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

Aqueous SDS micelle-promoted acid-catalyzed domino ABB' imino Diels-Alder reaction: a mild and efficient synthesis of privileged 2-methyl-tetrahydroquinoline scaffolds

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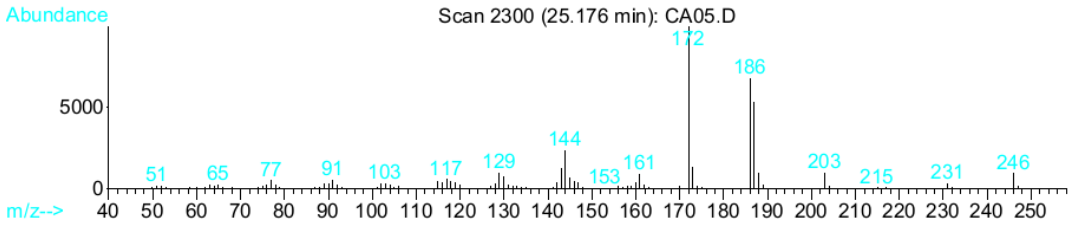
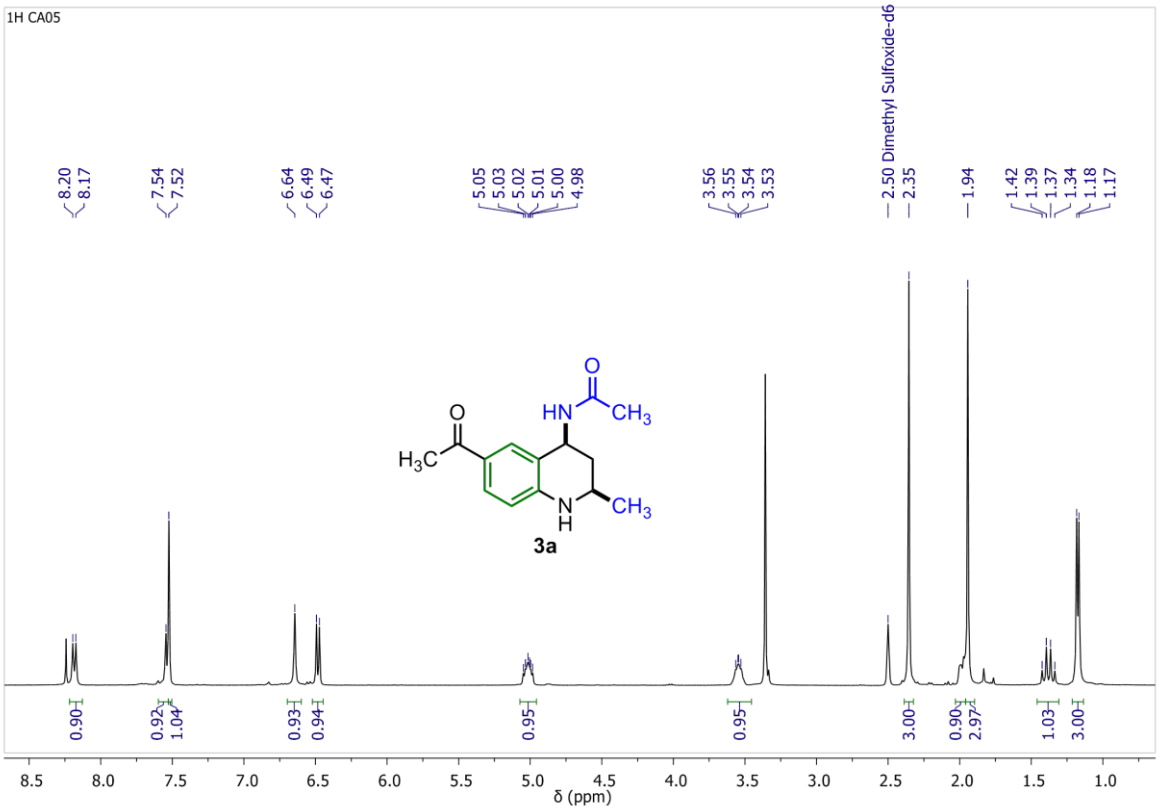
1. General experimental details

The reagents were of synthesis degree and were used without previous purification. The melting points (uncorrected) were determined with a Fisher-Johns melting point apparatus. The IR spectra were recorded on a Lumex Infralum FT-02 spectrophotometer in KBr and thin film. NMR (1D and 2D) spectra were recorded on Bruker Avance-400 spectrometer. Chemical shifts are reported in ppm (δ) relative to the solvent peak (2.50 and 7.26 ppm for DMSO-d_6 and $CDCl_3$ for protons, respectively). A Agilent Technologies 6890 plus Gas Chromatograph interfaced to an Agilent Technologies MSD 5963 Selective Detector (MSD) with a Chemstation Data system G17001DA was used for MS identification at 70 eV using a 60 m capillary column coated with HP-5 [5 %-phenyl-poly(dimethyl-siloxane)]. Elemental analyses were performed on a Perkin Elmer 2400 Series II analyzer and were within ± 0.4 of theoretical values. The reaction progress was monitored using thin layer chromatography on a silufol UV254 TLC aluminum sheet.

2. Copies of MS, ^{1}H NMR, ^{13}C NMR and 2D spectra of THQ compounds.

N-(6-Acetyl-2-methyl-1,2,3,4-tetrahydroquinolin-4-yl) acetamide, **3a**.





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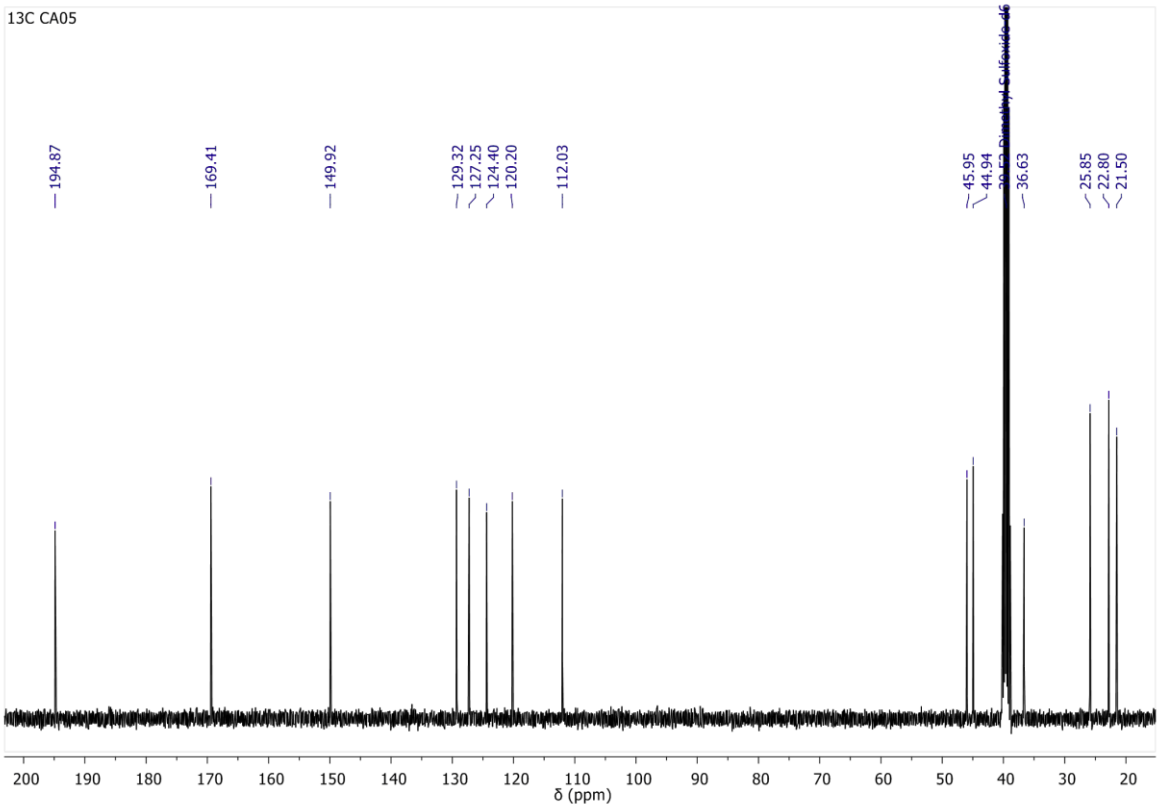

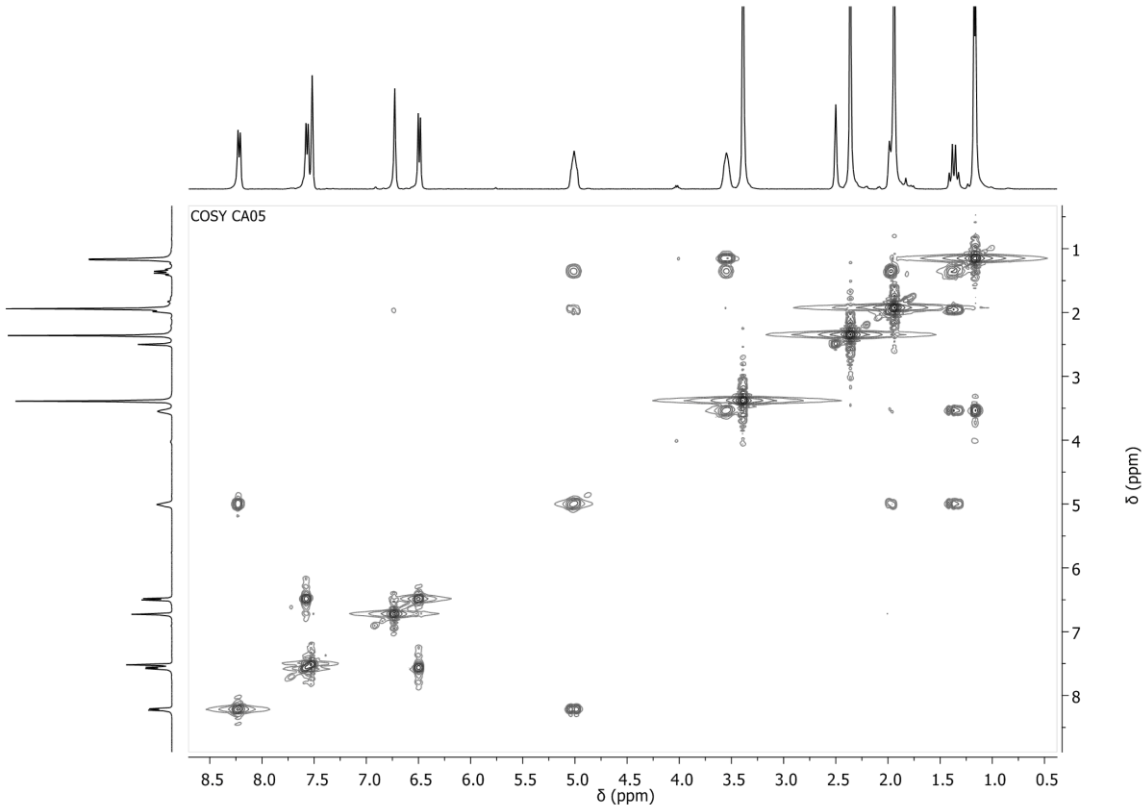

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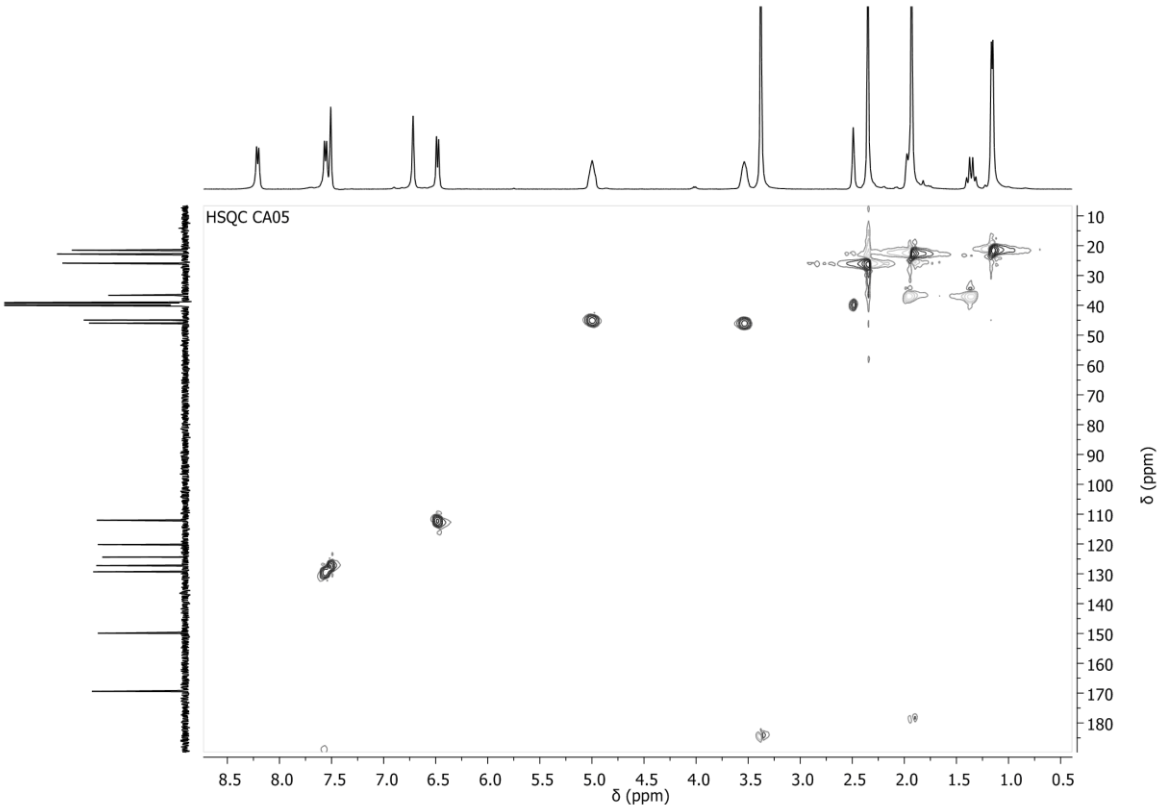

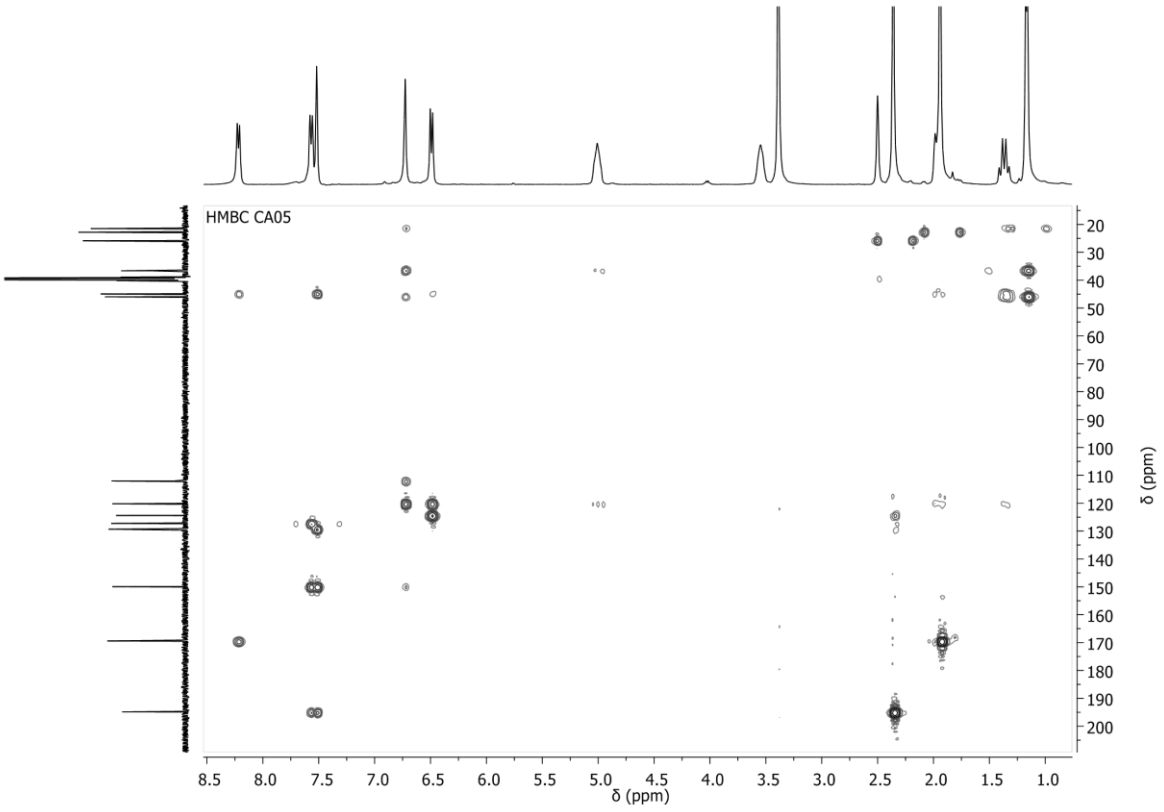

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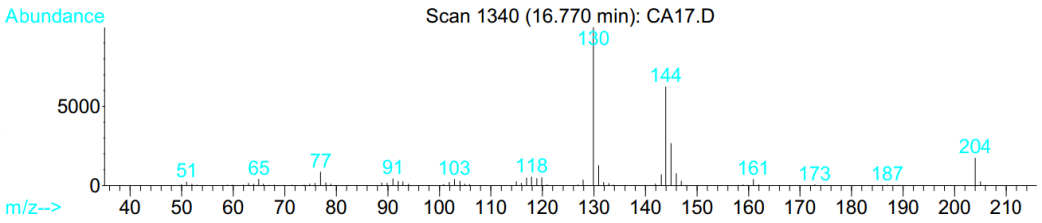

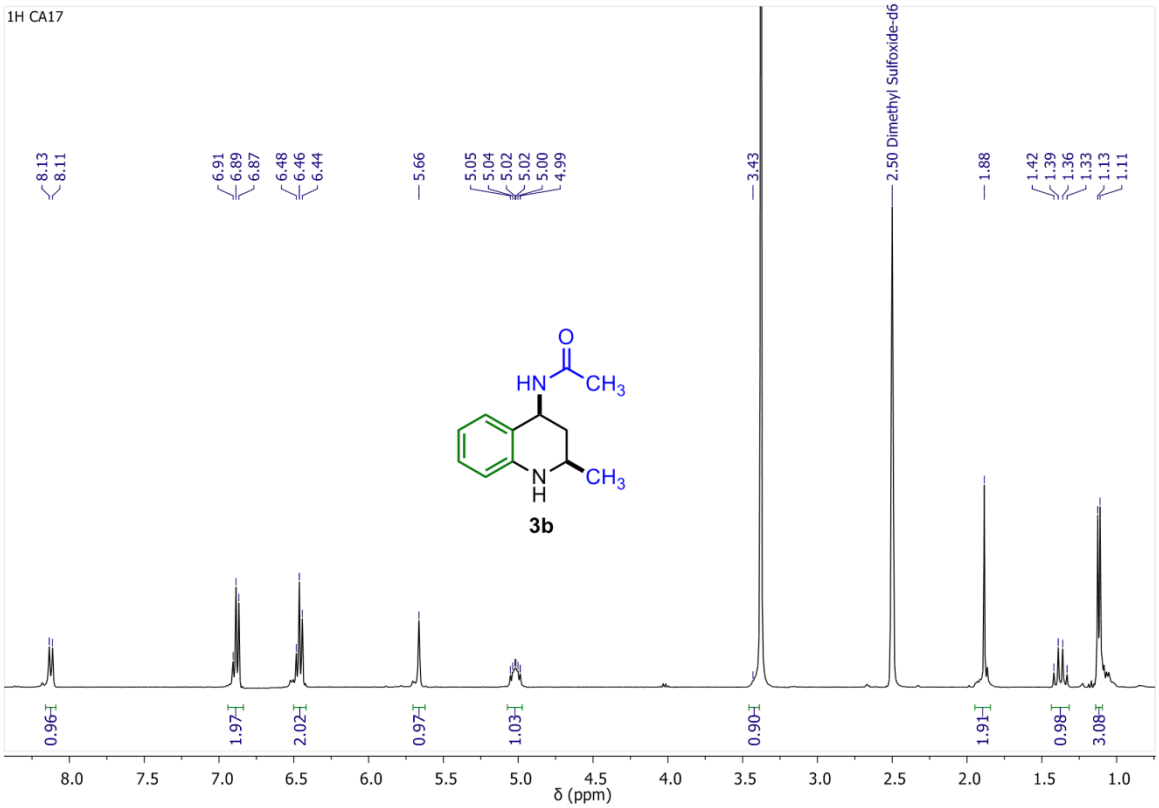

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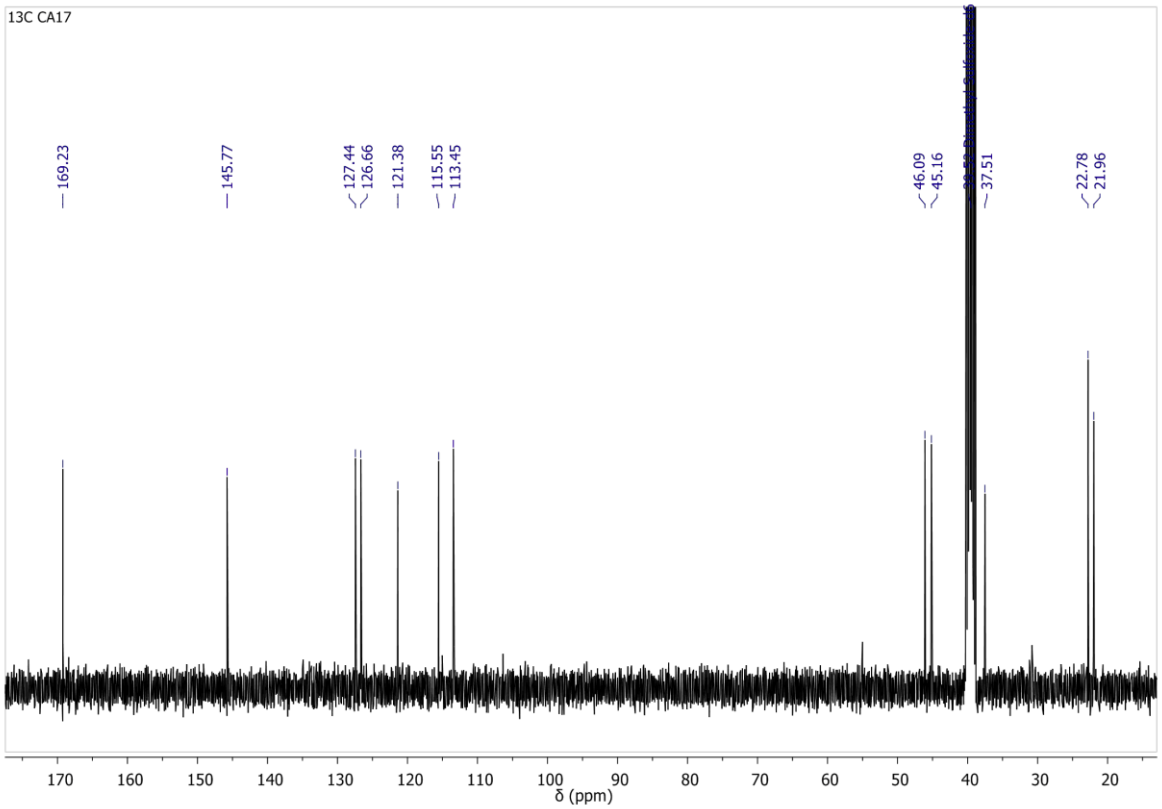

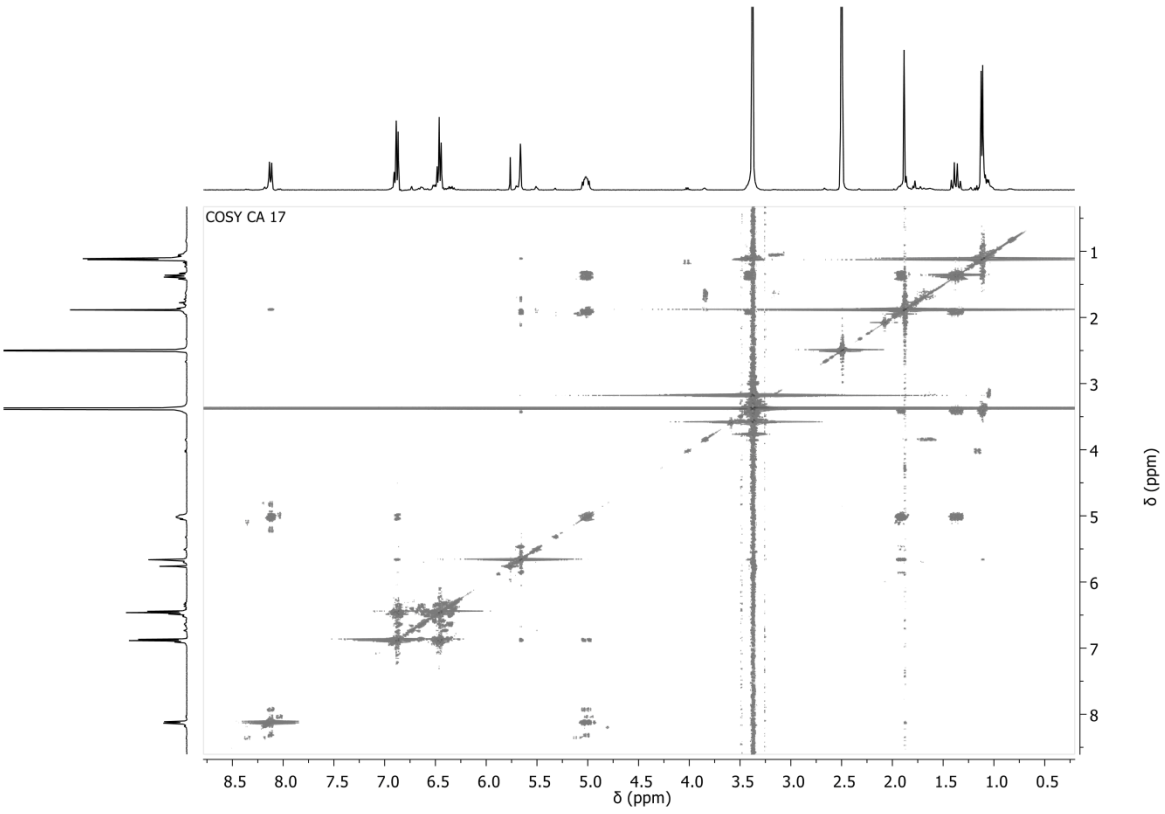

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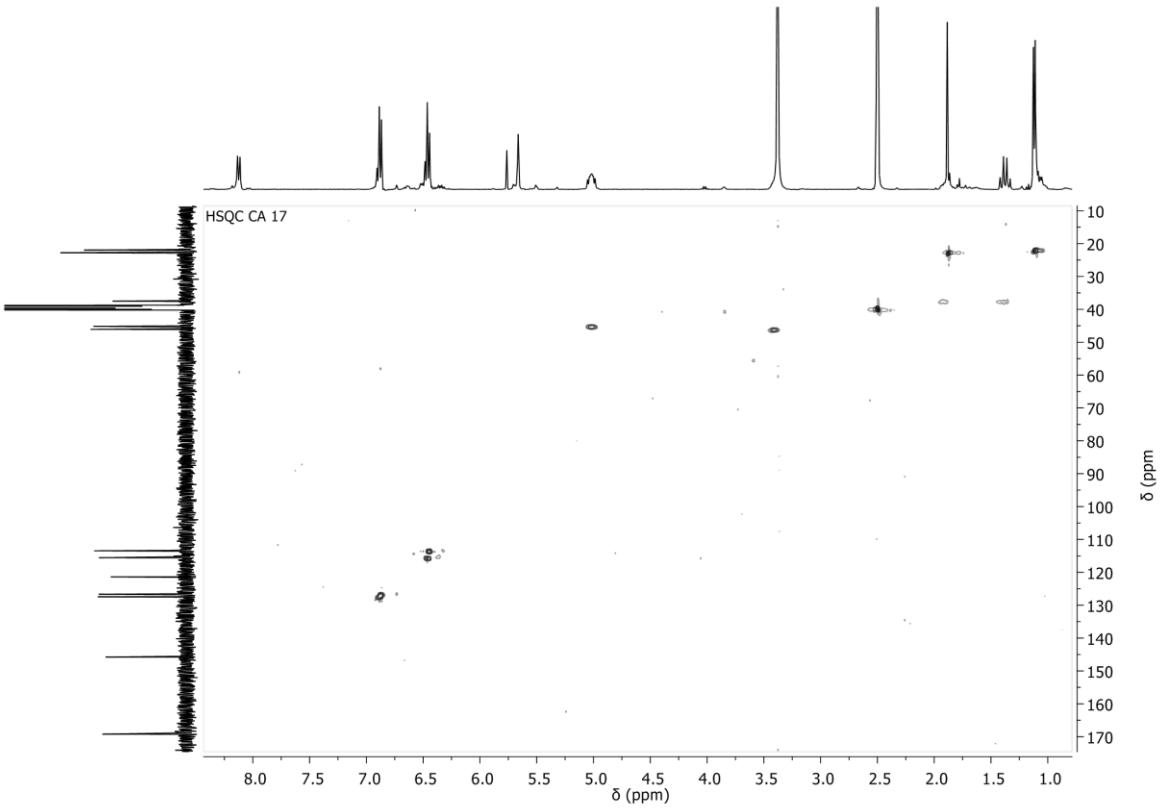

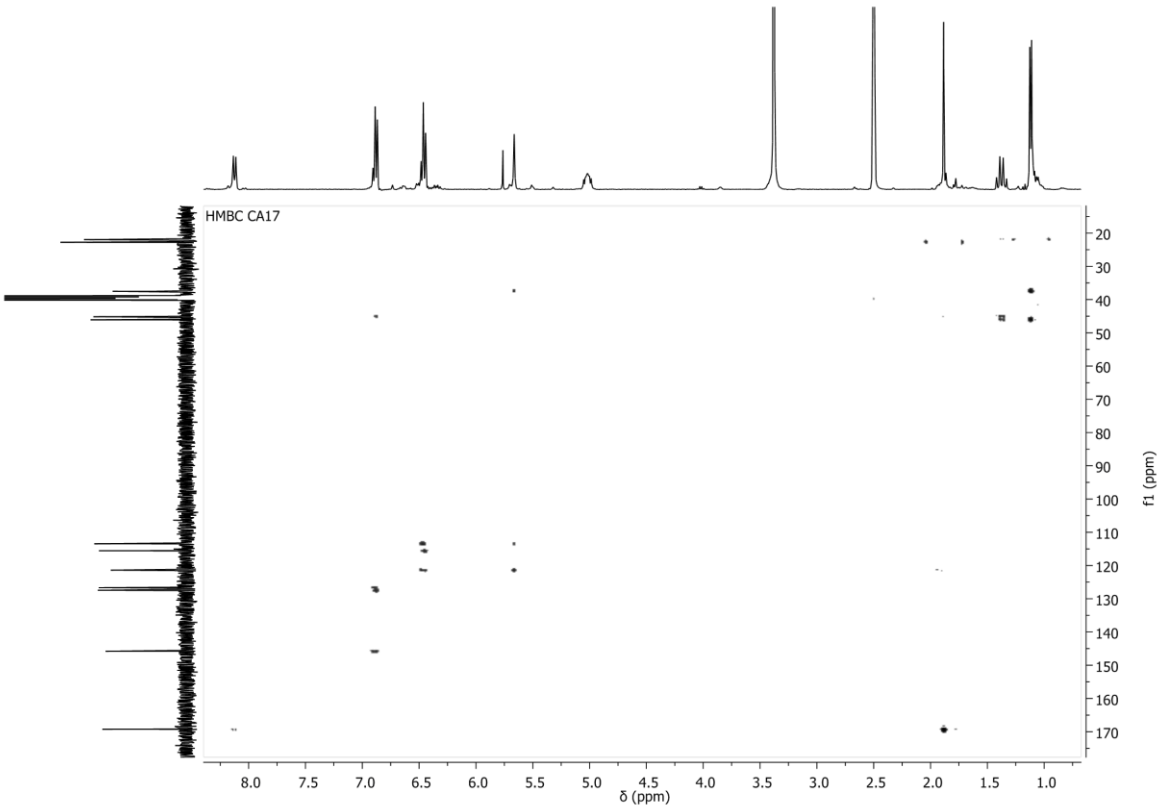

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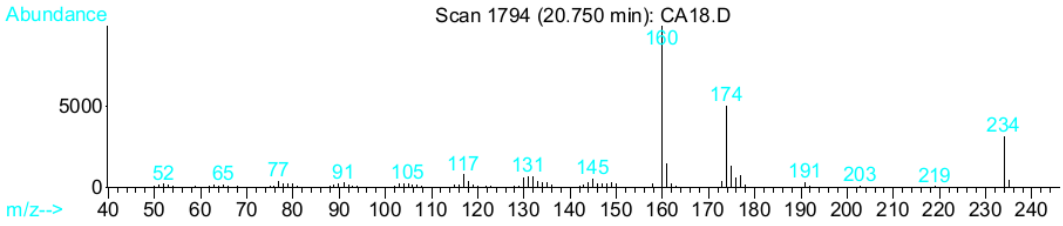

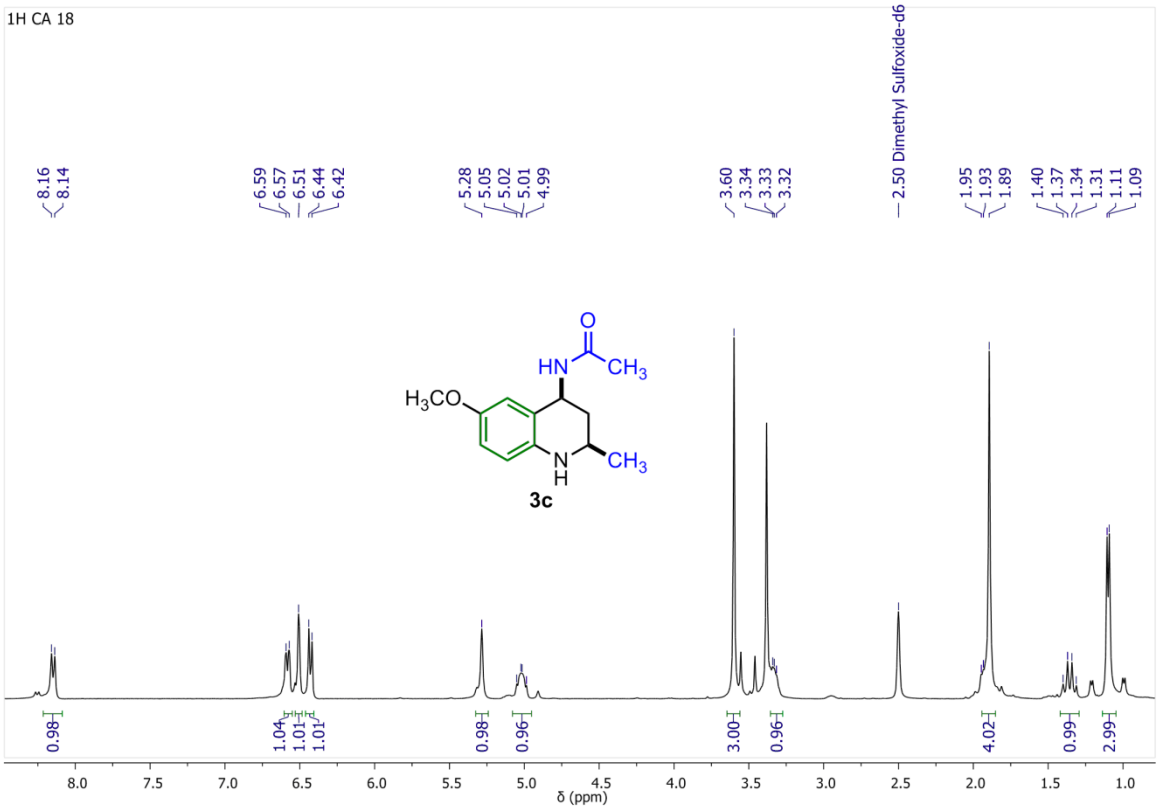

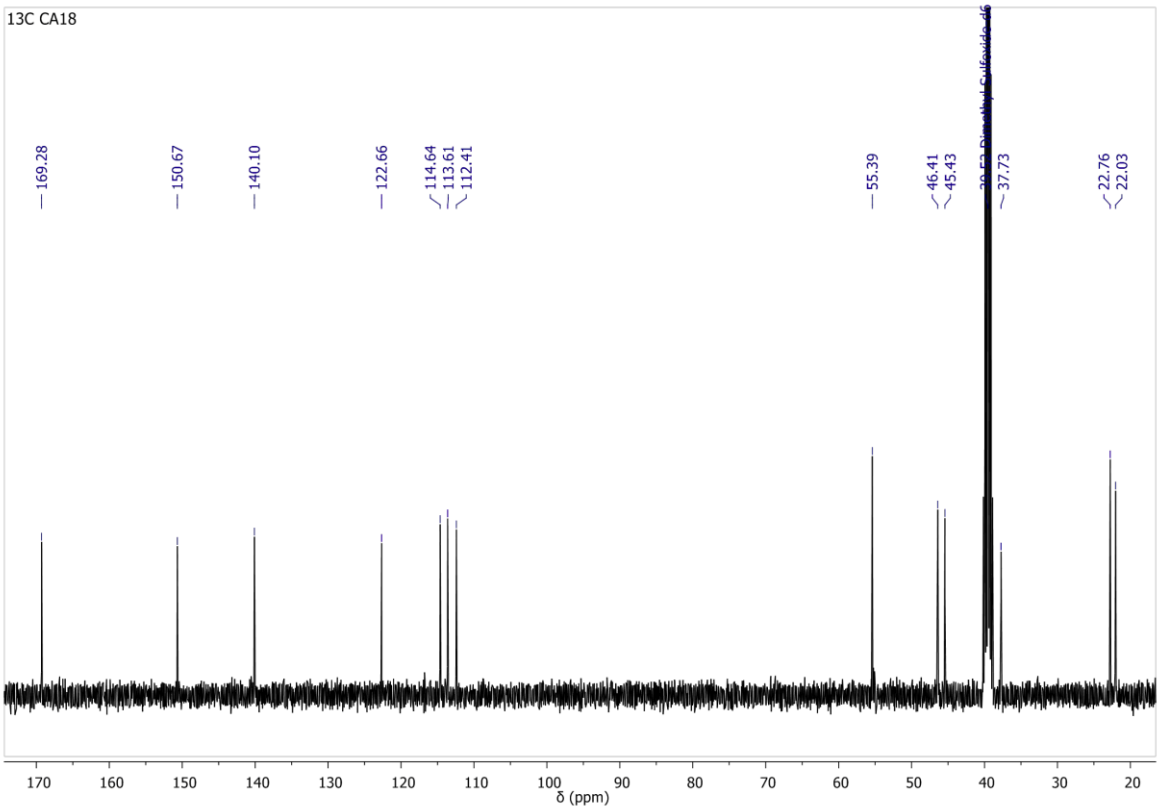
13C CA18
169.28
150.67
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113.61
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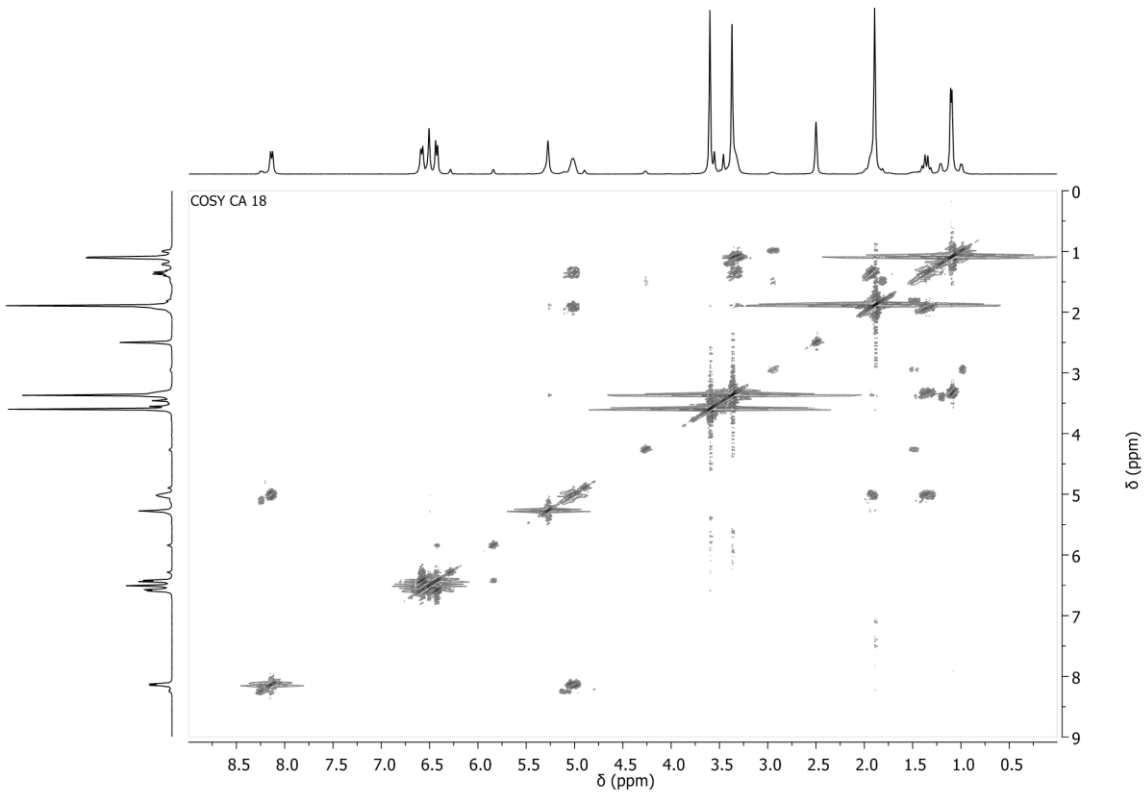
55.39
46.41
45.43
37.73
22.76
22.03
δ (ppm)


COSY CA 18
δ (ppm)
δ (ppm)

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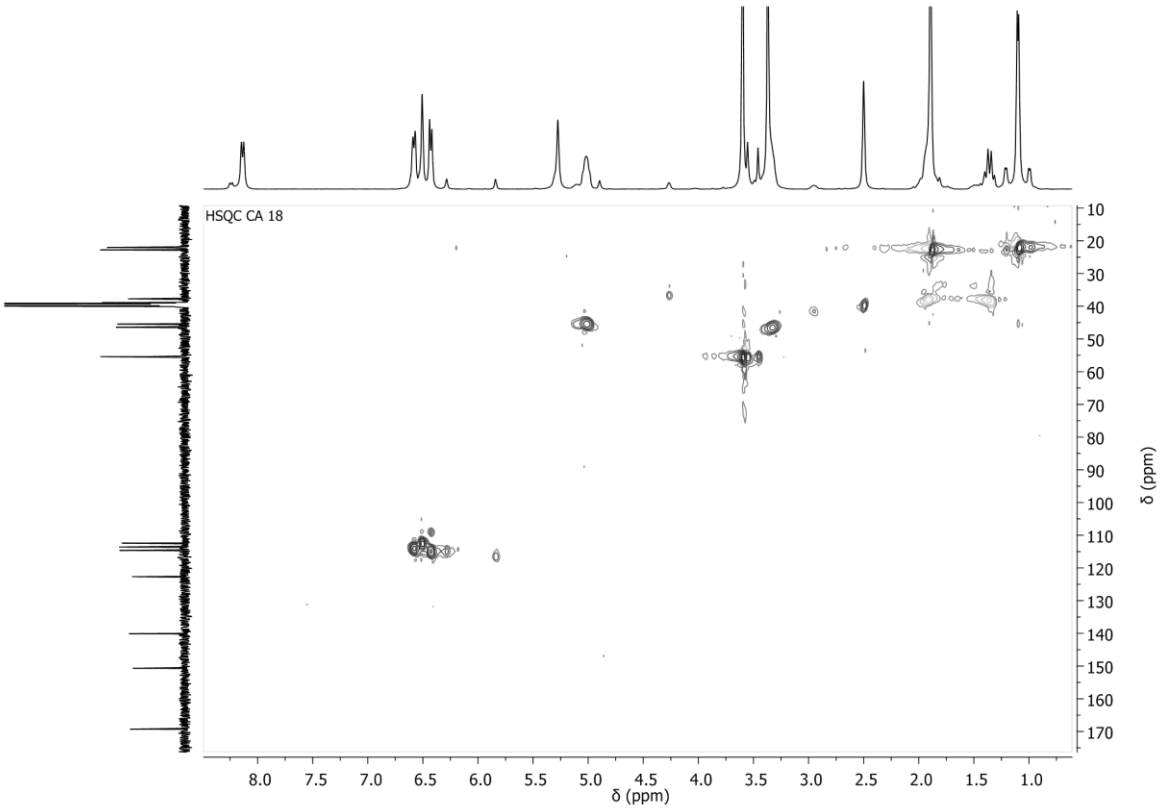

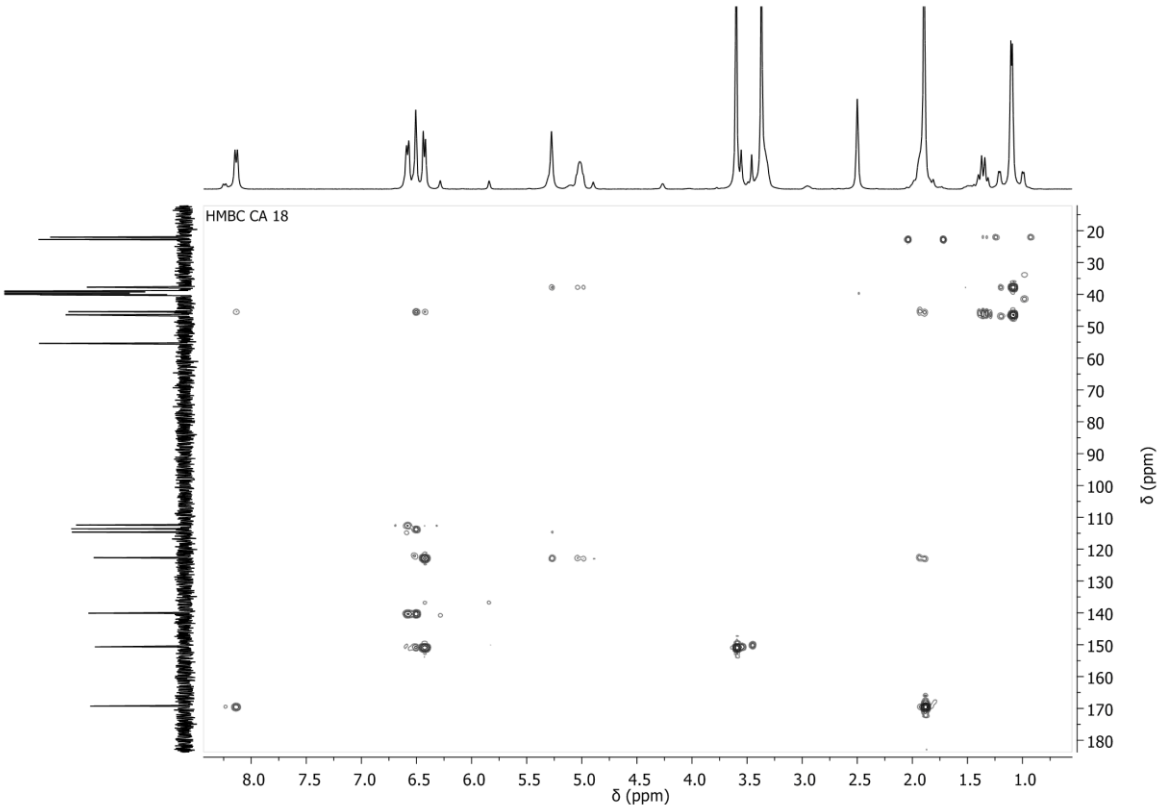

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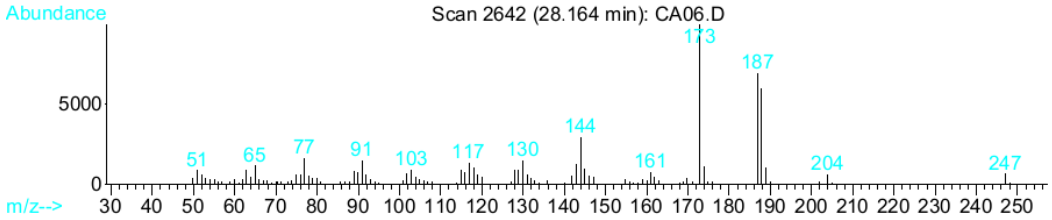

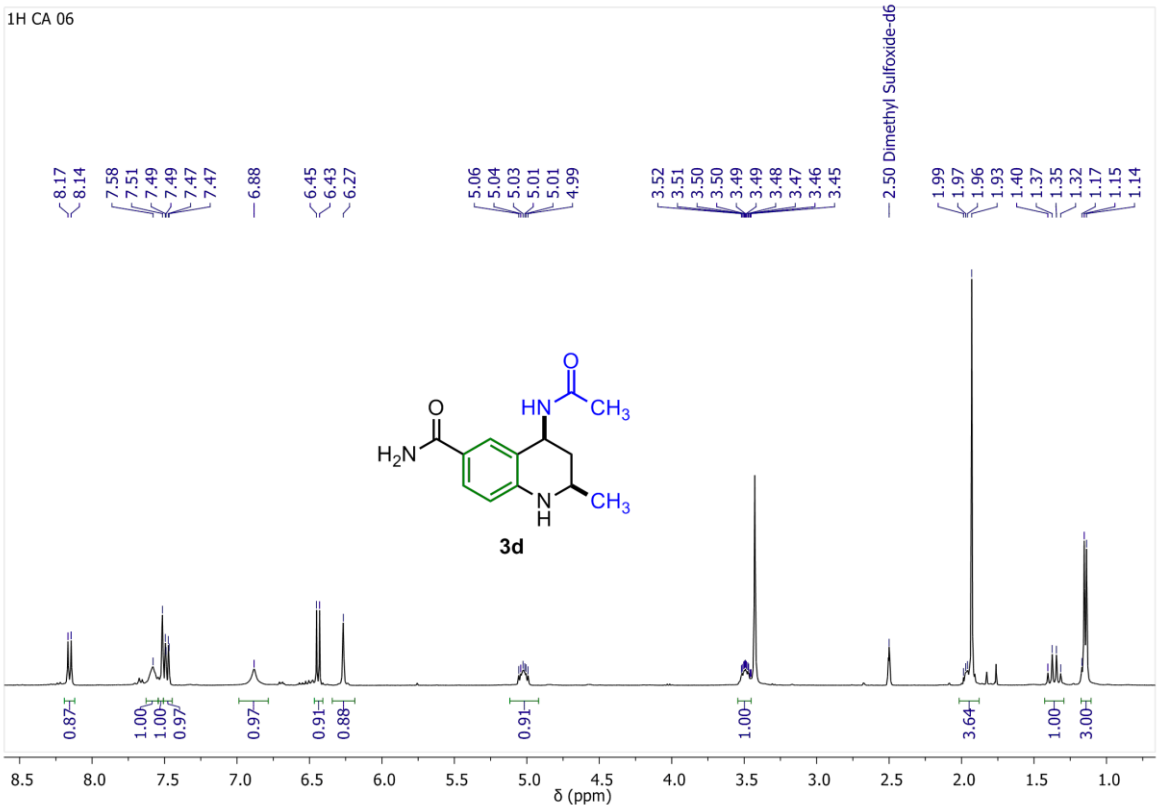

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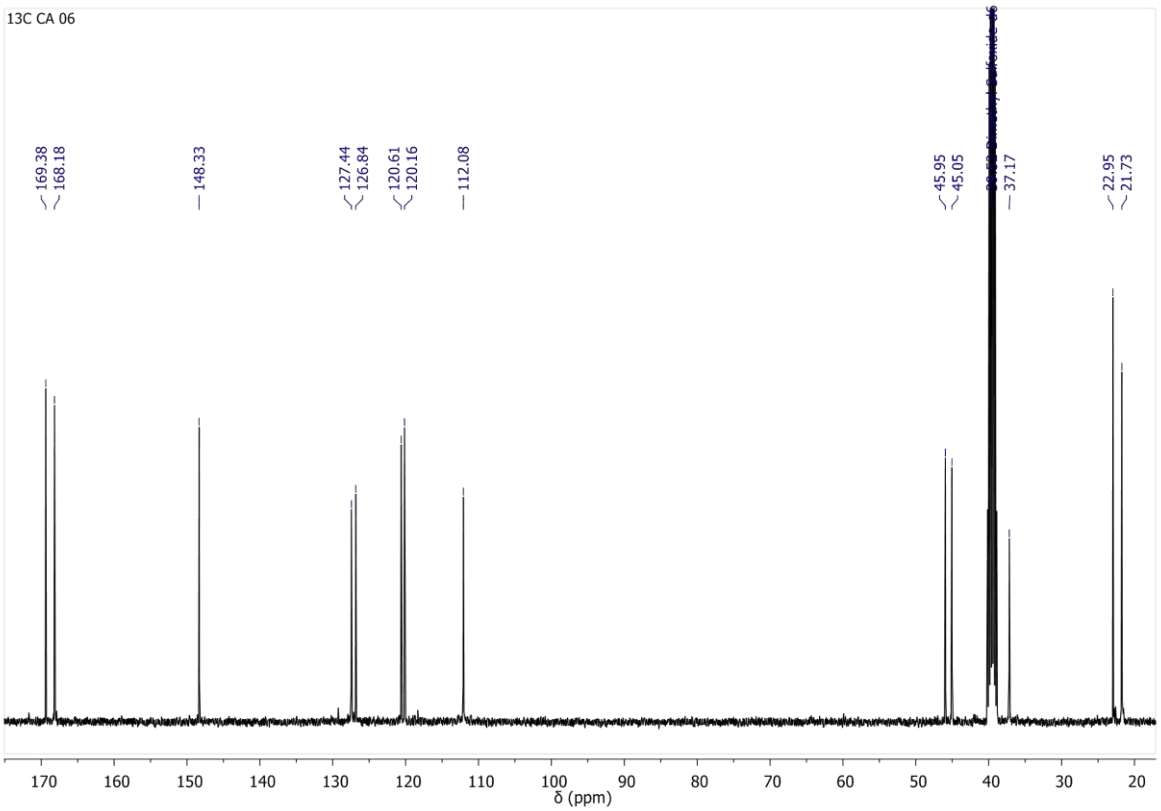

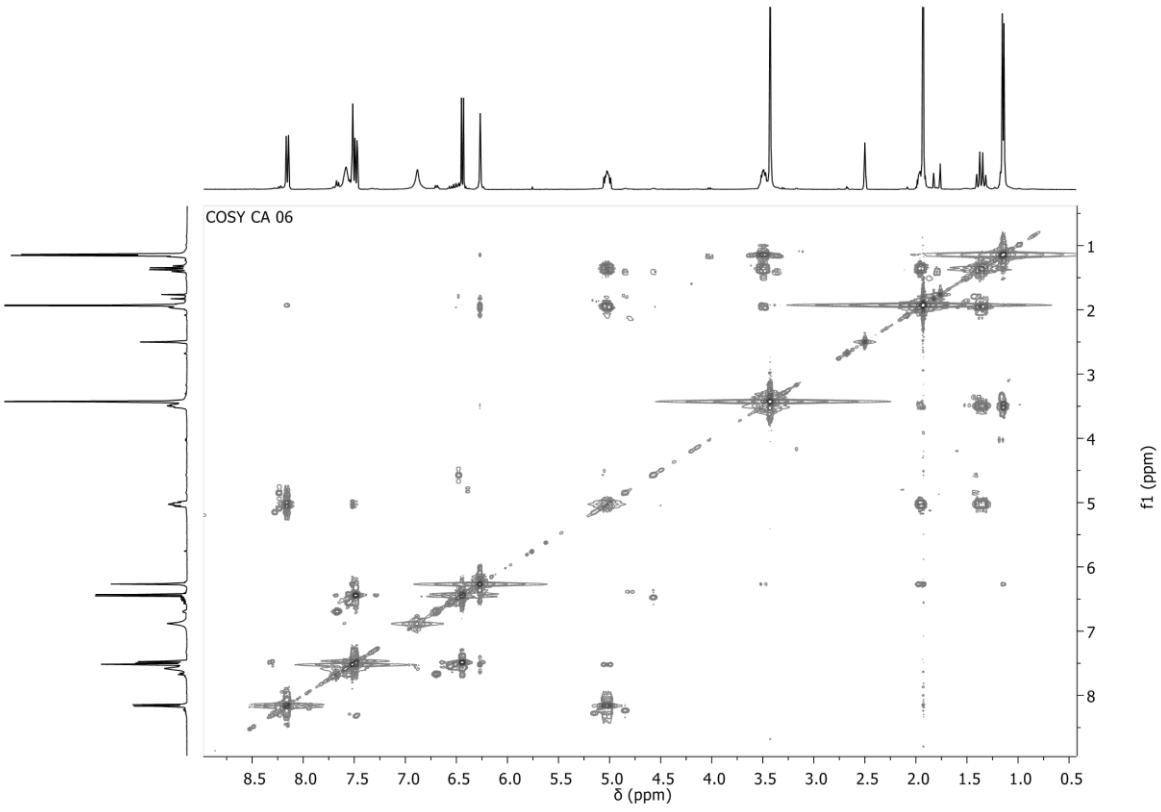

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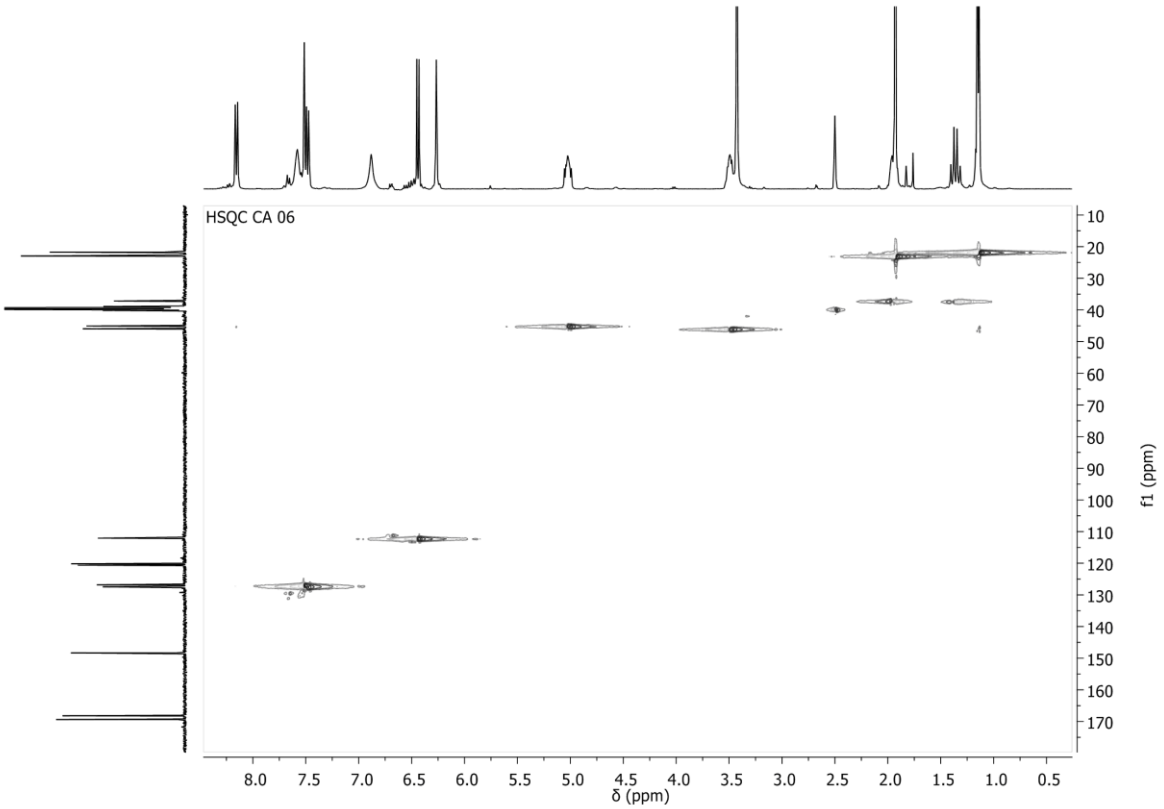

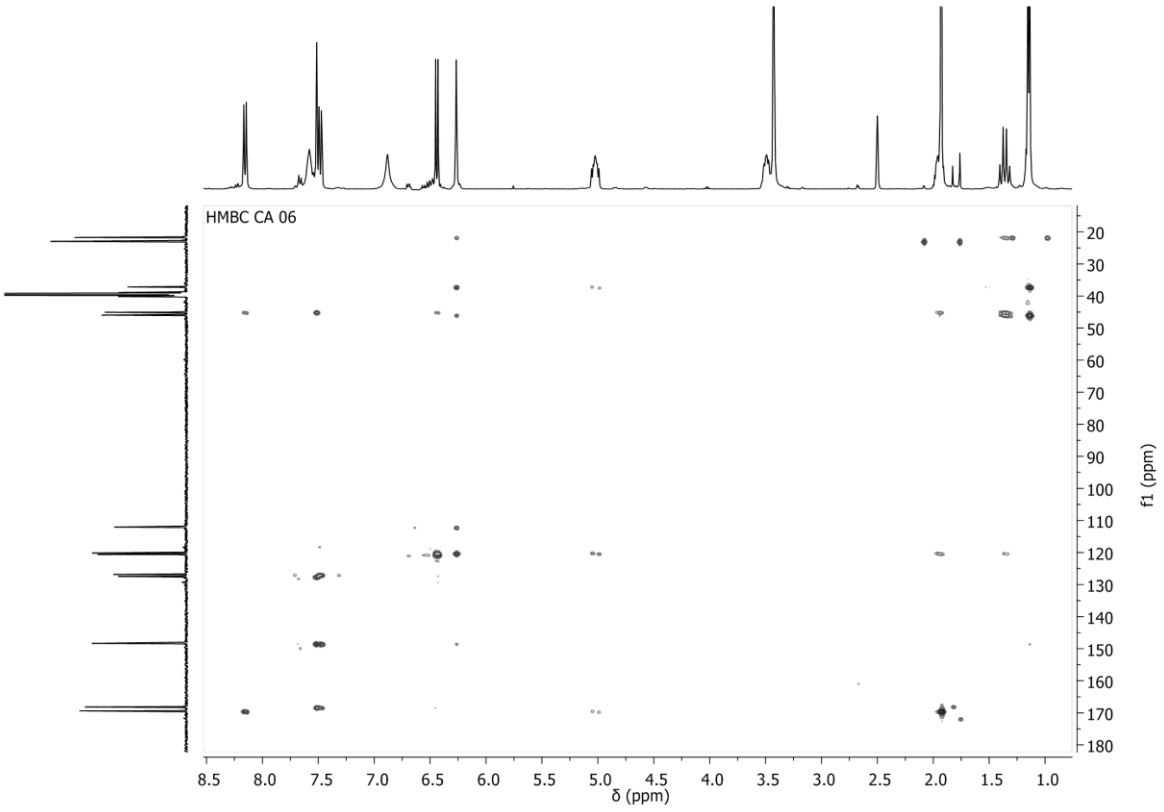

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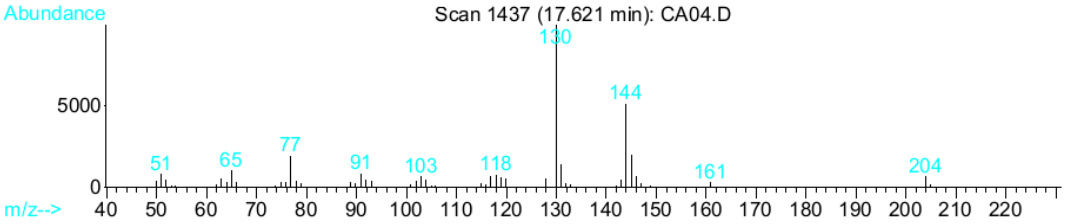

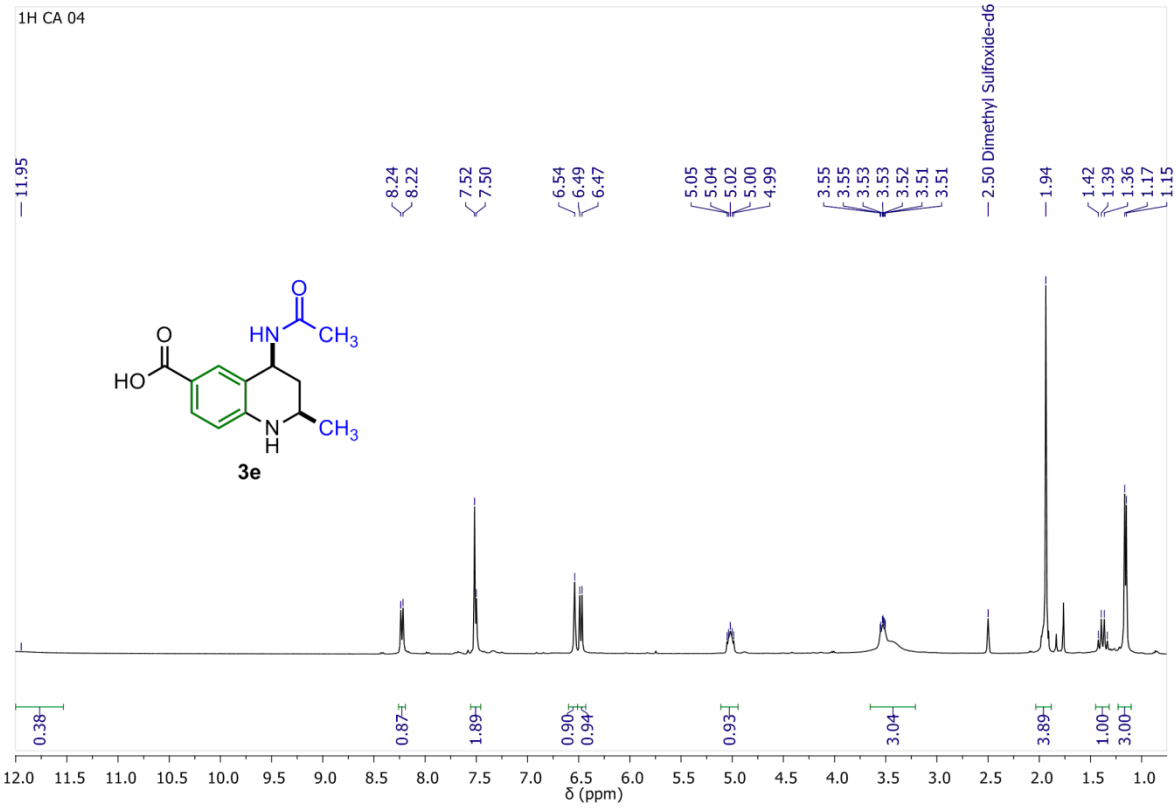

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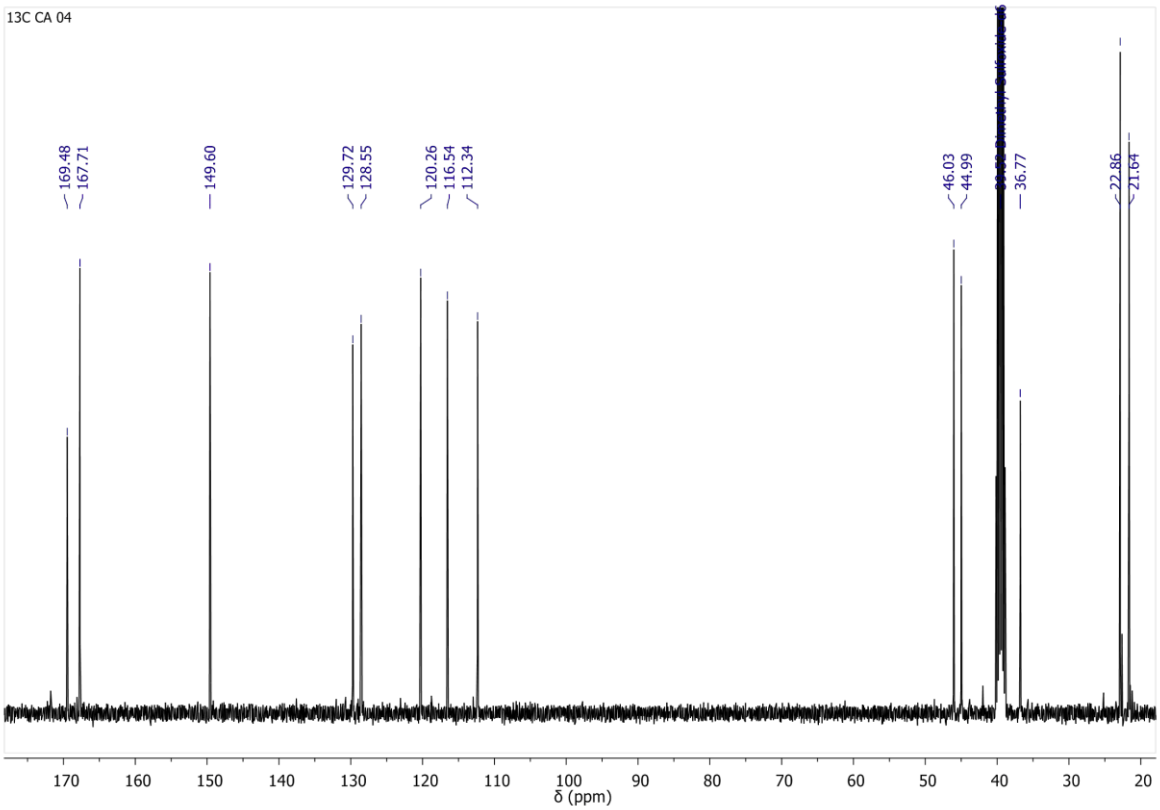

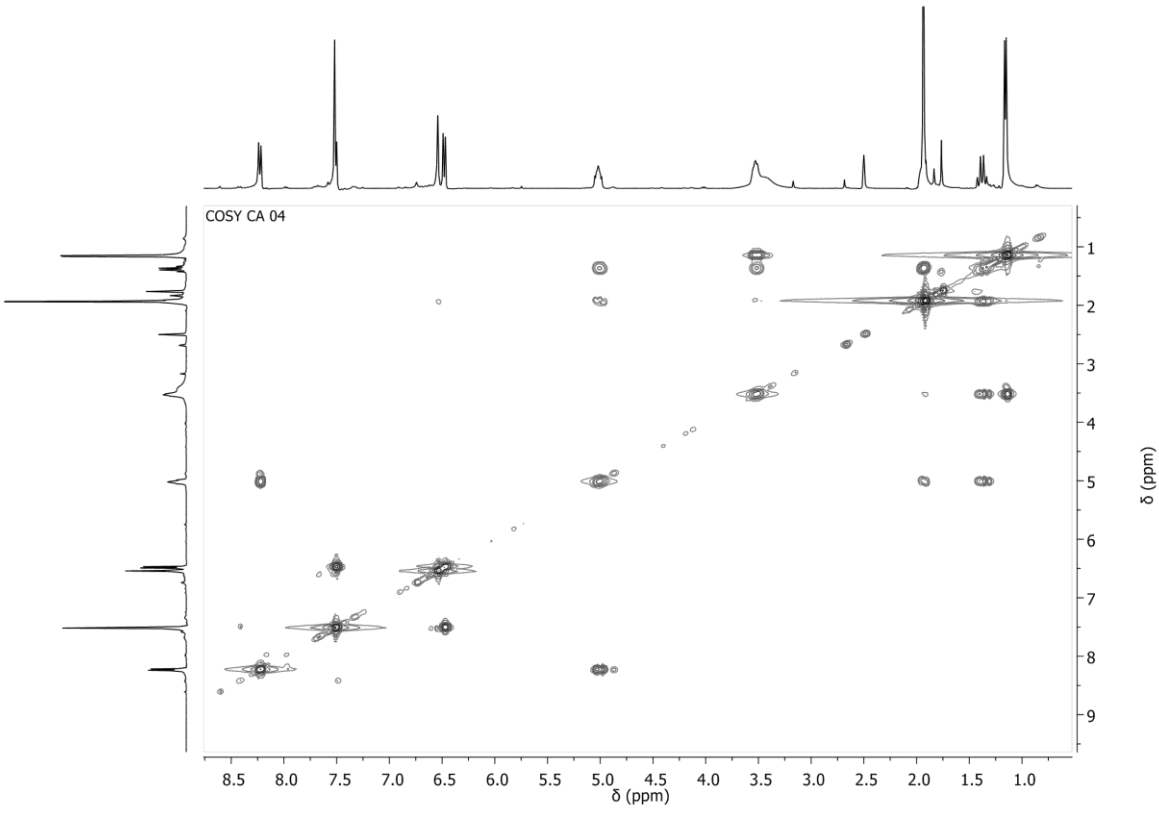

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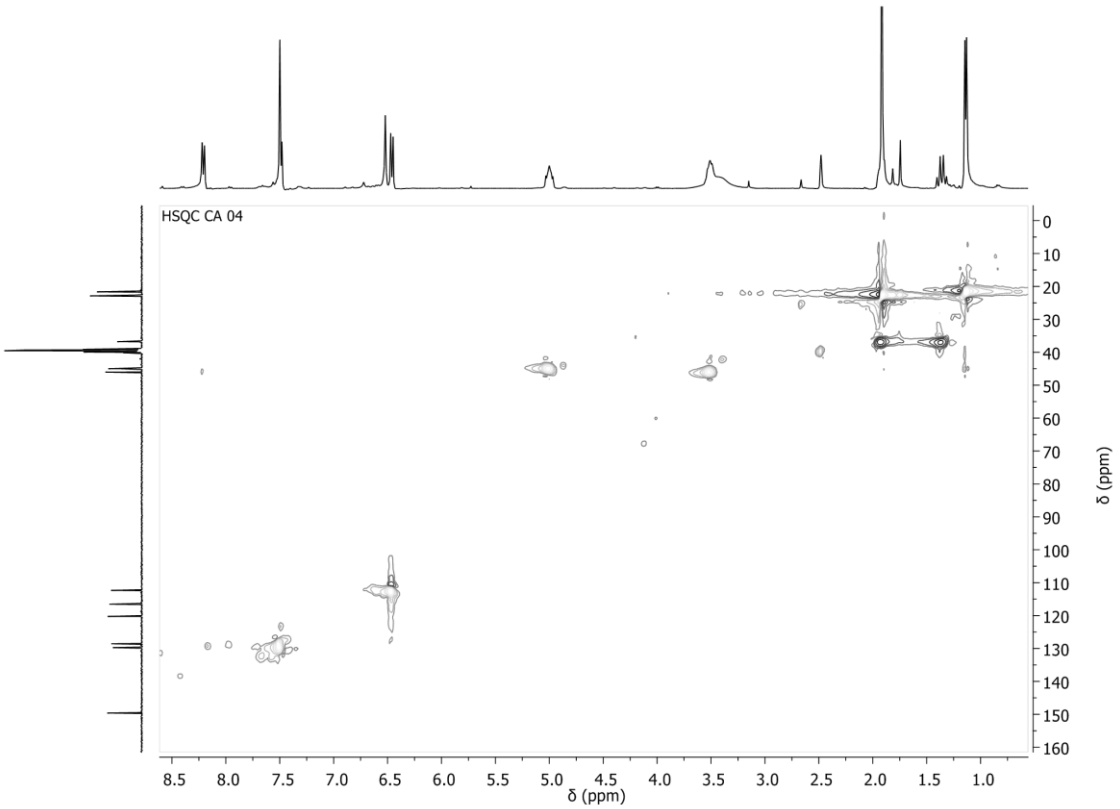

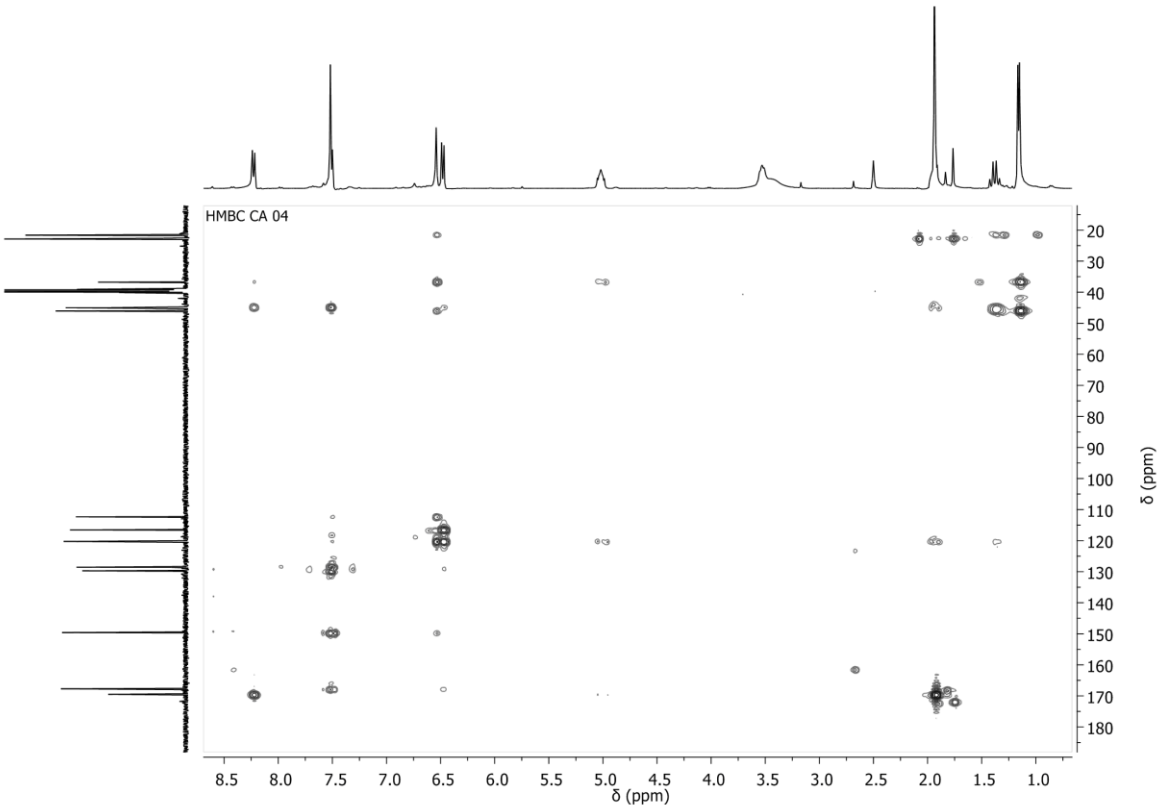

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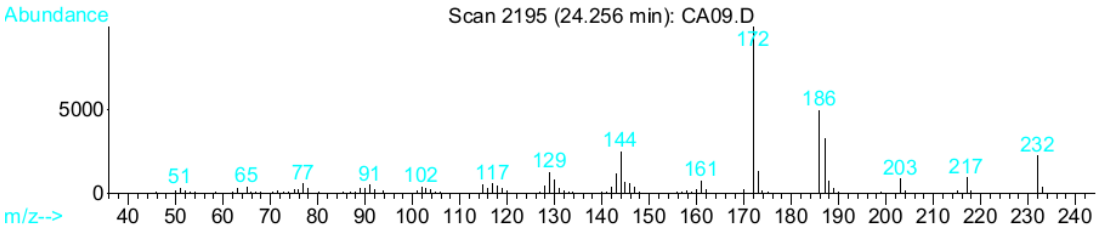
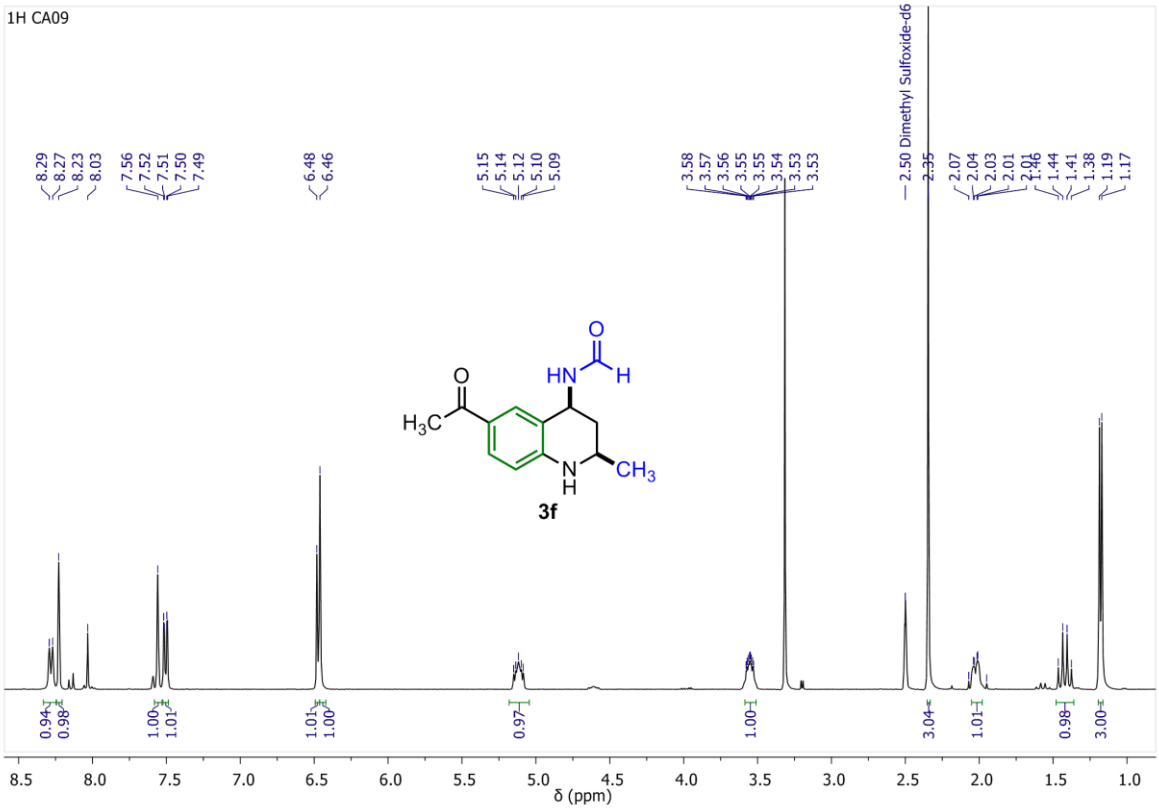
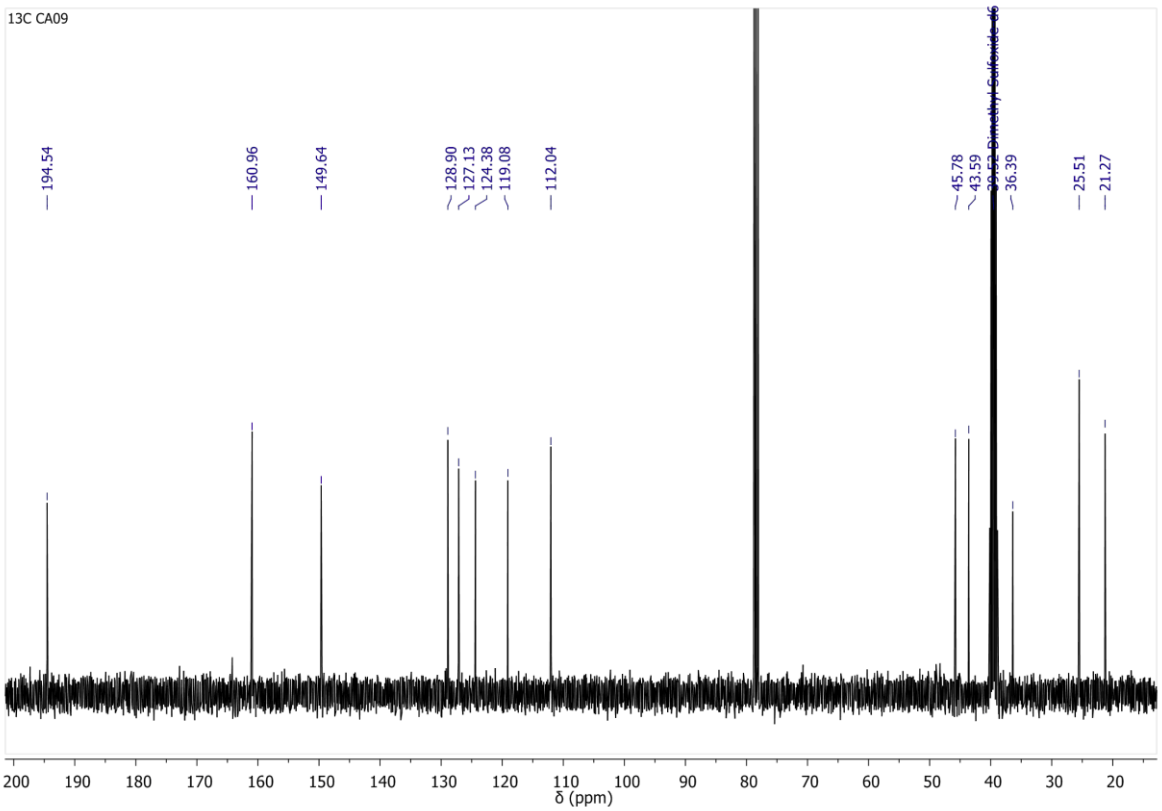




3f



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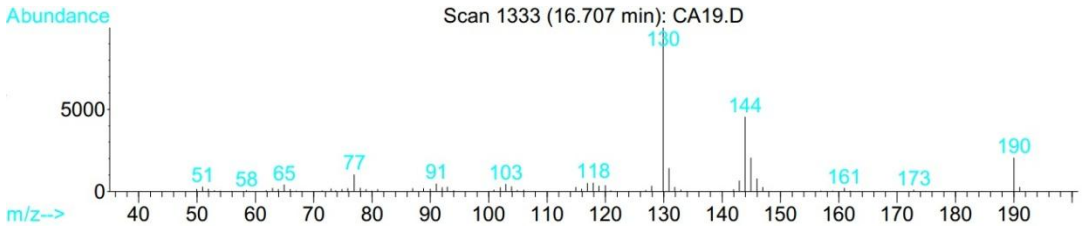

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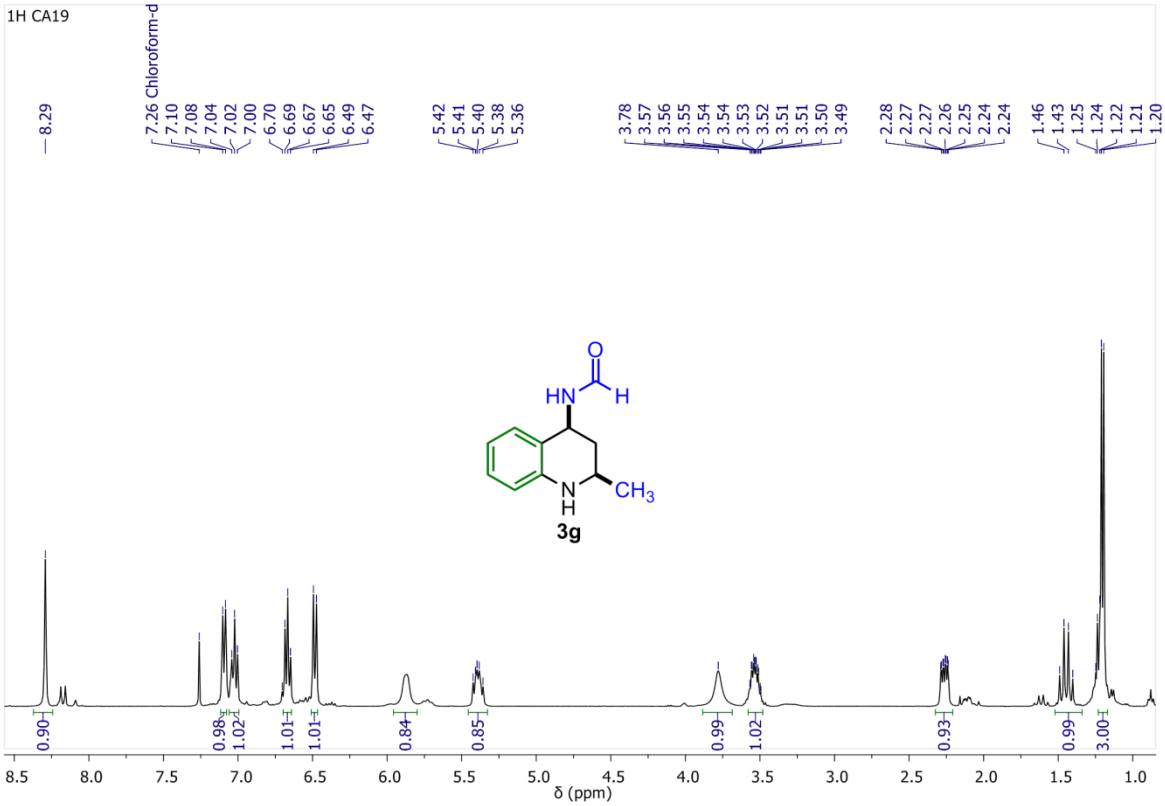

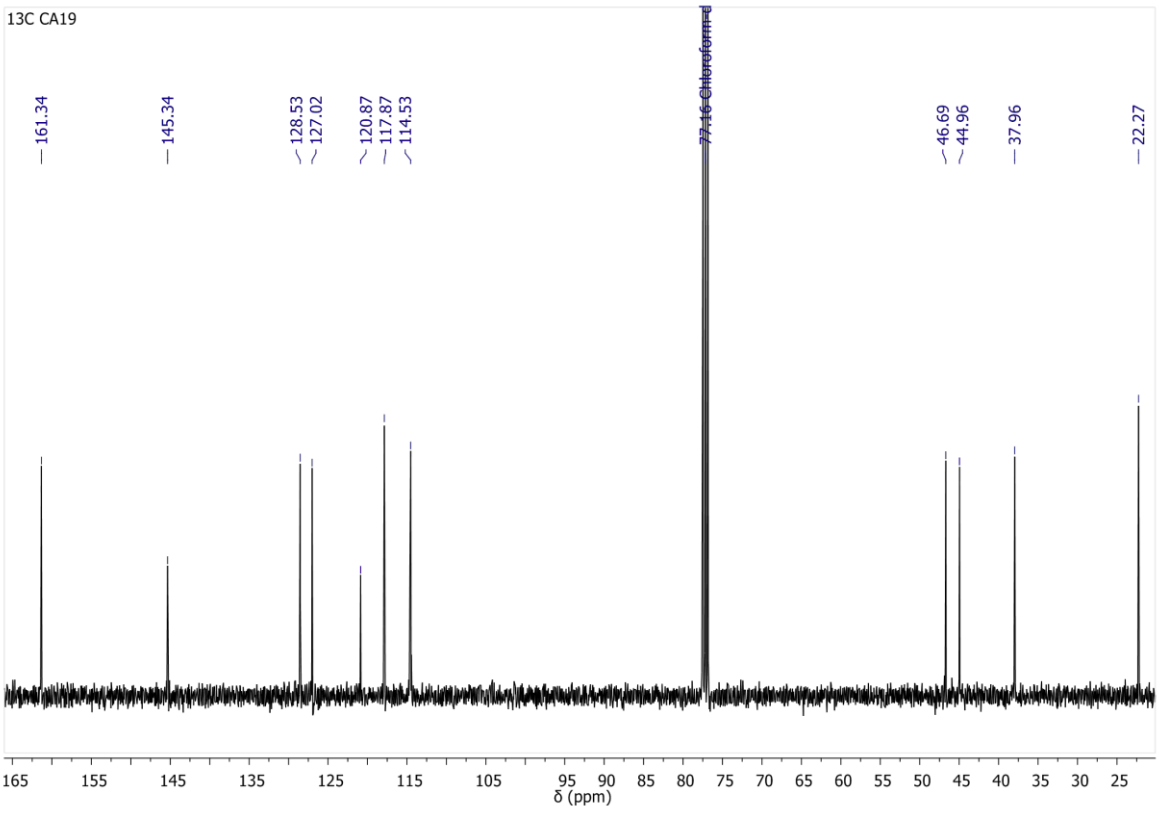

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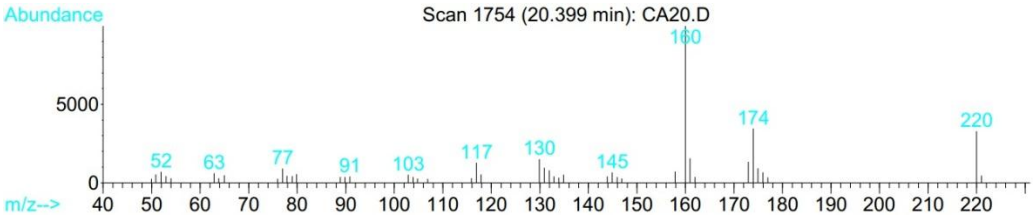

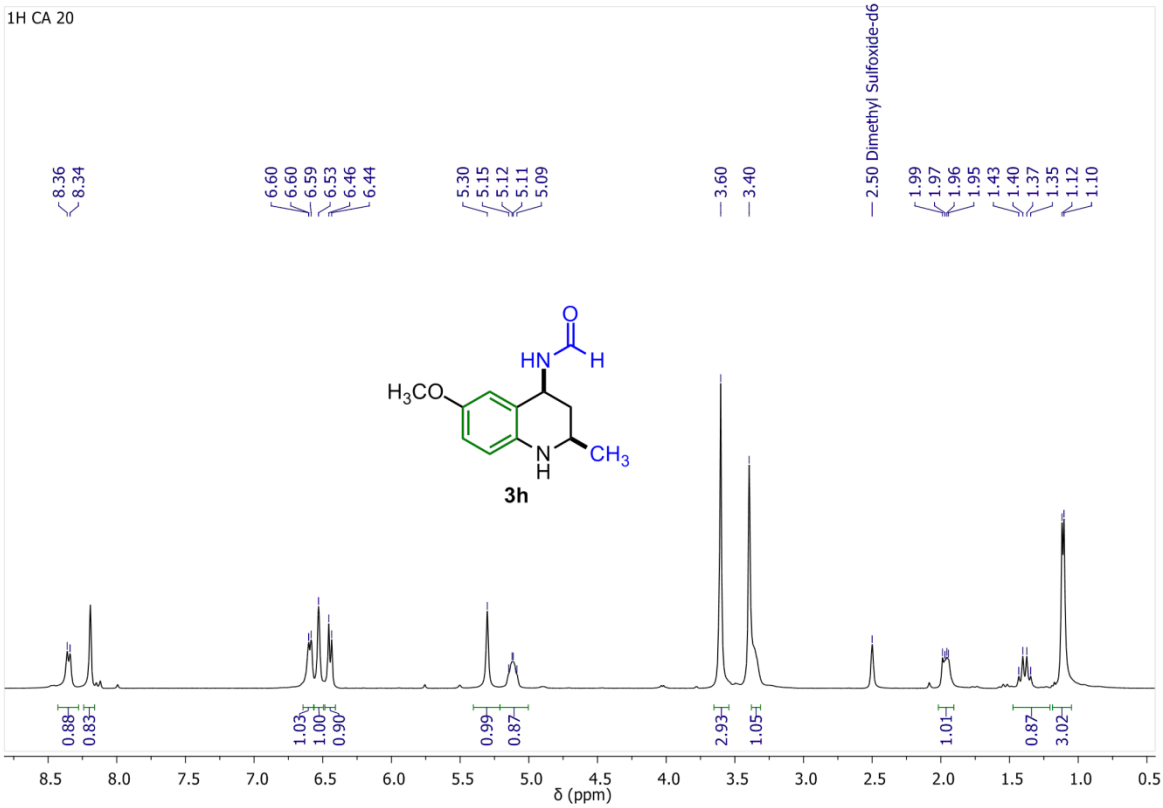

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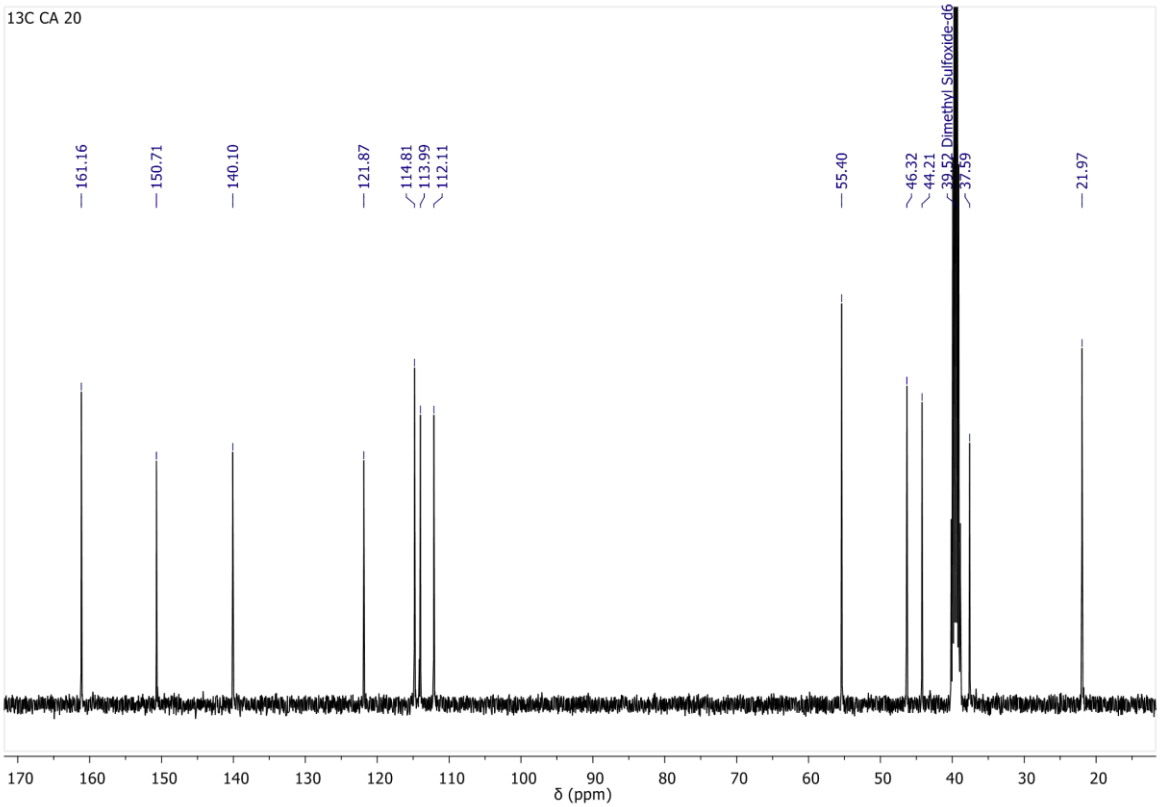

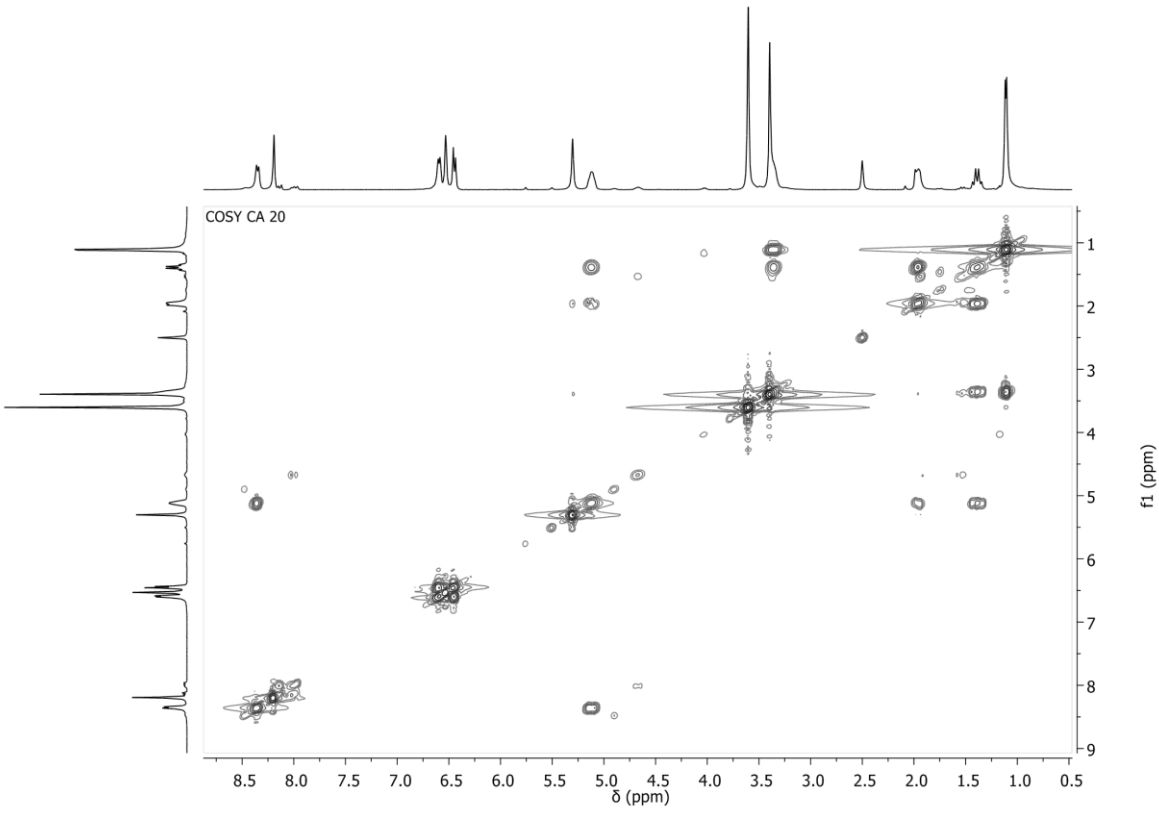

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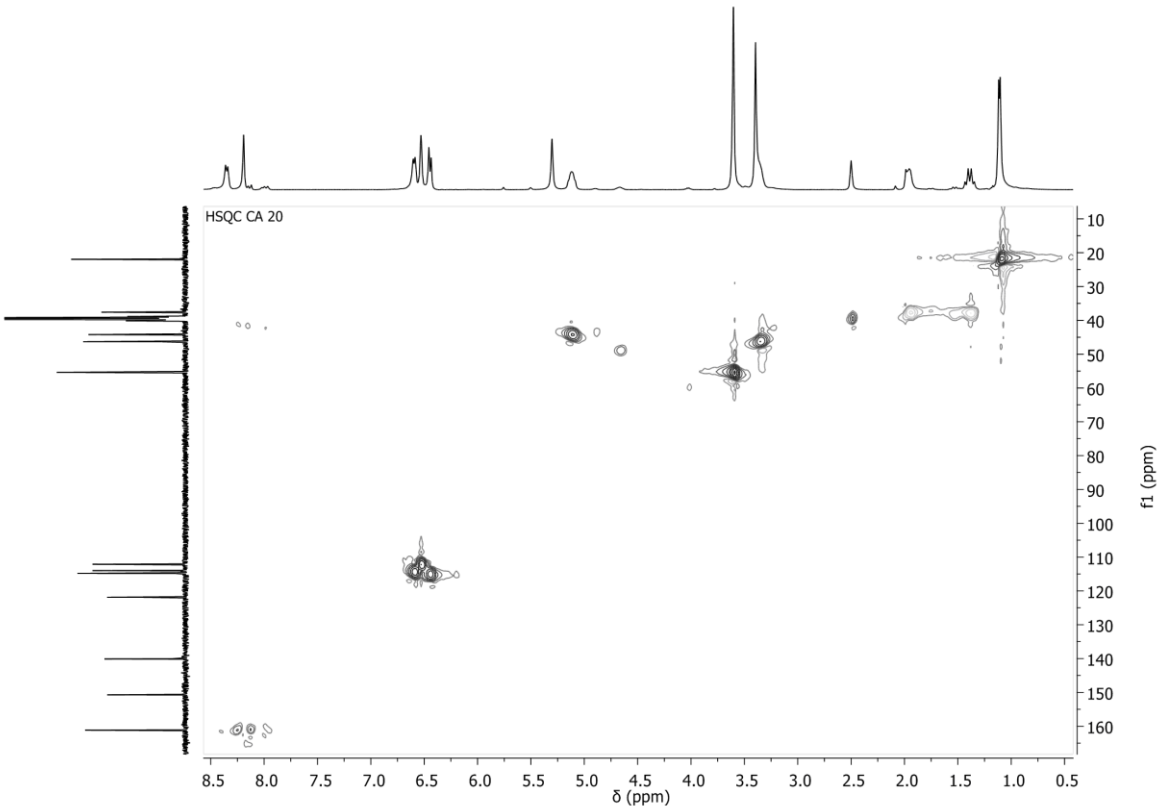

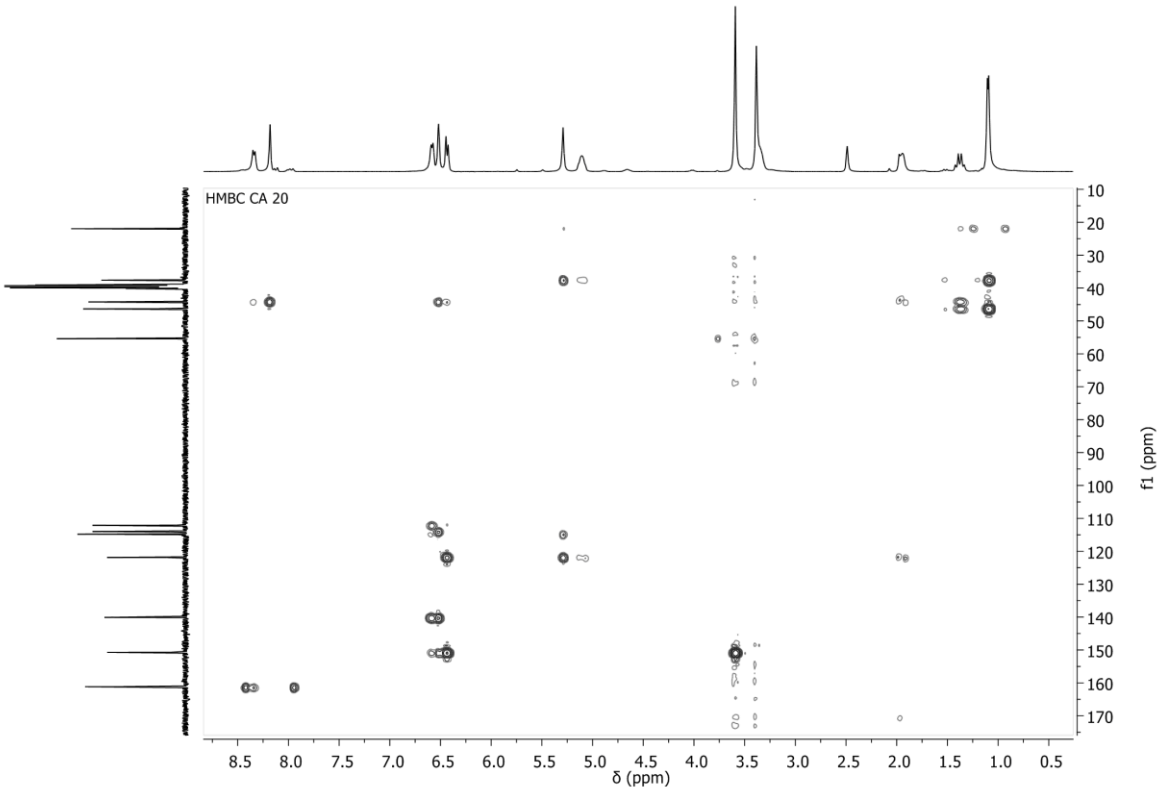

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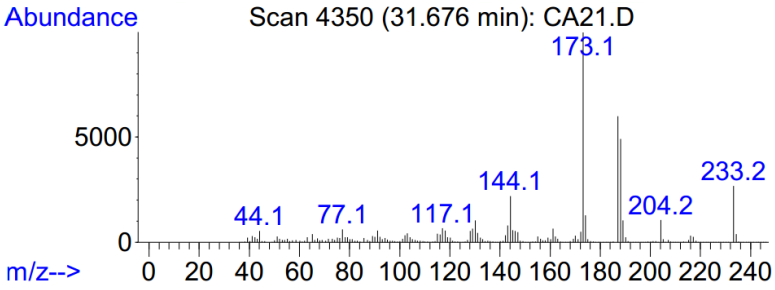

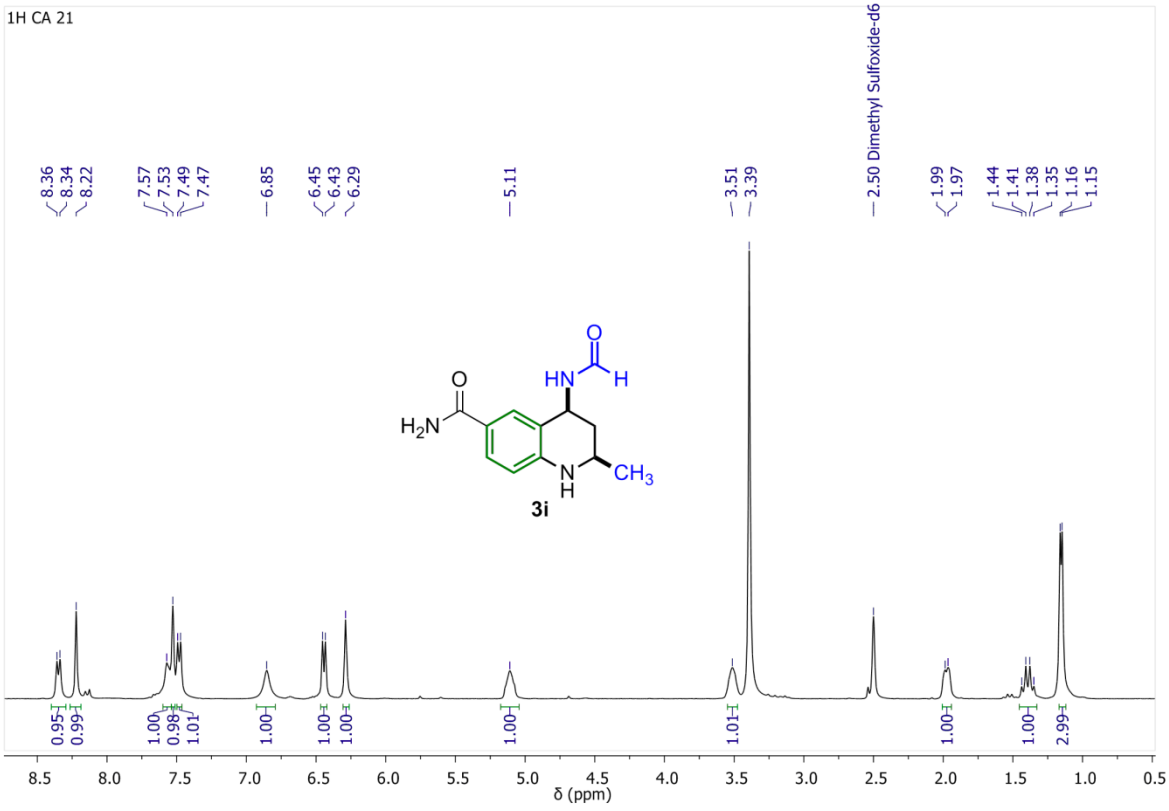

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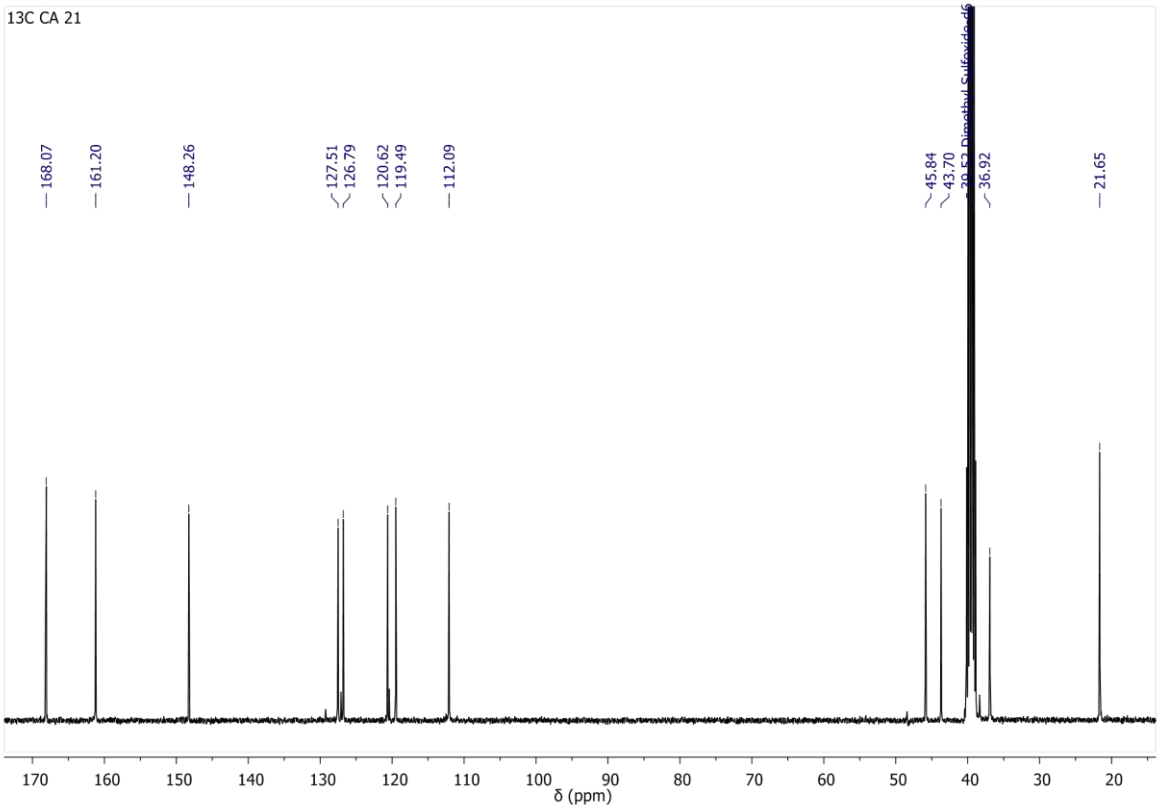

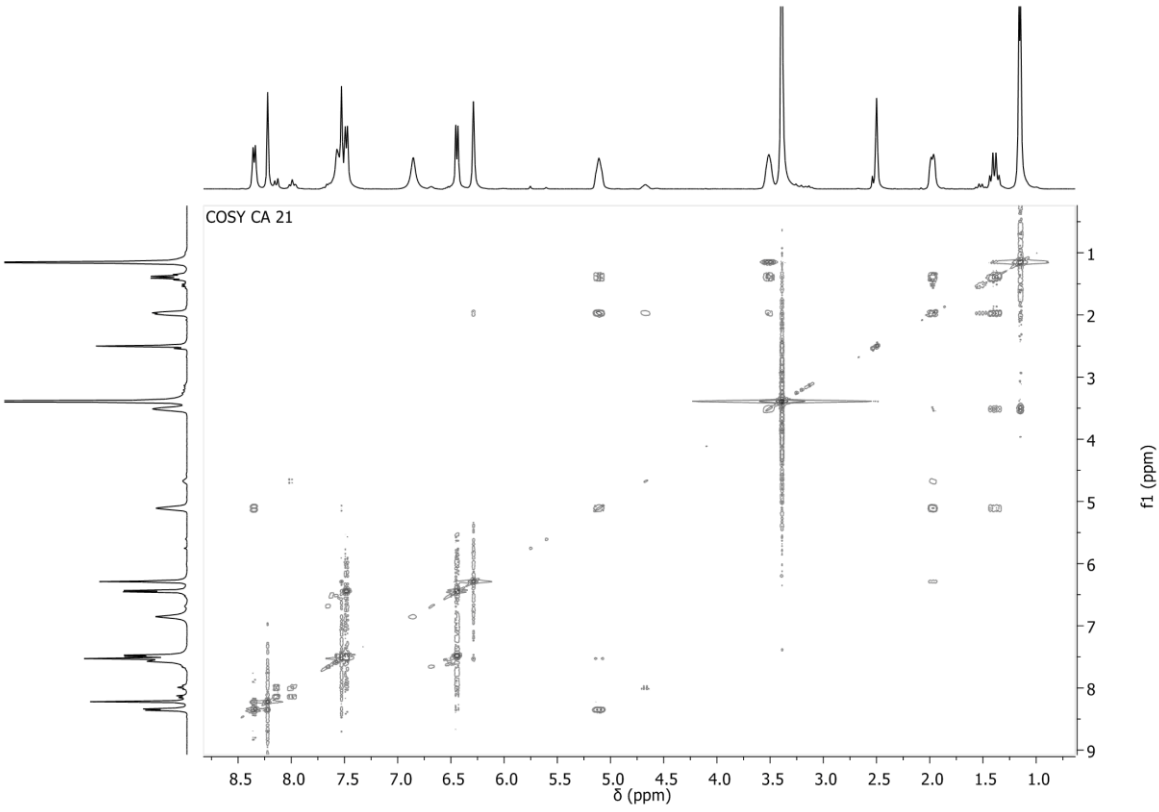

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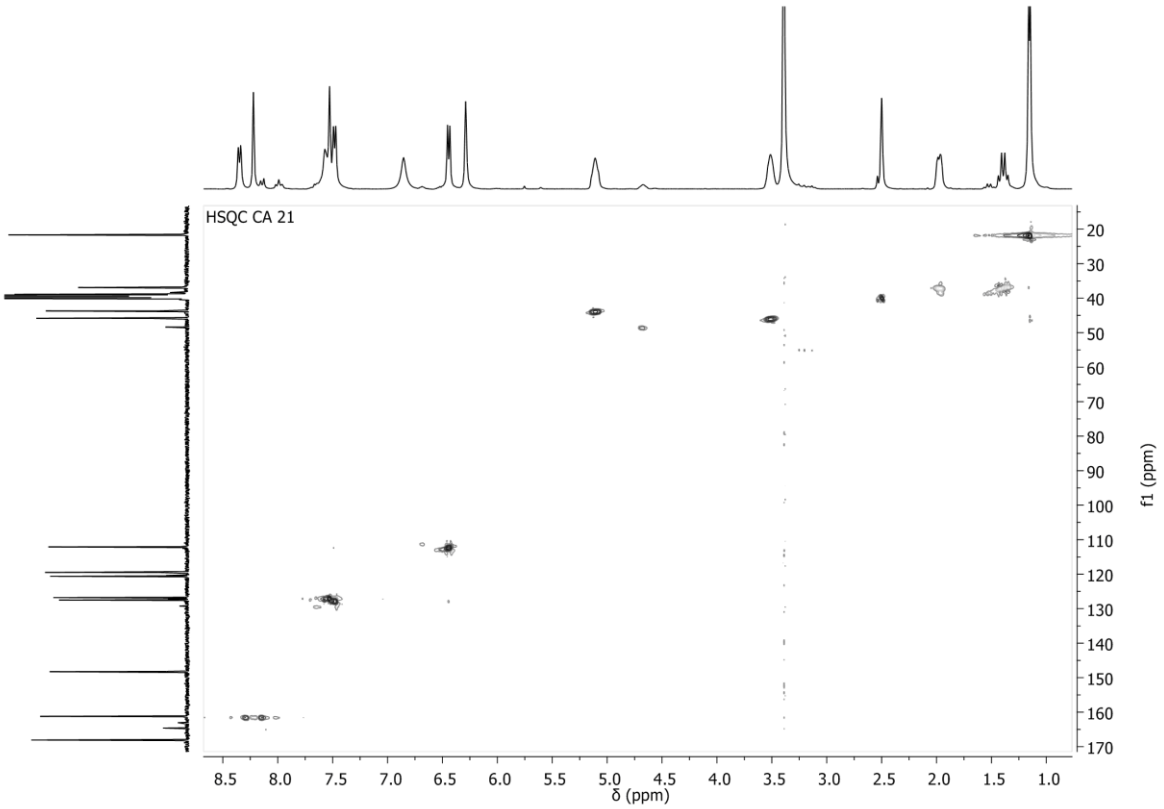
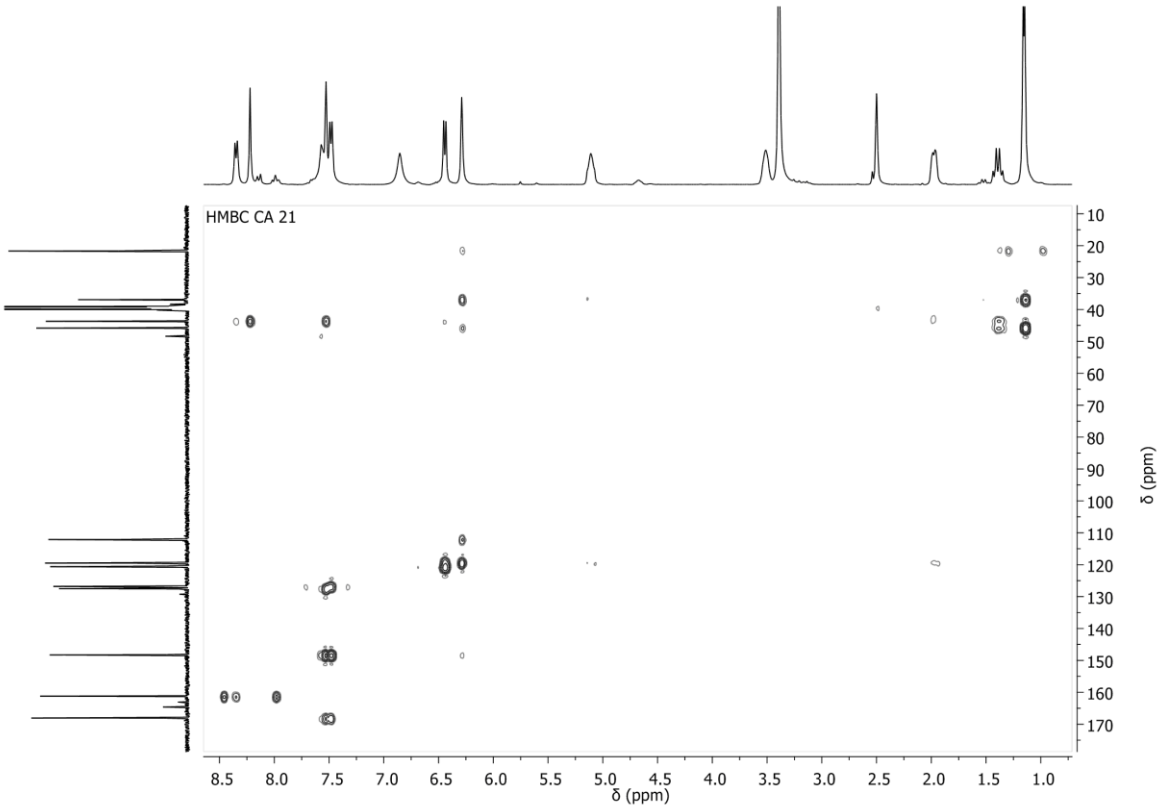
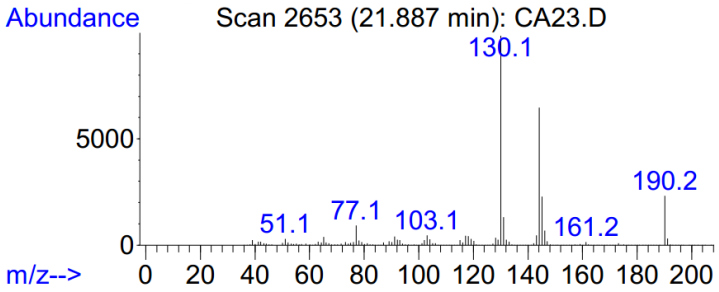
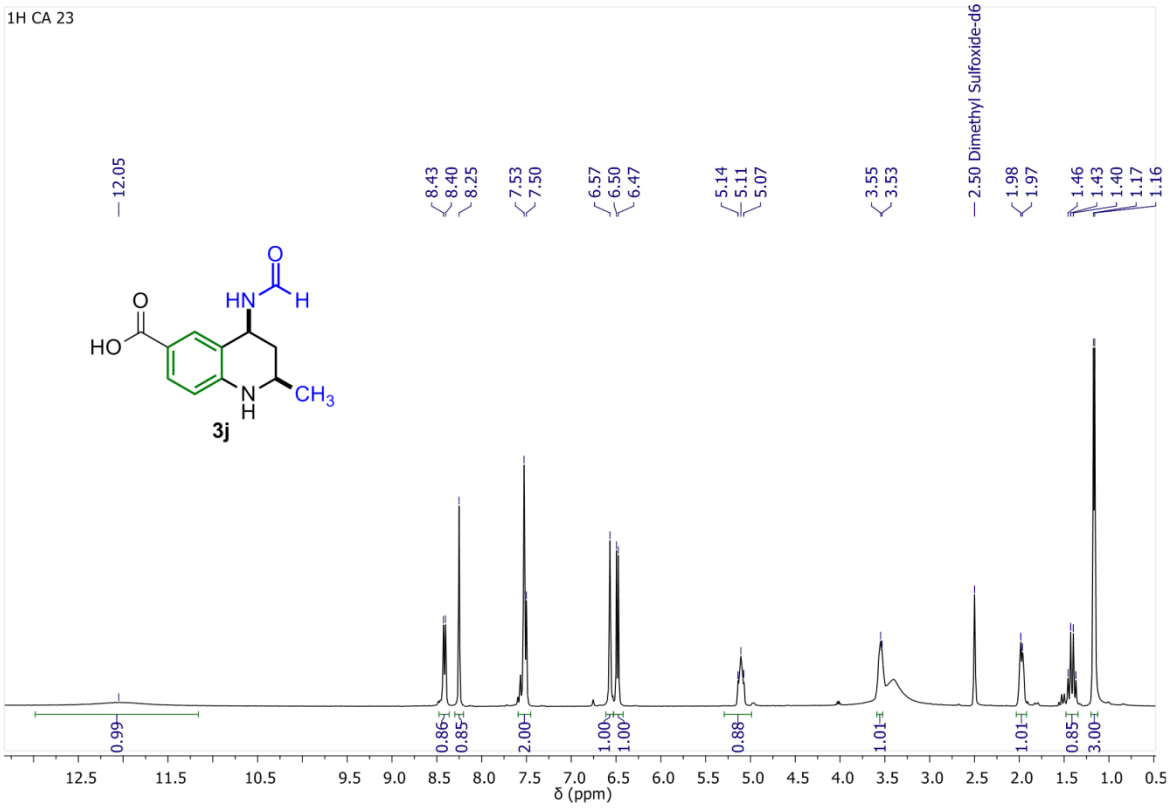




4-Formamido-2-methyl-1,2,3,4-tetrahydroquinoline-6-carboxylic acid, **3j**.





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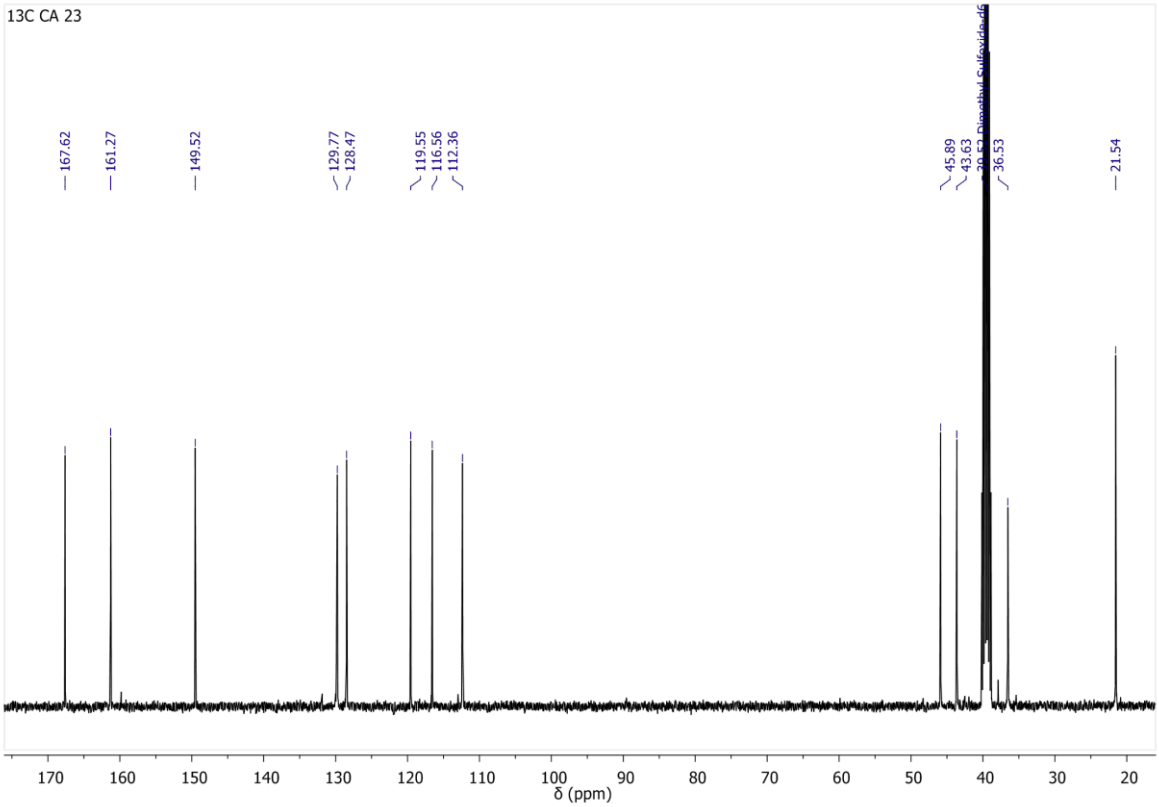
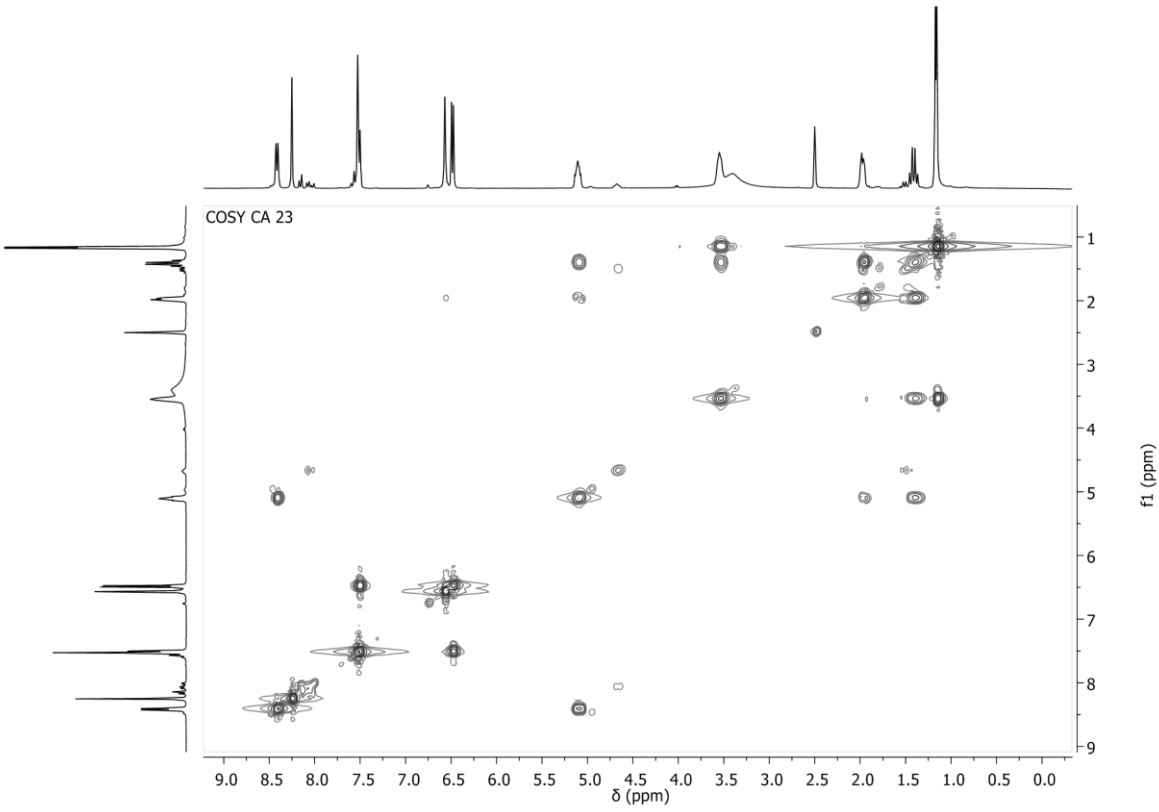
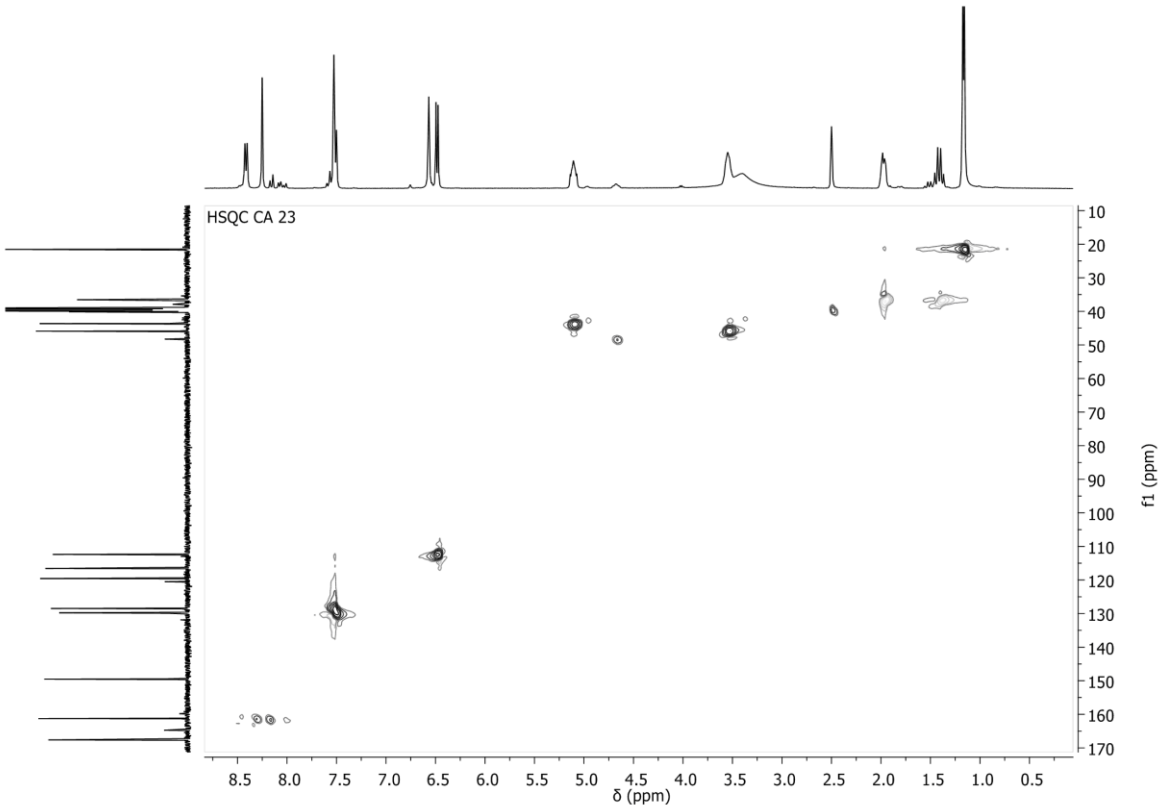
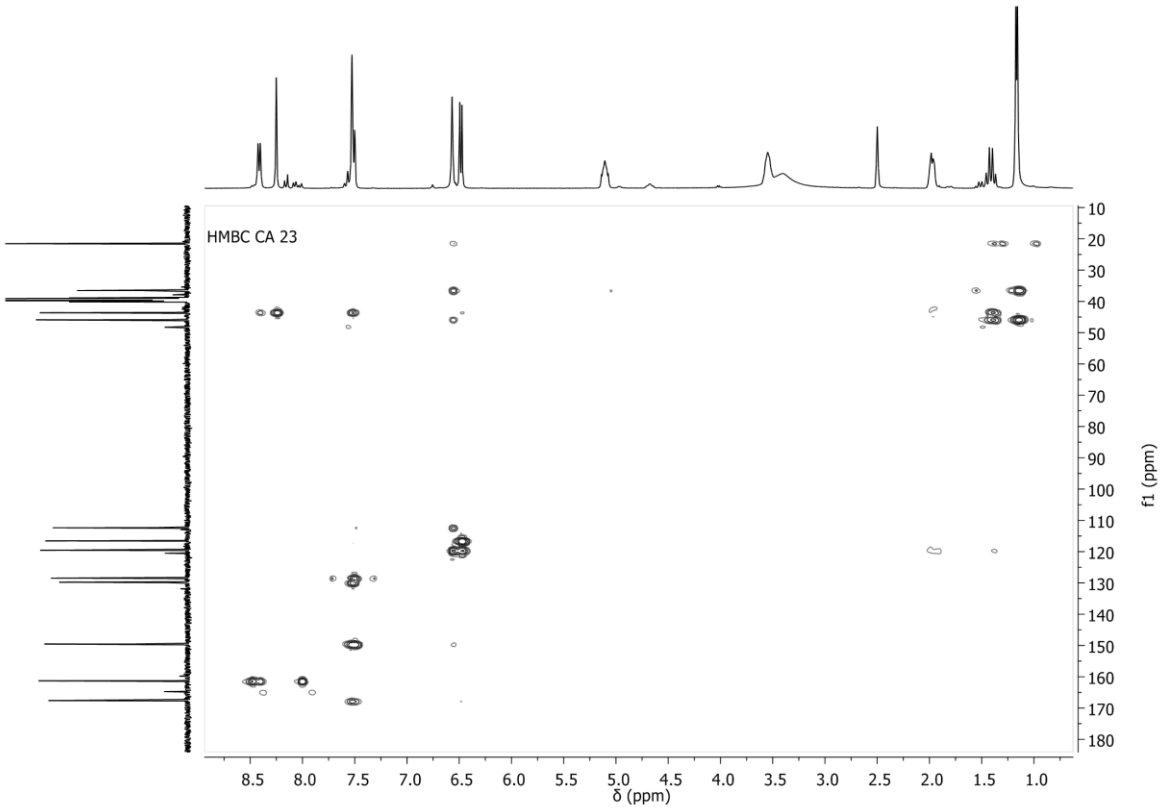





HSQC CA 23
f1 (ppm)
δ (ppm)


HMBC CA 23
f1 (ppm)
δ (ppm)

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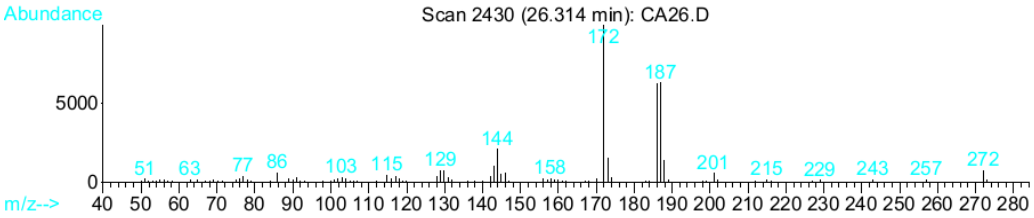
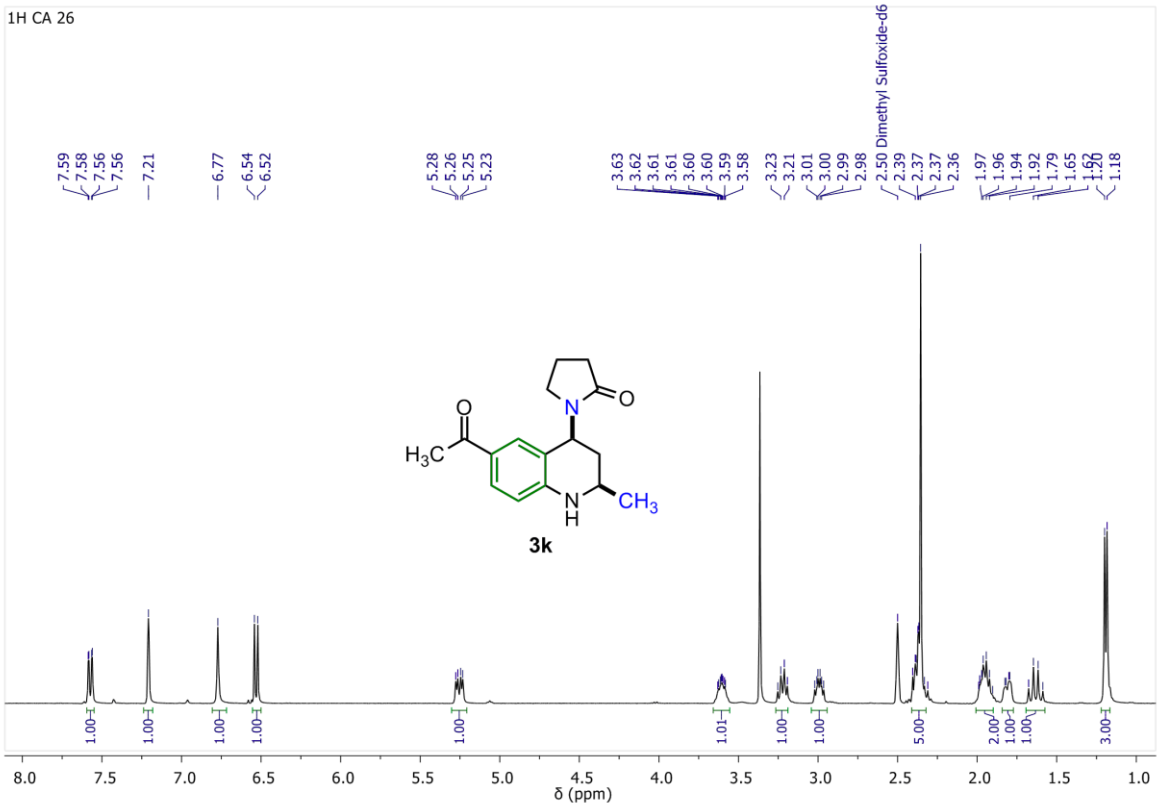
1-(6-Acetyl-2-methyl-1,2,3,4-tetrahydroquinolin-4-yl) pyrrolidin-2-one, **3k**.





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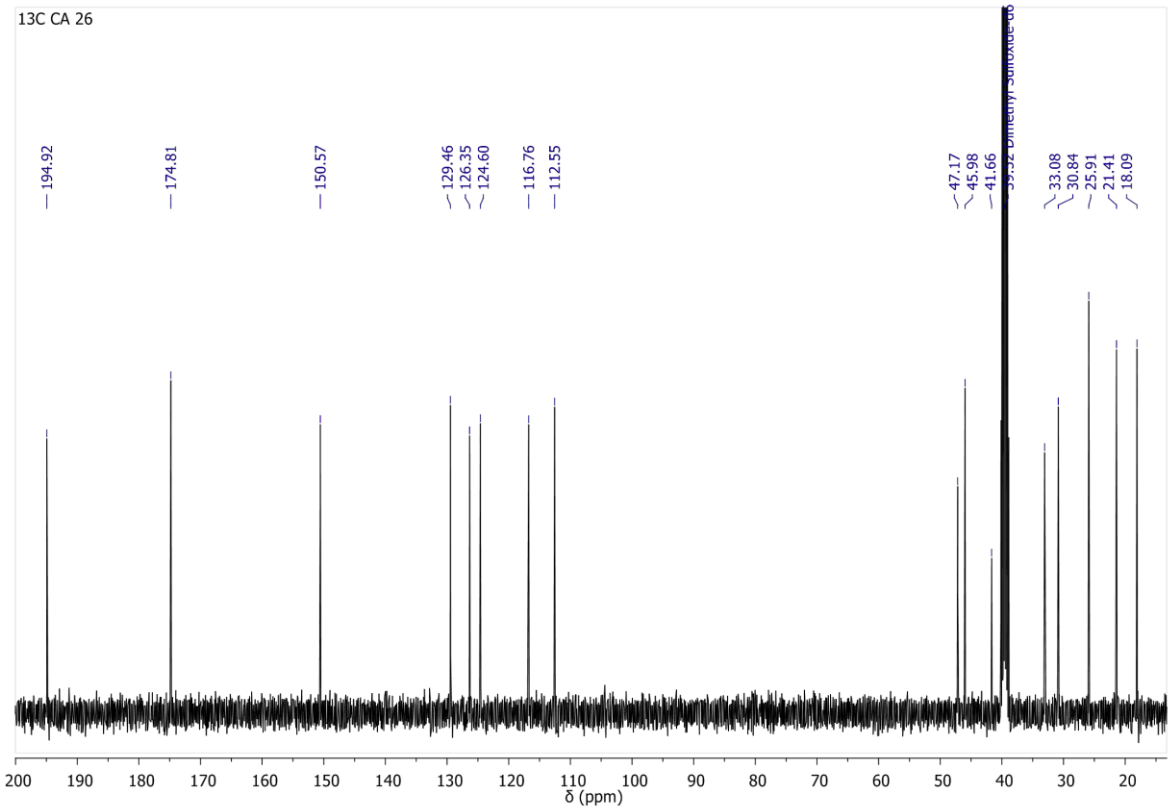
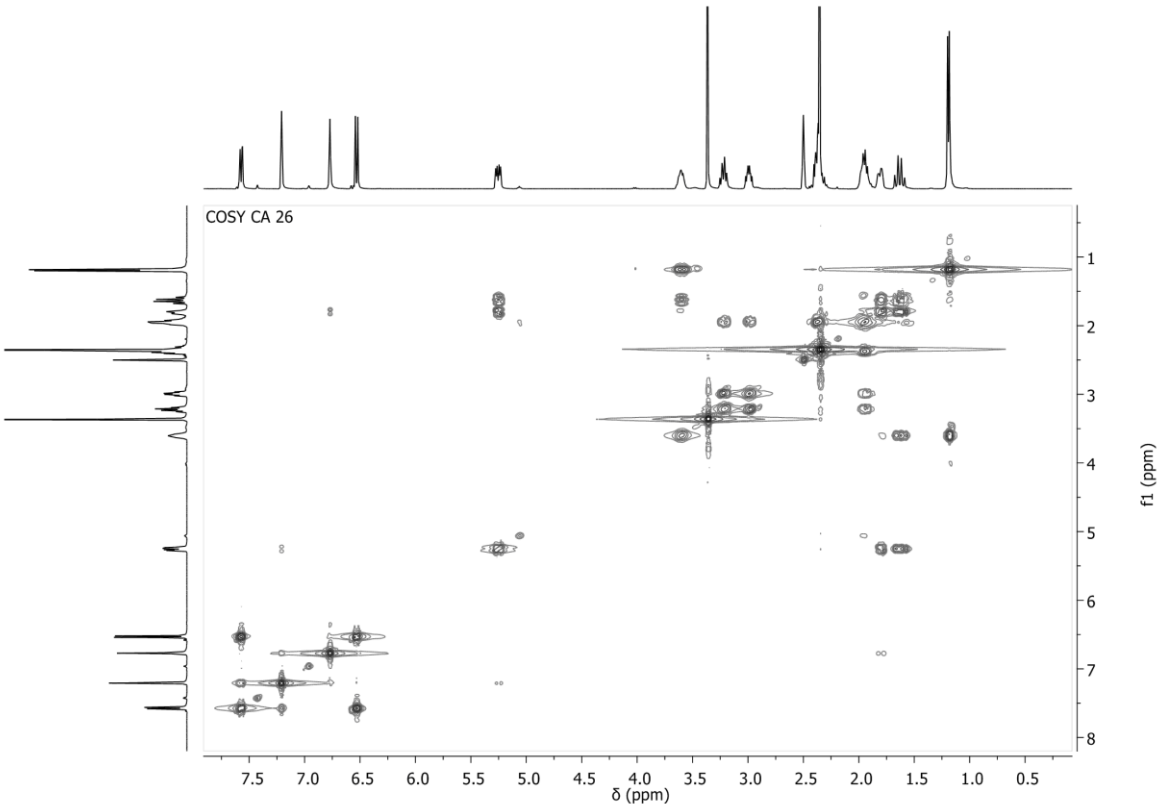
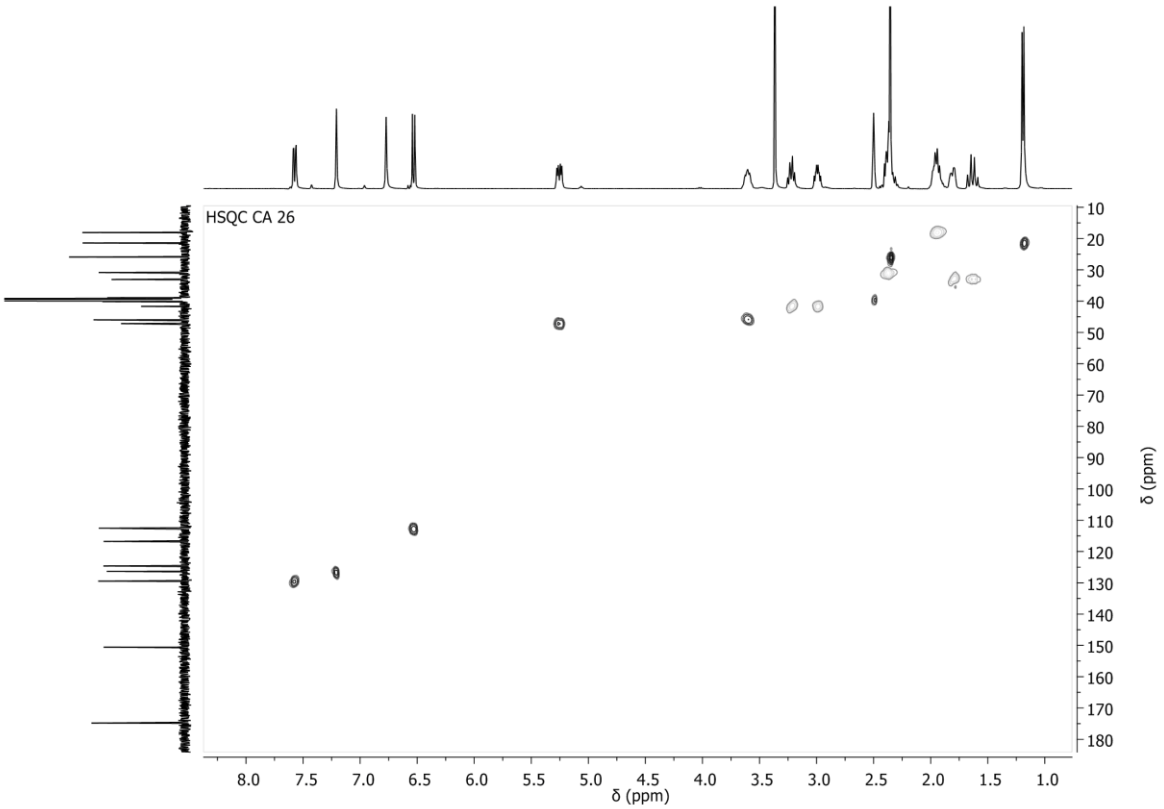
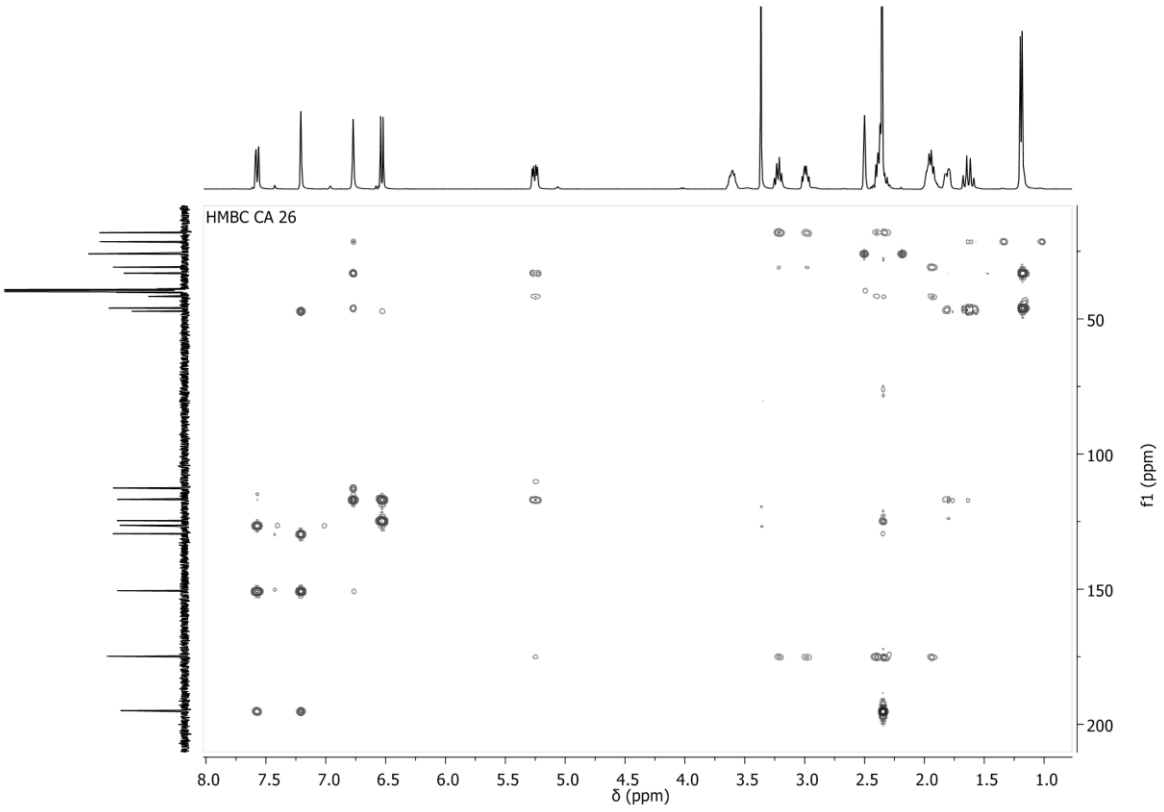
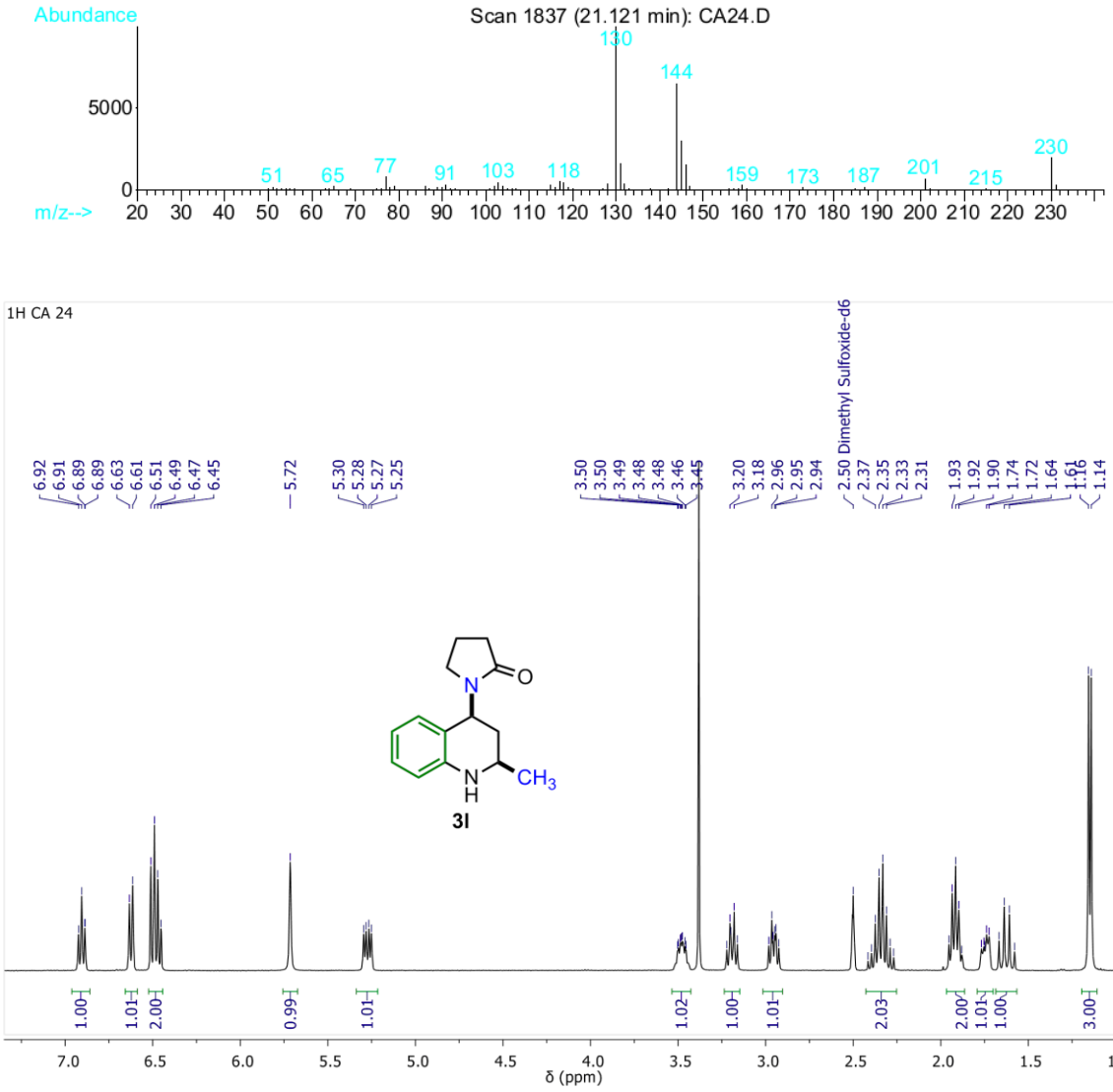





HSQC CA 26
δ (ppm)
δ (ppm)


HMBC CA 26
δ (ppm)
f1 (ppm)

1-(2-Methyl-1,2,3,4-tetrahydroquinolin-4-yl) pyrrolidin-2-one, **3l**.



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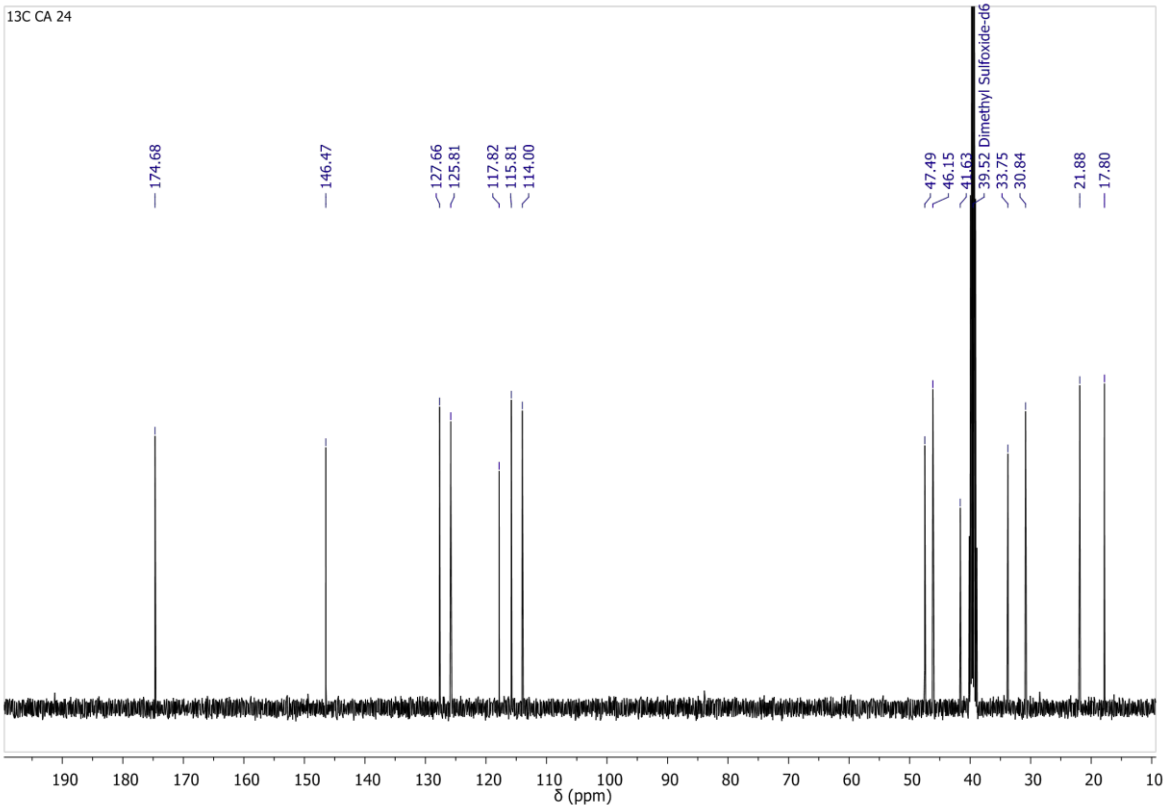

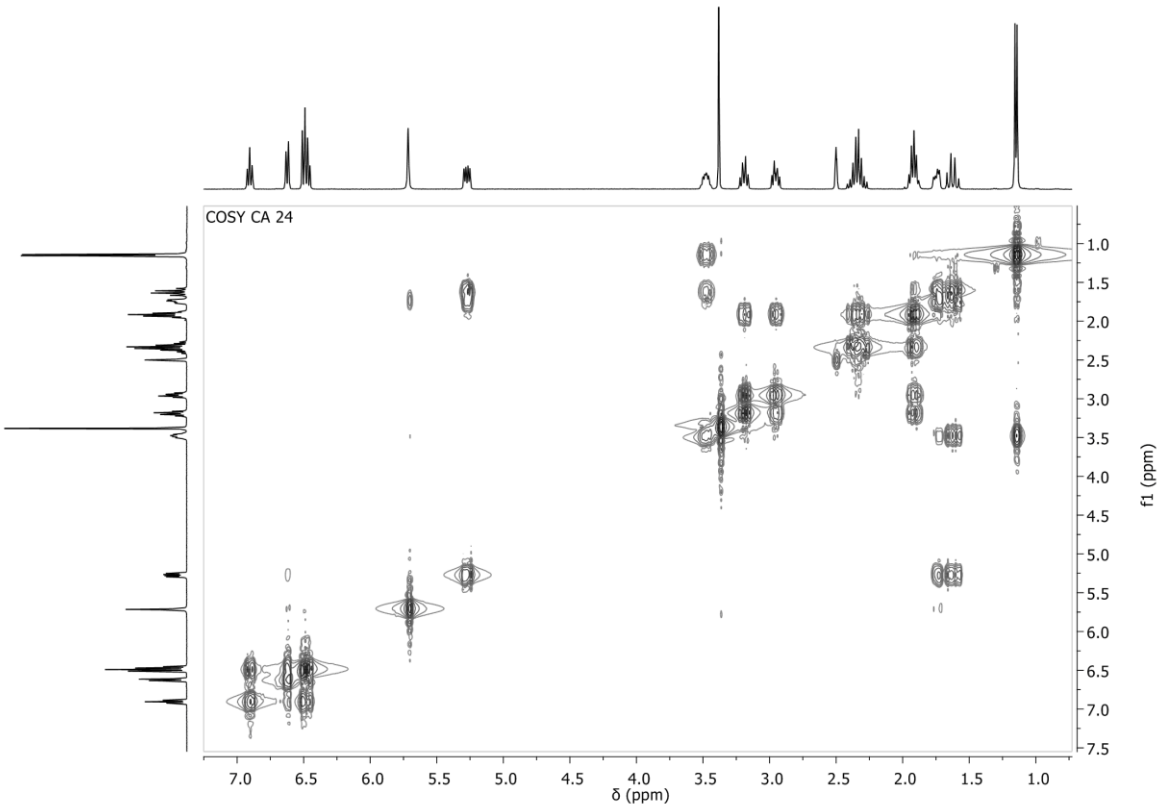

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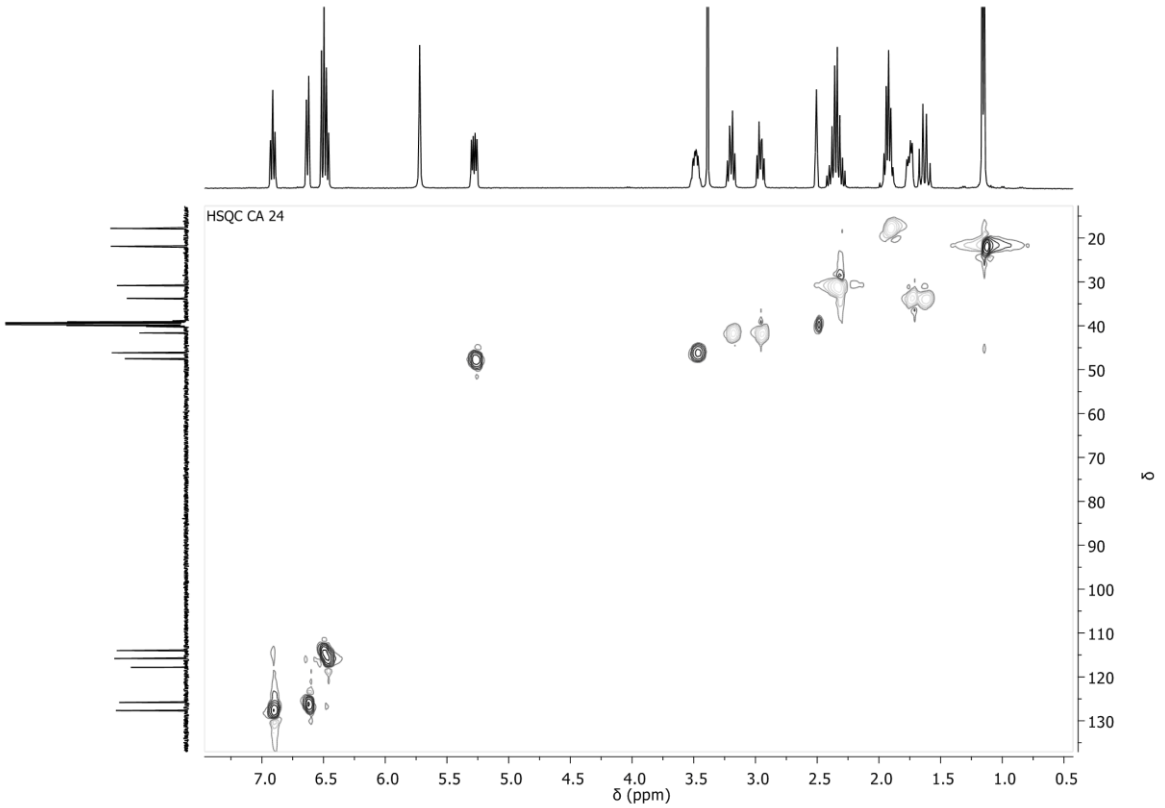
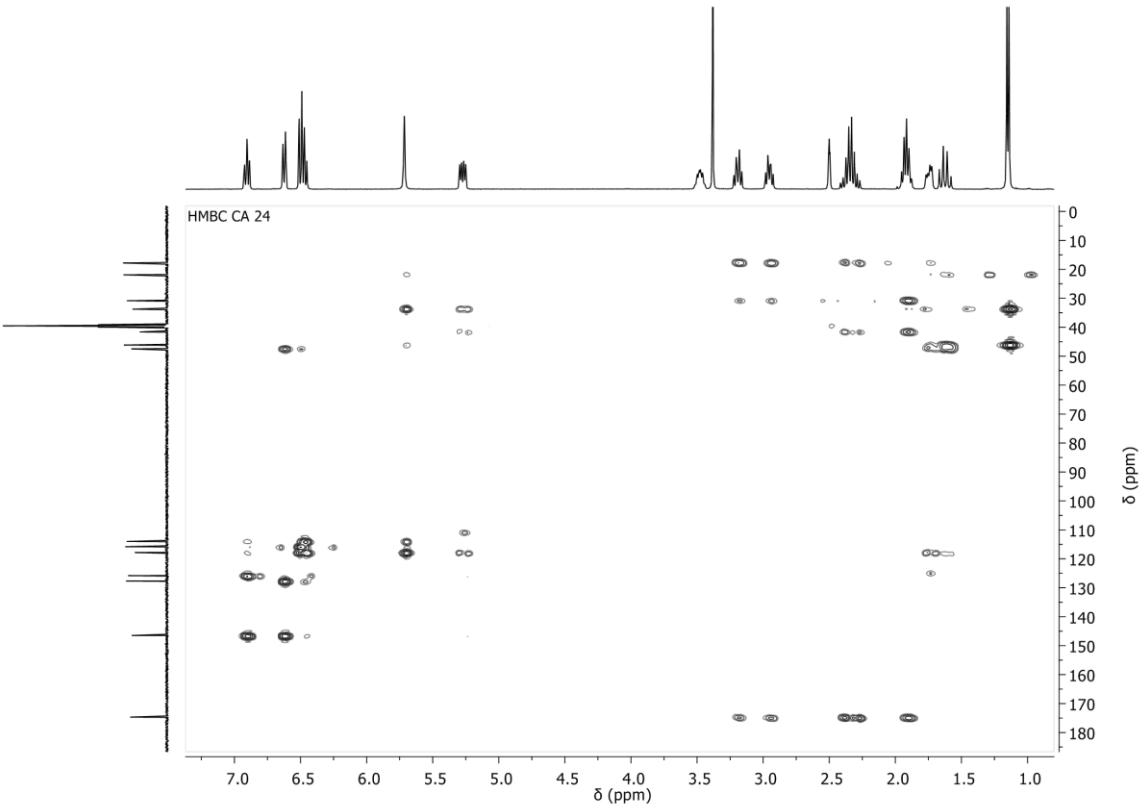
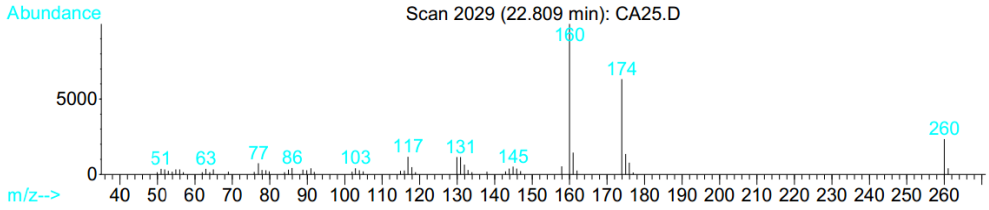
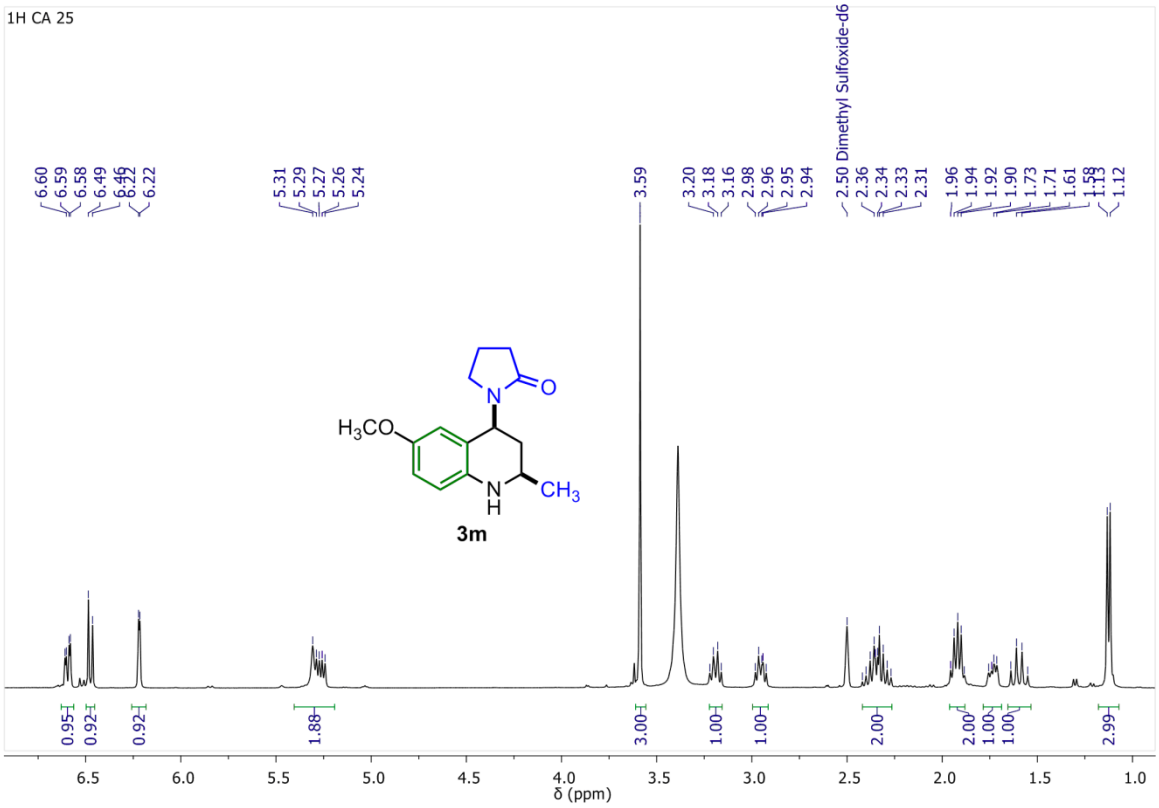




1-(6-Methoxy-2-methyl-1,2,3,4-tetrahydroquinolin-4-yl) pyrrolidin-2-one, **3m**.





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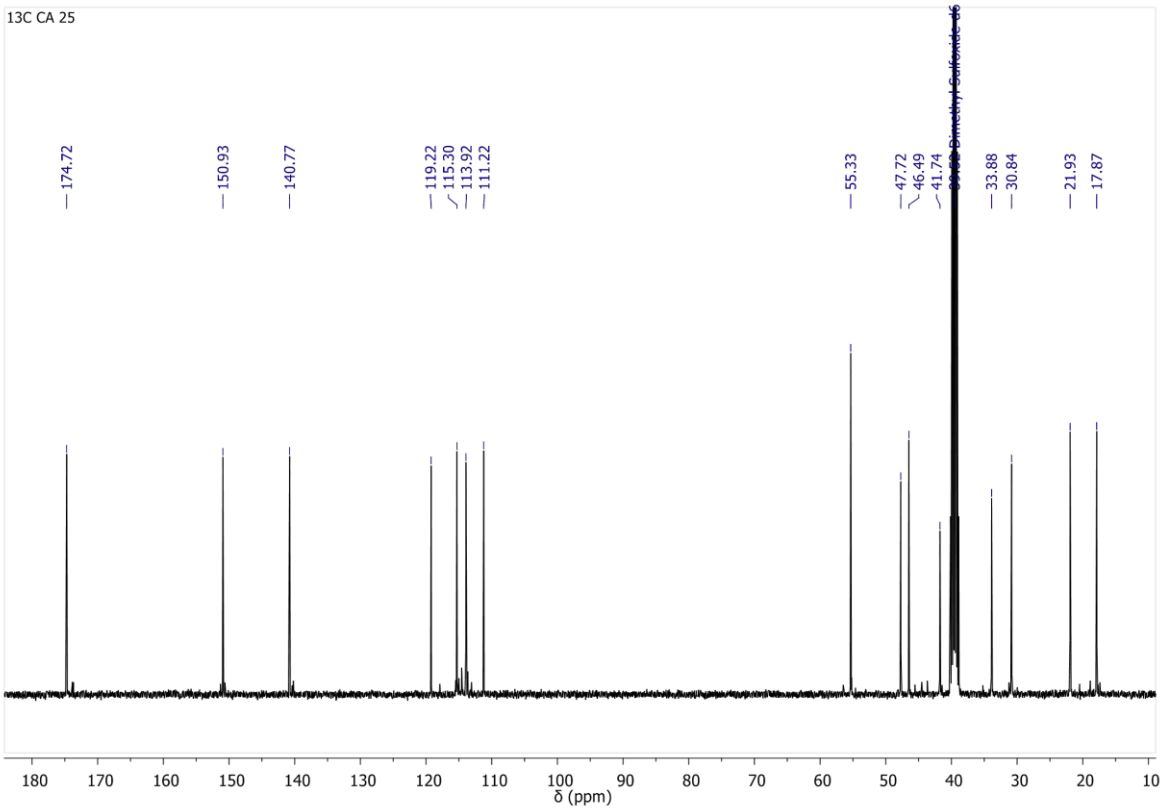

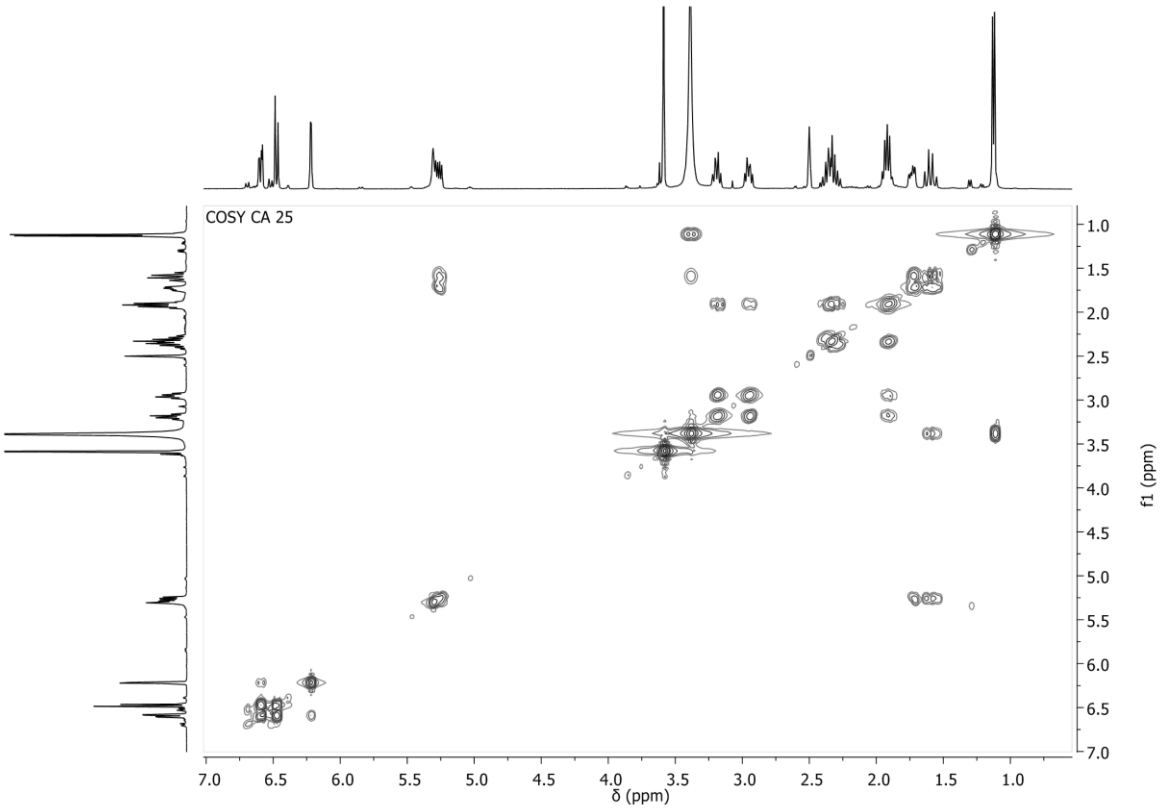

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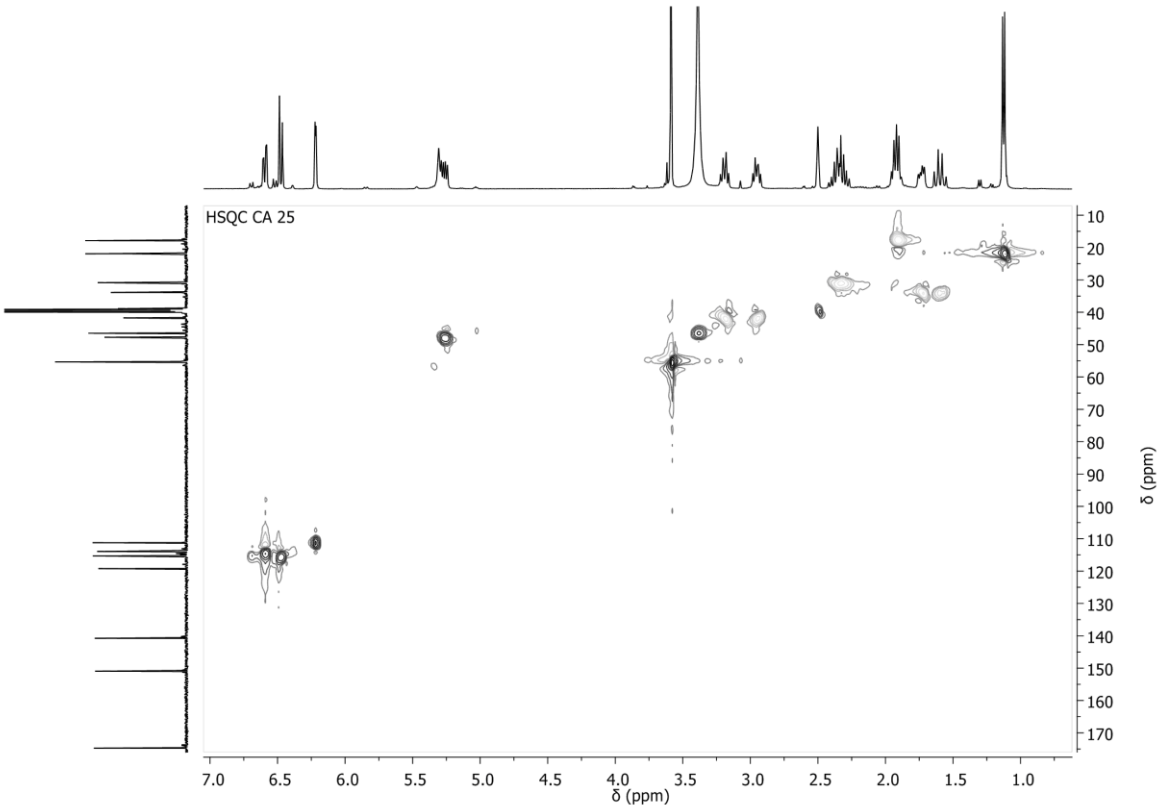
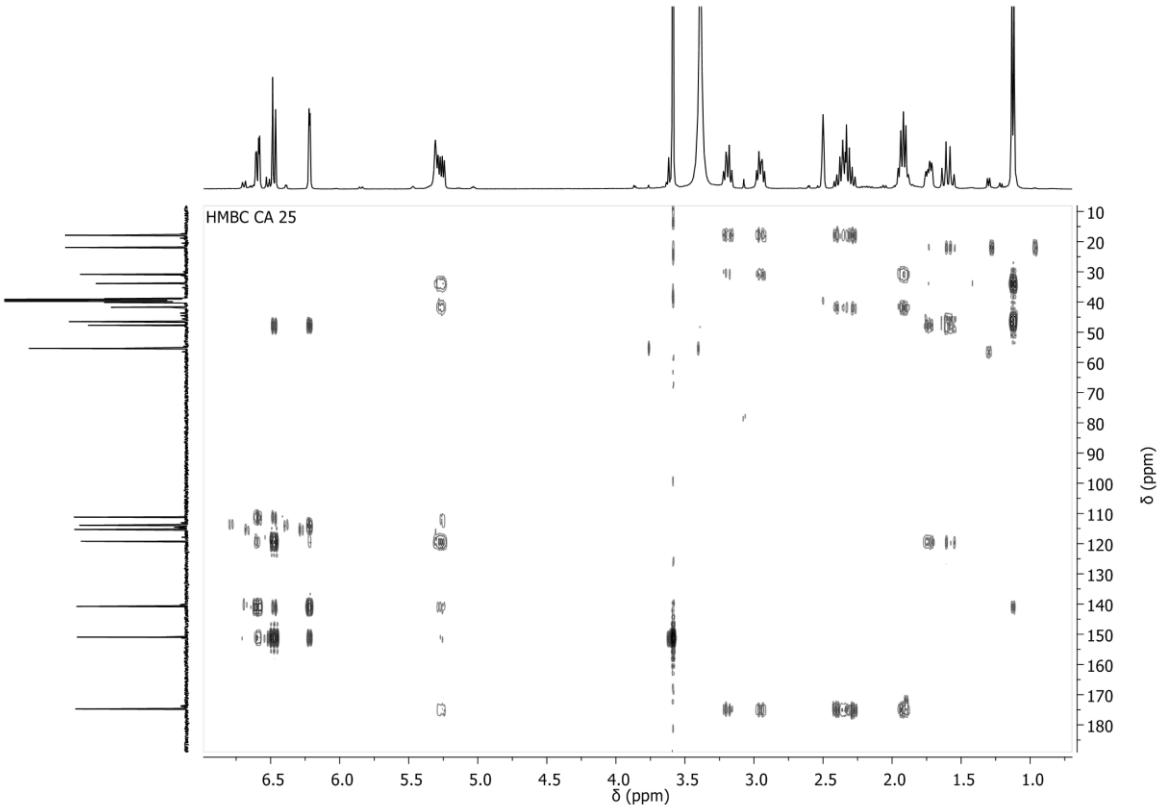
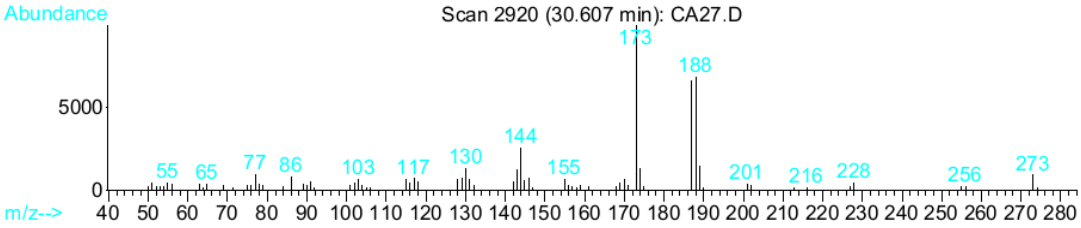
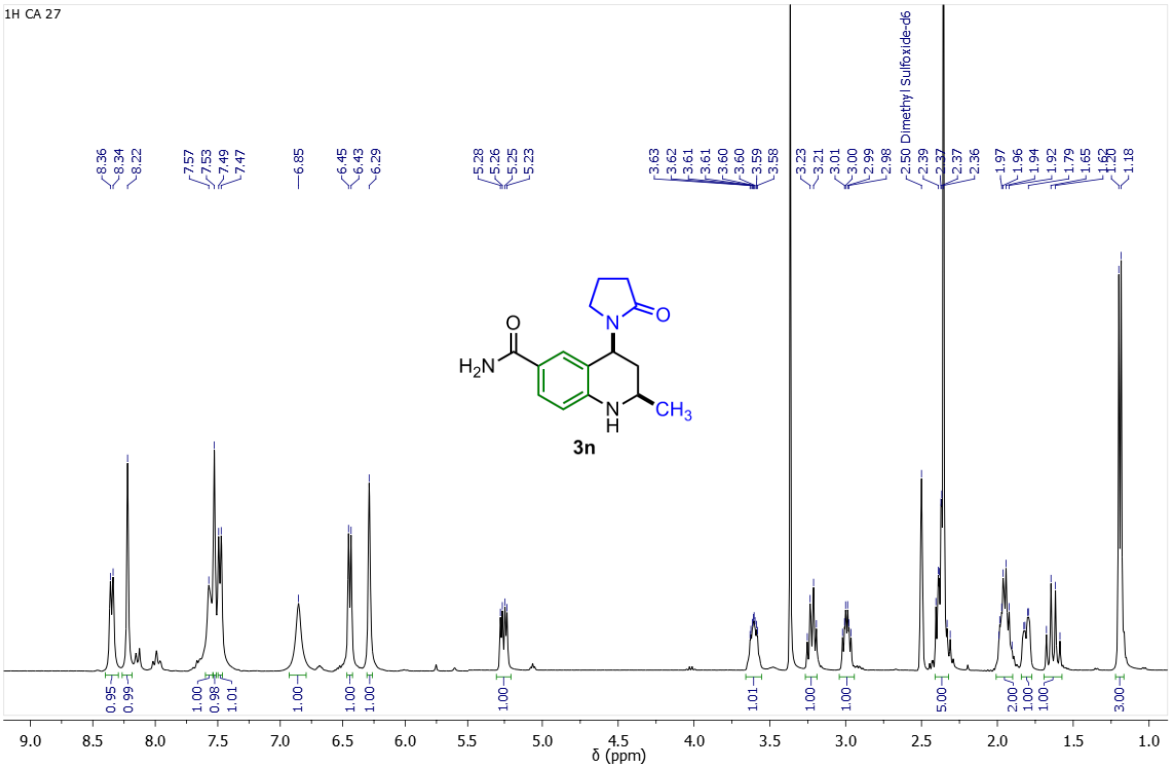


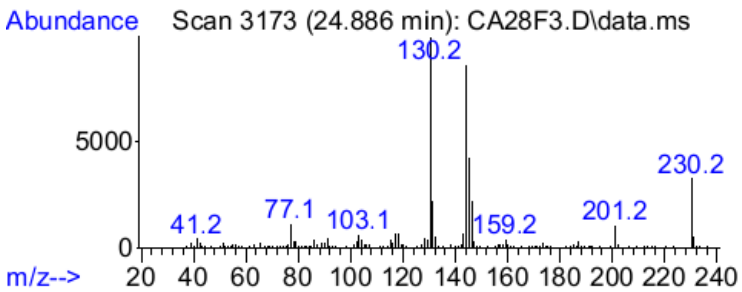


4-Methyl-4-(2-oxopyrrolidin-1-yl)-1,2,3,4-tetrahydro-quinoline-6-carboxamide, **3n**.





2-Methyl-4-(2-oxopyrrolidin-1-yl)-1,2,3,4-tetrahydroquinoline-6-carboxylic acid, **3o**.



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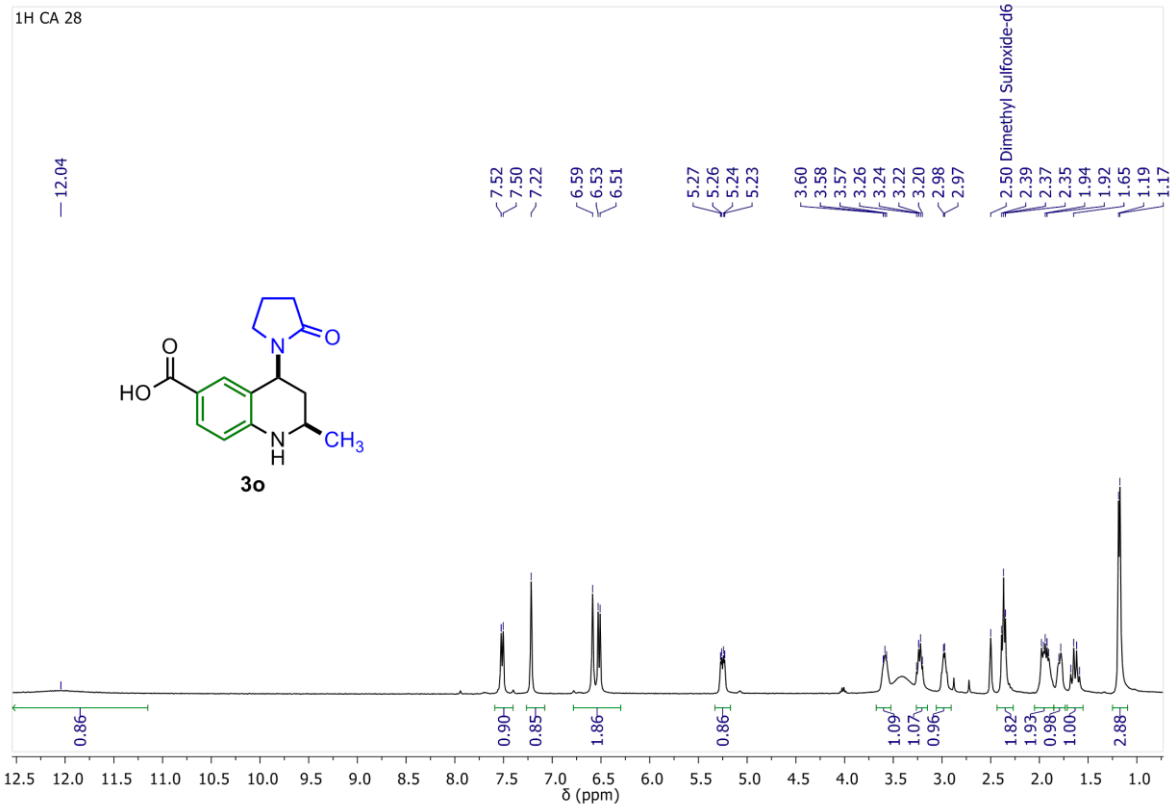

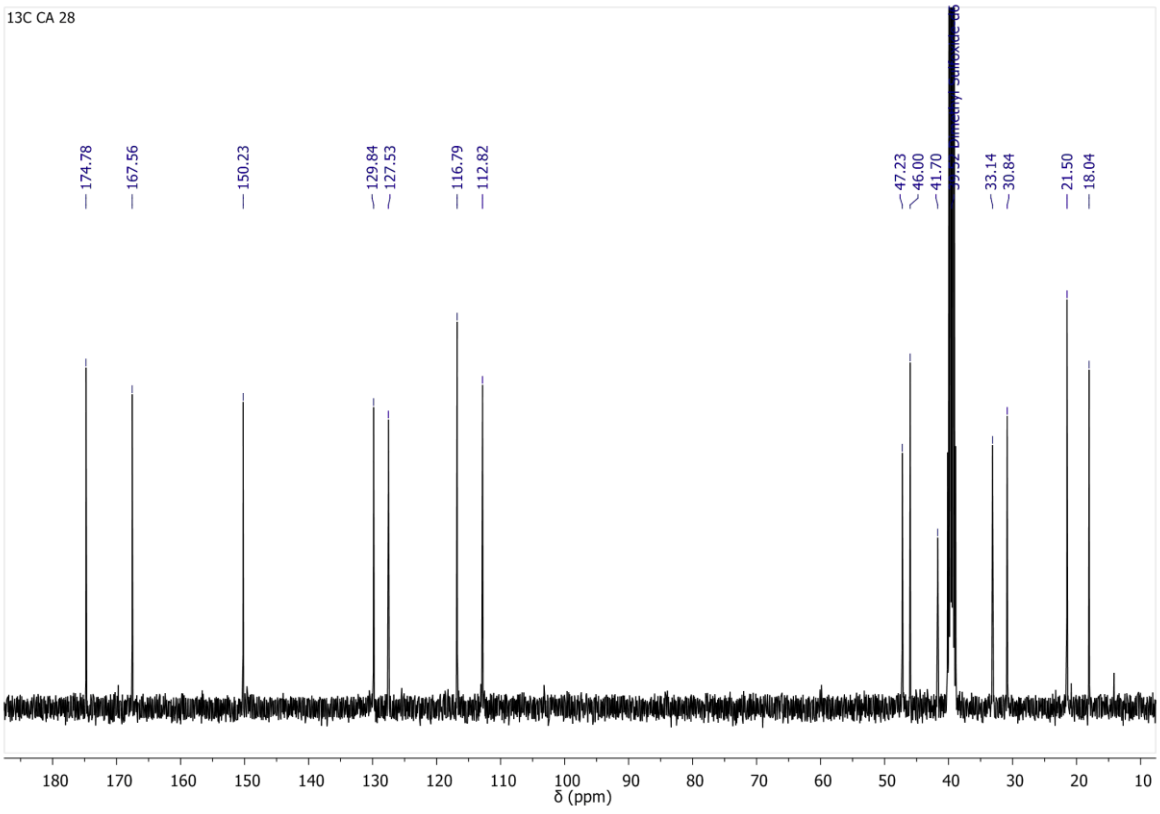

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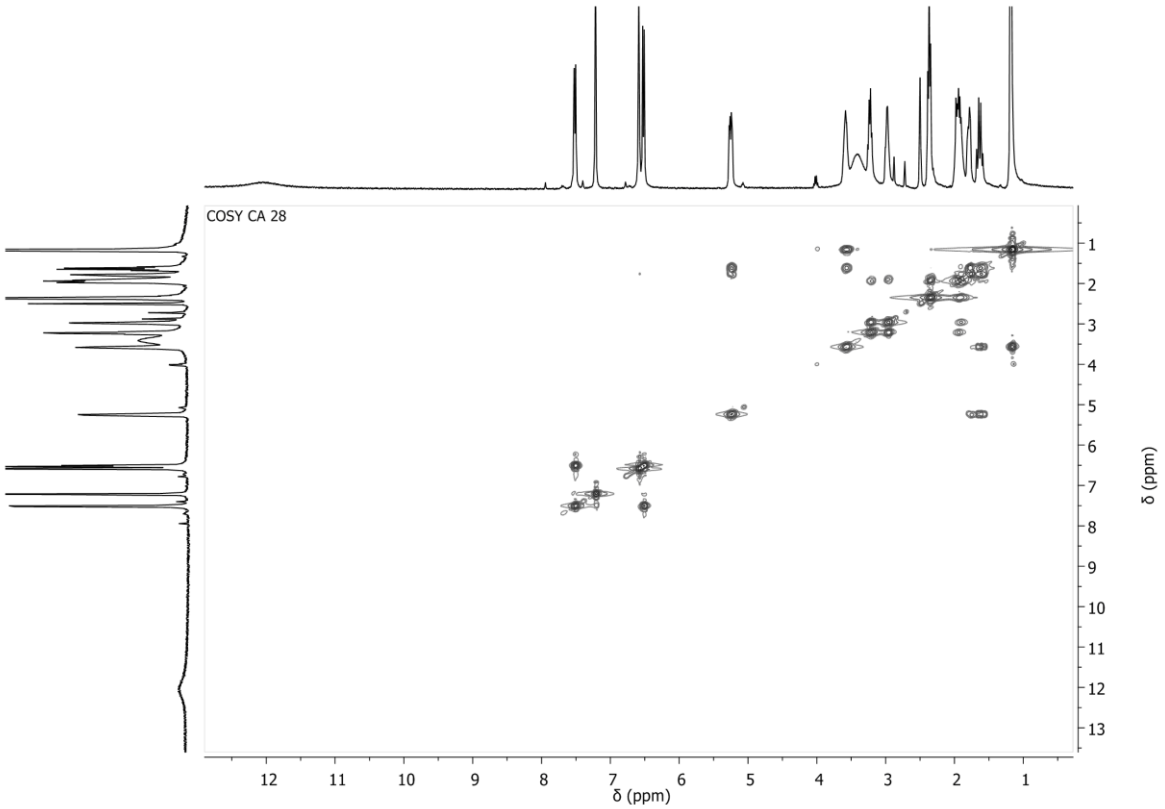

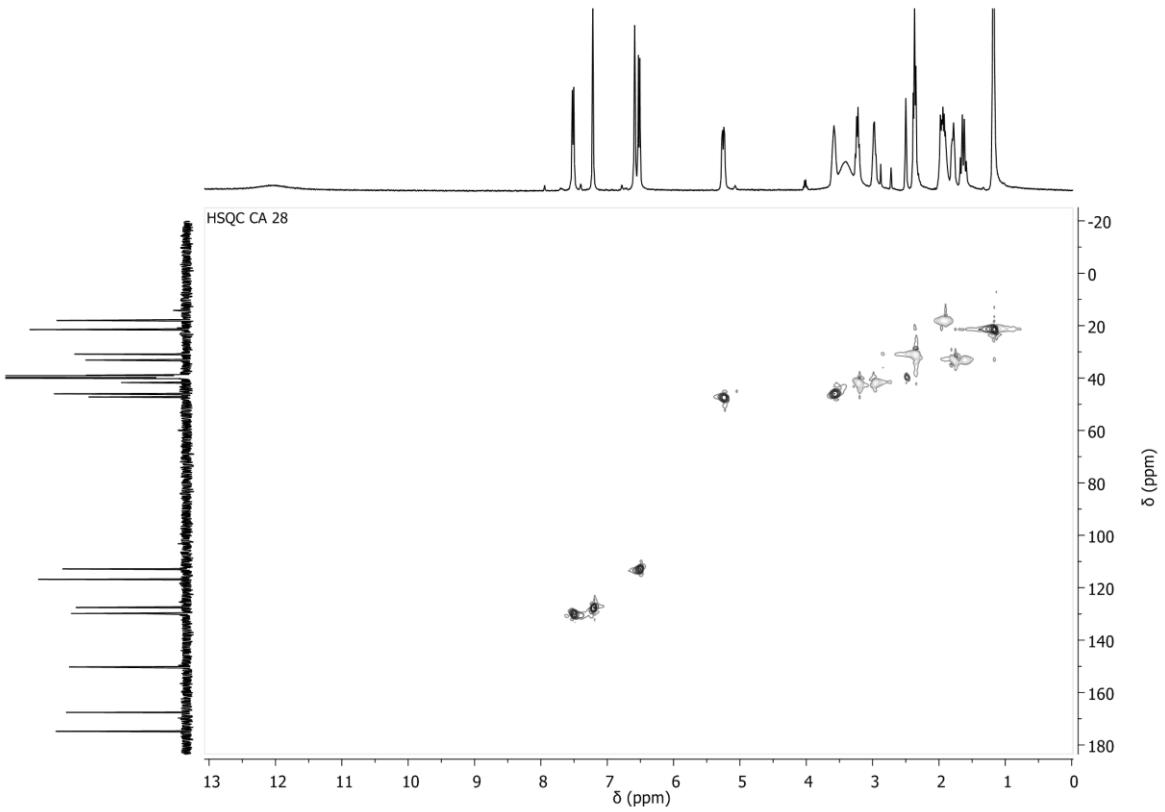

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