

Supplemental Information B

Pharmacophore-based Discovery of 2-(Phenylamino)Aceto-Hydrazides as Potent Eosinophil Peroxidase (EPO) Inhibitors

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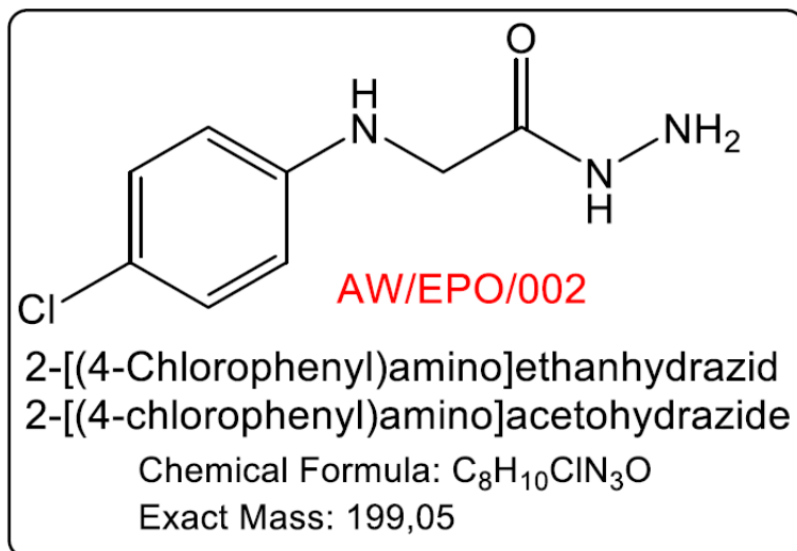
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Andreas Kubin, Planta Naturstoffe, Erlgasse 48, A-1120 Vienna, Austria, email: a.kubin@planta.at

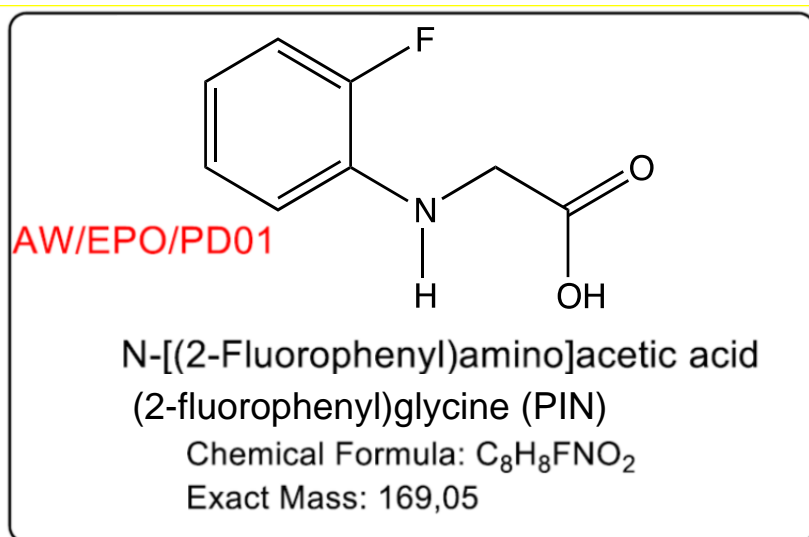
NMR and MS Analysis of the Lead Substances

MS analysis: MS spectra were redorded on a Bruker maXis HD™, ESI-qTOF

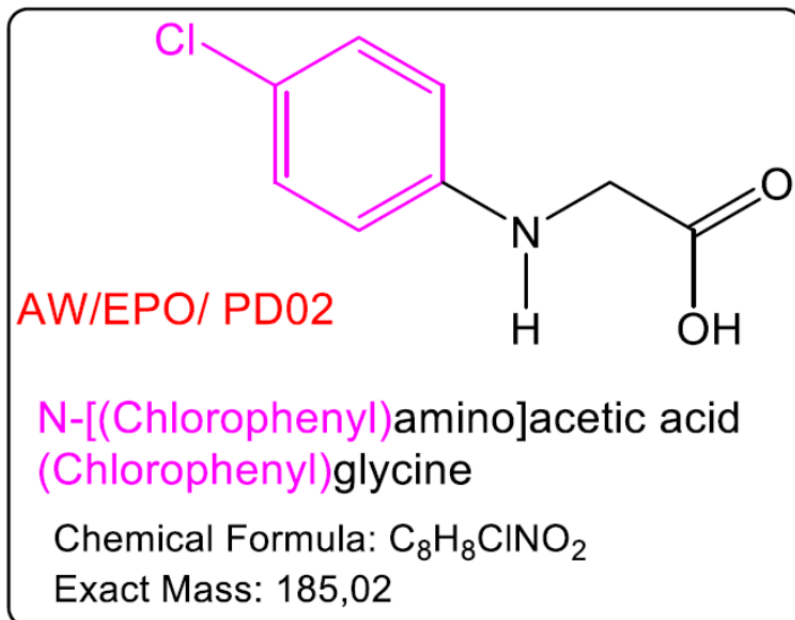
AW/EPO/002, 3.86 mg, 2-[(4-Chlorophenyl)amino]ethanhydrazid,
MS Analysis: MW = 199,60 g/mol



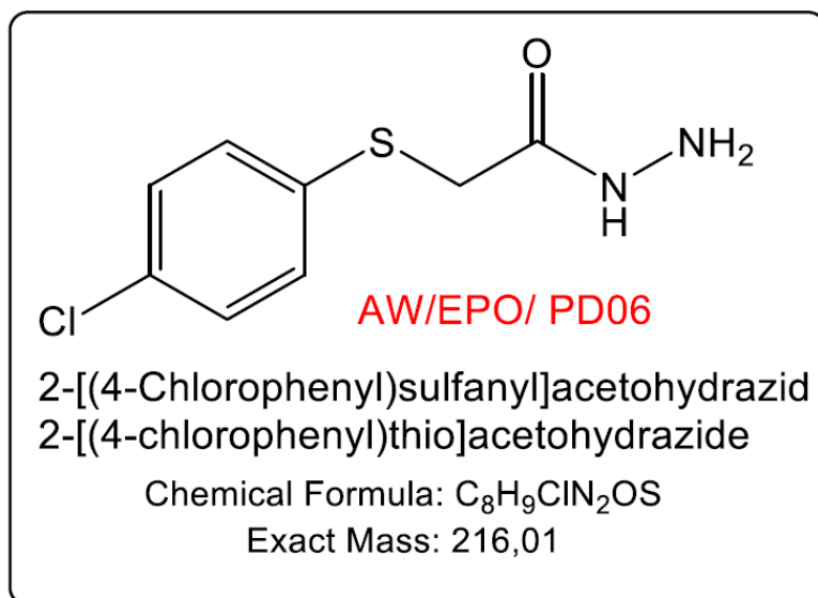
AW/EPO/PD01, 2,86 mg, N-[(2-Fluorophenyl)amino]acetic acid,
MS Analysis: MW = 191,2 g/mol



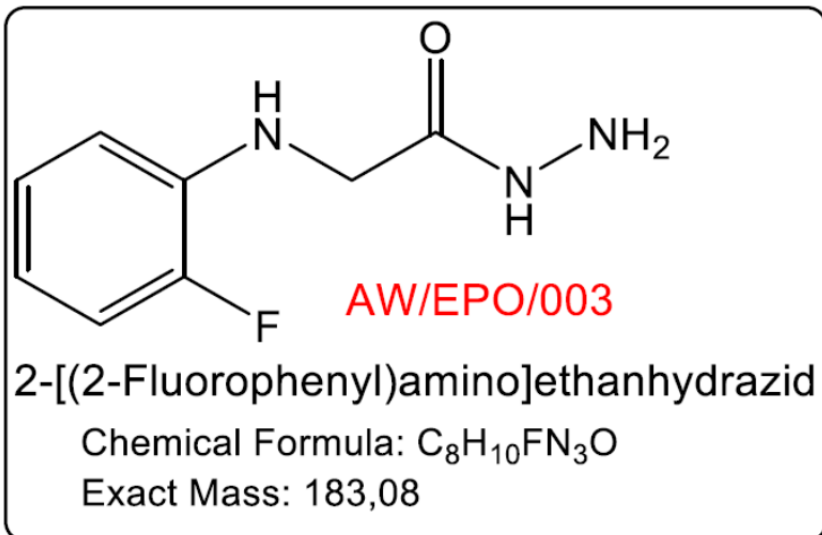
AW/EPO/ PD02, 4,62 mg, N-[(Chlorophenyl)amino]acetic acid,
MS Analysis: MW = 207,6 g/mol



AW/EPO/ PD06, 3.76 mg, 2-[(4-Chlorophenyl)sulfanyl]acetohydrazid,
MS Analysis: MW = 216,69 g/mol

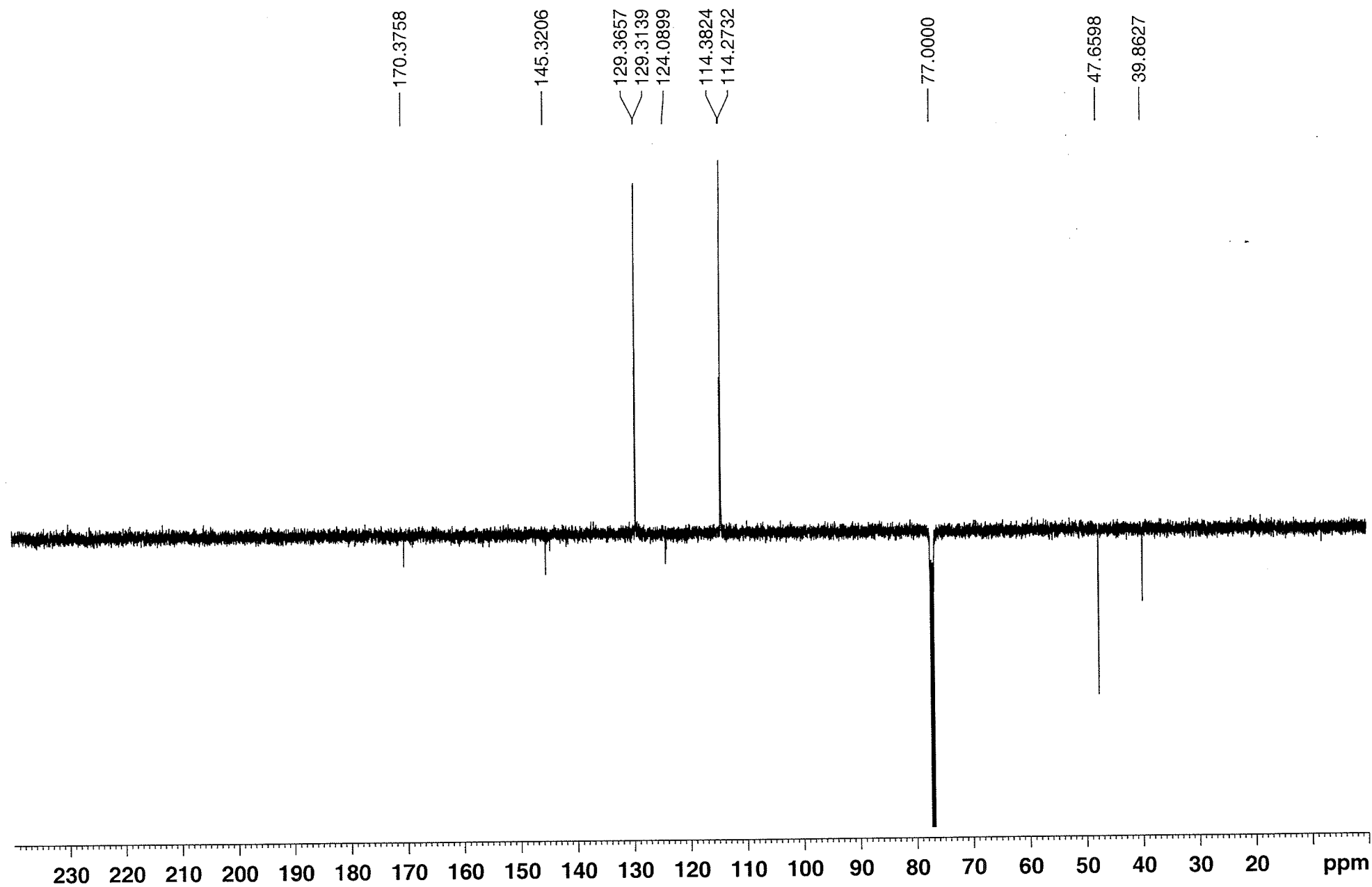


AW/EPO/003, 2,70 mg, 2-[(2-Fluorophenyl)amino]ethanhydrazid,
MS Analysis: MW = 183,19 g/mol

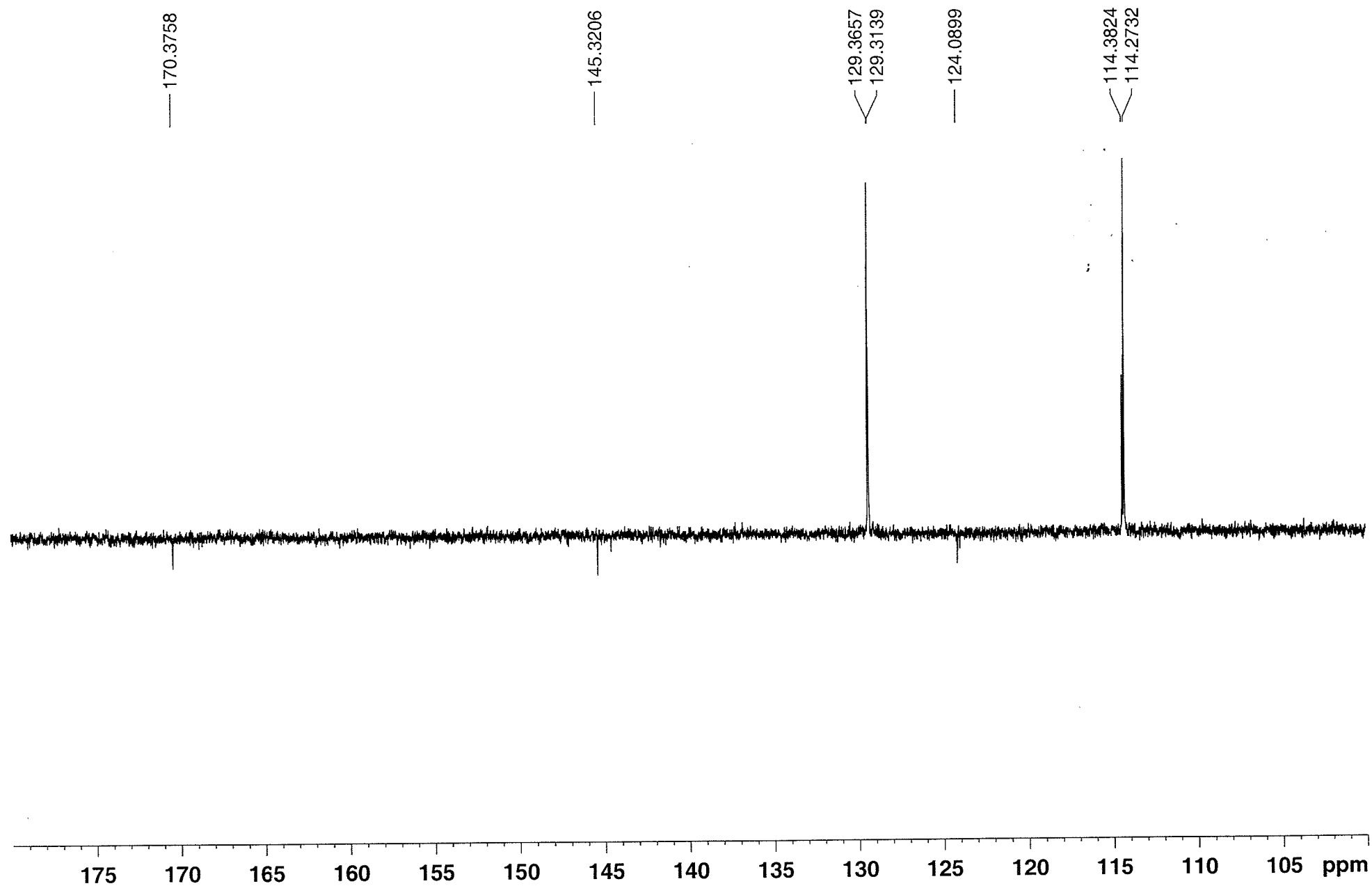


NMR analysis. NMR spectra were recorded on a Bruker Avance 500 NMR spectrometer (UltraShield) using a 5 mm switchable probe (TCI Prodigy Kryo-probe head, 5 mm, triple-resonance-invers-detection probe head) with z axis gradients and automatic tuning and matching accessory (Bruker BioSpin). The resonance frequency for ^1H NMR was 500.13 MHz and for ^{13}C NMR 125.75 MHz. All measurements were performed for a solution in fully deuterated chloroform or methanol at 298 K. Standard 1D and gradient-enhanced (ge) 2D experiments, like double quantum filtered (DQF) COSY, NOESY, HSQC, and HMBC, were used as supplied by the manufacturer. Chemical shifts are referenced internally to the residual, non-deuterated solvent signal for chloroform ^1H (δ 7.26 ppm) and to the carbon signal of the solvent for chloroform ^{13}C (δ 77.00 ppm).

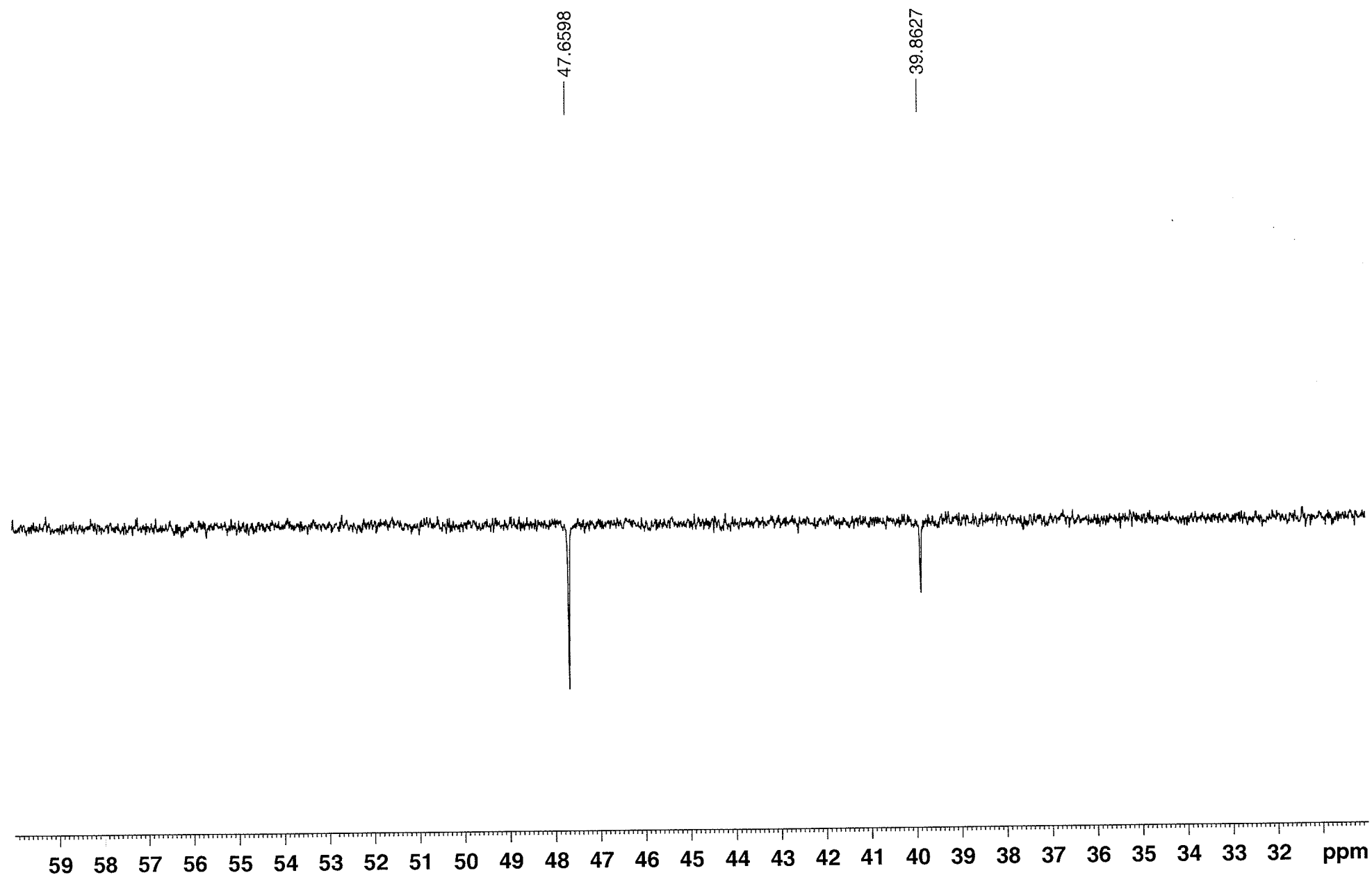
AWEPO002 in cdcl3 (APT) 2.11.2016

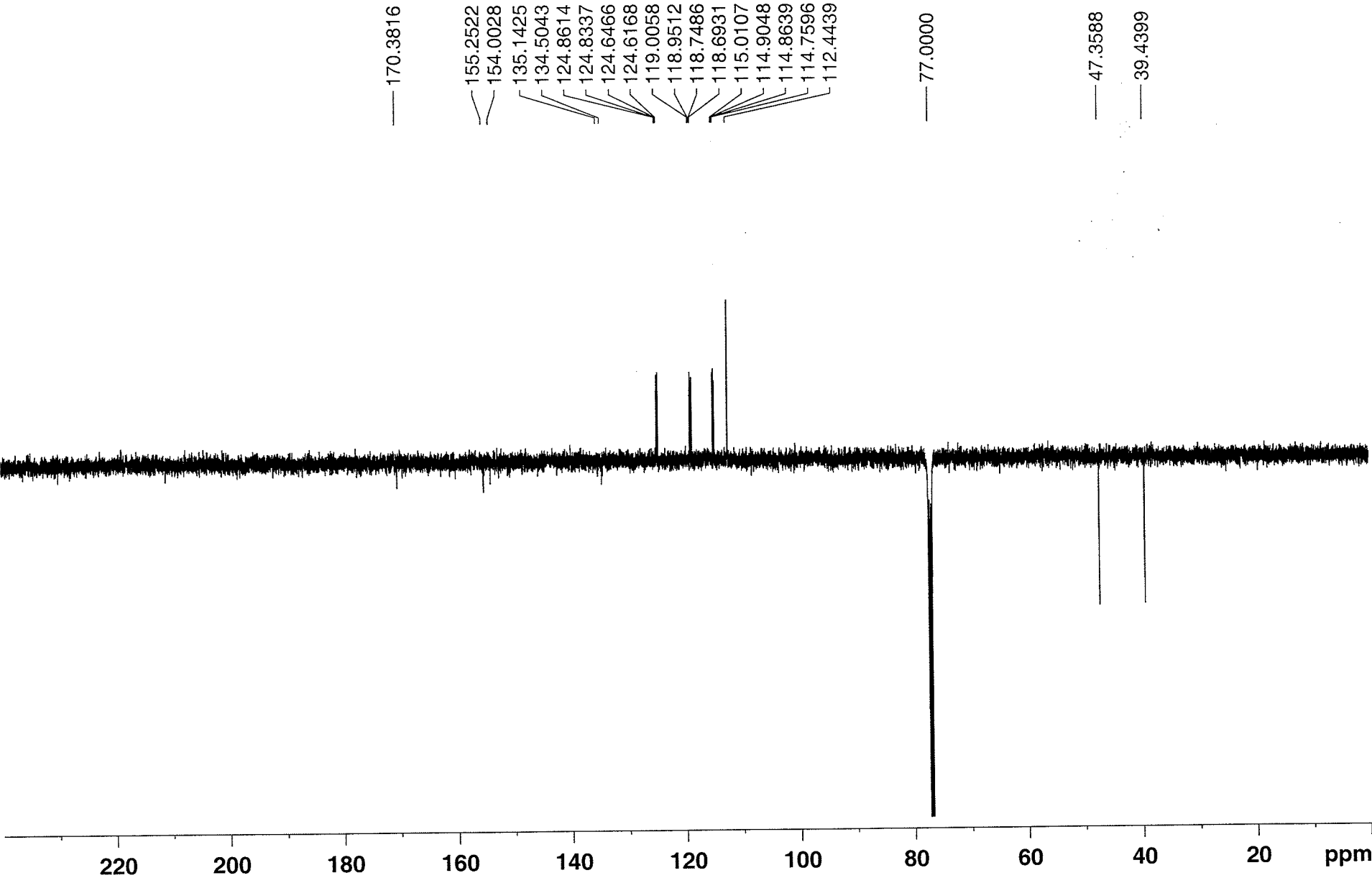


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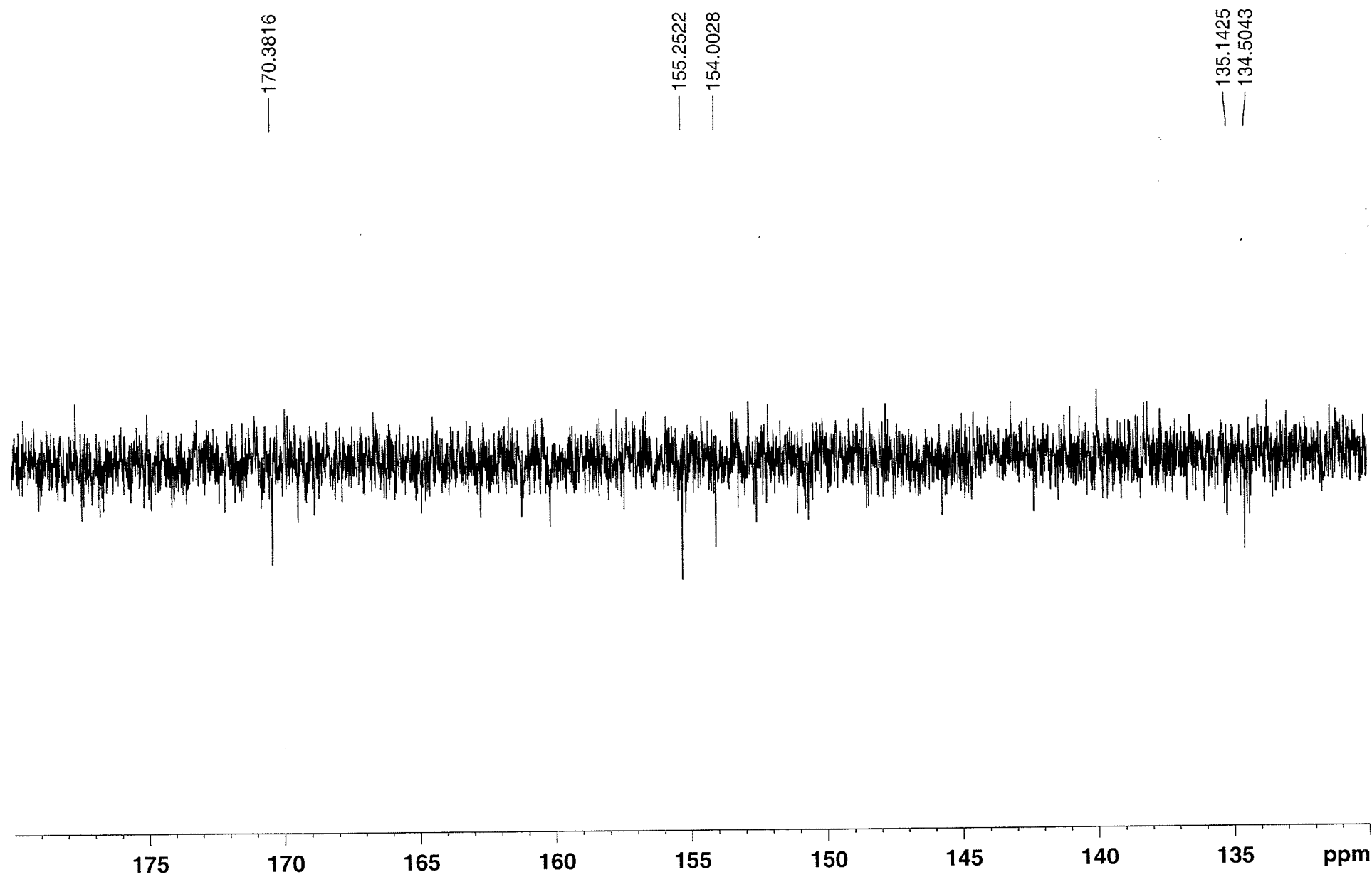


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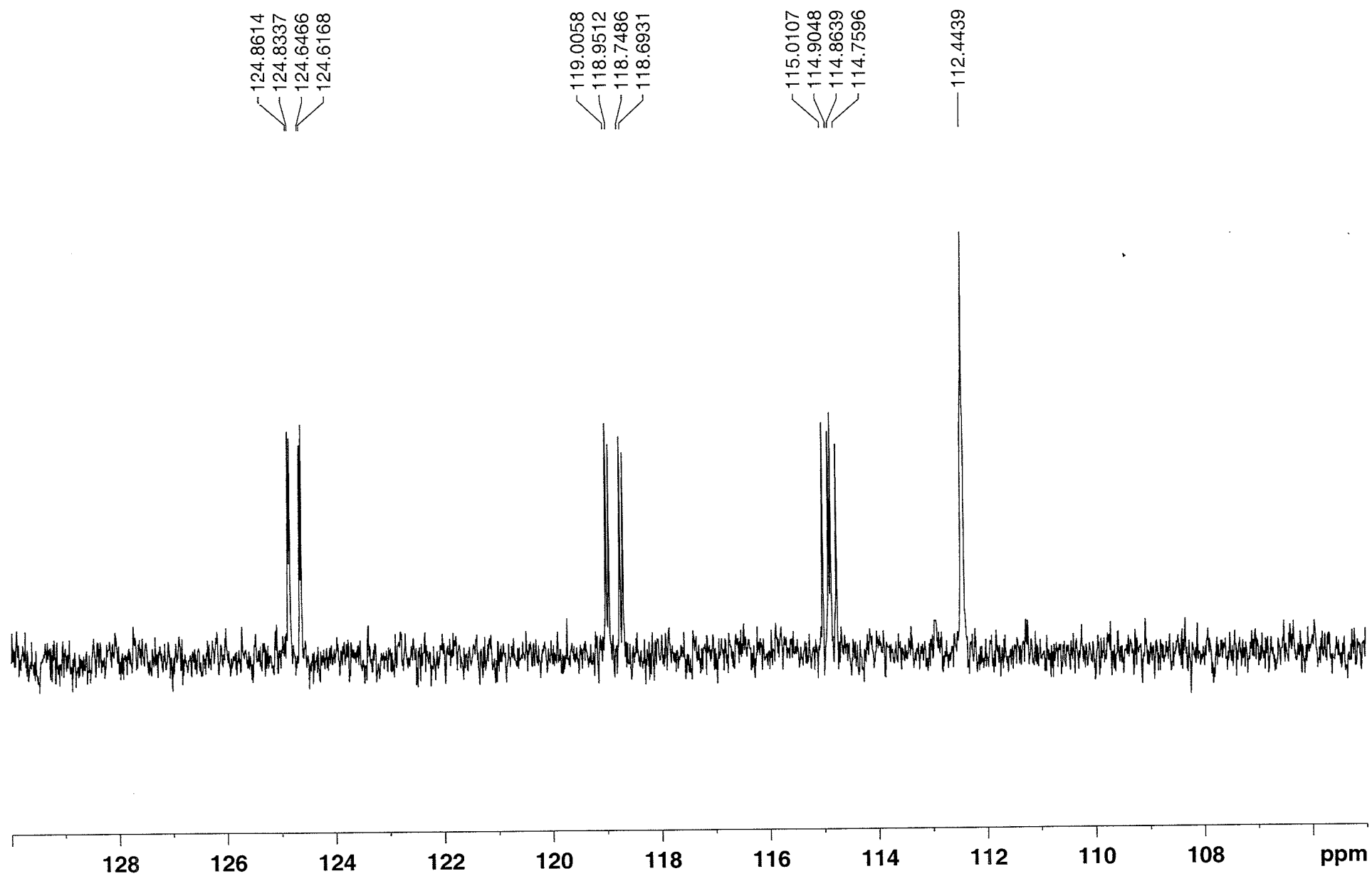




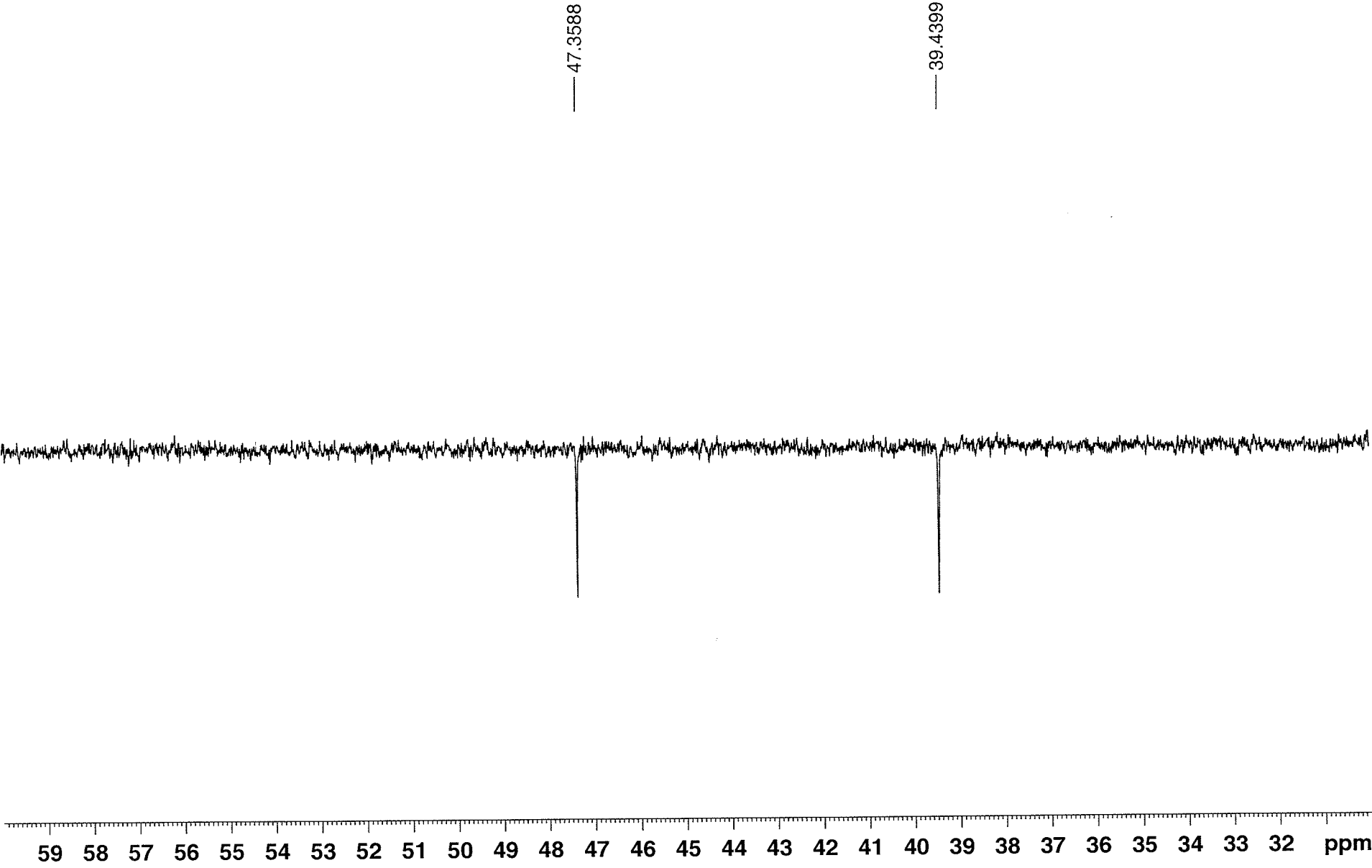
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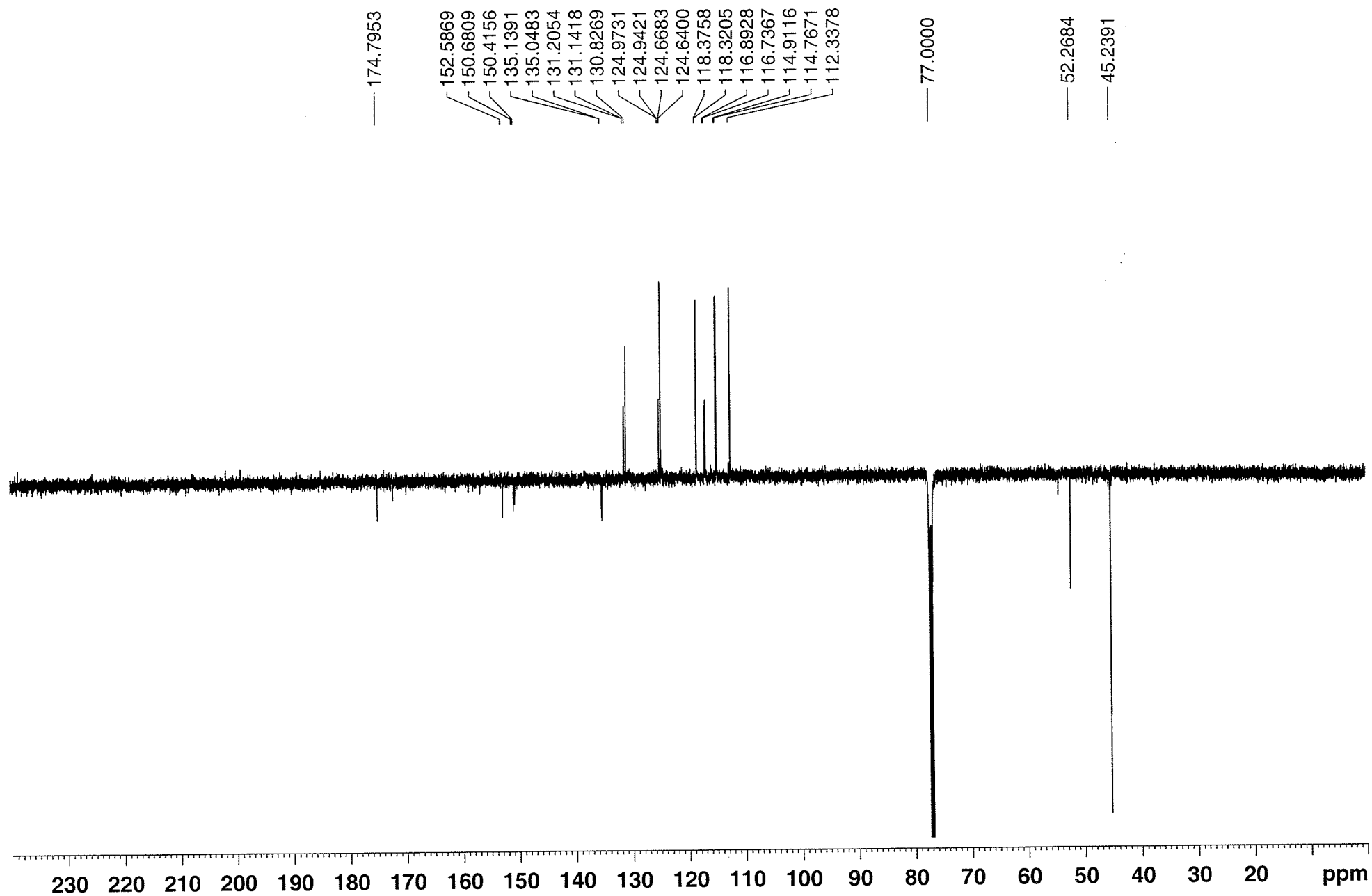
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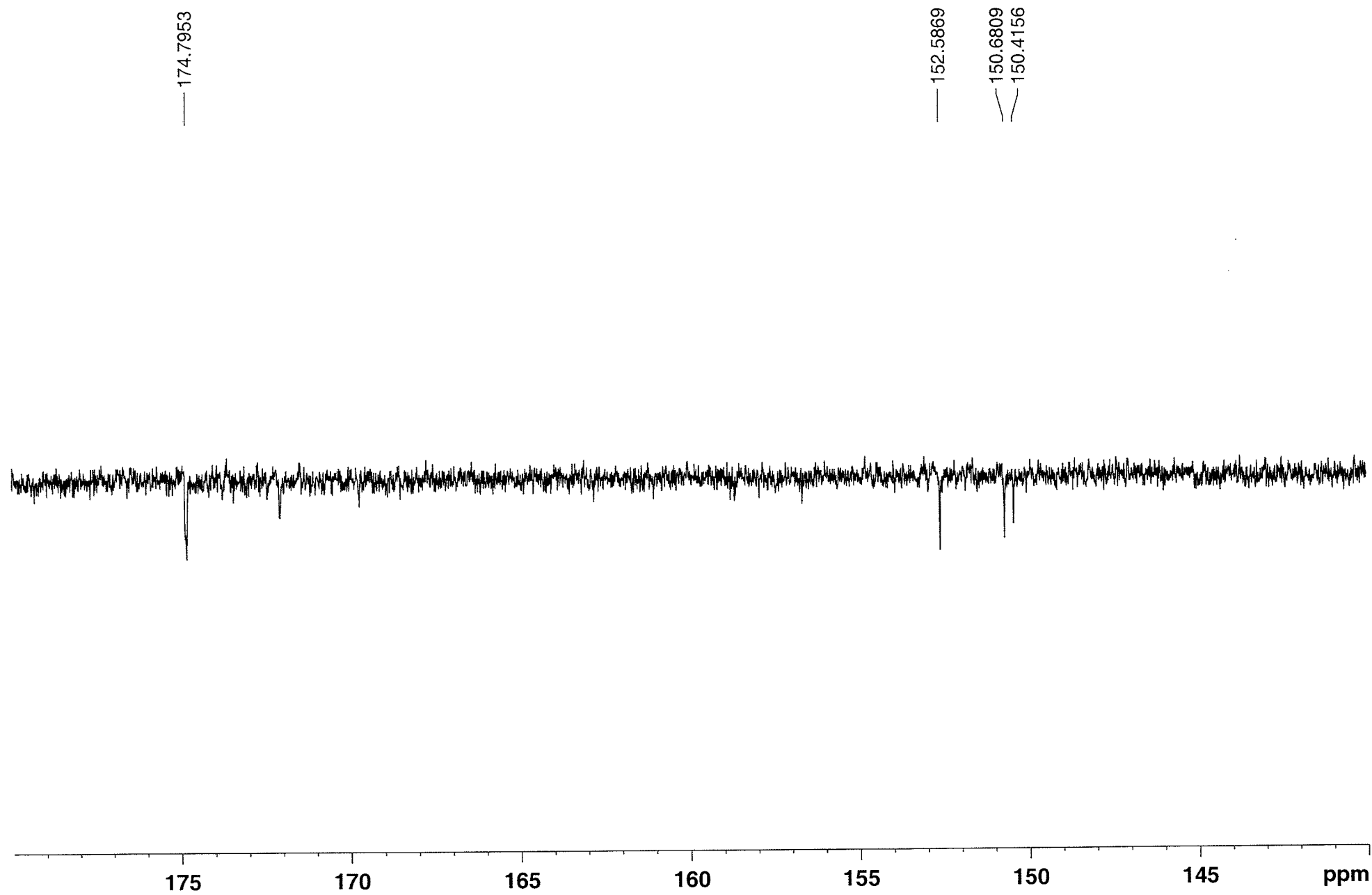
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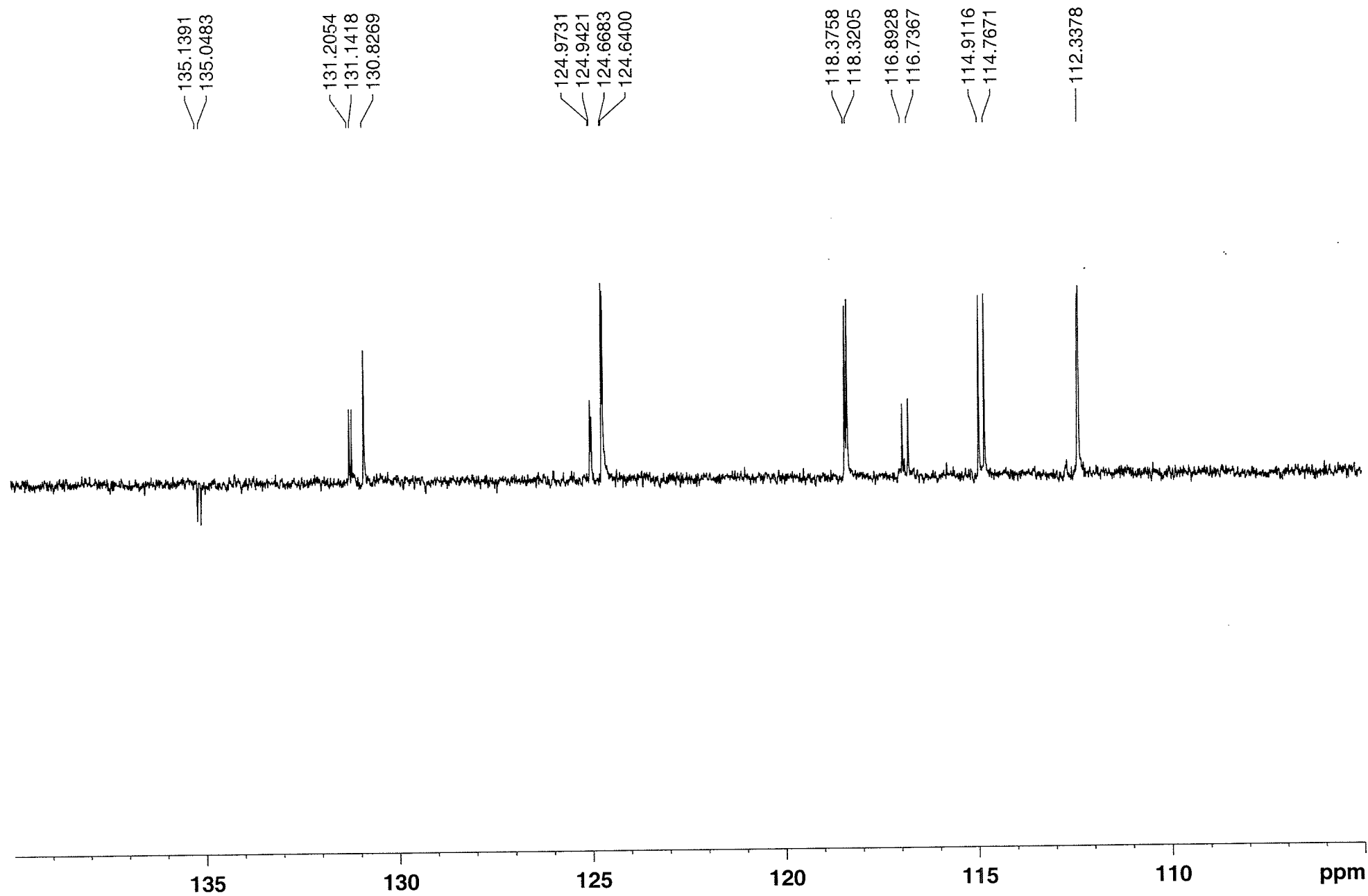
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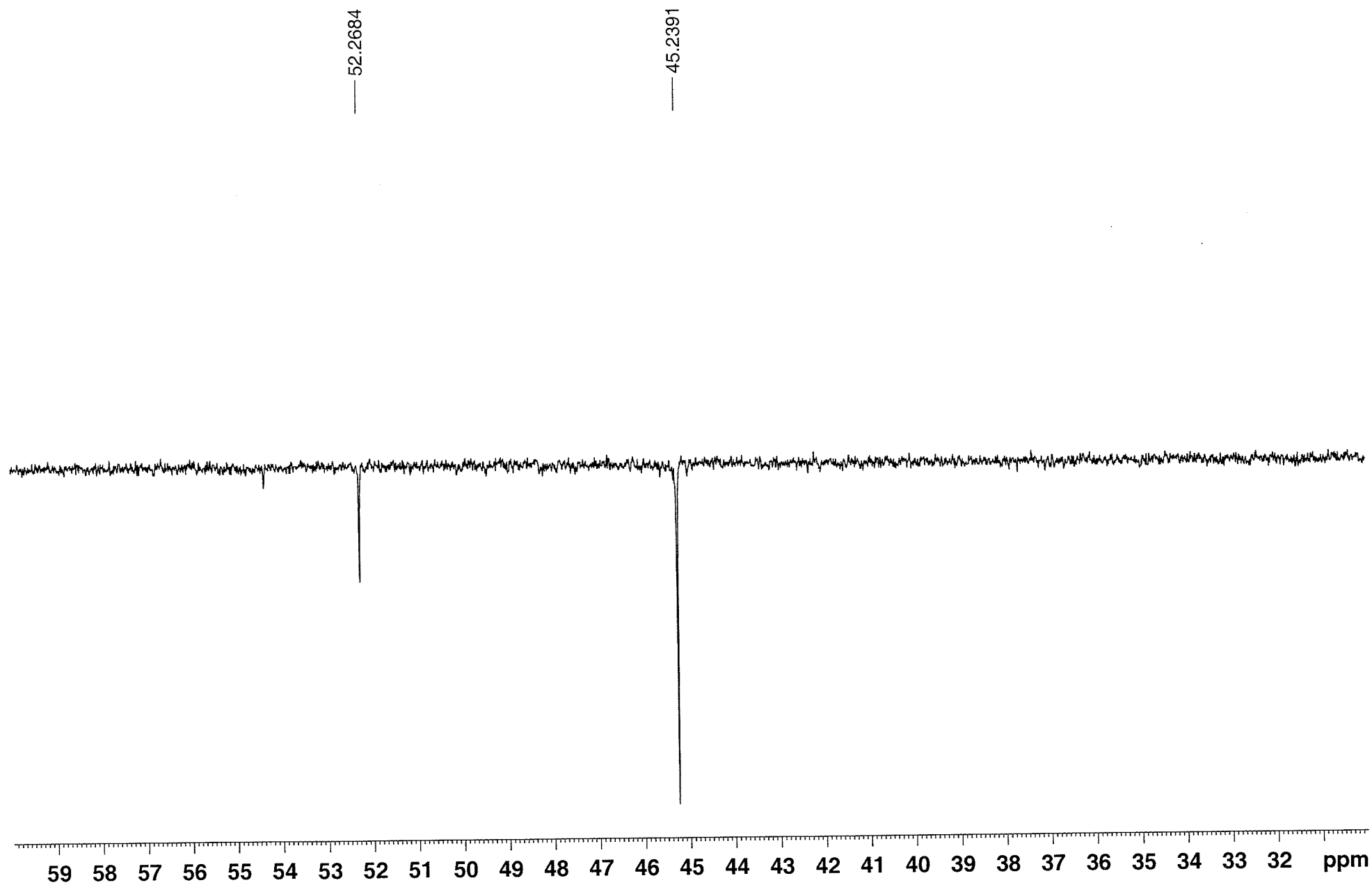
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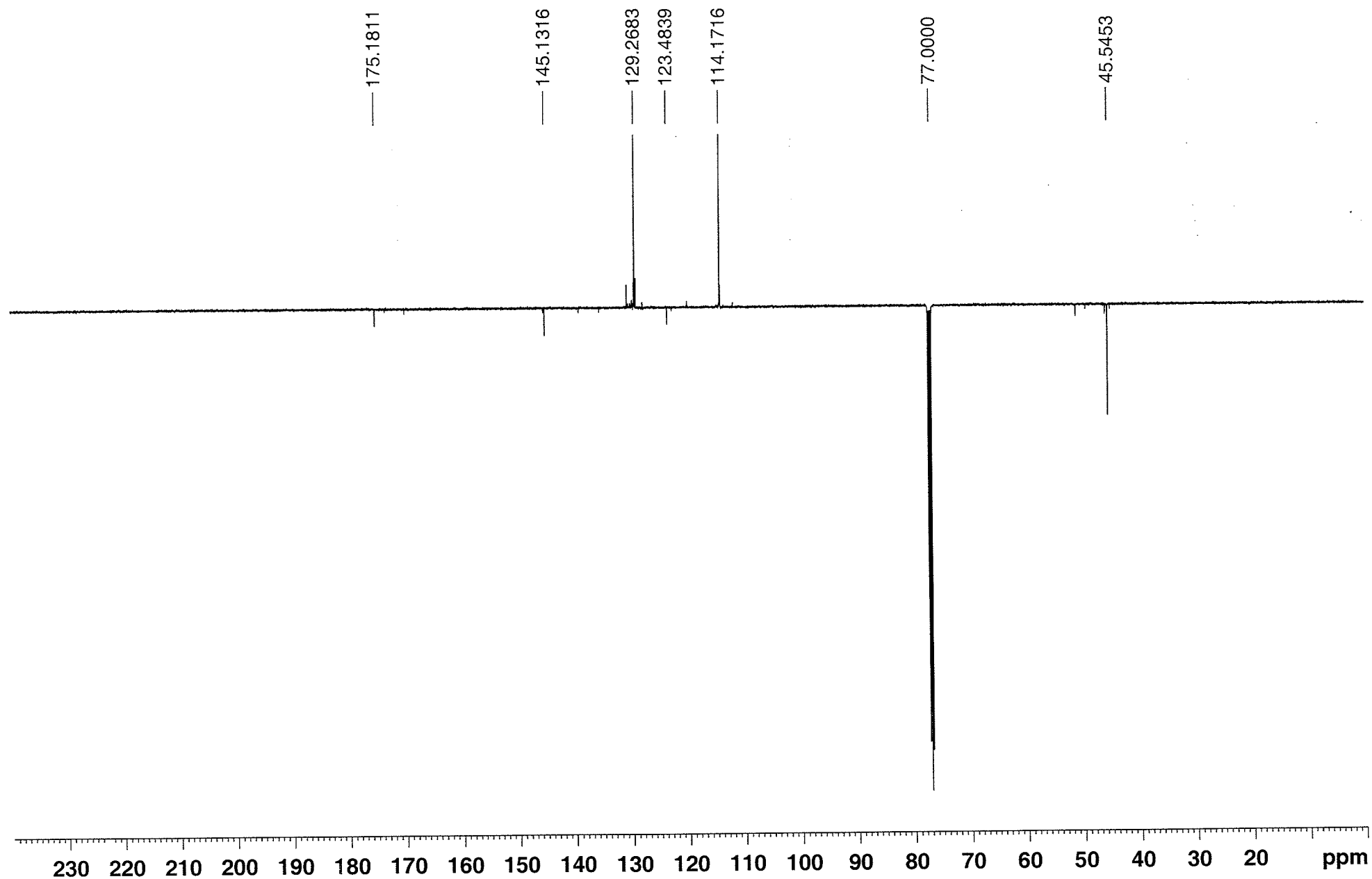
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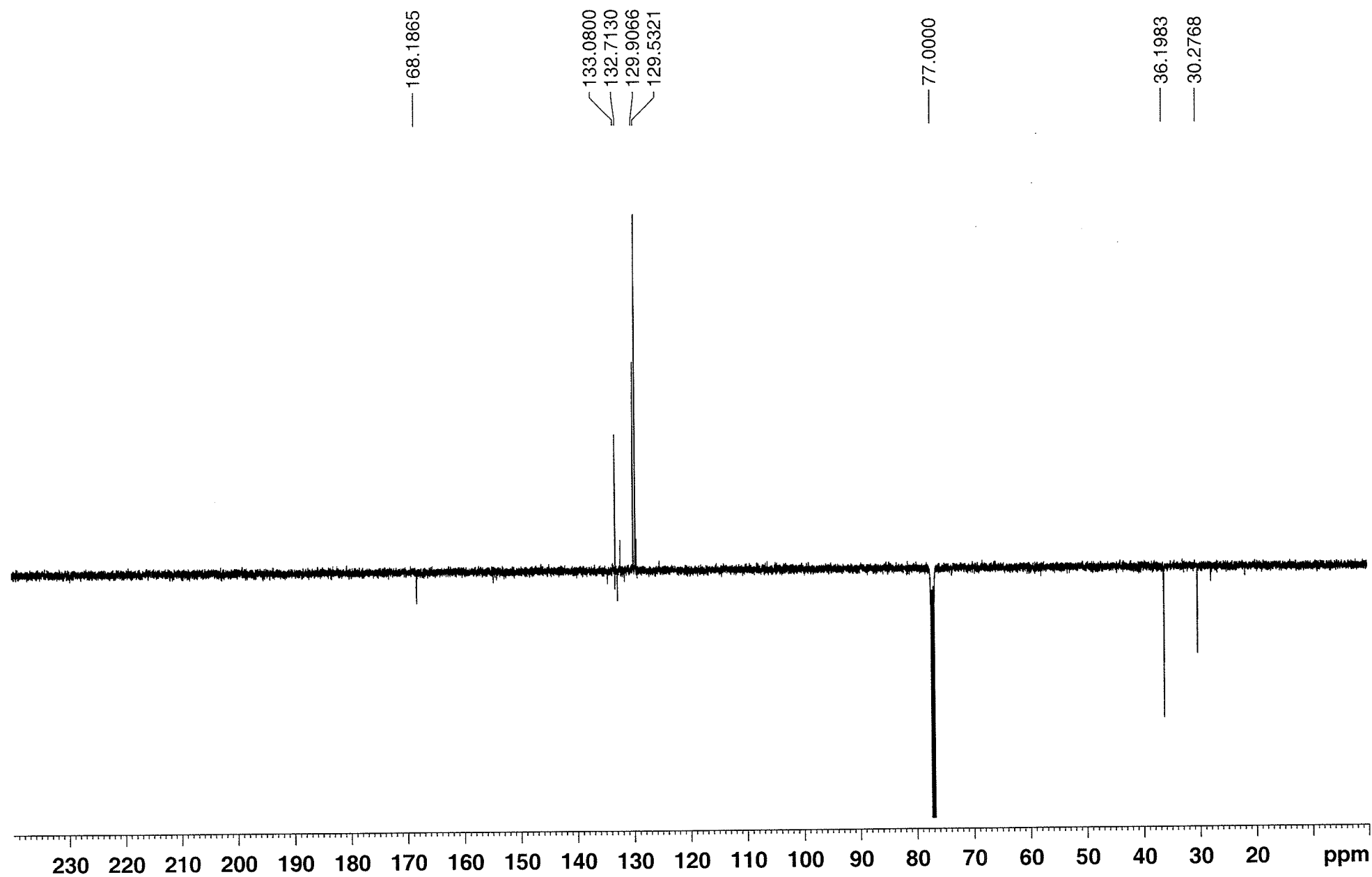
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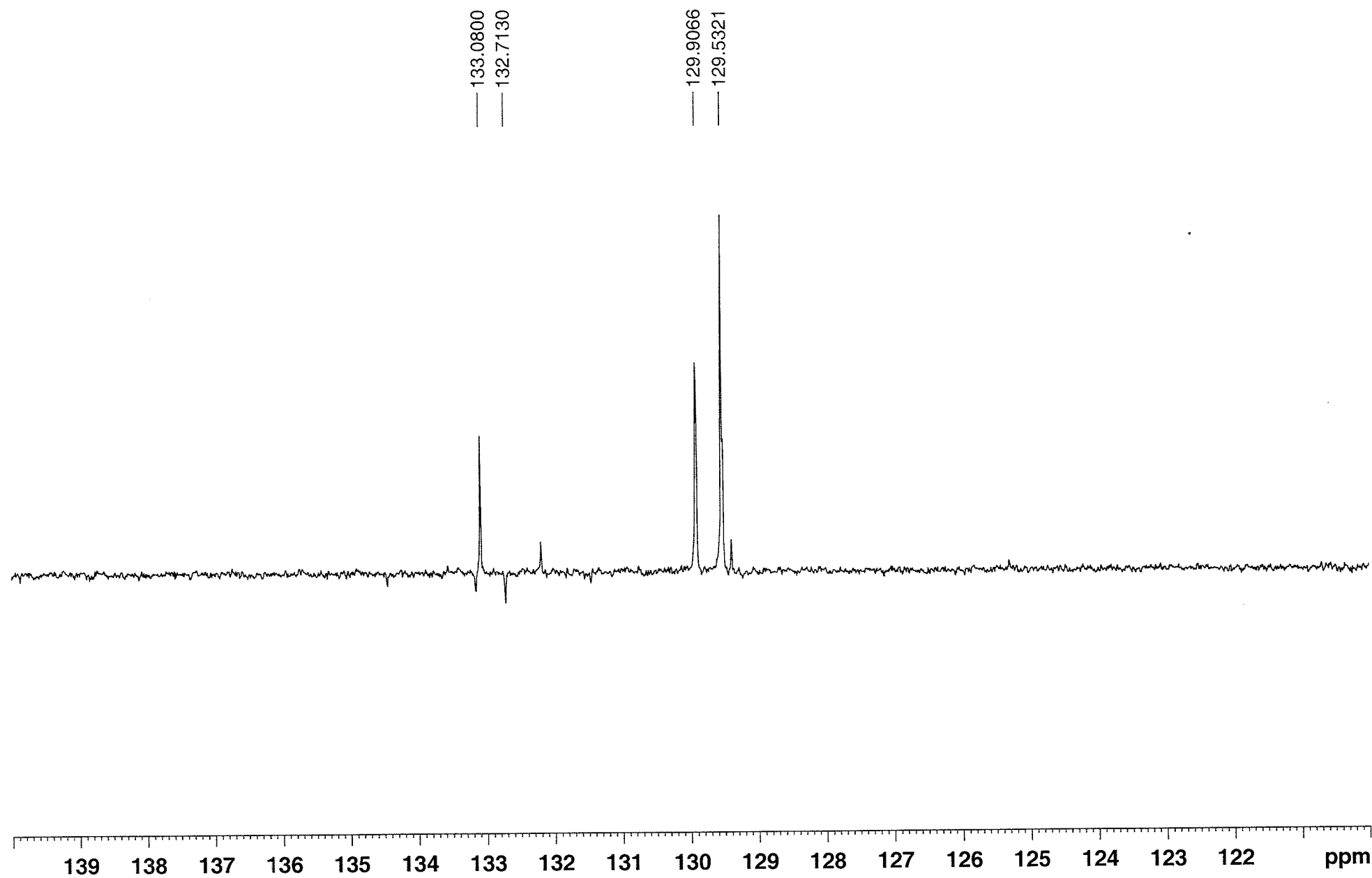
AWEPOpd02 in cdcl3 (APT) 2.11.2016



AWEPOpd06 in cdcl3 (APT) 2.11.2016



AWEPOpd06 in cdcl3 (APT) 2.11.2016



AWEPOpd06 in cdcl3 (APT) 2.11.2016

