

Structure–metabolism relationships of 4-pentenyl synthetic cannabinoid
receptor agonists using *in vitro* human hepatocyte incubations and high-
resolution mass spectrometry

Supplementary Information for Archives of Toxicology – NMR Spectra

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Xiongyu Wu³, Johan Dahlén³, Lorna A Nisbet¹, Craig McKenzie^{1,4}, Henrik Gréen^{1,5,*}

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² Division of Clinical Chemistry and Pharmacology, Department of Biomedical and Clinical
Sciences, Linköping University, Linköping, Sweden

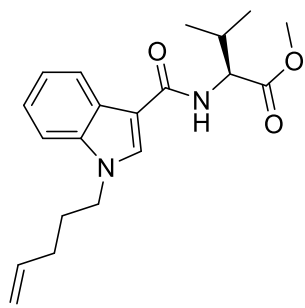
³ Department of Physics, Chemistry and Biology, Linköping University, Linköping, Sweden

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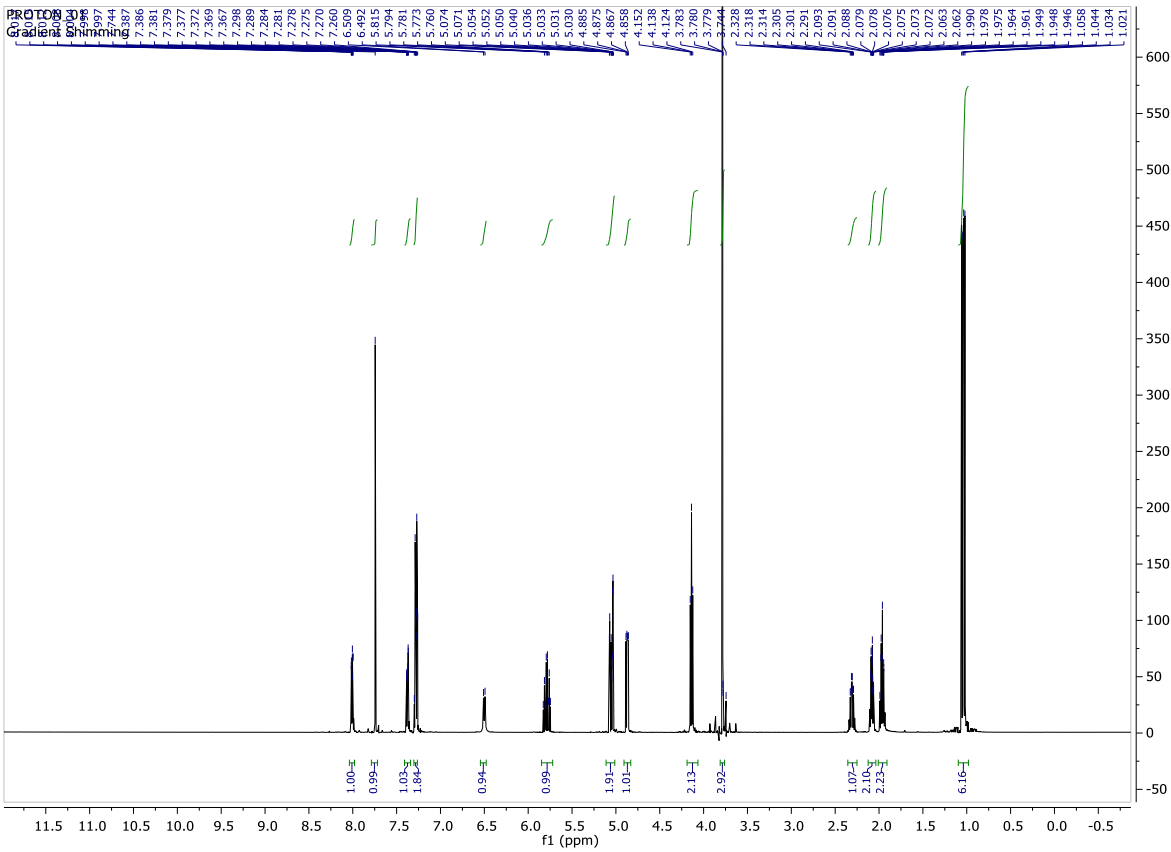
⁵ Department of Forensic Genetics and Forensic Toxicology, National Board of Forensic
Medicine, Linköping, Sweden

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henrik.green@liu.se

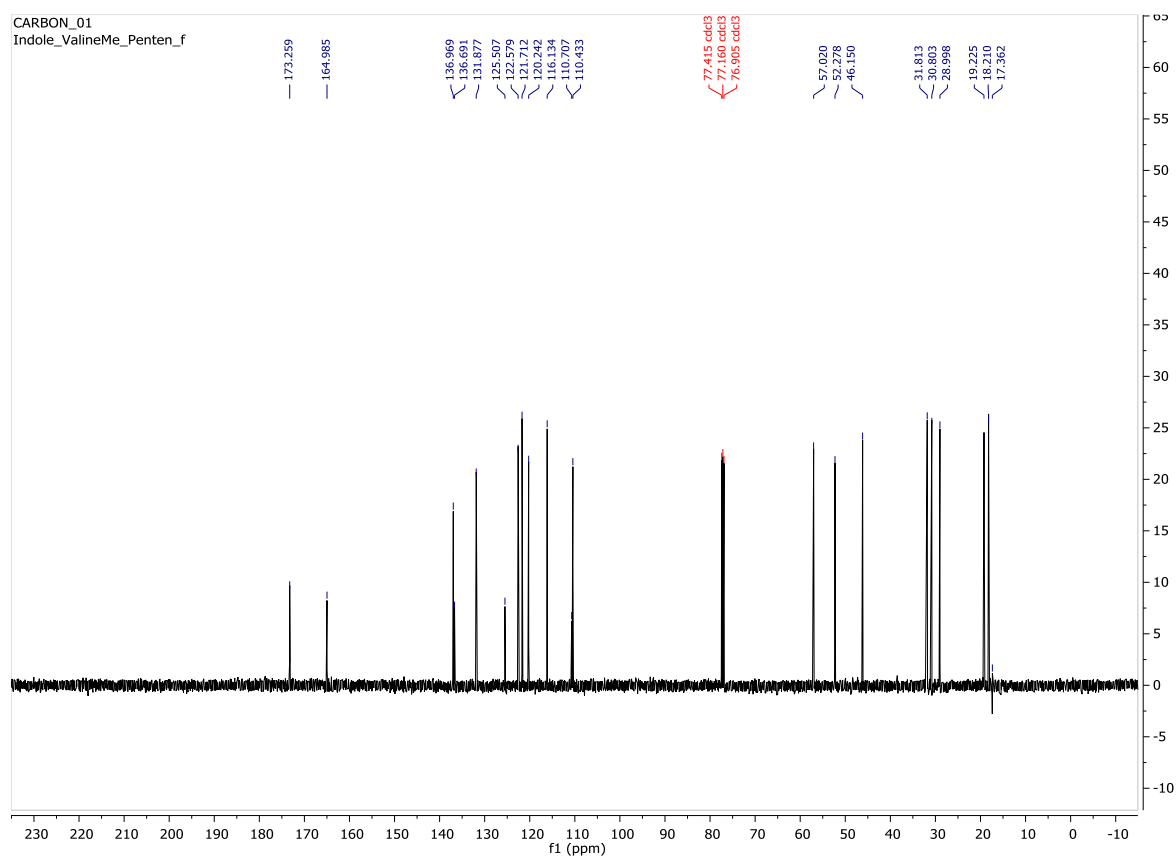
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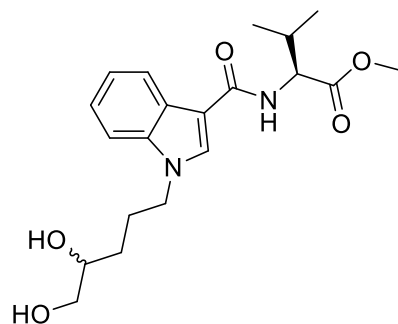
¹H-NMR Spectrum



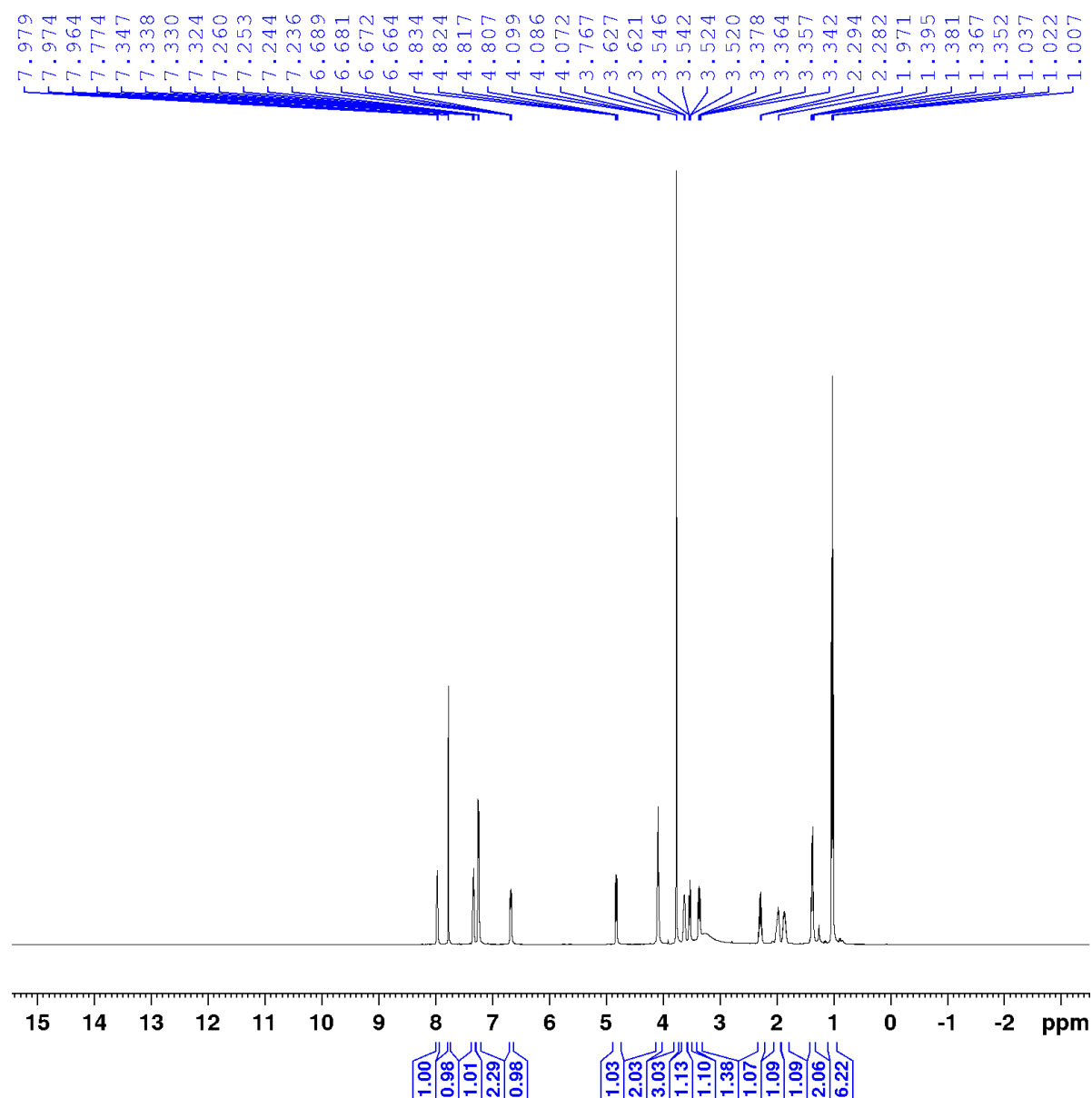
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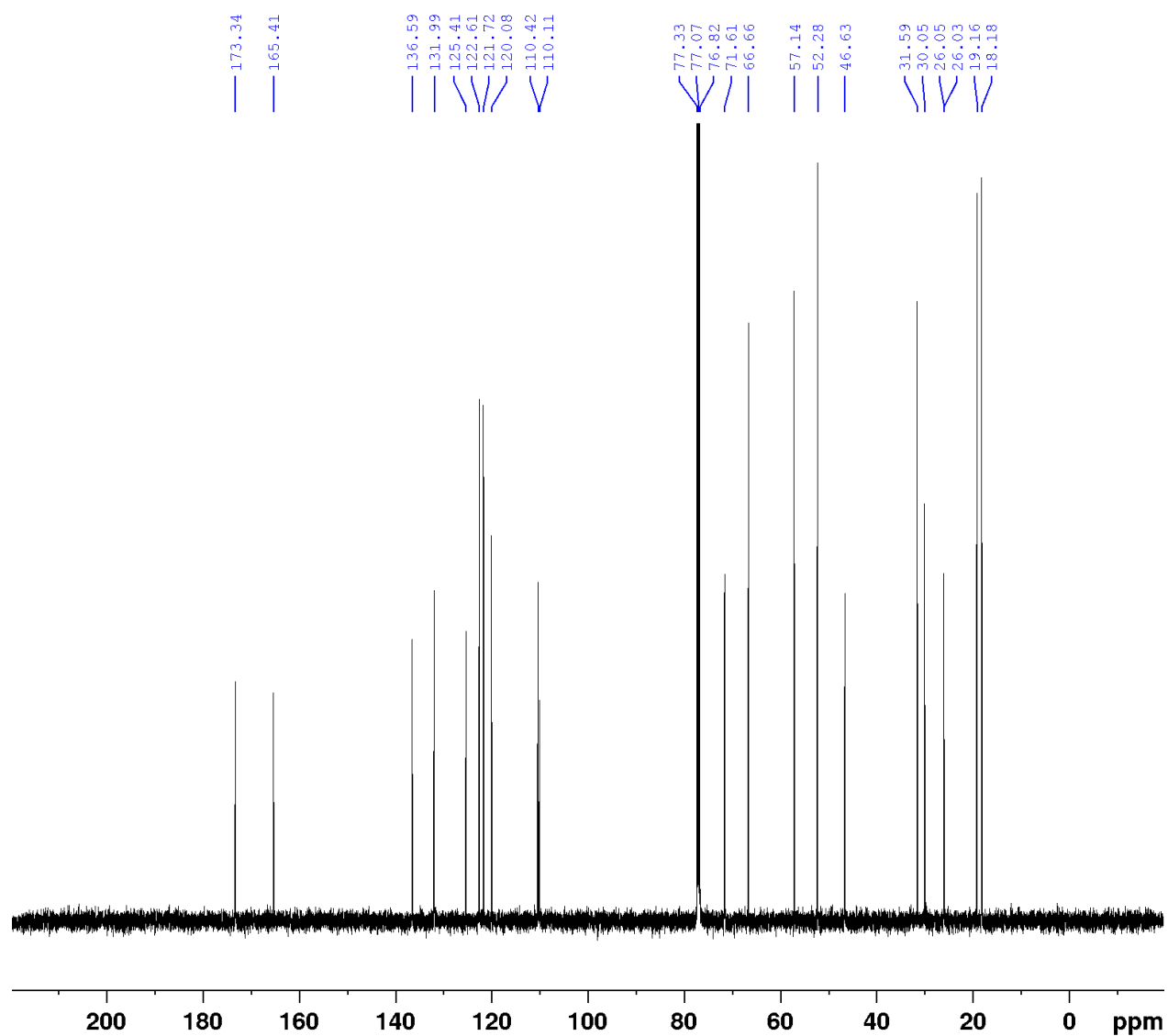
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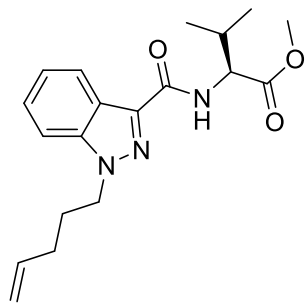
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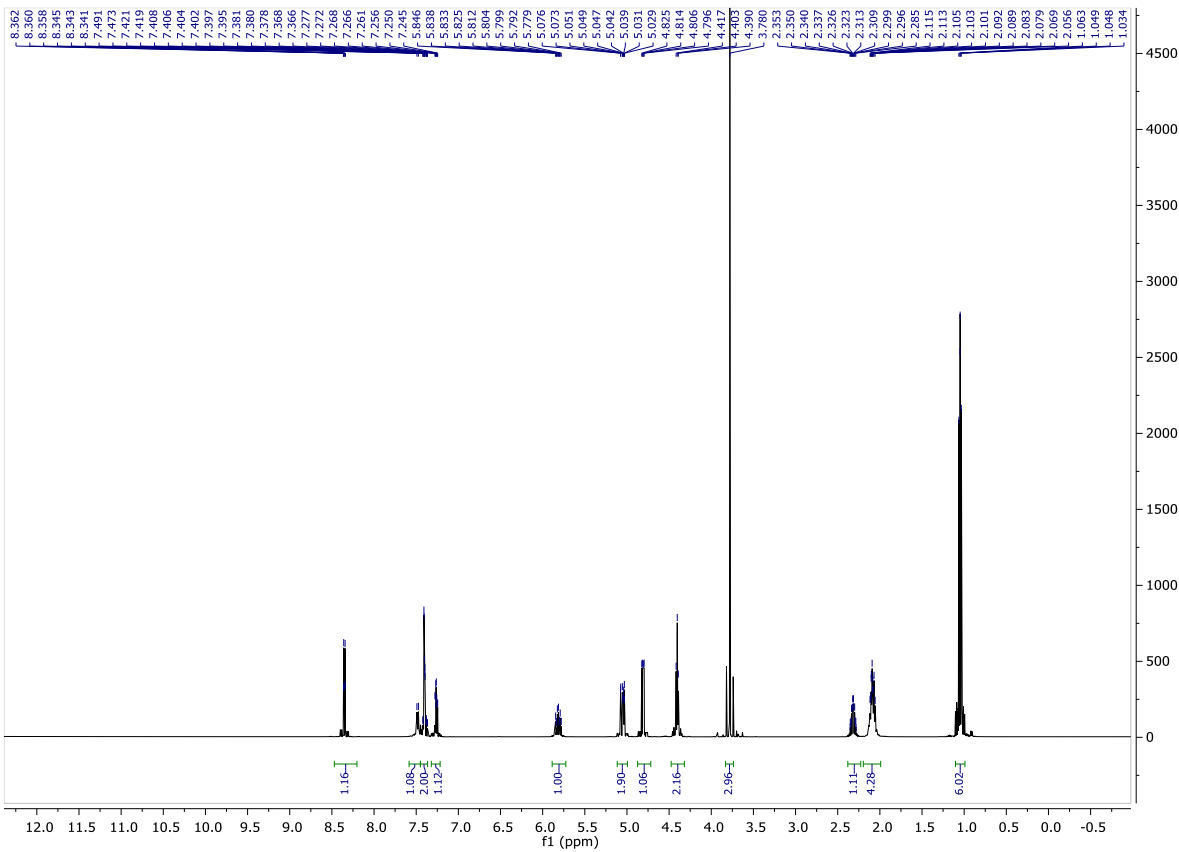
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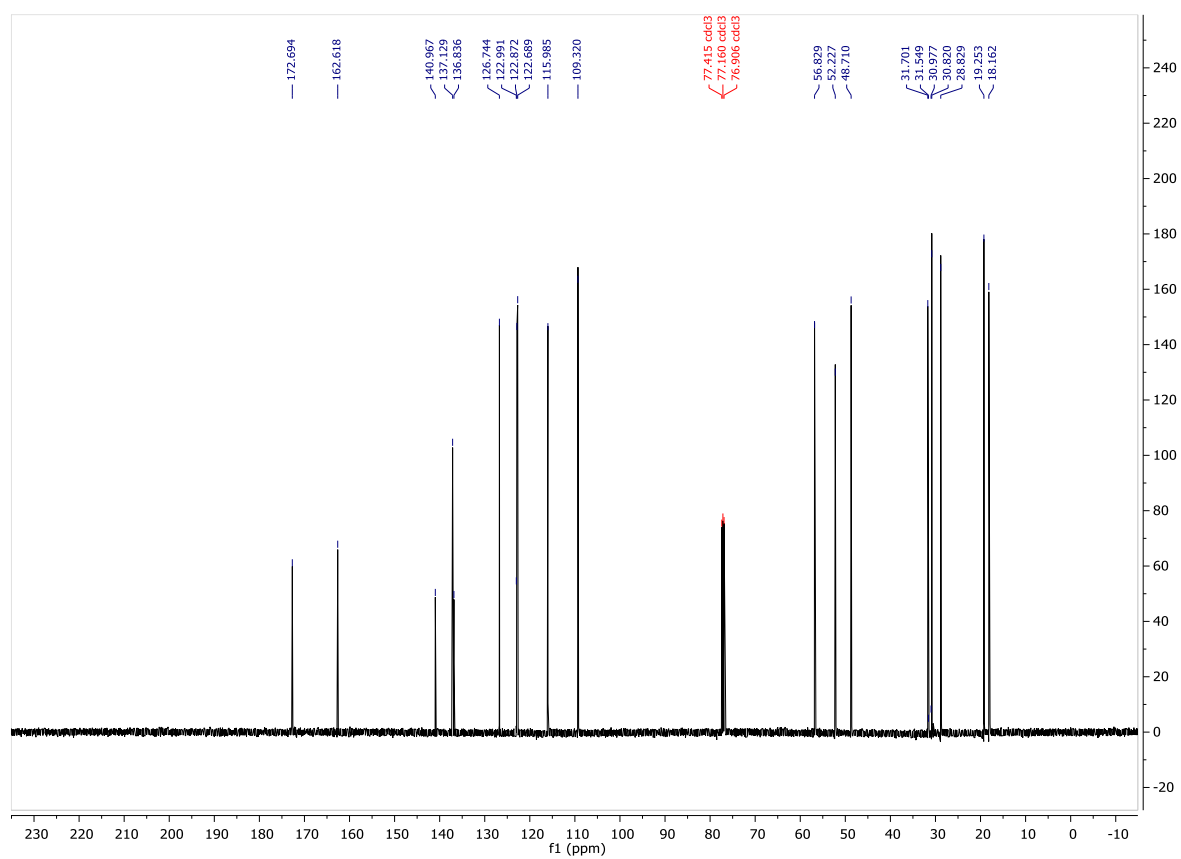
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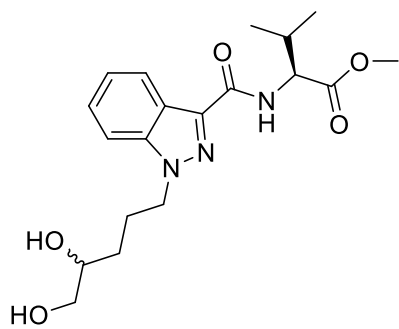
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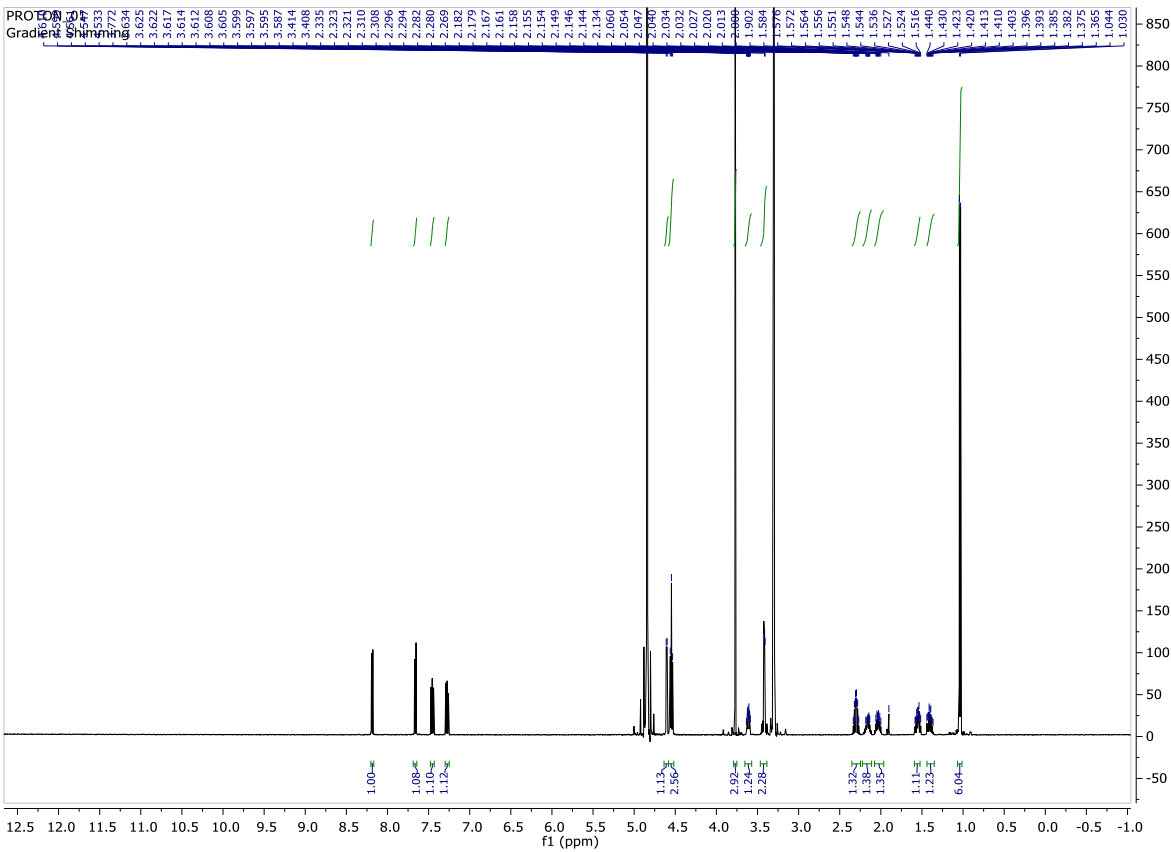
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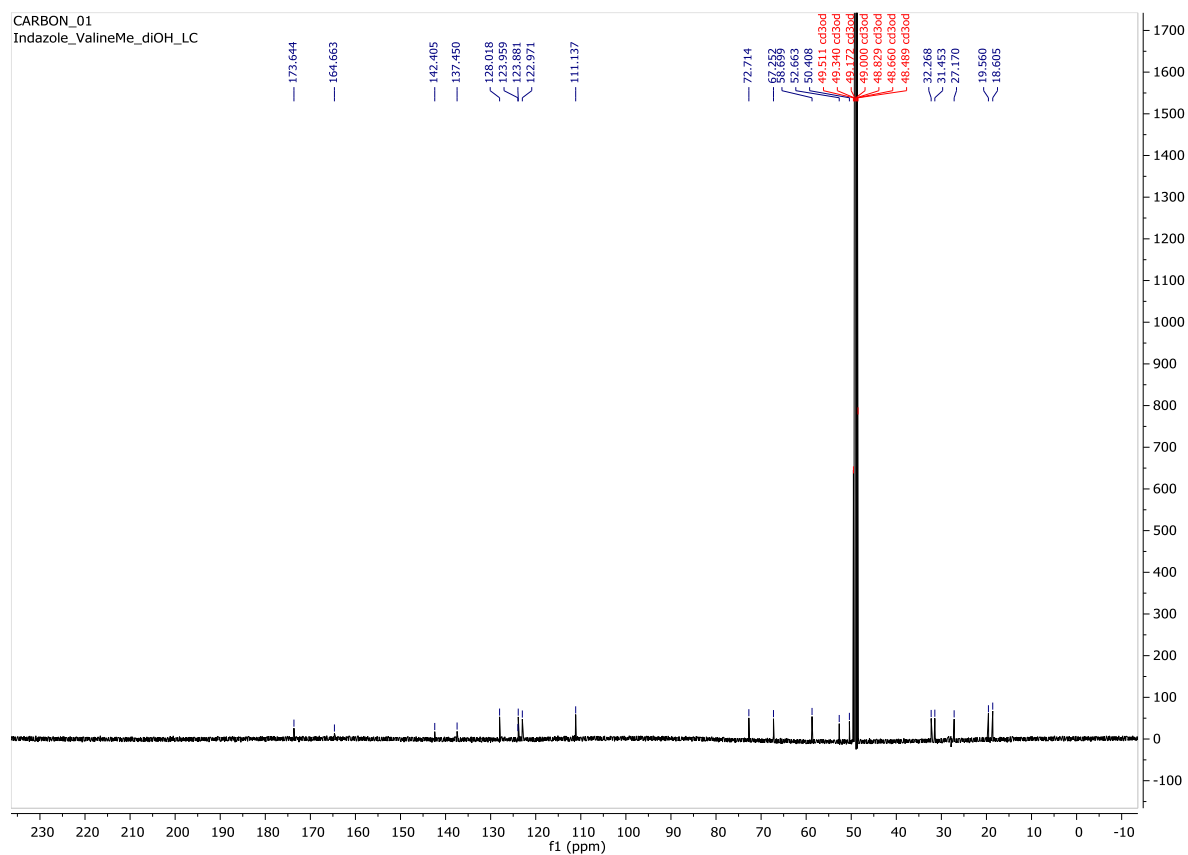
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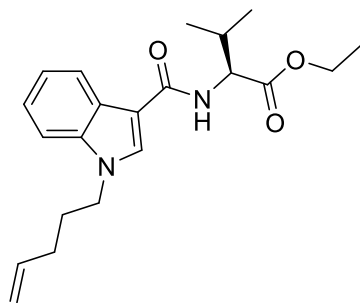
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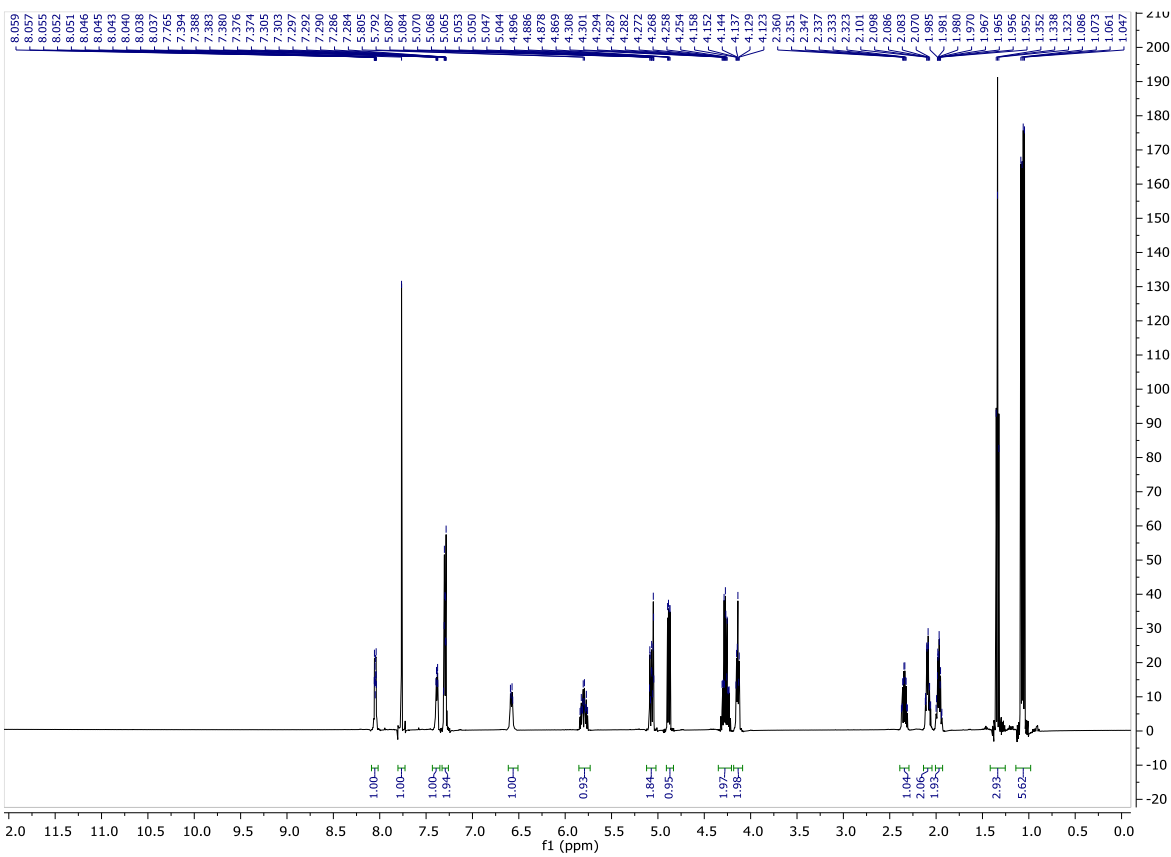
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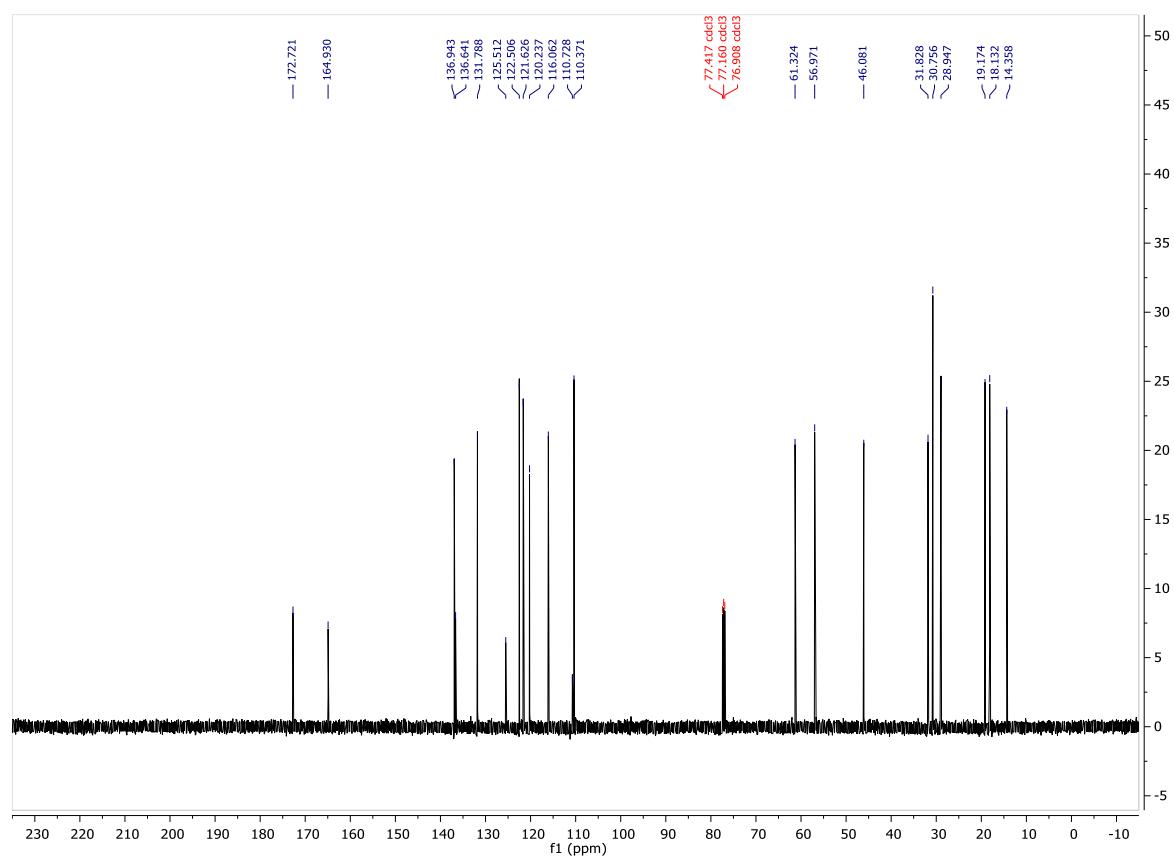
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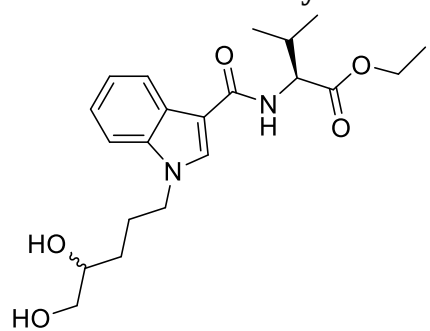
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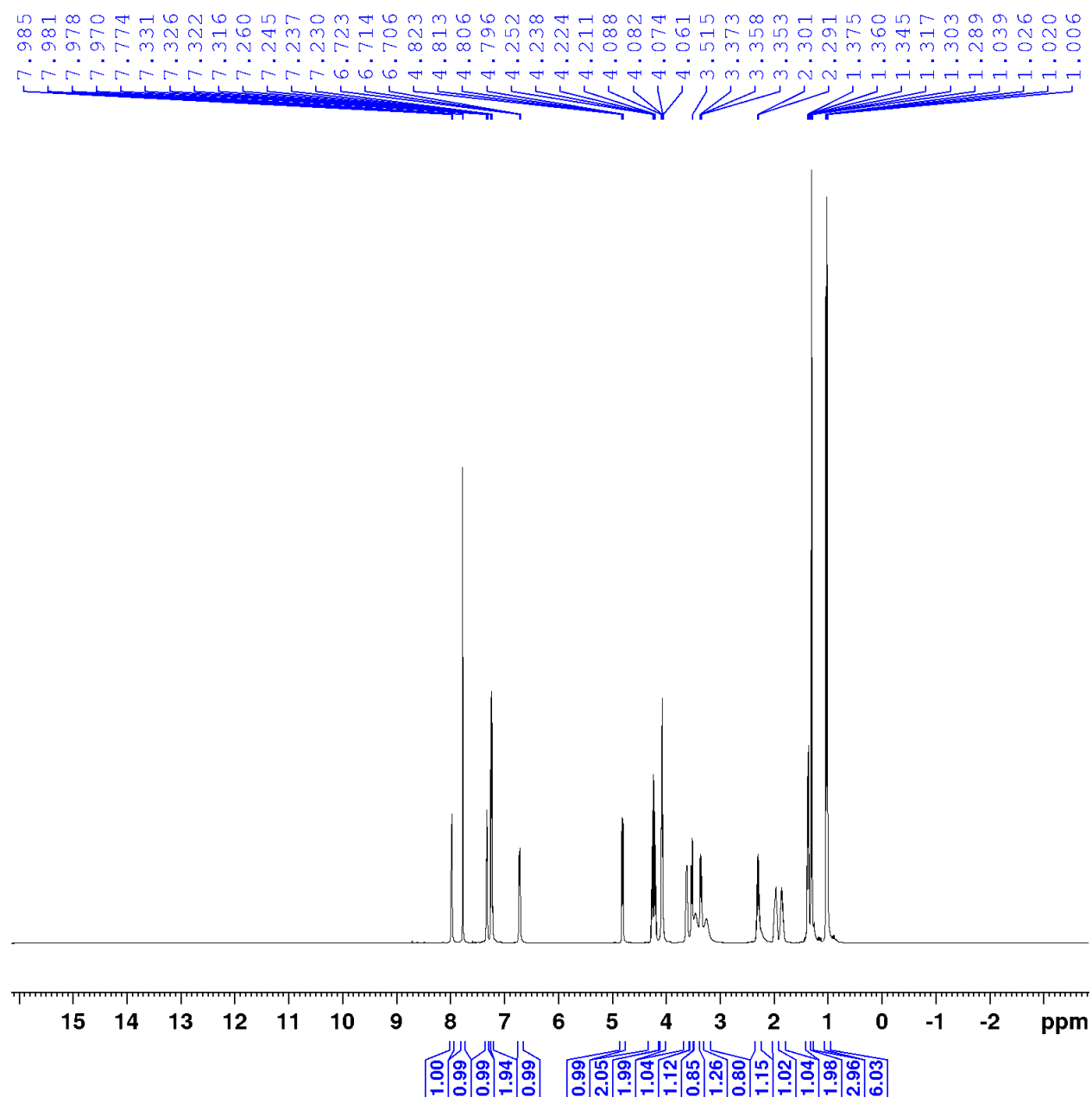
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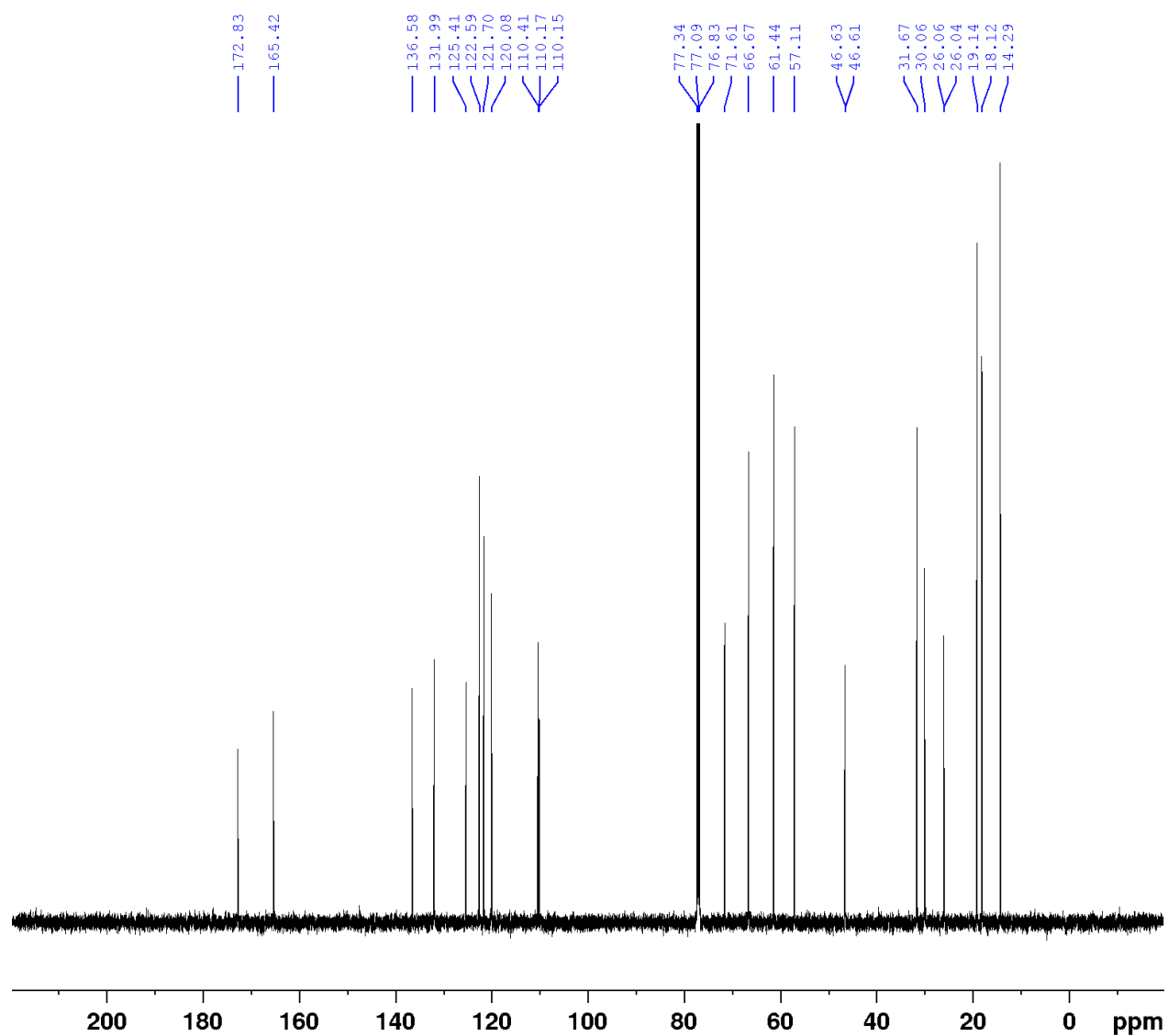
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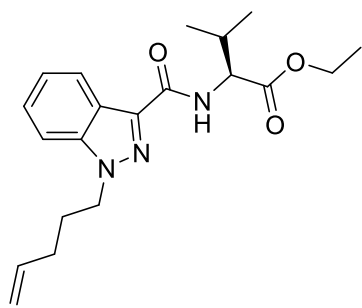
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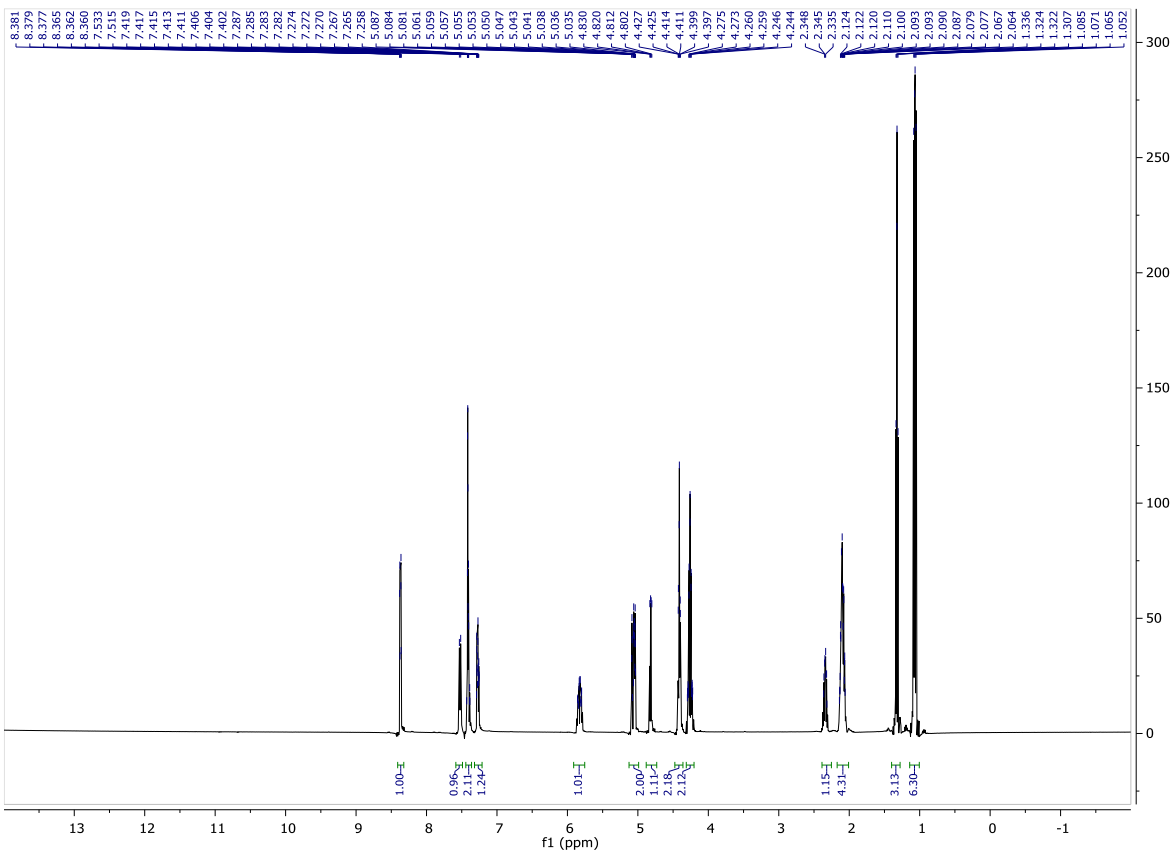
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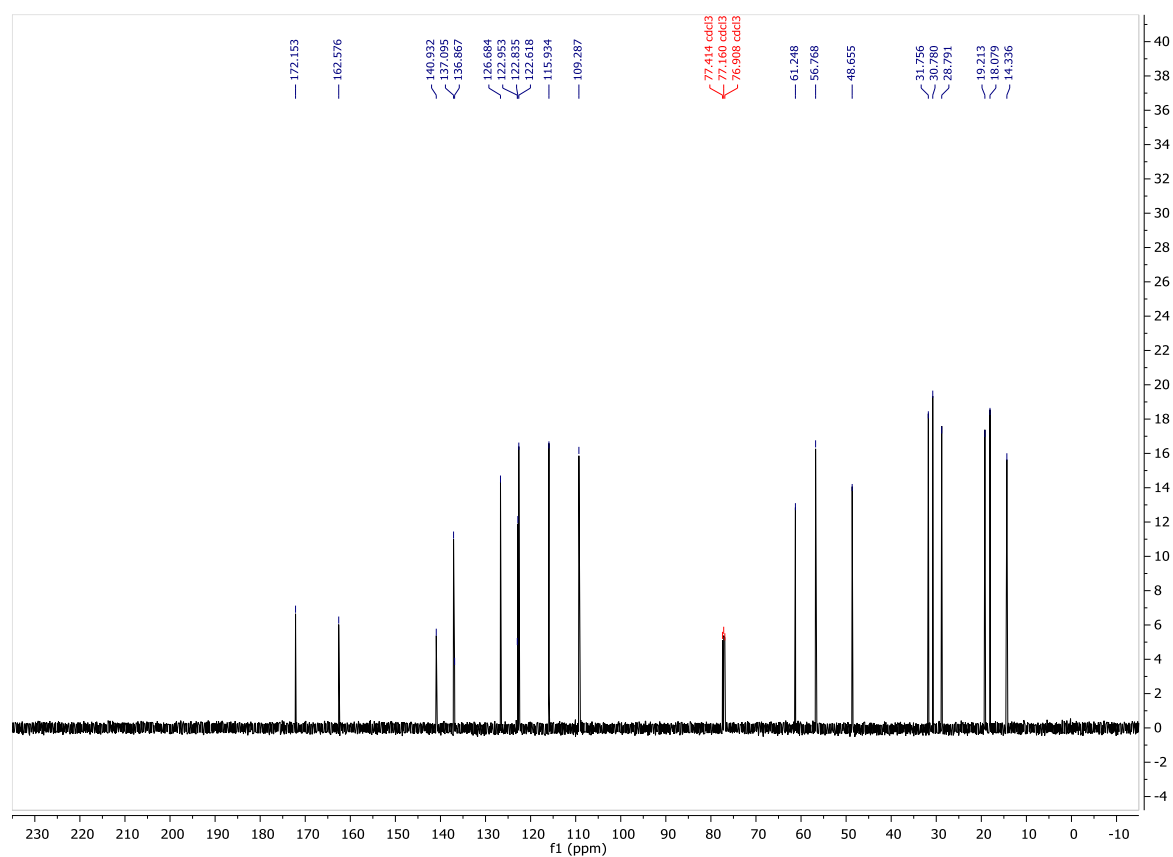
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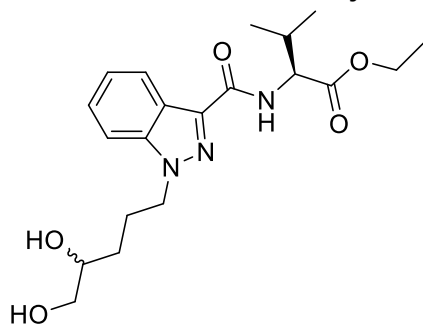
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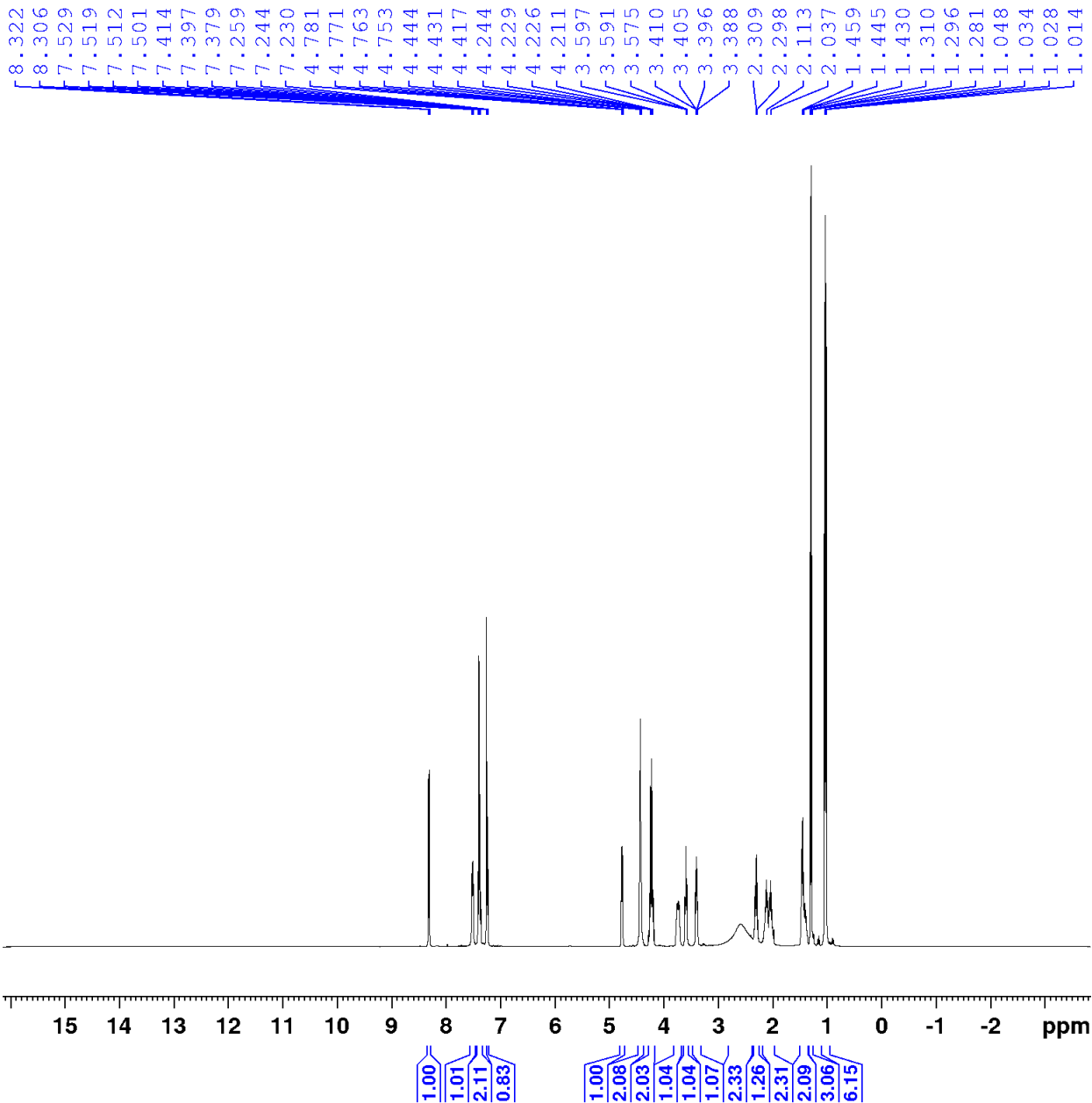
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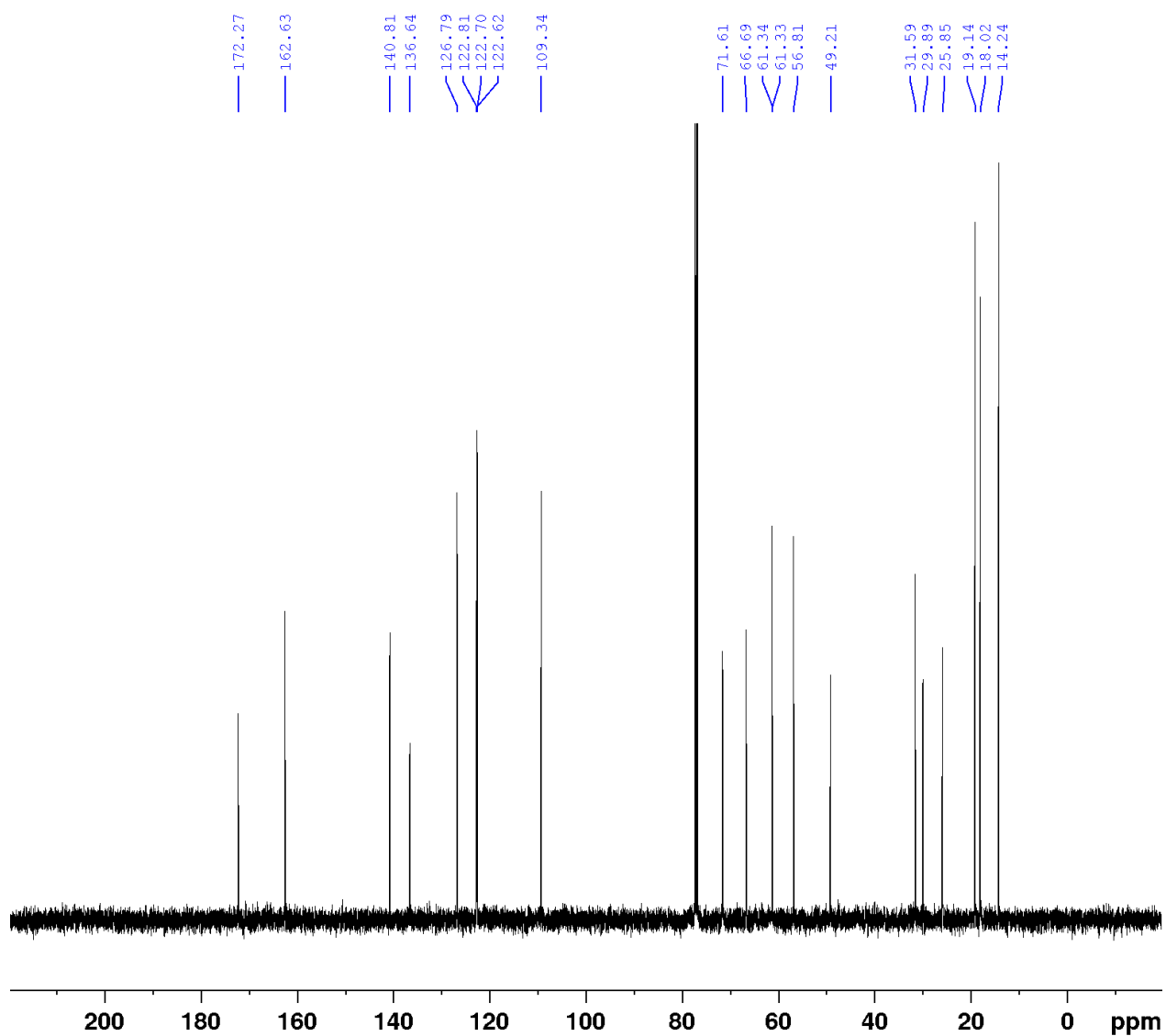
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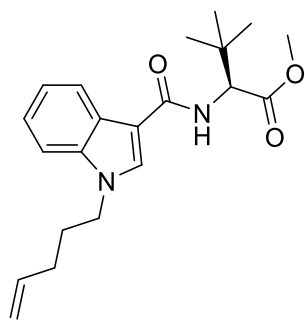
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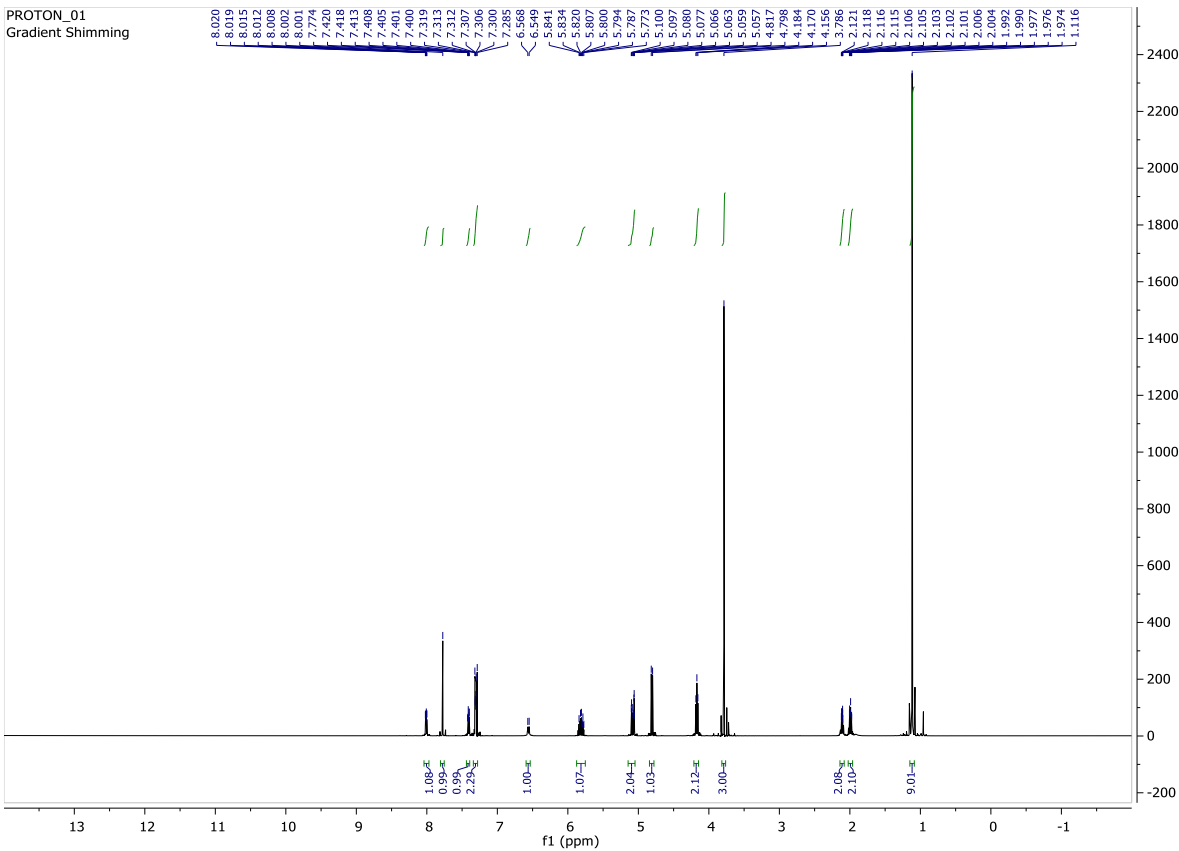
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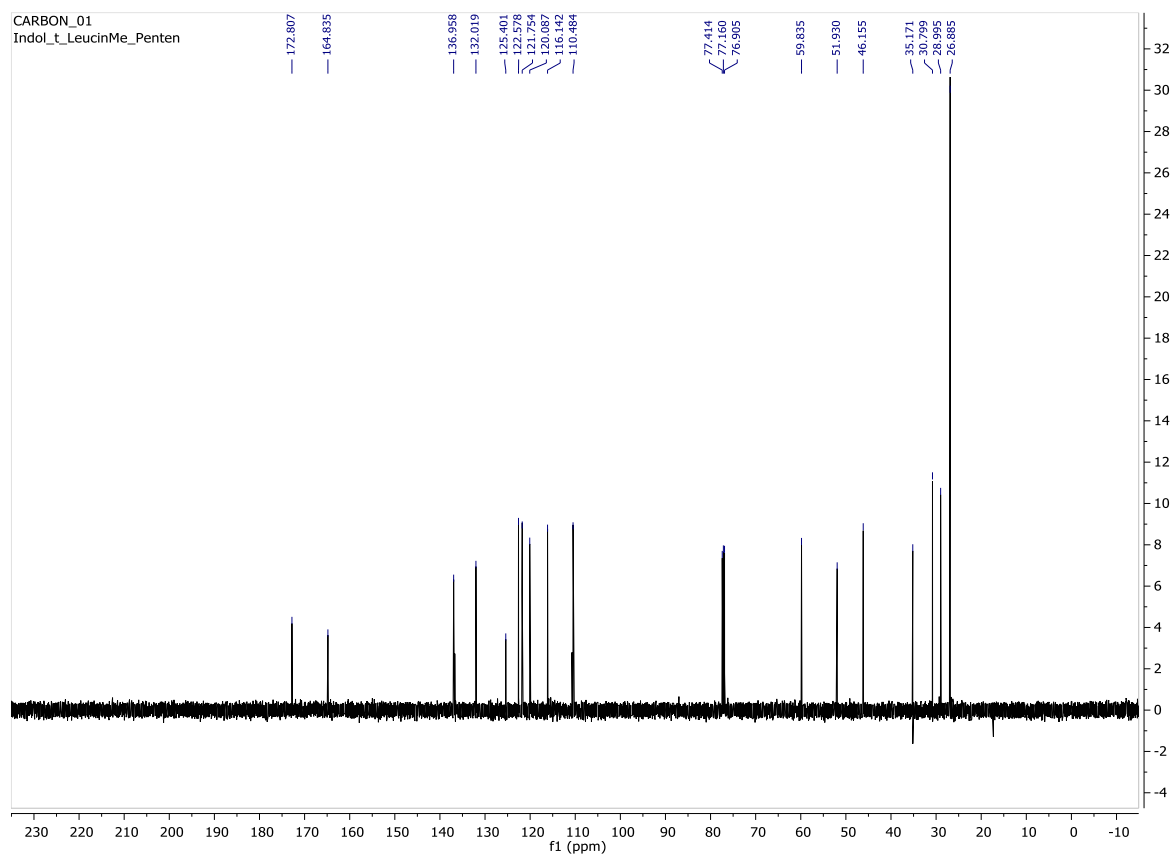
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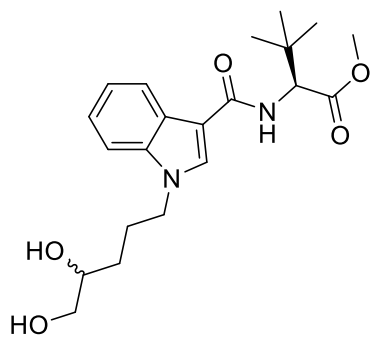
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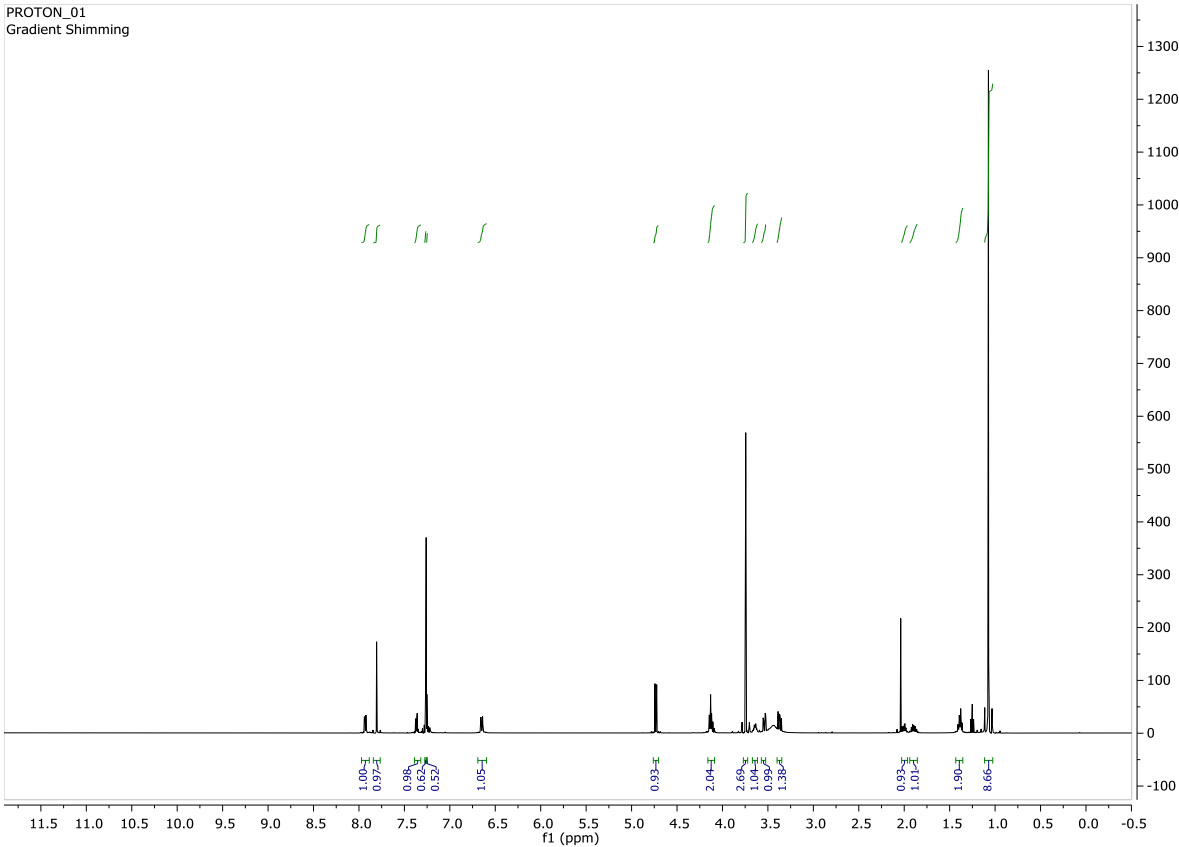
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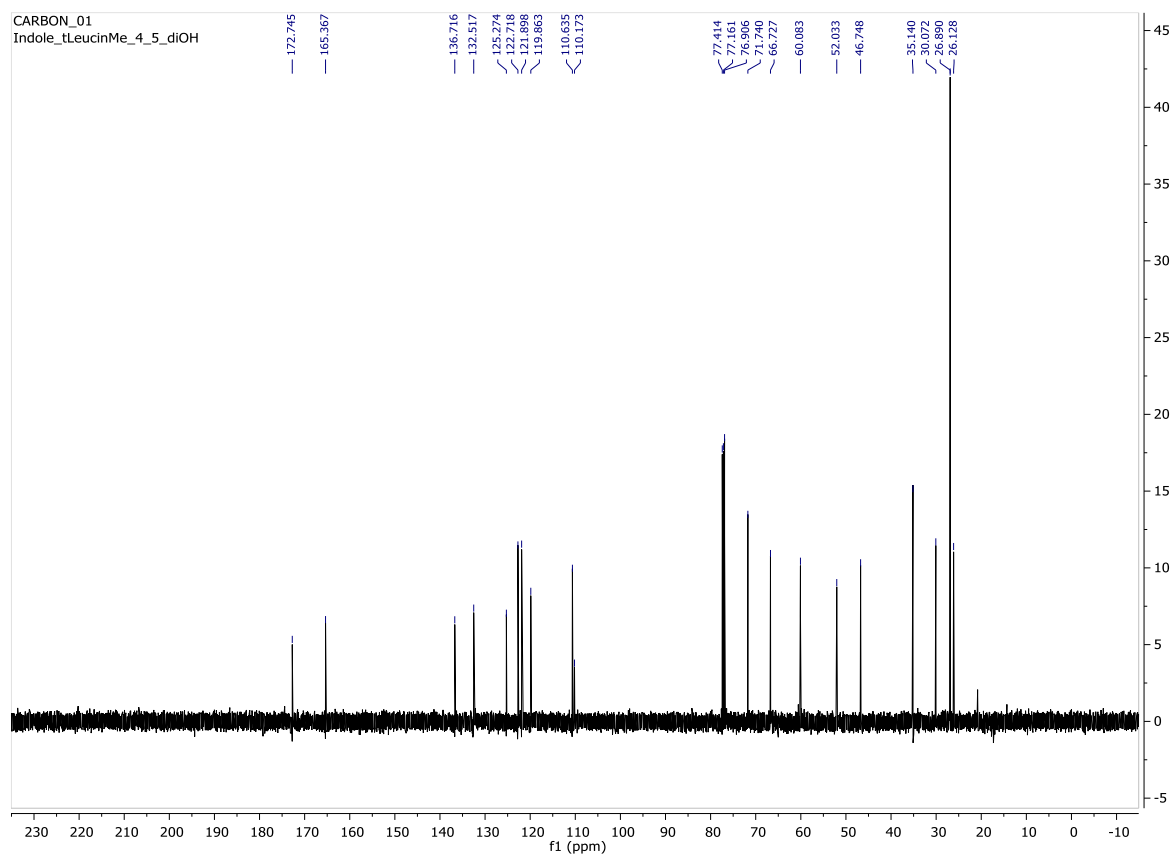
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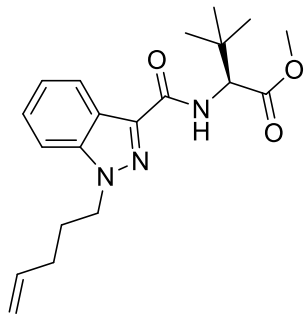
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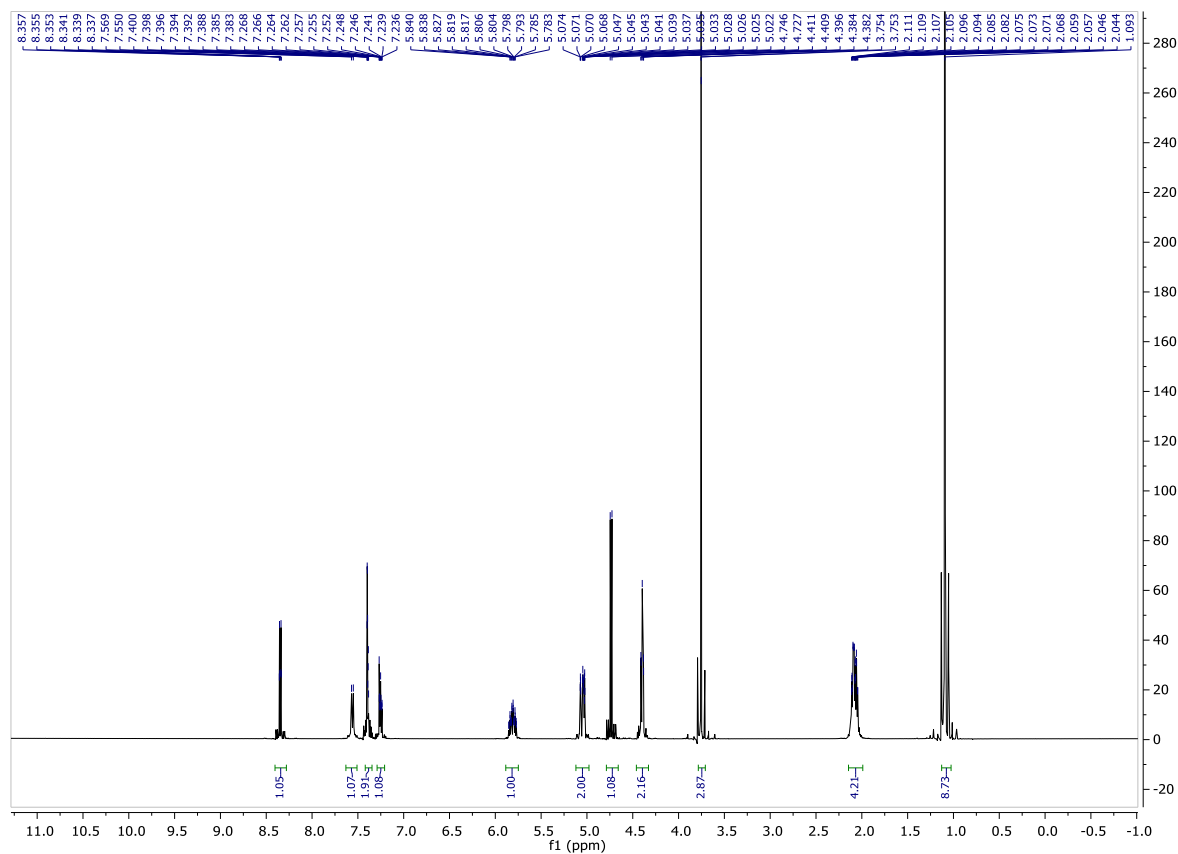
^{13}C -NMR Spectrum



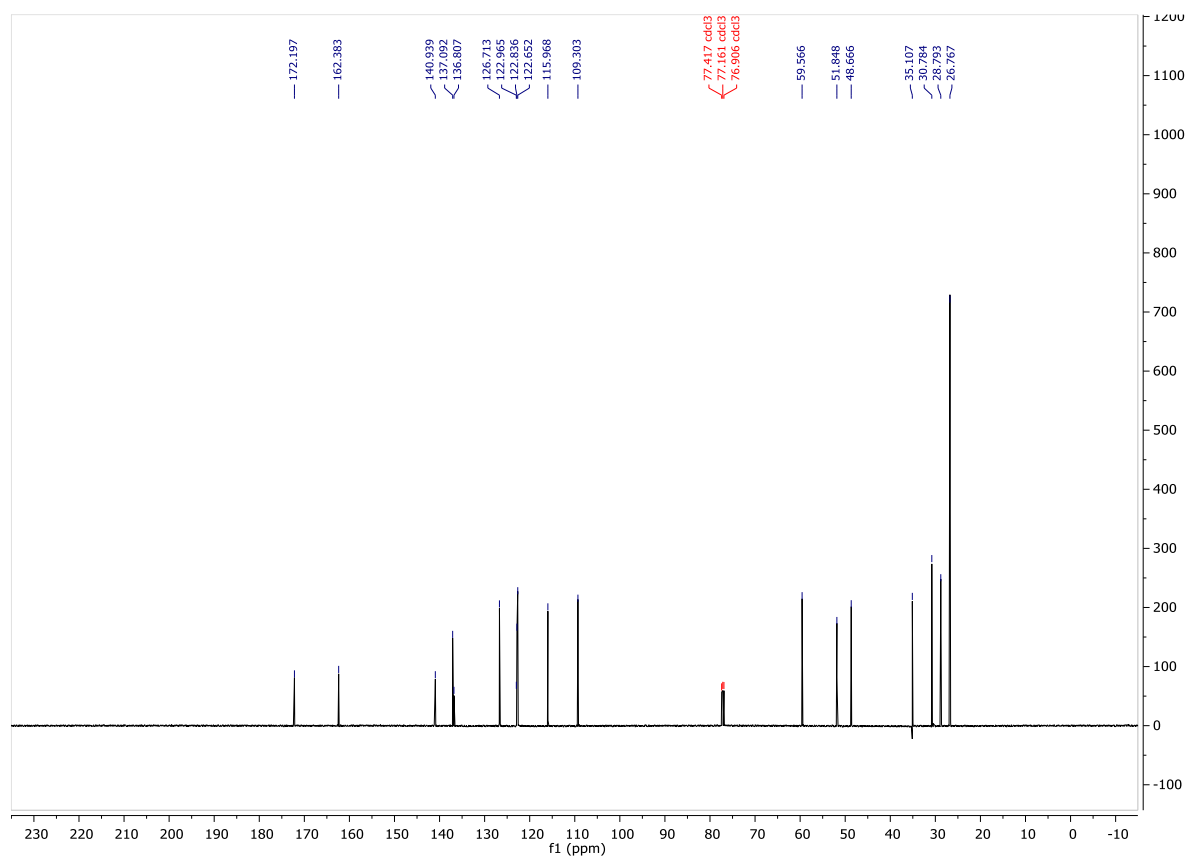
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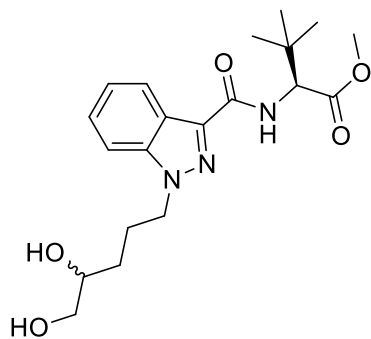
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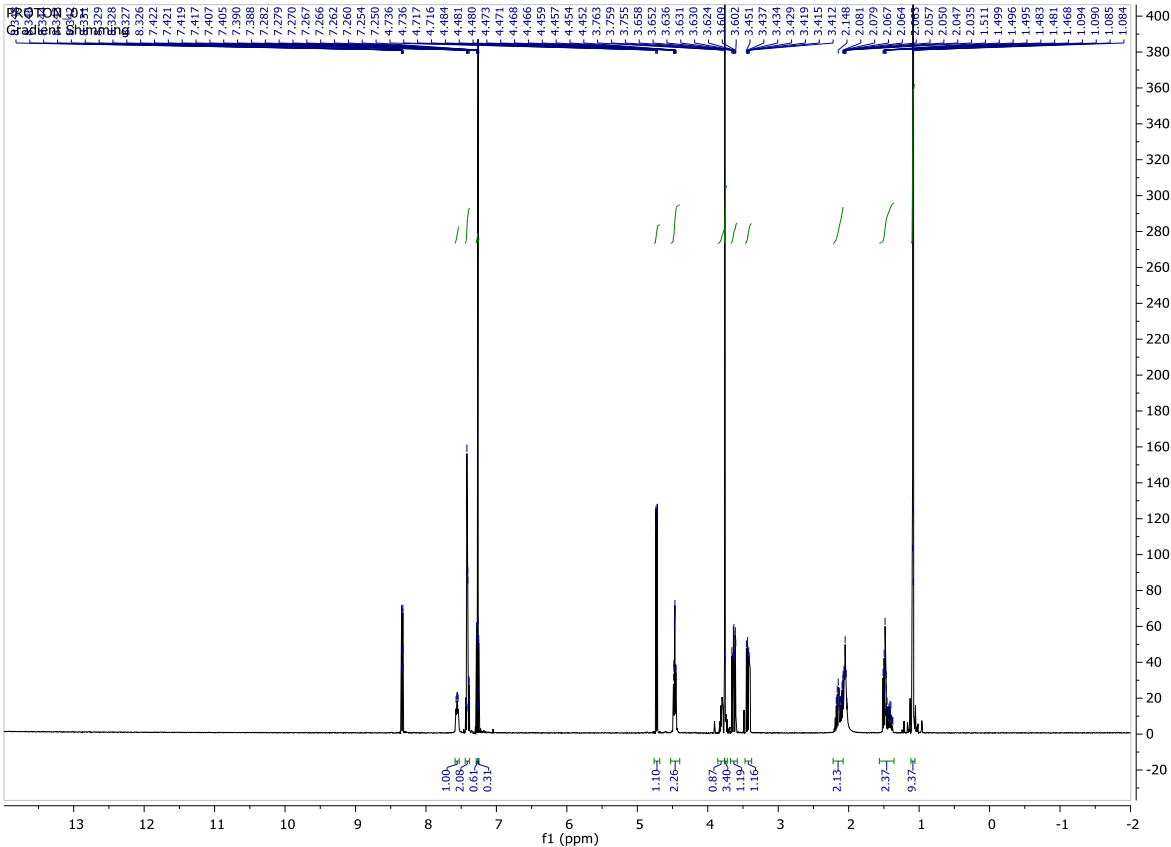
^{13}C -NMR Spectrum



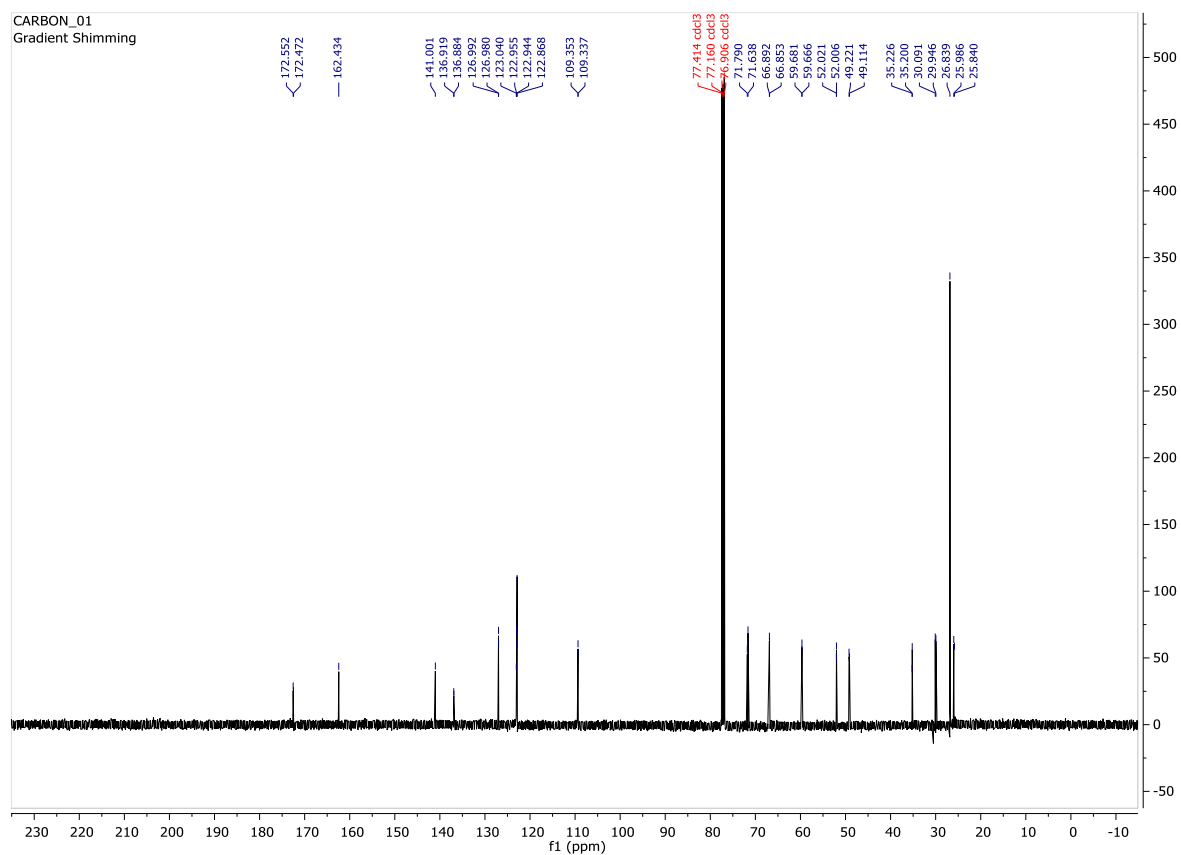
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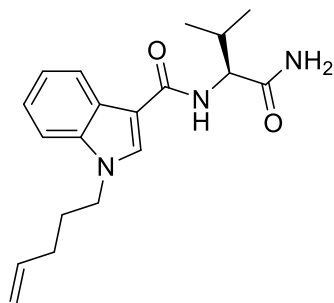
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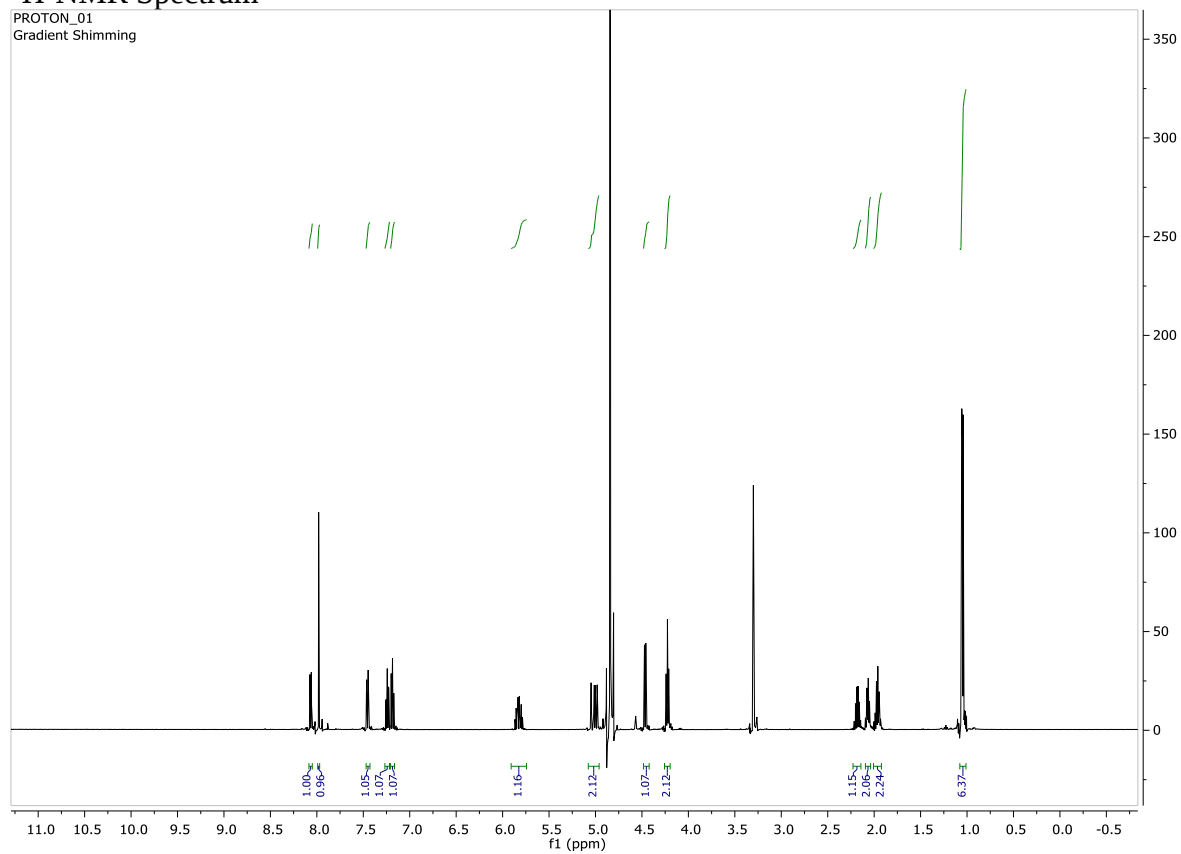
^{13}C -NMR Spectrum



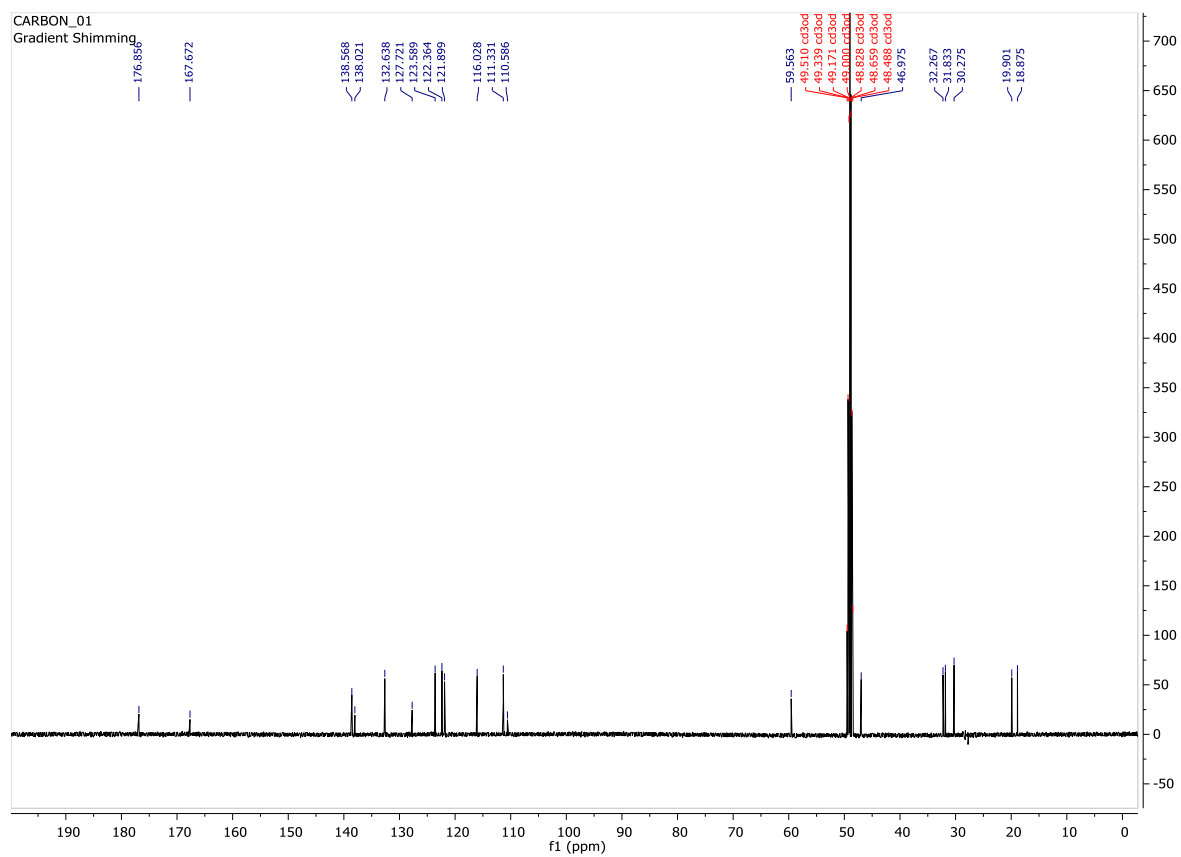
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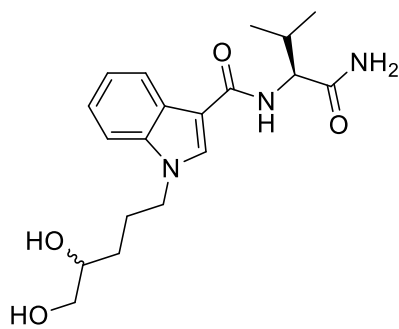
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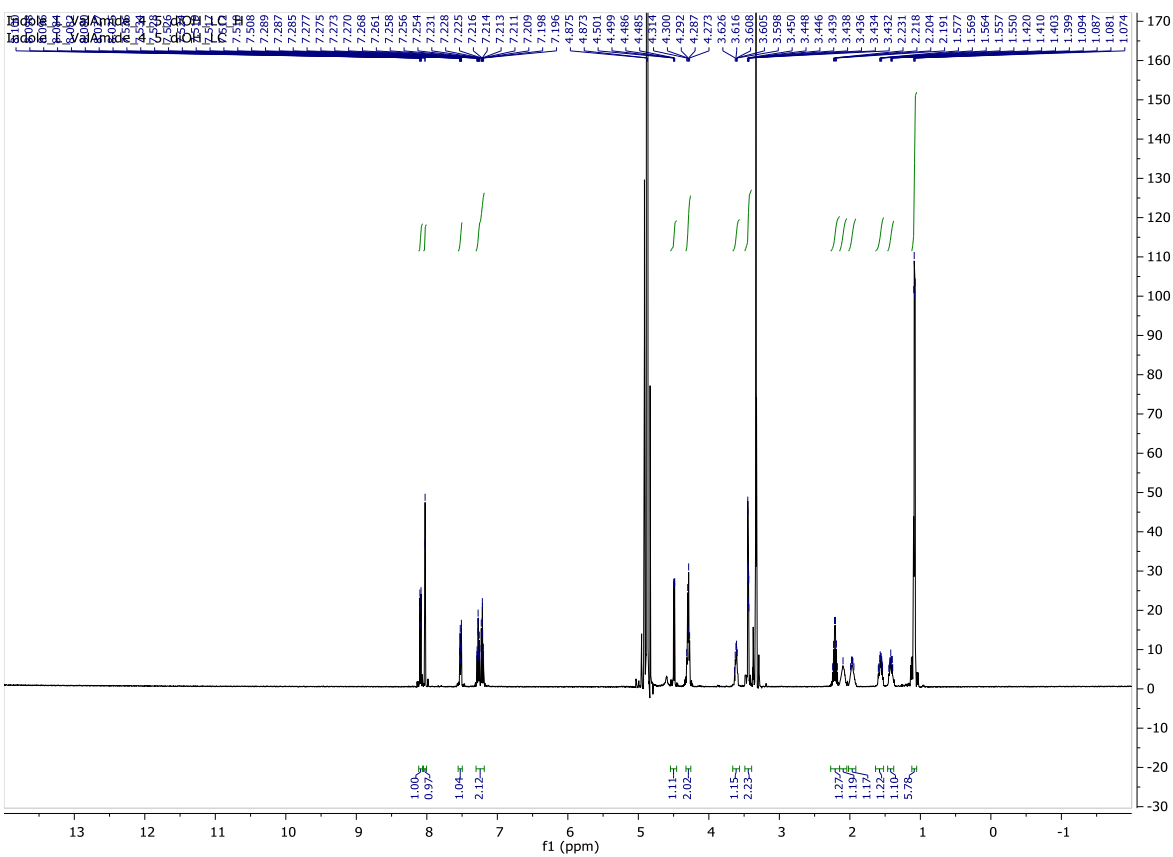
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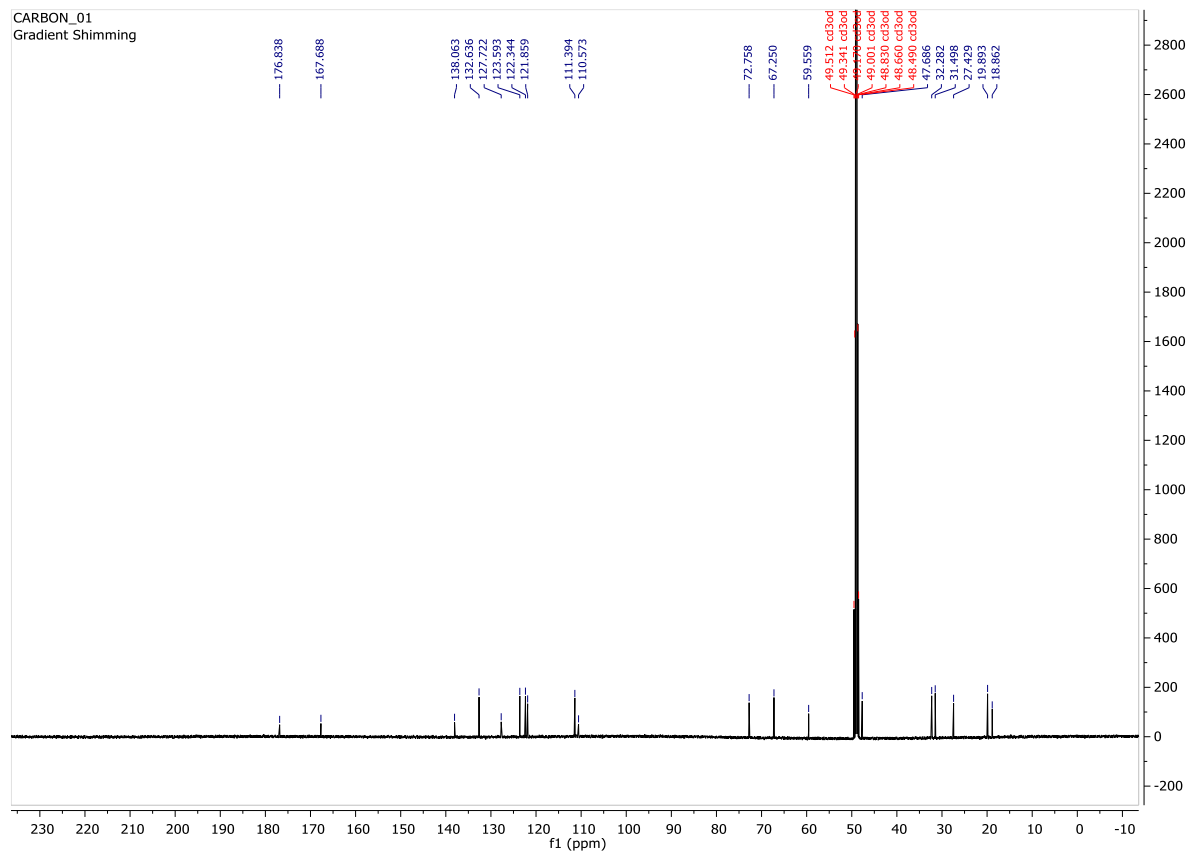
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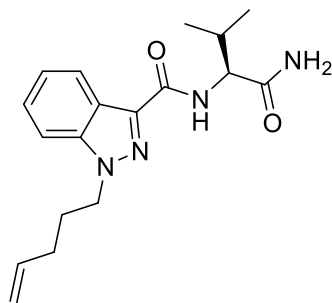
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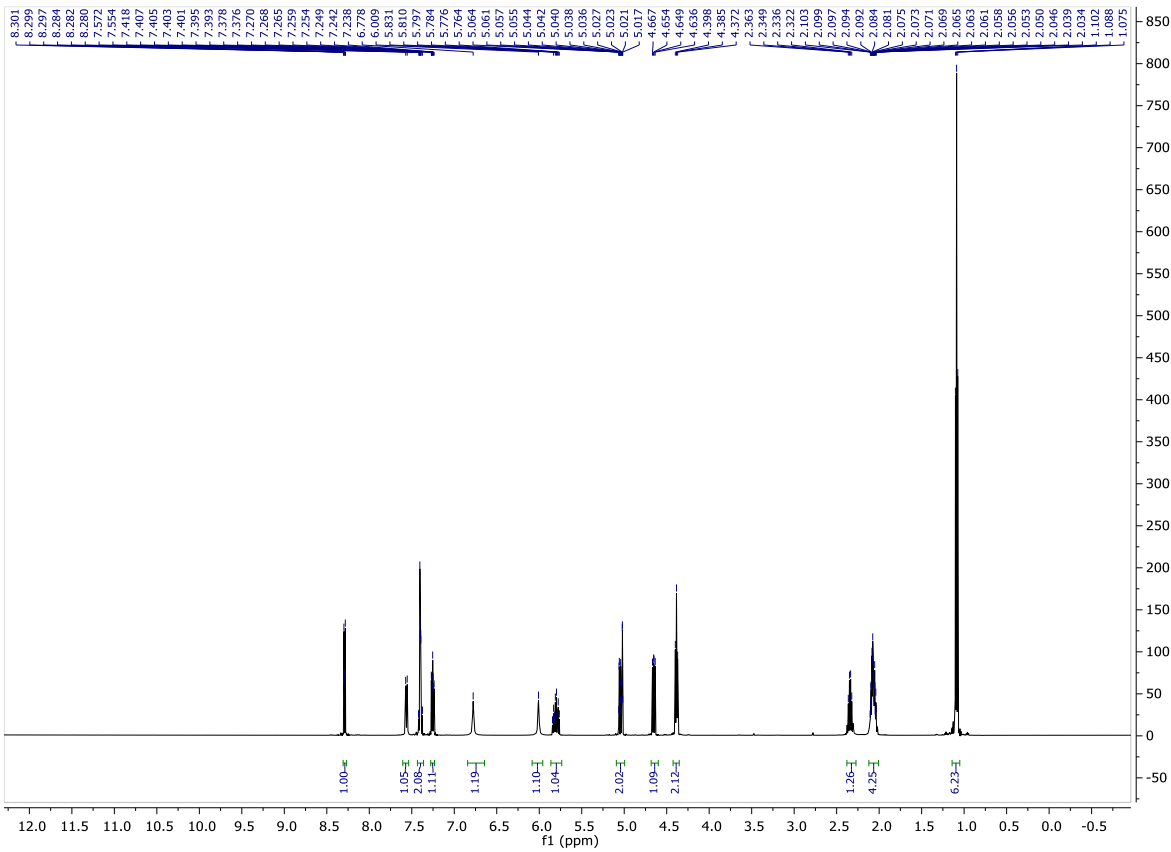
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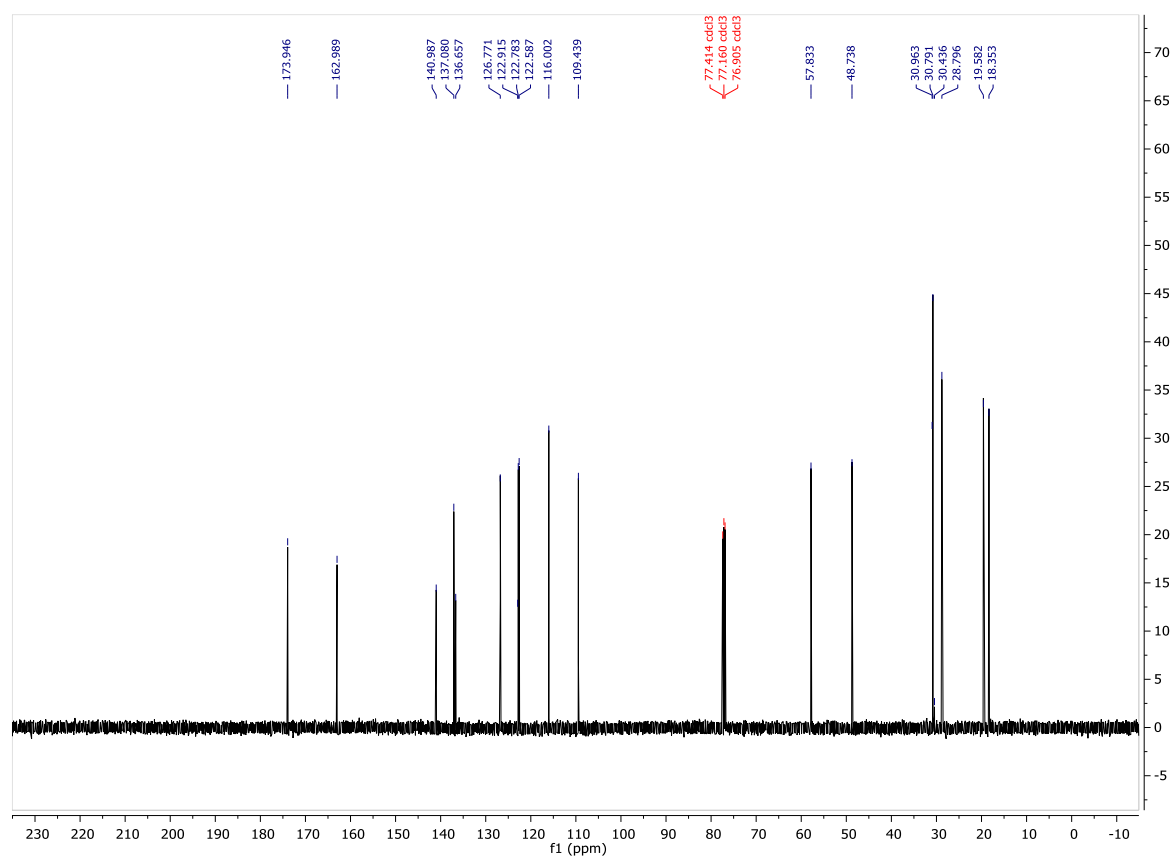
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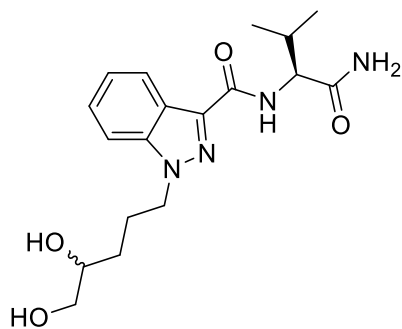
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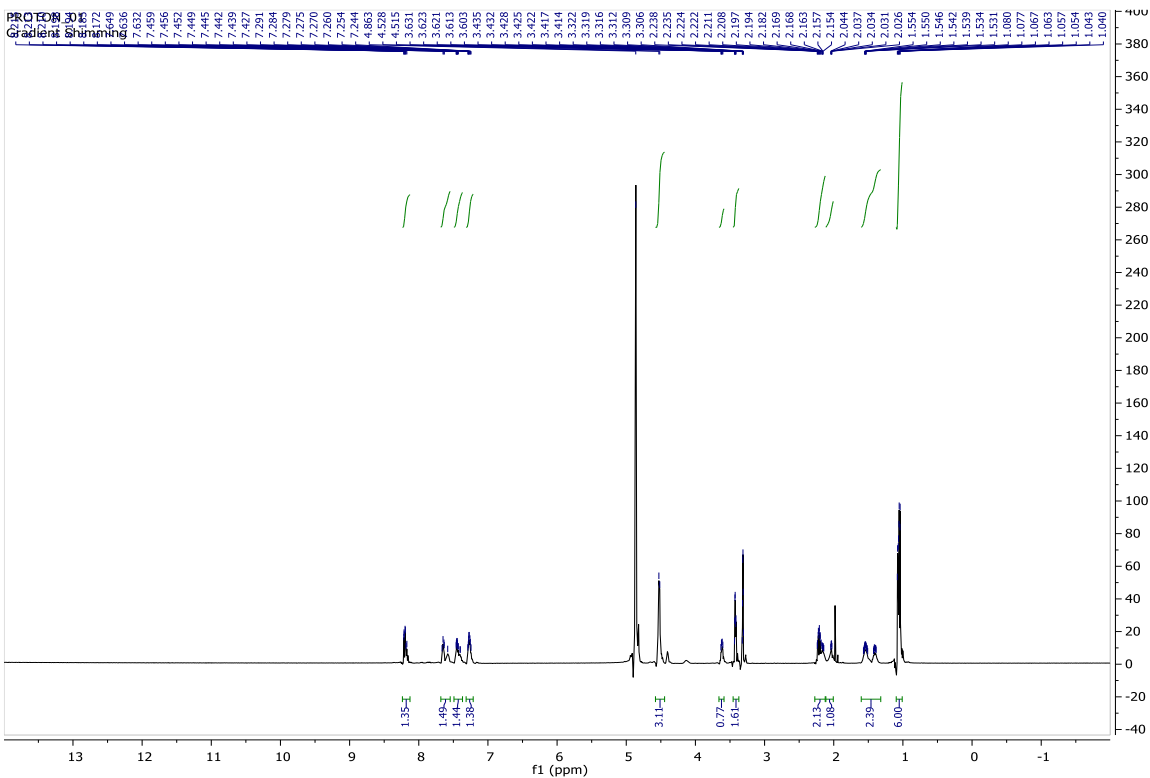
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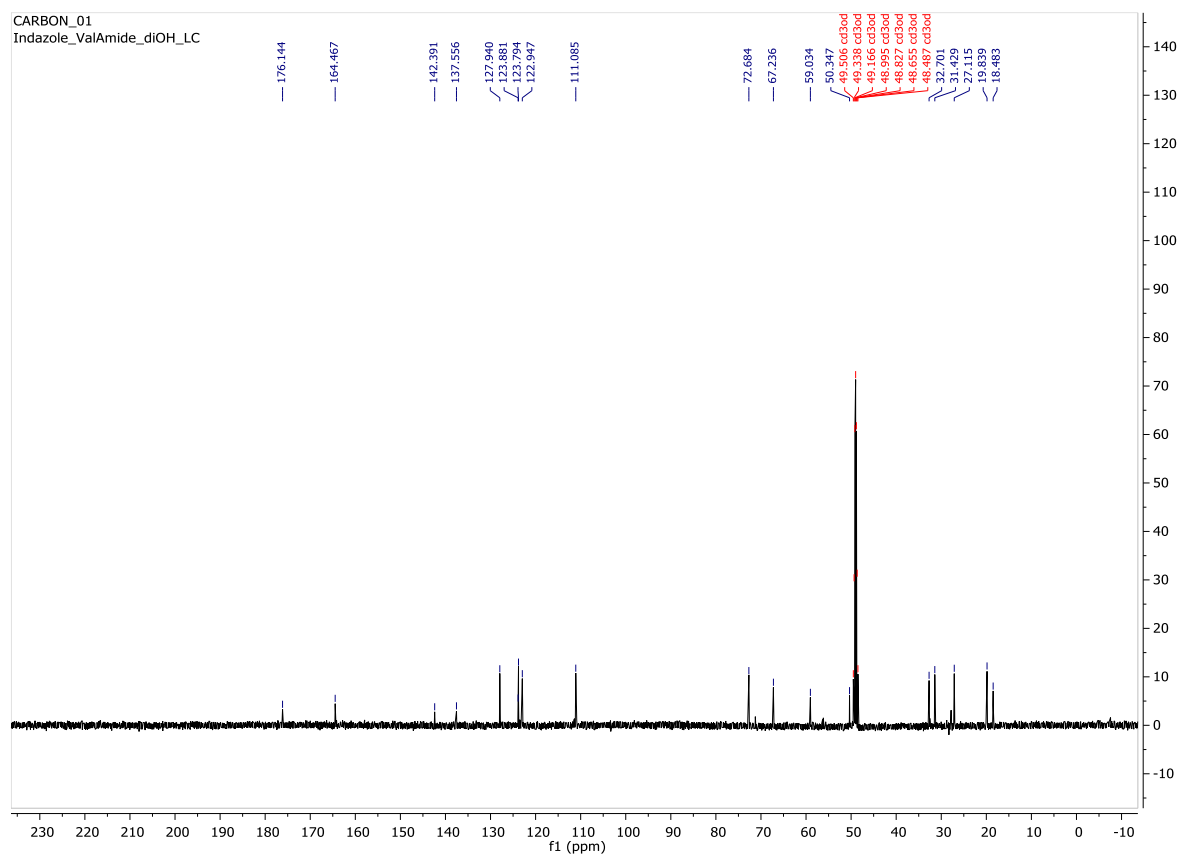
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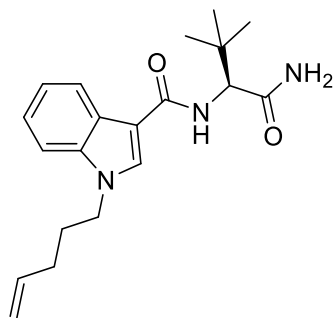
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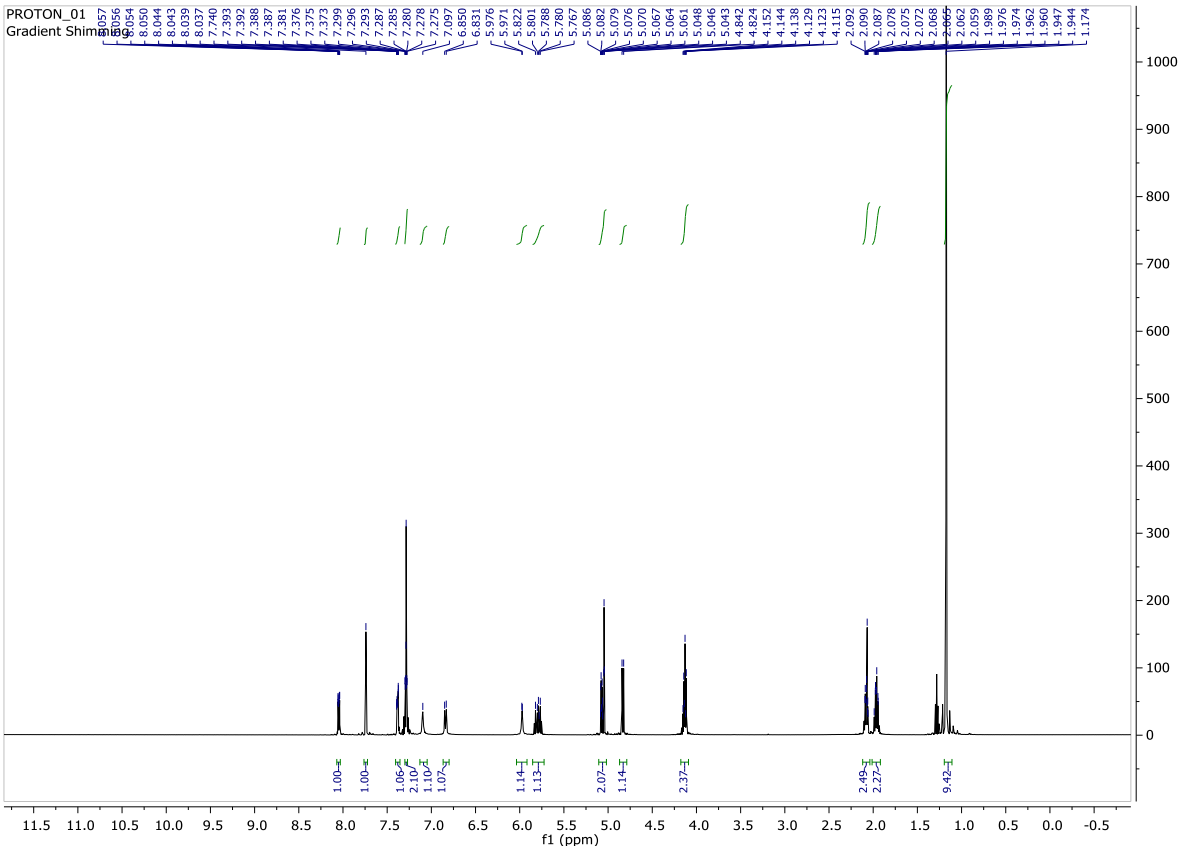
^{13}C -NMR Spectrum



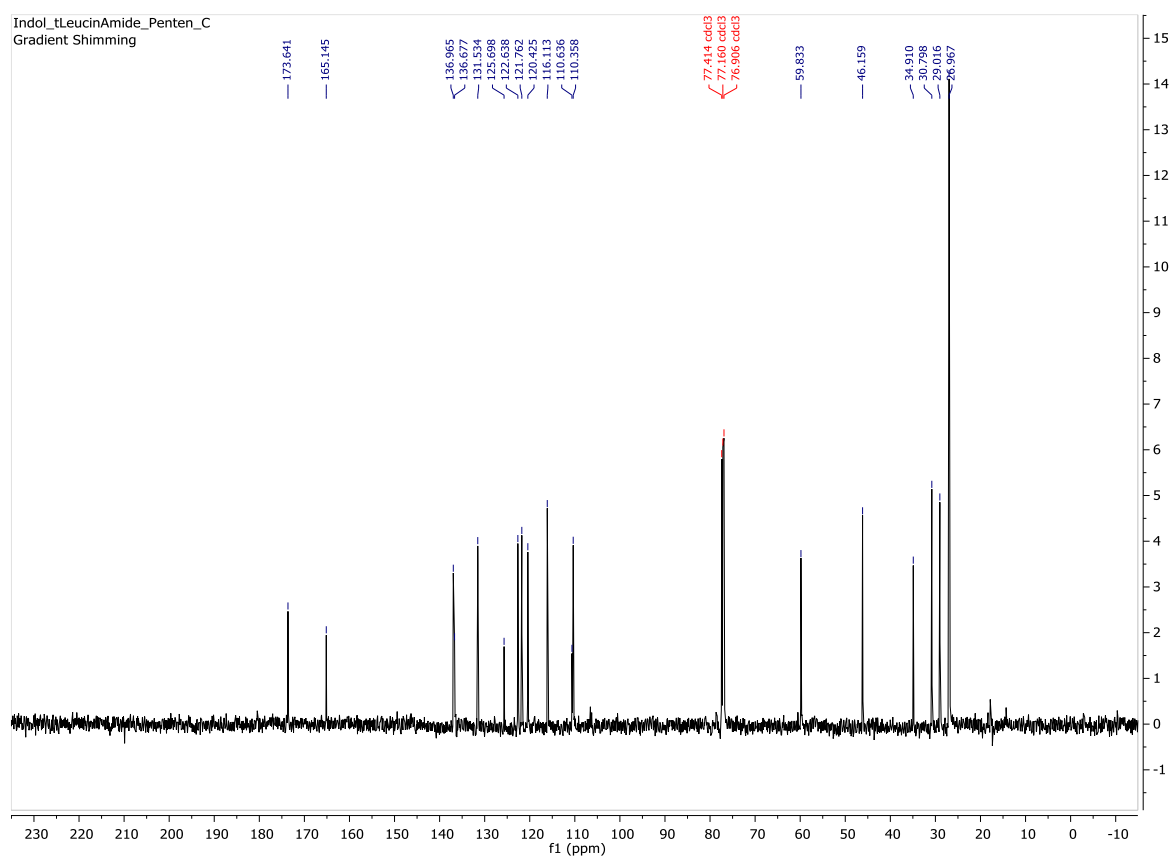
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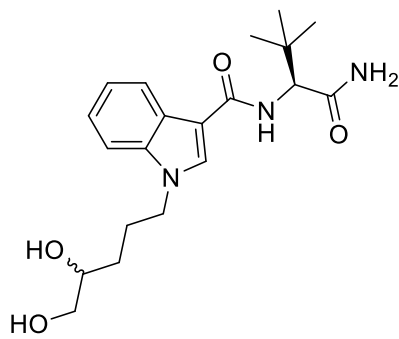
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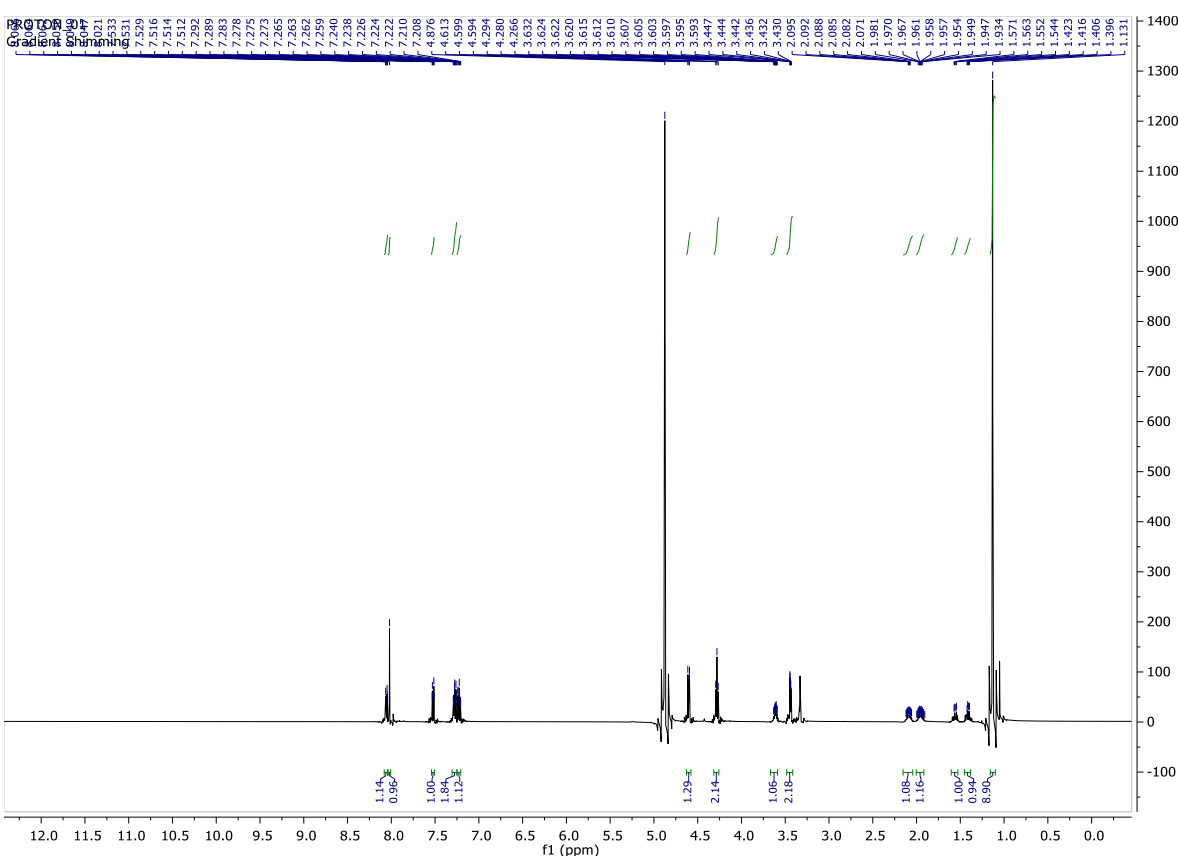
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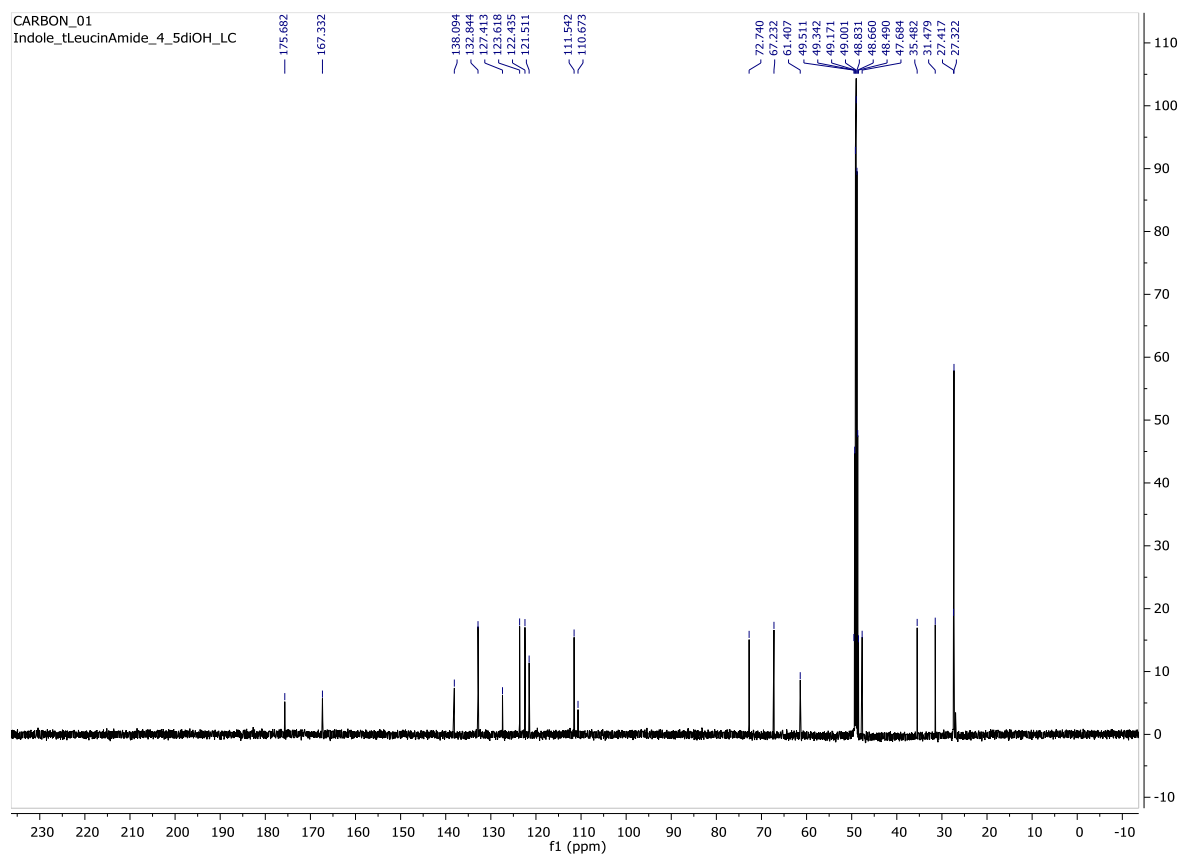
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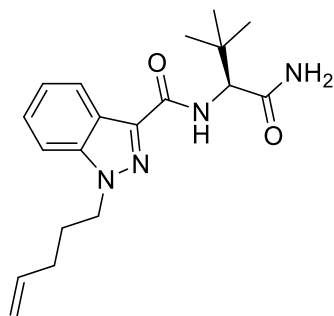
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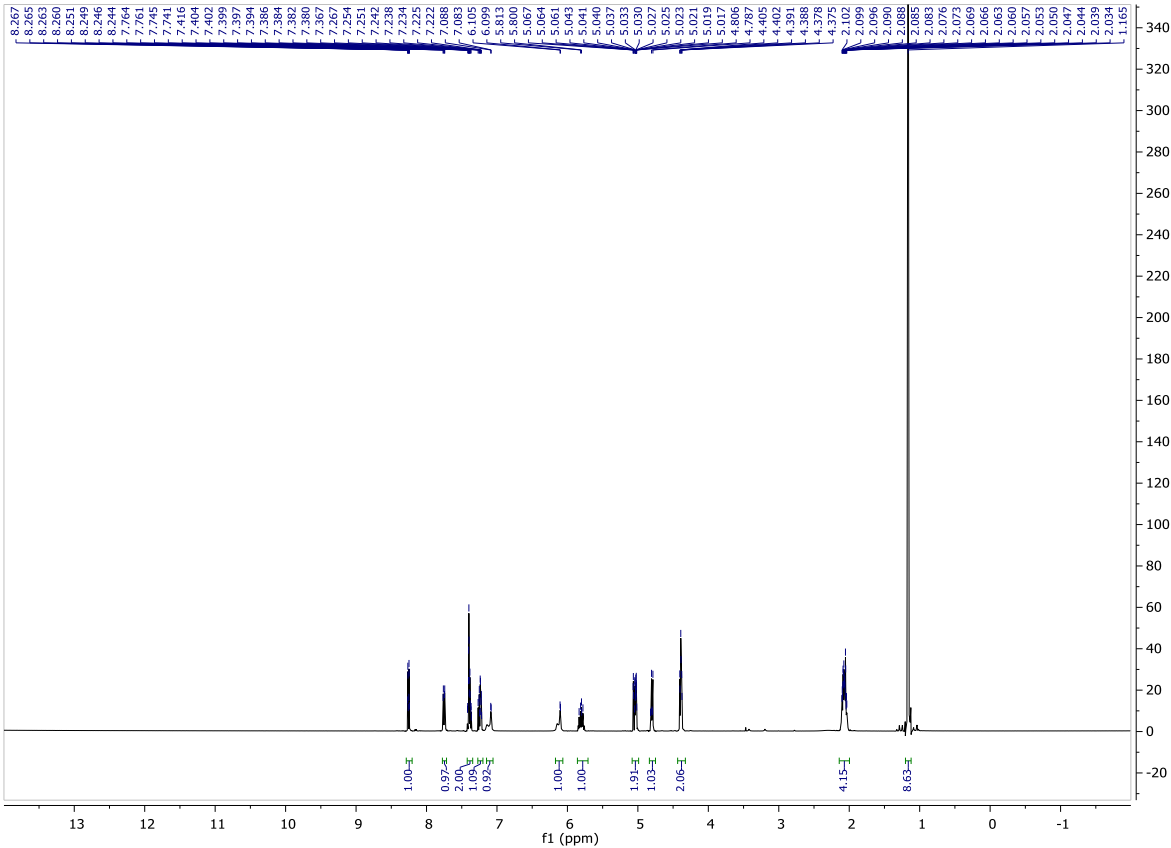
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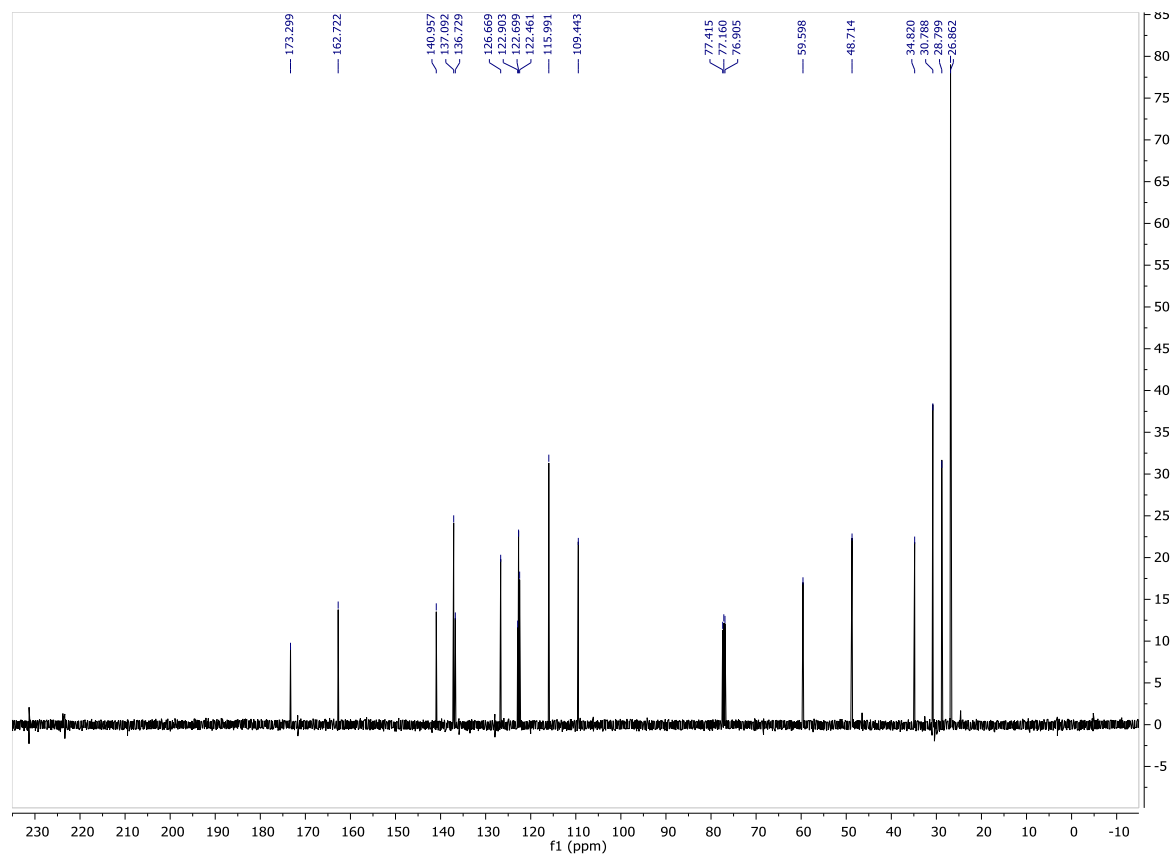
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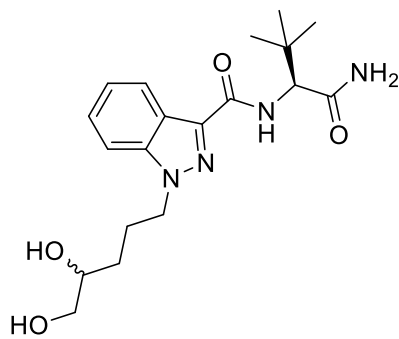
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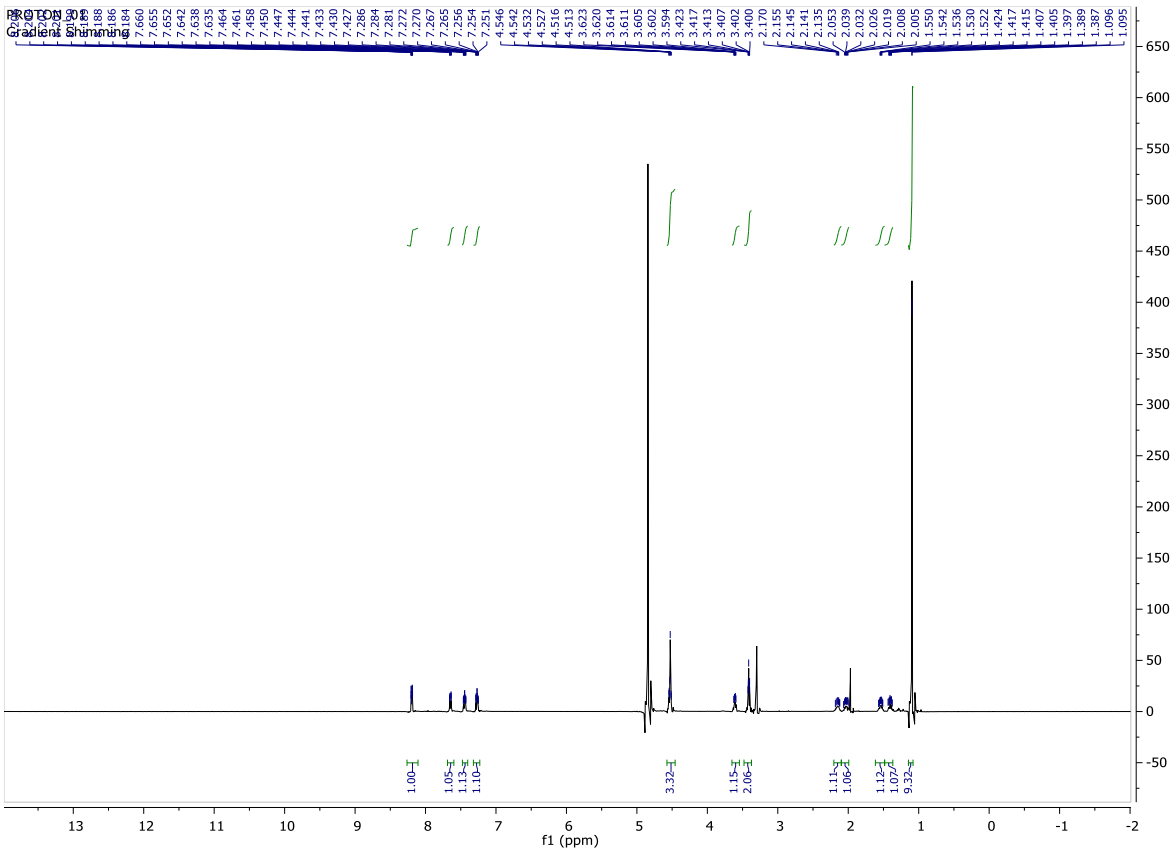
^{13}C -NMR Spectrum



ADB-4en-PINACA dihydrodiol (J2)



¹H-NMR Spectrum



^{13}C -NMR Spectrum

