Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

SUPPORTING INFORMATION

Base-modified NAD and AMP derivatives and their activity against bacterial DNA ligases

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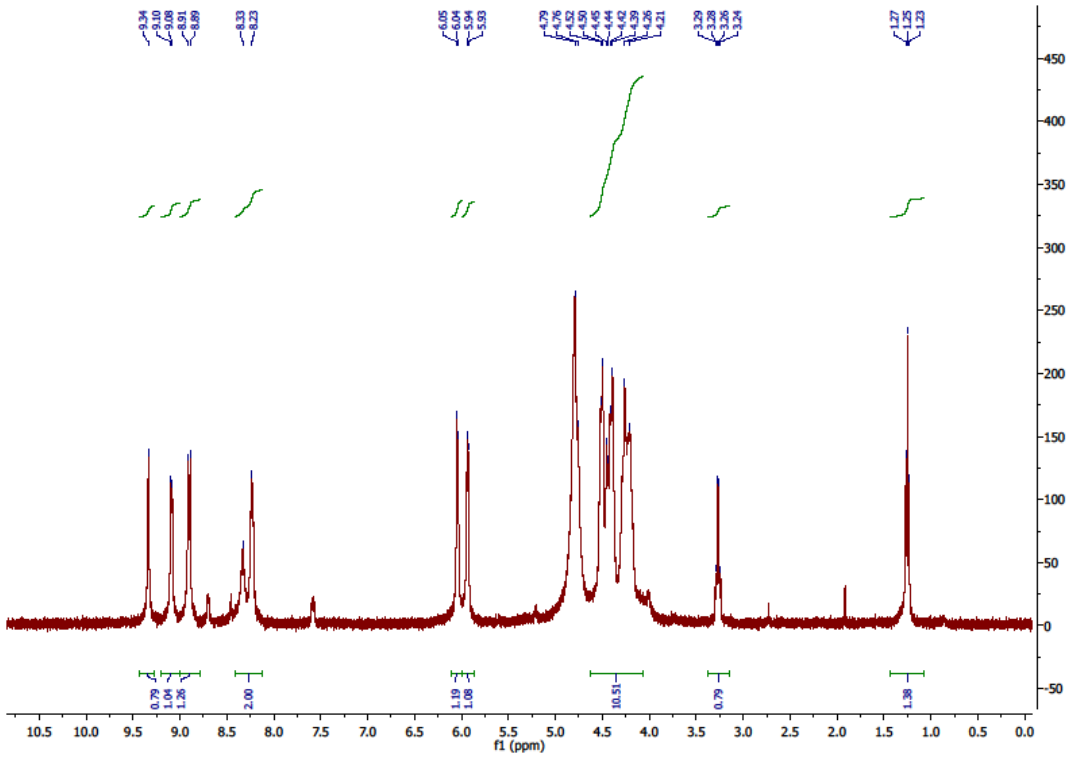
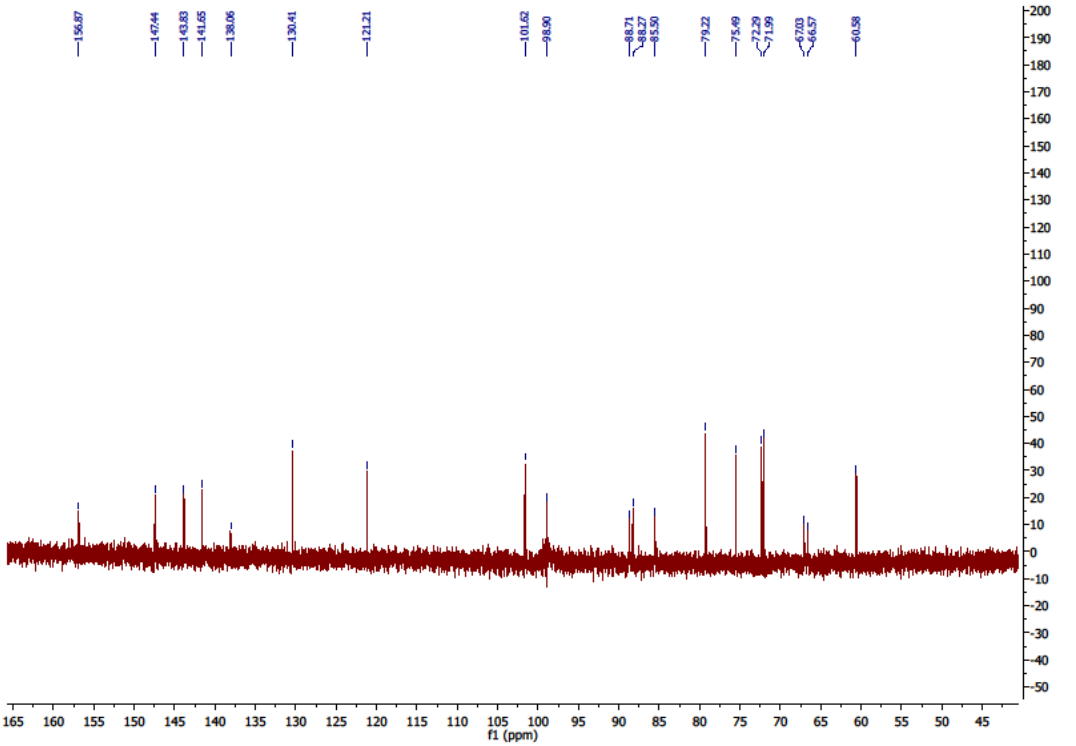
CONTENT

(1) NMR spectra

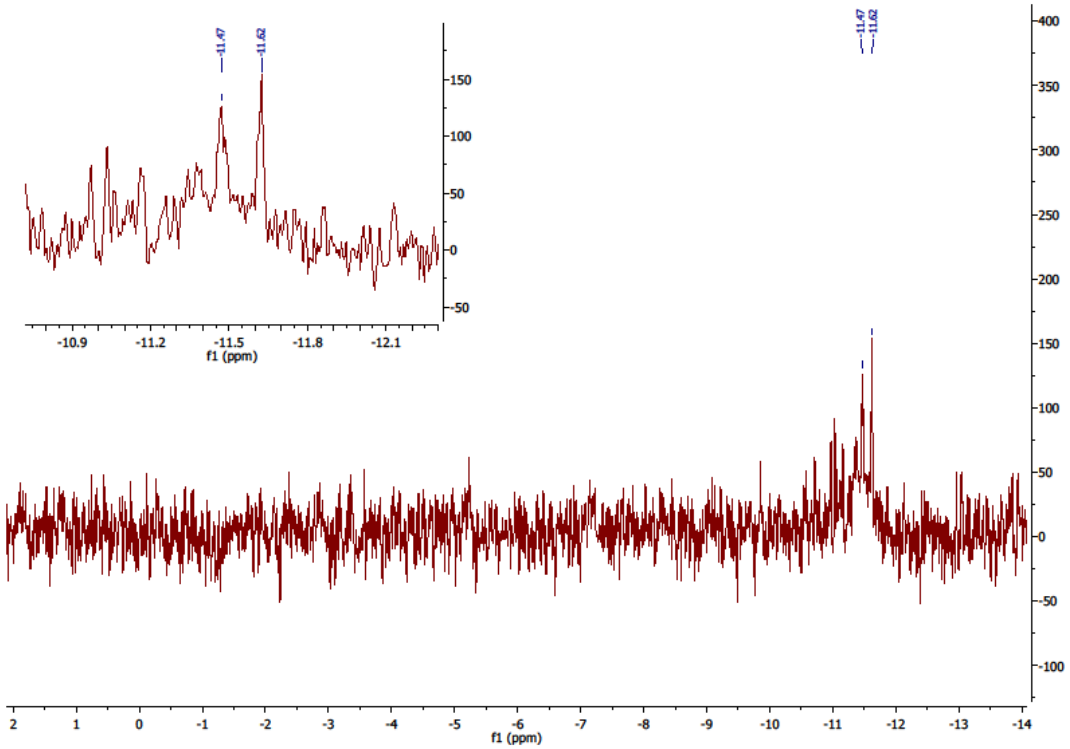
^{1}H NMR: 1a



^{13}C NMR: 1a



^{31}P NMR: 1a



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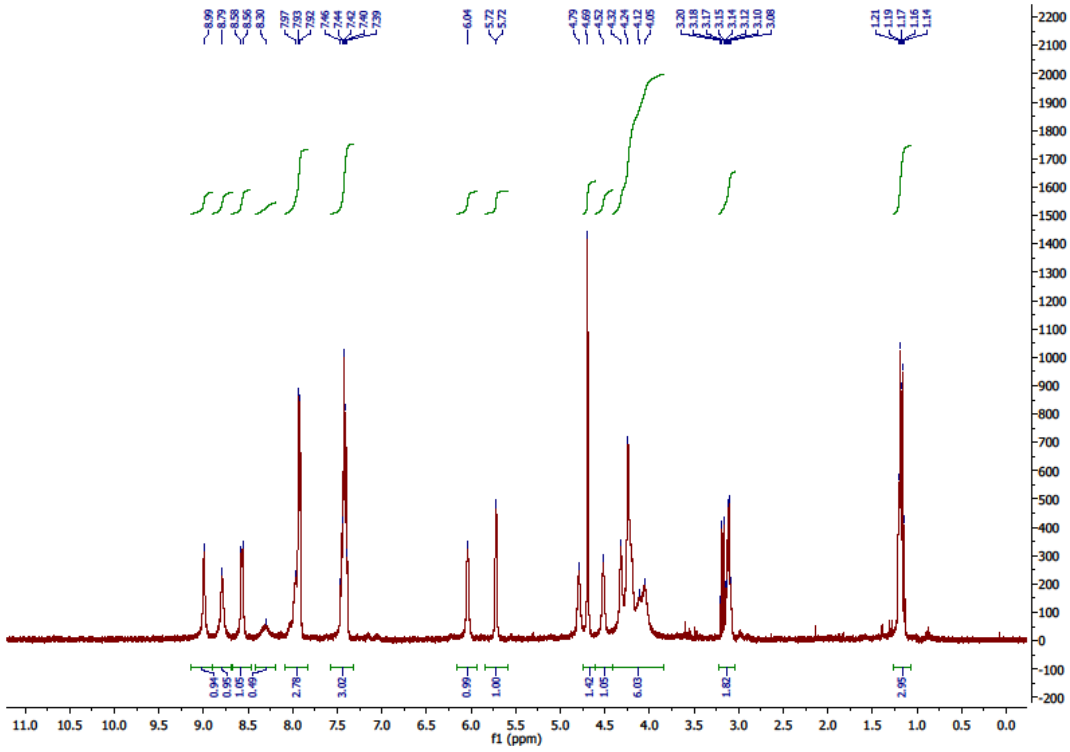

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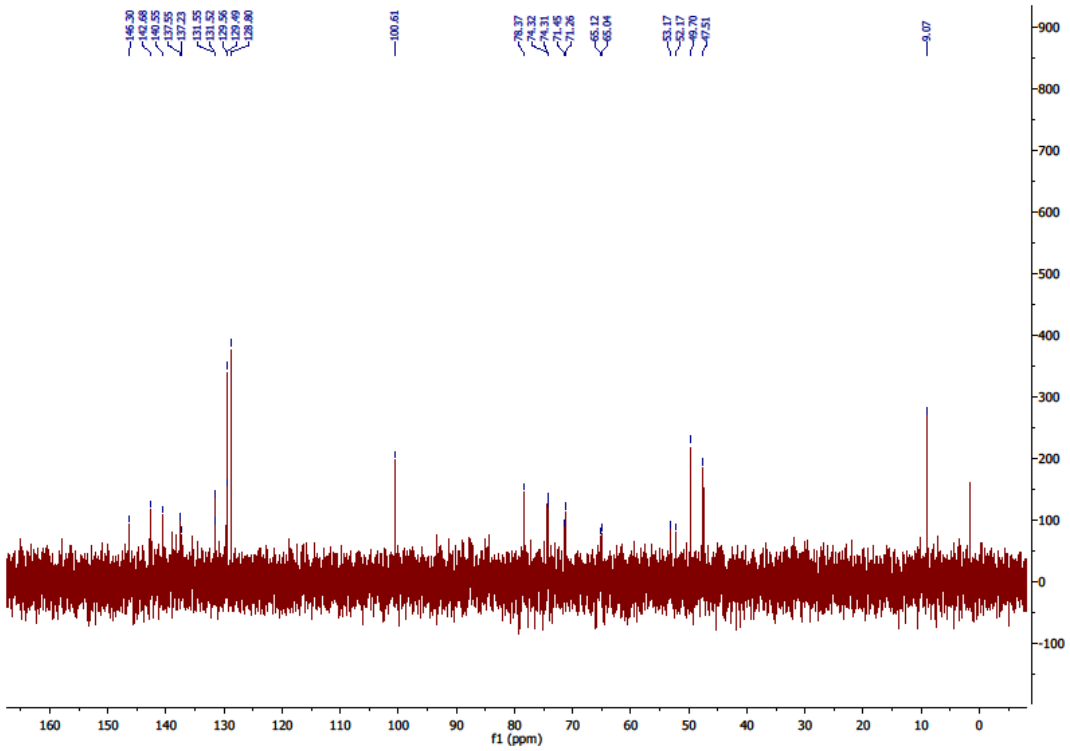
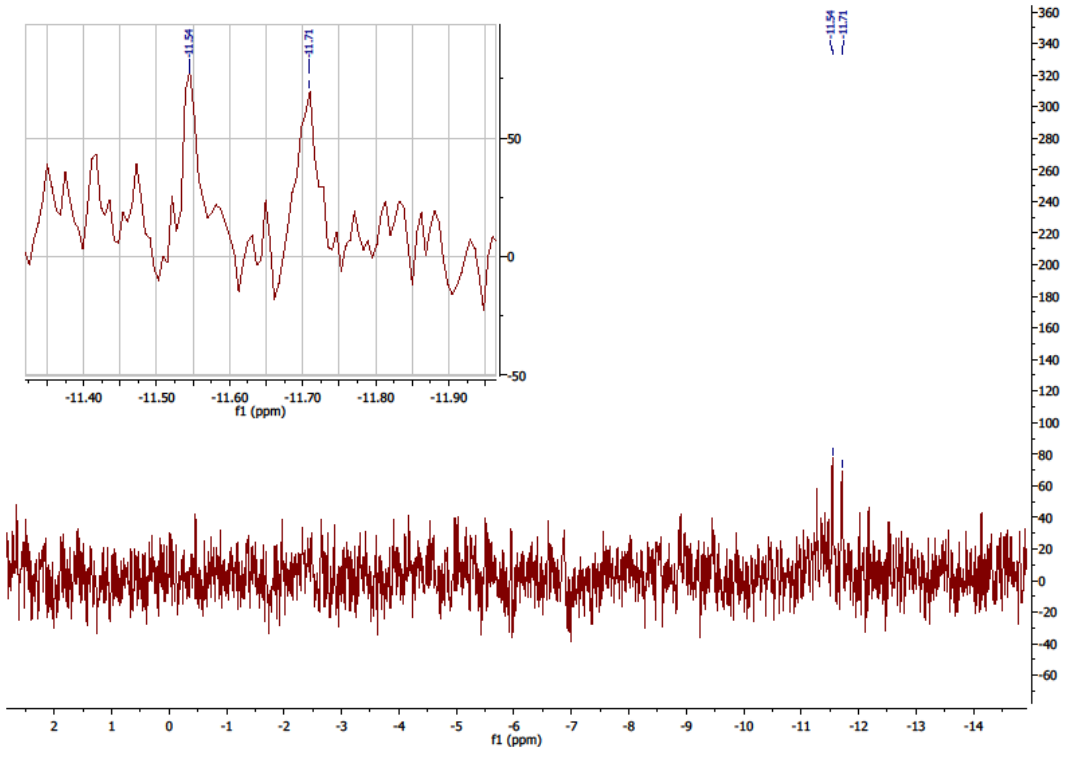


^{31}P NMR: 1b



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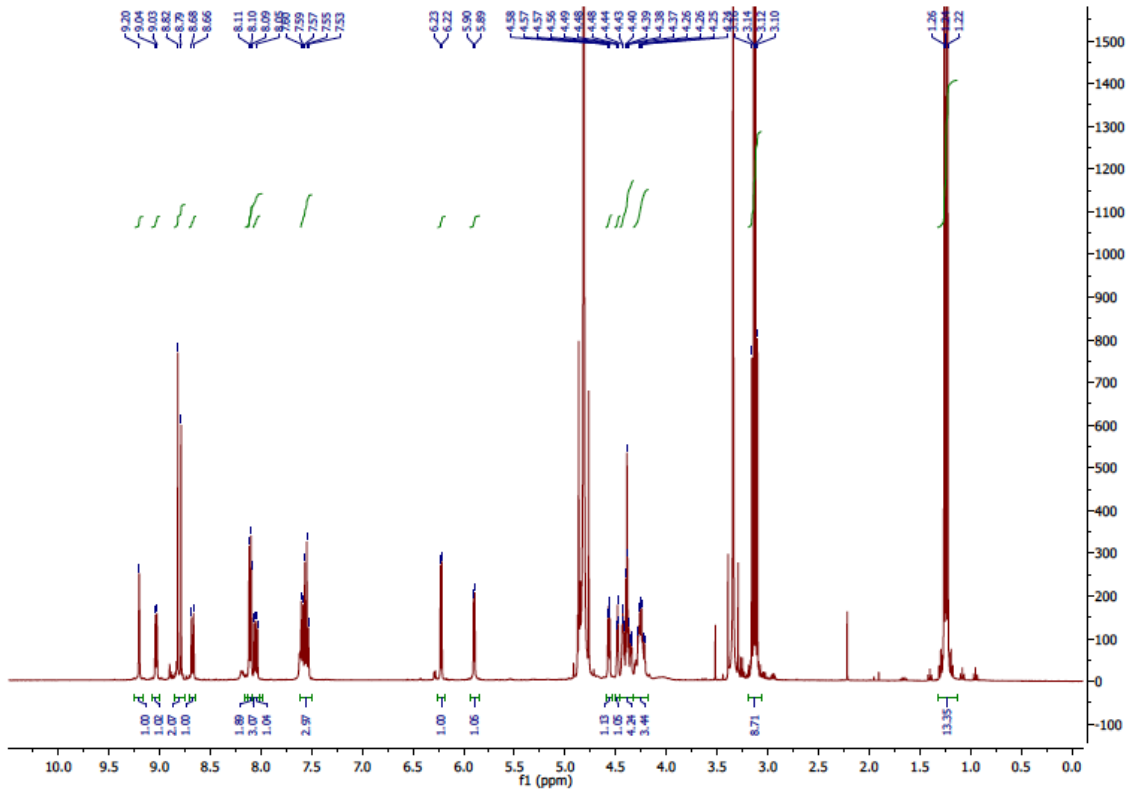

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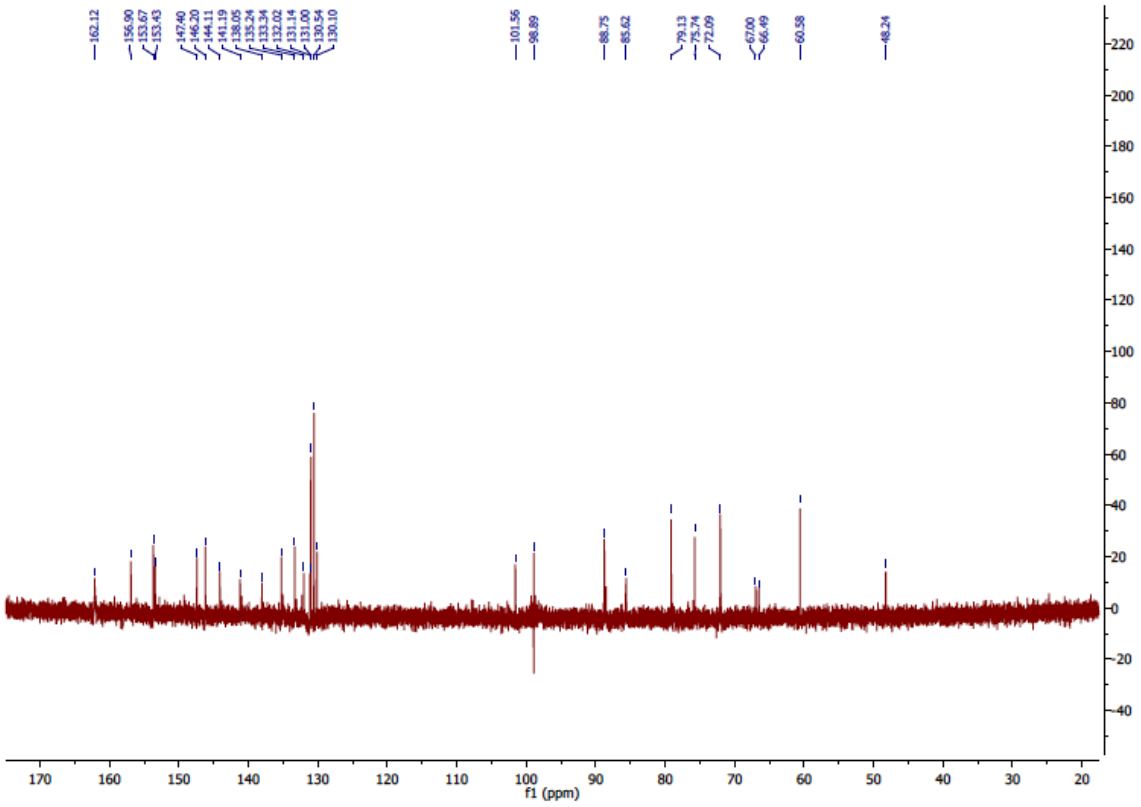

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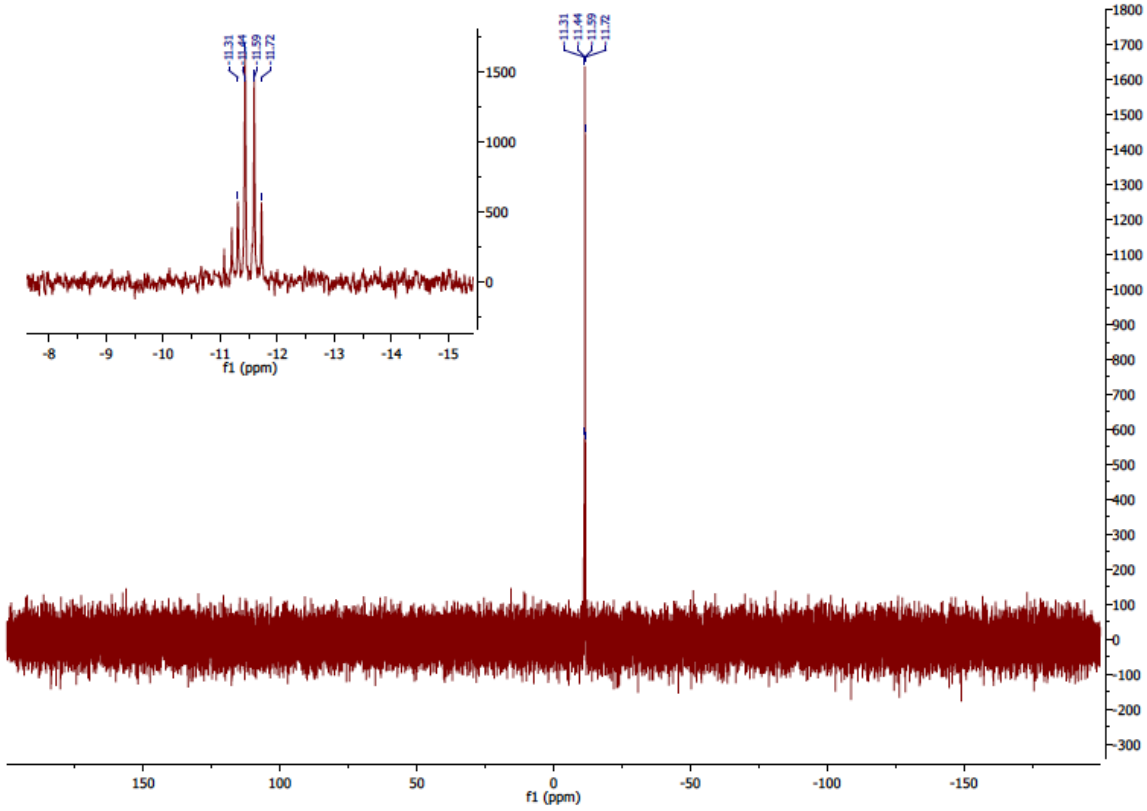

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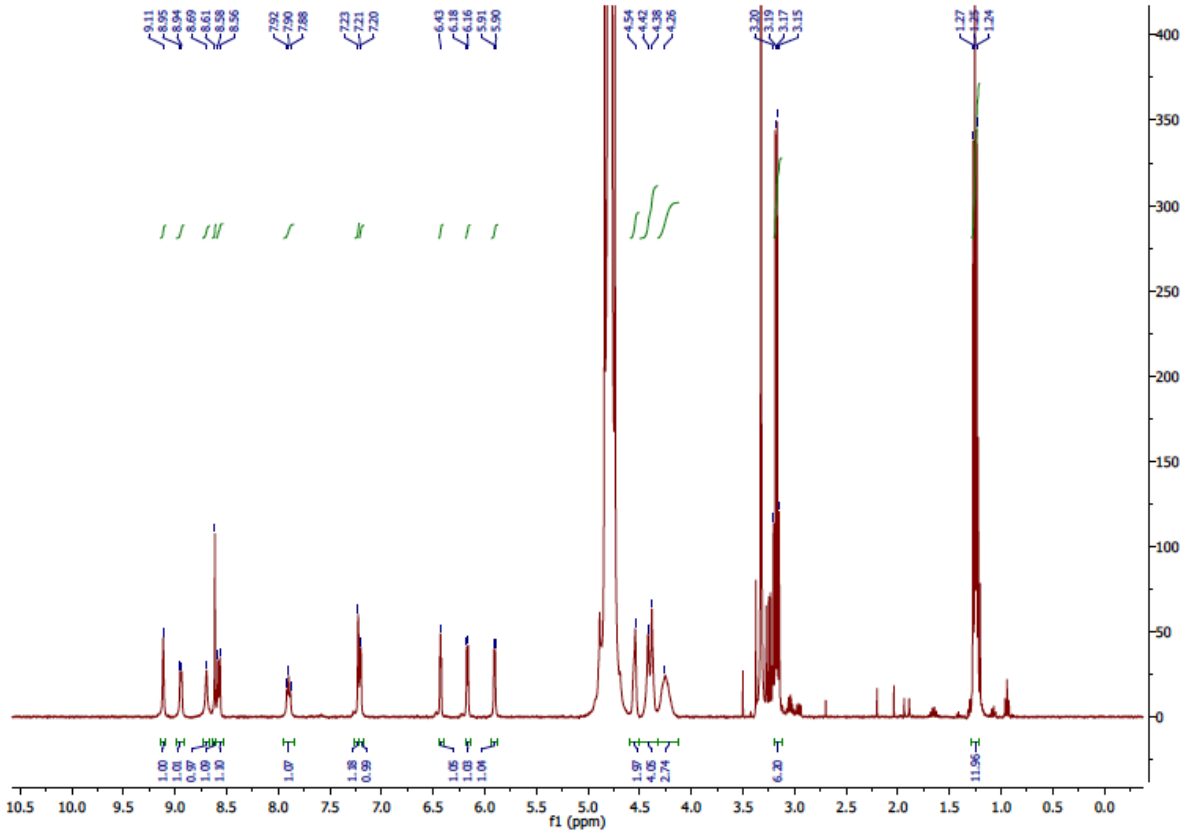

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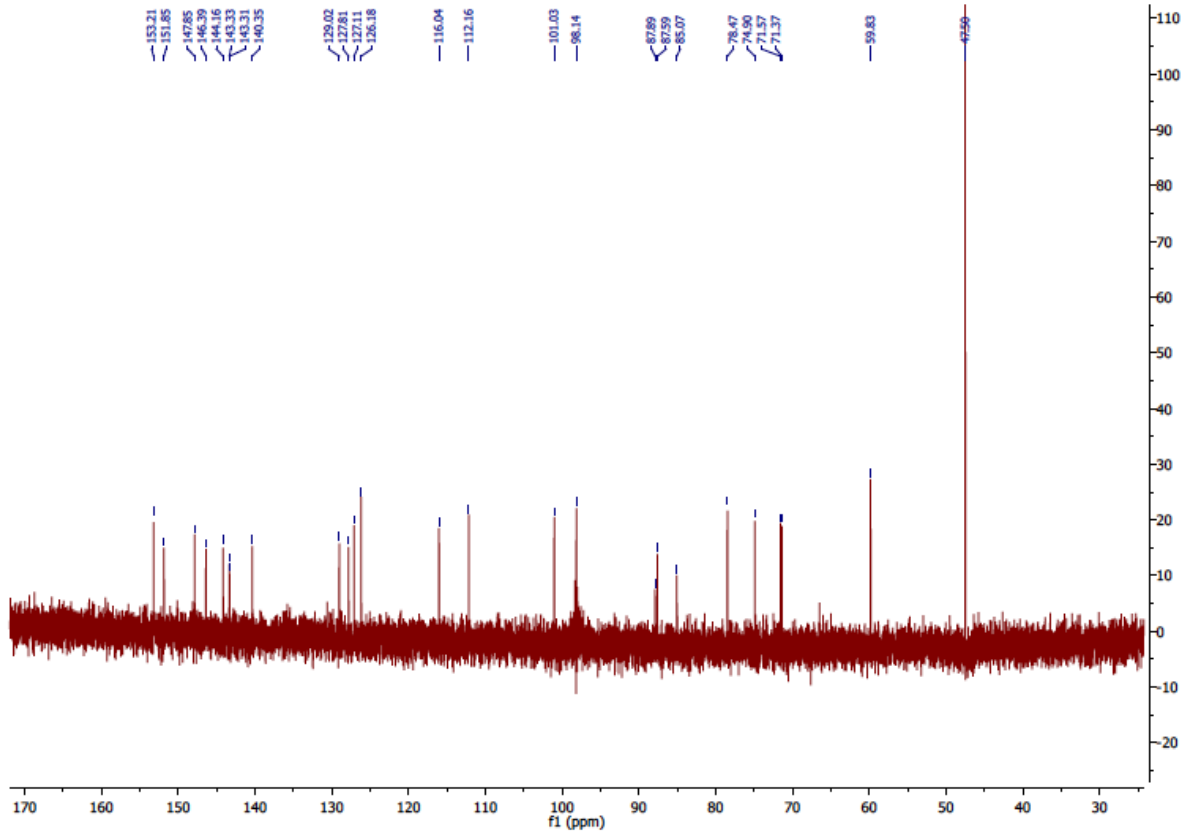

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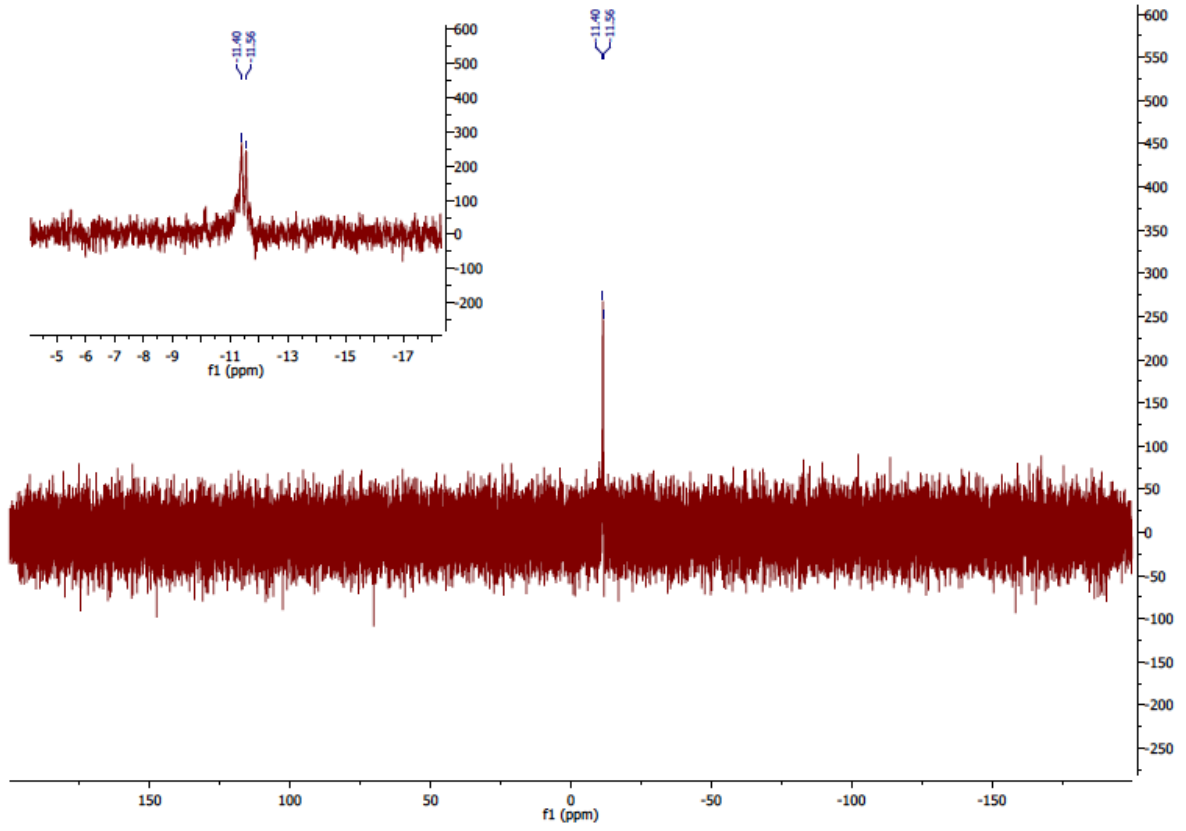

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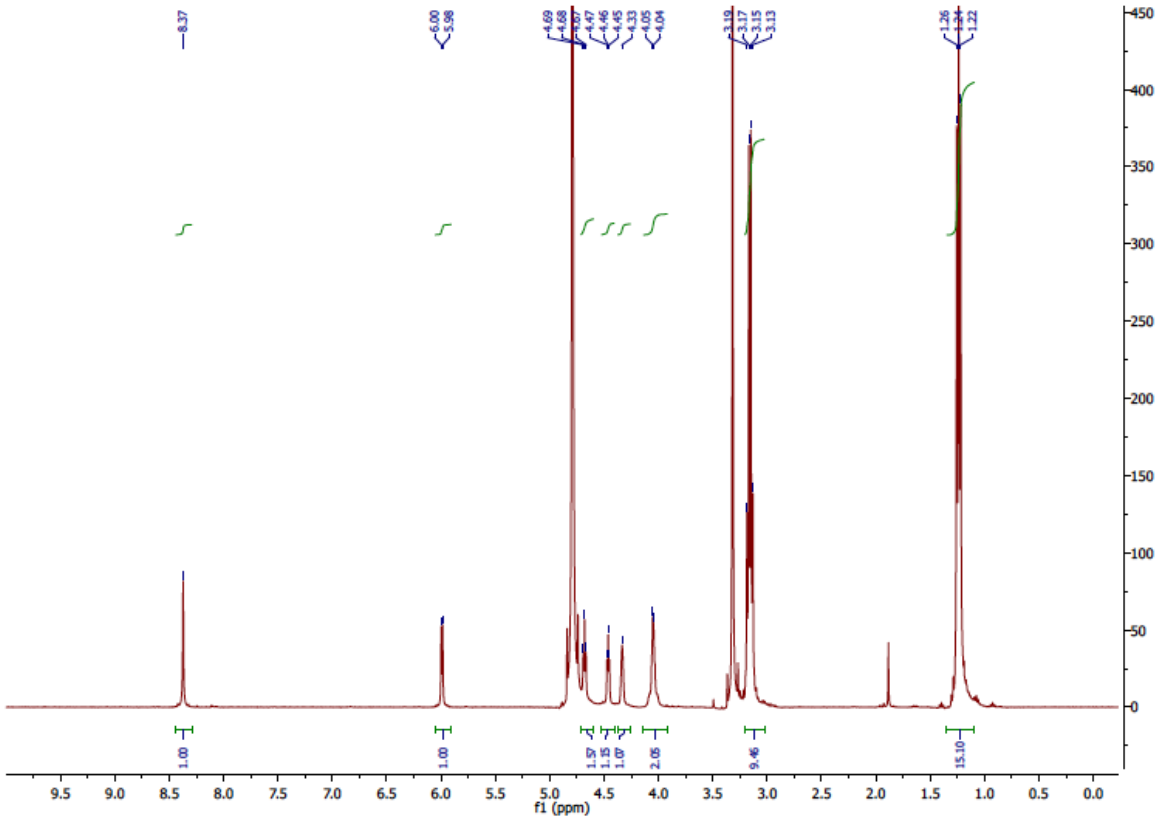

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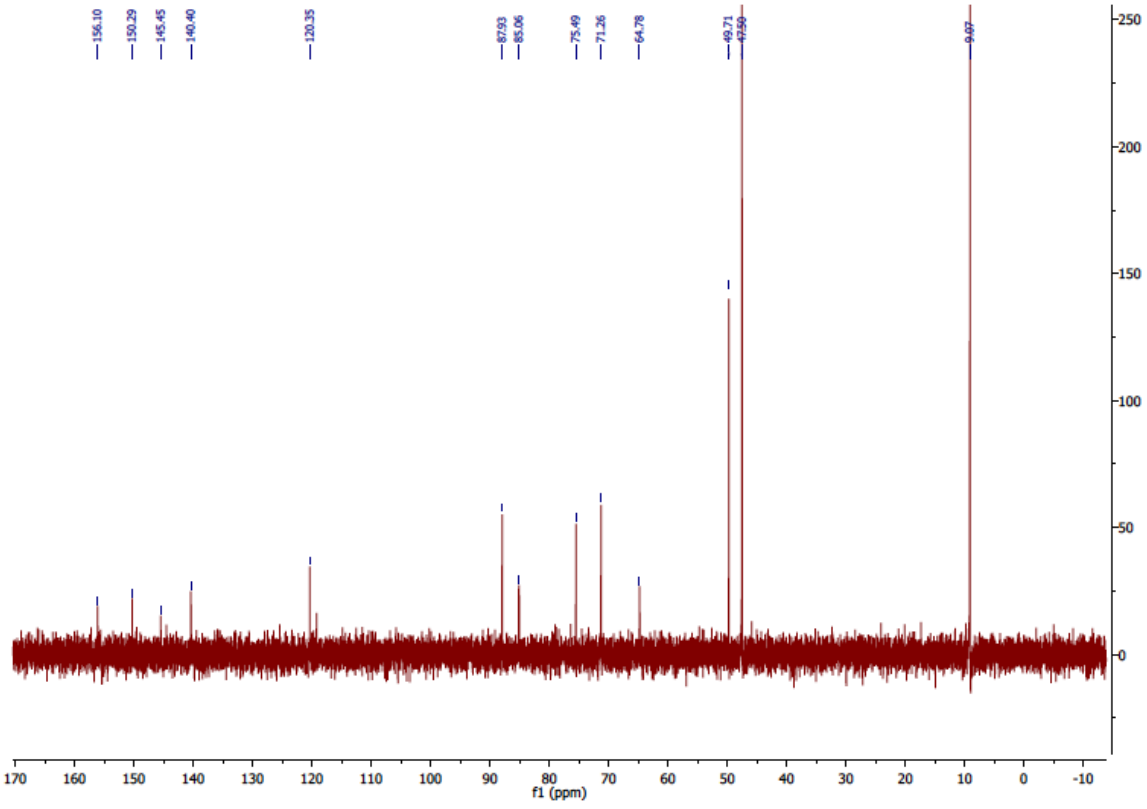

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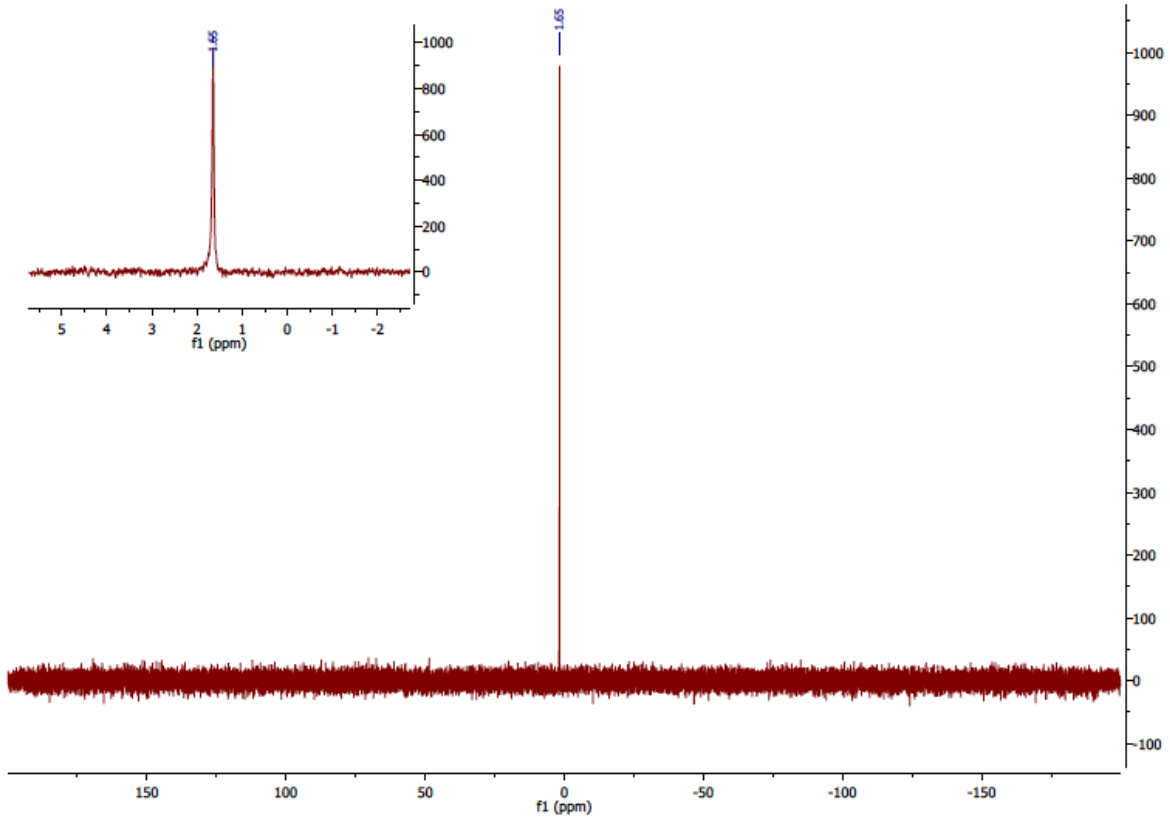

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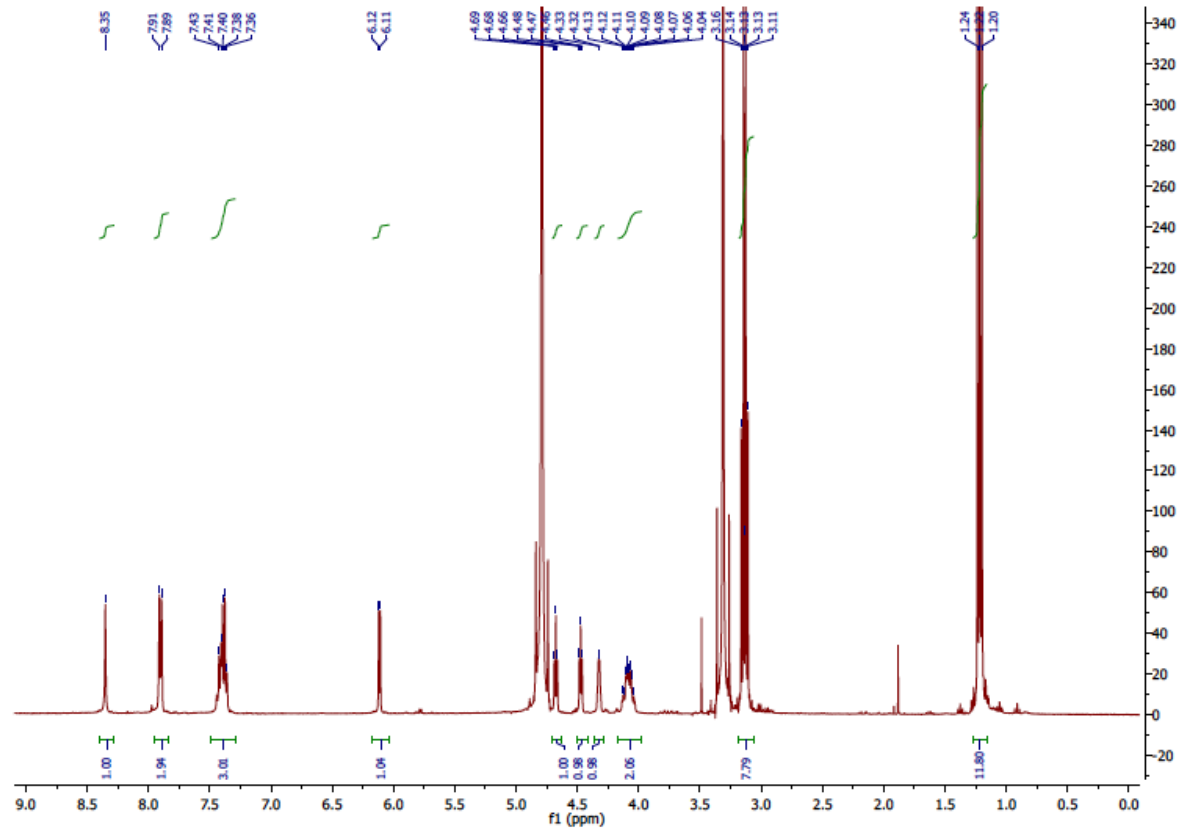

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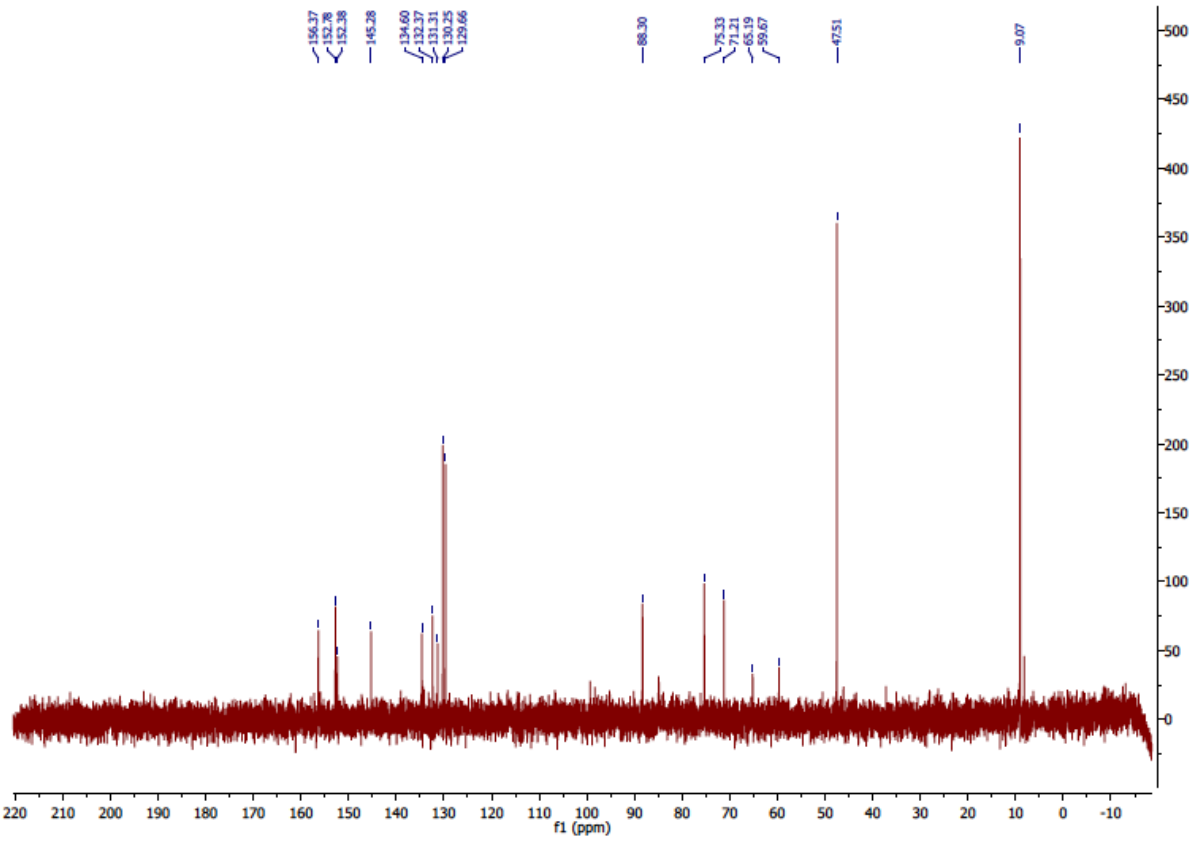

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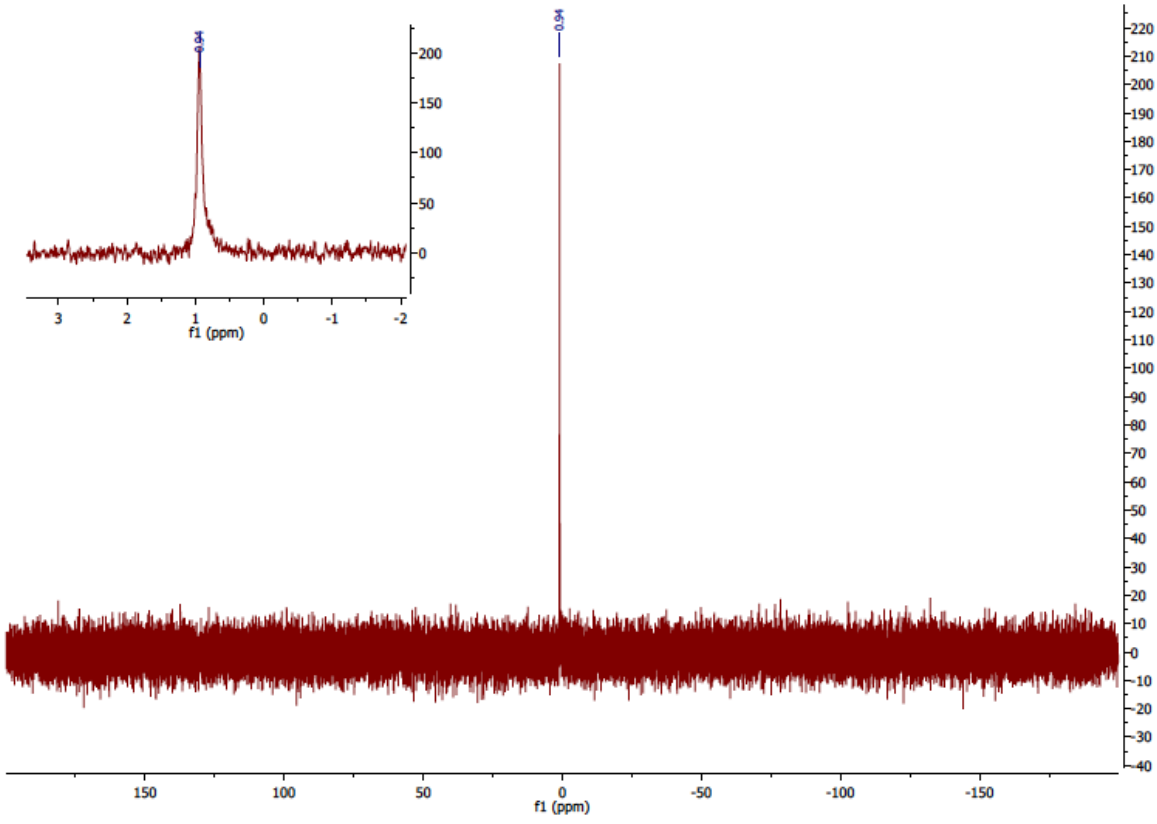

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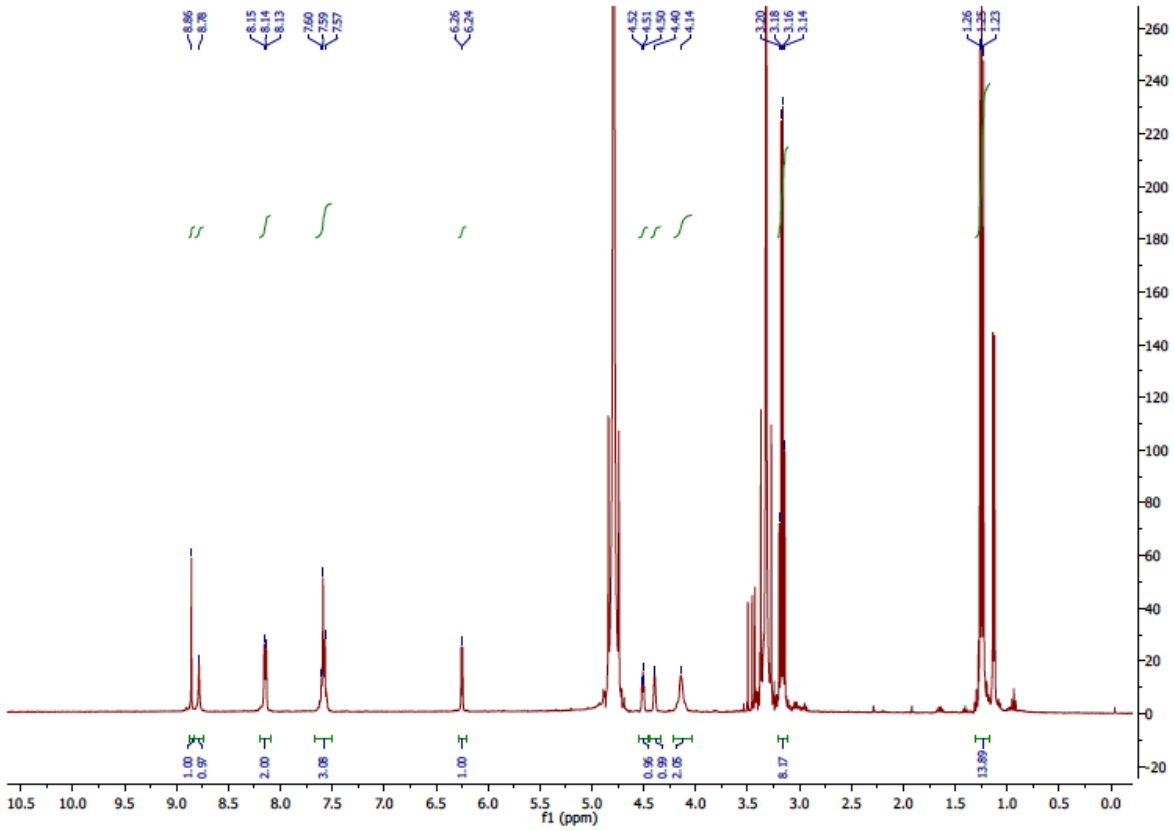

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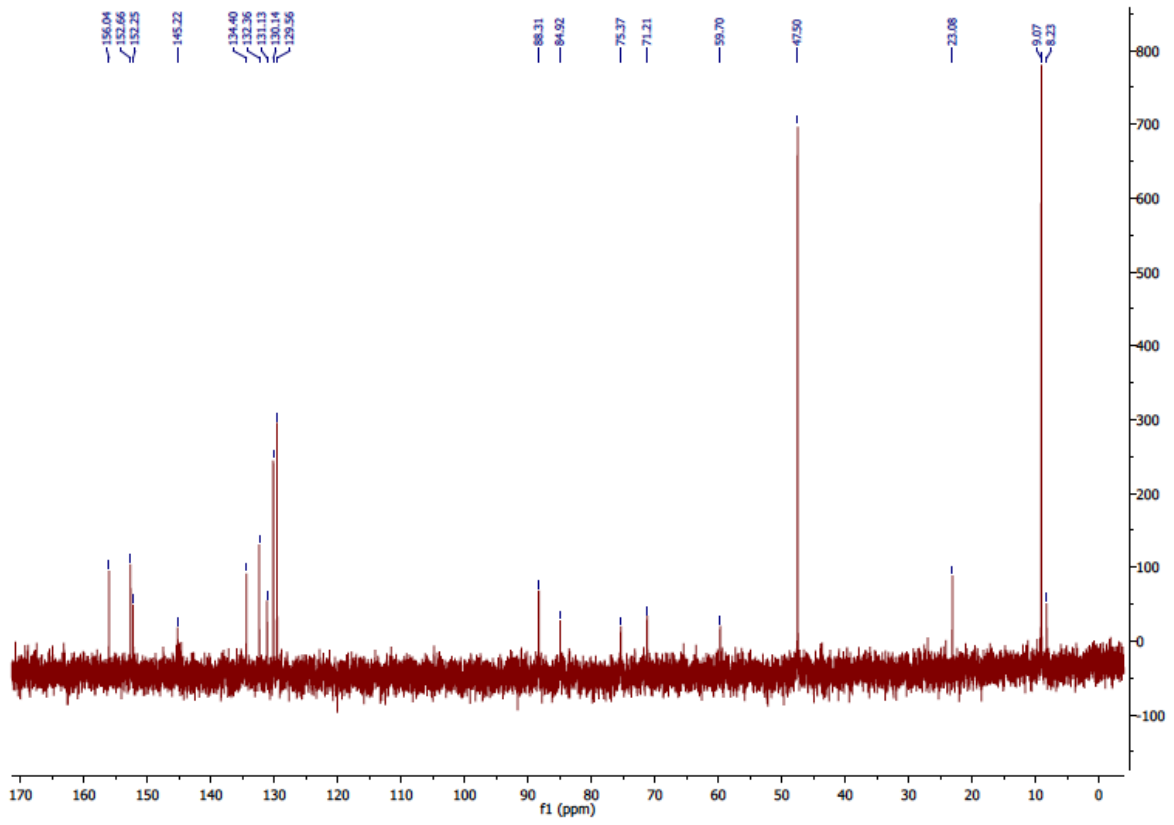

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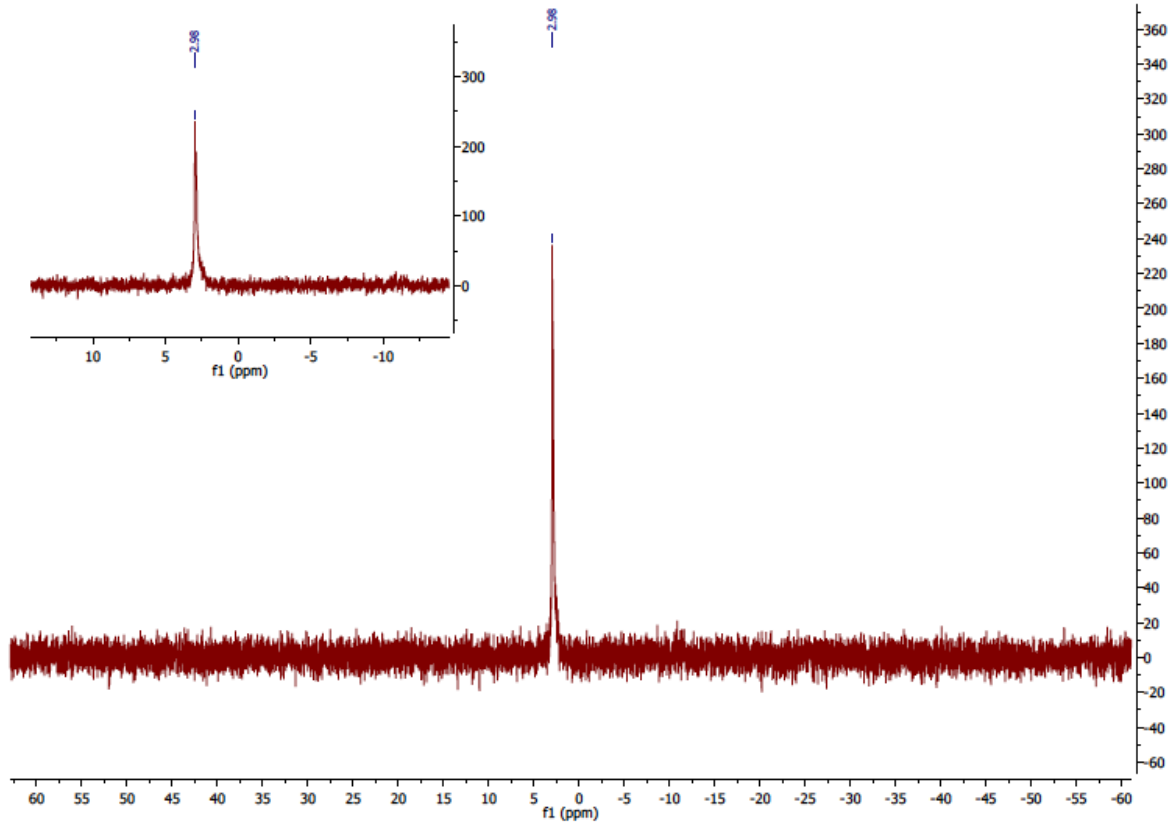

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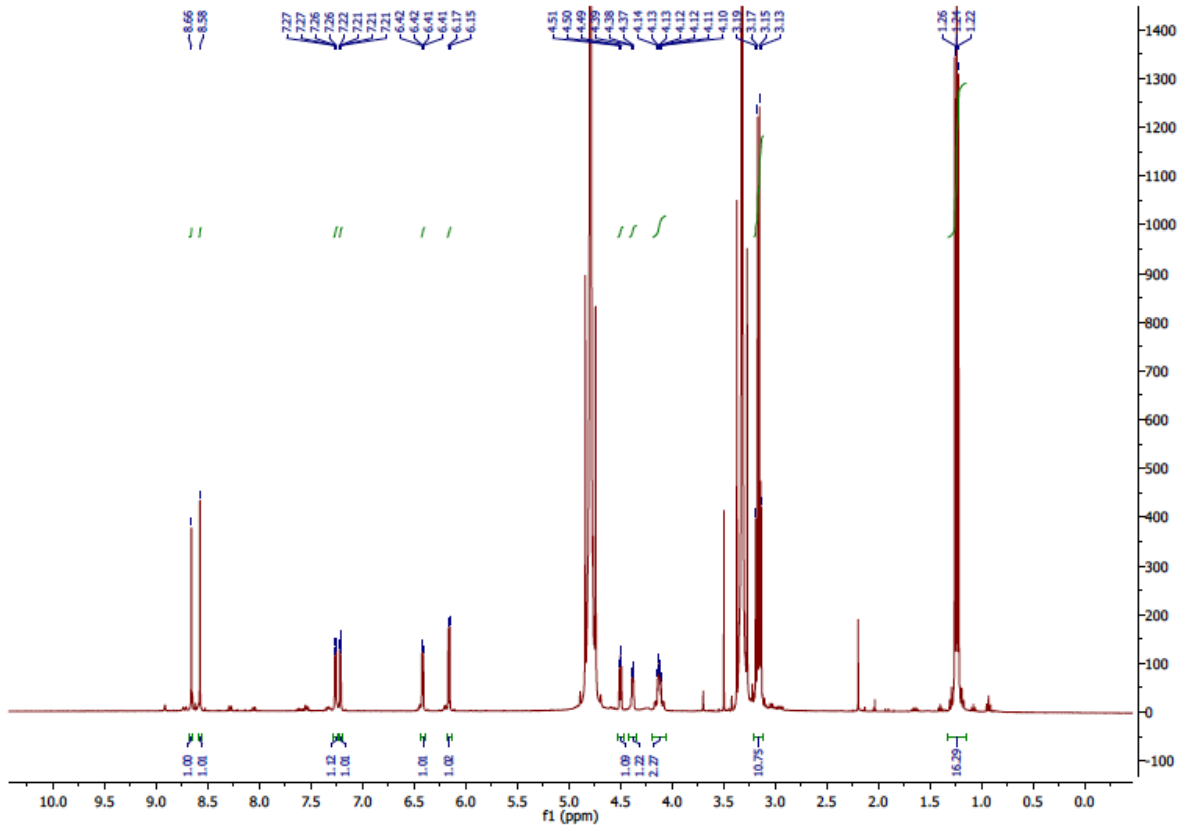

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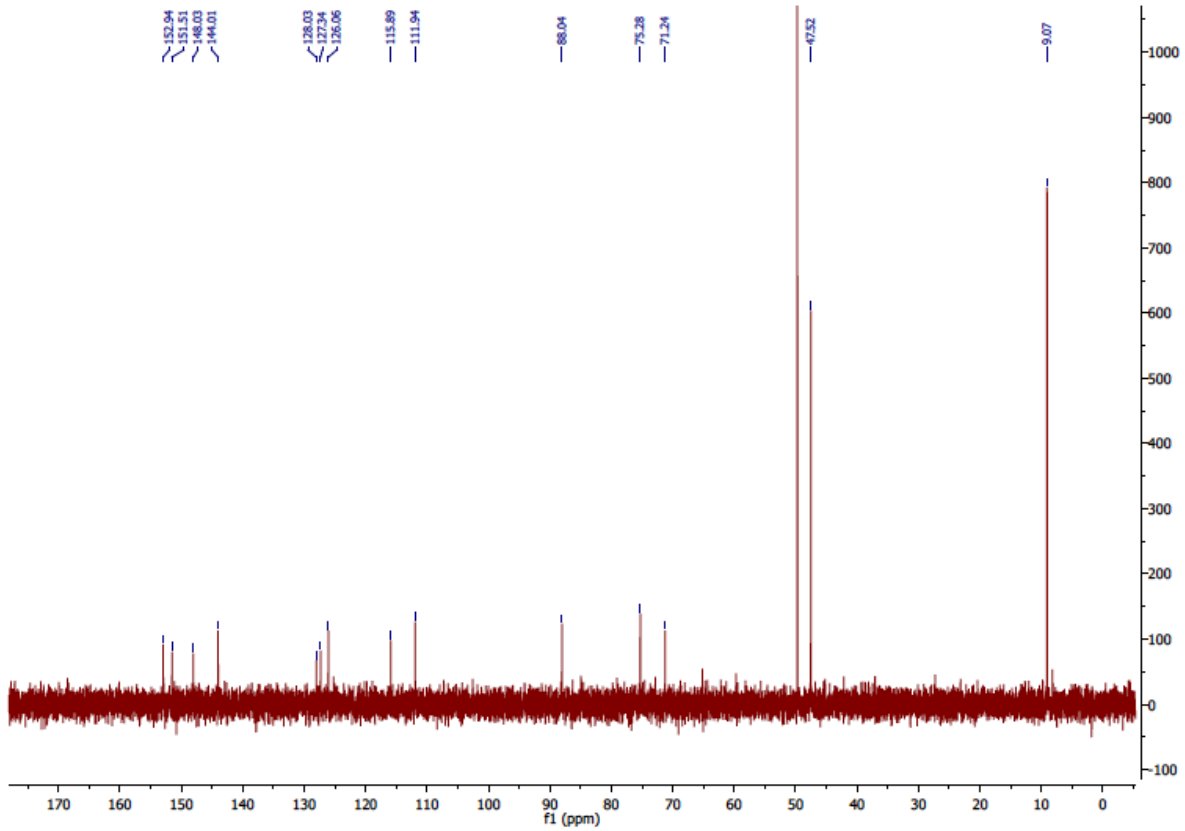

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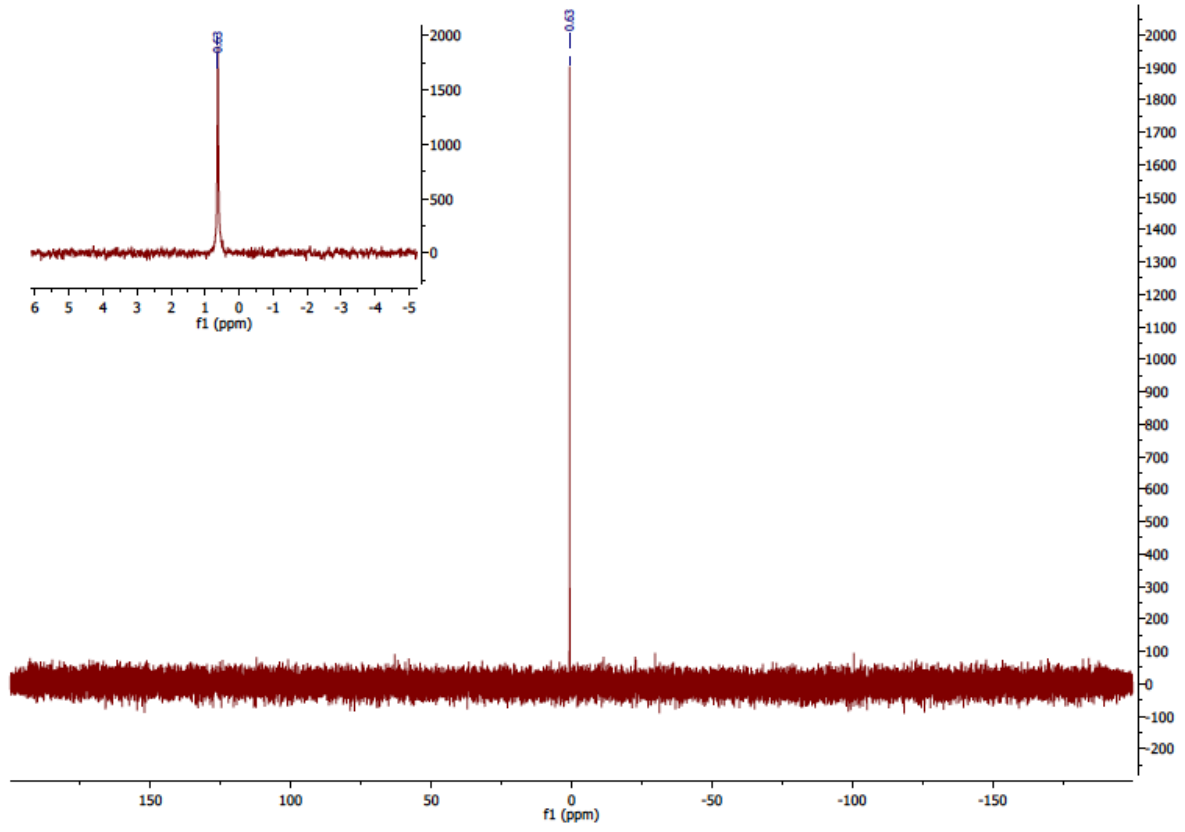

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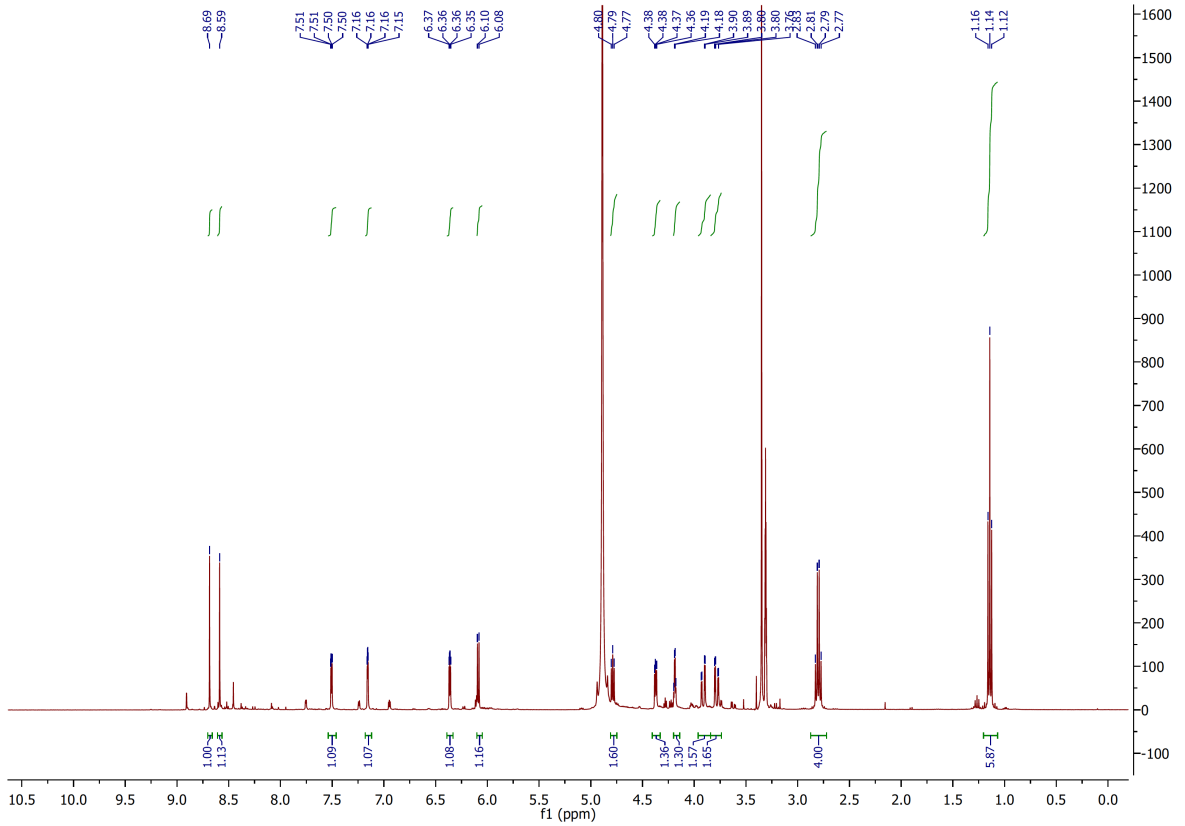

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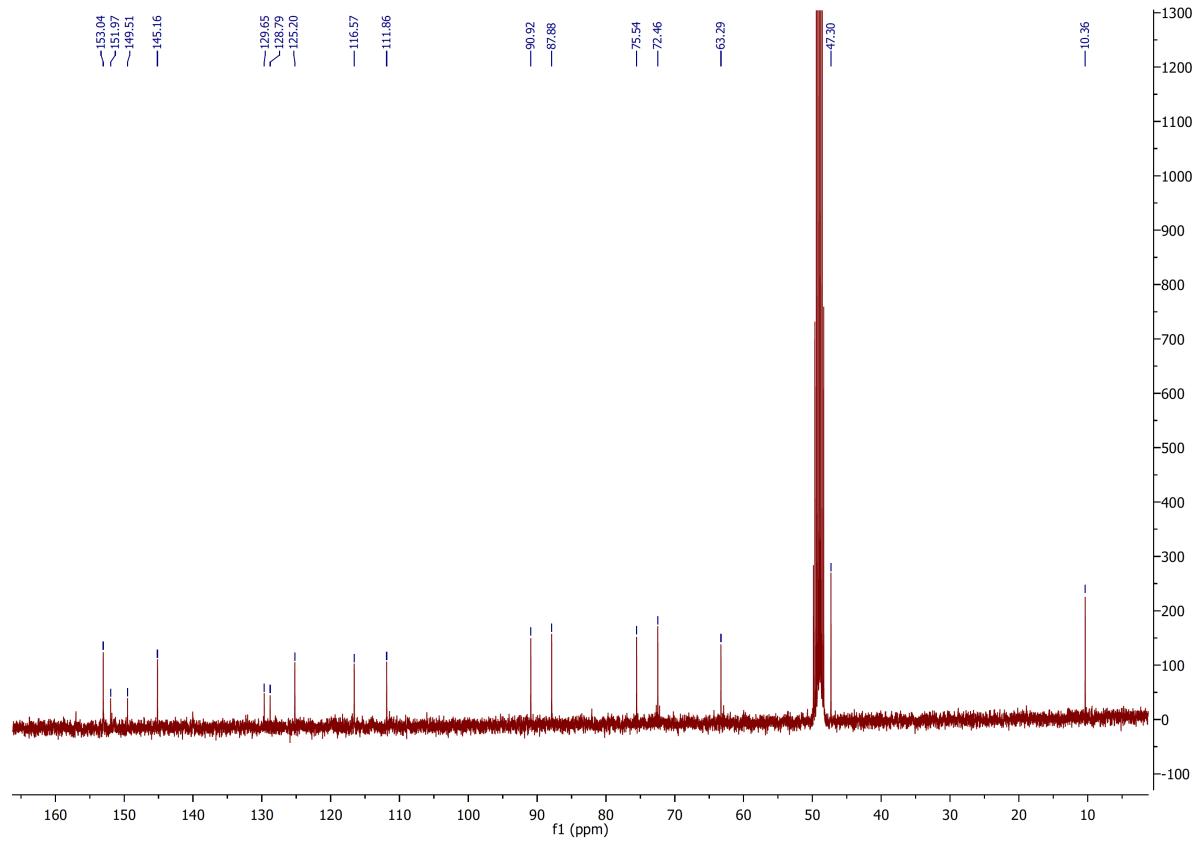

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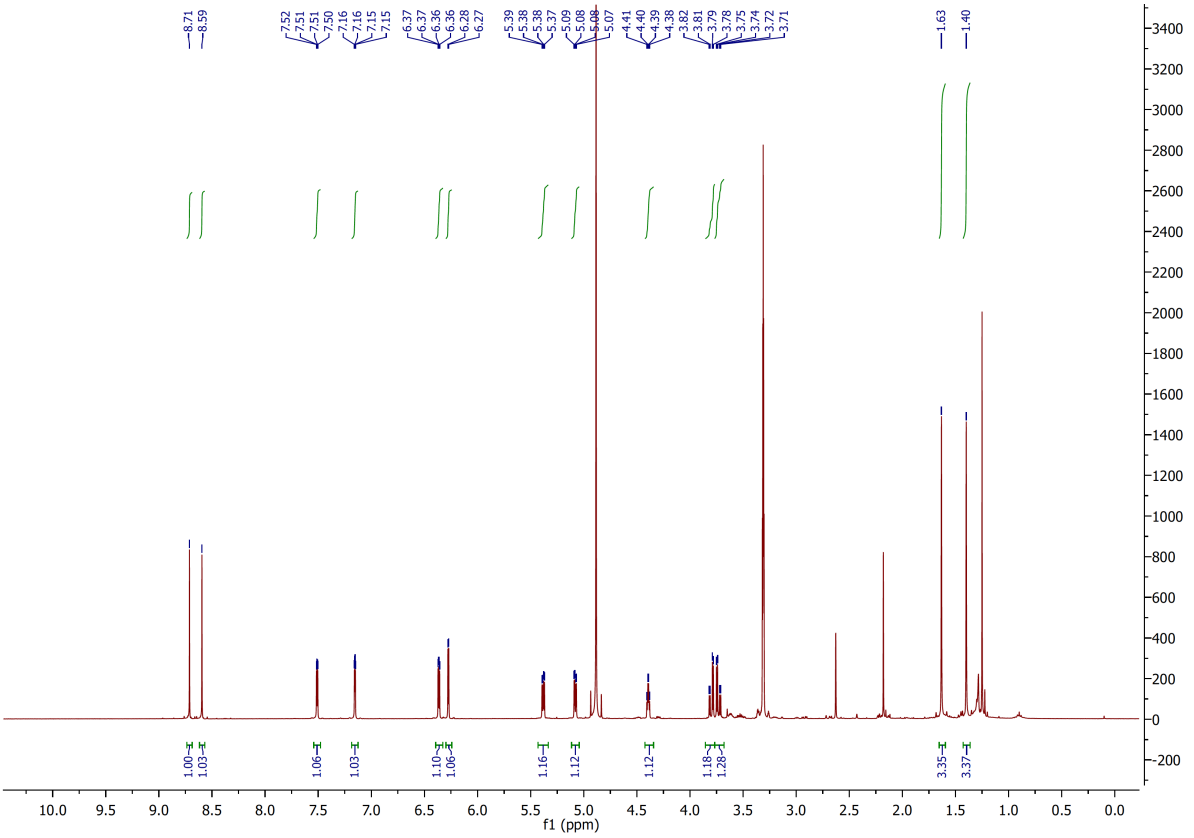

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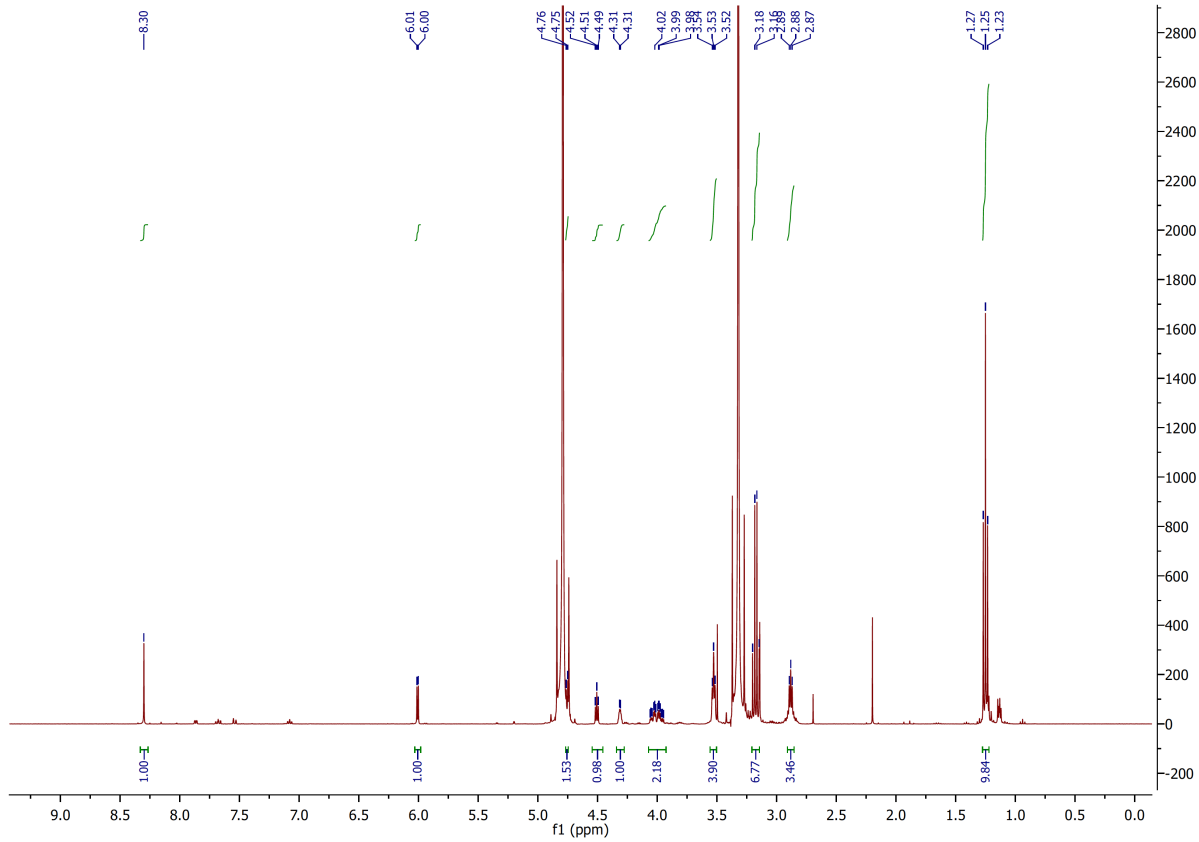

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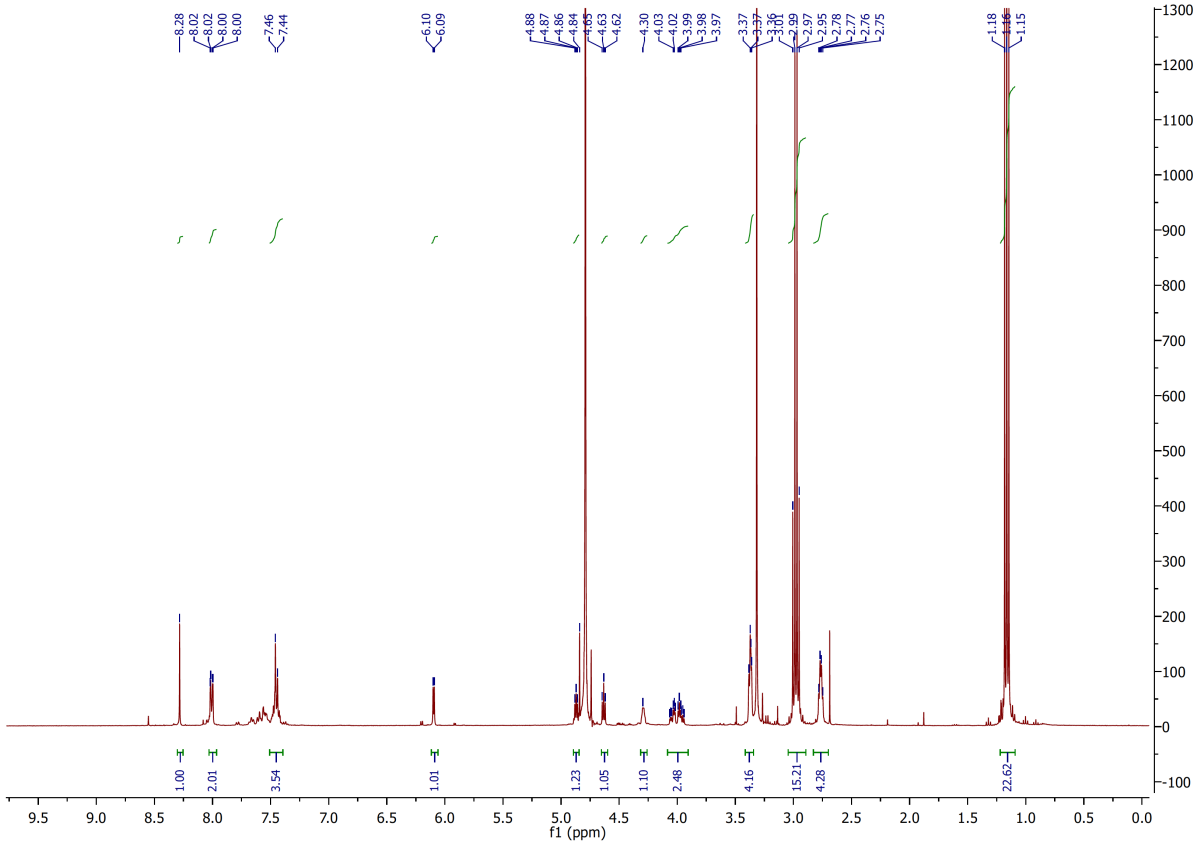
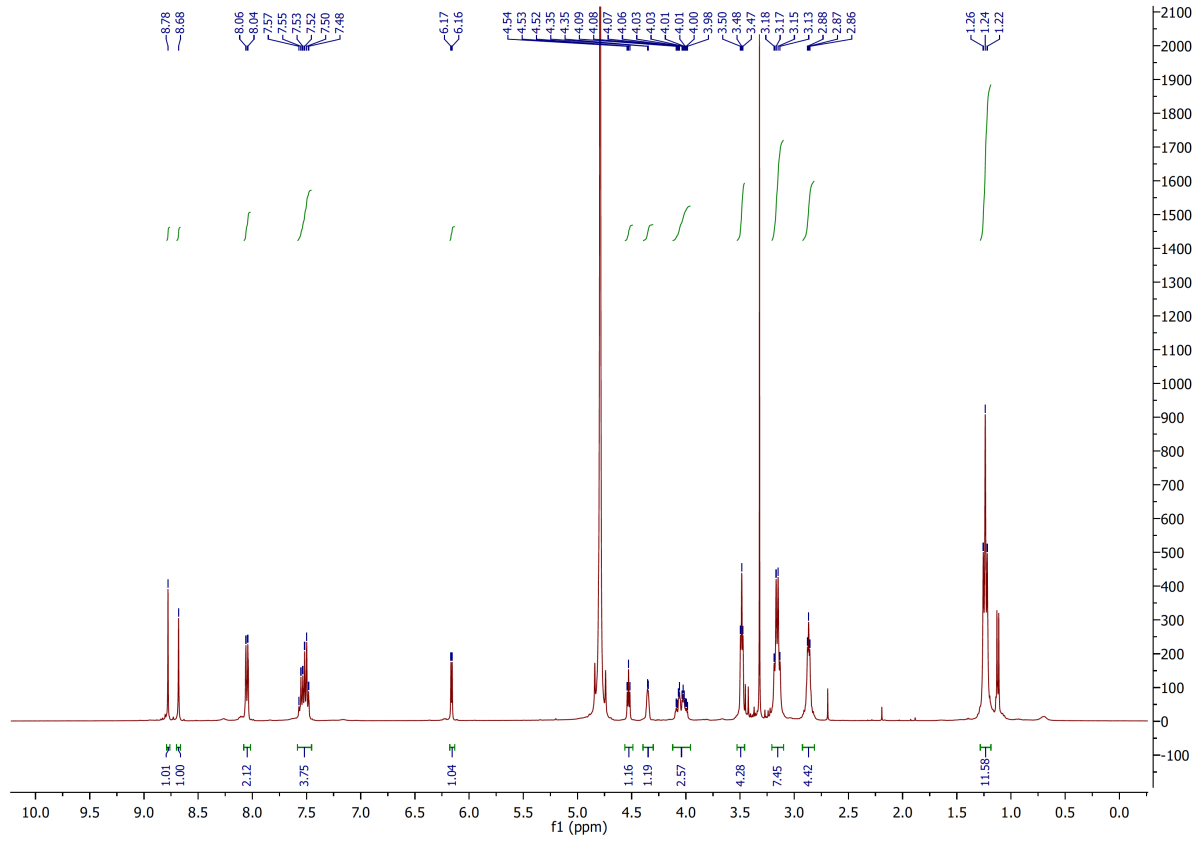


^{1}H NMR: 13a



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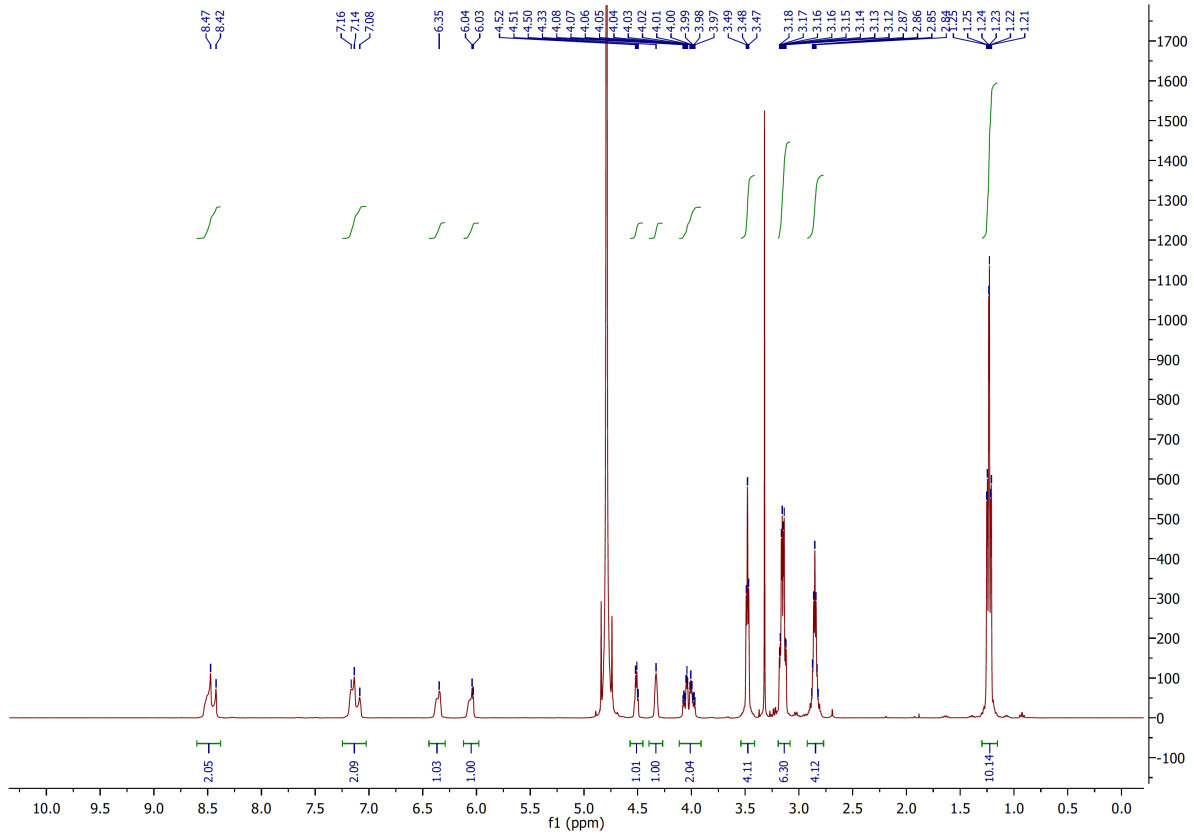
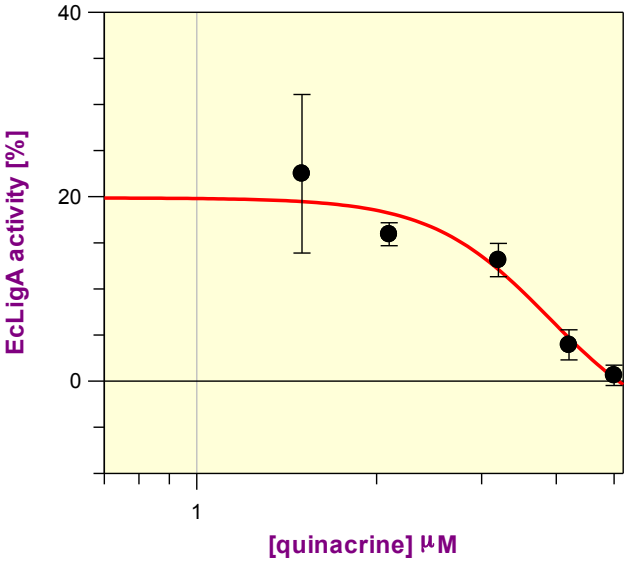
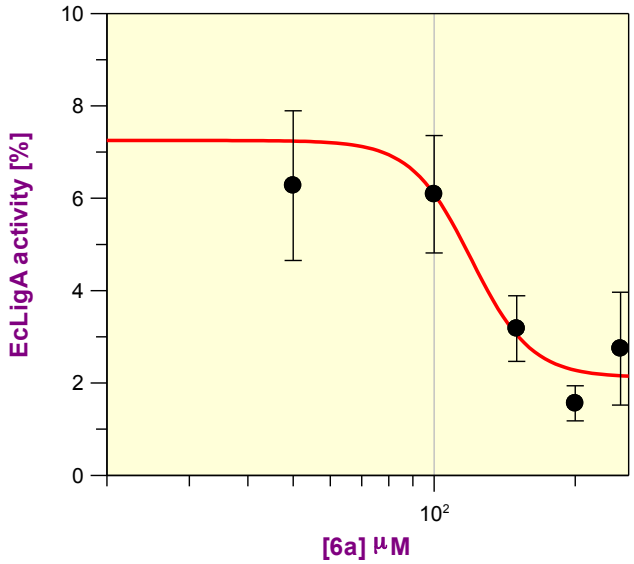


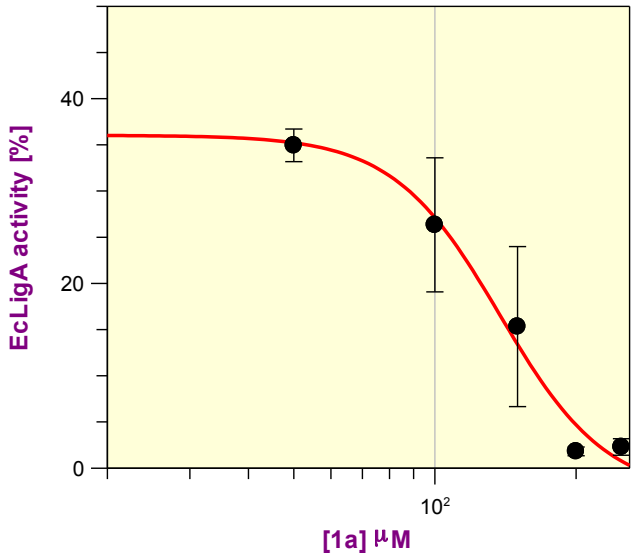
(2) Concentration-response curves from IC_{50} experiments



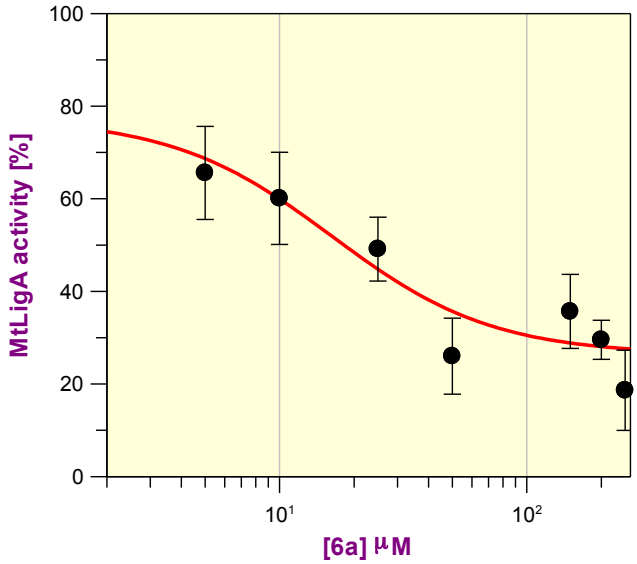
IC_{50} estimation for quinacrine against EcLigA. Conditions: DNA substrate (0.5 µM), *β*-NAD^+ (26 µM), EcLigA (0.07 µM), quinacrine·2HCl (0 - 5 µM) in 1 x buffer (30 mM Tris/HCl pH 8, 4 mM $MgCl_2$, 1 mM DTT, 50 µg/mL BSA) incubated at 30 °C under shaking and sampled at 5 min; all concentrations are final concentrations. Bars indicate mean values ± S.D. of triplicate experiments.



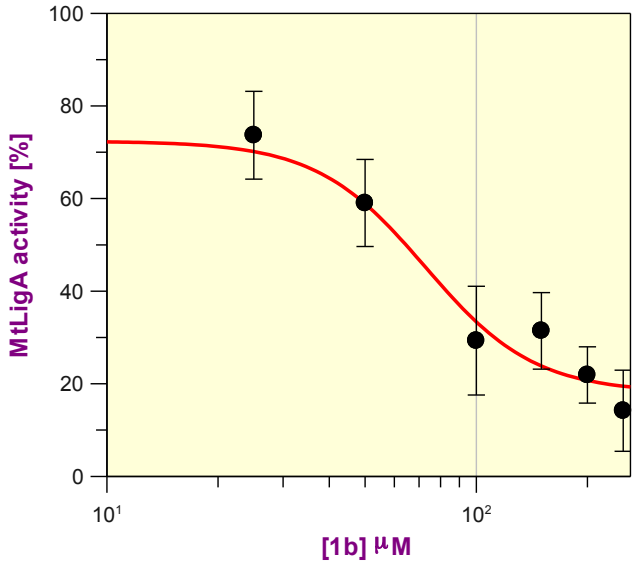
IC_{50} estimation for 2-iodo AMP **6a** against EcLigA. Conditions: DNA substrate (0.5 µM), *β*-NAD^+ (26 µM), EcLigA (0.07 µM), **6a** (0 - 250 µM) in 1 x buffer (30 mM Tris/HCl pH 8, 4 mM $MgCl_2$, 1 mM DTT, 50 µg/mL BSA) incubated at 30 °C under shaking and sampled at 5 min; all concentrations are final concentrations. Bars indicate mean values ± S.D. of triplicate experiments.



IC_{50} estimation for 2-iodo NAD^+ **1a** against EcLigA. Conditions: DNA substrate (0.5 µM), *β*-NAD^+ (26 µM), EcLigA (0.07 µM), **1a** (0 - 250 µM) in 1 x buffer (30 mM Tris/HCl pH 8, 4 mM $MgCl_2$, 1 mM DTT, 50 µg/mL BSA) incubated at 30 °C under shaking and sampled at 5 min; all concentrations are final concentrations. Bars indicate mean values ± S.D. of triplicate experiments.



IC_{50} estimation for 2-iodo AMP **6a** against MtLigA. Conditions: DNA substrate (0.5 µM), *β*-NAD^+ (26 µM), MtLigA (0.17 µM), **6a** (0 - 250 µM) in 1 x buffer (30 mM Tris/HCl pH 8, 4 mM $MgCl_2$, 1 mM DTT, 50 µg/mL BSA) incubated at 30 °C under shaking and sampled at 5 min; all concentrations are final concentrations. Bars indicate mean values ± S.D. of triplicate experiments.



IC_{50} estimation for 2-phenyl NAD^+ **1b** against MtLigA. Conditions: DNA substrate (0.5 µM), *β*-NAD^+ (26 µM), MtLigA (0.17 µM), **1b** (0 - 250 µM) in 1 x buffer (30 mM Tris/HCl pH 8, 4 mM $MgCl_2$, 1 mM DTT, 50 µg/mL BSA) incubated at 30 °C under shaking and sampled at 5 min; all concentrations are final concentrations. Bars indicate mean values ± S.D. of triplicate experiments.