An Efficient Synthesis of 3,5-Bis-Aminated Pyrazolo[1,5-*a*]pyrimidines: Microwave Assisted Copper Catalyzed C-3 Amination of 5-Amino-3-Bromo-substituted Precursors

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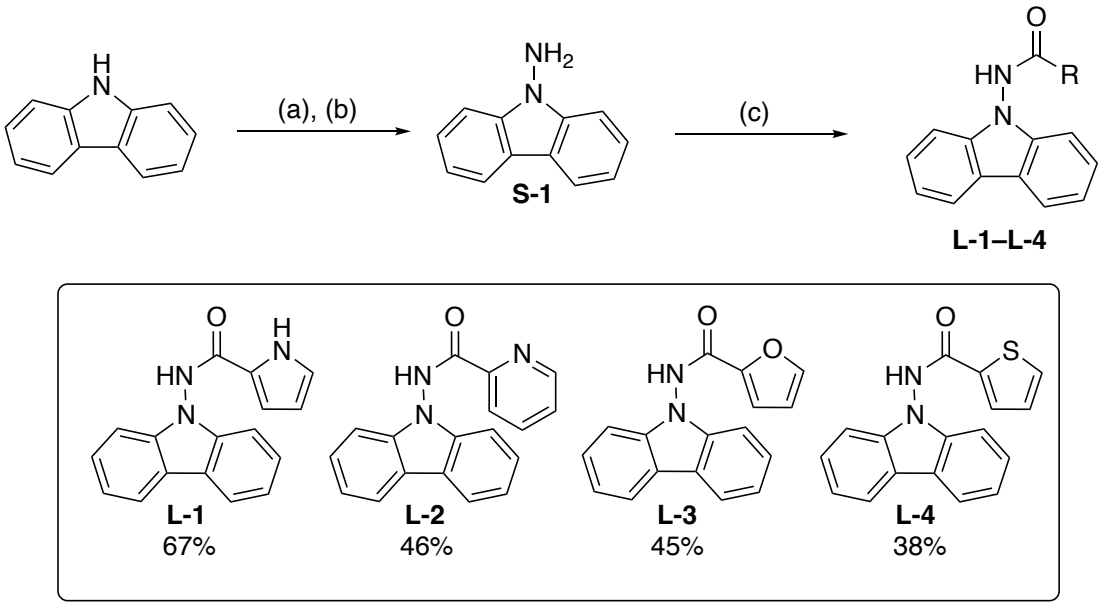
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General Experimental

Reactions described in the Supplementary Materials section were performed in flame- or oven-dried round-bottom flasks using solvents directly as supplied by commercial vendors, or dried as needed over standard drying agents, depending on the moisture sensitivity of the particular reaction. All other reagents were used directly as supplied without additional drying or purification. ^{1}H NMR and ^{13}C NMR spectra were determined in $CDCl_3$ or DMSO-d_6 using internal references: δ 7.27 or 2.50 (^{1}H), δ 77.23 or 39.52 (^{13}C), respectively. High resolution mass spectra were obtained using fast atom bombardment electrospray (ES) ionization techniques and had errors of less than ± 5 ppm.

Ligand Synthesis

Ligands **L-1**, **L-2**, **L-3**, and **L-4** were prepared via a modification of the method of Huang and co-workers, where we employed Ph_3P/NIS to generate a reactive acyl iodide intermediate[1, 2] to achieve the desired amidation (Scheme S1). In our hands, the method of Huang and co-workers which employed $SOCl_2$ for generating an acyl chloride consistently gave yields <35%, even after rigorous drying of glassware, solvents, and reagents. The Ph_3P/NIS method was more reproducible, and ligands were obtained in 38-67% (ave = 49%).



Scheme S1. Reagents and conditions: (a) $NaNO_2$, AcOH:DMSO (1:1); 0°C–RT; (b) Zn, EtOH:AcOH (4:1), 0°C–RT, 5 h; (c) RCO_2H (1.3 equiv.), Ph_3P (1.5 equiv.), NIS (1.5 equiv.), CH_3CN, 0°C – RT, 16 h.

N-Nitroso-9H-carbazole

N-Nitroso-9H-carbazole was prepared via the method of Huang and co-workers (1 g, 97%).[3] An exhaustive search of CAS SciFinder (Oct. 2024) revealed that although the ^1H characterization data for this compound has been reported, ^{13}C NMR data was missing. We report such data for archival purposes.

^1H NMR ($CDCl_3$, 500 MHz) δ 8.59–8.58 (m, 1H), 8.26 (d, J = 8.0 Hz; 1H), 7.97–7.93 (m, 2H), 7.57 (dt, J = 8.3, 1.0 Hz; 1H), 7.53–7.48 (m, 3H), ^{13}C NMR ($CDCl_3$, 125 MHz) δ 138.5, 132.7, 128.5, 128.1, 127.4, 126.2, 125.3, 124.8, 120.3, 119.8, 116.5, 112.3; HRMS Calcd. for $C_{12}H_9N_2O$ [M+H]: 197.0715; Found: 197.0721 (Δ = 3.0 ppm).

N-Amino-9H-carbazole **(S-1)**

N-Amino 9H-carbazole (**S-1**) was prepared following a modification of the method of Cui et al.[4] To a stirred solution of N-nitrosocarbazole (500 mg, 2.55 mmol), in EtOH:AcOH (4:1)(15 mL) at 0 °C was added Zn dust (670 mg, 10.5 mmol, 4 equiv.) in four aliquots over 1 hour (one aliquot every 15 min). The resulting mixture was allowed to warm to RT and stirred for 5 h. The crude reaction mixture was poured into EtOAc (20 mL), partitioned with H_2O (20 mL), and washed with $NaHCO_3$ (sat'd) (2 X 40 mL). The organic layer was dried over $MgSO_4$, filtered,

and then evaporated under reduced pressure. Purification via column chromatography (10% EtOAc/Hexanes) gave **S-1** (0.399 g, 2.2 mmol, 86%).

^{1}H NMR (DMSO-d_6, 500 MHz) δ 8.11 (d, J = 8.0 Hz, 2H), 7.60 (d, J = 8.5 Hz, 2H), 7.46 (dt, J = 8.0, 1.0 Hz, 2H), 7.17 ('t', J = 7.8 Hz, 2H), 5.83 (s, 2H); ^{13}C NMR (DMSO-d_6, 125 MHz) δ 141.6, 125.9, 120.4, 120.2, 119.0, 109.5; HRMS Calcd. for $C_{12}H_{10}N_2$ [M+H]: 183.0922; Found: 183.0929 (Δ = 3.8 ppm).

N-(9H-Carbazol-9-yl)-1H-pyrrole-2-carboxamide (L-1)

A solution of 1*H*-pyrrole-2-carboxylic acid (79 mg, 0.71 mmol, 1.3 equiv), N-iodosuccinimide (187 mg, 0.83 mmol, 1.5 equiv), and Ph_3P (218 mg, 0.83 mmol, 1.5 equiv), in CH_3CN (3 mL), was stirred under Argon at ambient temperature for 30 minutes. N-amino-9H-carbazole (100 mg, 0.55 mmol) was added, and the mixture stirred for an additional 16 h. Solvents were removed under reduced pressure and the crude residue purified via chromatography (20% EtOAc/Hexanes) to give **L-1** (101 mg, 0.37 mmol, 67%).

^{1}H NMR (DMSO-d_6, 500 MHz) δ 11.84 (s, 1H), 11.36 (s, 1H), 8.21 (d, J = 7.7 Hz, 2H), 7.46 (dt, J = 8.1, 1.0 Hz, 2H), 7.36 (d, J = 8.1 Hz, 2H), 7.28 ('t', J = 7.8 Hz, 2H), 7.20 (bs, 1H), 7.07 (bs, 1H), 6.27 (bs, 1H); ^{13}C NMR (DMSO-d_6, 125 MHz) δ 160.8, 140.7, 126.7, 123.8, 123.7, 121.1, 120.9, 120.4, 112.5, 109.8, 109.1; HRMS Calcd. for $C_{17}H_{14}N_3O$ [M+H]: 276.1137; Found: 276.1130 (Δ = 2.5 ppm).

N-(9H-Carbazol-9-yl)picolinamide (L-2)

Similar to **L-1**; N-aminocarbazole (100 mg, 0.55 mmol), picolinic acid (87 mg, 0.71 mmol, 1.3 equiv), N-iodosuccinimide (187 mg, 0.83 mmol, 1.5 equiv), Ph_3P (218 mg, 0.83 mmol, 1.5 equiv); **L-2** (73 mg, 0.25 mmol, 46%).

^{1}H NMR (DMSO-d_6, 500 MHz) δ 12.14 (s, 1H), 8.83 (d, J = 4.7 Hz, 1H), 8.20 (d, J = 7.7 Hz, 2H), 8.12–8.10 (m, 2H), 7.78–7.75 (m, 1H), 7.44 (t, J = 7.2 Hz, 2H), 7.33 (d, J = 8.0 Hz, 2H), 7.26 ('t', J = 7.5 Hz, 2H); ^{13}C NMR (DMSO-d_6, 125 MHz) δ 163.4, 148.4, 148.1, 139.2, 137.5, 127.0, 125.5, 122.3, 120.1, 119.8, 119.3, 108.1; HRMS Calcd. for $C_{18}H_{14}N_3O$ [M+H]: 288.1137; Found: 288.1134 (Δ = 1.0 ppm).

N-(9H-Carbazol-9-yl)furan-2-carboxamide (L-3)

Similar to **L-1**; N-aminocarbazole (100 mg, 0.55 mmol), furan-2-carboxylic acid (79 mg, 0.71 mmol, 1.3 equiv), N-iodosuccinimide (187 mg, 0.83 mmol, 1.5 equiv), Ph_3P (218 mg, 0.83 mmol, 1.5 equiv); **L-3** (68 mg, 0.25 mmol, 45%)

^{1}H NMR (DMSO-d_6, 500 MHz) δ 11.8 (bs, 1H), 8.20 (d, J = 7.8 Hz, 2H), 8.06 (d, J = 0.9 Hz, 2H), 7.47 - 7.44 (m, 3H), 7.37 (d, J = 8.1 Hz, 2H), 7.28 (ddd, J = 7.8, 7.1, 0.6 Hz, 2H), 6.80 (dd, J = 3.4, 1.7 Hz, 1H); ^{13}C NMR (DMSO-d_6, 125 MHz) δ 156.8, 145.9, 144.9, 139.3, 125.6, 120.1, 119.8, 119.5, 115.4, 111.7, 108.1; HRMS Calcd. for $C_{17}H_{13}N_2O_2$ [M+H]: 277.0977; Found: 277.0989 (Δ = 4.3 ppm).

N-(9H-Carbazol-9-yl)thiophene-2-carboxamide (L-4)

Similar to **L-1**; N-aminocarbazole (100 mg, 0.55 mmol), thiophene-2-carboxylic acid (91 mg, 0.71 mmol, 1.3 equiv), N-iodosuccinimide (187 mg, 0.83 mmol, 1.5 equiv), Ph_3P (218 mg, 0.83 mmol, 1.5 equiv); **L-4** (61 mg, 0.21 mmol, 38%).

^{1}H NMR (DMSO-d_6, 500 MHz) δ 11.9 (bs, 1H), 8.20 (d, J = 7.6 Hz, 2H), 8.14 ('s', 1H), 8.01 (d, J = 4.5 Hz, 1H), 7.47 ('t', J = 7.5 Hz, 2H), 7.39 (d, J = 8.0 Hz, 2H), 7.33 (d, J = 4.6 Hz, 1H), 7.28 ('t', J = 7.4 Hz, 1H); ^{13}C NMR (DMSO-d_6, 125 MHz) δ 160.4, 139.3, 135.4, 132.1, 129.5, 127.9, 125.7, 120.1, 119.9, 119.5, 108.1; HRMS Calcd. for $C_{17}H_{13}N_2OS$ [M+H]: 293.0749; Found: 293.0755 (Δ = 2.0 ppm).

Optimization of C-3 Amination

Reactions were set up according to the manuscript General Procedure for 3,5-bis-aminopyrazolo[1,5-*a*]pyrimidines **30**, reproduced below for clarity. After reacting at the specified temperatures, at timed intervals (as indicated in Table 1, see manuscript), the reactions were cooled to RT and analyzed by ^{1}H NMR. Various bases, solvents, and ligands were also evaluated (Table 1, manuscript).

General Procedure:

A solution of 3-Bromo-5-(pyrrolidin-1-yl)pyrazolo[1,5-*a*]pyrimidine (**29a**) (50 mg, 0.19 mmol), morpholine (25 mg, 0.29 mmol, 1.5 equiv.), **L-1** (6 mg, 0.02 mmol, 10 mol%), CuI (2 mg, 0.01 mmol, 5 mol%), and K_2CO_3 (52 mg, 0.38 mmol, 2 equiv.), in diethyleneglycol (DEG, 1 mL) was

stirred in a 10 mL microwave reactor vessel and heated at various temperatures and for varying lengths of time. Solvents, bases, and ligands were also varied (see Table 1, manuscript).

After the reaction had cooled to RT, an aliquot of reaction mix (approx. 200 μL) was directly mixed with DMSO-d_6 to prepare an NMR sample consisting of DEG:DMSO-d_6 (approx. 1:10, DEG:DMSO-d_6). Resonances Ha were normalized, then comparative integrations were used to determine the relative ratios of **29a**, **30e**, and **31** (see pp. 164-169).

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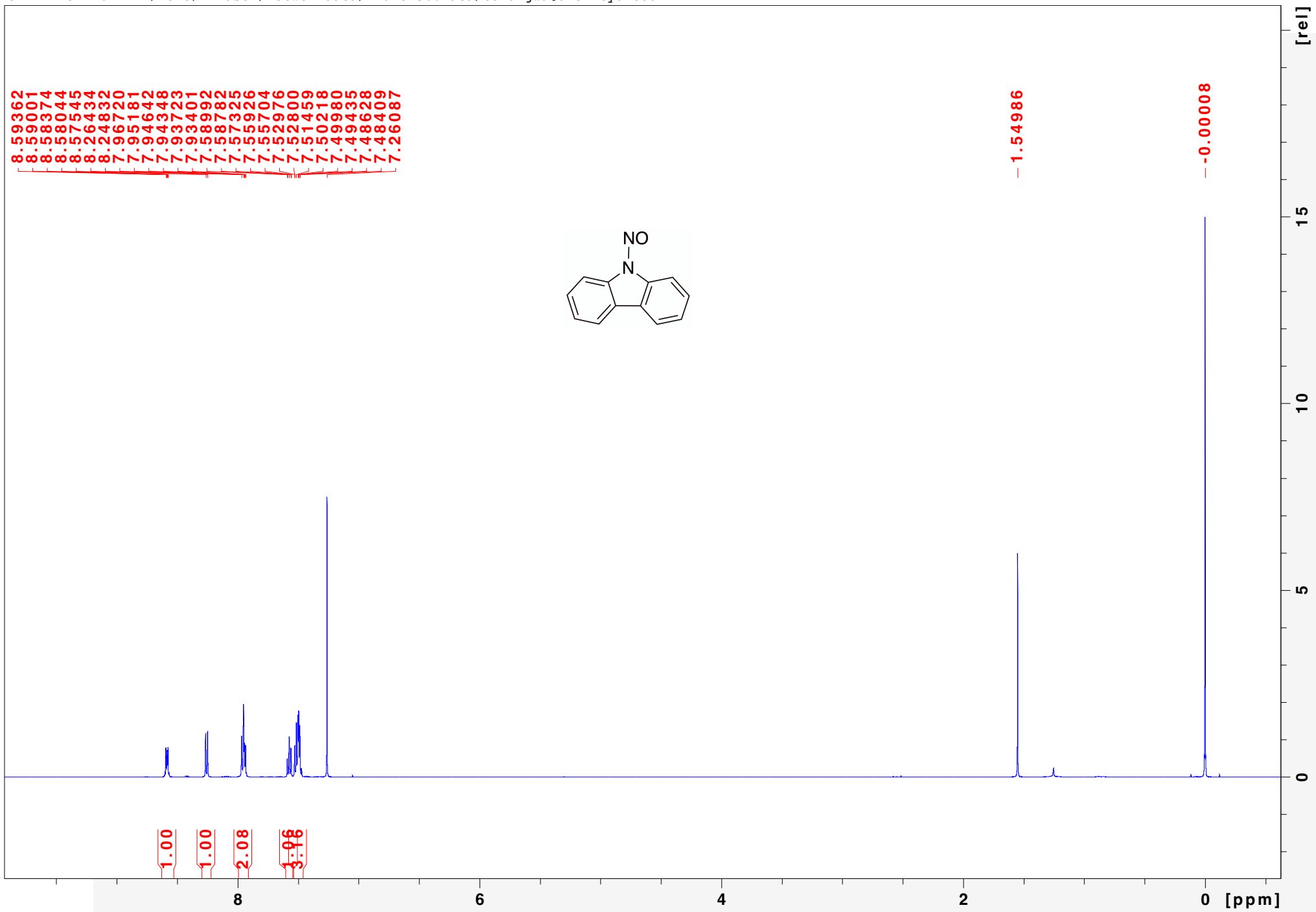
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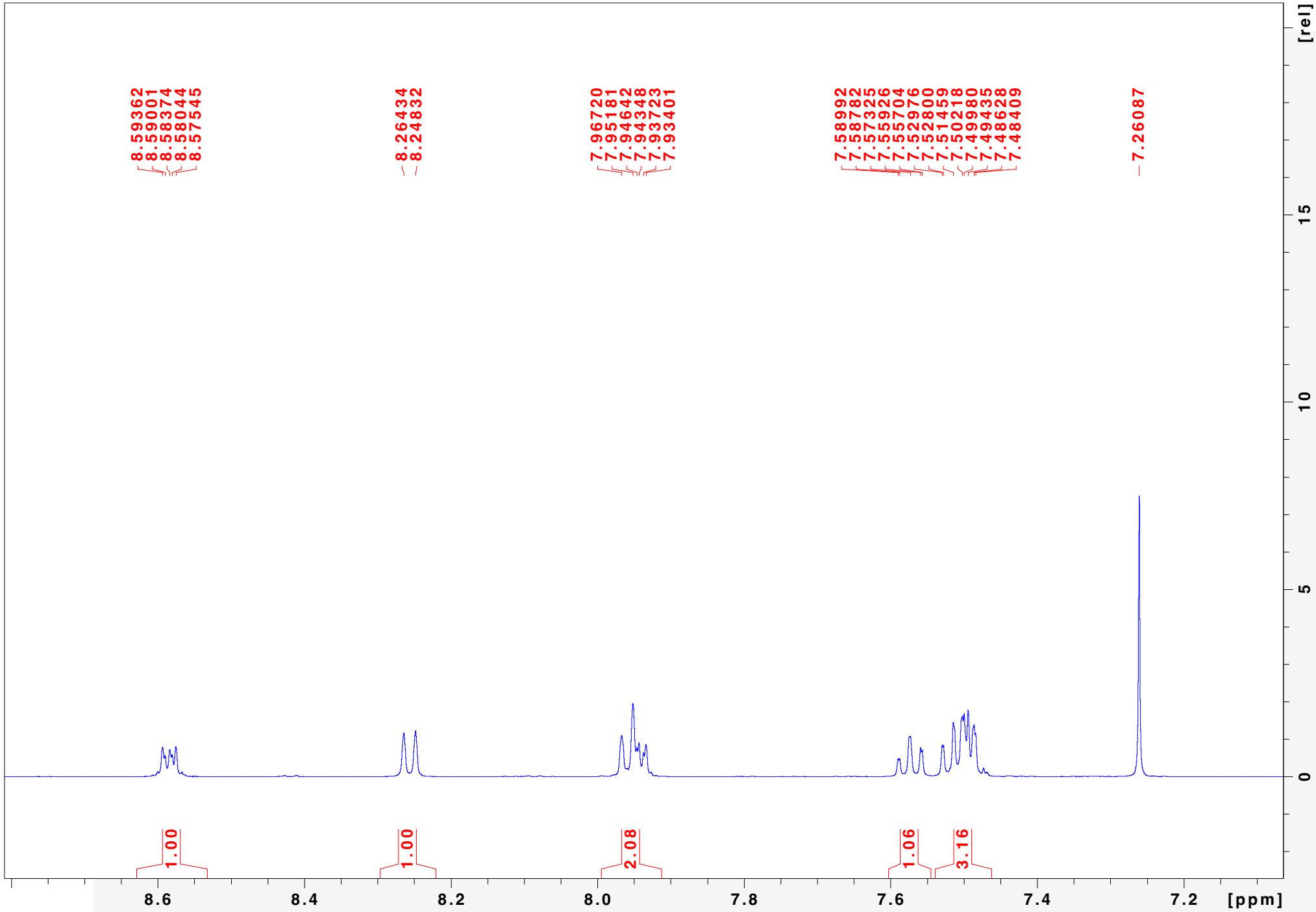
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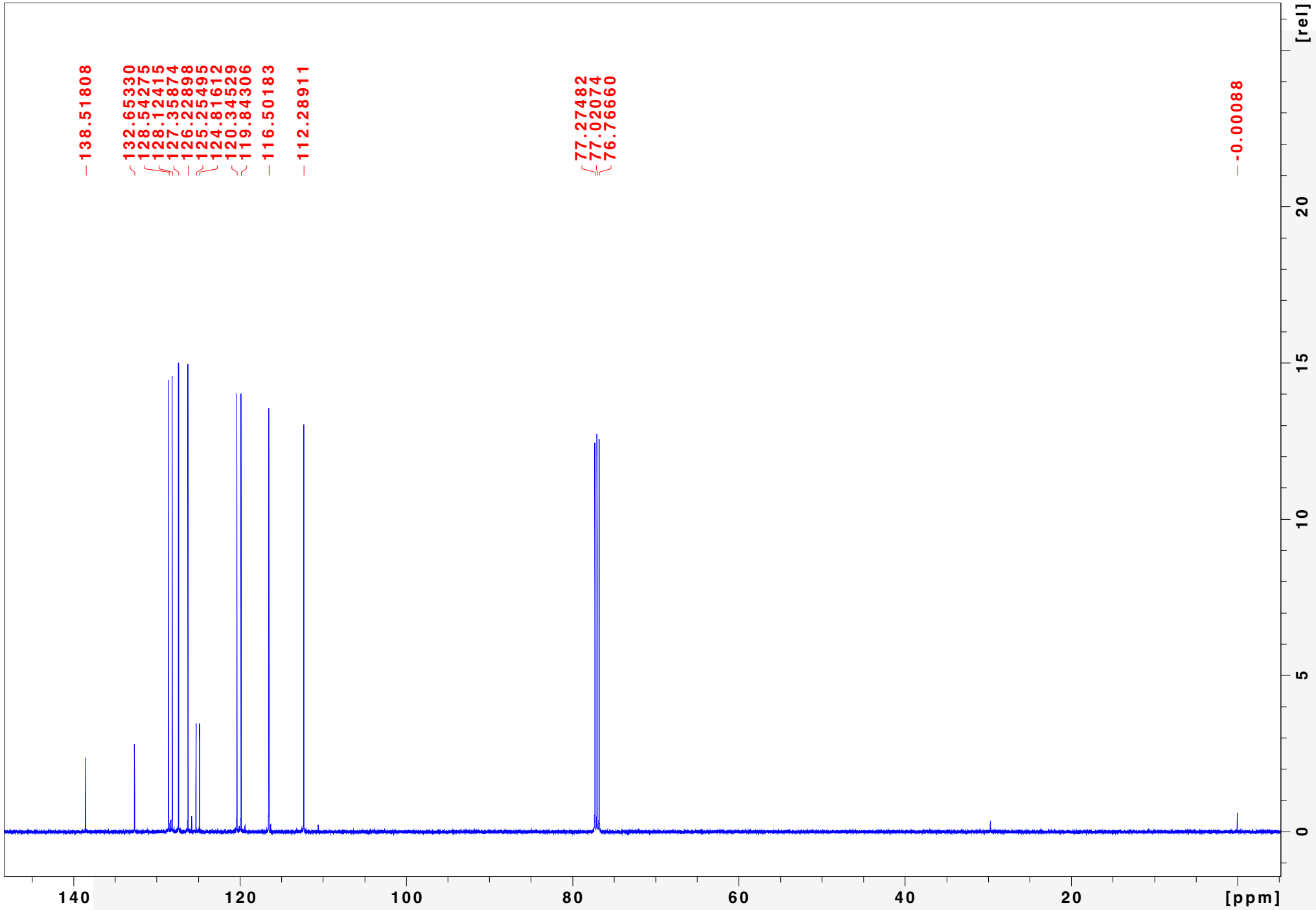
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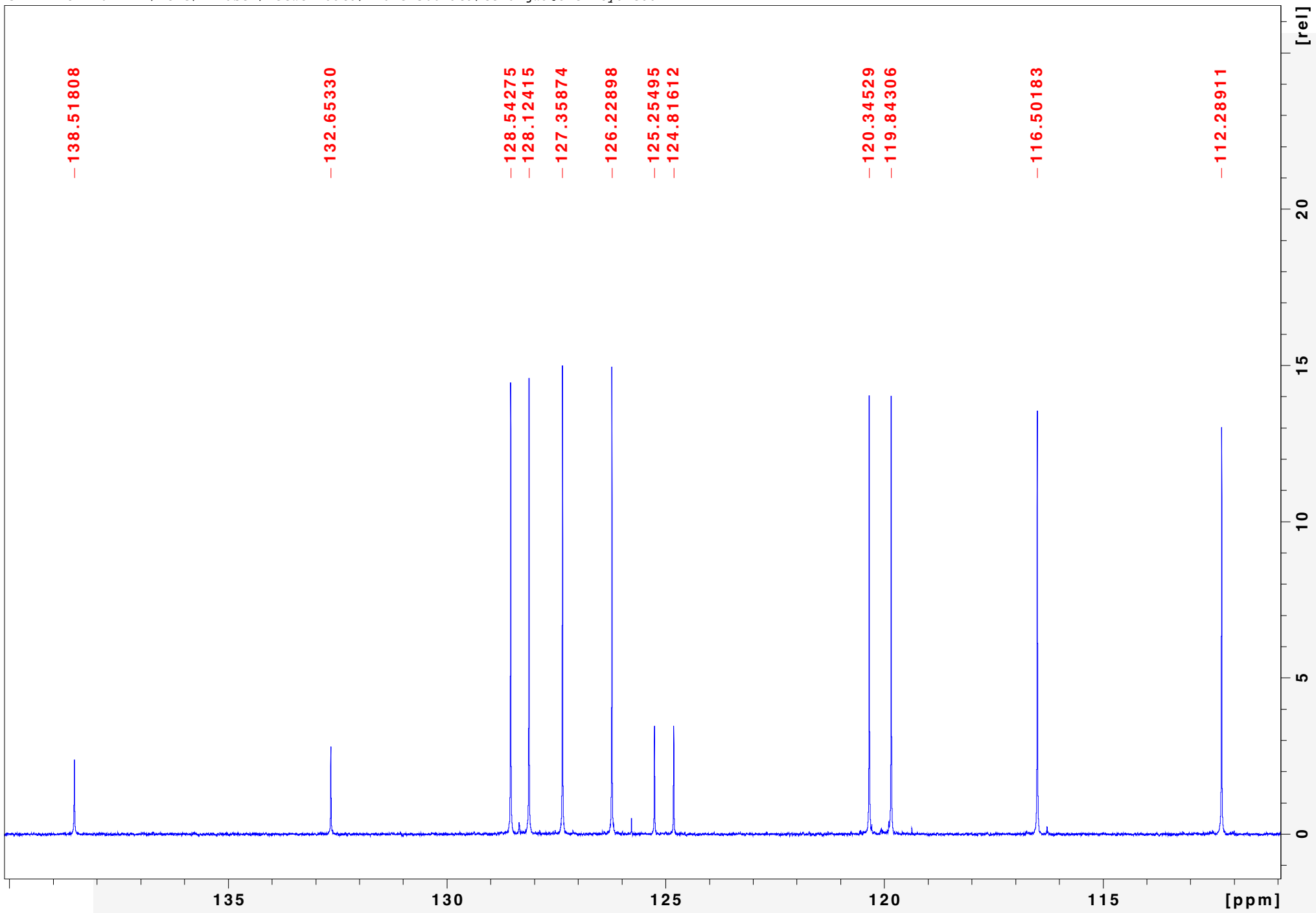
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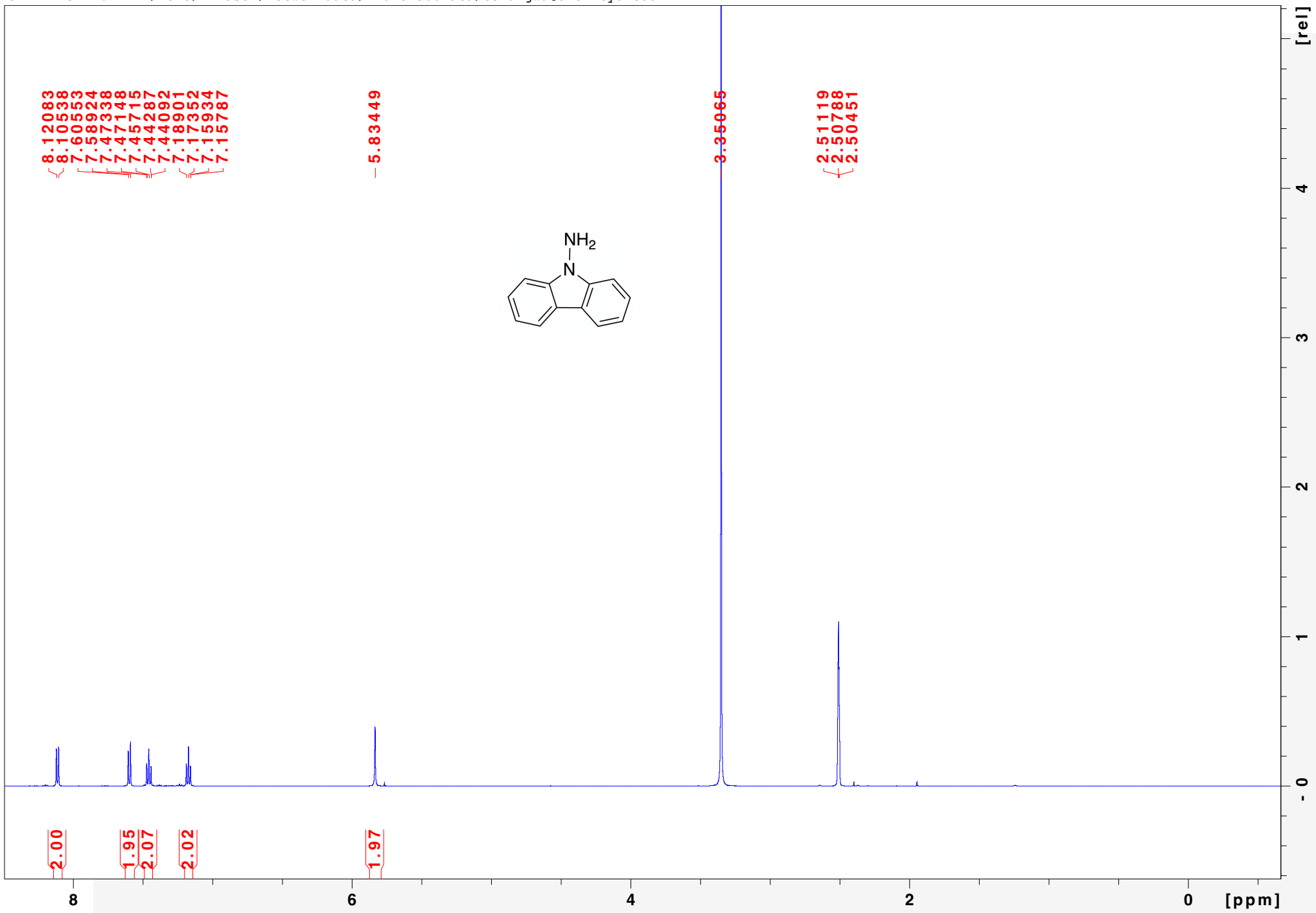
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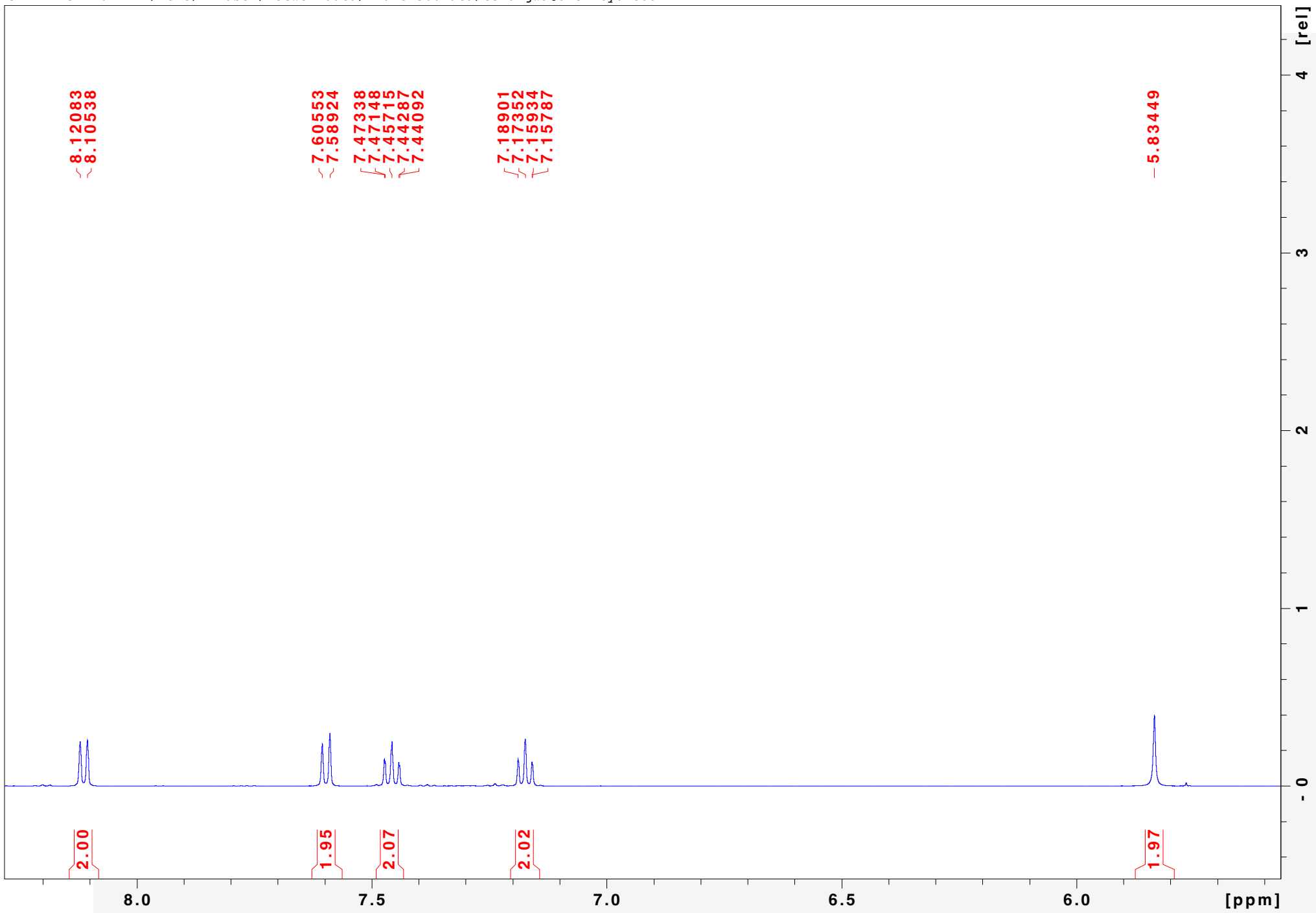
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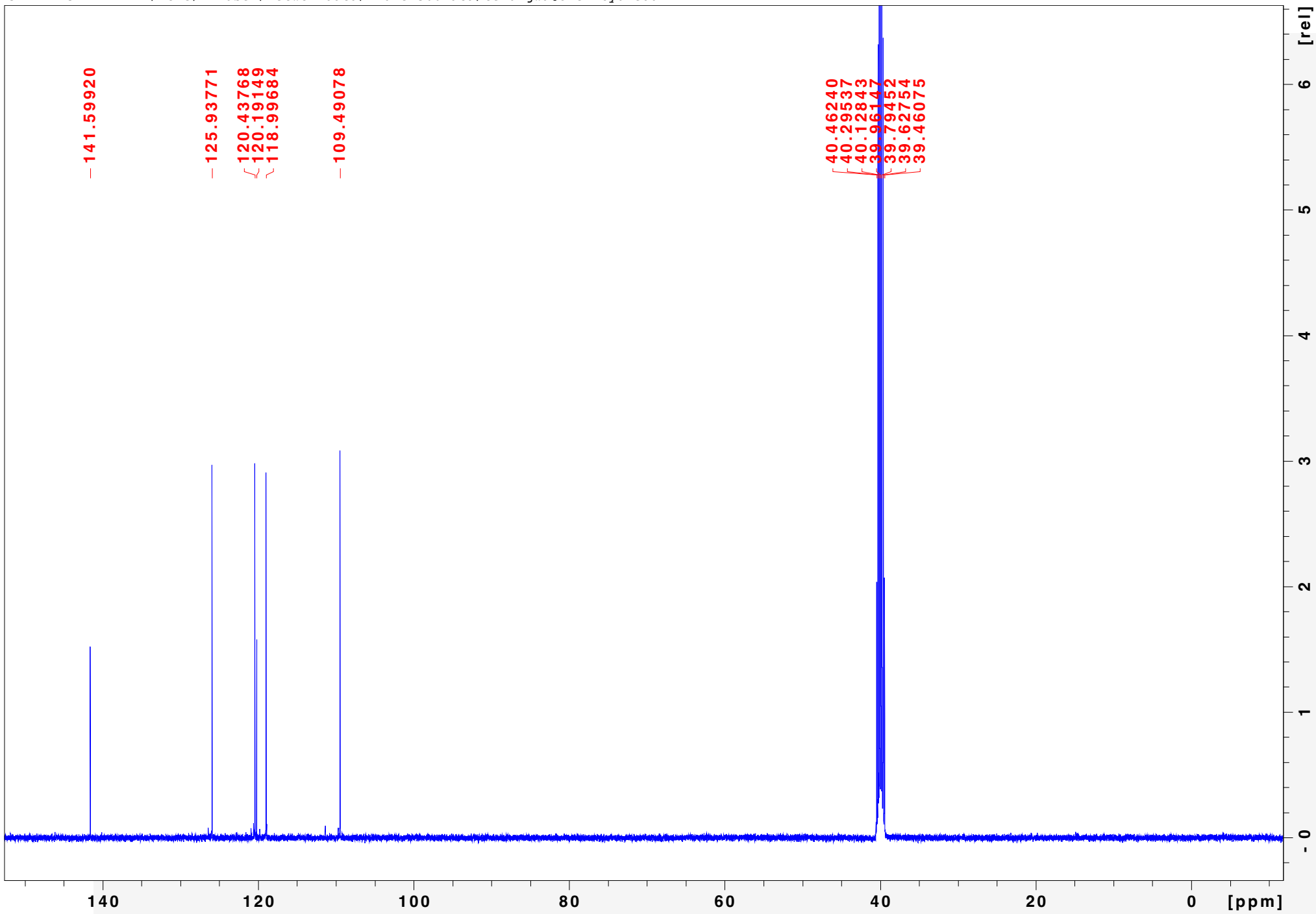
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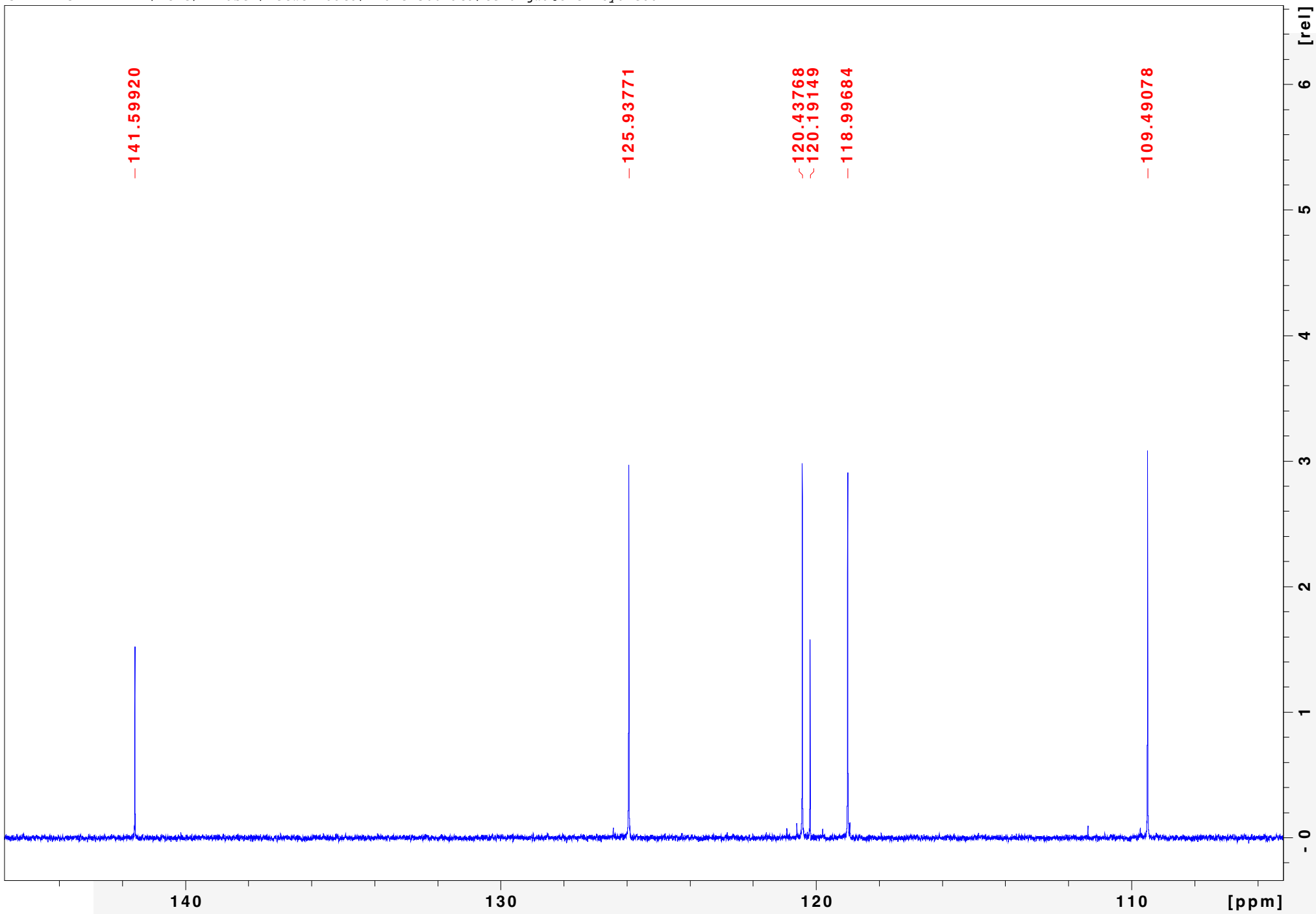
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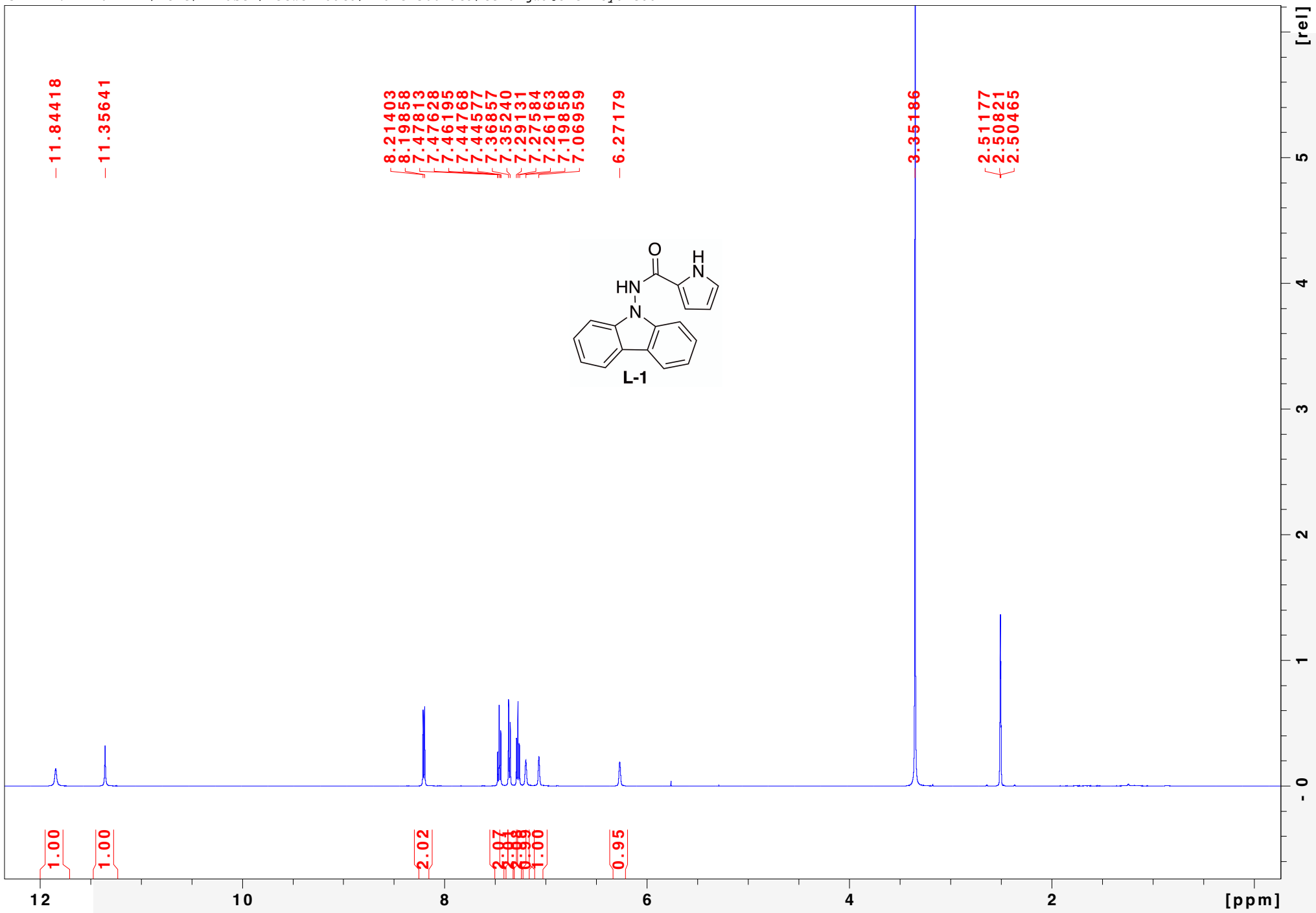
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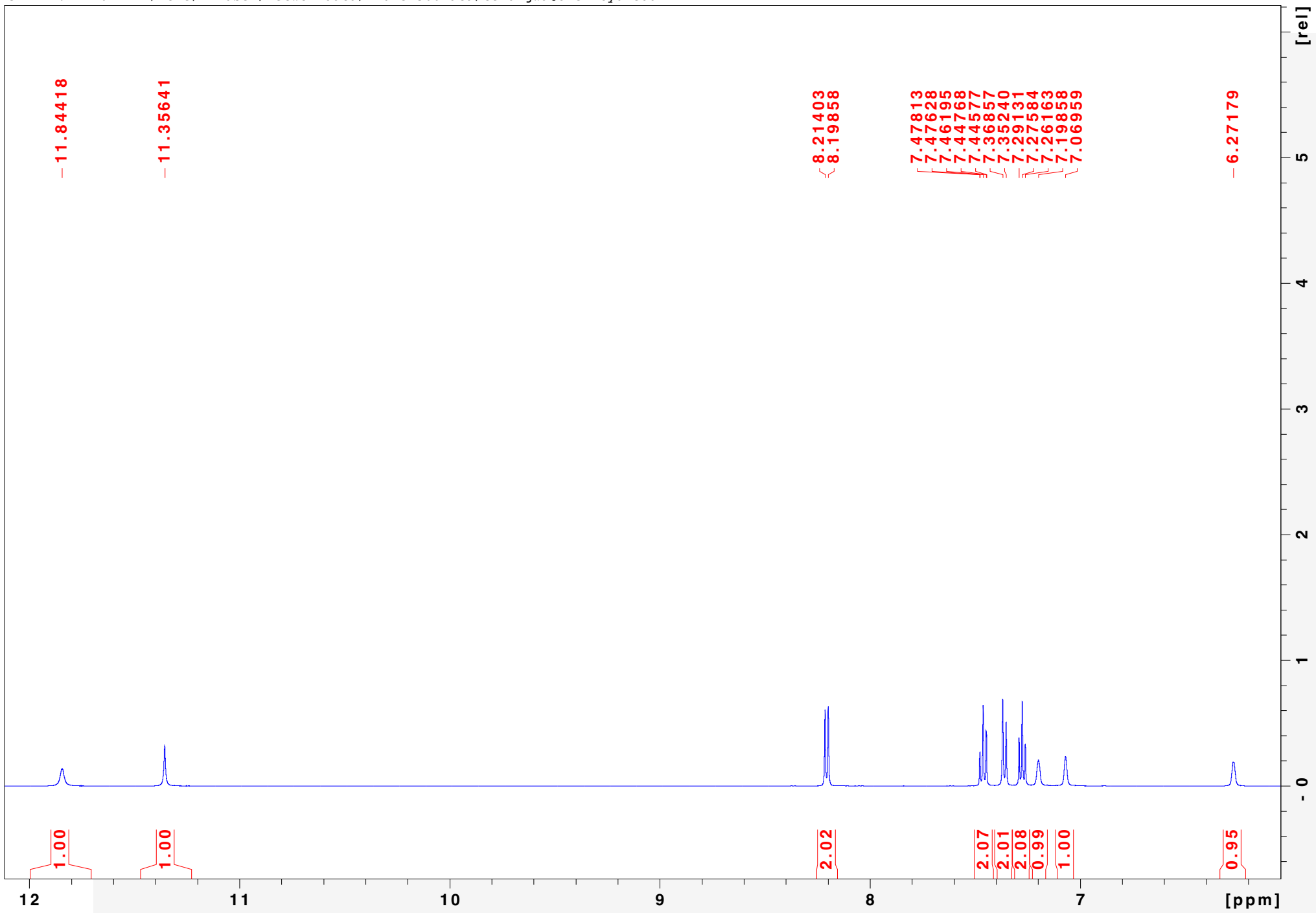
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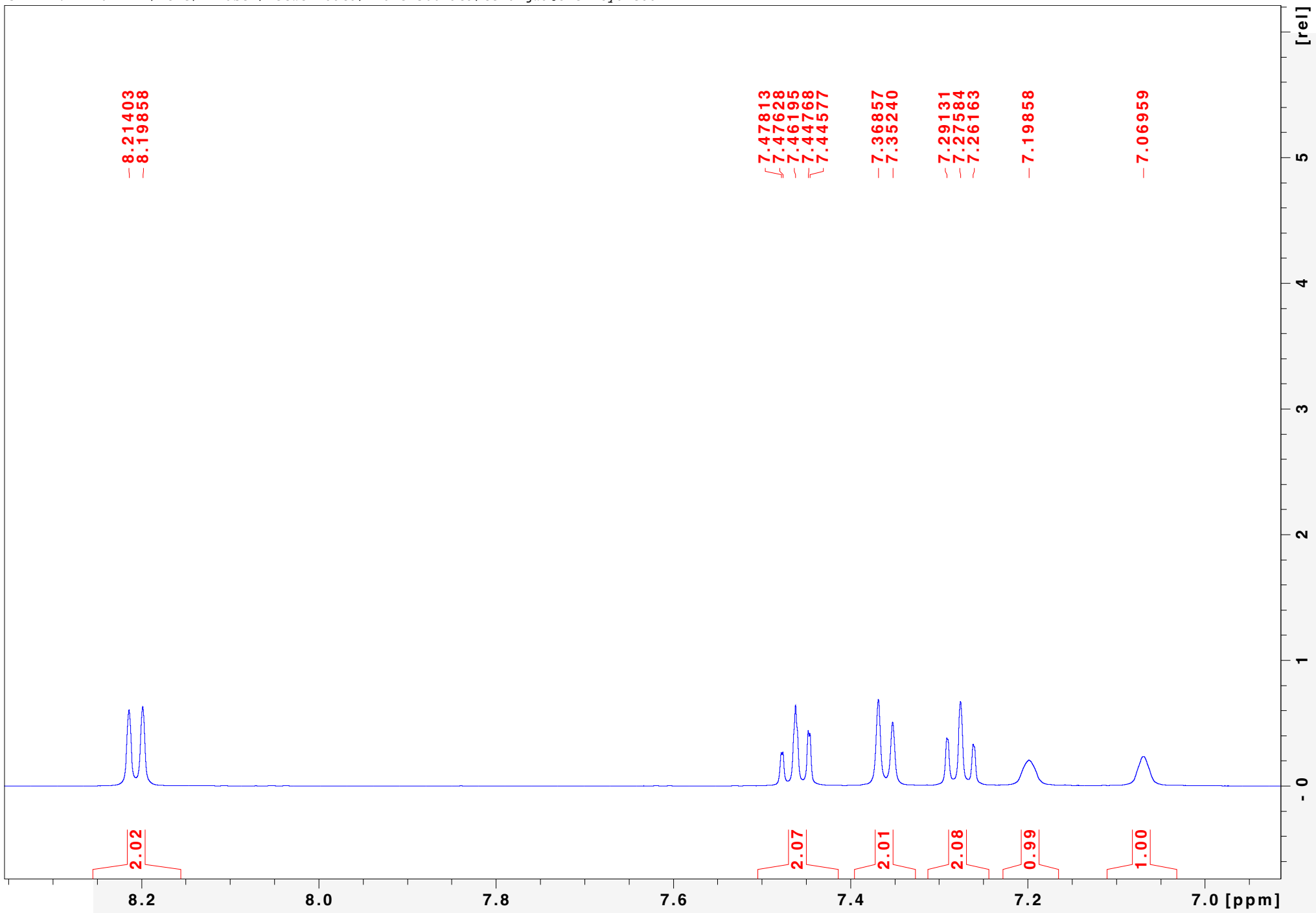
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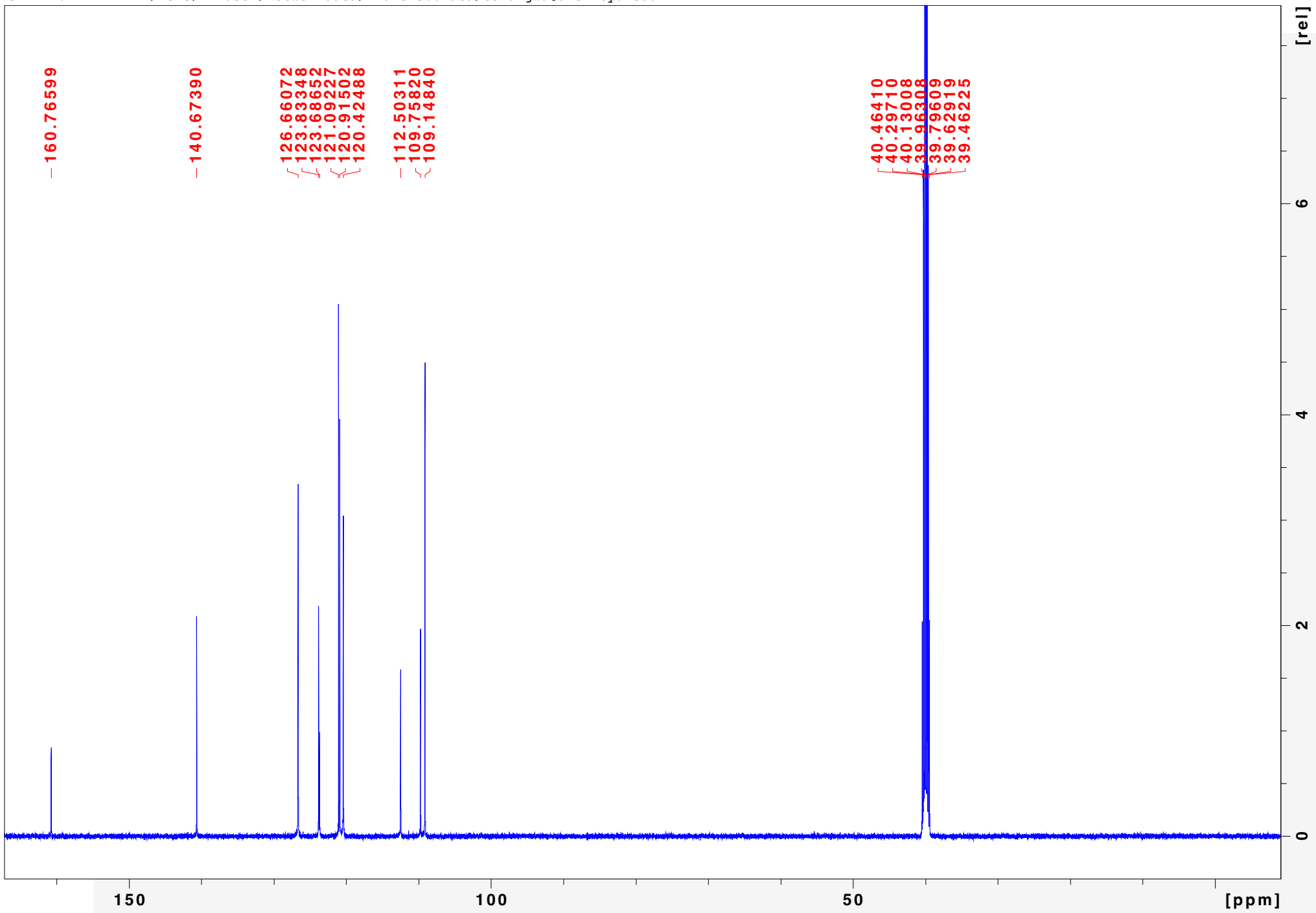
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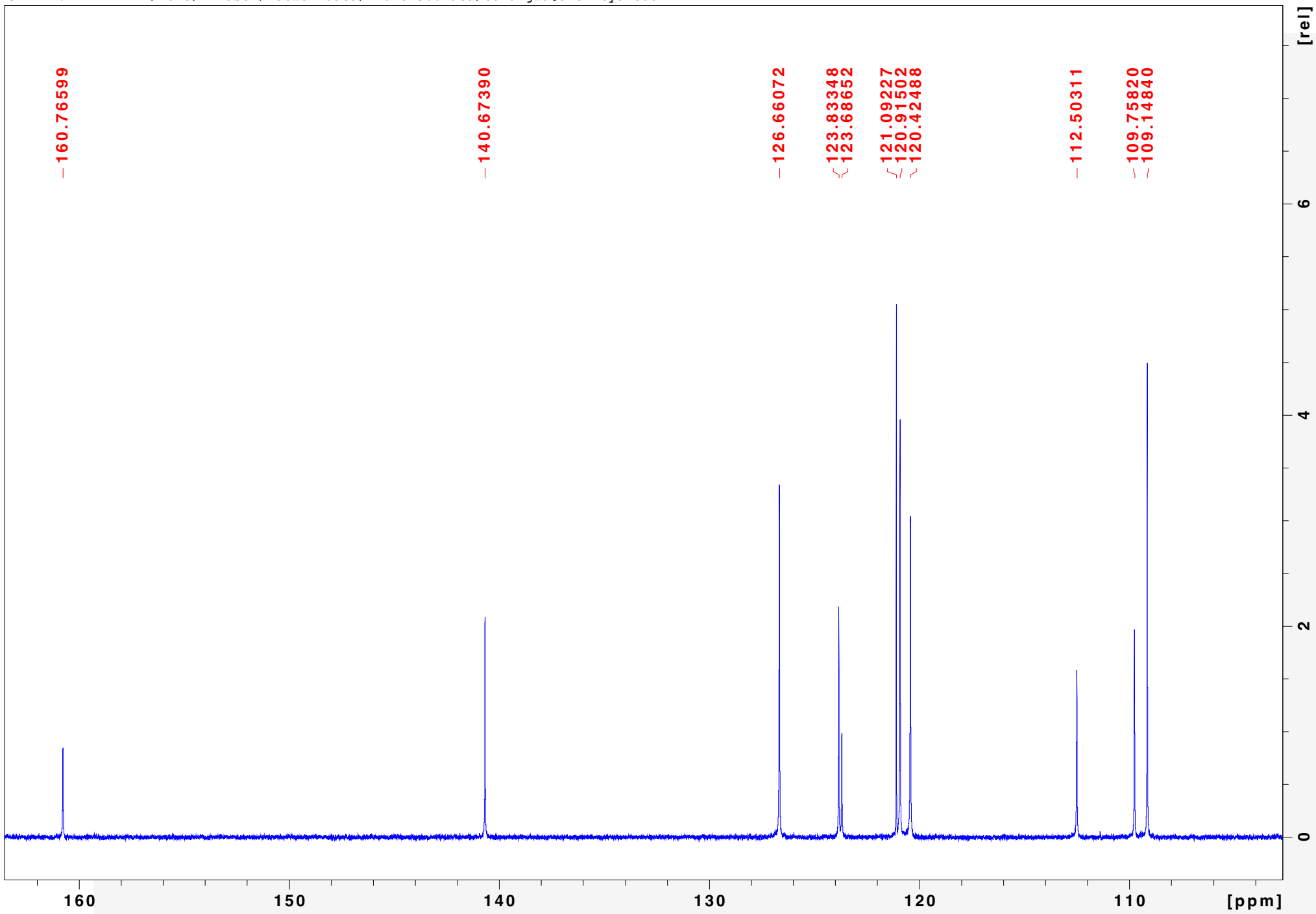
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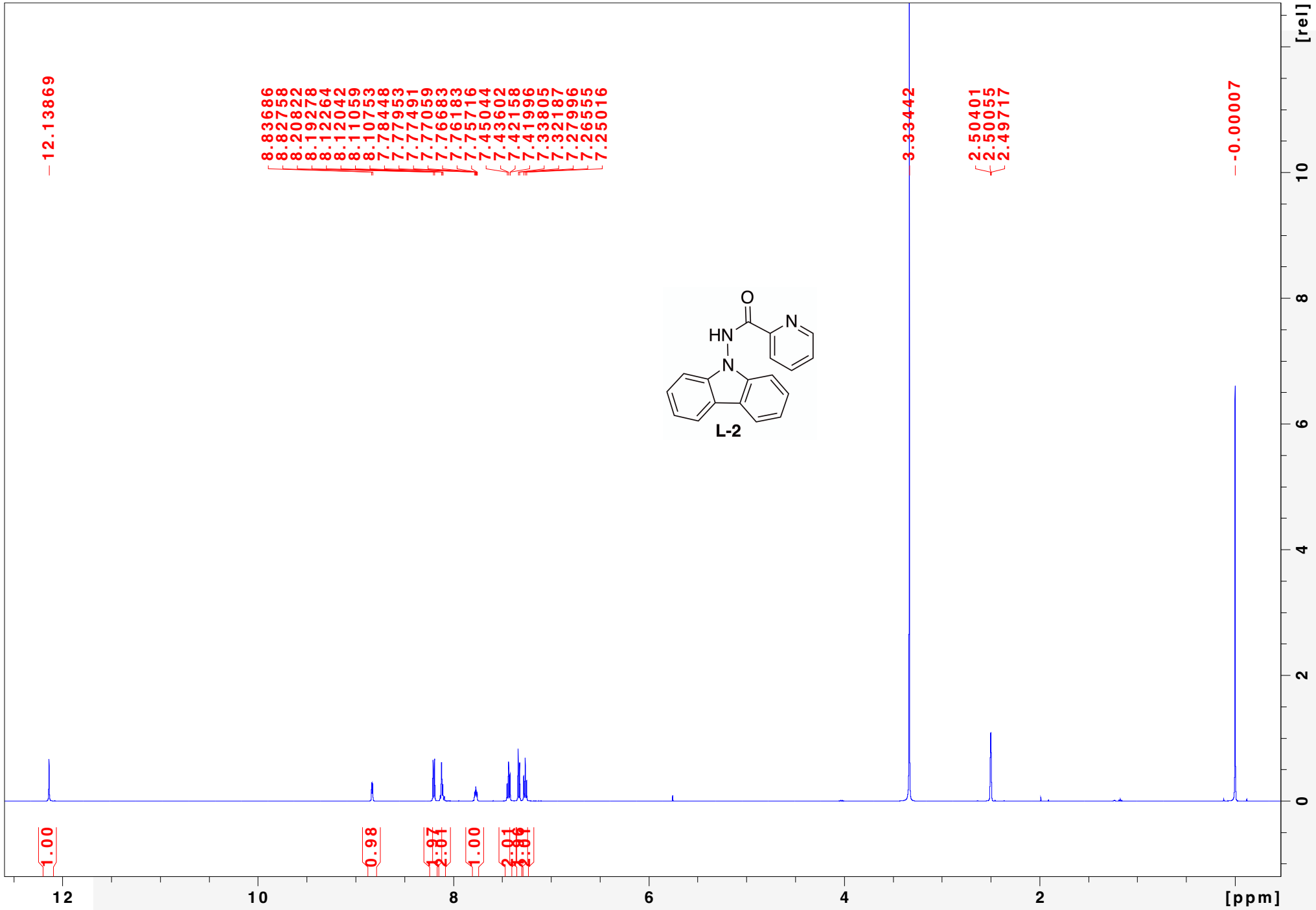
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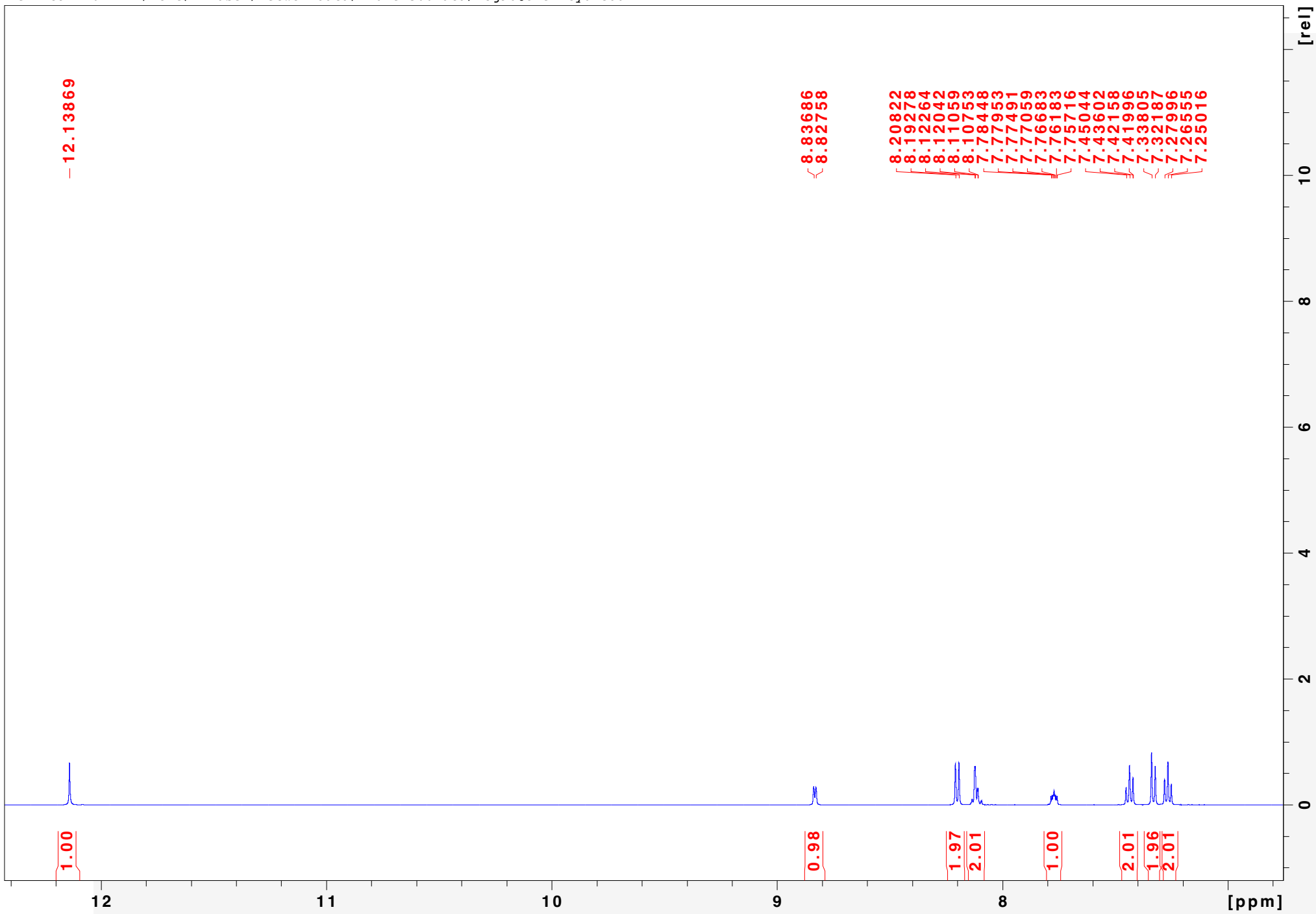


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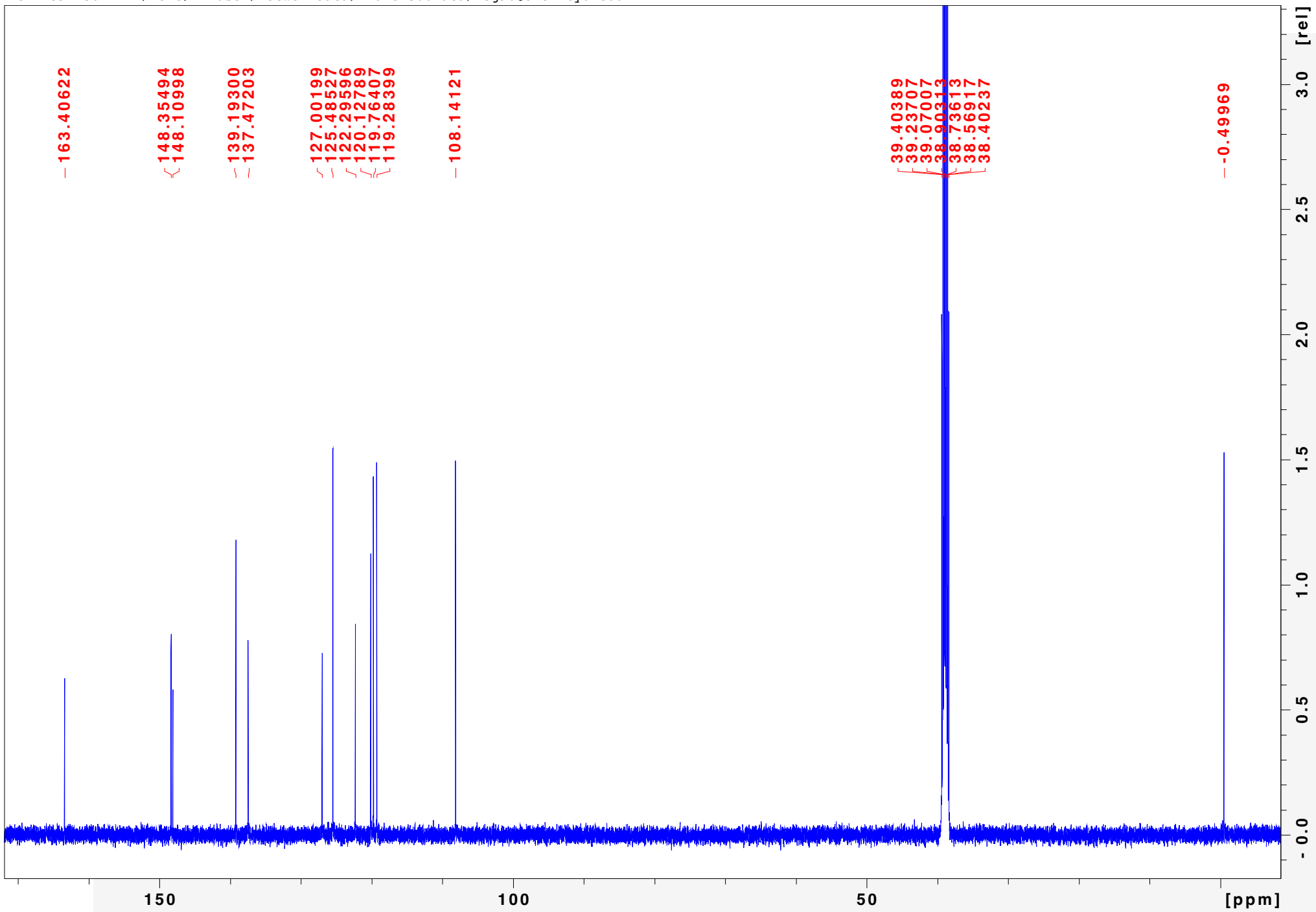


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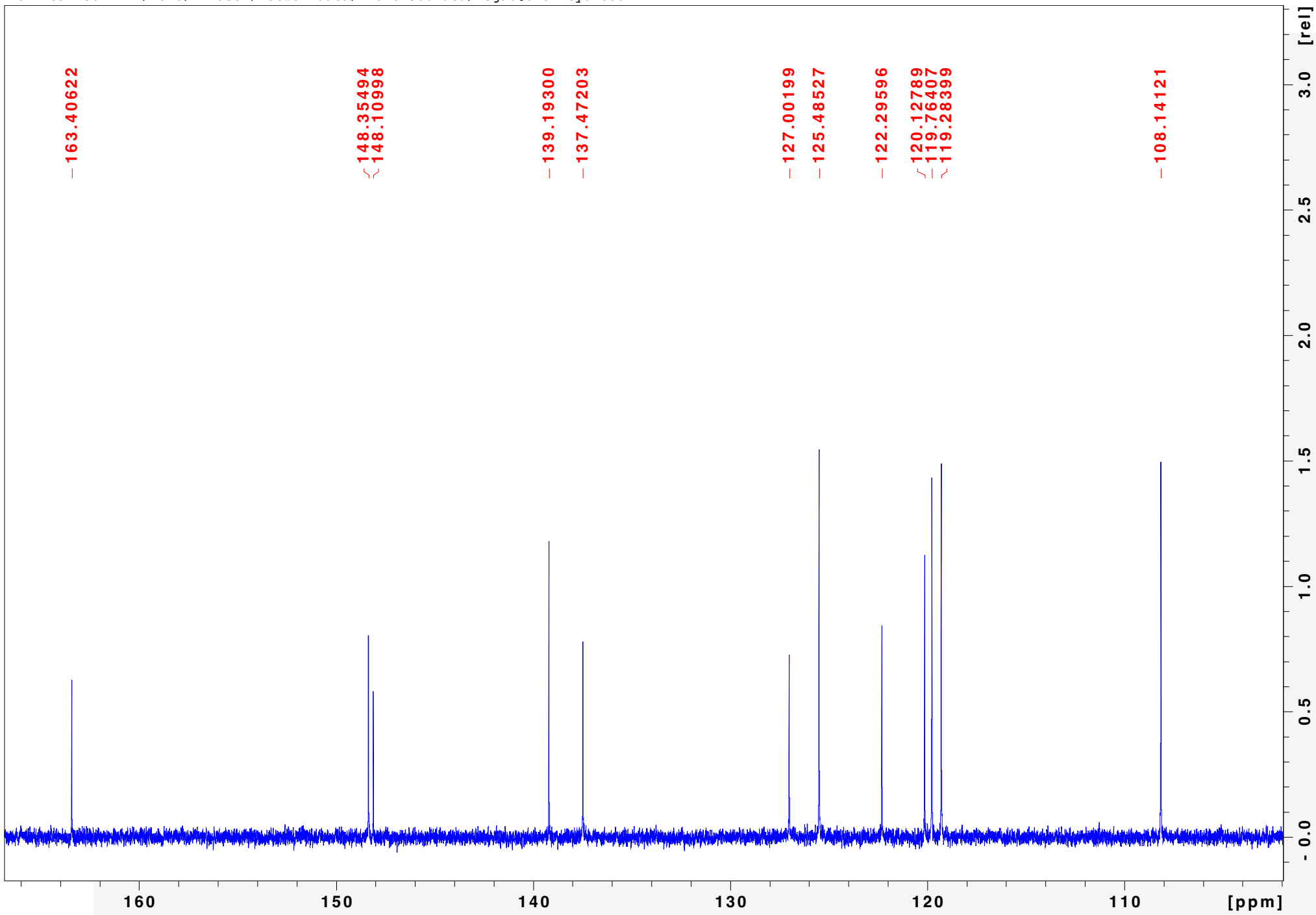



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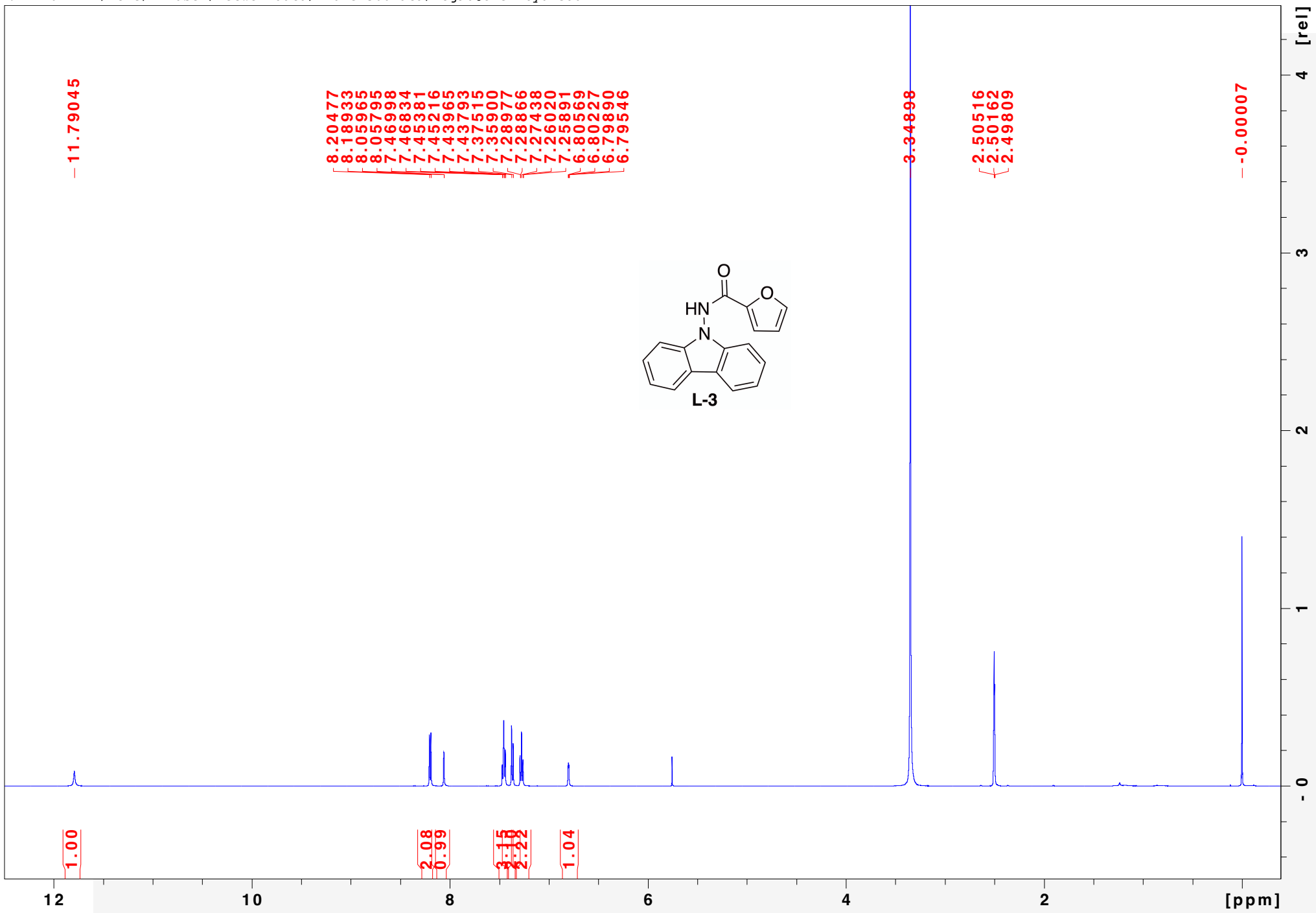
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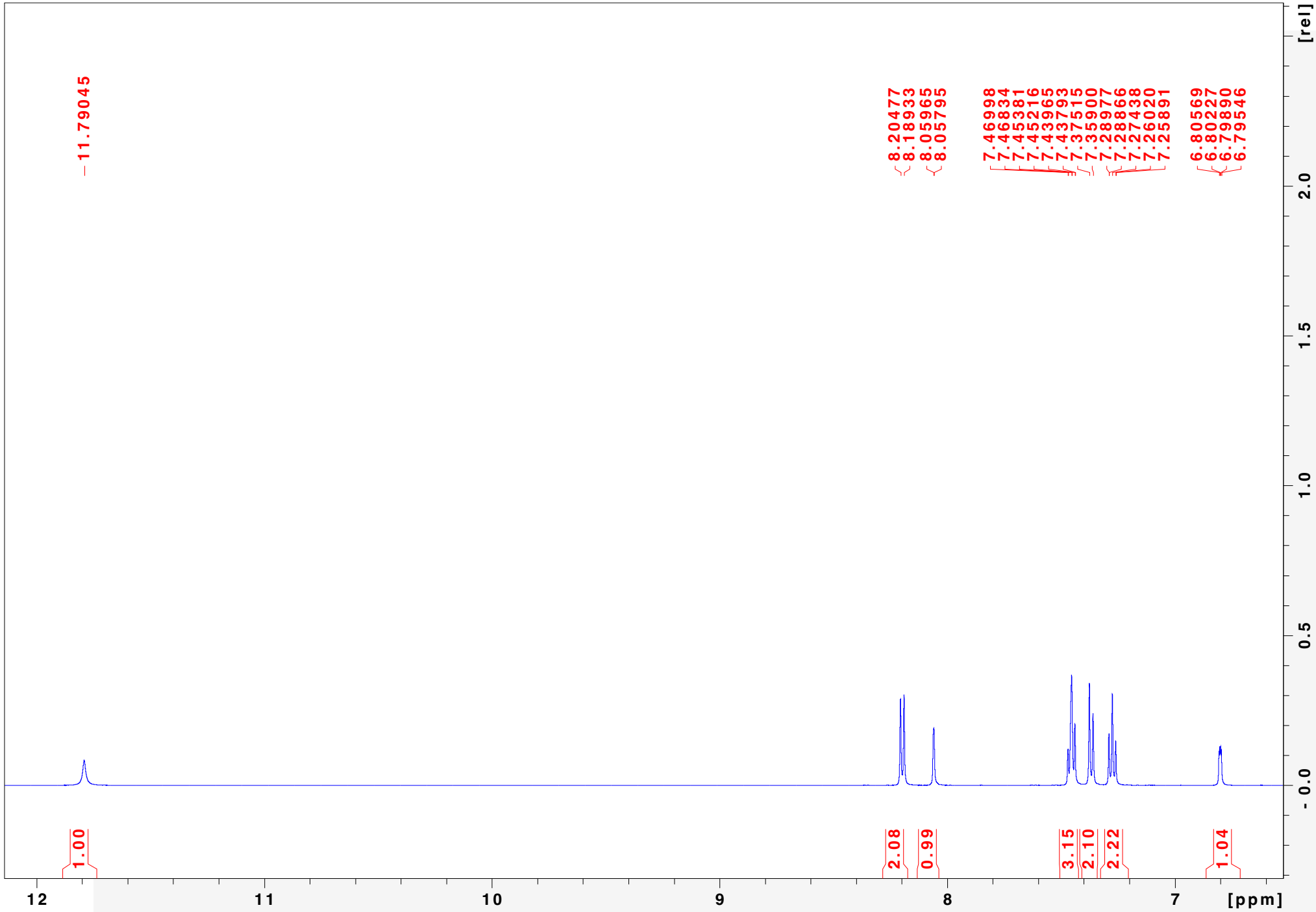
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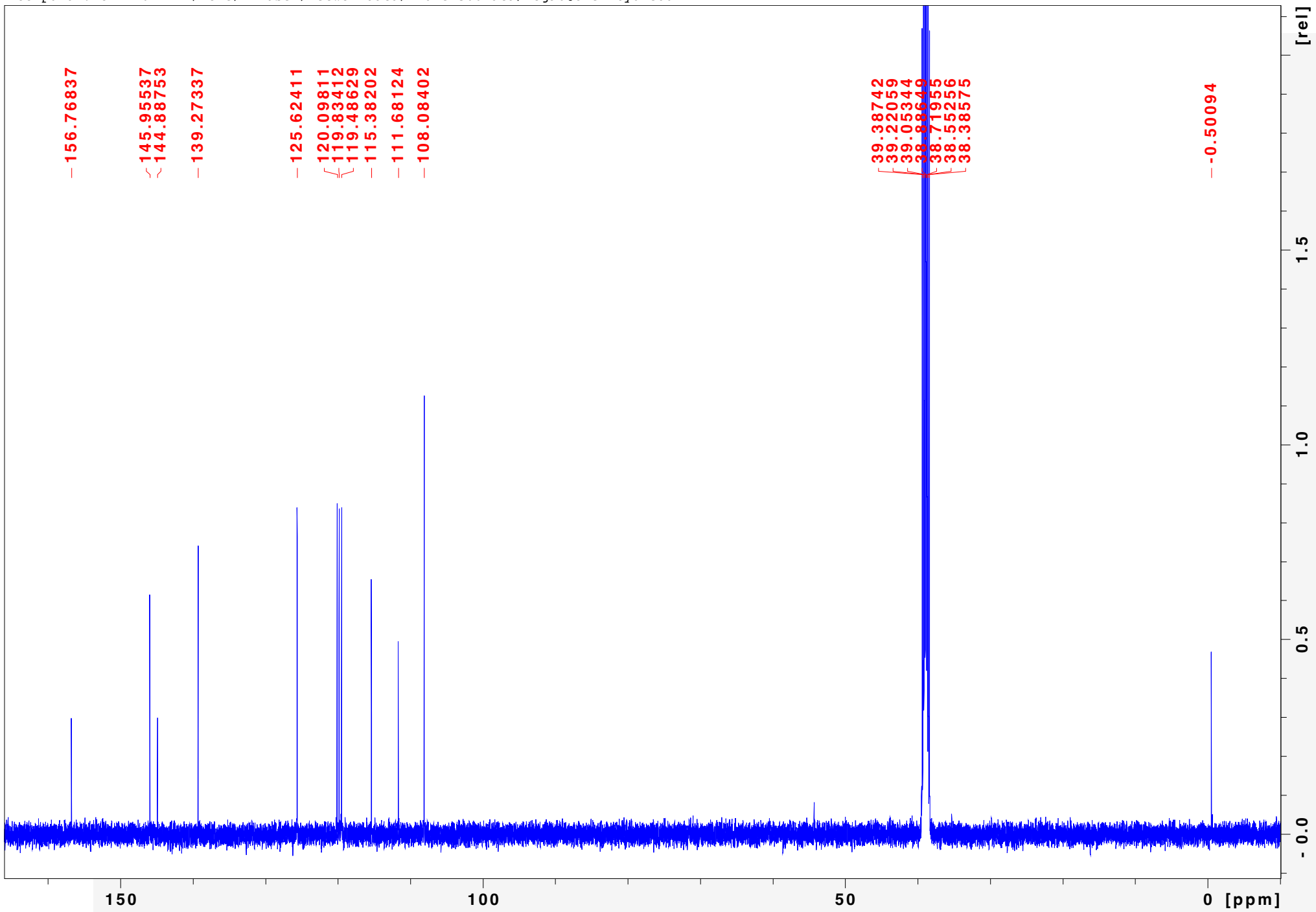
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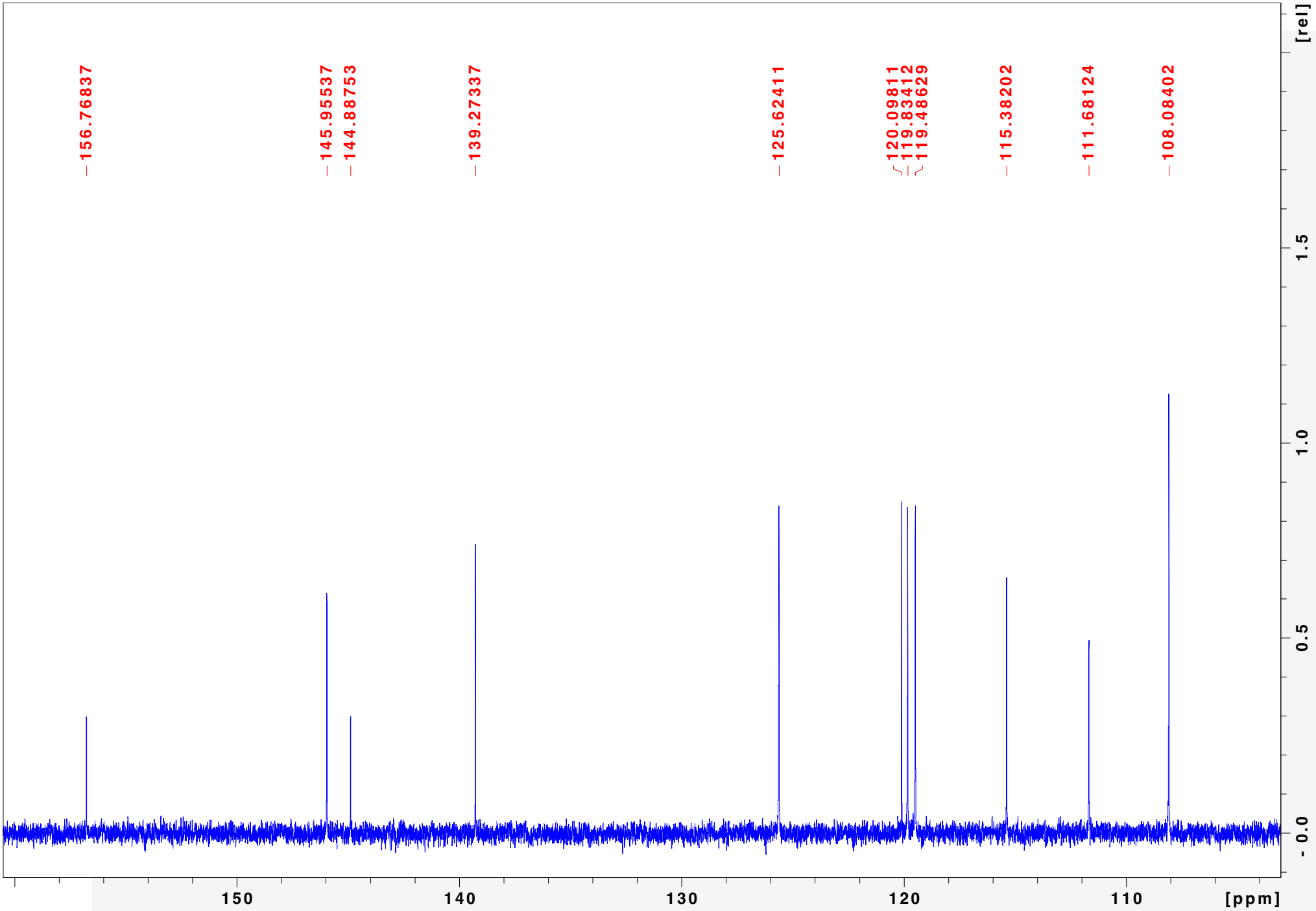
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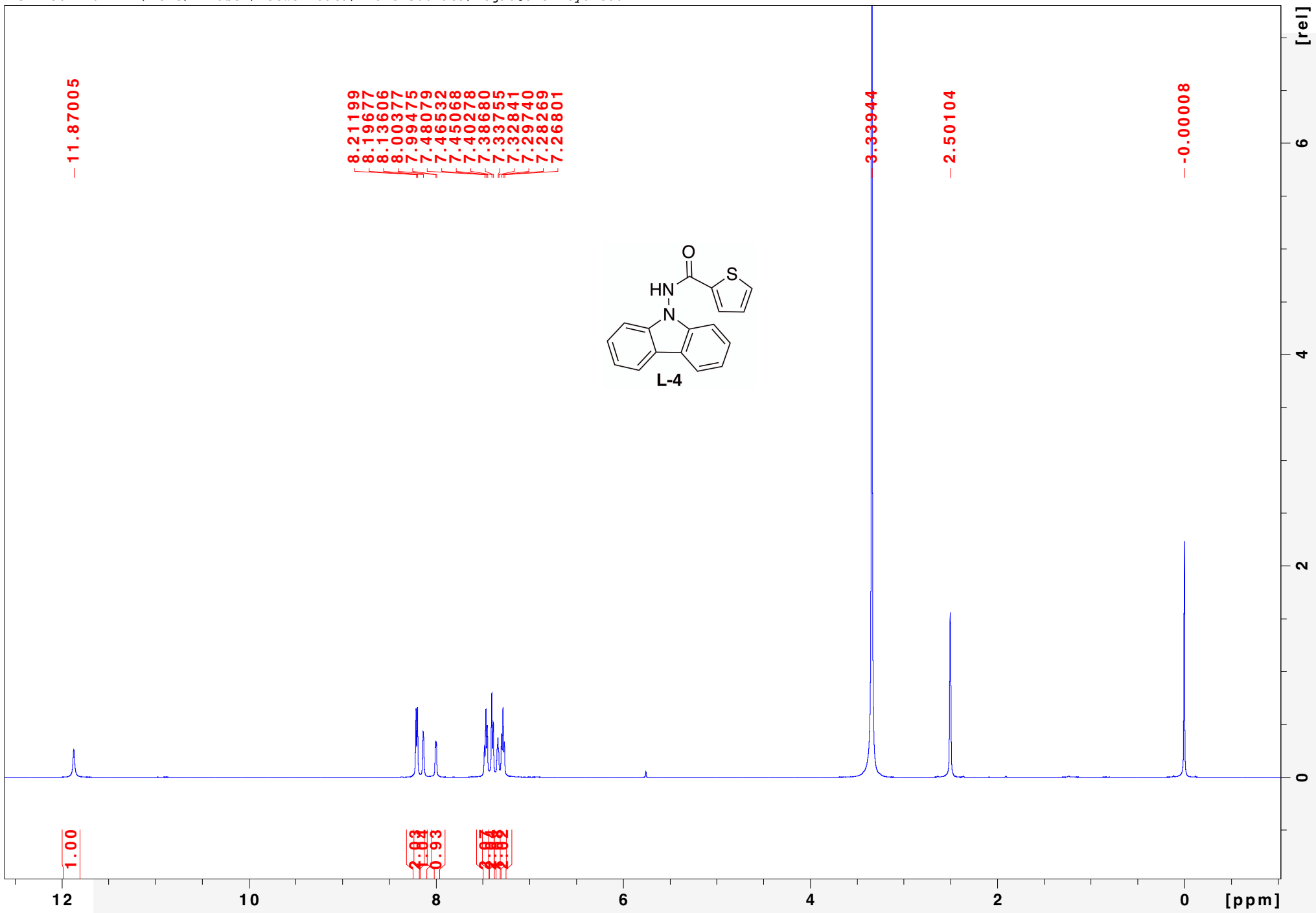
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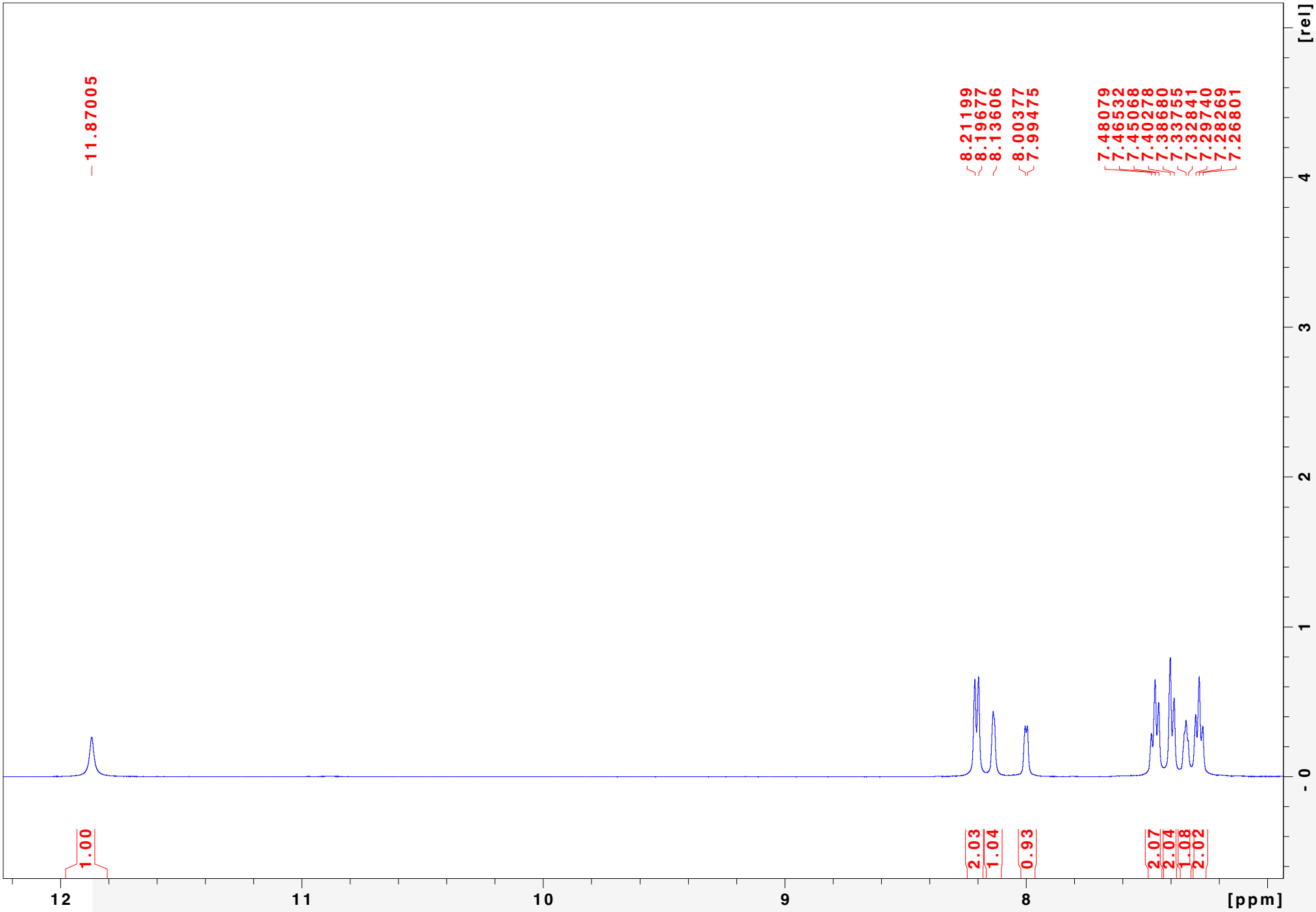
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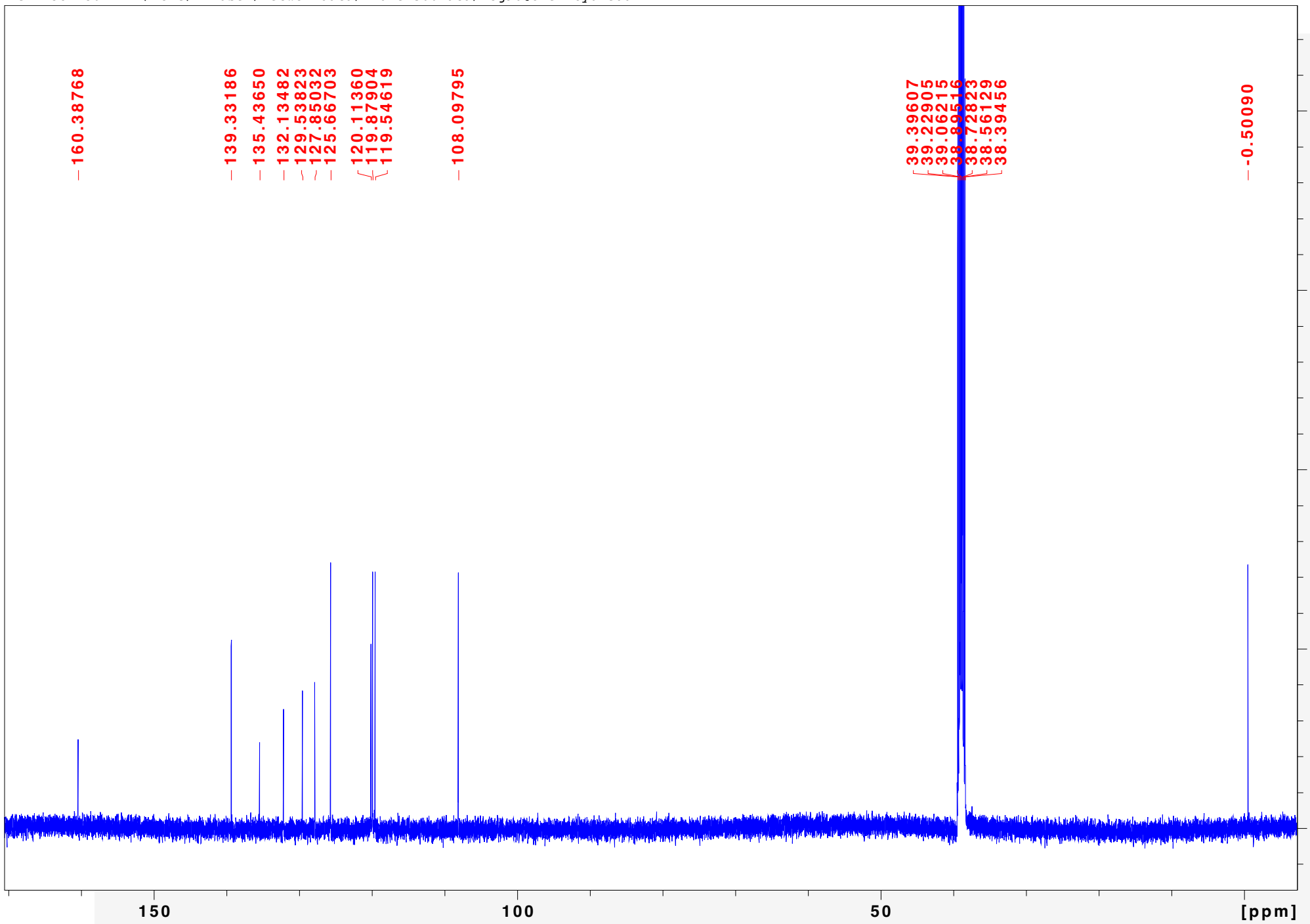


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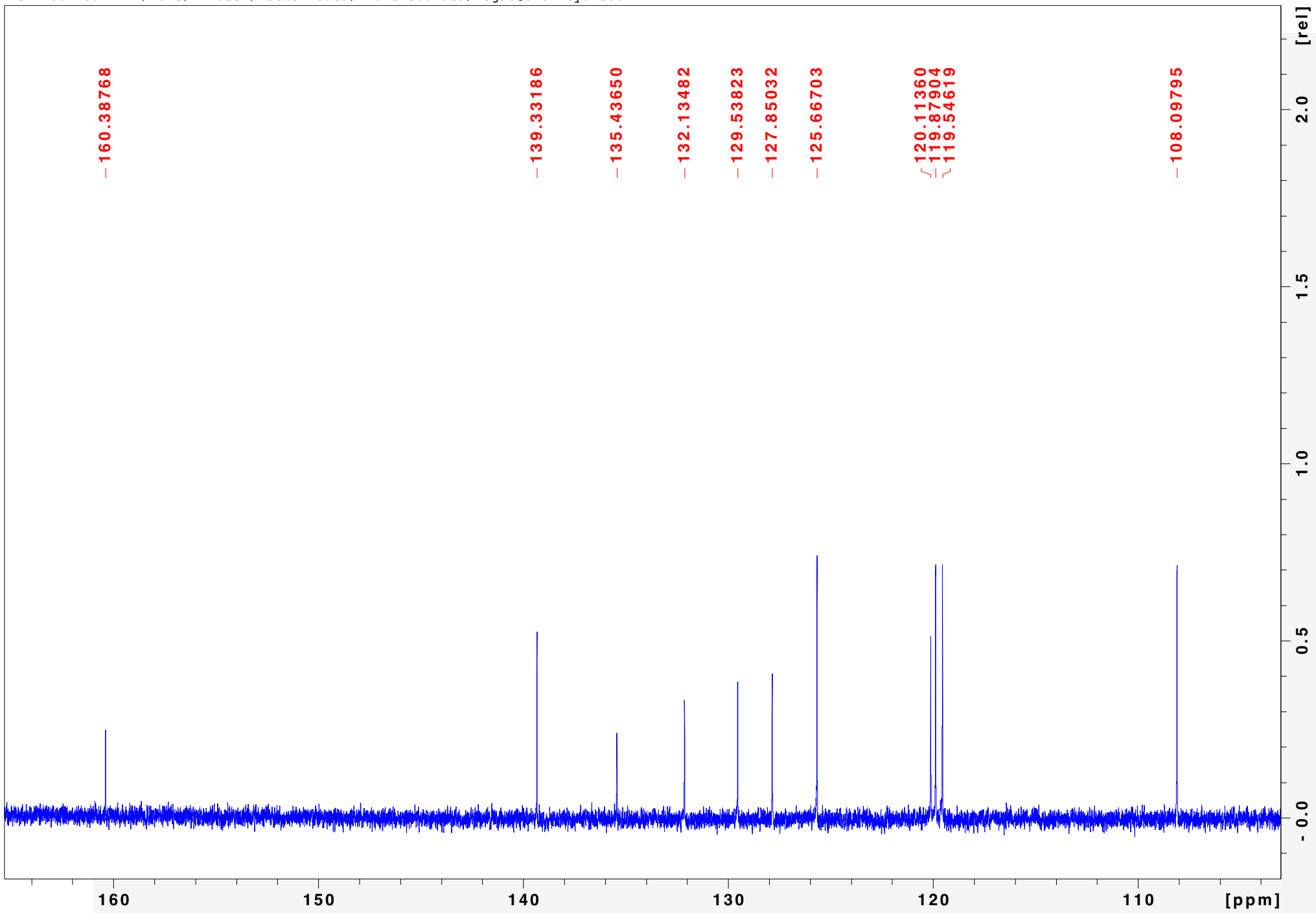


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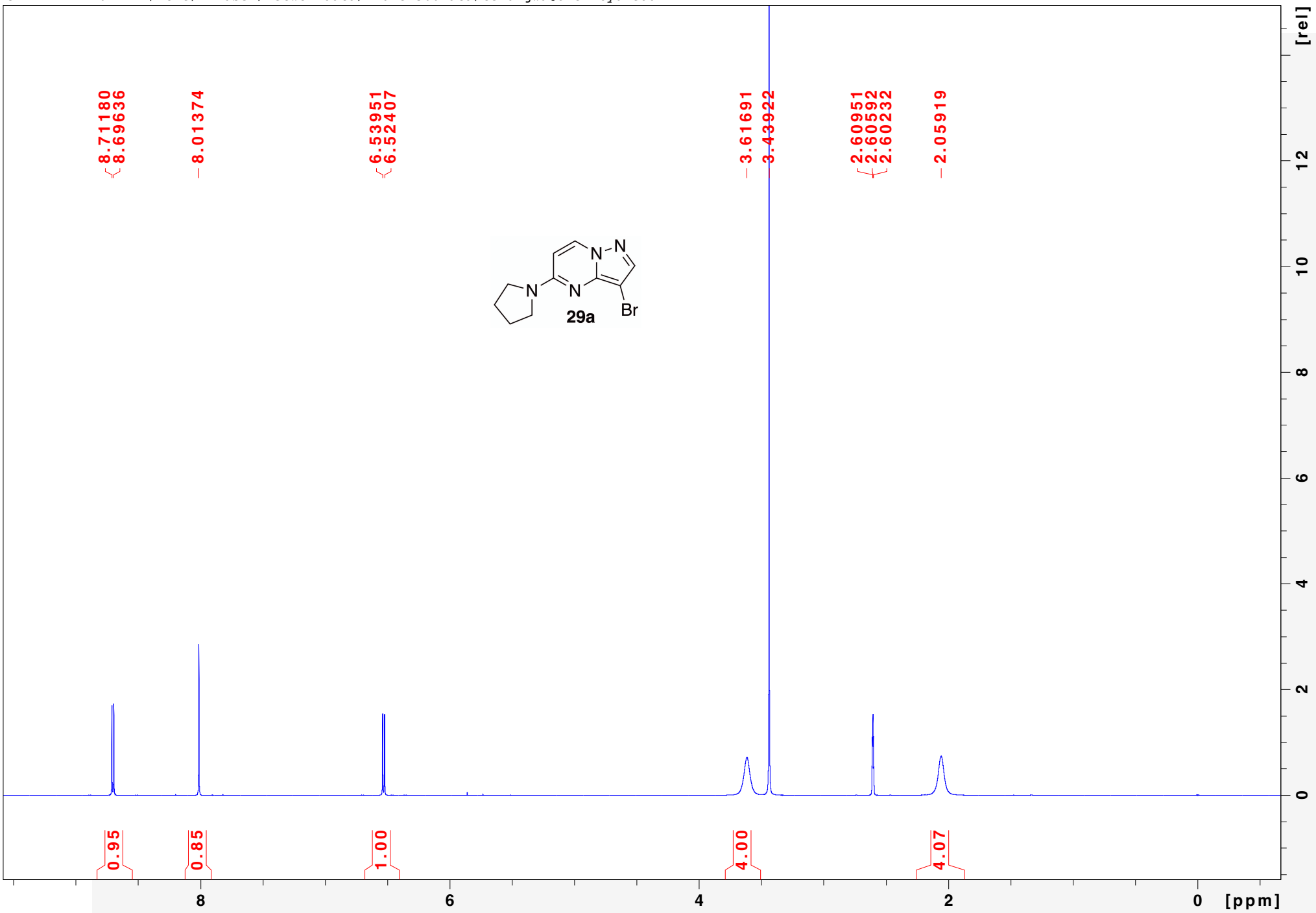



LG-I-38 30 1 /home/nmruser/networkdata/Bruker500Data/log96@chem.byu.edu
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132.13482
129.53823
127.85032
125.66703
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119.87904
119.54619
108.09795
39.39607
39.22905
39.06215
38.89516
38.72823
38.56129
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150
100
50
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[rel]
2.0
1.5
1.0
0.5
- 0.0

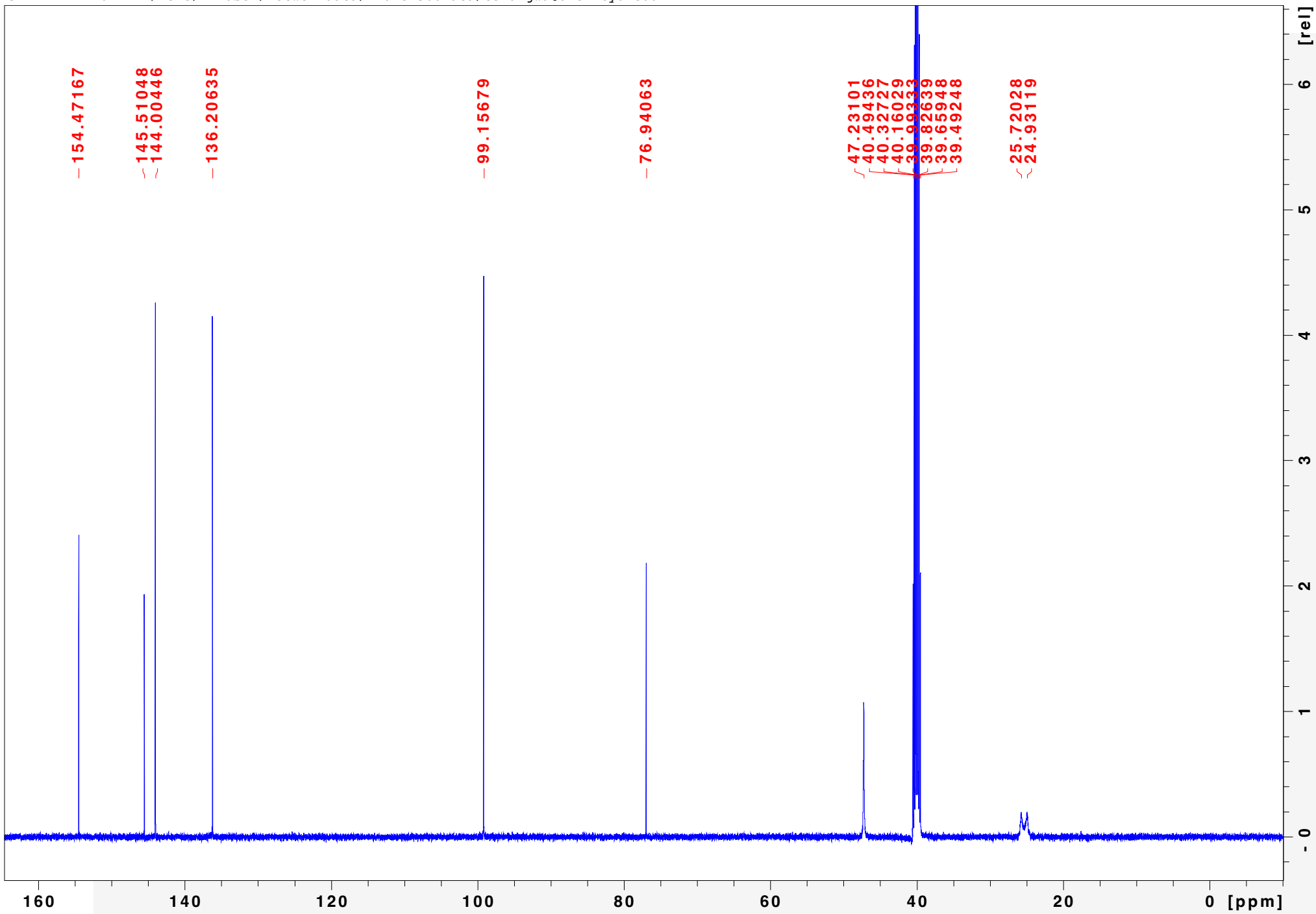
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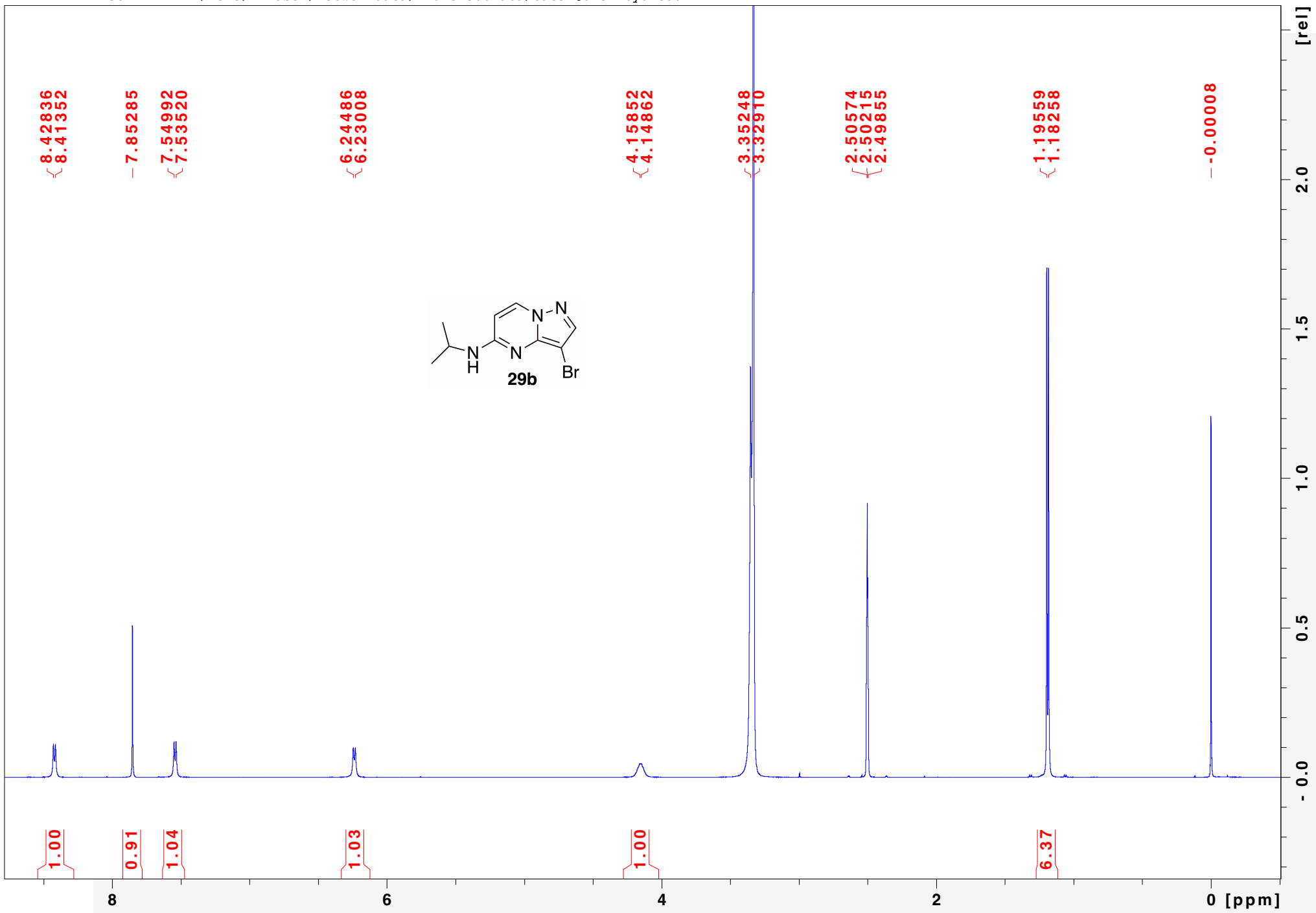
JI-II-44 10 1 /home/nmruser/networkdata/Bruker500Data/terungwa@chem.byu.edu



JI-II-44 20 1 /home/nmruser/networkdata/Bruker500Data/terungwa@chem.byu.edu

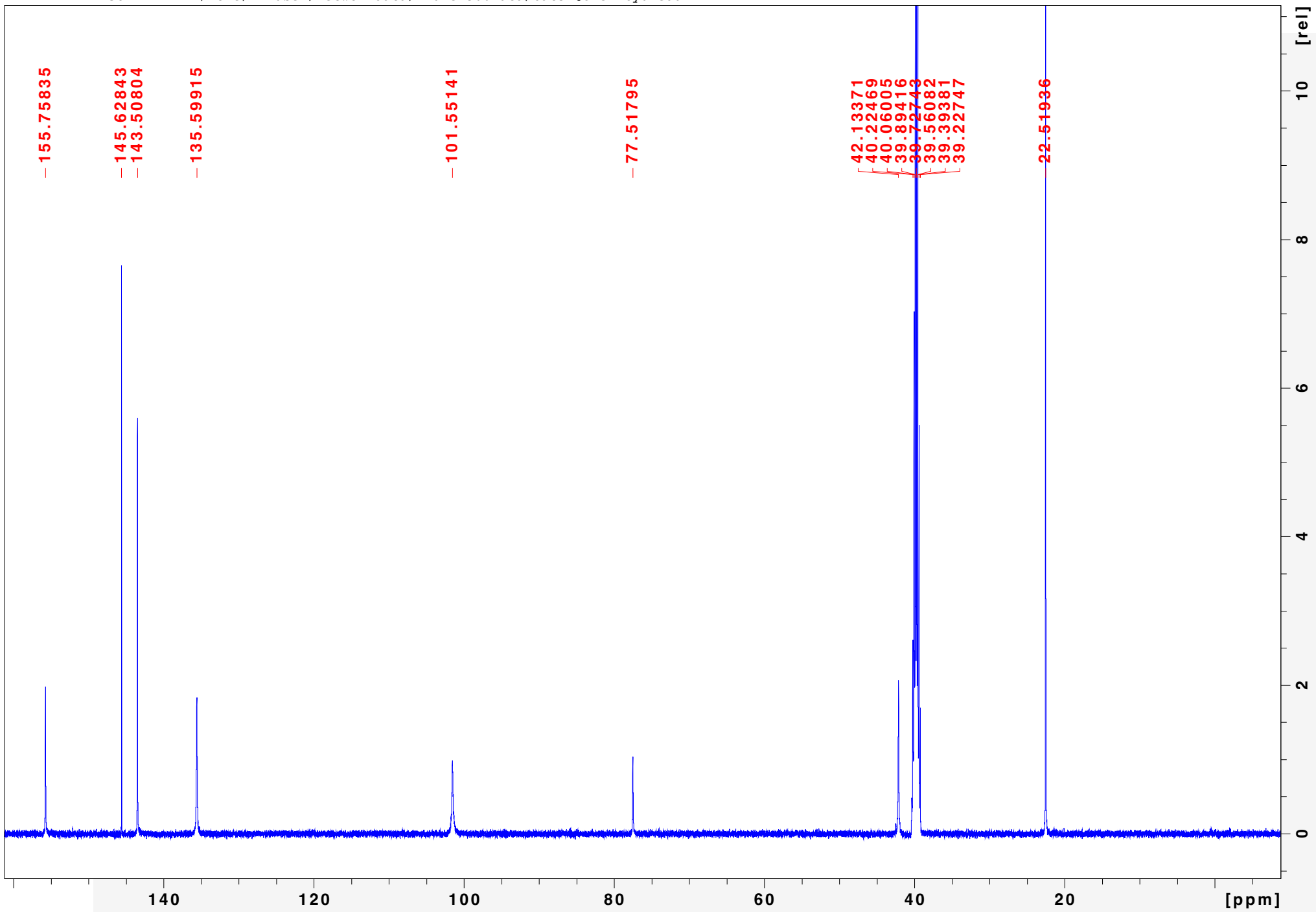


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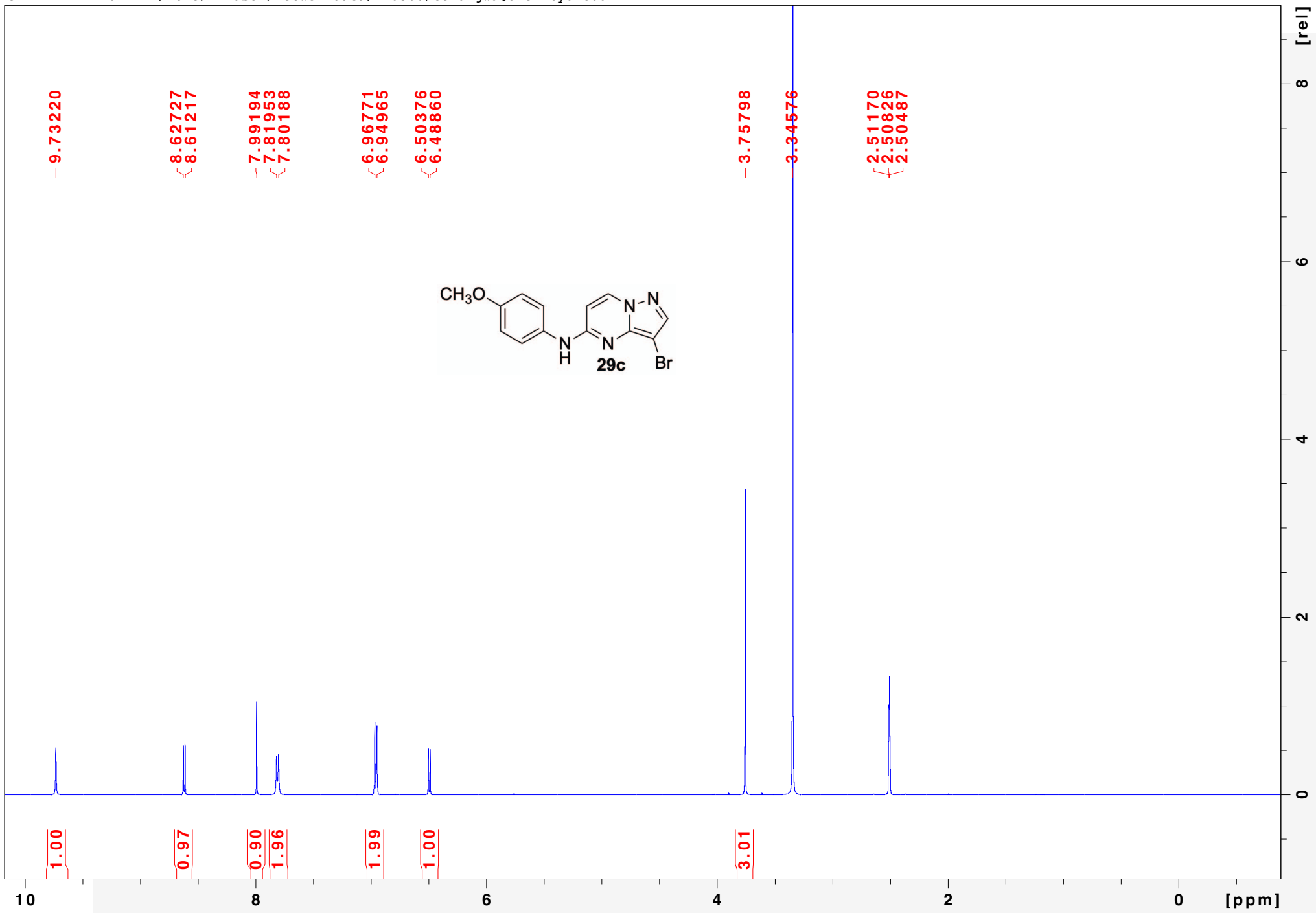


29b

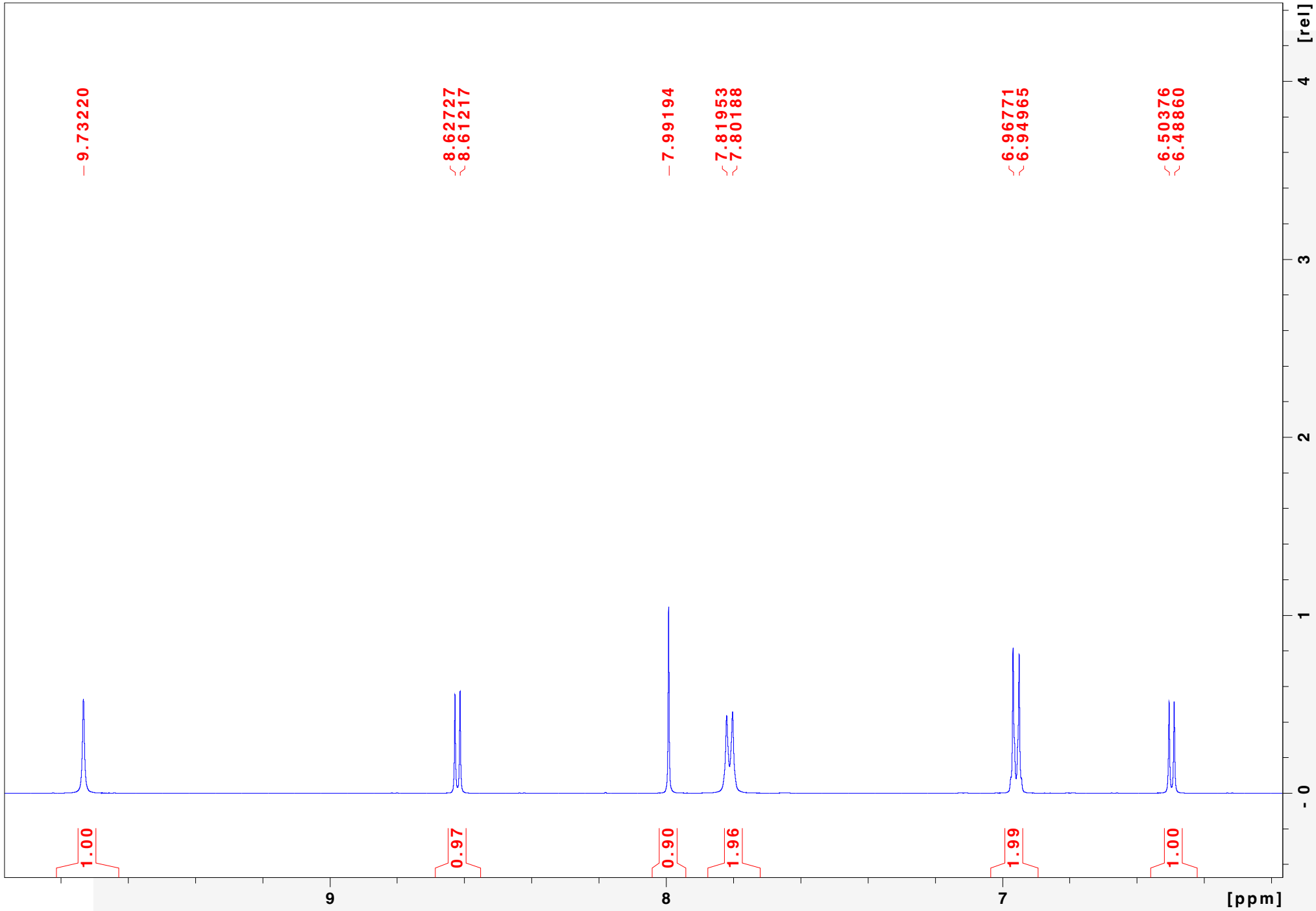
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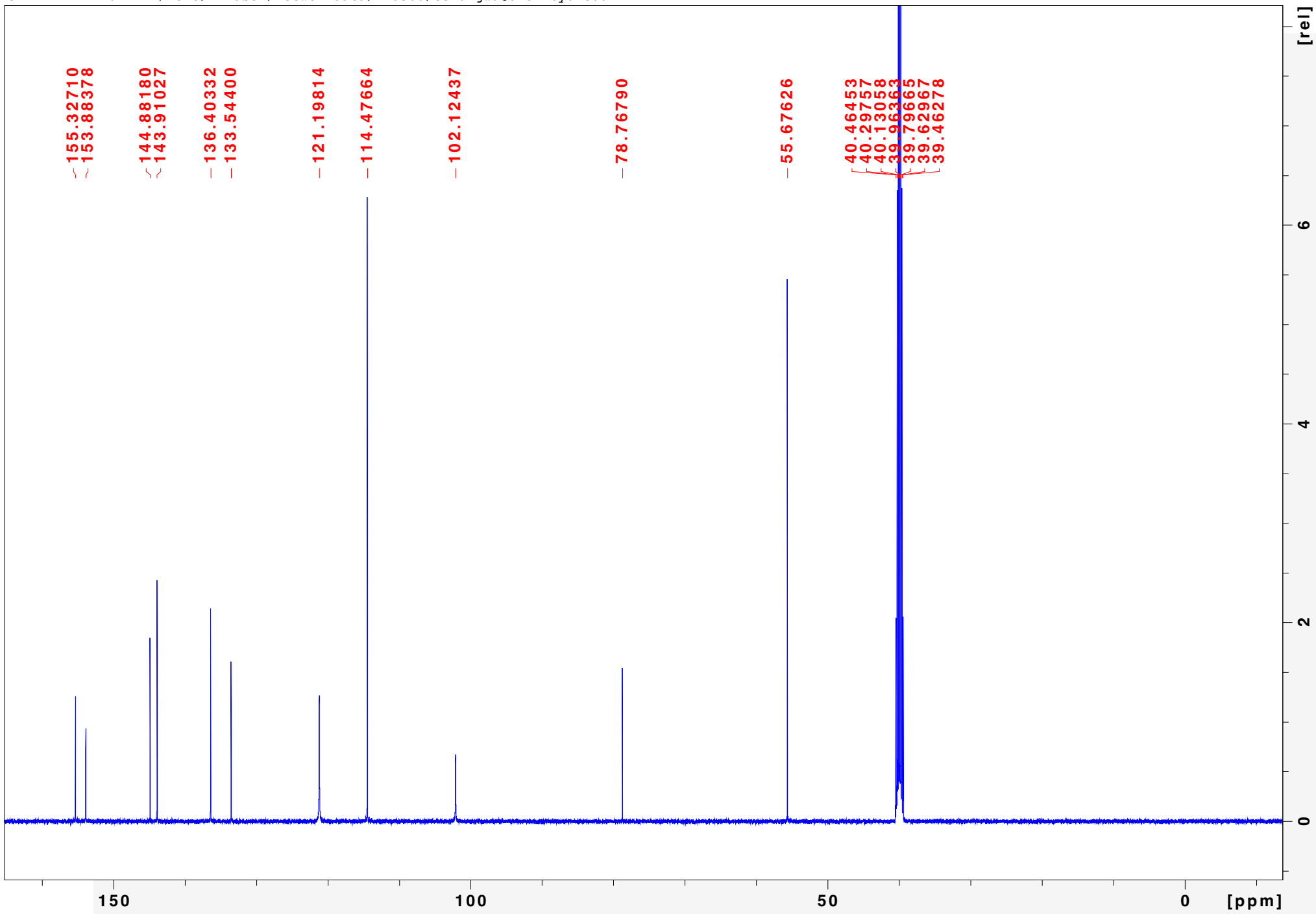
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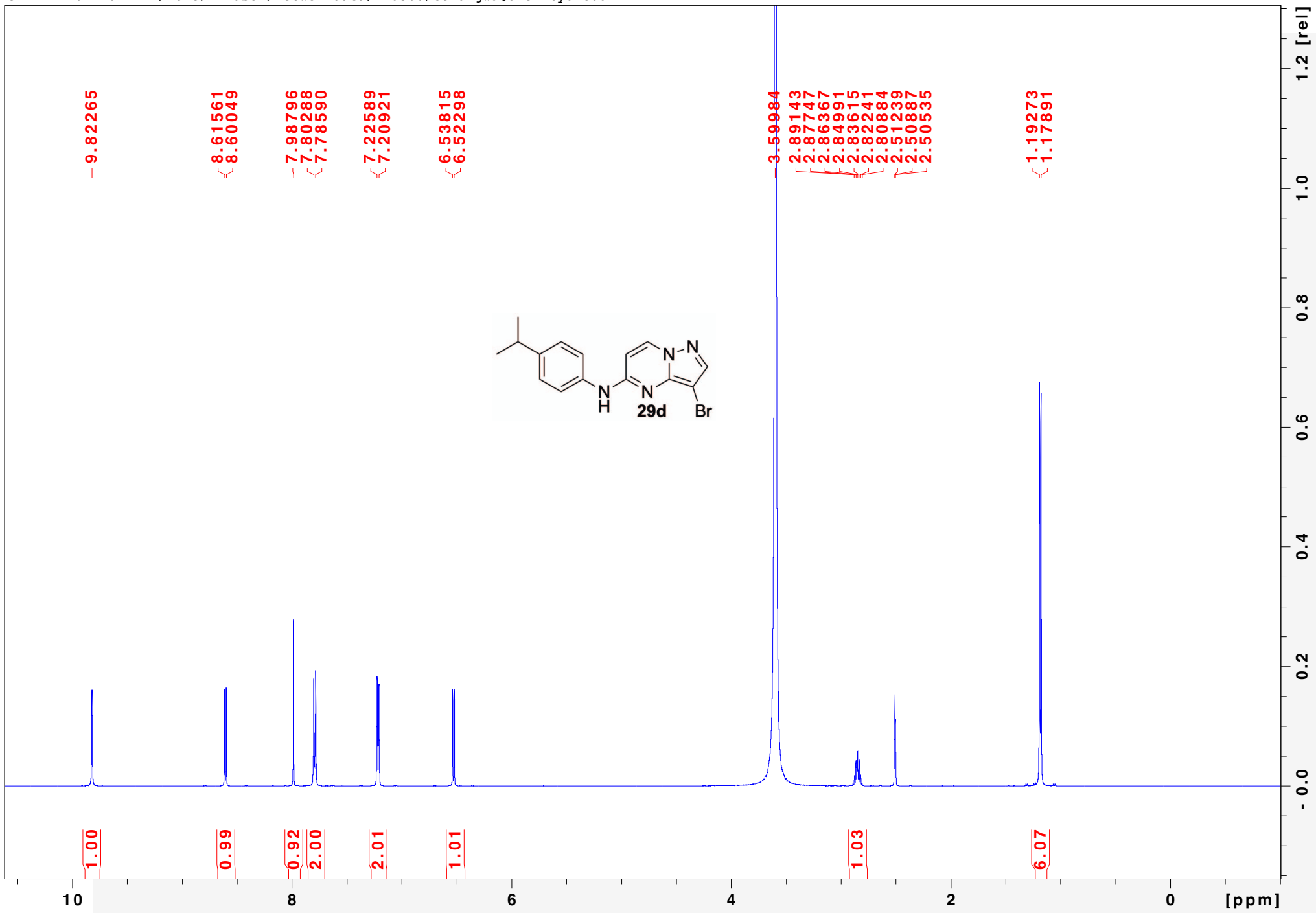
JI-III-41 10 1 /home/nmruser/networkdata/Bru500/terungwa@chem.byu.edu



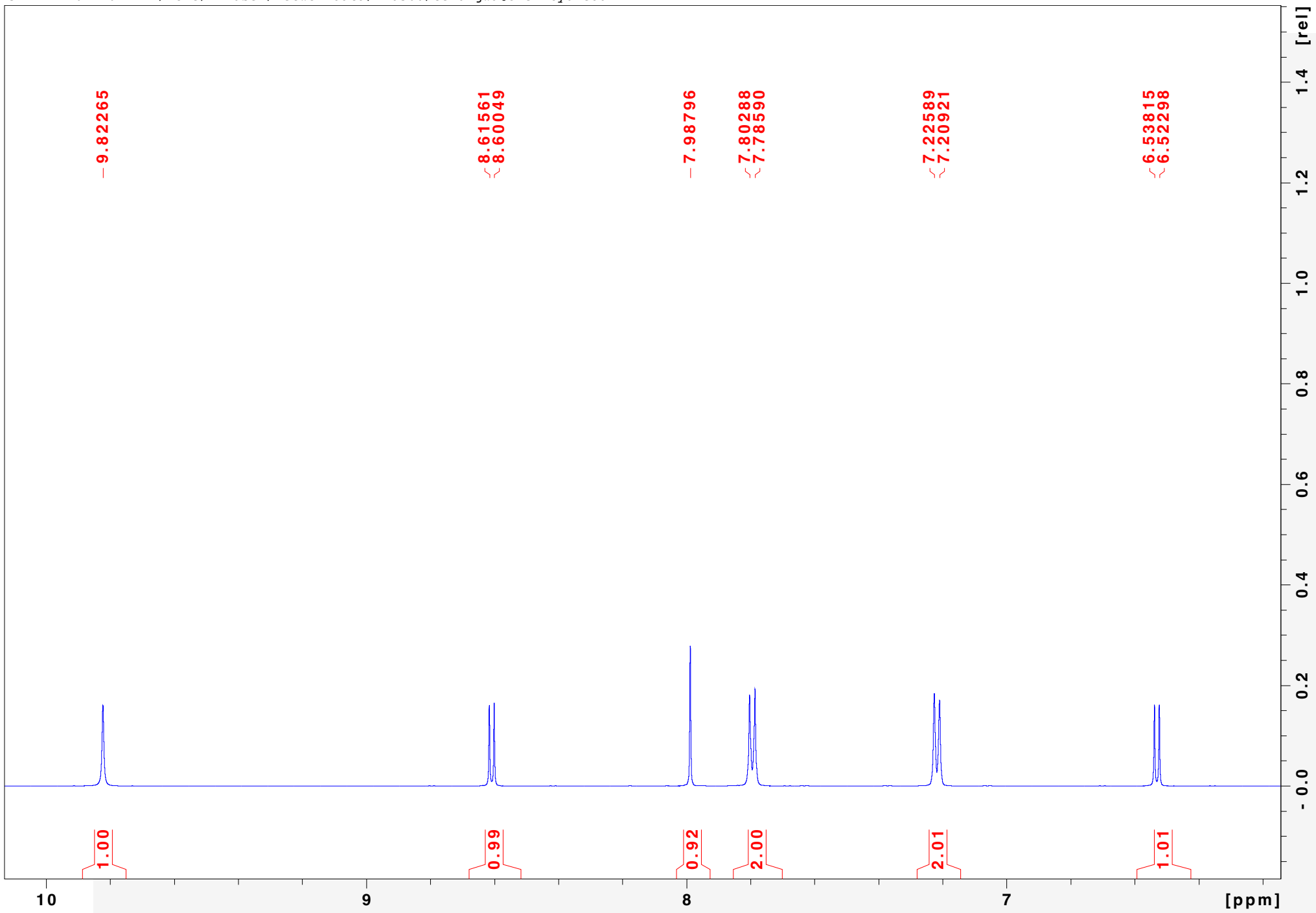
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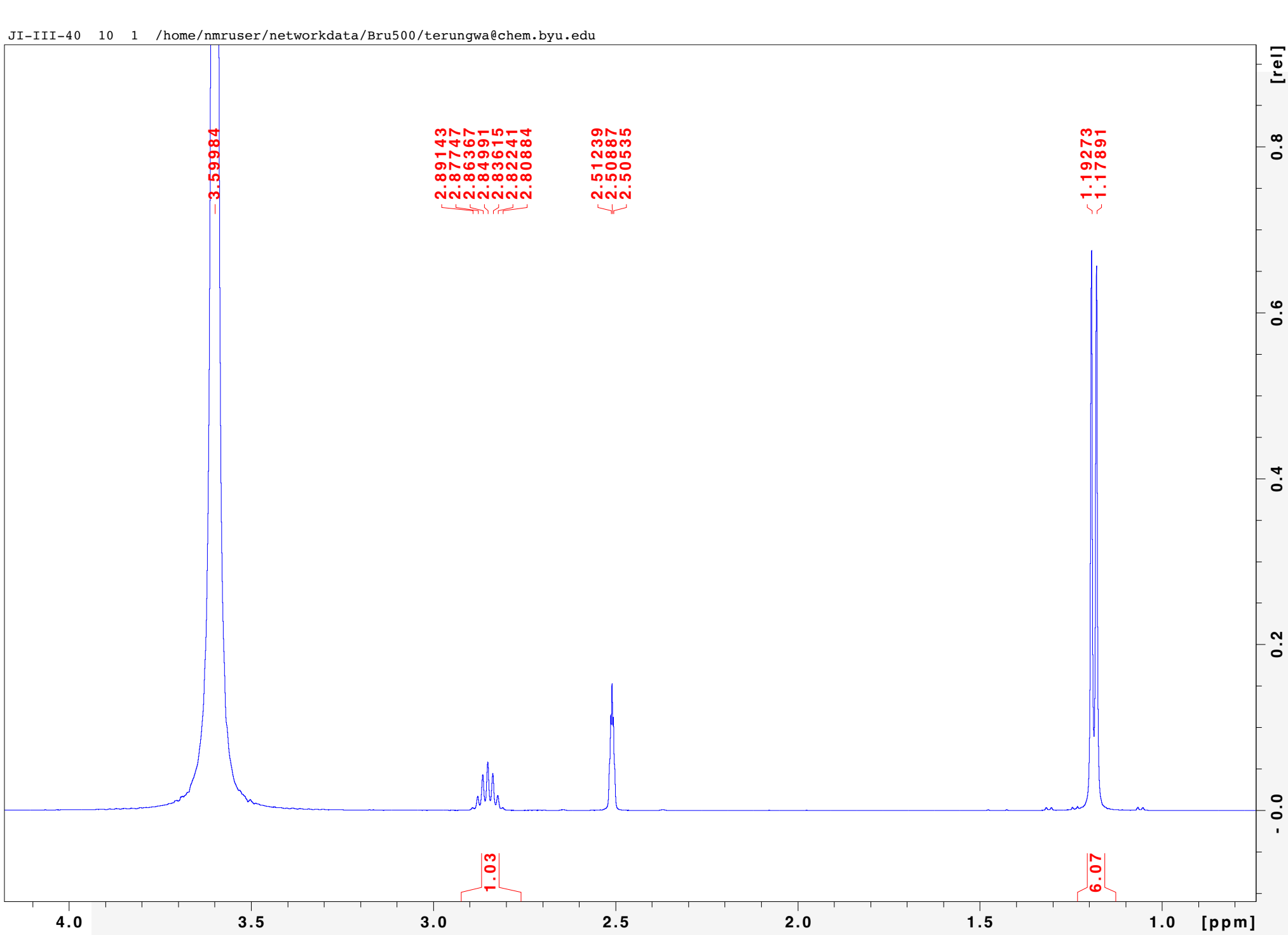


JI-III-40 10 1 /home/nmruser/networkdata/Bru500/terungwa@chem.byu.edu

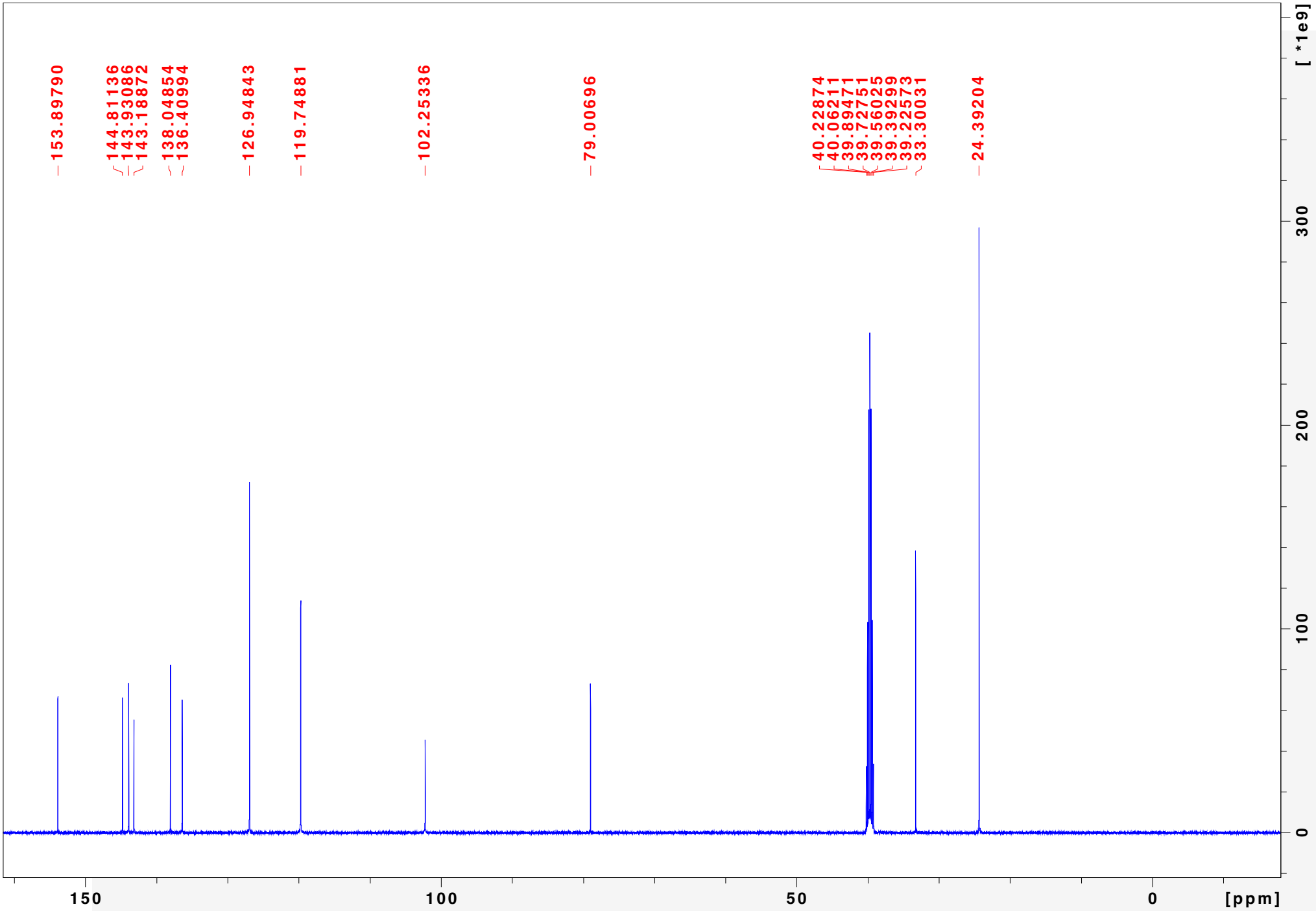


JI-III-40 10 1 /home/nmruser/networkdata/Bru500/terungwa@chem.byu.edu

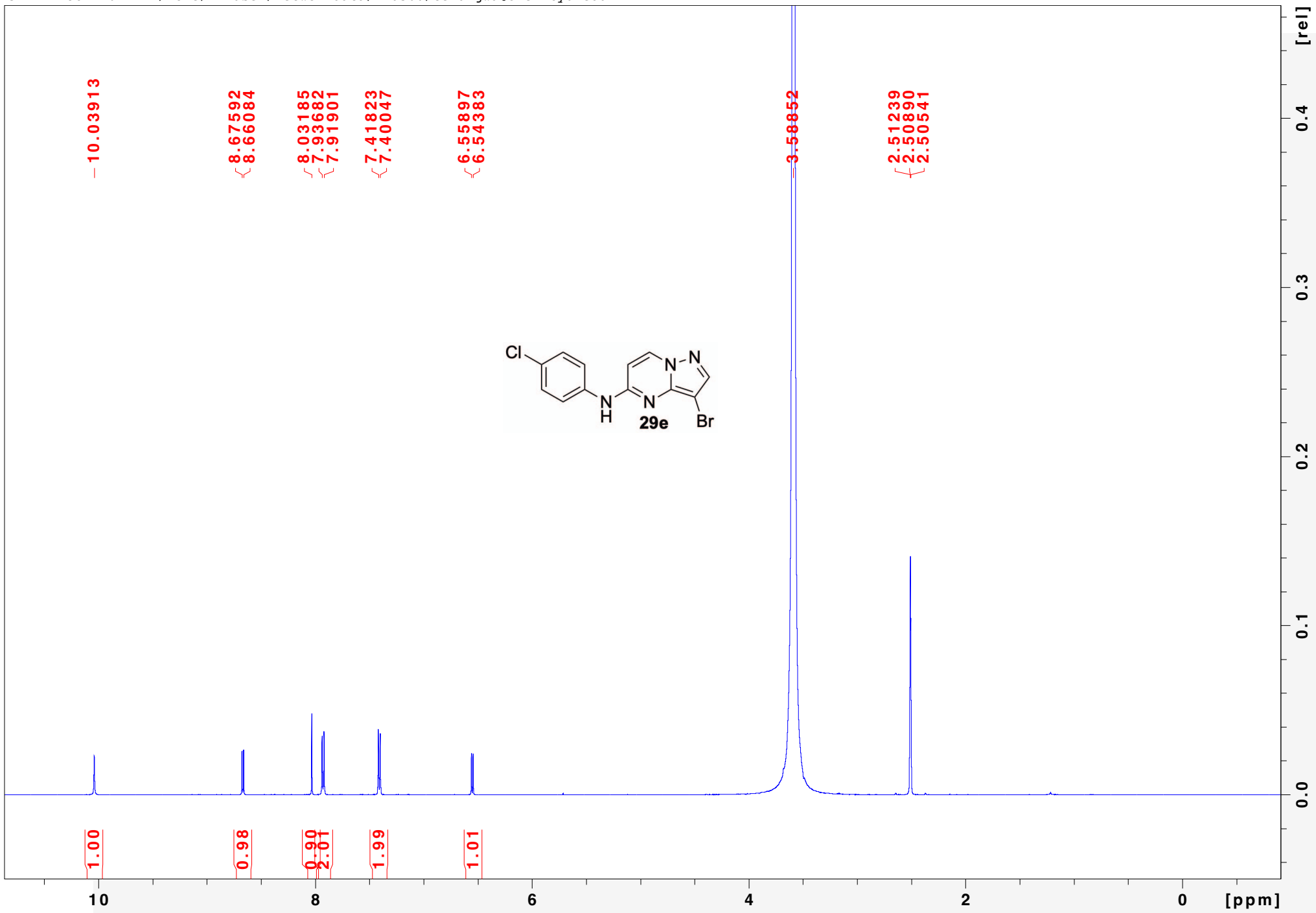



JI-III-40 10 1 /home/nmruser/networkdata/Bru500/terungwa@chem.byu.edu
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2.86367
2.84991
2.83615
2.82241
2.80884
2.51239
2.50887
2.50535
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1.17891
1.03
6.07
4.0
3.5
3.0
2.5
2.0
1.5
1.0
[ppm]
[rel]
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0.6
0.4
0.2
- 0.0

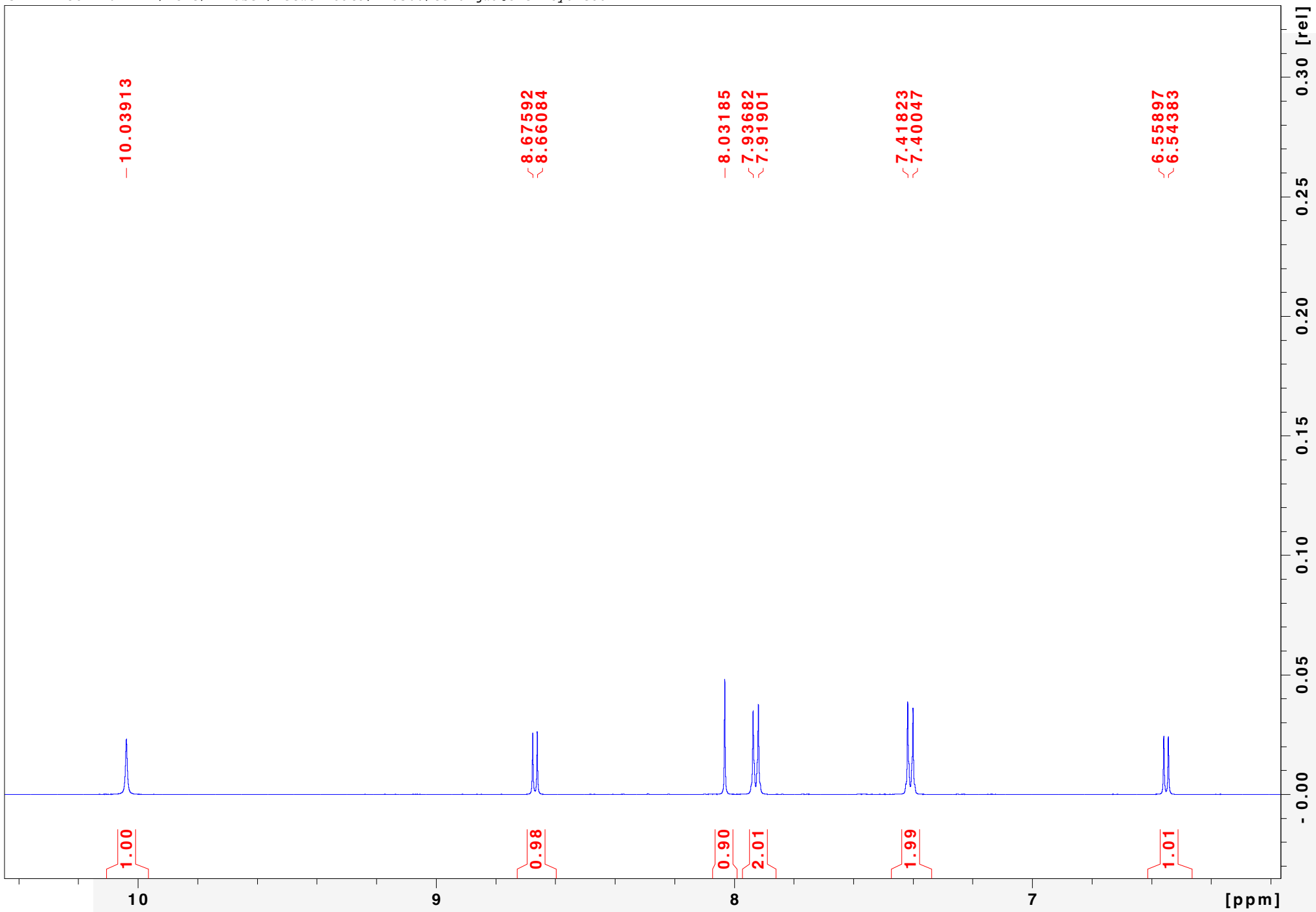
JI-III-40 20 1 /home/nmruser/networkdata/Bru500/terungwa@chem.byu.edu



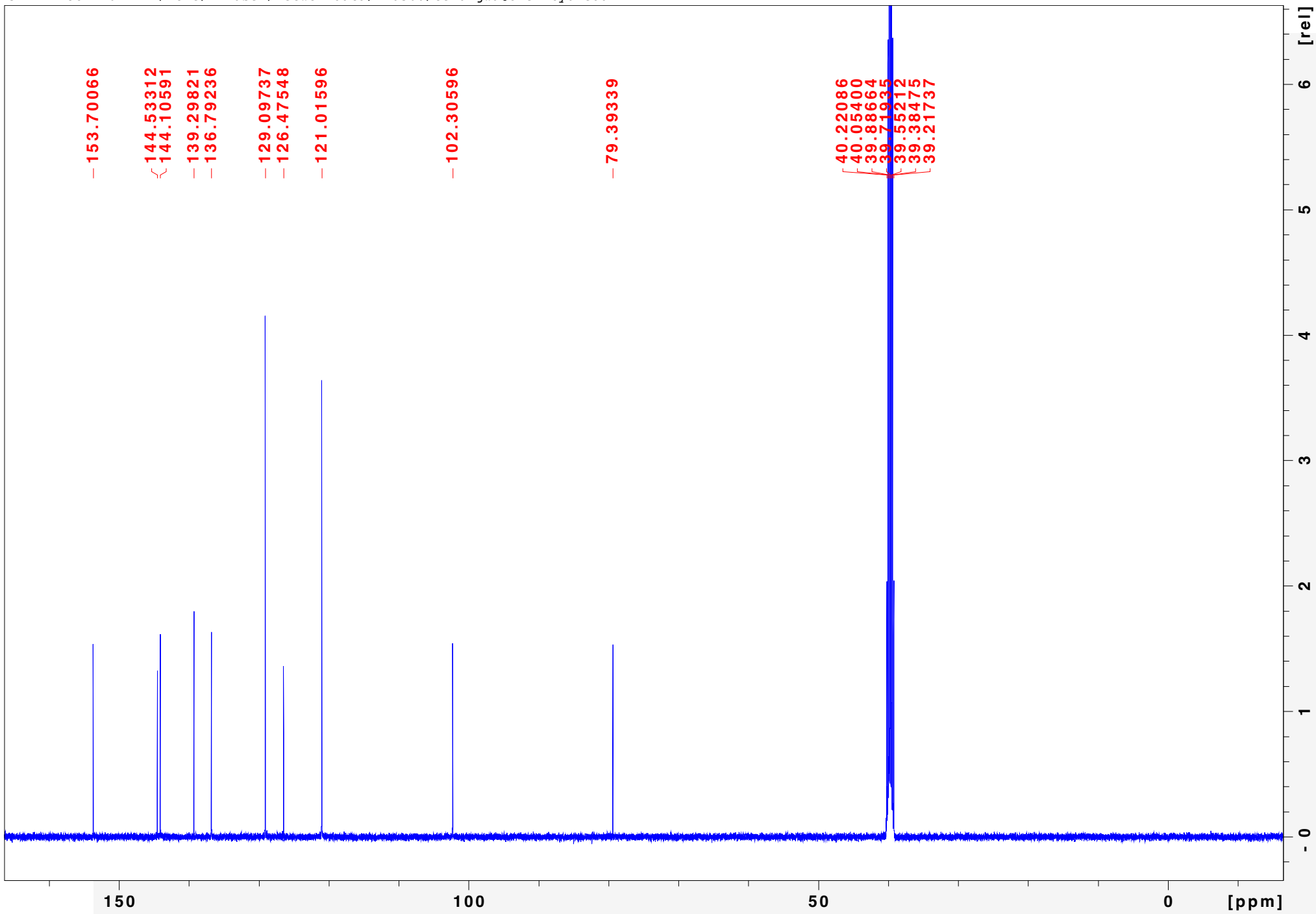
JI-III-38 10 1 /home/nmruser/networkdata/Bru500/terungwa@chem.byu.edu



JI-III-38 10 1 /home/nmruser/networkdata/Bru500/terungwa@chem.byu.edu



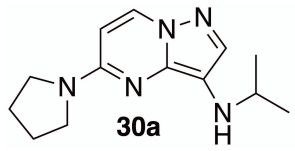
JI-III-38 20 1 /home/nmruser/networkdata/Bru500/terungwa@chem.byu.edu



JI-II-120 20 1 /home/nmruser/networkdata/terungwa@chem.byu.edu

PROTON DMSO /opt/nmrdata terungwa@chem.byu.edu 1

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6.2421
6.2267
3.4727
3.4586
3.4449
3.4329
3.4229
3.4132
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1.9307
1.0790
1.0664



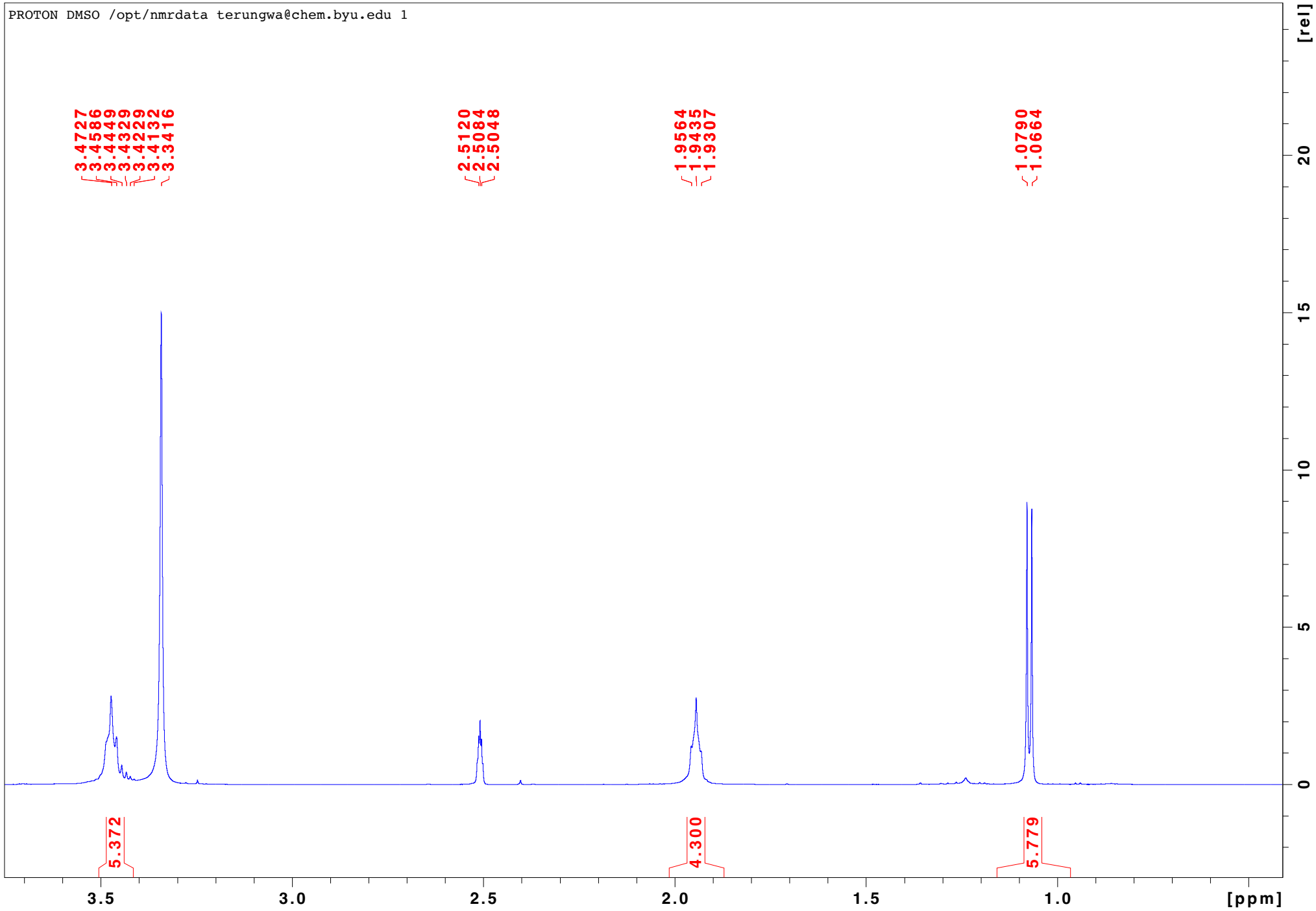
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5.779

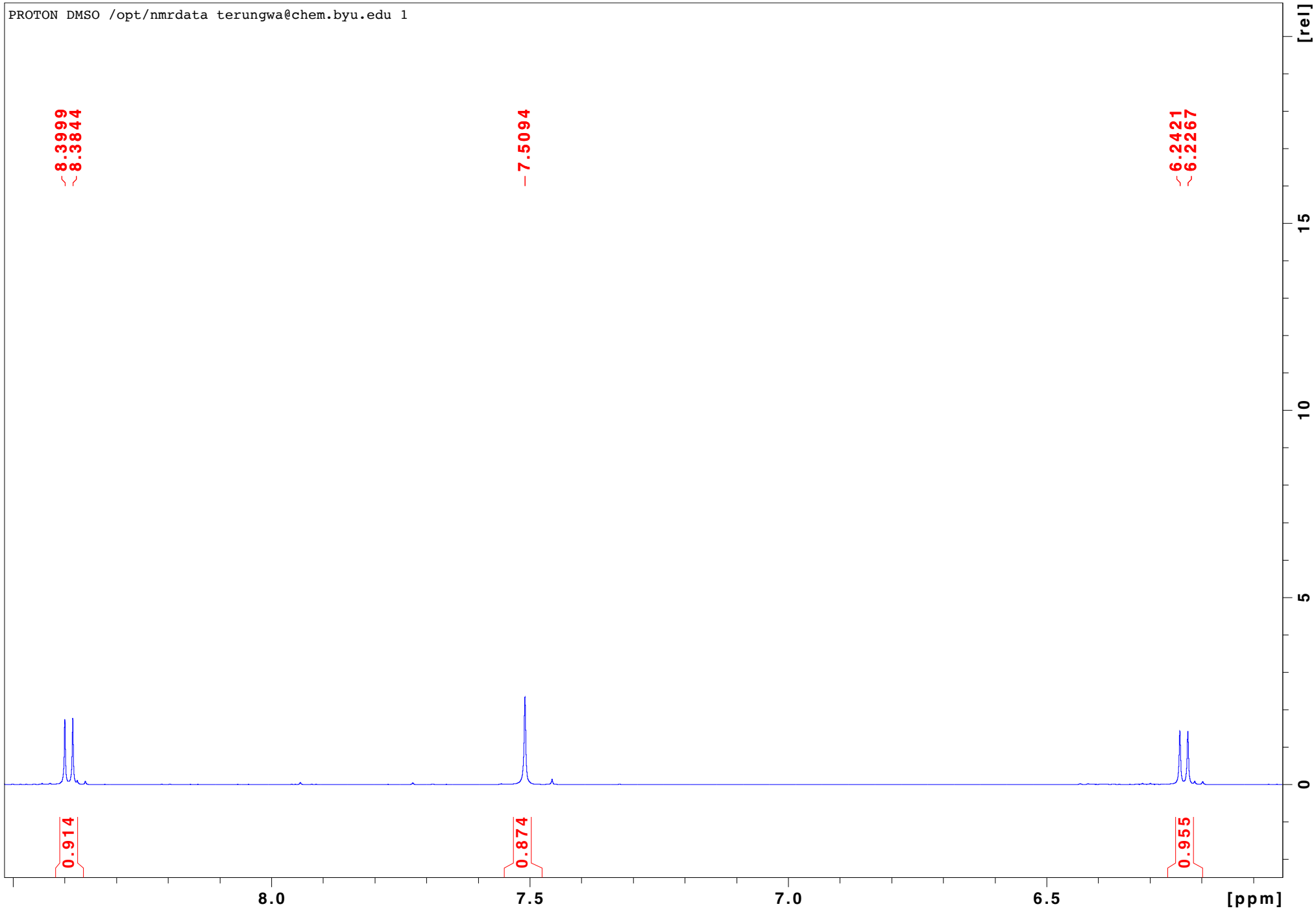
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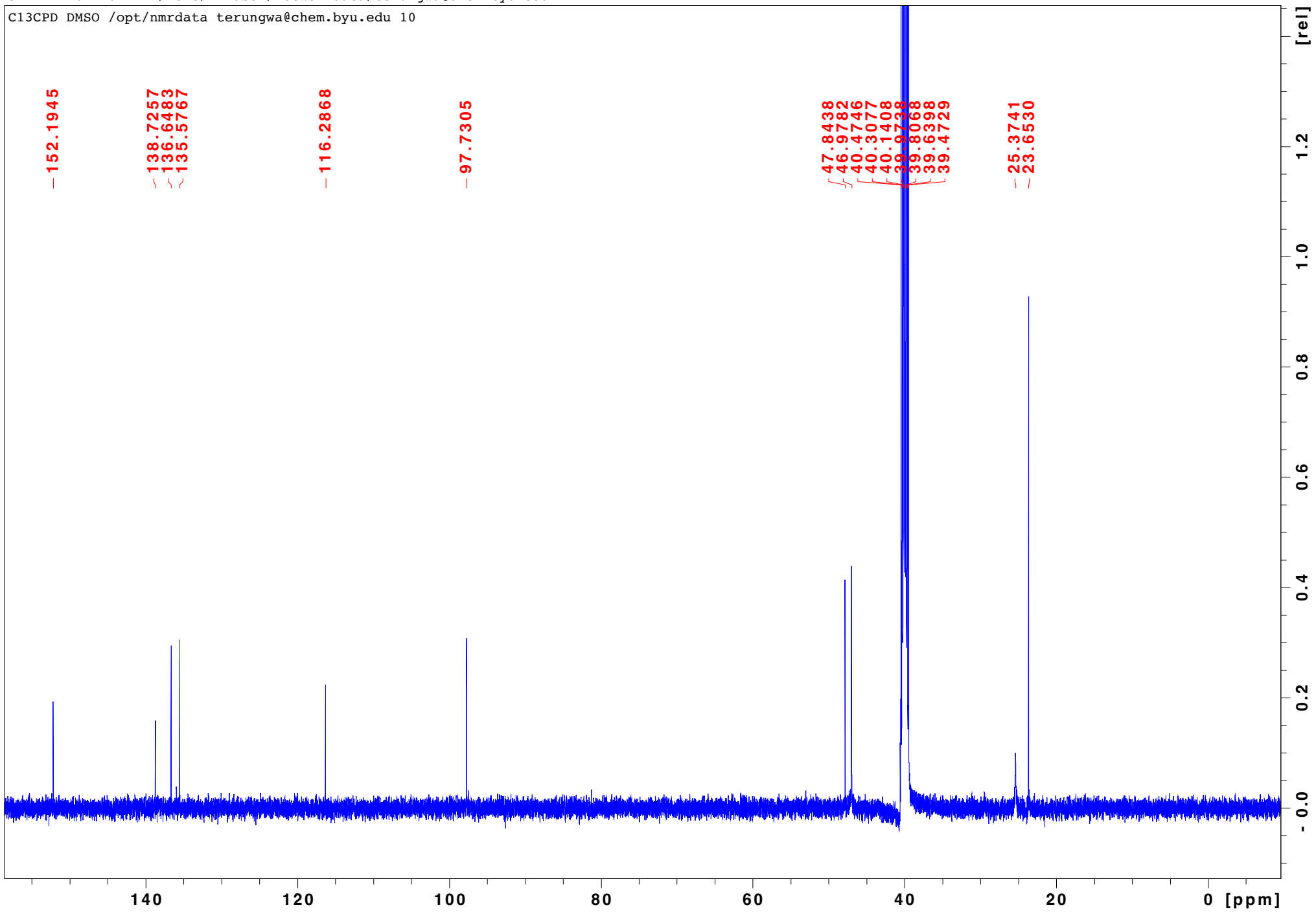
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JI-II-120 20 1 /home/nmruser/networkdata/terungwa@chem.byu.edu



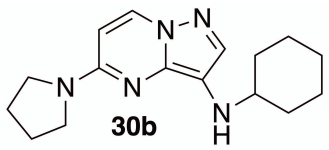
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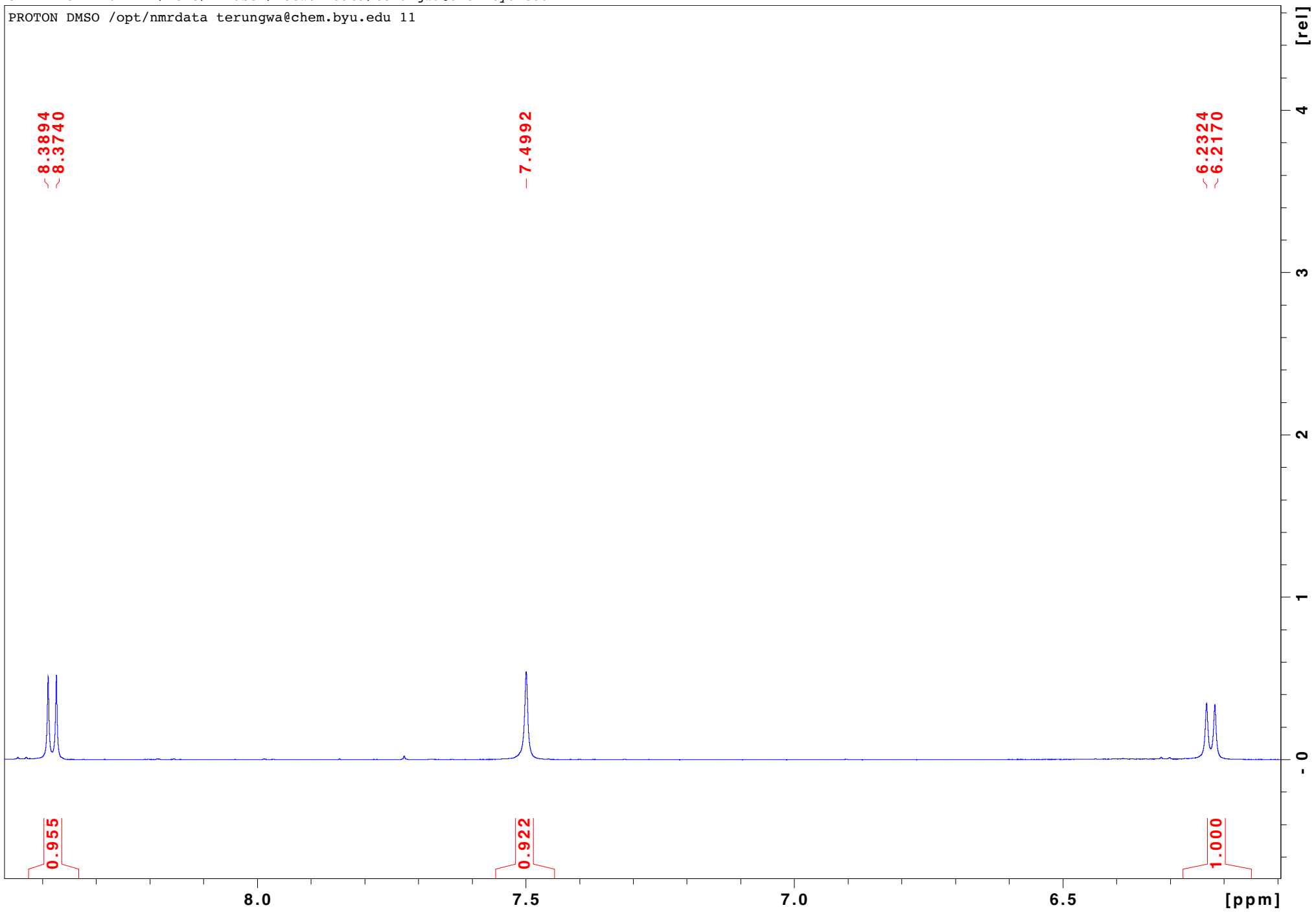


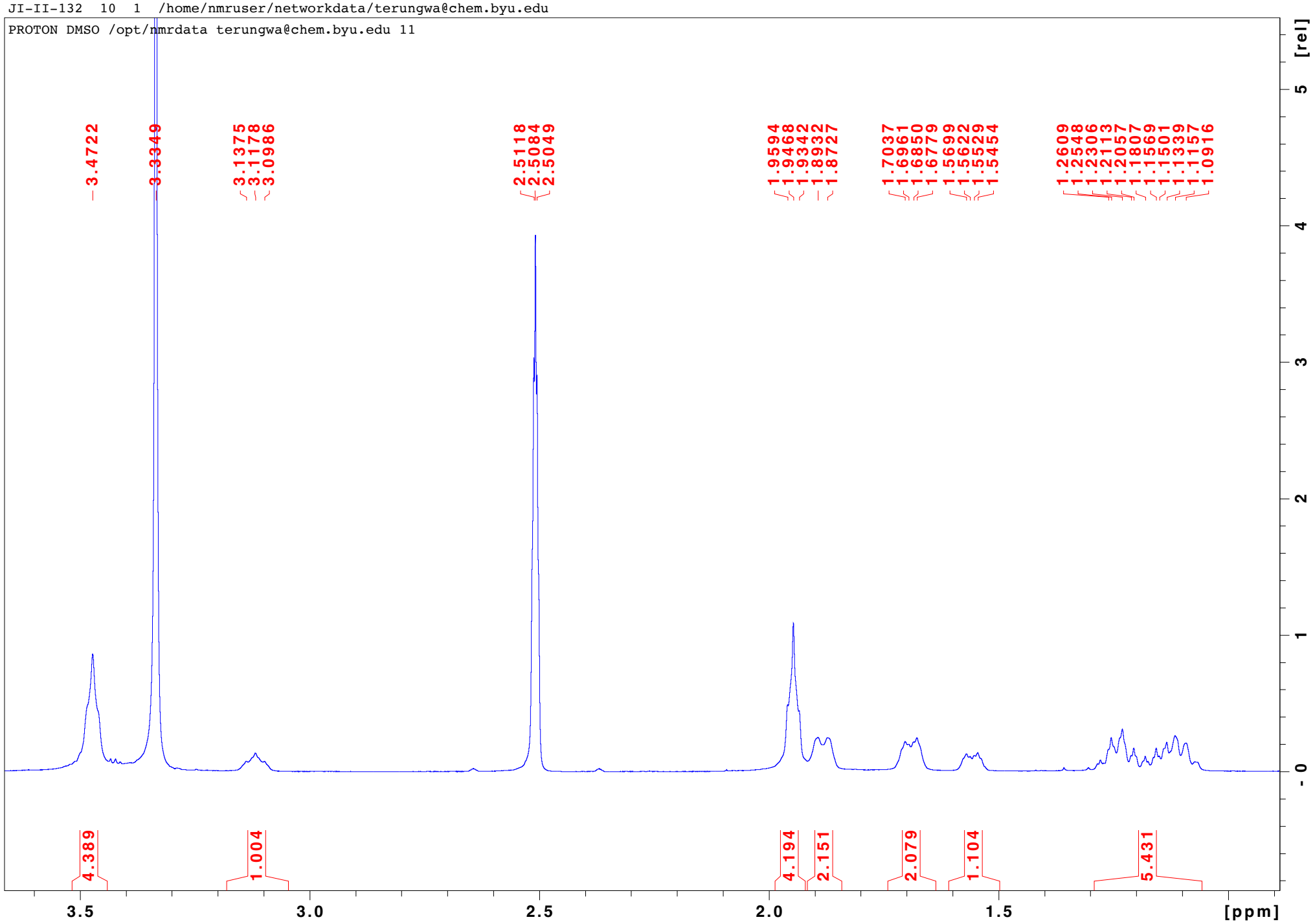

JI-II-120 40 1 /home/nmruser/networkdata/terungwa@chem.byu.edu
C13CPD DMSO /opt/nmrdata terungwa@chem.byu.edu 10
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135.5767
116.2868
97.7305
47.8438
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40.3077
40.1408
39.8068
39.6398
39.4729
25.3741
23.6530
[rel]
1.2
1.0
0.8
0.6
0.4
0.2
- 0.0
140
120
100
80
60
40
20
0 [ppm]

JI-II-132 10 1 /home/nmruser/networkdata/terungwa@chem.byu.edu

PROTON DMSO /opt/nmrdata terungwa@chem.byu.edu 11

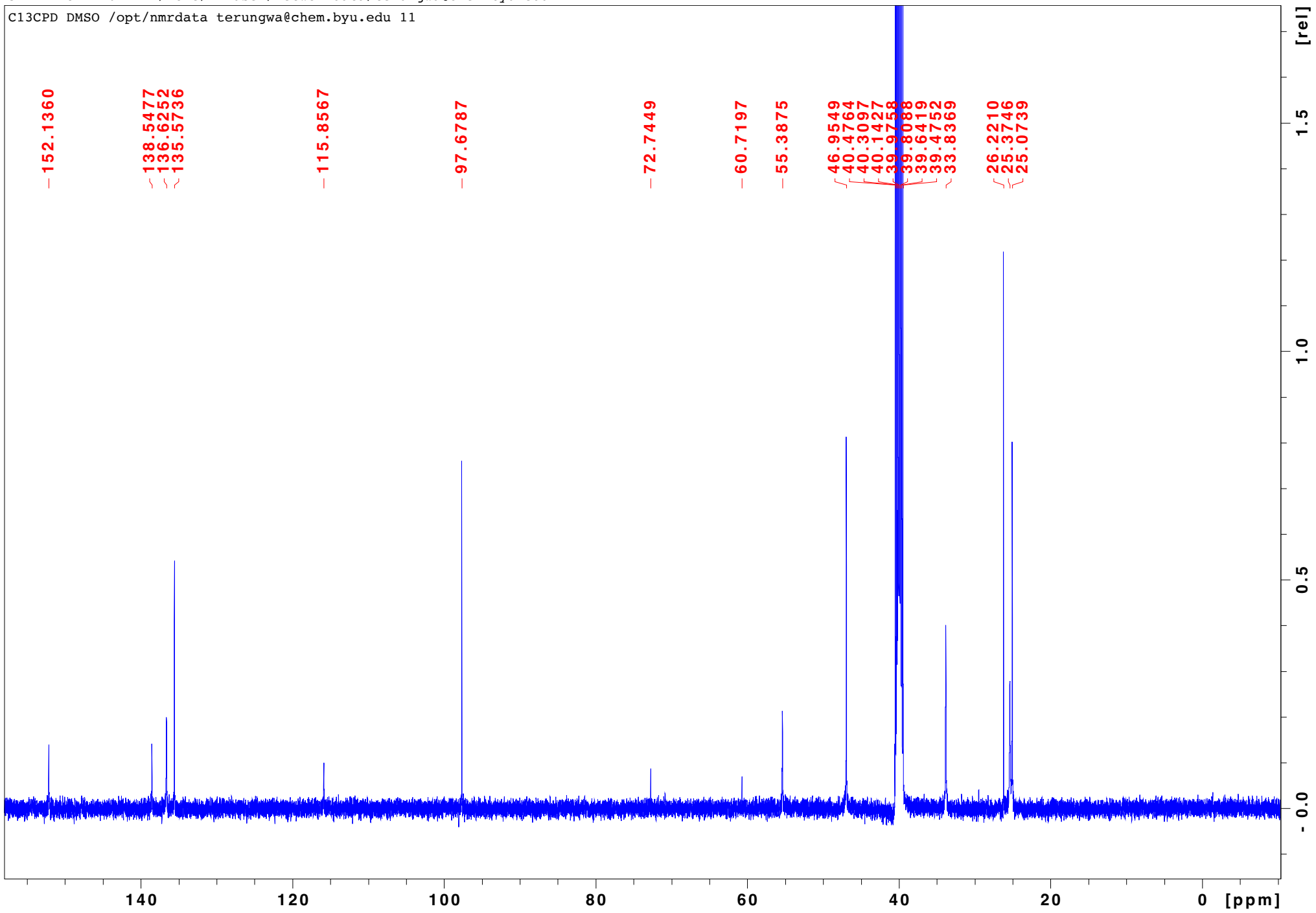



JI-II-132 10 1 /home/nmruser/networkdata/terungwa@chem.byu.edu
PROTON DMSO /opt/nmrdata terungwa@chem.byu.edu 11
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6.2324
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0.922
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7.5
7.0
6.5
[ppm]
[rel]
- 0
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2
3
4

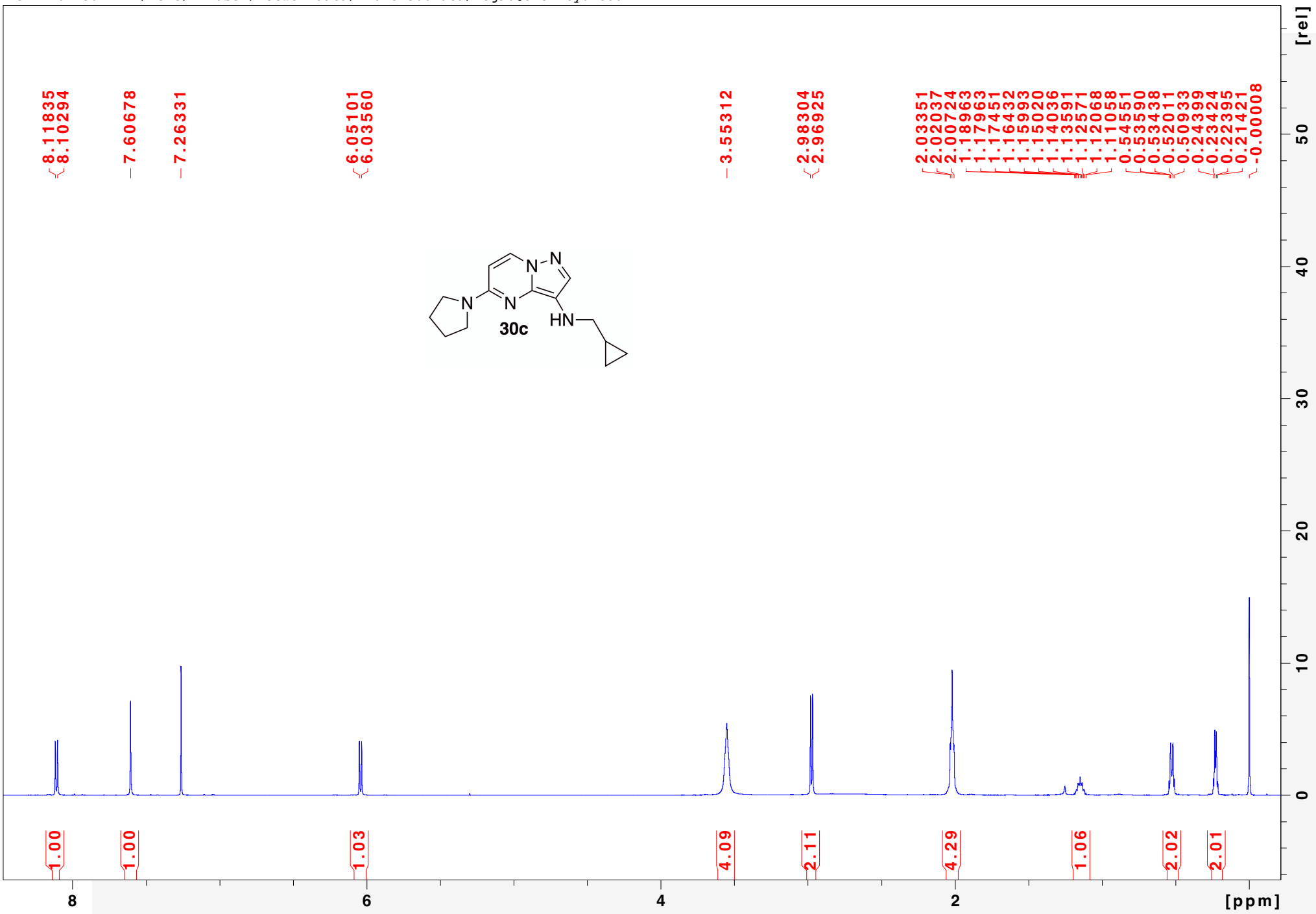

JI-II-132 10 1 /home/nmruser/networkdata/terungwa@chem.byu.edu
PROTON DMSO /opt/nmrdata terungwa@chem.byu.edu 11
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3.3349
3.1375
3.1178
3.0986
2.5118
2.5084
2.5049
1.9594
1.9468
1.9342
1.8932
1.8727
1.7037
1.6961
1.6850
1.6779
1.5699
1.5622
1.5529
1.5454
1.2609
1.2548
1.2306
1.2113
1.2057
1.1807
1.1569
1.1501
1.1339
1.1157
1.0916
4.389
1.004
4.194
2.151
2.079
1.104
5.431
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3.0
2.5
2.0
1.5
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- 0
1
2
3
4
5
[rel]

JI-II-132 20 1 /home/nmruser/networkdata/terungwa@chem.byu.edu

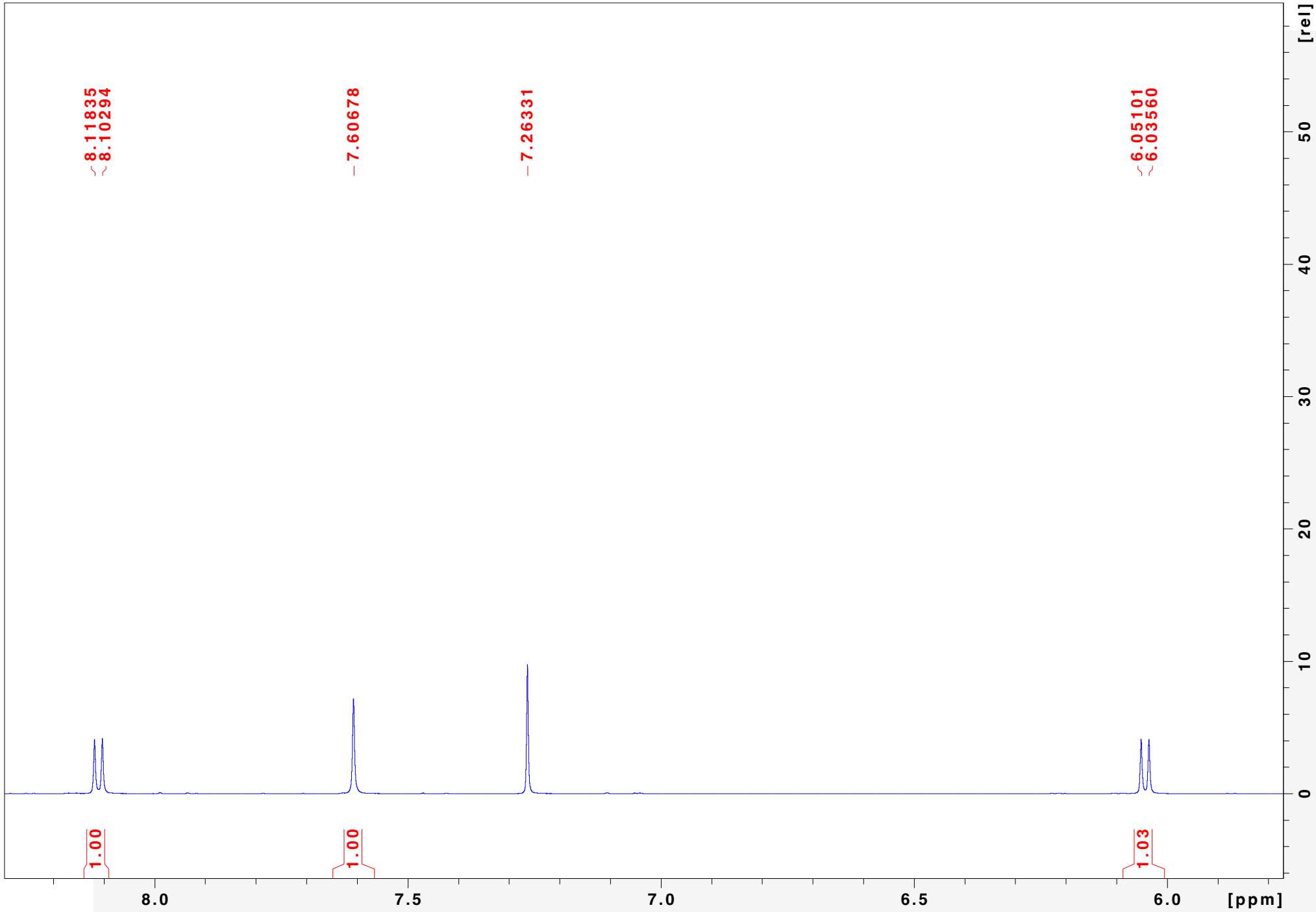
C13CPD DMSO /opt/nmrdata terungwa@chem.byu.edu 11



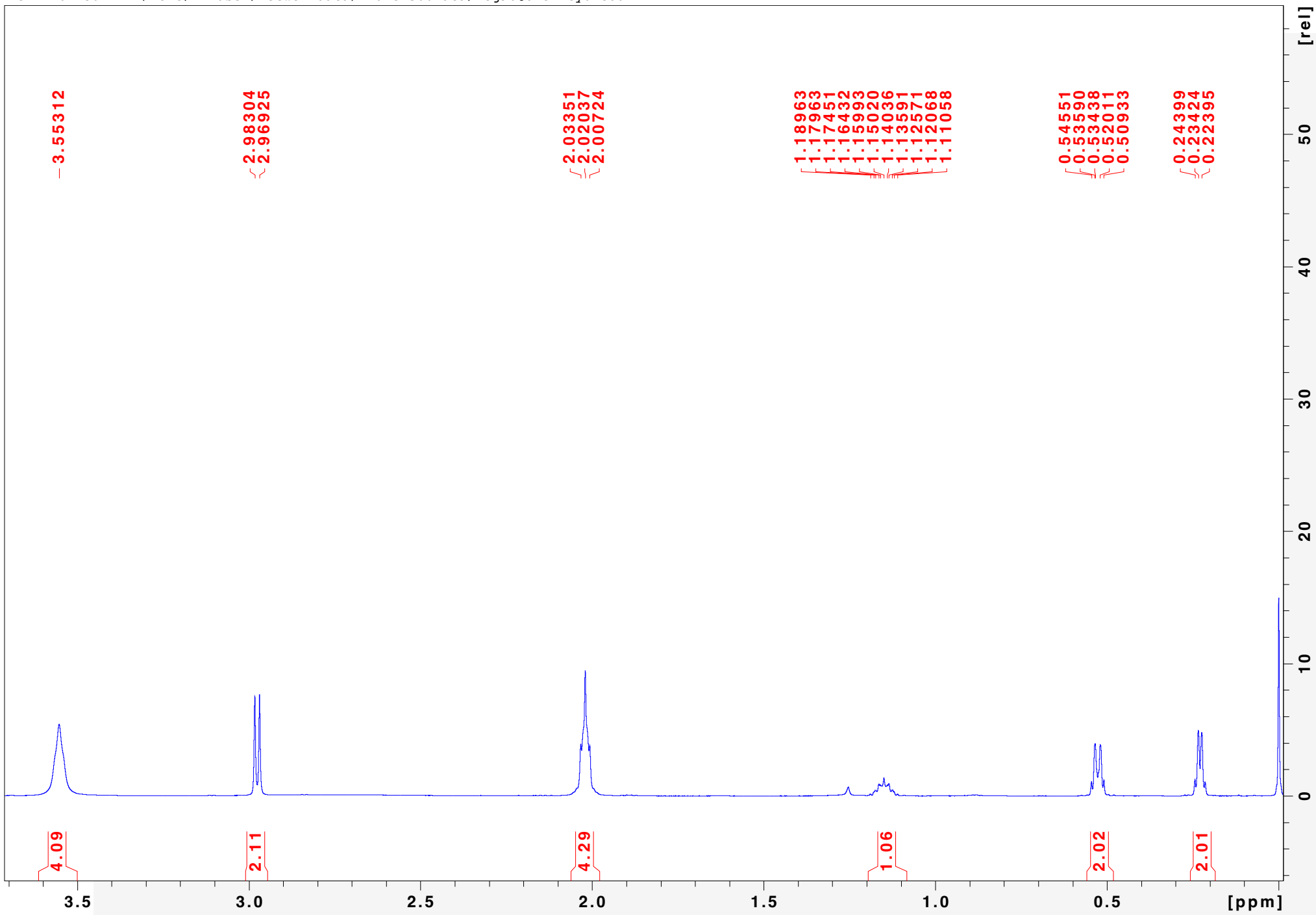
LG-I-46 30 1 /home/nmruser/networkdata/Bruker500Data/log96@chem.byu.edu



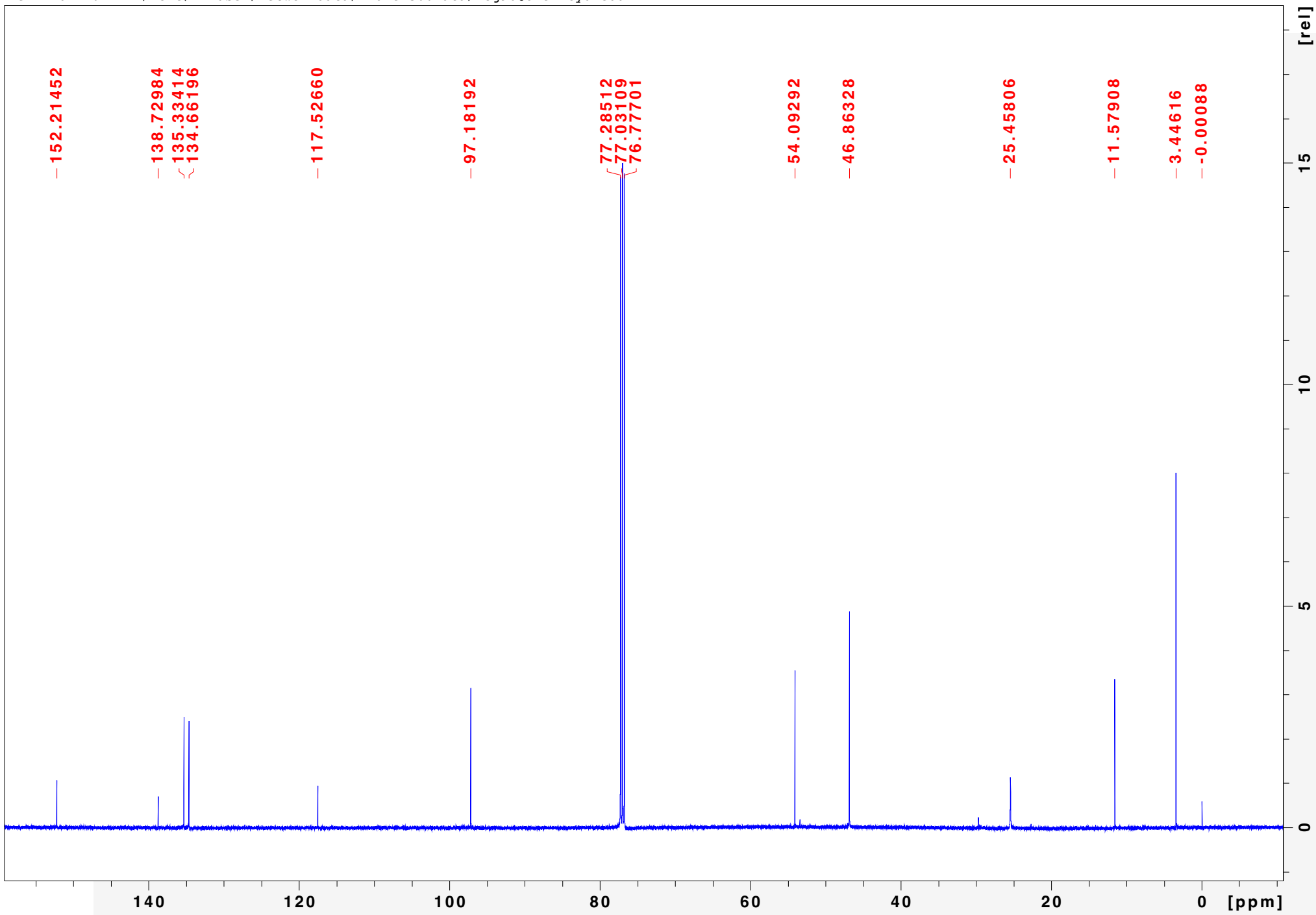
LG-I-46 30 1 /home/nmruser/networkdata/Bruker500Data/log96@chem.byu.edu



LG-I-46 30 1 /home/nmruser/networkdata/Bruker500Data/log96@chem.byu.edu



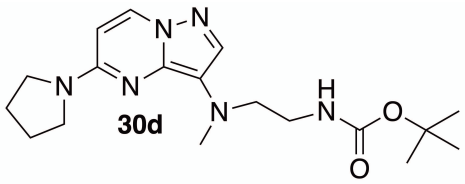
LG-I-46 20 1 /home/nmruser/networkdata/Bruker500Data/log96@chem.byu.edu



JI-II-131 40 1 /home/nmruser/networkdata/terungwa@chem.byu.edu

PROTON CDCl3 /opt/nmrdata terungwa@chem.byu.edu 6

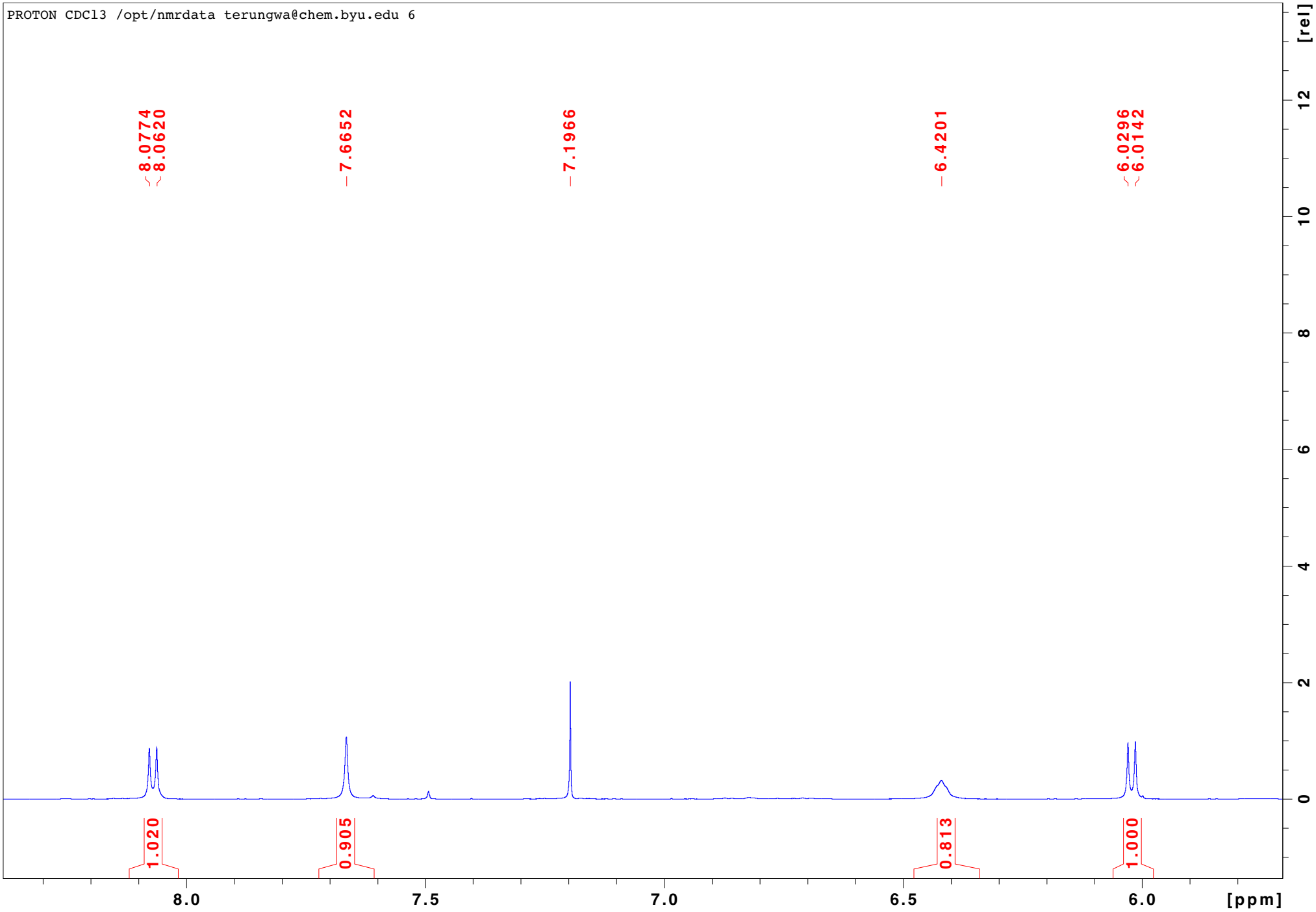
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7.6652
7.1966
6.4201
6.0296
6.0142
3.5414
3.5296
3.1198
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3.0986
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2.9733
2.9625
2.9525
2.7708
1.9668
1.3759



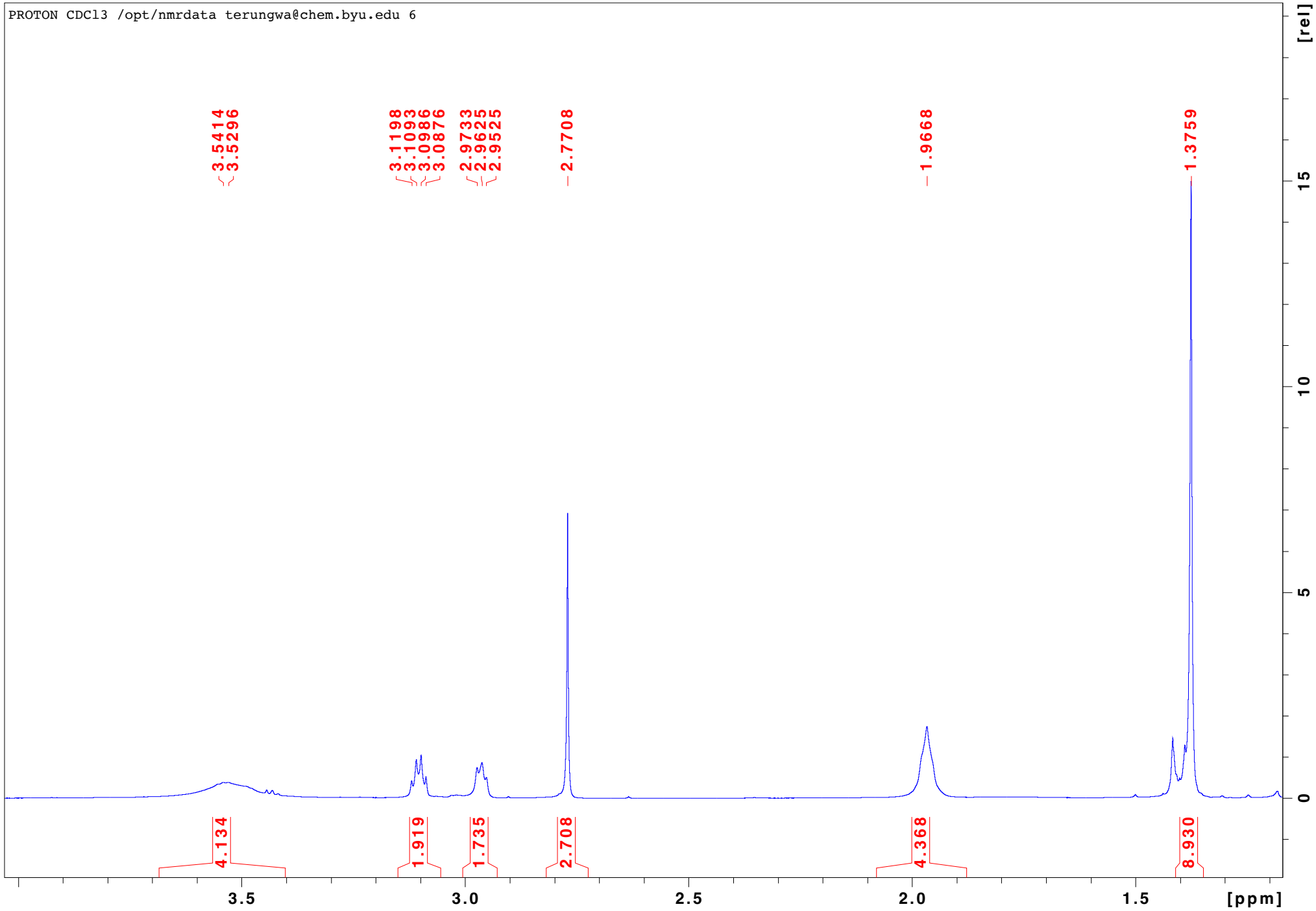
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0.905
0.813
1.000
4.134
1.919
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8.930

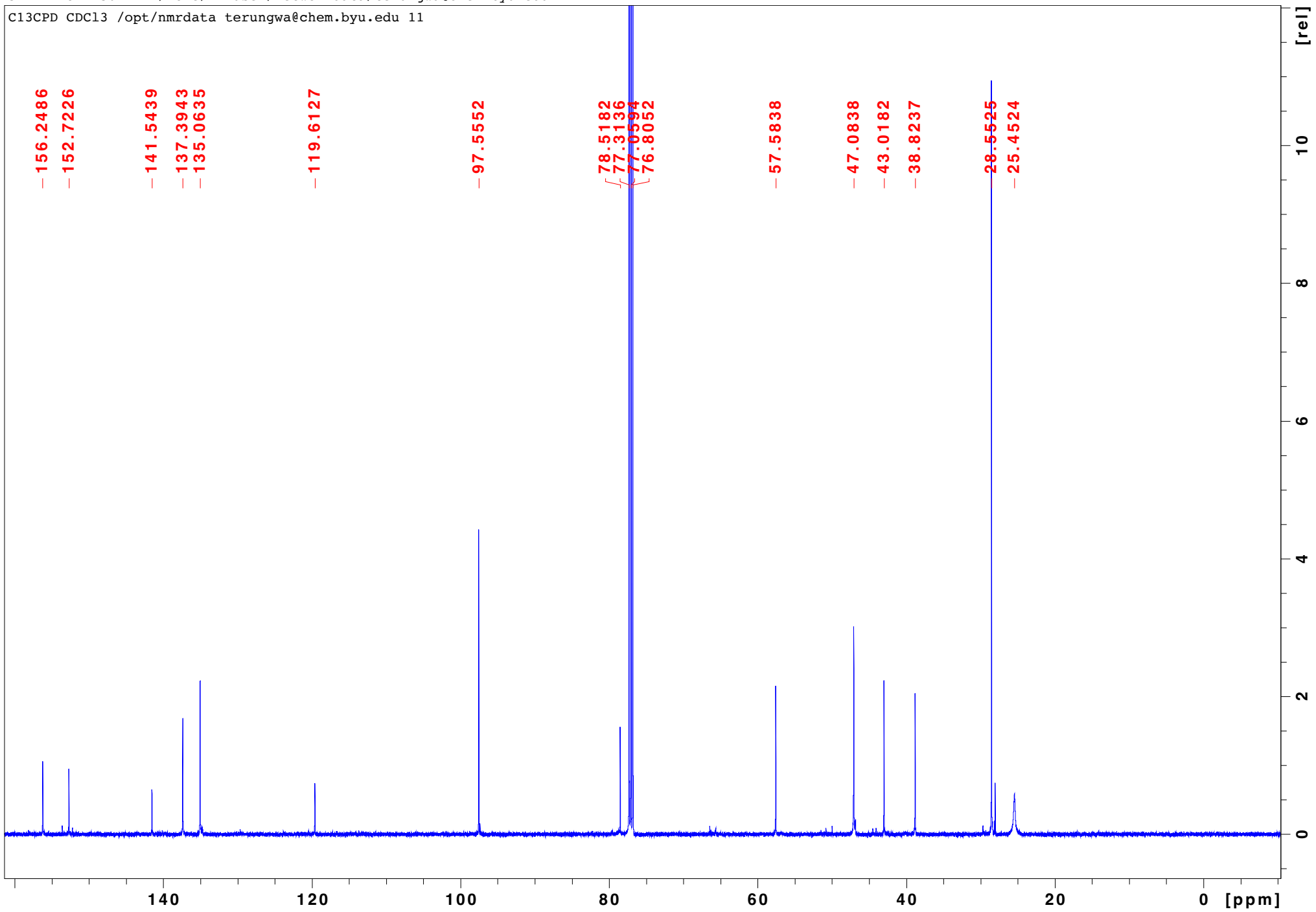
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10
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0
8
6
4
2
0
[ppm]

JI-II-131 40 1 /home/nmruser/networkdata/terungwa@chem.byu.edu



JI-II-131 40 1 /home/nmruser/networkdata/terungwa@chem.byu.edu

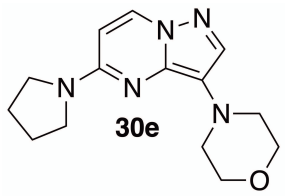



JI-II-131 50 1 /home/nmruser/networkdata/terungwa@chem.byu.edu
C13CPD CDCl3 /opt/nmrdata terungwa@chem.byu.edu 11
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137.3943
135.0635
119.6127
97.5552
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76.8052
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47.0838
43.0182
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28.5525
25.4524
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2
4
6
8
10
140
120
100
80
60
40
20
0
[ppm]

JI-II-49 40 1 /home/nmruser/networkdata/terungwa@chem.byu.edu

PROTON DMSO /opt/nmrdata terungwa@chem.byu.edu 17

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8.4442
7.5853
6.3080
6.2926
3.7423
3.7331
3.7238
3.4831
3.4700
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2.5050
1.9466



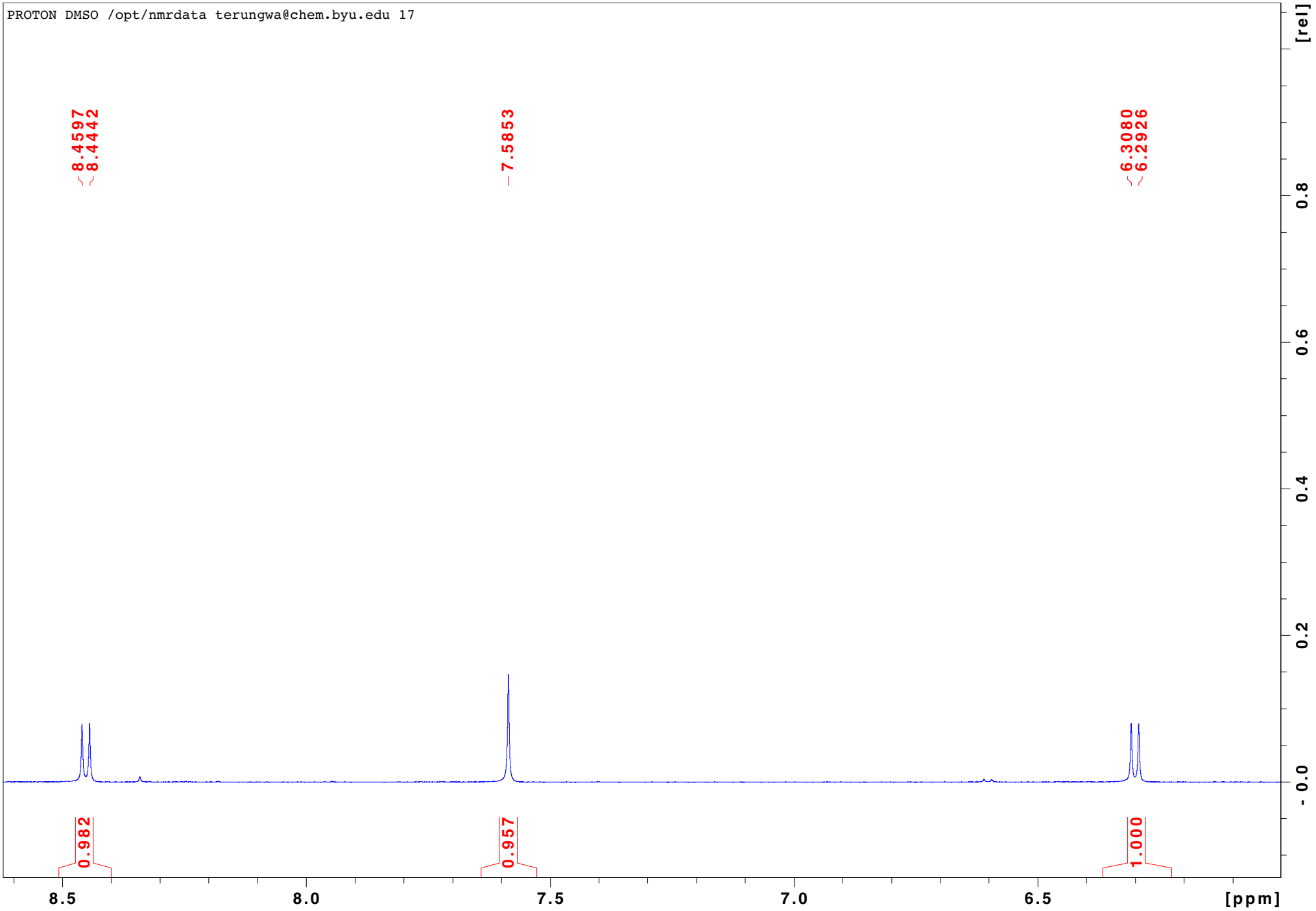
30e

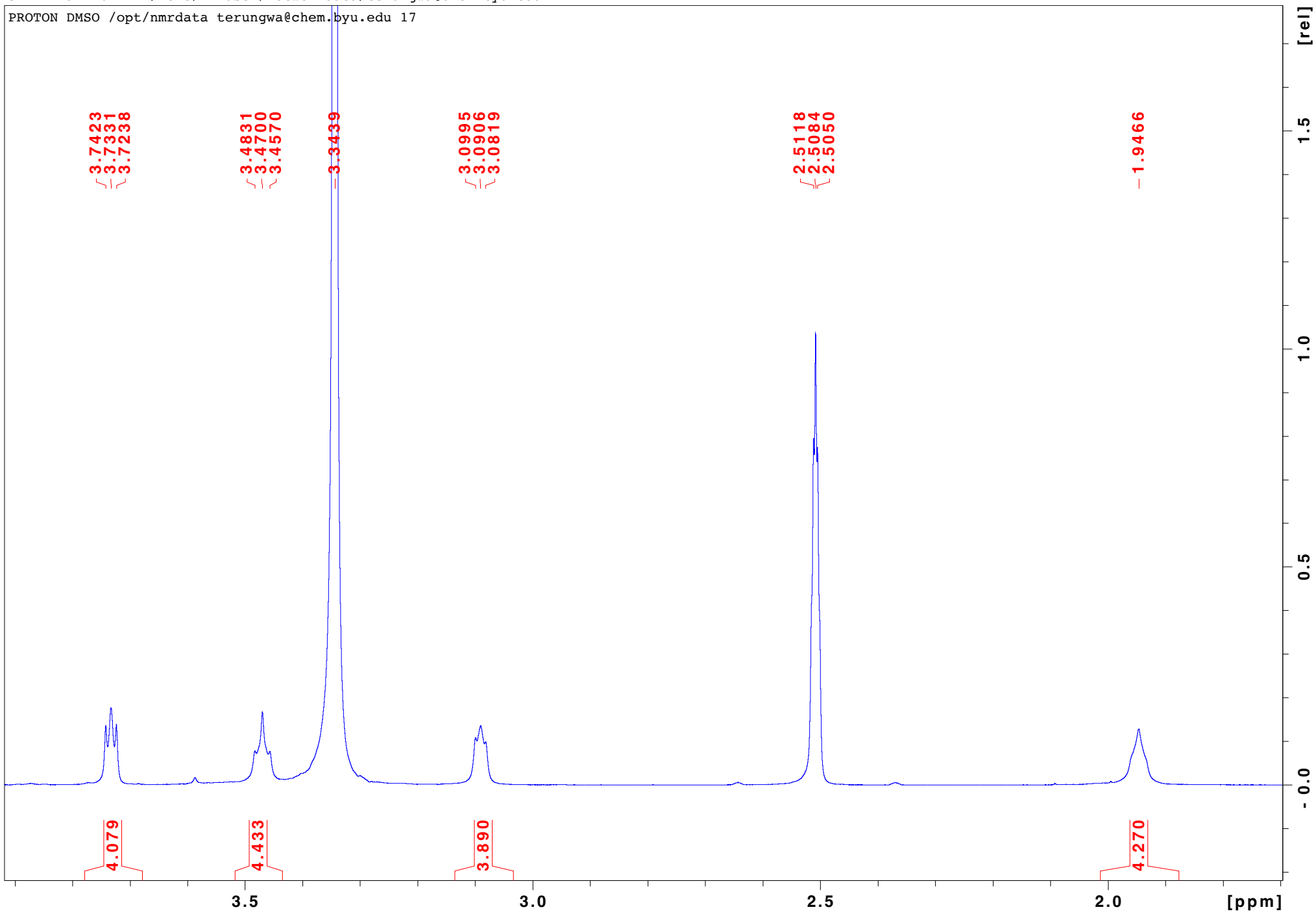
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4.079
4.433
3.890
4.270

8
6
4
2
[ppm]

[rel]
2.0
1.5
1.0
0.5
- 0.0

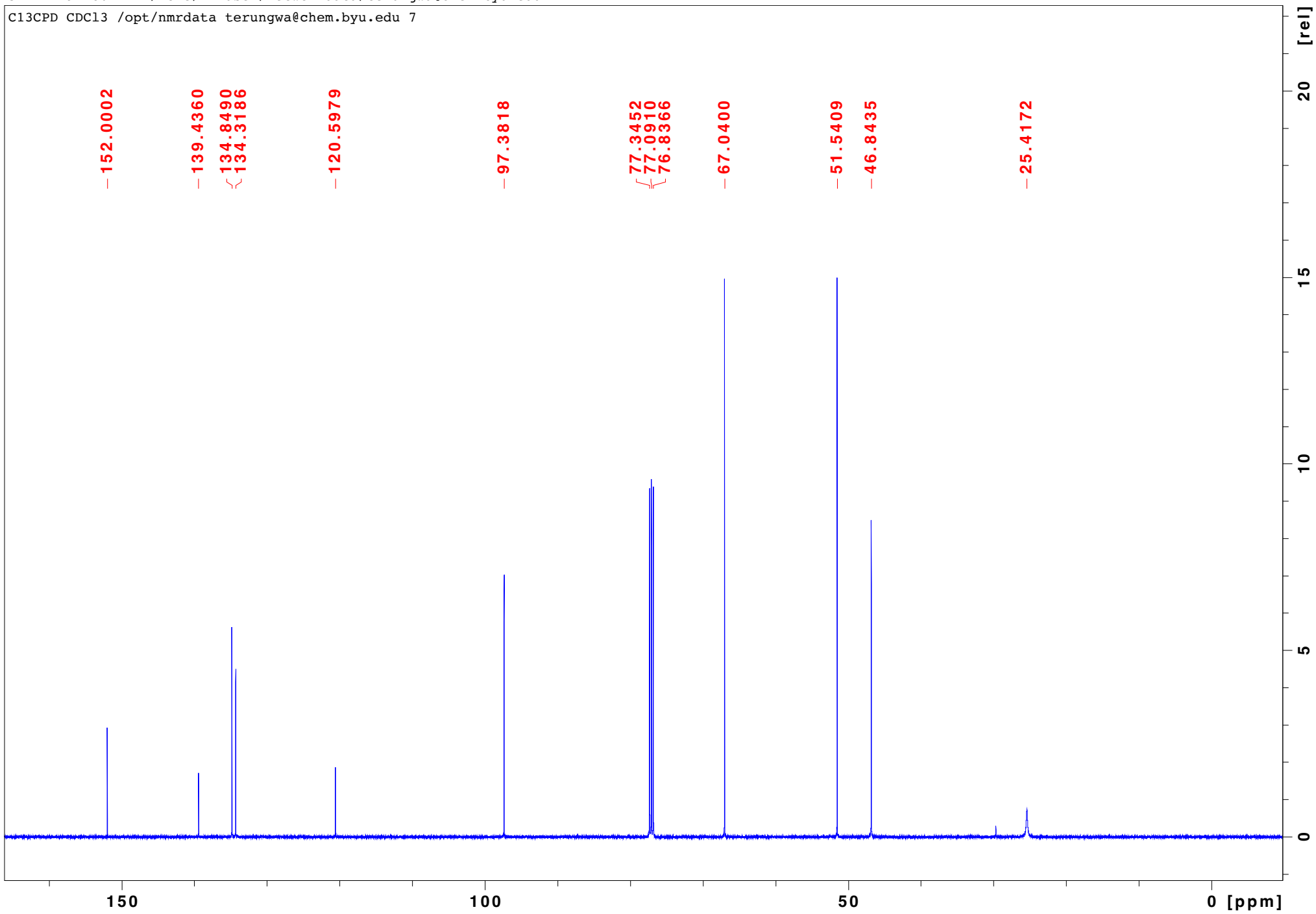
JI-II-49 40 1 /home/nmruser/networkdata/terungwa@chem.byu.edu




JI-II-49 40 1 /home/nmruser/networkdata/terungwa@chem.byu.edu
PROTON DMSO /opt/nmrdata terungwa@chem.byu.edu 17
3.7423
3.7331
3.7238
3.4831
3.4700
3.4570
3.3439
3.0995
3.0906
3.0819
2.5118
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4.079
4.433
3.890
4.270
3.5
3.0
2.5
2.0
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[rel]
1.5
1.0
0.5
- 0.0

JI-II-49 80 1 /home/nmruser/networkdata/terungwa@chem.byu.edu

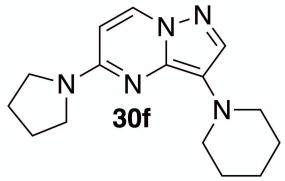
C13CPD CDCl3 /opt/nmrdata terungwa@chem.byu.edu 7



JI-II-133 10 1 /home/nmruser/networkdata/terungwa@chem.byu.edu

PROTON DMSO /opt/nmrdata terungwa@chem.byu.edu 6

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6.2844
6.2690
3.4829
3.4700
3.4570
3.3550
3.0588
3.0486
3.0383
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2.5051
1.9478
1.6498
1.6382
1.6273
1.6166
1.6052
1.5089
1.4967
1.4858
1.4742
1.4629

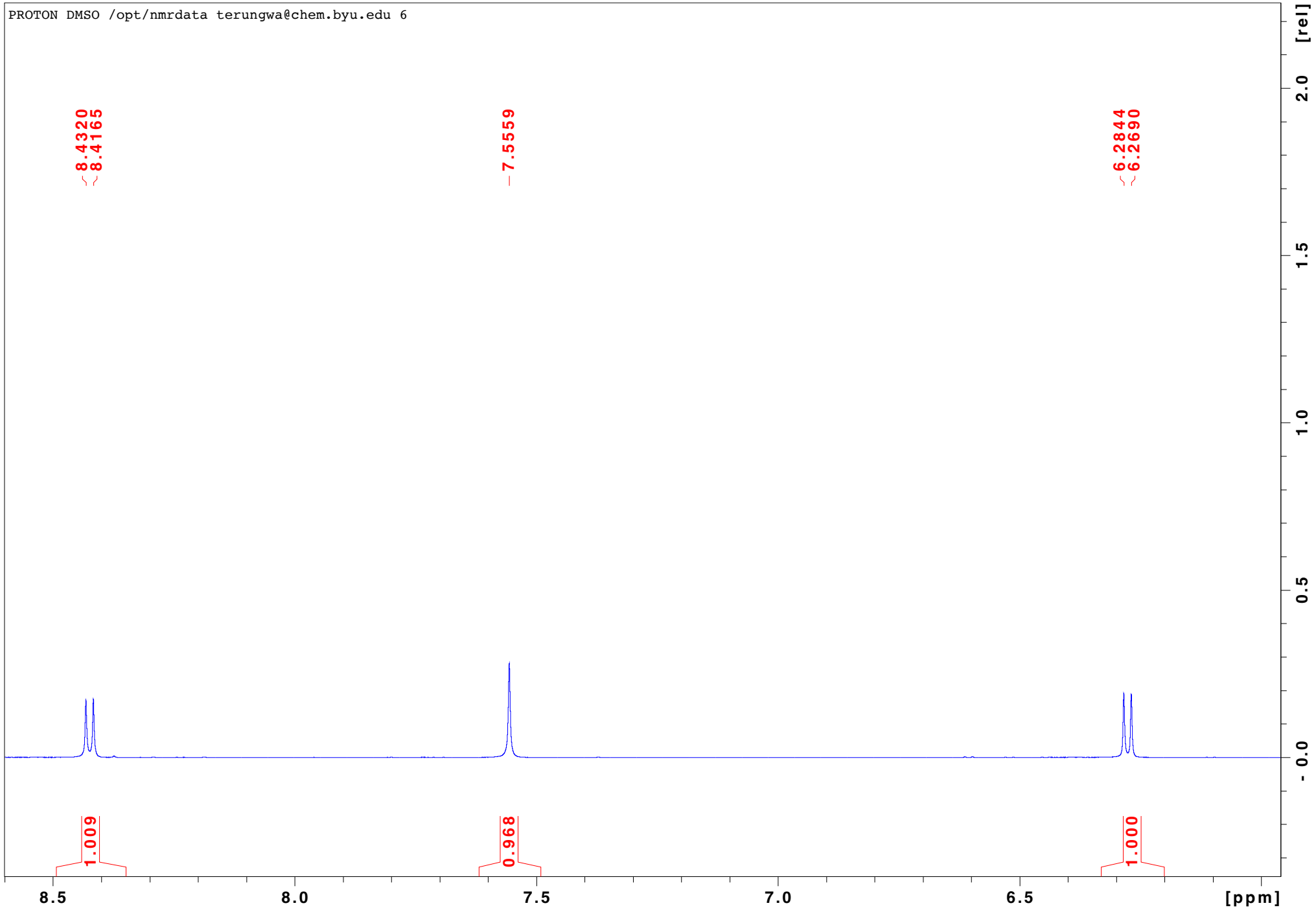


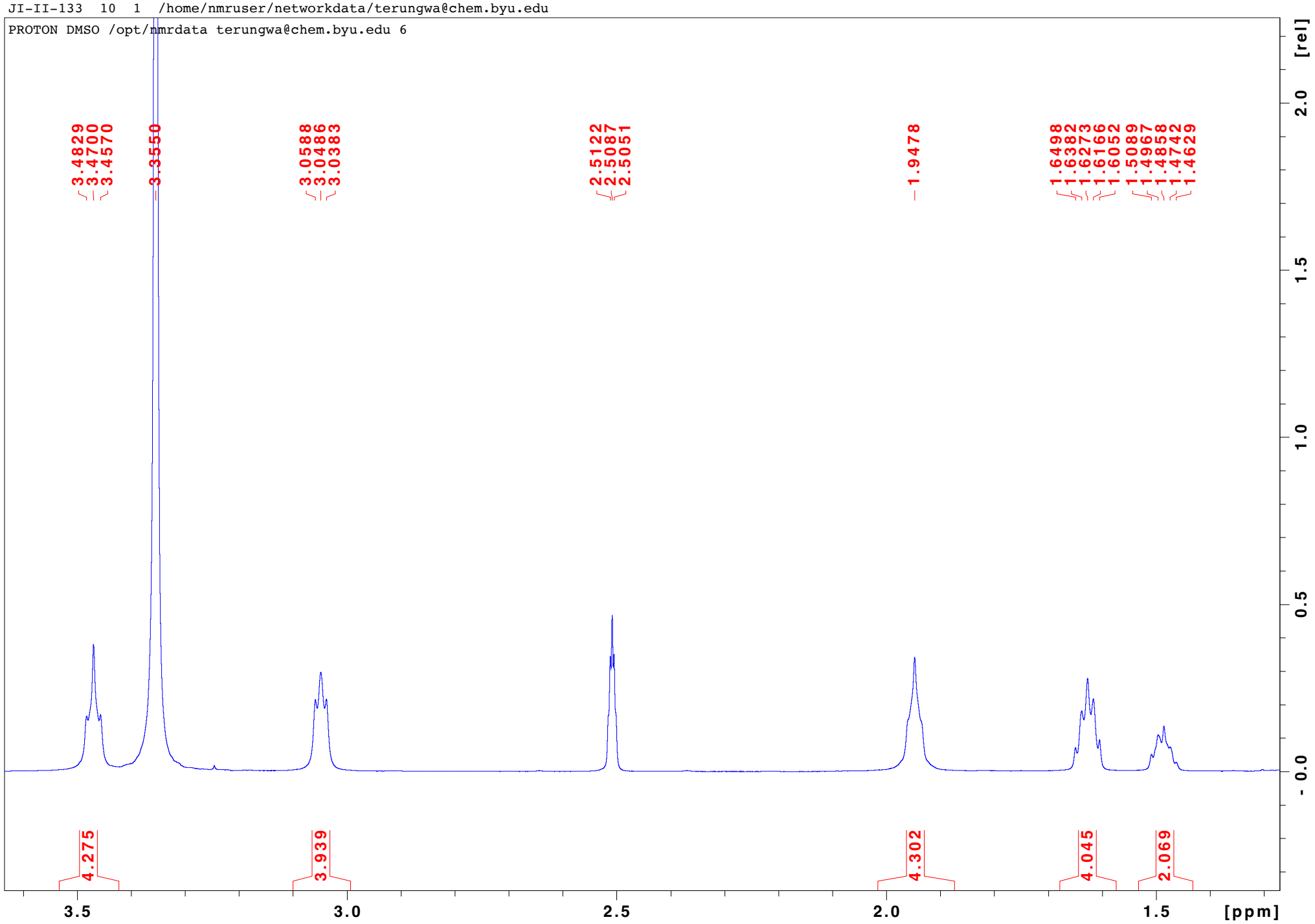
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1.000
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4.302
4.045
2.069

8
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4
2
0
[ppm]

[rel]
2.5
2.0
1.5
1.0
0.5
- 0.0

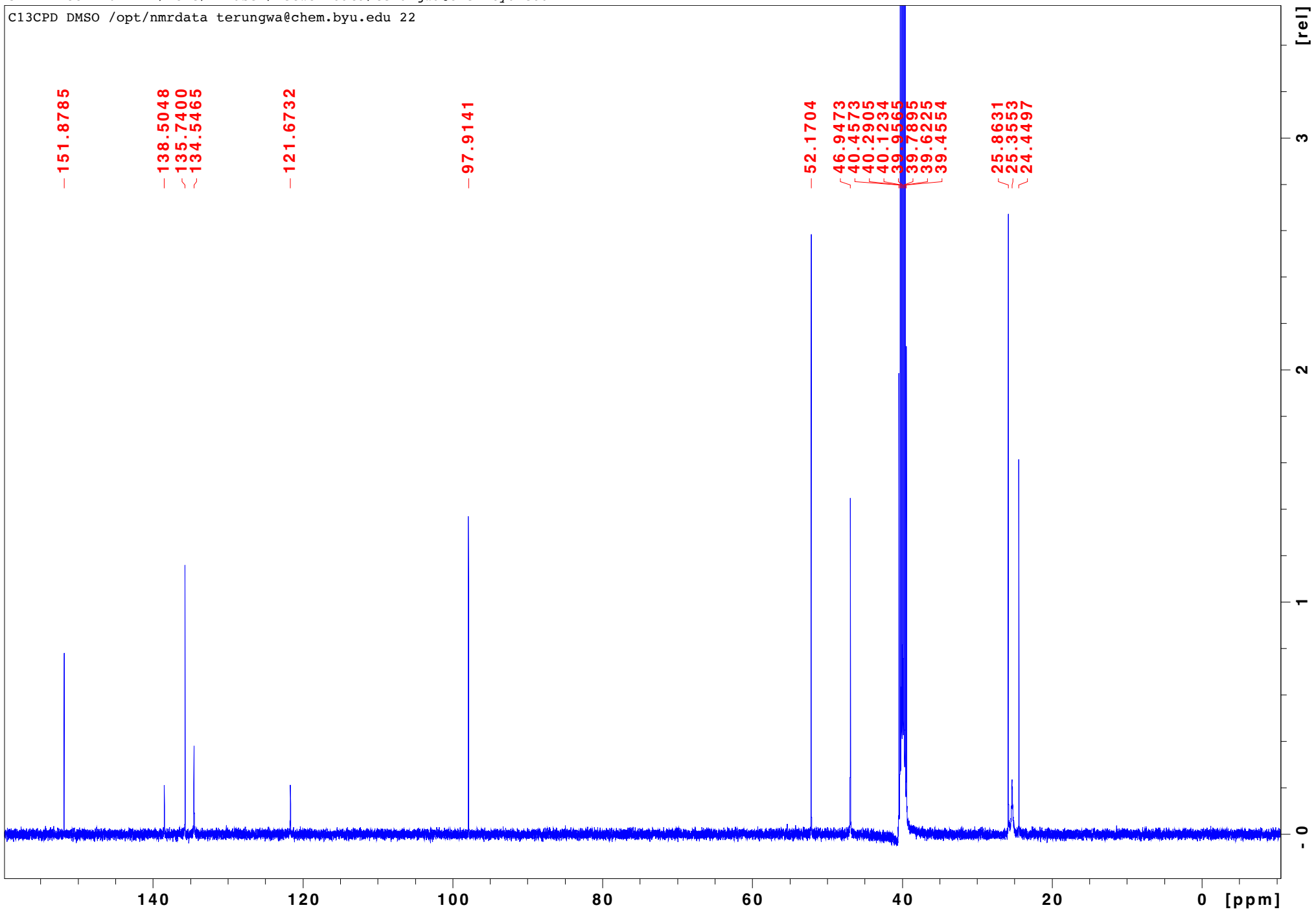
JI-II-133 10 1 /home/nmruser/networkdata/terungwa@chem.byu.edu



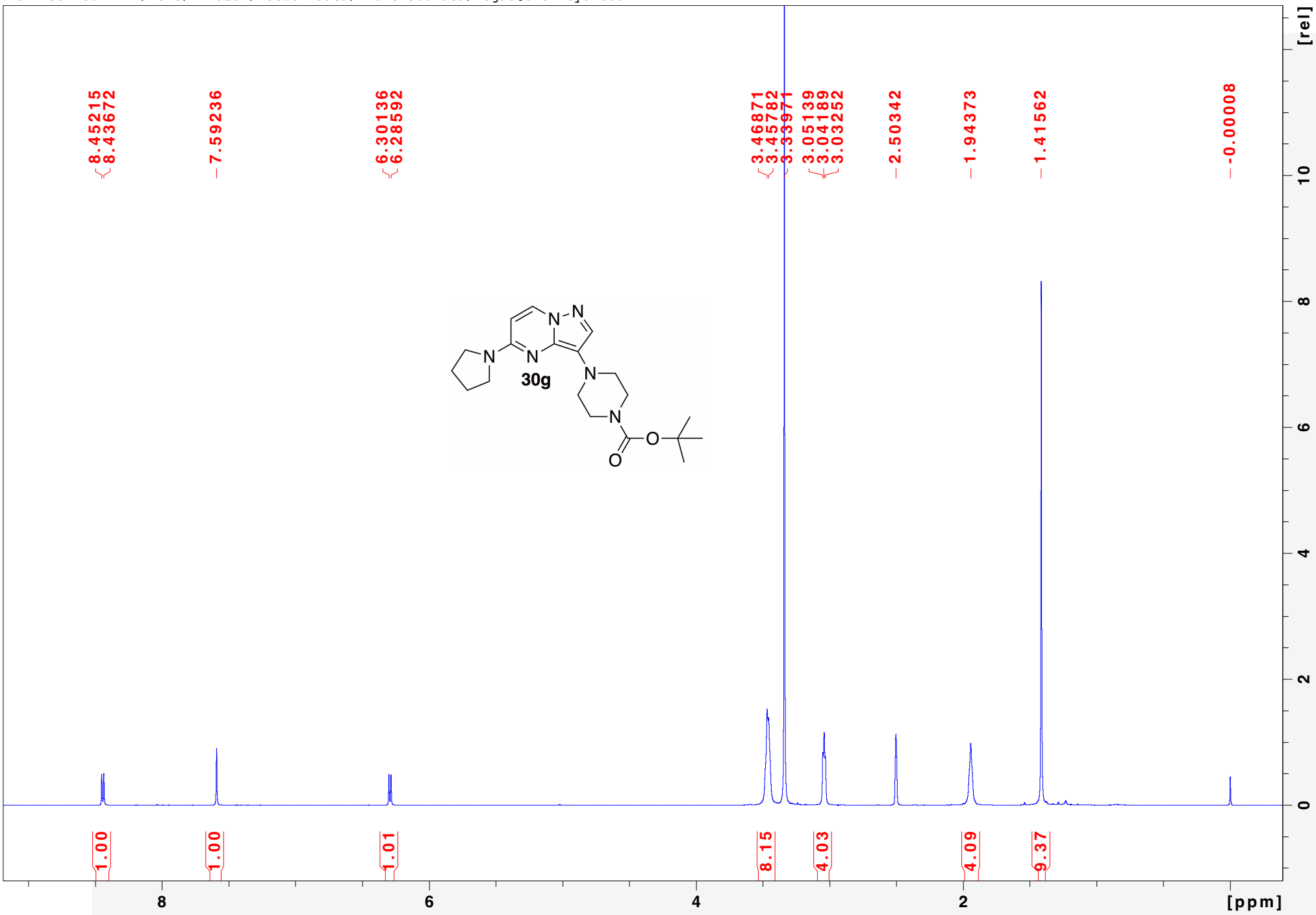

JI-II-133 10 1 /home/nmruser/networkdata/terungwa@chem.byu.edu
PROTON DMSO /opt/nmrdata terungwa@chem.byu.edu 6
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3.4700
3.4570
3.3550
3.0588
3.0486
3.0383
2.5122
2.5087
2.5051
1.9478
1.6498
1.6382
1.6273
1.6166
1.6052
1.5089
1.4967
1.4858
1.4742
1.4629
4.275
3.939
4.302
4.045
2.069
3.5
3.0
2.5
2.0
1.5
[ppm]
- 0.0
0.5
1.0
1.5
2.0
[rel]

JI-II-133 20 1 /home/nmruser/networkdata/terungwa@chem.byu.edu

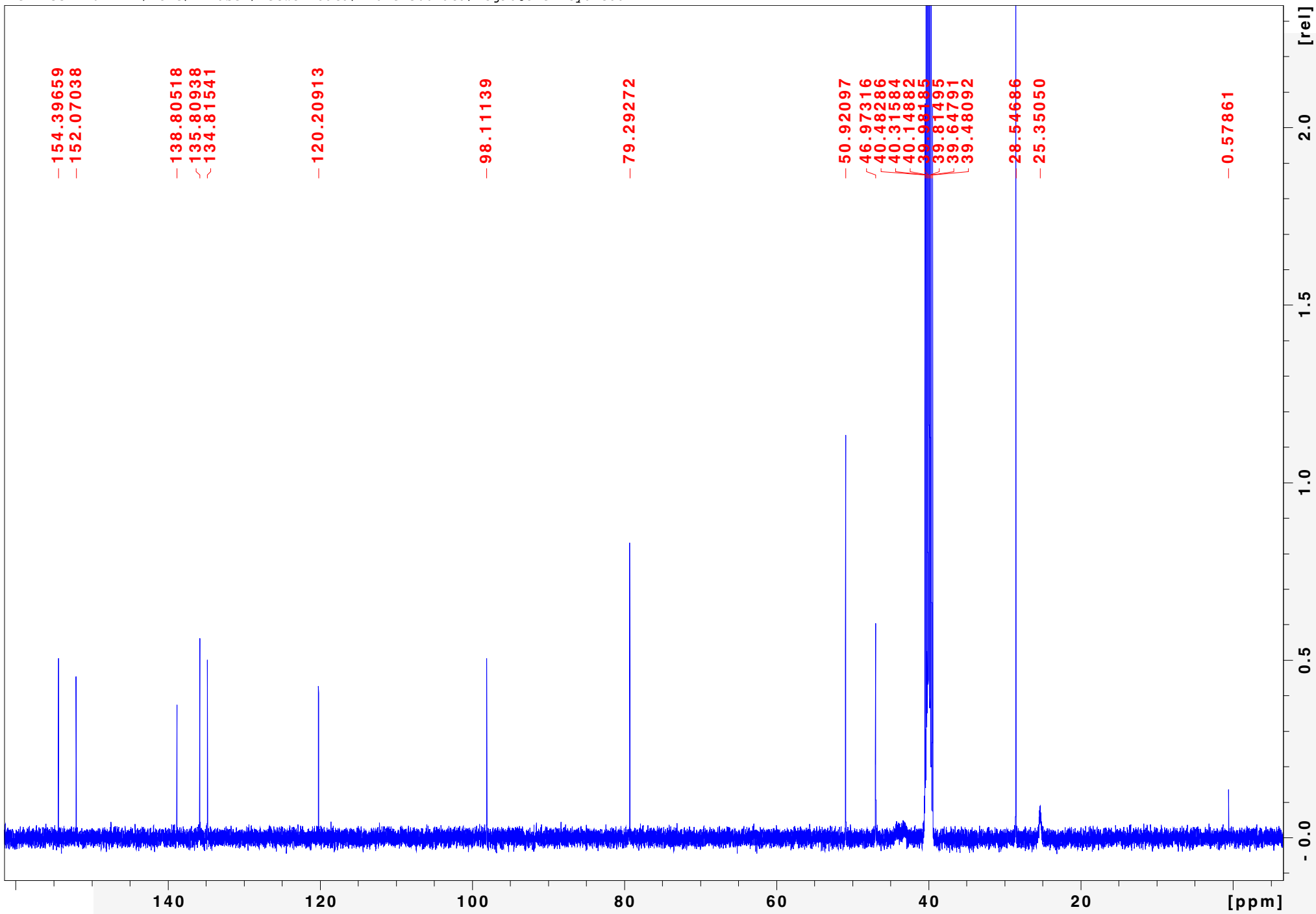
C13CPD DMSO /opt/nmrdata terungwa@chem.byu.edu 22



LG-I-55 30 1 /home/nmruser/networkdata/Bruker500Data/log96@chem.byu.edu

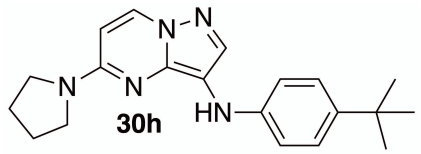


LG-I-55 20 1 /home/nmruser/networkdata/Bruker500Data/log96@chem.byu.edu



JI-II-116 20 1 /home/nmruser/networkdata/terungwa@chem.byu.edu

PROTON DMSO /opt/nmrdata terungwa@chem.byu.edu 22



30h

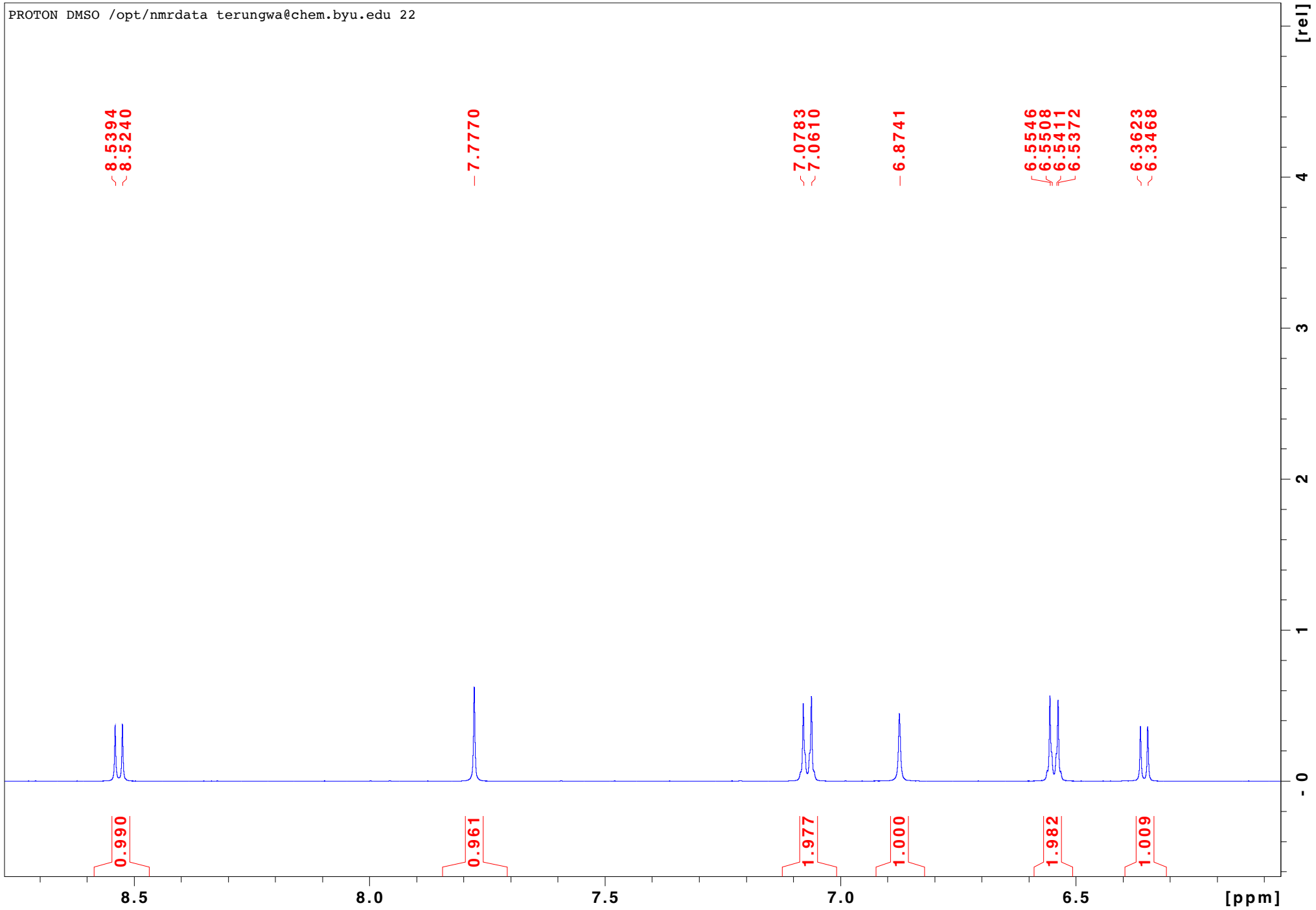
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8.5240
7.7770
7.0783
7.0610
6.8741
6.5546
6.5508
6.5411
6.5372
6.3623
6.3468
3.4655
3.4524
3.4394
3.3355
2.5120
2.5084
2.5048
1.9226
1.2097

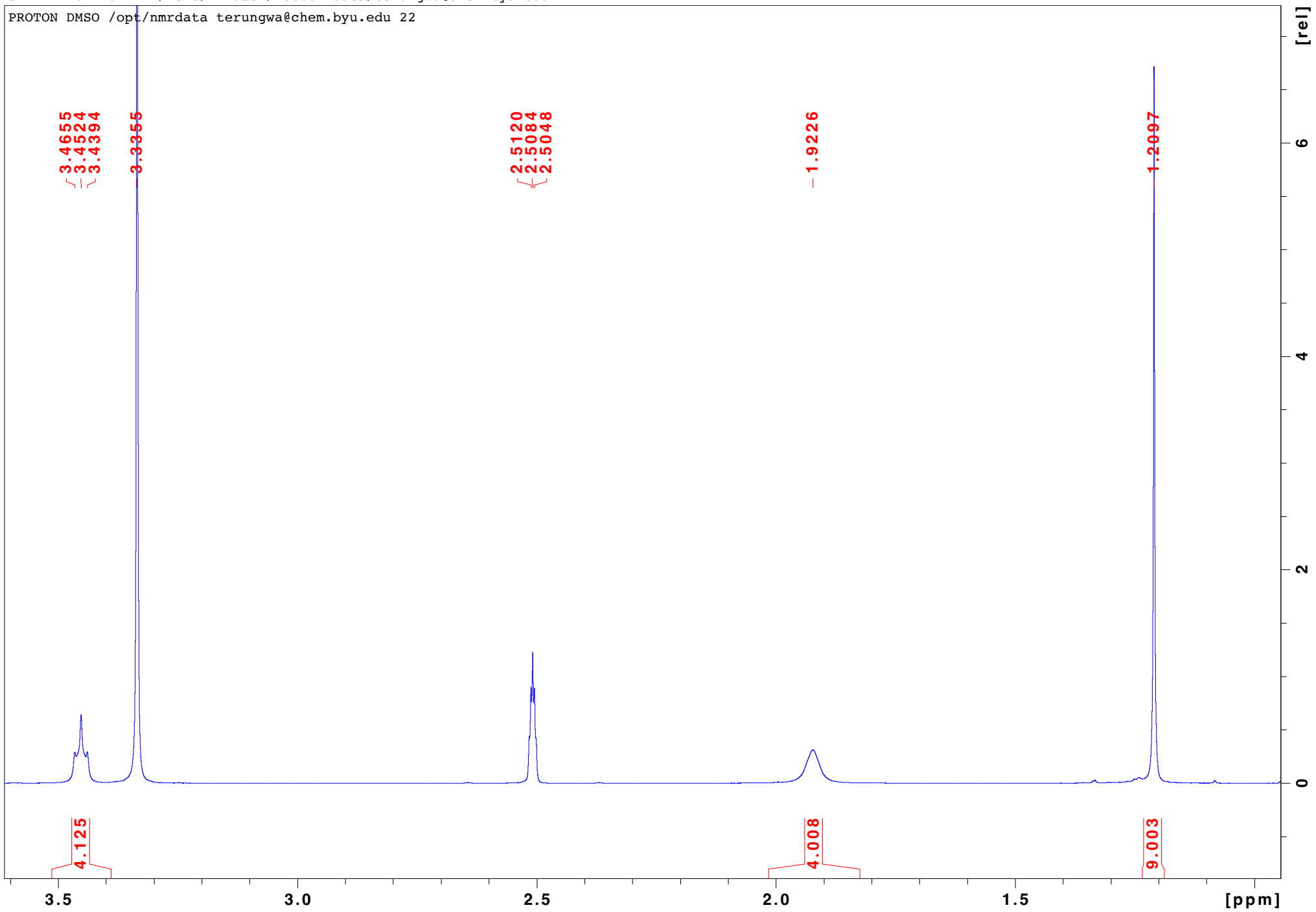
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1.982
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4.125
4.008
9.003

8 6 4 2 0 [ppm]

0 2 4 6 8 [rel]

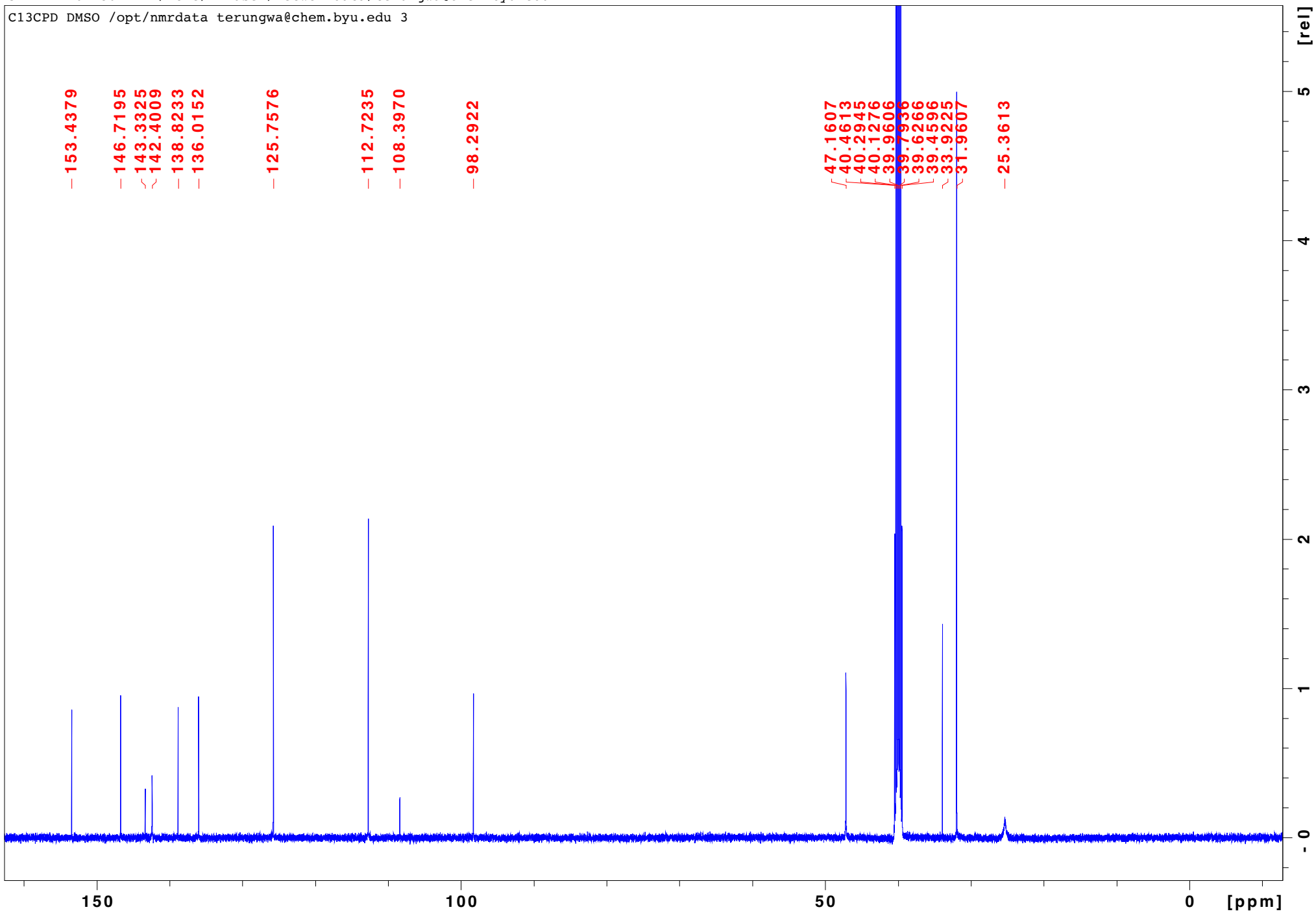
JI-II-116 20 1 /home/nmruser/networkdata/terungwa@chem.byu.edu




JI-II-116 20 1 /home/nmruser/networkdata/terungwa@chem.byu.edu
PROTON DMSO /opt/nmrdata terungwa@chem.byu.edu 22
3.4655
3.4524
3.4394
3.3355
2.5120
2.5084
2.5048
1.9226
1.2097
4.125
4.008
9.003
3.5
3.0
2.5
2.0
1.5
[ppm]
[rel]
0
2
4
6

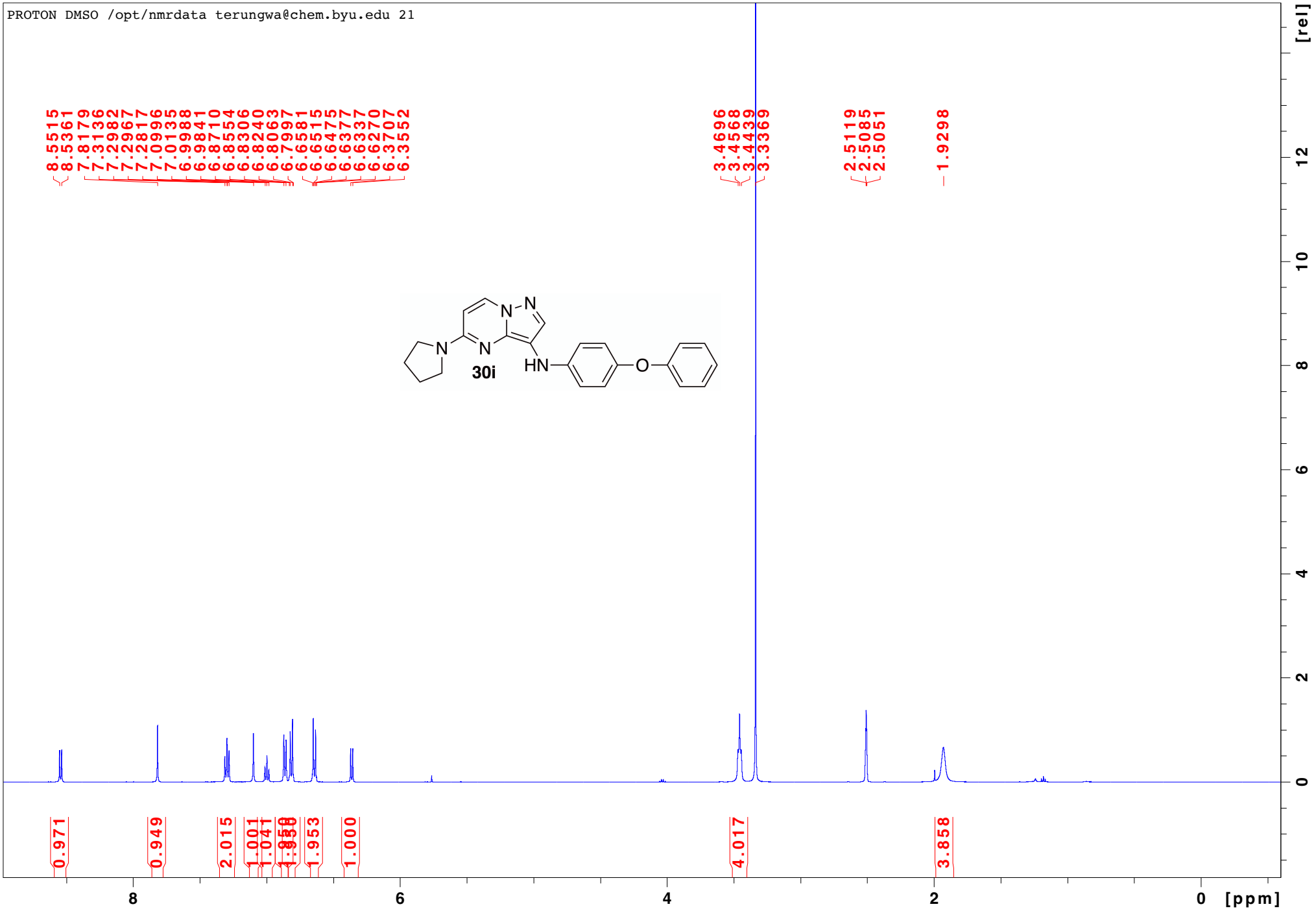
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C13CPD DMSO /opt/nmrdata terungwa@chem.byu.edu 3

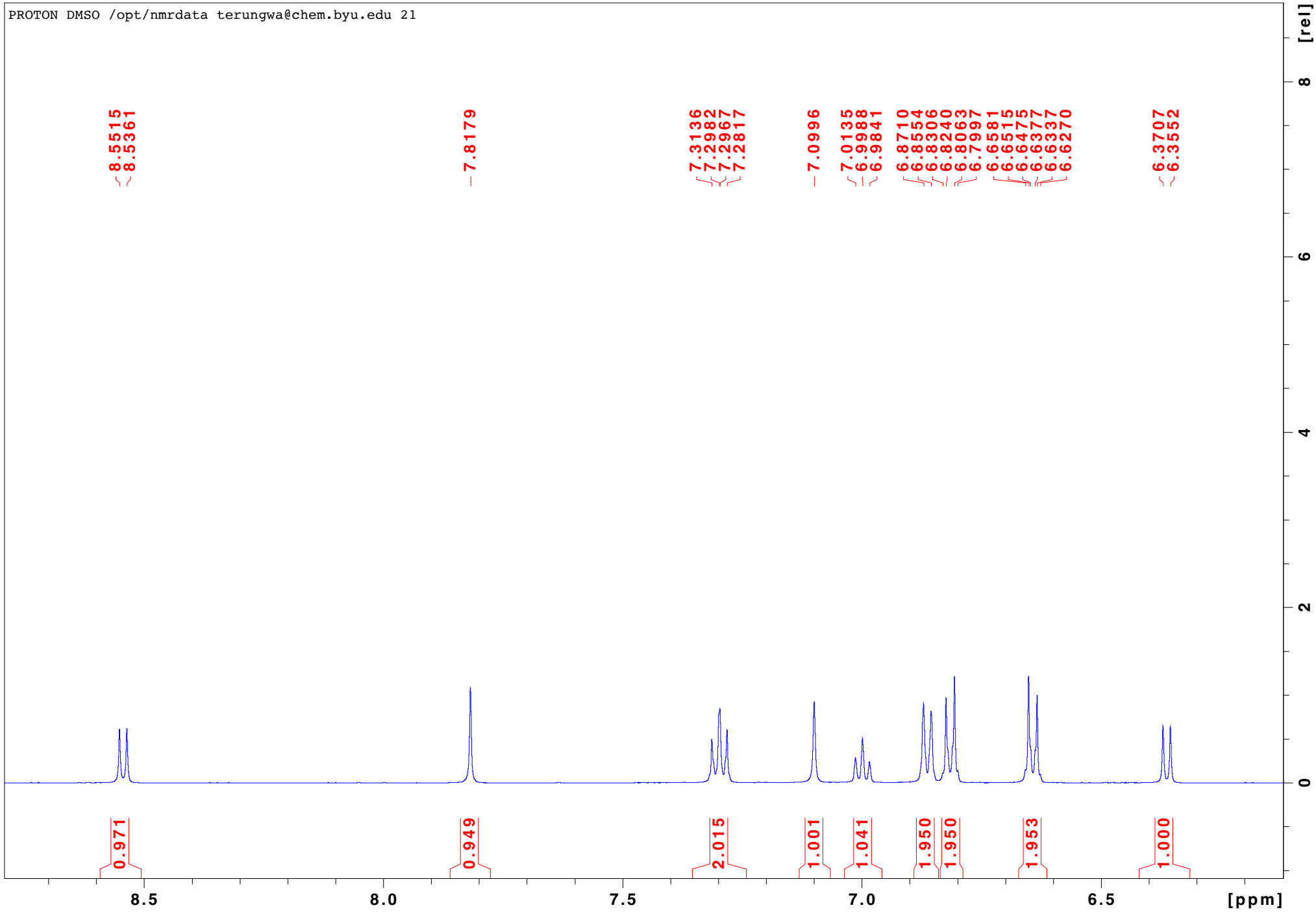


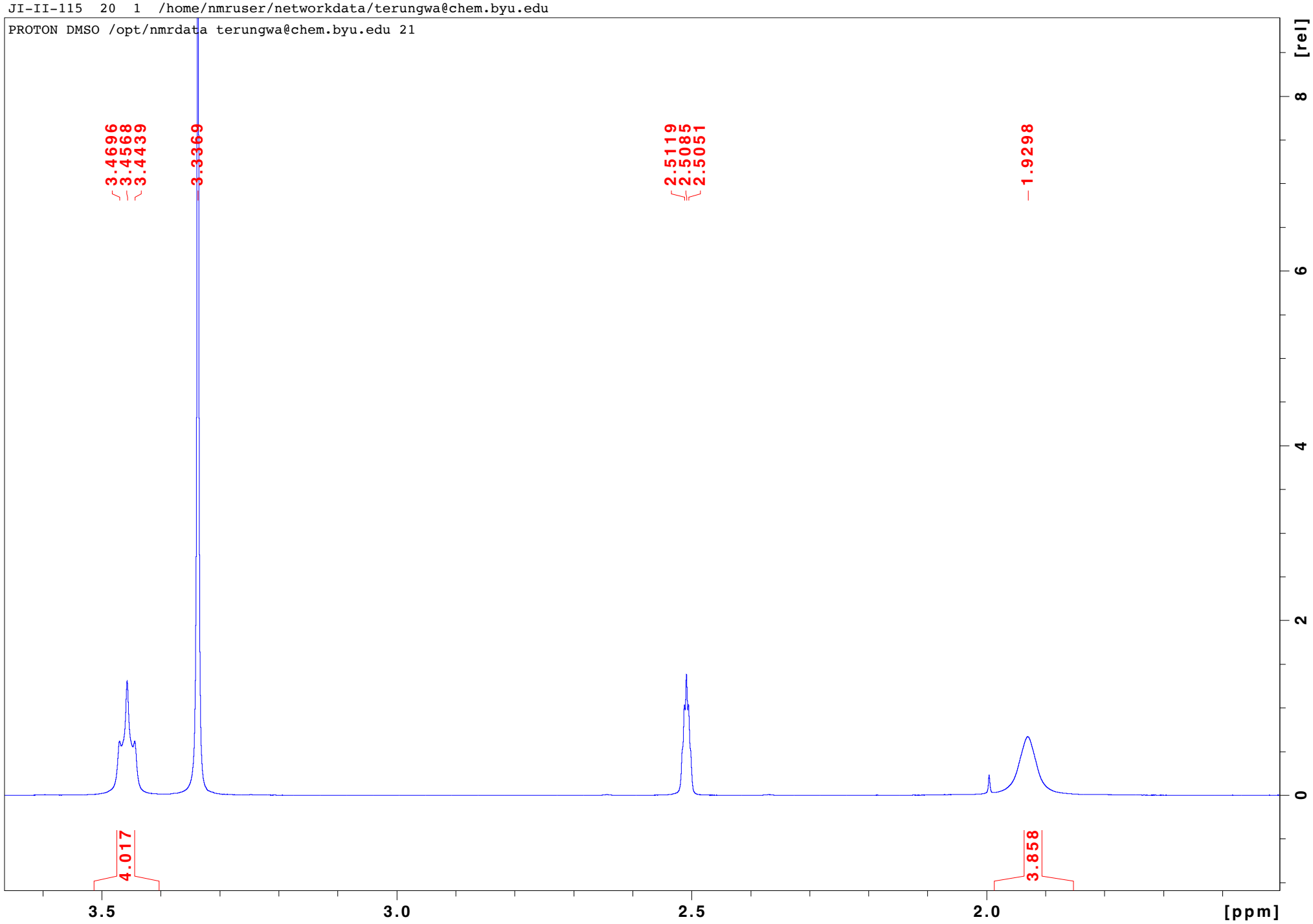
JI-II-115 20 1 /home/nmruser/networkdata/terungwa@chem.byu.edu

PROTON DMSO /opt/nmrdata terungwa@chem.byu.edu 21



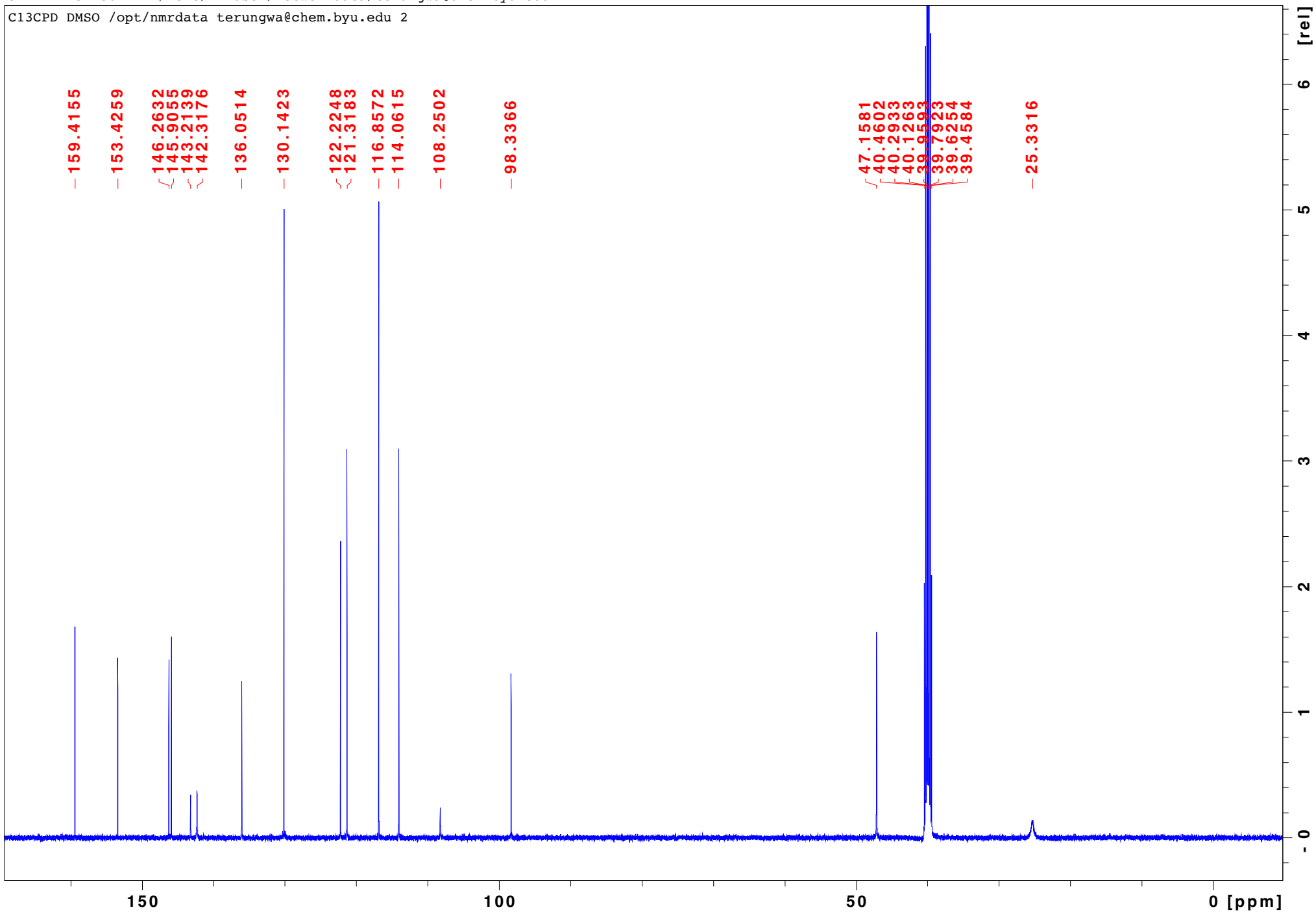
JI-II-115 20 1 /home/nmruser/networkdata/terungwa@chem.byu.edu




JI-II-115 20 1 /home/nmruser/networkdata/terungwa@chem.byu.edu
PROTON DMSO /opt/nmrdata terungwa@chem.byu.edu 21
3.4696
3.4568
3.4439
3.3369
2.5119
2.5085
2.5051
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4.017
3.858
3.5
3.0
2.5
2.0
[ppm]
0
2
4
6
8
[rel]

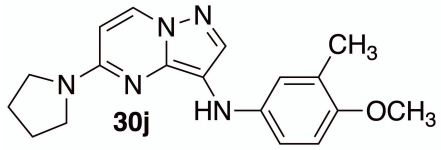
JI-II-115 30 1 /home/nmruser/networkdata/terungwa@chem.byu.edu

C13CPD DMSO /opt/nmrdata terungwa@chem.byu.edu 2



JI-II-117 10 1 /home/nmruser/networkdata/terungwa@chem.byu.edu

PROTON DMSO /opt/nmrdata terungwa@chem.byu.edu 9

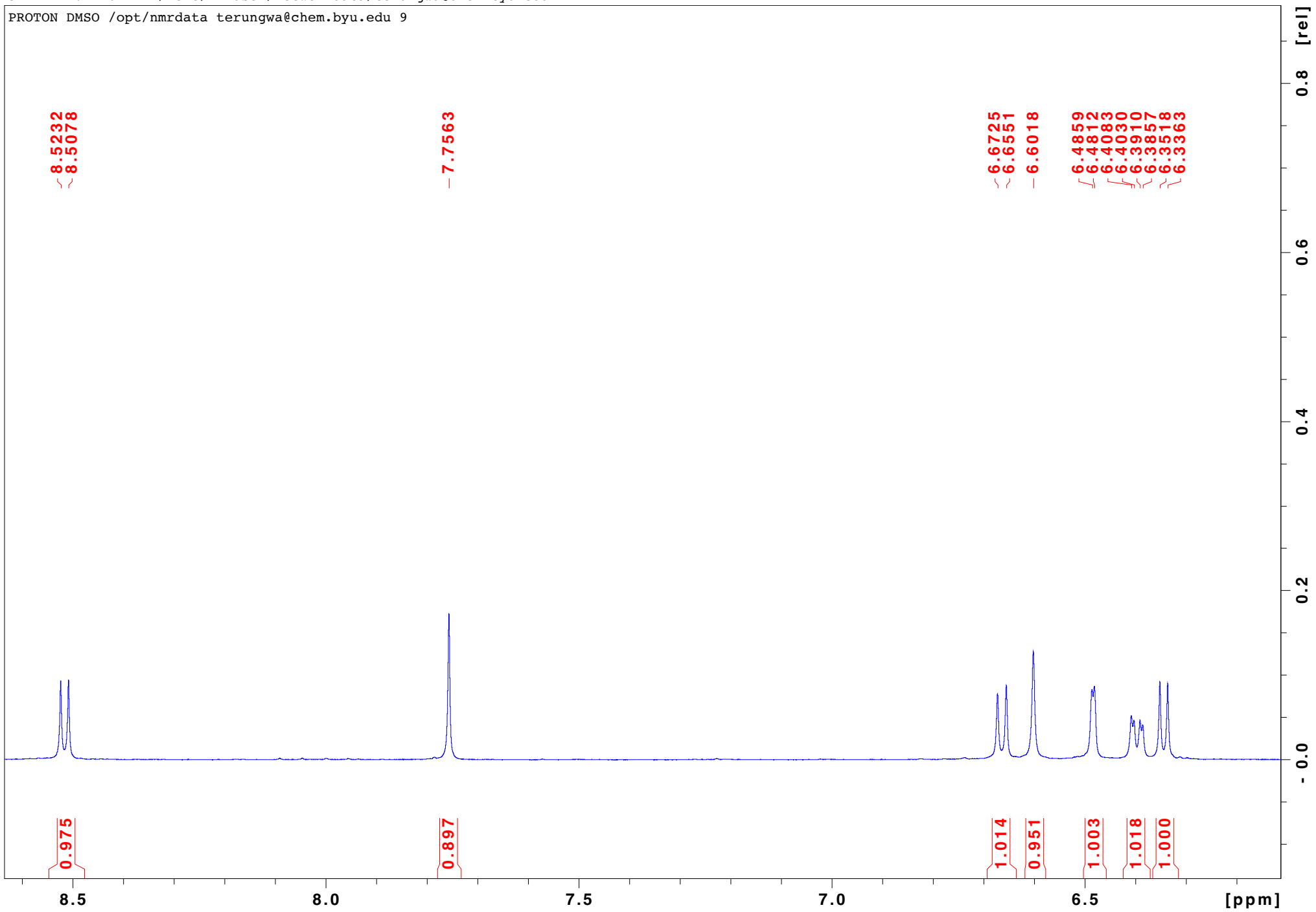


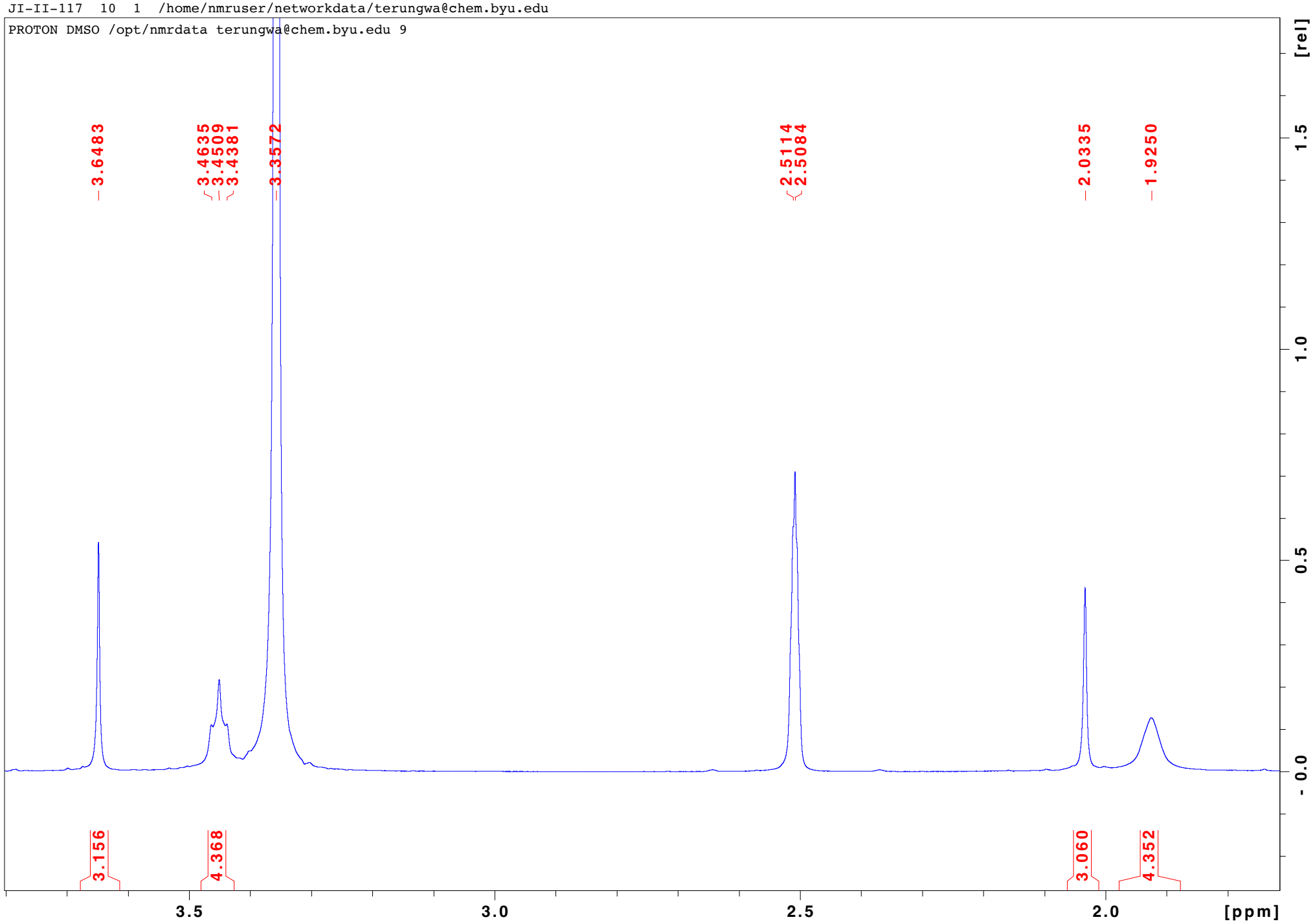
30j

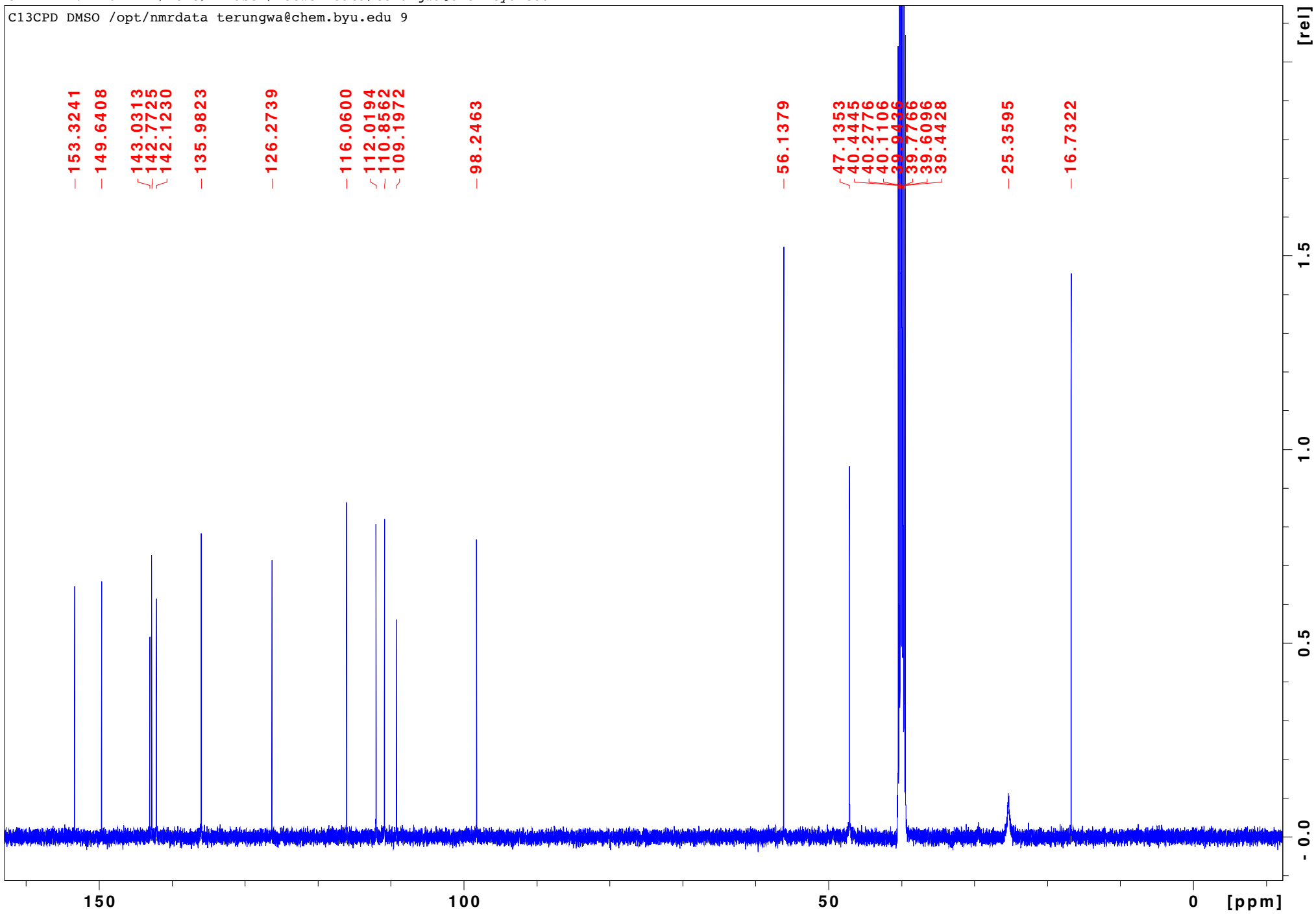
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8.5078
7.7563
6.6725
6.6551
6.6018
6.4859
6.4812
6.4083
6.4030
6.3910
6.3857
6.3518
6.3363
3.6483
3.4635
3.4509
3.4381
3.3572
2.5114
2.5084
2.0335
1.9250

0.975
0.897
3.156
4.368
3.060
4.352

[rel]
1.5
1.0
0.5
- 0.0
8
6
4
2
0
[ppm]


JI-II-117 10 1 /home/nmruser/networkdata/terungwa@chem.byu.edu
PROTON DMSO /opt/nmrdata terungwa@chem.byu.edu 9
8.5232
8.5078
7.7563
6.6725
6.6551
6.6018
6.4859
6.4812
6.4083
6.4030
6.3910
6.3857
6.3518
6.3363
0.975
0.897
1.014
0.951
1.003
1.018
1.000
8.5
8.0
7.5
7.0
6.5
[ppm]
- 0.0
0.2
0.4
0.6
0.8
[rel]

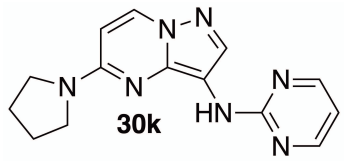

JI-II-117 10 1 /home/nmruser/networkdata/terungwa@chem.byu.edu
PROTON DMSO /opt/nmrdata terungwa@chem.byu.edu 9
3.6483
3.4635
3.4509
3.4381
3.3572
2.5114
2.5084
2.0335
1.9250
3.156
4.368
3.060
4.352
3.5
3.0
2.5
2.0
[ppm]
[rel]
1.5
1.0
0.5
- 0.0


JI-II-117 20 1 /home/nmruser/networkdata/terungwa@chem.byu.edu
C13CPD DMSO /opt/nmrdata terungwa@chem.byu.edu 9
153.3241
149.6408
143.0313
142.7725
142.1230
135.9823
126.2739
116.0600
112.0194
110.8562
109.1972
98.2463
56.1379
47.1353
40.4445
40.2776
40.1106
39.9436
39.7766
39.6096
39.4428
25.3595
16.7322
[rel]
1.5
1.0
0.5
- 0.0
150
100
50
0
[ppm]

JI-II-123 20 1 /home/nmruser/networkdata/terungwa@chem.byu.edu

PROTON DMSO /opt/nmrdata terungwa@chem.byu.edu 5

8.5378
8.5224
8.3209
8.3118
8.3024
7.9529
6.6679
6.6584
6.6489
6.3623
6.3469
3.4820
3.4688
3.4556
3.3526
2.5120
2.5085
2.5050
1.9317
1.2393

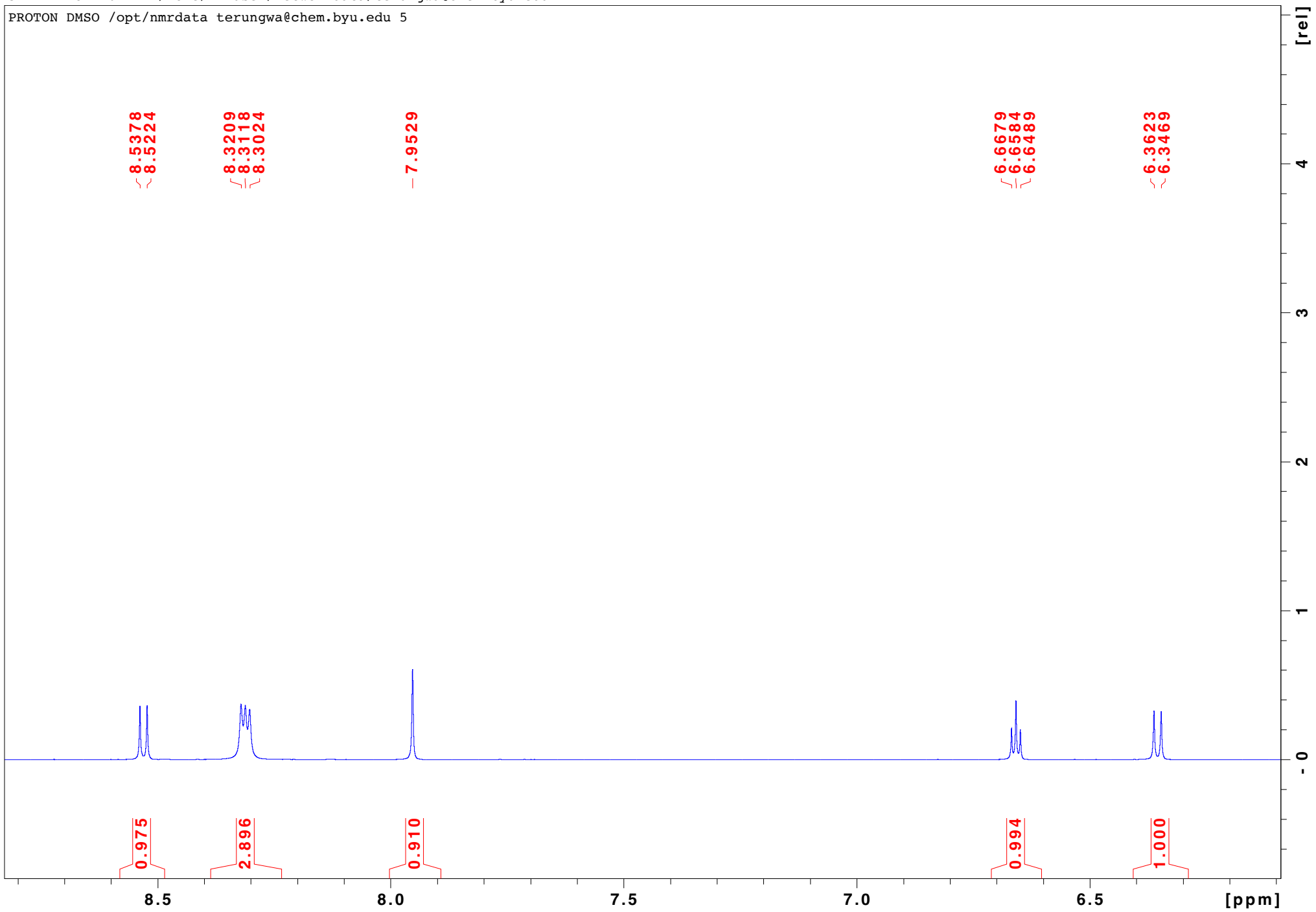


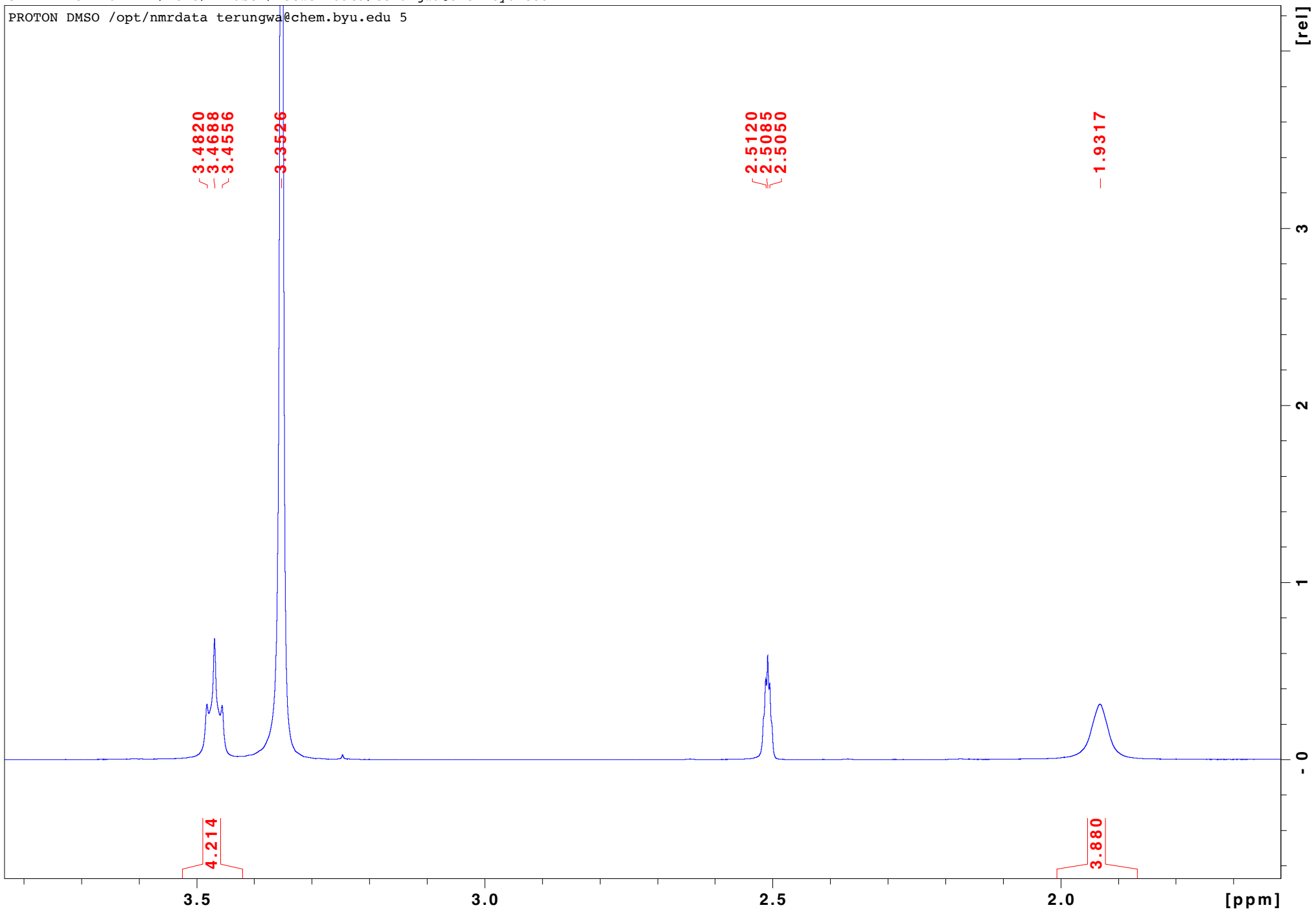
30k

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2.896
0.910
0.994
1.000
4.214
3.880

8
6
4
2
0 [ppm]

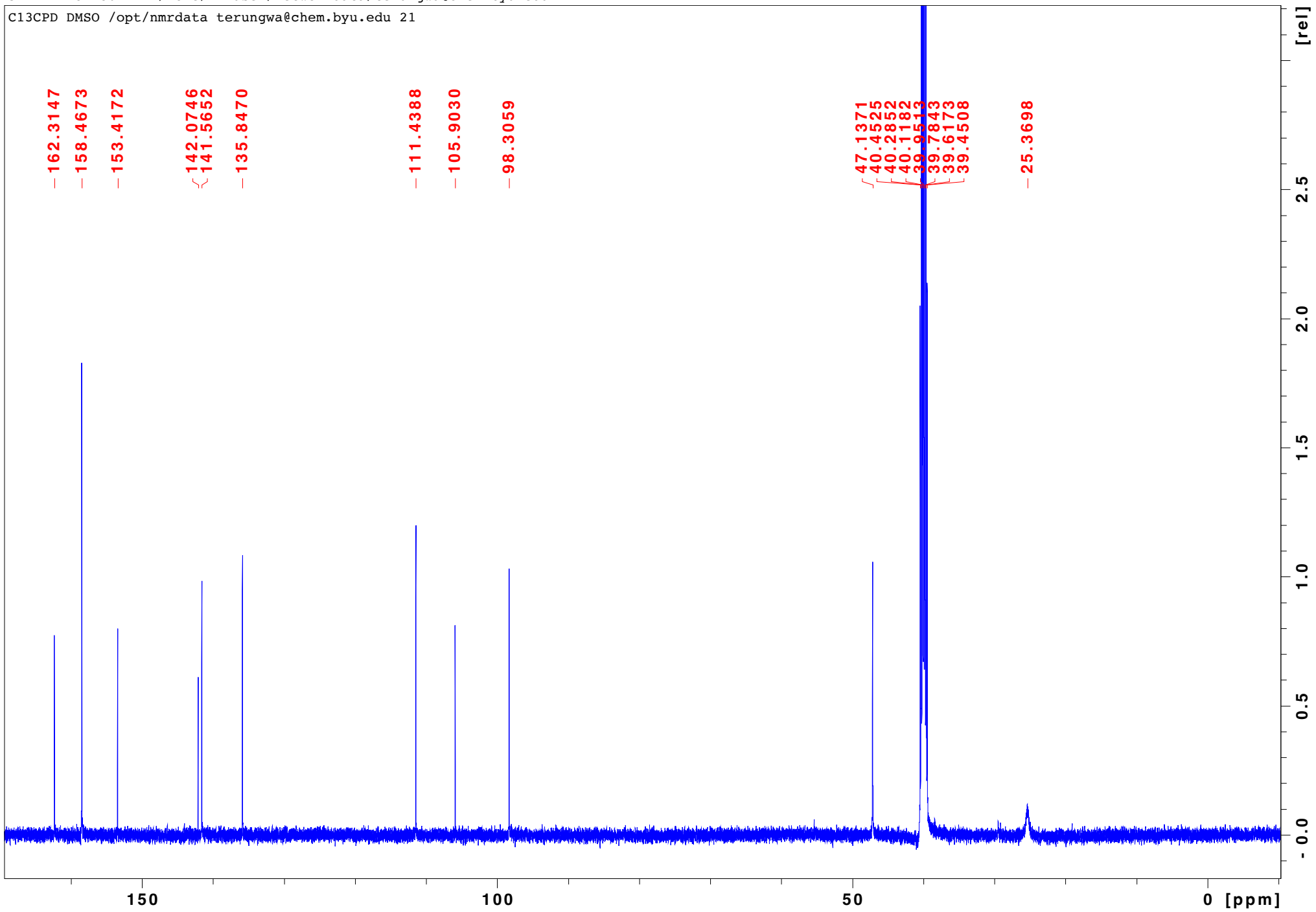
- 0
1
2
3
4
[rel]


JI-II-123 20 1 /home/nmruser/networkdata/terungwa@chem.byu.edu
PROTON DMSO /opt/nmrdata terungwa@chem.byu.edu 5
8.5378
8.5224
8.3209
8.3118
8.3024
7.9529
6.6679
6.6584
6.6489
6.3623
6.3469
0.975
2.896
0.910
0.994
1.000
8.5
8.0
7.5
7.0
6.5
[ppm]
[rel]
- 0
1
2
3
4


JI-II-123 20 1 /home/nmruser/networkdata/terungwa@chem.byu.edu
PROTON DMSO /opt/nmrdata terungwa@chem.byu.edu 5
3.4820
3.4688
3.4556
3.3526
2.5120
2.5085
2.5050
1.9317
4.214
3.880
3.5
3.0
2.5
2.0
[ppm]
[rel]
- 0
1
2
3

JI-II-123 30 1 /home/nmruser/networkdata/terungwa@chem.byu.edu

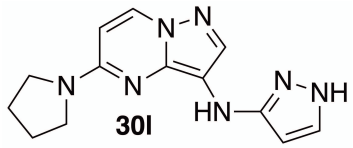
C13CPD DMSO /opt/nmrdata terungwa@chem.byu.edu 21



JI-II-125 20 1 /home/nmruser/networkdata/terungwa@chem.byu.edu

PROTON DMSO /opt/nmrdata terungwa@chem.byu.edu 3

8.6489
8.6333
7.9957
7.2595
7.2559
6.4751
6.4595
5.6471
5.4147
5.4110
3.4995
3.3412
2.5119
2.5084
2.5048
1.9730



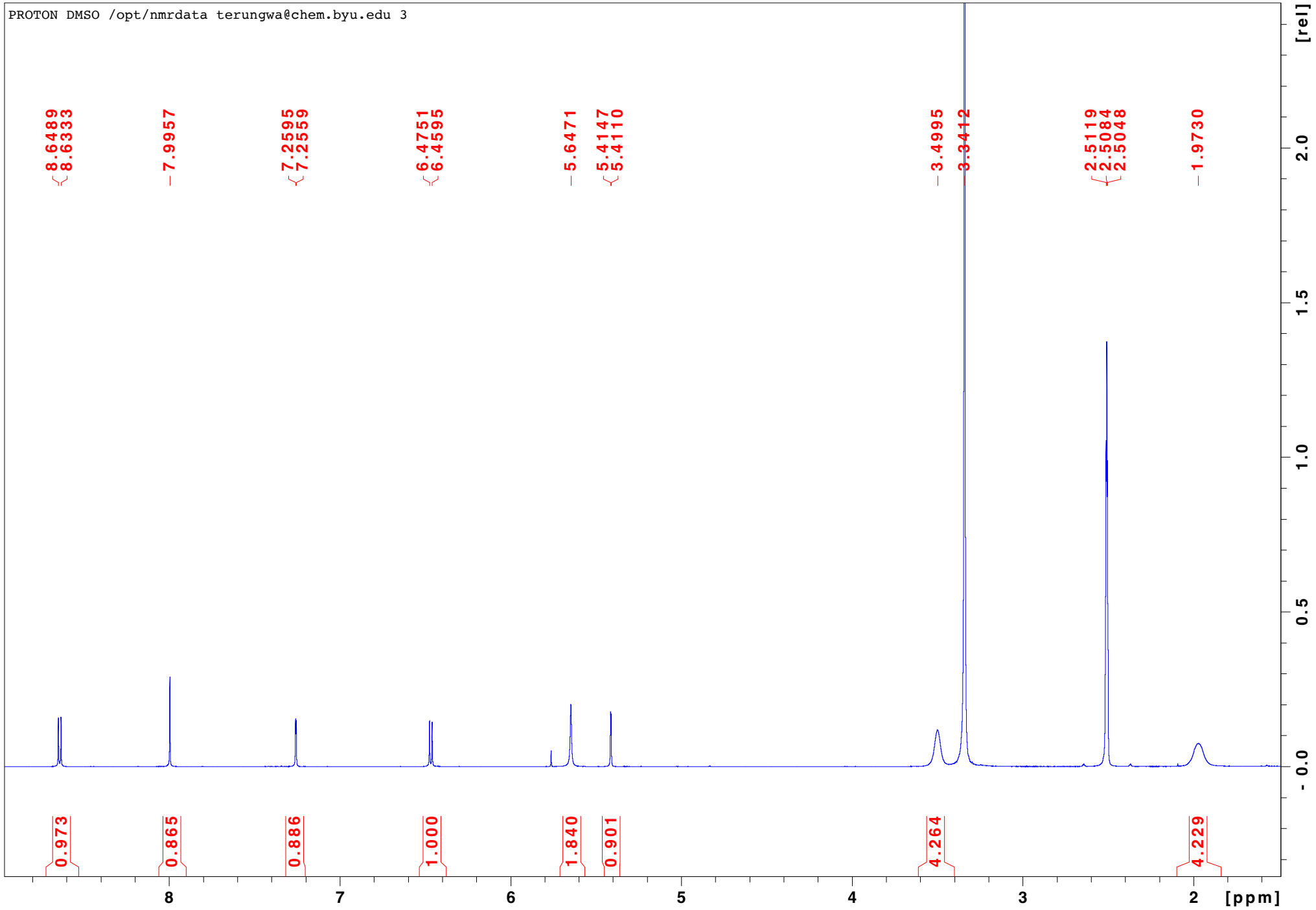
30l

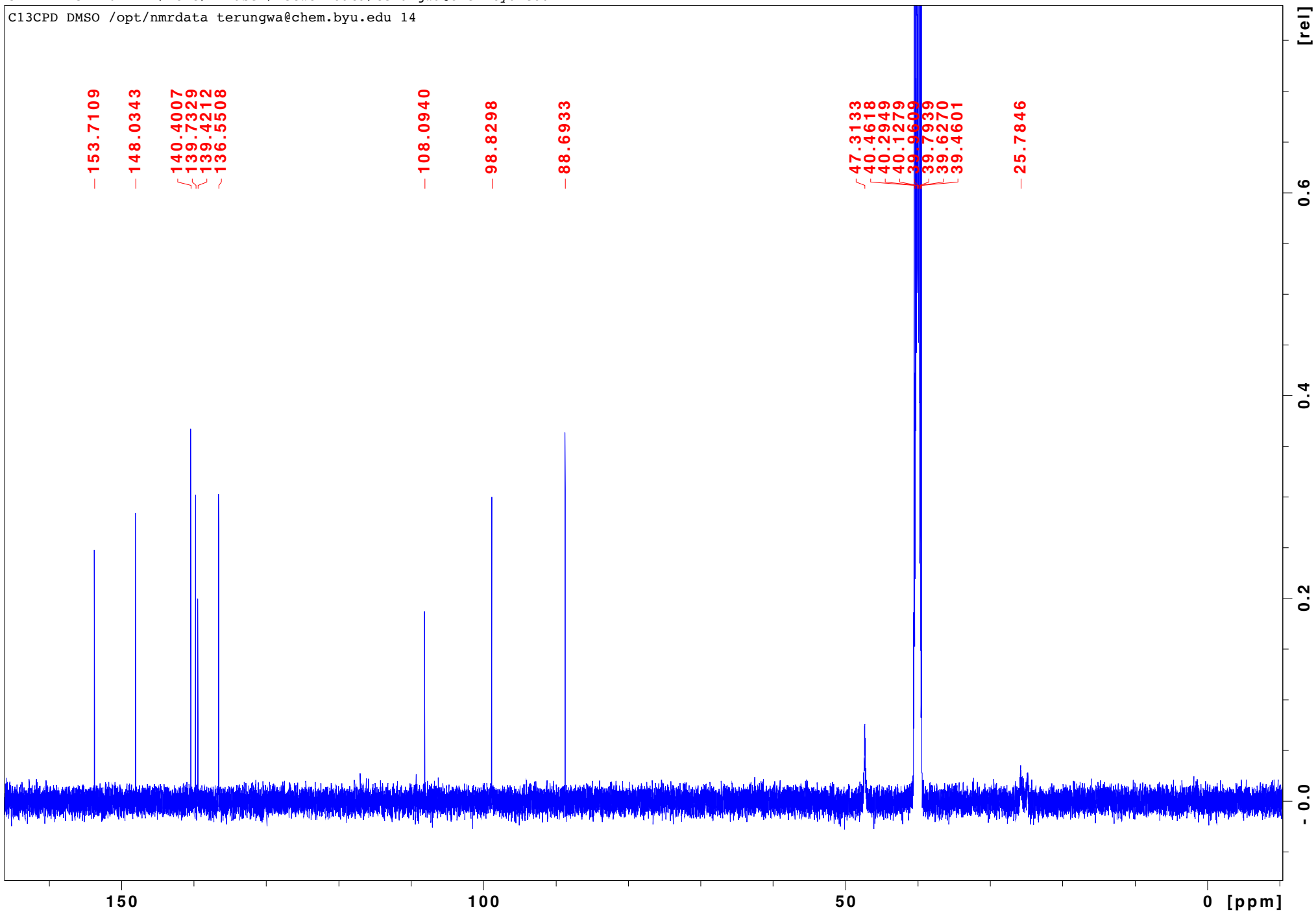
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0.901
4.264
4.229

[rel]
2.0
1.5
1.0
0.5
- 0.0

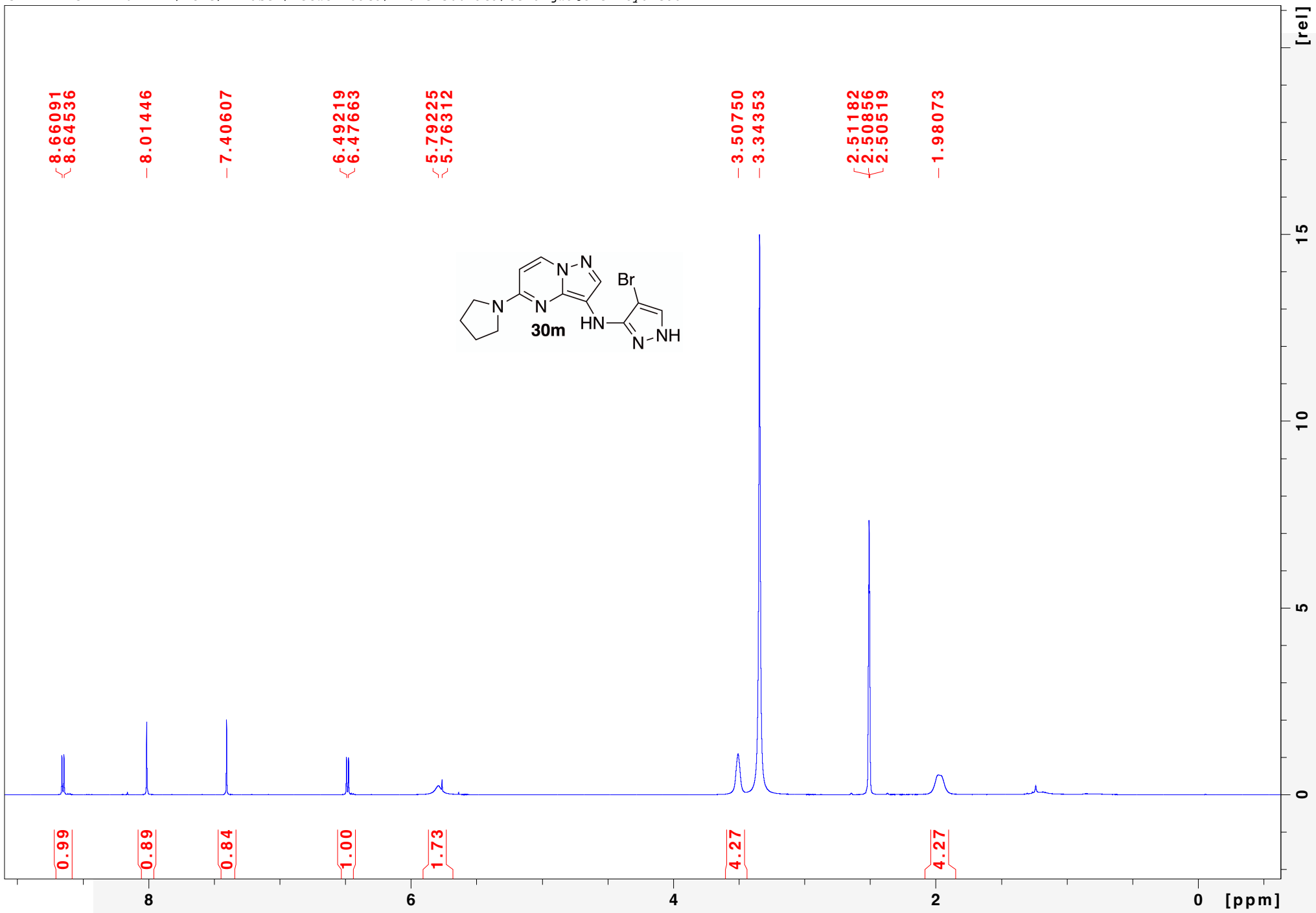
8
6
4
2
0
[ppm]

JI-II-125 20 1 /home/nmruser/networkdata/terungwa@chem.byu.edu

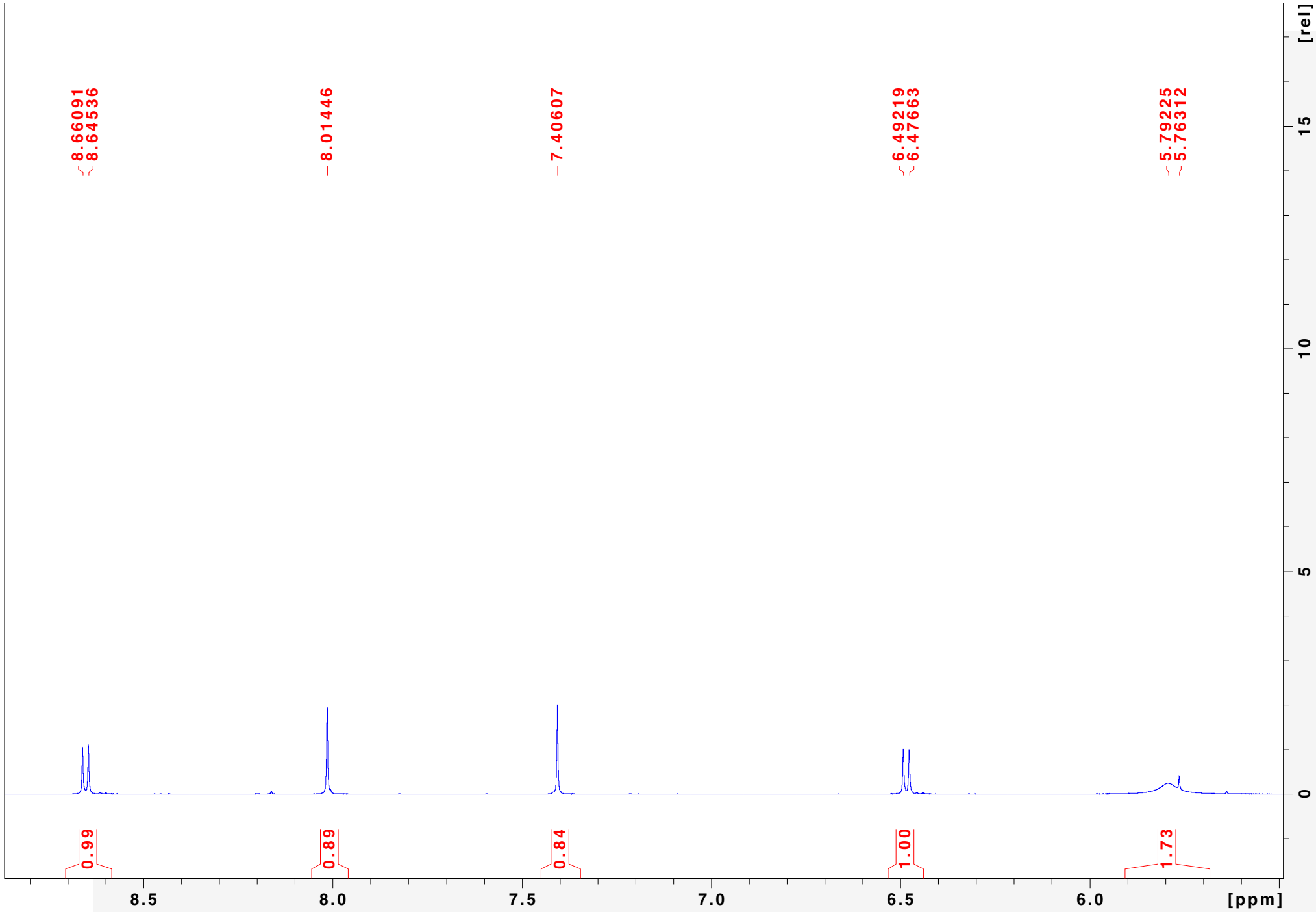



JI-II-125 40 1 /home/nmruser/networkdata/terungwa@chem.byu.edu
C13CPD DMSO /opt/nmrdata terungwa@chem.byu.edu 14
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148.0343
140.4007
139.7329
139.4212
136.5508
108.0940
98.8298
88.6933
47.3133
40.4618
40.2949
40.1279
39.9609
39.7939
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39.4601
25.7846
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0.6
0.4
0.2
- 0.0
150
100
50
0 [ppm]

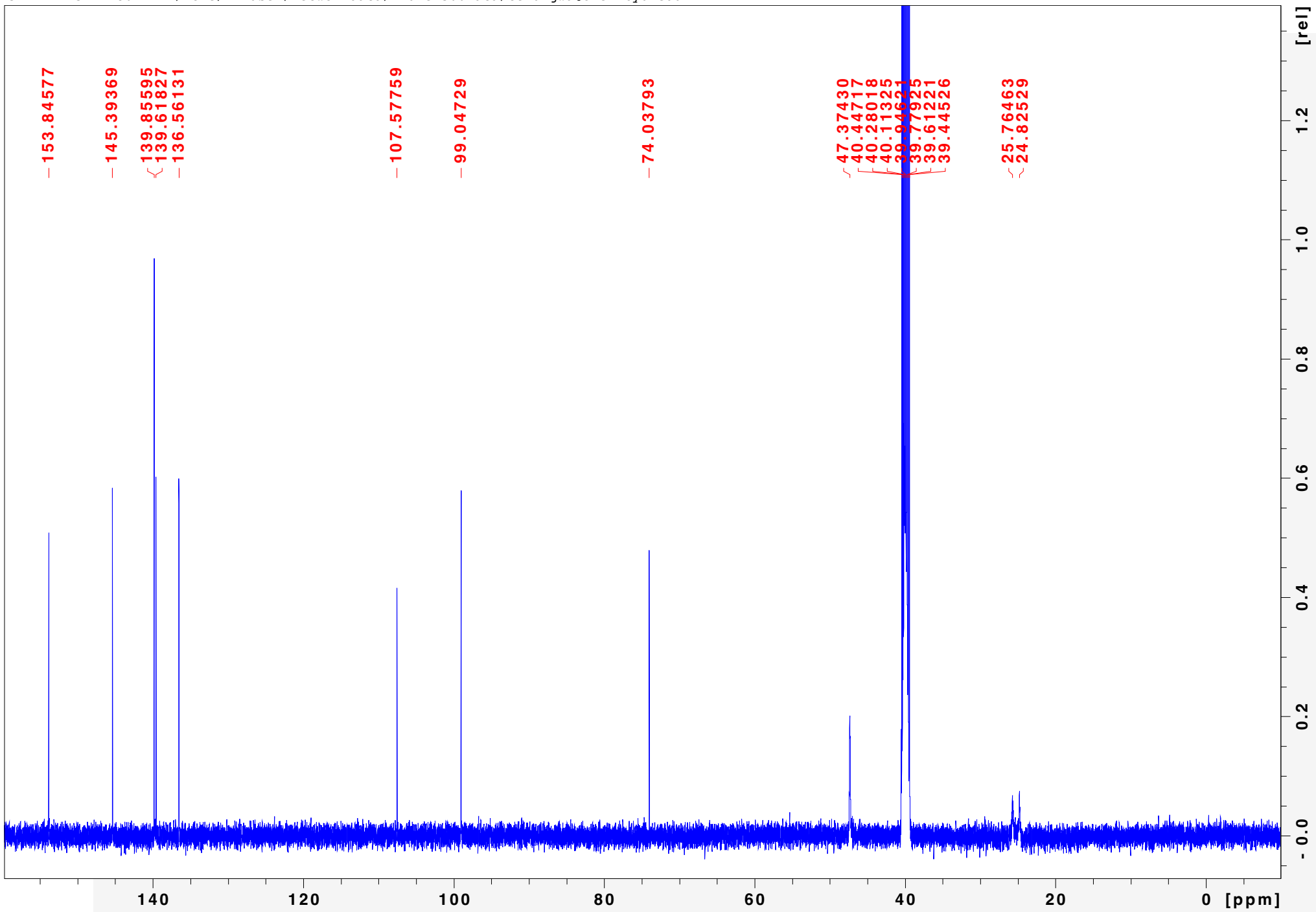
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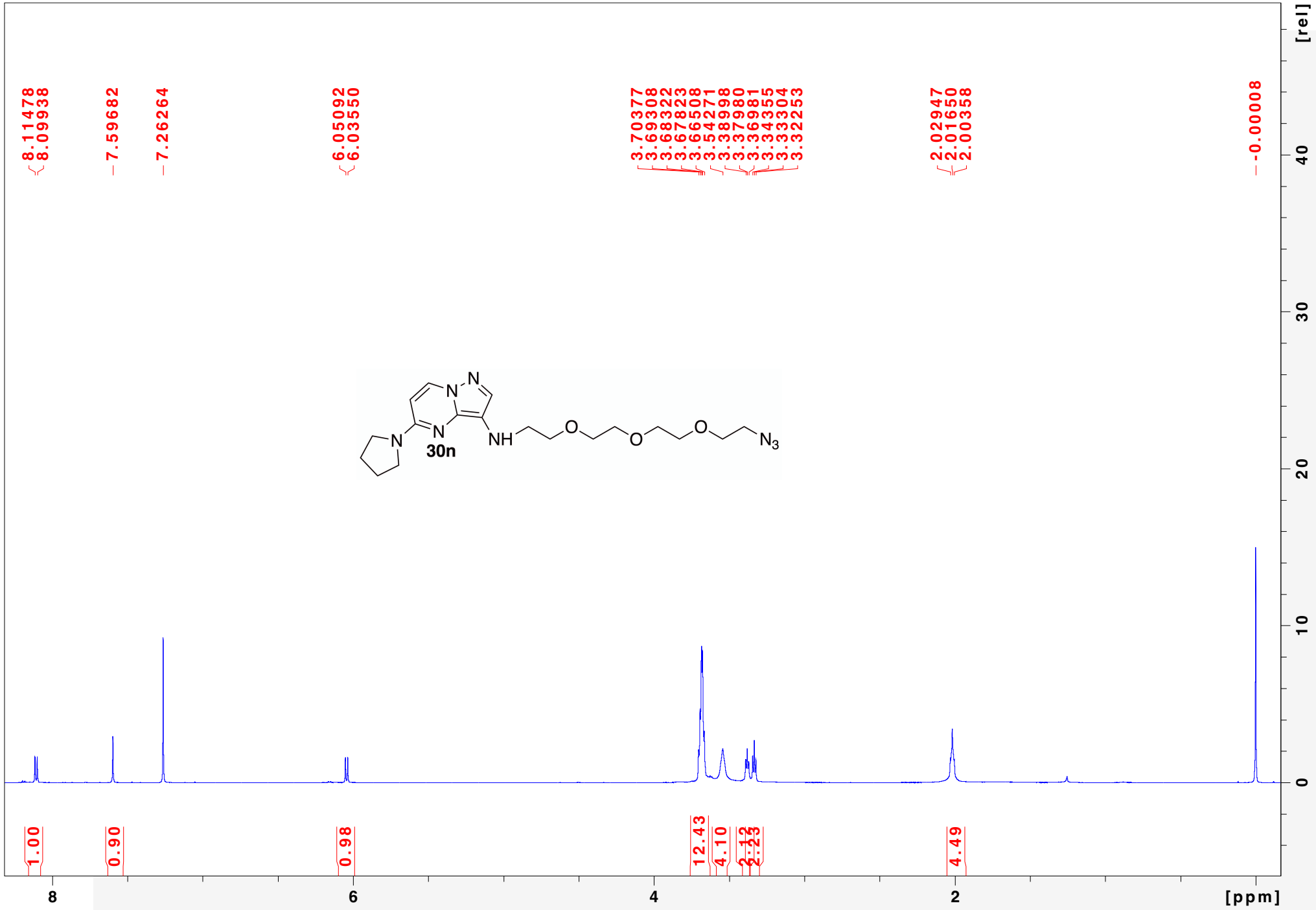
JI-II-125Br 10 1 /home/nmruser/networkdata/Bruker500Data/terungwa@chem.byu.edu

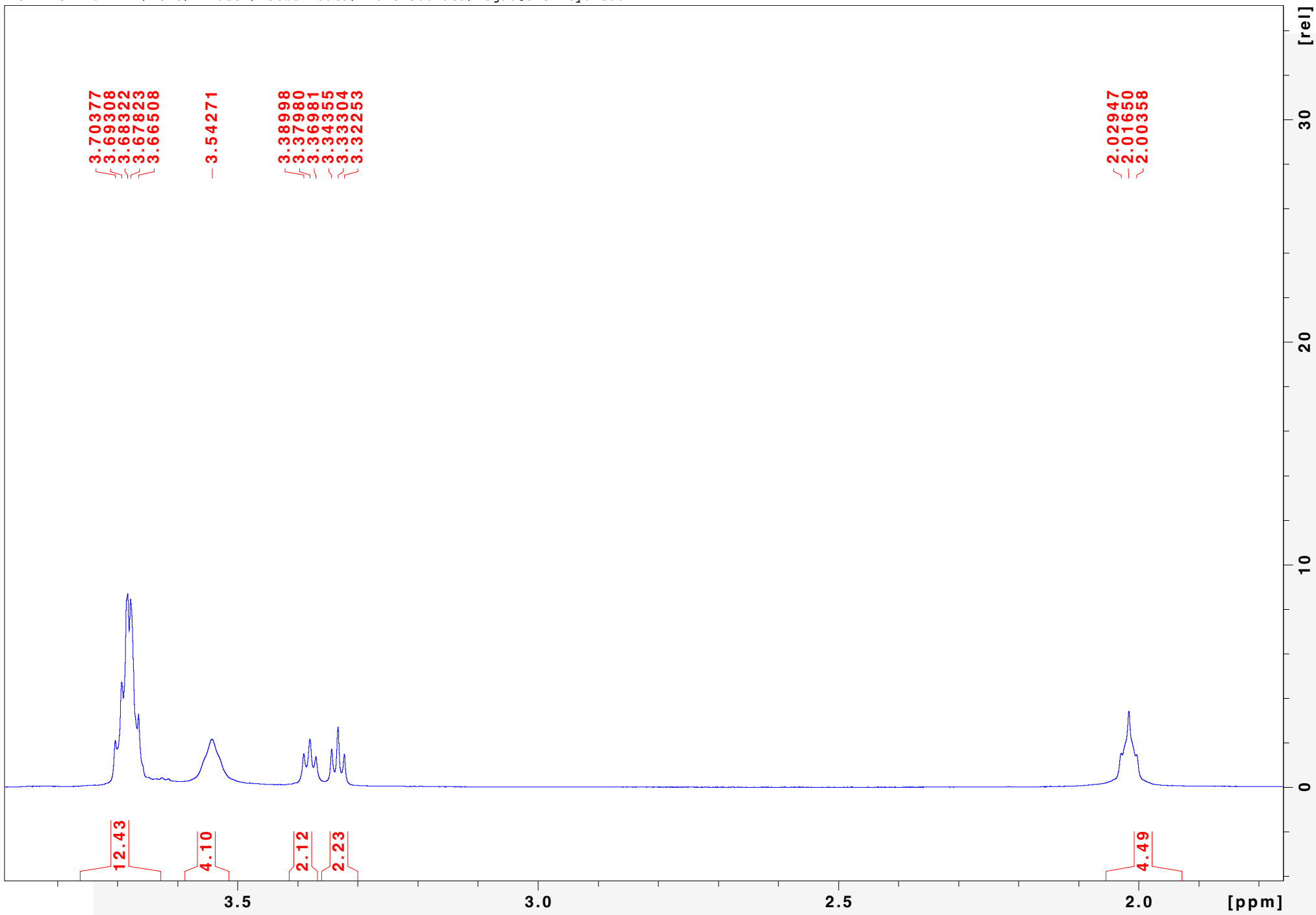


JI-II-125Br 30 1 /home/nmruser/networkdata/Bruker500Data/terungwa@chem.byu.edu

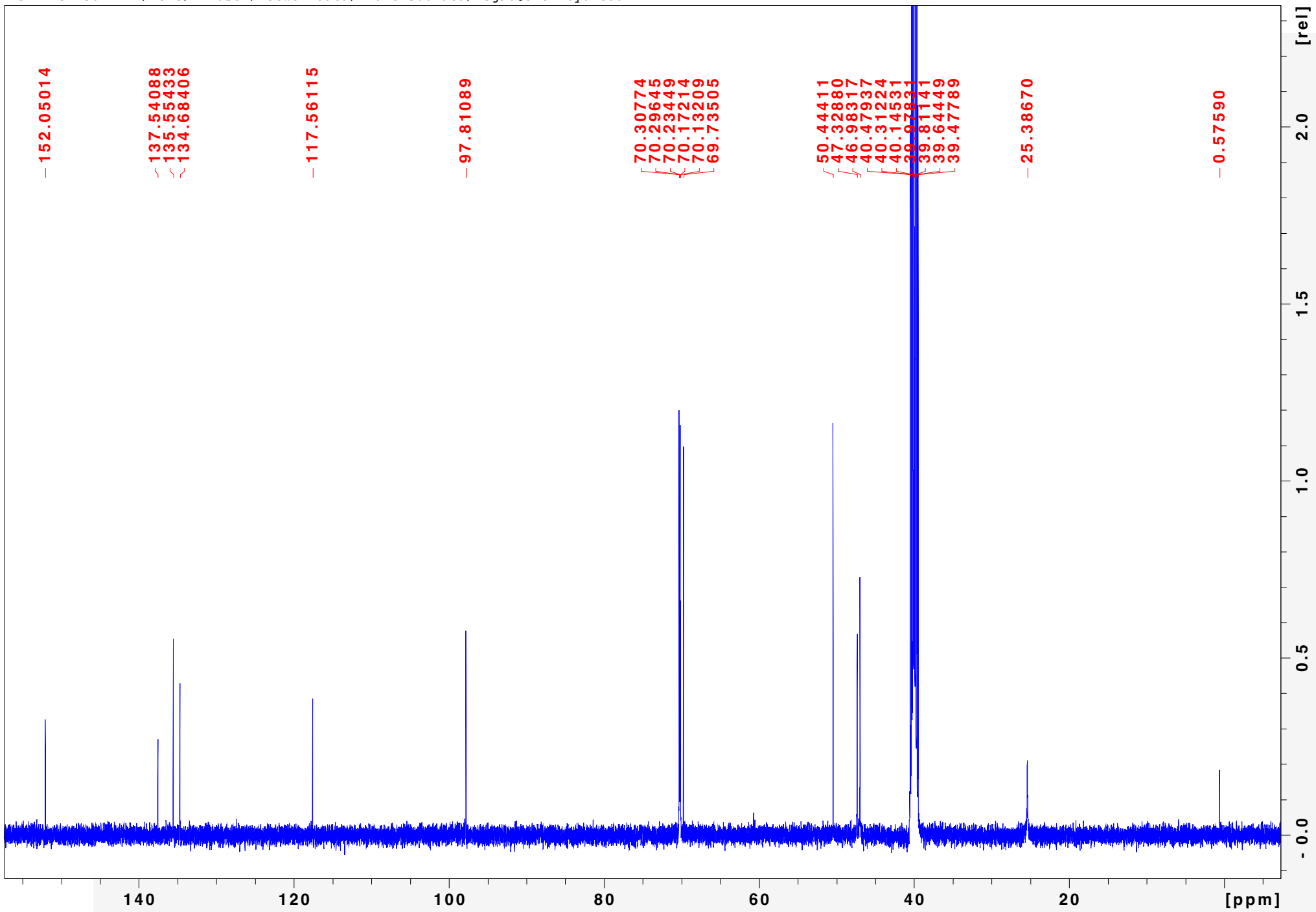


LG-I-43 40 1 /home/nmruser/networkdata/Bruker500Data/log96@chem.byu.edu

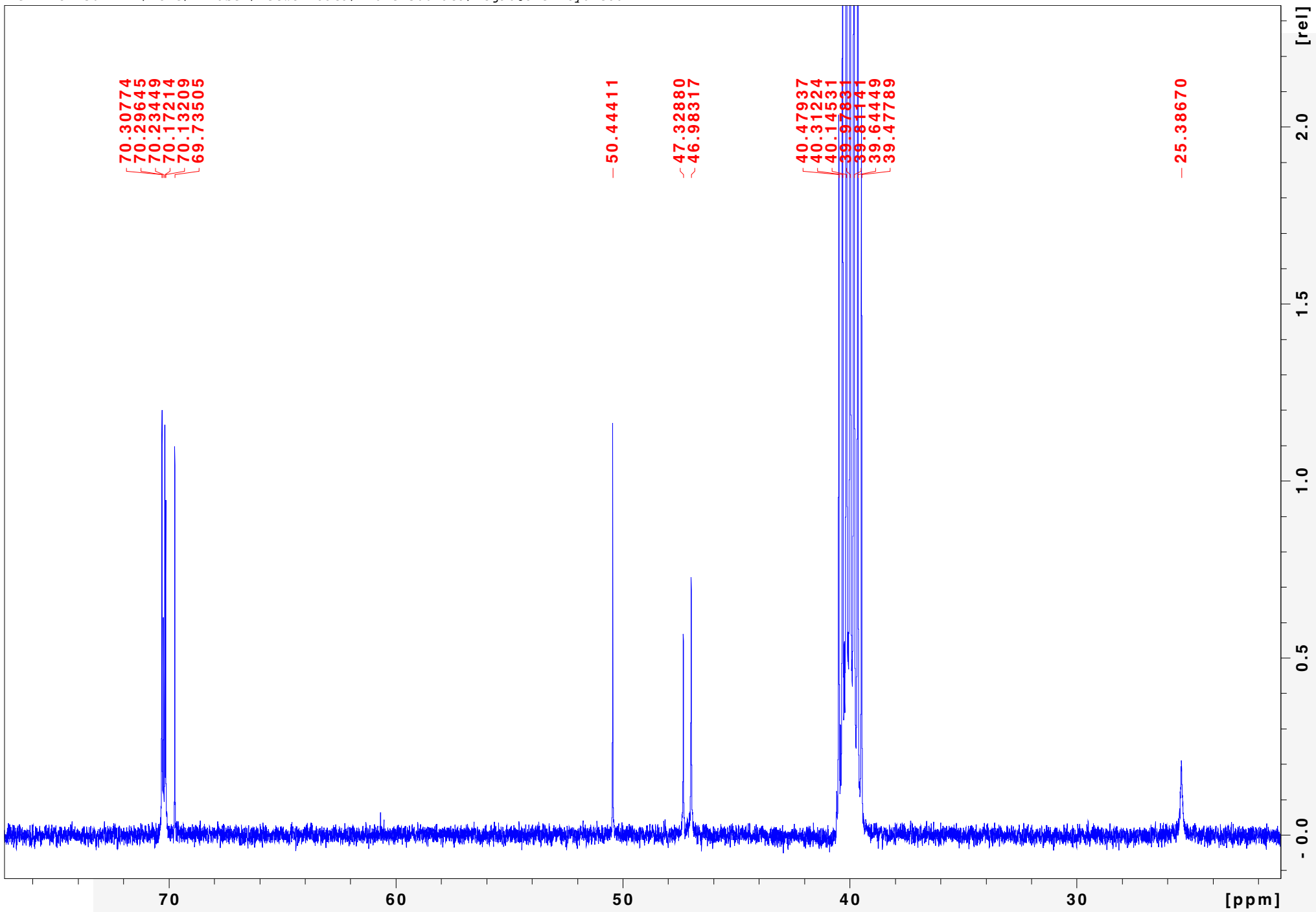



LG-I-43 40 1 /home/nmruser/networkdata/Bruker500Data/log96@chem.byu.edu
3.70377
3.69308
3.68322
3.67823
3.66508
3.54271
3.38998
3.37980
3.36981
3.34355
3.33304
3.32253
2.02947
2.01650
2.00358
12.43
4.10
2.12
2.23
4.49
[rel]
[ppm]
3.5
3.0
2.5
2.0
0
10
20
30

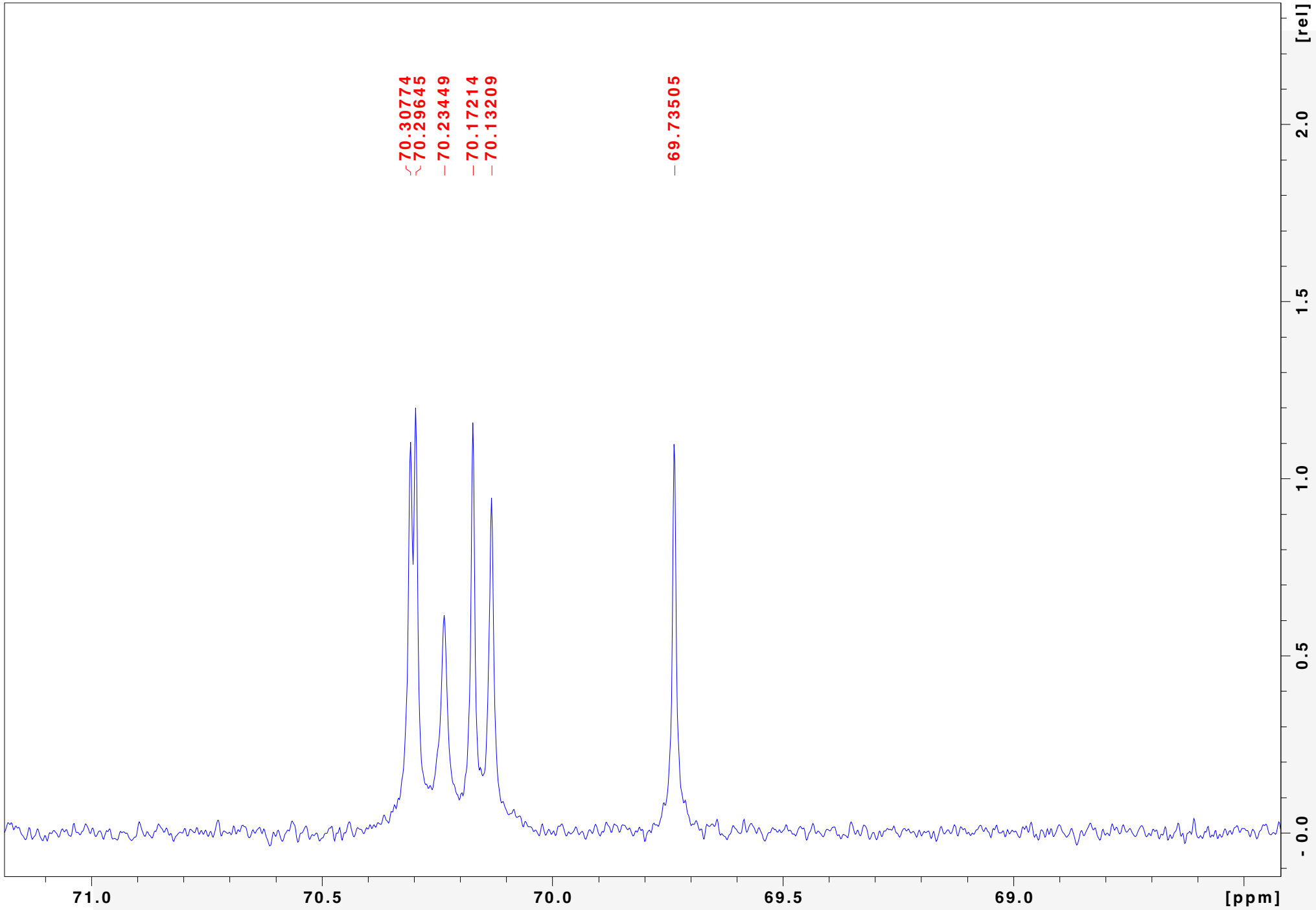
LG-I-43 50 1 /home/nmruser/networkdata/Bruker500Data/log96@chem.byu.edu



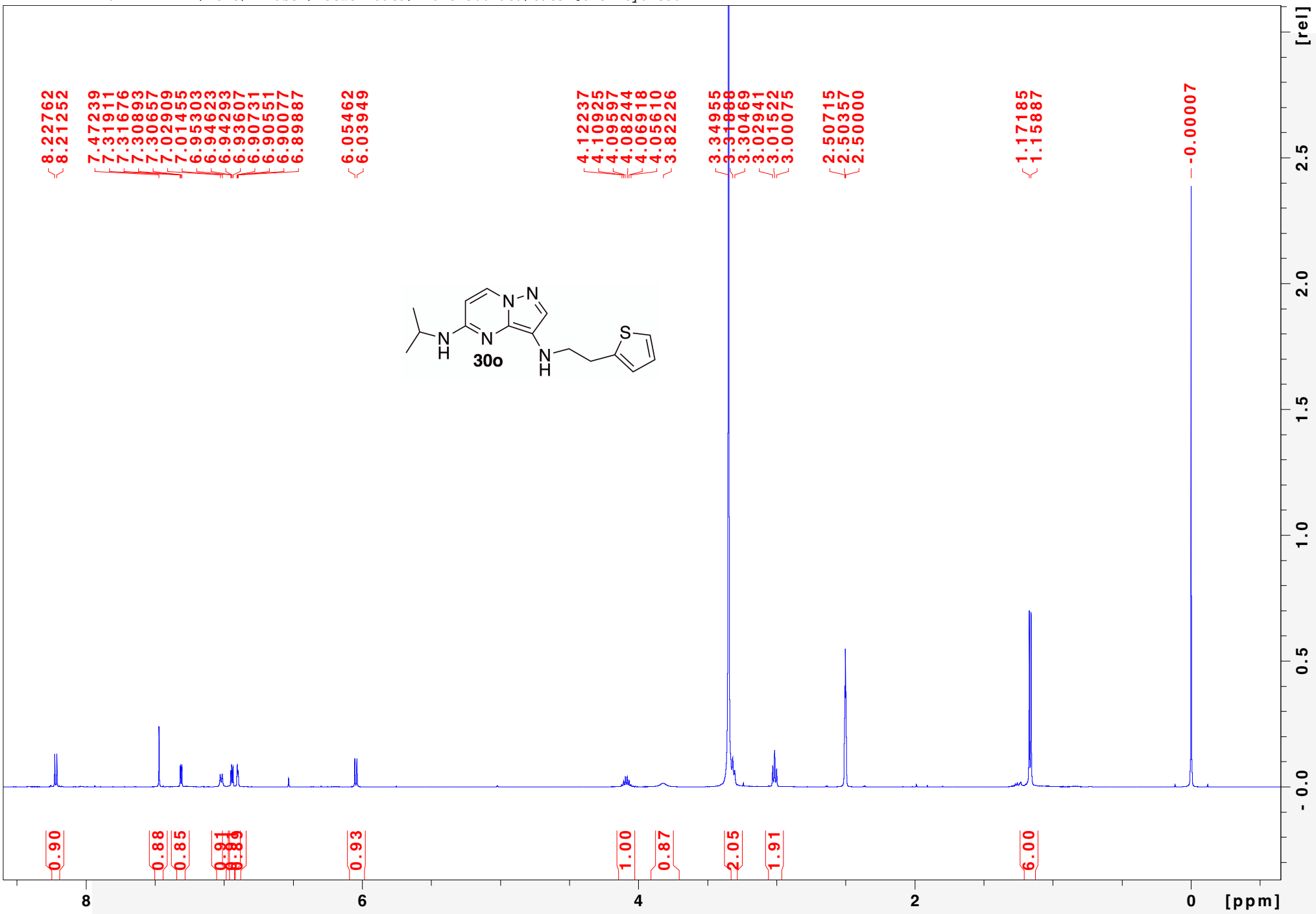
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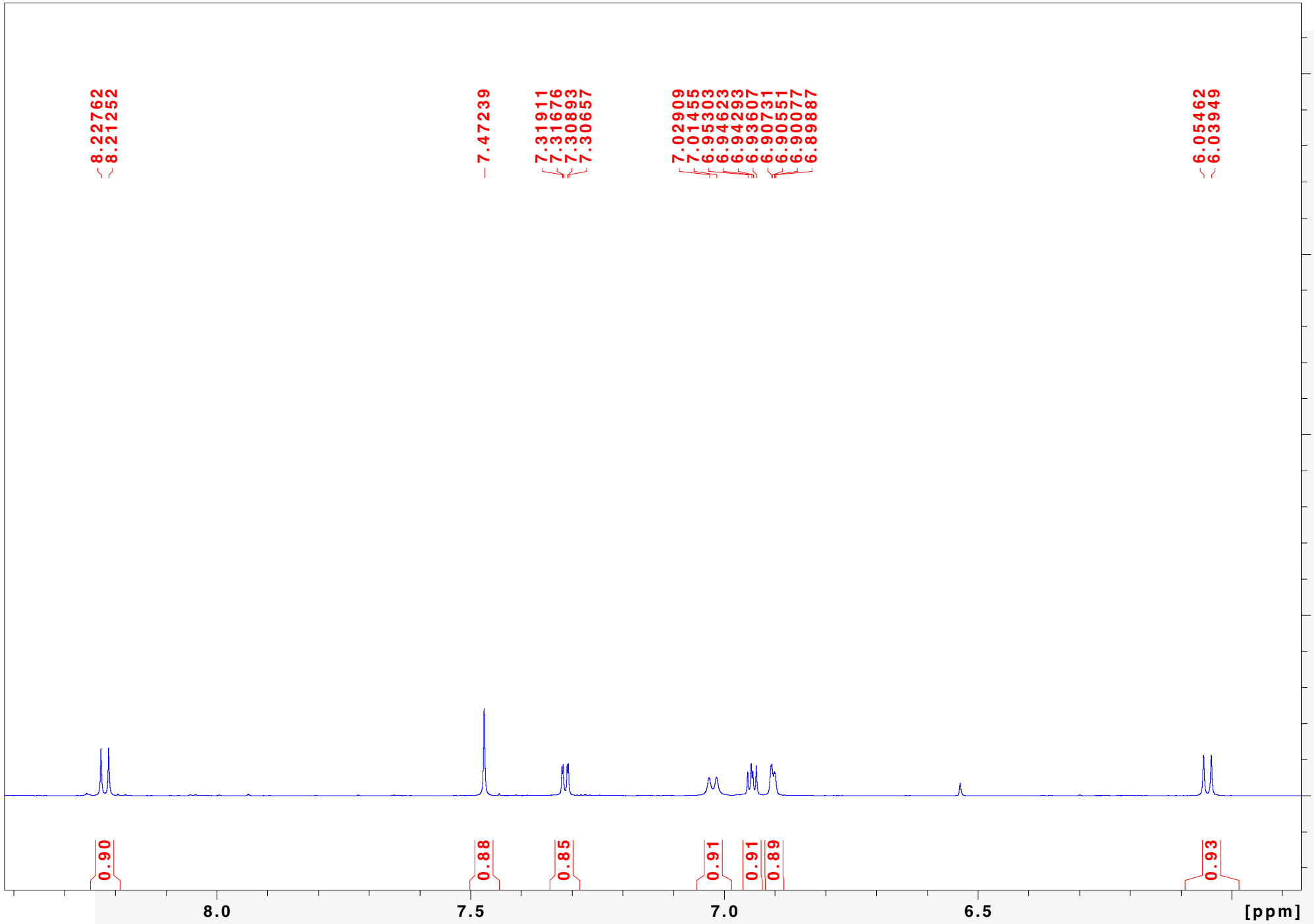
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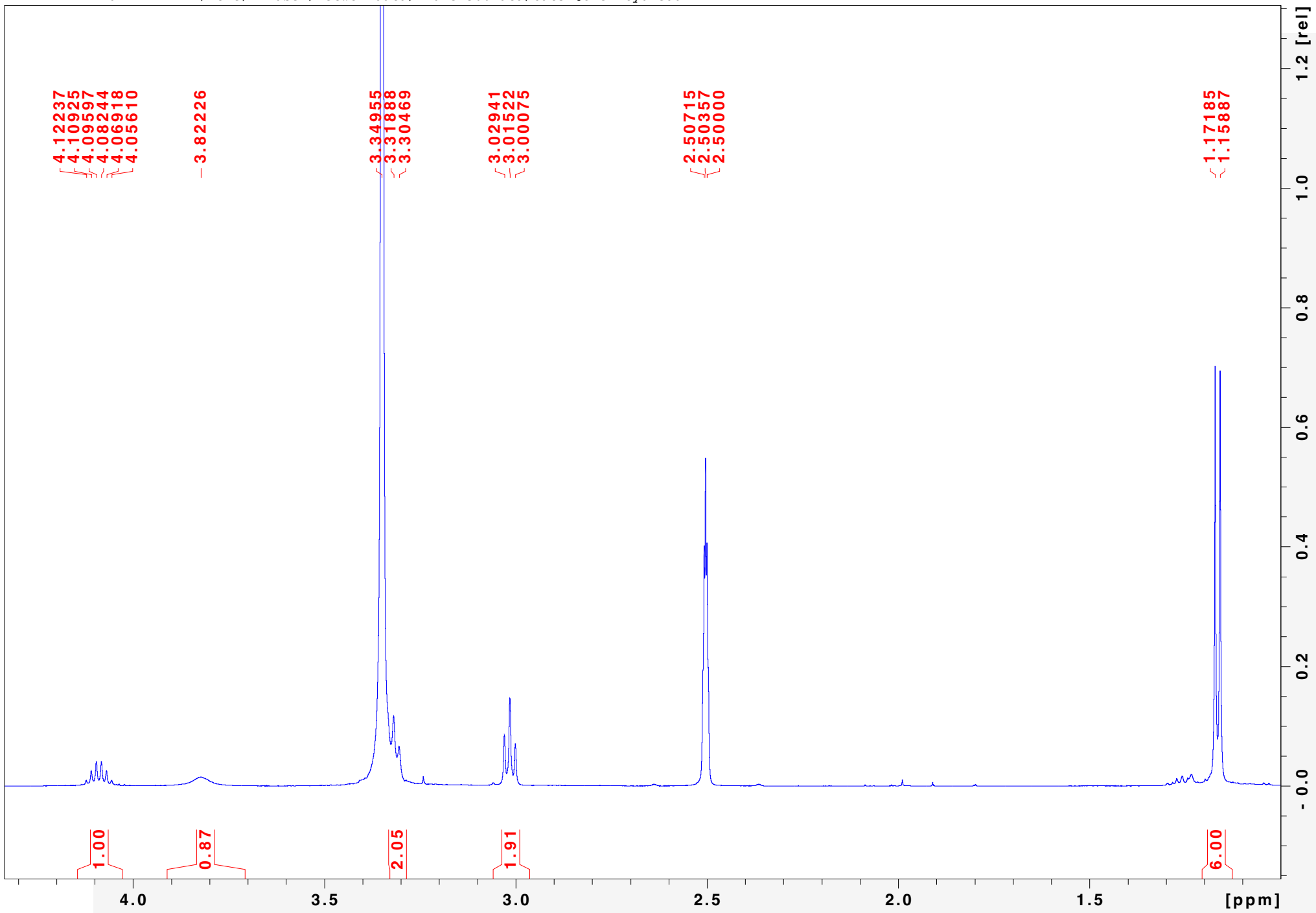


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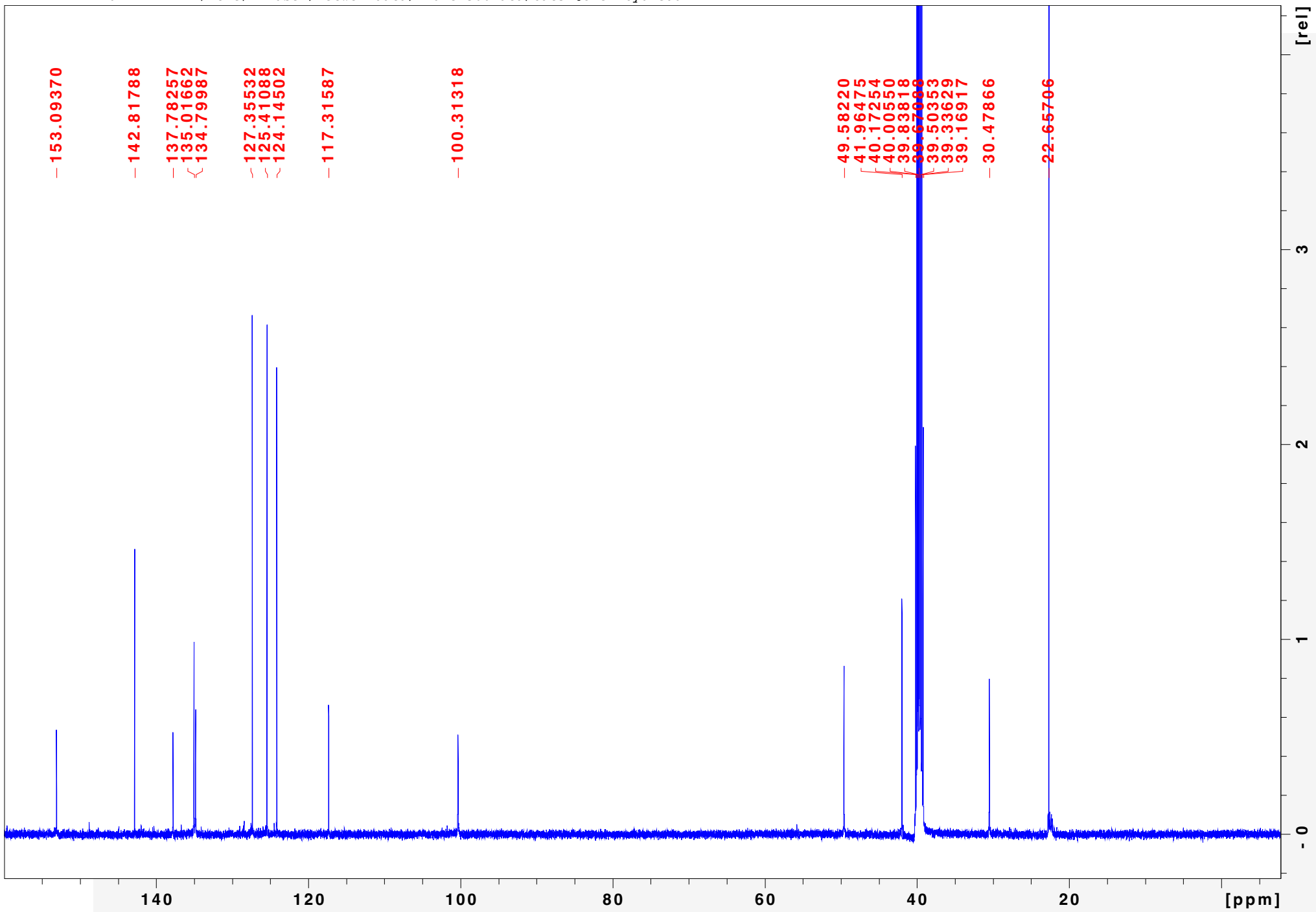


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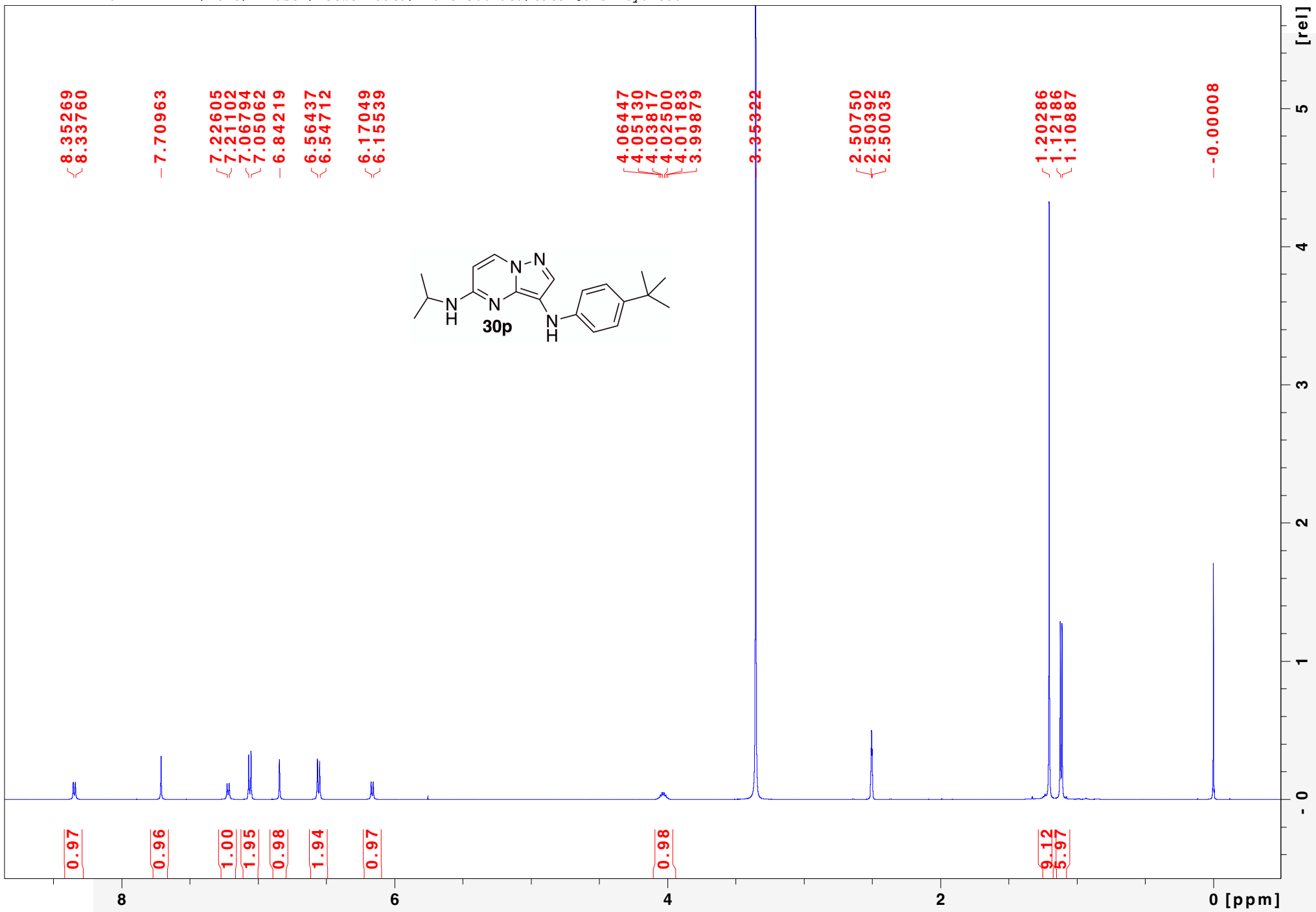



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4.05610
3.82226
3.34955
3.31888
3.30469
3.02941
3.01522
3.00075
2.50715
2.50357
2.50000
1.17185
1.15887
1.00
0.87
2.05
1.91
6.00
4.0
3.5
3.0
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1.5
[ppm]
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0.6
0.8
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1.2 [rel]

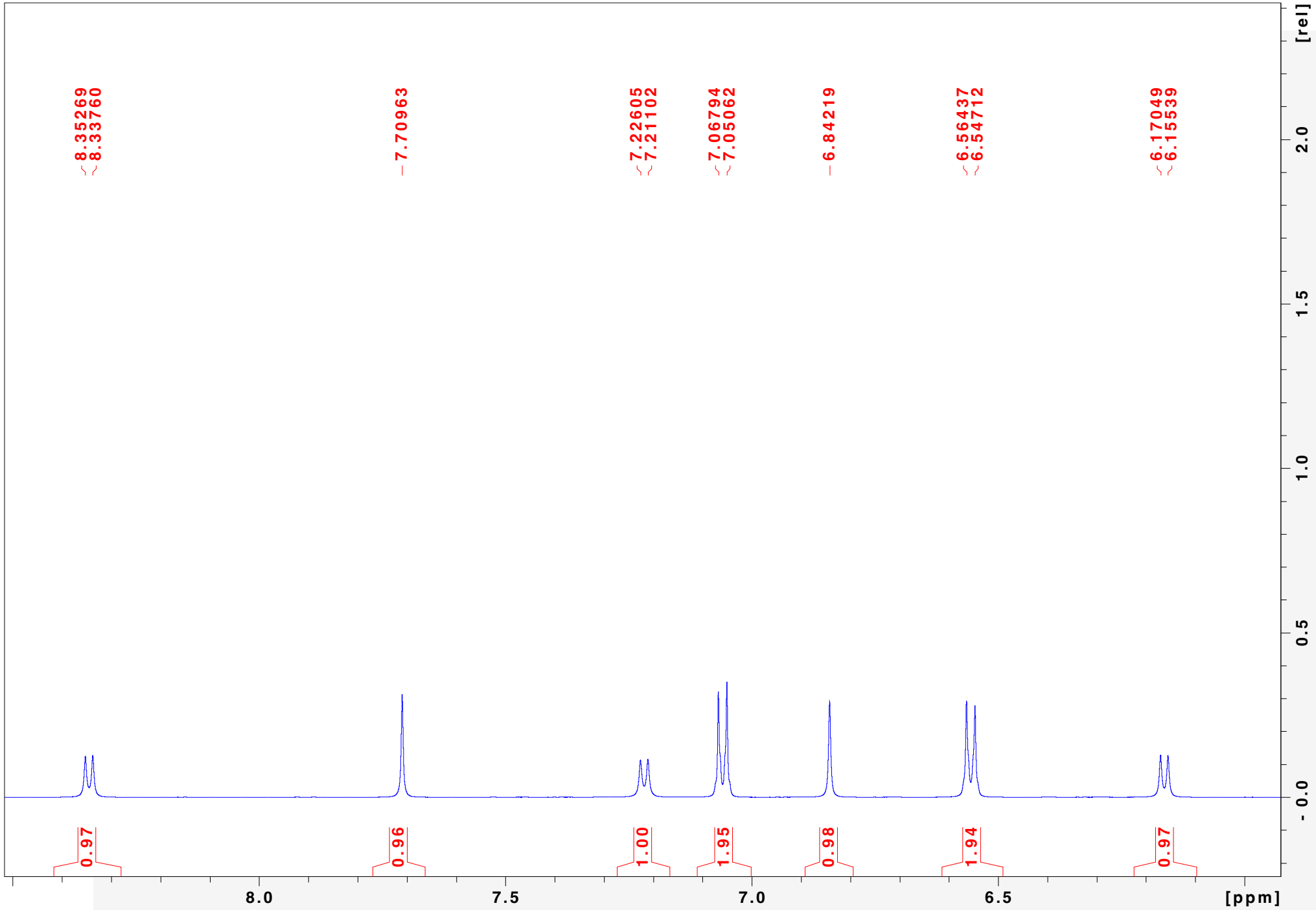
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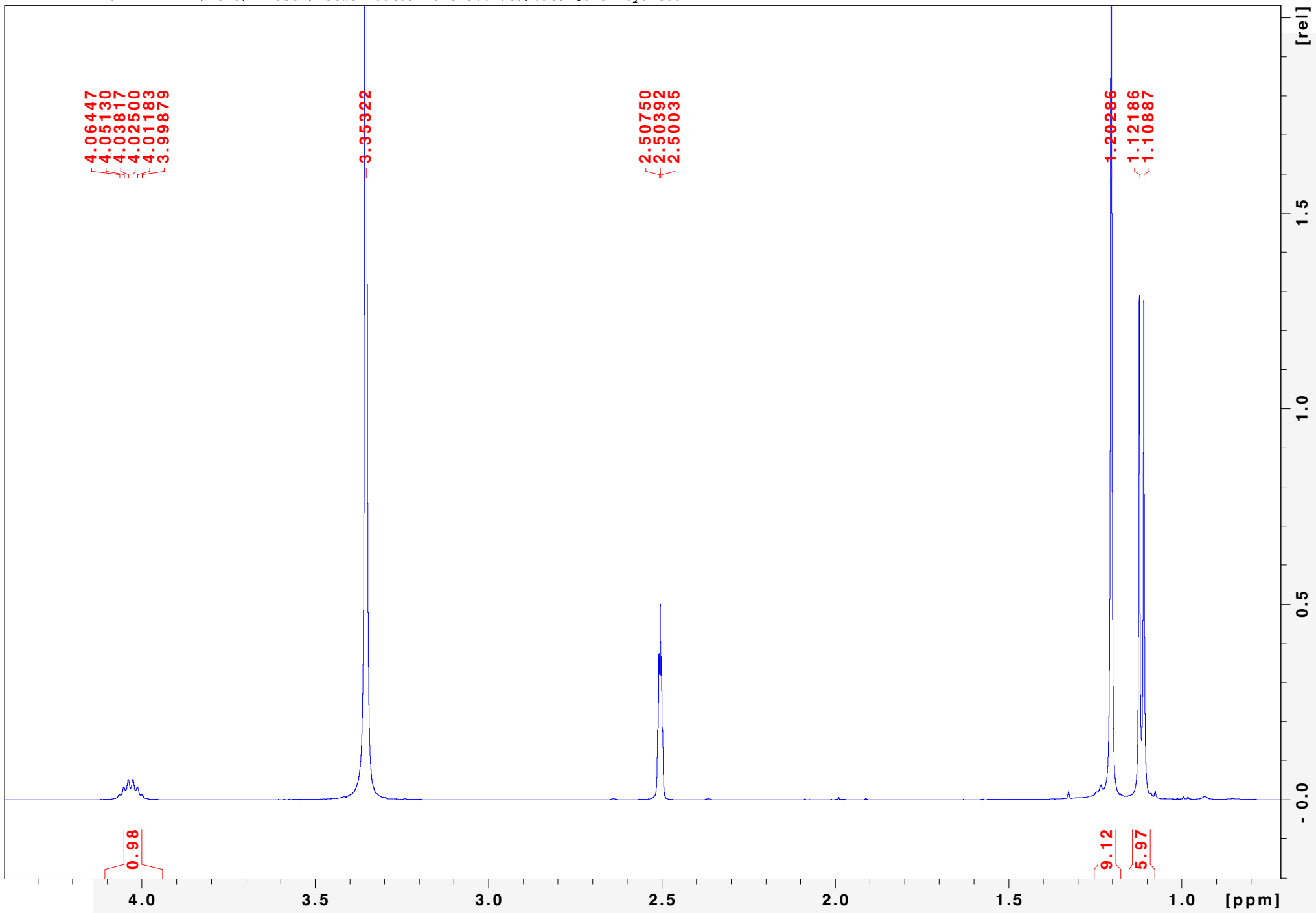


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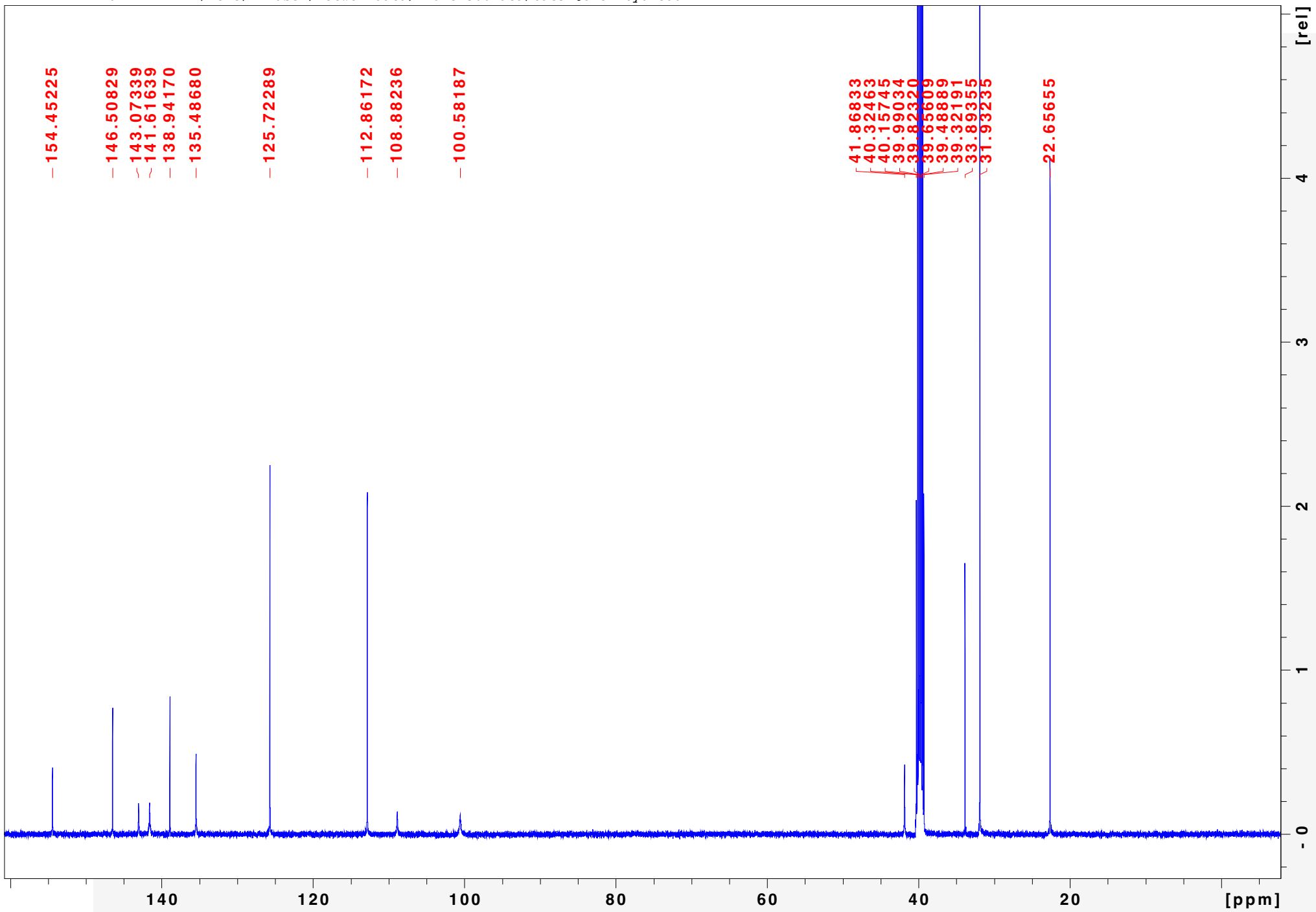


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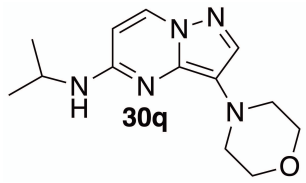

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2.50750
2.50392
2.50035
1.20286
1.12186
1.10887
0.98
9.12
5.97
4.0
3.5
3.0
2.5
2.0
1.5
1.0
[ppm]
[rel]
1.5
1.0
0.5
- 0.0

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"BAT - II - 60" 1 1 /home/nmruser/networkdata/Bruker500Data/bat54@chem.byu.edu

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7.52639
7.14604
7.13214
6.12083
6.10569
4.05991
4.04681
4.03369
4.02051
4.00738
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3.34694
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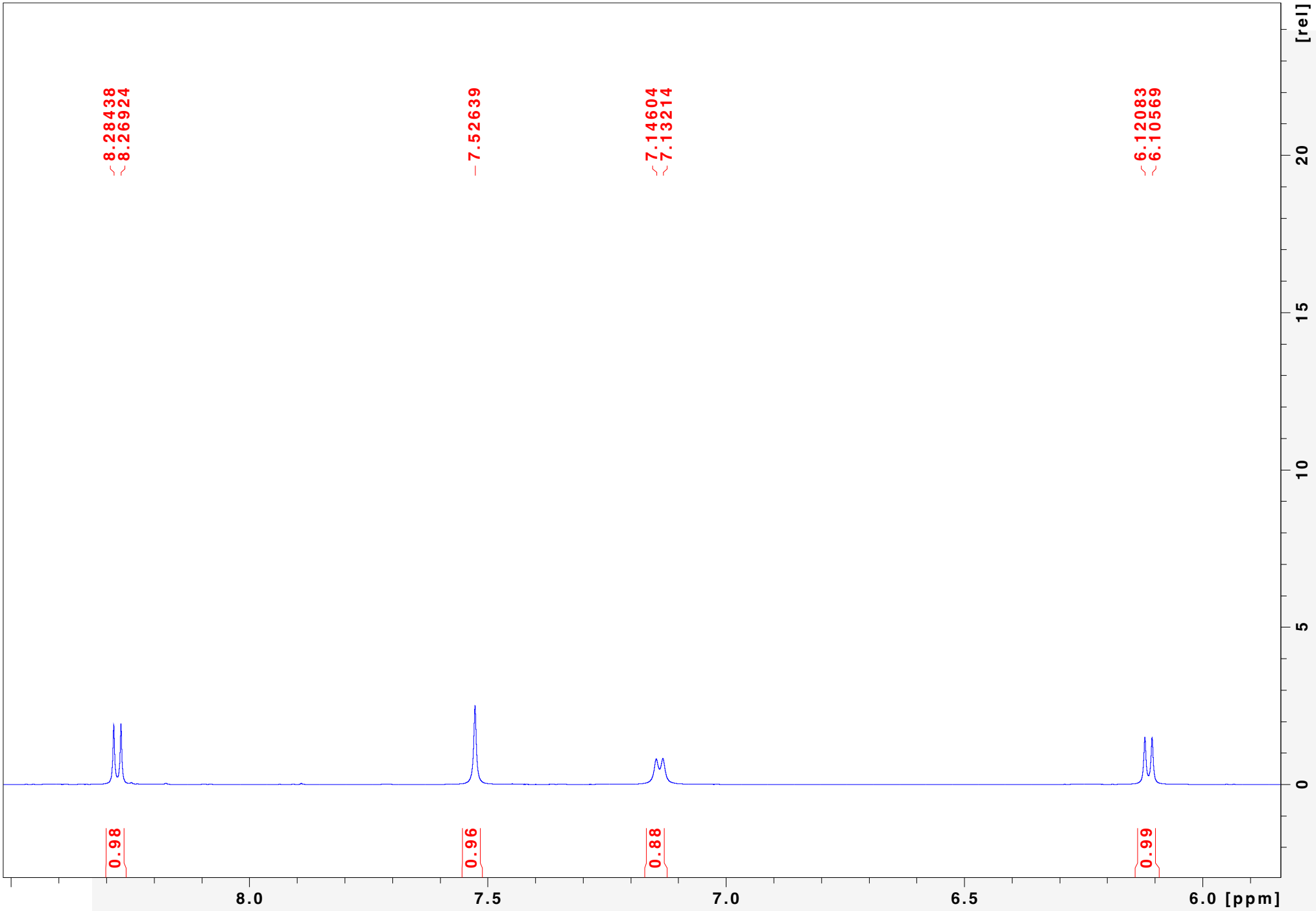
30q

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6.00

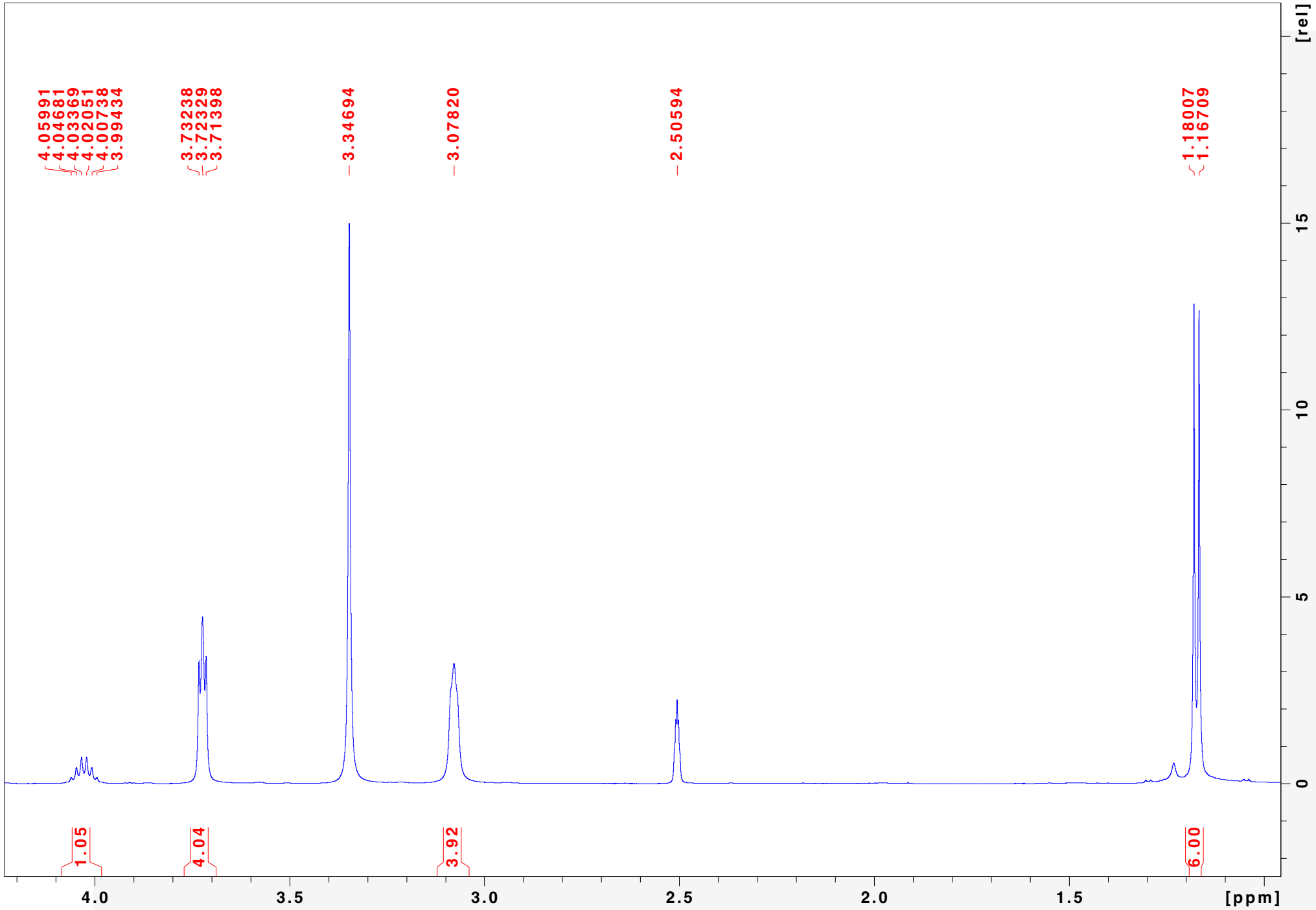
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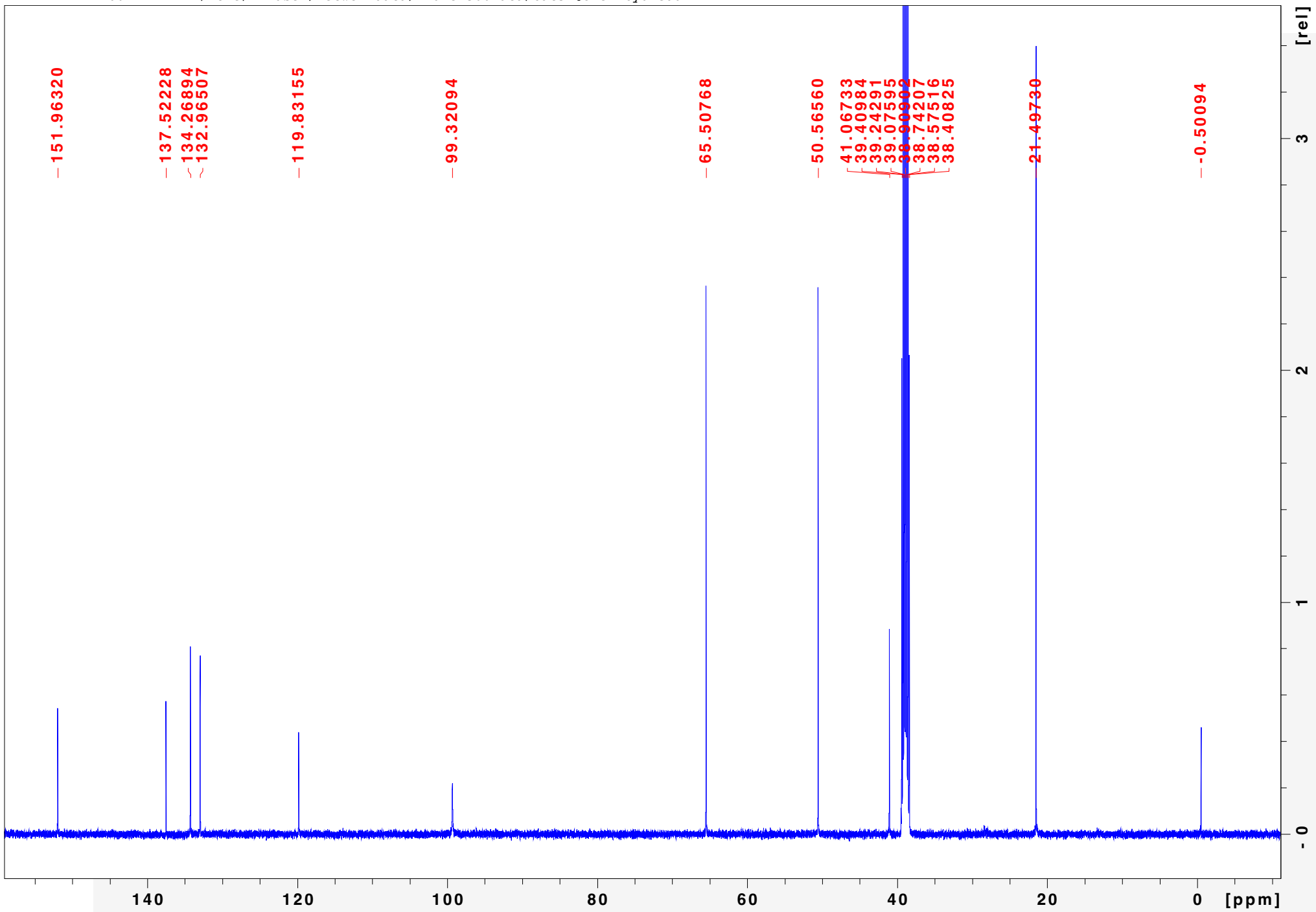
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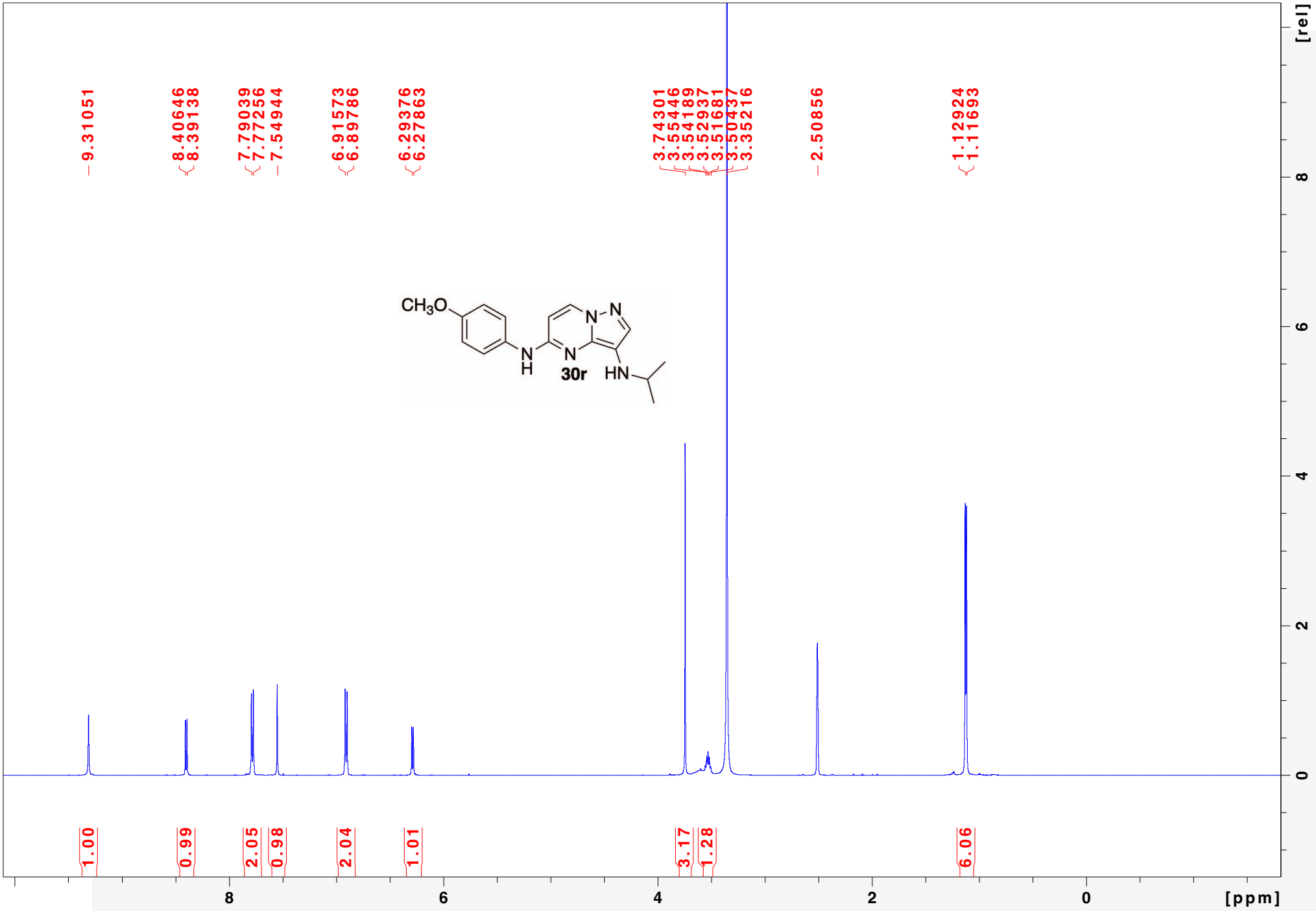
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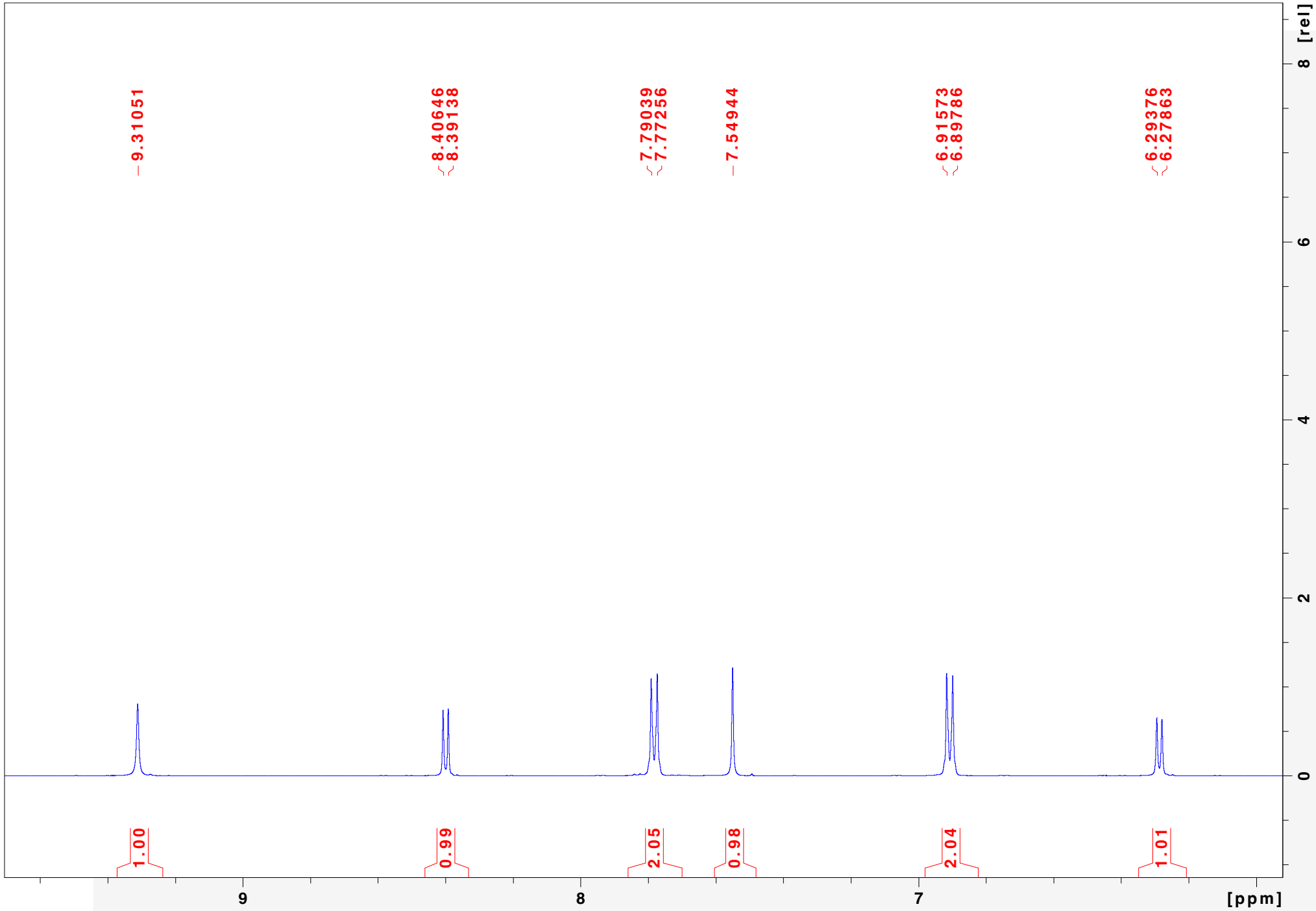
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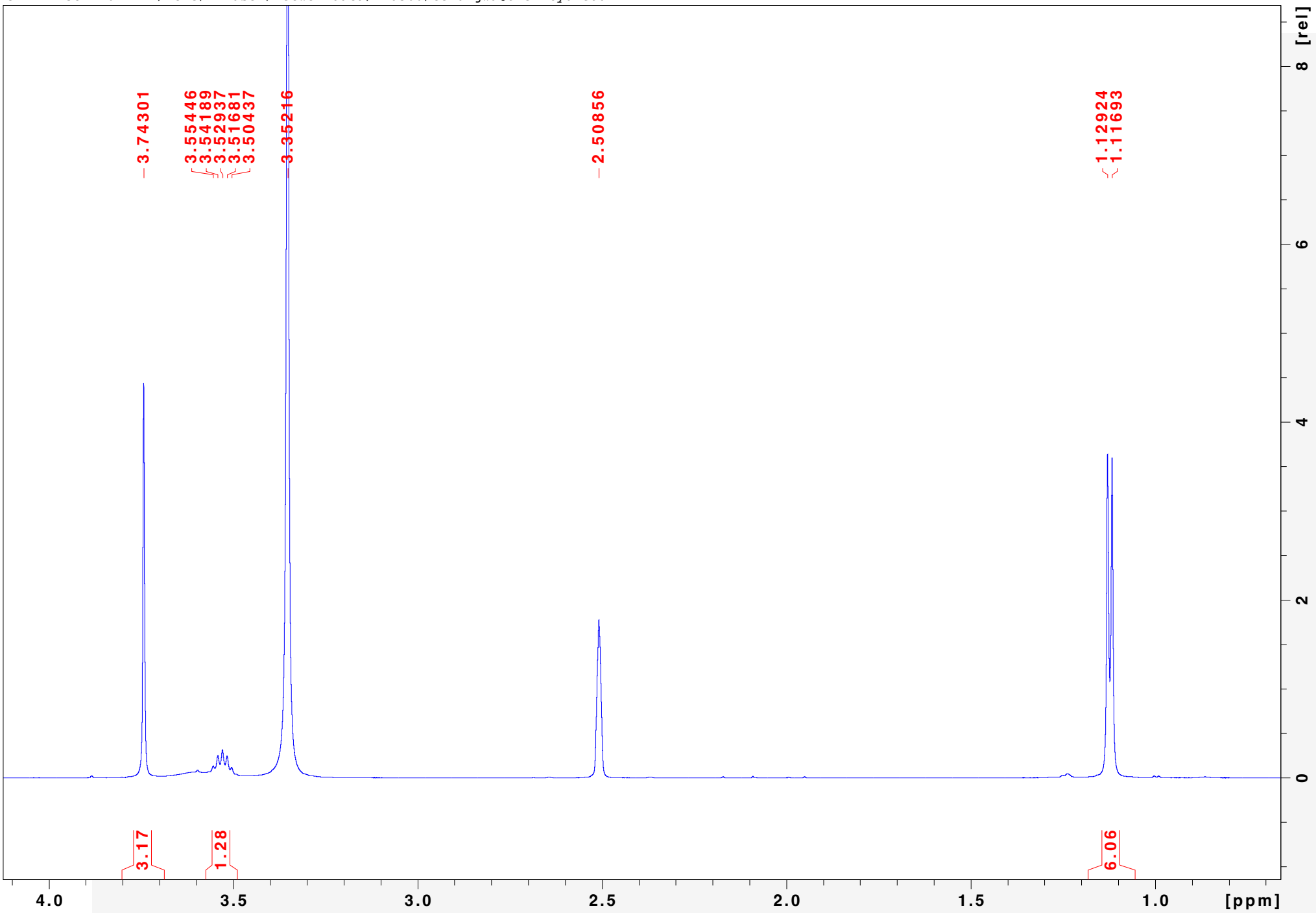
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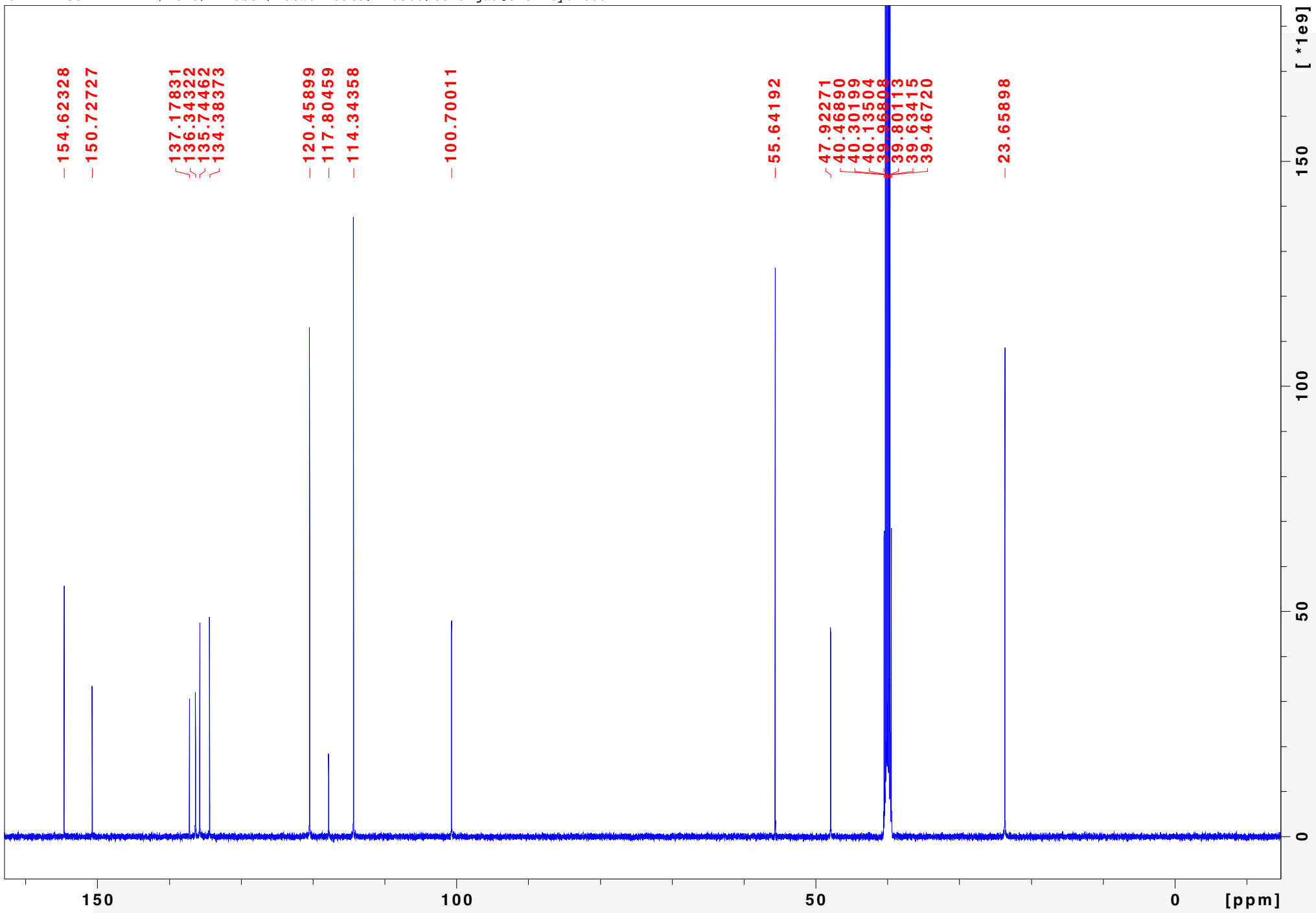
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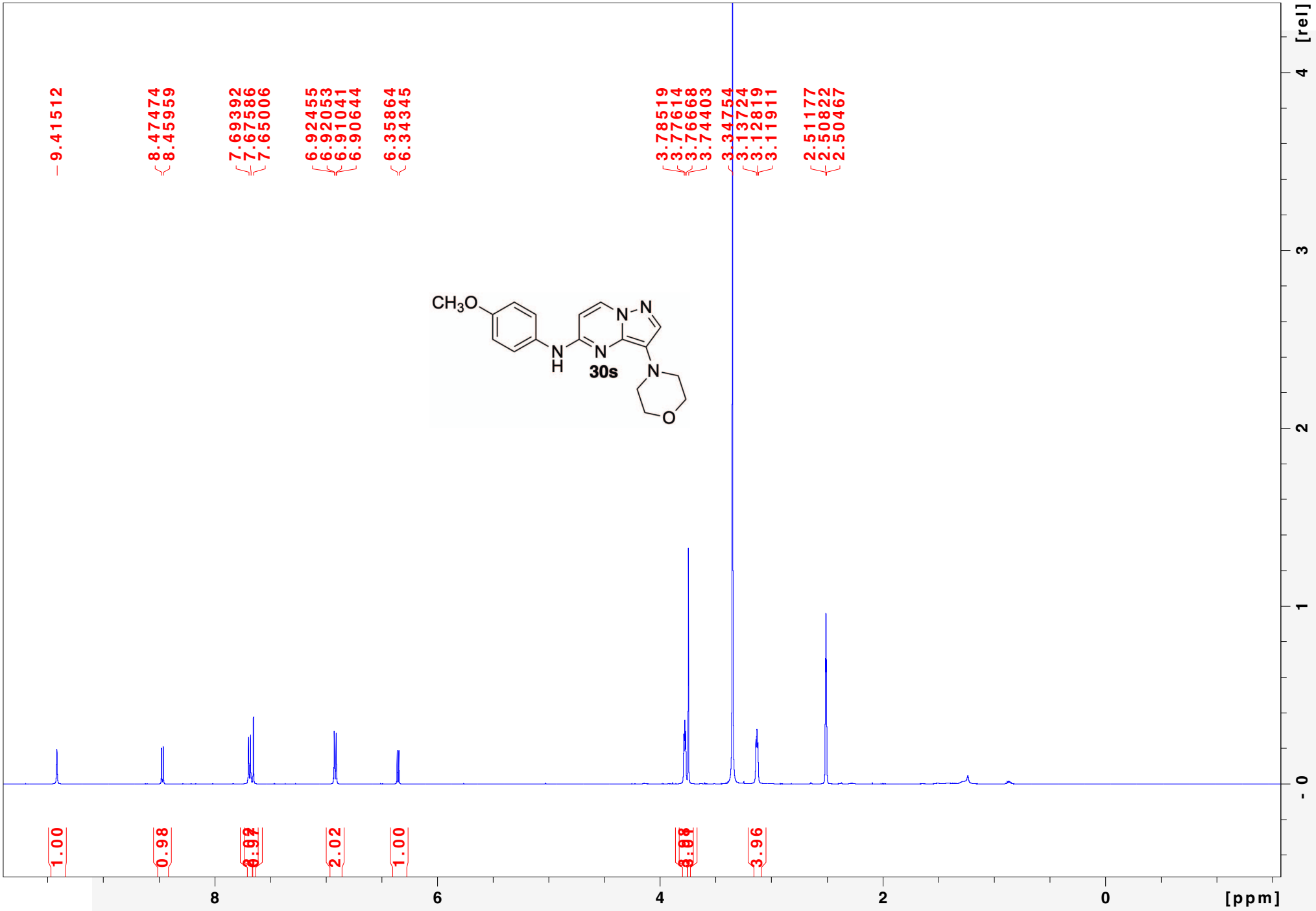
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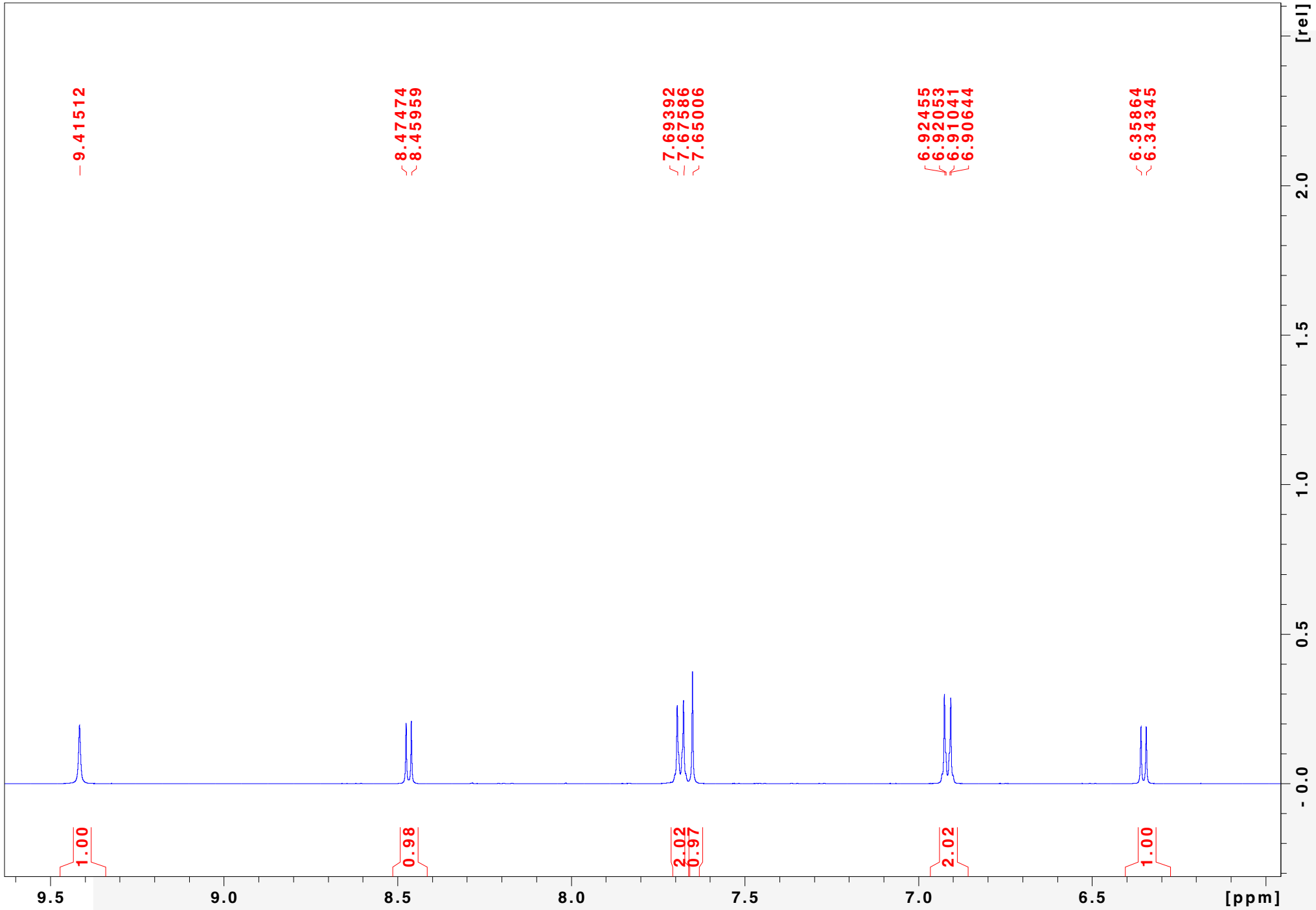
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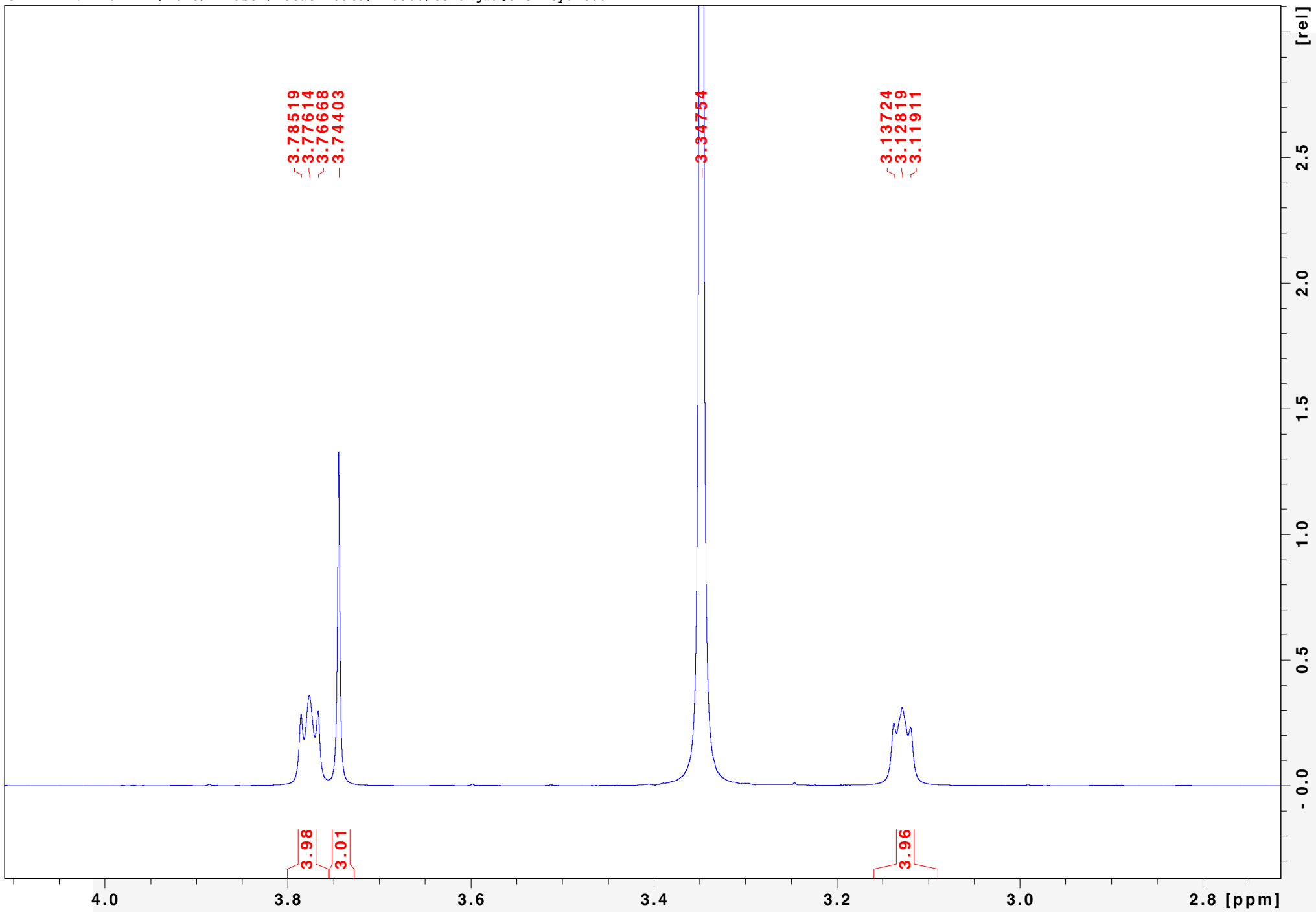


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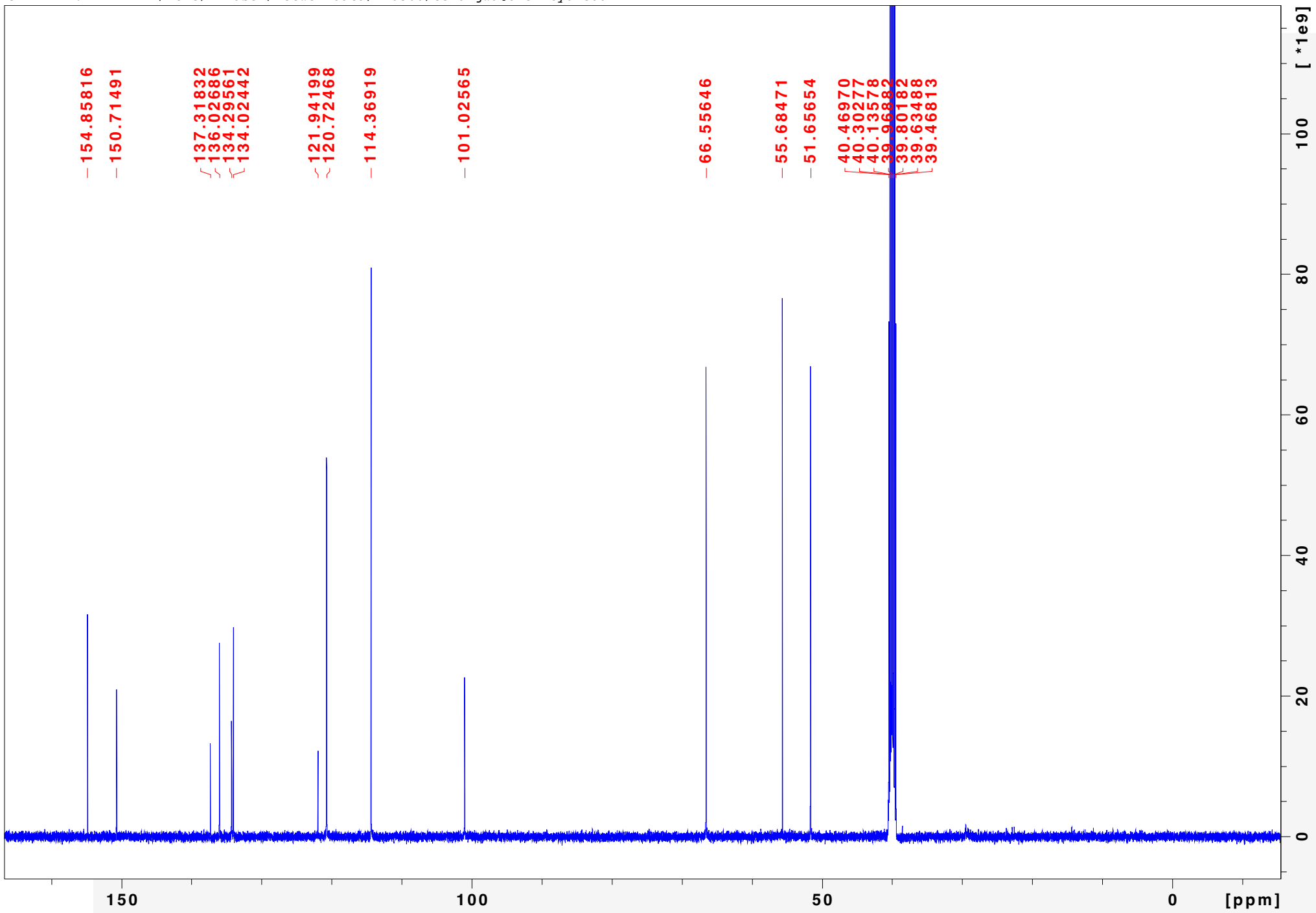


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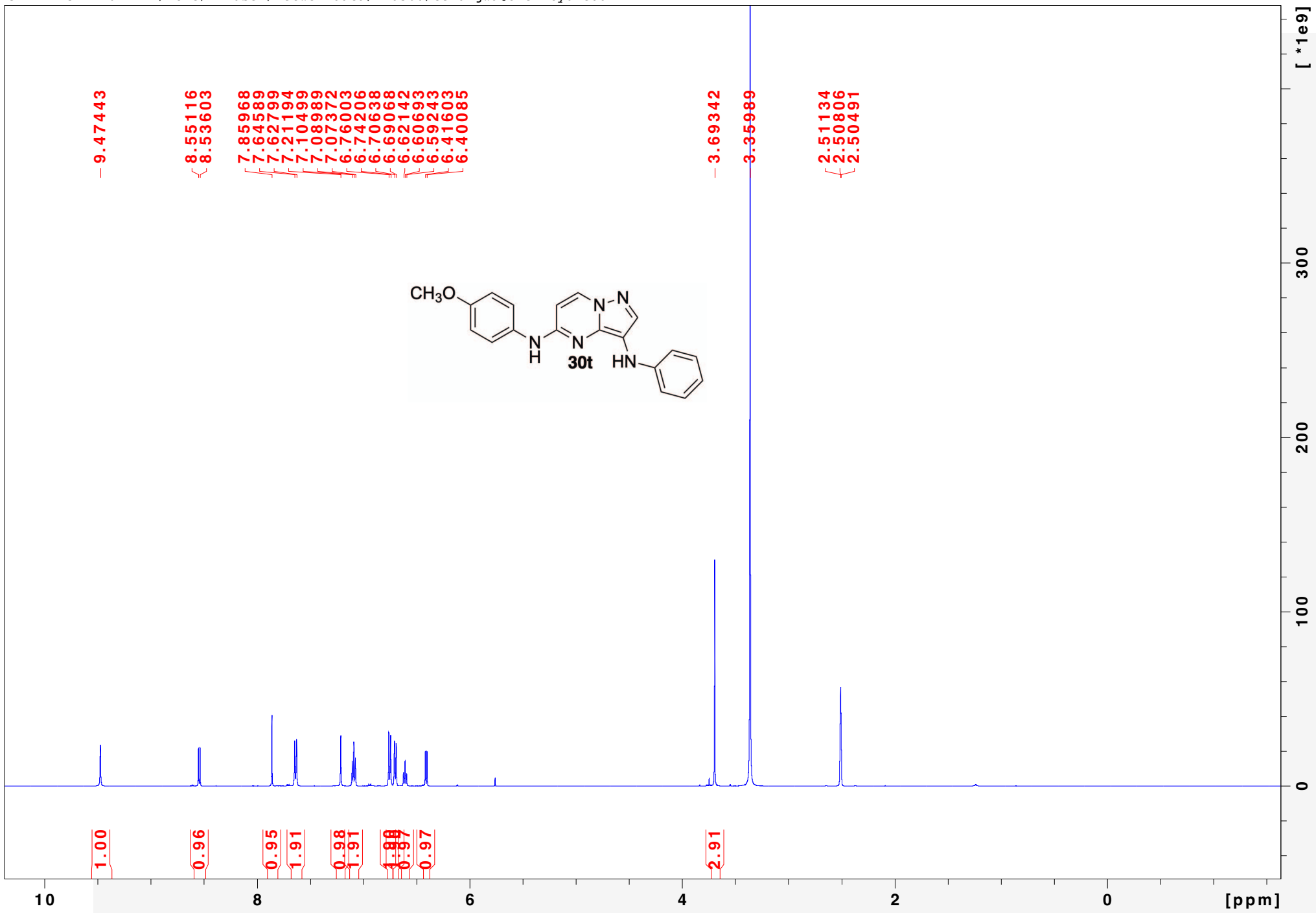



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3.8
3.6
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3.0
2.8 [ppm]
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1.0
0.5
- 0.0

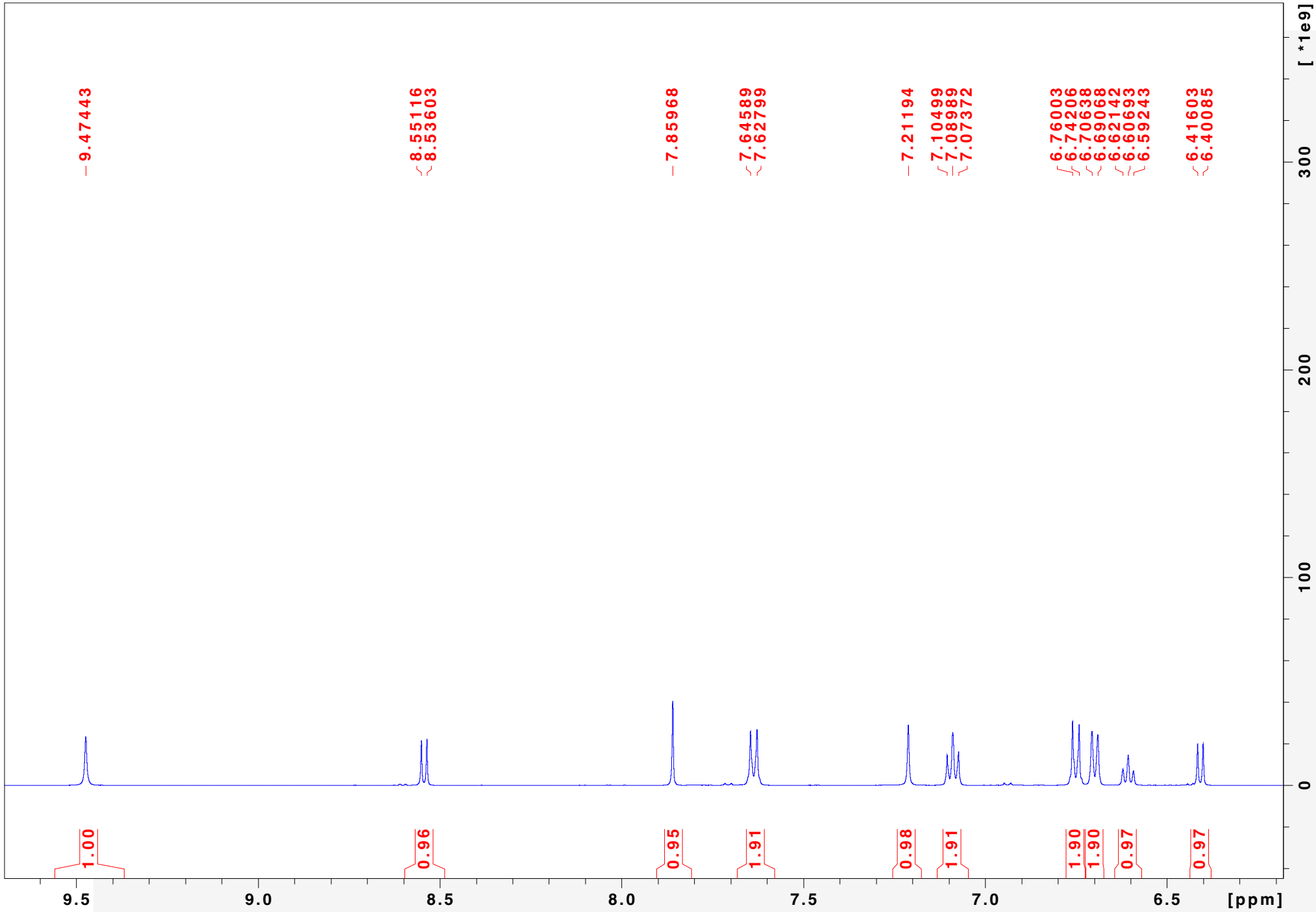
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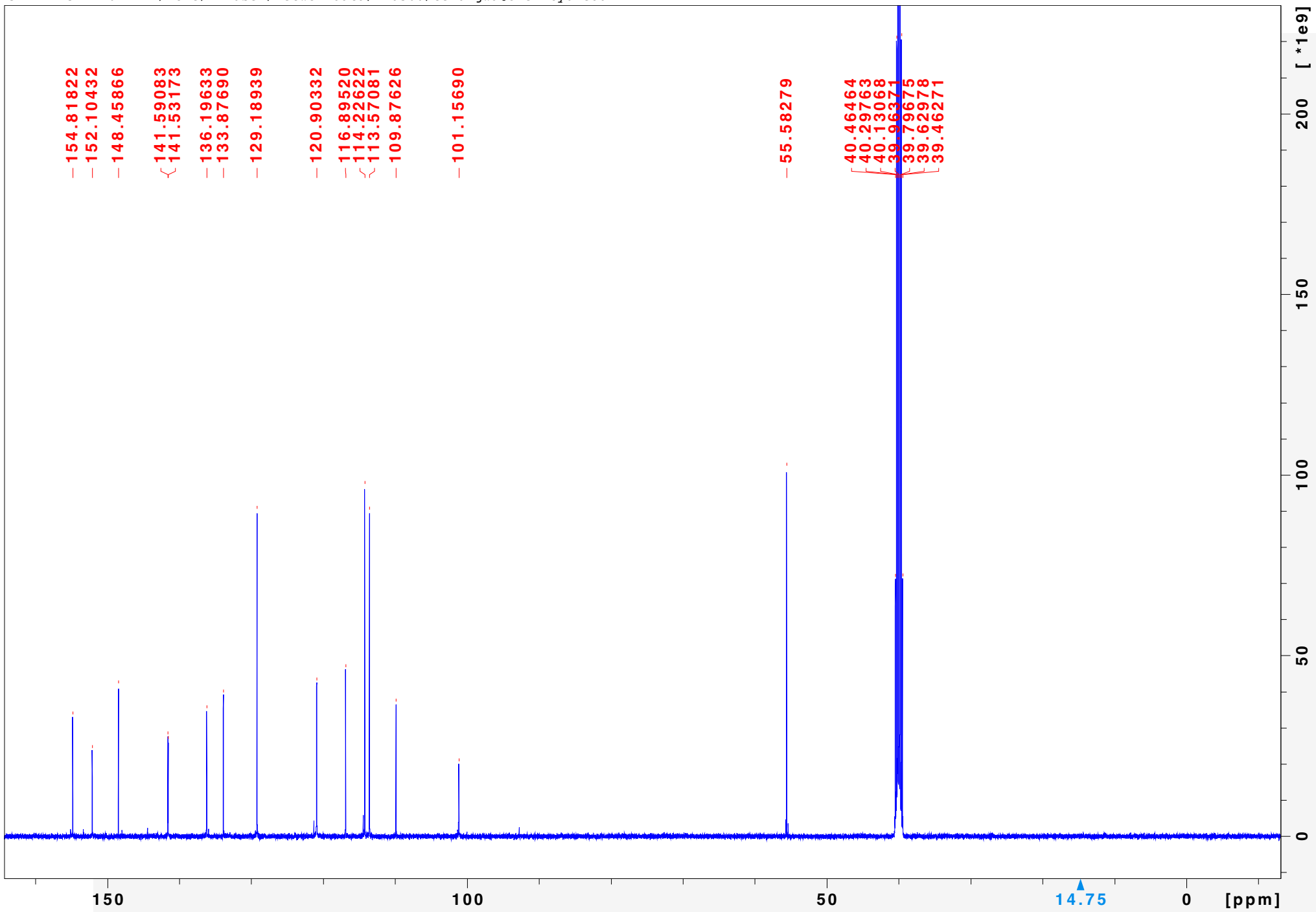
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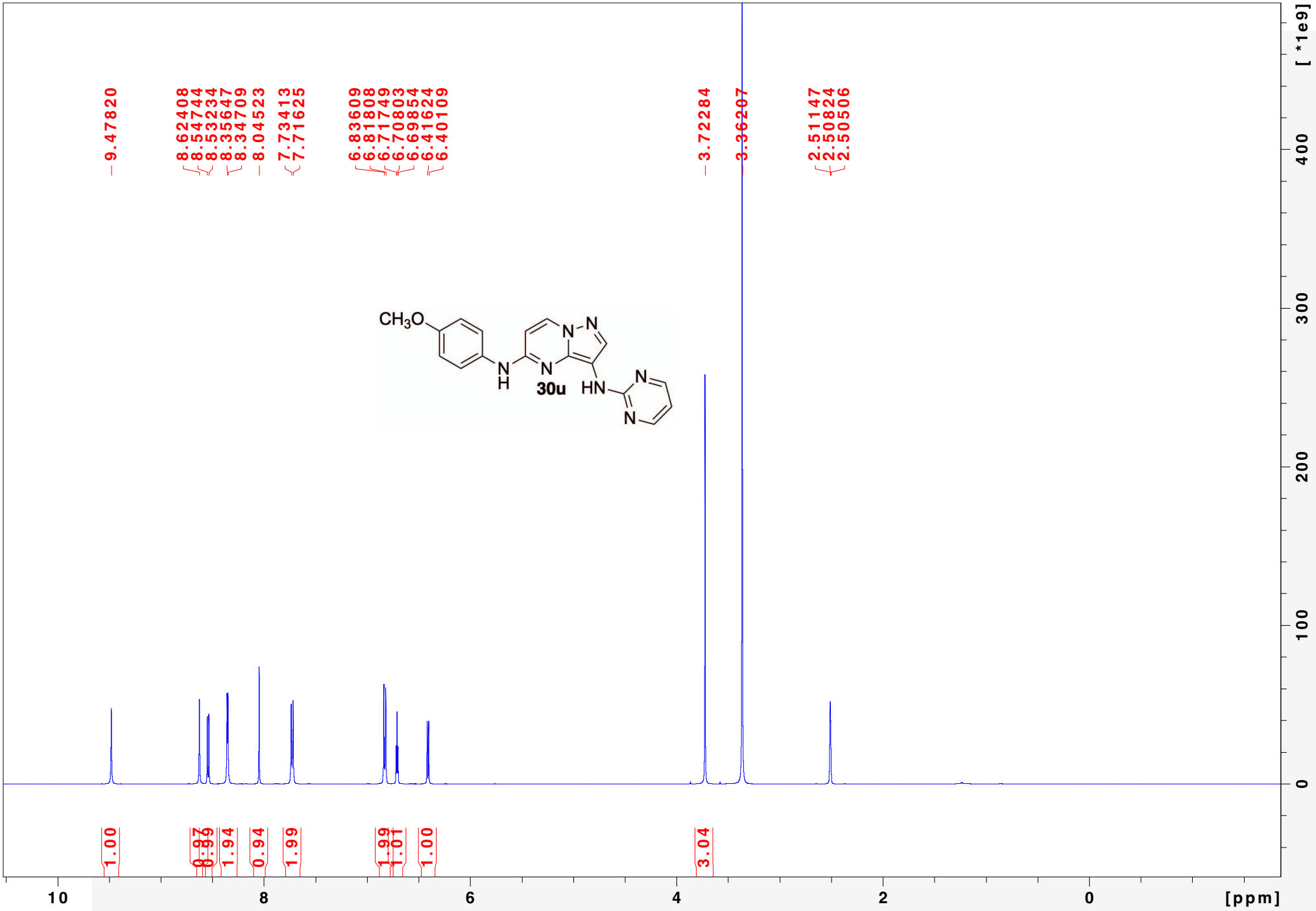
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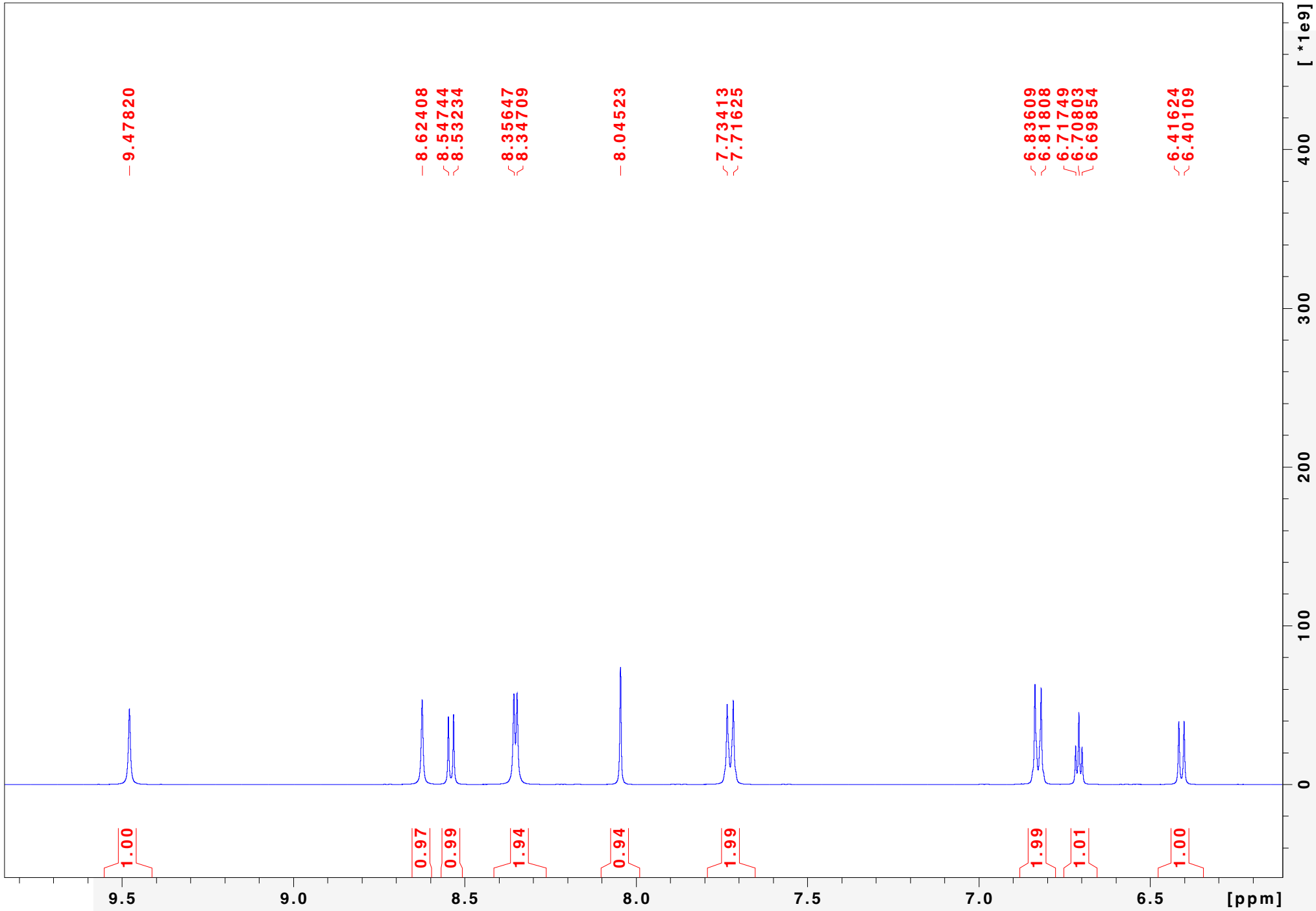
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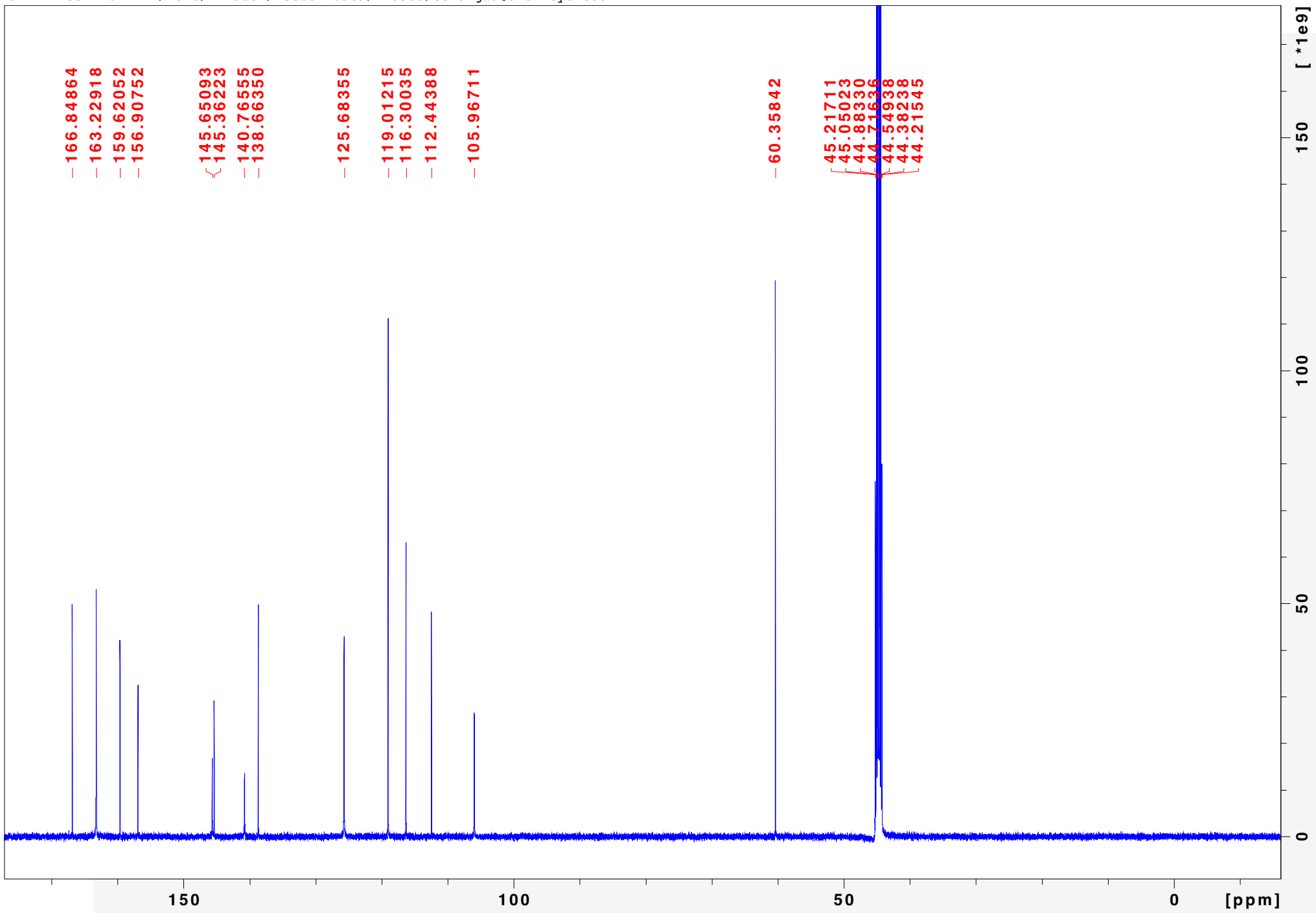
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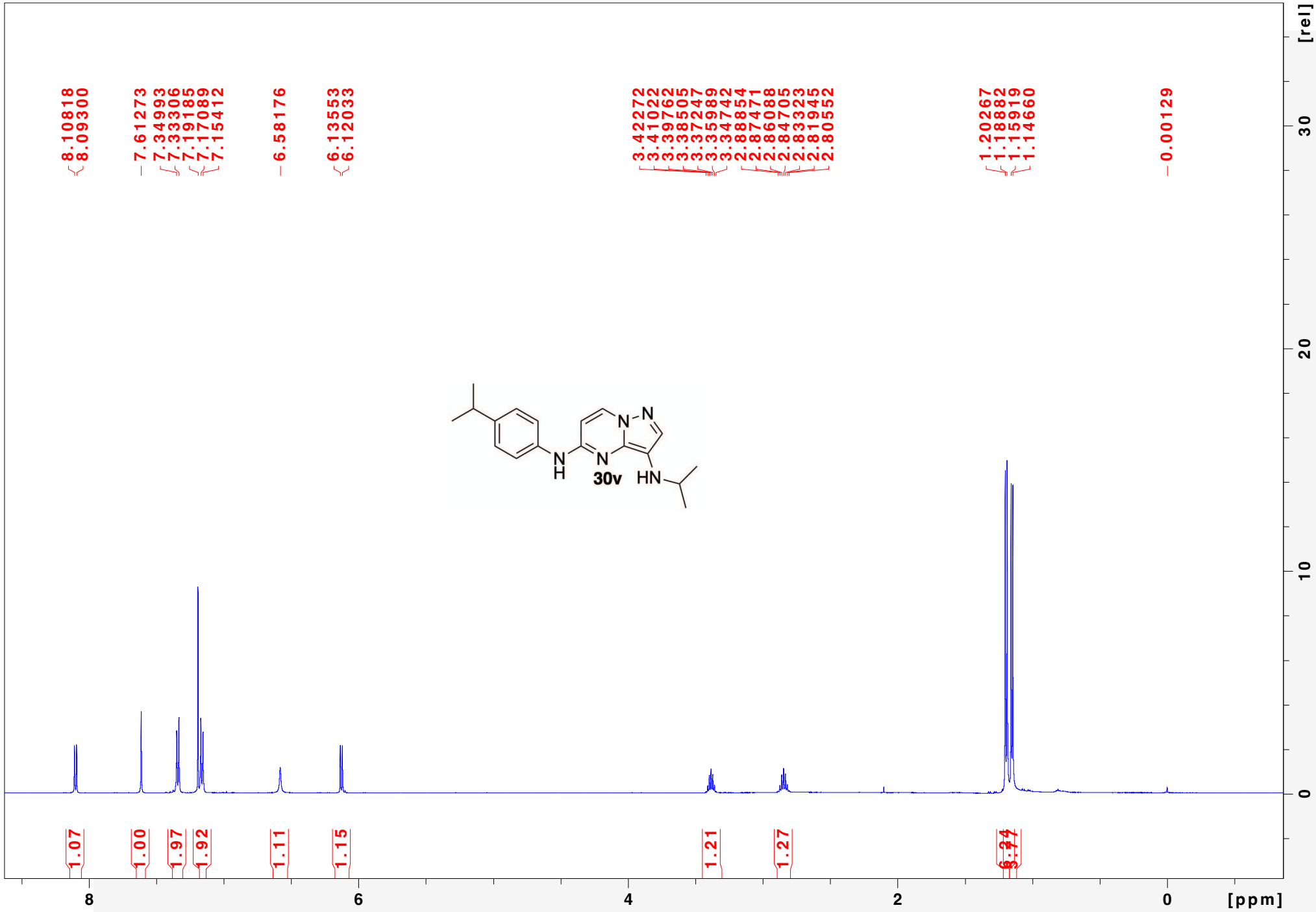
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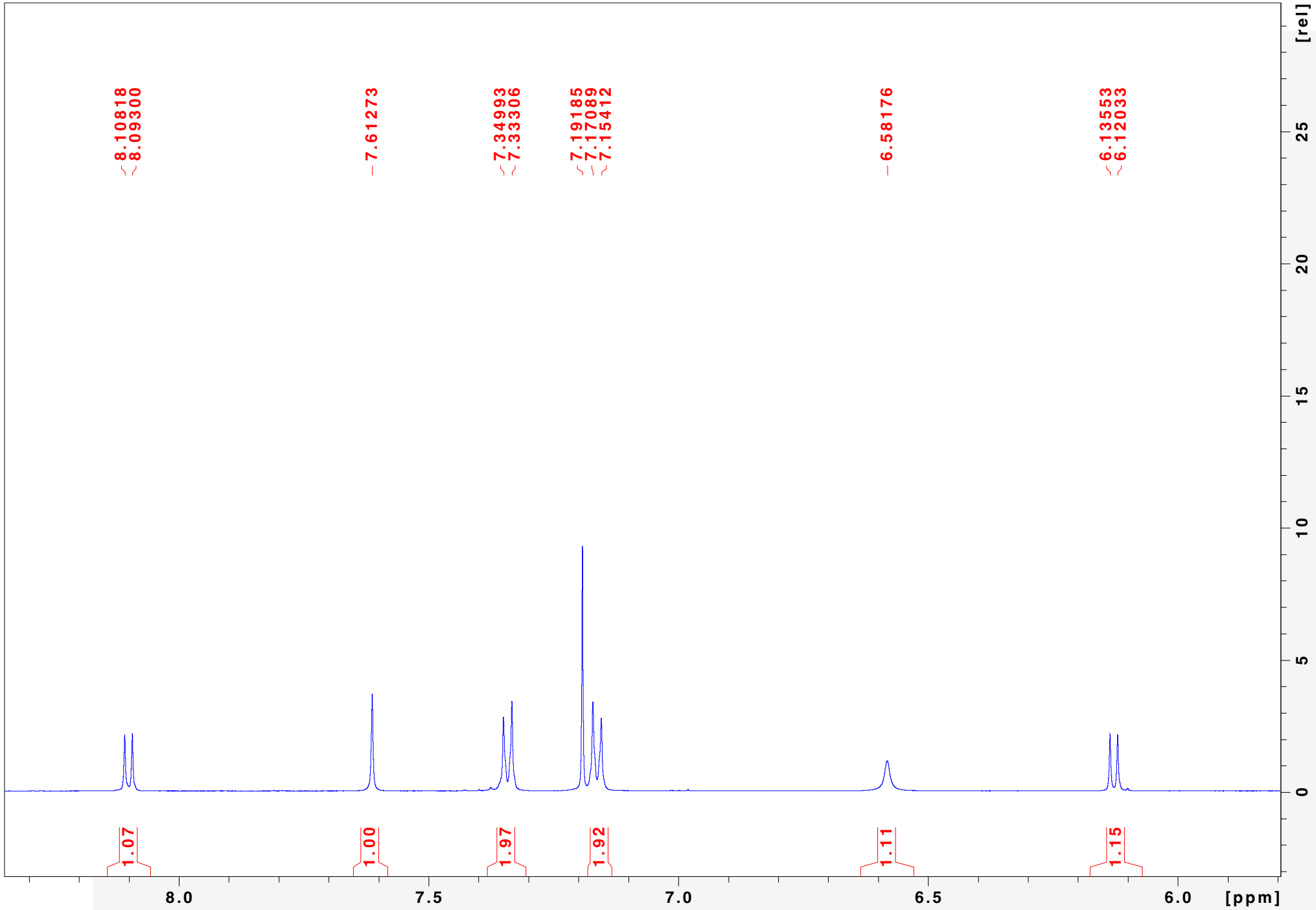
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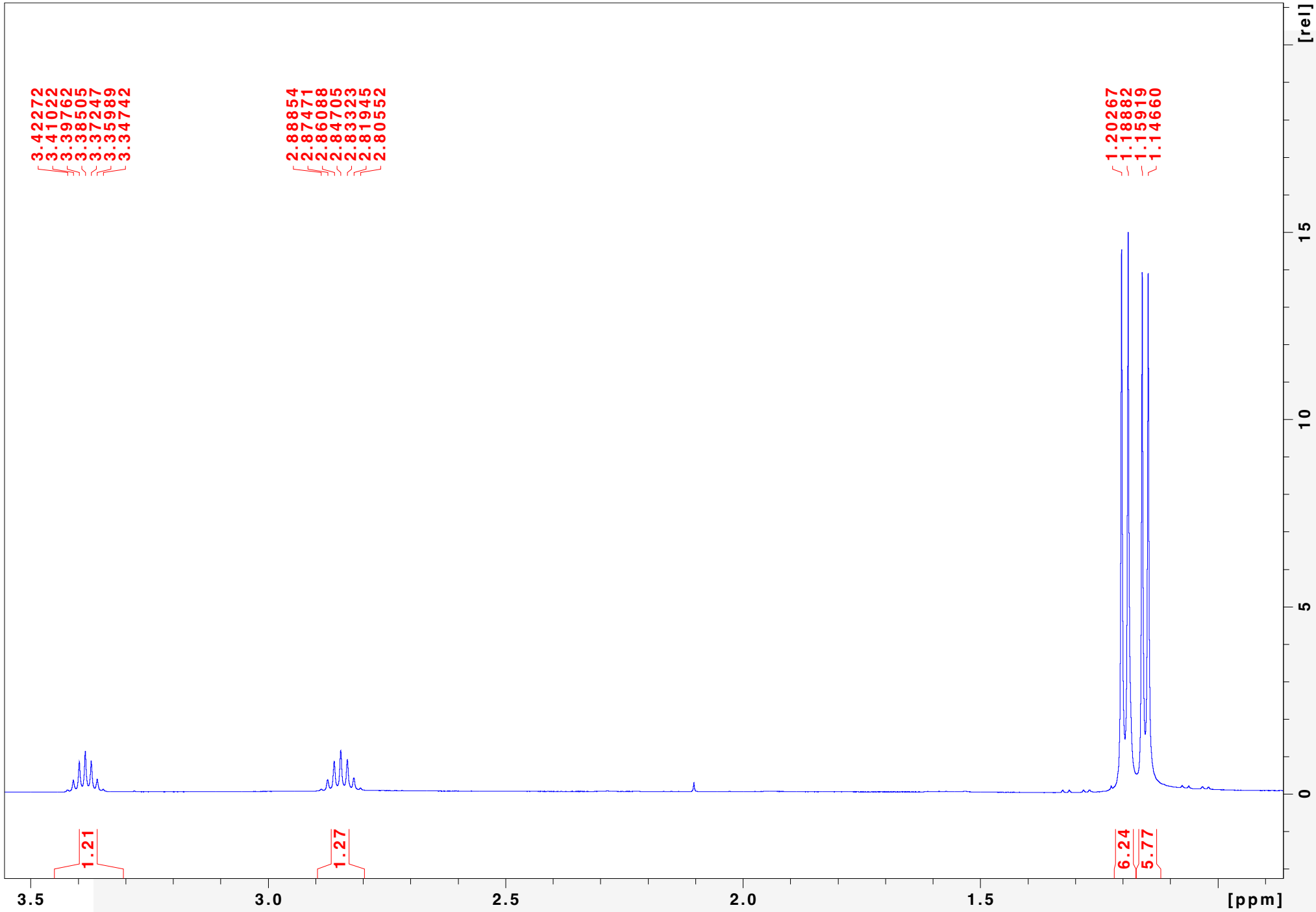
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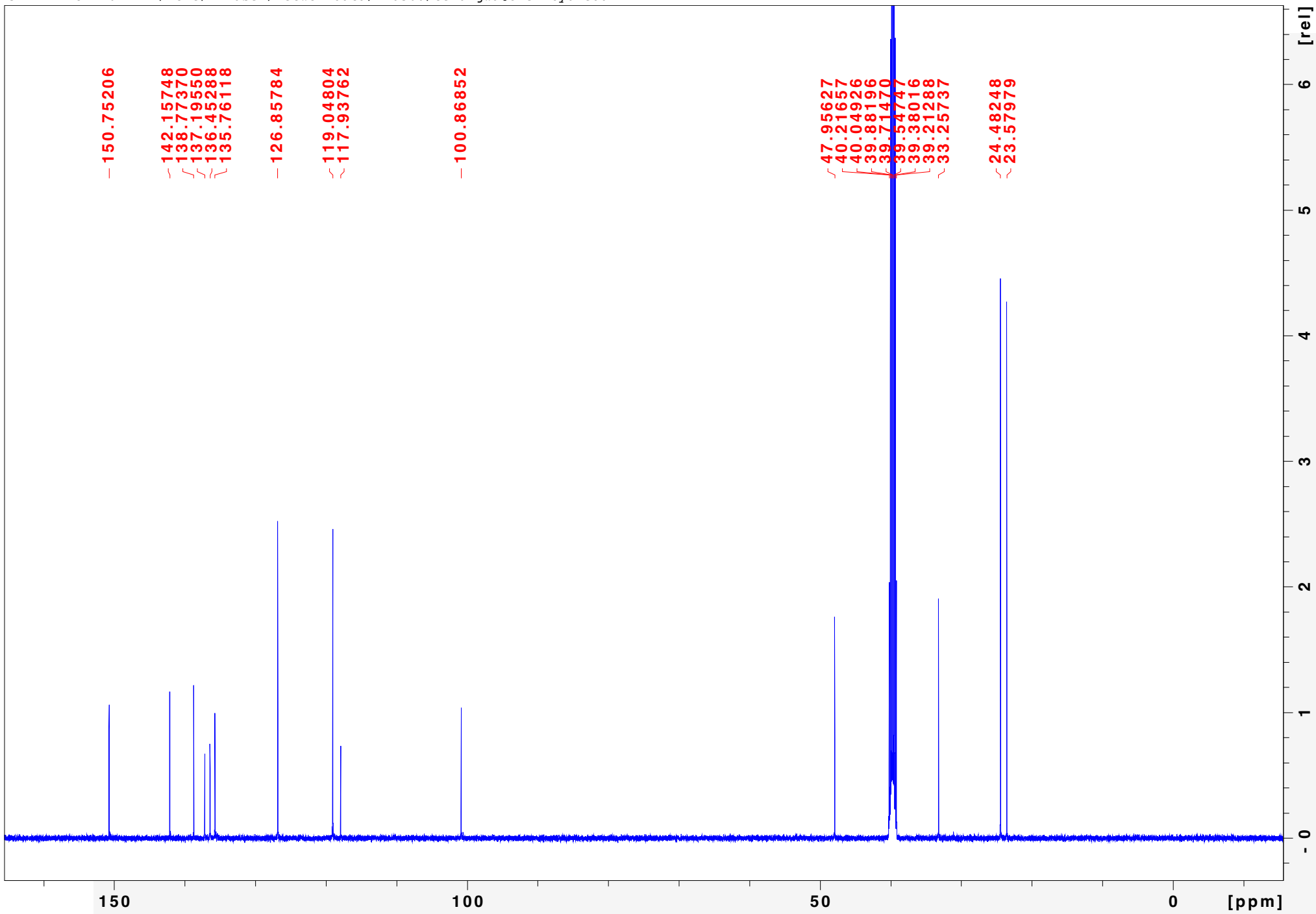
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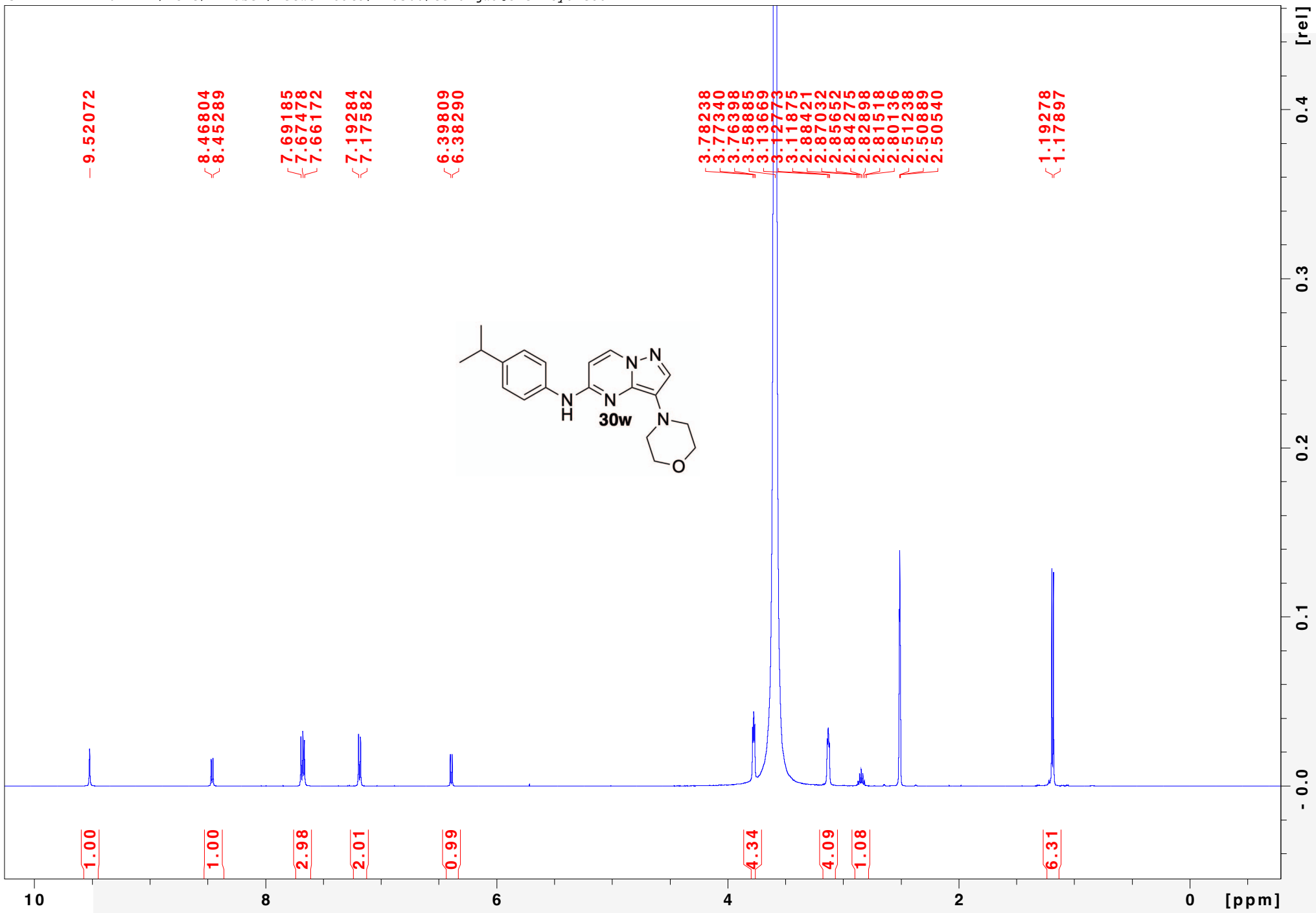
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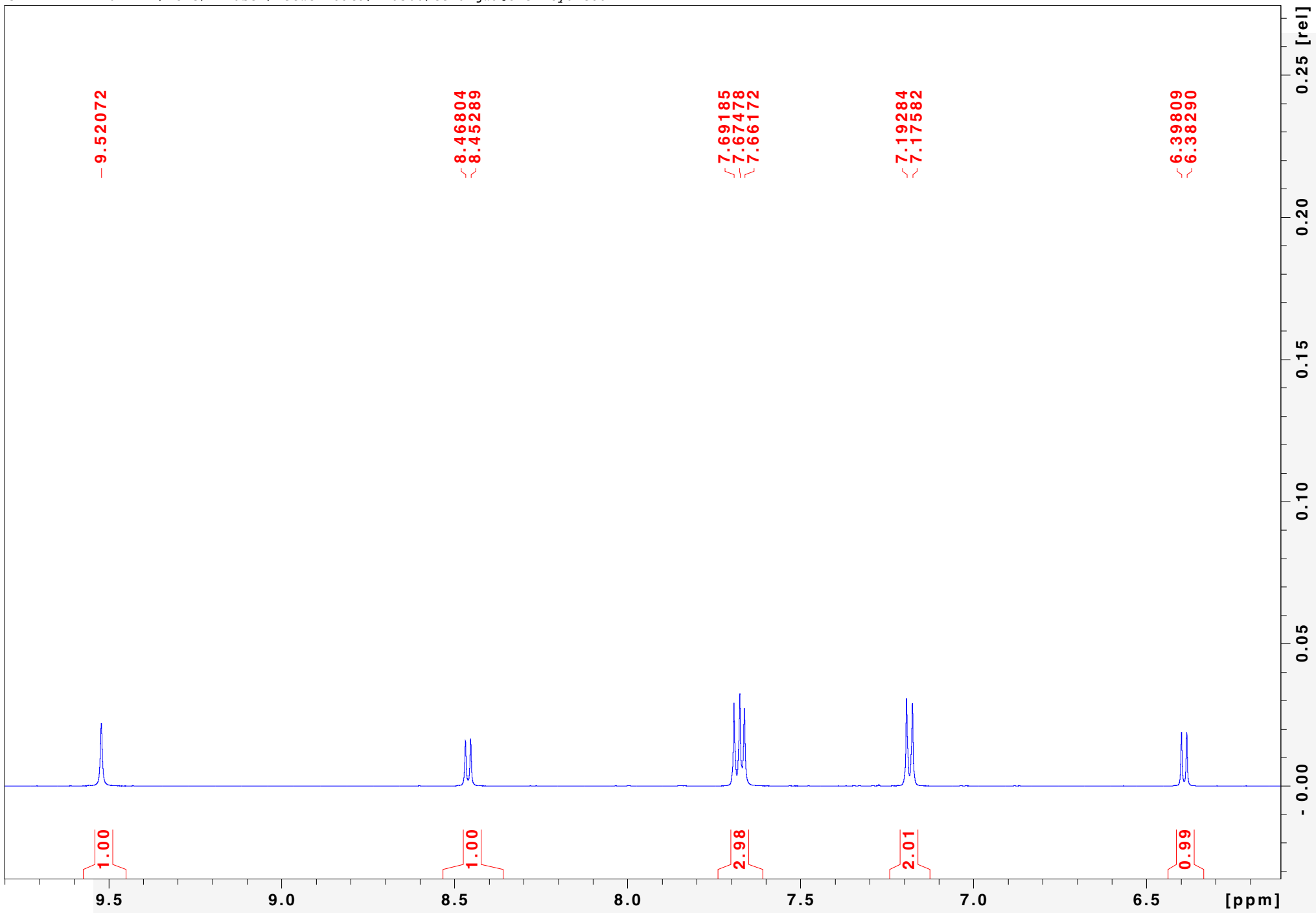


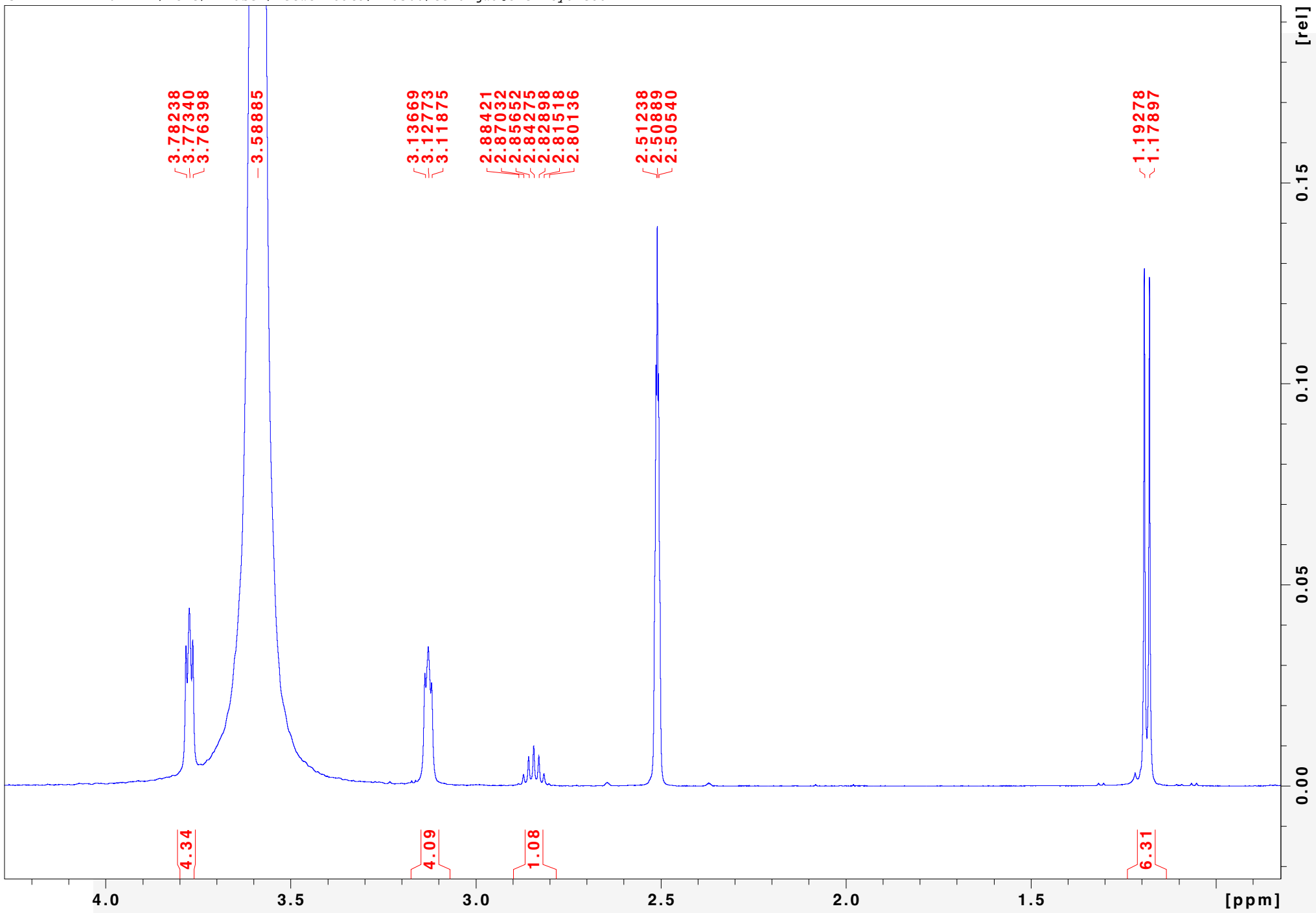
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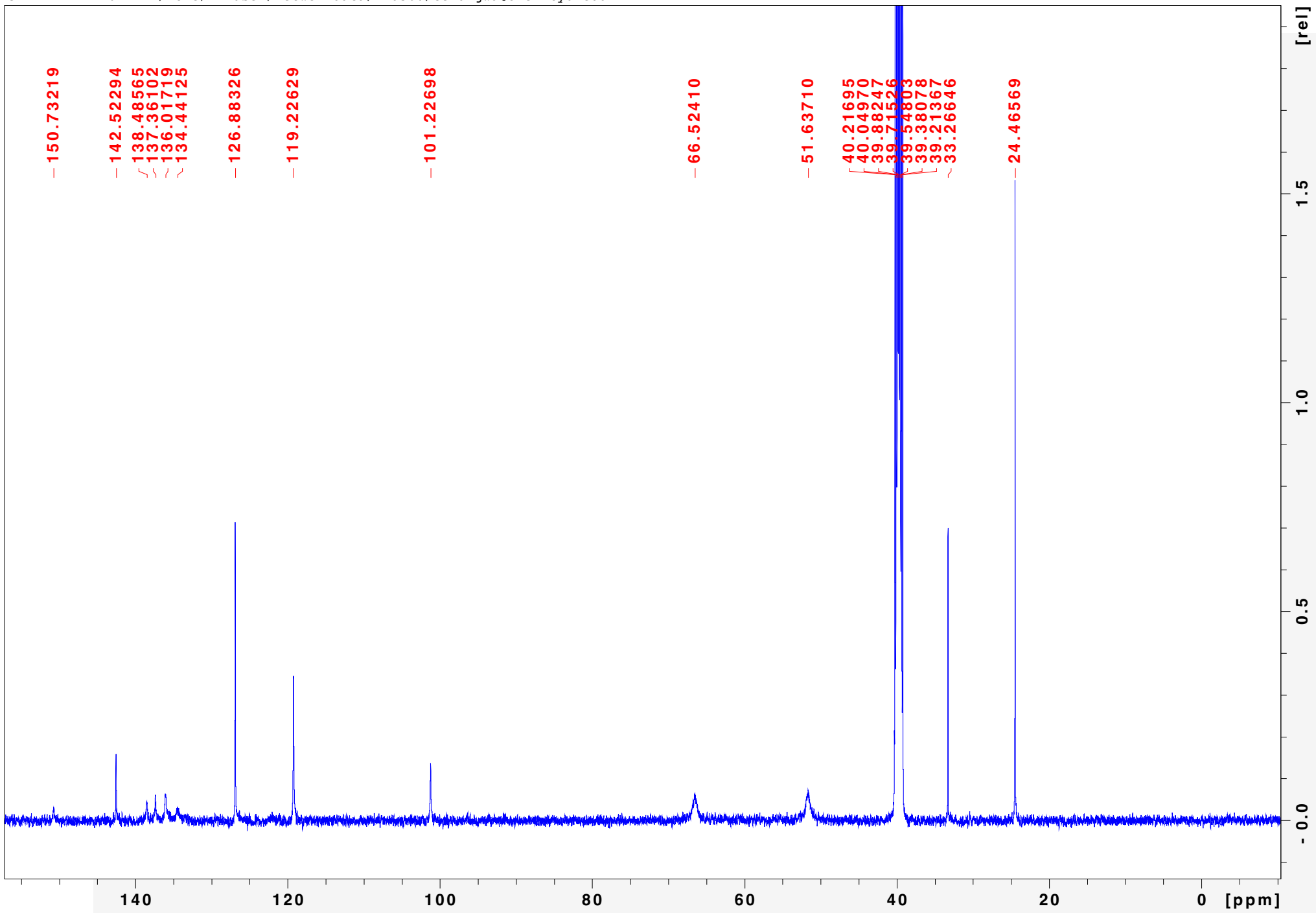
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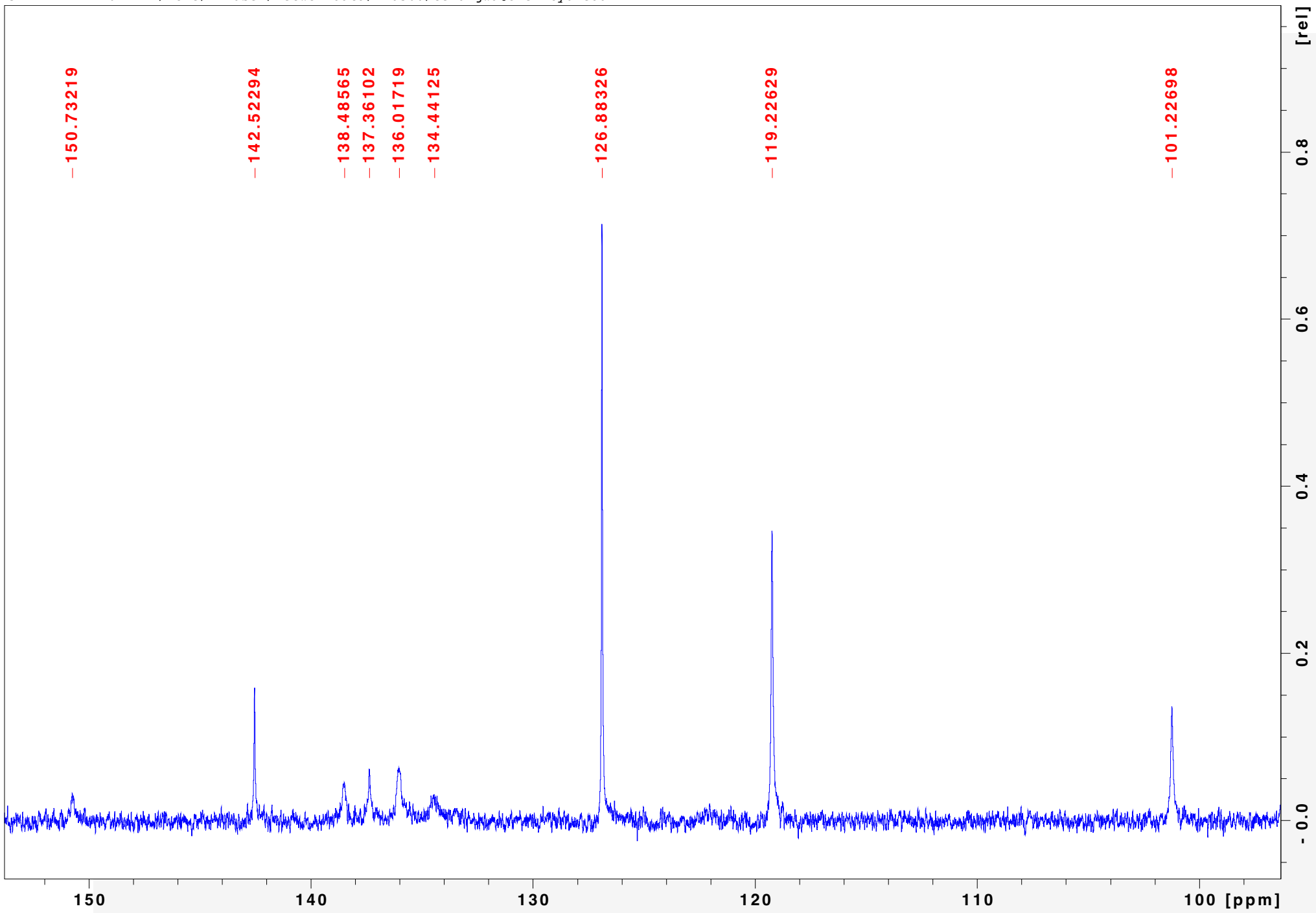

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7.66172
7.19284
7.17582
6.39809
6.38290
1.00
1.00
2.98
2.01
0.99
9.5
9.0
8.5
8.0
7.5
7.0
6.5
[ppm]
0.25 [rel]
0.20
0.15
0.10
0.05
- 0.00


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3.11875
2.88421
2.87032
2.85652
2.84275
2.82898
2.81518
2.80136
2.51238
2.50889
2.50540
1.19278
1.17897
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1.08
6.31
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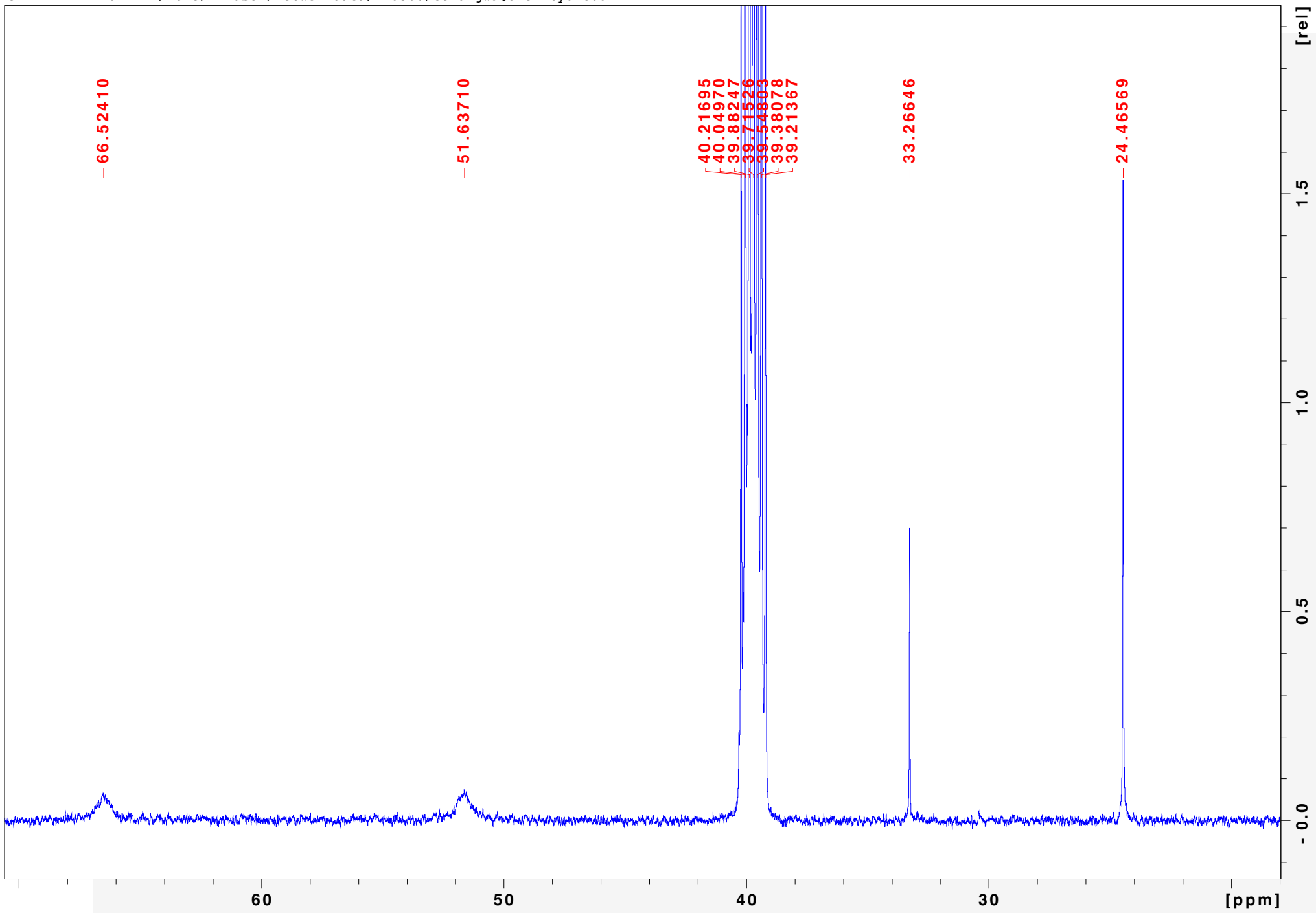
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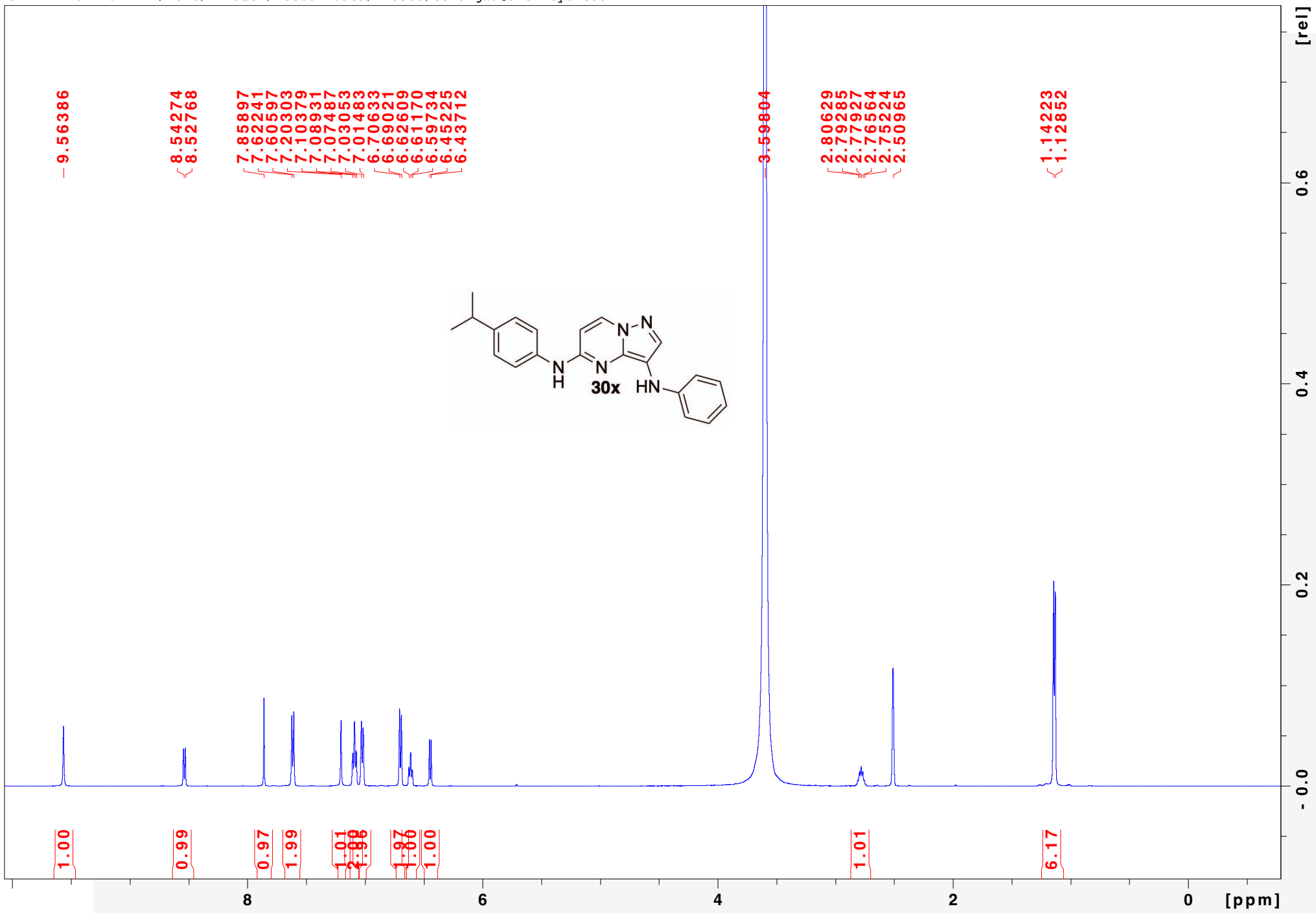
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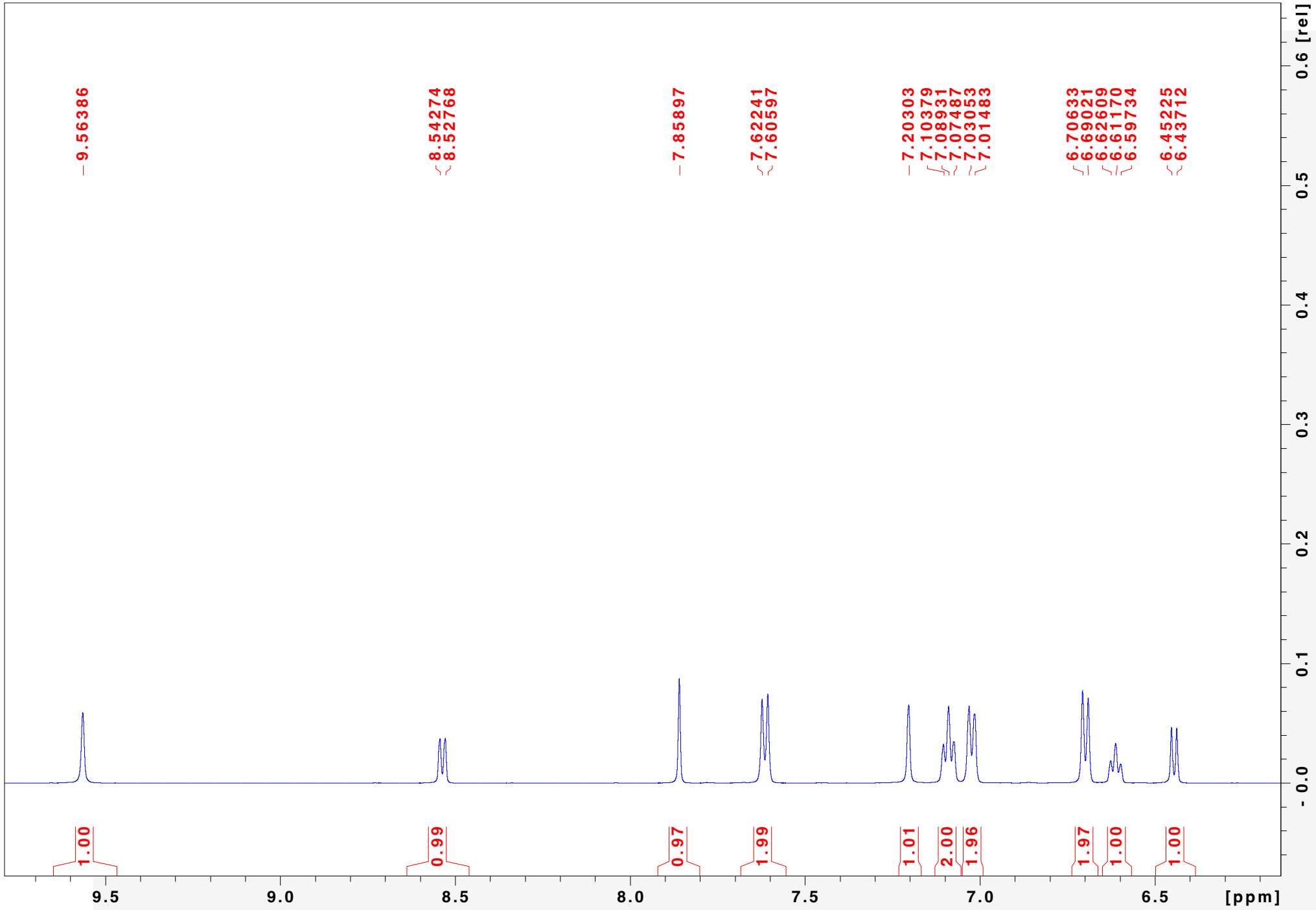
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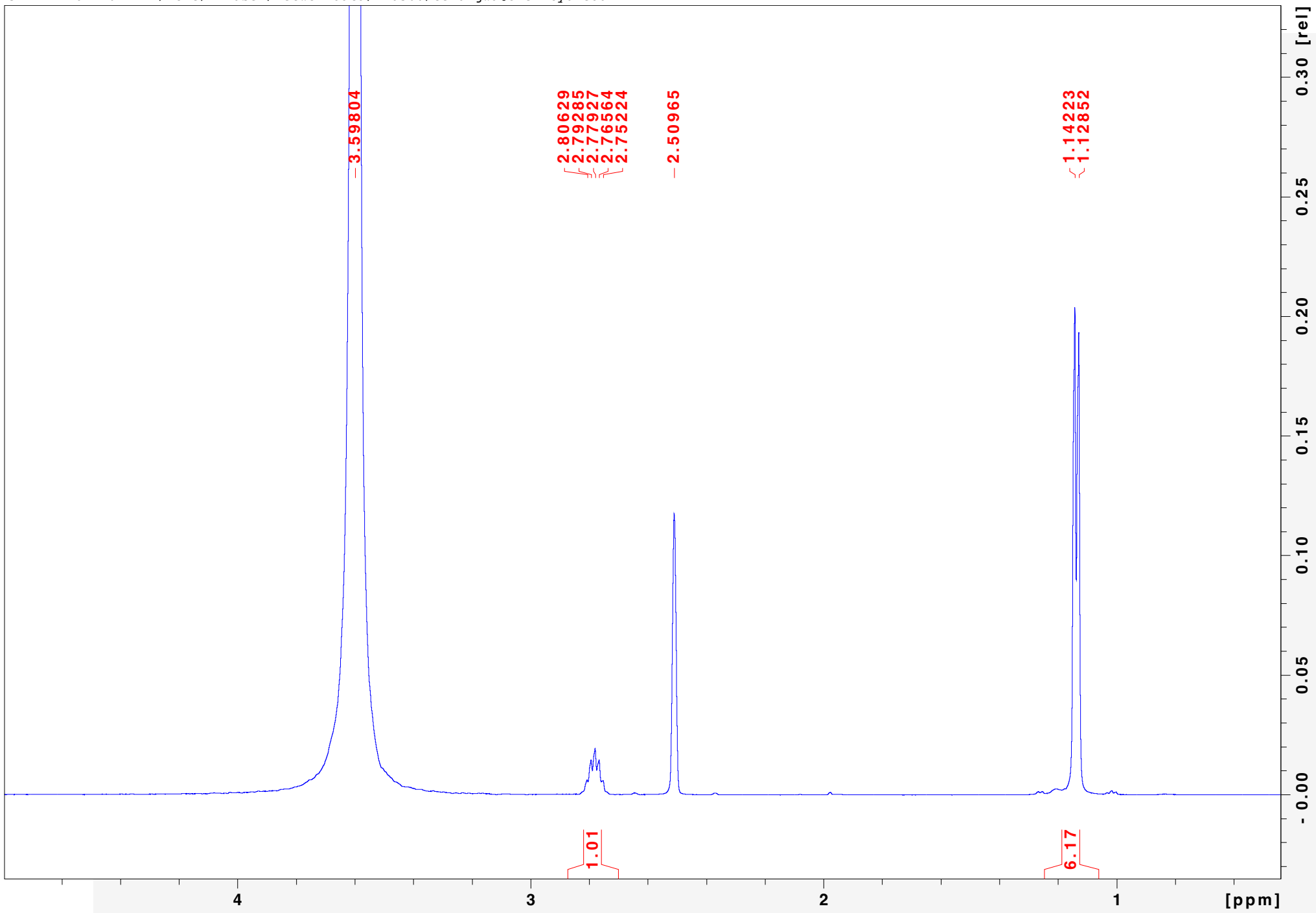
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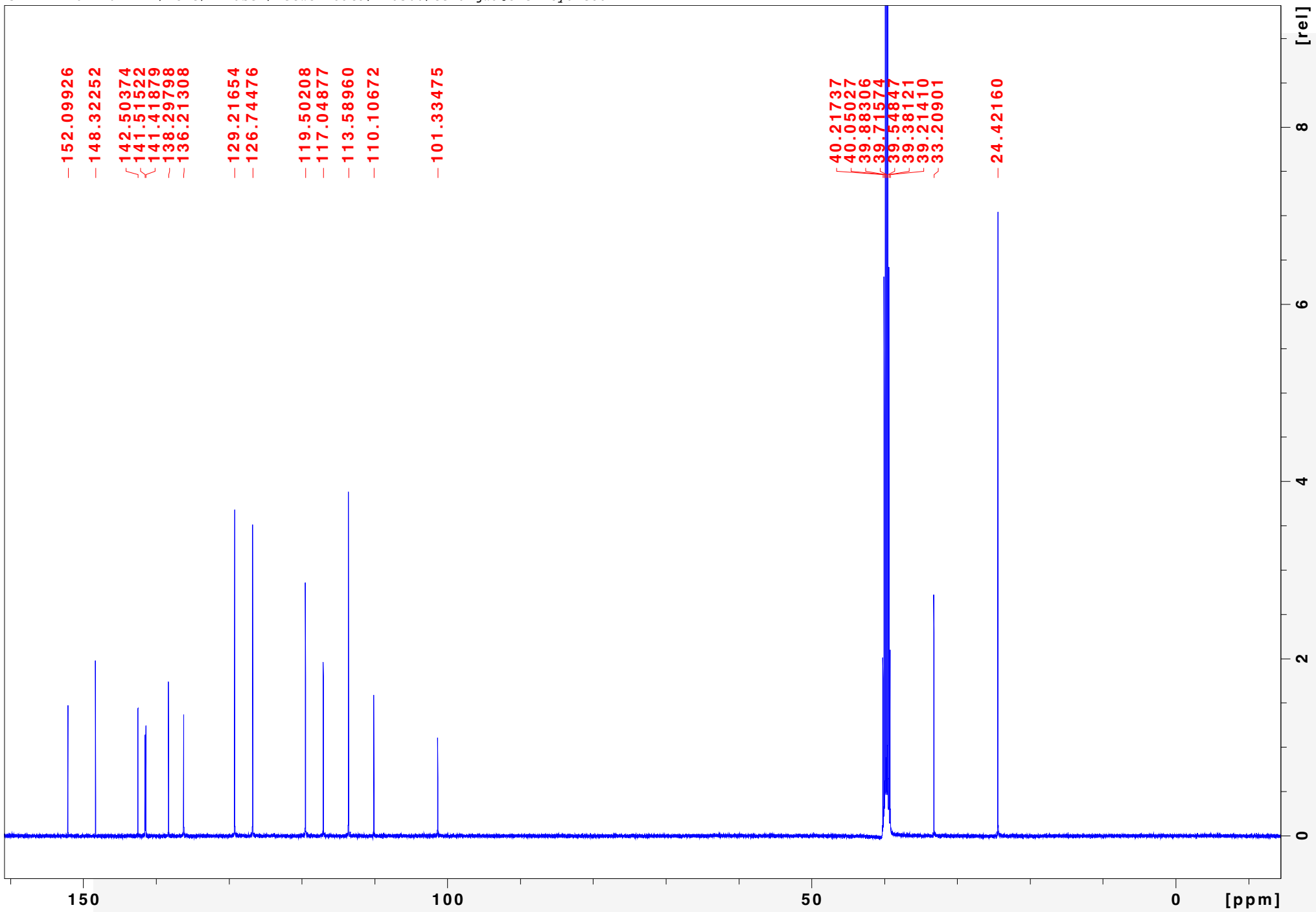
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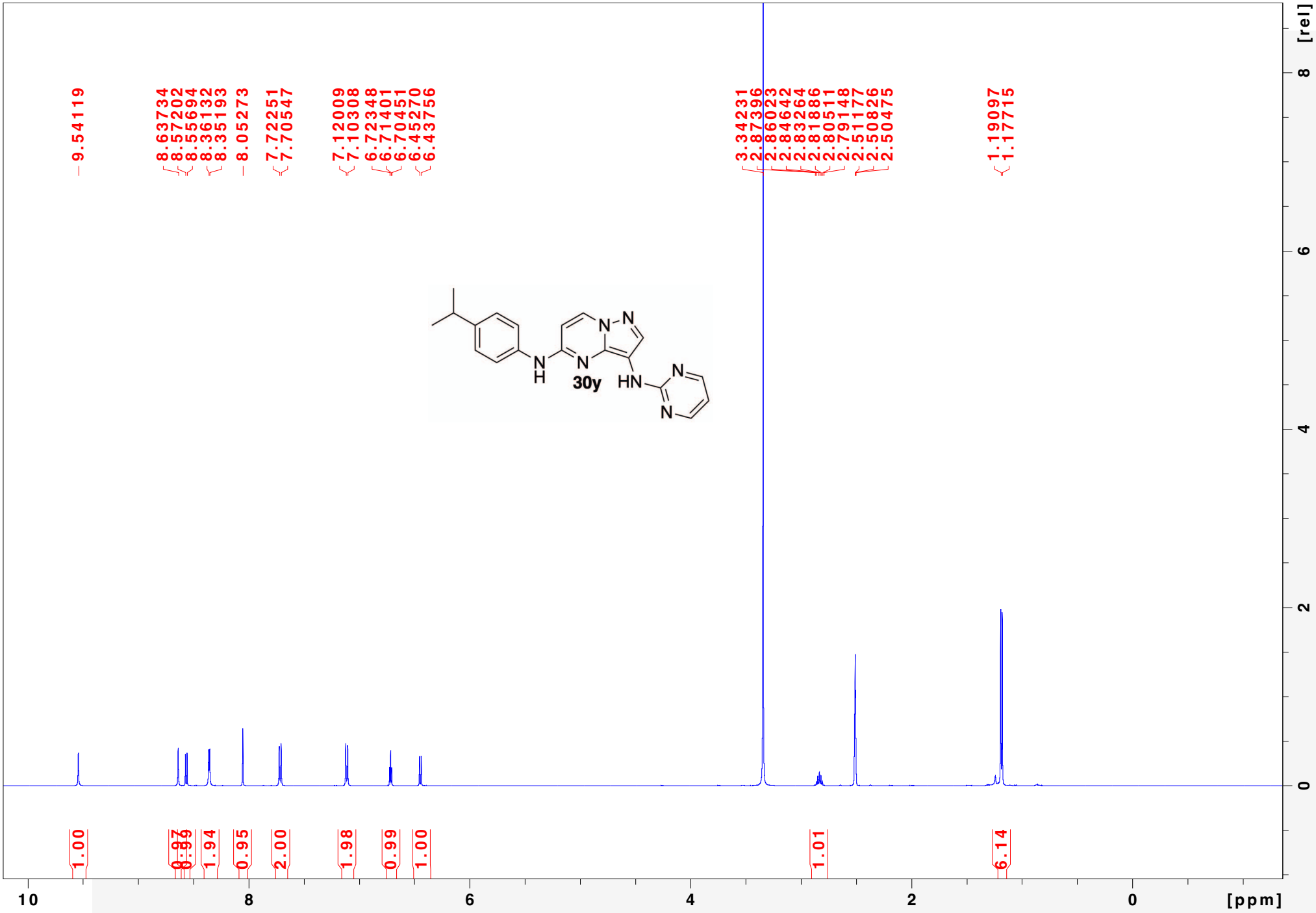
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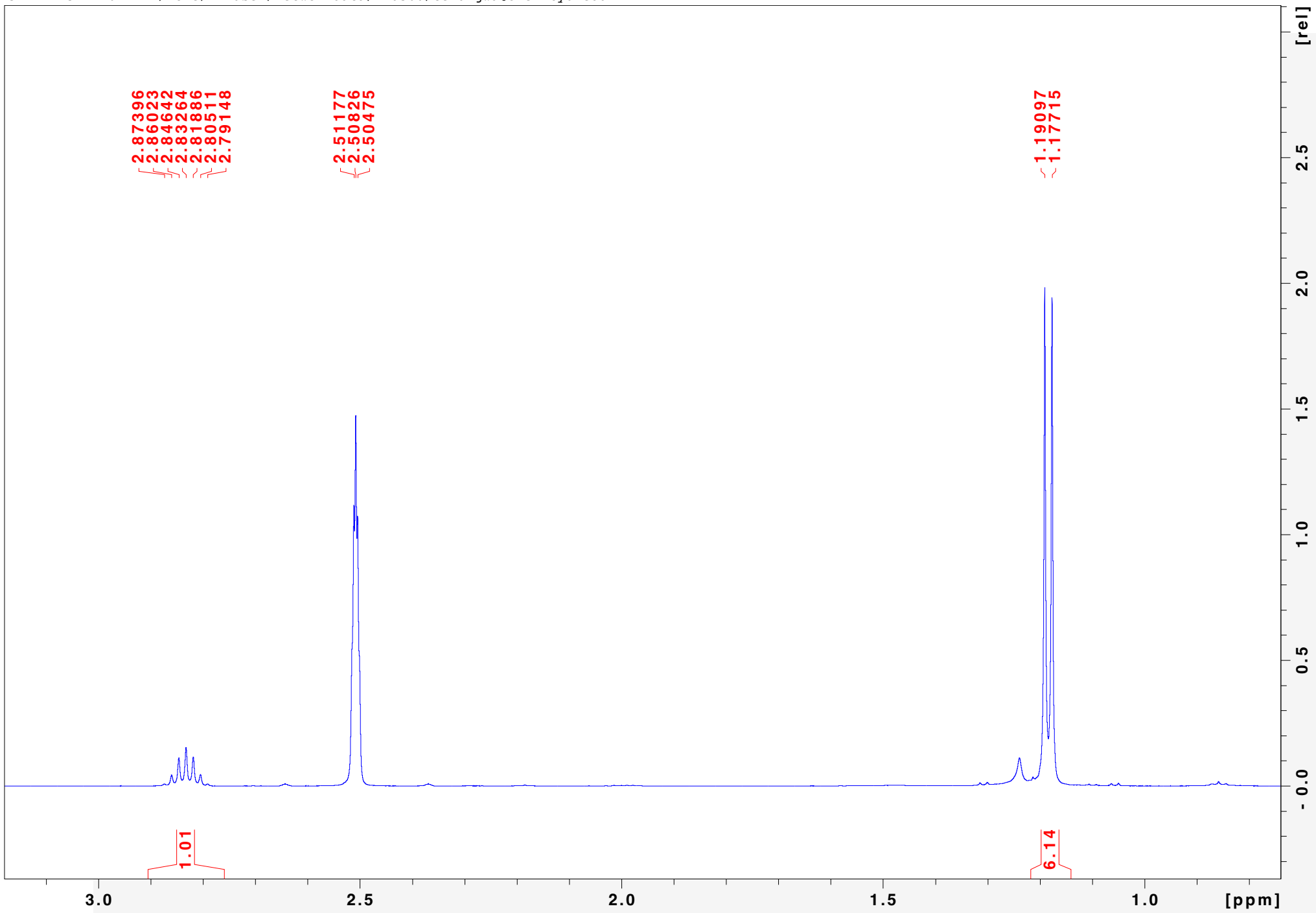
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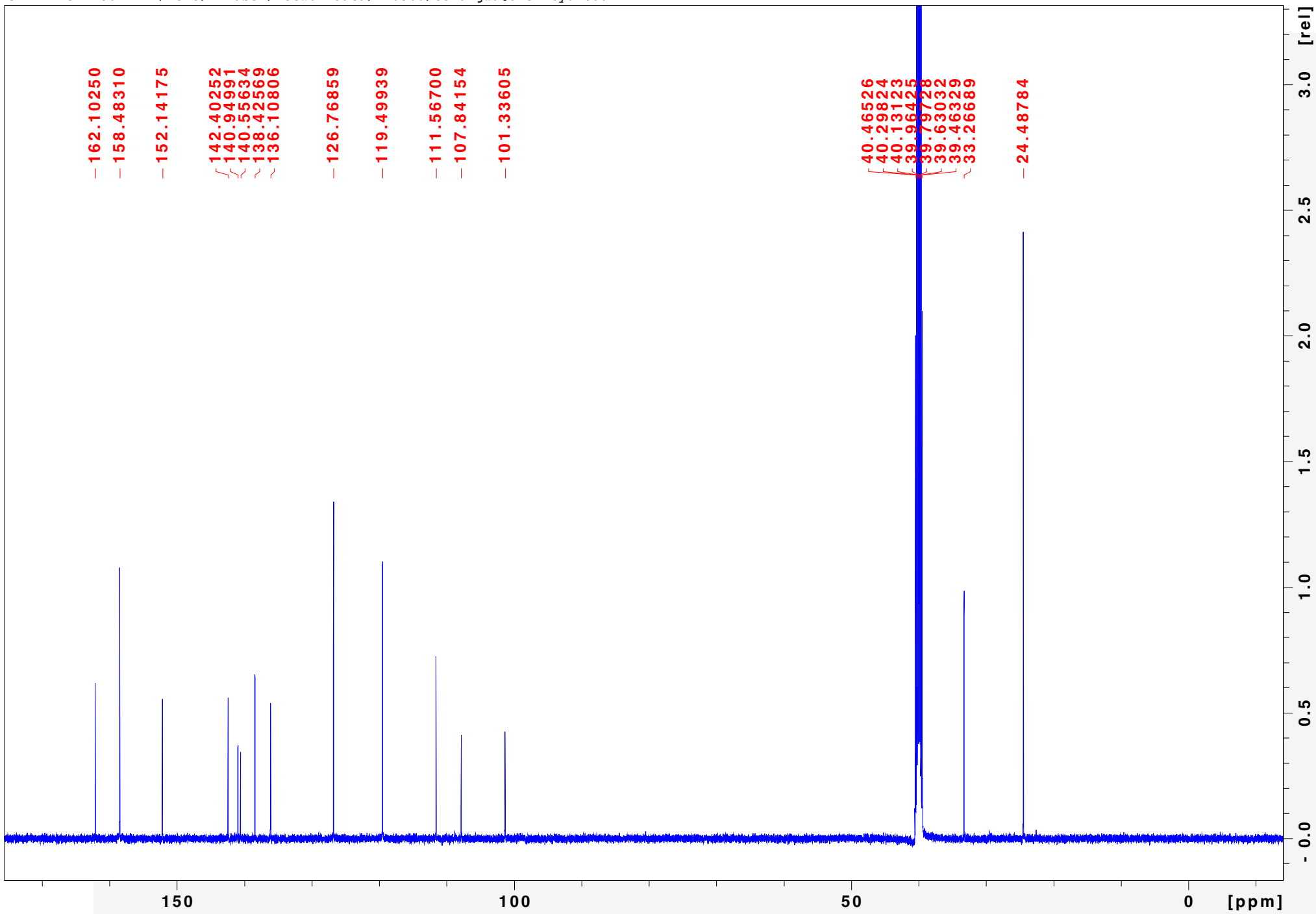
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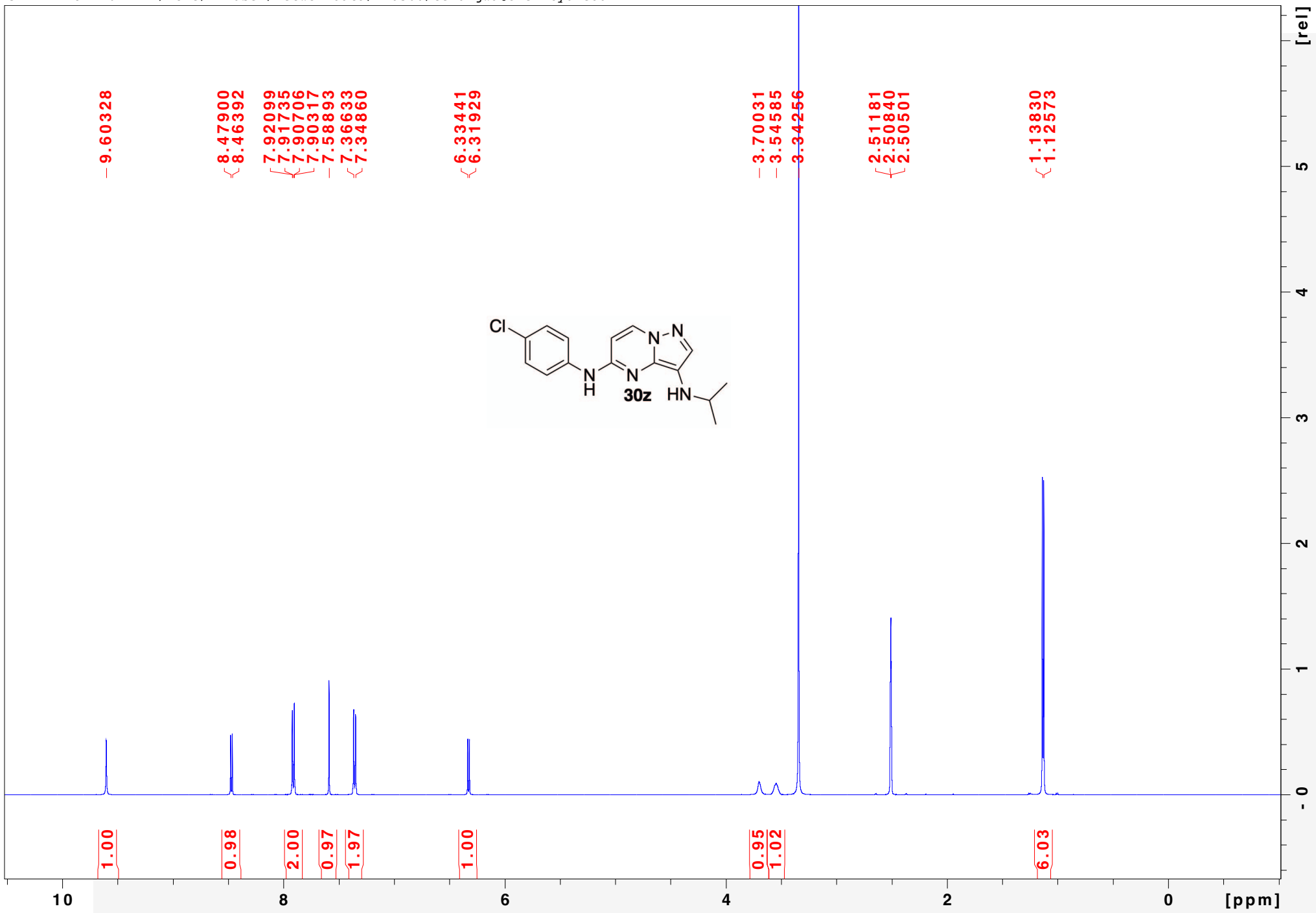
JI-III-51 20 1 /home/nmruser/networkdata/Bru500/terungwa@chem.byu.edu



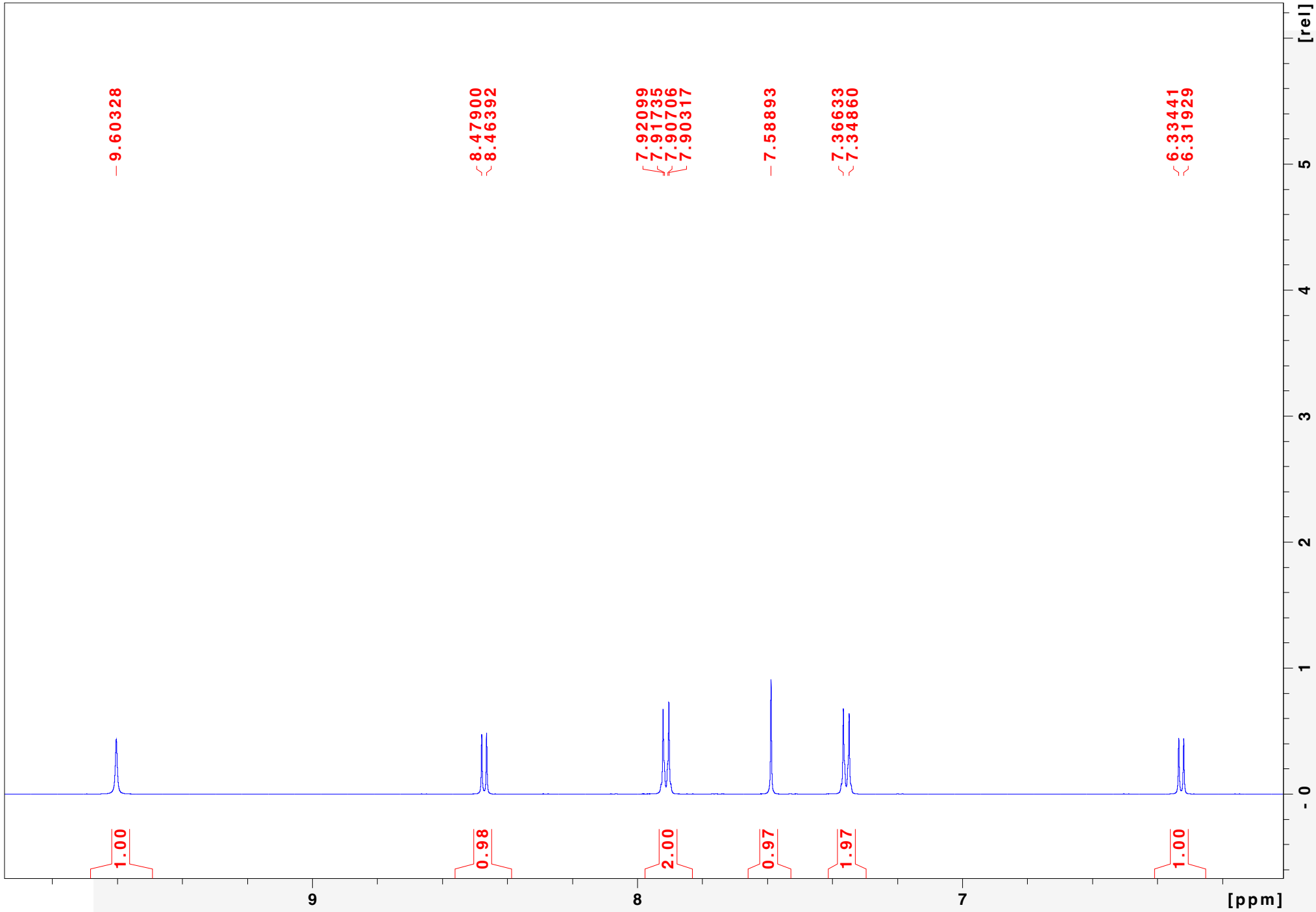
JI-III-51 30 1 /home/nmruser/networkdata/Bru500/terungwa@chem.byu.edu

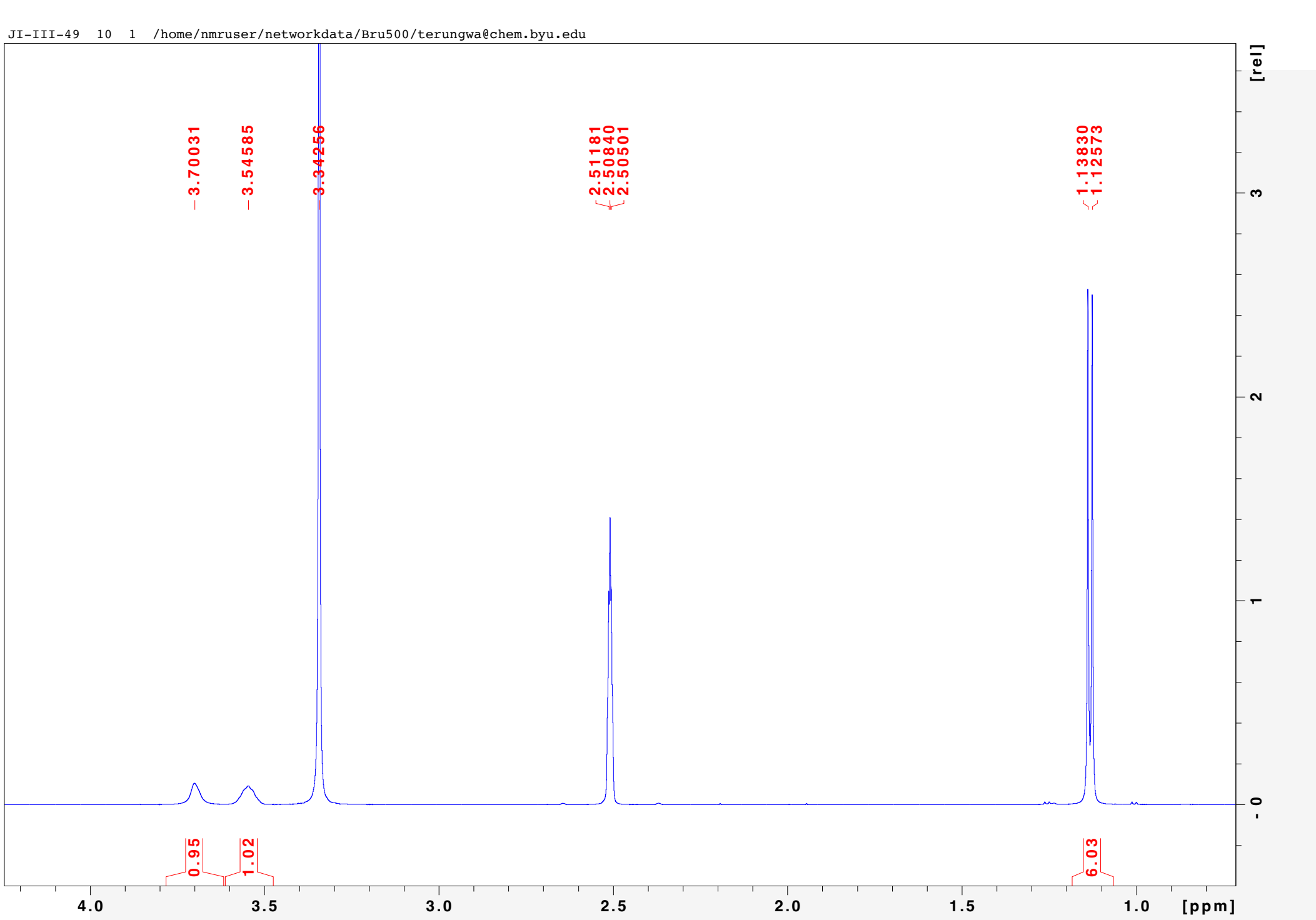


JI-III-49 10 1 /home/nmruser/networkdata/Bru500/terungwa@chem.byu.edu

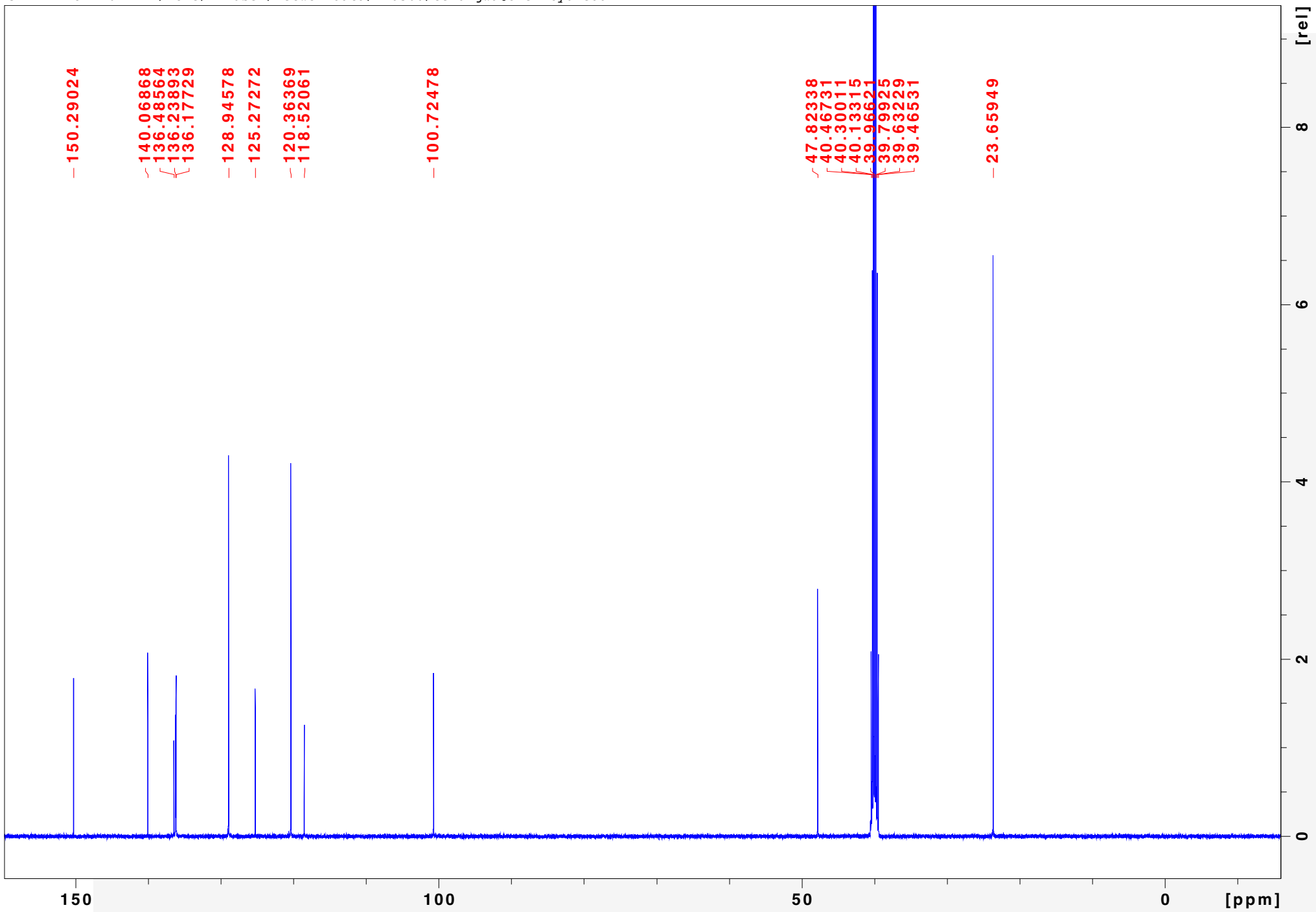


JI-III-49 10 1 /home/nmruser/networkdata/Bru500/terungwa@chem.byu.edu

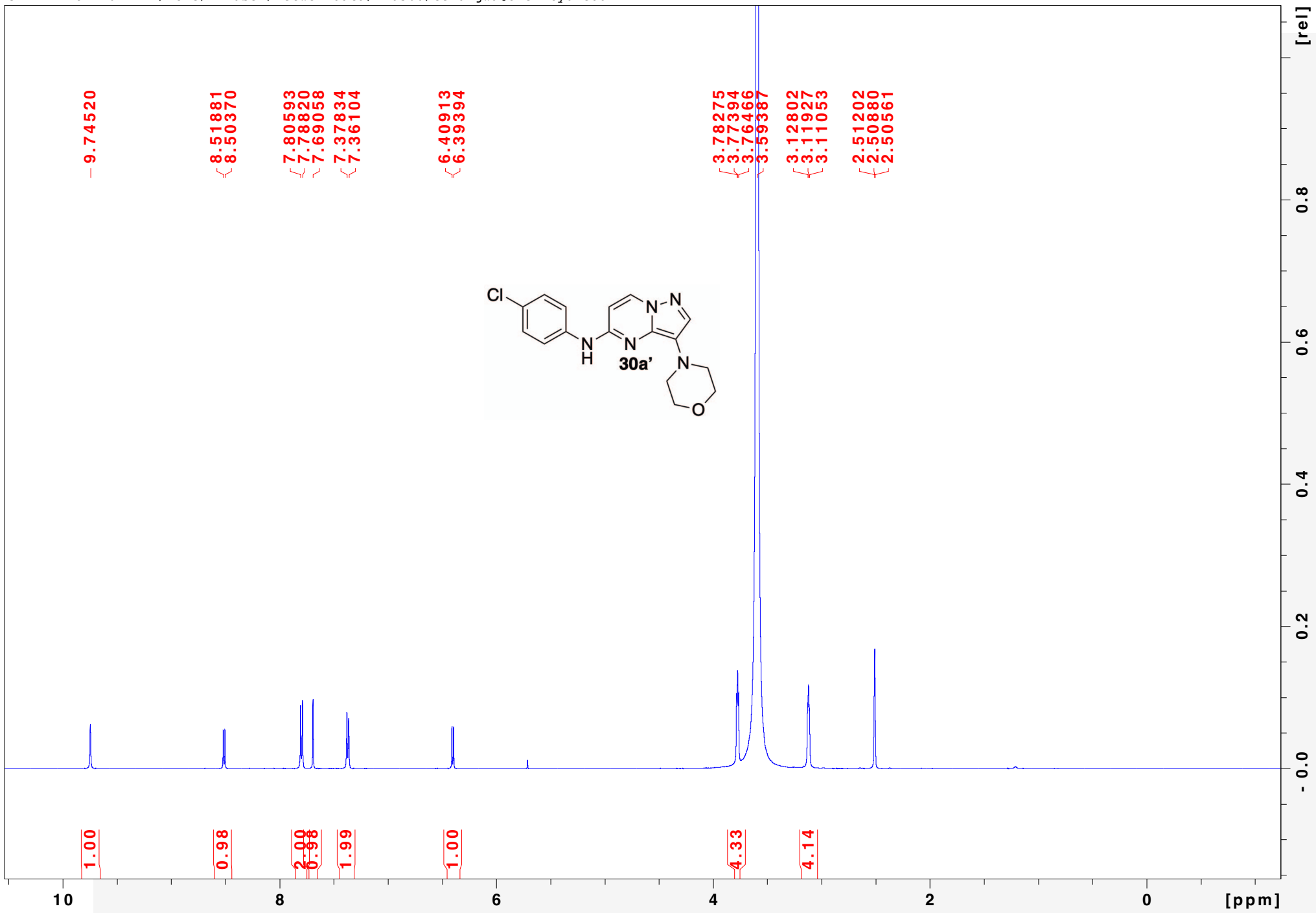



JI-III-49 10 1 /home/nmruser/networkdata/Bru500/terungwa@chem.byu.edu
3.70031
3.54585
3.34256
2.51181
2.50840
2.50501
1.13830
1.12573
0.95
1.02
6.03
4.0
3.5
3.0
2.5
2.0
1.5
1.0
[ppm]
[rel]
0
1
2
3

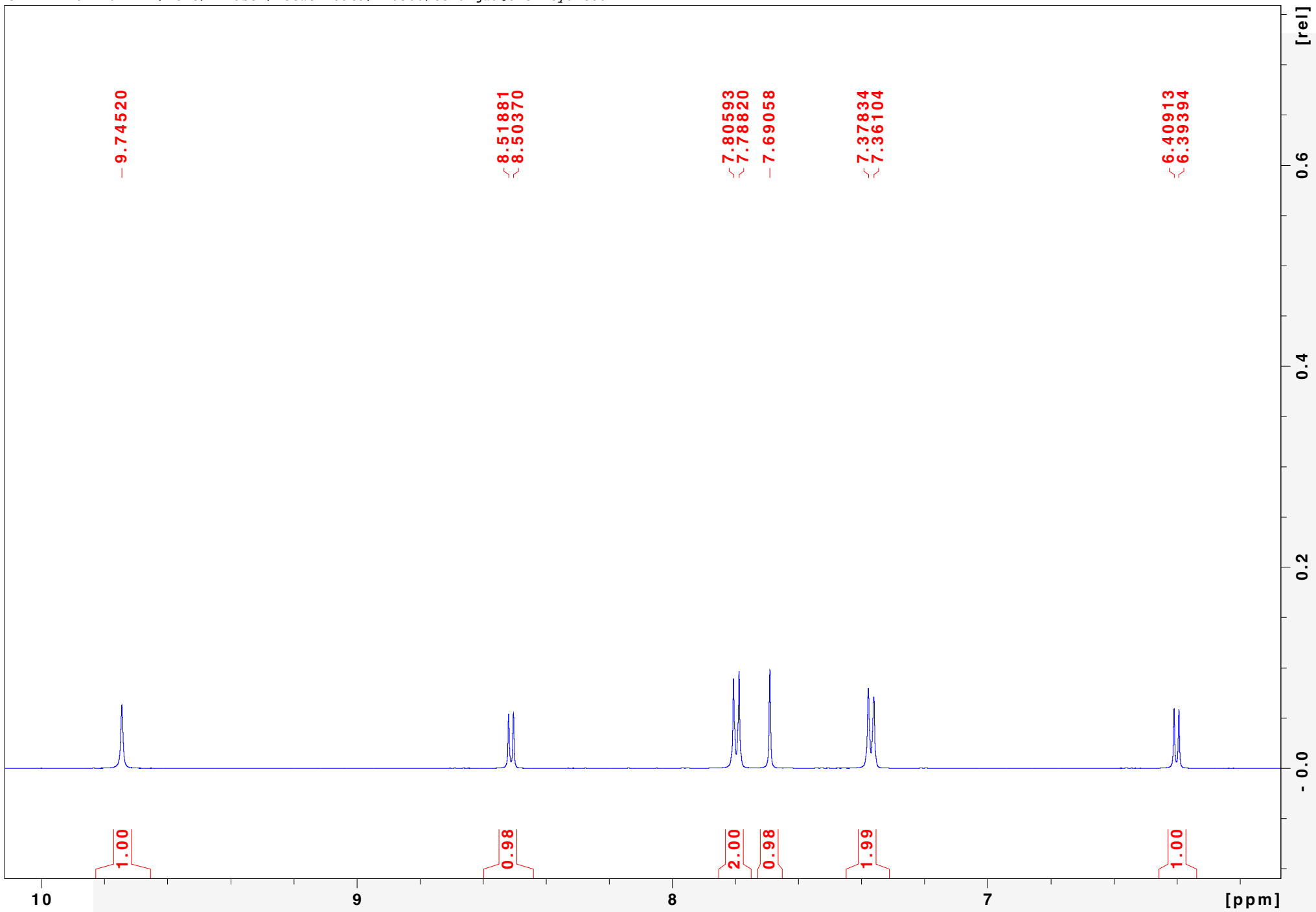
JI-III-49 20 1 /home/nmruser/networkdata/Bru500/terungwa@chem.byu.edu

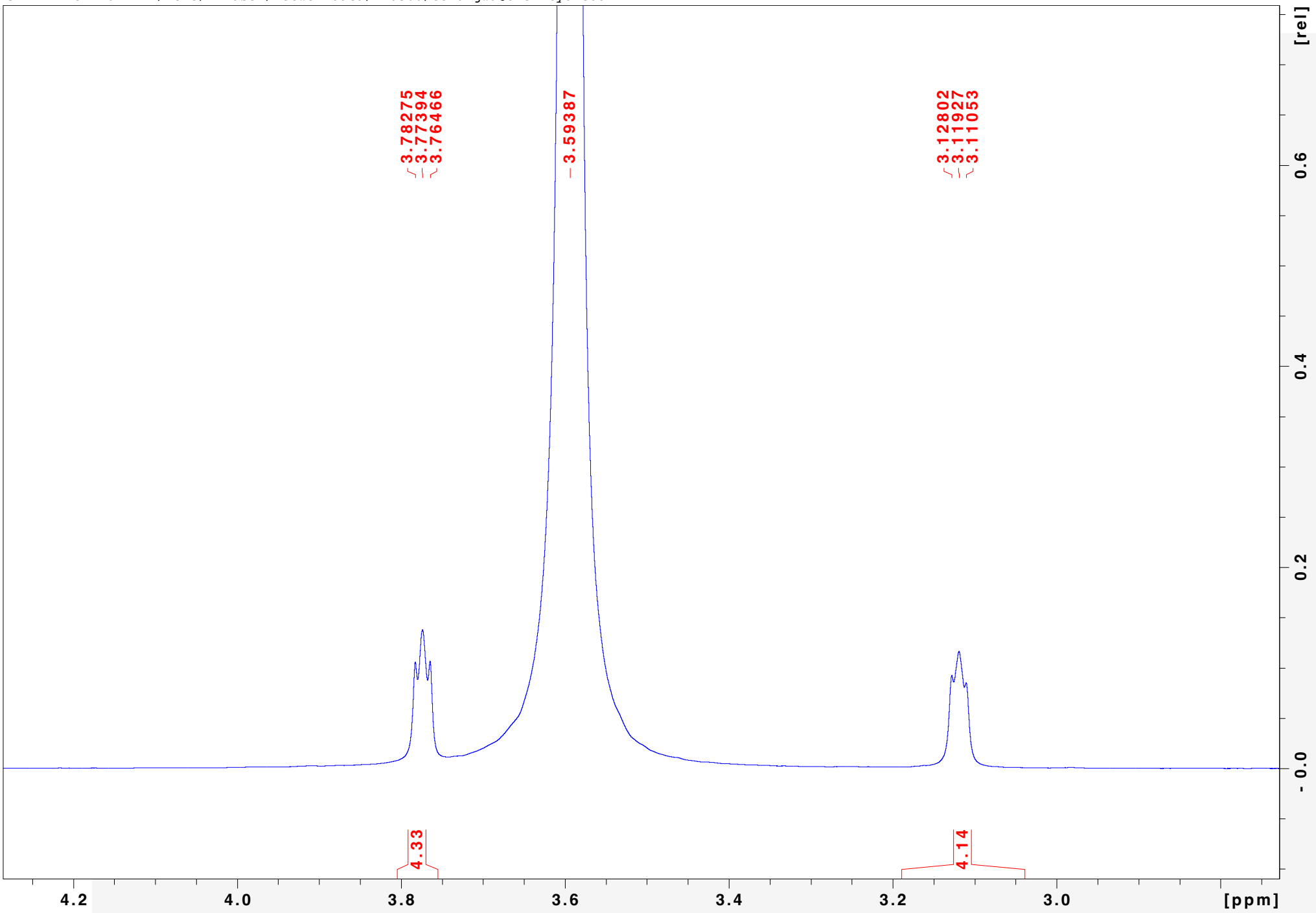


JI-III-48 10 1 /home/nmruser/networkdata/Bru500/terungwa@chem.byu.edu

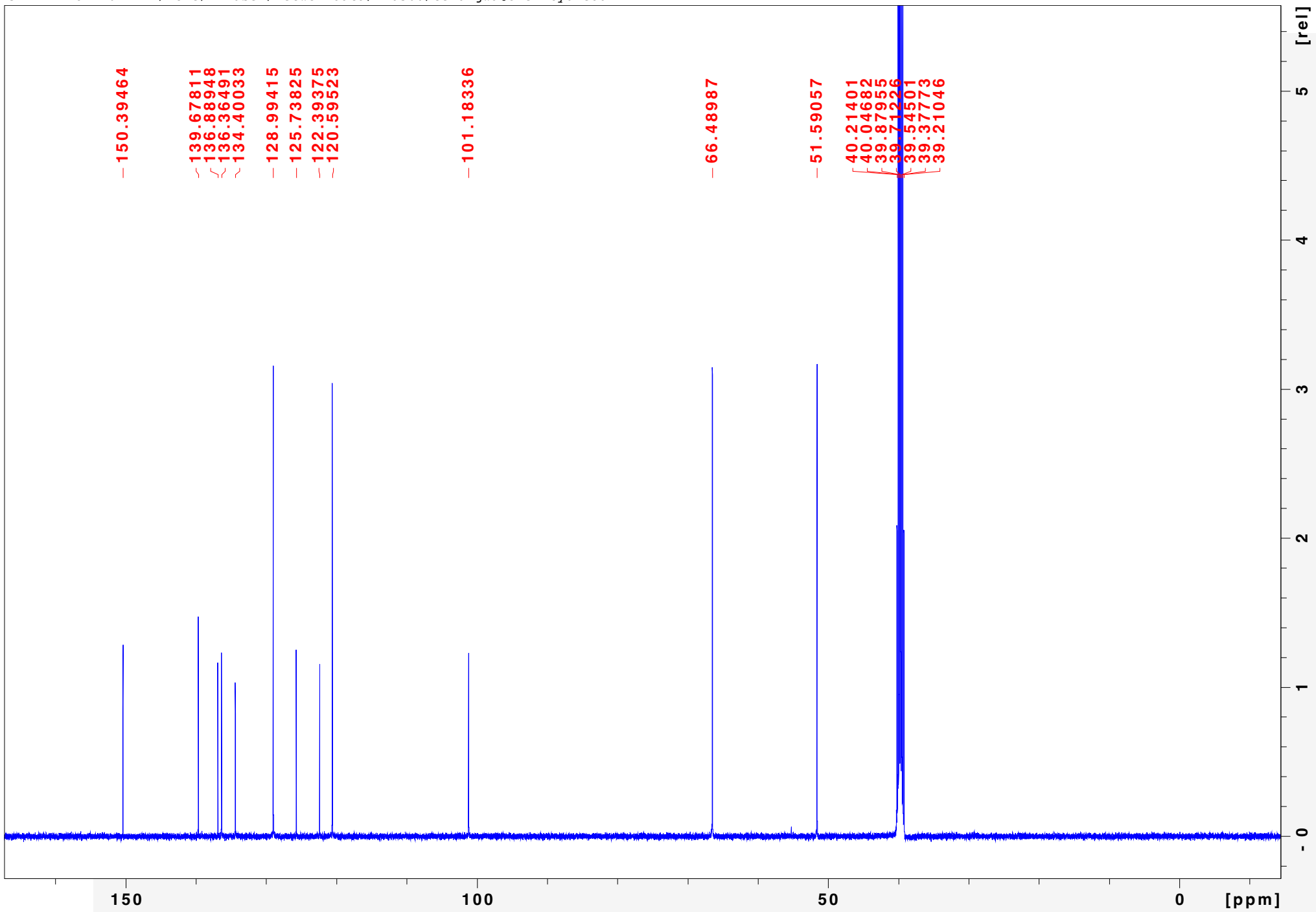


JI-III-48 10 1 /home/nmruser/networkdata/Bru500/terungwa@chem.byu.edu

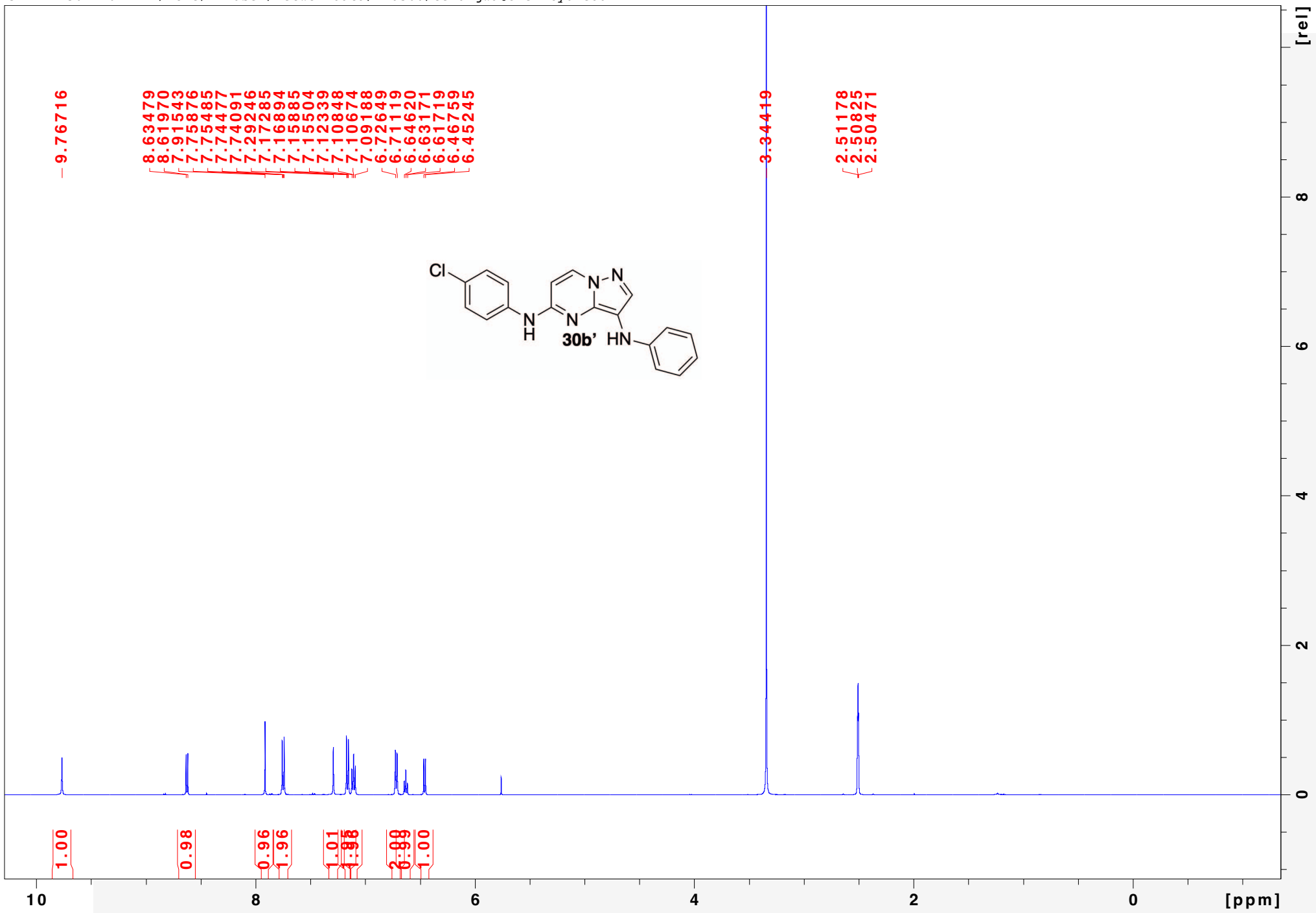



JI-III-48 10 1 /home/nmruser/networkdata/Bru500/terungwa@chem.byu.edu
3.78275
3.77394
3.76466
3.59387
3.12802
3.11927
3.11053
4.33
4.14
4.2
4.0
3.8
3.6
3.4
3.2
3.0
[ppm]
[rel]
0.6
0.4
0.2
- 0.0

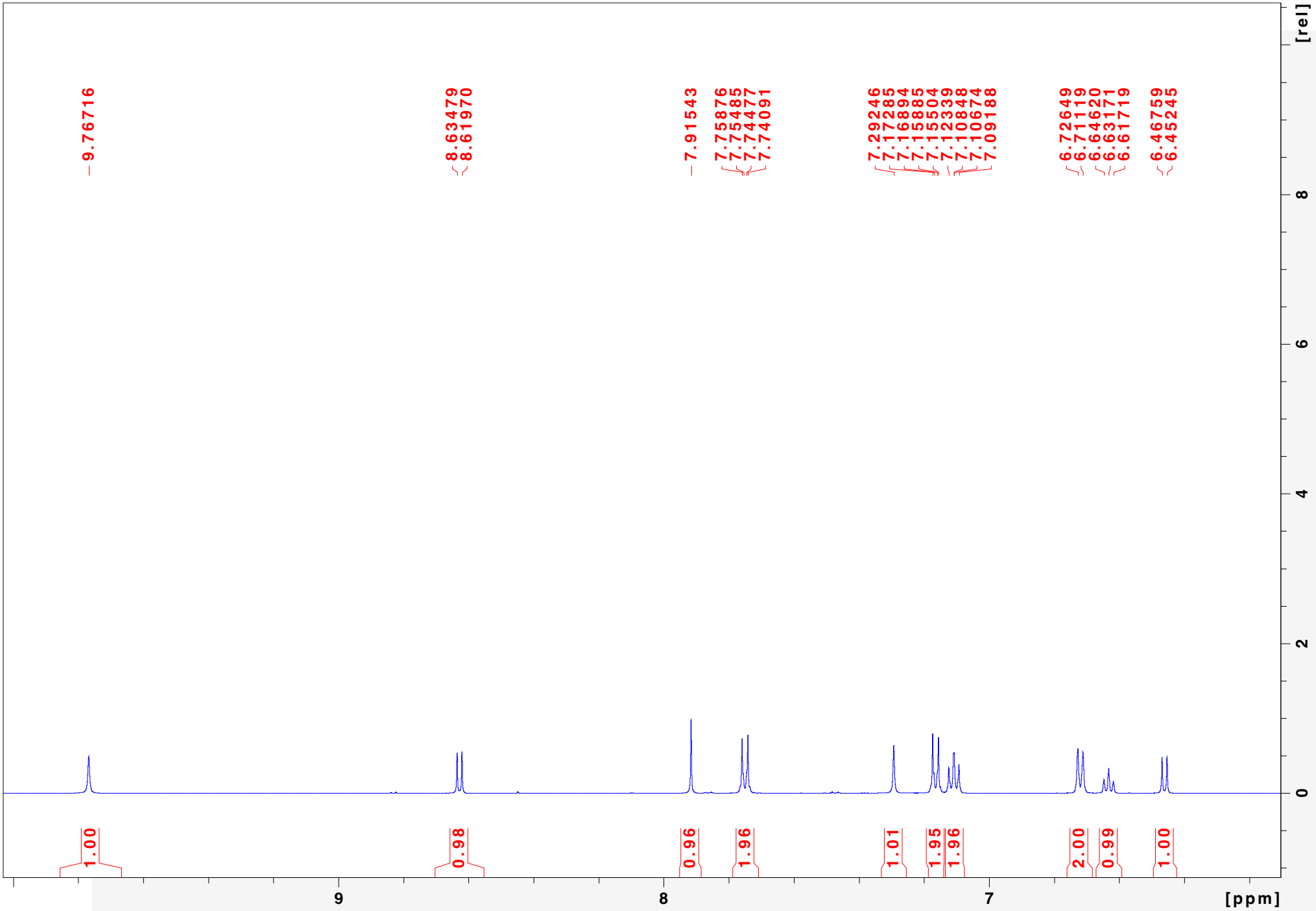
JI-III-48 20 1 /home/nmruser/networkdata/Bru500/terungwa@chem.byu.edu



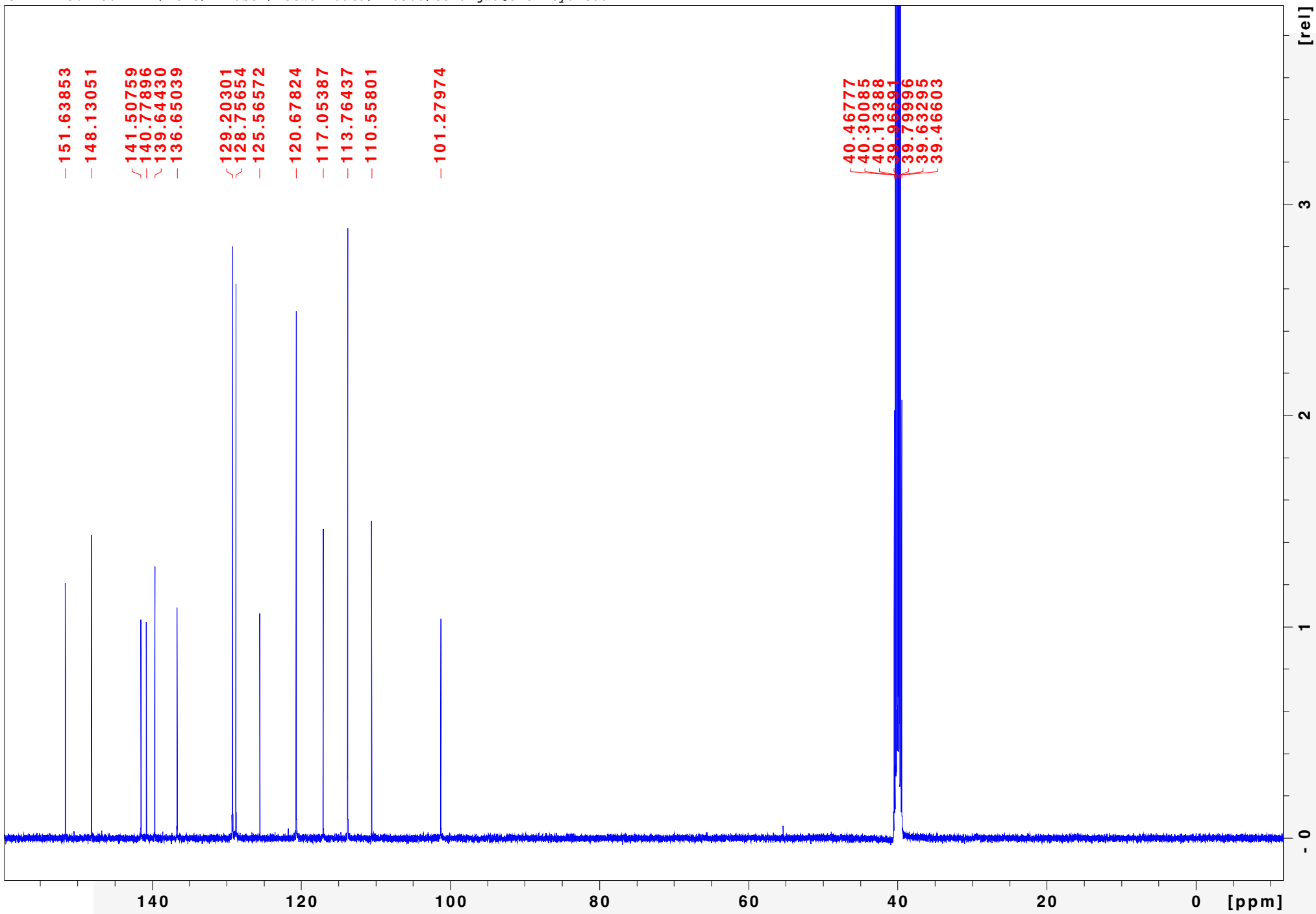
JI-III-50 20 1 /home/nmruser/networkdata/Bru500/terungwa@chem.byu.edu



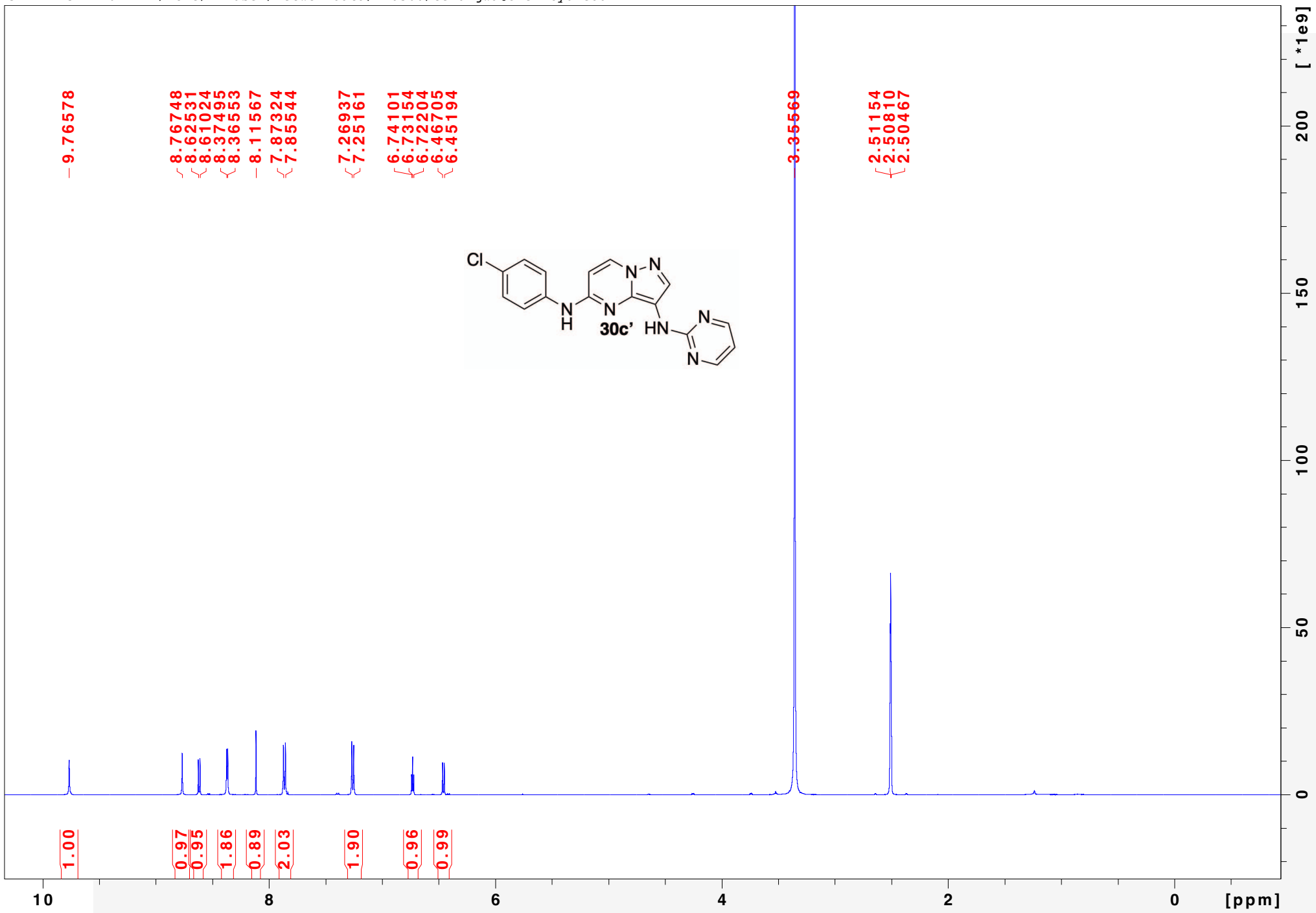
JI-III-50 20 1 /home/nmruser/networkdata/Bru500/terungwa@chem.byu.edu



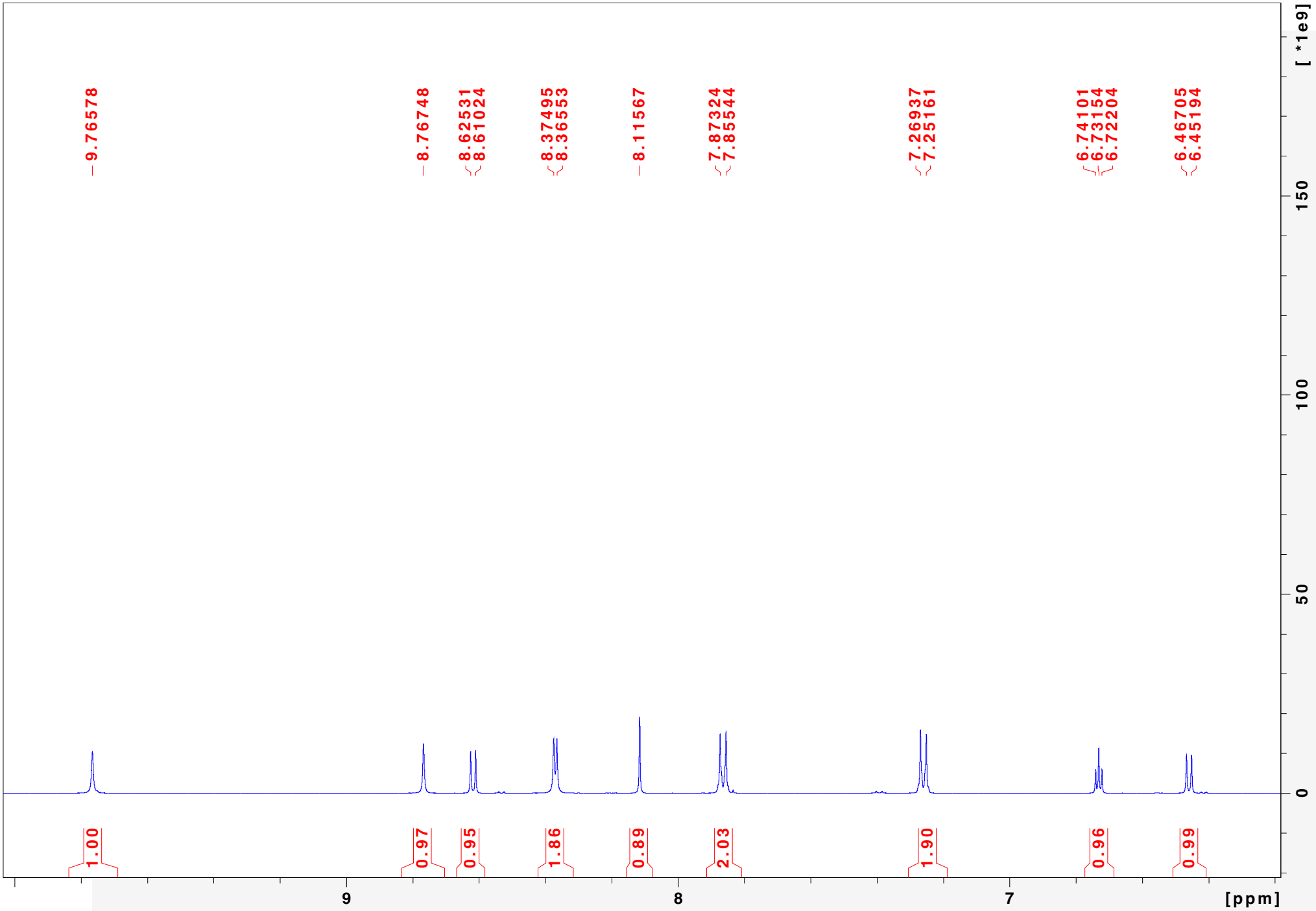
JI-III-50 30 1 /home/nmruser/networkdata/Bru500/terungwa@chem.byu.edu



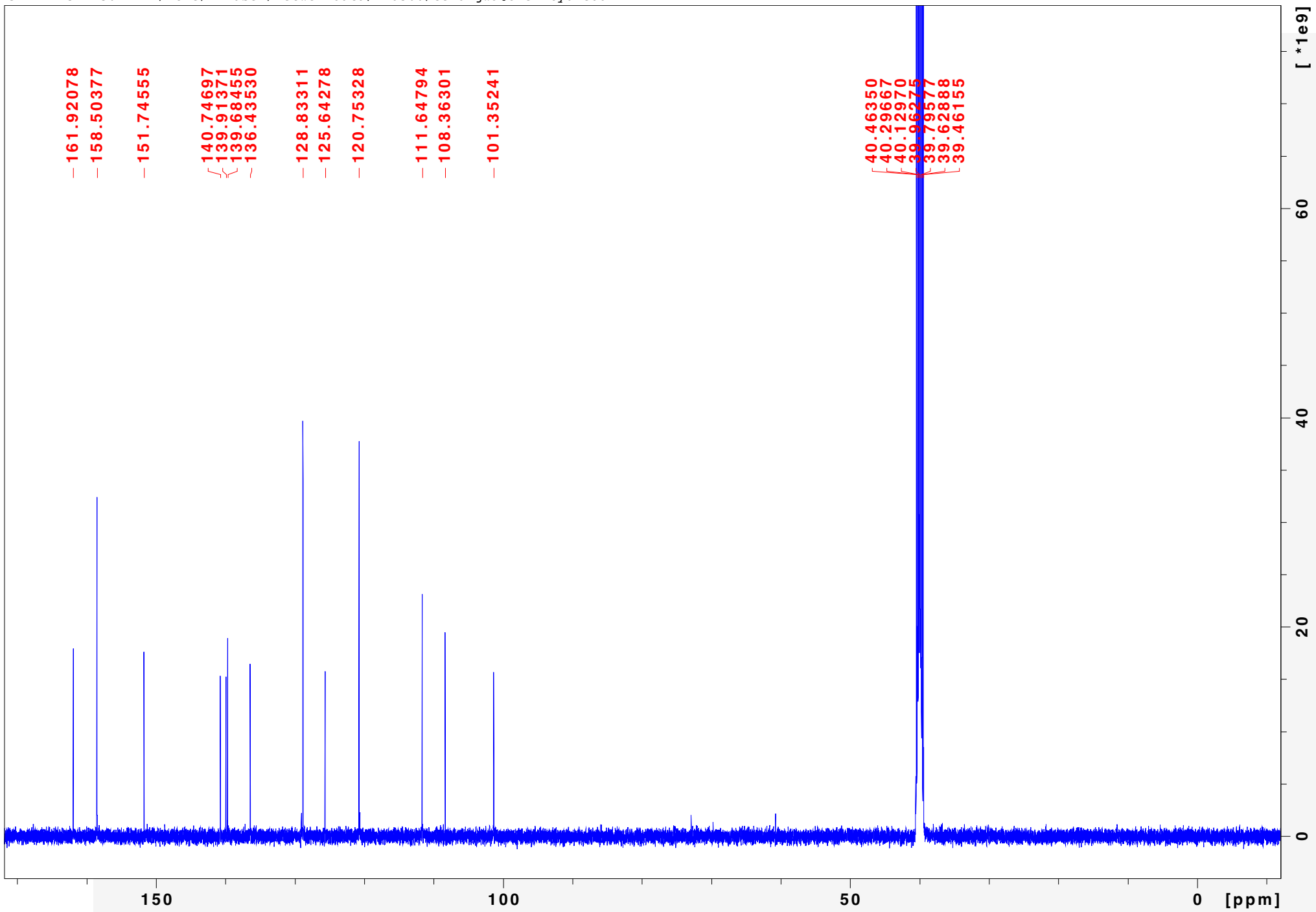
JI-III-52 40 1 /home/nmruser/networkdata/Bru500/terungwa@chem.byu.edu



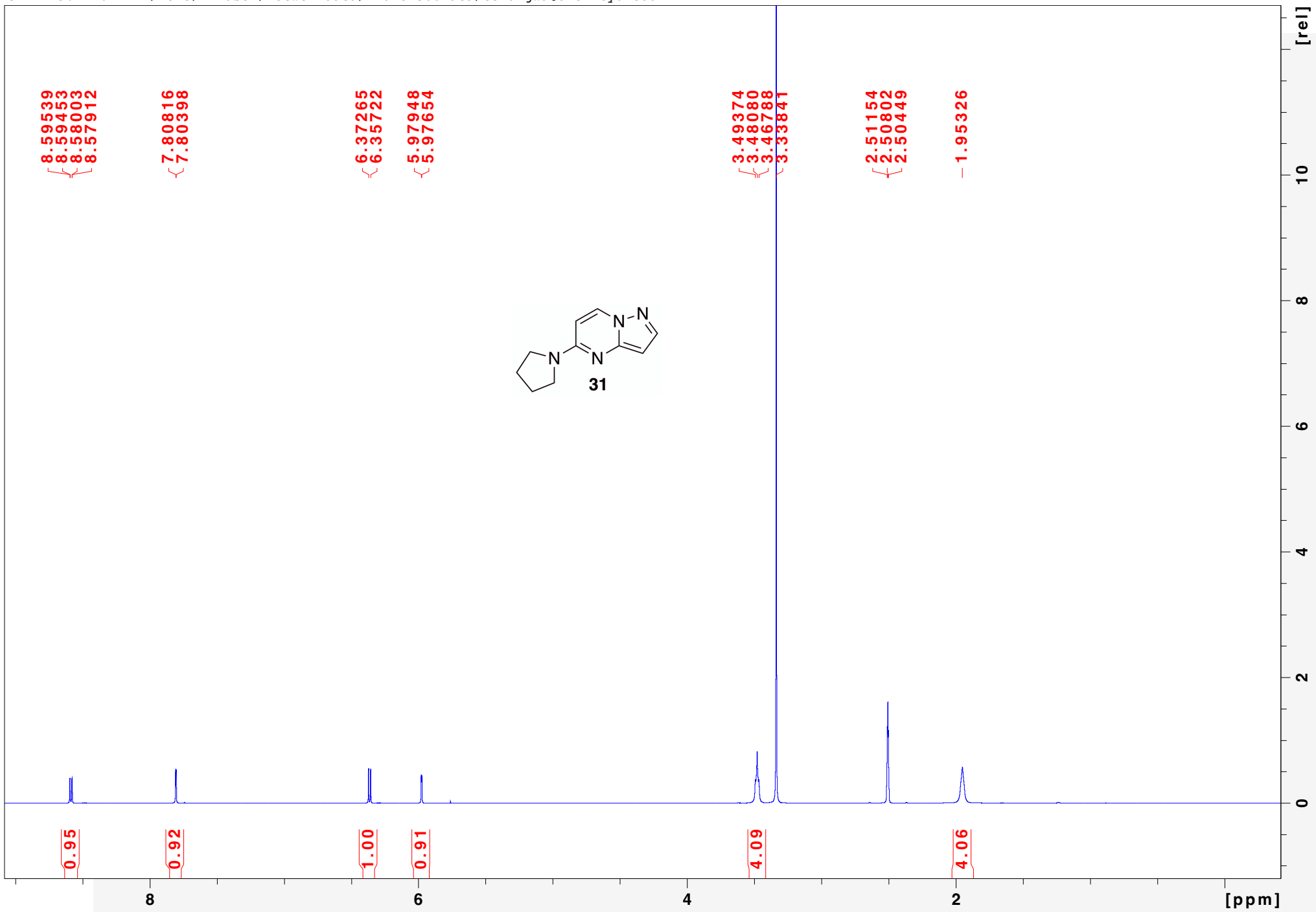
JI-III-52 40 1 /home/nmruser/networkdata/Bru500/terungwa@chem.byu.edu



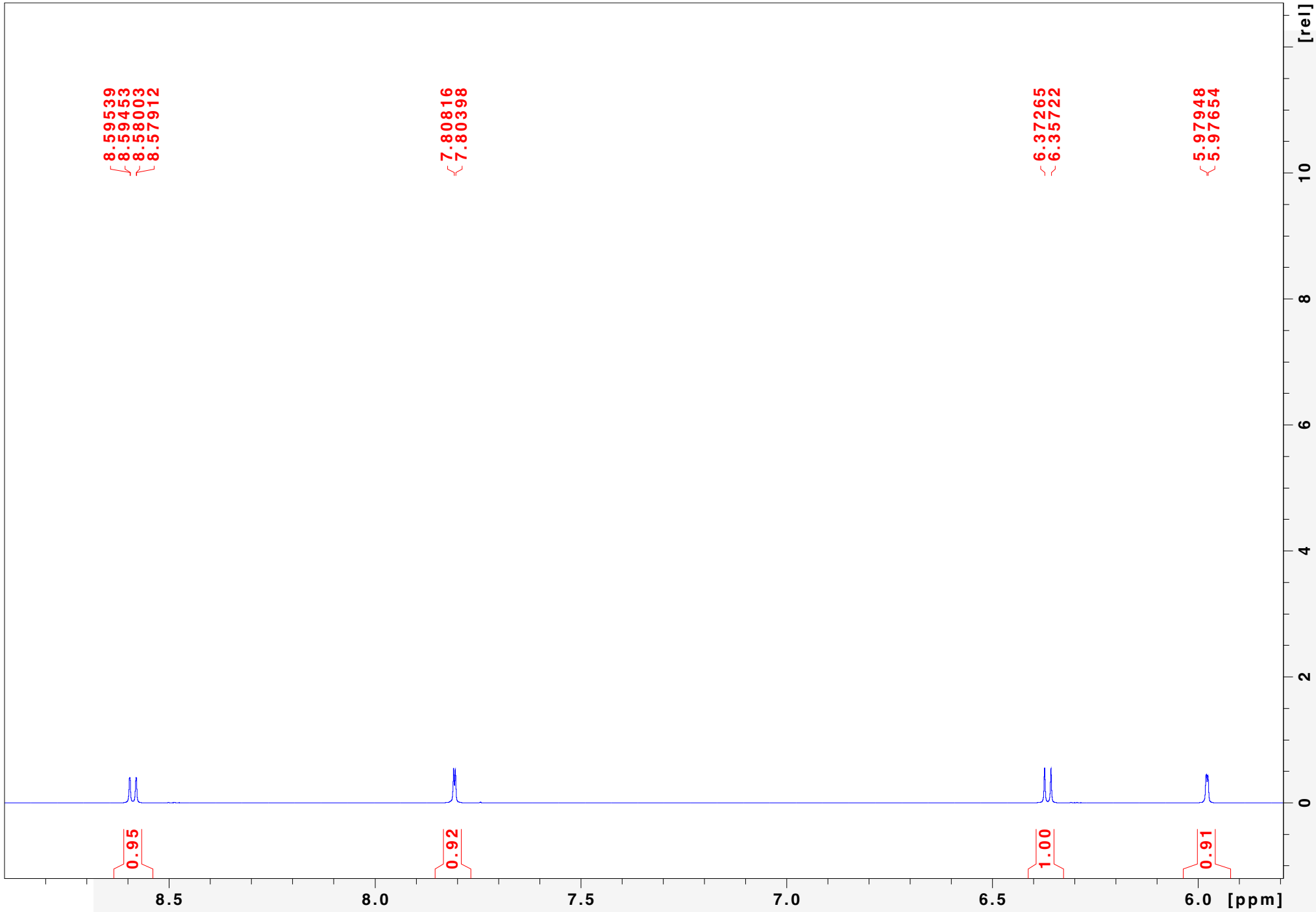
JI-III-52 50 1 /home/nmruser/networkdata/Bru500/terungwa@chem.byu.edu



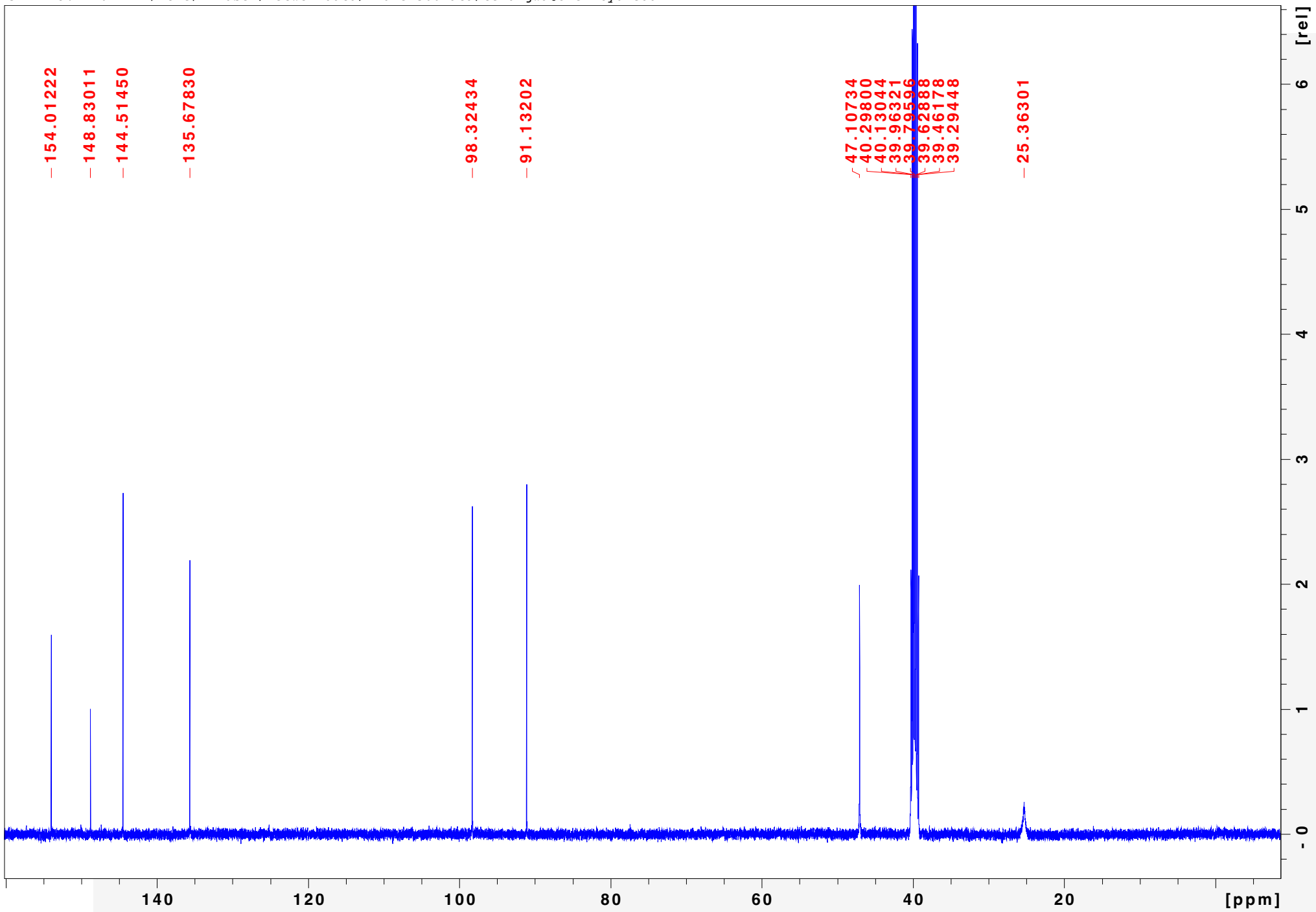
JI-II-97 10 1 /home/nmruser/networkdata/Bruker500Data/terungwa@chem.byu.edu



JI-II-97 10 1 /home/nmruser/networkdata/Bruker500Data/terungwa@chem.byu.edu



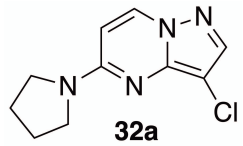
JI-II-97 20 1 /home/nmruser/networkdata/Bruker500Data/terungwa@chem.byu.edu



JI-II-111 10 1 /home/nmruser/networkdata/terungwa@chem.byu.edu

PROTON DMSO /opt/nmrdata terungwa@chem.byu.edu 12

8.6022
8.5867
7.9258
6.4494
6.4340
3.5199
3.3351
2.5113
2.5077
2.5041
1.9624



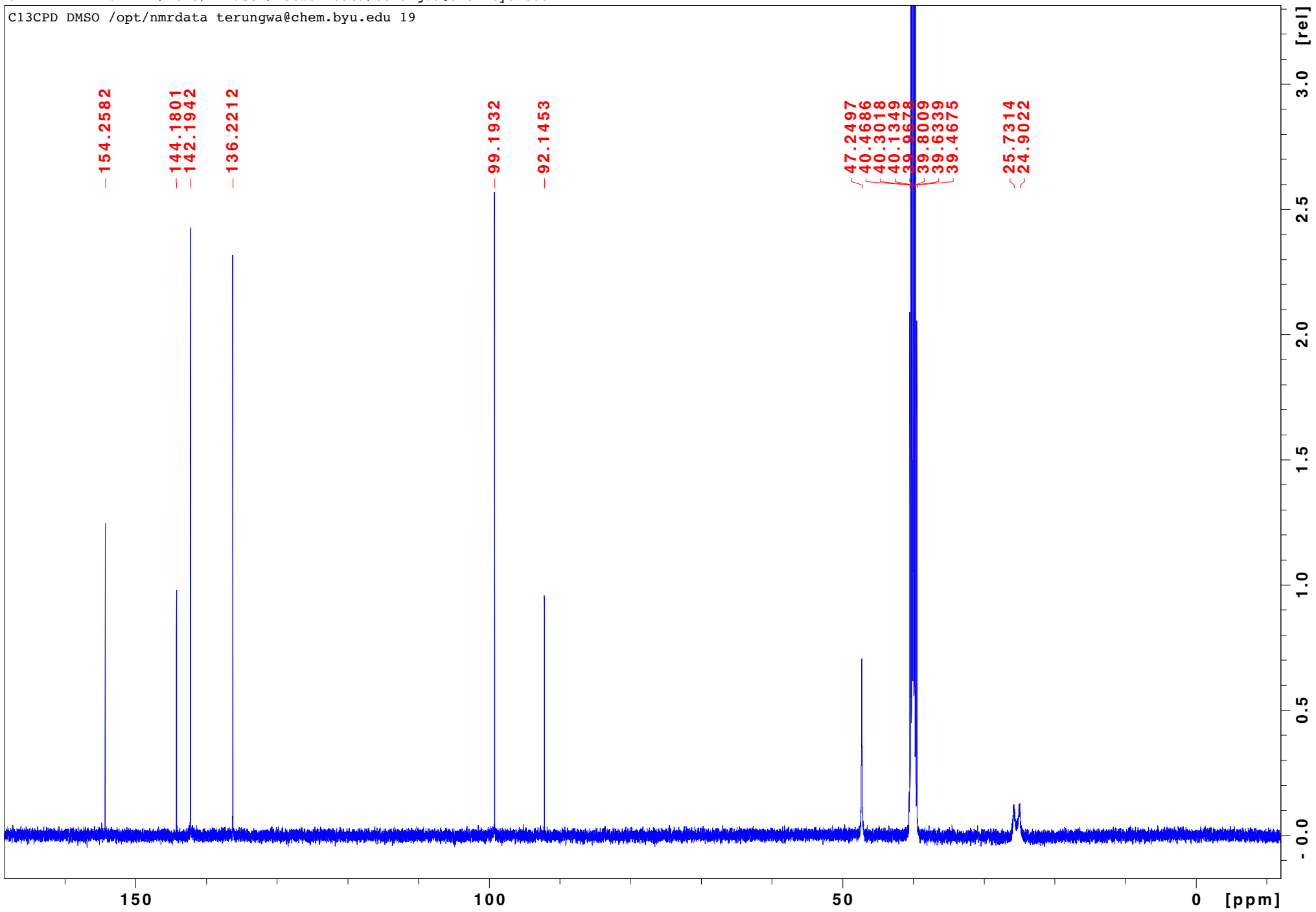
32a

1.000
0.886
1.056
4.278
4.262

[rel]
[ppm]

JI-II-111 20 1 /home/nmruser/networkdata/terungwa@chem.byu.edu

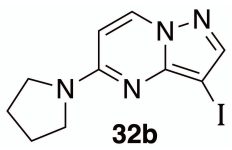
C13CPD DMSO /opt/nmrdata terungwa@chem.byu.edu 19



JI-II-112 10 1 /home/nmruser/networkdata/terungwa@chem.byu.edu

PROTON DMSO /opt/nmrdata terungwa@chem.byu.edu 14

8.6038
8.5884
7.8684
6.4075
6.3921
3.5208
3.3369
2.5113
2.5078
2.5042
1.9611

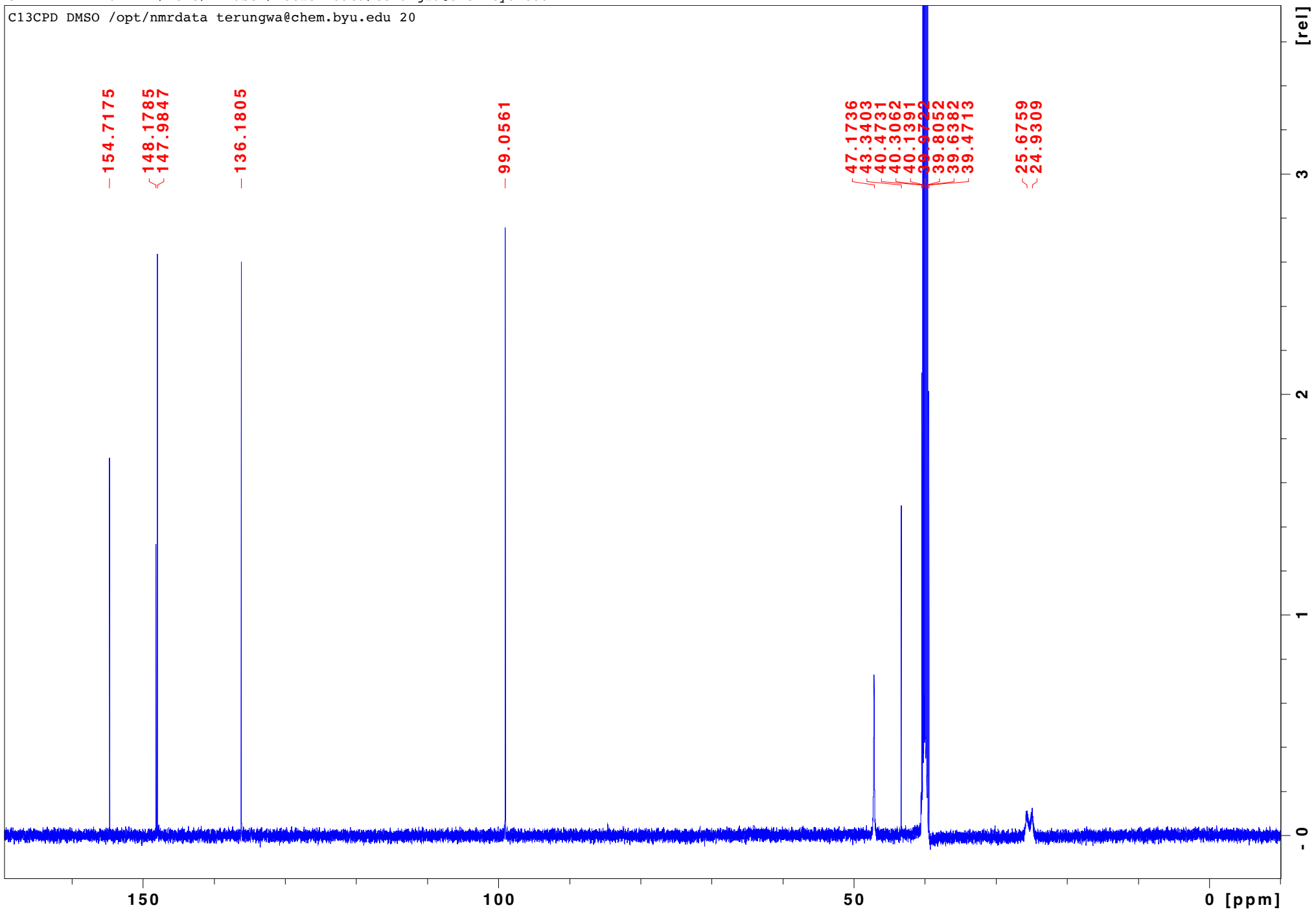


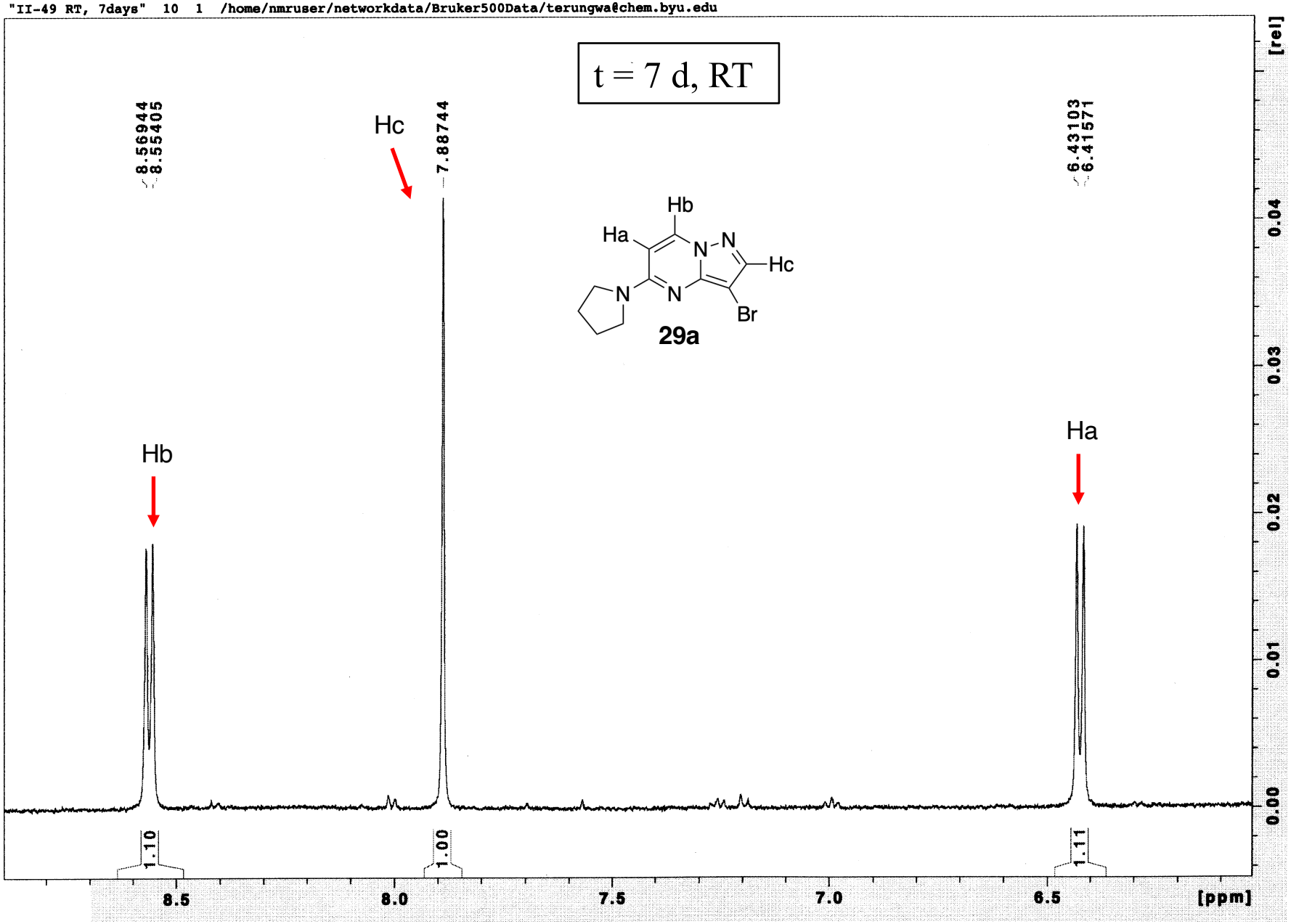
32b

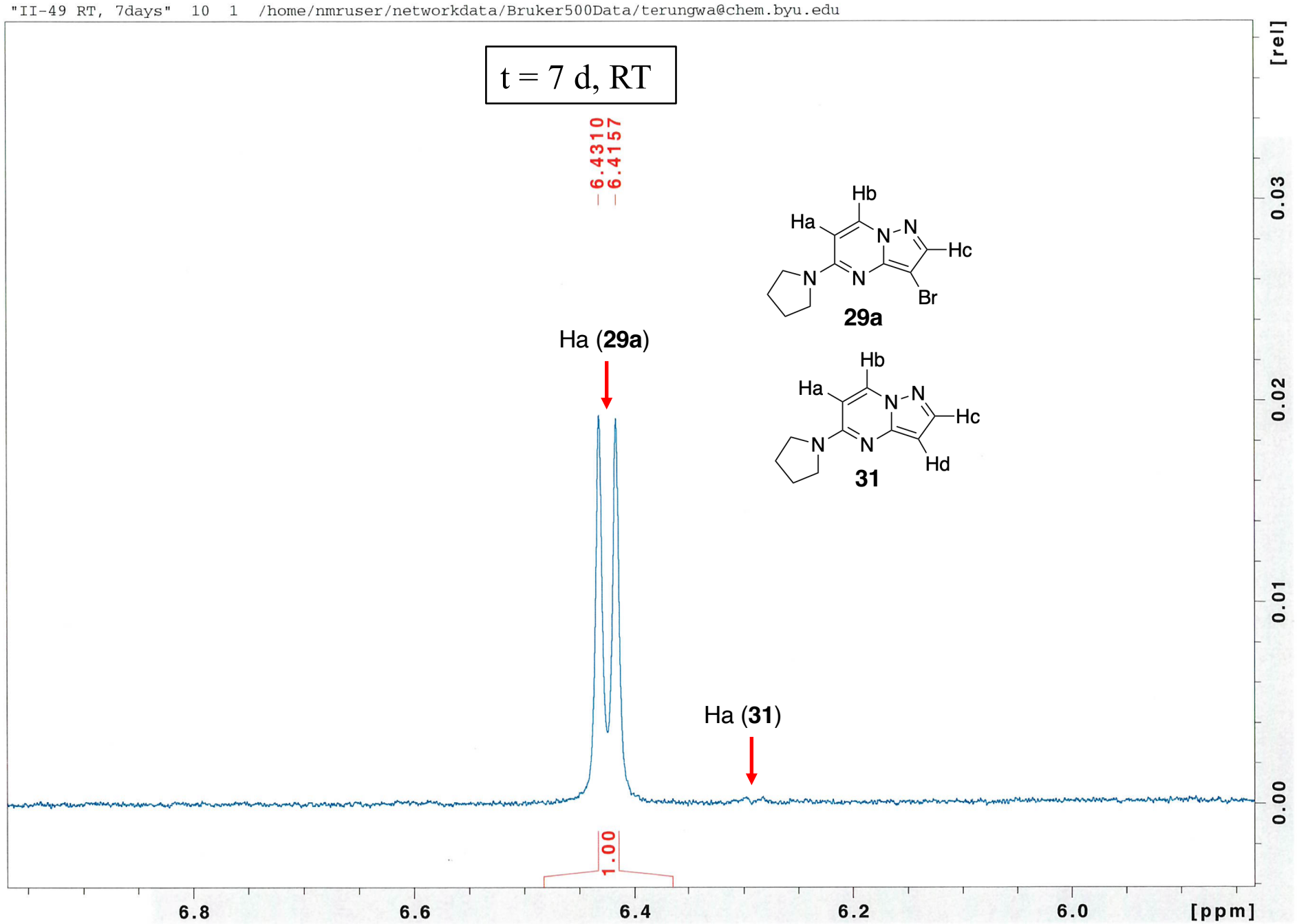
0.979
0.859
1.000
4.131
4.133

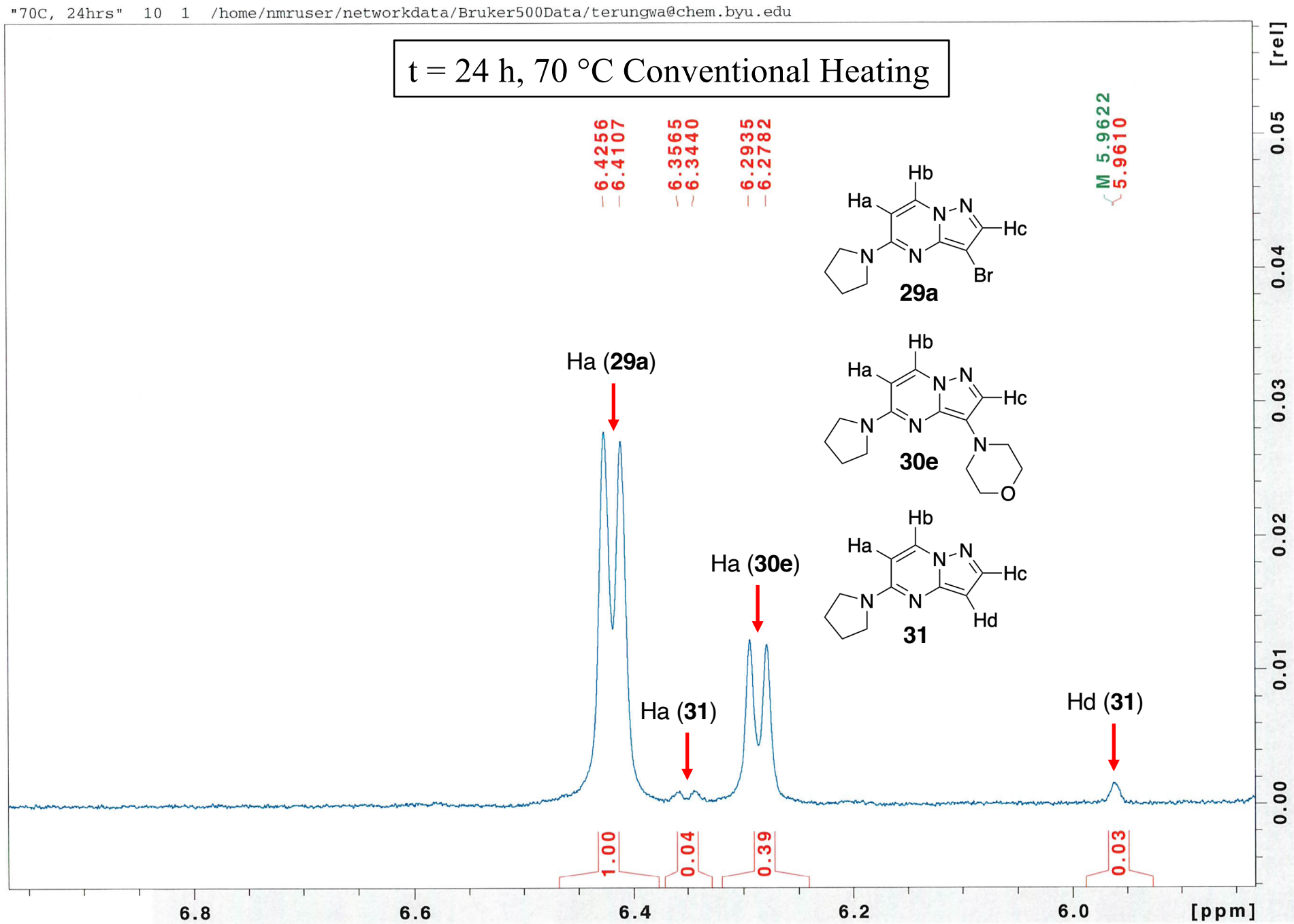
8
6
4
2
0
[ppm]

0
2
4
6
8
10
[rel]

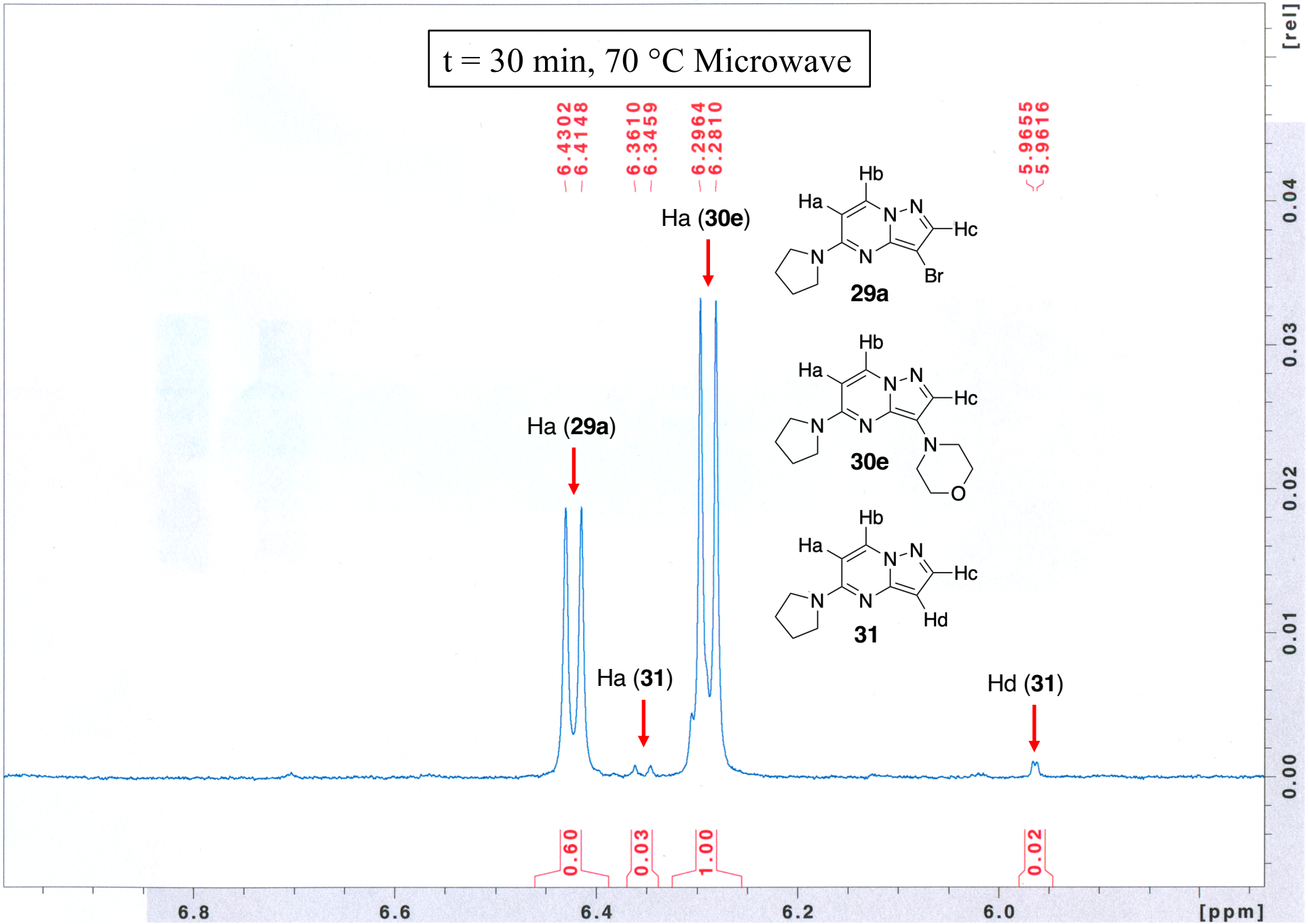

JI-II-112 20 1 /home/nmruser/networkdata/terungwa@chem.byu.edu
C13CPD DMSO /opt/nmrdata terungwa@chem.byu.edu 20
154.7175
148.1785
147.9847
136.1805
99.0561
47.1736
43.3403
40.4731
40.3062
40.1391
39.8052
39.6382
39.4713
25.6759
24.9309
[rel]
3
2
1
- 0
150
100
50
0 [ppm]

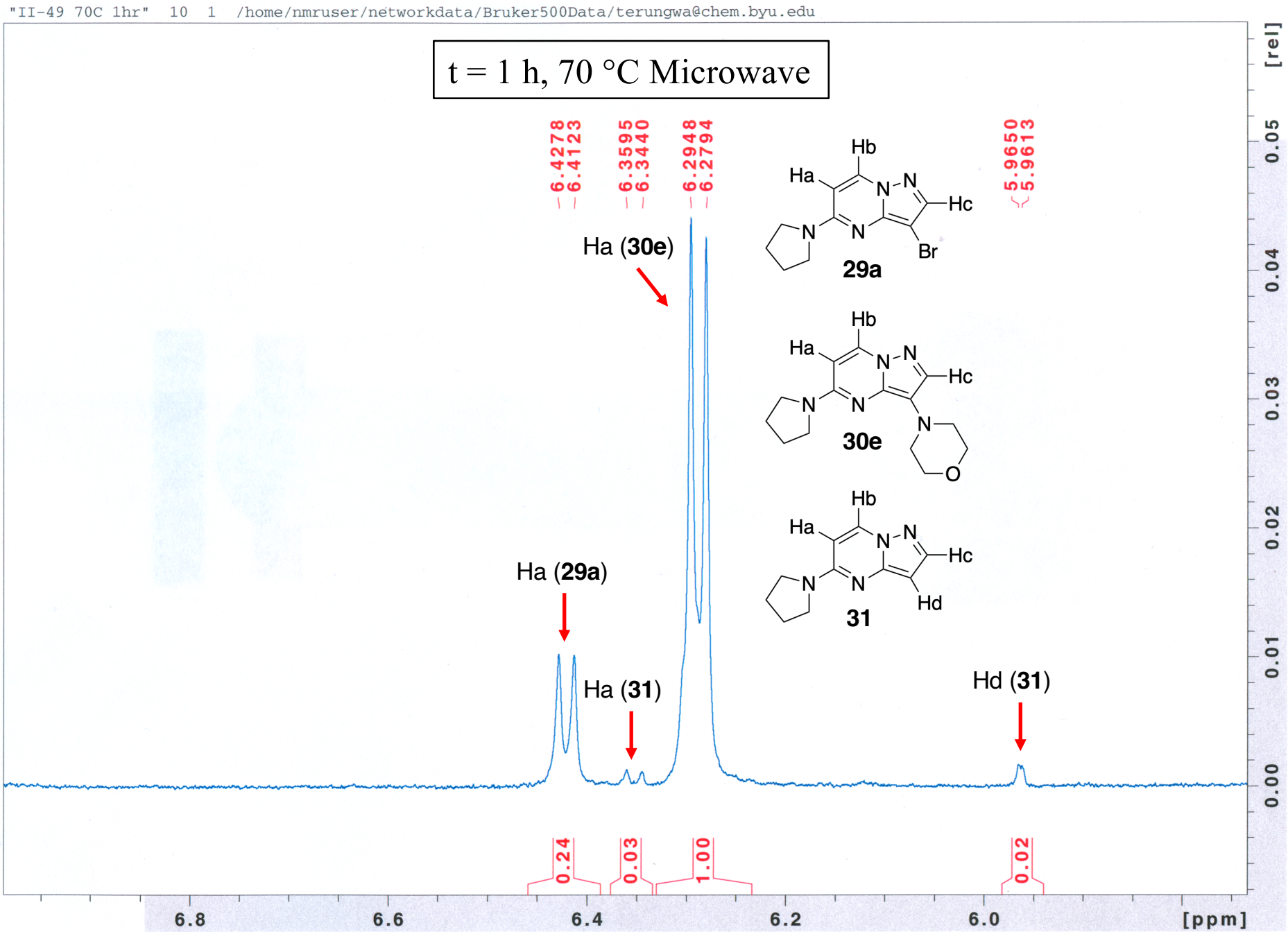

"II-49 RT, 7days" 10 1 /home/nmruser/networkdata/Bruker500Data/terungwa@chem.byu.edu
t = 7 d, RT
8.56944
8.55405
Hc
7.88744
6.43103
6.41571
Hb
Ha
Hc
N
N
N
N
Br
29a
Hb
Ha
1.10
1.00
1.11
8.5
8.0
7.5
7.0
6.5
[ppm]
[rel]
0.04
0.03
0.02
0.01
0.00

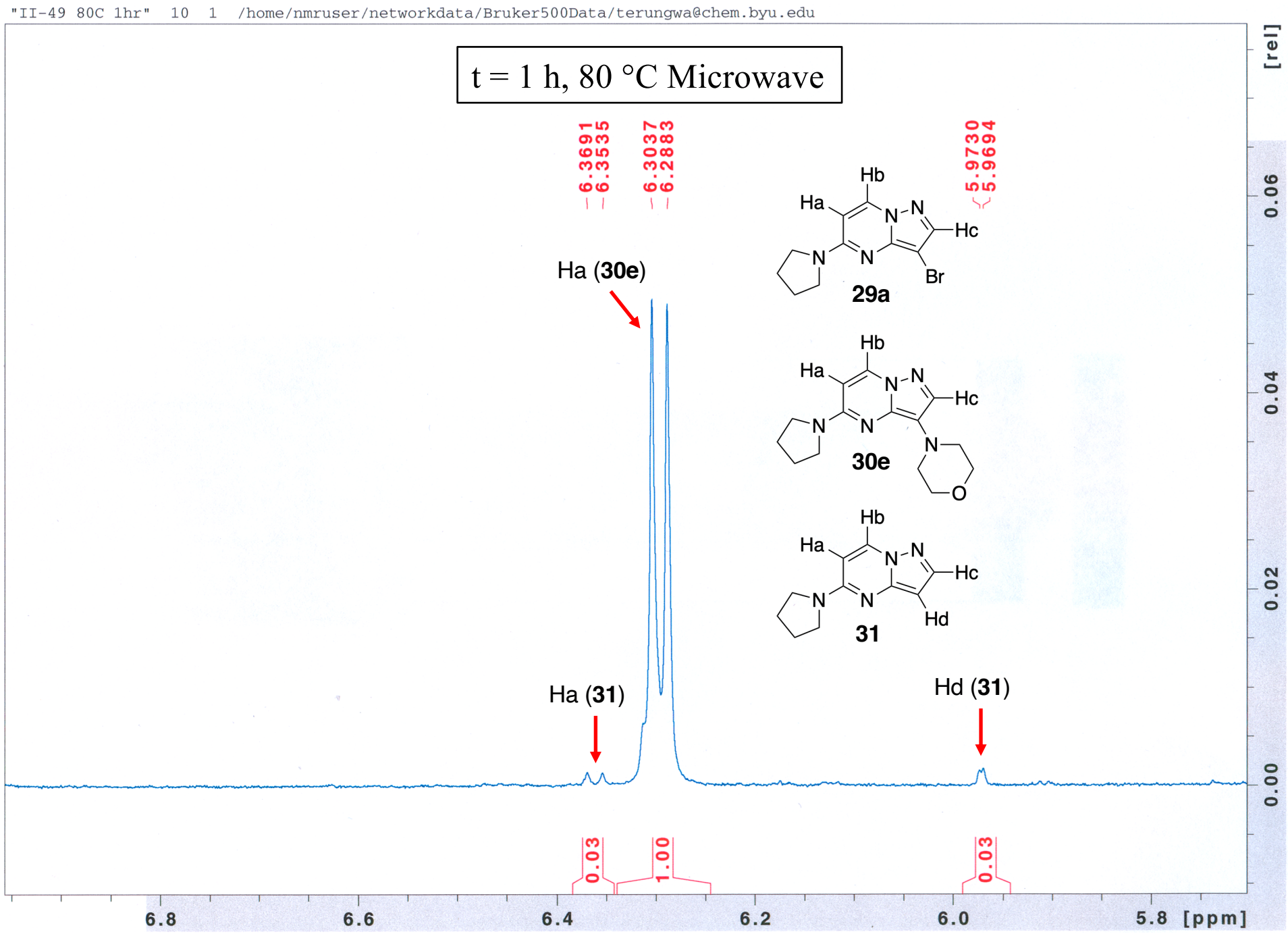

"II-49 RT, 7days" 10 1 /home/nmruser/networkdata/Bruker500Data/terungwa@chem.byu.edu
t = 7 d, RT
6.4310
6.4157
Hb
Ha
N
N
Hc
N
N
Br
29a
Ha (29a)
Hb
Ha
N
N
Hc
N
N
Hd
31
Ha (31)
1.00
6.8
6.6
6.4
6.2
6.0
[ppm]
[rel]
0.03
0.02
0.01
0.00


"70C, 24hrs" 10 1 /home/nmruser/networkdata/Bruker500Data/terungwa@chem.byu.edu
t = 24 h, 70 °C Conventional Heating
6.4256
6.4107
6.3565
6.3440
6.2935
6.2782
M 5.9622
5.9610
Hb
Ha
Hc
Br
29a
Ha (29a)
Hb
Ha
Hc
30e
Ha (30e)
Hb
Ha
Hc
Hd
31
Ha (31)
Hd (31)
1.00
0.04
0.39
0.03
6.8
6.6
6.4
6.2
6.0
[ppm]
[rel]
0.05
0.04
0.03
0.02
0.01
0.00

"II-49 70C 30min" 10 1 /home/nmruser/networkdata/Bruker500Data/terungwa@chem.byu.edu




"II-49 70C 1hr" 10 1 /home/nmruser/networkdata/Bruker500Data/terungwa@chem.byu.edu
t = 1 h, 70 °C Microwave
6.4278
6.4123
6.3595
6.3440
6.2948
6.2794
5.9650
5.9613
Ha (30e)
Ha (29a)
Ha (31)
Hd (31)
Hb
Ha
Hc
Br
29a
30e
Hd
31
0.24
0.03
1.00
0.02
6.8
6.6
6.4
6.2
6.0
[ppm]
[rel]
0.05
0.04
0.03
0.02
0.01
0.00


"II-49 80C 1hr" 10 1 /home/nmruser/networkdata/Bruker500Data/terungwa@chem.byu.edu
t = 1 h, 80 °C Microwave
6.3691
6.3535
6.3037
6.2883
5.9730
5.9694
Ha (30e)
Hb
Ha
Hc
Br
29a
30e
Hd
31
Ha (31)
Hd (31)
0.03
1.00
0.03
6.8
6.6
6.4
6.2
6.0
5.8 [ppm]
[rel]
0.06
0.04
0.02
0.00