Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Progress towards water-soluble triazole-based selective MMP-2 inhibitors

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SUPPORTING INFORMATION

Table of Content

Time evolution of the MMP-2 backbone atoms RMSD of the MD trajectory

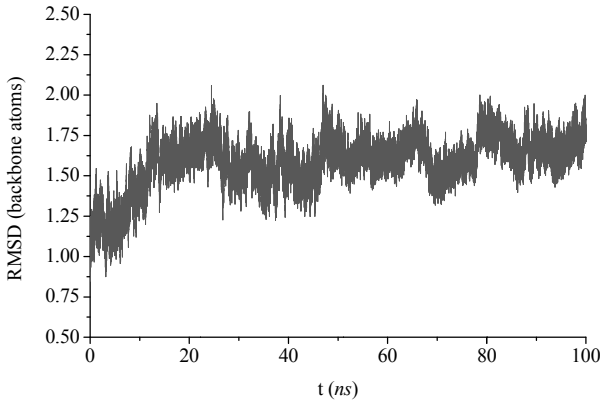
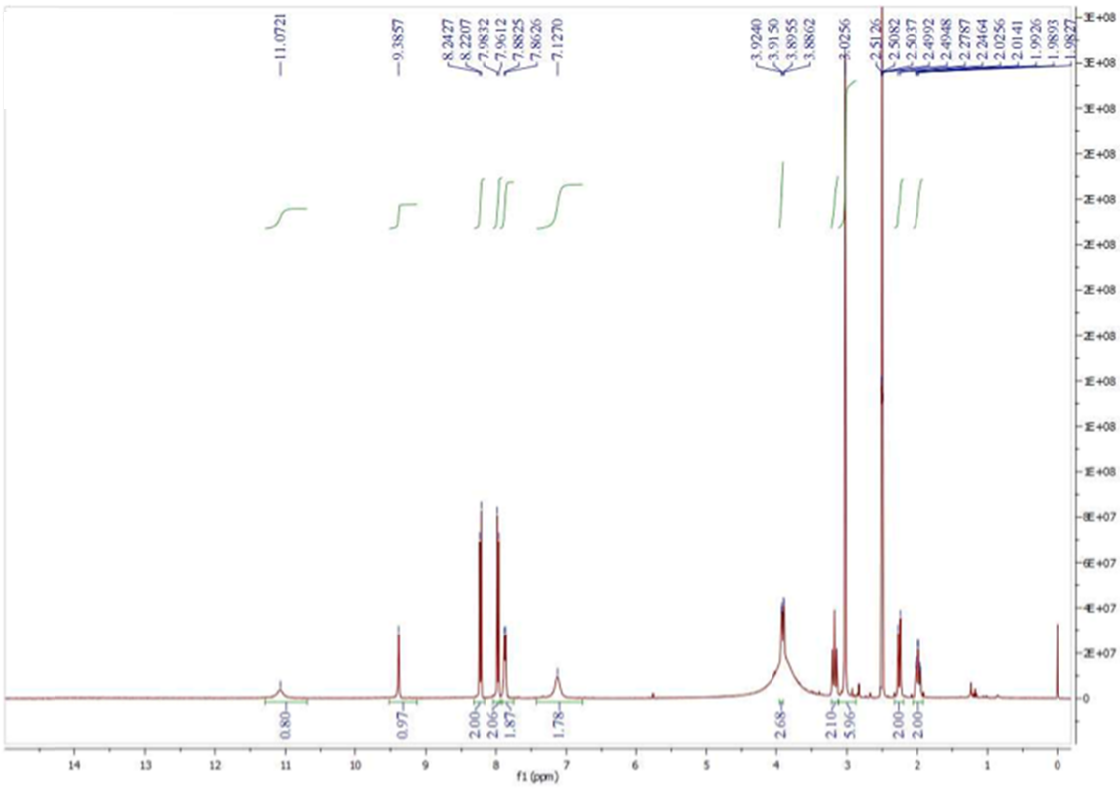
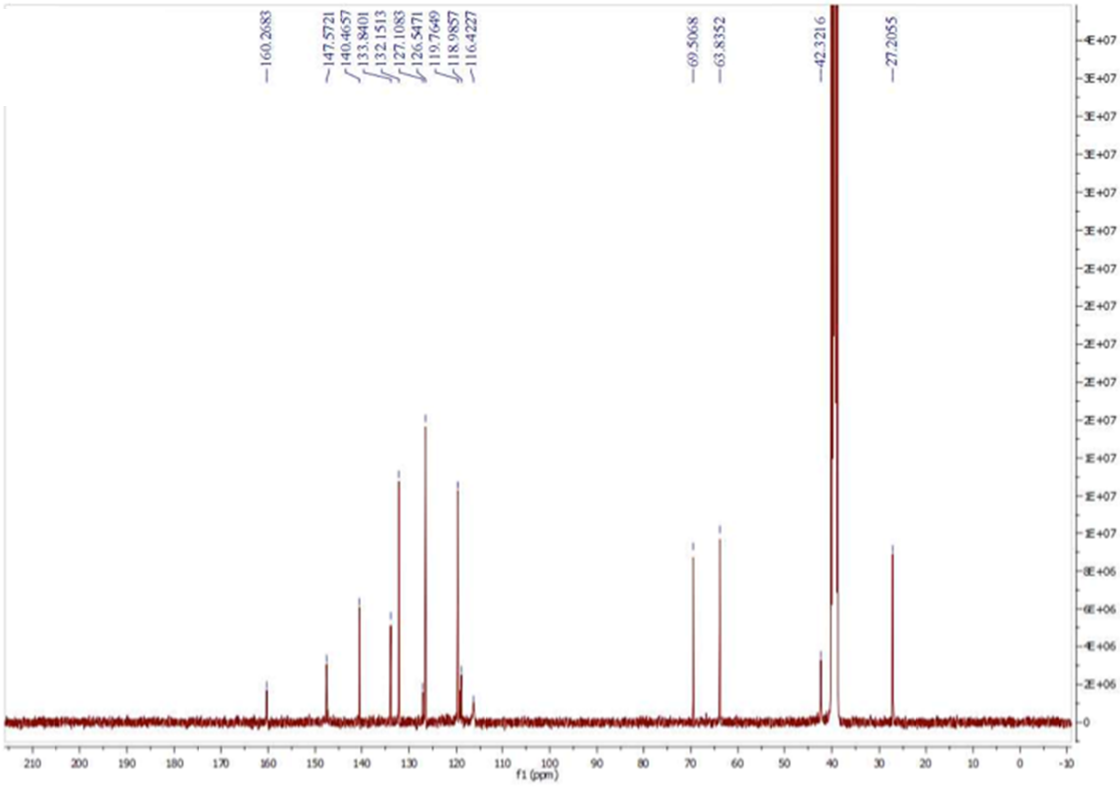


Figure S1. Time evolution of the Root-Mean-Square Deviation (RMSD, in Å) for the protein backbone atoms (except the *N*-term coil) of the MD trajectory.

^{1}H and ^{13}C NMR spectra of 1e-i and 13a-j

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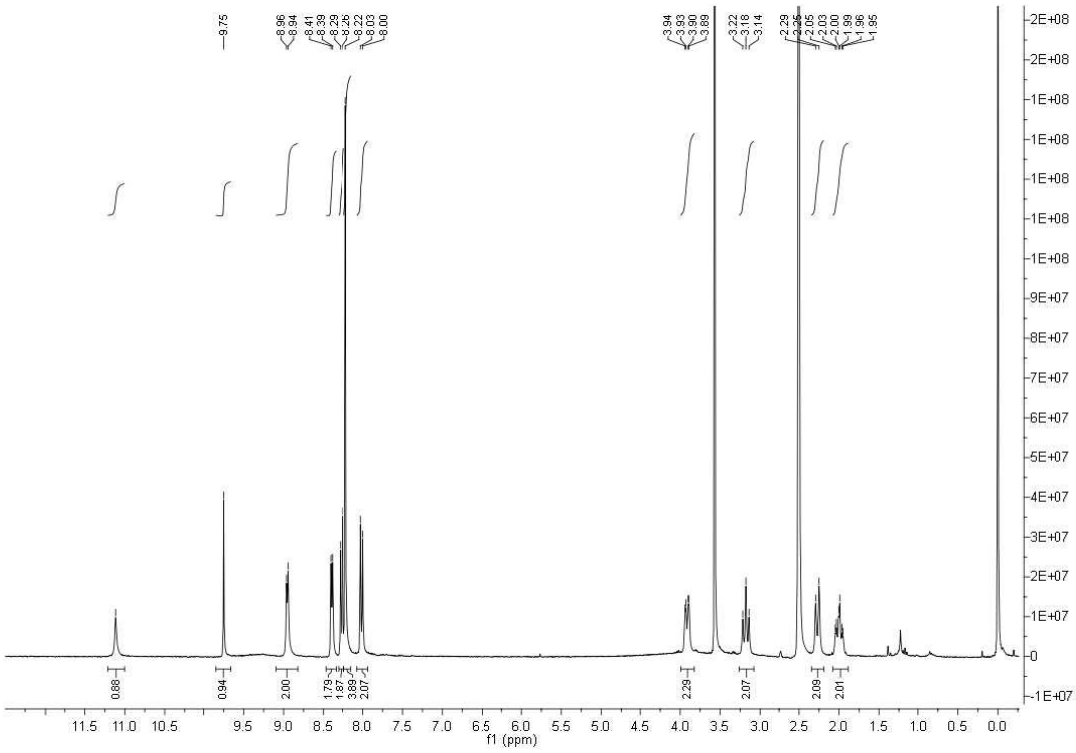
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3.22
3.18
3.14
2.29
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2.03
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1.95
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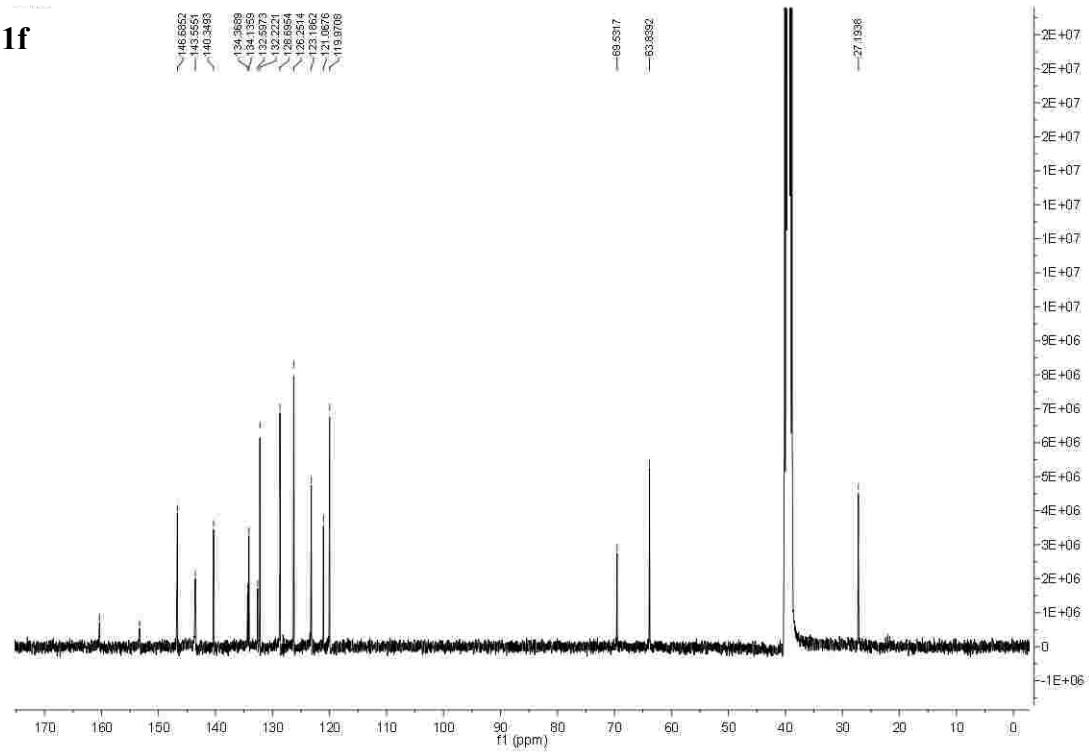
2.01
f1 (ppm)

1f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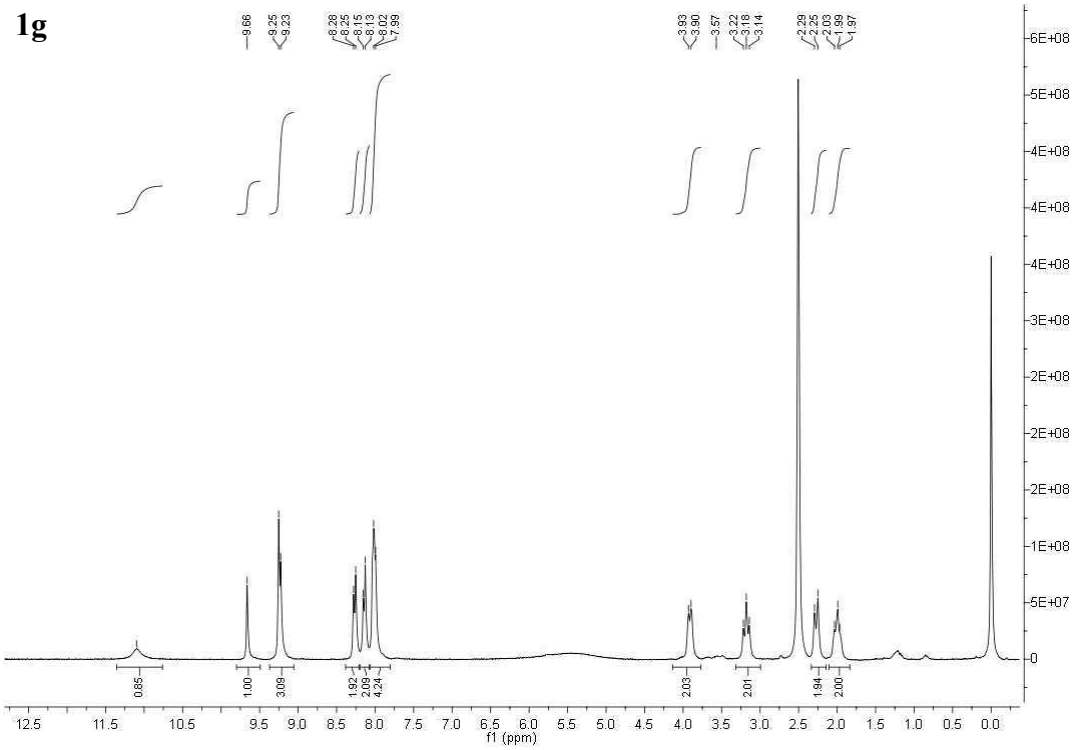
1g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2.29
2.25
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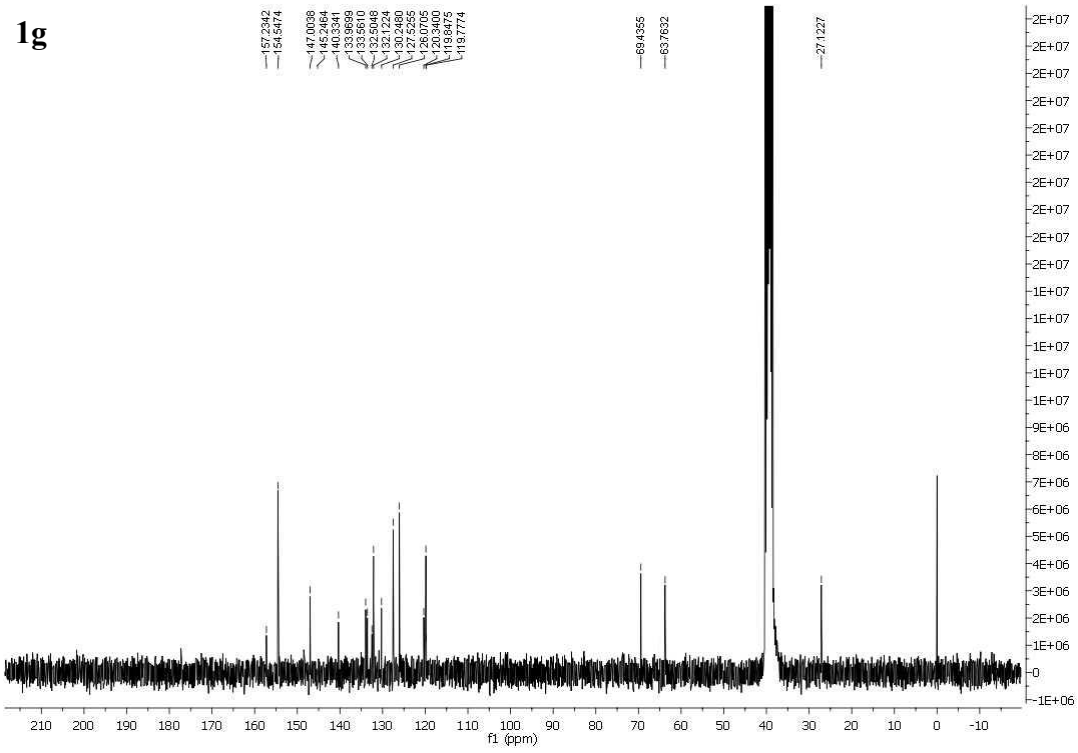
1g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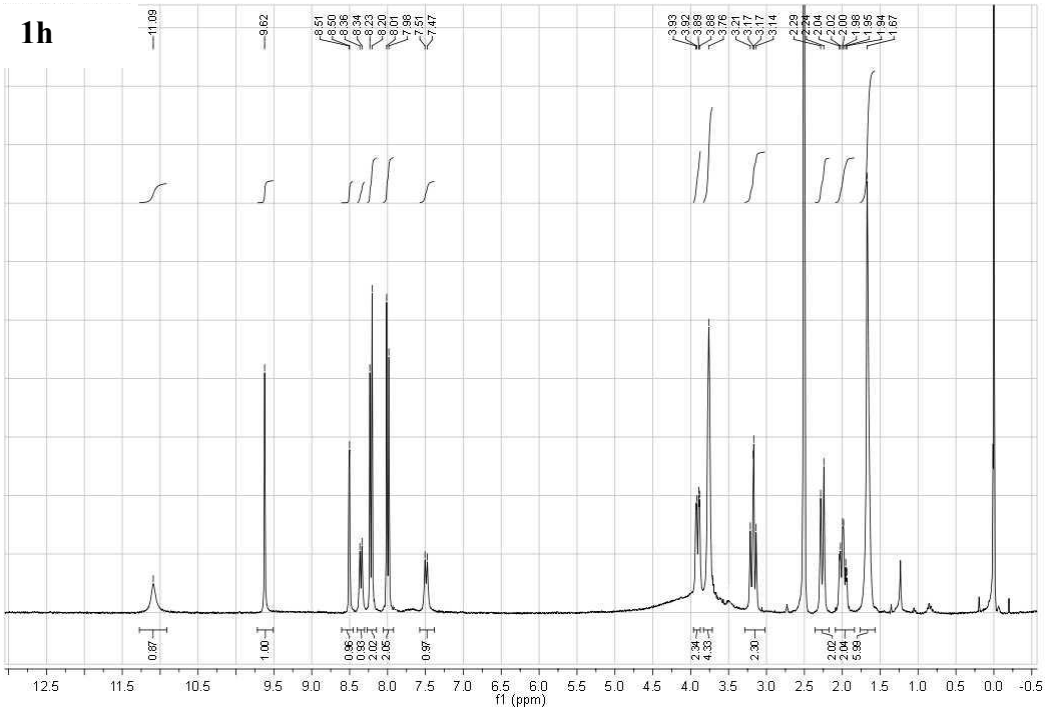
1h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2.02
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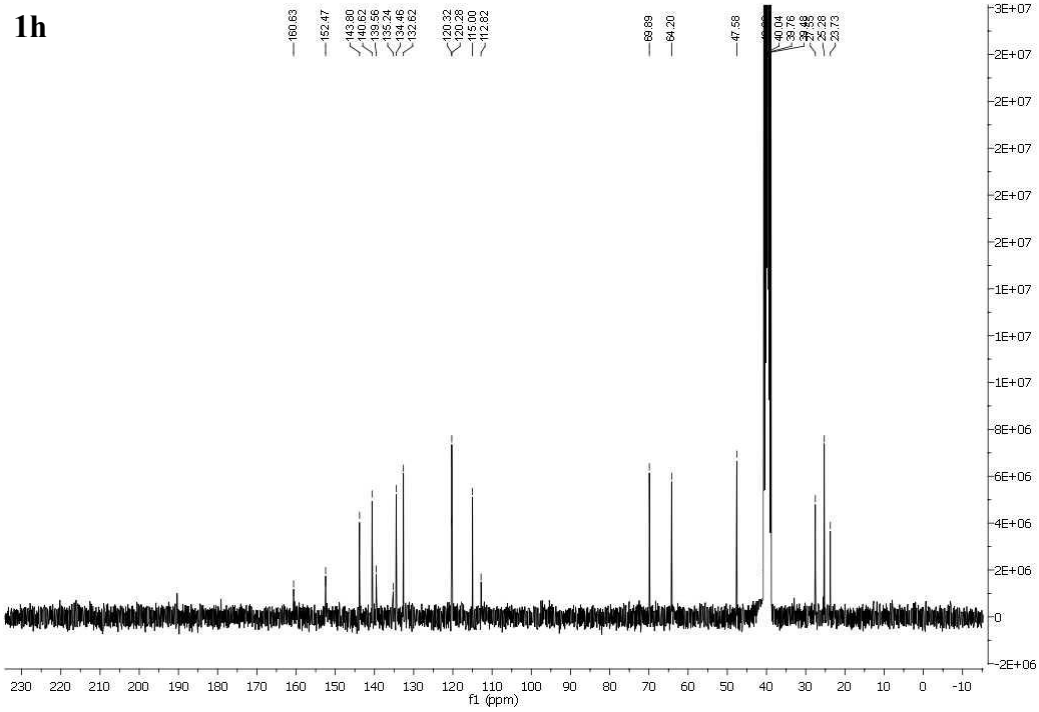
1h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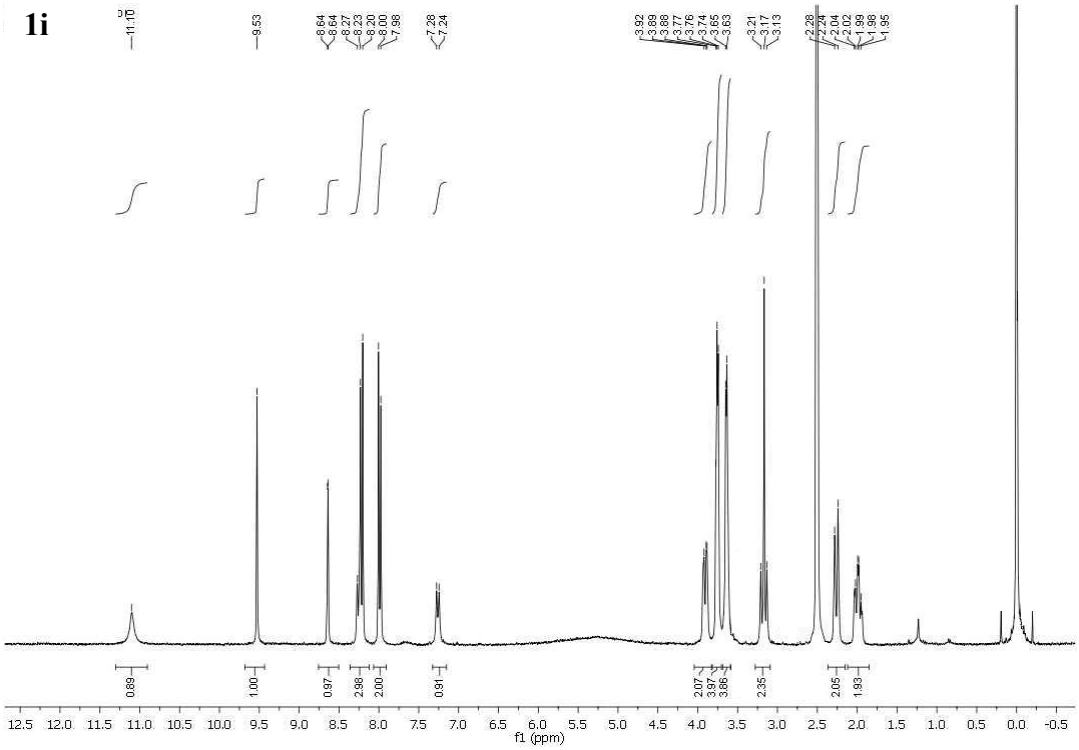
1i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3.17
3.13
2.28
2.24
2.04
2.02
2.02
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1.95
0.89
1.00
0.97
2.98
2.00
0.91
2.07
3.97
3.86
2.35
2.05
1.93
12.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
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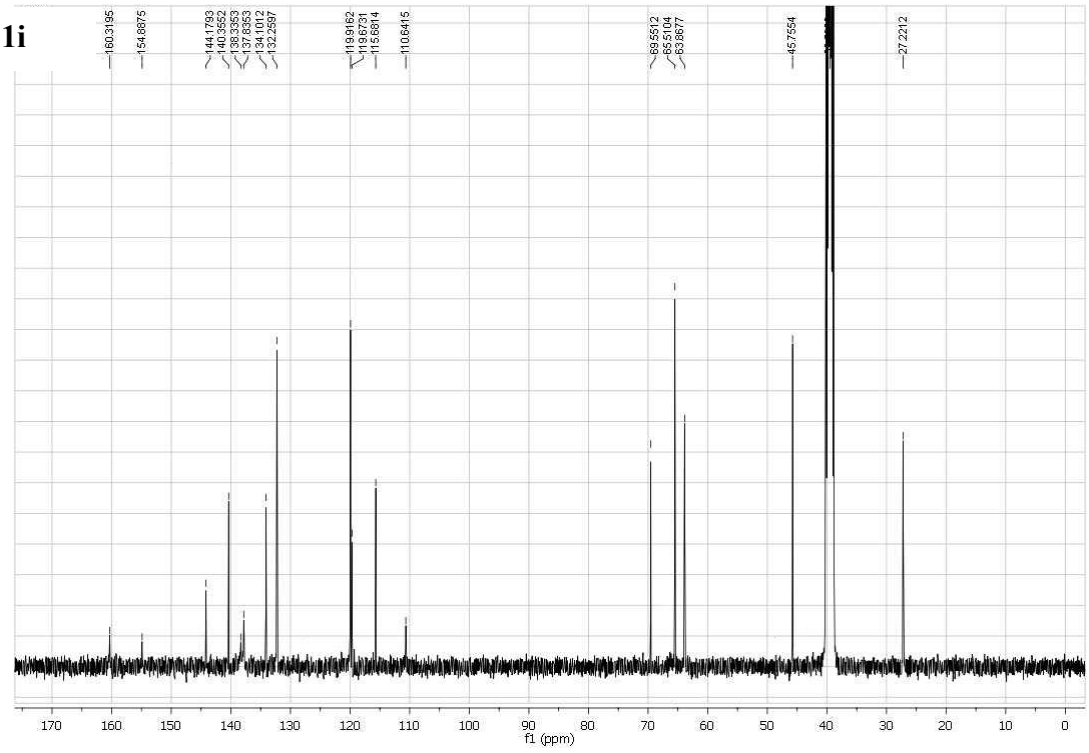
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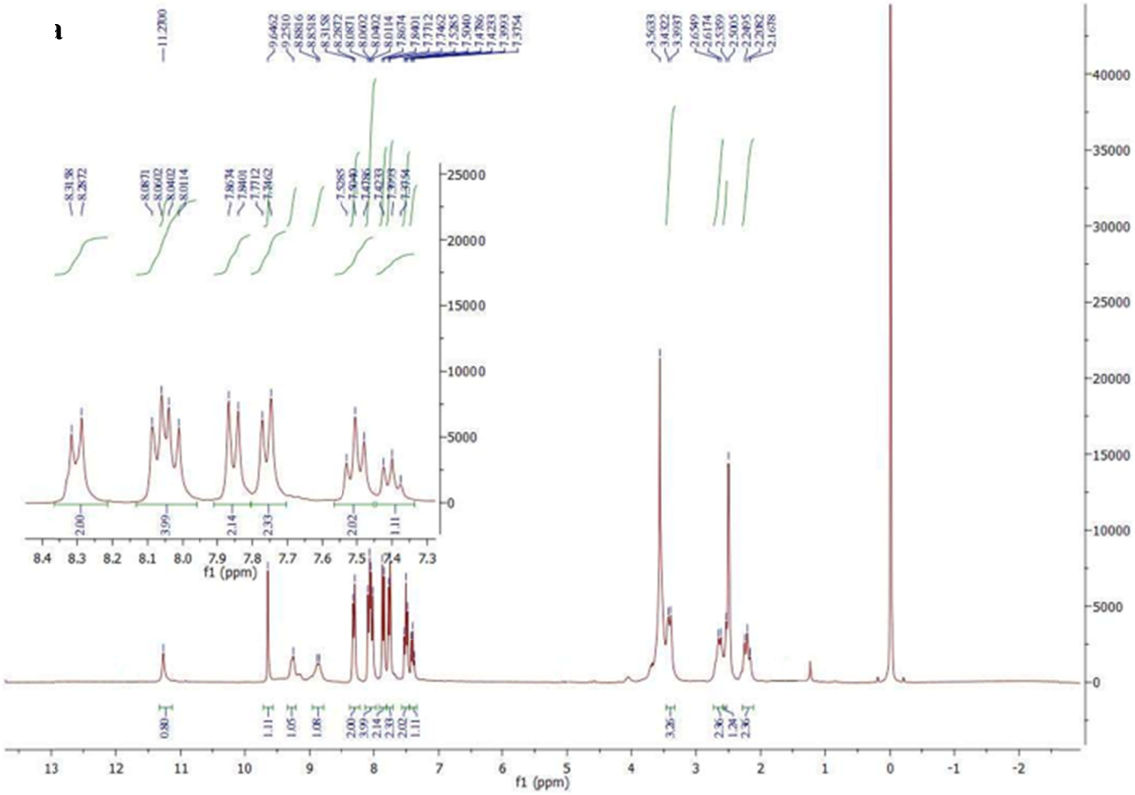
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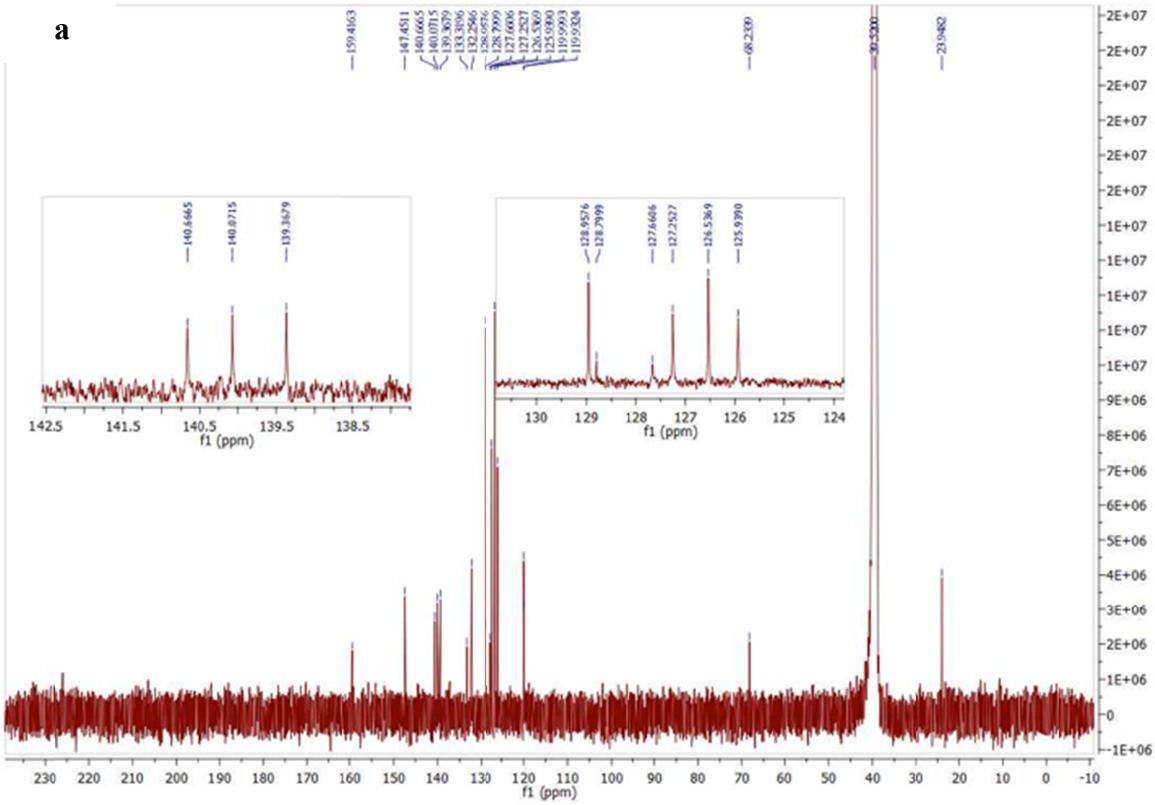
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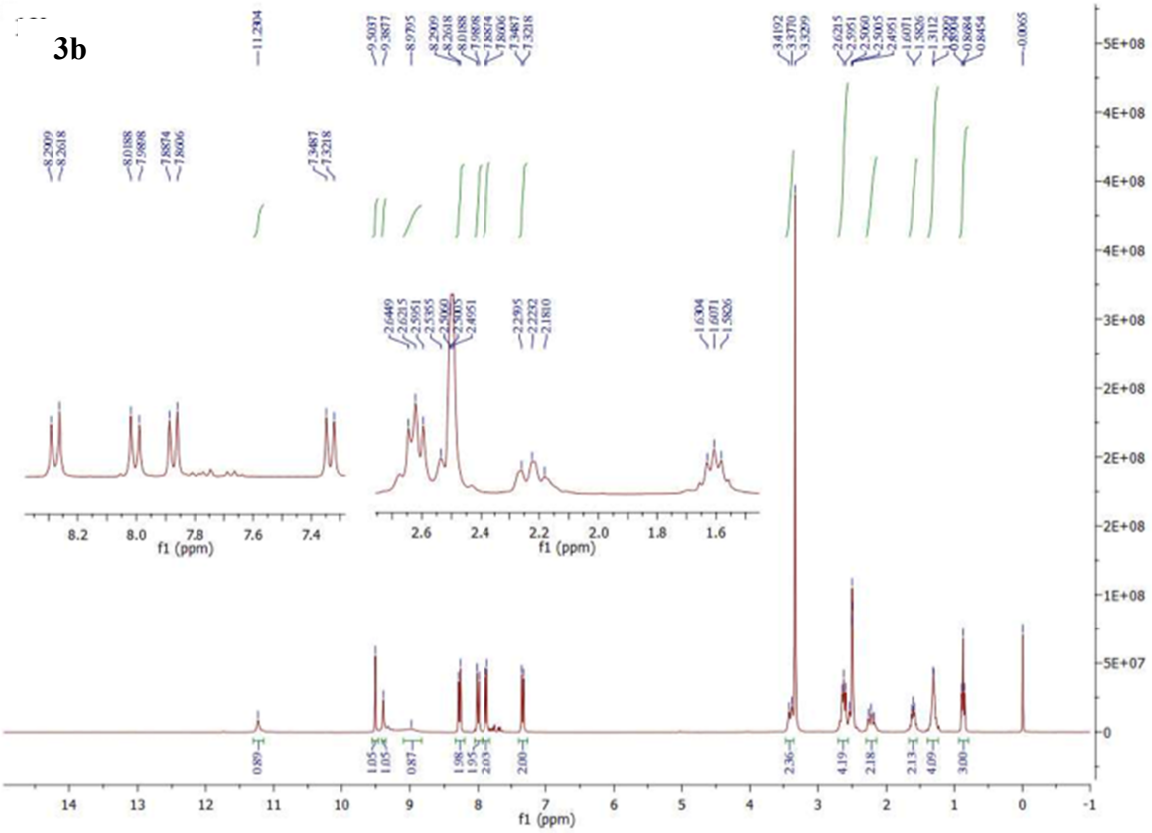

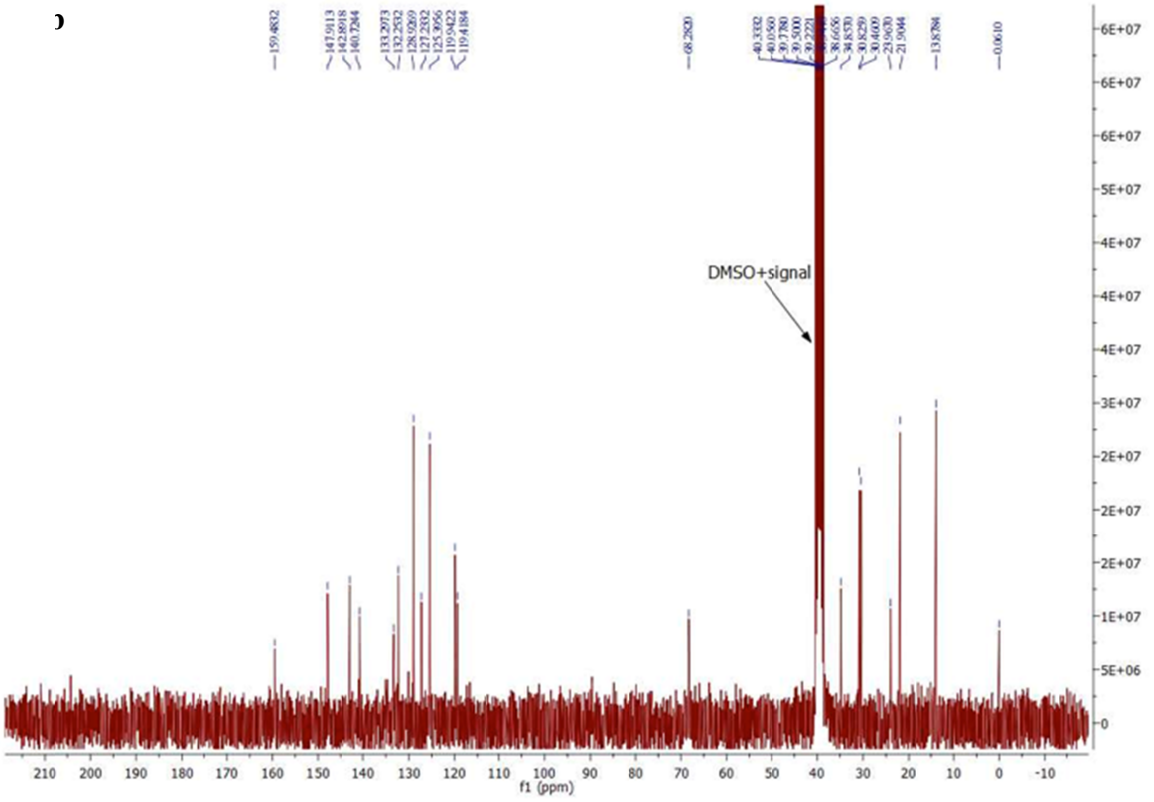

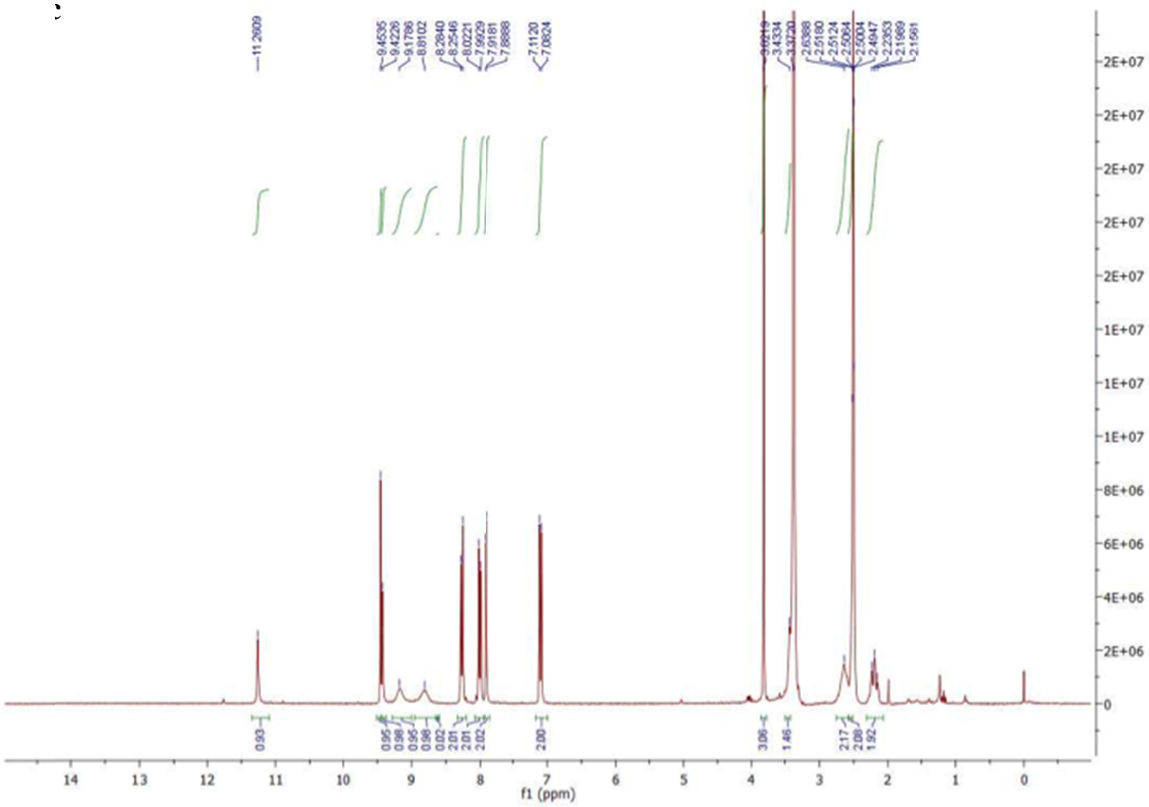
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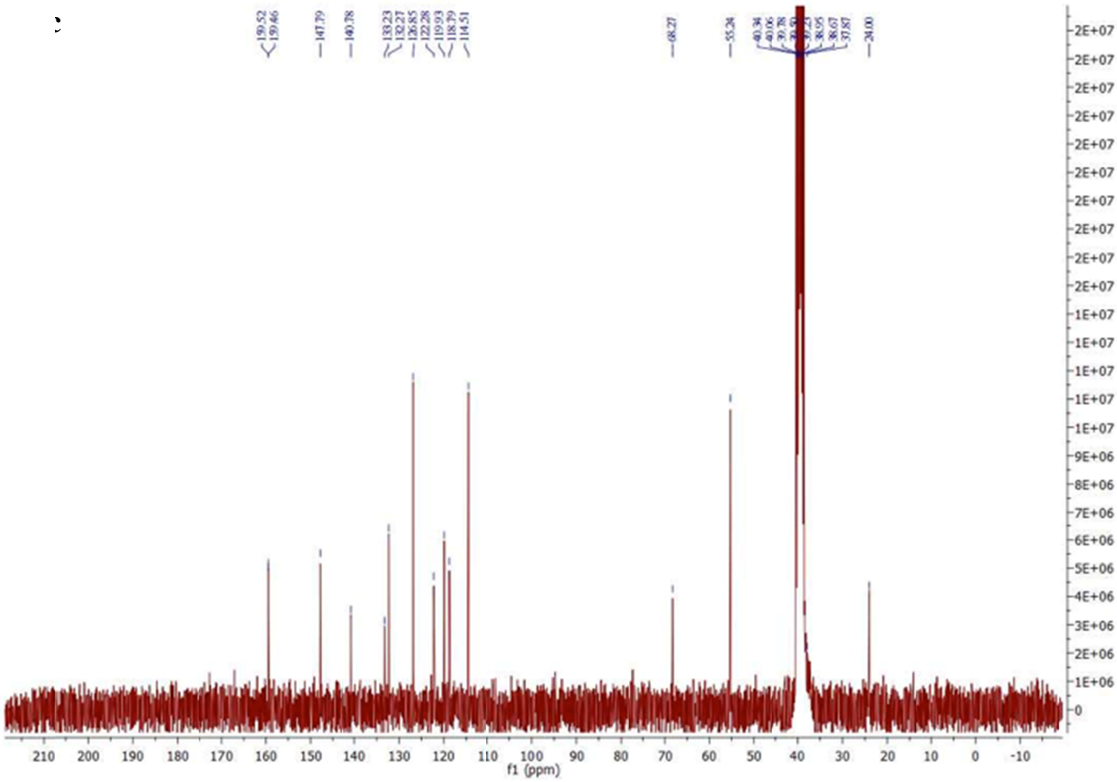
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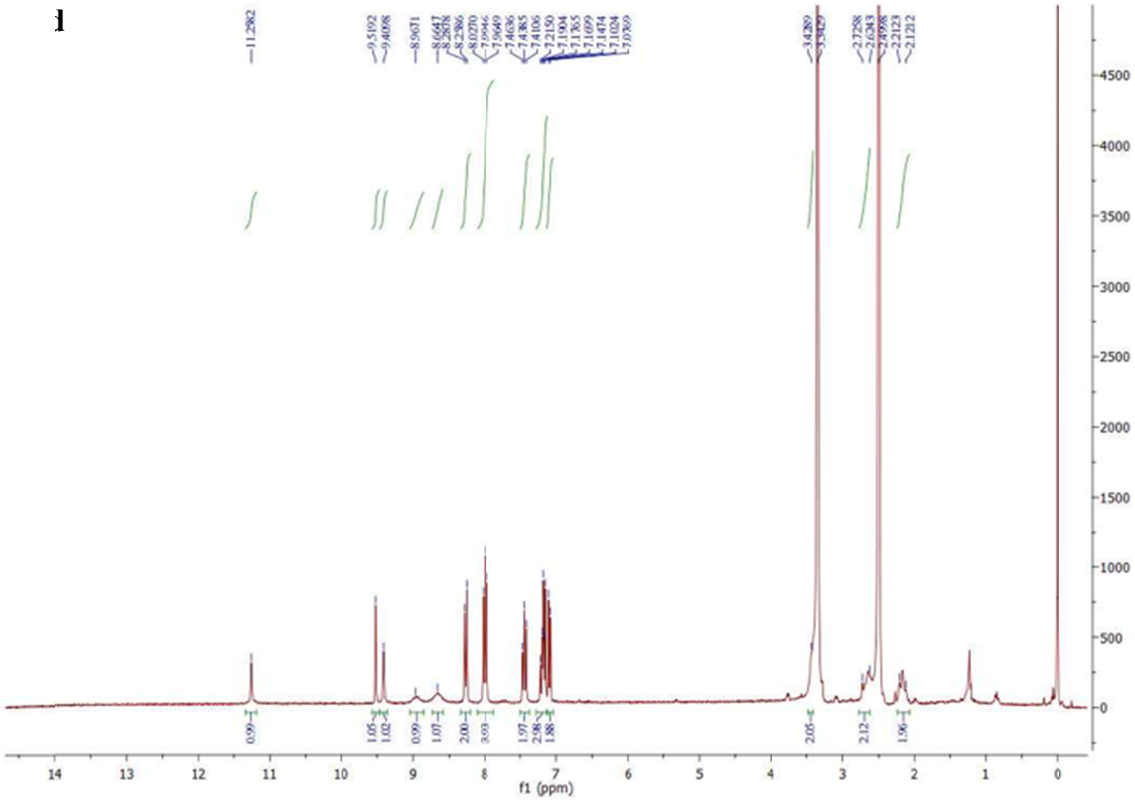
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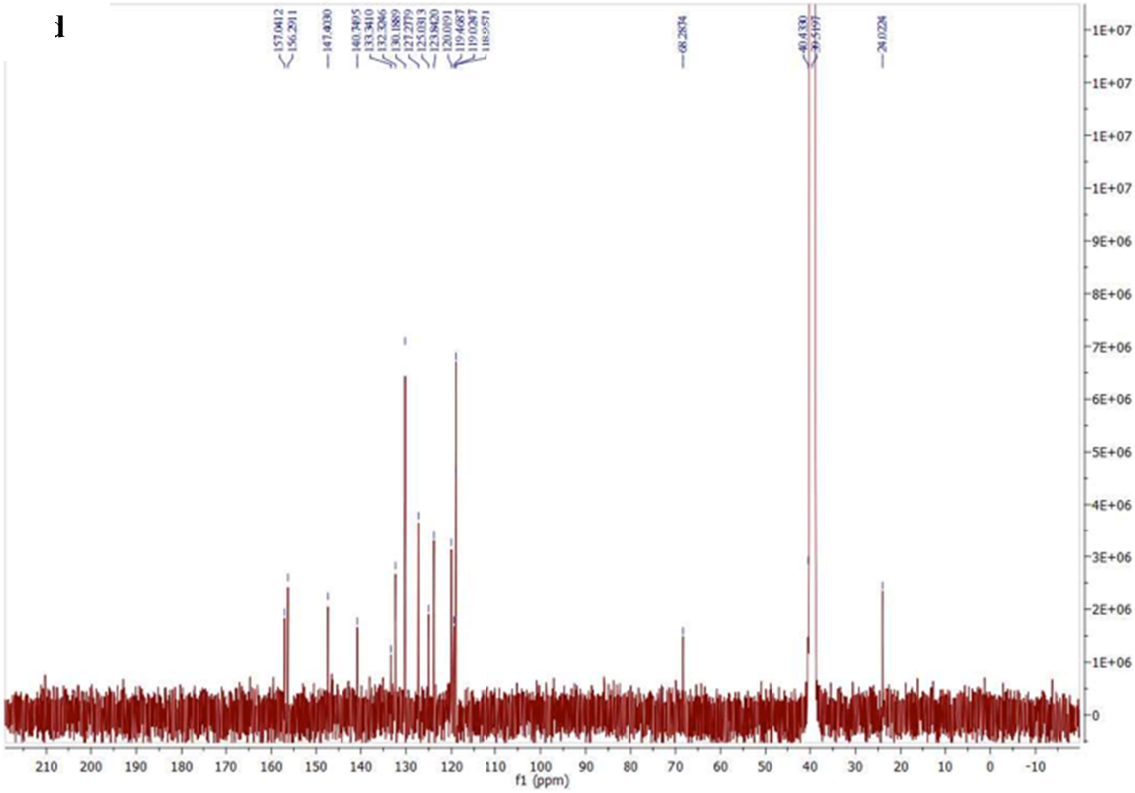
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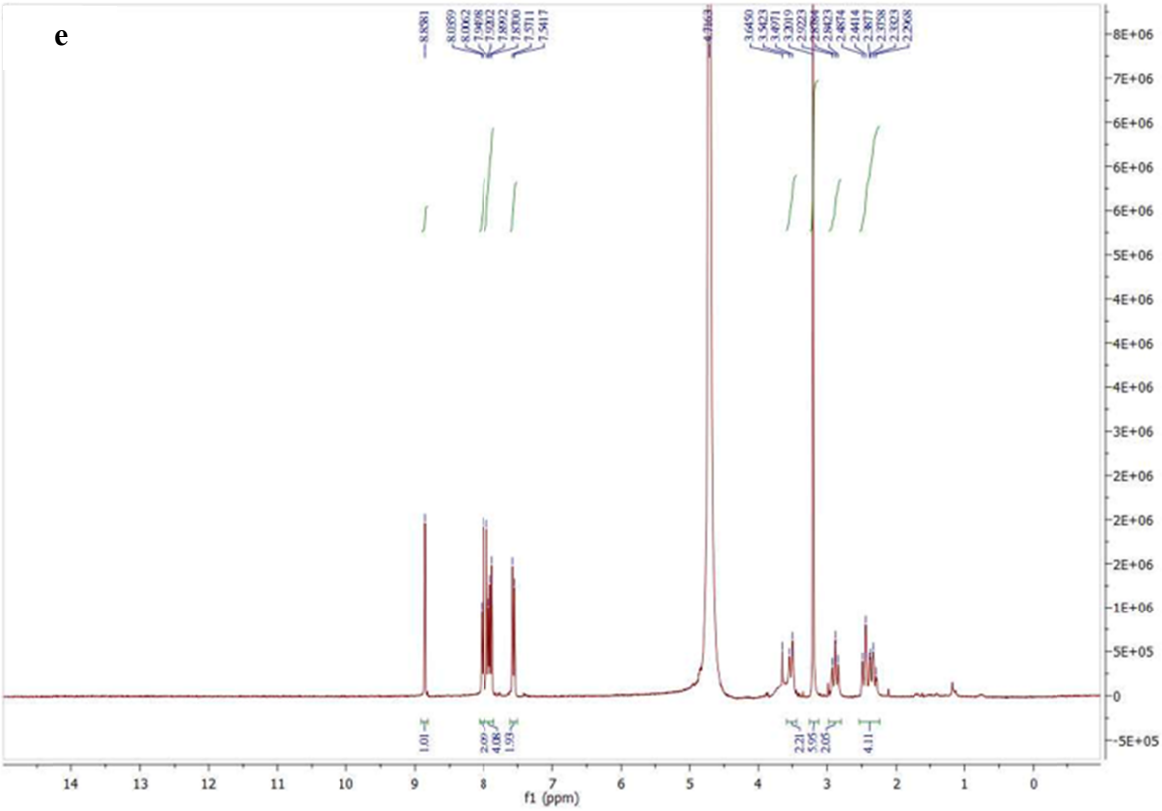

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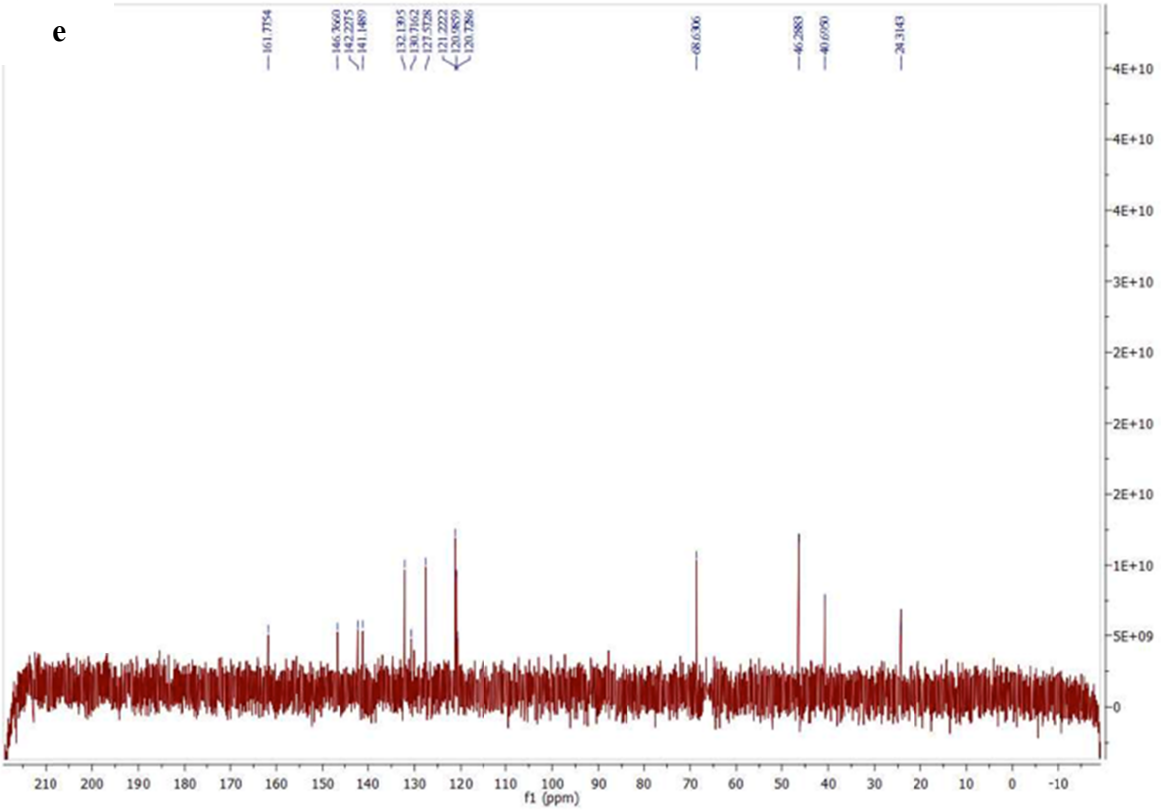

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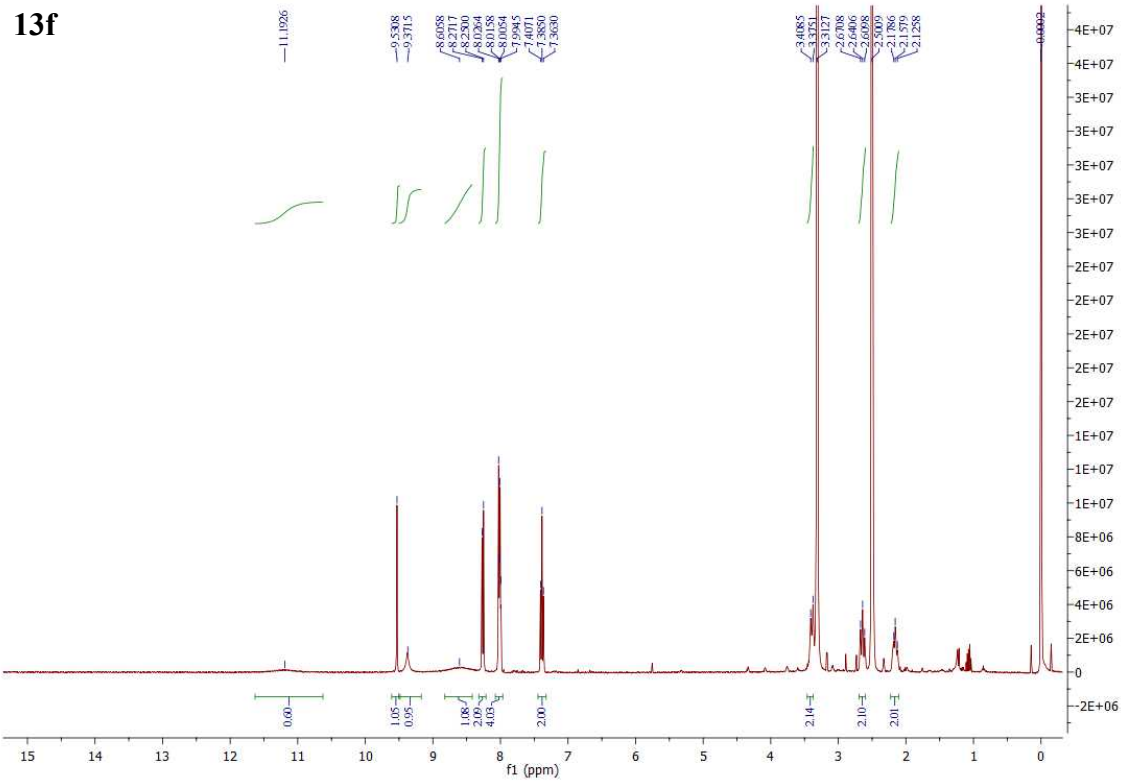
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2.6406
2.6098
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2.1786
2.1579
2.1258
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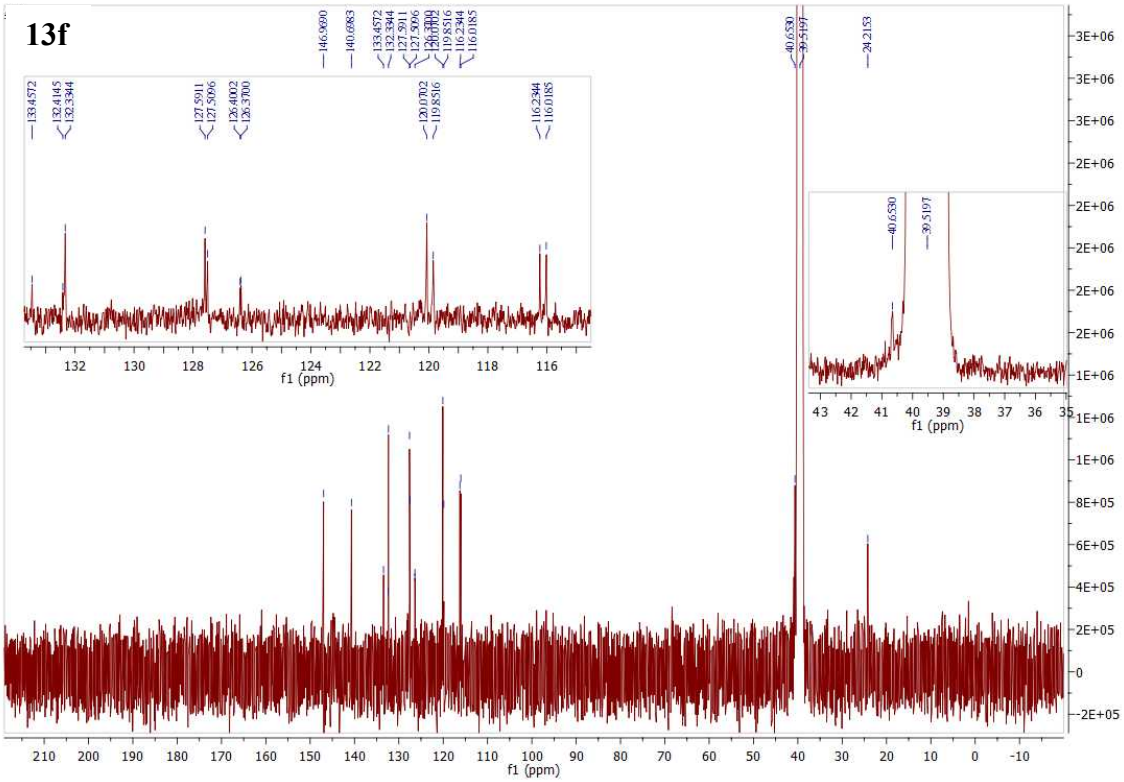
f1 (ppm)

13f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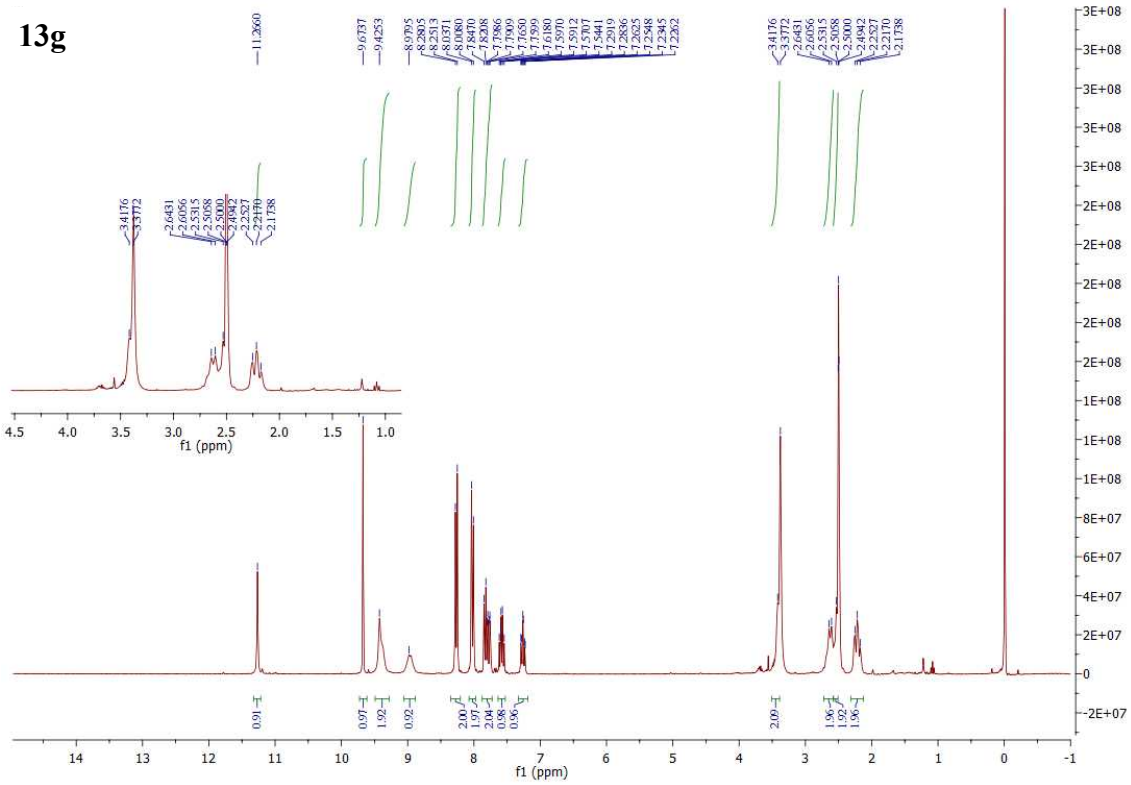
13g



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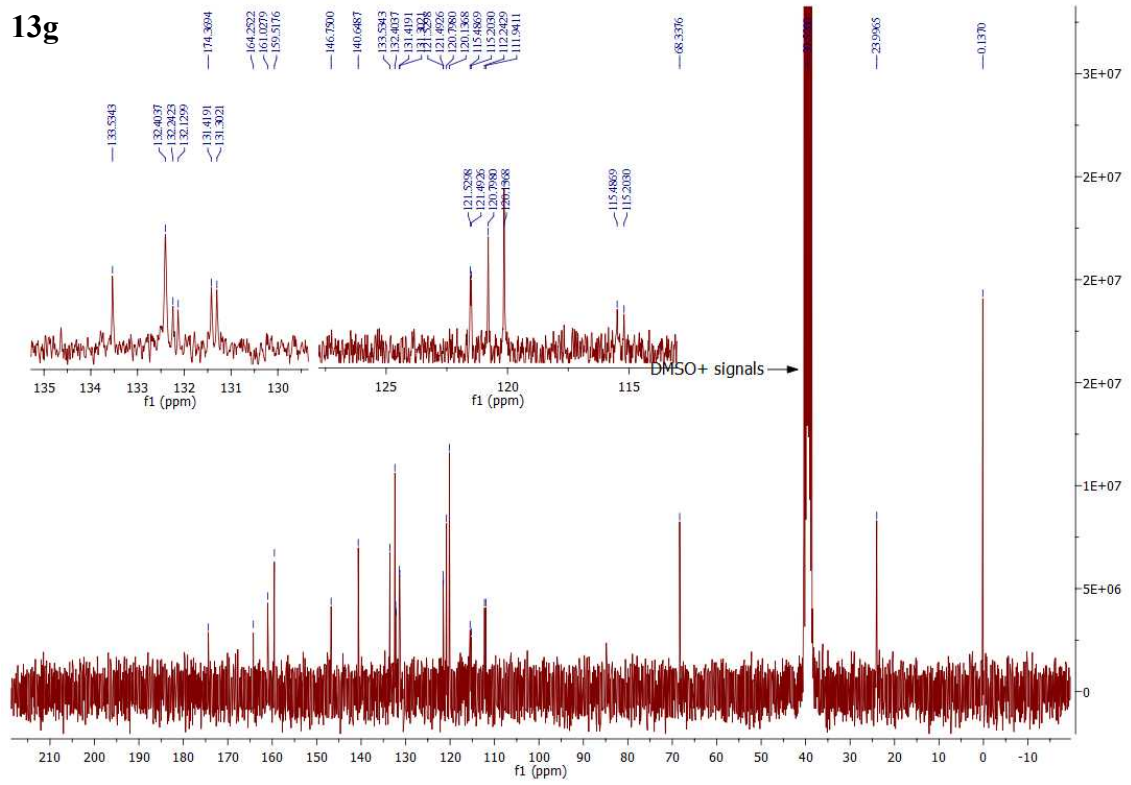

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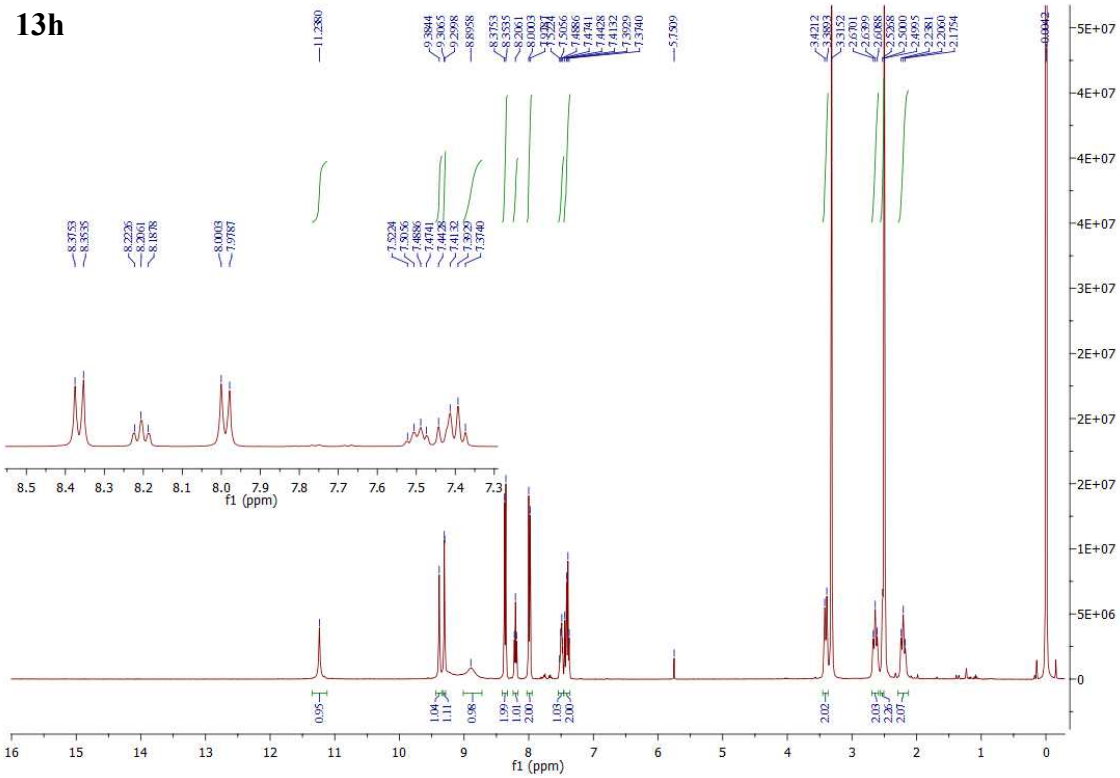

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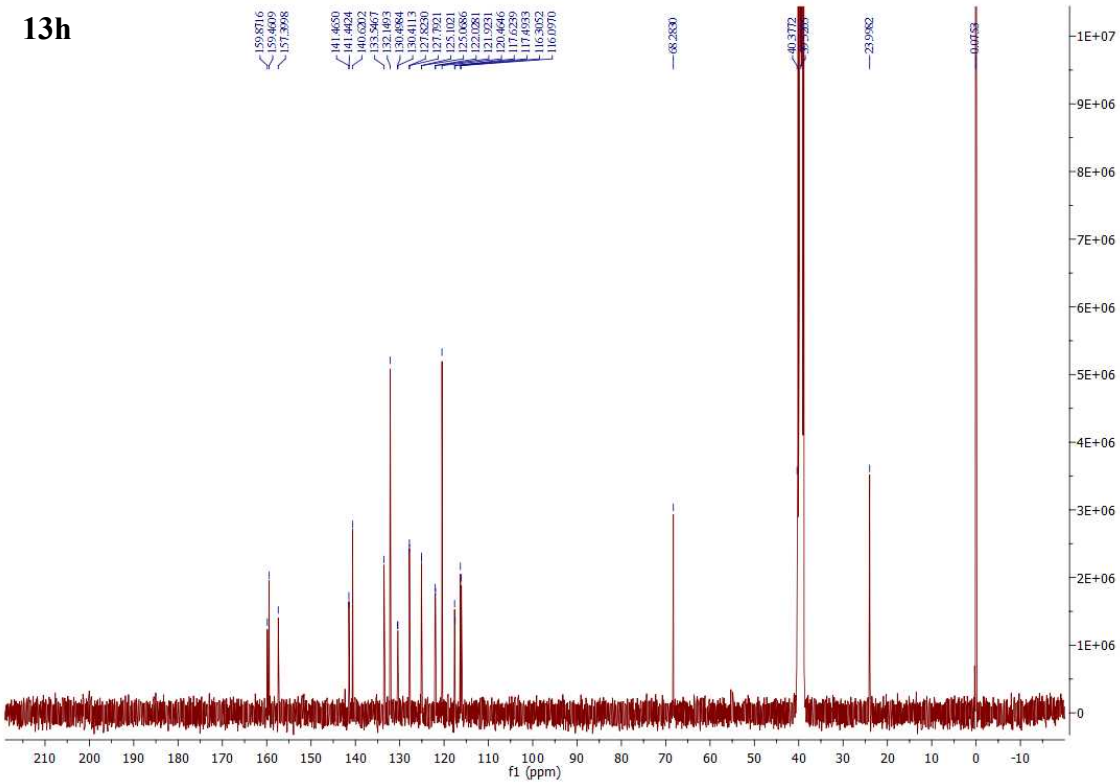

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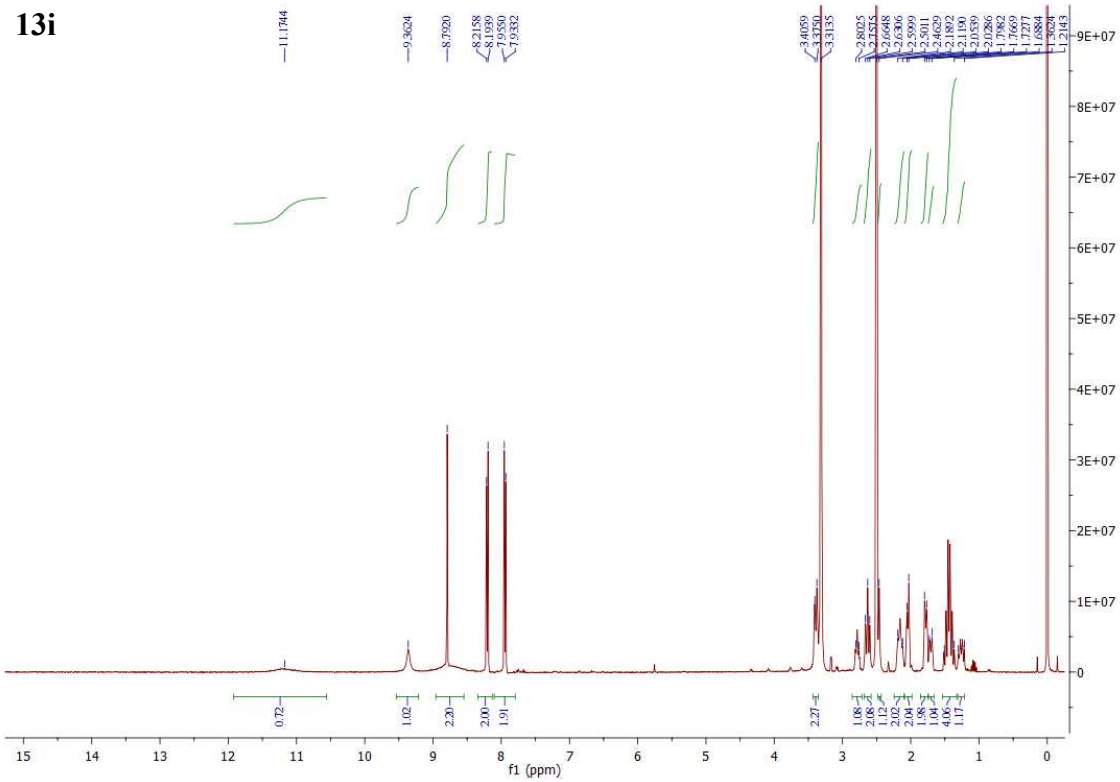
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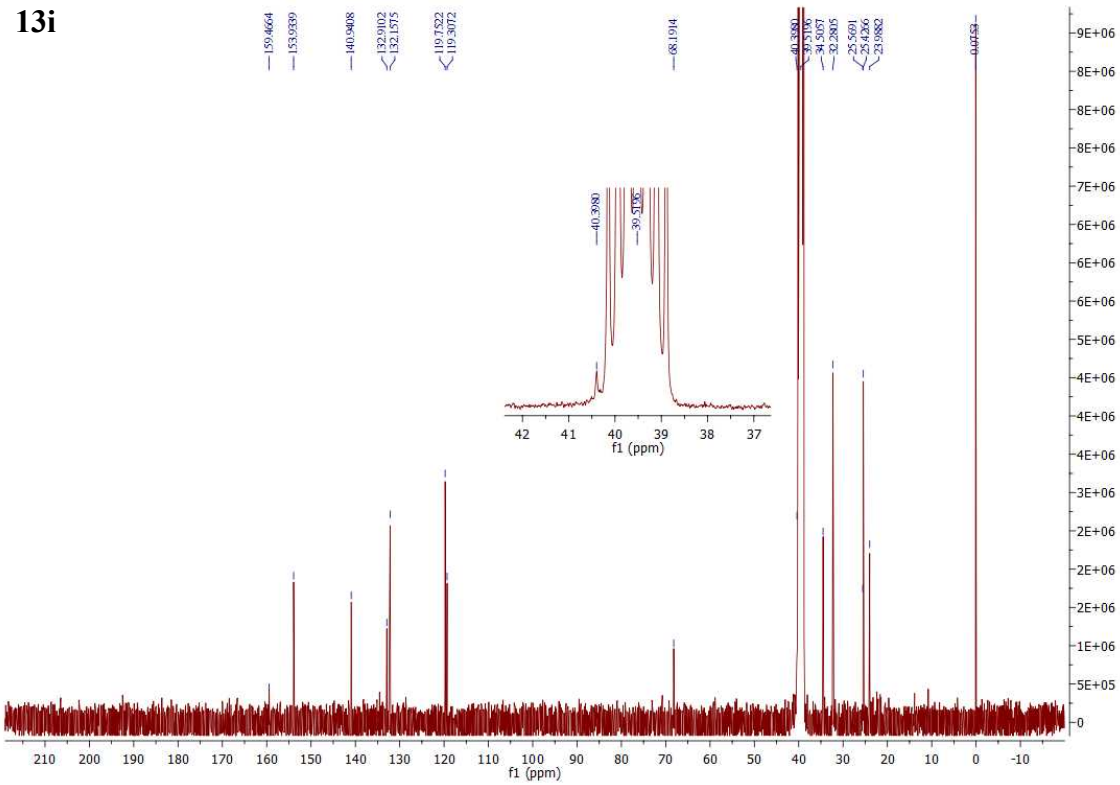
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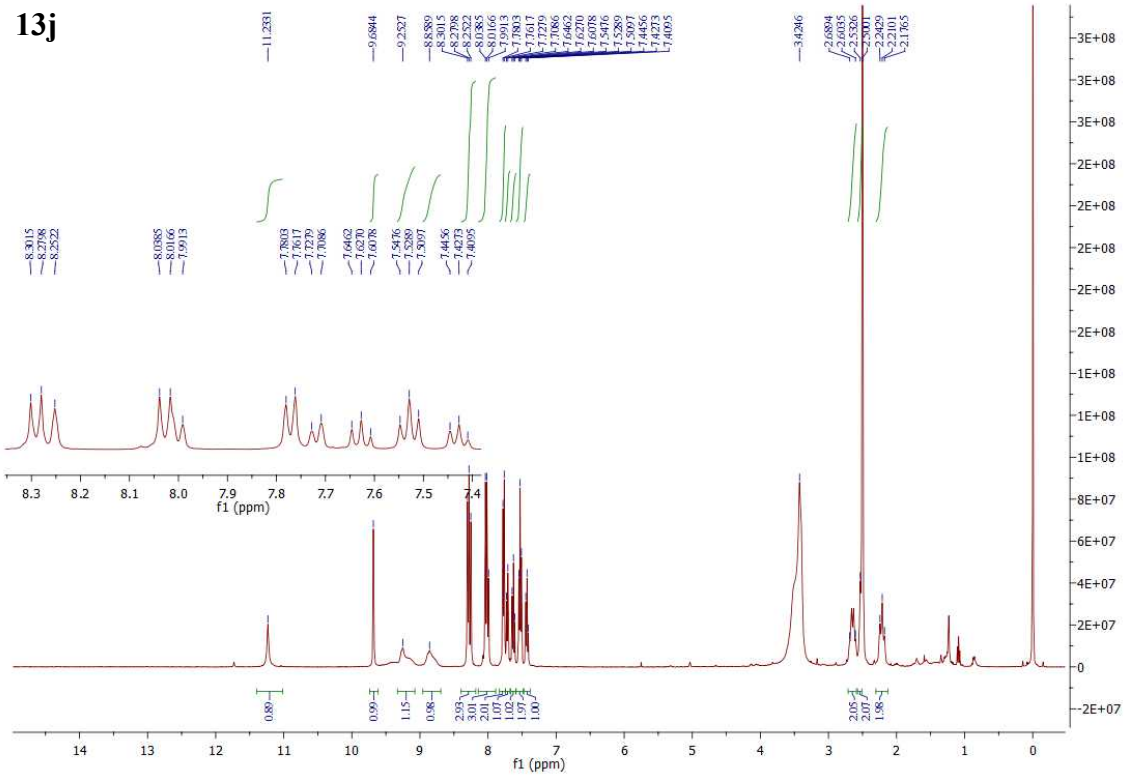

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