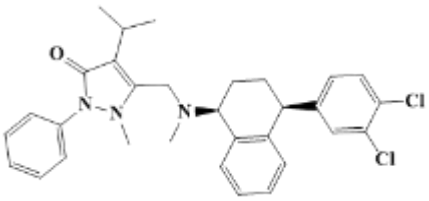
Supplementary data



Sertraline – methyl-propyphenazone (SER-MP)

Purification

The compound was purified by column chromatography over silica gel, mobile phase dichloromethane (DCM), and then 9:1 DCM/ethyl acetate. The obtained purity, as an oily substance, reached 98.8%, as determined by HPLC-DAD at 254 nm.

High-Resolution Mass of SER-MP

Instrument

Thermo Scientific LTQ-XL Orbitrap mass spectrometer coupled with Accela autosampler and Accela pump (San Jose, CA, USA). The ion source; electrospray ionization (ESI) compartment. The system was controlled with Xcalibur® Thermo Fisher Scientific Inc, version 2.07 SP1. Spray voltage, 5.0 kv, sheath gas flow rate, 42 mL/min, auxiliary gas, 5 mL/min, capillary voltage, 60v, capillary temperature, 335 °C, scan range, 100 - 700 m/z. The collision energy was 35 v. Column, Eclipse Plus C18, 3.5 µm, 4.6X100 mm (Agilent, Palo Alto, USA), column oven, 25 °C. The mobile system comprised acetonitrile (90%), water containing 0.1% glacial acetic acid 100% (10%). The flow rate was 400 µL/min. A positive ESI-MS mode was applied.

Result

The delta mass = +*m/z* 534.20789- 534.20038 = *m/z* 0.00751

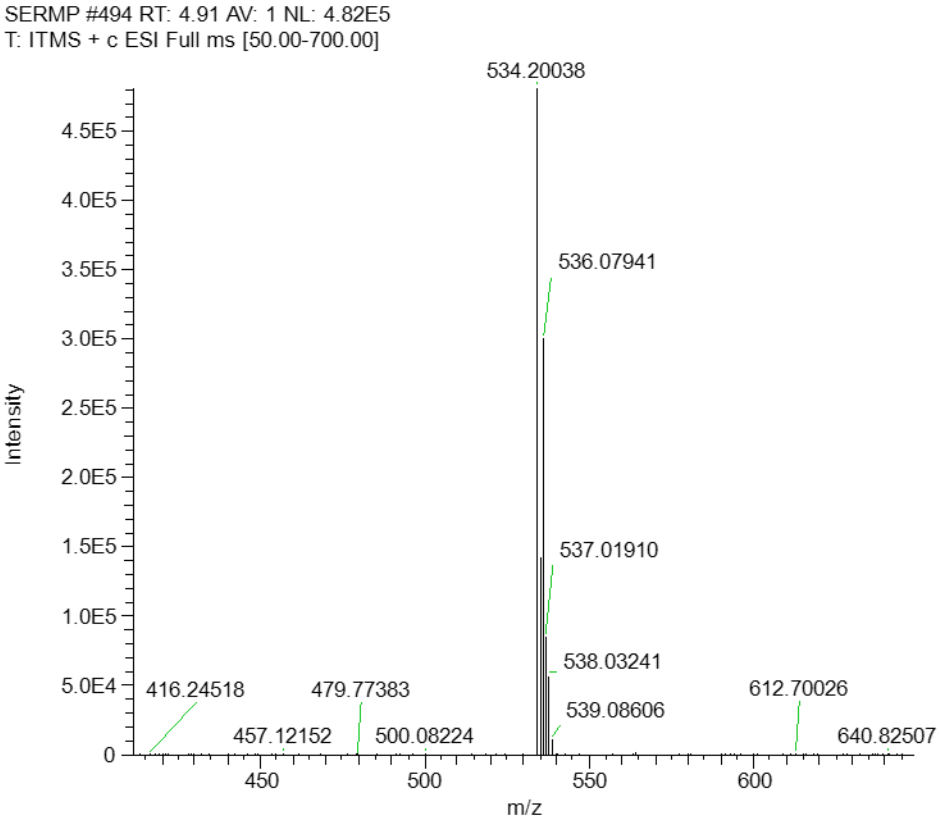


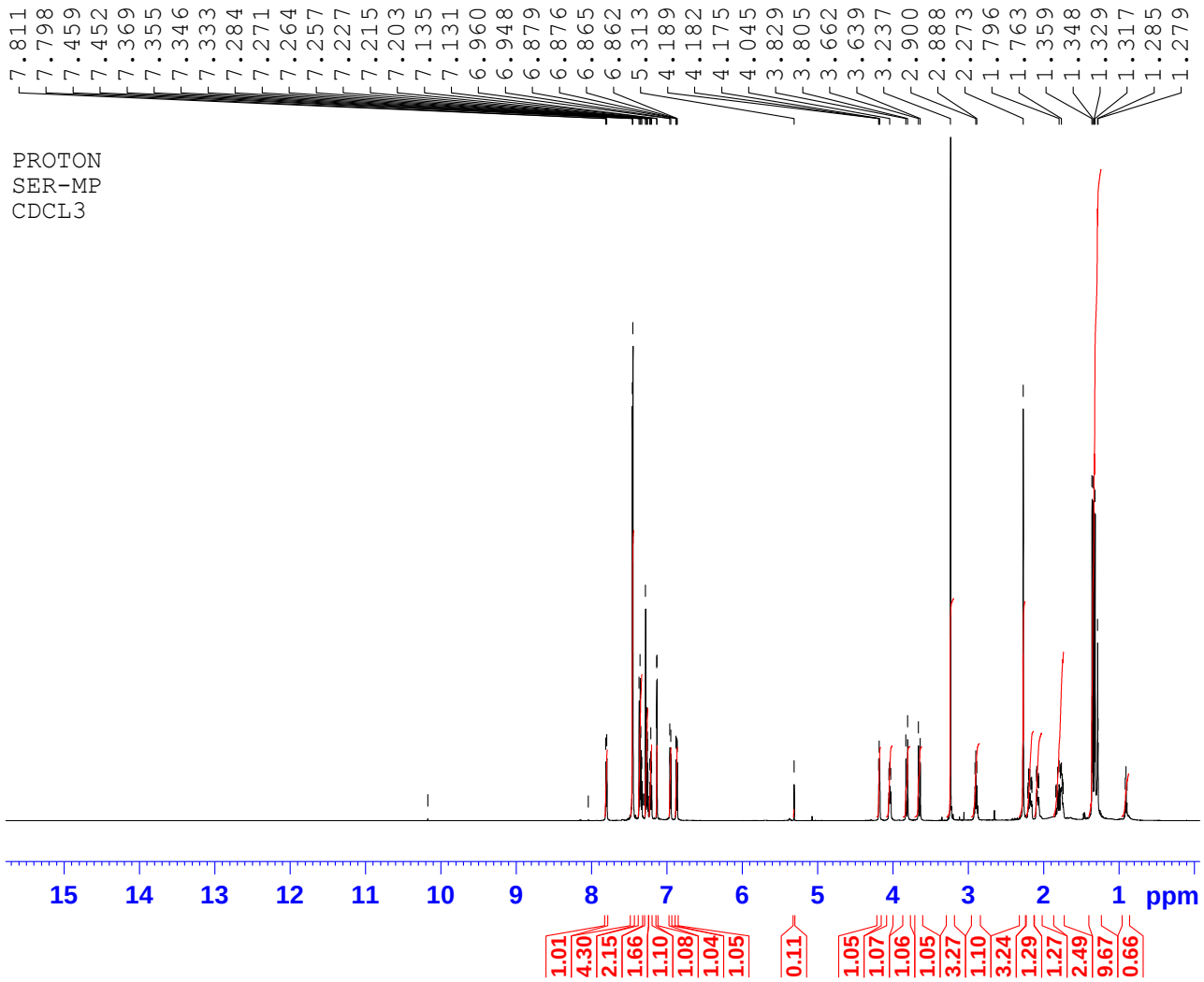
Fig. S1. Mass spectrum of SER-MP

^{1}H-NMR & ^{13}C-NMR analysis

The 1H-NMR and 13C-NMR analysis was repeated using Nuclear Magnetic Resonance, Ultra Shield 600, Bruker, Billerica, Massachusetts, United States.
The 600 MHz NMR data was added (Fig. S2 & Fig. S3).
Adjusted paragraph:
^{1}H NMR (600 MHz, CDCl3) δ 7.81 (d, J = 7.8 Hz, 1H), 7.49 – 7.43 (m, 4H), 7.38 – 7.32 (m, 2H), 7.27 – 7.24 (m, 1H), 7.22 (t, J = 7.2 Hz, 1H), 7.13 (d, J = 6.8 Hz, 1H), 6.95 (d, J = 7.2 Hz, 1H), 6.87 (dd, J = 6.6, 8.4 Hz, 1H), 4.18 (t, J = 4.2 Hz, 1H), 4.09 – 4.01 (m, 1H), 3.82 (d, J = 14.4 Hz, 1H), 3.65 (d, J = 13.8 Hz, 1H), 3.24 (s, 3H), 2.90 (t, J = 7.2 Hz, 1H), 2.27 (s, 3H), 2.32 – 2.31 (m, 1H), 2.30 – 2.22 (m, 1H), 1.86 – 1.73 (m, 2H), 1.35 (d, J = 6.6 Hz, 3H), 1.32 (d, J = 7.2 Hz, 3H) (Fig. S2).

^{13}C NMR (150 MHz, CDCl3) δ 165.39, 152.18, 147.44, 138.82, 138.50, 135.52, 129.19, 128.37, 128.32, 127.40, 126.21, 123.70, 118.22, 60.25, 48.32, 43.76, 37.01, 36.36, 30.18, 29.92, 24.75, 21.44, 21.41, 15.46 (Fig. S3).

Fig. S2. ^{1}H NMR spectrum of SER-MP in CDCl3



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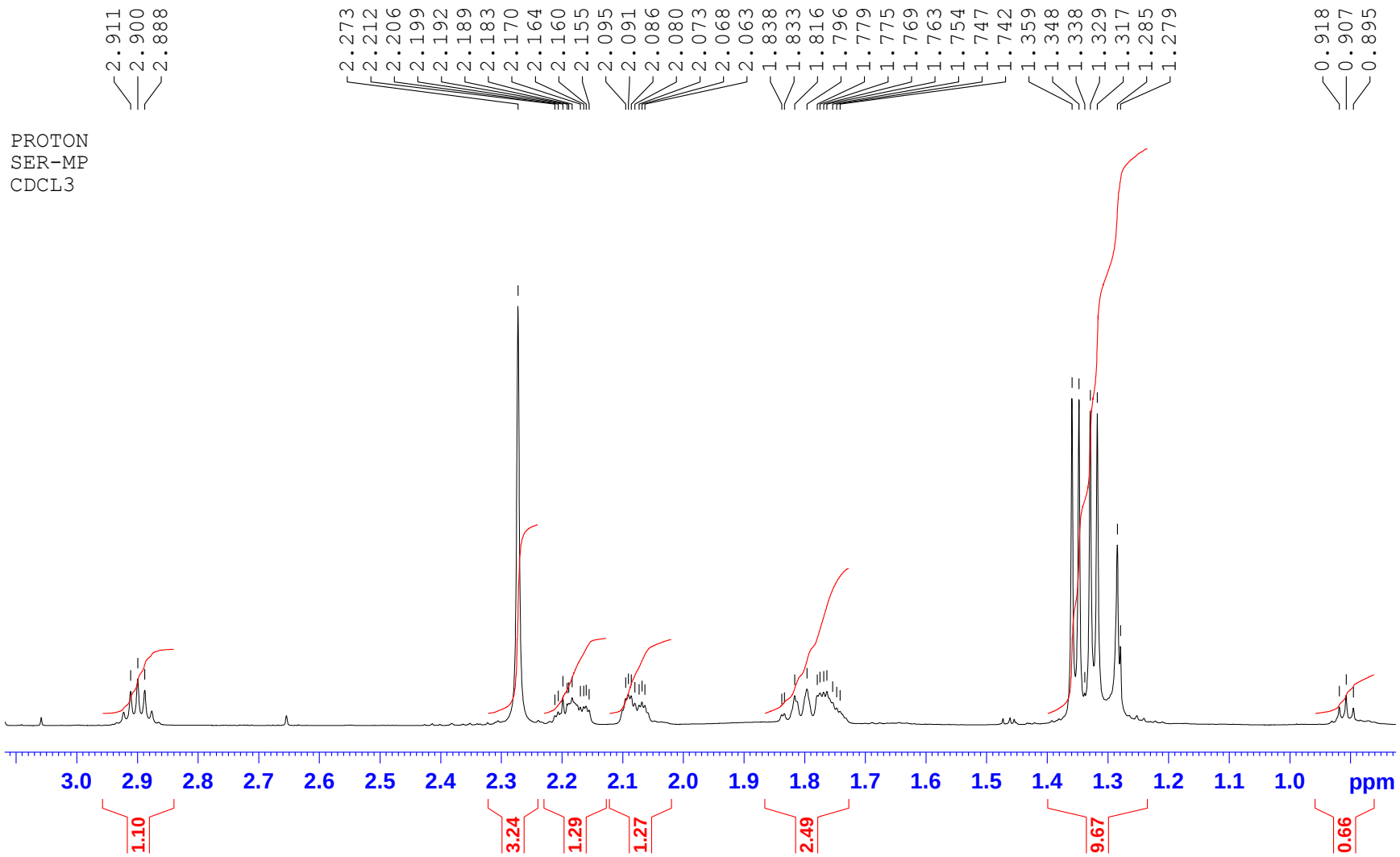
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1.775
1.769
1.763
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1.747
1.742
1.359
1.348
1.338
1.329
1.317
1.285
1.279
0.918
0.907
0.895
PROTON
SER-MP
CDCL3
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2.9
2.8
2.7
2.6
2.5
2.4
2.3
2.2
2.1
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1.7
1.6
1.5
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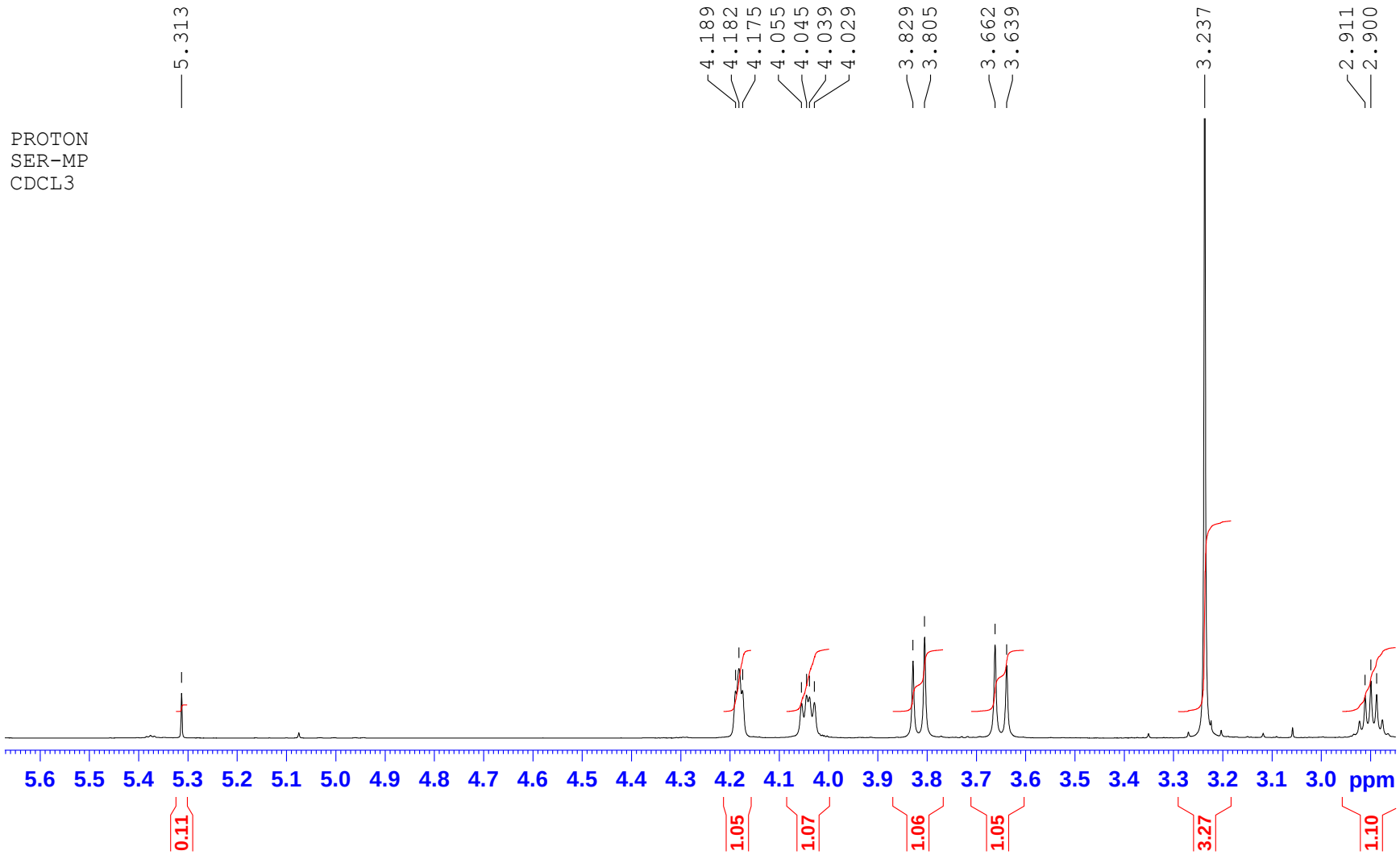
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3.237
2.911
2.900
PROTON
SER-MP
CDCL3
5.6 5.5 5.4 5.3 5.2 5.1 5.0 4.9 4.8 4.7 4.6 4.5 4.4 4.3 4.2 4.1 4.0 3.9 3.8 3.7 3.6 3.5 3.4 3.3 3.2 3.1 3.0 ppm
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1.07
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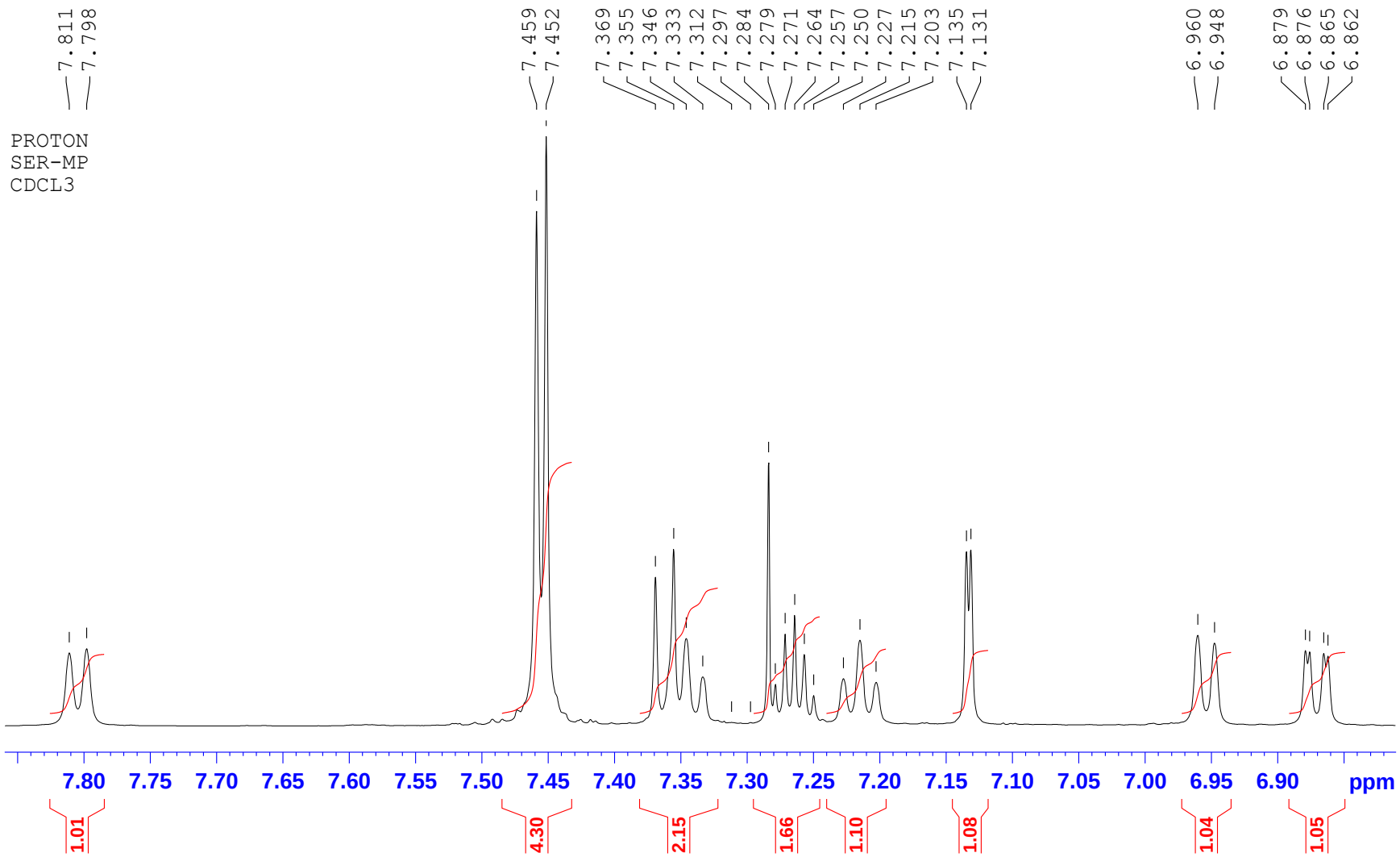
1.10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7.257
7.250
7.227
7.215
7.203
7.135
7.131
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6.876
6.865
6.862
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7.10
7.05
7.00
6.95
6.90
ppm
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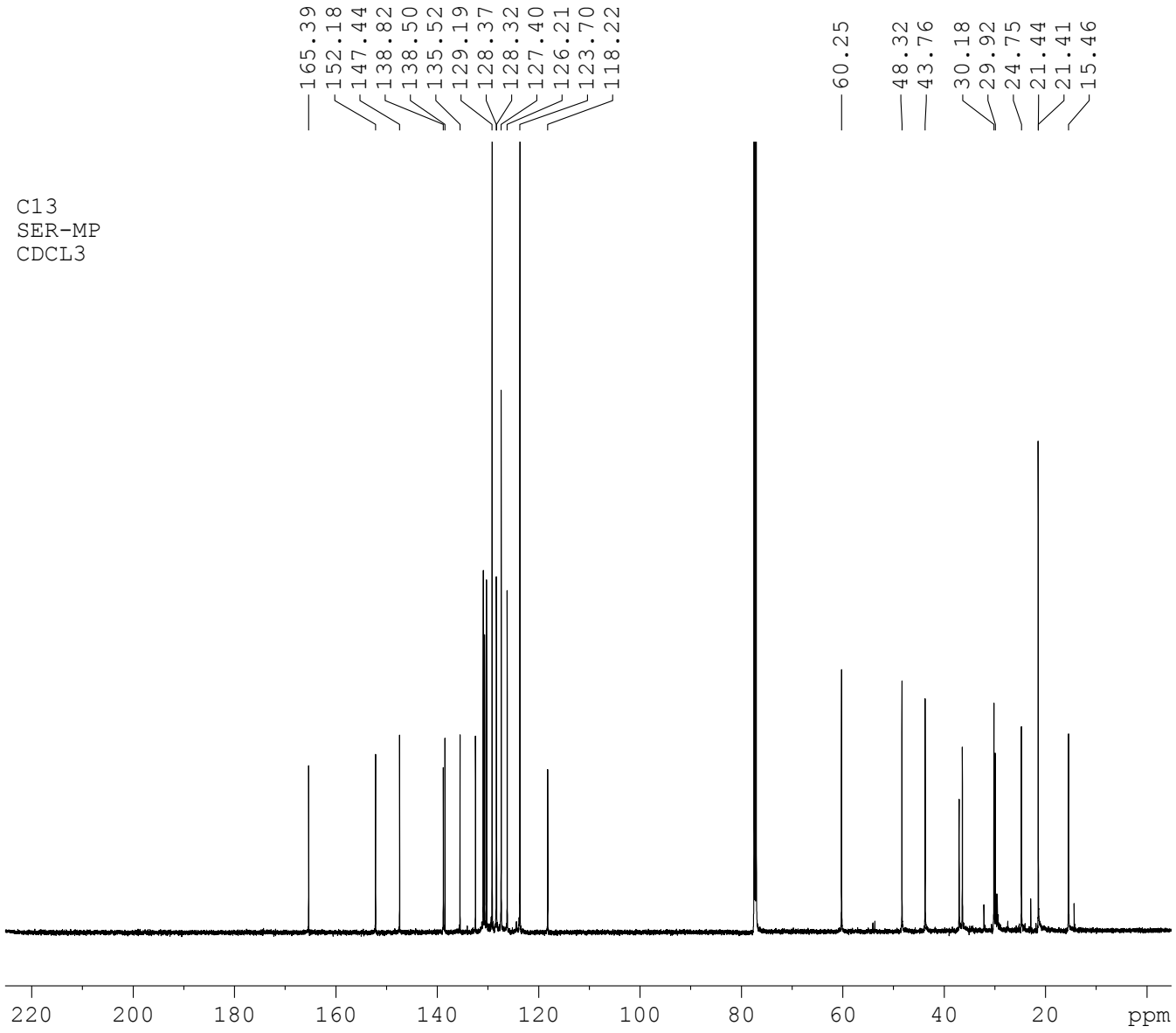
1.10
1.08
1.04
1.05

.Fig. S3. ^{13}C NMR spectrum of SER-MP in CDCl3



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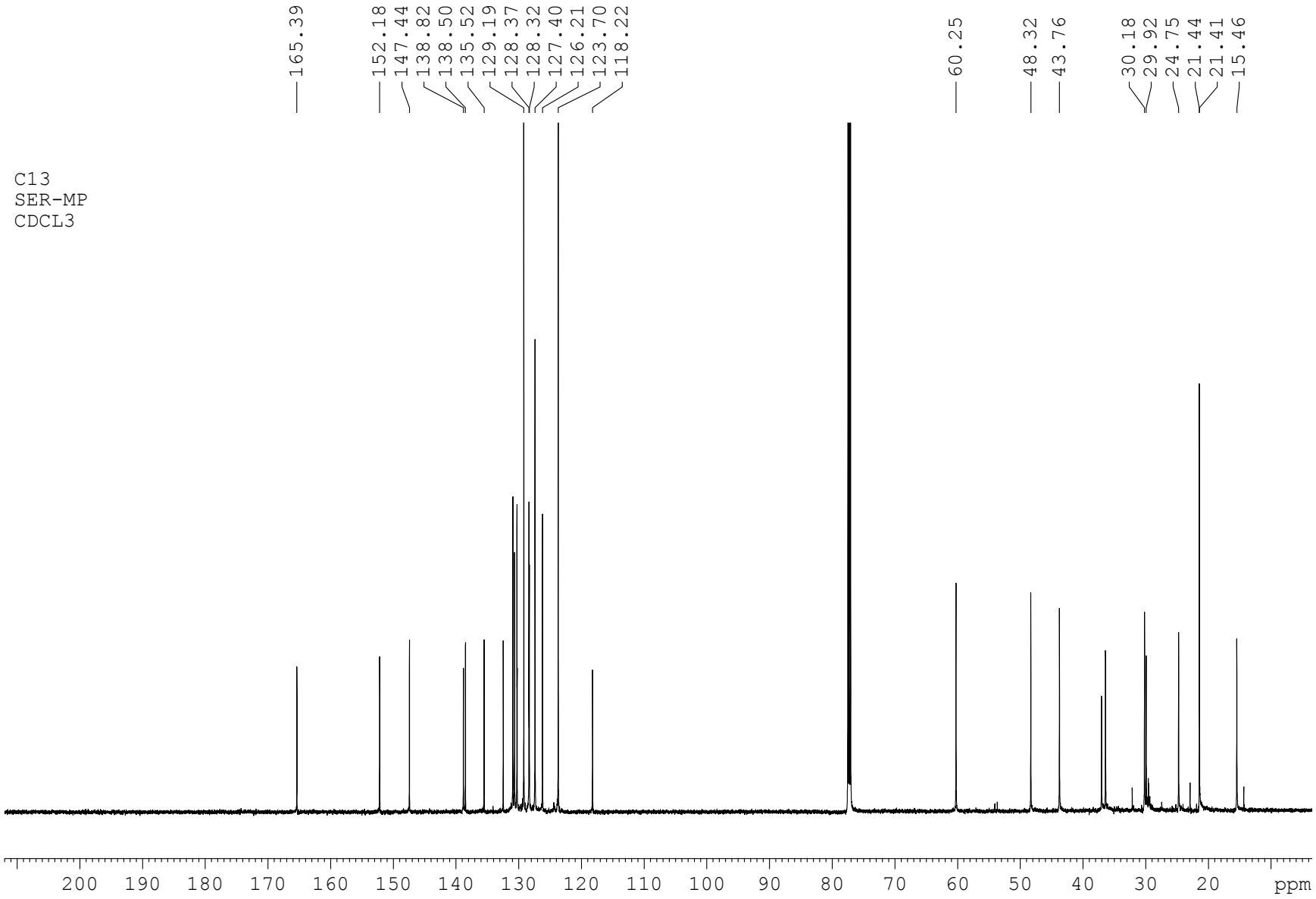
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43.76
30.18
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C13
SER-MP
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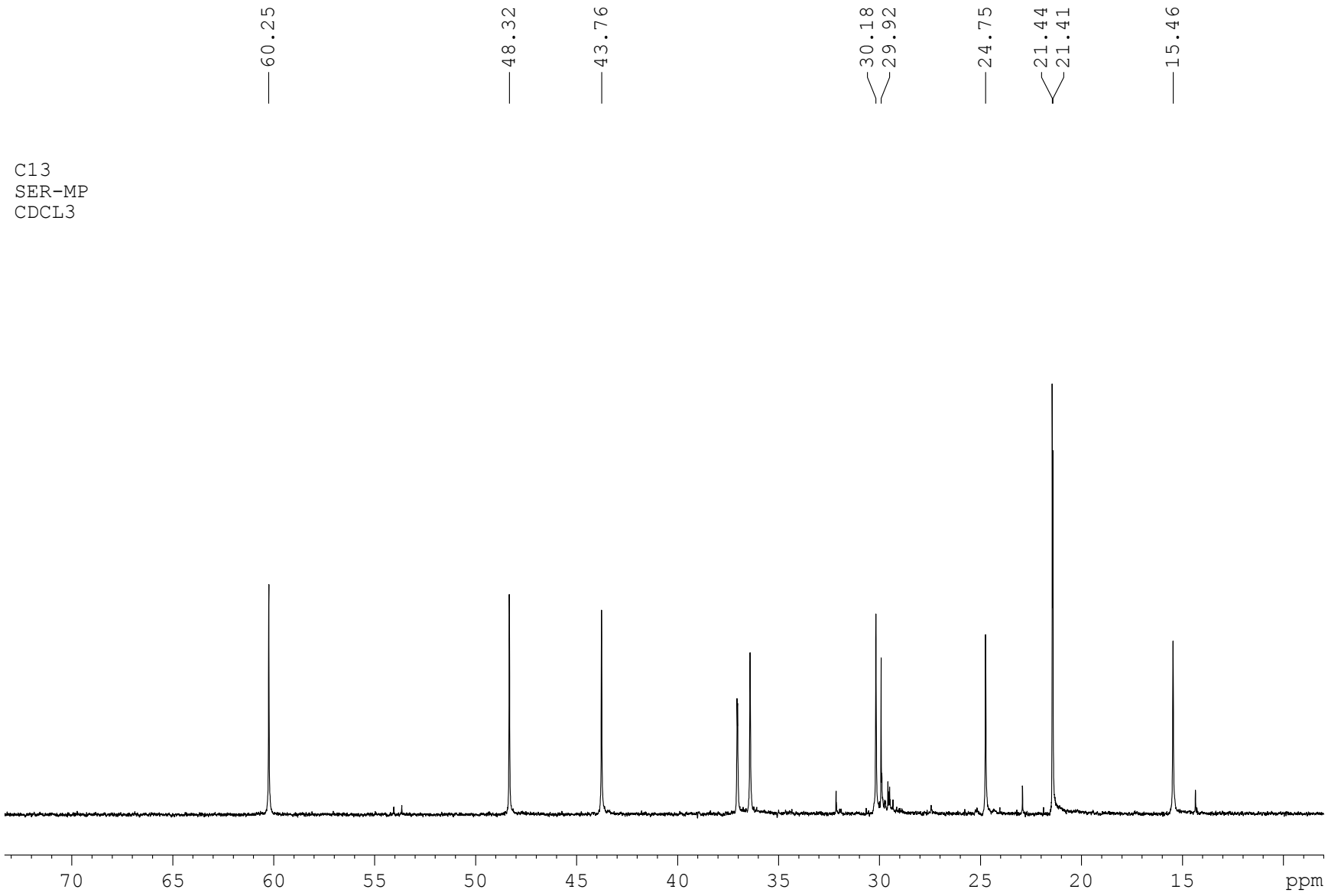
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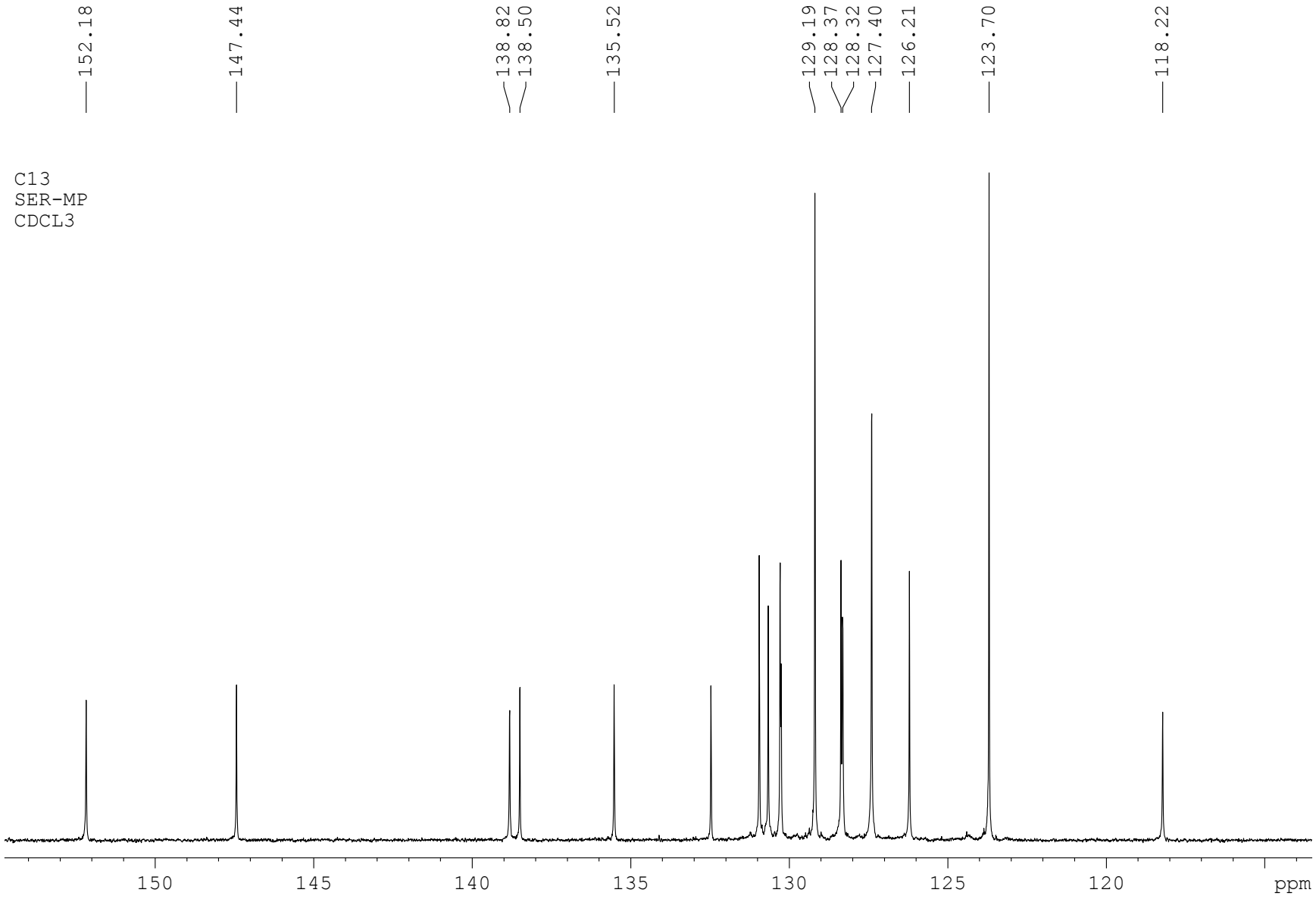
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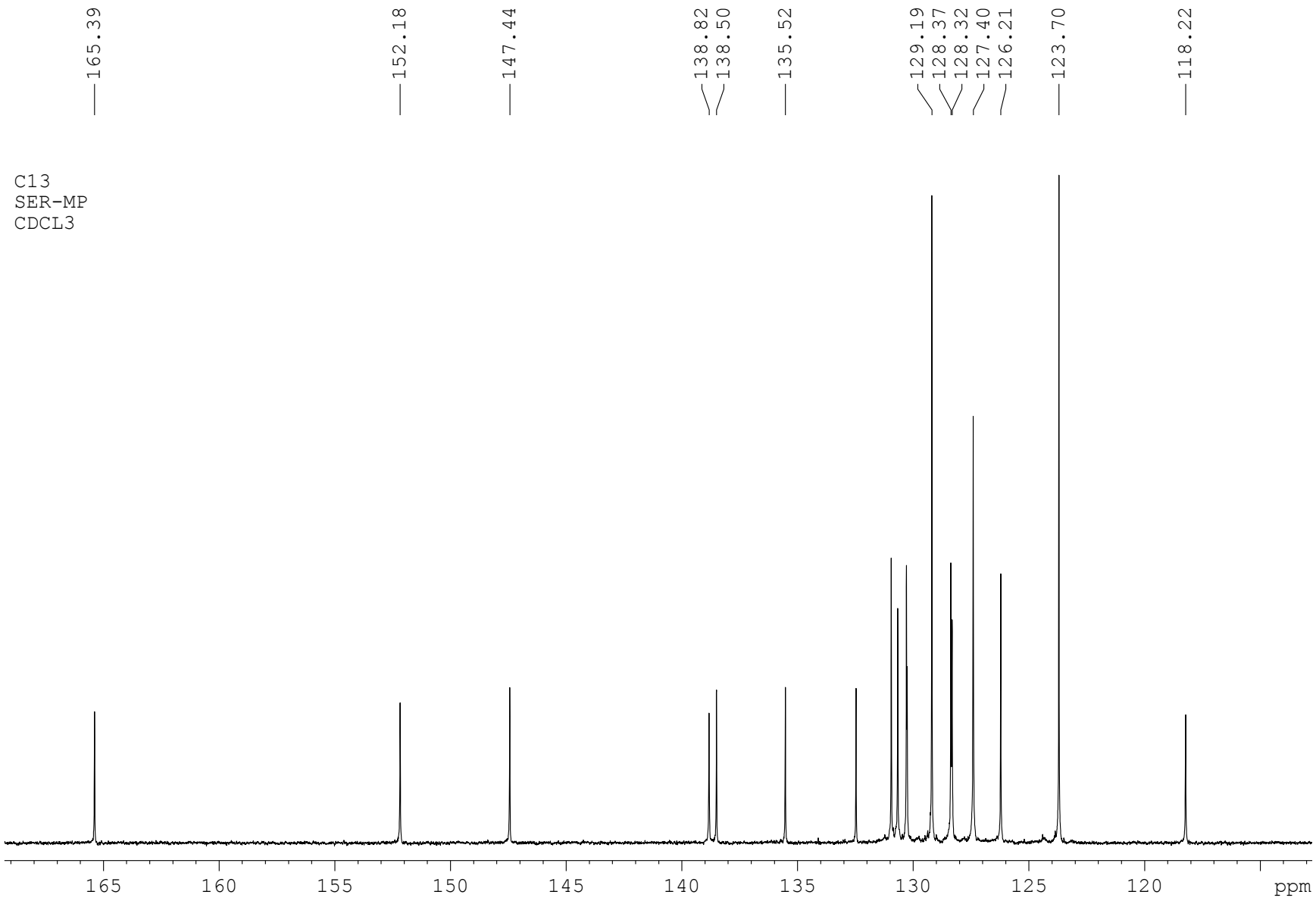
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