

Supplementary Materials

Importance of the proximity and orientation of ligand-linkage to the design of cinnamate-GW9662 hybrid compounds as covalent PPAR γ agonists

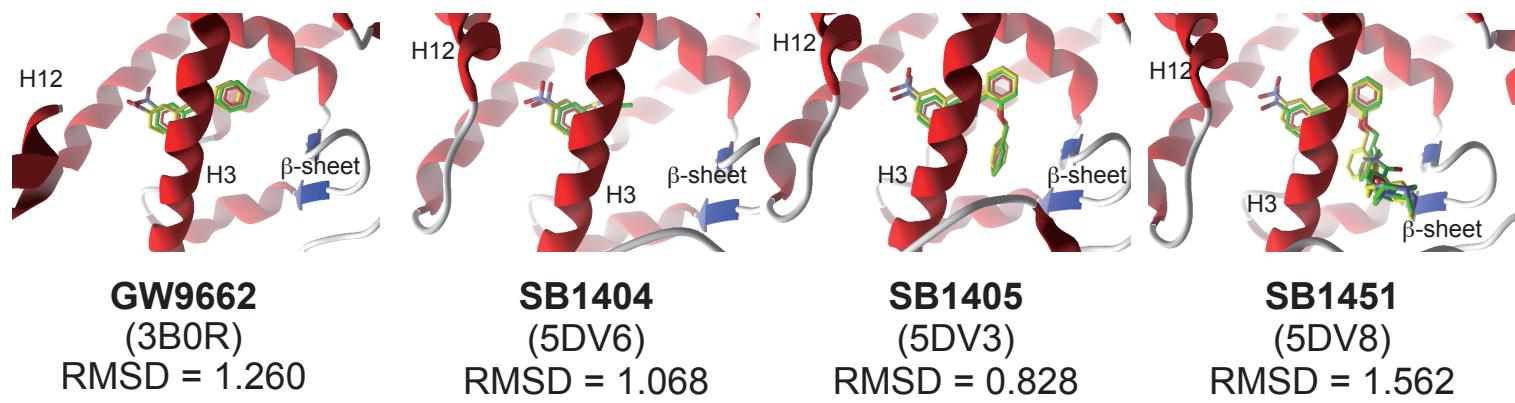
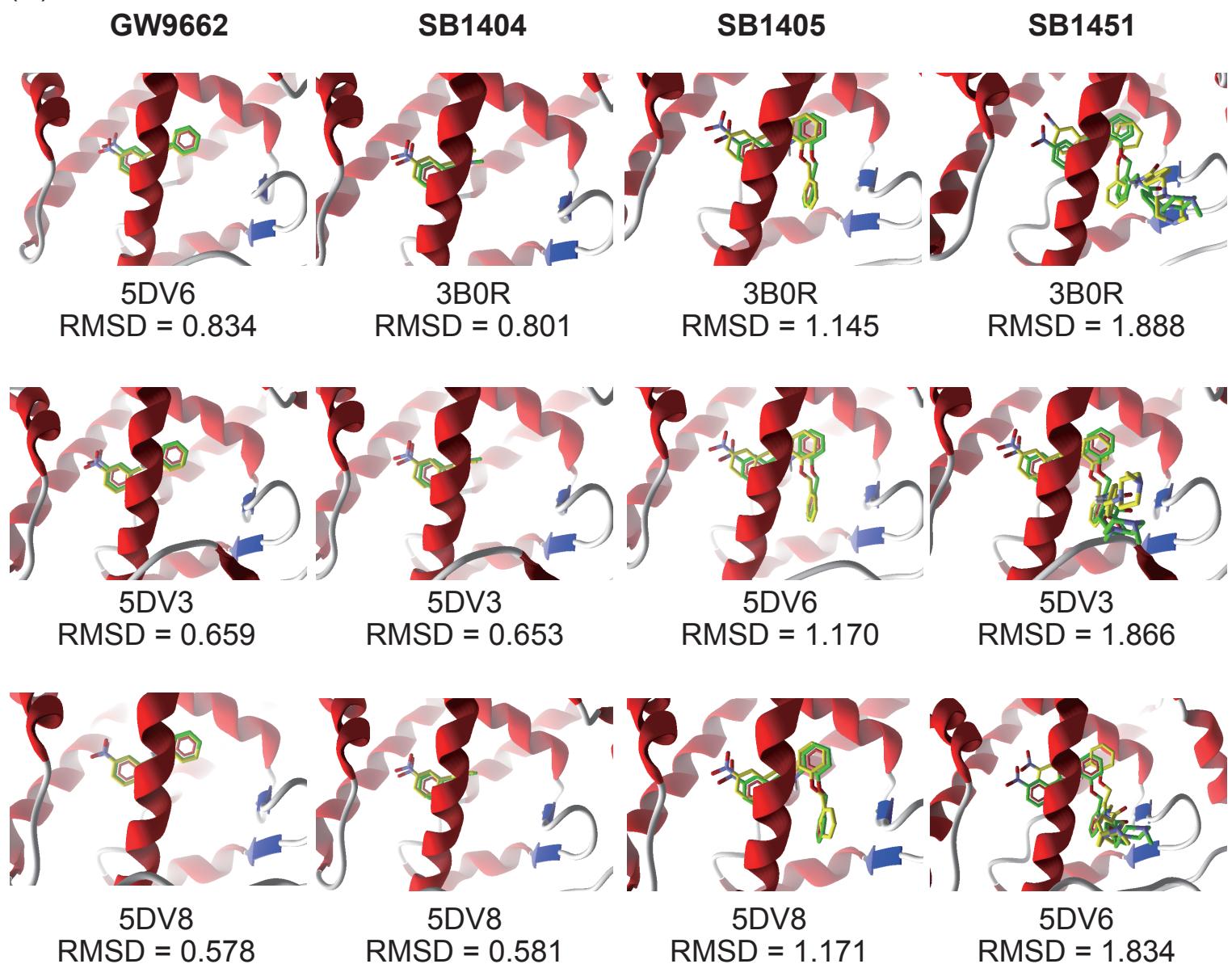
Yuki Utsugi^{1,2}, Hirona Kobuchi³, Yukio Kawamura³, Ahmed Salahelden Aboelhamd Atito², Masaya Nagao⁴, Hiroko Isoda^{2,5,6}, and Yusaku Miyamae^{2,4,6*}

^aCollege of Agro-Biological Resources Sciences, University of Tsukuba,

^bMaster's/Doctoral Program in Life Science Innovation, School of Integrative and Global Majors, University of Tsukuba, ^cDepartment of Food and Nutrition, Faculty of Home Economics, Kyoto Women's University, ^dGraduate School of Biostudies, Kyoto University, ^eAlliance for Research on the Mediterranean and North Africa, University of Tsukuba, ^fFaculty of Life and Environmental Sciences, University of Tsukuba. E-mail: miyamae.yusaku.fw@u.tsukuba.ac.jp

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(A)**(B)**

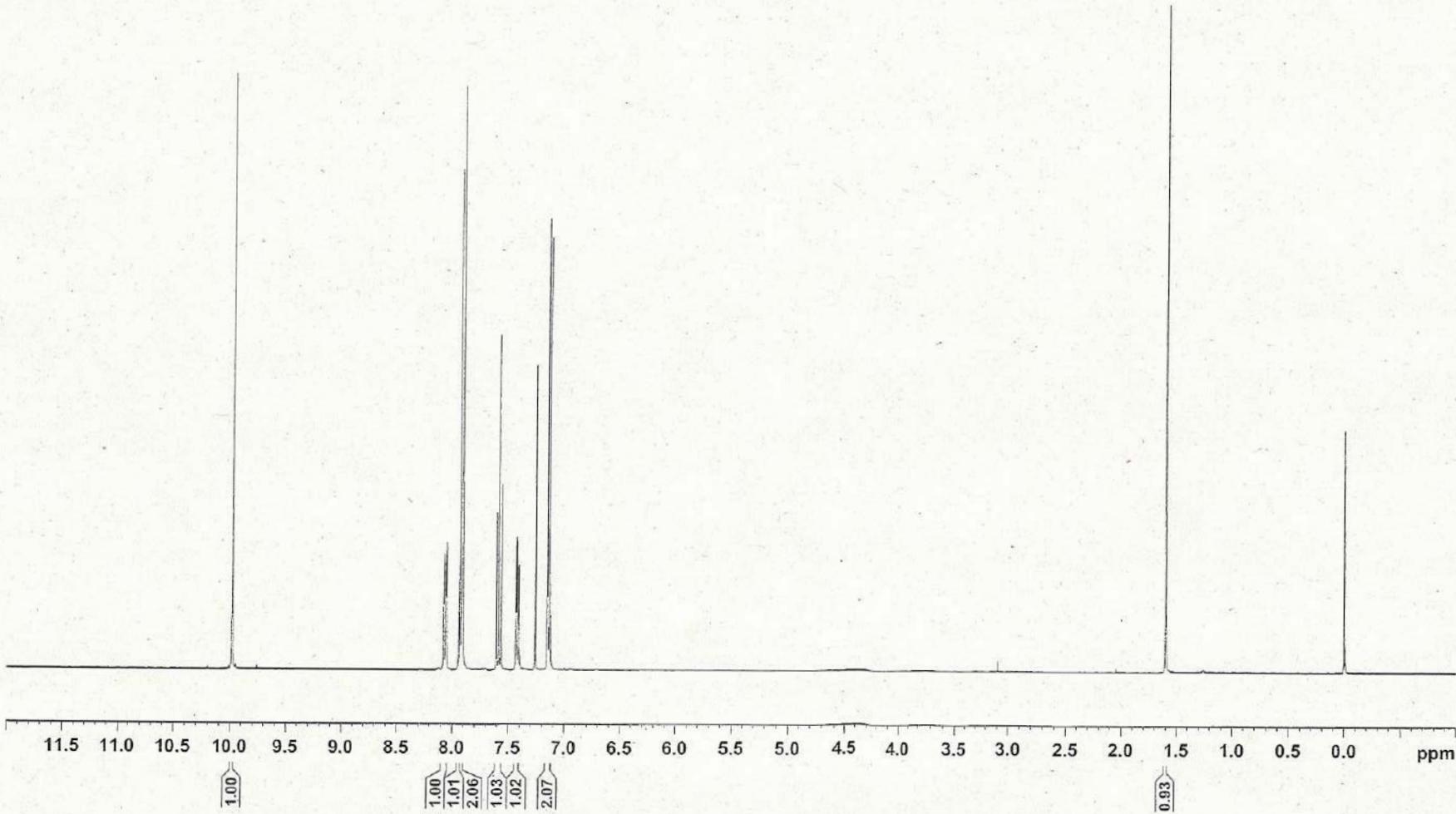
Supplementary Figure 1. Validation of docking protocol. (A) The indicated ligands were docked into the original protein crystal structures. The reported binding manners and predicted docking poses were displayed in green and yellow, respectively. (B) The ligands were docked in the crystal structures other than originally reported structural data. The reported binding manners and predicted docking poses were displayed in green and yellow, respectively.

3994.7758
3235.3393
3233.2181
3232.2976
3227.1346
3226.2141
3225.0134
3224.0929
3180.4278
3177.9063
3175.8651
3171.1024
3169.1413
3167.9006
3165.6193
3036.9053
3028.7006
2976.7907
2975.9102
2974.3894
2973.5089
2968.6261
2967.7055
2966.2247
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2867.1277
2865.3041
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2862.6451
2857.8024
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2853.3198

641.1285

0.0000

400 MHz ^1H NMR spectrum of compound **6a** in CDCl_3



— 190.5667

— 161.3130

— 156.4128

— 149.4374

— 132.5628

— 132.1862

— 130.8141

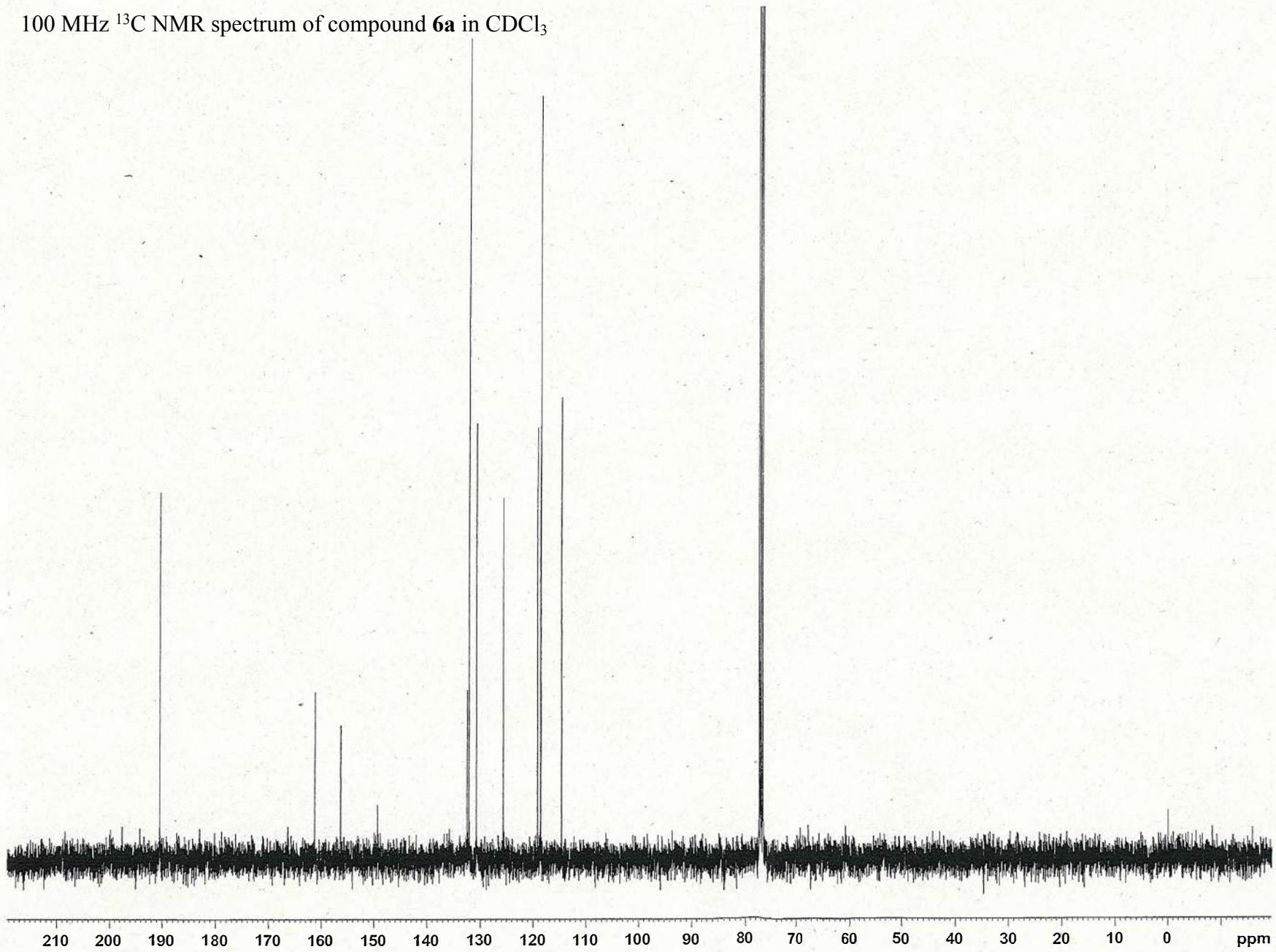
— 125.7755

— 119.3132

— 118.6951

— 114.7562

100 MHz ^{13}C NMR spectrum of compound **6a** in CDCl_3

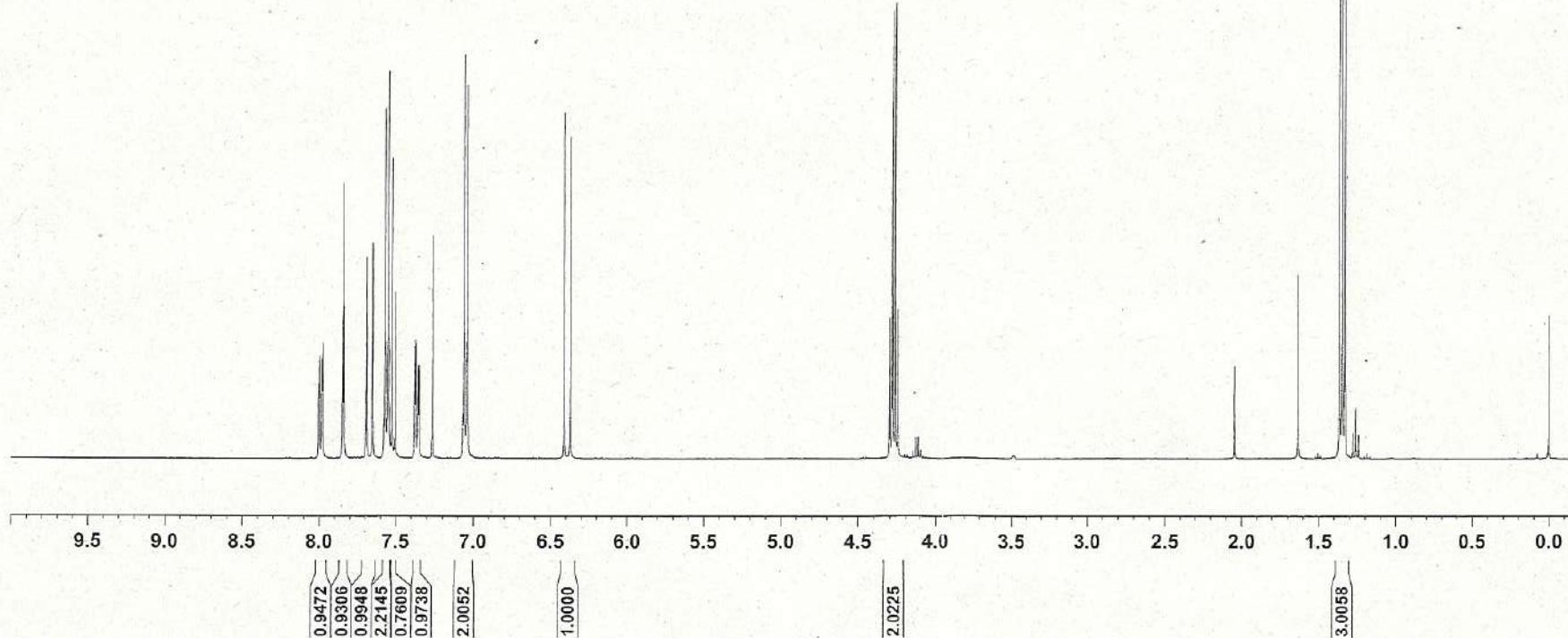


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3137.6432
3079.7299
3063.7207
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3020.6960
3012.4512
3004.2465
2953.8976
2952.9771
2951.4562
2950.5757
2945.6528
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2943.2515
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2908.5515
2826.8246
2824.8234
2820.1007
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2550.6658

1721.5093
1714.3852
1707.2612
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538.6295
531.5055

400 MHz ^1H NMR spectrum of compound **7a** in CDCl_3



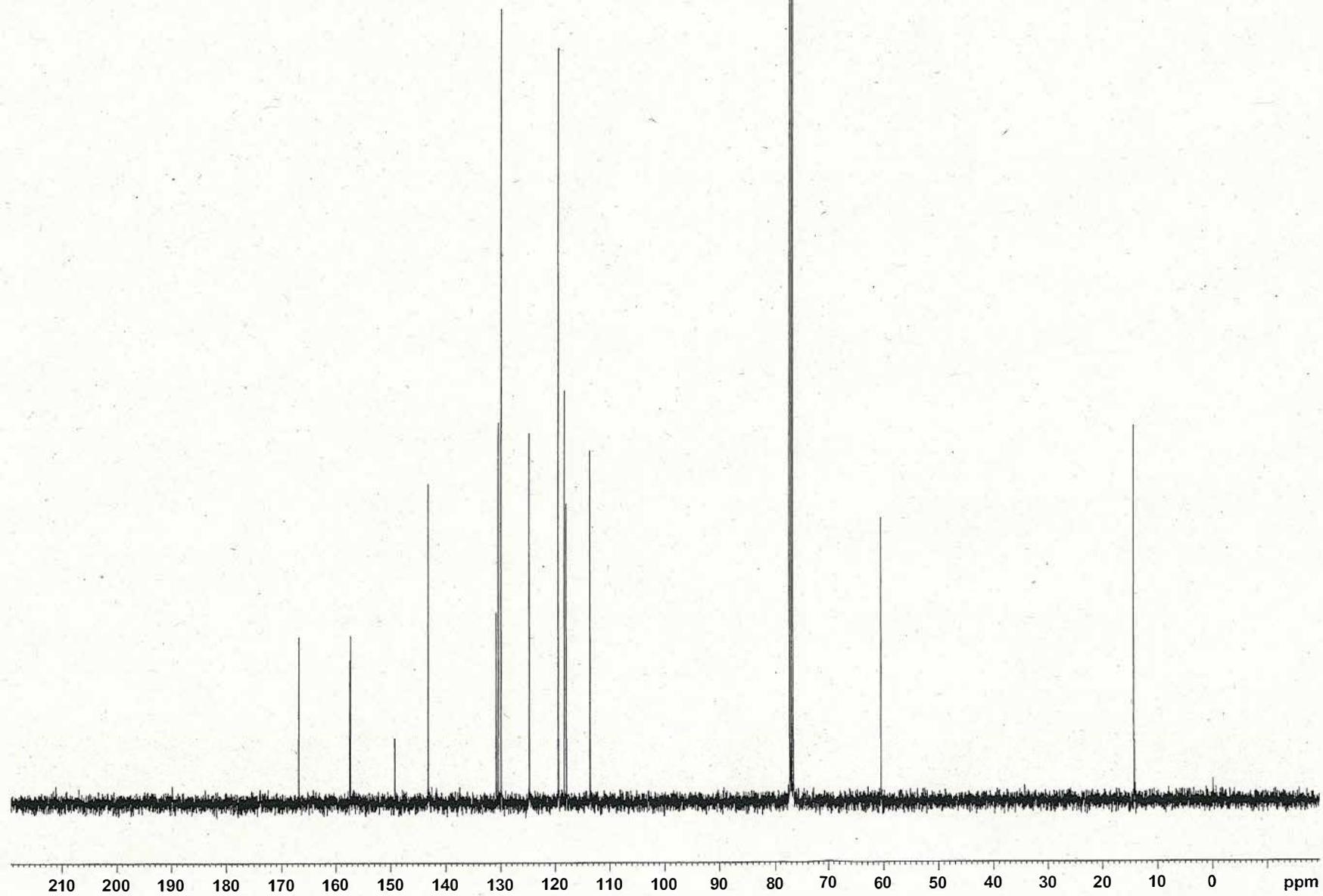
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—< 157.3894
— 149.3266
— 143.2559

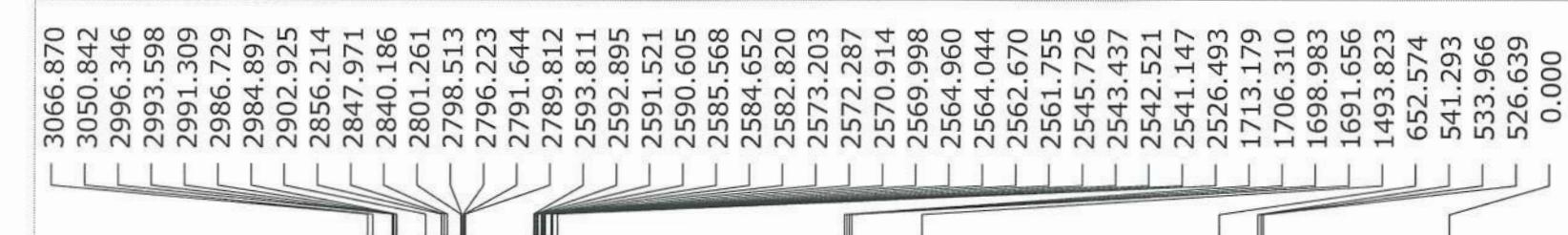
—> 130.8916
—< 130.5049
—> 129.9948
—< 124.8190
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—< 113.6421

— 60.5288

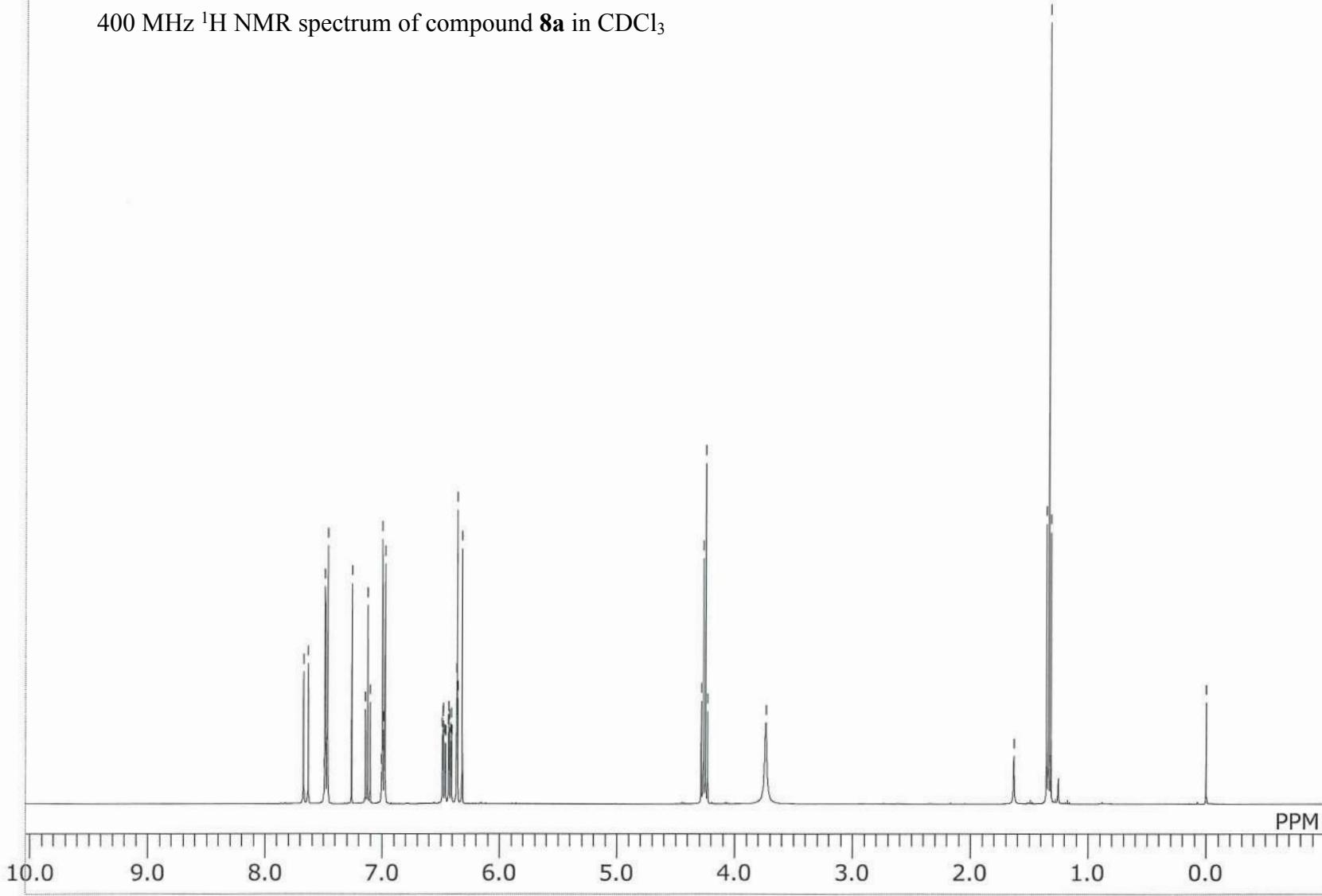
— 14.2964

100 MHz ^{13}C NMR spectrum of compound **7a** in CDCl_3

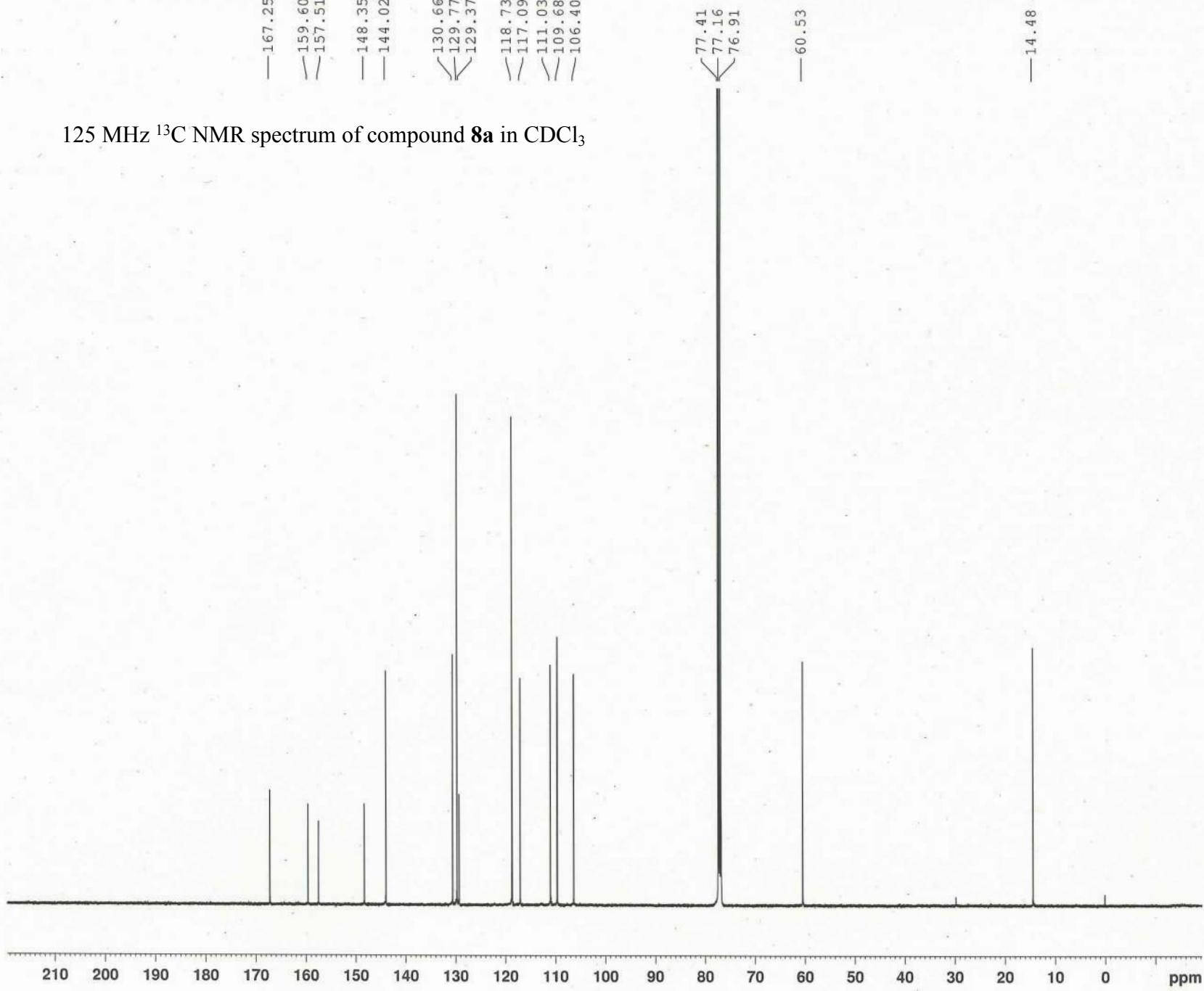


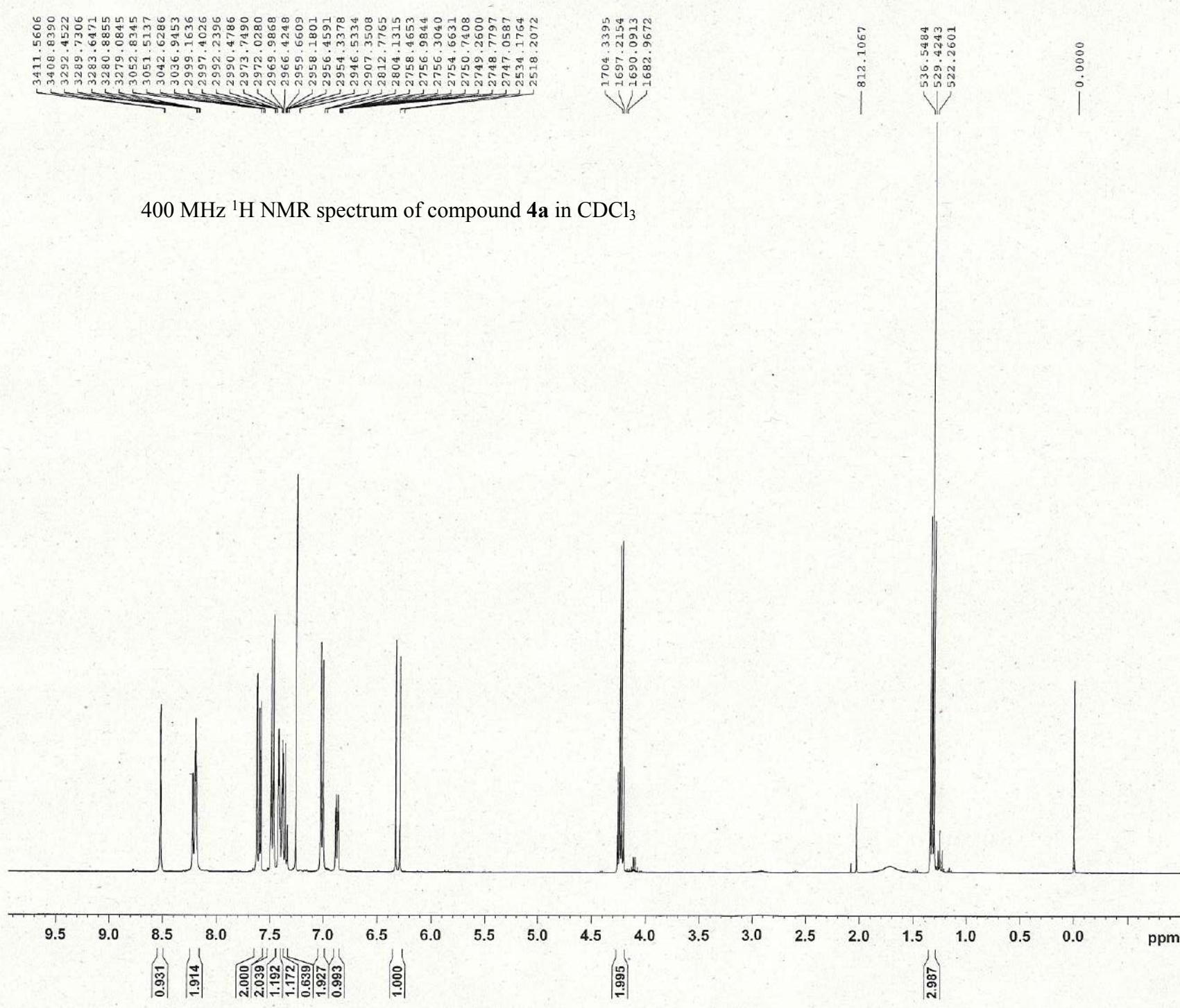


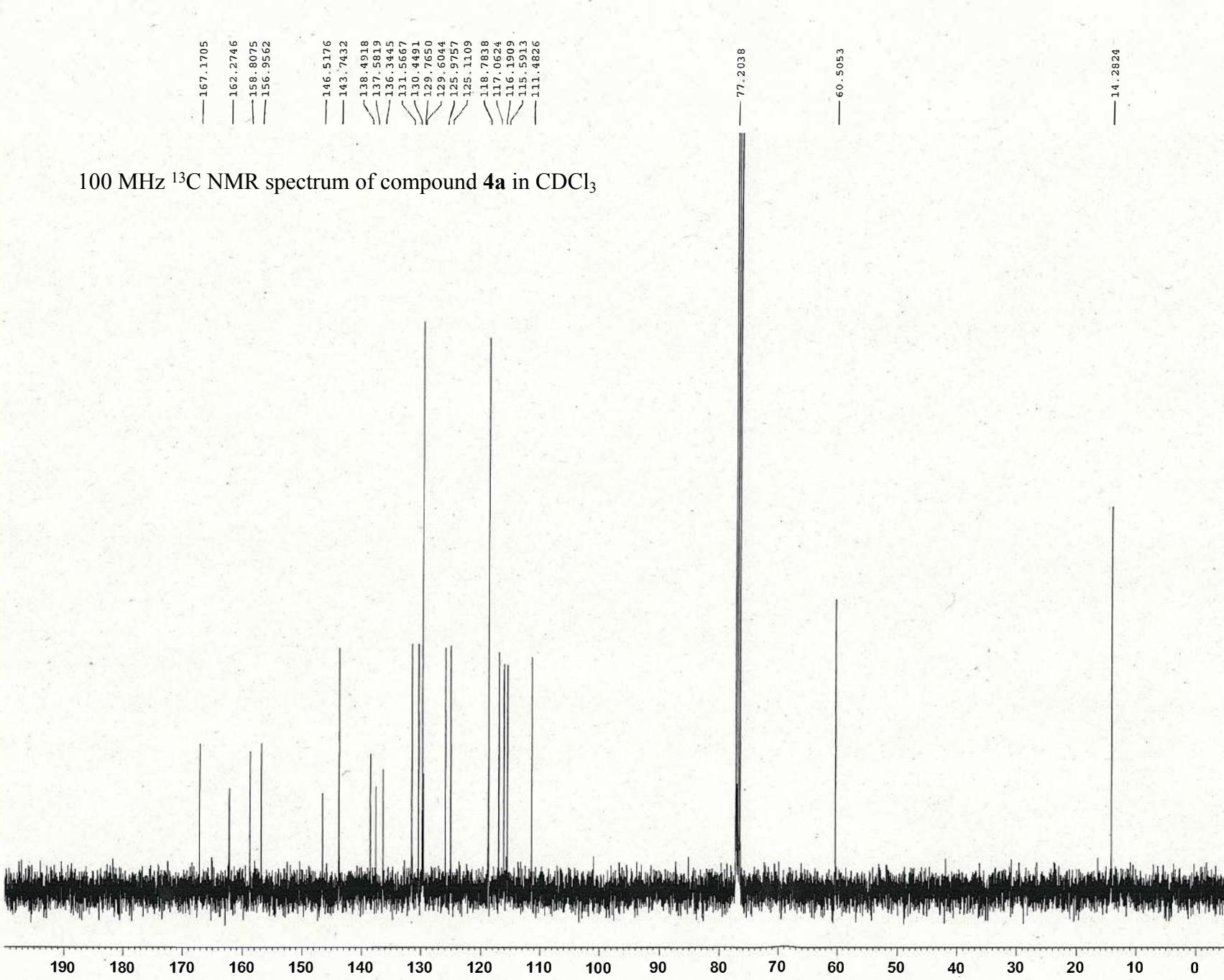
400 MHz ^1H NMR spectrum of compound **8a** in CDCl_3

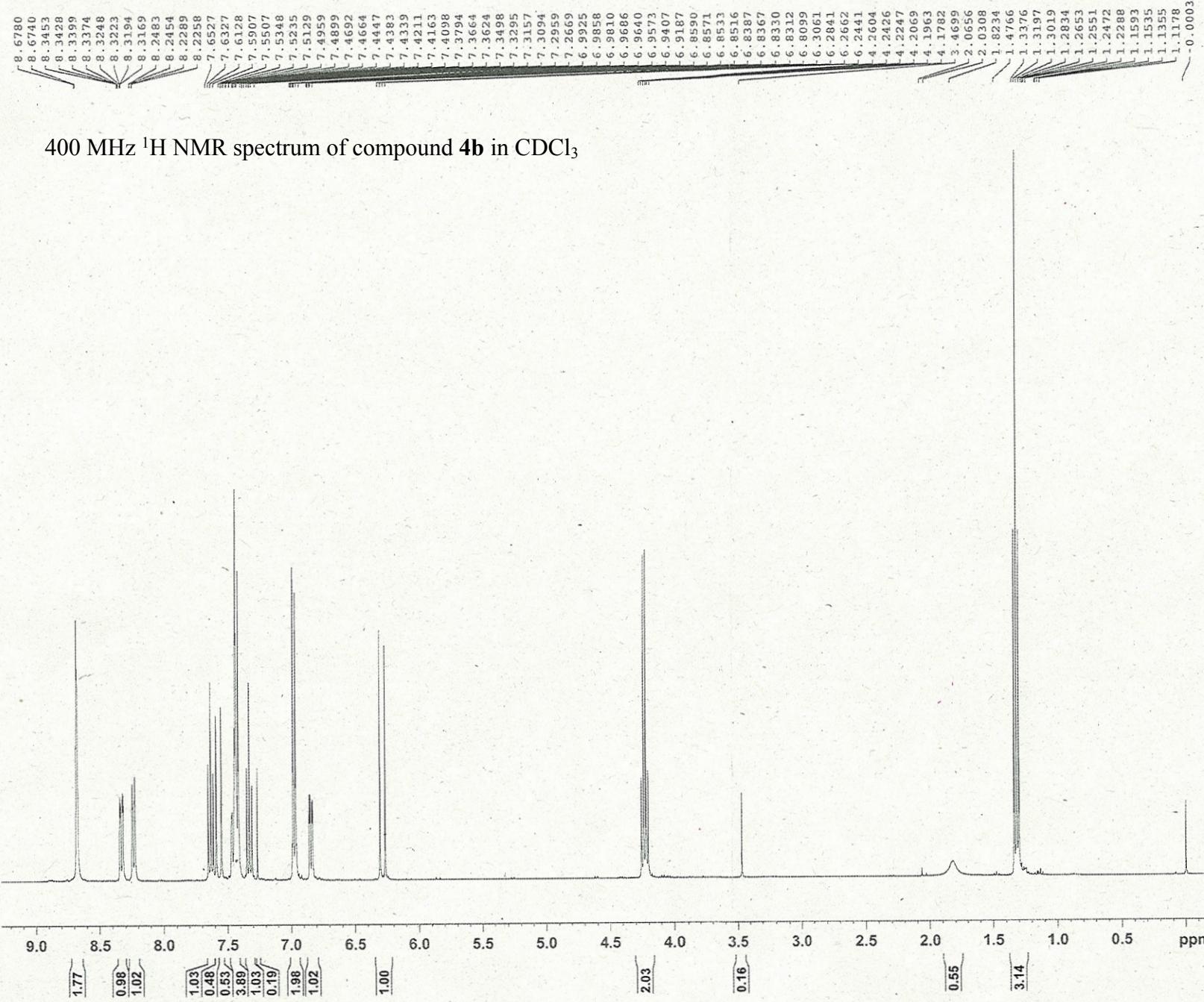


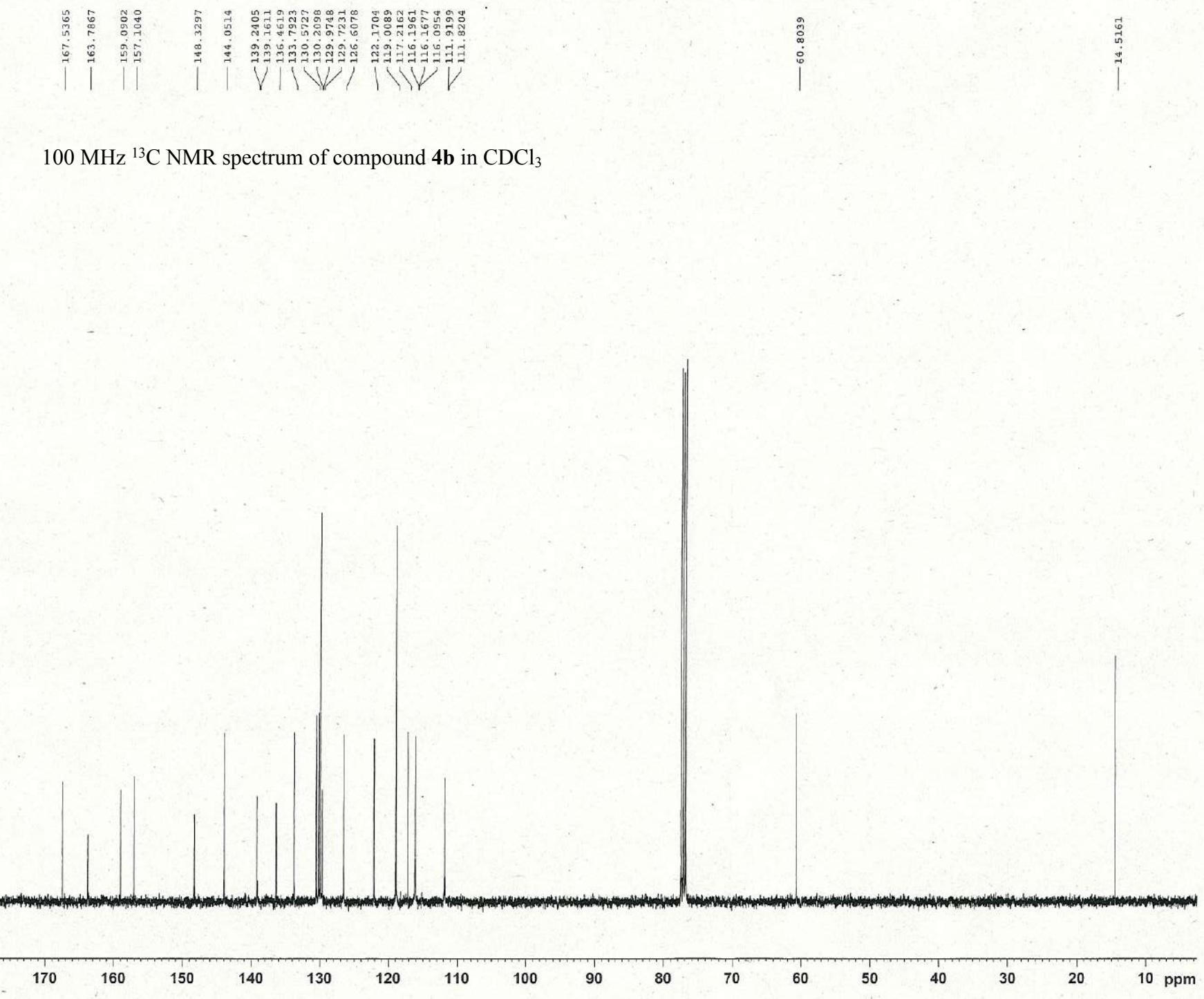
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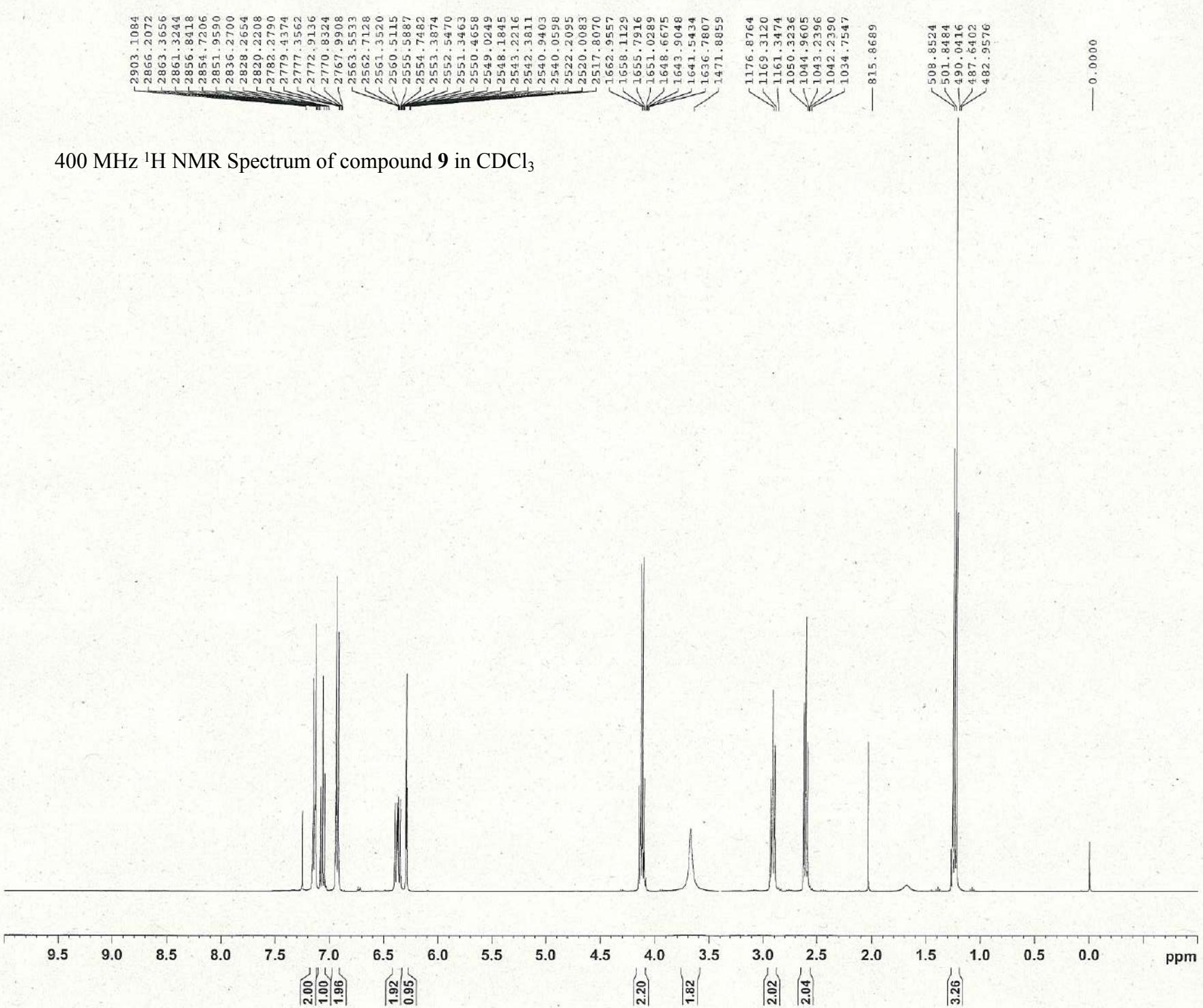


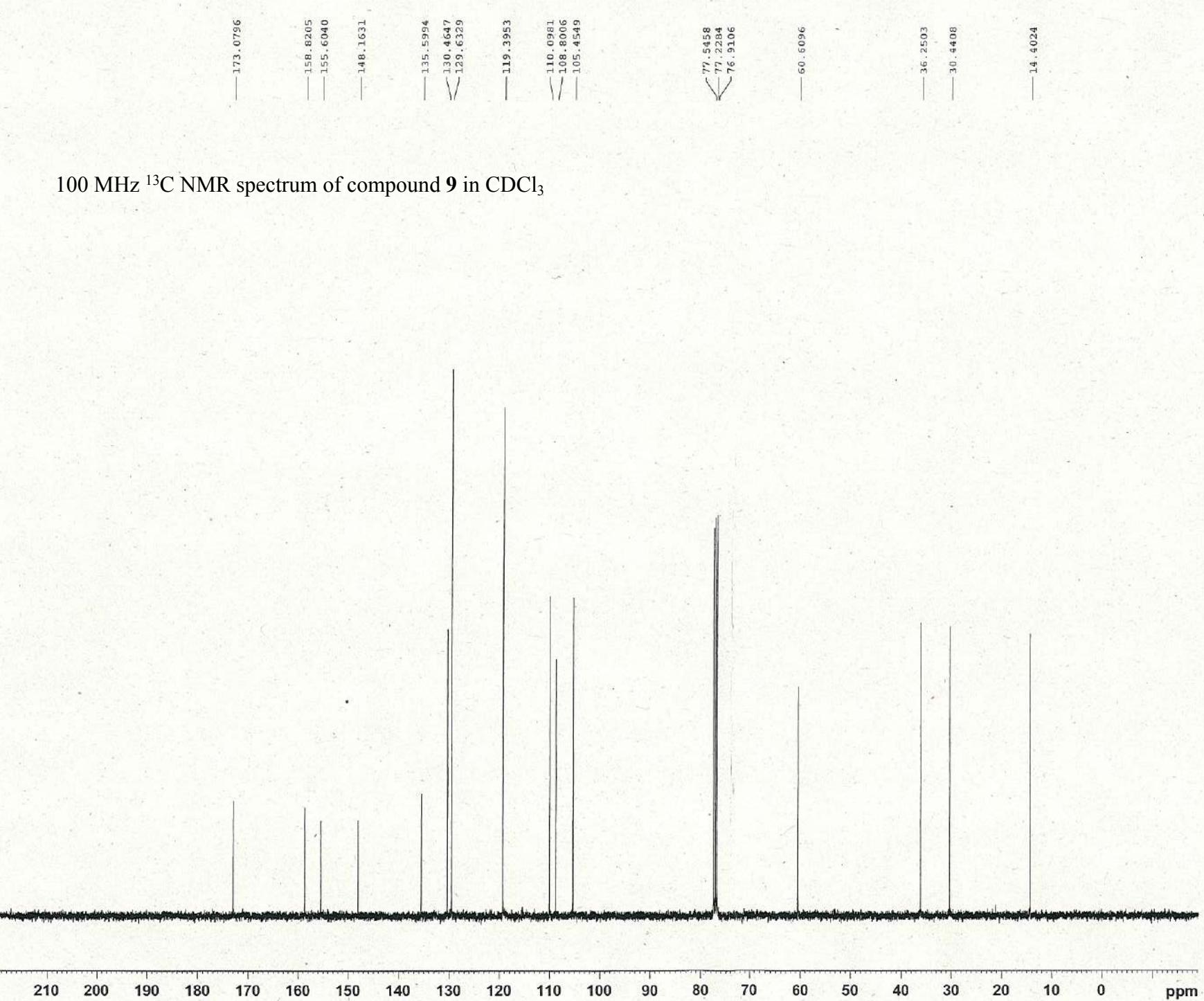


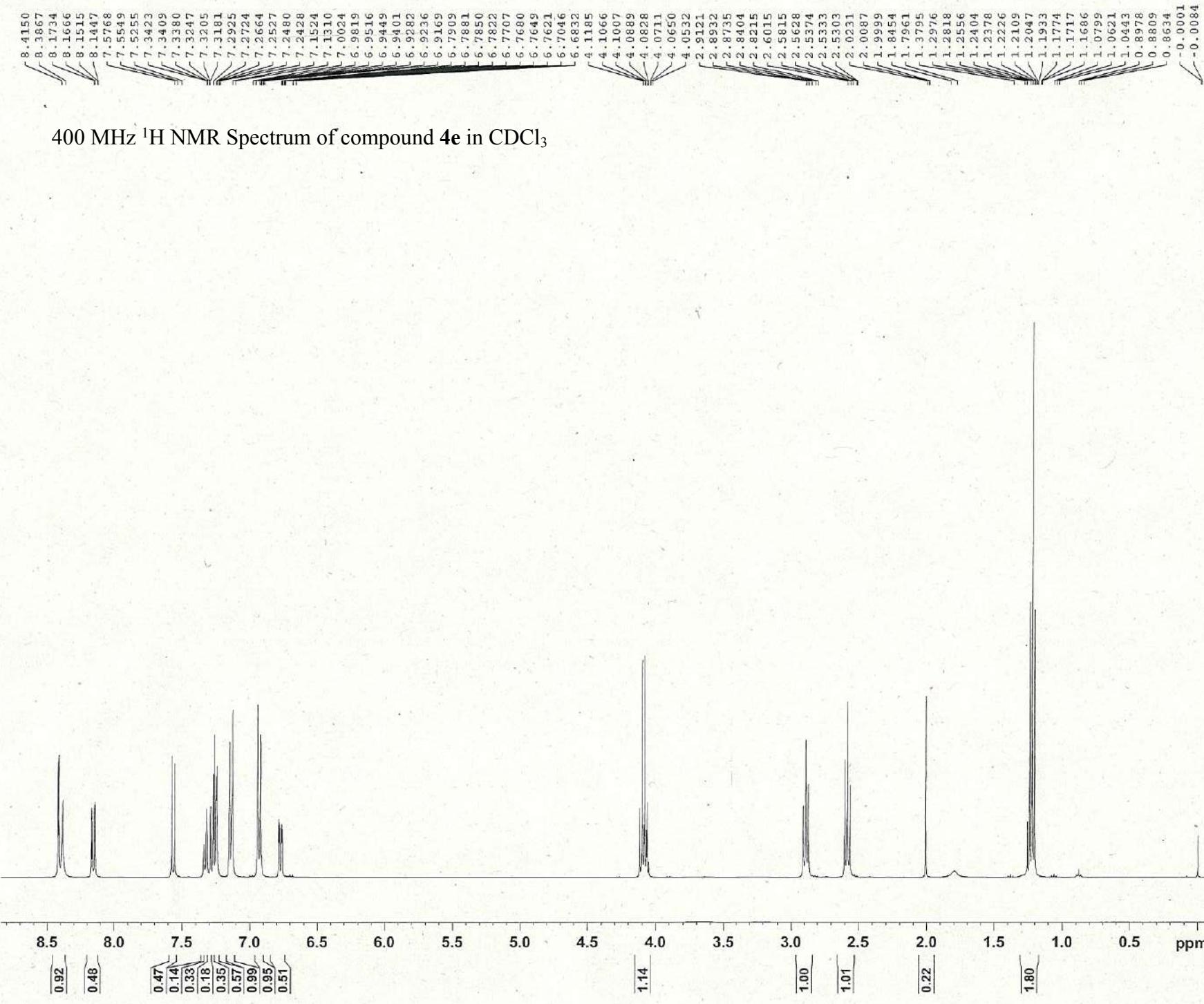


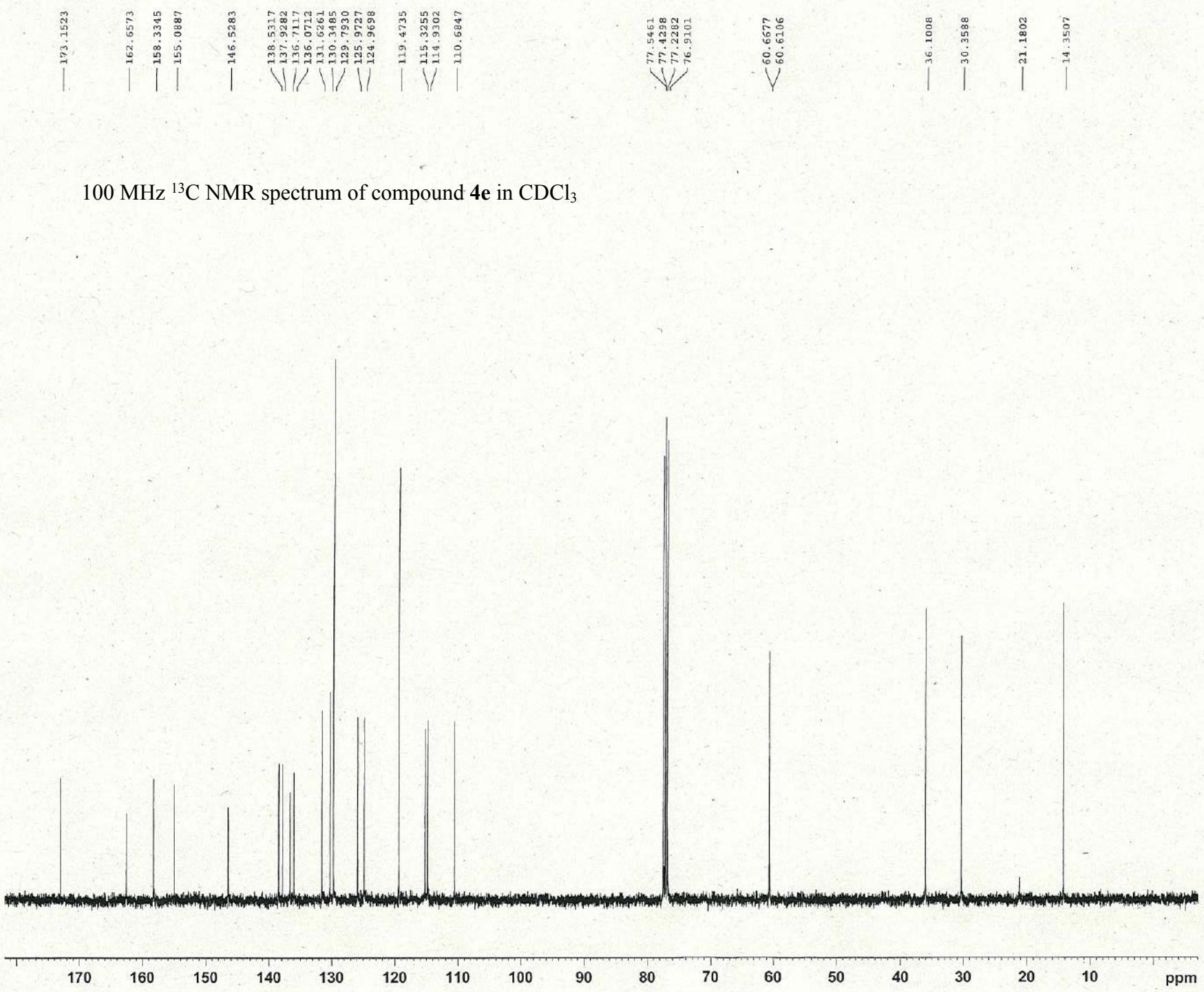




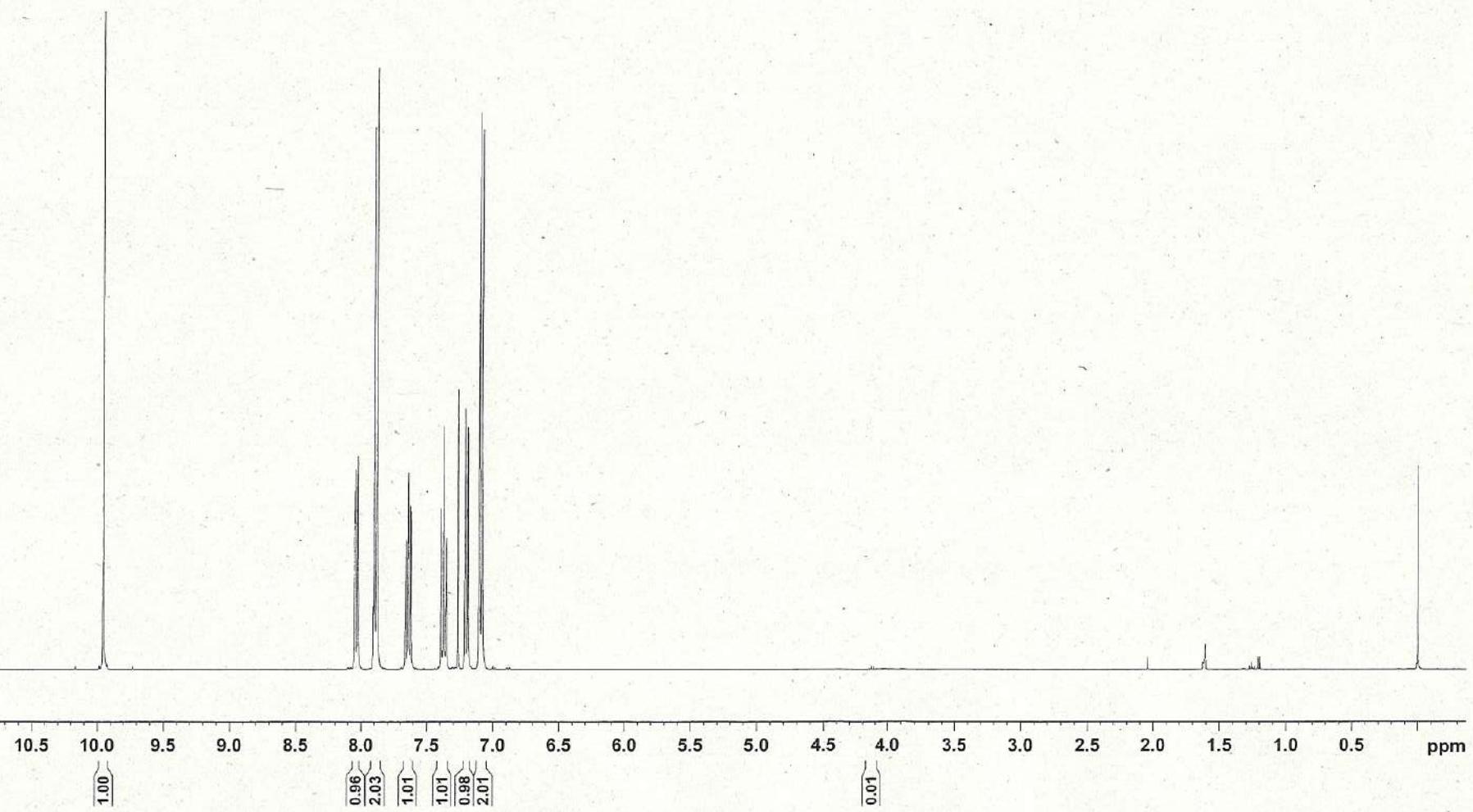








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3164.9789
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3161.0568
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3068.4834
3066.8025
3060.8791
3060.2787
3059.3582
3058.6378
3052.7544
3051.0734
2960.6615
2959.3807
2952.4968
2951.9765
2951.3361
2944.9725
2943.7317
2908.3914
2887.3794
2886.1787
2879.0946
2877.3339
2846.4358
2843.8744
2837.0304
2835.2294
2832.7880

400 MHz ^1H NMR Spectrum of compound **6b** in CDCl_3 

— 190.7723

— 161.9477

— 148.5142

— 142.4645

— 134.8580

— 132.4438

— 132.2318

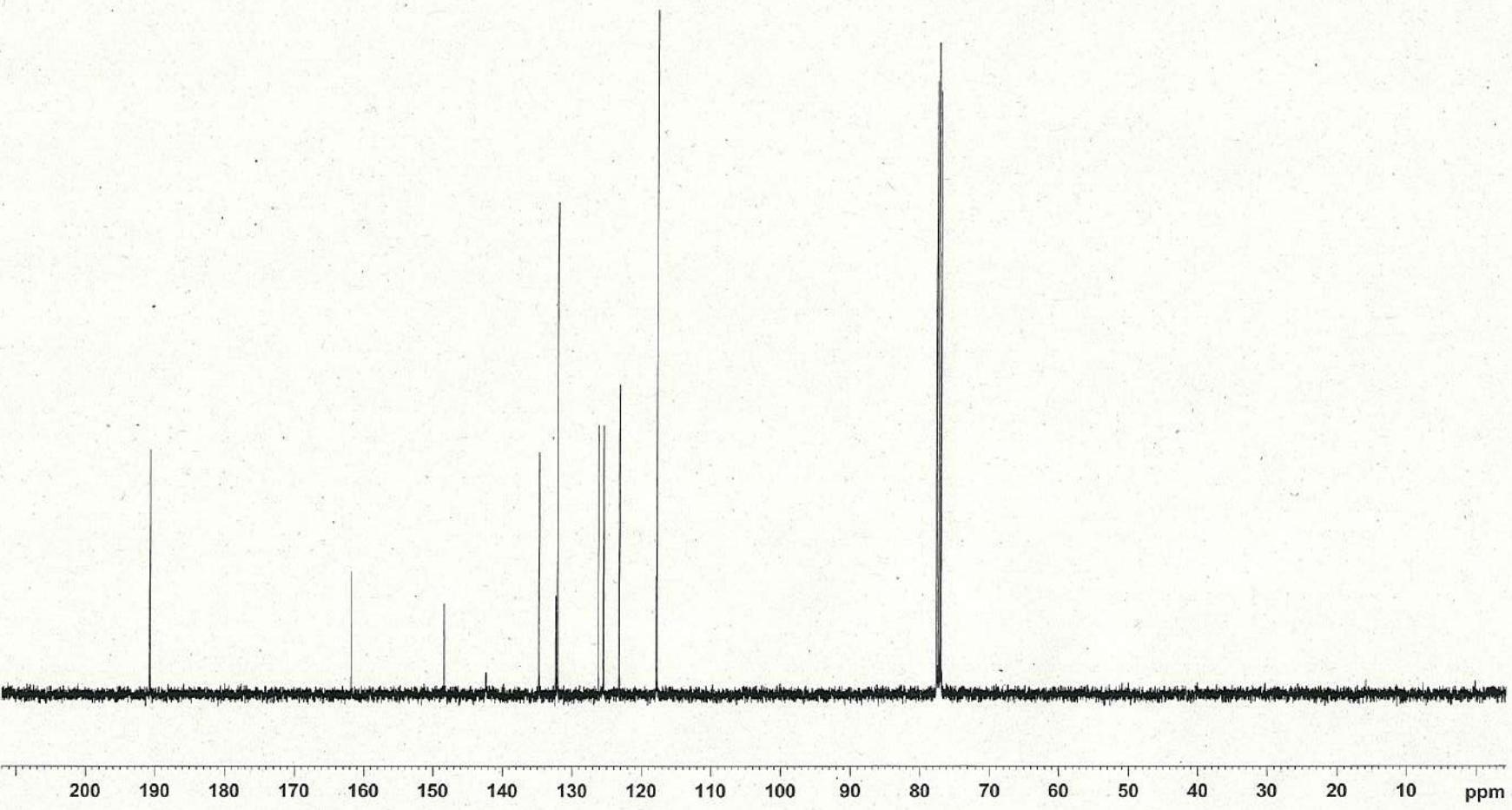
— 126.2761

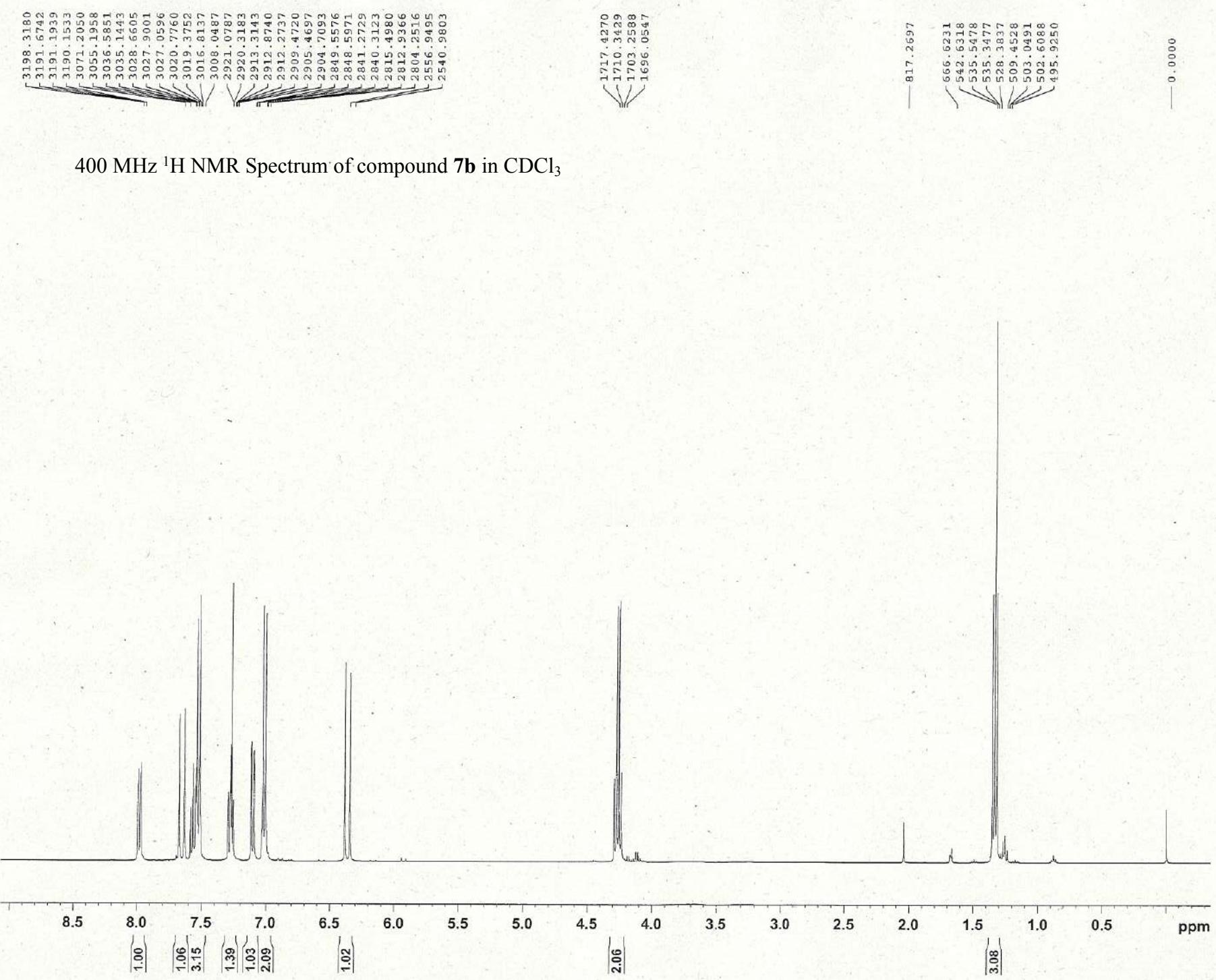
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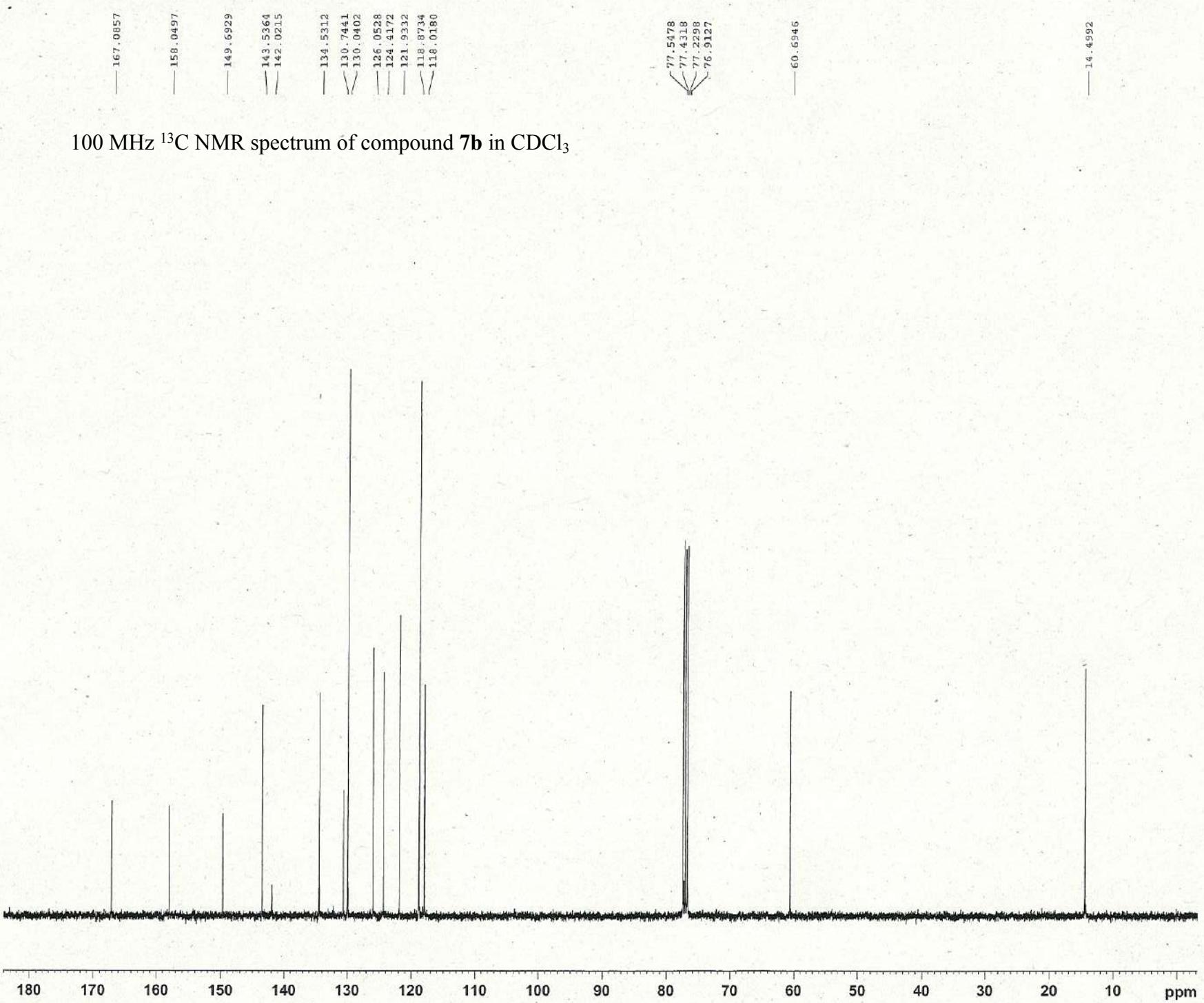
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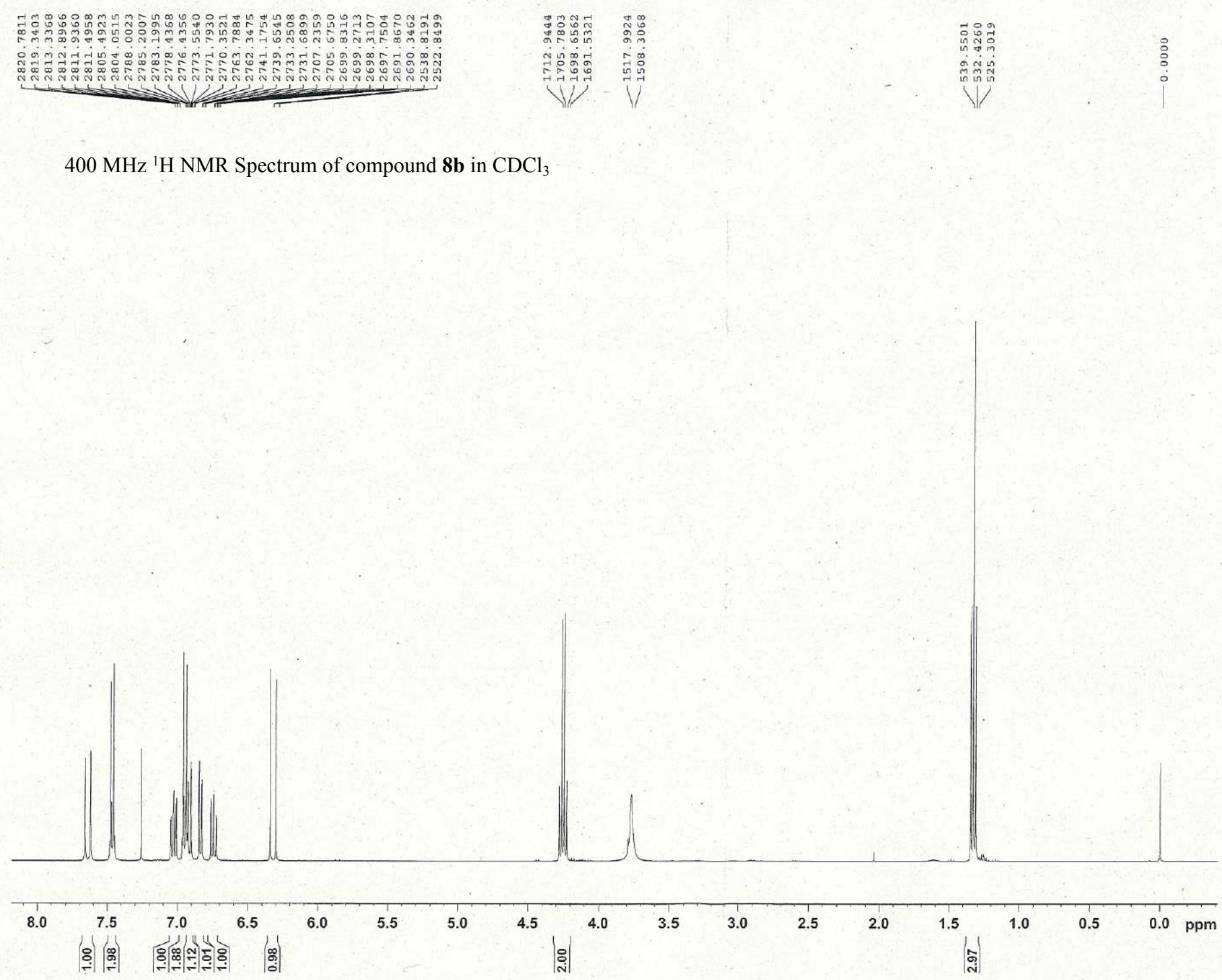
— 117.9198

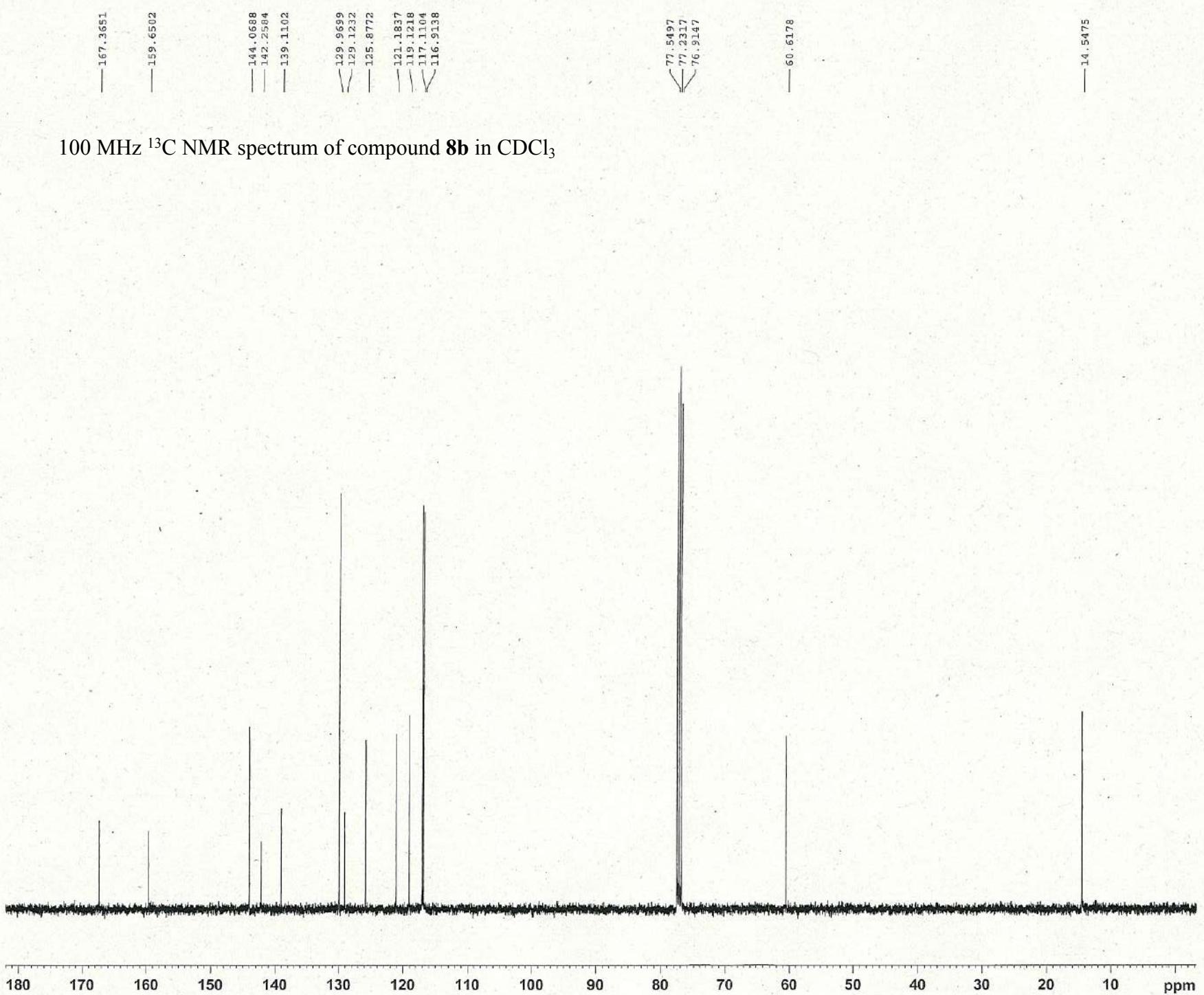
100 MHz ^{13}C NMR spectrum of compound **6b** in CDCl_3

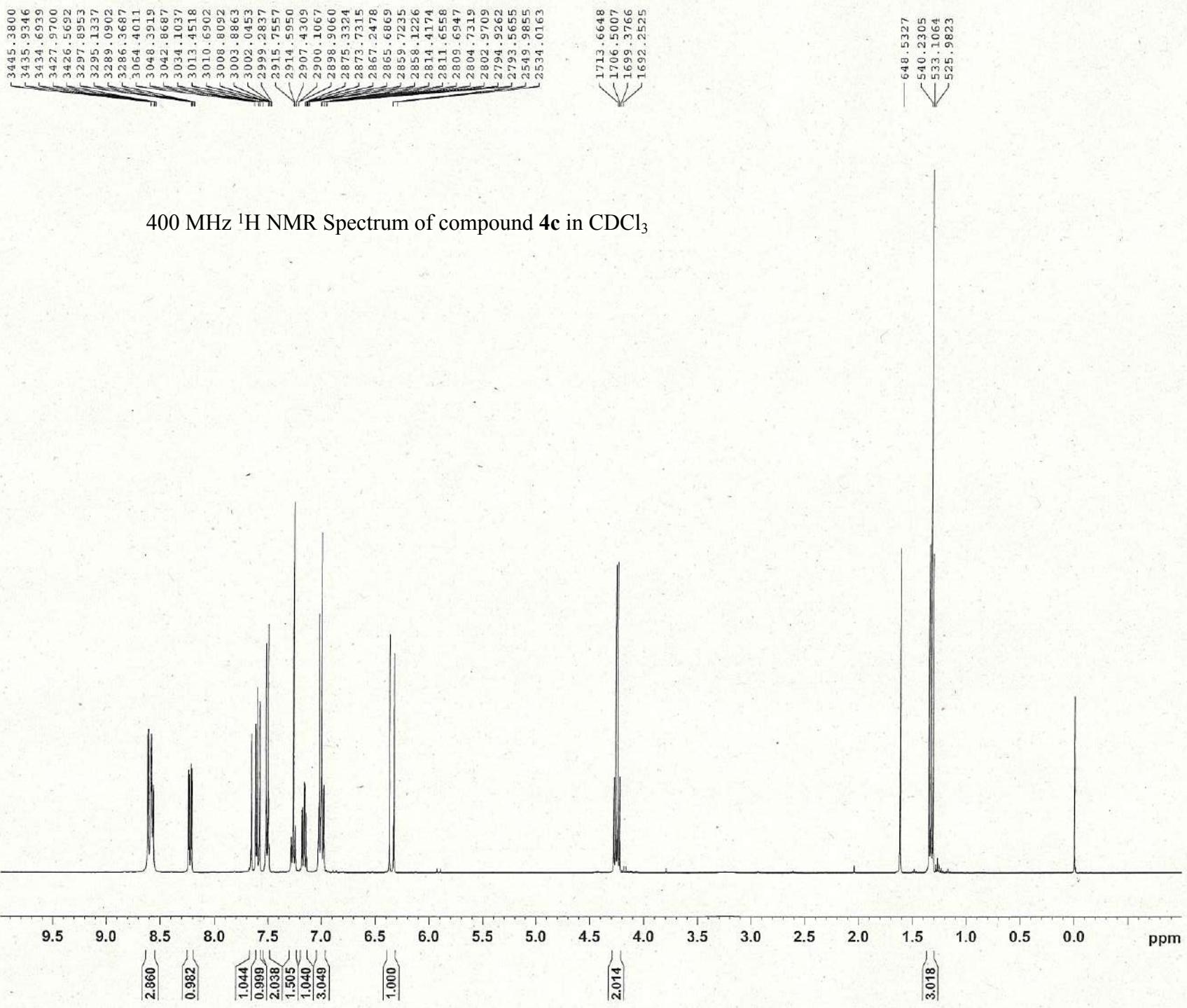


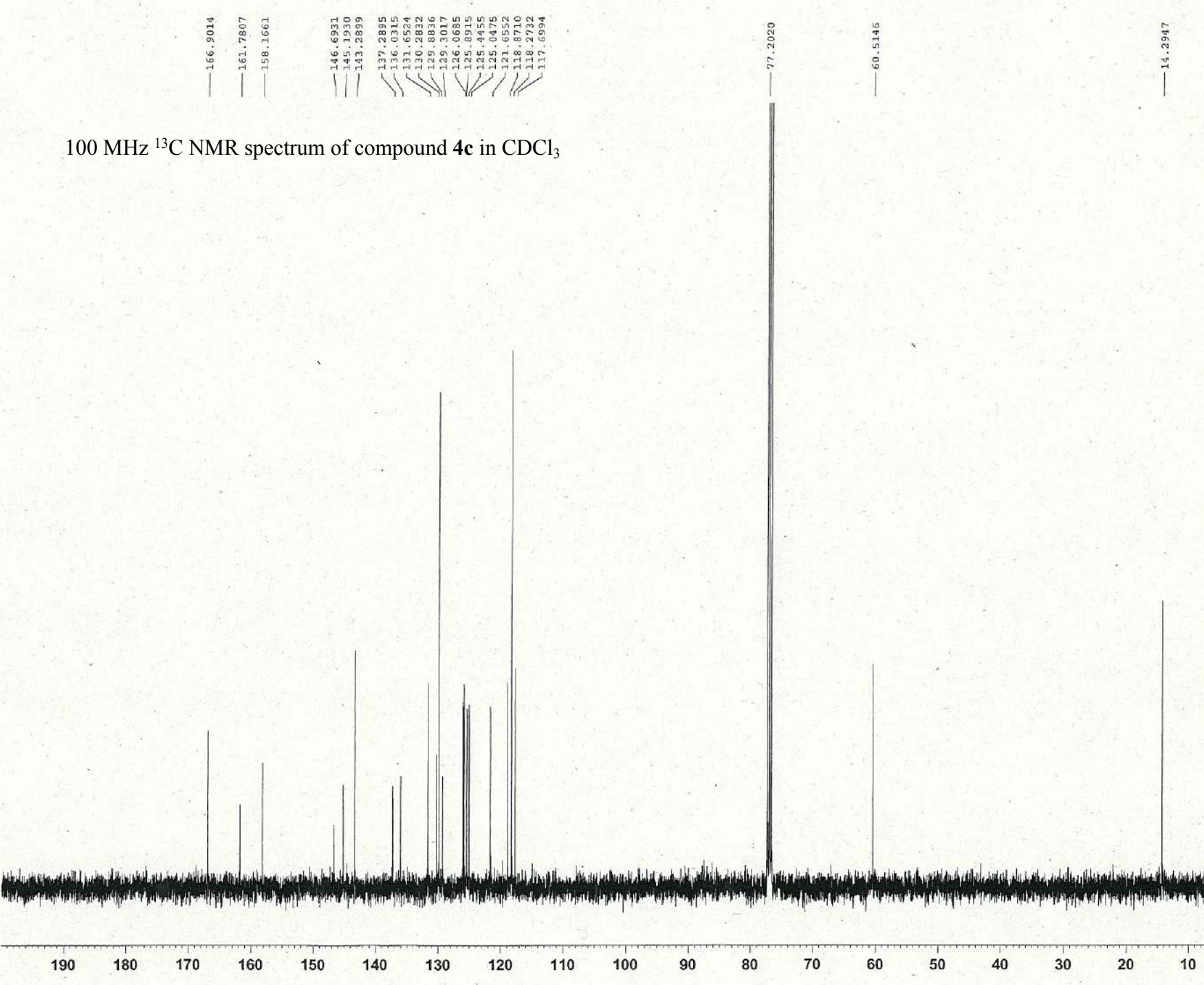












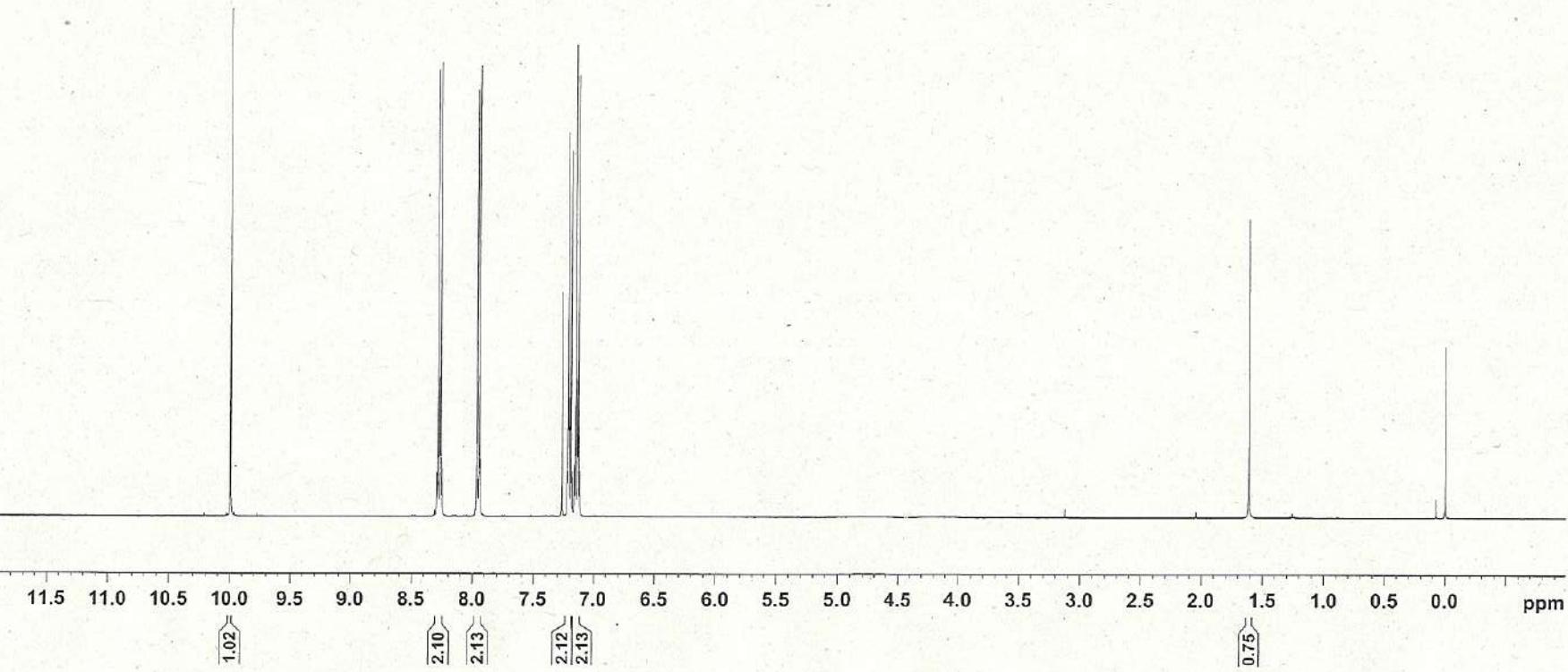
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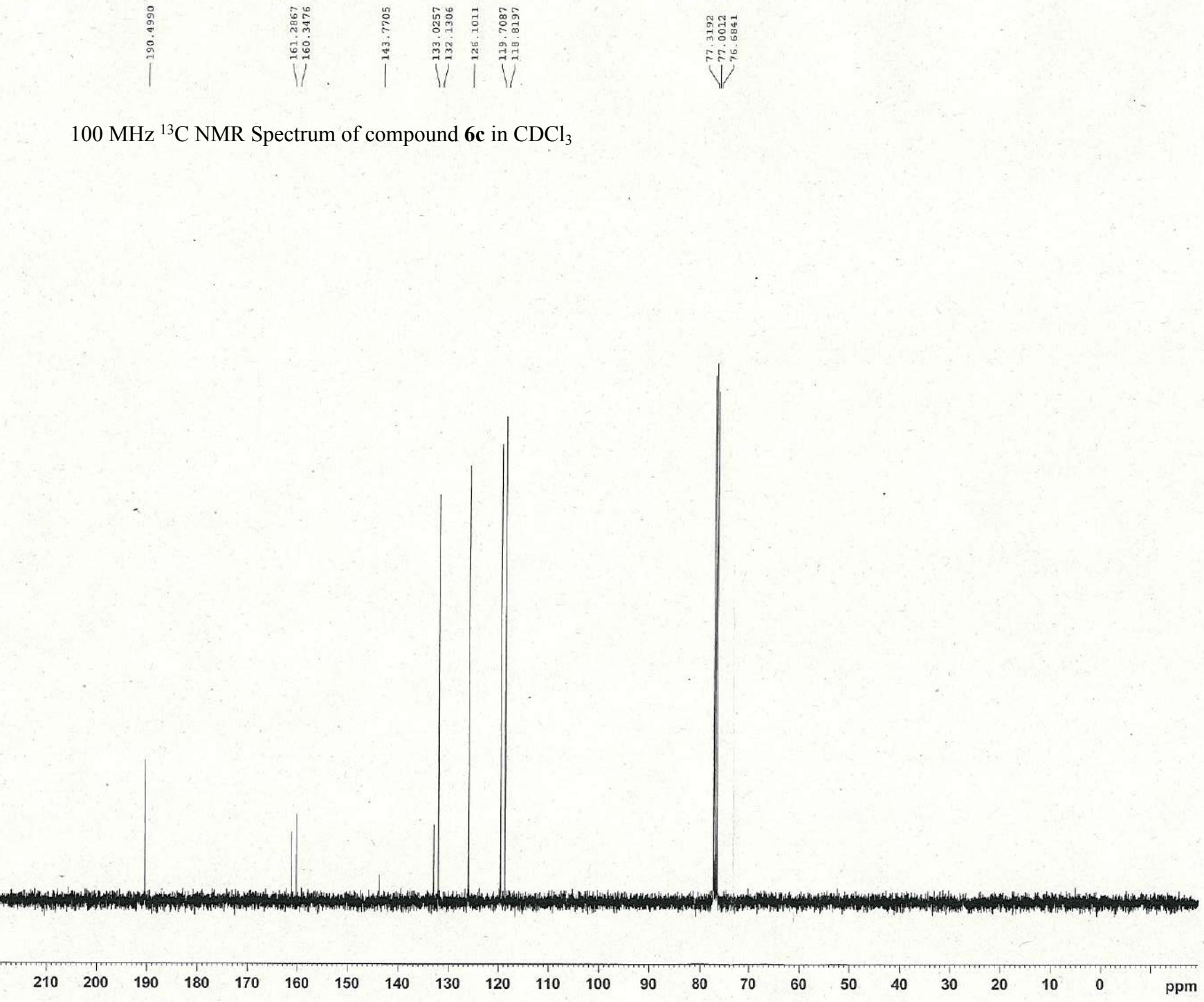
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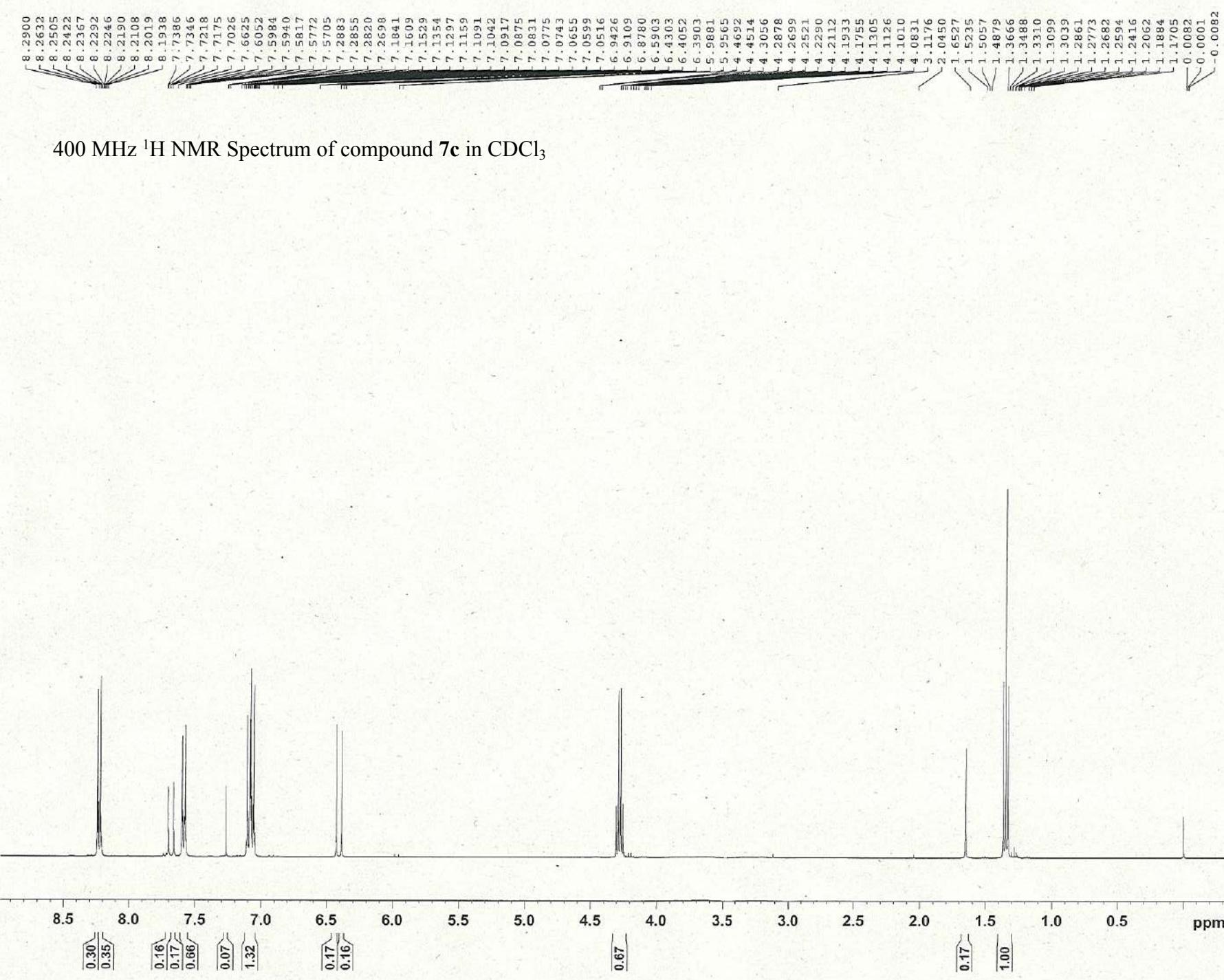
— 645.6911

— 0.0400

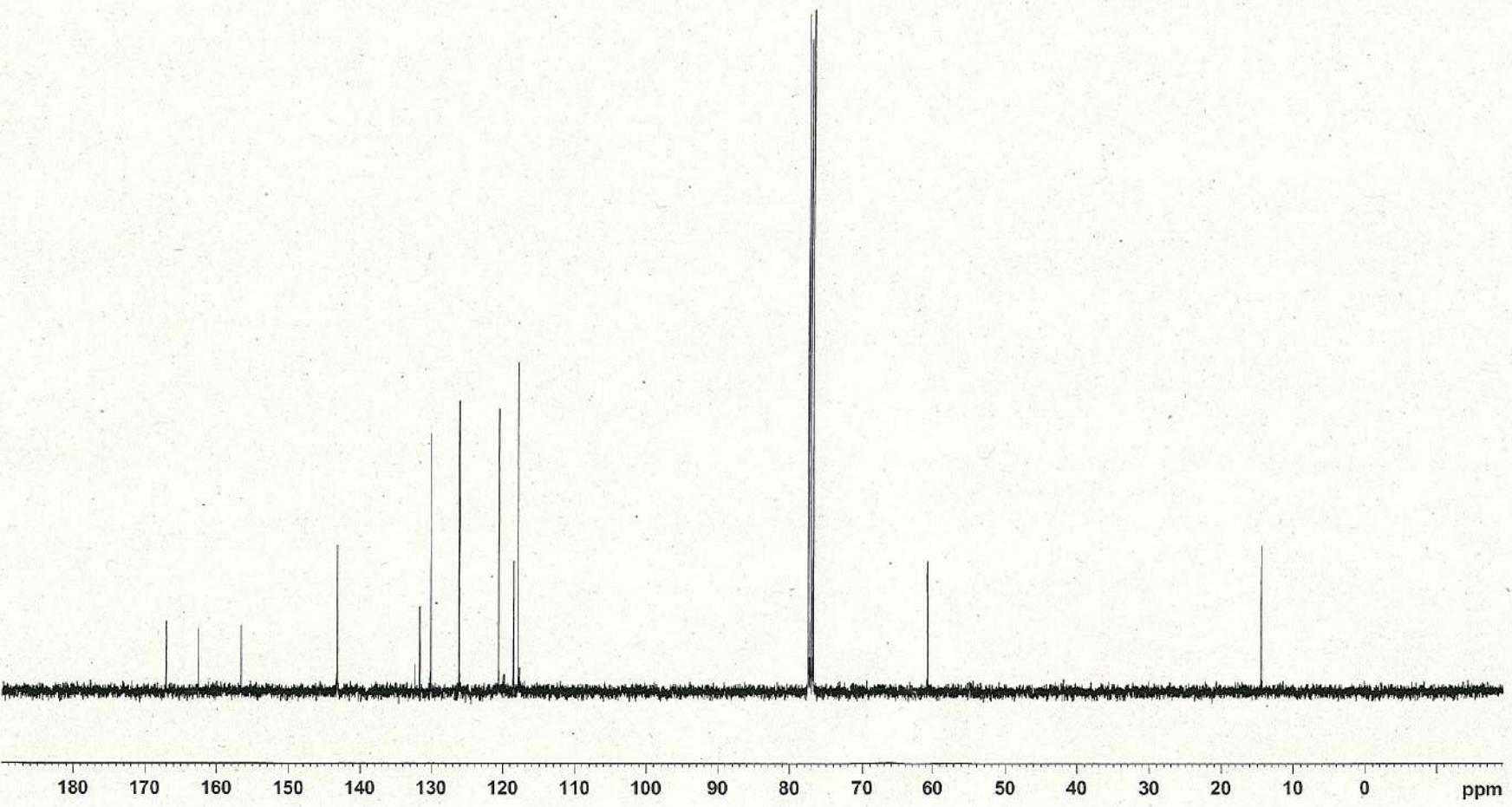
400 MHz ^1H NMR Spectrum of compound **6c** in CDCl_3

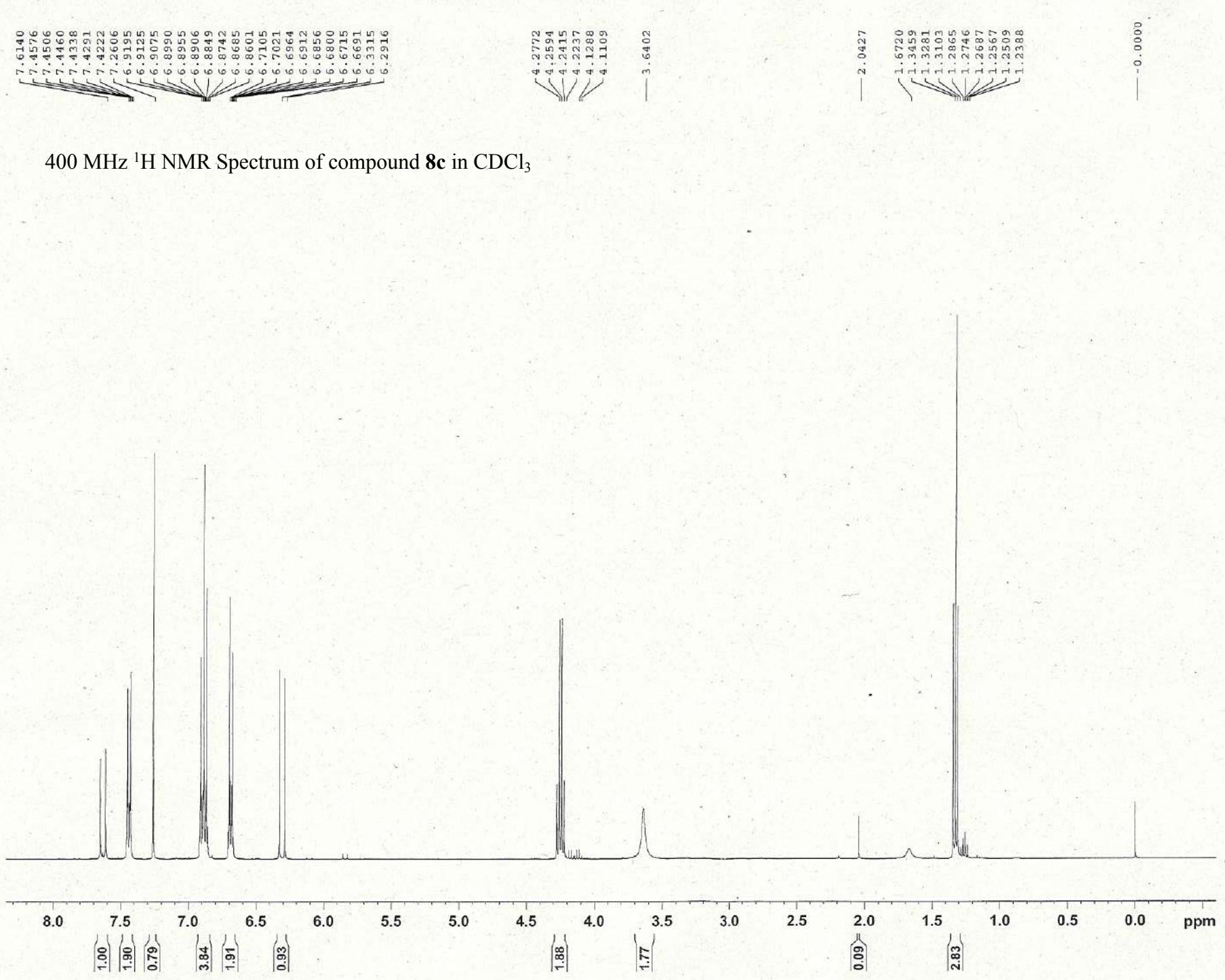


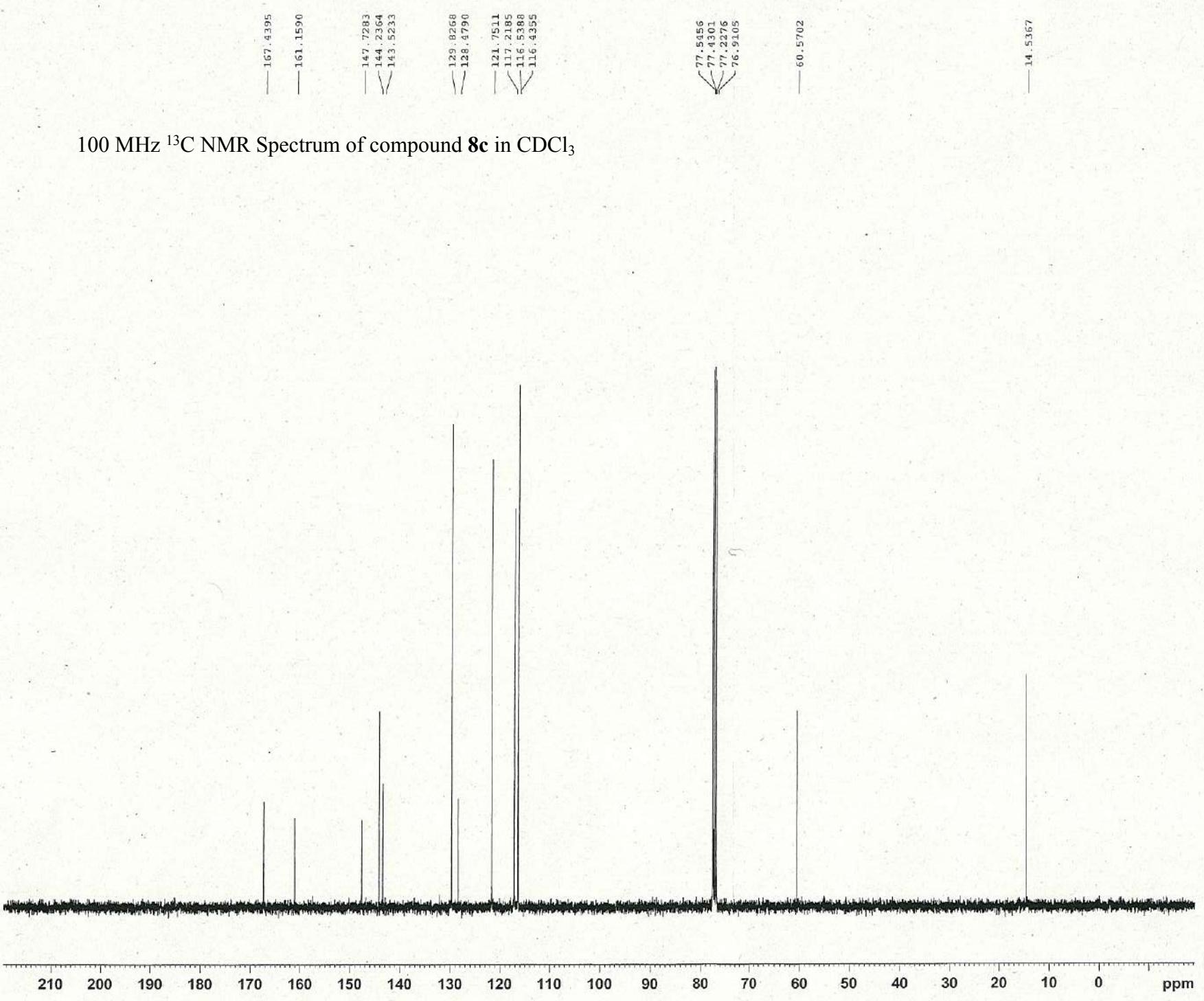


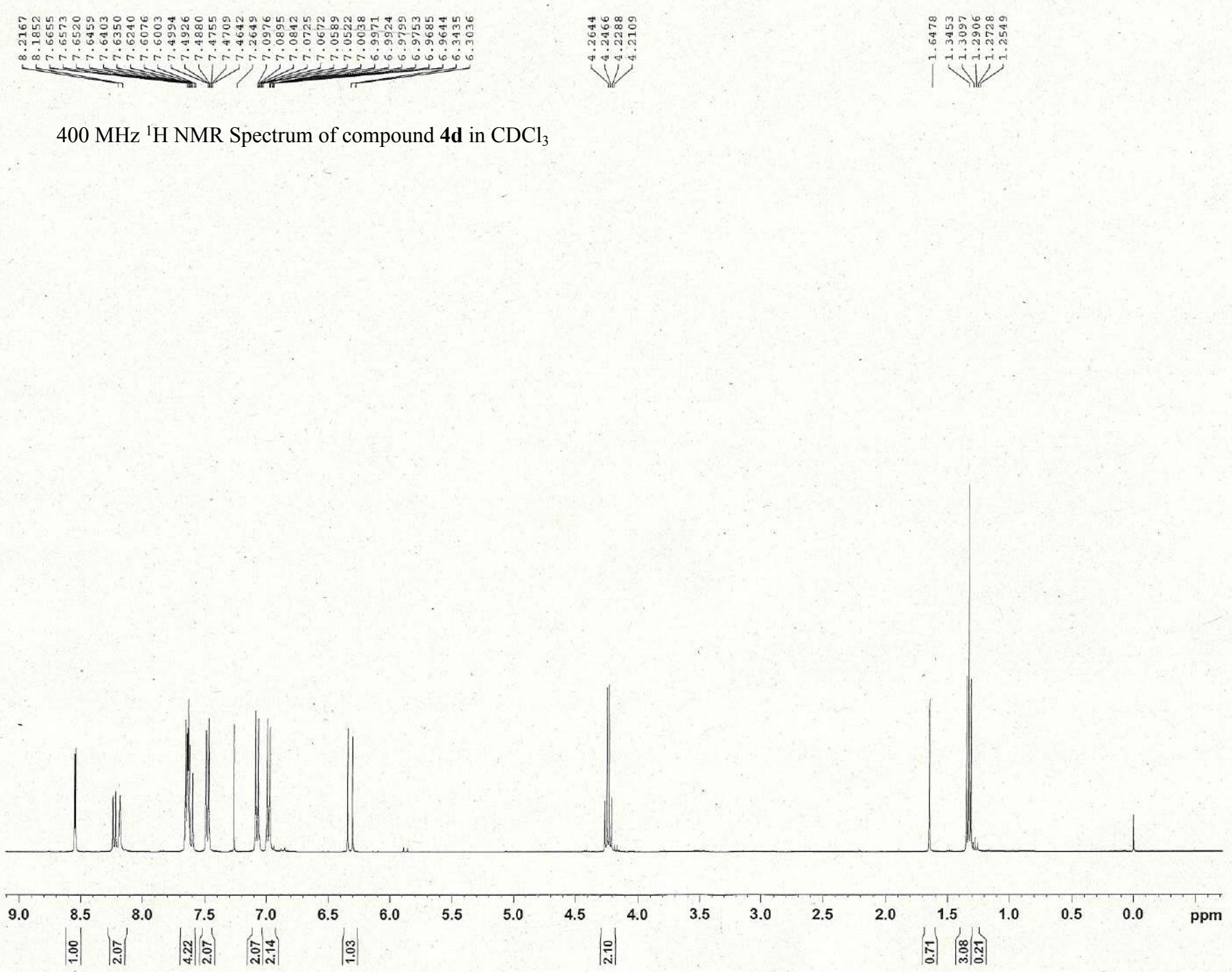


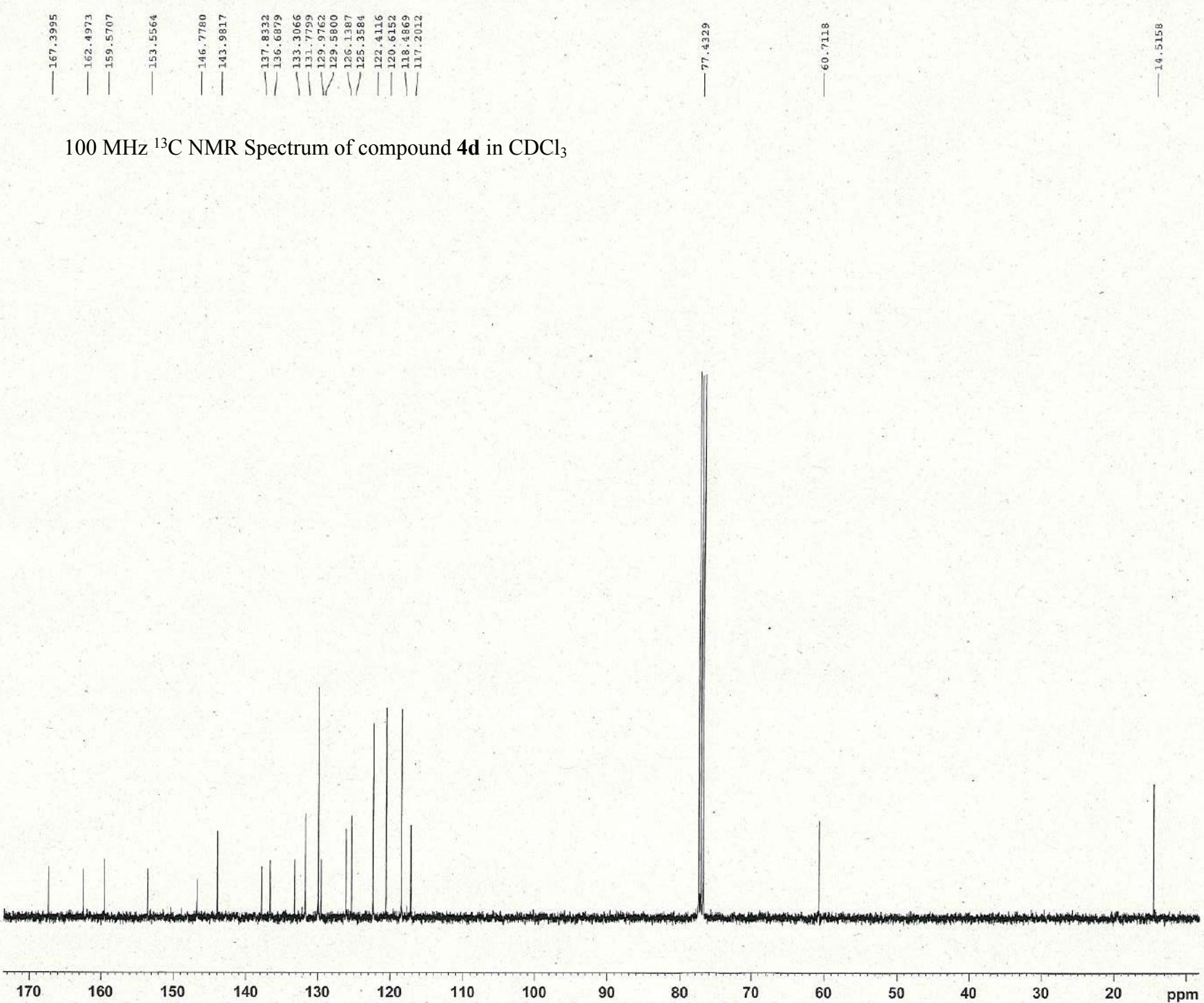
100 MHz ^{13}C NMR Spectrum of compound **7c** in CDCl_3

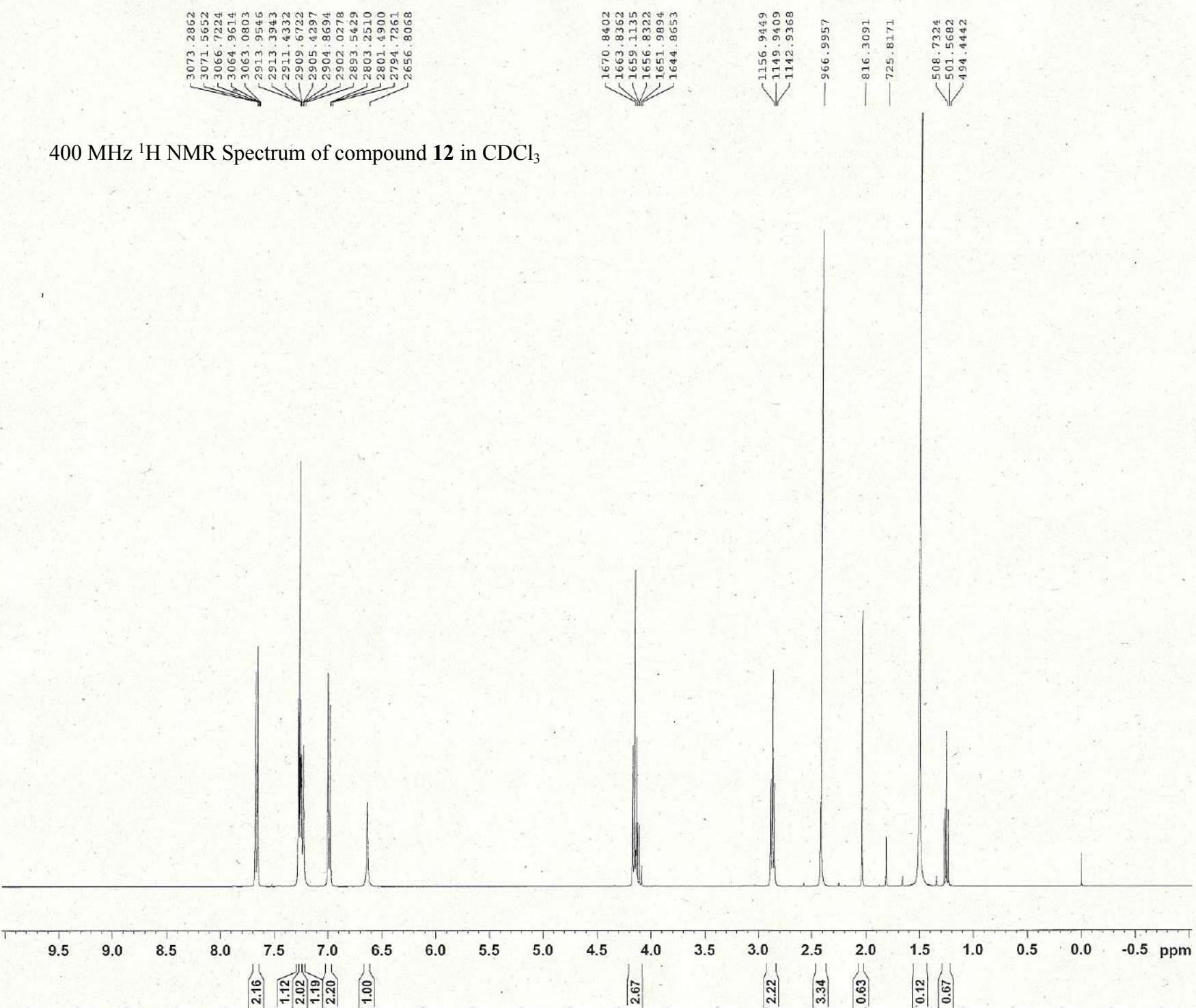




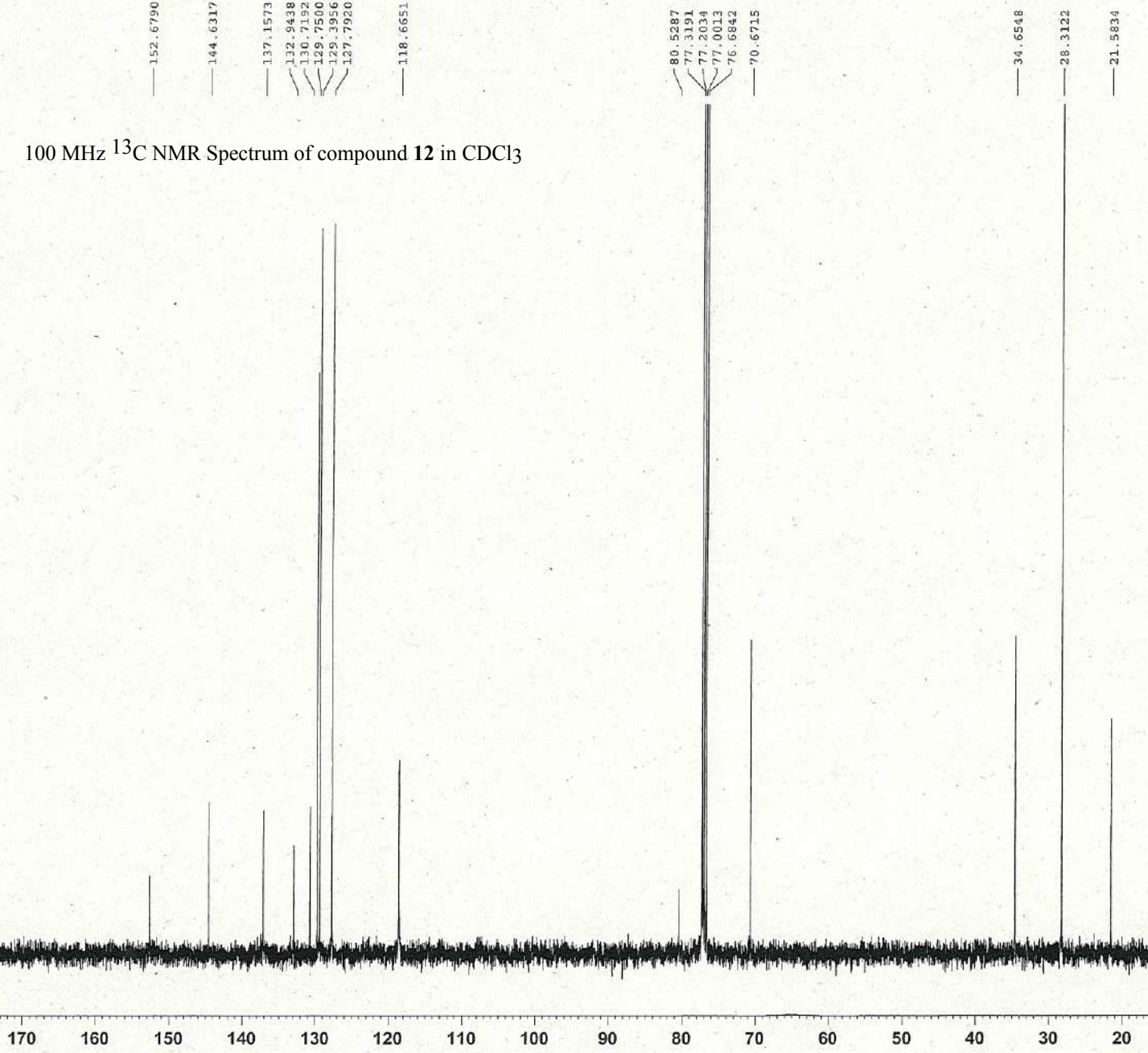








100 MHz ^{13}C NMR Spectrum of compound **12** in CDCl_3



1.000

3950.7505

400 MHz ^1H NMR Spectrum of compound **13** in CDCl_3

2.106

2.103

2.206

2.124

0.878

2.148

2.197

9.951

605.7881

0.0400

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— 19201.0102

— 16489.7241

— 15376.3970

— 13785.8952
— 13311.4679
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— 13074.0562
— 13029.9434

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— 7781.1528
— 7749.2706
— 7717.2678
— 6948.9274

— 3509.5260

— 2849.7740

100 MHz ^{13}C NMR Spectrum of compound **13** in CDCl_3

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2985.3956
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2980.7529
2977.7501
2973.8690
2971.1074
2929.8037
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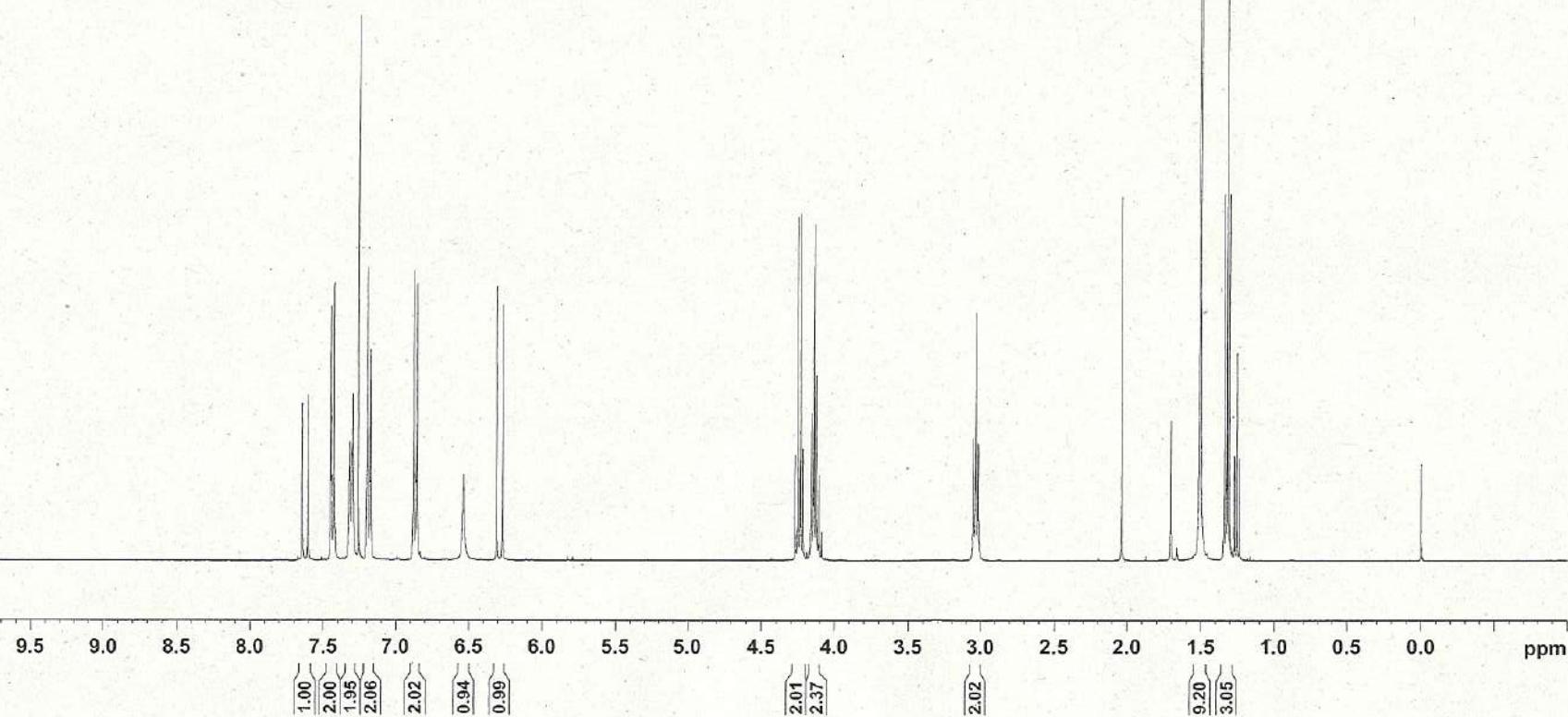
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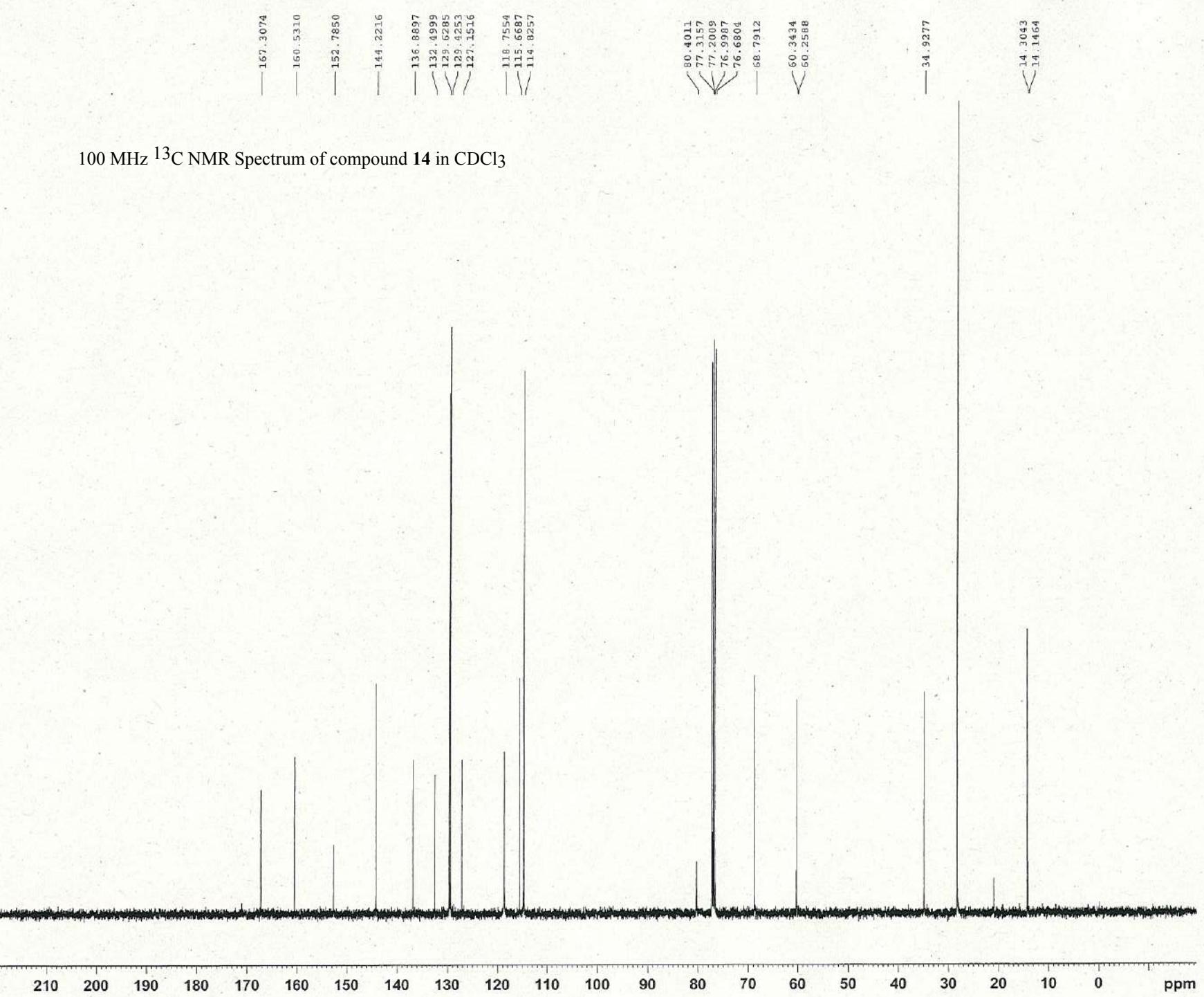
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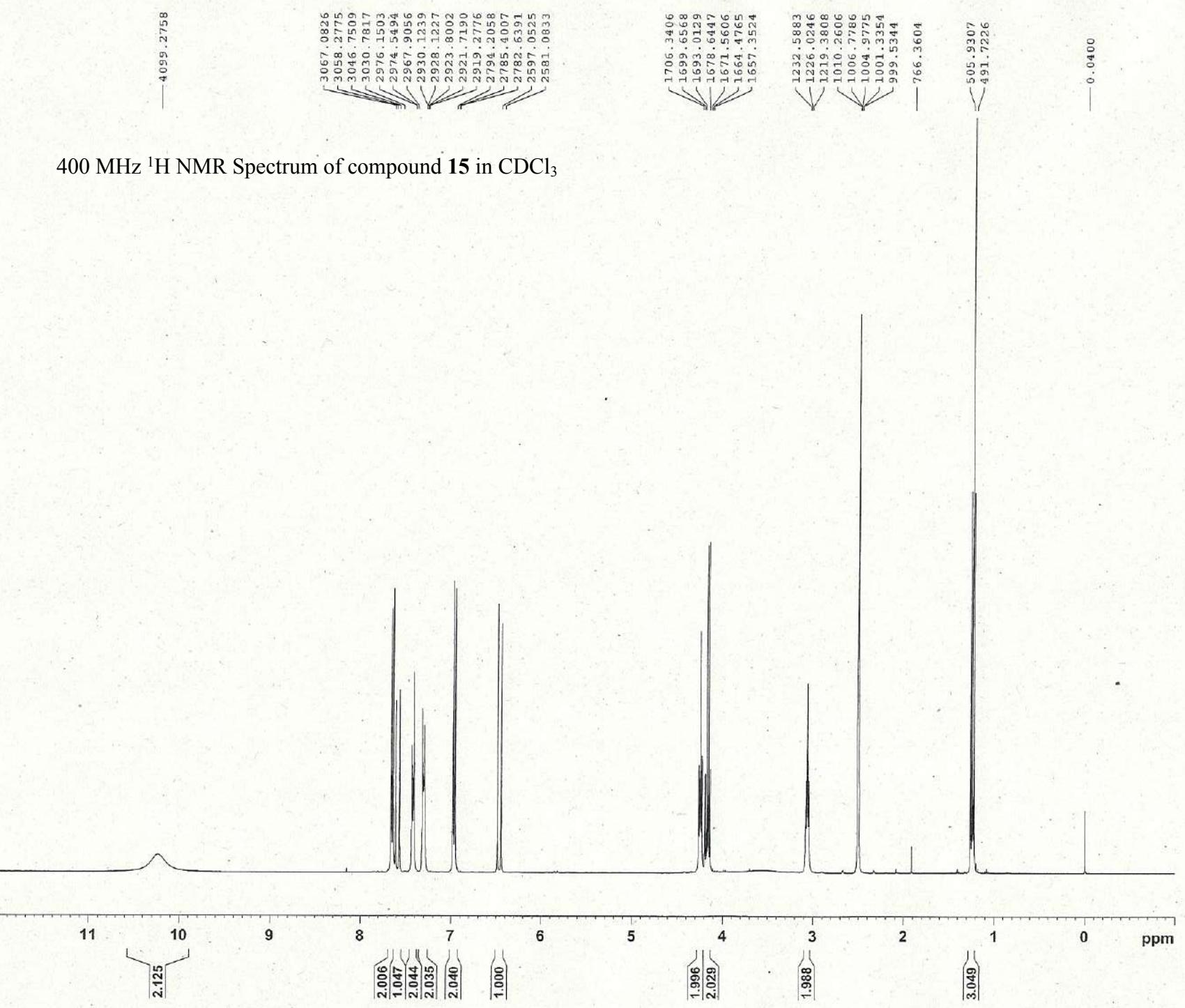
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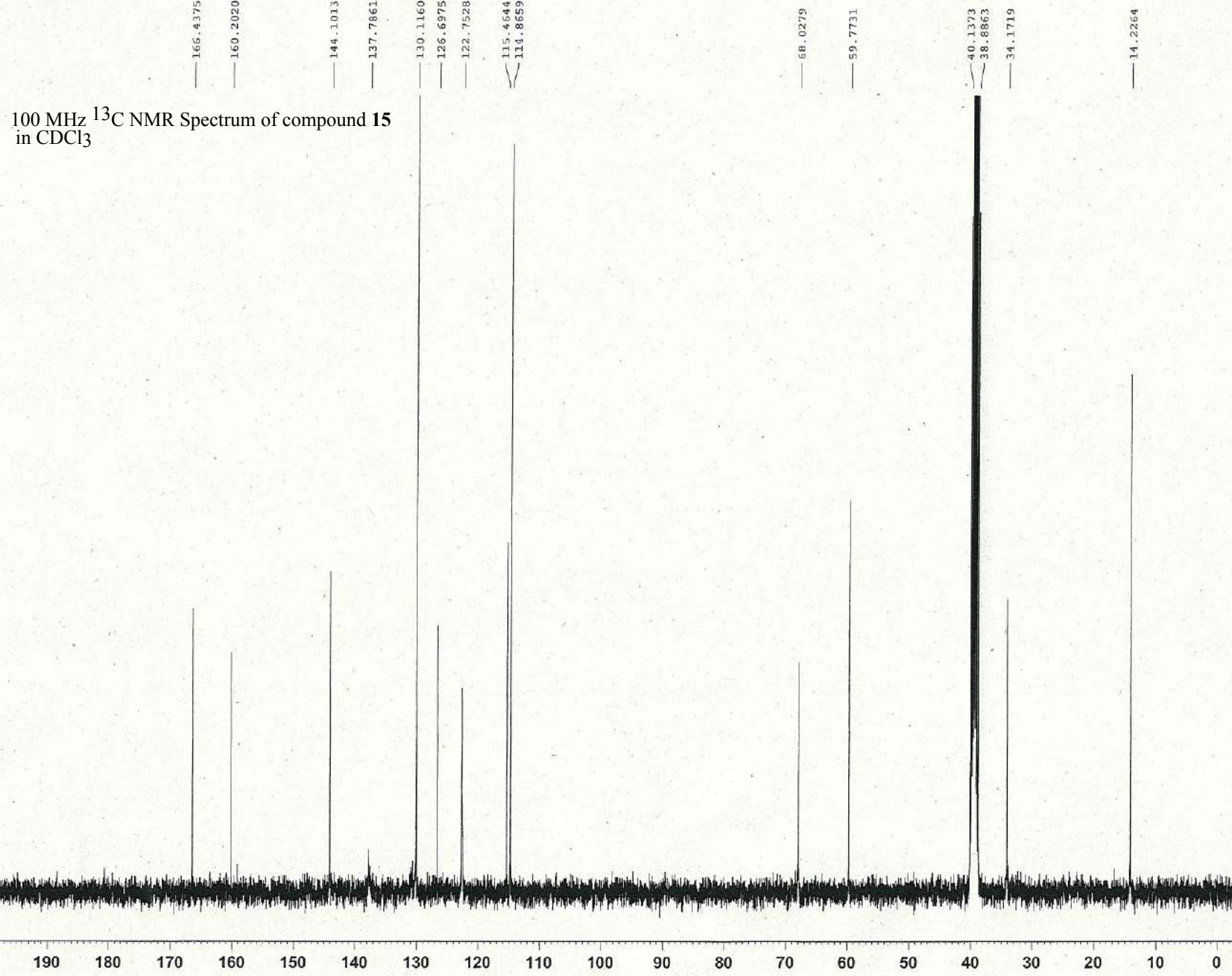
400 MHz ^1H NMR Spectrum of compound **14** in CDCl_3







100 MHz ^{13}C NMR Spectrum of compound **15**
in CDCl_3



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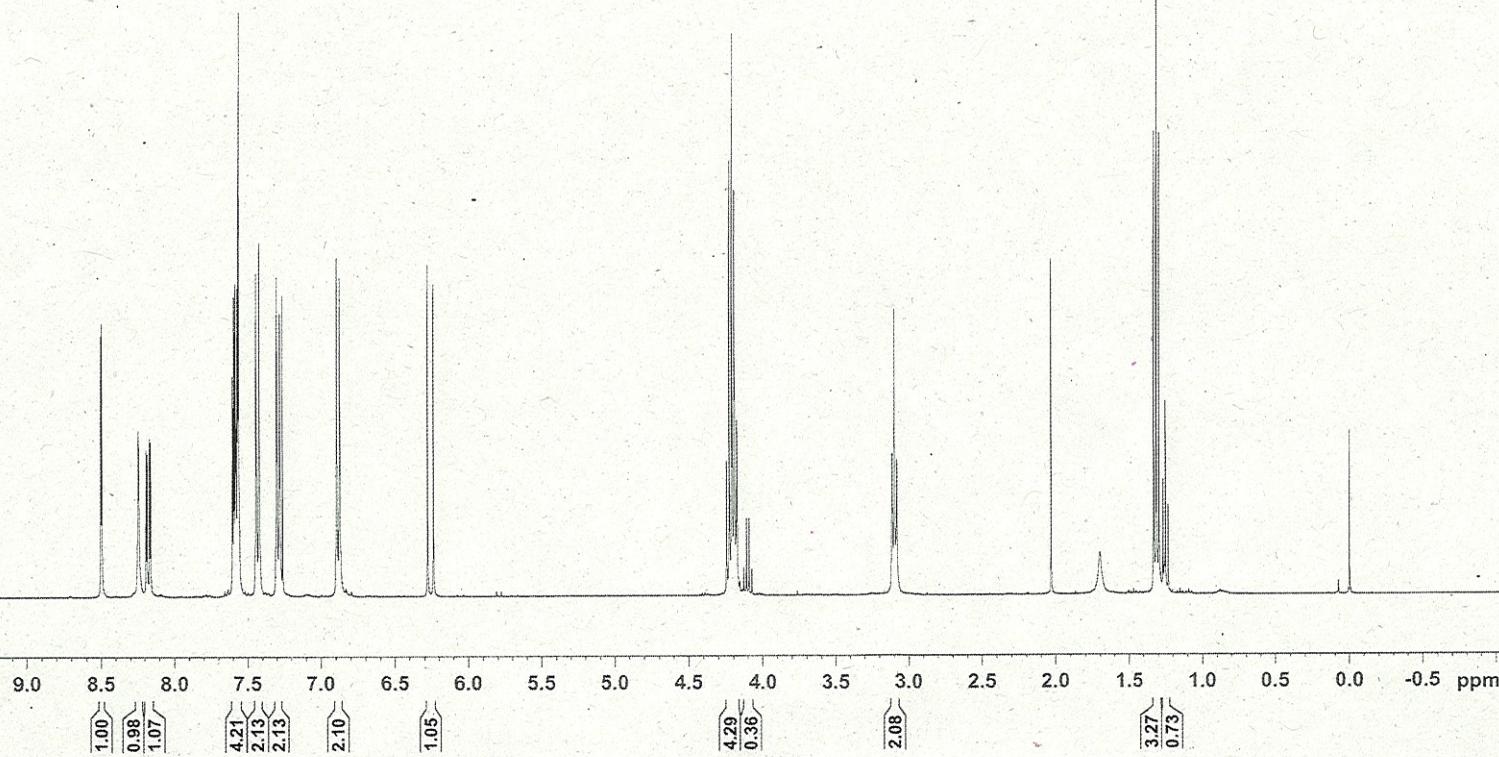
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0.0000

400 MHz ^1H NMR spectrum of compound **16** in CDCl_3



100 MHz ^{13}C NMR spectrum of compound **16** in CDCl_3

