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Supporting Information

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Metal-Catalyzed One-Pot Synthesis of Tetrazines Directly from Aliphatic Nitriles and Hydrazine**

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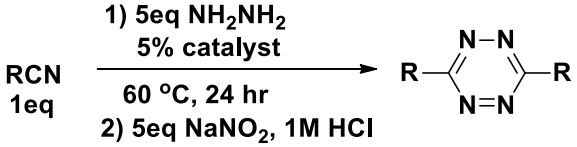
General Methods

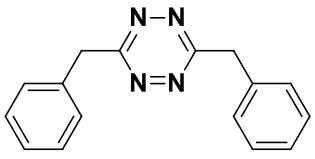
All chemicals were received from commercial sources and used without further purification. Thin layer chromatography (TLC) was performed on silica gel. Chromatographic purifications were conducted using 40-63 μm silica gel. All mixtures of solvents are given in *v*/*v* ratio. ^{1}H and ^{13}C NMR spectroscopy was performed on a Varian NMR at 500 (^{1}H) or 125 (^{13}C) MHz and a Jeol NMR at 500 (^{1}H) or 125 (^{13}C) MHz. All ^{13}C NMR spectra were proton decoupled. **Caution!** Anhydrous hydrazine (used for all tetrazine syntheses) is highly reactive to oxidizing agents and should be handled with care. **Caution!** 1,2,4,5-tetrazines are nitrogen rich molecules that can be highly reactive. Although we experienced no difficulty or accidents while performing the following syntheses at the scales noted, caution should be exercised particularly if attempting scale up.

Experimental Section

1. General procedure for synthesis of 3,6-dialkyl 1,2,4,5-tetrazine:

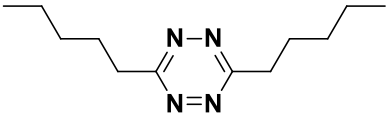


To a 10 mL microwave reaction tube equipped with a stir bar, 0.05 mmol of catalyst, 1.0 mmol of alkyl nitrile, and 0.16 mL (5 mmol) of anhydrous hydrazine was added. The vessel was sealed and the mixture was stirred in an oil bath at 60°C for 24 hours. After reaction, the seal was removed and the reaction solution was cooled to room temperature (when using benzyl cyanide as substrate, 2 mL DMF was added to dissolve the formed solid intermediate). Sodium nitrite (5 mmol, 345 mg) in 5 mL of water was slowly added to the solution and followed by slow addition of 1M HCl during which the solution turned bright red in color and gas evolved. Addition of 1M HCl continued until gas evolution ceased and the pH value is 3. (**Caution**! This step generates a large amount of toxic nitrogen oxide gasses and should be performed in a well ventilated fume hood). The mixture was extracted with CH_2Cl_2 and the organic phase dried over sodium sulfate. The solvent was removed using rotary evaporation and the residue purified using silica column chromatography. For applications requiring the absence of trace metals, we suggest washing the organic phase with an aqueous solution of EDTA prior to purification.

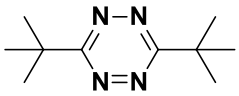


3,6-dibenzyl-1,2,4,5-tetrazine: The title product was purified as a purple solid after silica column chromatography (Hexane:EtOAc=20:1). Yield: 70% ($Zn(OTf)_2$); 95% ($Ni(OTf)_2$). ^{1}H NMR (500 MHz, $CDCl_3$) δ 7.39-7.43 (4H, m), 7.29-

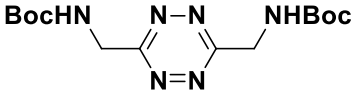
7.34 (4H, m), 7.22-7.28 (2H, m), 4.60 (4H, s); ^{13}C NMR (125 MHz, $CDCl_3$) δ 169.31, 135.91, 129.34, 129.01, 127.49, 41.35; HRMS $[M+H]^+$ m/z calcd. for $[C_{16}H_{15}N_4]^+$ 263.1289, found 263.1291.



3,6-dipentyl-1,2,4,5-tetrazine: The title product was purified as a red oil after silica column chromatography (Hexane). Yield: 59% ($Zn(OTf)_2$); trace ($Ni(OTf)_2$). ^{1}H NMR (500 MHz, $CDCl_3$) δ 3.29 (4H, t, J = 7.5 Hz), 1.89-1.98 (4H, m), 1.32-1.46 (8H, m), 0.91 (6H, t, J = 7 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.36, 34.82, 31.43, 28.14, 22.45, 14.00; HRMS $[M+H]^+$ m/z calcd. for $[C_{12}H_{23}N_4]^+$ 223.1916, found 223.1917.

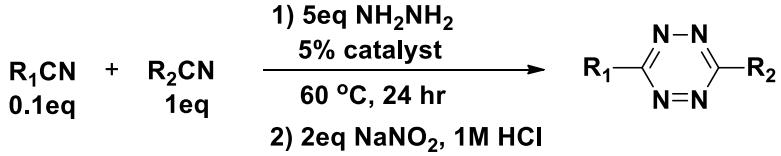


3,6-di-*tert*-butyl-1,2,4,5-tetrazine: The title product was purified as a purple solid after silica column chromatography (Hexane). Yield: 25% ($Zn(OTf)_2$); trace ($Ni(OTf)_2$). ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.58 (18H, s); ^{13}C NMR (125 MHz, $CDCl_3$) δ 175.12, 37.88, 29.30; HRMS $[M+H]^+$ m/z calcd. for $[C_{10}H_{19}N_4]^+$ 195.1603, found 195.1604.



di-*tert*-butyl ((1,2,4,5-tetrazine-3,6-diyl)bis(methylene))dicarbamate: The title product was purified as a red solid after silica column chromatography (hexane:EtOAc=2:1). Yield: 32% ($Zn(OTf)_2$). ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.45 (18H, s), 4.98 (4H, d, J = 10 Hz), 5.62 (2H, broad s); ^{13}C NMR (125 MHz, $CDCl_3$) δ 39.01, 51.15, 80.71, 141.01, 150.45; HRMS $[M+Na]^+$ m/z calcd. for $[C_{14}H_{24}N_6O_4Na]^+$ 363.1749, found 363.1751.

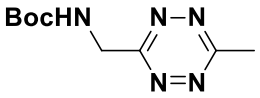
2. General procedure for synthesis of 3-alkyl-6-aryl or alkyl-1,2,4,5-tetrazine:



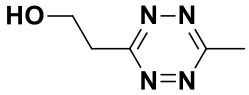
when R_1 is N-Boc-pyrrole, the Boc will be deprotected to give pyrrole

To a 10 mL microwave reaction tube equipped with a stir bar, 0.25 mmol of catalyst, 0.26 mL (5.0 mmol) of acetonitrile, 0.5 mmol of a second nitrile, and 0.8

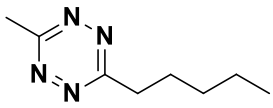
mL (25.0 mmol) of anhydrous hydrazine was added. The vessel was sealed and the mixture was stirred in an oil bath at 60°C for 24 hours. The reaction solution was cooled to room temperature and the seal was removed. Sodium nitrite (10 mmol, 690 mg) in 5 mL of water was slowly added to the solution followed by slow addition of 1M HCl during which the solution turned bright red in color and gas evolved. Addition of 1M HCl continued until gas evolution ceased and the pH value is 3. (**Caution**! This step generates a large amount of toxic nitrogen oxide gasses and should be performed in a well ventilated fume hood). The mixture was extracted with EtOAc and the organic phase dried over sodium sulfate. The EtOAc was removed using rotary evaporation and the residue purified using silica column chromatography.



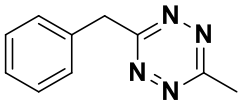
***tert*-butyl ((6-methyl-1,2,4,5-tetrazin-3-yl)methyl)carbamate:** The title product was purified as a red solid after silica column chromatography (Hexane:EtOAc=5:1). Yield: 36% ($Zn(OTf)_2$); 36% ($Ni(OTf)_2$). ^1H NMR (500 MHz, $CDCl_3$) δ 5.57 (1H, N-H, bs), 4.95 (2H, s), 3.08 (3H, s), 1.46 (9H, s). ^{13}C NMR (125 MHz, $CDCl_3$) δ 33.27, 38.99, 51.06, 80.61, 141.01, 149.52, 151.03; HRMS $[M+Na]^+$ m/z calcd. for $[C_9H_{15}N_5O_2Na]^+$ 248.1119, found 248.1118.



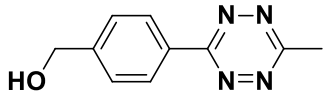
2-(6-methyl-1,2,4,5-tetrazin-3-yl)ethanol: Following the general procedure but the reaction time is 36hr. The title product was purified as a red liquid after silica column chromatography (Hexane:EtOAc=1:1). Yield: 36% ($Zn(OTf)_2$); 36% ($Ni(OTf)_2$). ^1H NMR (500 MHz, $CDCl_3$) δ 1.62 (1H, bs), 3.07 (3H, s), 3.57 (2H, t, J = 10 Hz), 4.26 (2H, t, J = 10 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ 35.07, 48.25, 66.20, 112.98, 152.35, 152.69; HRMS $[M+H]^+$ m/z calcd. for $[C_5H_9N_4O]^+$ 141.0770, 141.0771.



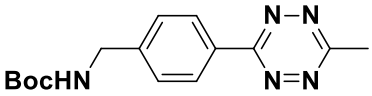
3-methyl-6-pentyl-1,2,4,5-tetrazine: The title product was purified as a red liquid after silica column chromatography (Hexane:EtOAc=10:1). Yield: 40% ($Zn(OTf)_2$); 17% ($Ni(OTf)_2$). ^1H NMR (500 MHz, $CDCl_3$) δ 0.92 (3H, t, J = 10 Hz), 1.39 (4H, m), 1.93 (2H, m), 3.03 (3H, s) 3.28 (2H, t, J = 10 Hz). ^{13}C NMR (125 MHz, $CDCl_3$) δ 27.48, 33.24, 34.22, 38.79, 41.39, 44.12, 150.20, 152.50; HRMS $[M+H]^+$ m/z calcd. for $[C_8H_{15}N_4]^+$ 167.1289, found 167.1291.



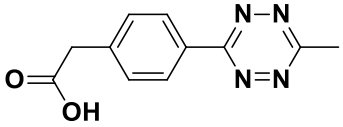
3-benzyl-6-methyl-1,2,4,5-tetrazine: The title product was purified as a red liquid after silica column chromatography (Hexane:EtOAc=10:1). Yield: 40% ($Zn(OTf)_2$); 20% ($Ni(OTf)_2$). ^1H NMR (400 MHz, $CDCl_3$) δ 3.01 (3H, s), 4.61 (2H, s), 7.23-7.26 (1H, m), 7.29-7.33 (2H, m) 7.39-7.42 (2H, m); ^{13}C NMR (100 MHz, $CDCl_3$) δ 22.05, 42.13, 128.28, 128.83, 130.13, 168.46, 169.90; HRMS $[M+H]^+$ m/z calcd. for $[C_{10}H_{11}N_4]^+$ 187.0977, 187.0978.



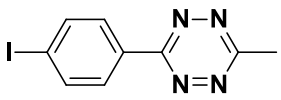
(4-(6-methyl-1,2,4,5-tetrazin-3-yl)phenyl)methanol: The title product was purified as a purple solid after silica column chromatography (Hexane:EtOAc=2:1). Yield: 27% ($Zn(OTf)_2$); 66% ($Ni(OTf)_2$). ^1H NMR (500 MHz, $CDCl_3$) δ 3.10 (3H, m), 4.84 (2H, s), 7.58 (2H, m), 8.59 (2H, d, J = 10 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 33.38, 68.12, 118.38, 118.94, 121.08, 132.91, 147.50, 150.14; HRMS $[M+H]^+$ m/z calcd. for $[C_{10}H_{11}N_4O]^+$ 203.0924, found 203.0927.



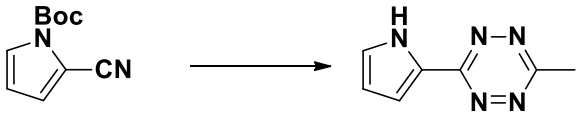
***tert*-butyl 4-(6-methyl-1,2,4,5-tetrazin-3-yl)benzylcarbamate:** The title product was purified as a red solid after silica column chromatography (Hexane:EtOAc=4:1). Yield: 30% ($Zn(OTf)_2$); 68% ($Ni(OTf)_2$). ^1H NMR (500 MHz, $CDCl_3$) δ 1.48 (9H, s), 3.09 (3H, s), 4.43 (2H, d, J = 5 Hz), 4.97 (1H, bs), 7.50 (2H, d, J = 10 Hz), 8.56 (2H, d, J = 5 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 32.25, 38.06, 50.80, 79.14, 117.74, 117.84, 119.89, 130.54, 140.12, 146.42, 149.08; HRMS $[M+Na]^+$ m/z calcd. for $[C_{15}H_{19}N_5O_2Na]^+$ 324.1429, 324.1431.



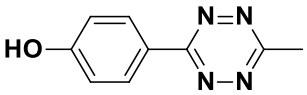
2-(4-(6-methyl-1,2,4,5-tetrazin-3-yl)phenyl)acetic acid: The title product was purified as a purple solid after silica column chromatography (CH_2Cl_2:MeOH=15:1). Yield: 70% ($Zn(OTf)_2$); 70% ($Ni(OTf)_2$). ^1H NMR (500 MHz, $CDCl_3$) δ 3.93 (3H, s), 4.48 (2H, s), 7.47 (2H, d, J = 5 Hz), 8.31 (2H, d, J = 5 Hz); ^{13}C NMR (125 MHz, CD_3OD) δ 35.73, 53.18, 121.99, 124.01, 124.41, 132.35, 151.10, 153.85, 159.56; HRMS $[M+H]^+$ m/z calcd. for $[C_{11}H_{11}N_4O_2]^+$ 231.0879, 231.0877.



3-(4-(iodomethyl)phenyl)-6-methyl-1,2,4,5-tetrazine: The title product was purified as a purple solid after silica column chromatography (Hexane:EtOAc=60:1). Yield: 40% ($Ni(OTf)_2$). ^1H NMR (500 MHz, $CDCl_3$) δ 3.10 (3H, s), 7.95 (2H, d, J = 10 Hz), 8.32 (2H, d, J = 10 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 33.37, 96.57, 119.81, 121.41, 127.25, 147.41, 150.40; HRMS $[M+H]^+$ m/z calcd. for $[C_9H_8IN_4]^+$ 298.9788, found 298.9783.

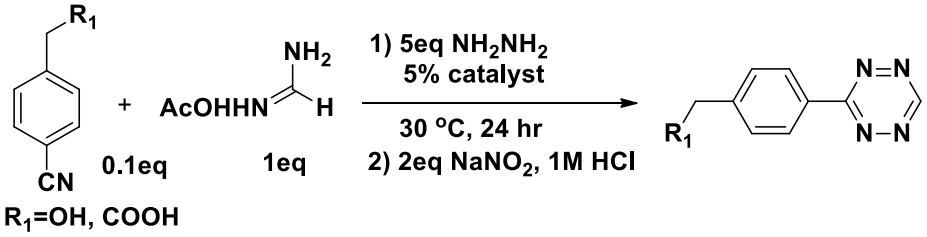


3-methyl-6-(1H-pyrrol-2-yl)-1,2,4,5-tetrazine: The title product was purified as a orange solid after silica column chromatography (Hexane:EtOAc=8:1). Yield: 58% ($Ni(OTf)_2$). ^1H NMR (500 MHz, $CDCl_3$) δ 3.00 (3H, s), 6.44 (1H, m), 7.14 (1H, s), 7.41 (1H, m), 9.72 (1H, bs); ^{13}C NMR (125 MHz, $CDCl_3$) δ 22.10, 112.96, 115.57, 125.20, 160.05, 166.66; HRMS $[M+H]^+$ m/z calcd. for $[C_7H_8N_5]^+$ 162.0772, found 162.0774.



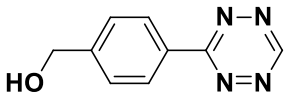
4-(6-methyl-1,2,4,5-tetrazin-3-yl)phenol: The title product was purified as a orange solid after silica column chromatography (Hexane:EtOAc=8:1). Yield: 30% ($Ni(OTf)_2$); 43% ($Zn(OTf)_2$). ^1H NMR (500 MHz, $CDCl_3$) δ 3.07 (3H, s), 5.23 (1H, S), 7.03 (2H, d, J = 10 Hz), 8.52 (2H, d, J = 10 Hz); ^{13}C NMR (125 MHz, CD_3OD) δ 20.88, 117.14, 124.30, 130.74, 163.12, 165.18, 167.84; HRMS $[M+H]^+$ m/z calcd. for $[C_9H_9N_4O]^+$ 189.0771, found 189.0766.

3. General procedure for synthesis of 3-H-6-aryl-1,2,4,5-tetrazine:

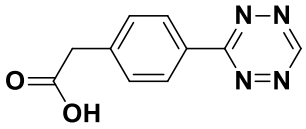


To a 10 mL microwave reaction tube equipped with a stir bar, 0.125 mmol of $Ni(OTf)_2$, 0.27g (2.5 mmol) of formamidine acetate, benzonitrile (0.25 mmol), and 0.40 mL (12.5 mmol) of anhydrous hydrazine was added. The vessel was sealed and the mixture was stirred at 30°C for 24 hours. Sodium nitrite (5 mmol, 345 mg) in 5 mL of water was slowly added to the solution and followed by slow addition

of 1M HCl during which the solution turned bright red in color and gas evolved. Addition of 1M HCl continued until gas evolution ceased and the pH value is 3. (**Caution**! This step generates a large amount of toxic nitrogen oxide gasses and should be performed in a well ventilated fume hood). The mixture was extracted with EtOAc and the organic phase dried over sodium sulfate. The EtOAc was removed using rotary evaporation and the residue purified using silica column chromatography.

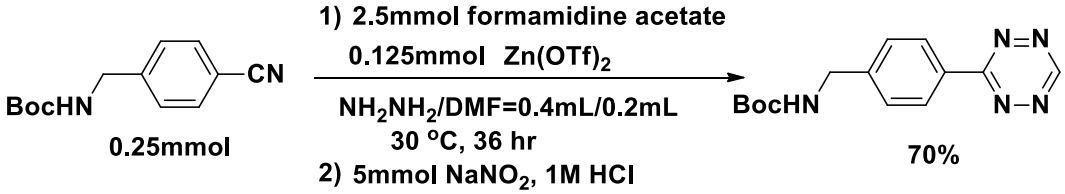


(4-(1,2,4,5-tetrazin-3-yl)phenyl)methanol: The title product was purified as a red solid after silica column chromatography (Hexane:EtOAc=2:1). Yield: 64% ($Ni(OTf)_2$). ^1H NMR (500 MHz, $CDCl_3$) δ 4.87 (3H, s), 7.63 (2H, dd, J = 10 Hz, 5 Hz), 8.64 (2H, d, J = 10 Hz); ^{13}C NMR (125 MHz, $CDCl_3$) δ 68.00, 118.29, 119.12, 120.85, 133.44, 142.54, 149.37; HRMS $[M-H]^-$ m/z calcd. for $[C_9H_7N_4O]^-$ 187.0626, found 187.0625.



2-(4-(1,2,4,5-tetrazin-3-yl)phenyl)acetic acid: The title product was purified as a red solid after silica column chromatography (CH_2Cl_2:MeOH=15:1). Yield: 74% ($Ni(OTf)_2$). ^1H NMR (500 MHz, $CDCl_3$) δ 3.81 (2H, s), 7.56 (2H, d, J = 10 Hz), 8.62 (2H, d, J = 10 Hz), 10.23 (1H, s); ^{13}C NMR (125 MHz, CD_3OD) δ 52.42, 122.10, 124.02, 124.38, 132.18, 146.12, 152.88, 158.77; HRMS $[M+H]^+$ m/z calcd. for $[C_{10}H_9N_4O_2]^+$ 217.0717, found 217.0720.

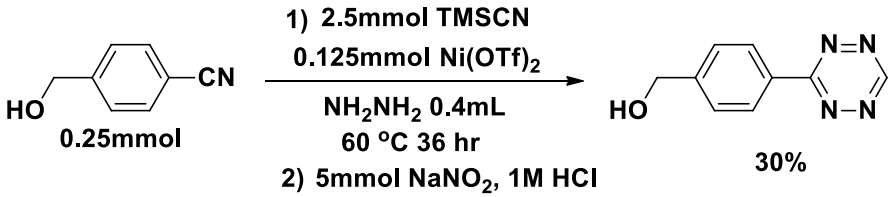
4. Synthesis of *tert*-butyl 4-(1,2,4,5-tetrazin-3-yl)benzylcarbamate
This substrate cannot be dissolved in NH_2NH_2 at room temperature, which resulted in very low yields when using the above reaction conditions. We modified the reaction conditions, using $Zn(OTf)_2$ as catalyst and added a minimal amount of DMF to dissolve the substrate followed by gentle heating at 30°C for 36 hours, and subsequent work up following the above procedure to recover our desired product in 70% yield.



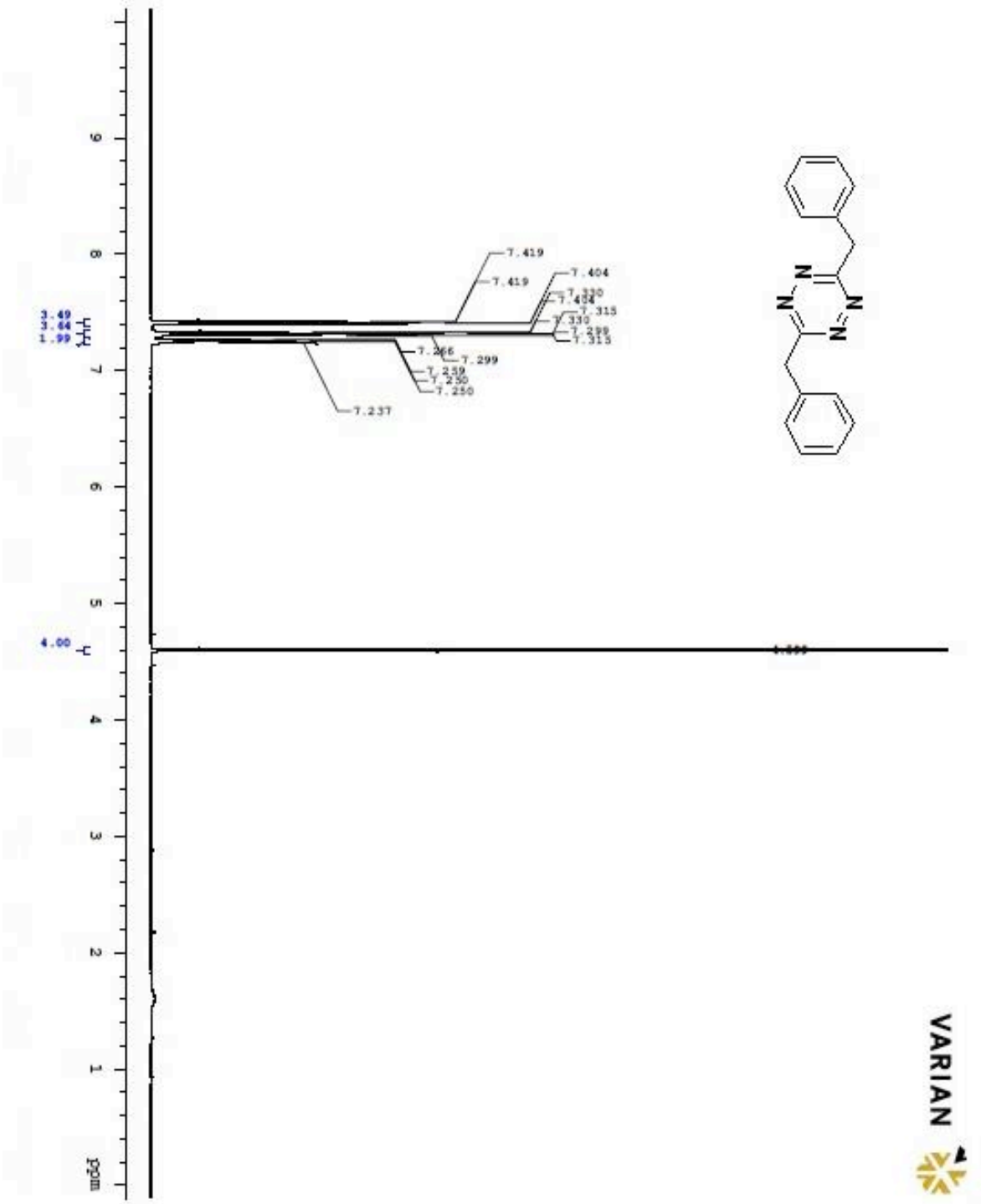
To a 10 mL microwave reaction tube equipped with a stir bar, 0.125 mmol of $Zn(OTf)_2$, 0.27g (2.5 mmol) of formamidine acetate, 58mg (0.25 mmol) nitrile,

0.20 mL DMF, and 0.40 mL (12.5 mmol) of anhydrous hydrazine was added. The vessel was sealed and the mixture was stirred in an oil bath at 30°C for 36 hours. The reaction solution was cooled to room temperature and the seal was removed. Sodium nitrite (5.0 mmol, 345 mg) in 5 mL of water was slowly added to the solution and followed by slow addition of 1M HCl during which the solution turned bright red in color and gas evolved. Addition of 1M HCl continued until gas evolution ceased and the pH value is 3. (**Caution**! This step generates a large amount of toxic nitrogen oxide gasses and should be performed in a well ventilated fume hood). The mixture was extracted with EtOAc and the organic phase dried over sodium sulfate. The EtOAc was removed using rotary evaporation and the residue purified using silica column chromatography (Hexane:EtOAc=7:1) to give 50 mg product as red solid, the yield is 70%. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.49 (9H, s), 4.45 (2H, d, J = 5 Hz), 4.97 (1H, bs), 7.53 (2H, d, J = 10 Hz), 8.60 (2H, d, J = 10 Hz), 10.21 (1H, s); ^{13}C NMR (125 MHz, $CDCl_3$) δ 39.07, 51.82, 118.84, 119.19, 120.76, 132.11, 141.12, 142.56, 149.36; HRMS $[M+Na]^+$ m/z calcd. for $[C_{14}H_{17}N_5O_2Na]^+$ 310.1276, found 310.1274.

5. General procedure for synthesis of 3-H-6-aryl-1,2,4,5-tetrazine using trimethylsilyl cyanide as a nitrile source.



To a 10 mL microwave reaction tube equipped with a stir bar, 0.125 mmol of $Ni(OTf)_2$, 33mg 4-(hydroxymethyl)benzonitrile (0.25 mmol), 0.40 mL (12.5 mmol) of anhydrous hydrazine, and 0.25g (2.5 mmol) of trimethylsilyl cyanide was added (**Caution**! Trimethylsilyl cyanide is an extremely toxic reagent and should be handled with great care). The vessel was sealed and the mixture was stirred in an oil bath at 60°C for 36 hours. The reaction solution was cooled to room temperature and the seal was removed. Sodium nitrite (5 mmol, 345 mg) in 5 mL of water was slowly added to the solution and followed by slow addition of 1M HCl during which the solution turned bright red in color and gas evolved. Addition of 1M HCl continued until gas evolution ceased and the pH value is 3. (**Caution**! This step generates a large amount of toxic nitrogen oxide gasses and should be performed in a well ventilated fume hood). The mixture was extracted with EtOAc and the organic phase dried over sodium sulfate. The EtOAc was removed using rotary evaporation and the residue purified using silica column chromatography (Hexane:EtOAc=2:1) to give 14 mg product. Yield: 30%.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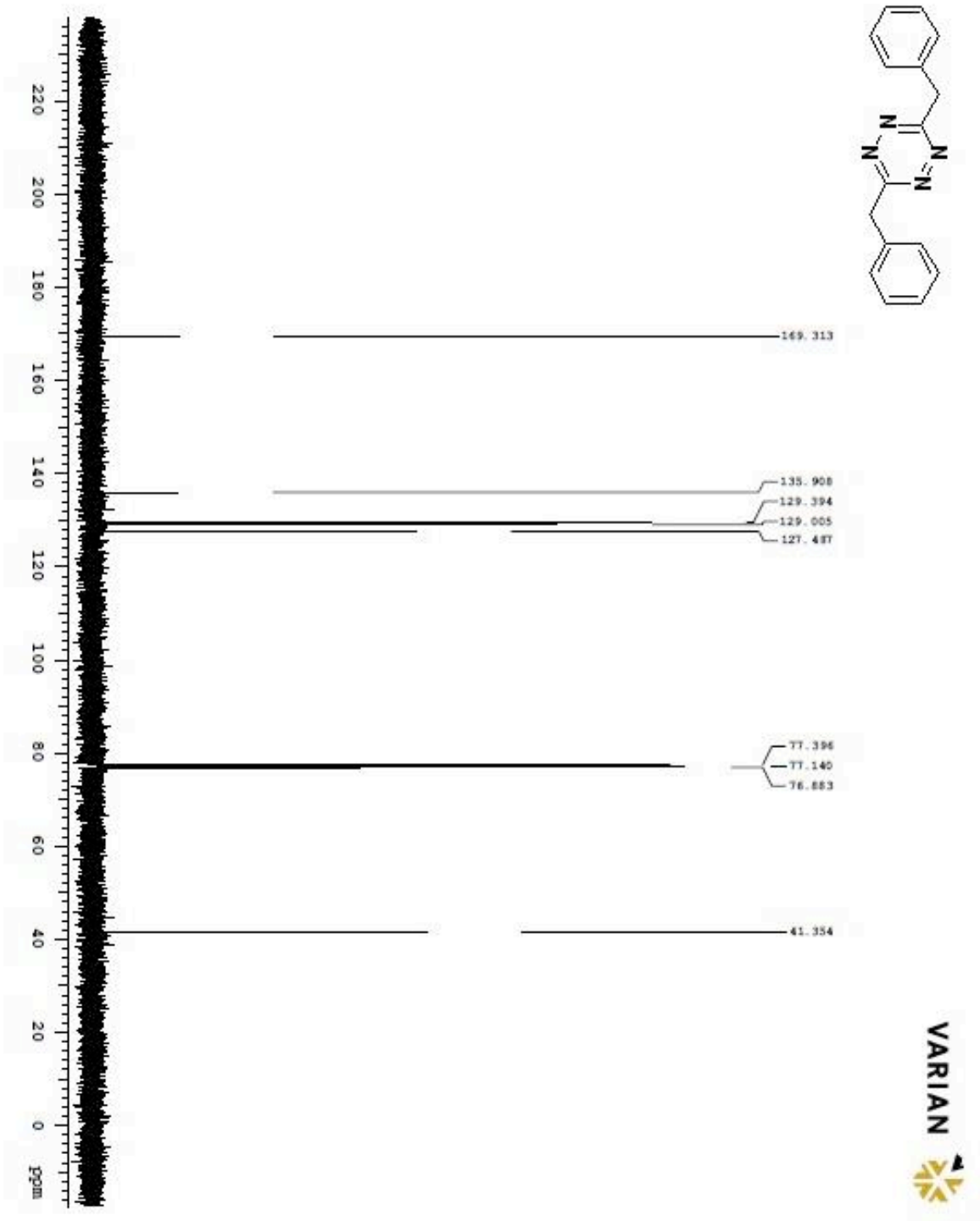
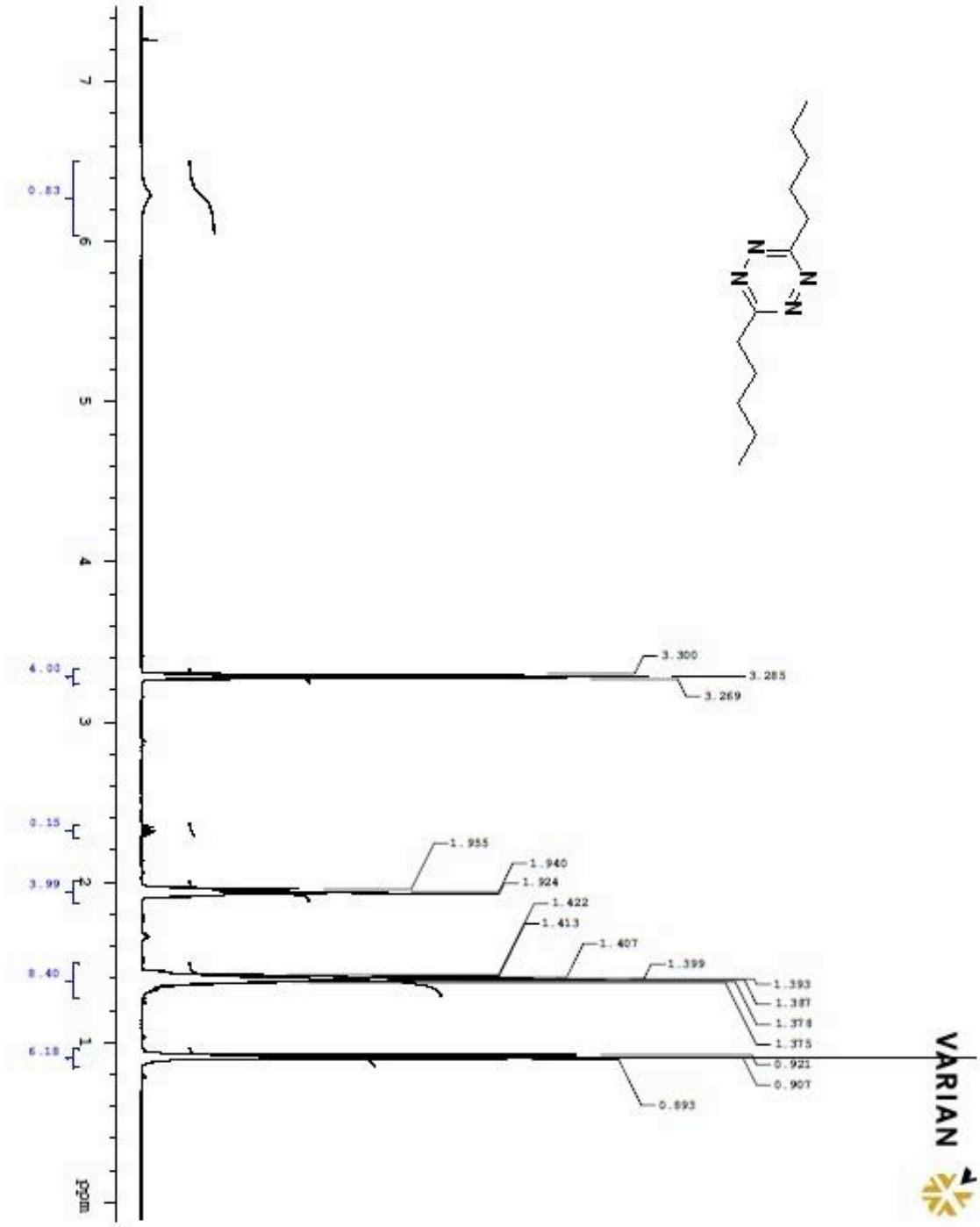
7.419
7.404
7.330
7.315
7.330
7.299
7.259
7.250
7.250
7.237
3.49
3.44
1.99
4.00
ppm
VARIAN


169.313
135.908
129.394
129.005
127.487
77.396
77.140
76.883
41.354
220
200
180
160
140
120
100
80
60
40
20
0
ppm
VARIAN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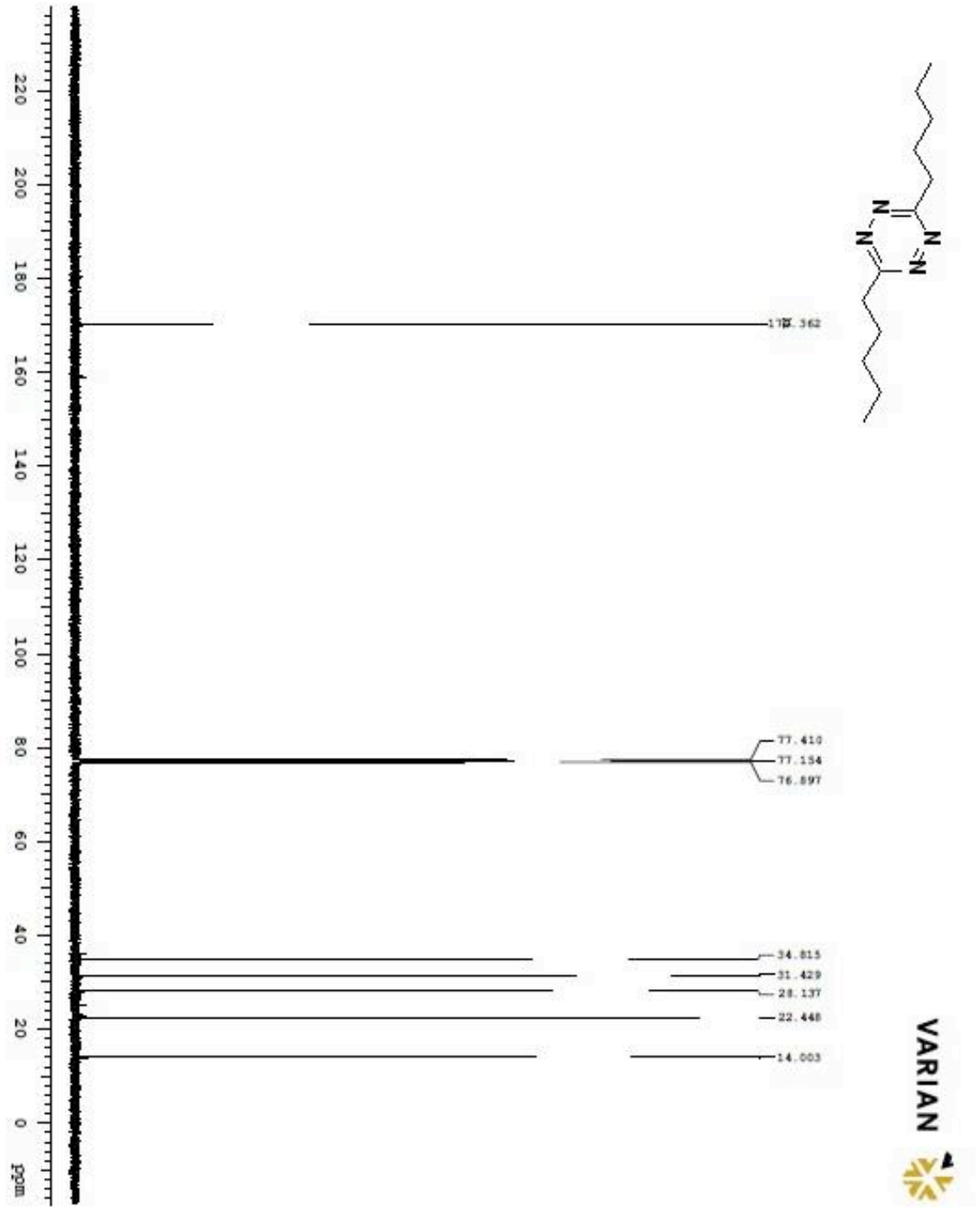
4.00
0.15
3.99
8.40
6.18
3.300
3.285
3.269
1.955
1.940
1.924
1.422
1.413
1.407
1.399
1.393
1.387
1.378
1.375
0.921
0.907
0.893
VARIAN


220
200
180
160
140
120
100
80
60
40
20
0
ppm
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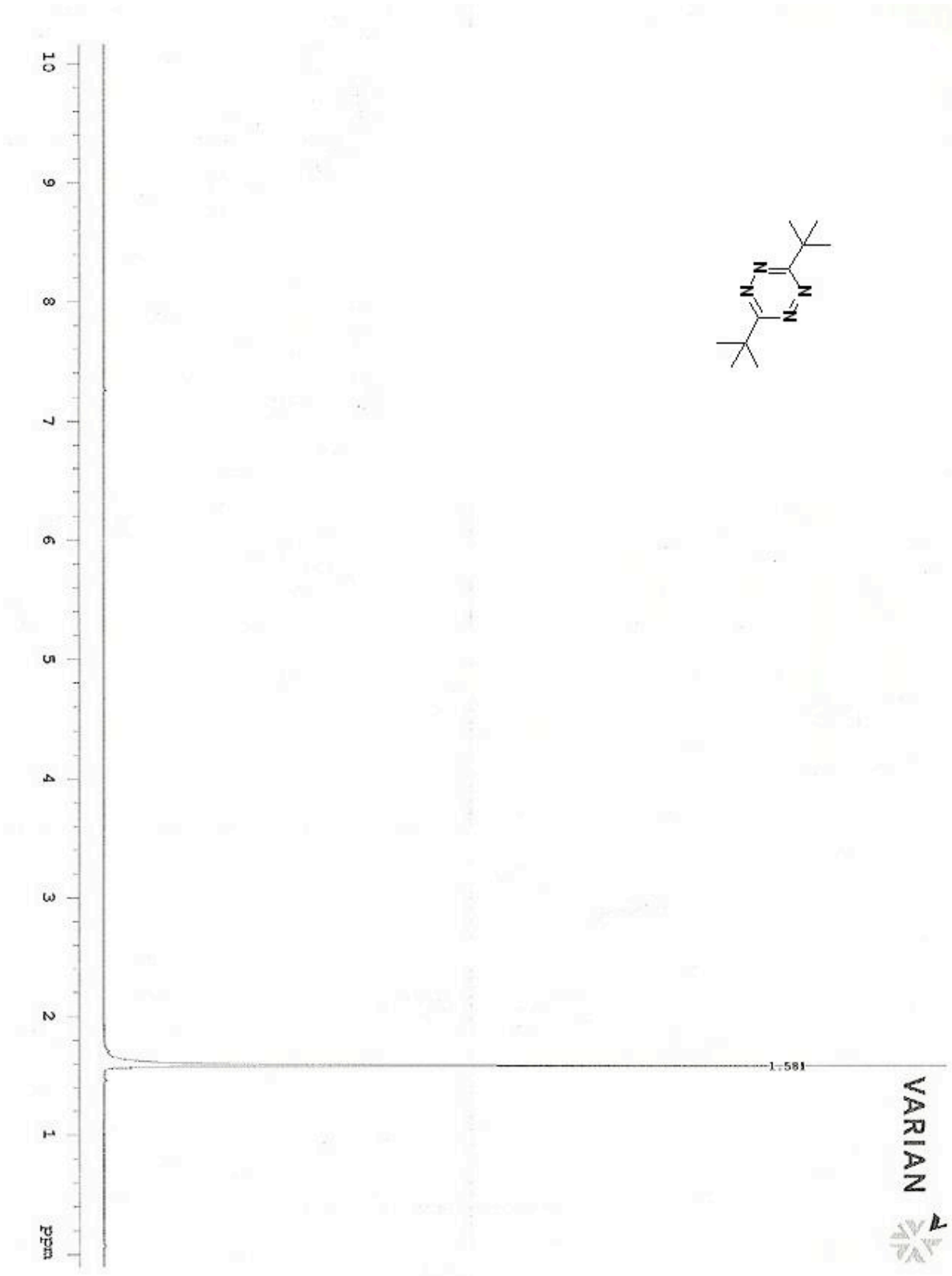
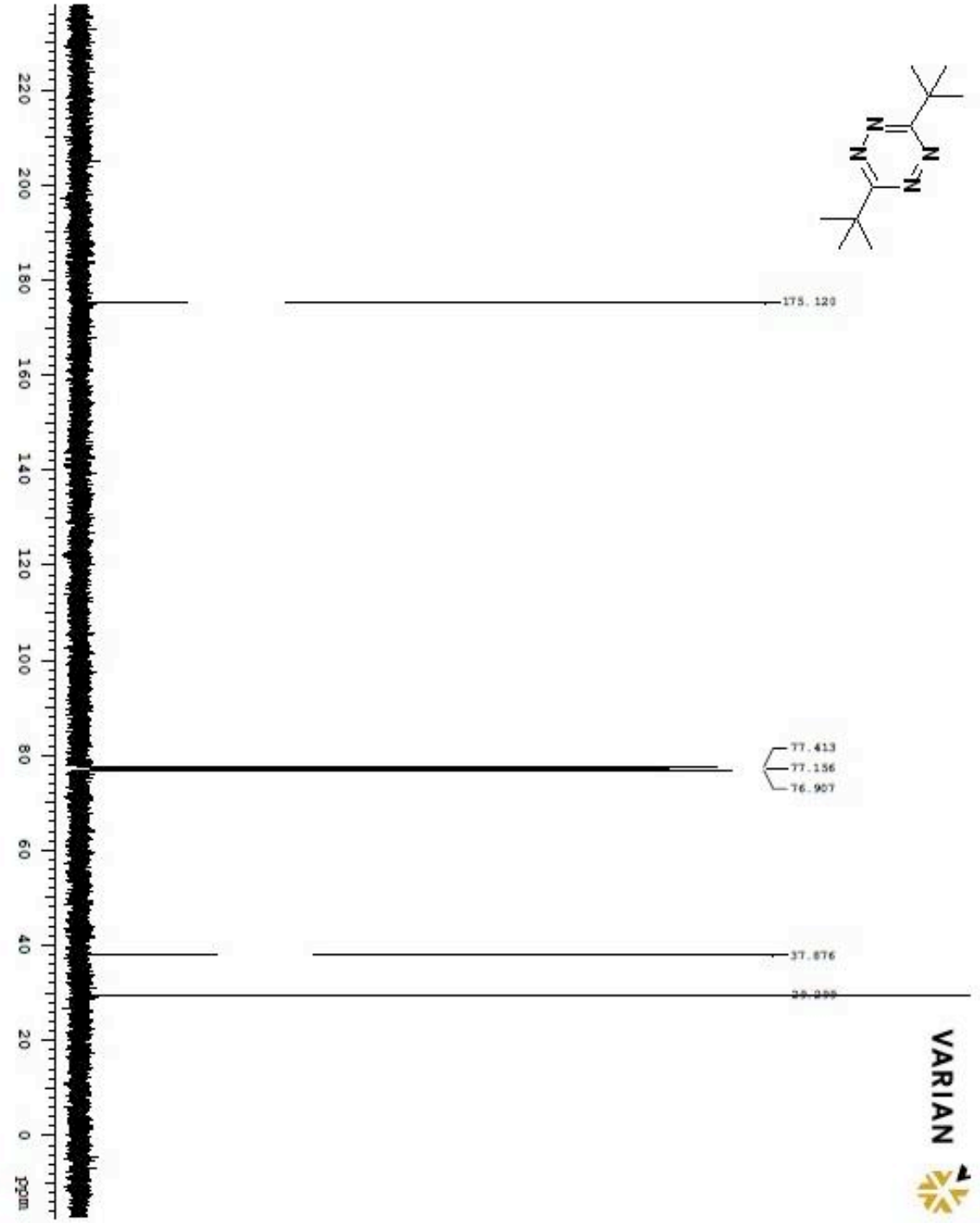
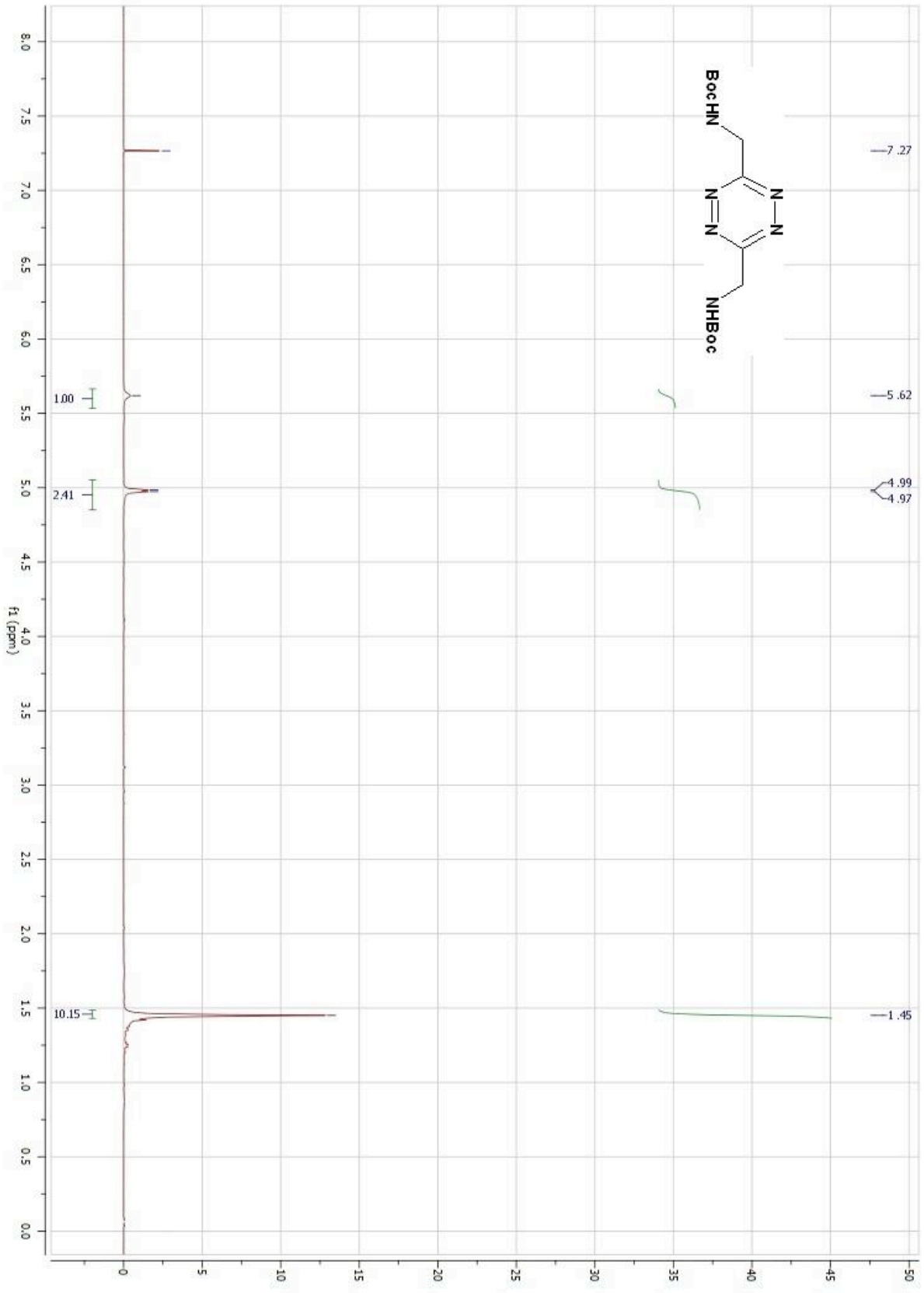
77.154
76.897
34.815
31.429
28.137
22.448
14.003
VARIAN


10
9
8
7
6
5
4
3
2
1
ppm
1.581
VARIAN


175.120
77.413
77.156
76.907
37.876
29.899
VARIAN
220
200
180
160
140
120
100
80
60
40
20
0
ppm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NHBoc
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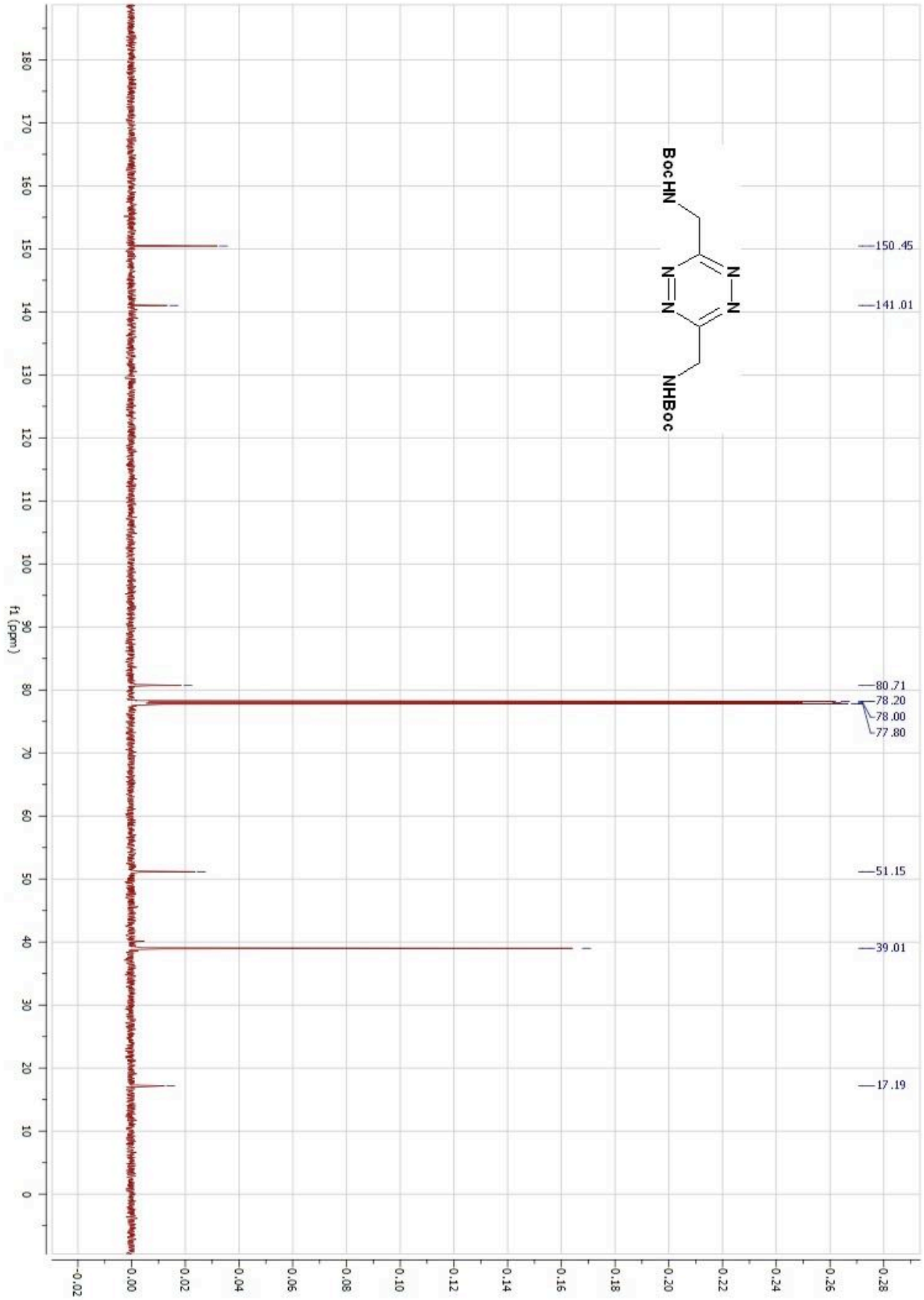
5.62
4.99
4.97
1.45
1.00
2.41
10.15
f1 (ppm)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NHBoc
N
N
N
N
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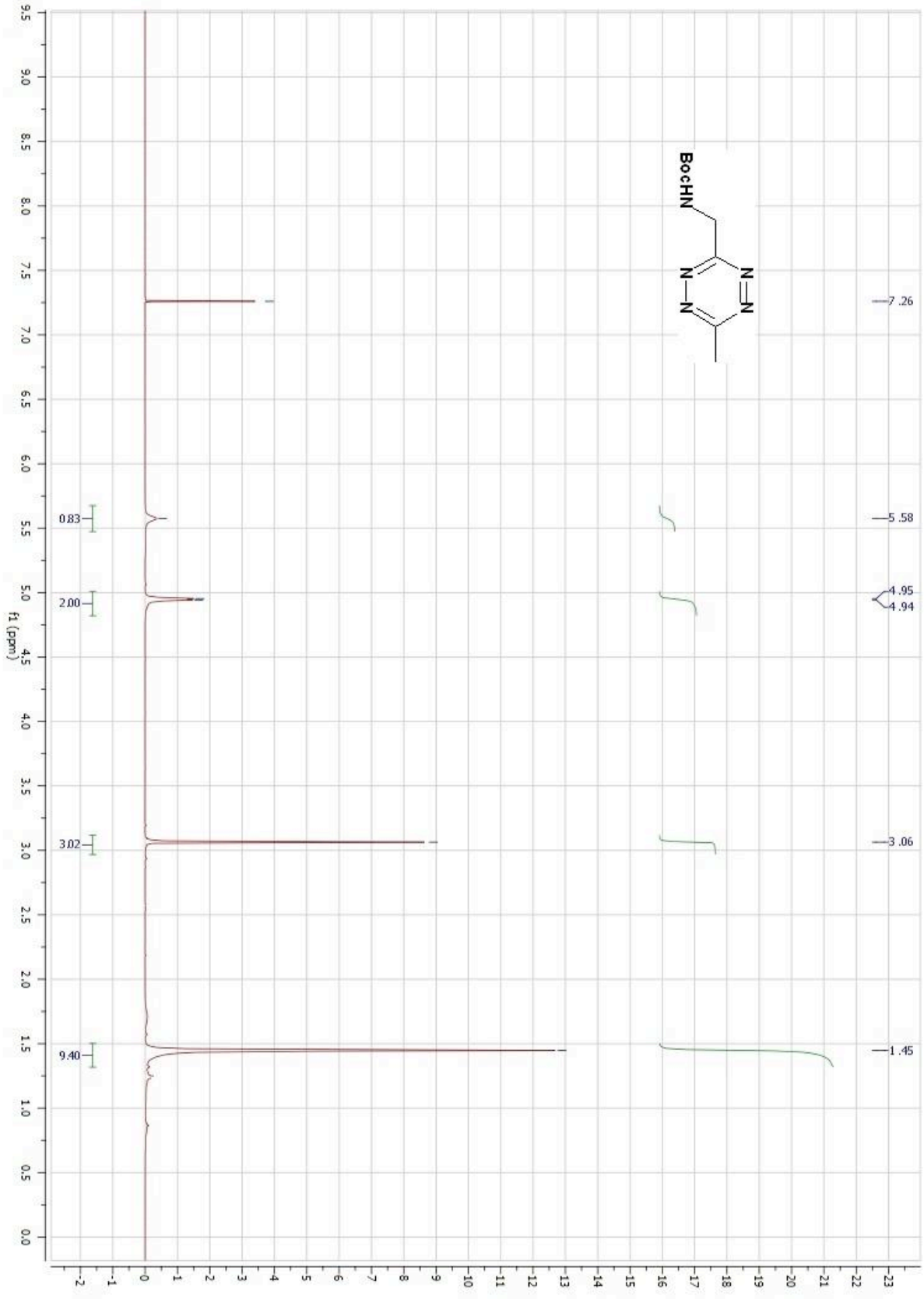
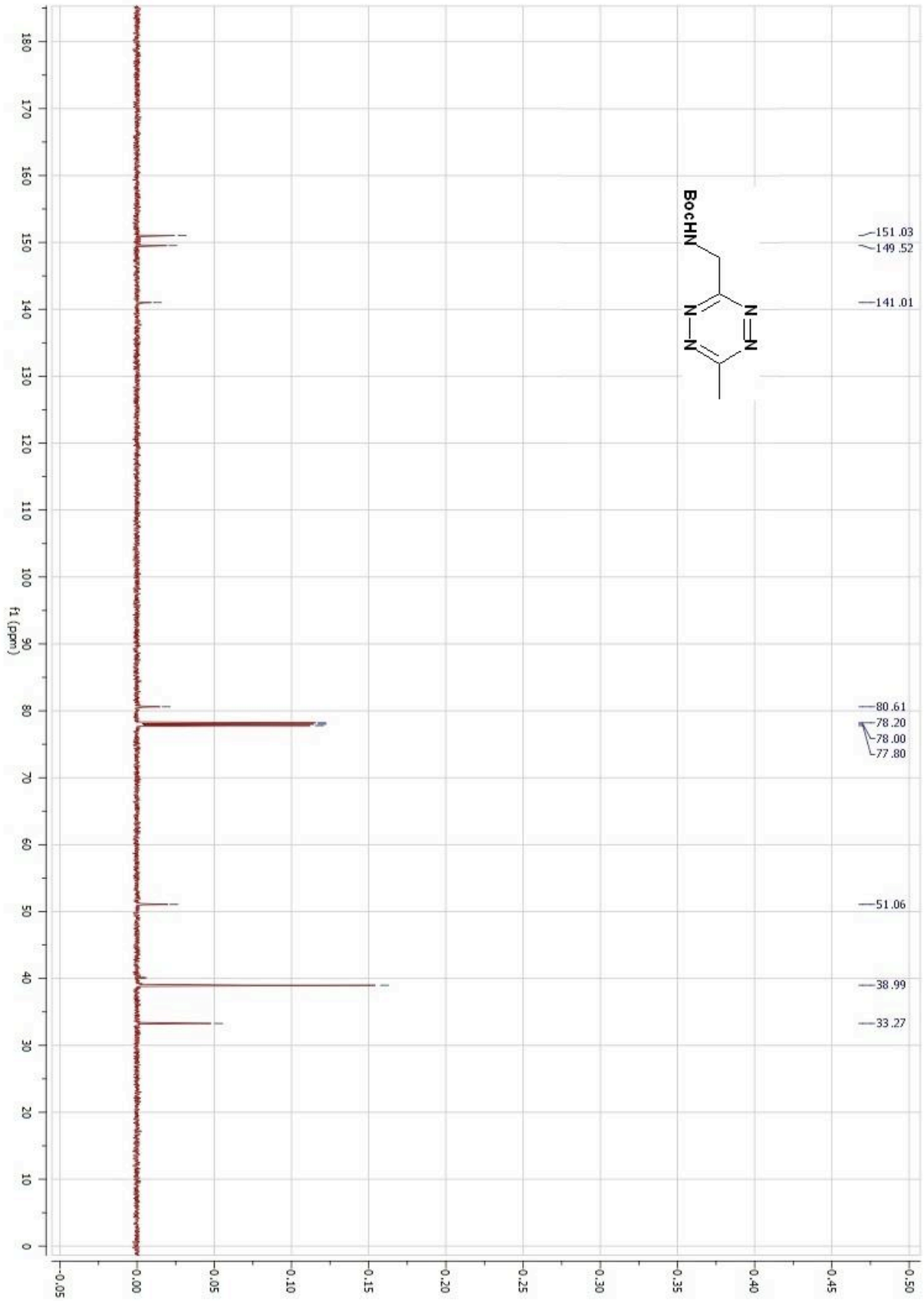
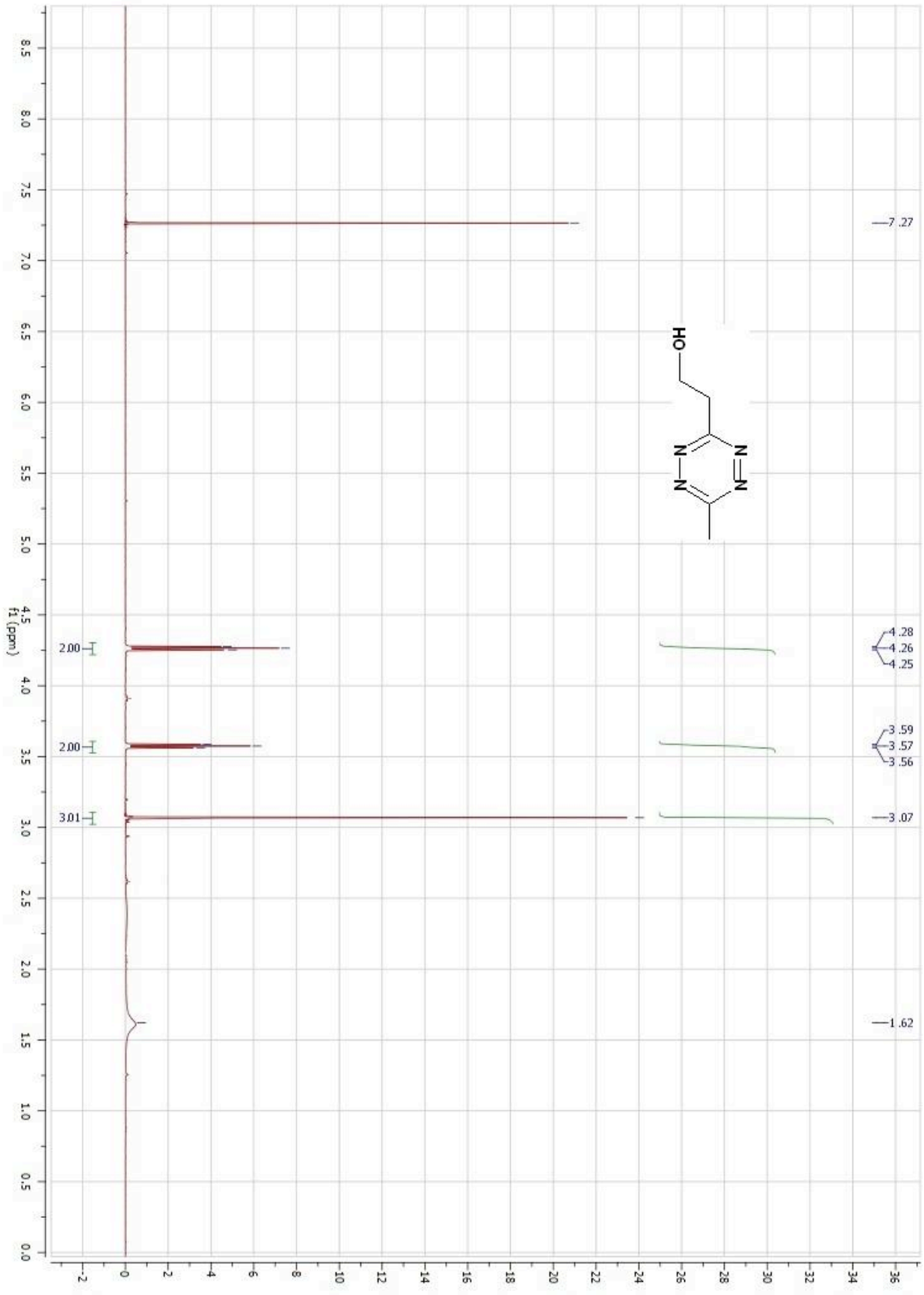
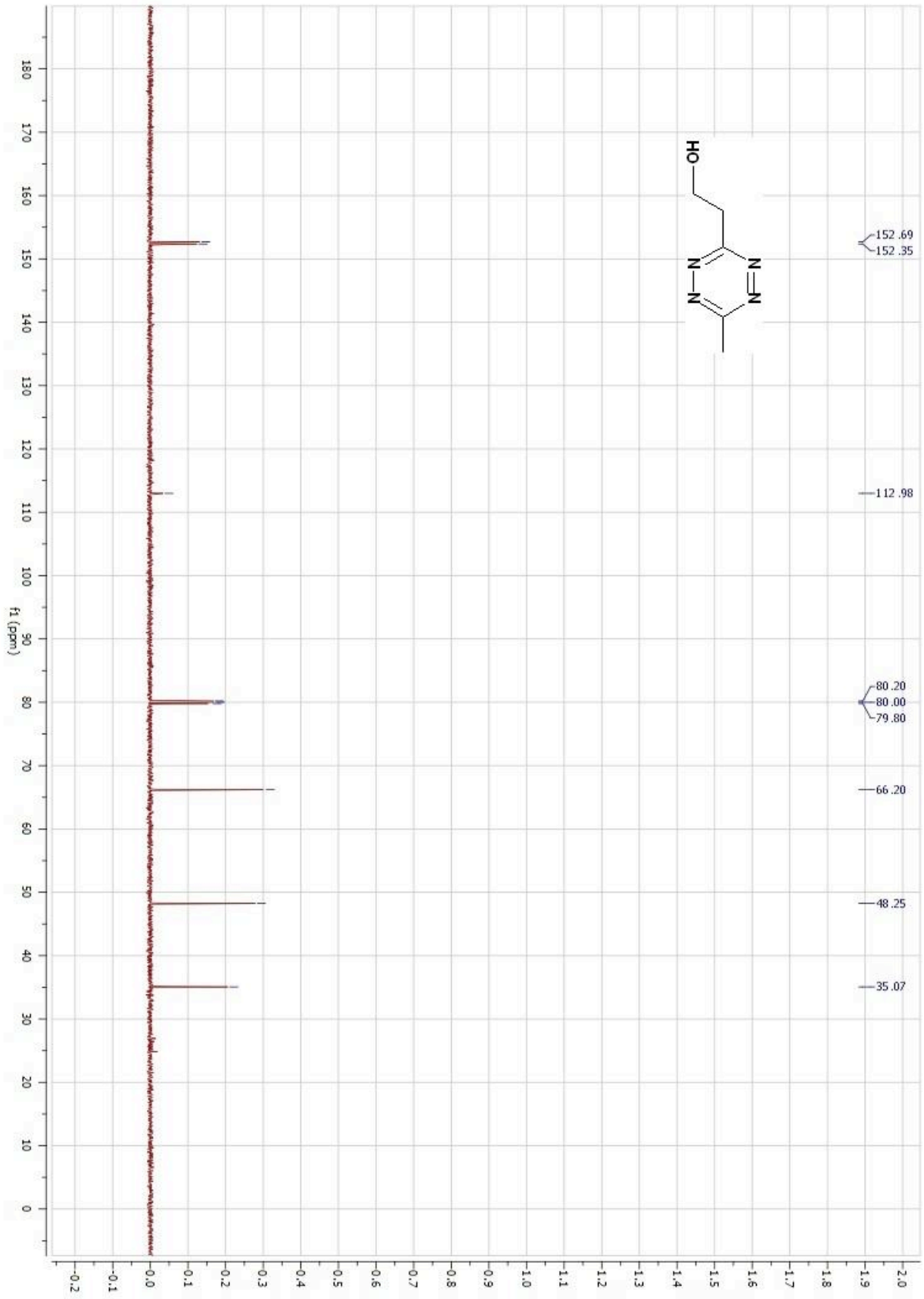
141.01
80.71
78.20
78.00
77.80
51.15
39.01
17.19
f1 (ppm)


BocHN
N
N
N
N
7.26
5.58
4.95
4.94
3.06
1.45
0.83
2.00
3.02
9.40
f1 (ppm)


BocHN
N
N
N
N
151.03
149.52
141.01
80.61
78.20
78.00
77.80
51.06
38.99
33.27
f1 (ppm)


f1 (ppm)
7.27
4.28
4.26
4.25
3.59
3.57
3.56
3.07
1.62
2.00
2.00
3.01
HO
N
N
N
N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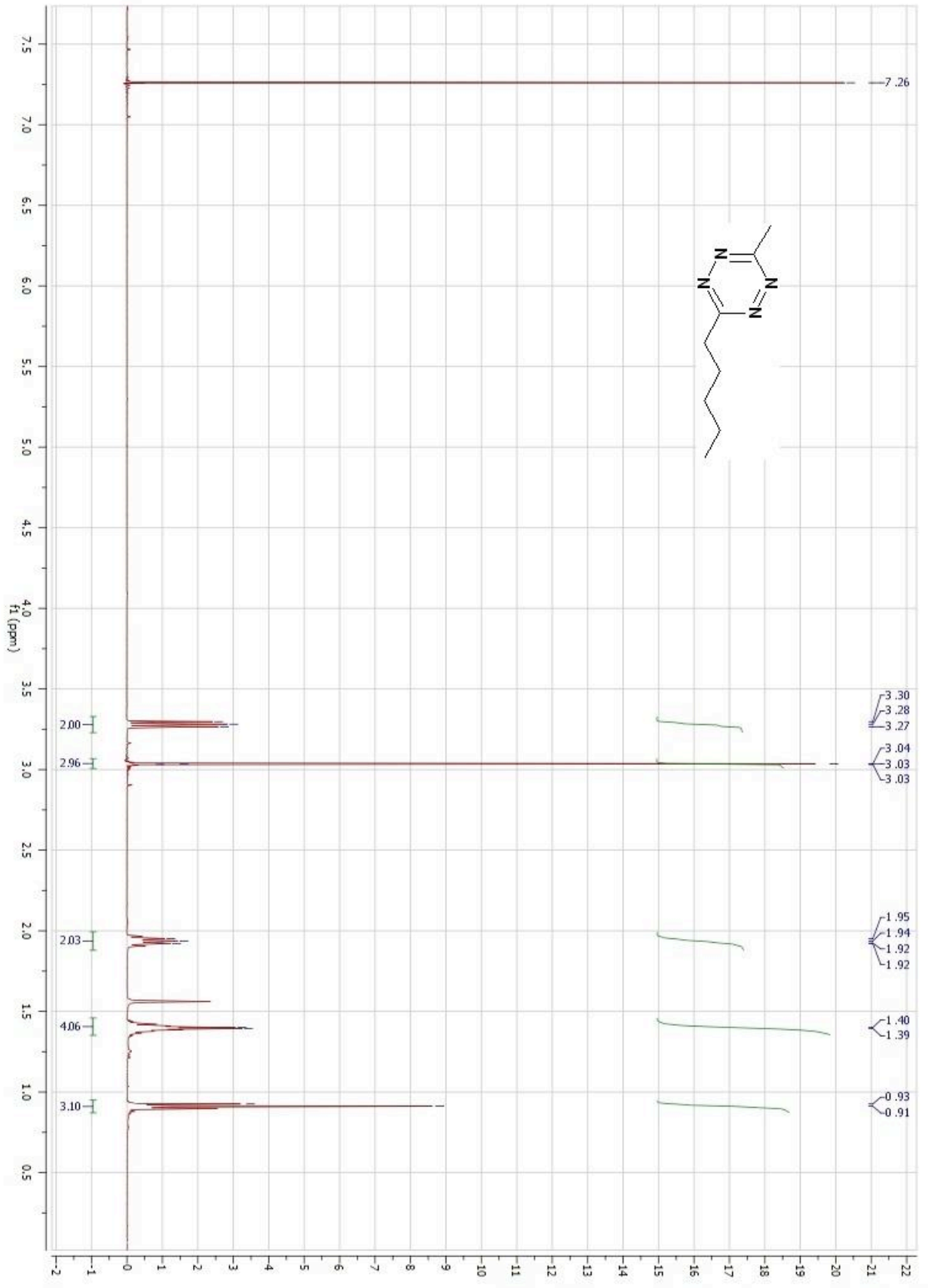
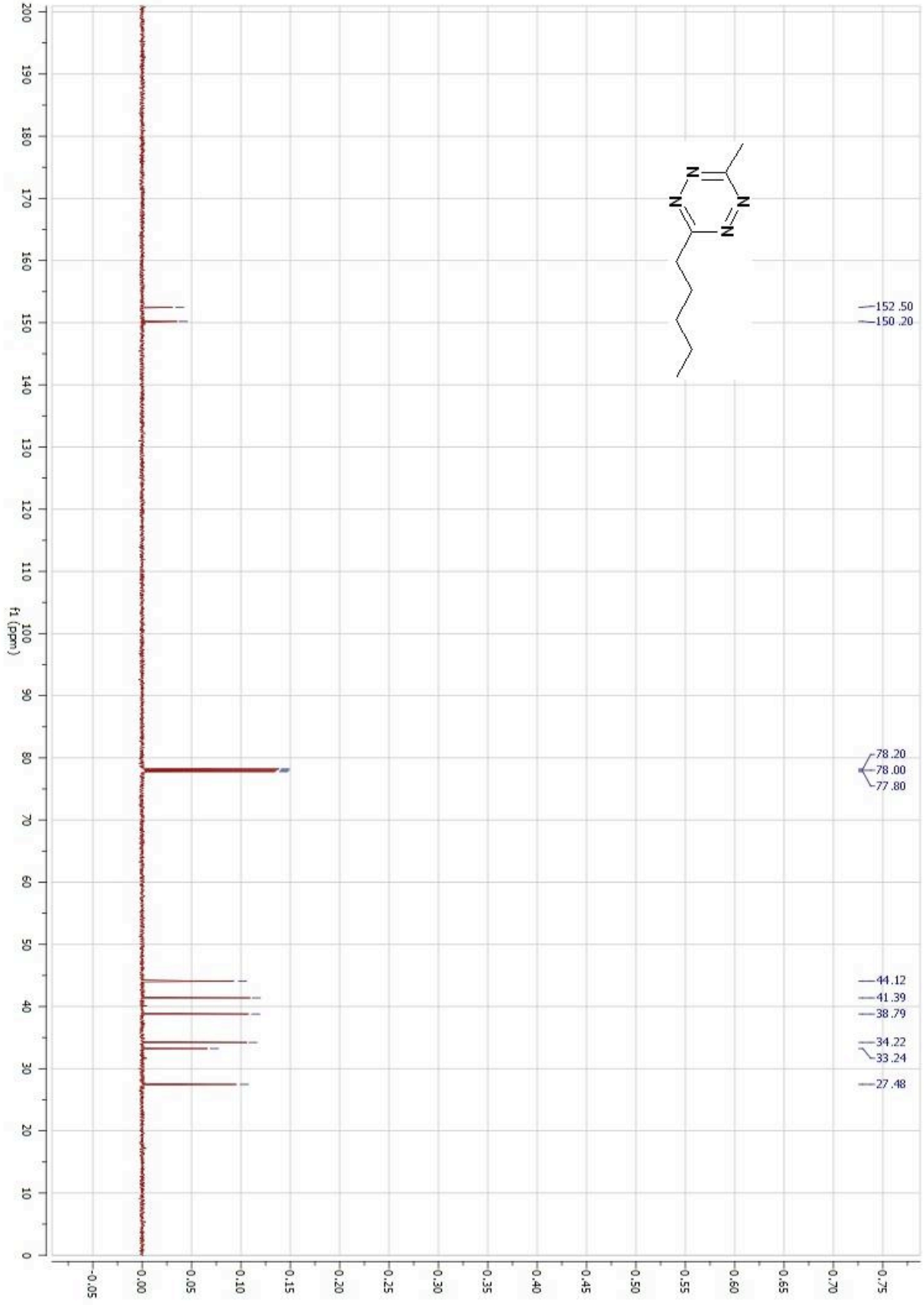
152.35
112.98
80.20
80.00
79.80
66.20
48.25
35.07
f1 (ppm)


7.26
3.30
3.28
3.27
3.04
3.03
3.03
1.95
1.94
1.92
1.92
1.40
1.39
0.93
0.91
2.00
2.96
2.03
4.06
3.10
f1 (ppm)


f1 (ppm)
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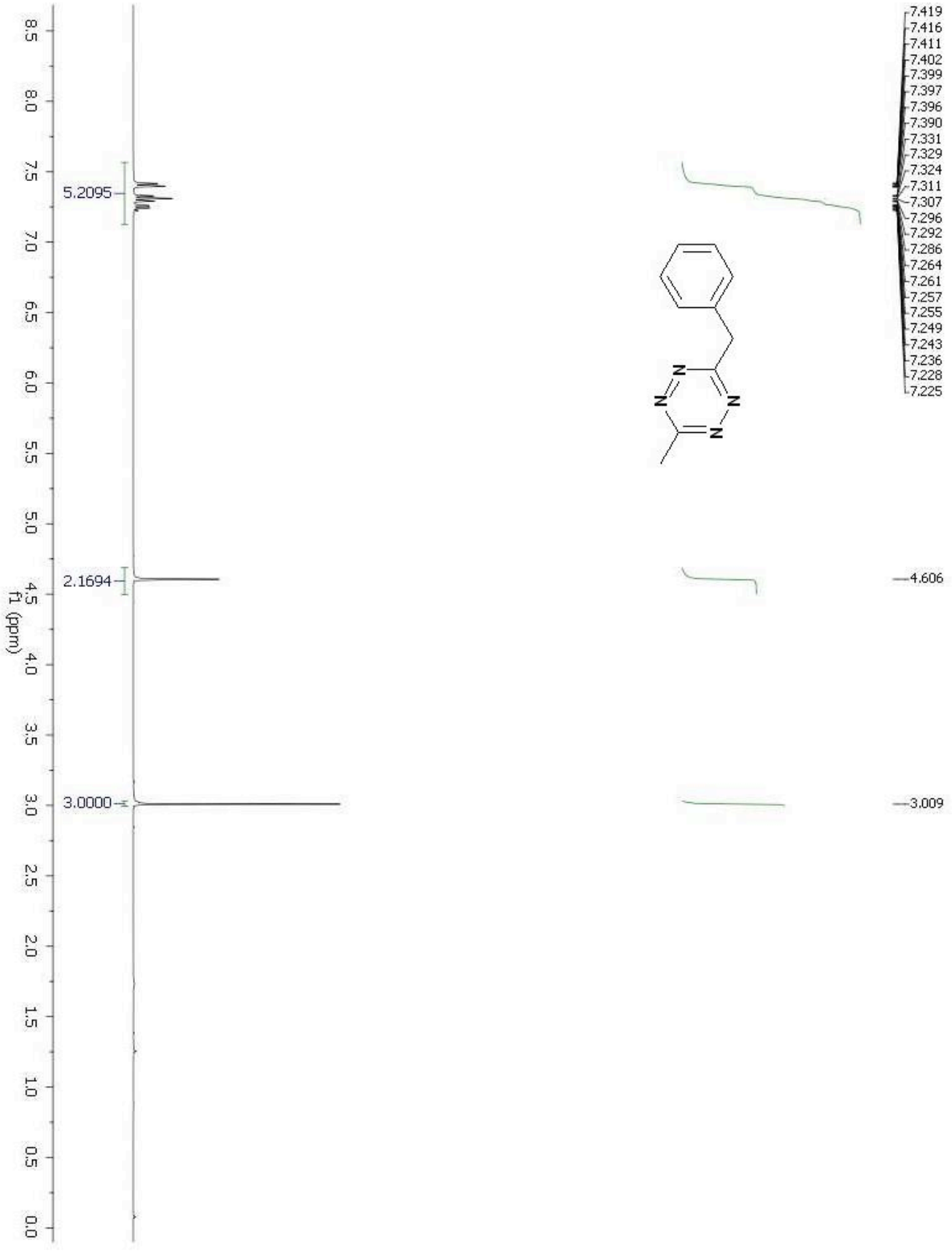
150.20
78.20
78.00
77.80
44.12
41.39
38.79
34.22
33.24
27.48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7.416
7.411
7.402
7.399
7.397
7.396
7.390
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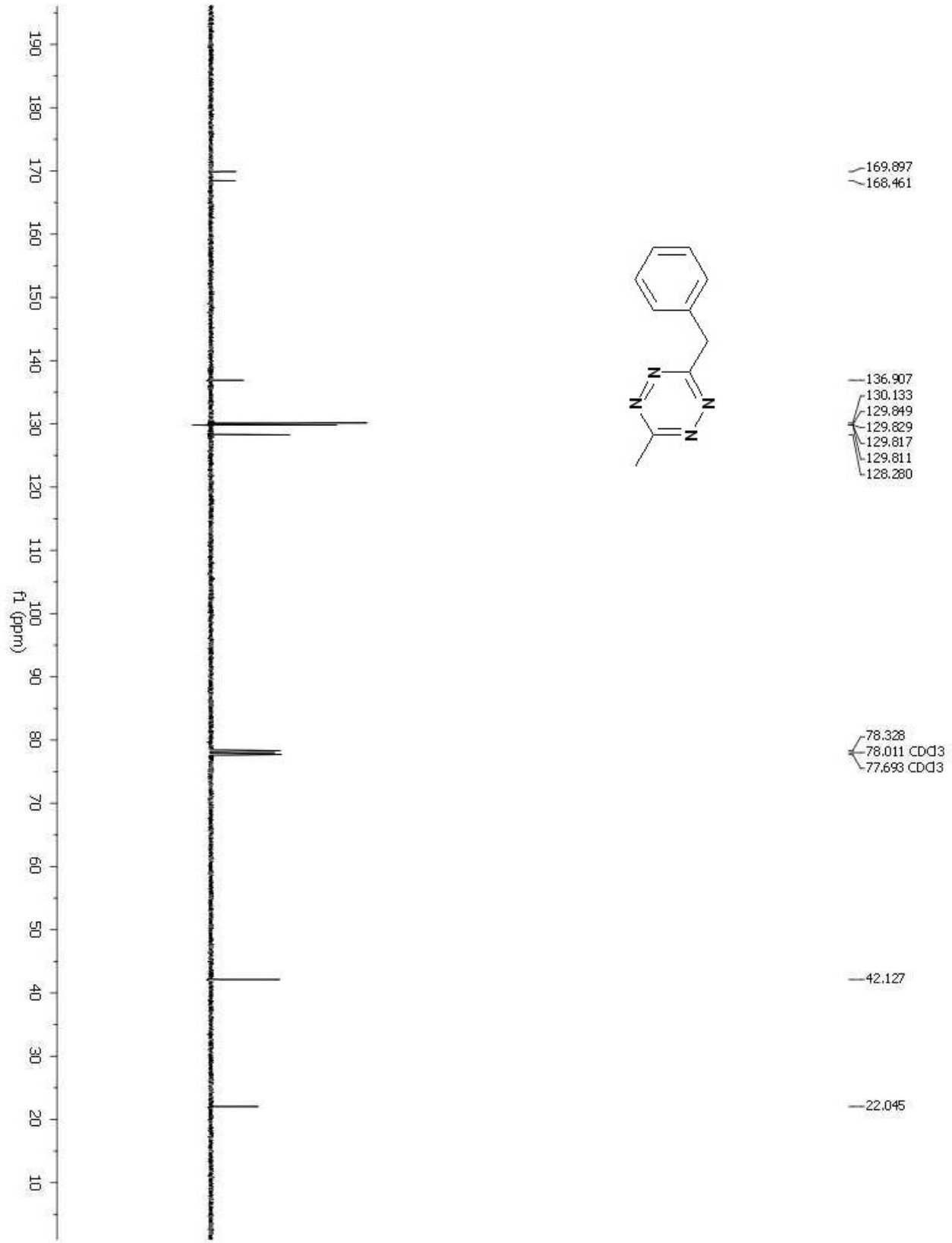
7.329
7.324
7.311
7.307
7.296
7.292
7.286
7.264
7.261
7.257
7.255
7.249
7.243
7.236
7.228
7.225
5.2095
2.1694
3.0000
4.606
3.009
f1 (ppm)


f1 (ppm)
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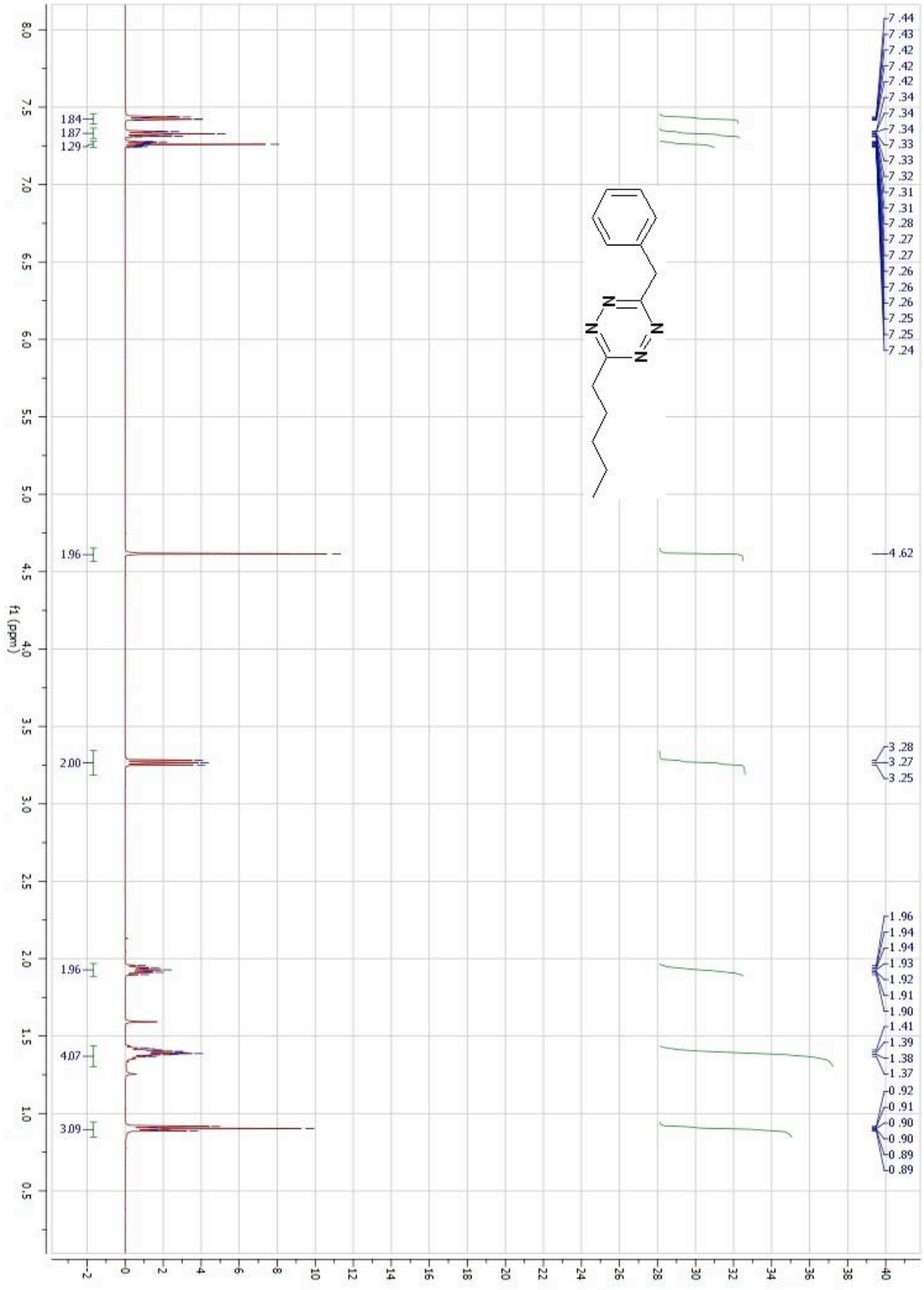
136.907
130.133
129.849
129.829
129.817
129.811
128.280
78.328
78.011 CDCl3
77.693 CDCl3
42.127
22.045


f1 (ppm)
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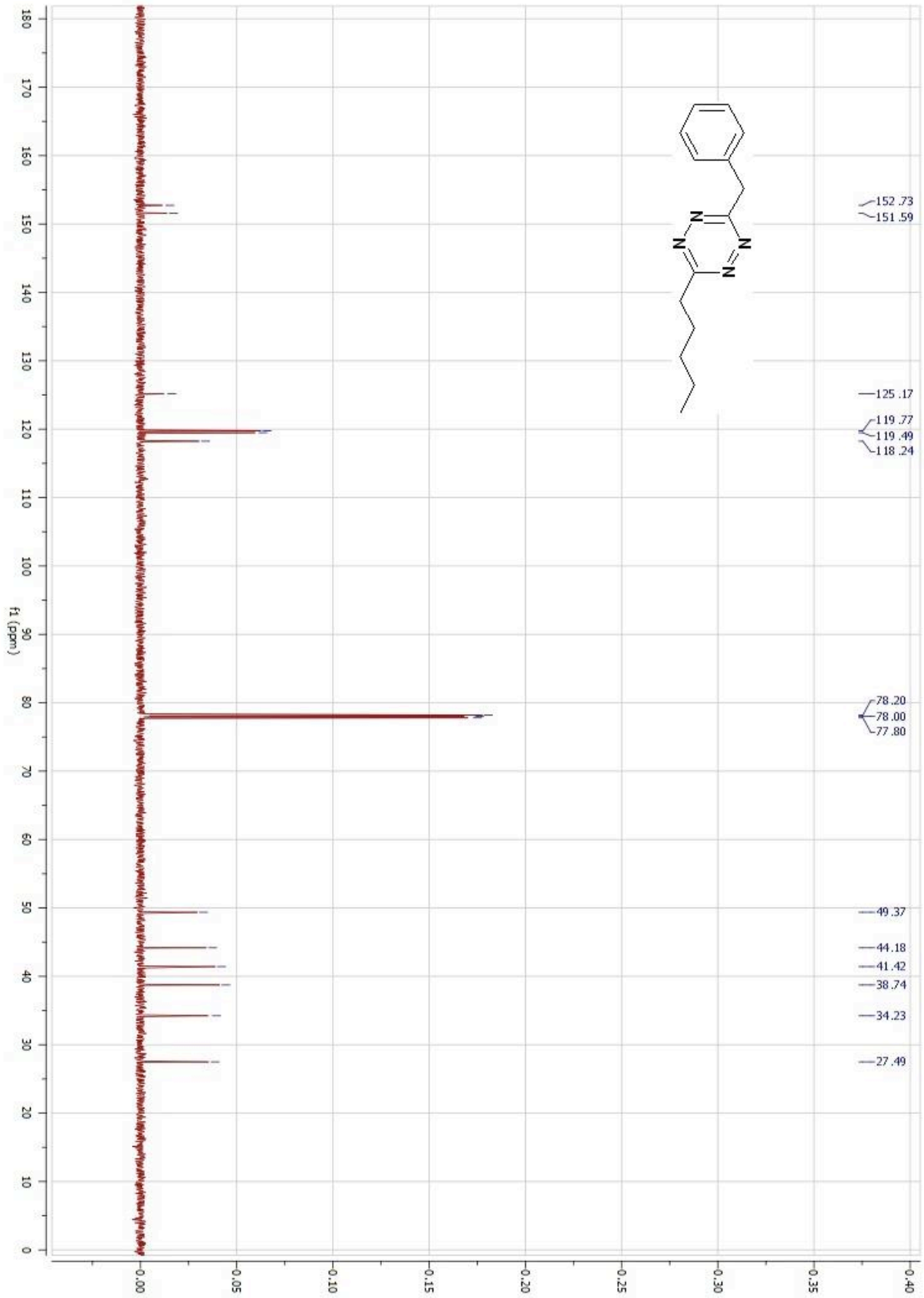
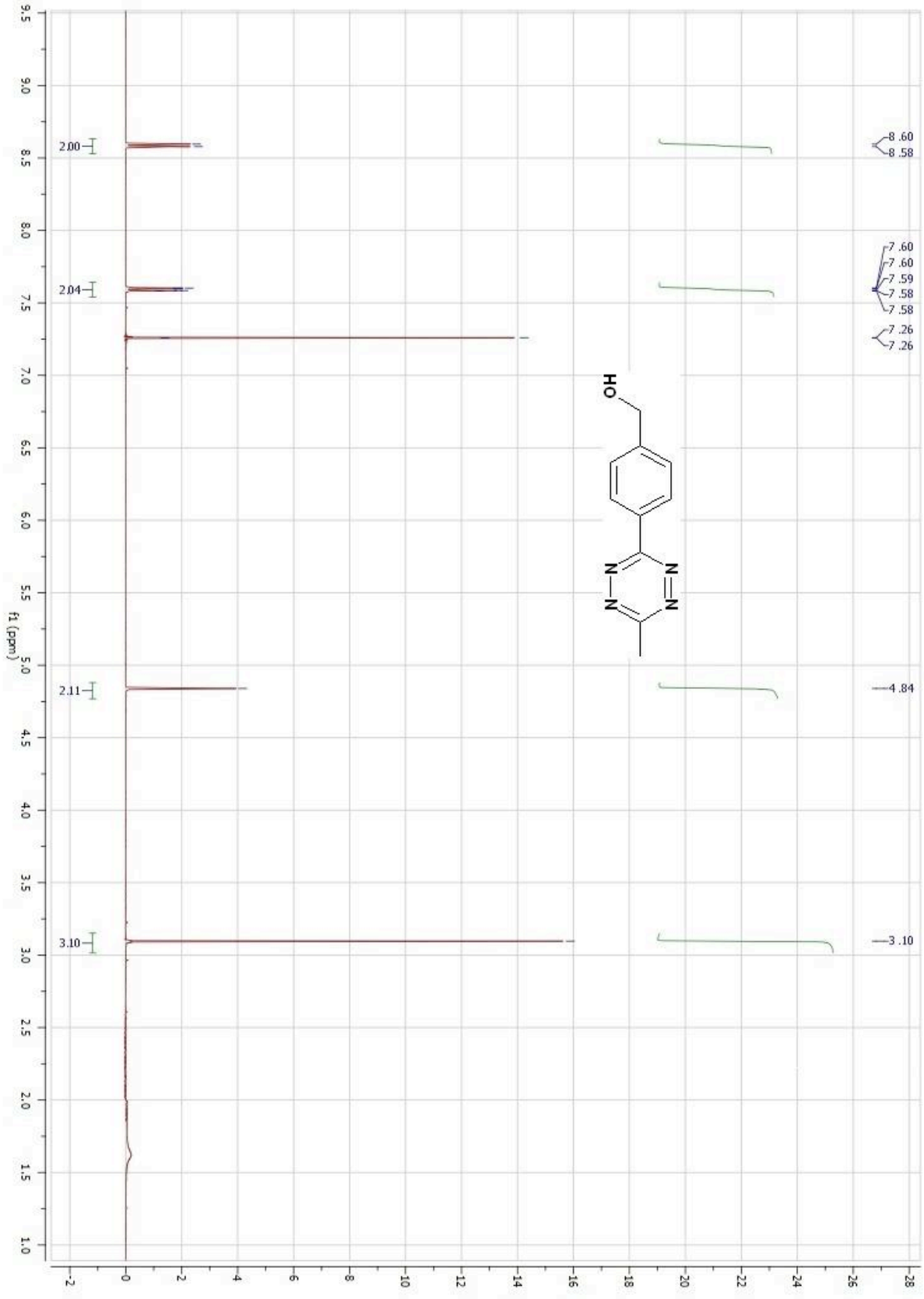
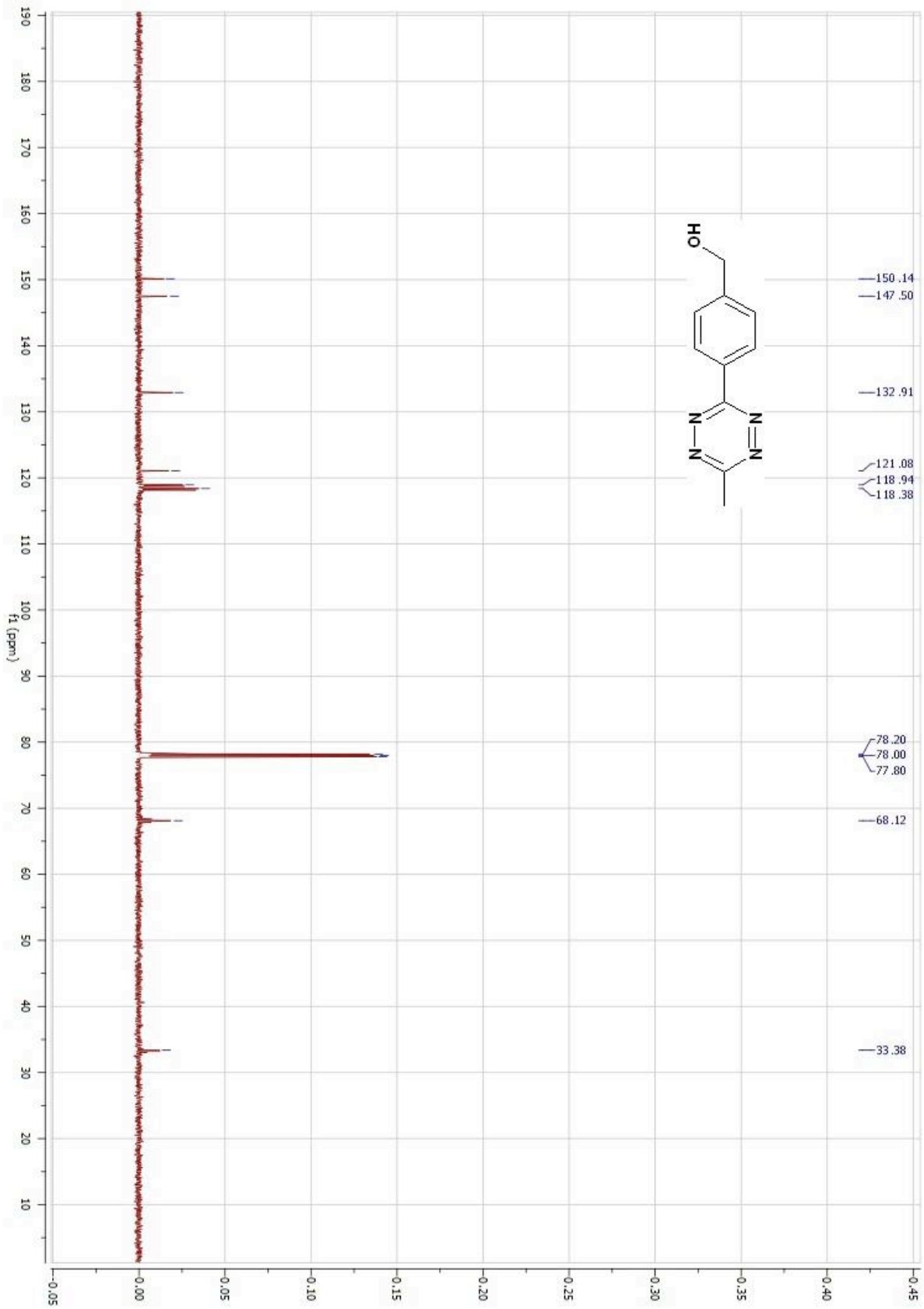
1.87
1.29
1.96
2.00
1.96
4.07
3.09
7.44
7.43
7.42
7.42
7.42
7.34
7.34
7.34
7.33
7.33
7.32
7.31
7.31
7.28
7.27
7.27
7.26
7.26
7.26
7.25
7.25
7.24
4.62
3.28
3.27
3.25
1.96
1.94
1.94
1.93
1.92
1.91
1.90
1.41
1.39
1.38
1.37
0.92
0.91
0.90
0.90
0.89
0.89


152.73
151.59
125.17
119.77
119.49
118.24
78.20
78.00
77.80
49.37
44.18
41.42
38.74
34.23
27.49
f1 (ppm)


8.60
8.58
7.60
7.60
7.59
7.58
7.58
7.26
7.26
4.84
3.10
2.00
2.04
2.11
3.10
HO
N
N
N
N
f1 (ppm)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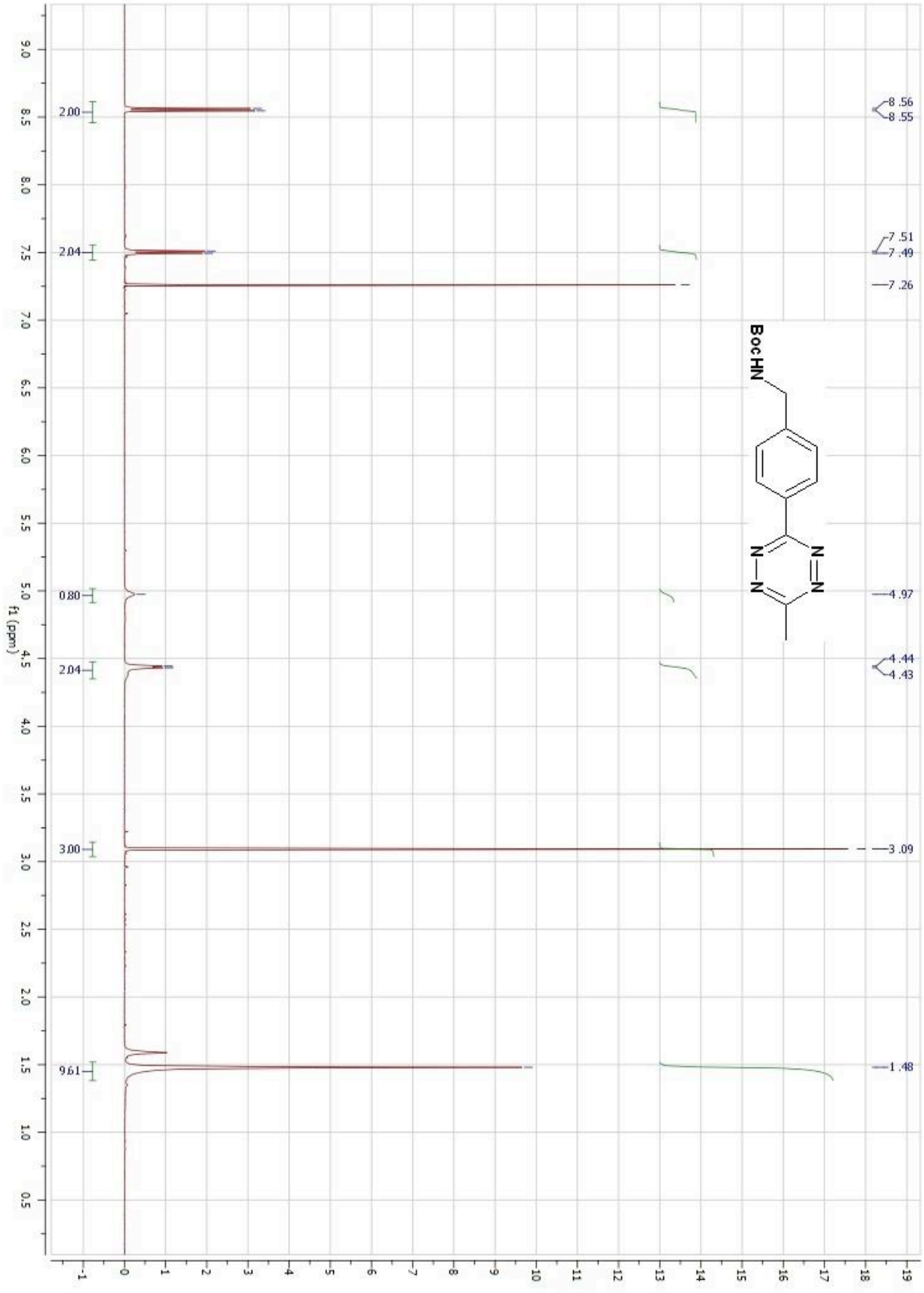
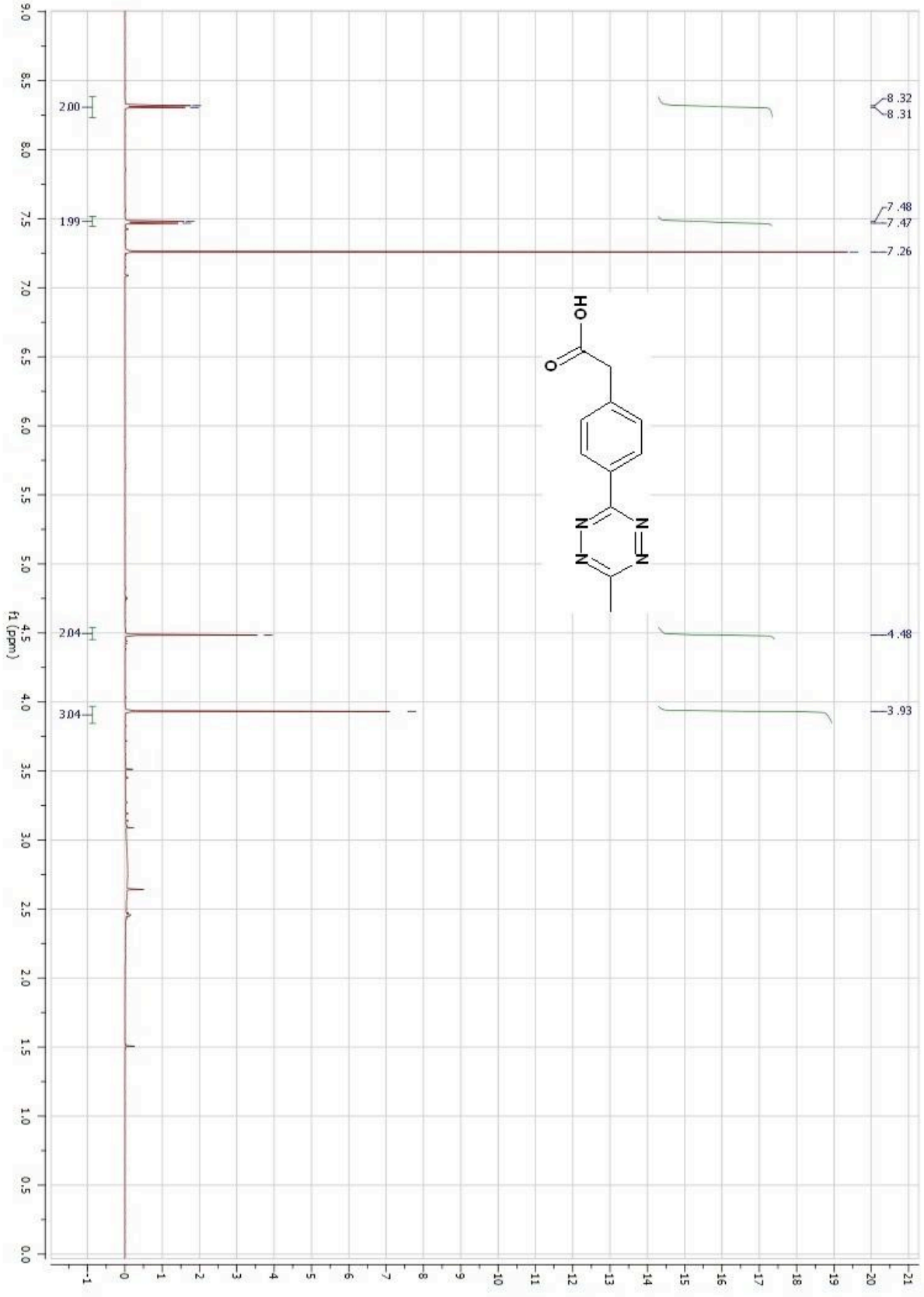
121.08
118.94
118.38
78.20
78.00
77.80
68.12
33.38
f1 (ppm)


8.56
8.55
7.51
7.49
7.26
4.97
4.44
4.43
3.09
1.48
2.00
2.04
0.80
2.04
3.00
9.61
Boc HN
N
N
N
N
f1 (ppm)


BocHN
N
N
N
N
149.08
146.42
140.12
130.54
119.89
117.84
117.74
79.14
77.20
77.00
76.80
50.80
38.06
32.25
f1 (ppm)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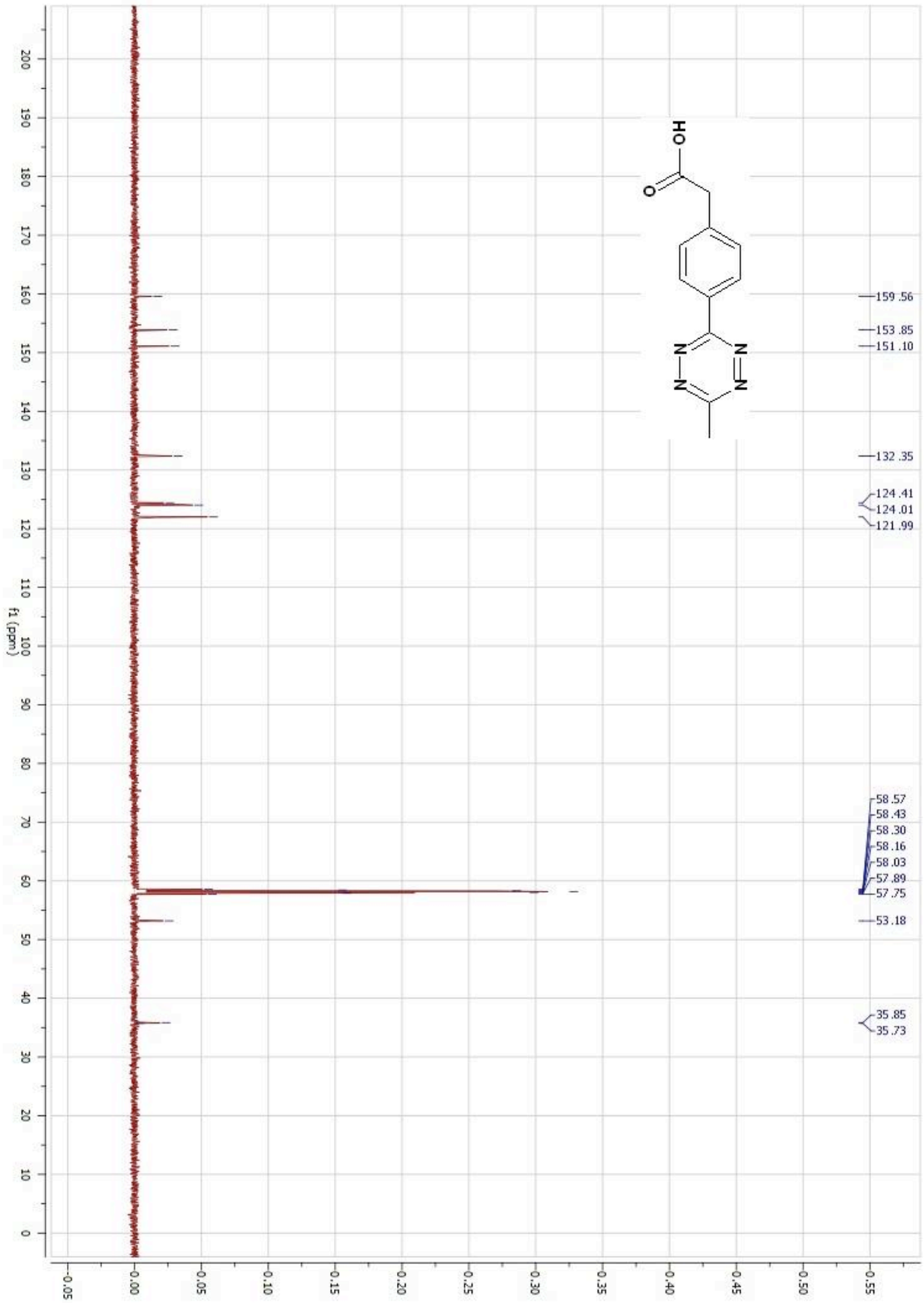
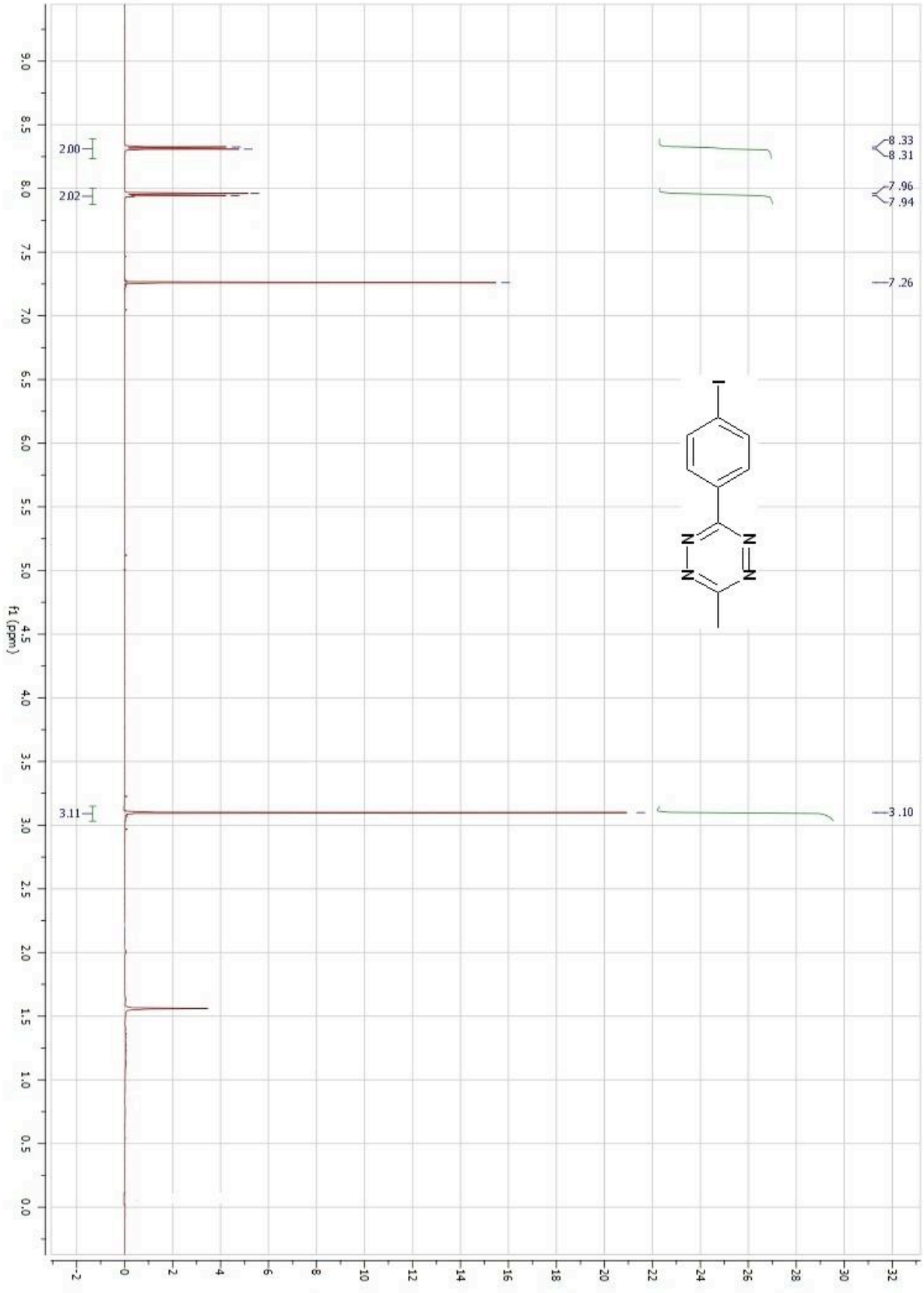
2.04
3.04
8.32
8.31
7.48
7.47
7.26
4.48
3.93
f1 (ppm)


159.56
153.85
151.10
132.35
124.41
124.01
121.99
58.57
58.43
58.30
58.16
58.03
57.89
57.75
53.18
35.85
35.73
f1 (ppm)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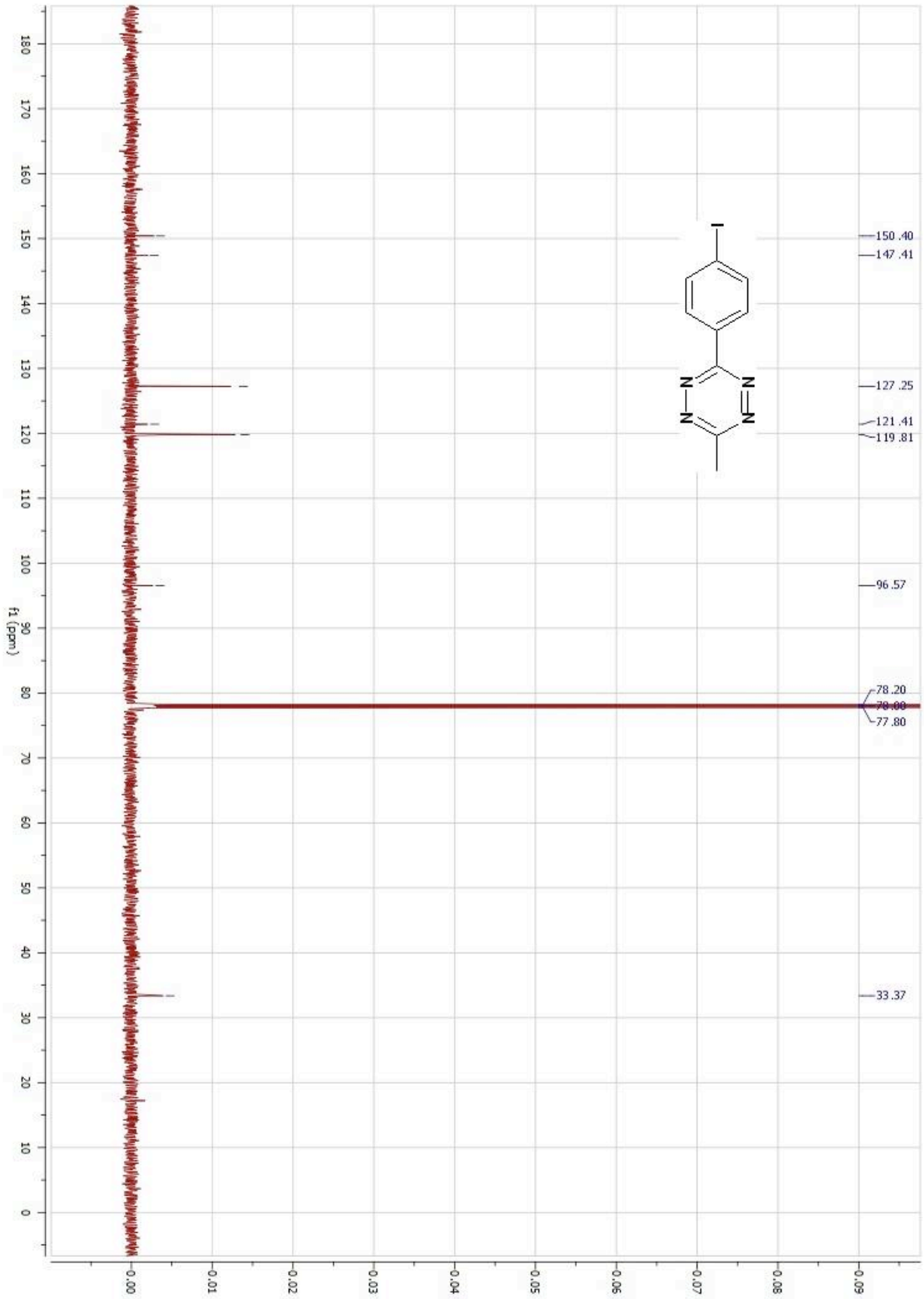
2.02
3.11
8.33
8.31
7.96
7.94
7.26
3.10
f1 (ppm)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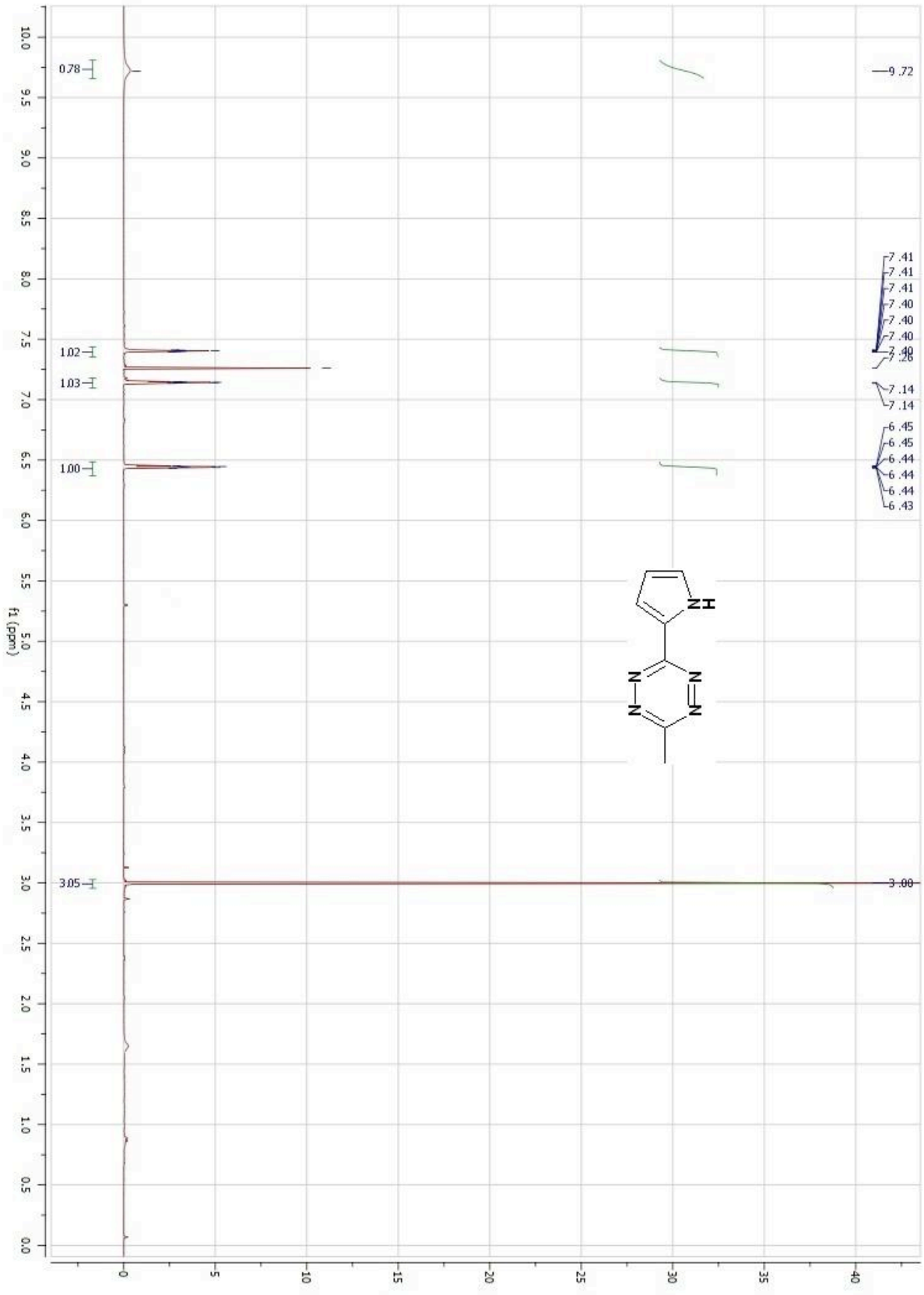
119.81
96.57
78.20
78.00
77.80
33.37
f1 (ppm)


0.78
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1.03
1.00
3.05
3.00
9.72
7.41
7.41
7.41
7.40
7.40
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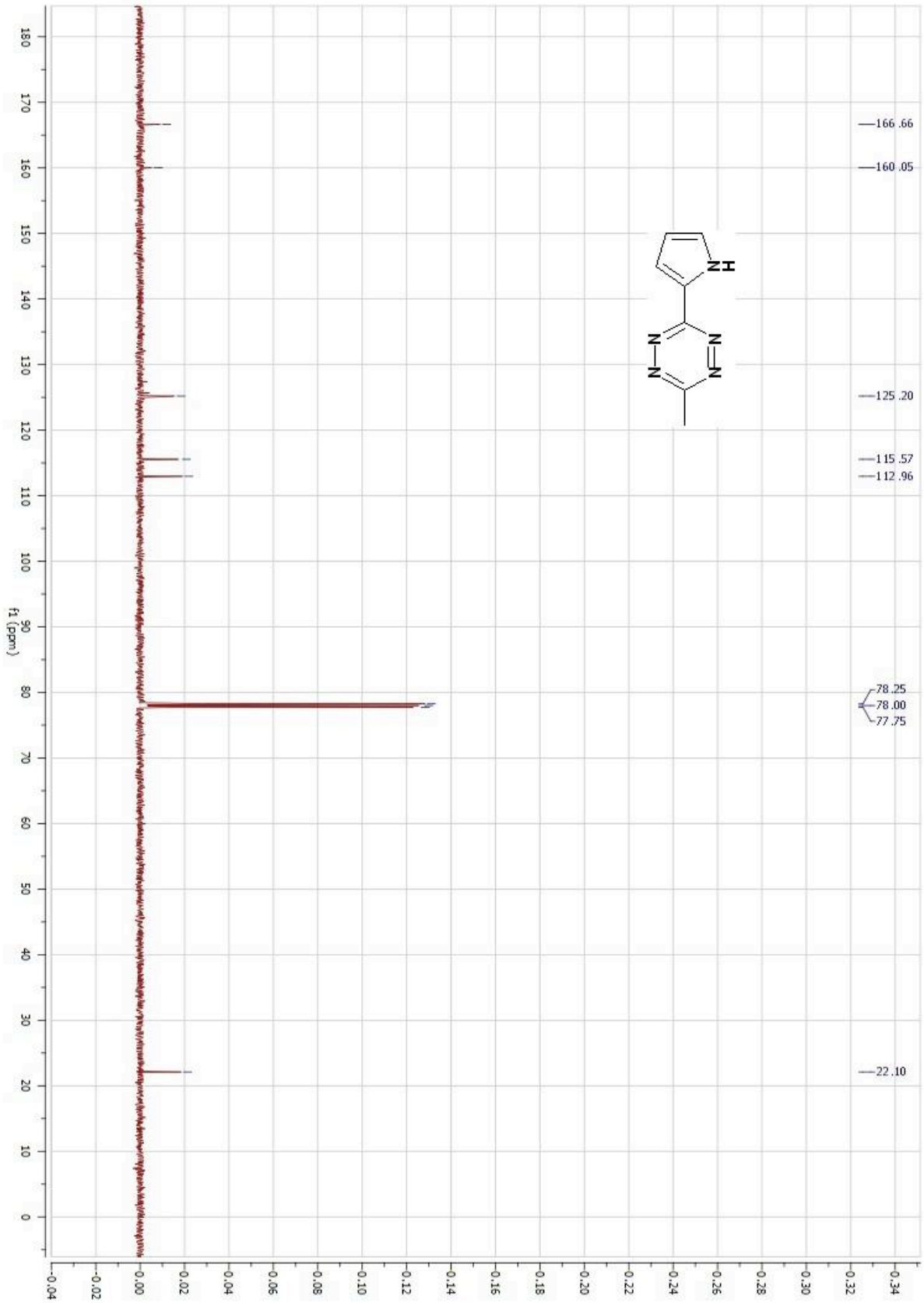
6.44
6.44
6.44
6.43
f1 (ppm)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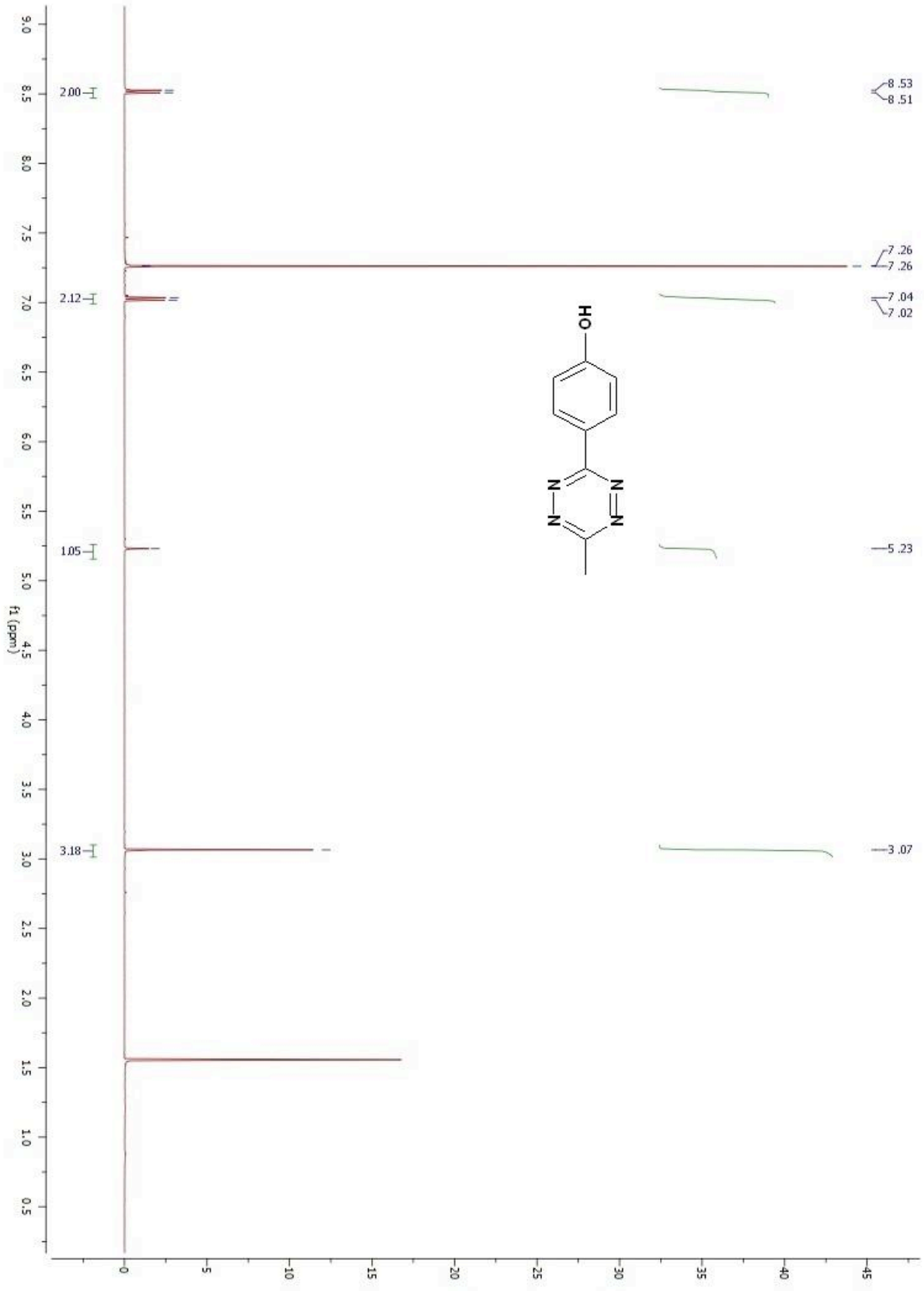
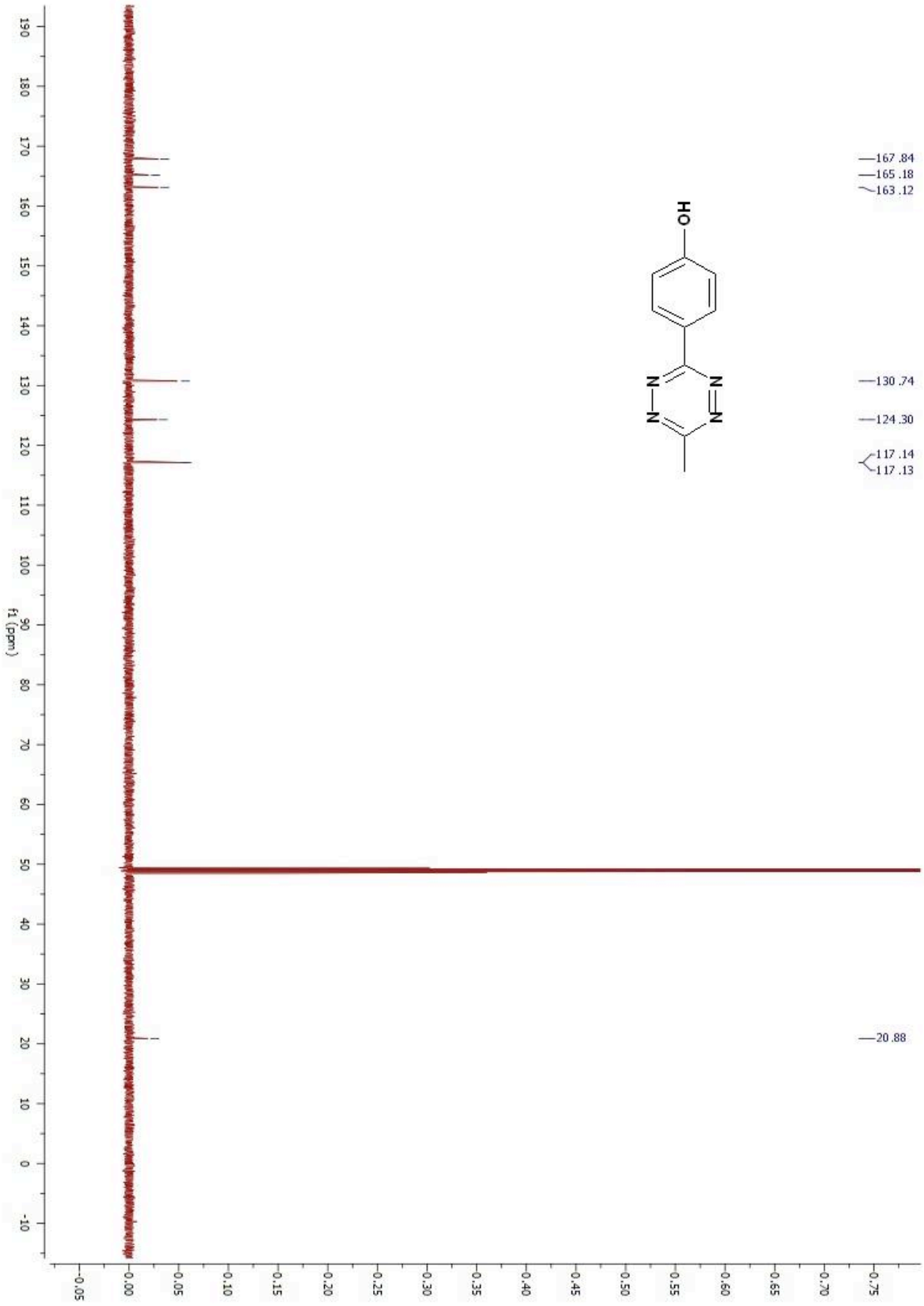
115.57
112.96
78.25
78.00
77.75
22.10
f1 (ppm)


2.00
2.12
1.05
3.18
8.53
8.51
7.26
7.26
7.04
7.02
5.23
3.07
OH
N
N
N
N
f1 (ppm)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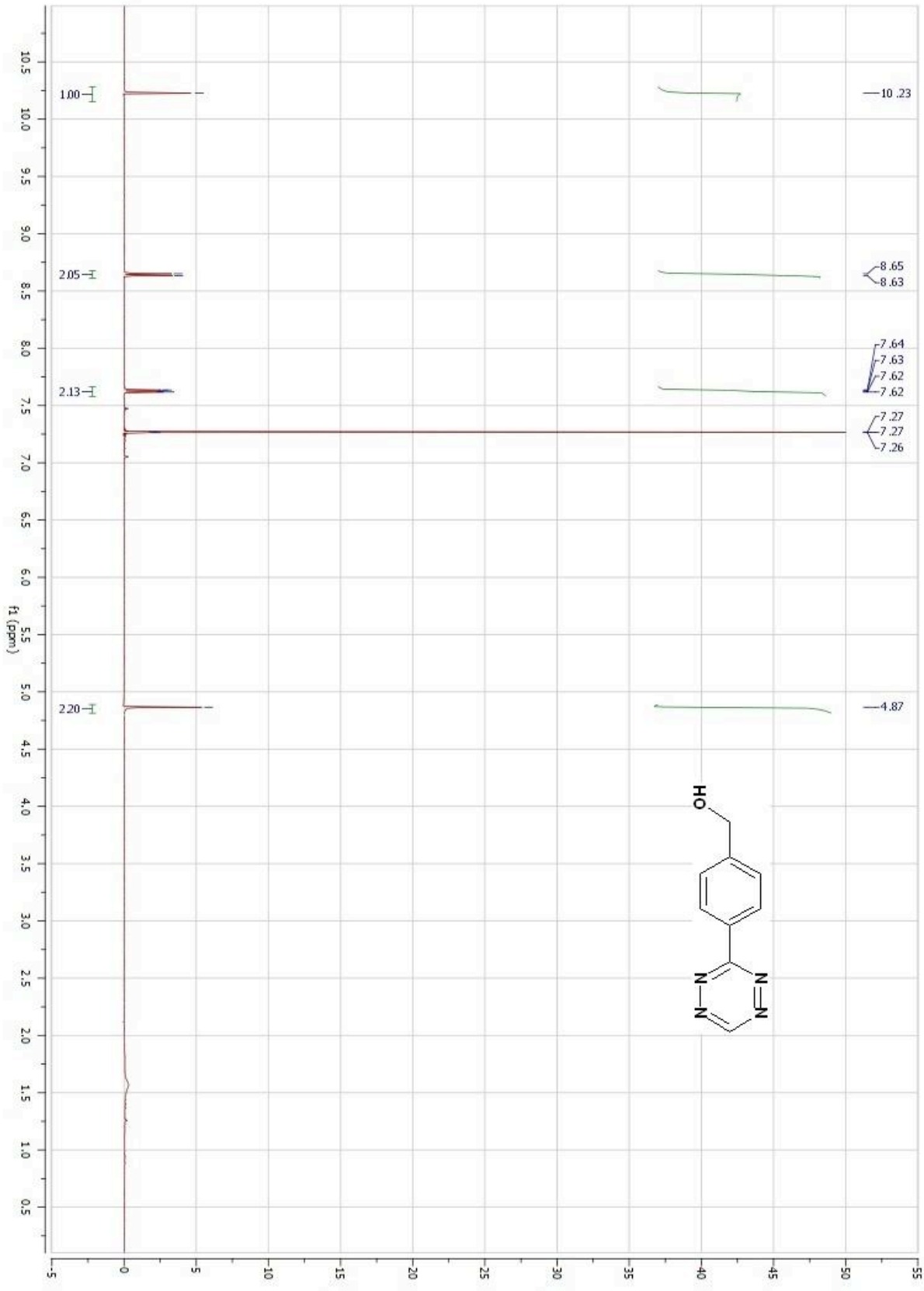
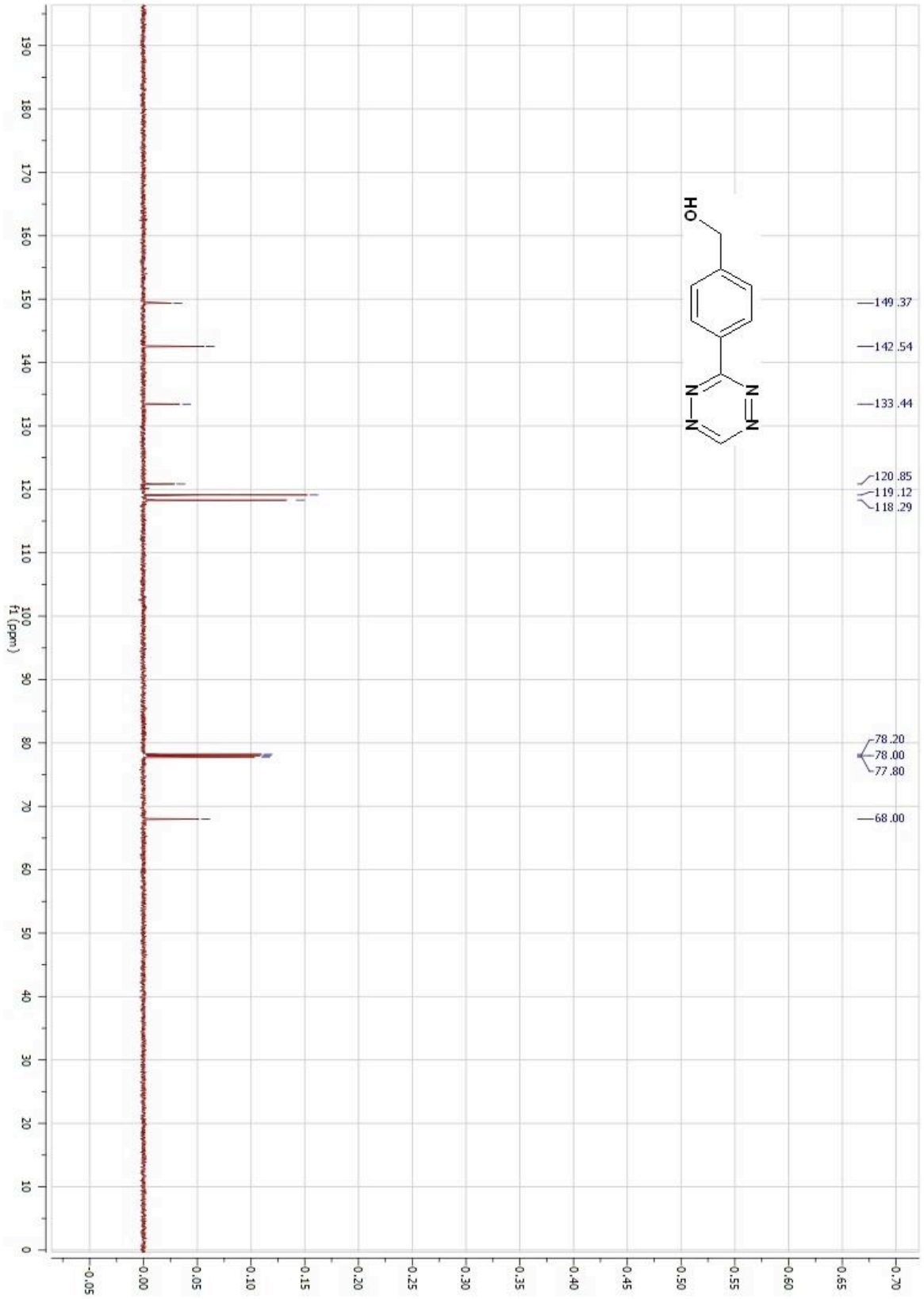
117.14
117.13
20.88
OH
N
N
N
N
f1 (ppm)


1.00
2.05
2.13
2.20
10.23
8.65
8.63
7.64
7.63
7.62
7.62
7.27
7.27
7.26
4.87
OH
N
N
N
N
f1 (ppm)


149.37
142.54
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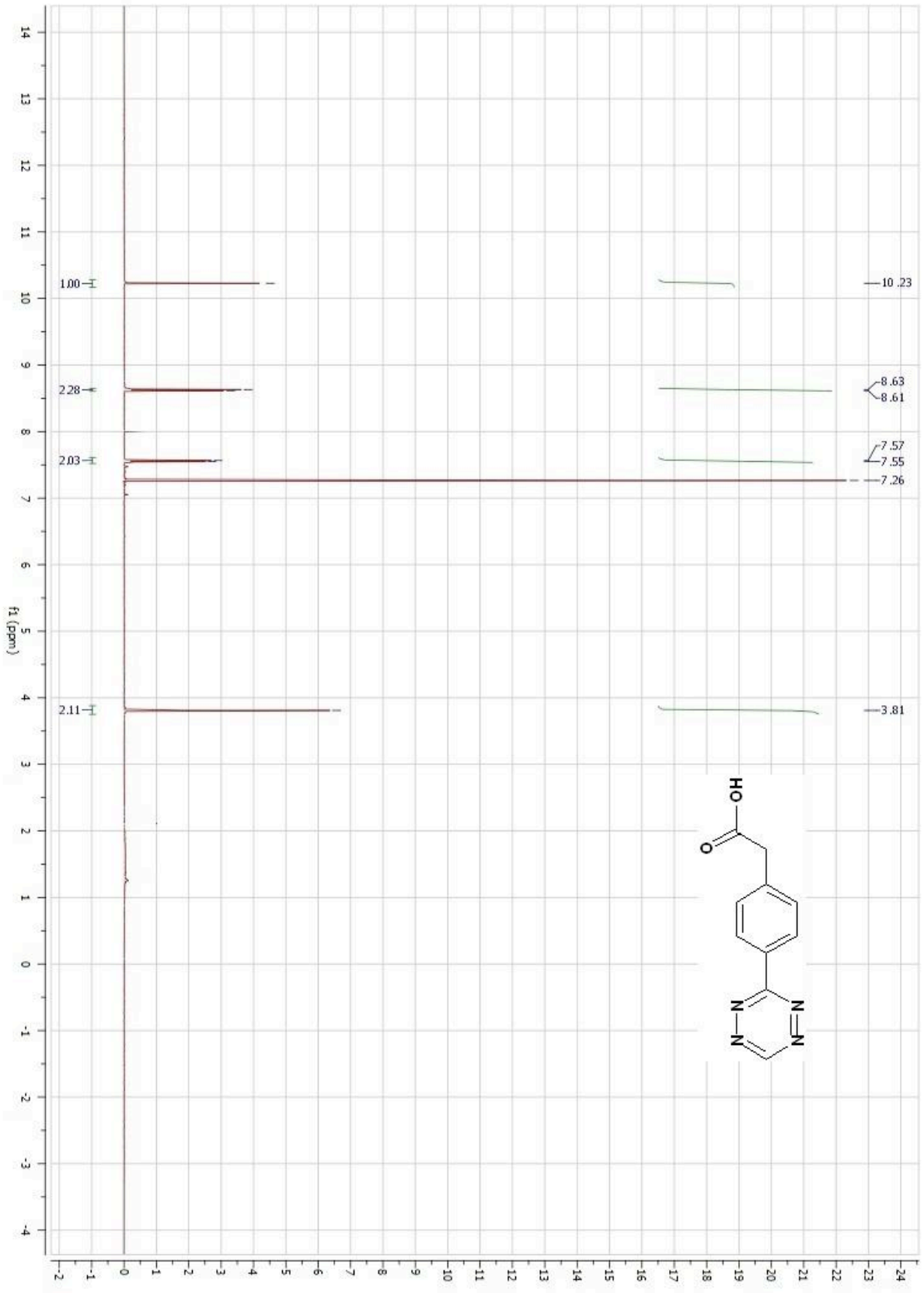
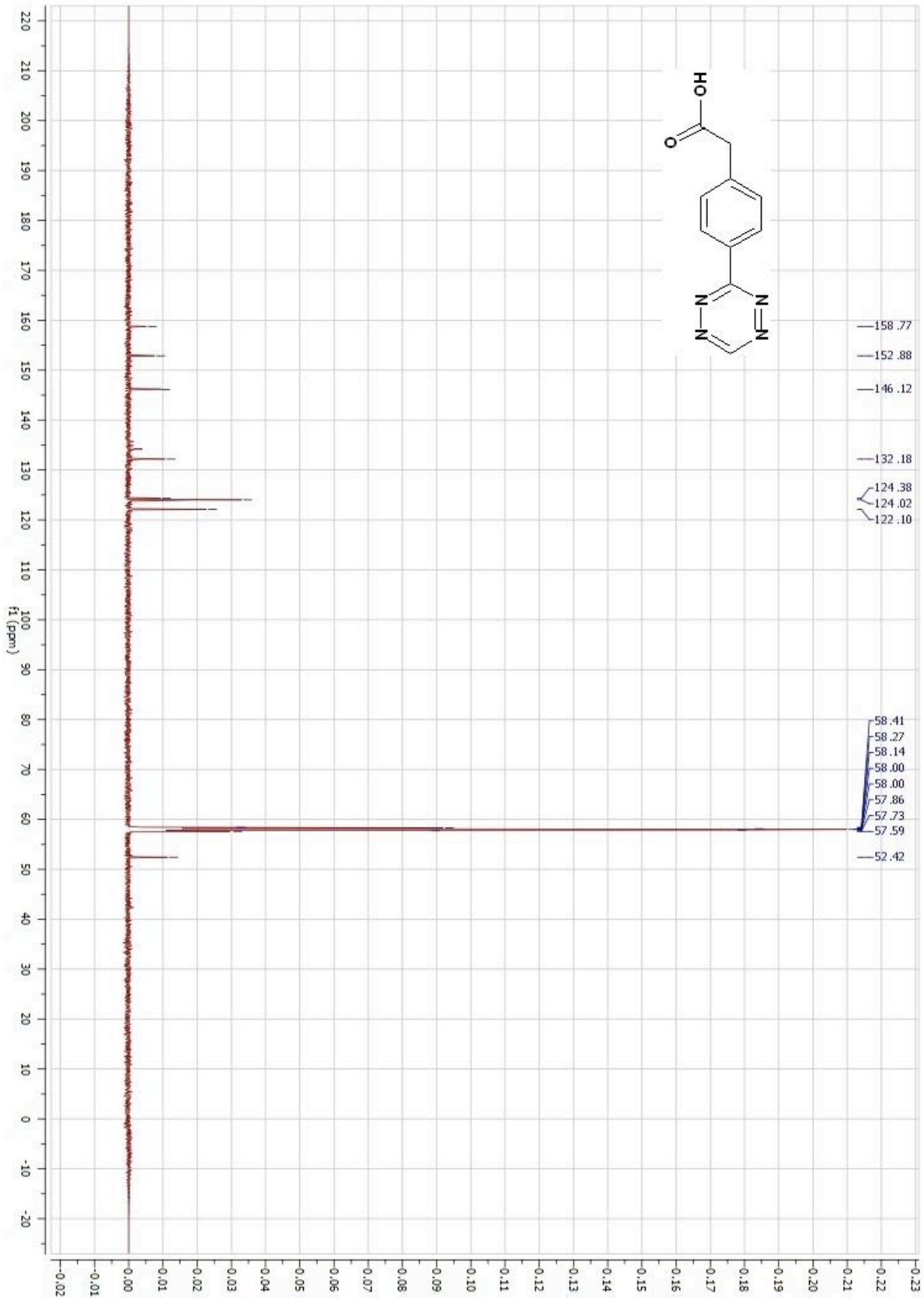
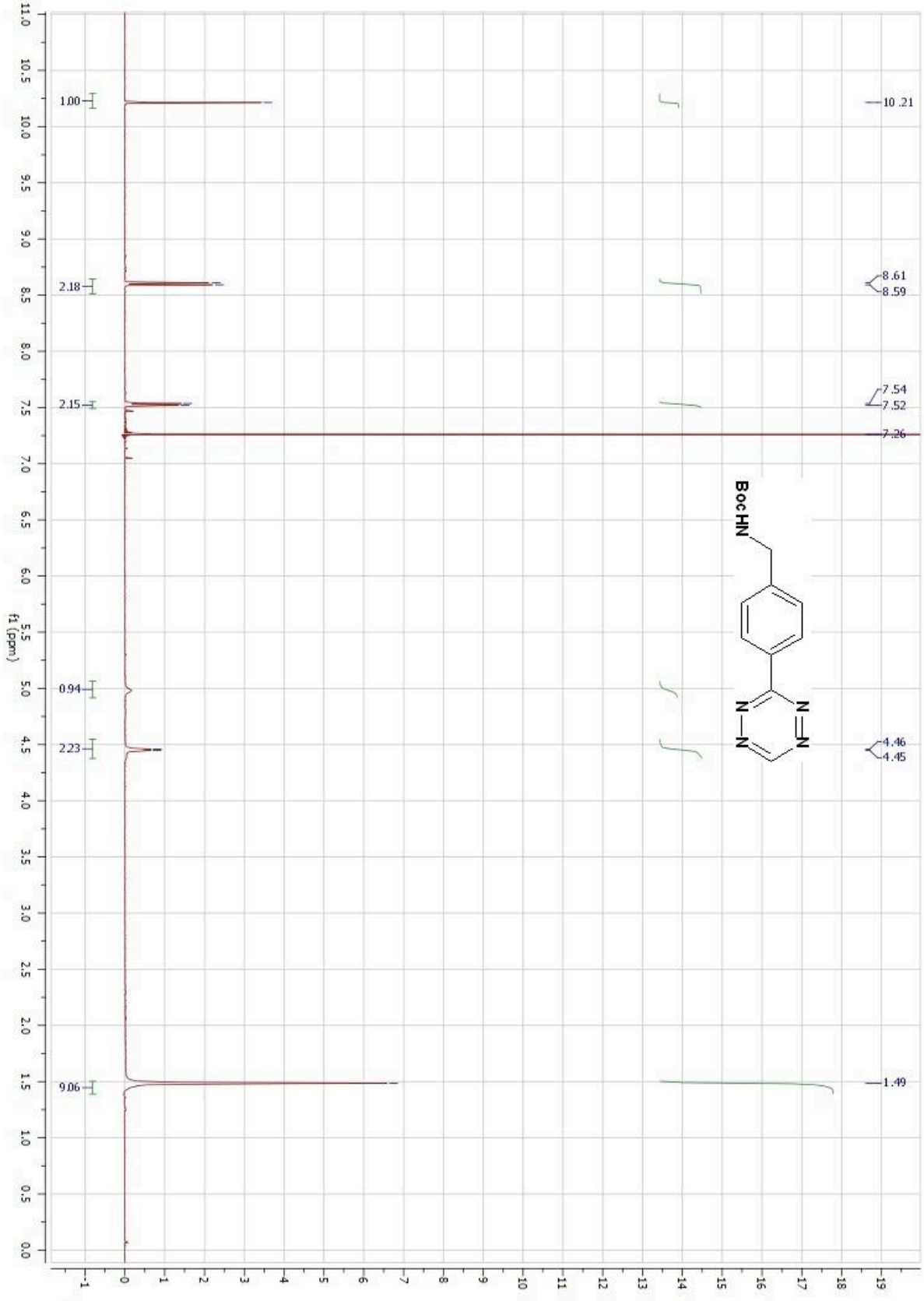
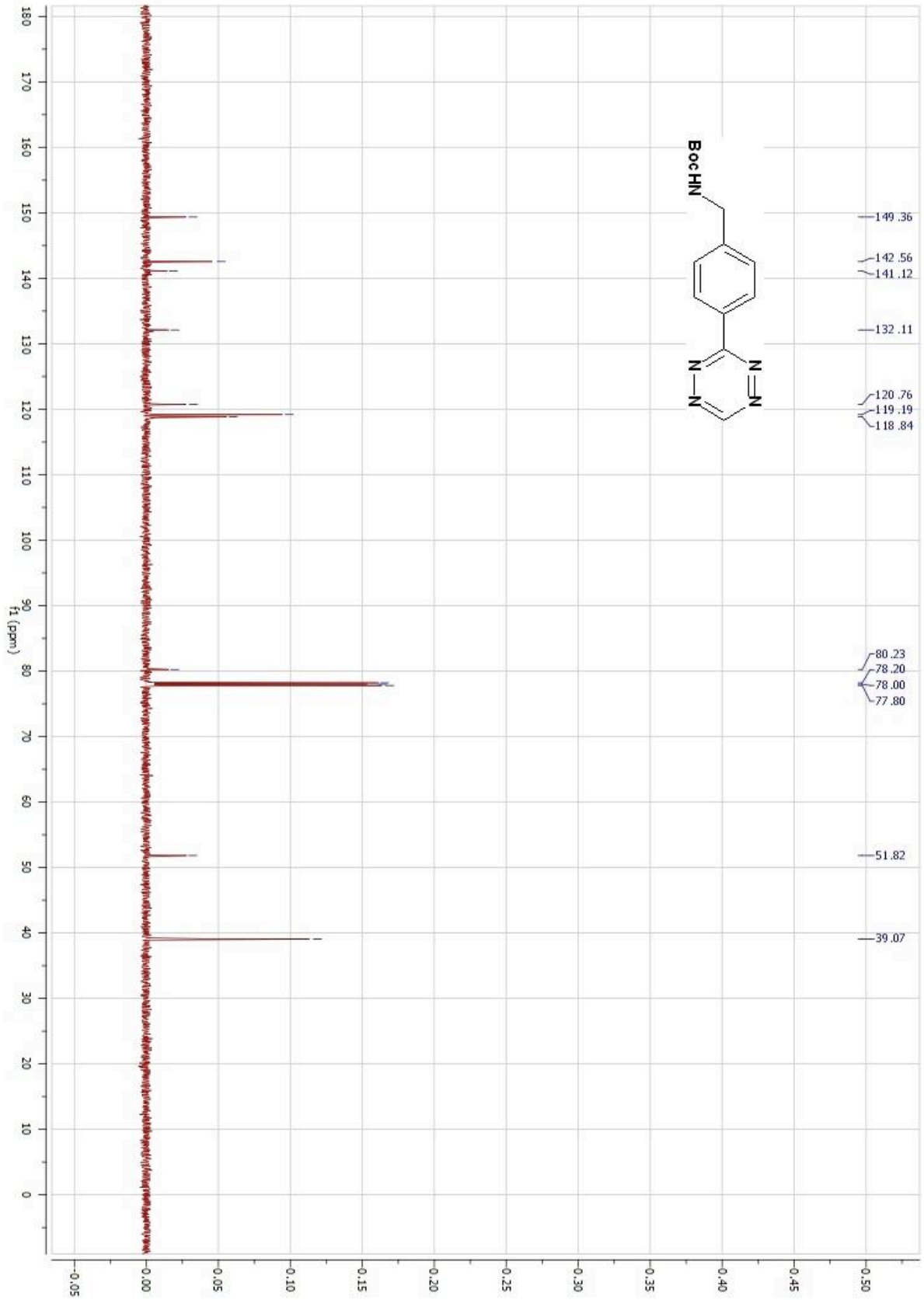
120.85
119.12
118.29
78.20
78.00
77.80
68.00
f1 (ppm)


1.00
2.28
2.03
2.11
10.23
8.63
8.61
7.57
7.55
7.26
3.81
f1 (ppm)
OH
O
N
N
N
N


158.77
152.88
146.12
132.18
124.38
124.02
122.10
58.41
58.27
58.14
58.00
58.00
57.86
57.73
57.59
52.42
f1 (ppm)


1.00
2.18
2.15
0.94
2.23
9.06
10.21
8.61
8.59
7.54
7.52
7.26
4.46
4.45
1.49
BocHN
N
N
N
N
f1 (ppm)


BocHN
N
N
N
N
149.36
142.56
141.12
132.11
120.76
119.19
118.84
80.23
78.20
78.00
77.80
51.82
39.07
f1 (ppm)