Supporting Information

Highly Sensitive AIEE Active Fluorescent Probe for Detection of Deferasirox: Extensive Experimental and Theoretical Studies

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SI-1. Instruments and reagents

The sensor **MPT** was characterized by performing ^{1}H NMR at 400 MHz, ^{13}C NMR and DEPT-135 at 100 MHz with the help of Bruker Avance III NMR spectrometer employing $CDCl_3$ as solvent and the reference compound was TMS (tetramethylsilane). NMR titration experiments were carried out in $CDCl_3$. The spectrofluorometer (FluoroMax-Plus-P-C, Horiba Jobin Yvon Technology, USA) was used to record the fluorescence emission spectra. The fluorescence studies were performed on solutions of sensor **MPT** in HPLC grade THF in order to detect the anticipated analyte. All chemicals and reagents, purchased from Daejung Chemicals & Metals (Korea), Oakwood Chemicals (USA), Sigma Aldrich (USA), and Alfa Aesar (UK), were employed directly without any further purification. Reagents and chemicals included diphenylacetic acid, potassium thiocyanate, 3,4 dimethoxyaniline, THF, dichloromethane, methanol, sodium bicarbonate, and distilled water. The plasma (P9523, MDL number: MFCD00131920) was purchased from Sigma Aldrich (USA).

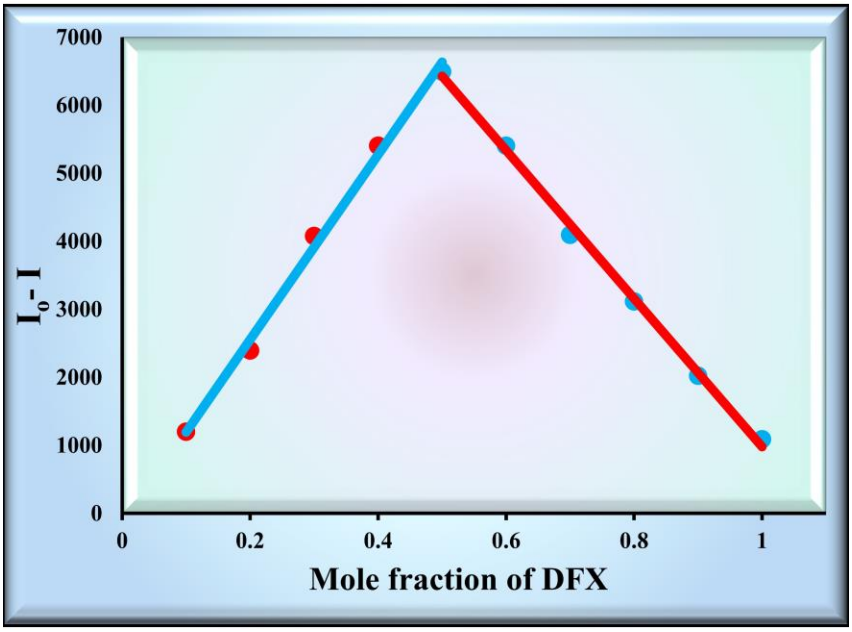

Fig. S 1. Jobs plot of sensor **MPT**-DFX complex in H_2O:THF (9:1, v/v)

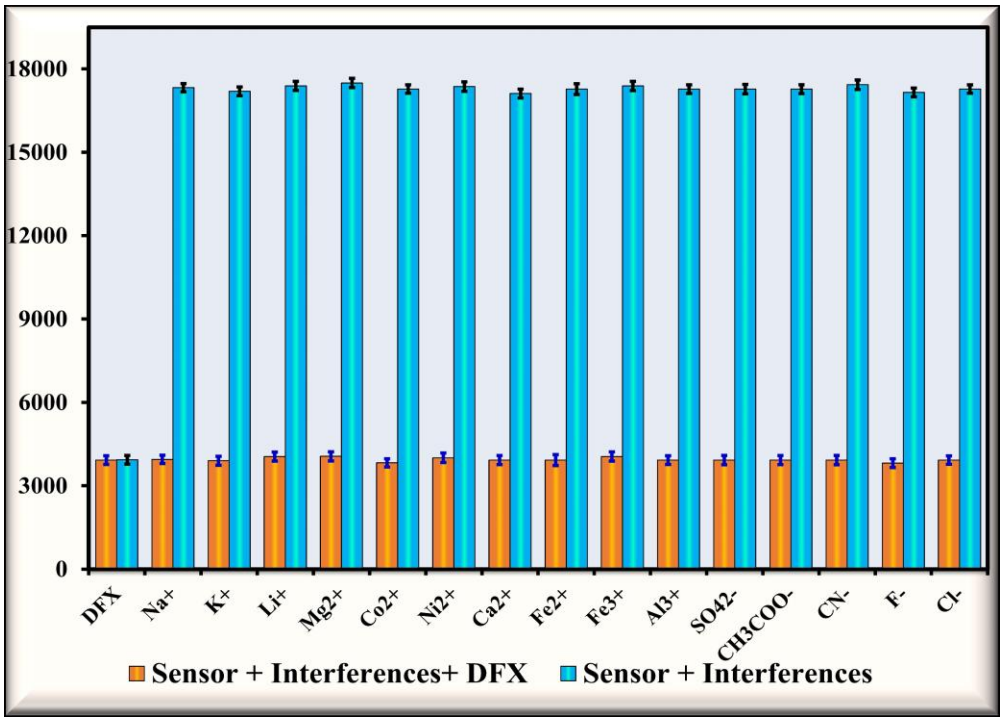

Fig. S 2. The emission response of sensor **MPT** towards DFX before and after adding some common interferences

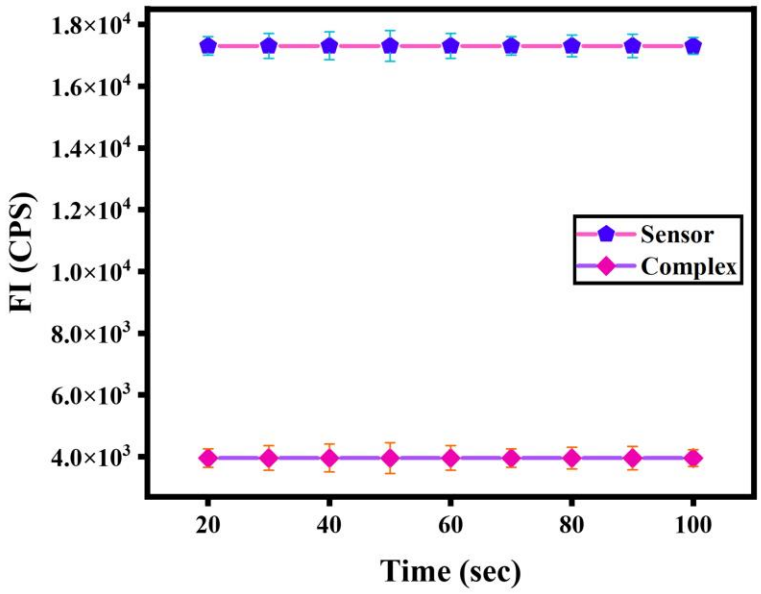

Fig. S 3. Photostability test of probe **MPT**

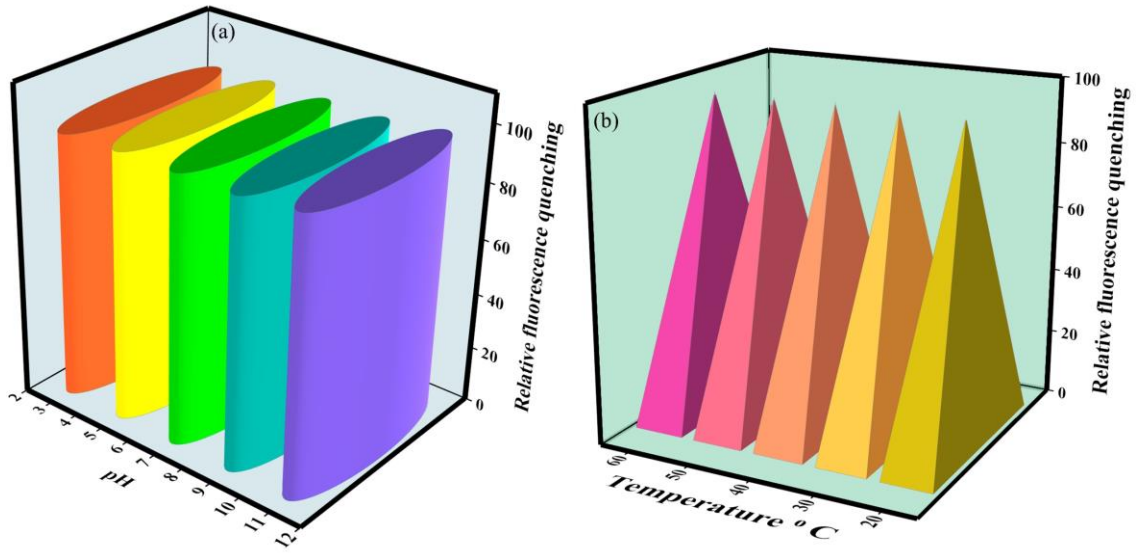

Fig. S 4. (a) Effect of pH and (b) Effect of temperature on the relative fluorescence quenching of sensor **MPT** towards DFX

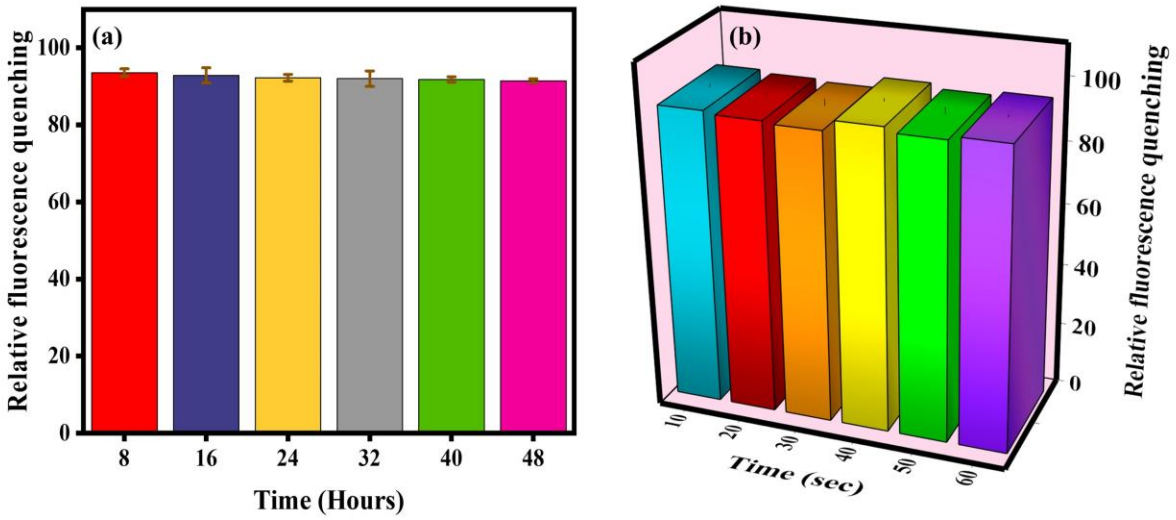

Fig. S 5. (a) Relative fluorescence quenching of **MPT** for DFX in the time interval of 8 – 48 hours and (b) Relative fluorescence quenching of **MPT** for DFX in the time interval of 10 – 60 sec.

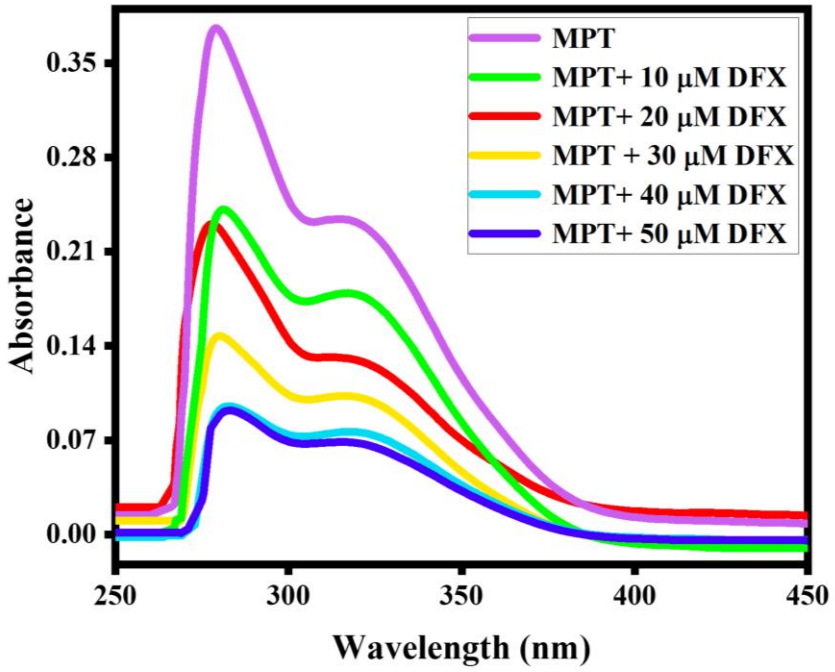

Fig. S 6. UV-*Vis.* absorbance of **MPT**-DFX

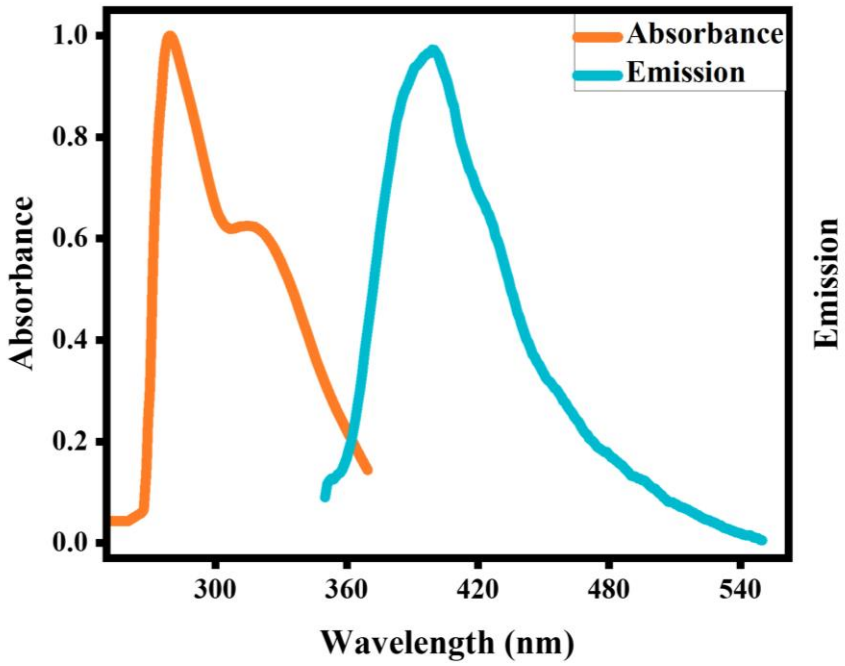

Fig. S 7. UV-*Vis* absorbance and fluorescence emission of sensor **MPT** in THF solution (10 µM)

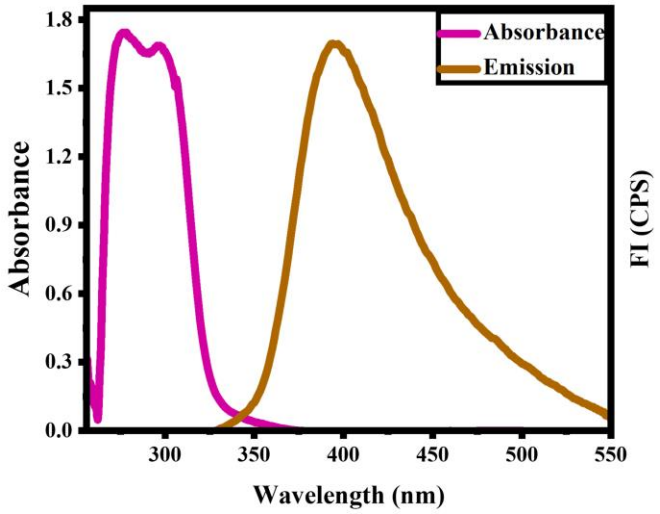

Fig. S 8. The absorbance of DFX and emission spectra of **MPT**

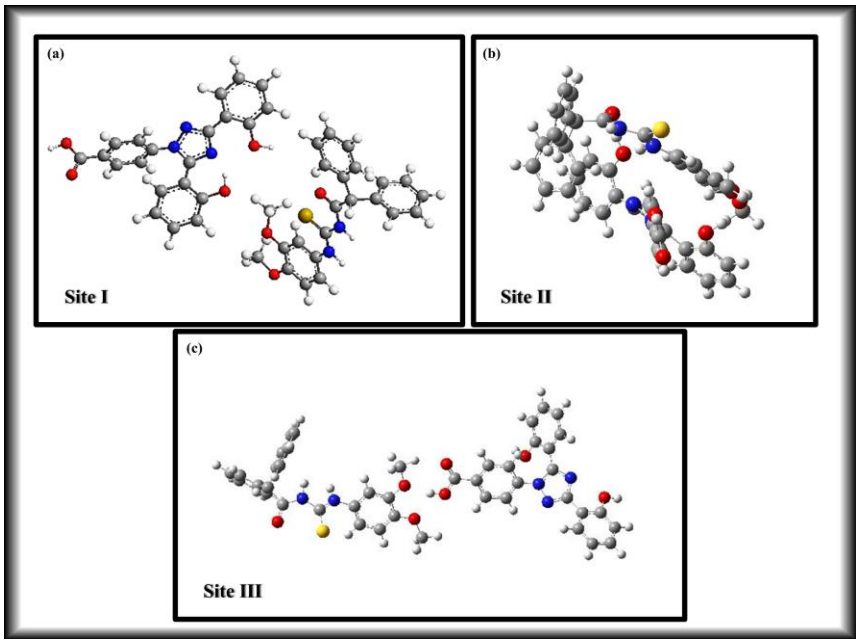

Fig. S 9. Optimized geometries of sensor **MPT** (a) Site I **MPT**-DFX (b) Site II **MPT**-DFX (c) Site III **MPT**-DFX

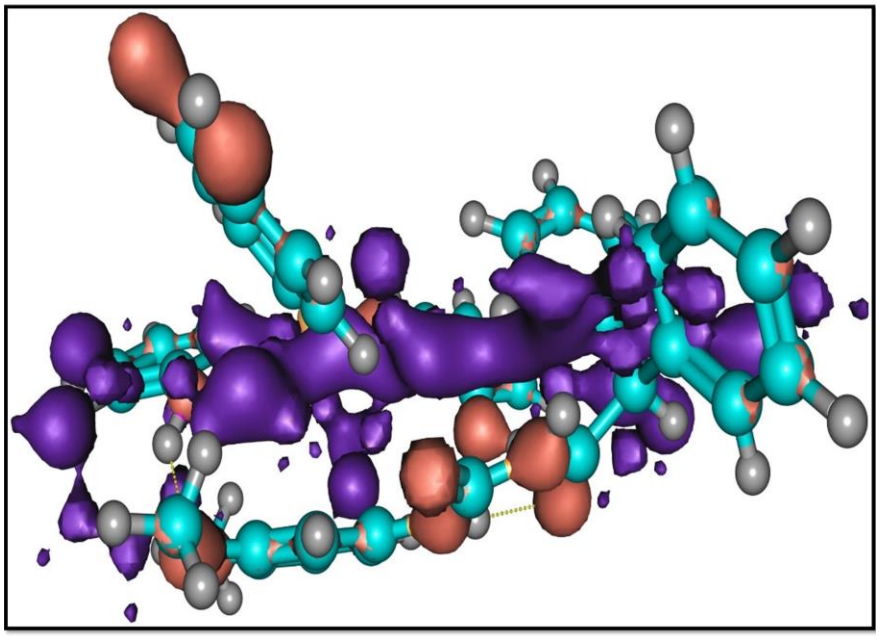

Figure S 10. Electron density difference image of **MPT**-DFX Complex

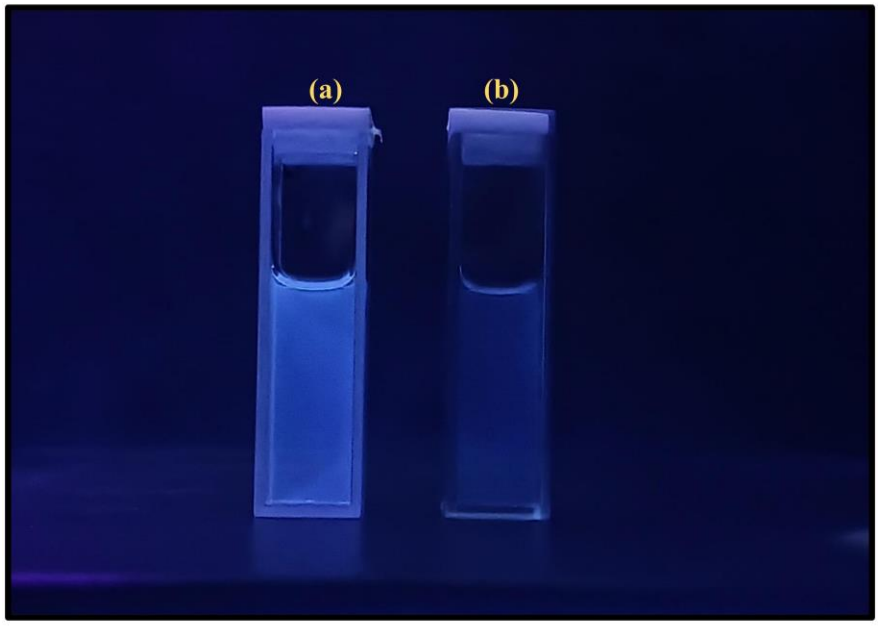

Fig. S 11. Bright fluorescence of **MPT** (a) before adding DFX and, (b) after adding DFX

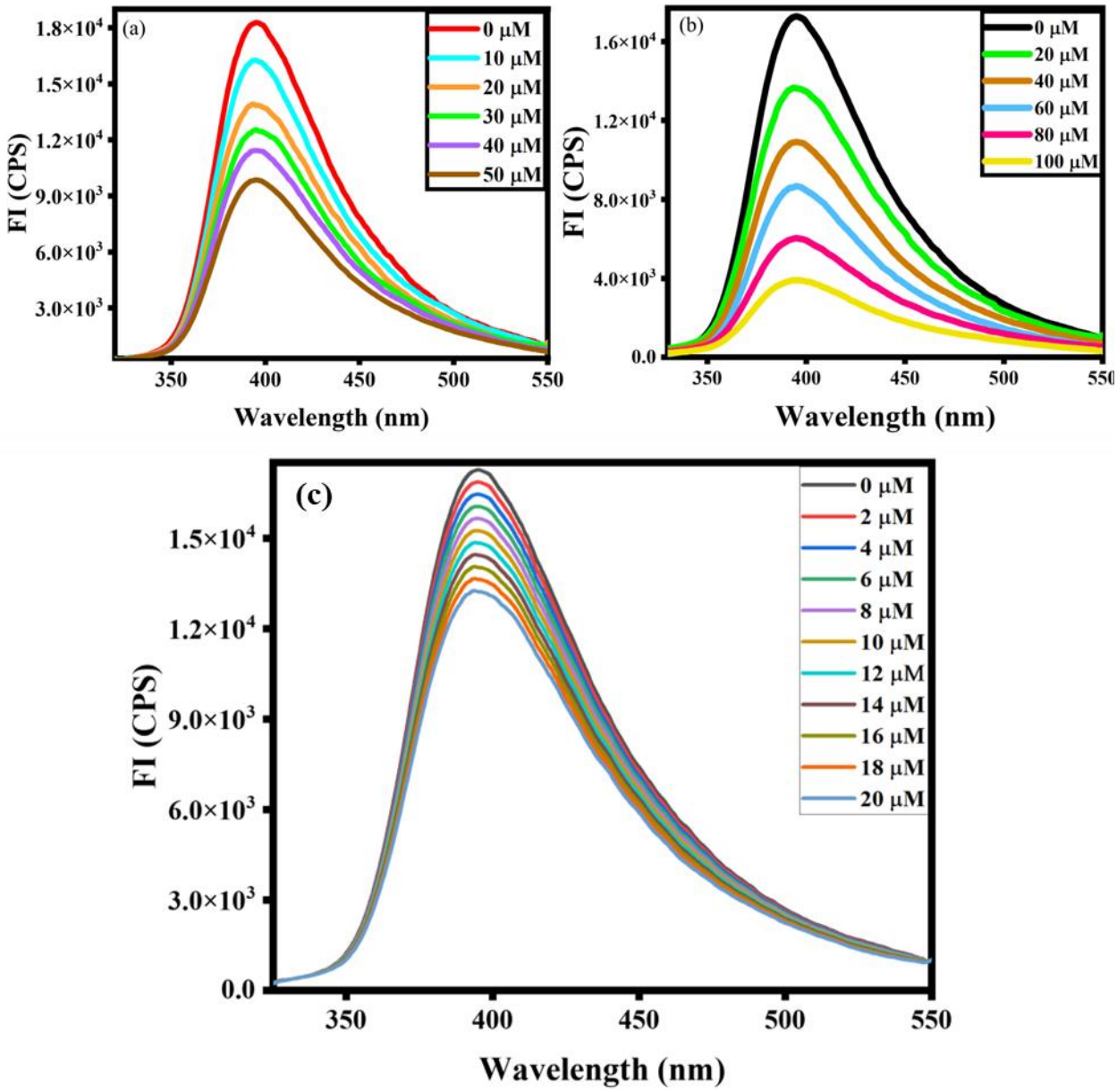

Fig. S 12. (a) Fluorescence relative emission of sensor **MPT** in plasma and (b) Real water sample (c) Fluorescence quenching observed in spiked artificial urine samples

Table. S 1 (a). The quantum yield of MPT in different water fractions and with DFX

Water Fraction	Quantum Yield	DFX Concentration(μM)	Quantum Yield
10	0.075	-	-
20	0.086	10	0.137
30	0.098	20	0.112
40	0.11	30	0.091
50	0.117	40	0.075
60	0.123	50	0.061
70	0.128	60	0.05
80	0.134	70	0.042
90	0.137	80	0.037
95	0.092	90	0.034
99	0.078	100	0.033

Table. S 1 (b). Comparison of sensor MPT with already reported DFX sensors

Sensor	LOD	Phenomenon	Reference
Carbamothioyl based sensor	175 nM (0.2 μM)	Fluorescence quenching	This work
Carbon dots probe and Cu^{2+} as medium	0.33 μg/mL (330 μM)	Fluorescence quenching	**[1]**
Dopamine-conjugated carbon dots	600 ng/mL (600 μM)	Fluorescence quenching	**[2]**

Carbon dots and Cu^{2+}-catalyzed oxidation of *o*-phenylenediamine	0.38 mg/mL (0.38 M)	Fluorescence quenching	**[3]**
"ON-OFF-ON" sensor for sequential detection of Fe^{3+} and deferasirox	0.14 ppm	Fluorescence enhancement	**[4]**
Poly(Allylaminehydrochloride)-Templated Copper Nanoclusters	0.1 μg/mL	Fluorescence quenching	**[5]**

Table. S 2. Spike and recovery experiment for detection of DFX in plasma

Spiked (μM)	Recovered (μM)	Recovery (%)	RSD (%)
10	10.4	104	1.21
20	19.7	98.5	1.18
30	30.6	102	1.26
40	41.4	103.5	1.2
50	51.8	103.6	1.29

Table. S 3. QTAIM analysis of **MPT**-DFX

BCPs	MPT-DFX	ρ(r) (a.u)	$\nabla^2\rho(r)$ (a.u)	G(r) (a.u)	V(r) (a.u)	H(r) (a.u)	-V/G	E_{int} (kcal/mol)
1	S…H	0.005	0.017	0.003	-0.002	-0.00106	0.68	-0.722

2	S... H	0.006	0.020	0.004	-0.003	0.00108	0.72	-0.878
3	H…C	0.004	0.011	0.002	-0.001	-0.00058	0.50	-0.314
4	O...H	0.025	0.076	0.020	-0.021	-0.00108	1.05	-6.589
5	C…H	0.006	0.021	0.004	-0.003	-0.00112	0.75	-0.941
6	O…O	0.010	0.046	0.010	-0.009	-0.00132	0.90	-2.823
7	C…N	0.004	0.012	0.002	-0.002	-0.00049	1.00	-0.628
8	O…H	0.028	0.094	0.023	-0.023	-0.00003	1.00	-7.216
9	H…O	0.013	0.042	0.010	-0.009	-0.00052	0.90	-2.824
10	C…O	0.009	0.028	0.006	-0.005	-0.00081	0.83	-1.569
11	C…N	0.004	0.011	0.002	-0.002	-0.00050	1.00	-0.628
12	N…H	0.006	0.020	0.004	-0.003	-0.00089	0.75	-0.941
13	C…H	0.007	0.021	0.004	-0.003	-0.00099	0.75	-0.941
14	C…C	0.006	0.019	0.004	-0.003	-0.00093	0.75	-0.941

Table. S 4. Spike and recovery values for DFX detection in real water samples

Spiked (µM)	Recovered (µM)	Recovery (%)	RSD (%)
20	19.8	99	1.24
40	40.5	101.3	1.2
60	60.9	101.5	1.32

80	81.3	101.6	1.29
100	102	102	1.17
120	121.2	101	1.19

Table S 5. Spike and recovery values for the detection of DFX in artificial urine samples

Spiked (µM)	Recovered (µM)	Recovery (%)	RSD (%)
2	1.99	99.5	0.52
4	3.96	99	0.45
6	5.87	97.8	0.4
8	7.93	99	0.35
10	9.48	94.8	0.32
12	11.79	98	0.29
14	13.92	99	0.28
16	15.89	99	0.3
18	17.9	99	0.35
20	19.73	98	0.4

References:

[1] W. Han, C. Miao, X. Zhang, Y. Lin, X. Hao, Z. Huang, S. Weng, X. Lin, X. Guo, J. Huang, A signal-off fluorescent strategy for deferasirox effective detection using carbon dots as probe and Cu^{2+} as medium, Anal. Chim. Acta, 1179 (2021) 338853, https://doi.org/10.1016/j.aca.2021.338853.

[2] C.-C. Wang, P.-T. Huang, H.-S. Kou, S.-M. Wu, Cu^{2+}-induced quenching and recovery of the luminescence of dopamine-conjugated carbon dots for sensing deferasirox in plasma, Sens. Actuators B Chem., 311 (2020) 127916, https://doi.org/10.1016/j.snb.2020.127916.

[3] C.-F. Miao, X.-Z. Guo, X.-T. Zhang, Y.-N. Lin, W.-D. Han, Z.-J. Huang, S.-H. Weng, Ratiometric fluorescence assay based on carbon dots and Cu^{2+}-catalyzed oxidation of O-phenylenediamine for the effective detection of deferasirox, RSC Adv., 11(55) (2021) 34525-34532, https://doi.org/10.1039/D1RA07078A.

[4] A.Y.A. Alzahrani, K.O. Khan, S. Rafique, H. Irshad, A.M. Khan, S.A. Shahzad, Theoretical and experimental studies on mechanochromic triphenylamine based fluorescent "ON-OFF-ON" sensor for sequential detection of Fe^{3+} and deferasirox, Spectrochim. Acta A Mol. Biomol. Spectrosc., 297 (2023) 122745, https://doi.org/10.1016/j.saa.2023.122745.

[5] H.-J. Lin, C.-C. Wang, H.-S. Kou, C.-W. Cheng, S.-M. Wu, Stable Luminescent Poly (Allylaminehydrochloride)-Templated Copper Nanoclusters for Selectively Turn-Off Sensing of Deferasirox in β-Thalassemia Plasma, Pharmaceuticals, 14(12) (2021) 1314, https://doi.org/10.3390/ph14121314.

SI-2. NMR spectra of the synthesized compound

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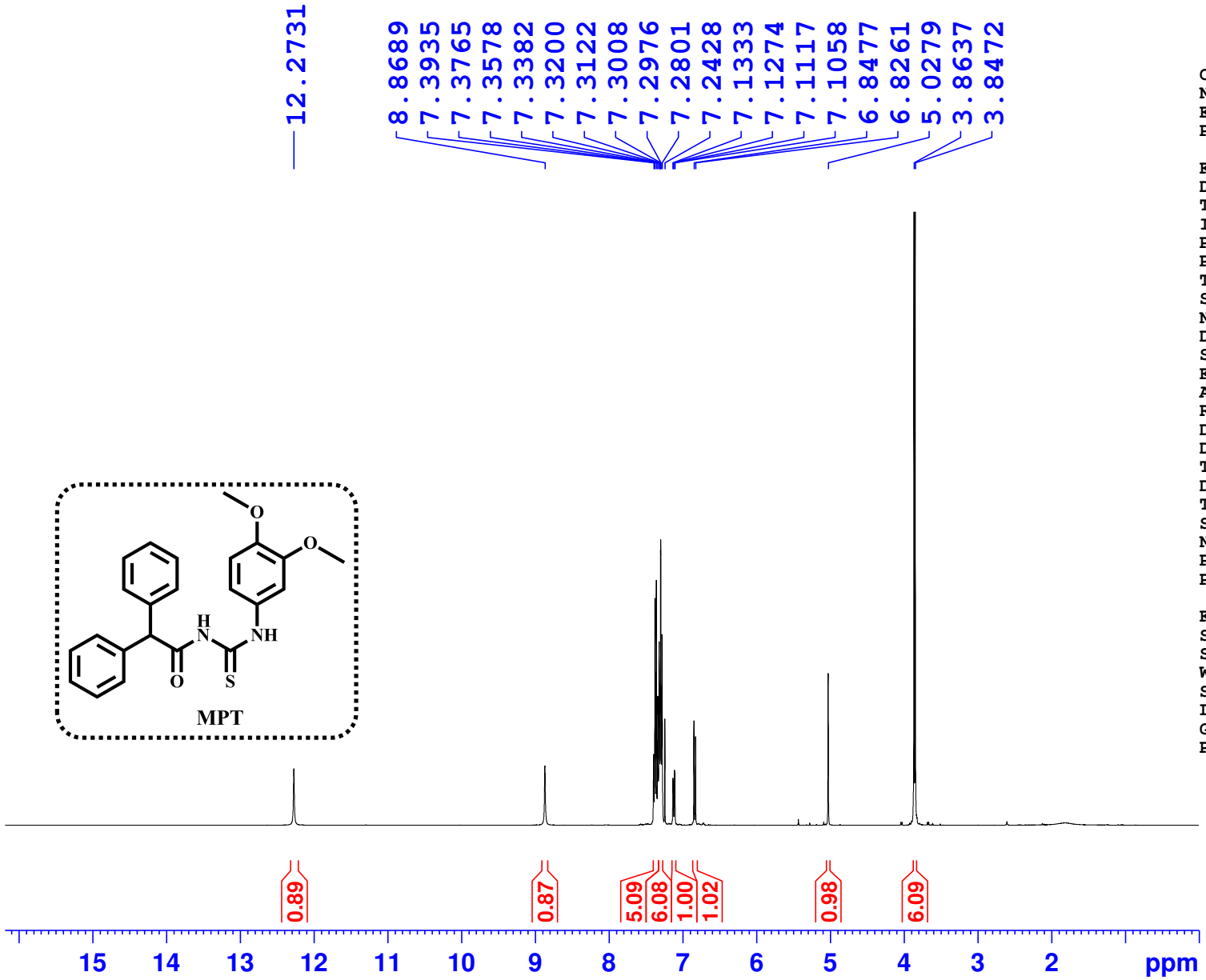


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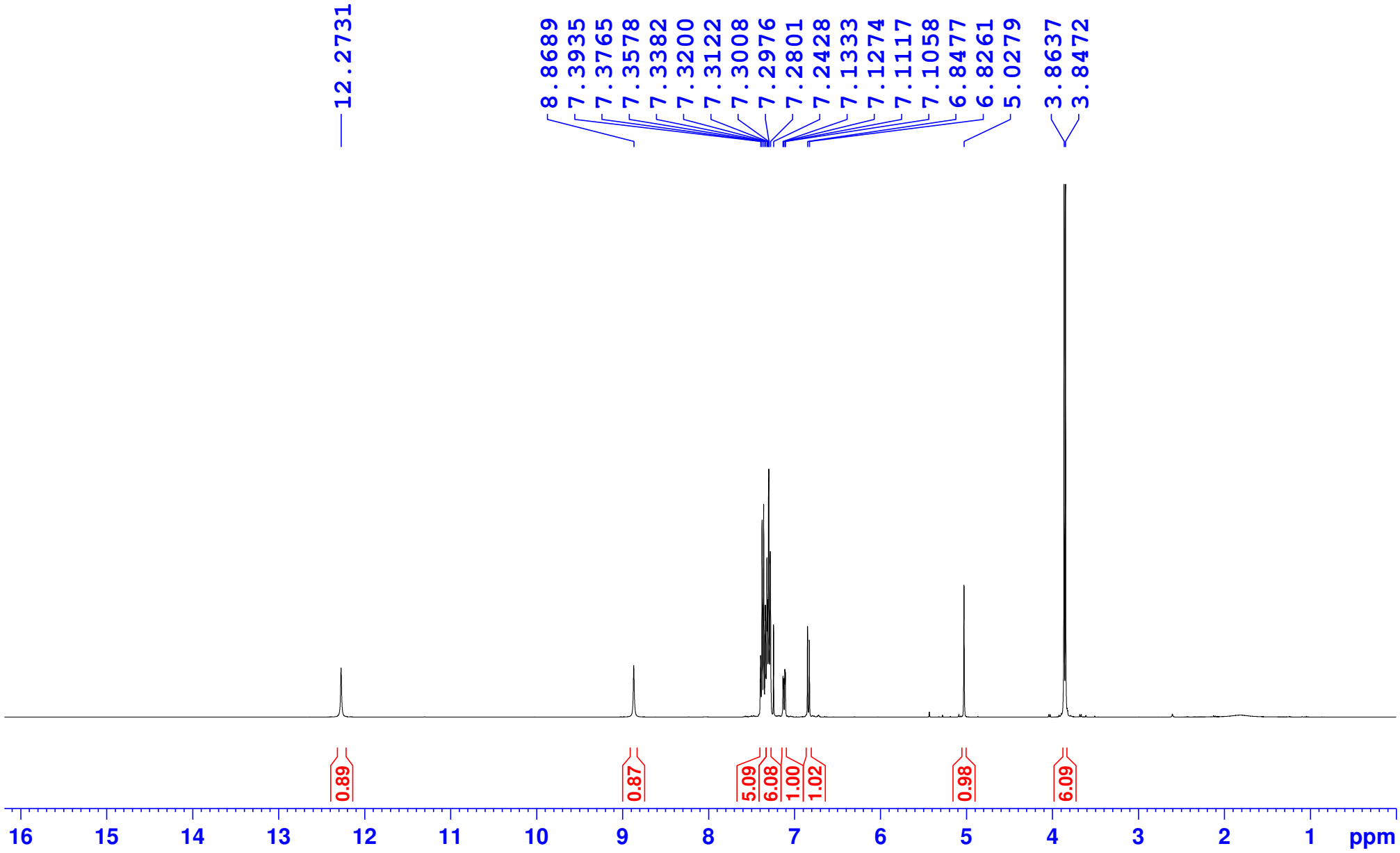

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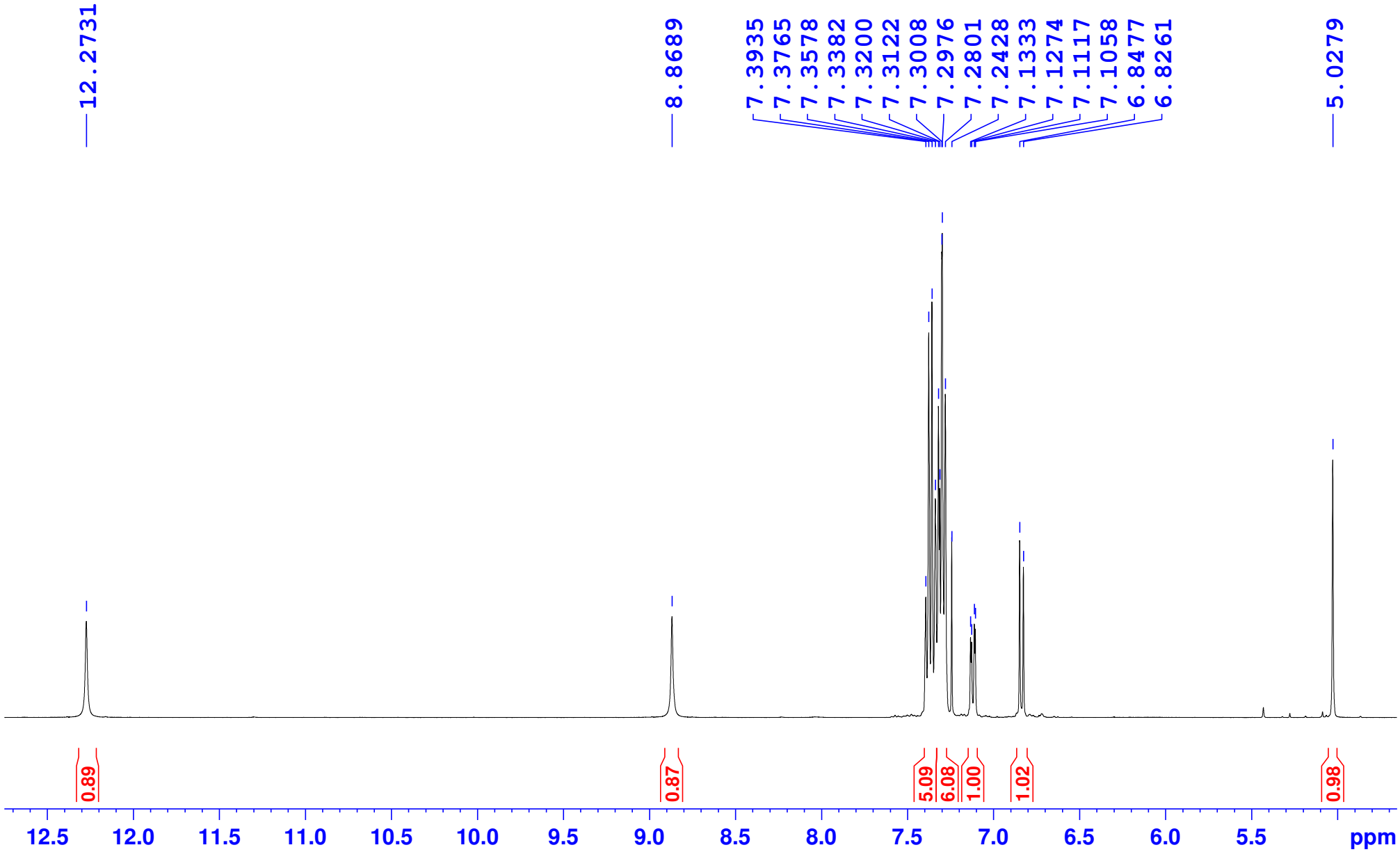

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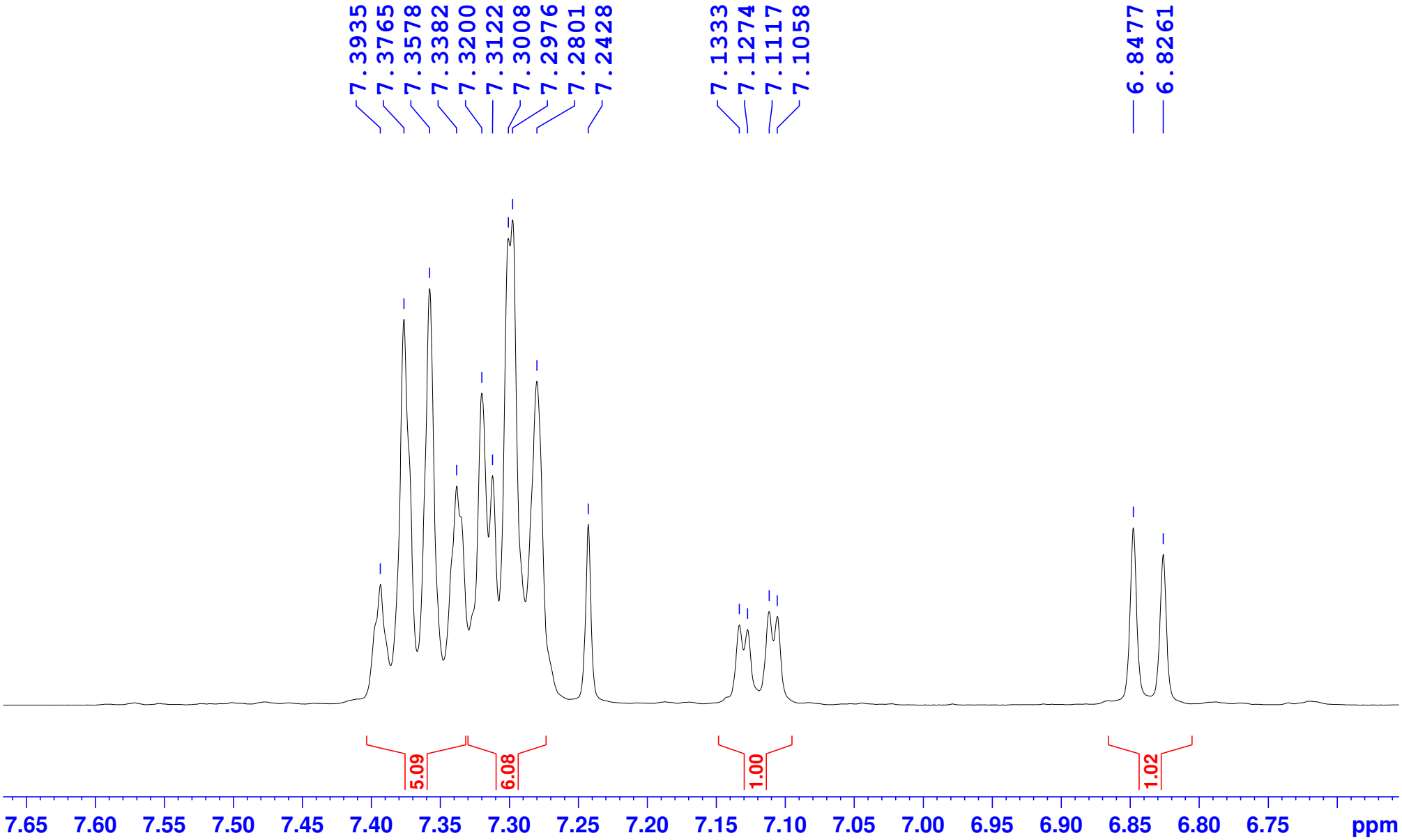

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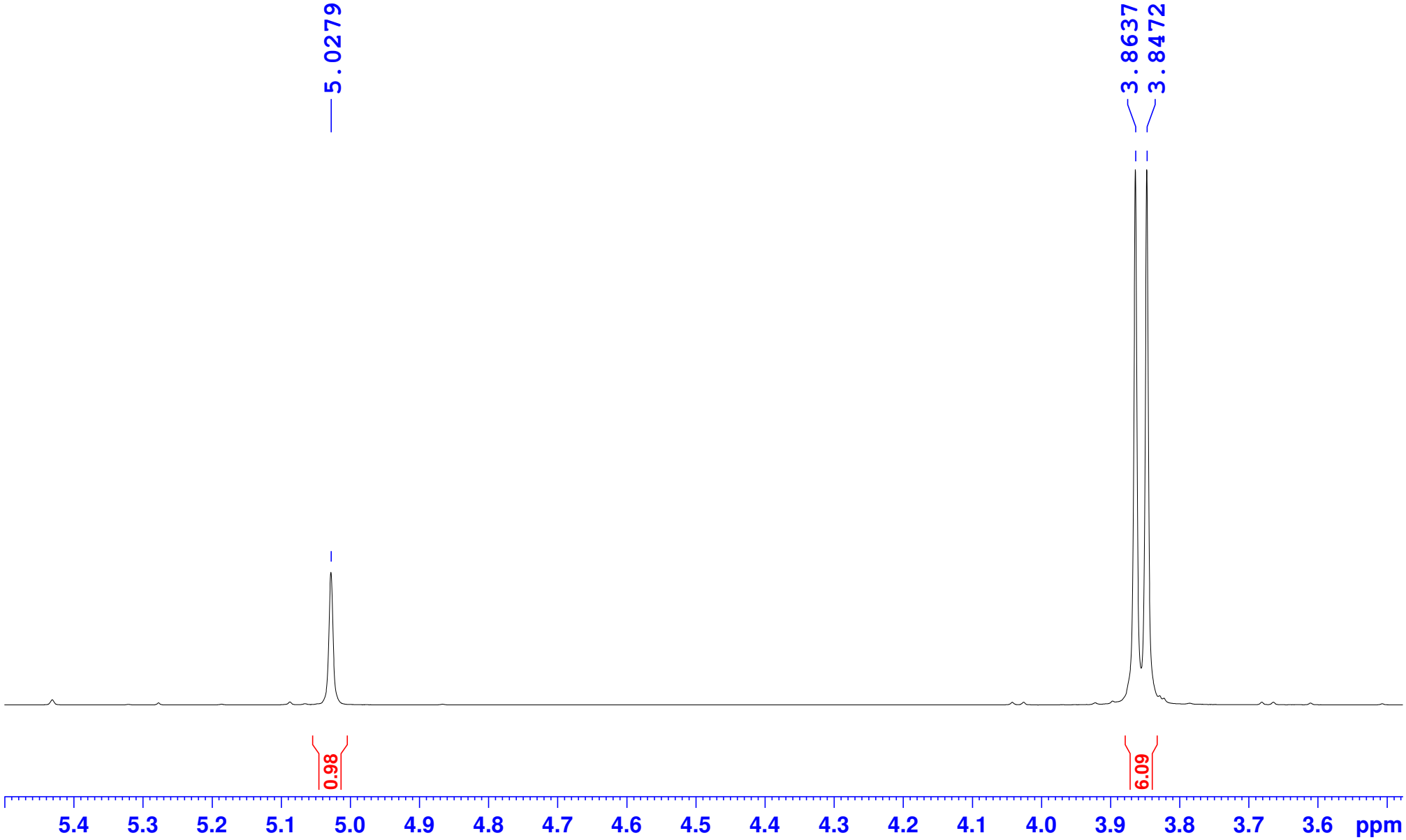

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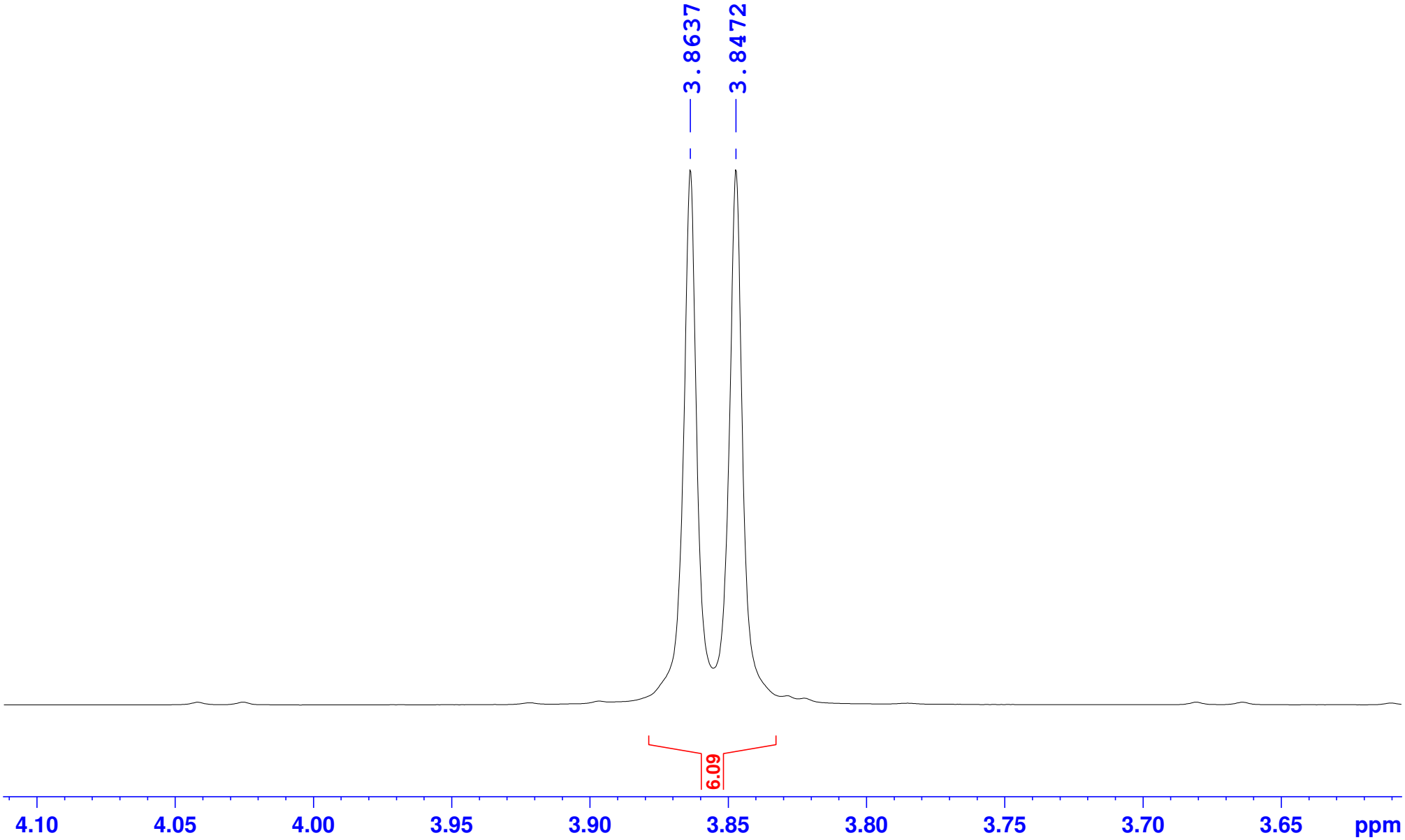

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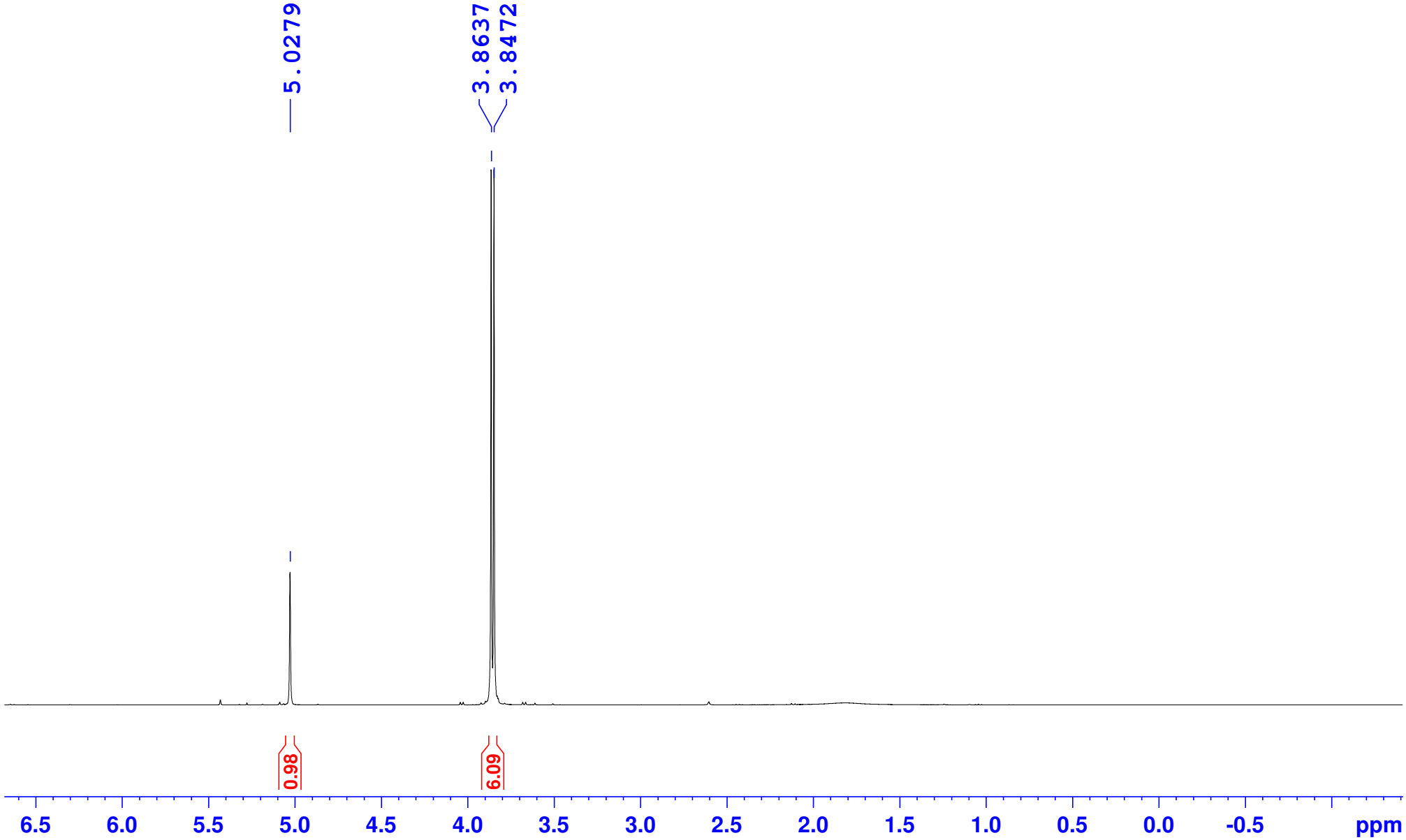

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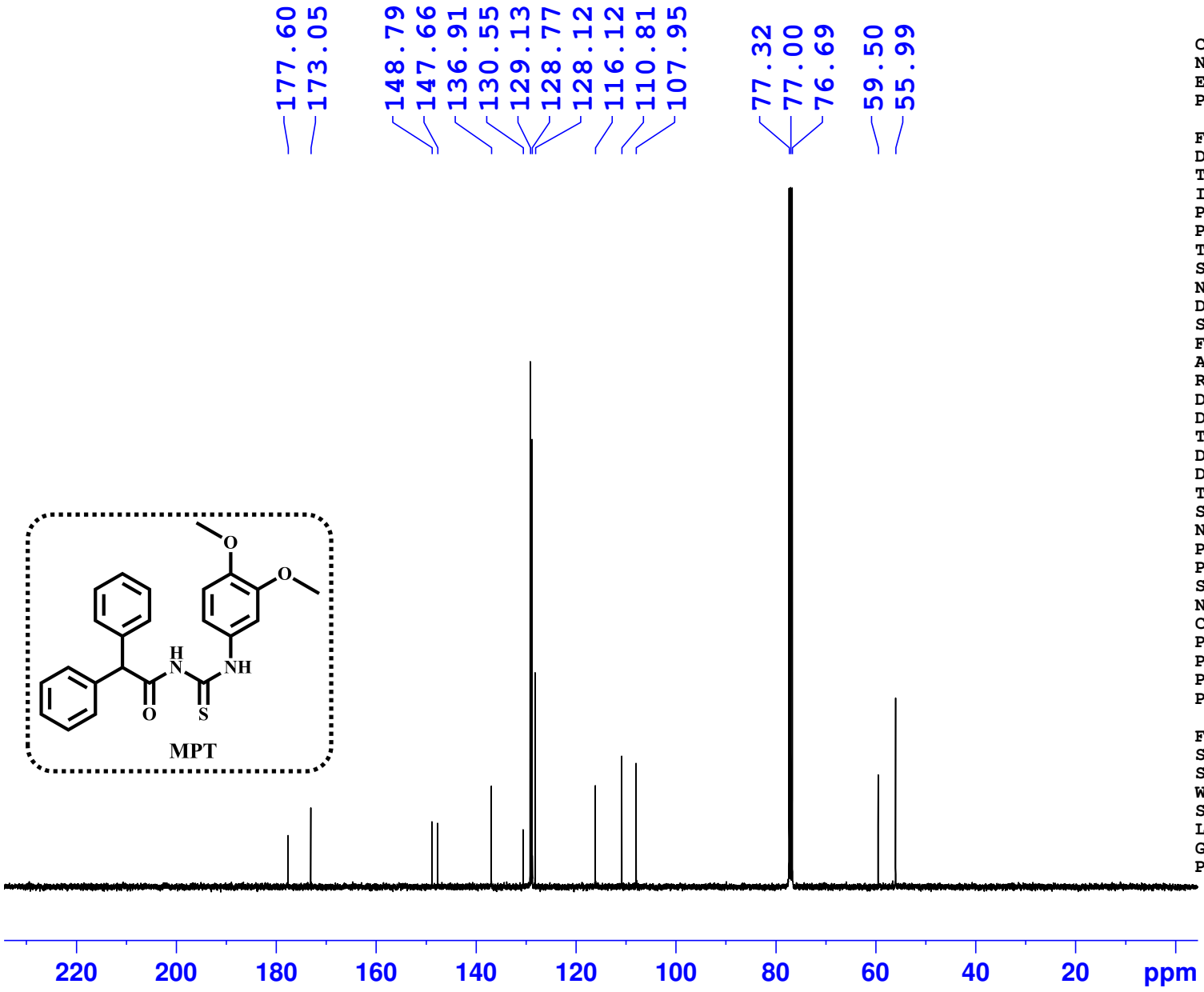


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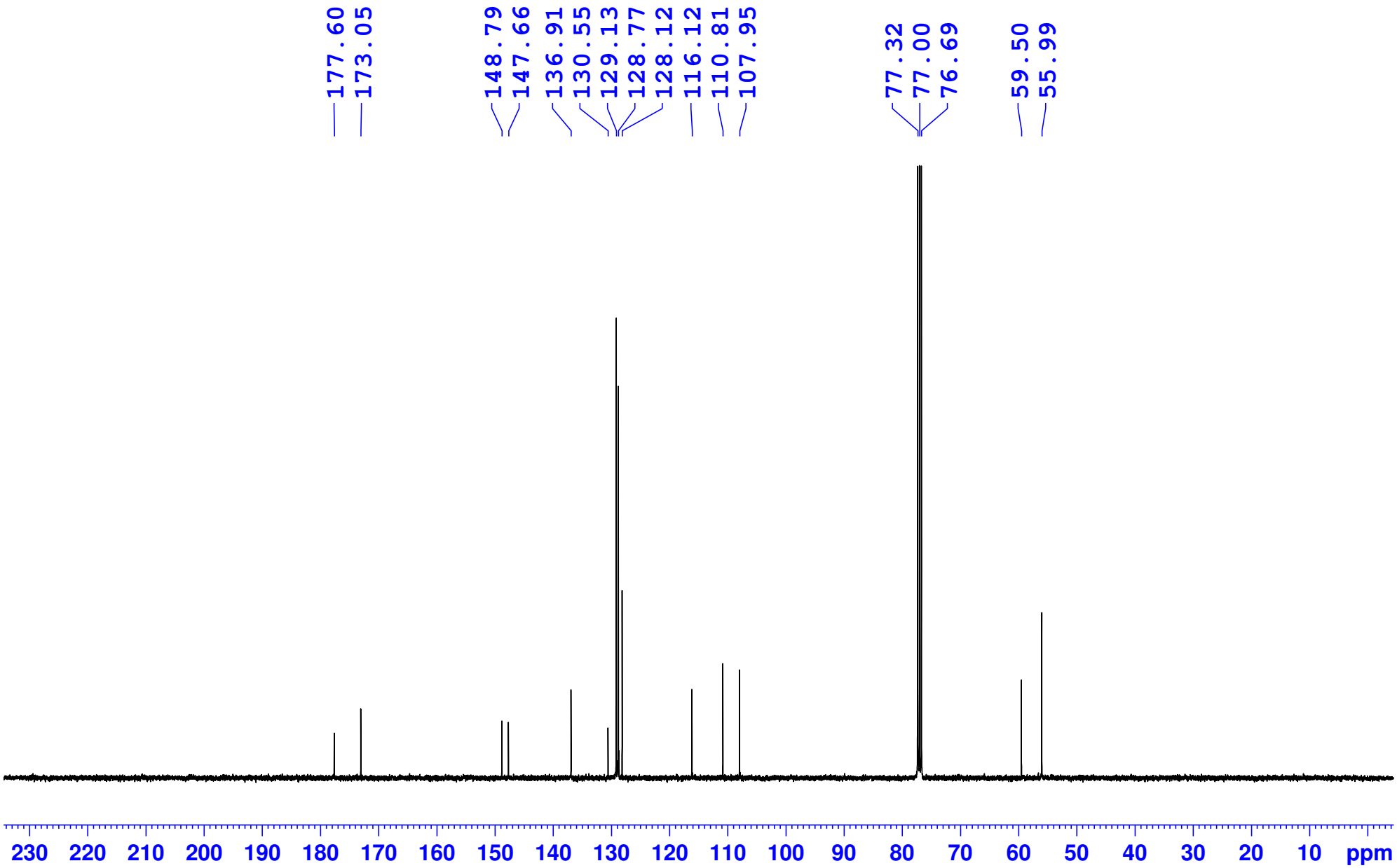

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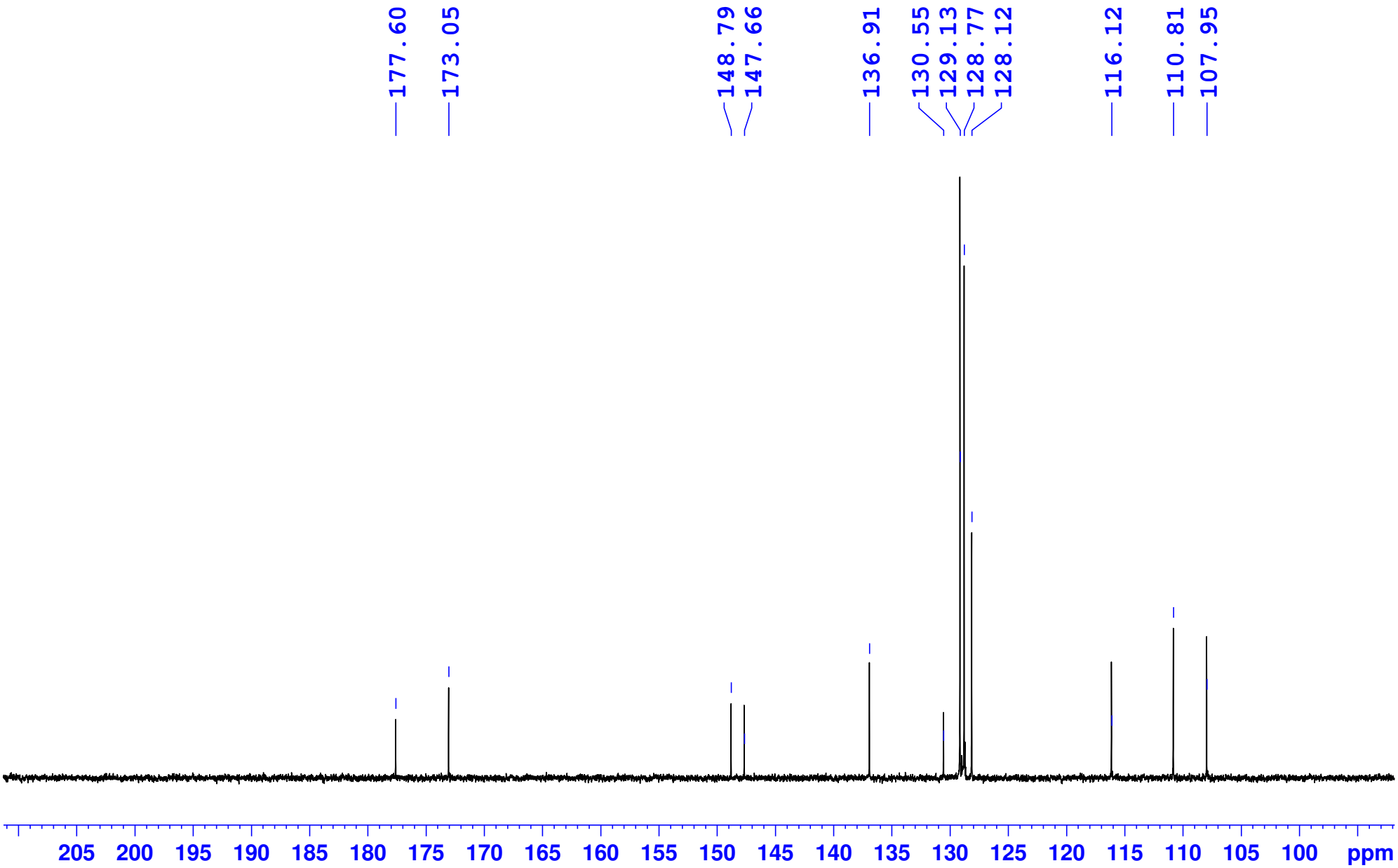

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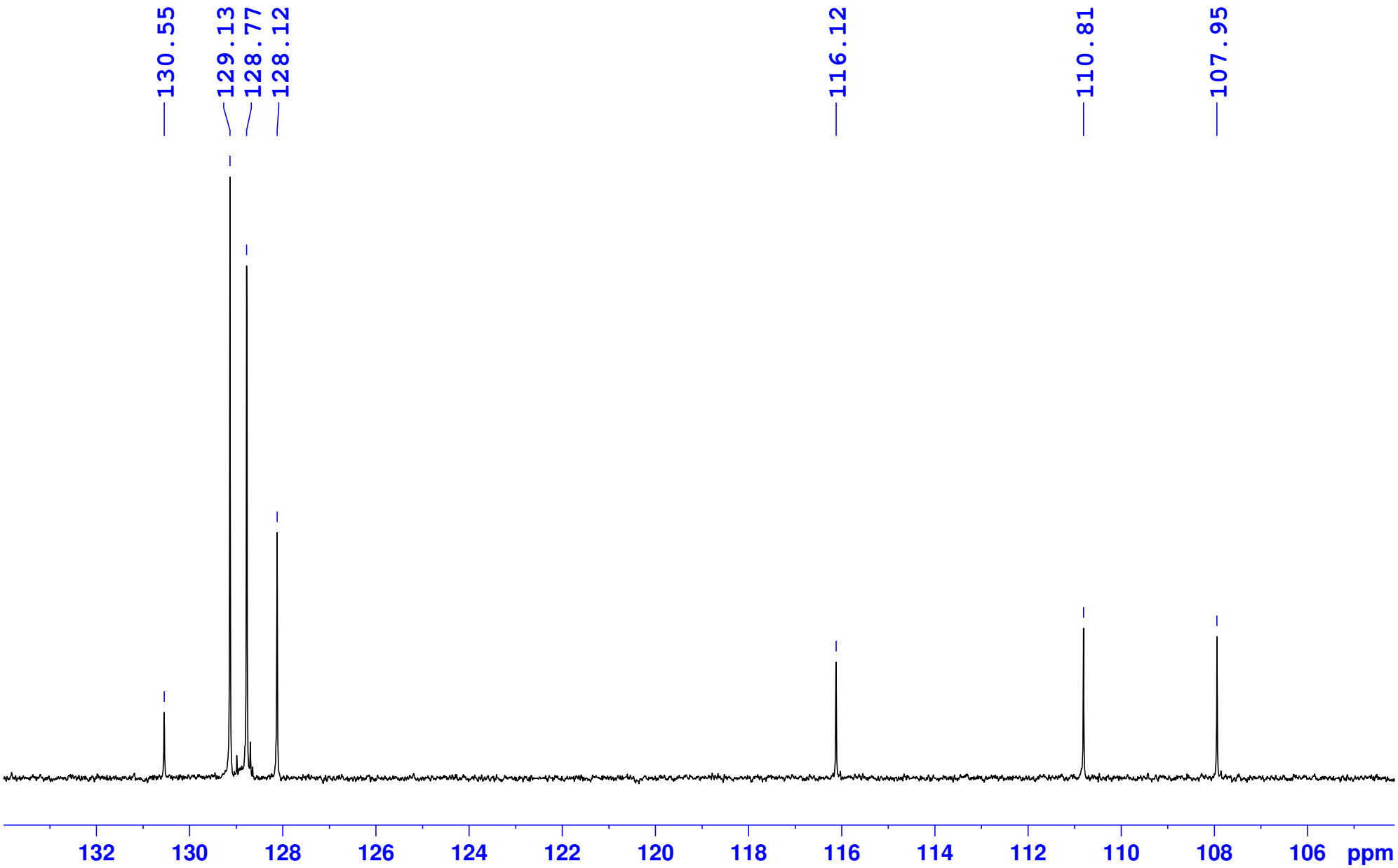

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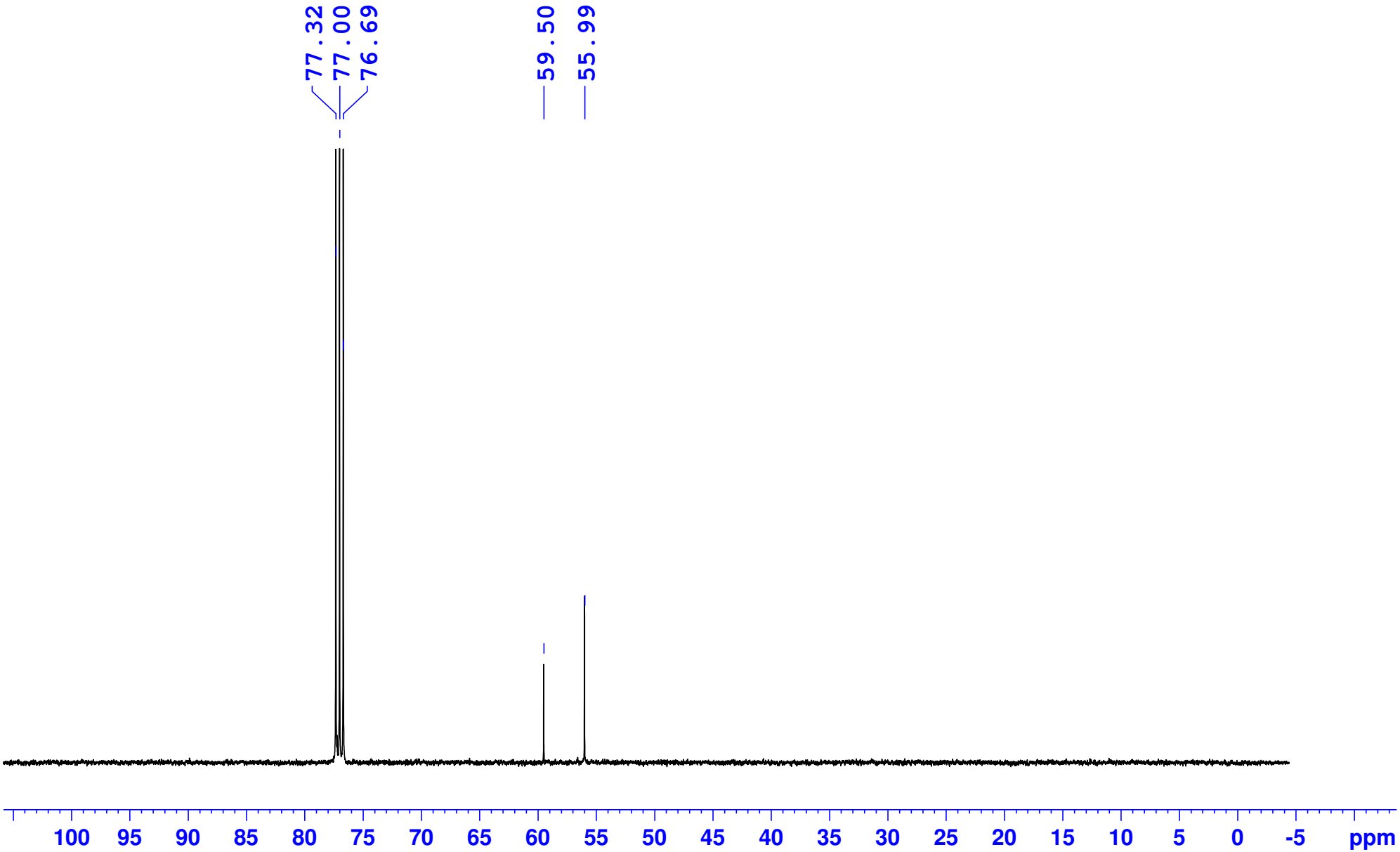

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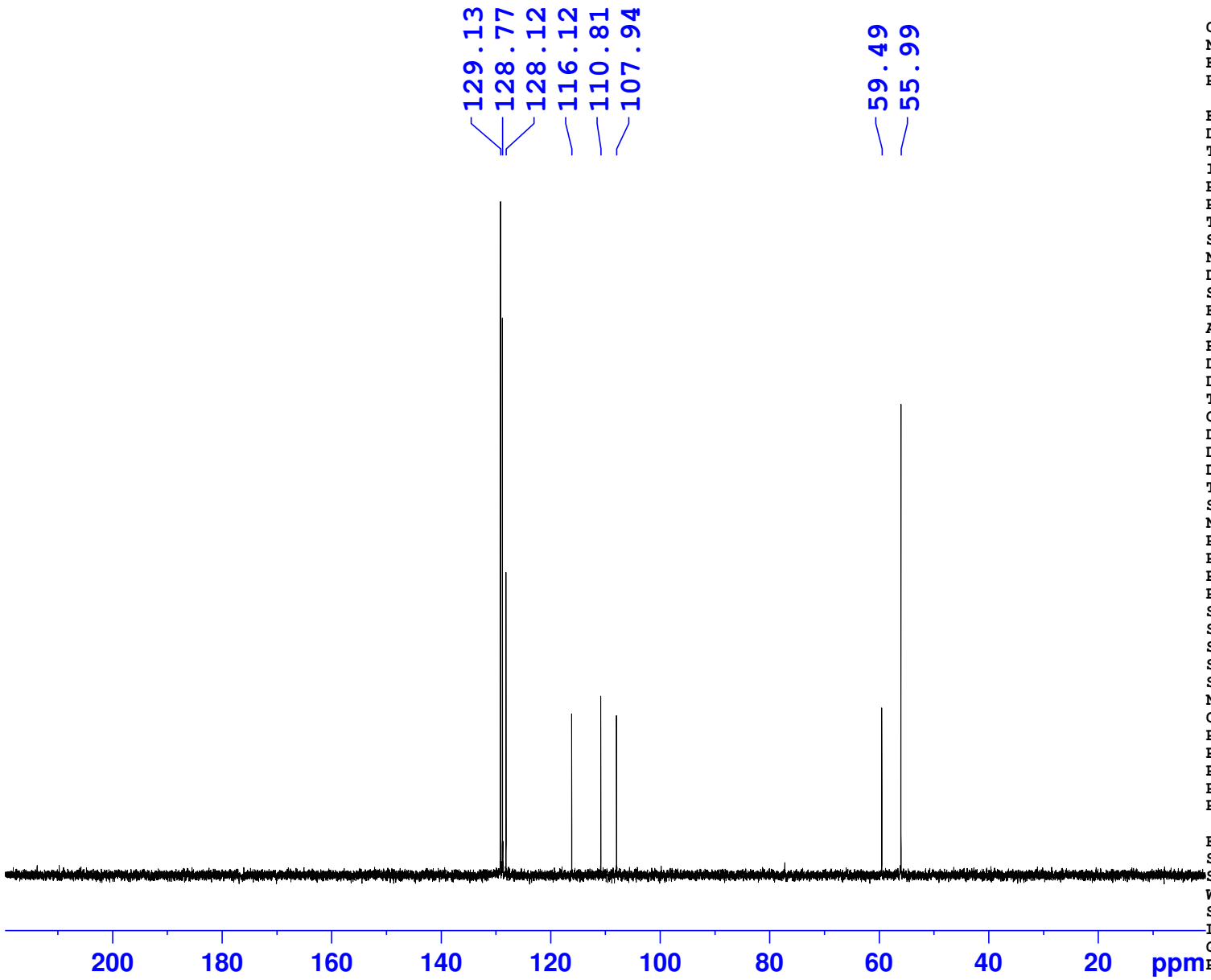


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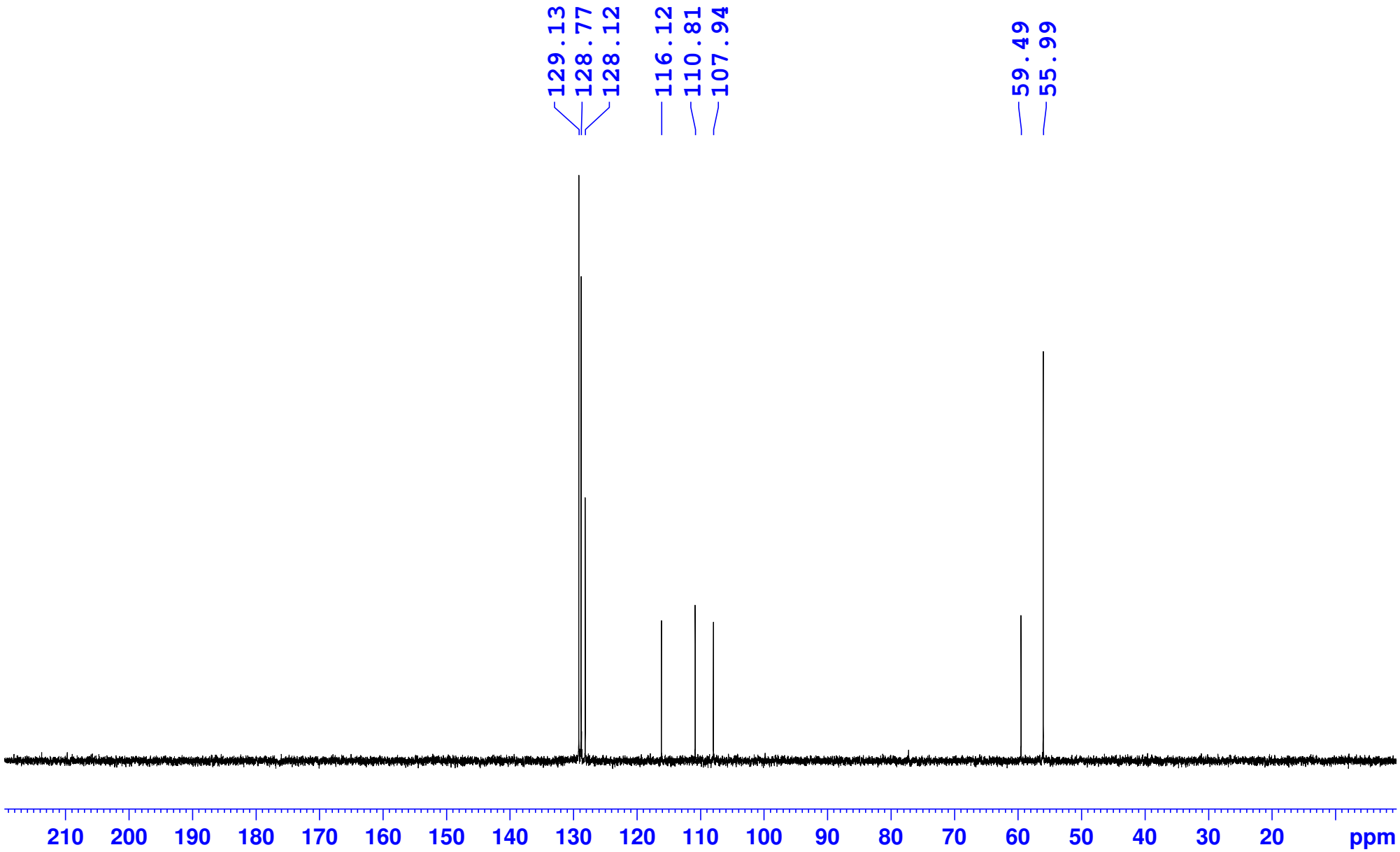

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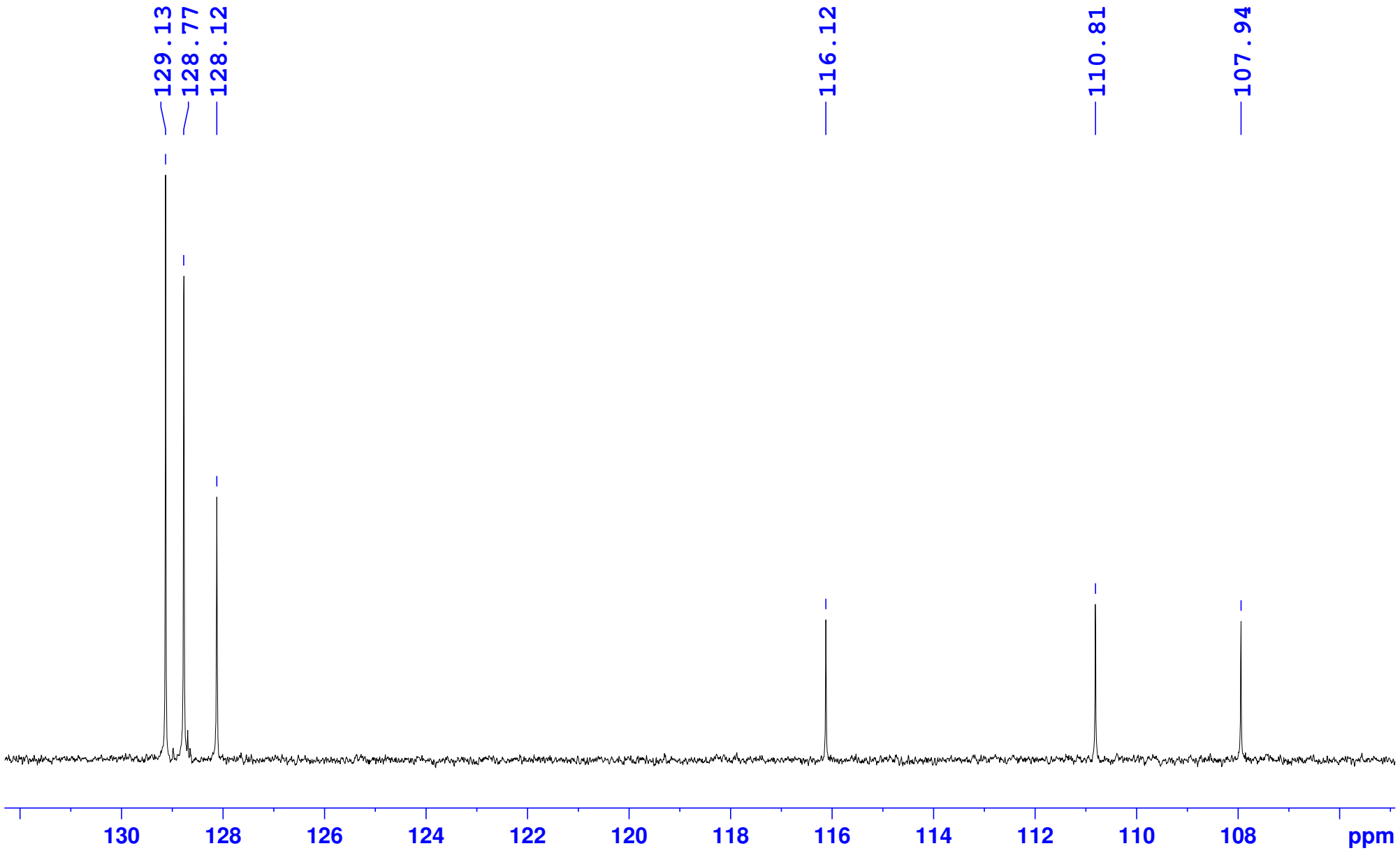

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