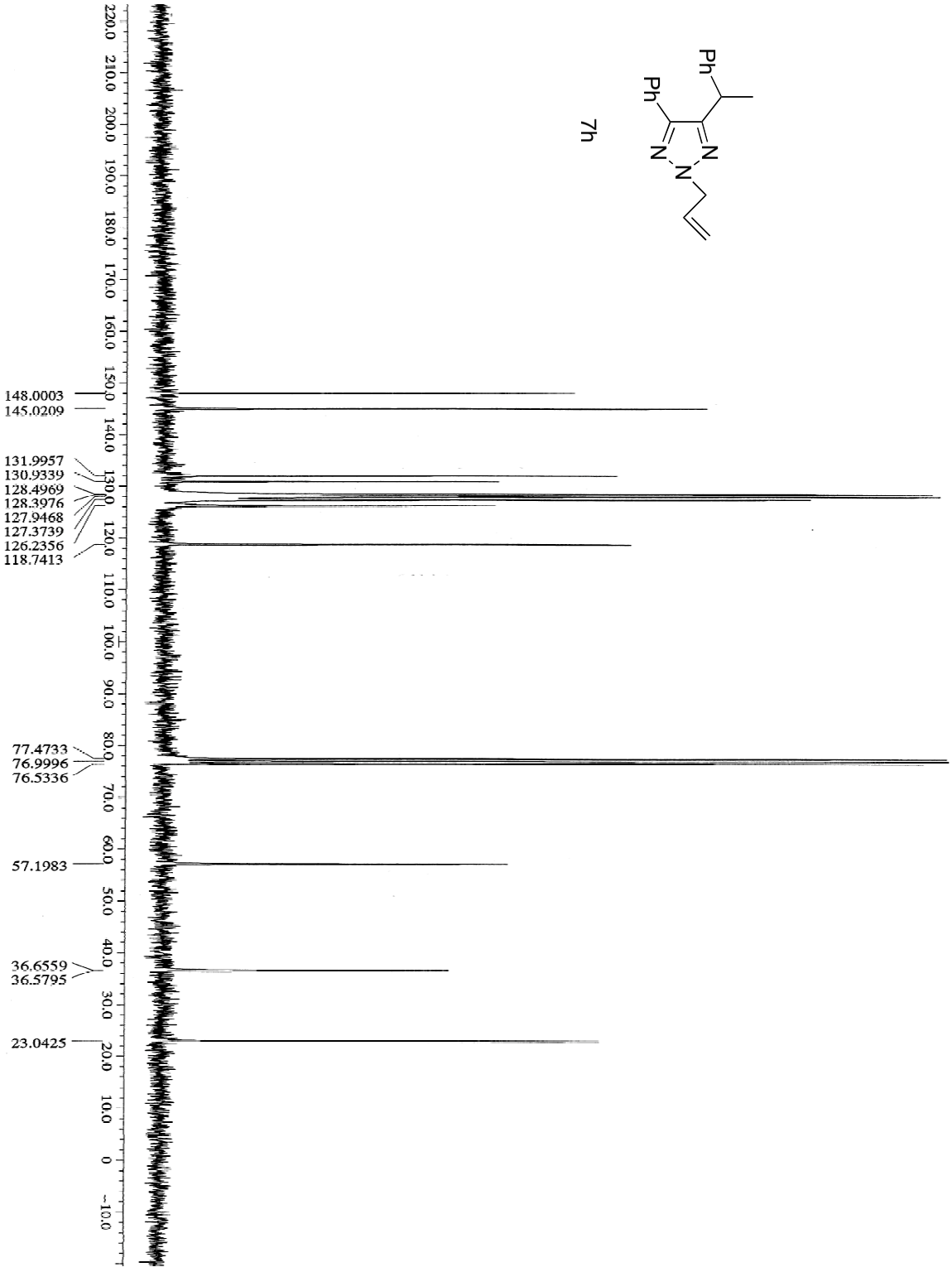
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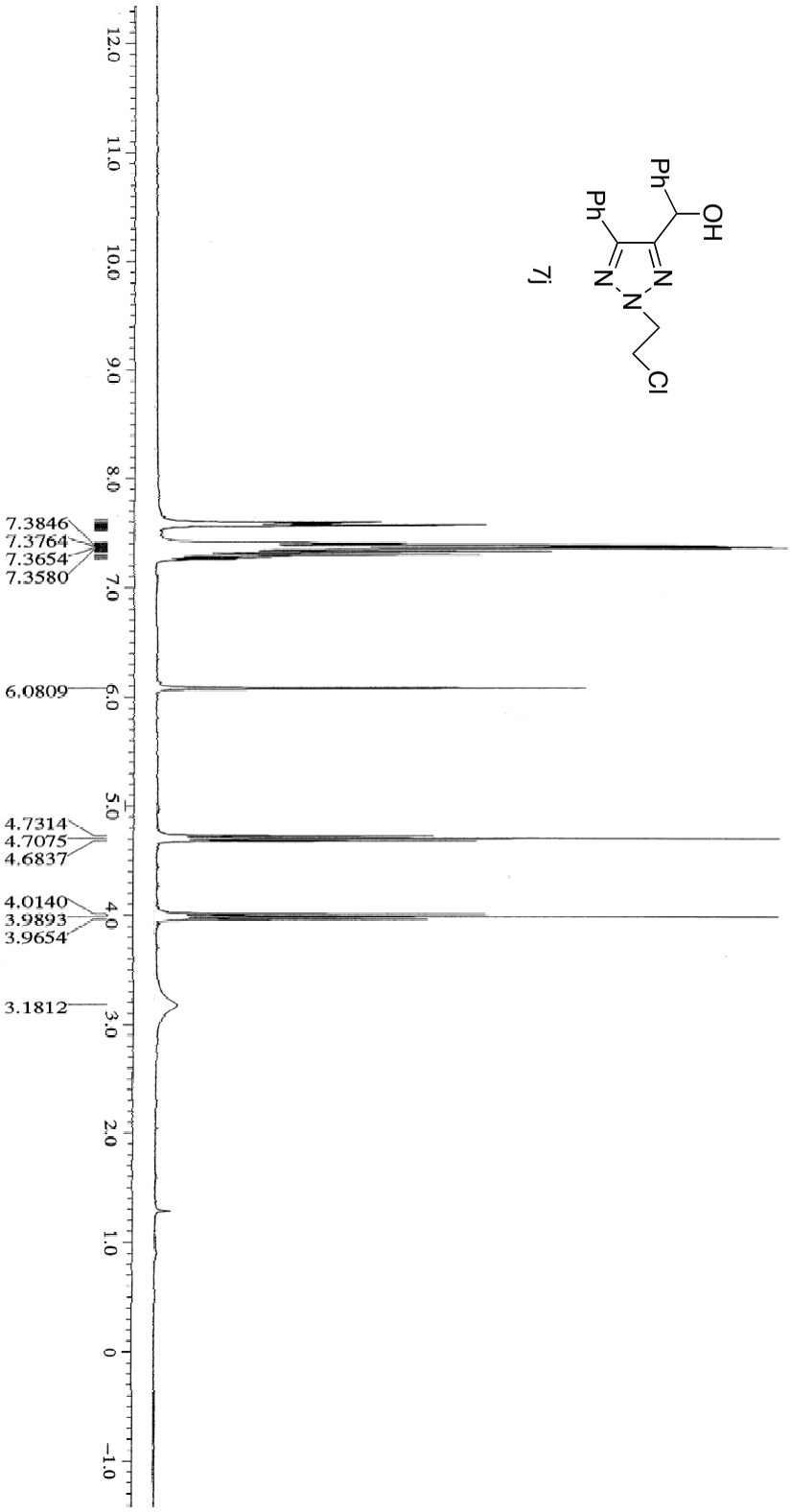
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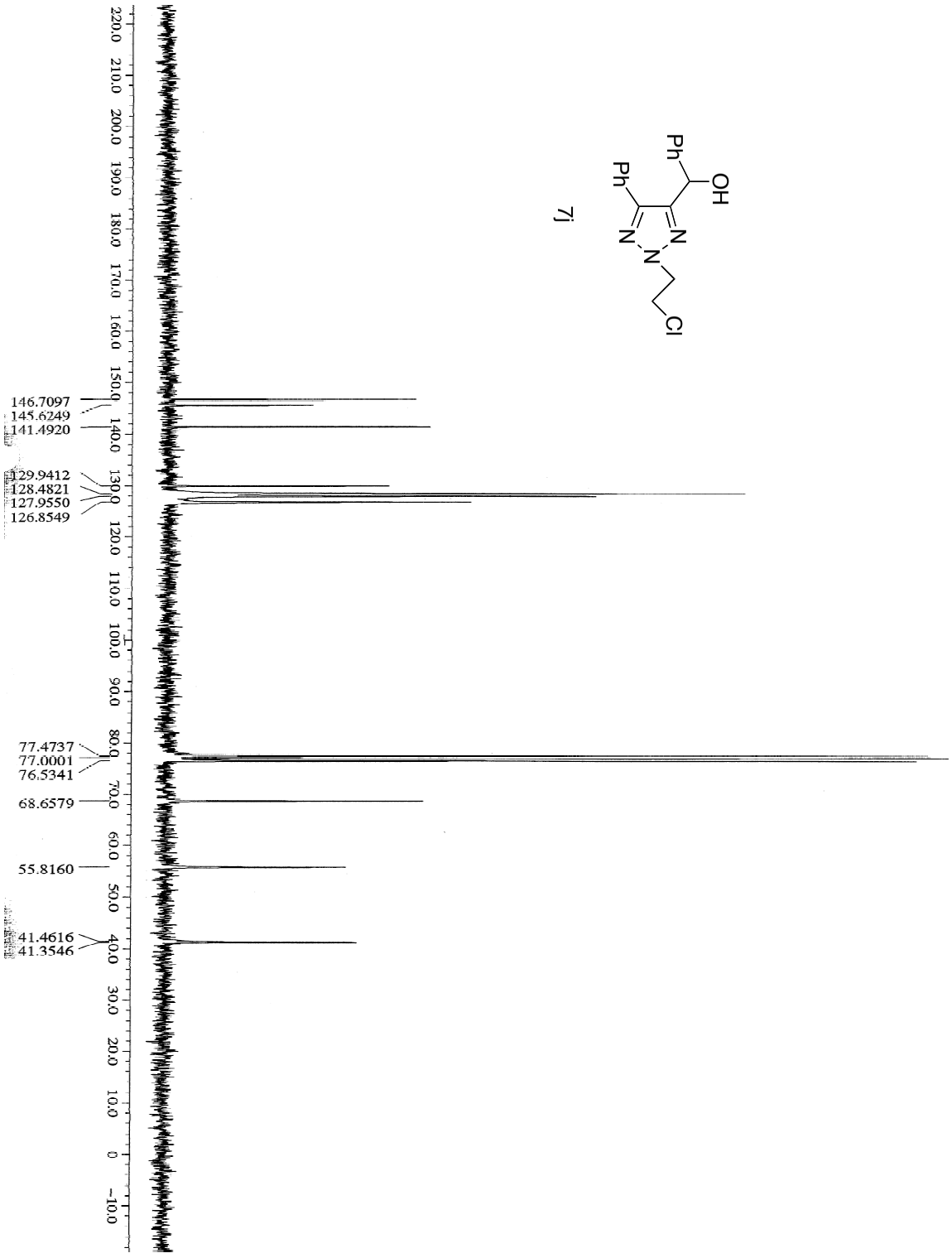
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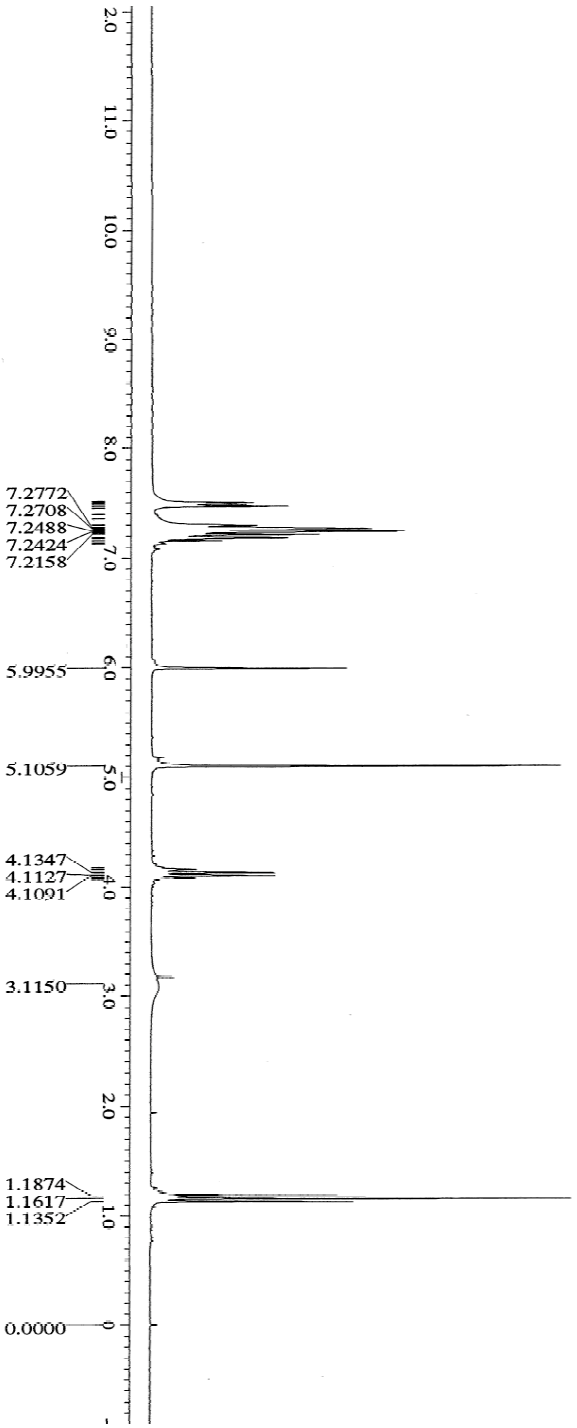
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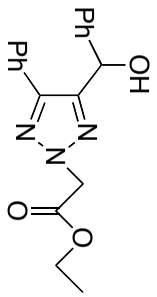
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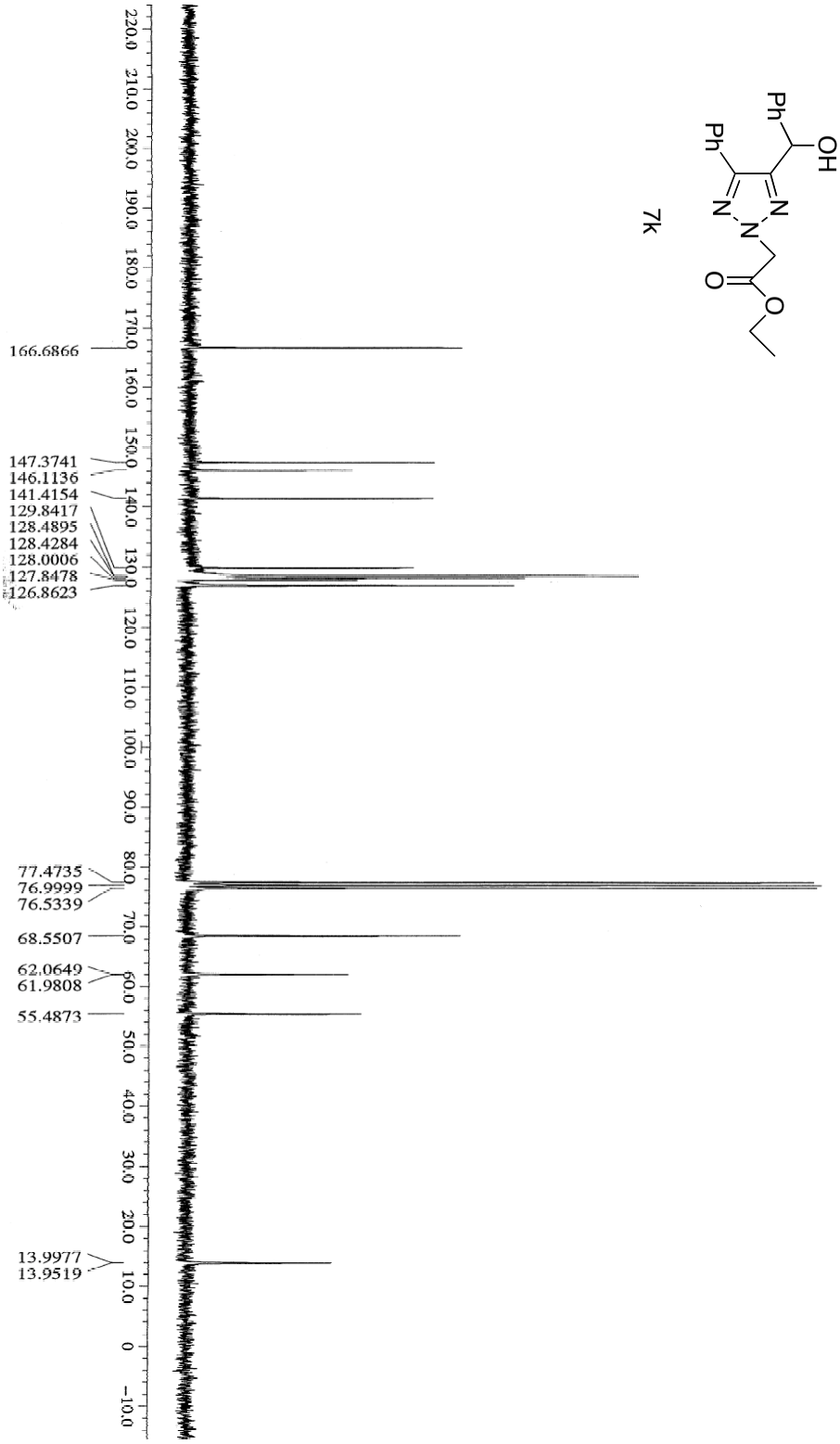
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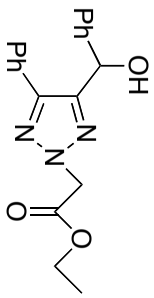
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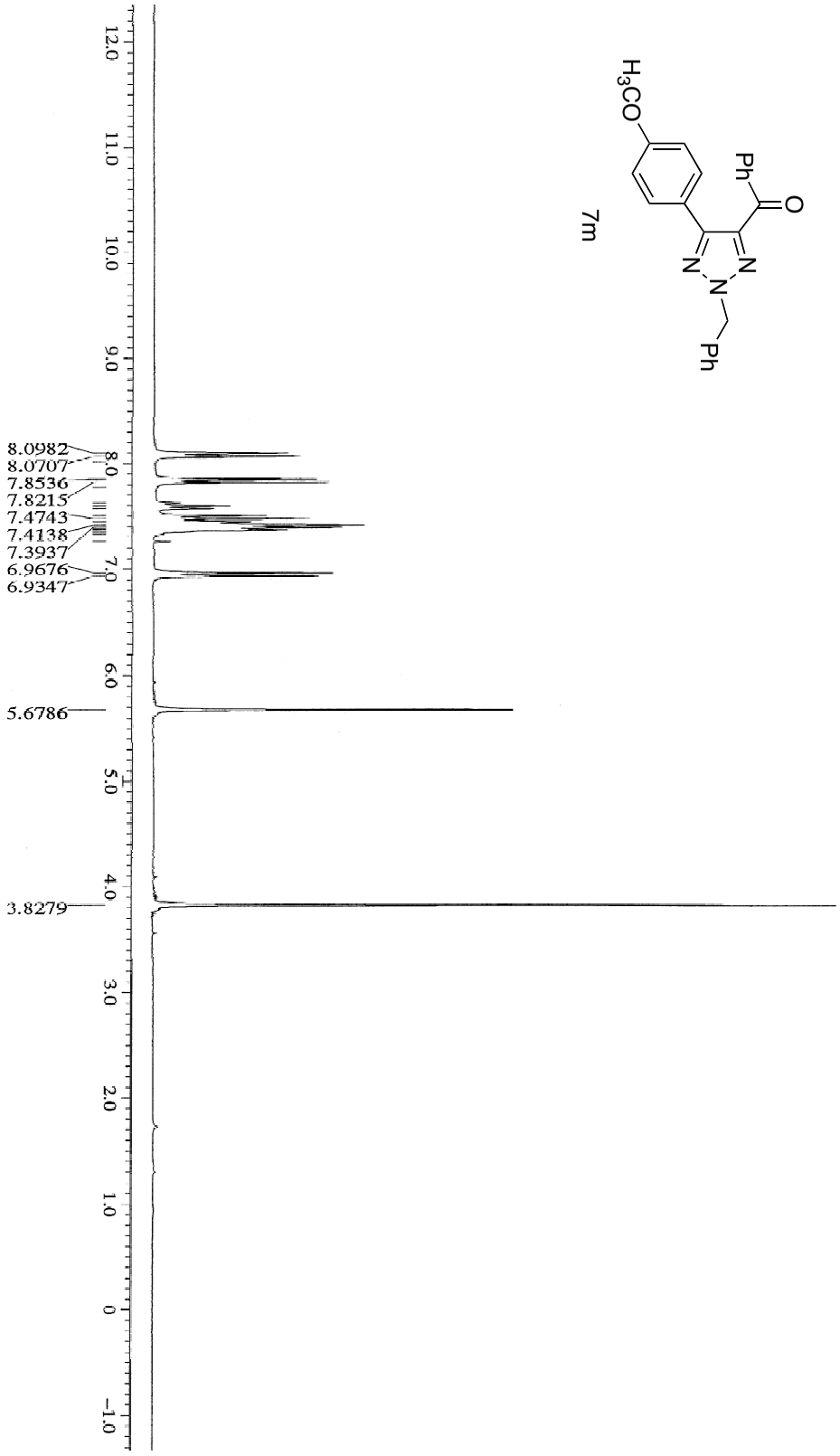
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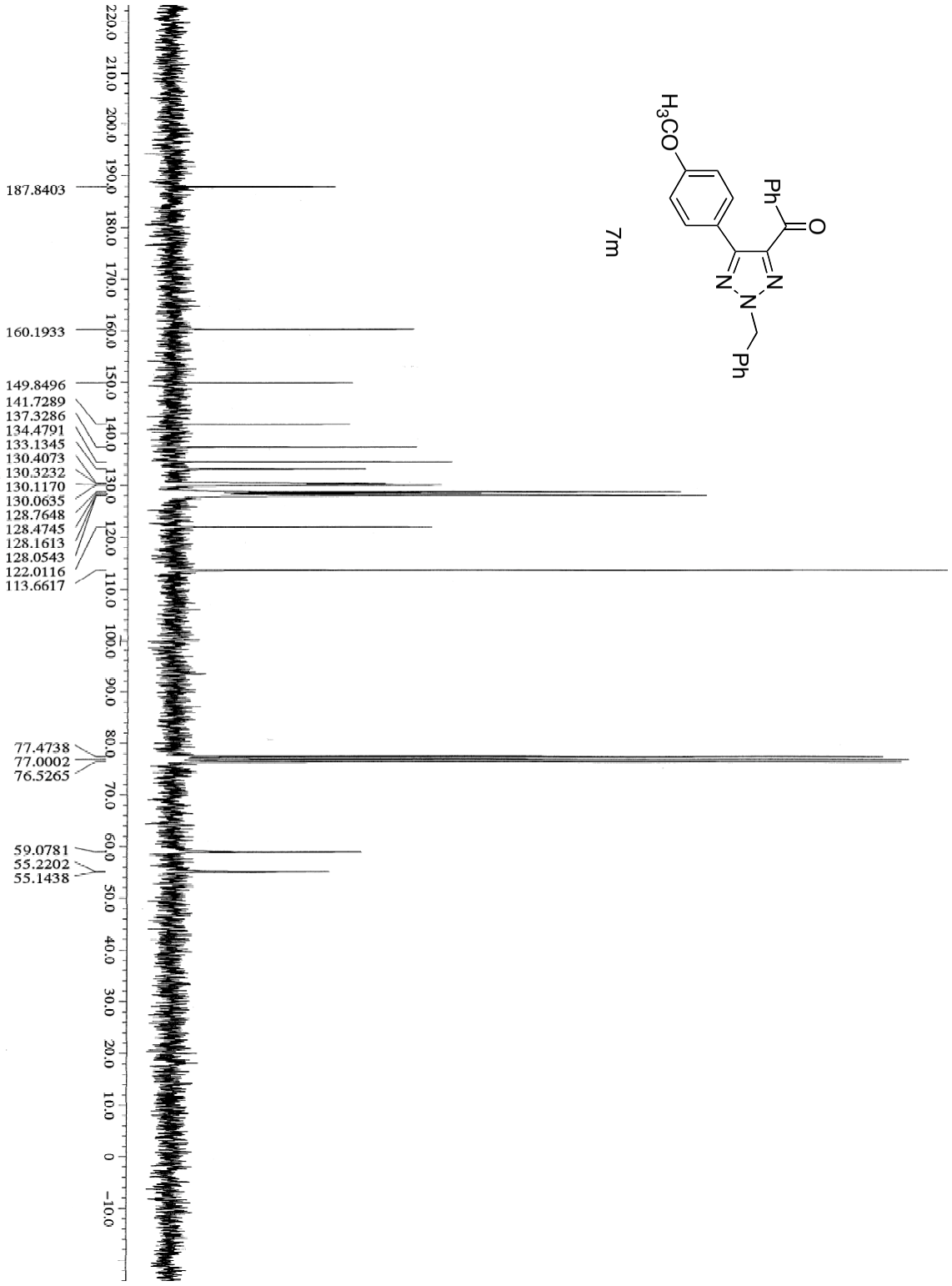
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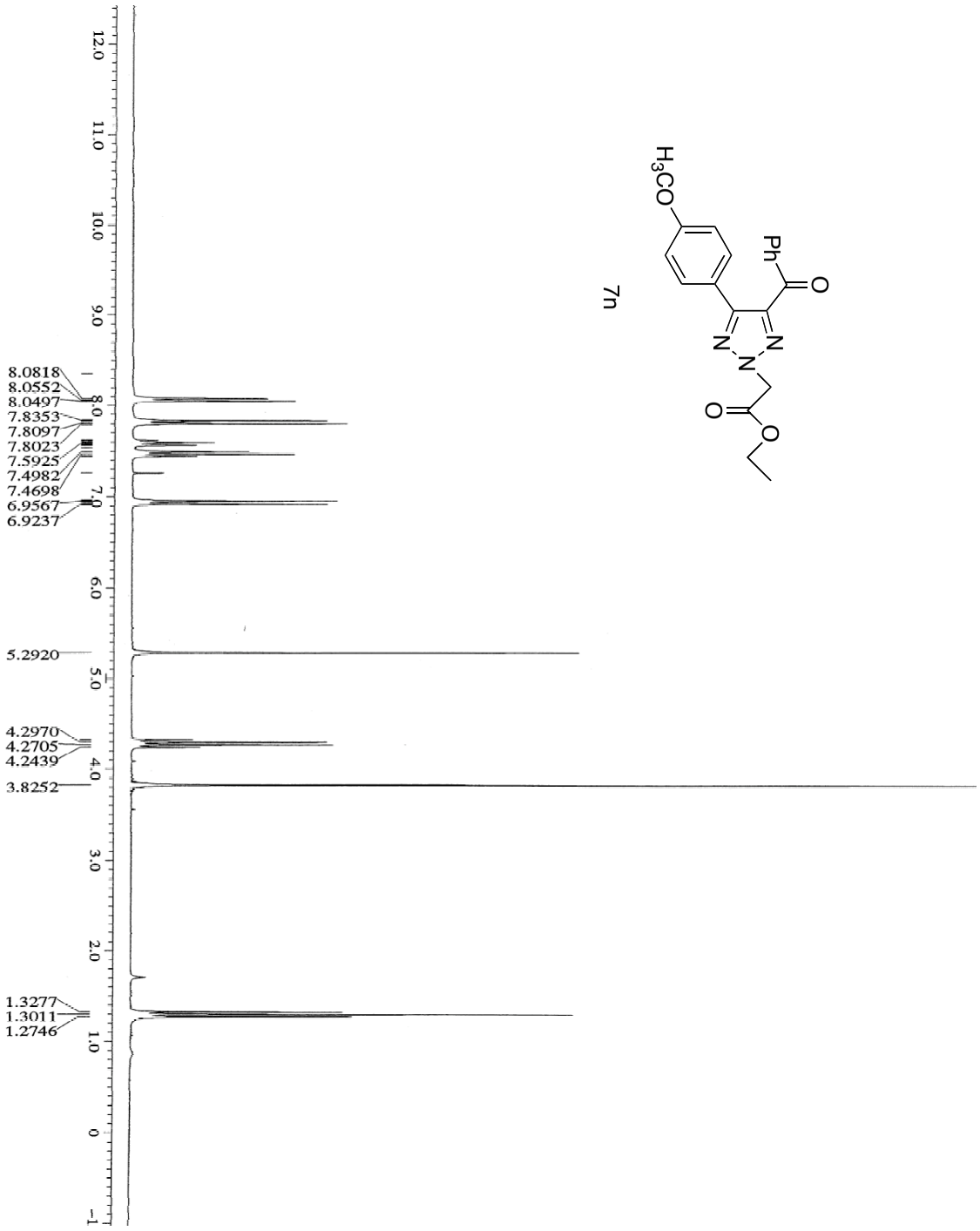
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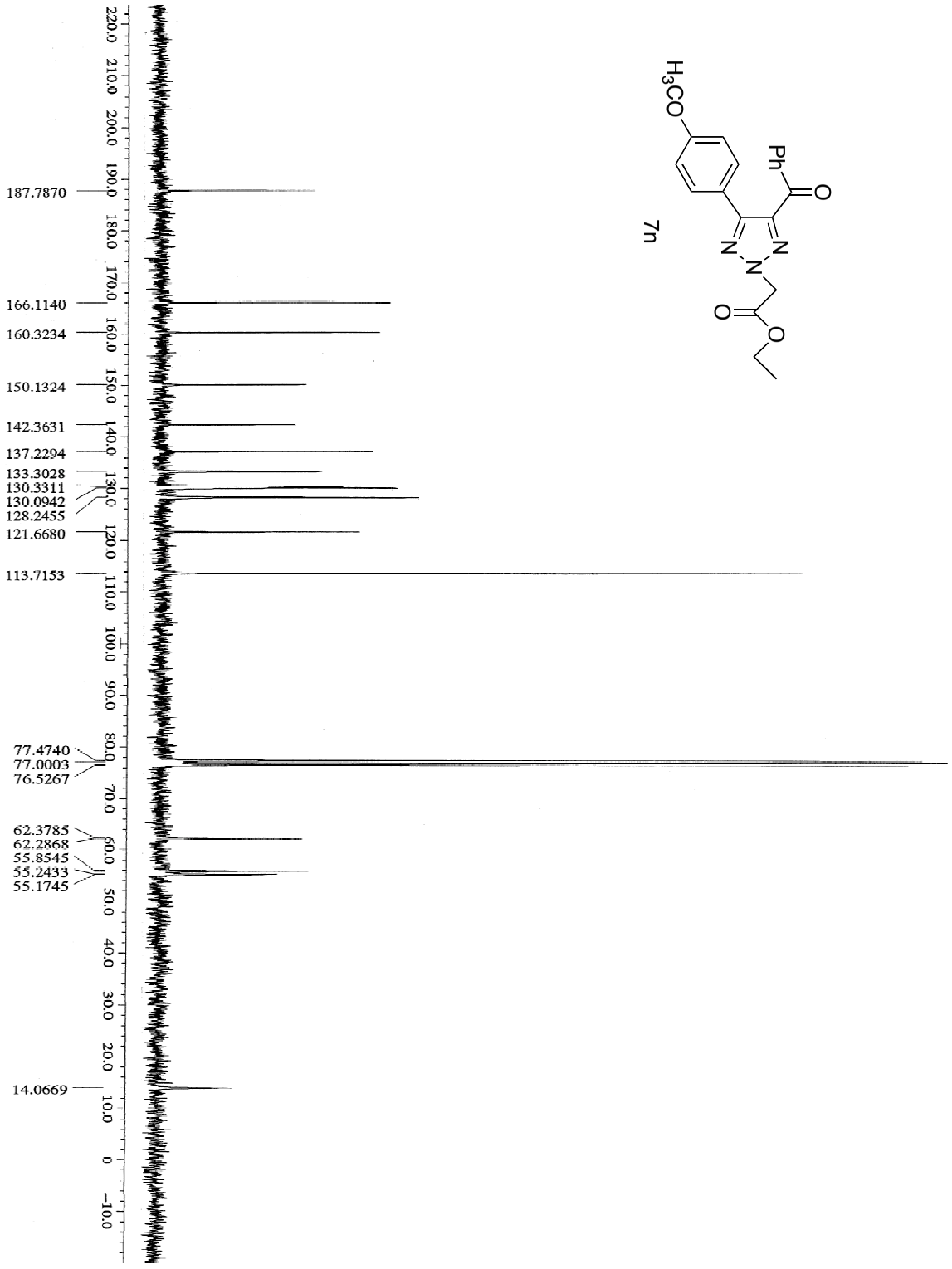
7n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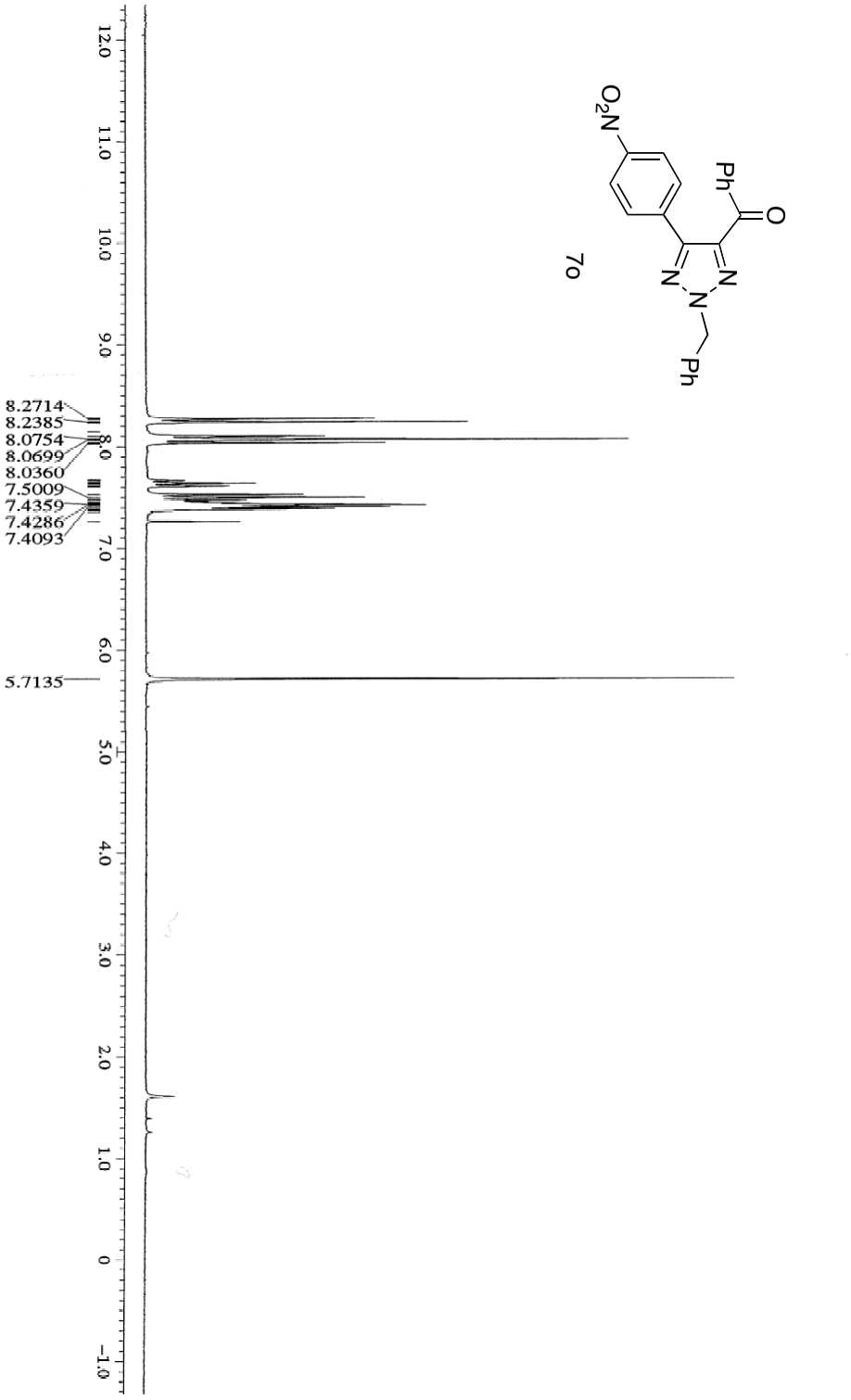
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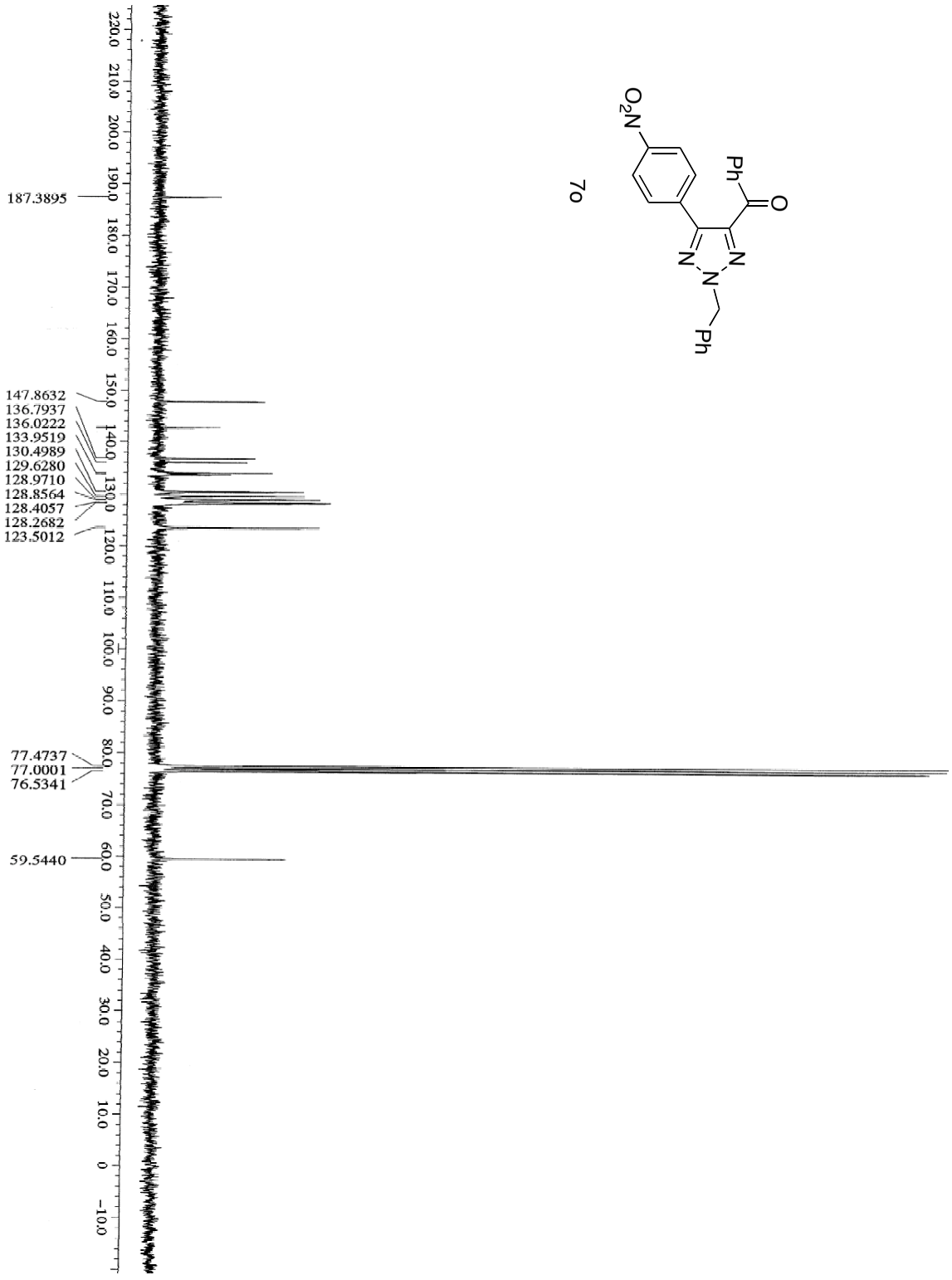
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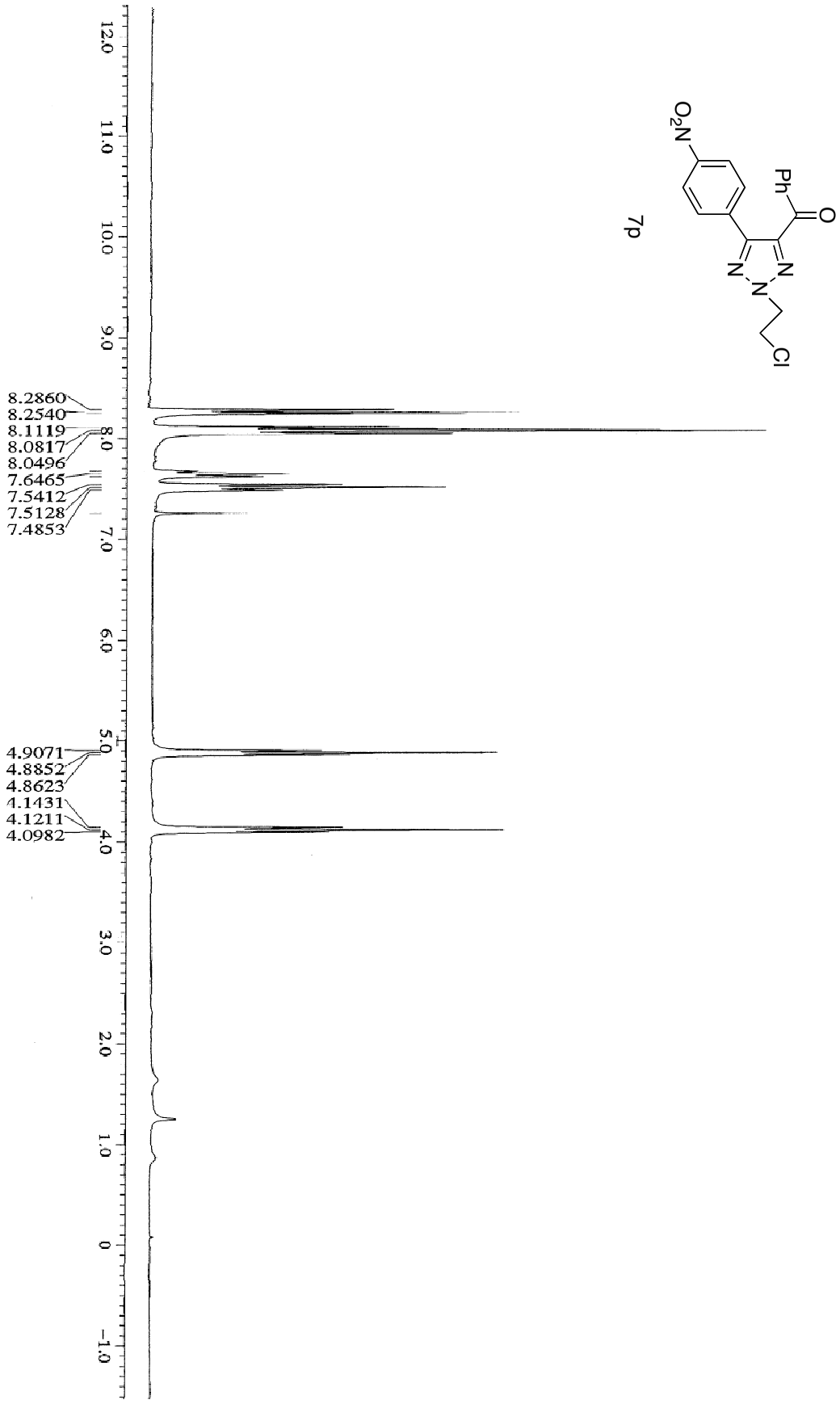
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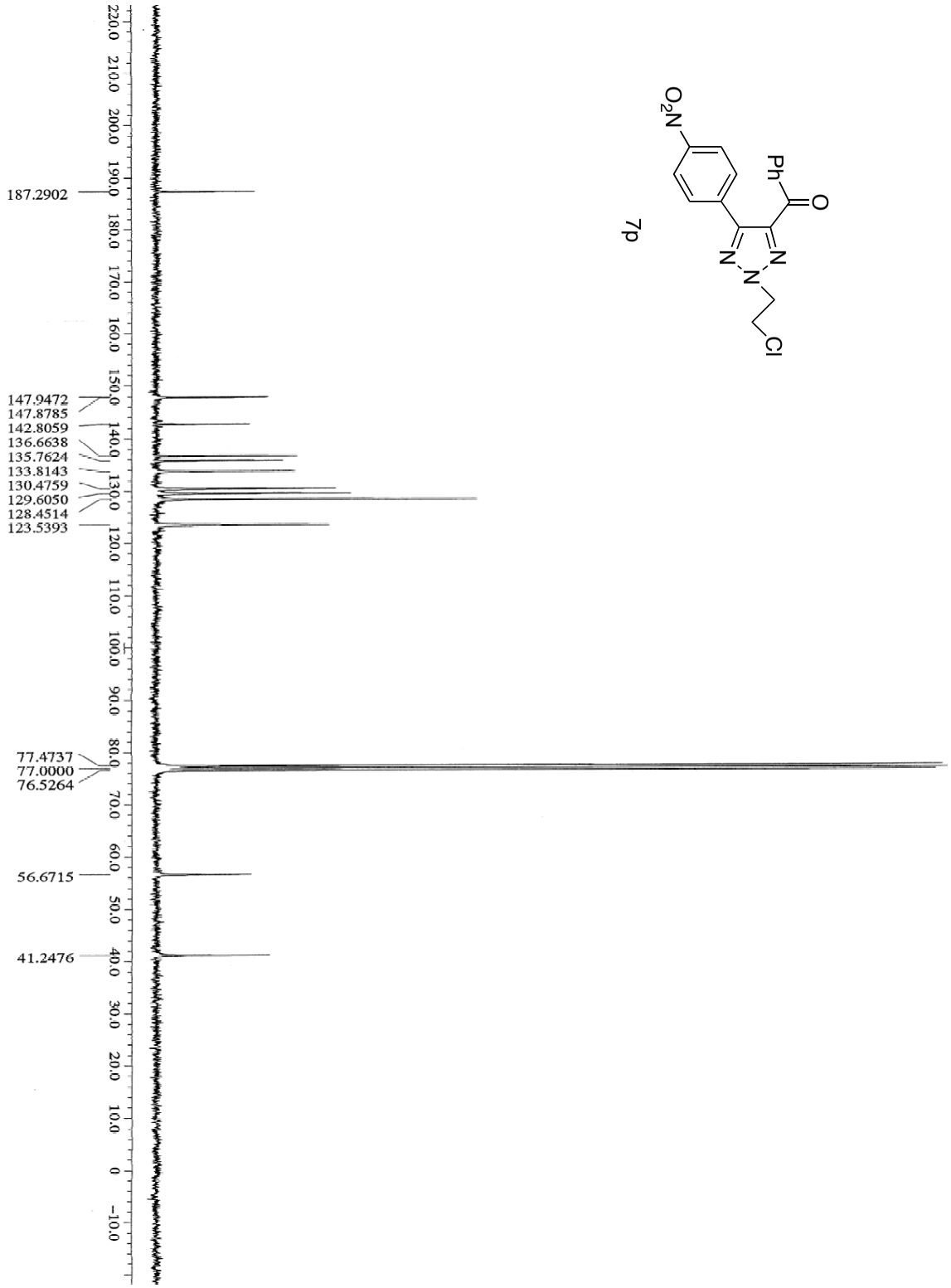
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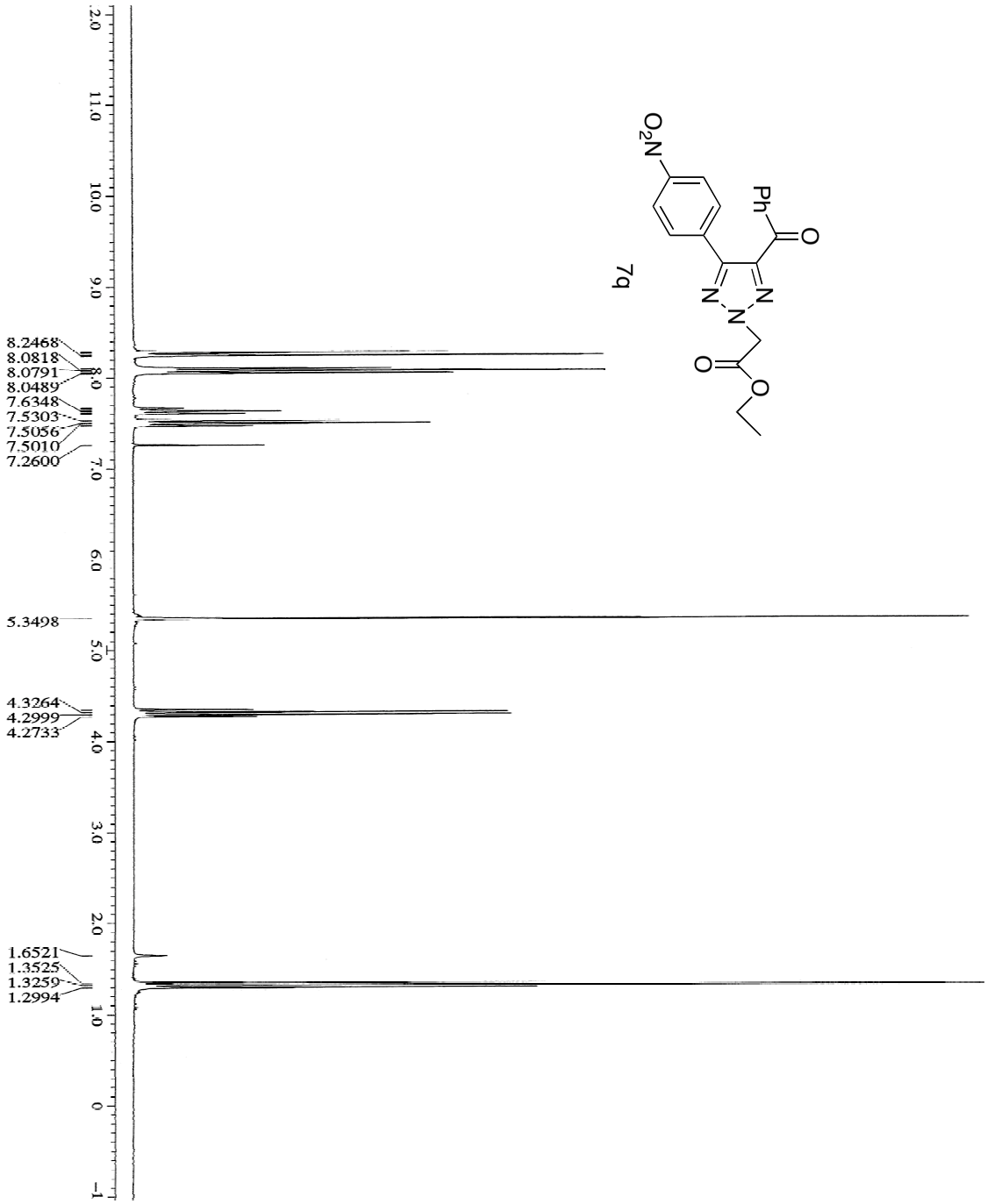
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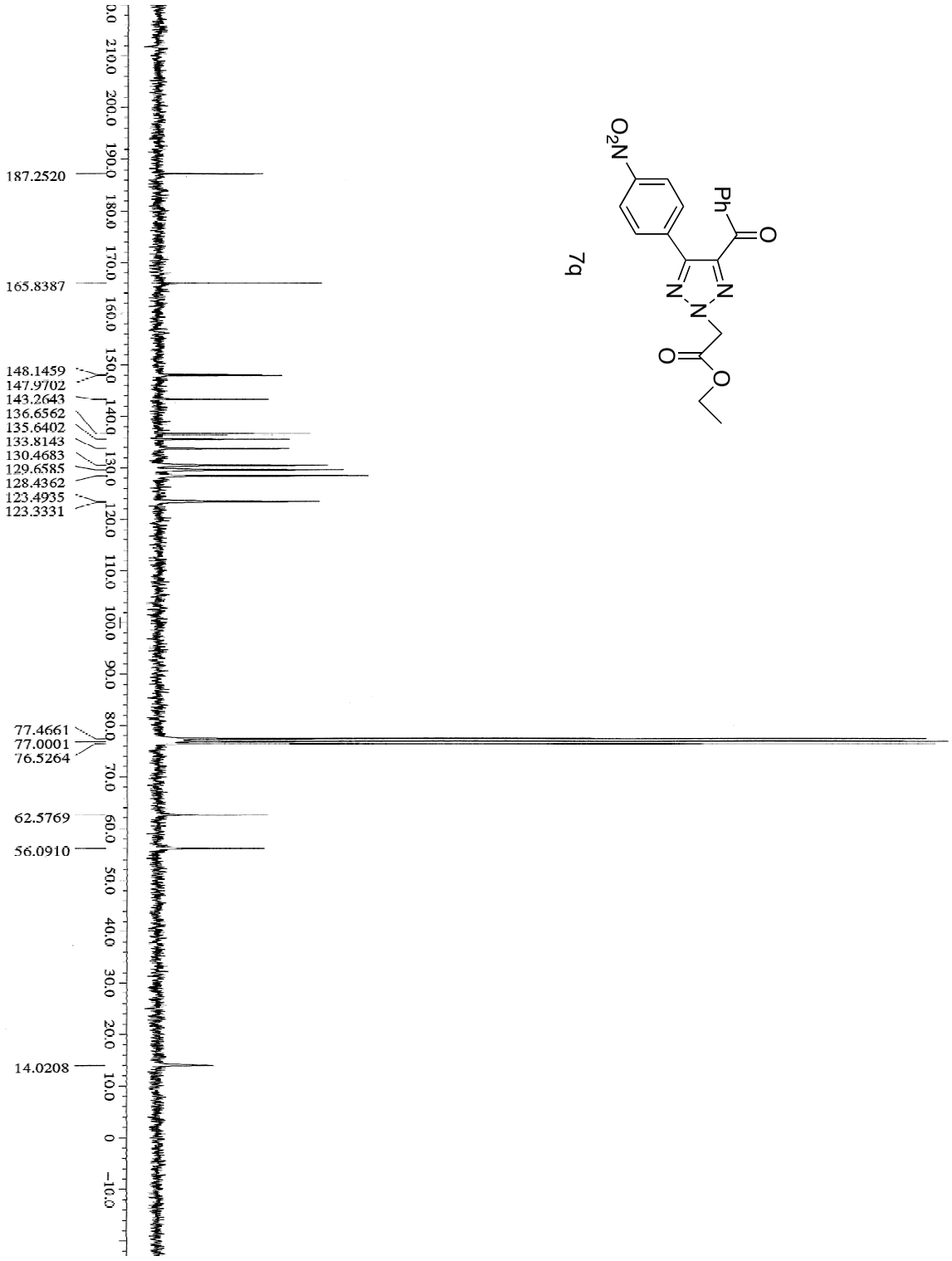
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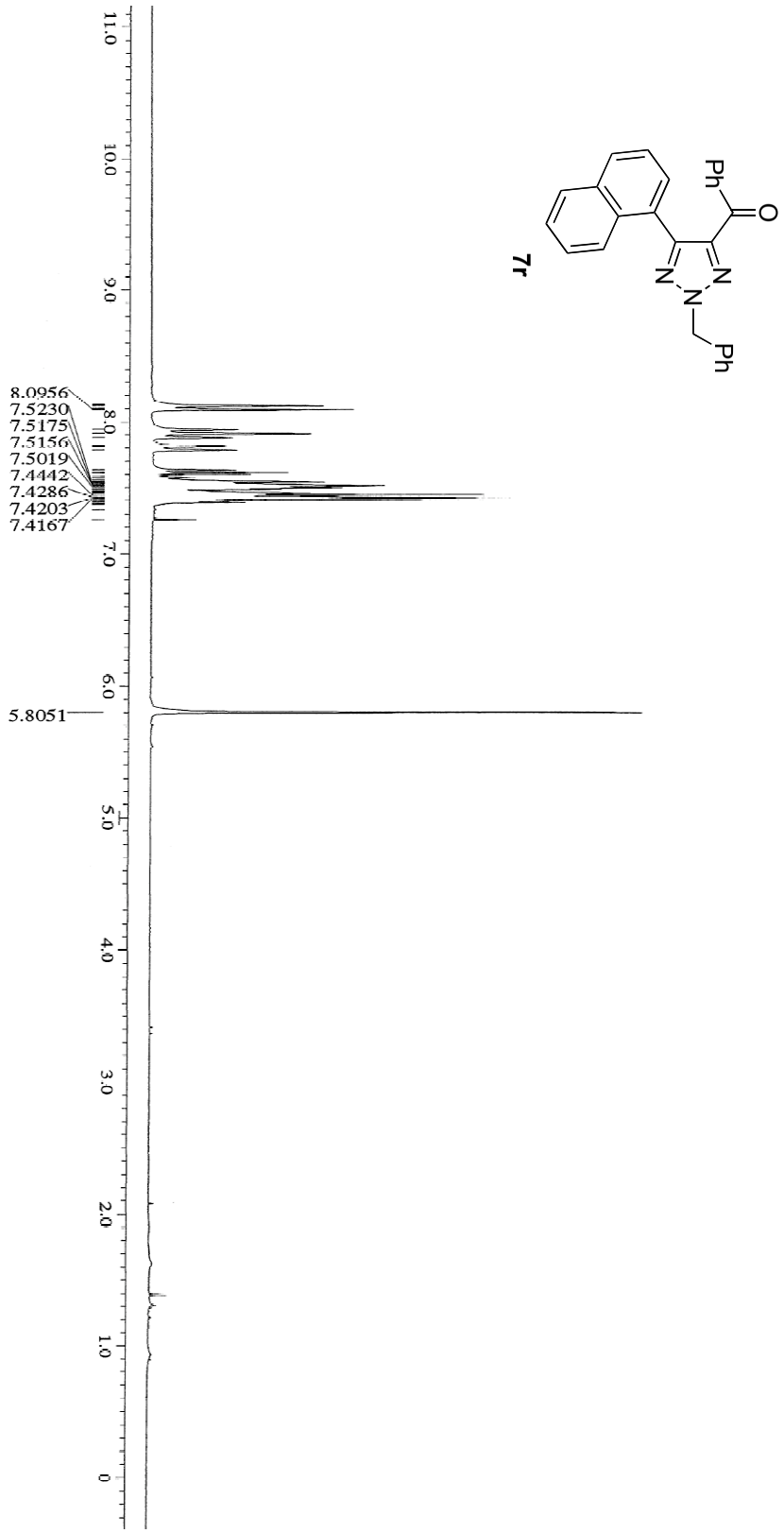
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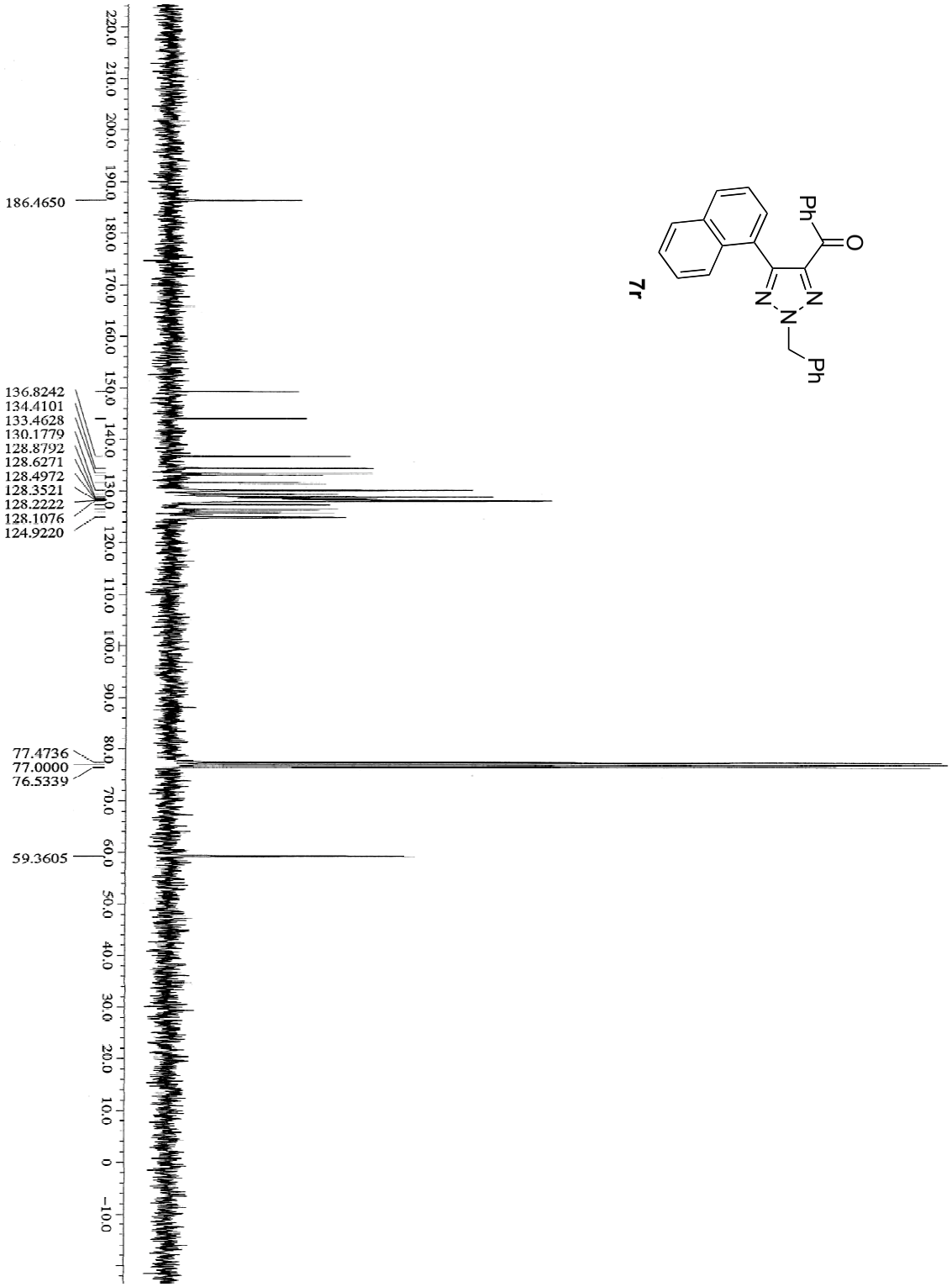
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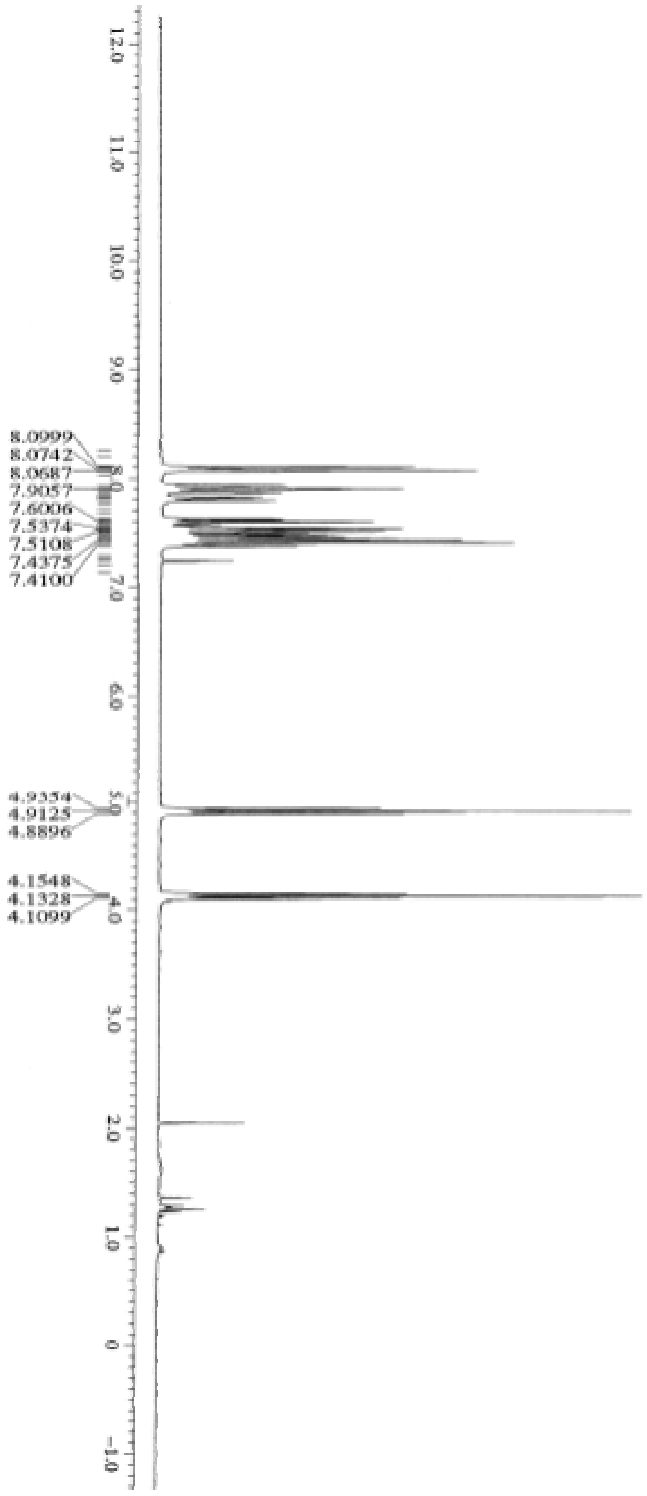
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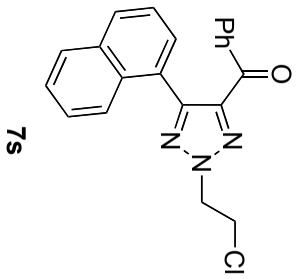
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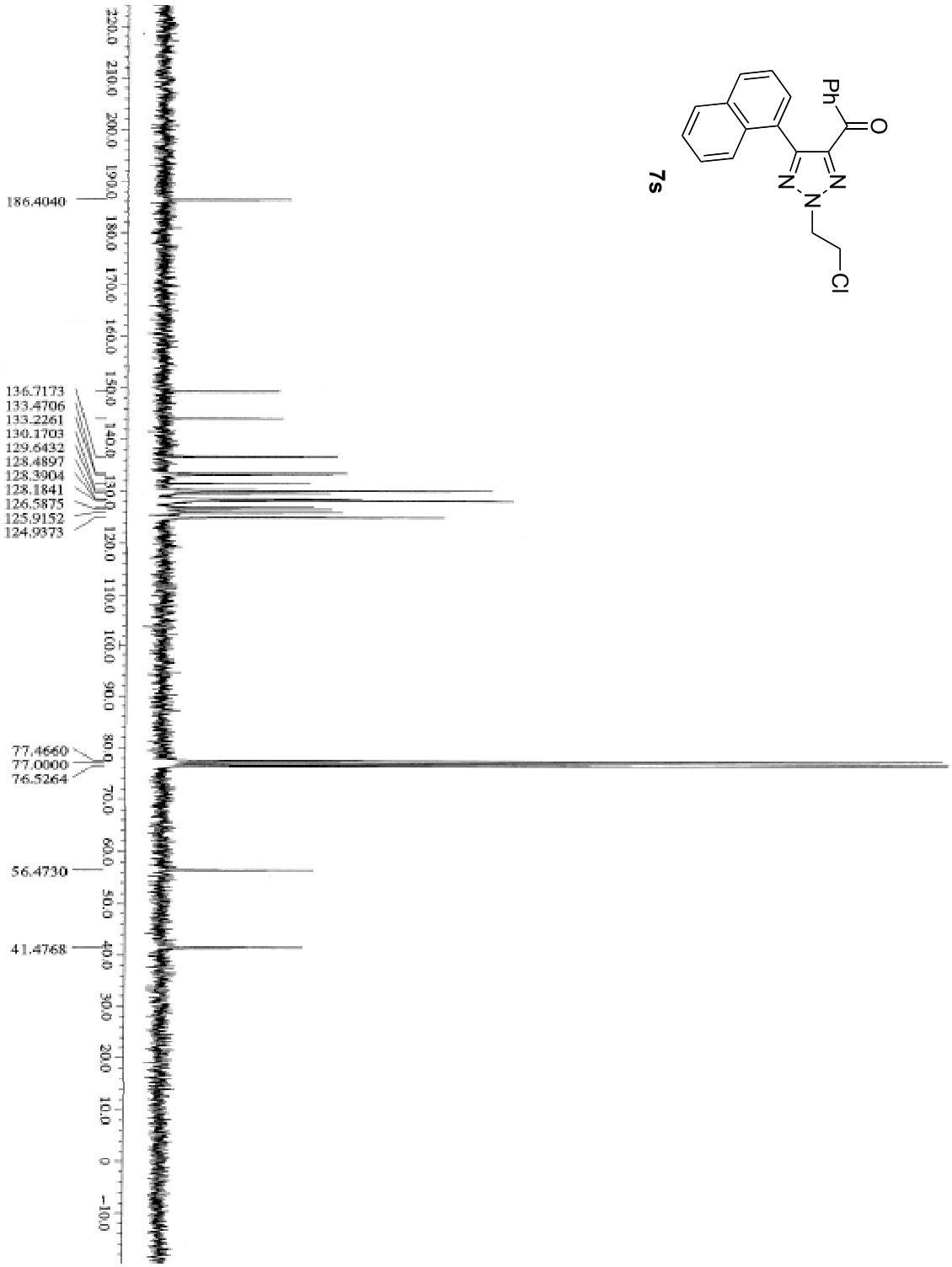
7s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124.9373
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77.0000
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41.4768
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190.0
180.0
170.0
160.0
150.0
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130.0
120.0
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90.0
80.0
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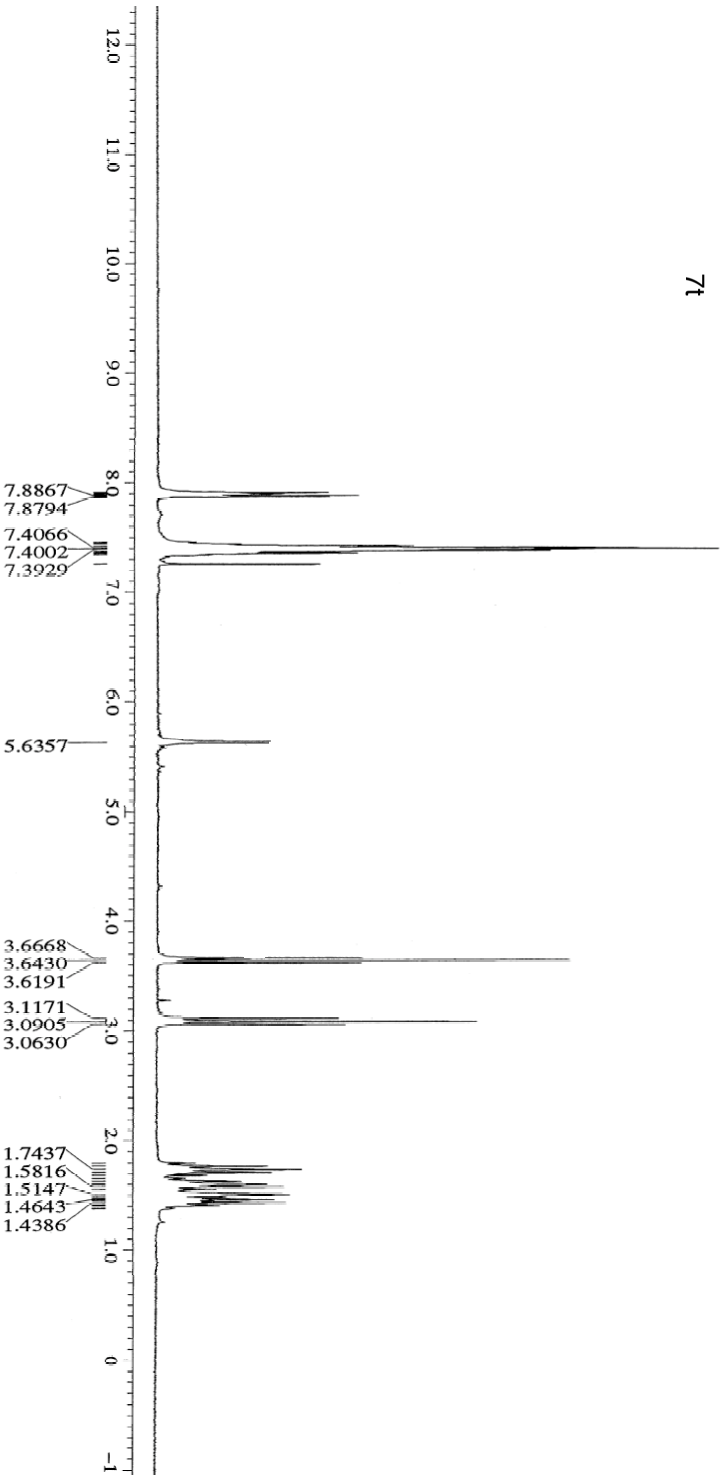
Cl

7s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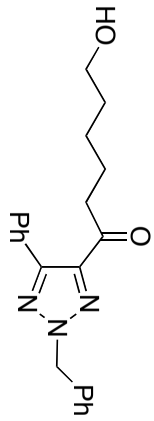
HO
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Ph
N
N
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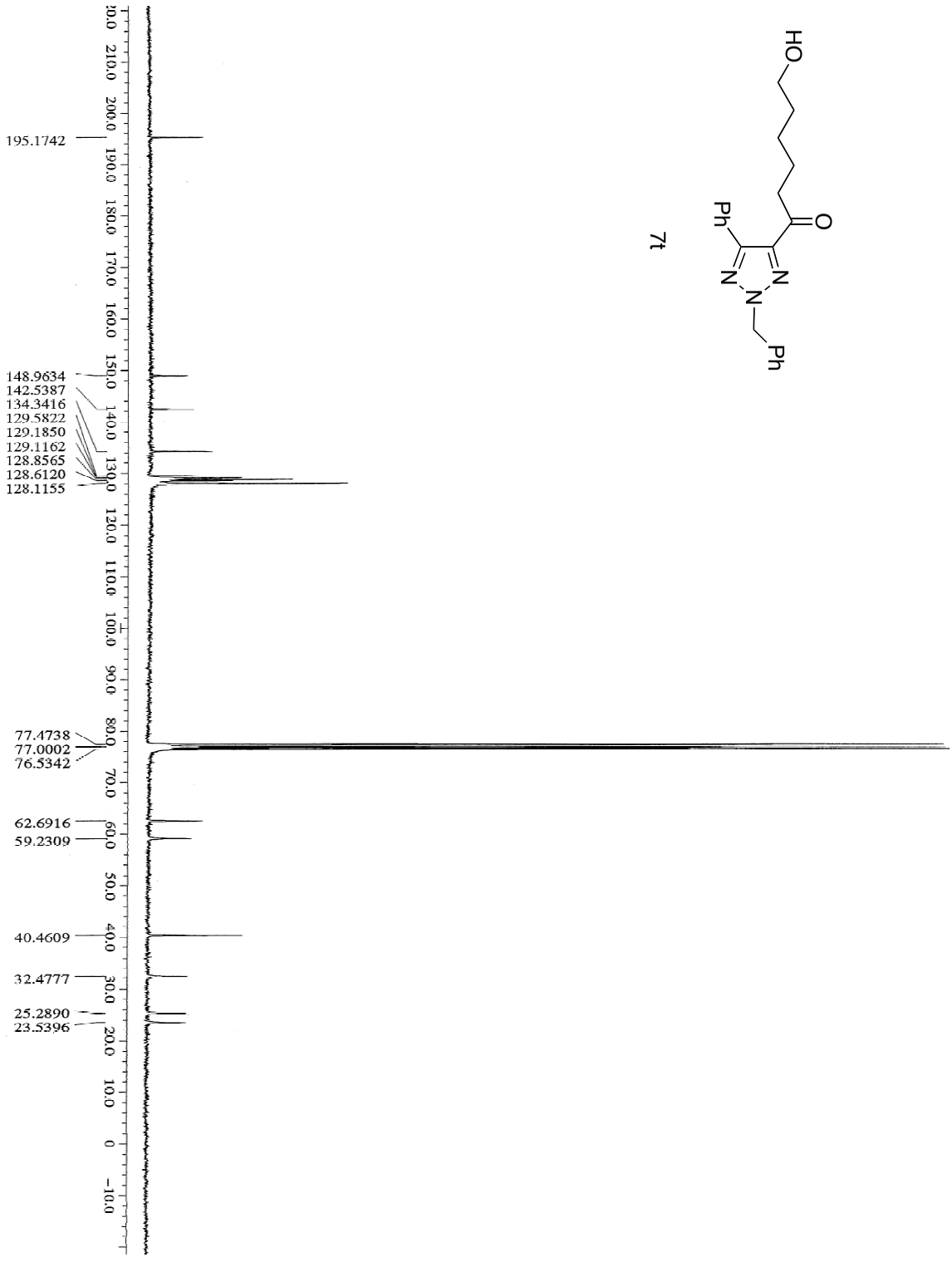
Ph

7t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77.0002
76.5342
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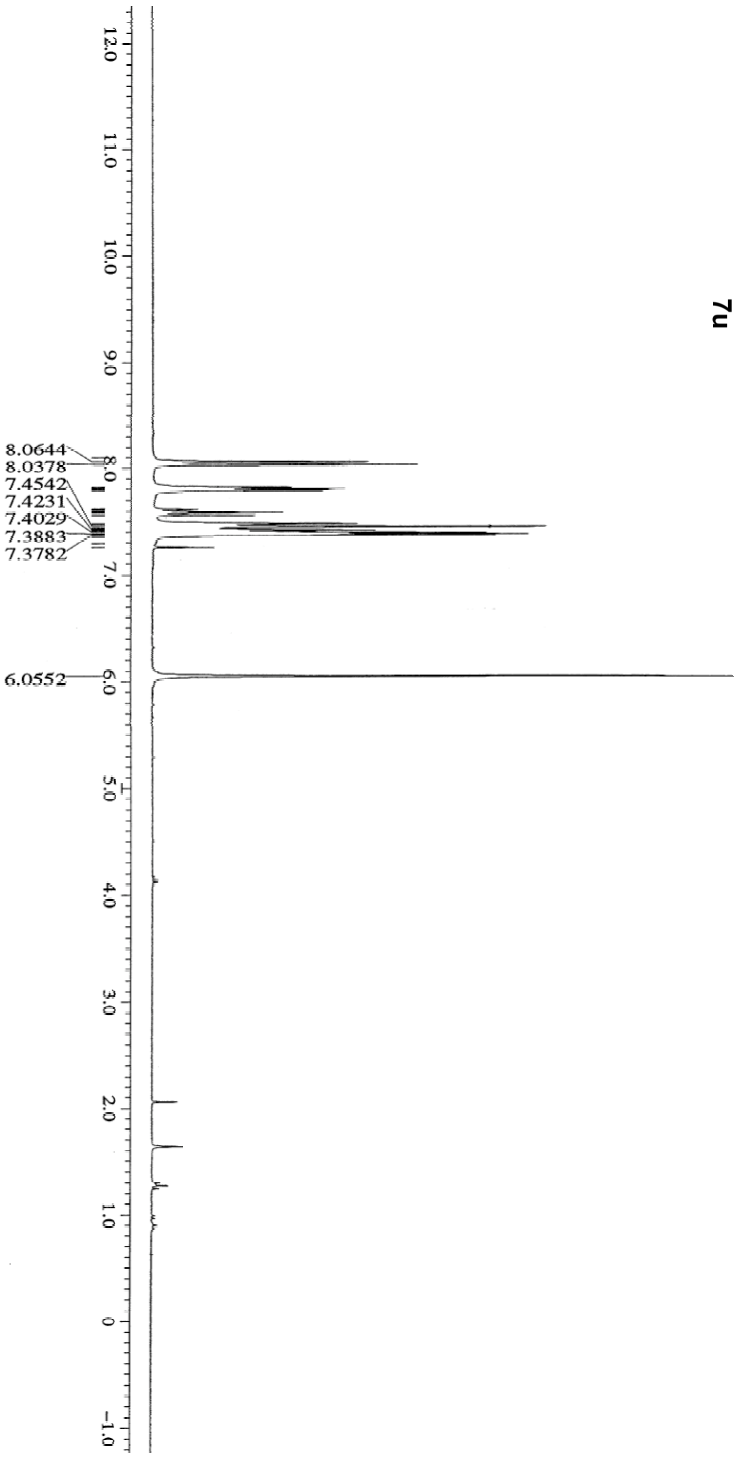
HO
O
Ph
N
N
N
Ph
7t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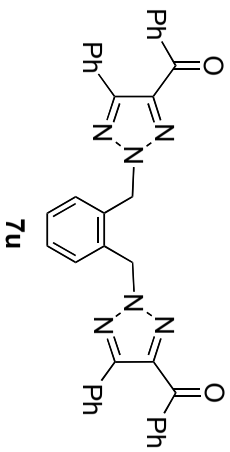
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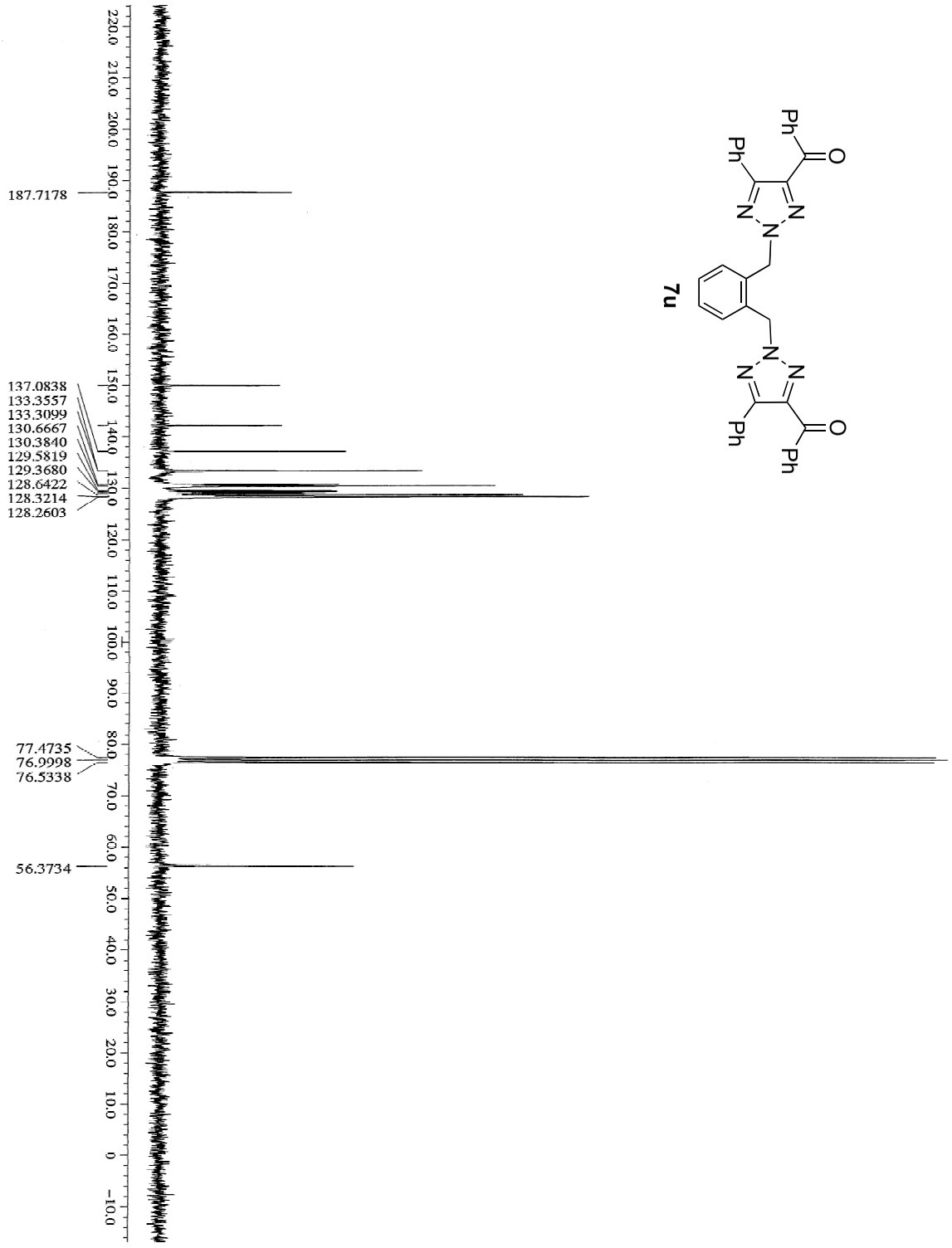
Ph

7u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120.0
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40.0
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Ph
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Ph
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N
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Ph
O
Ph

7u