An unprecedent reactivity of D-A cyclopronane derivatives: decyanation reaction

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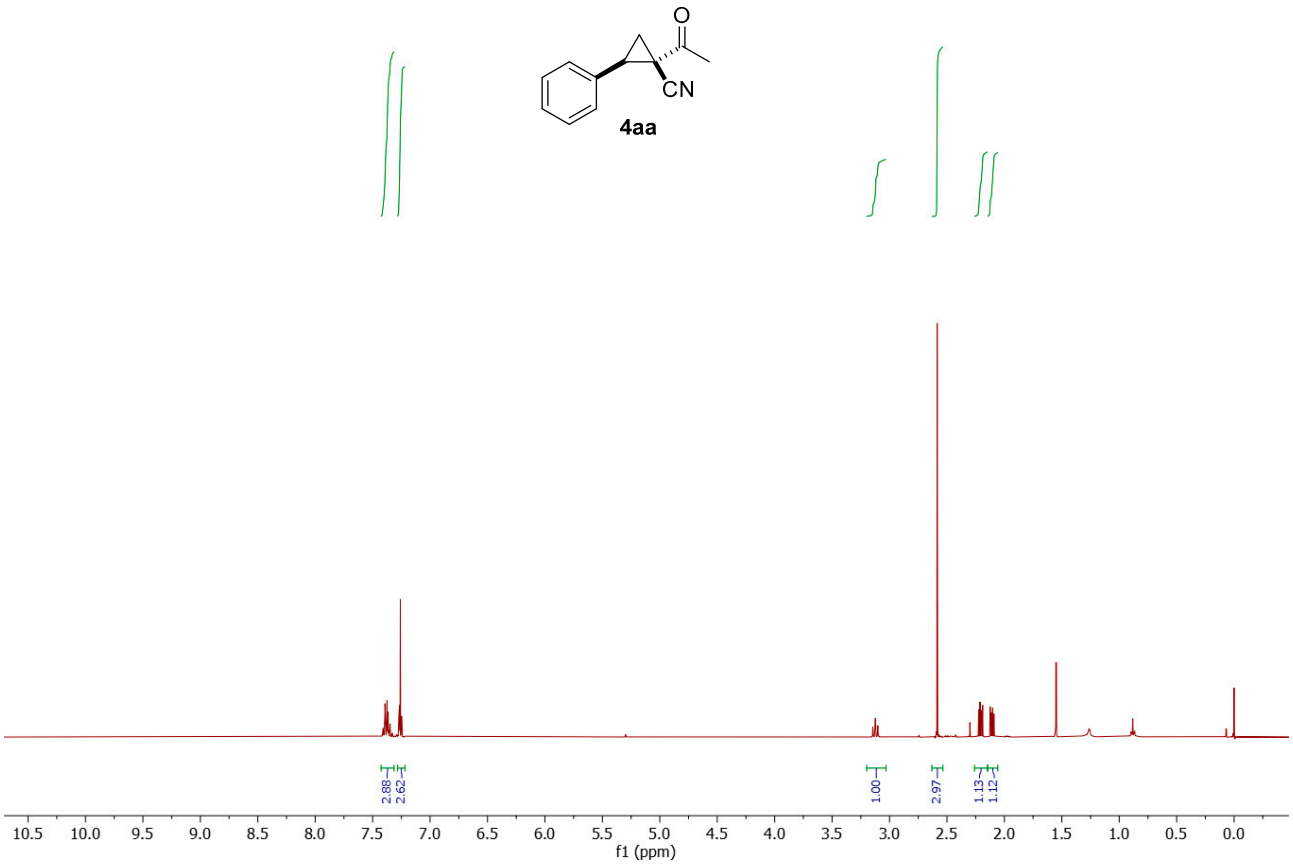
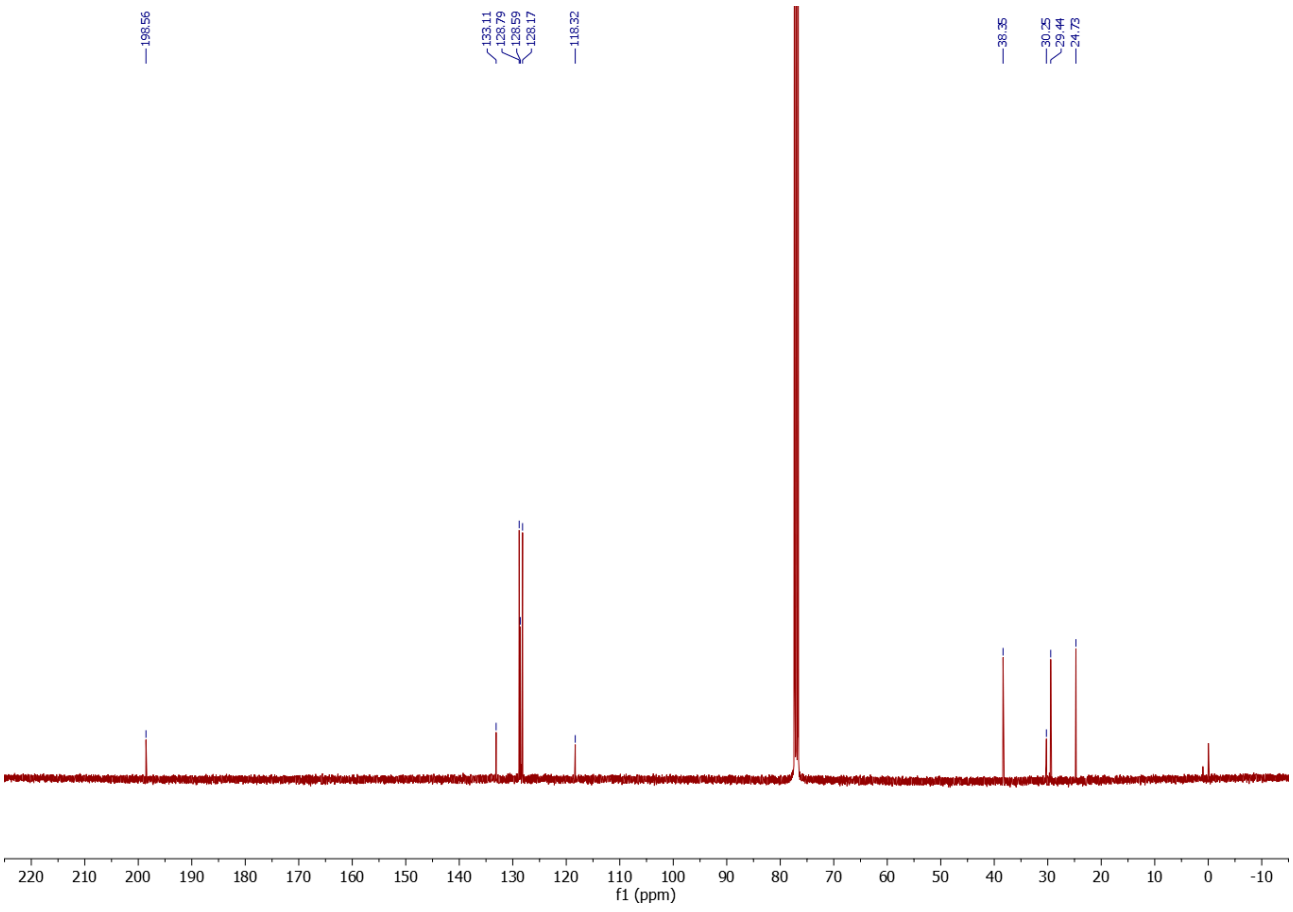
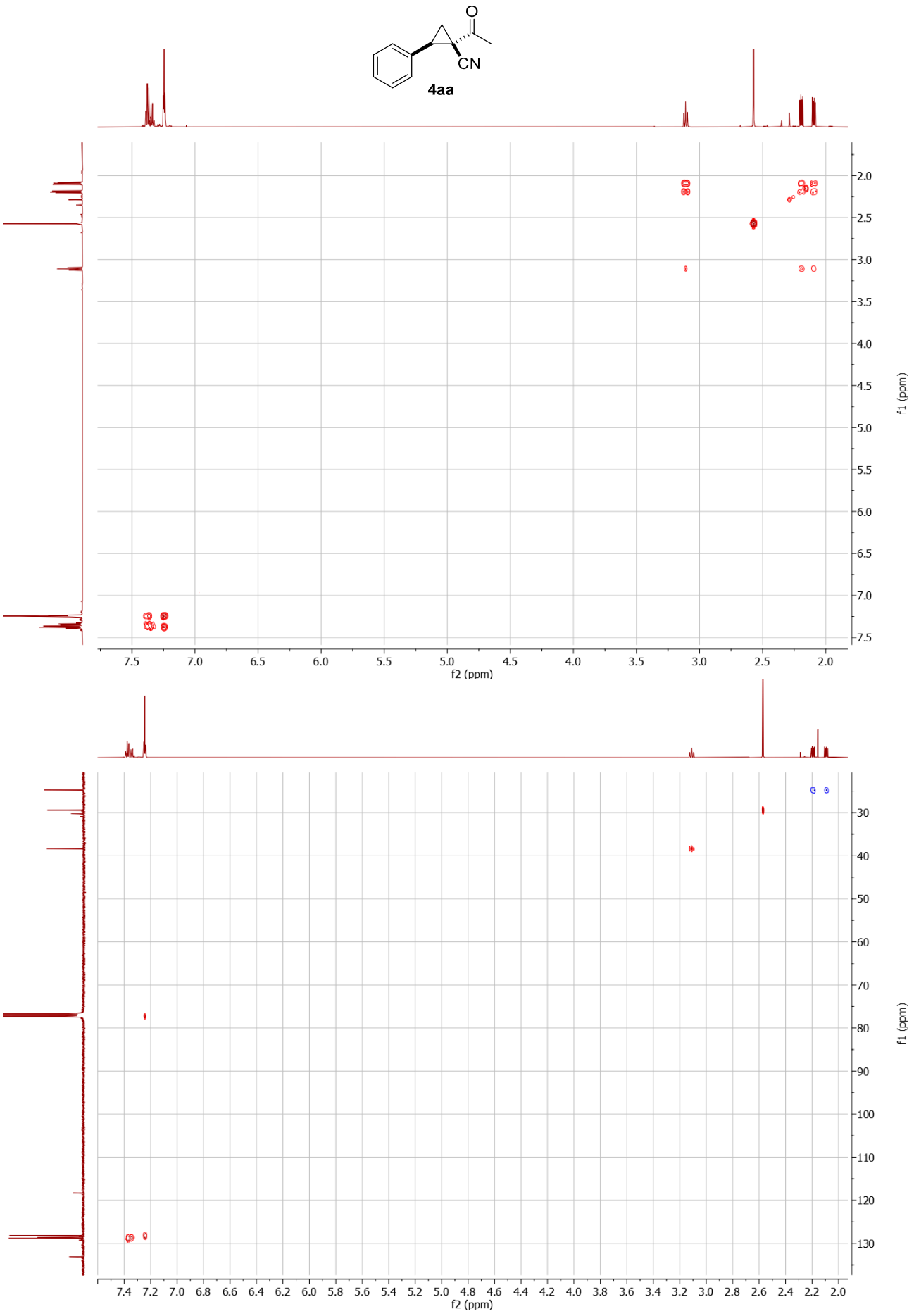
Supporting information

Selected NMR spectra

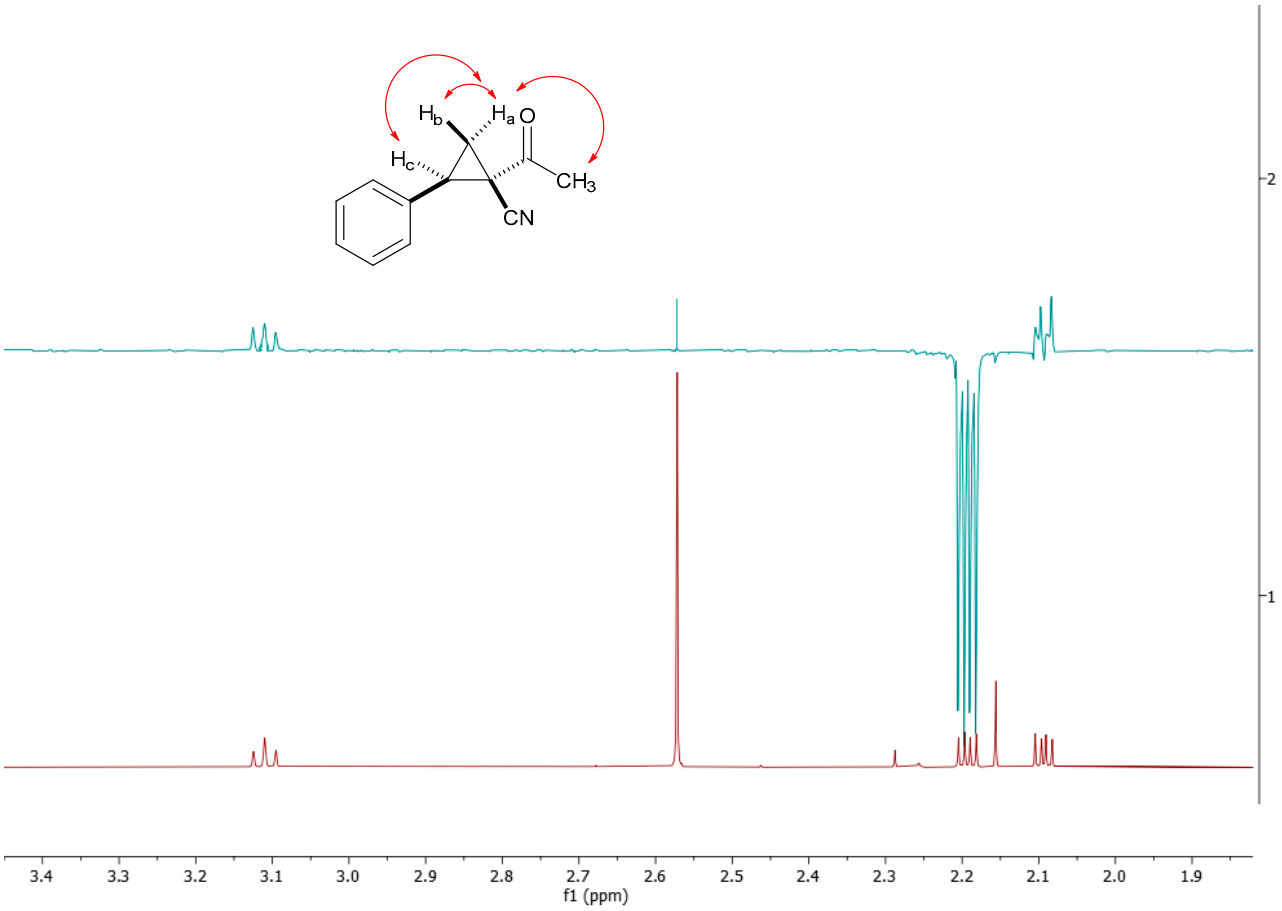
1-acetyl-2-phenylcyclopropane-1-carbonitrile 4aa



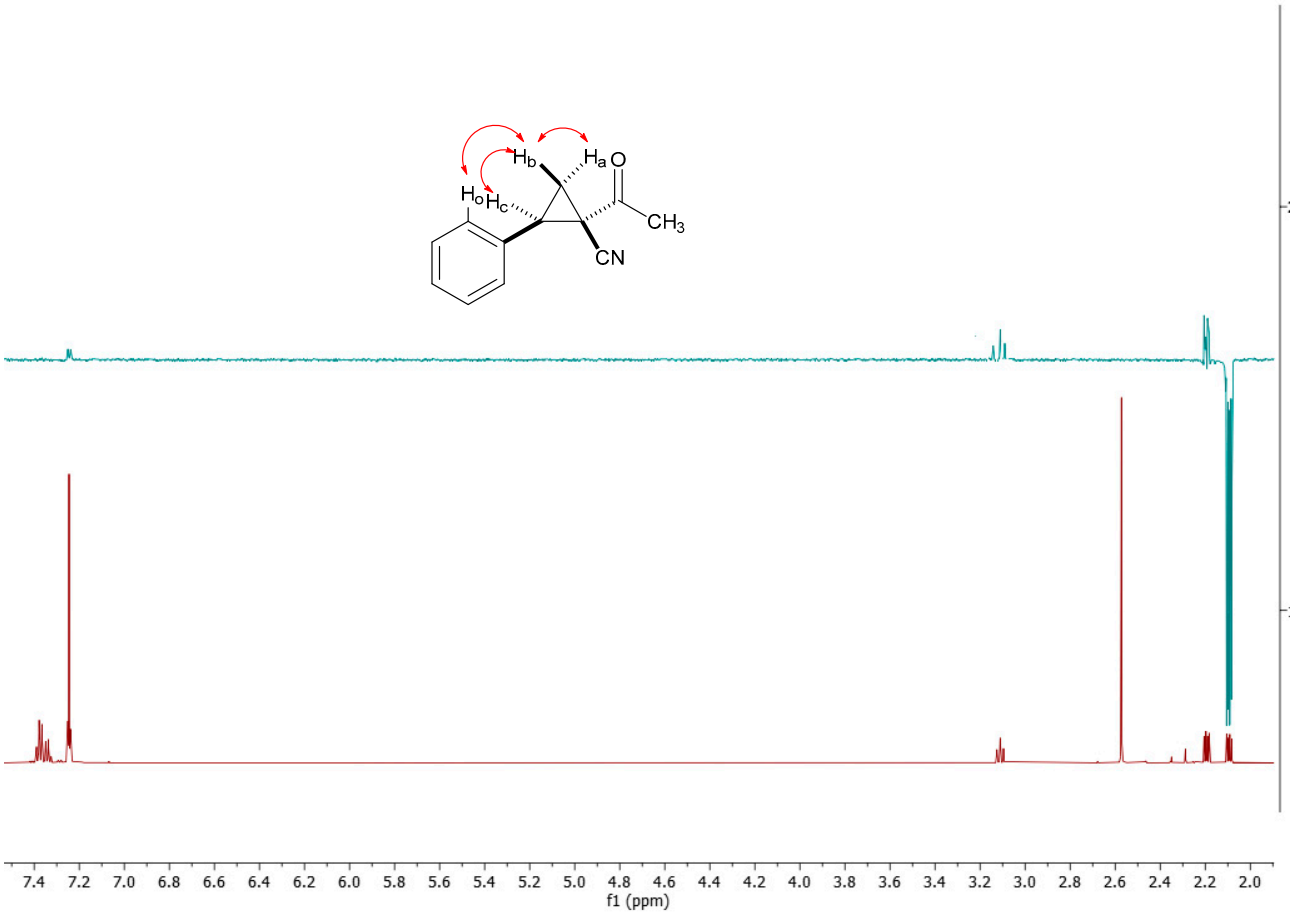



O
CN
4aa
f2 (ppm)
f1 (ppm)
f2 (ppm)
f1 (ppm)

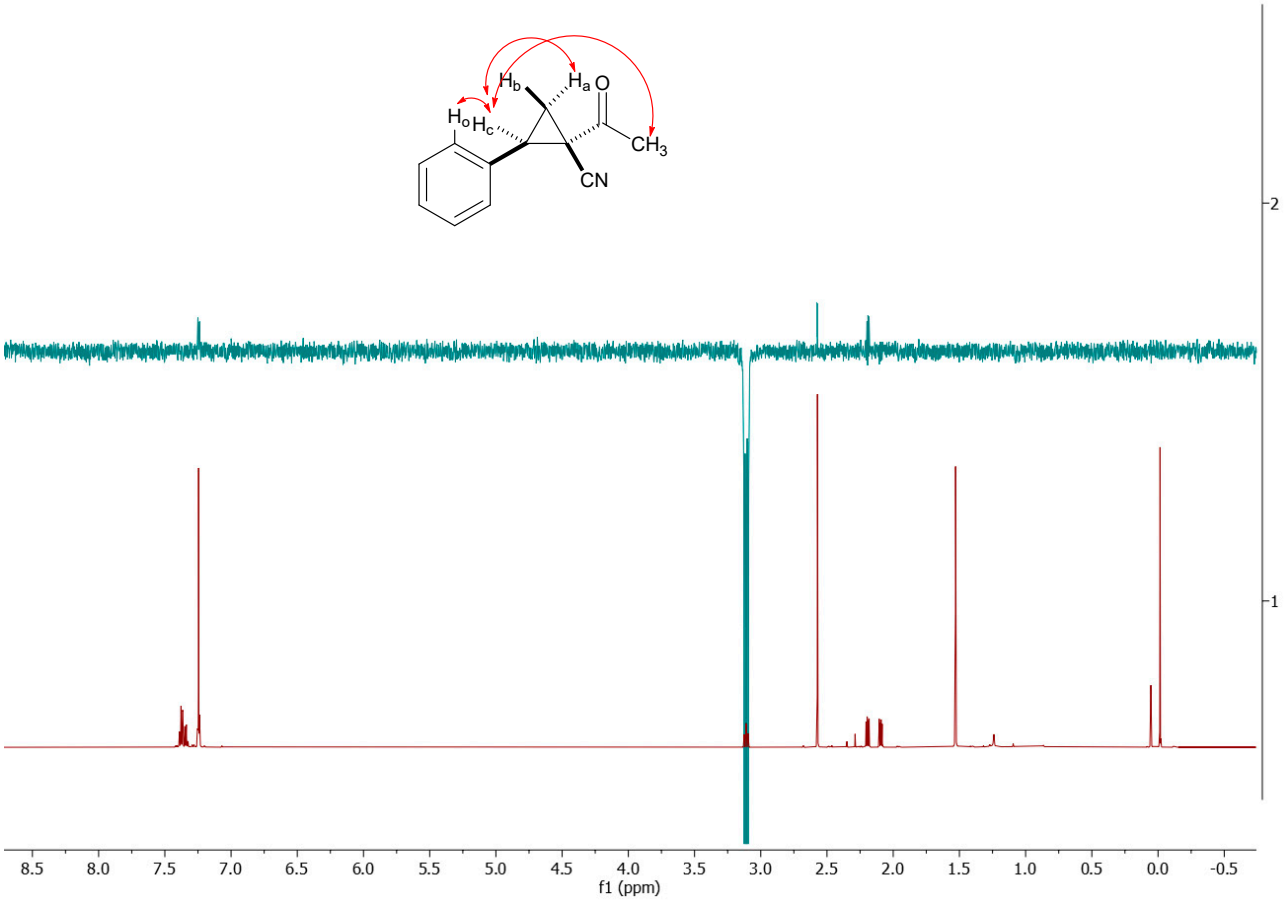
Irradiation of the H_a at 2.21 ppm gave NOE effect on the signal at 2.58 ppp assigned to CH_3, on the signal at 2.11 assigned to H_b and on the signal at 3.12 ppm assigned to H_c.



Irradiation of the H_b at 2.11 ppm gave NOE effect on the signal at 2.21 assigned to H_a, on the signal at 3.12 ppm assigned to H_c and on the signal at 7.20 ppm of the *ortho*-aromatic protons.



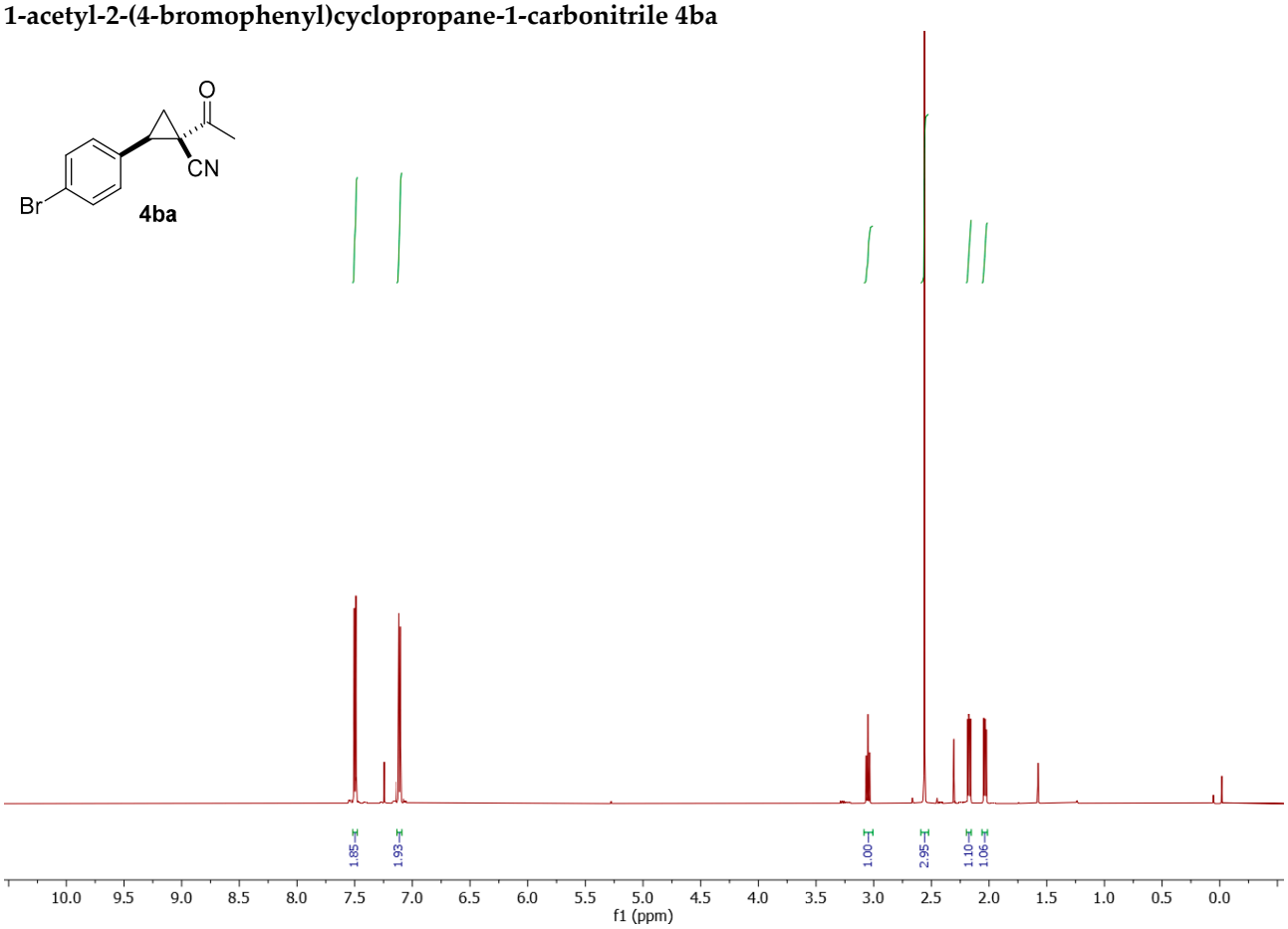
Irradiation of the H_c at 3.12 ppm gave NOE effect on the signal at 2.58 ppp assigned to CH_3, on the signal at 2.21 assigned to H_a and on the signal at 7.20 ppm of the *ortho*-aromatic protons.

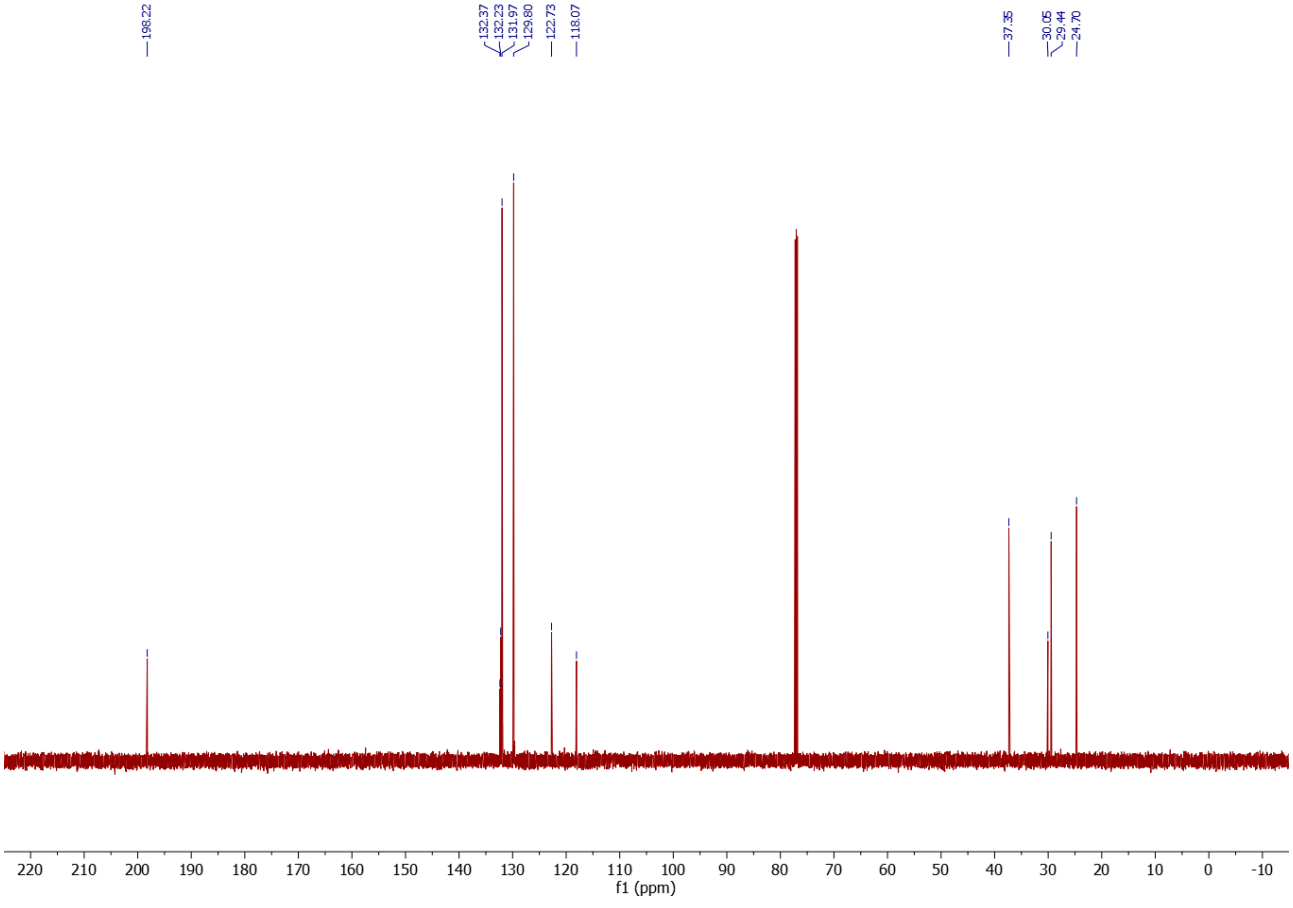


These results indicate a *cis*-relationship between H_c and CH_3 and thus, ultimately, a *trans* configuration of product **4aa**.

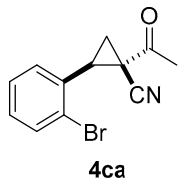
1-acetyl-2-(4-bromophenyl)cyclopropane-1-carbonitrile 4ba

4ba

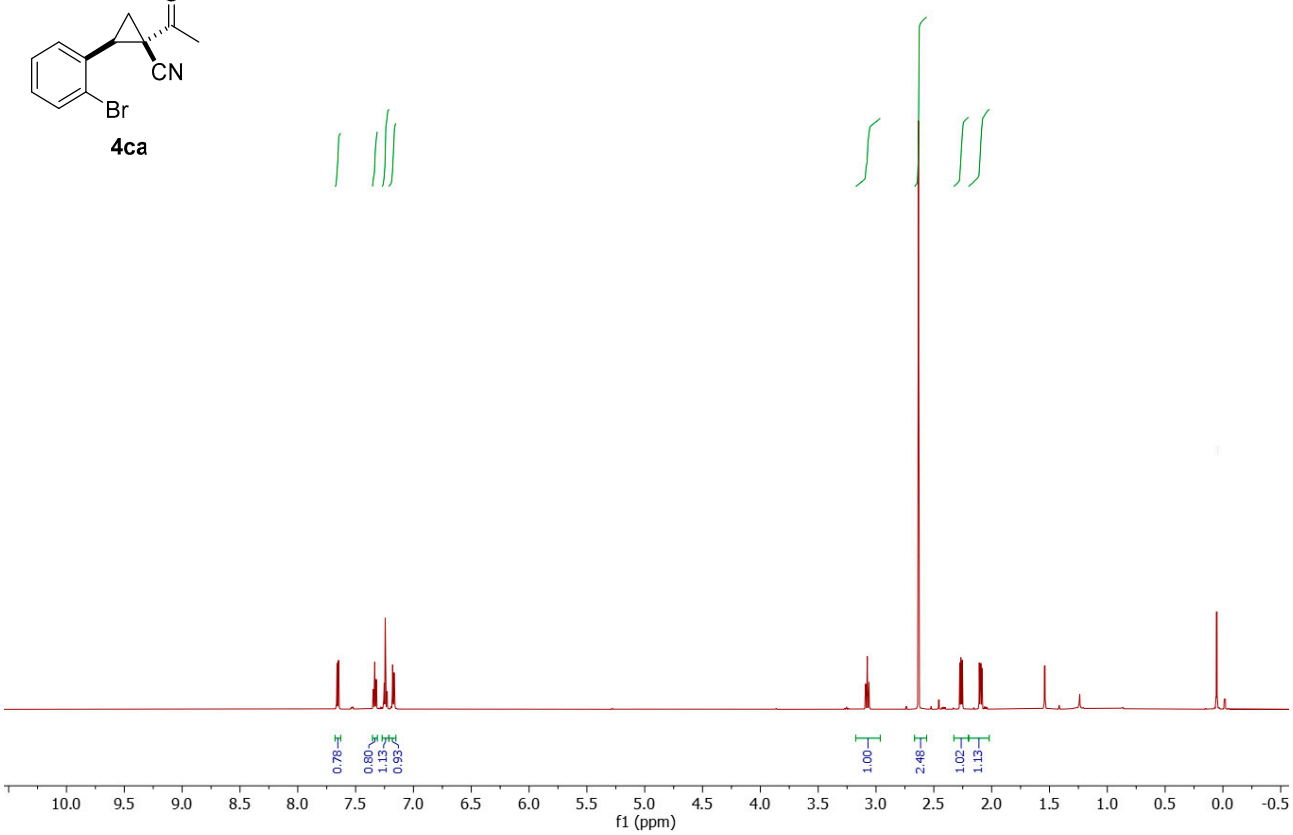


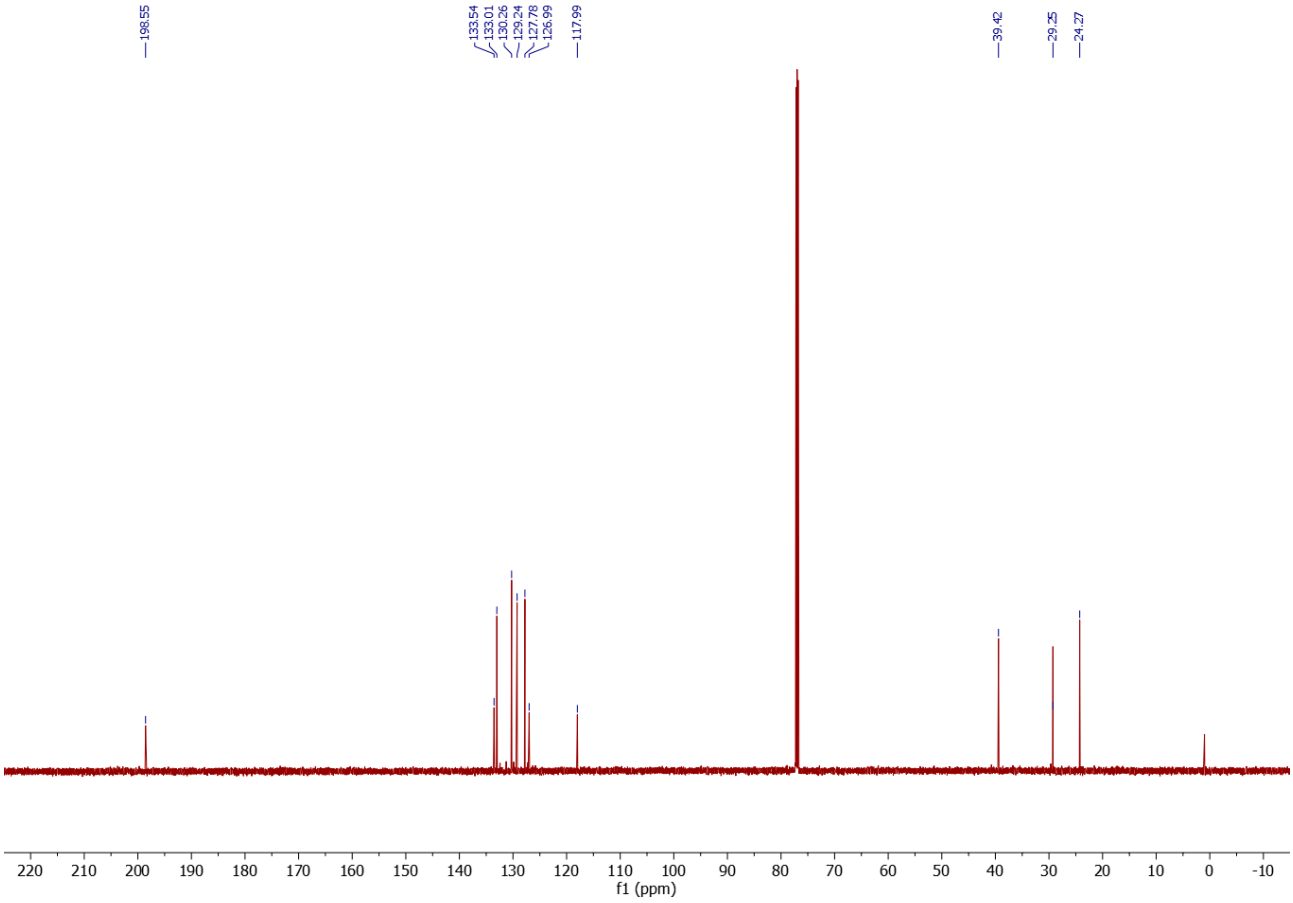


1-acetyl-2-(2-bromophenyl)cyclopropane-1-carbonitrile 4ca



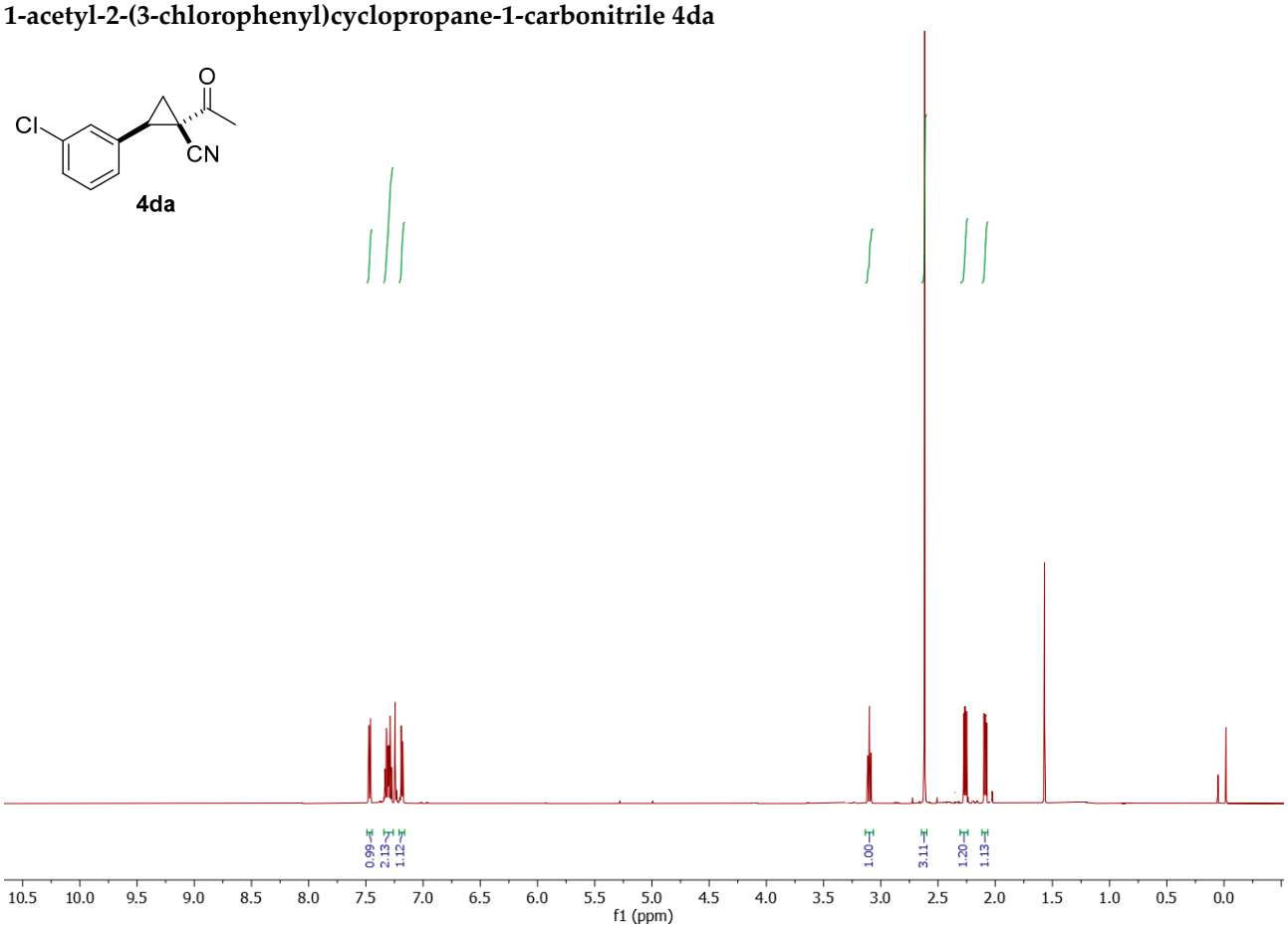
4ca

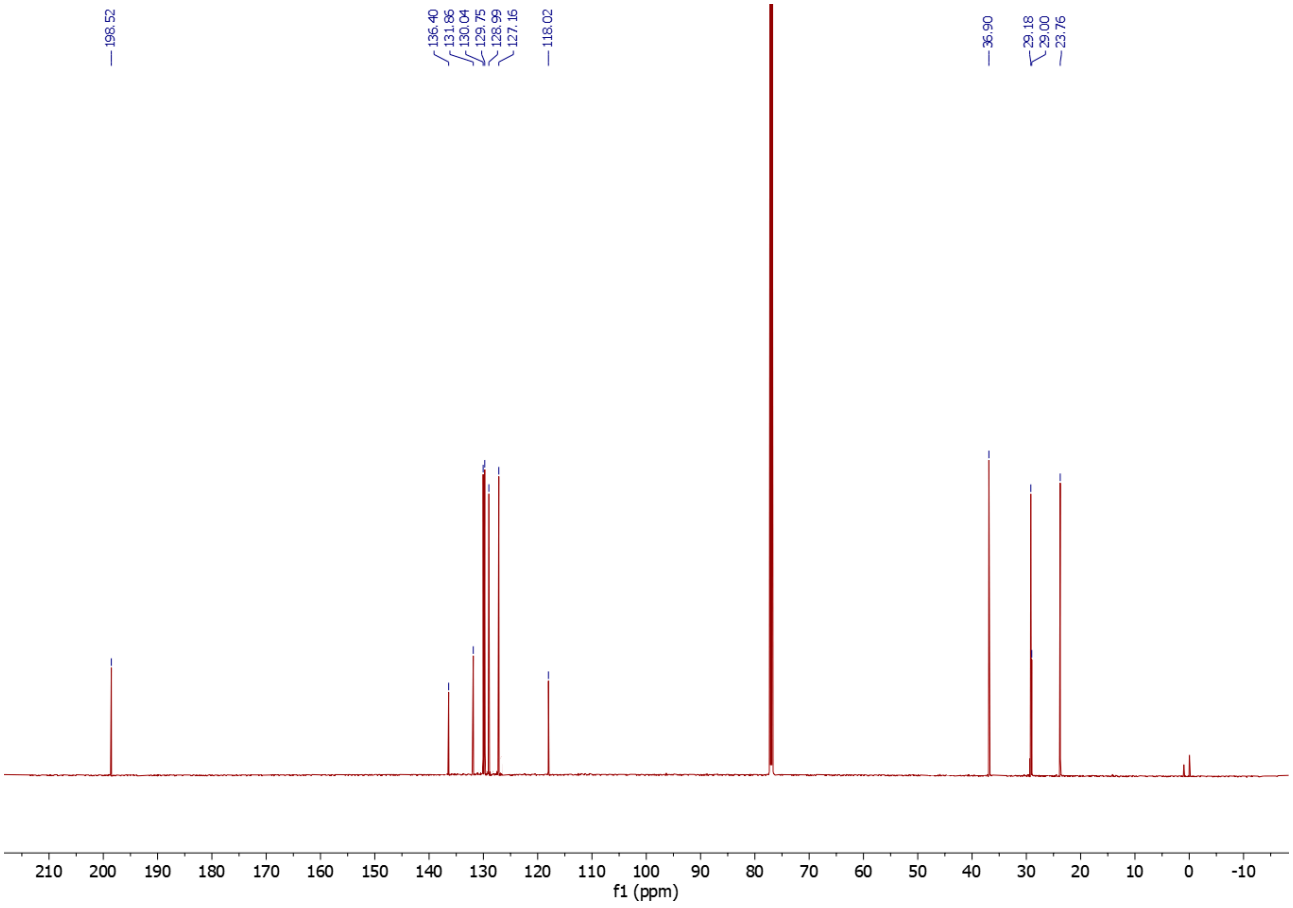




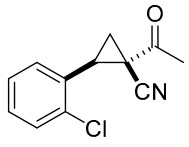
1-acetyl-2-(3-chlorophenyl)cyclopropane-1-carbonitrile 4da

4da

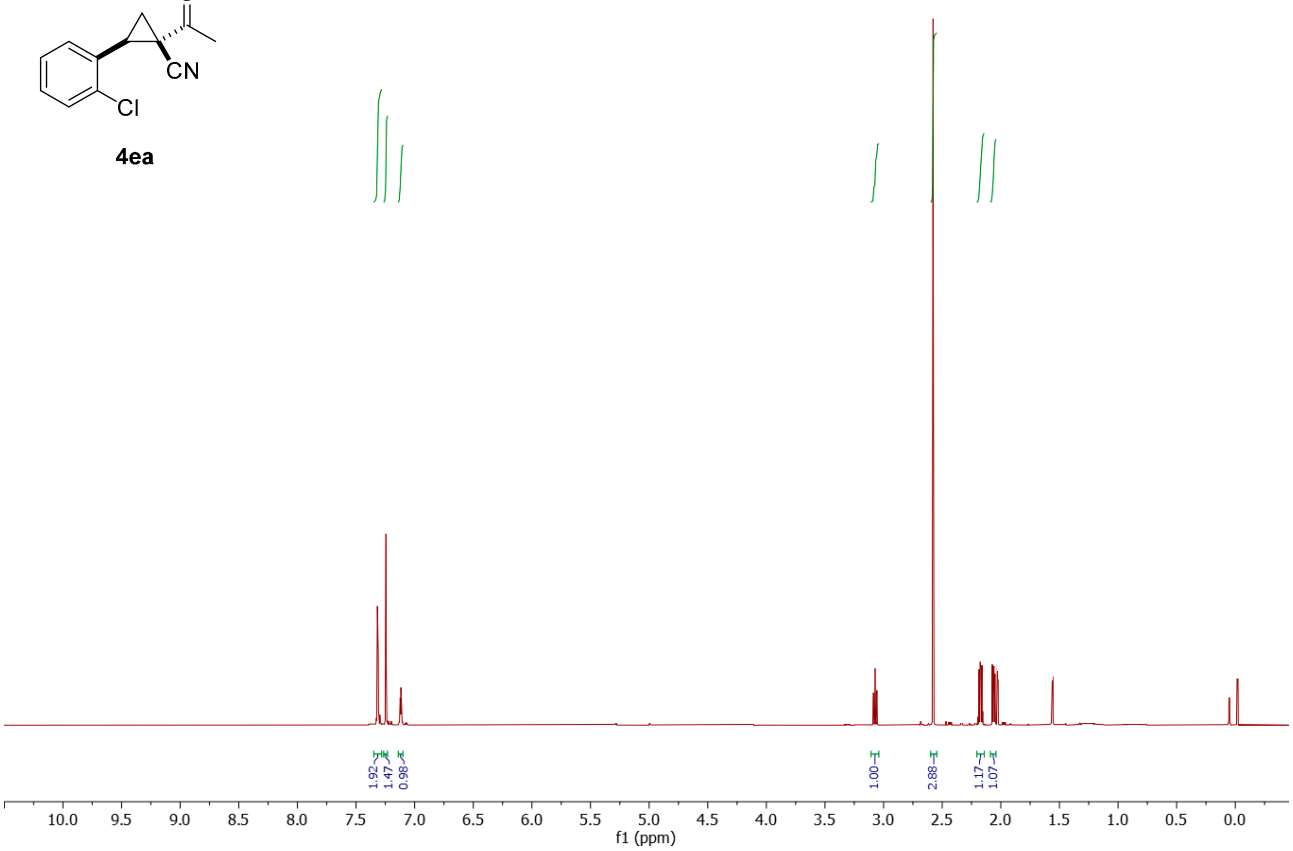


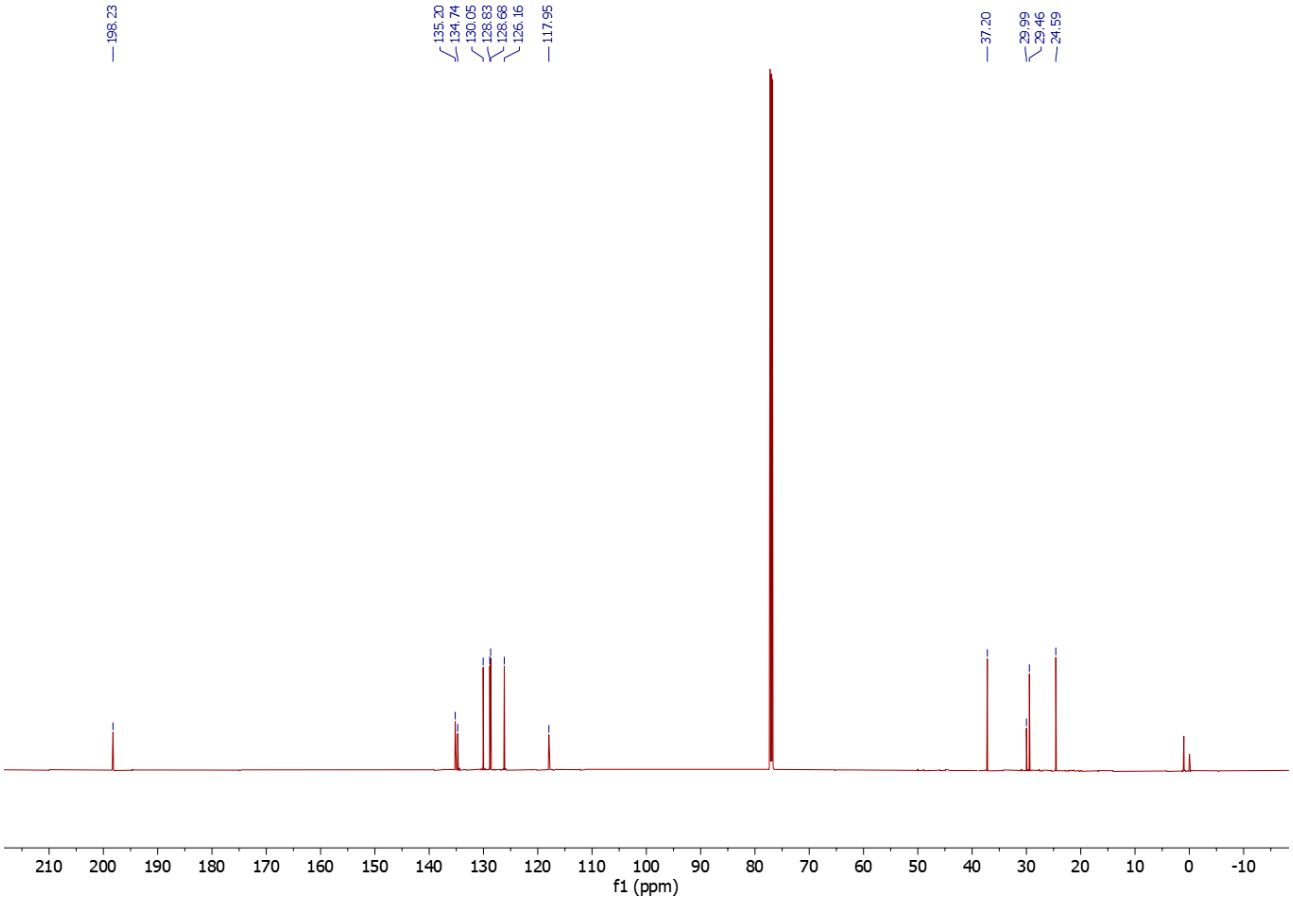


1-acetyl-2-(2-chlorophenyl)cyclopropane-1-carbonitrile 4ea

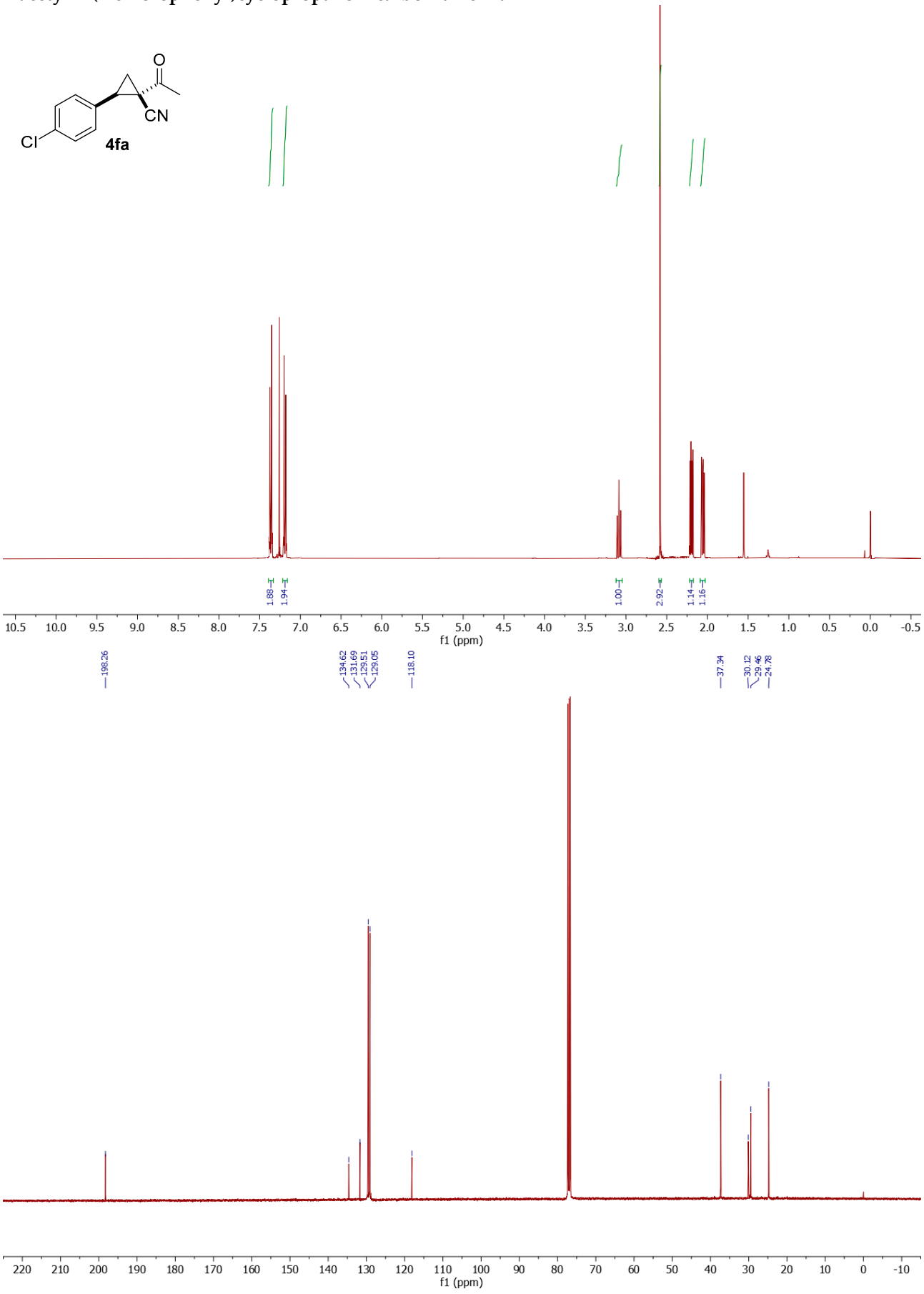


4ea

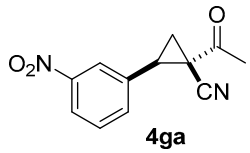




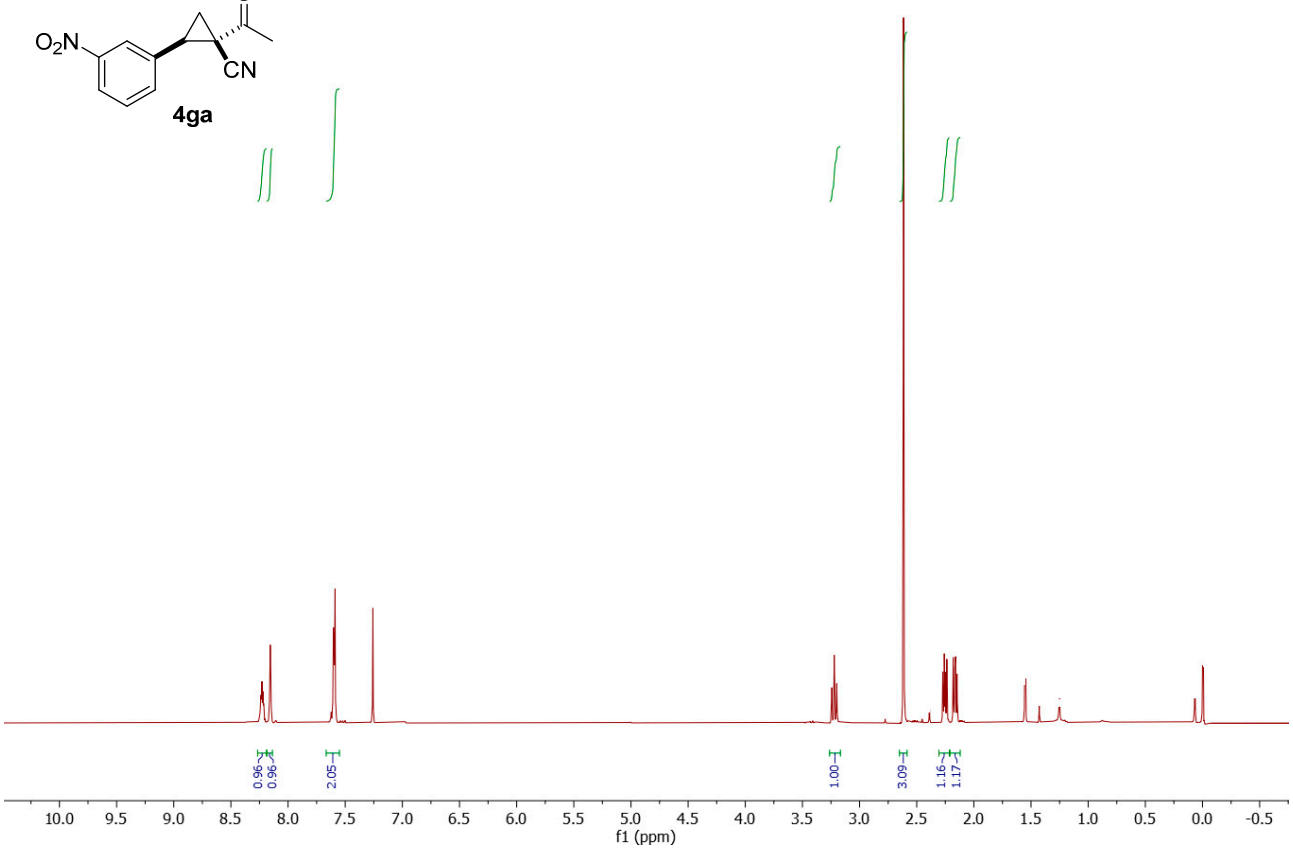
1-acetyl-2-(4-chlorophenyl)cyclopropane-1-carbonitrile 4fa

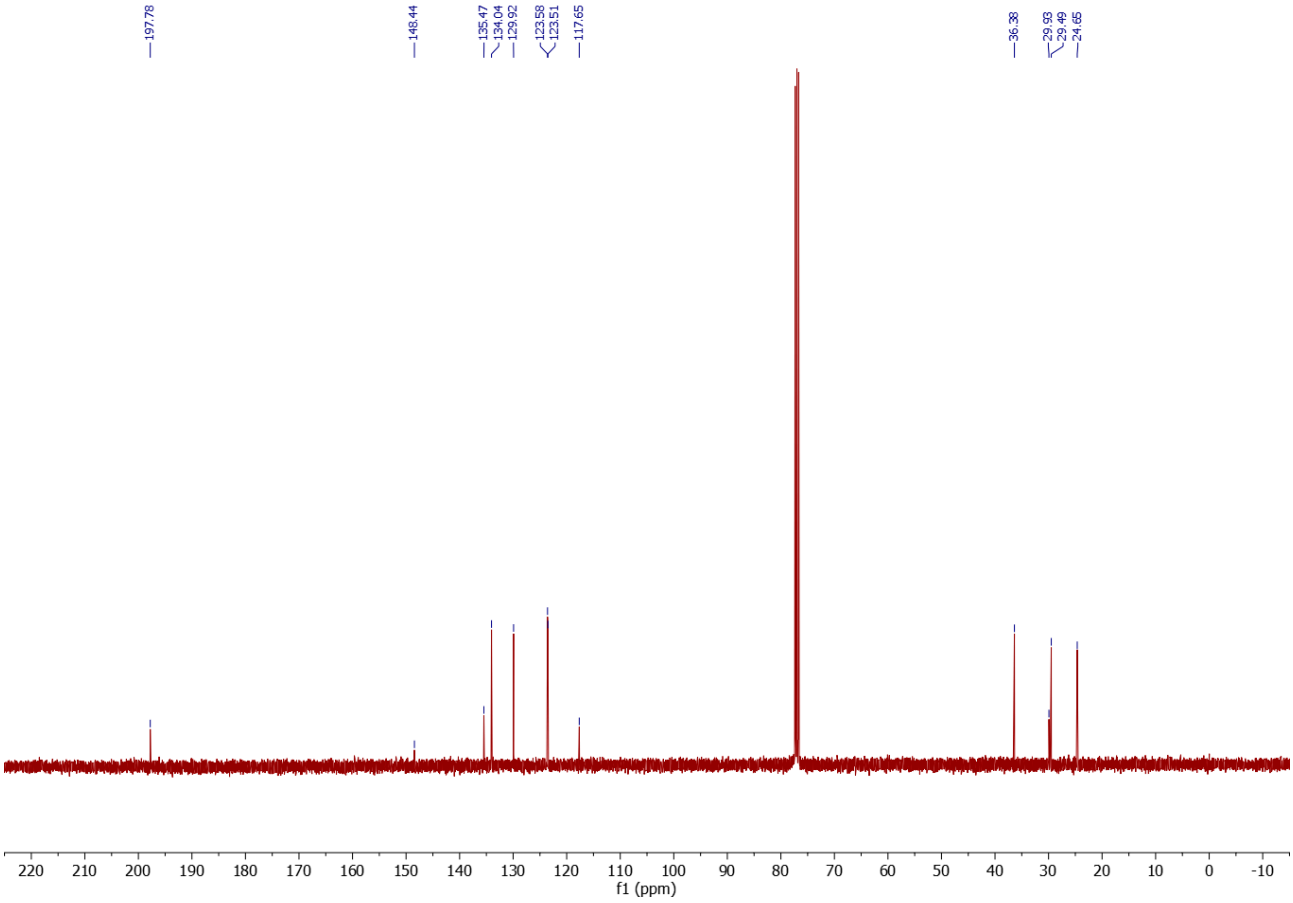


1-acetyl-2-(3-nitrophenyl)cyclopropane-1-carbonitrile 4ga



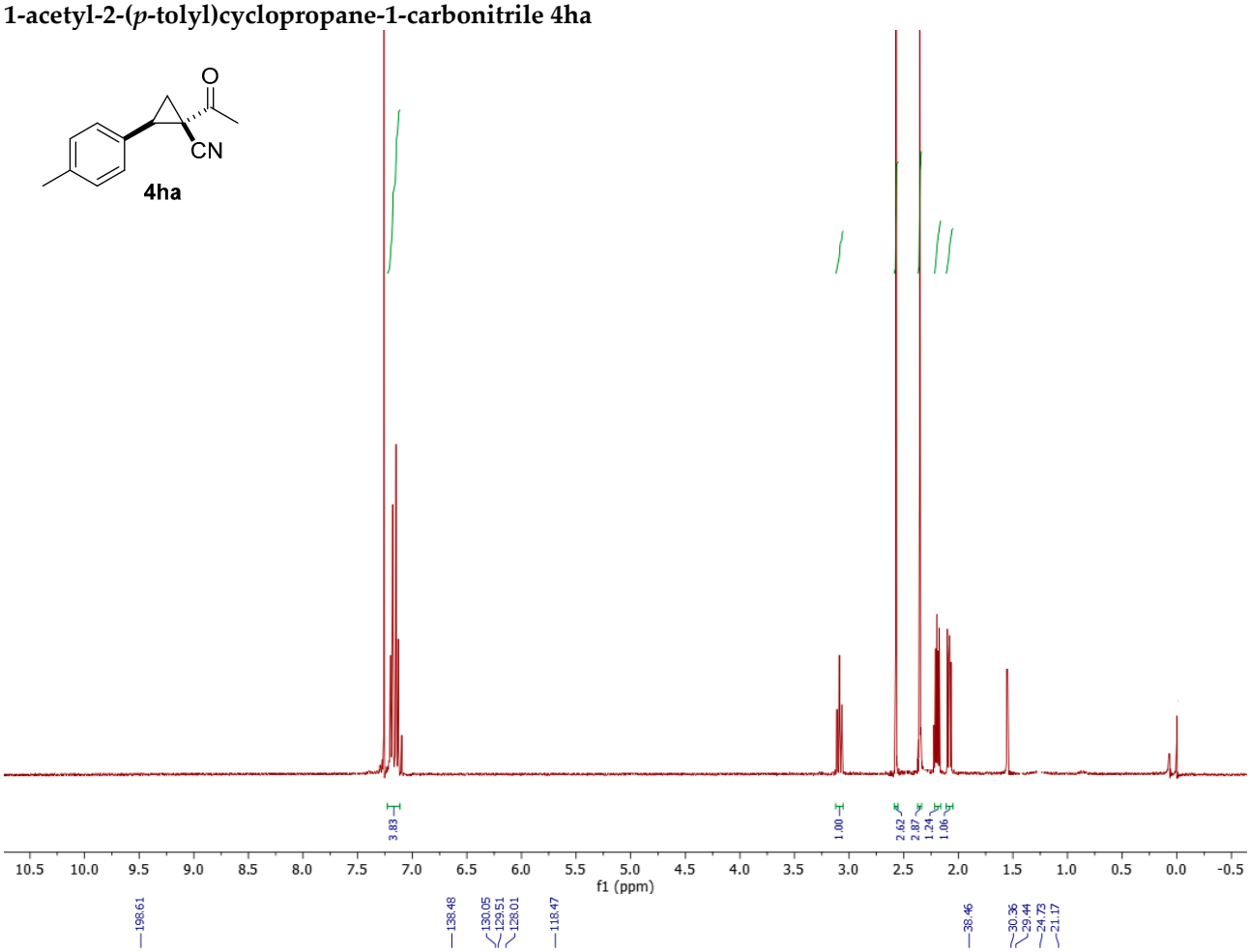
4ga

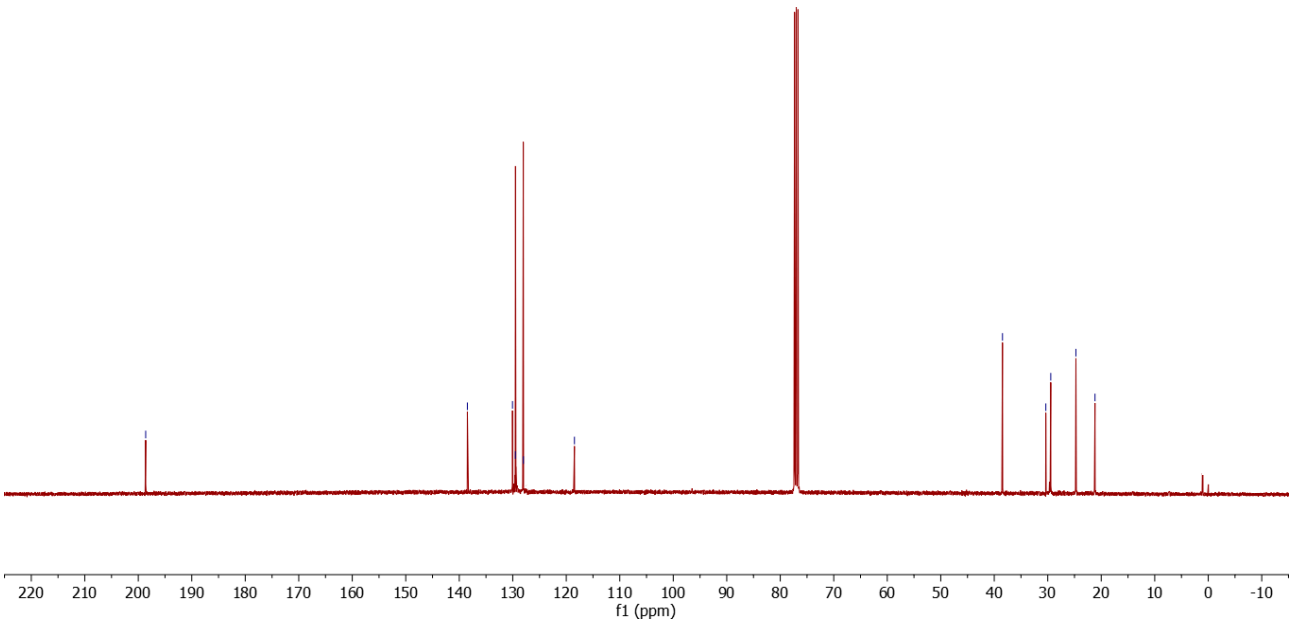




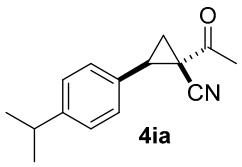
1-acetyl-2-(*p*-tolyl)cyclopropane-1-carbonitrile 4ha

4ha

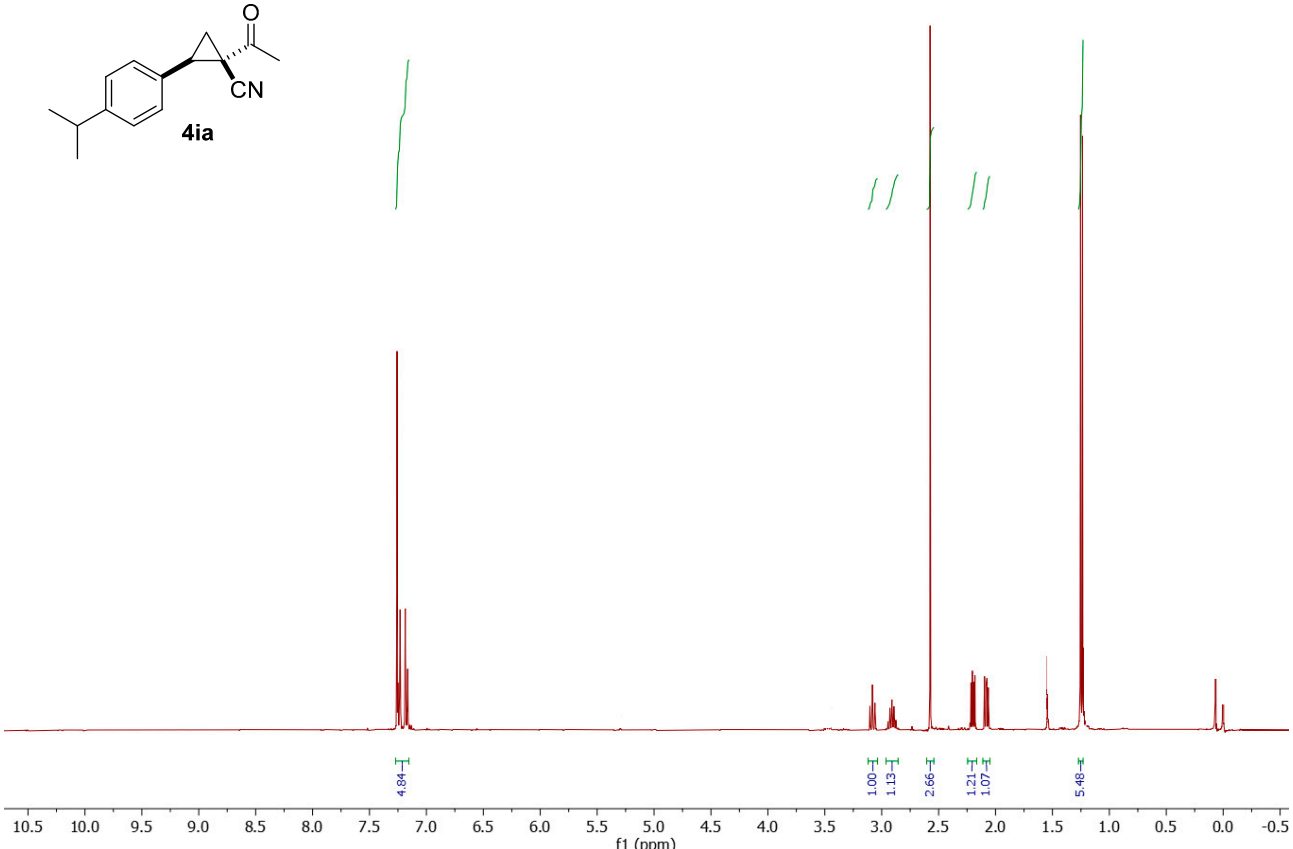


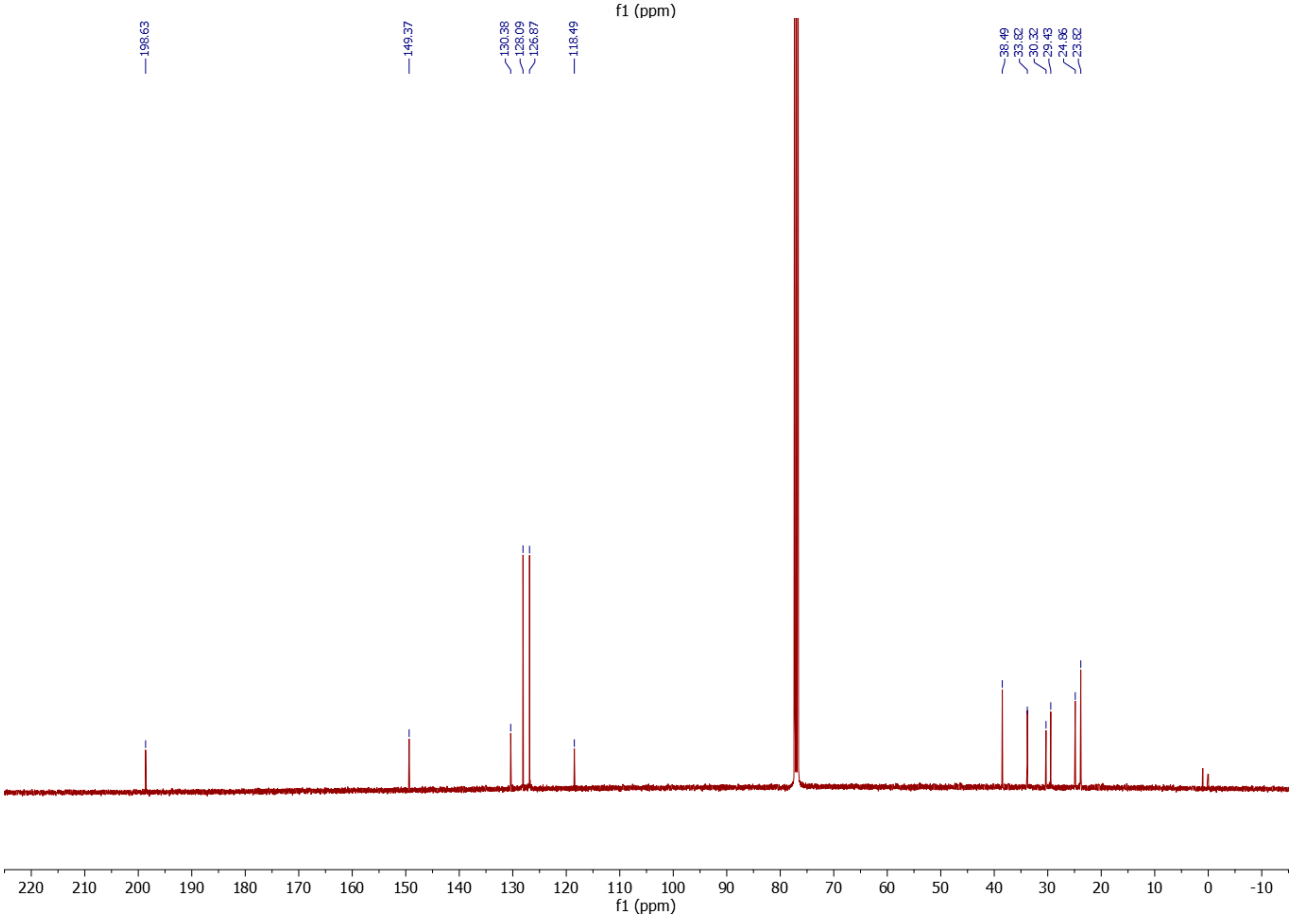


1-acetyl-2-(4-isopropylphenyl)cyclopropane-1-carbonitrile 4ia

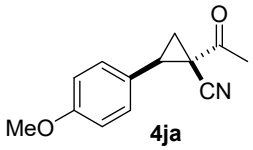


4ia

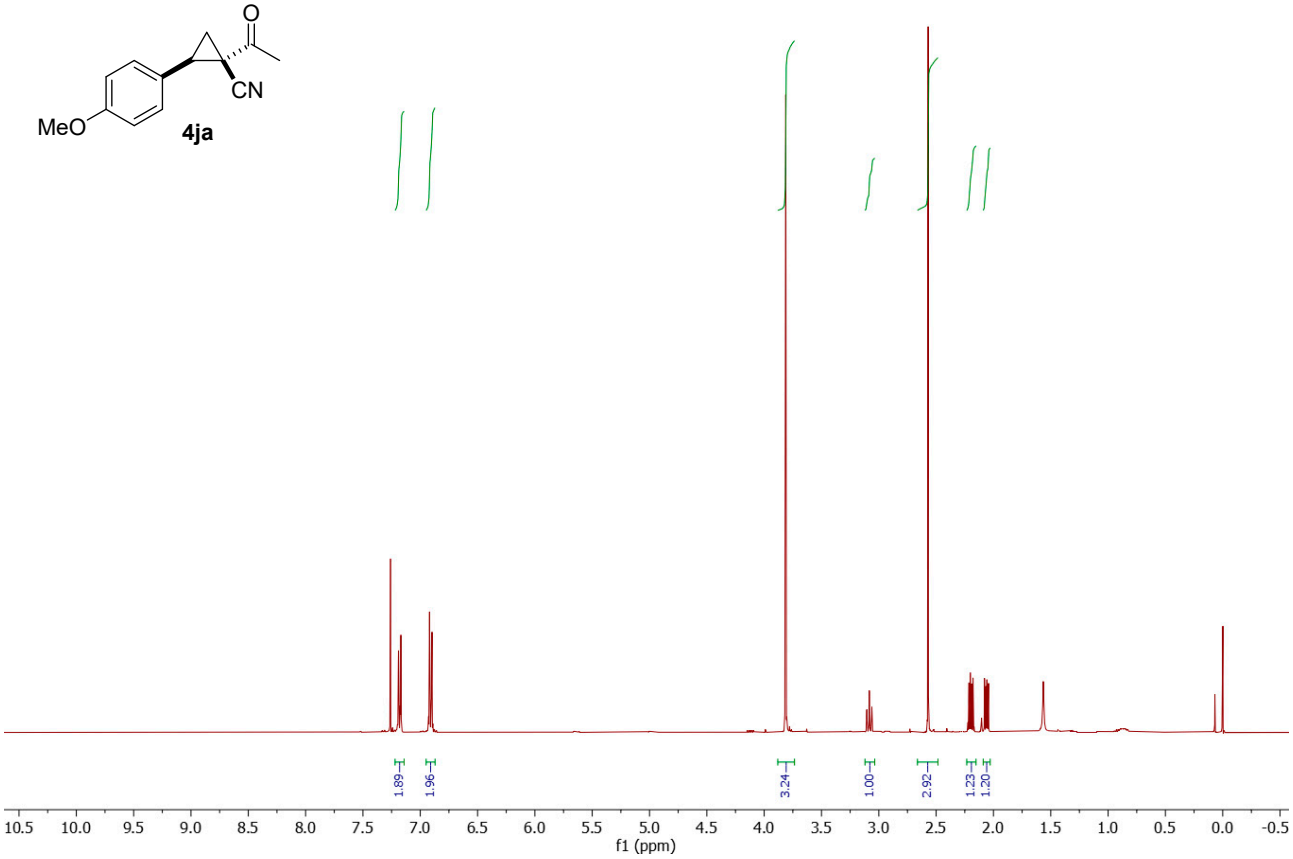


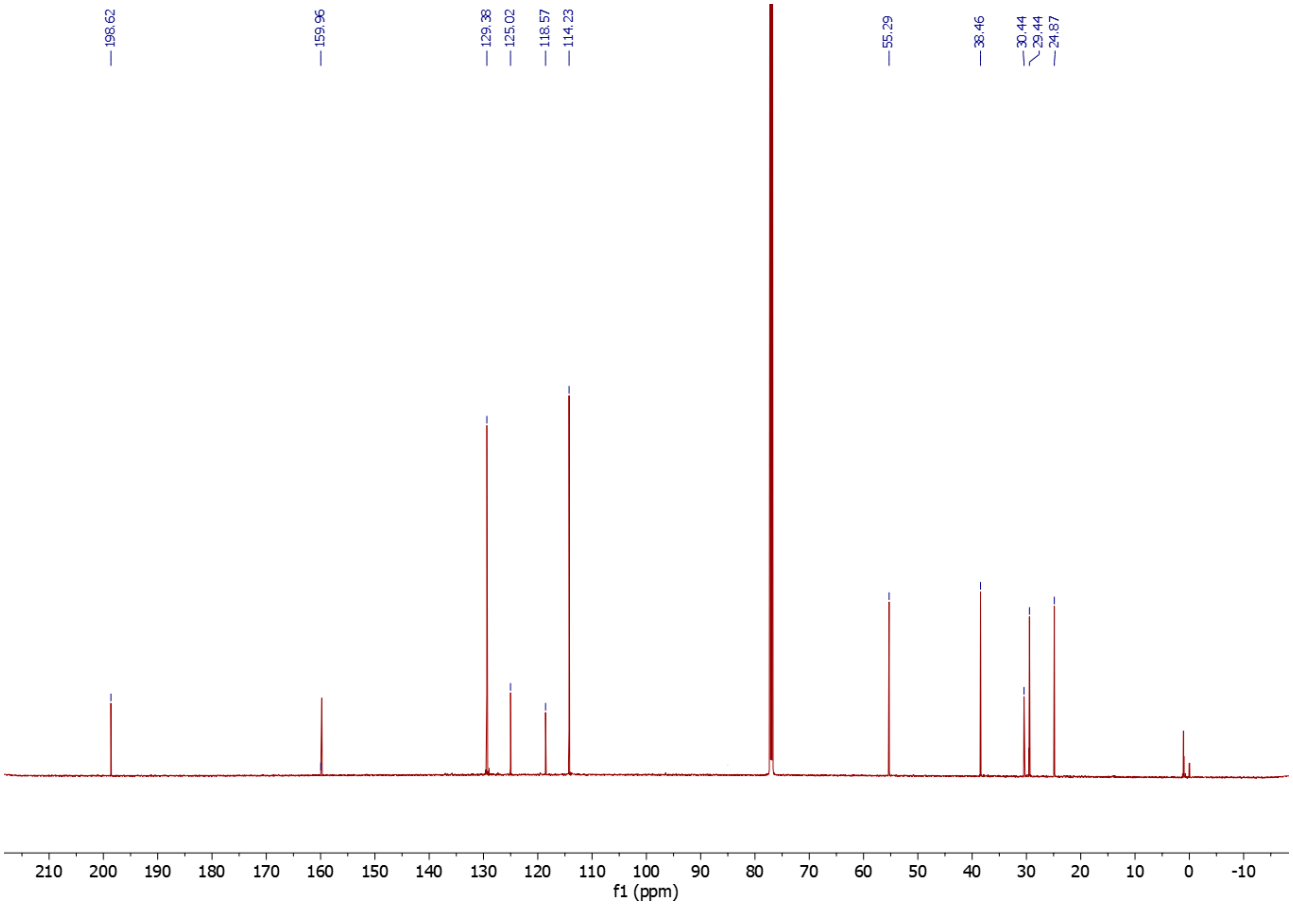


1-acetyl-2-(4-methoxyphenyl)cyclopropane-1-carbonitrile 4ja



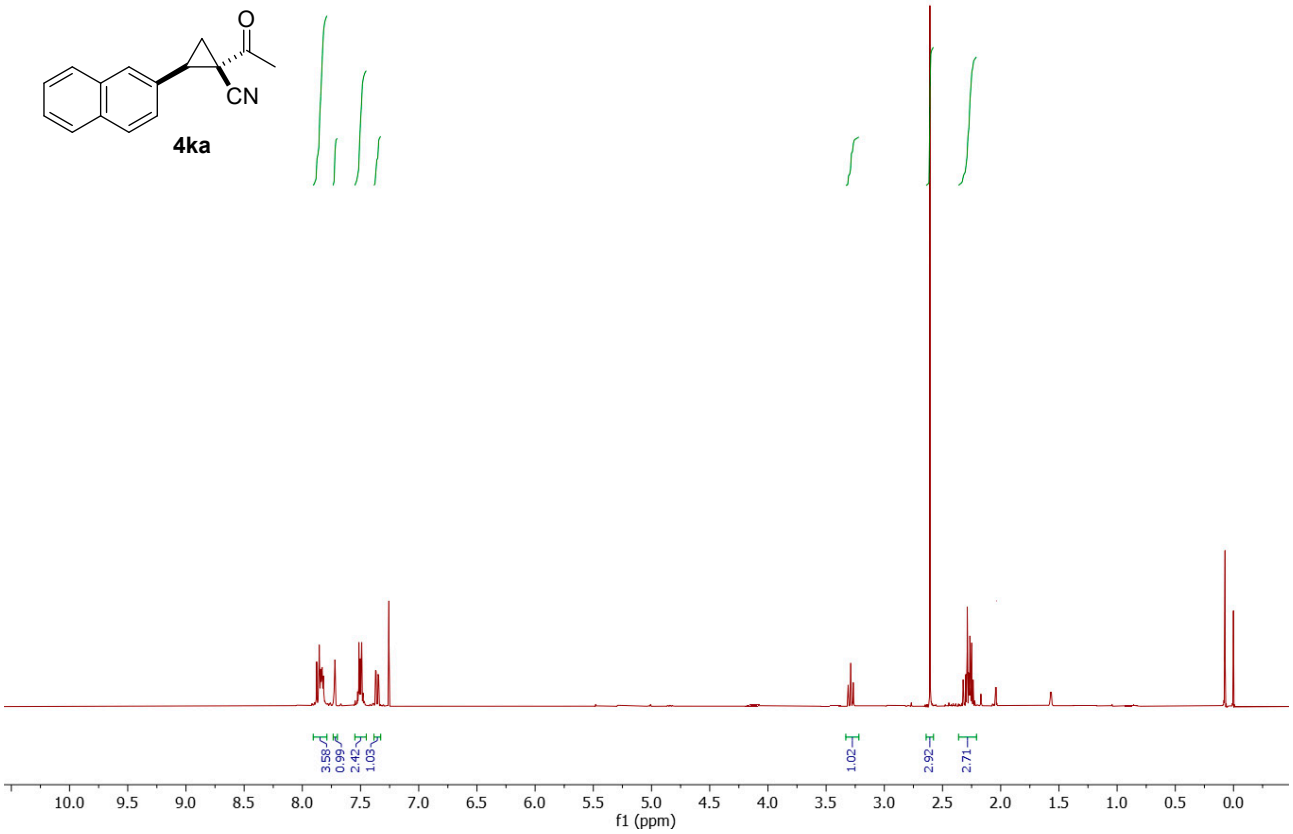
4ja

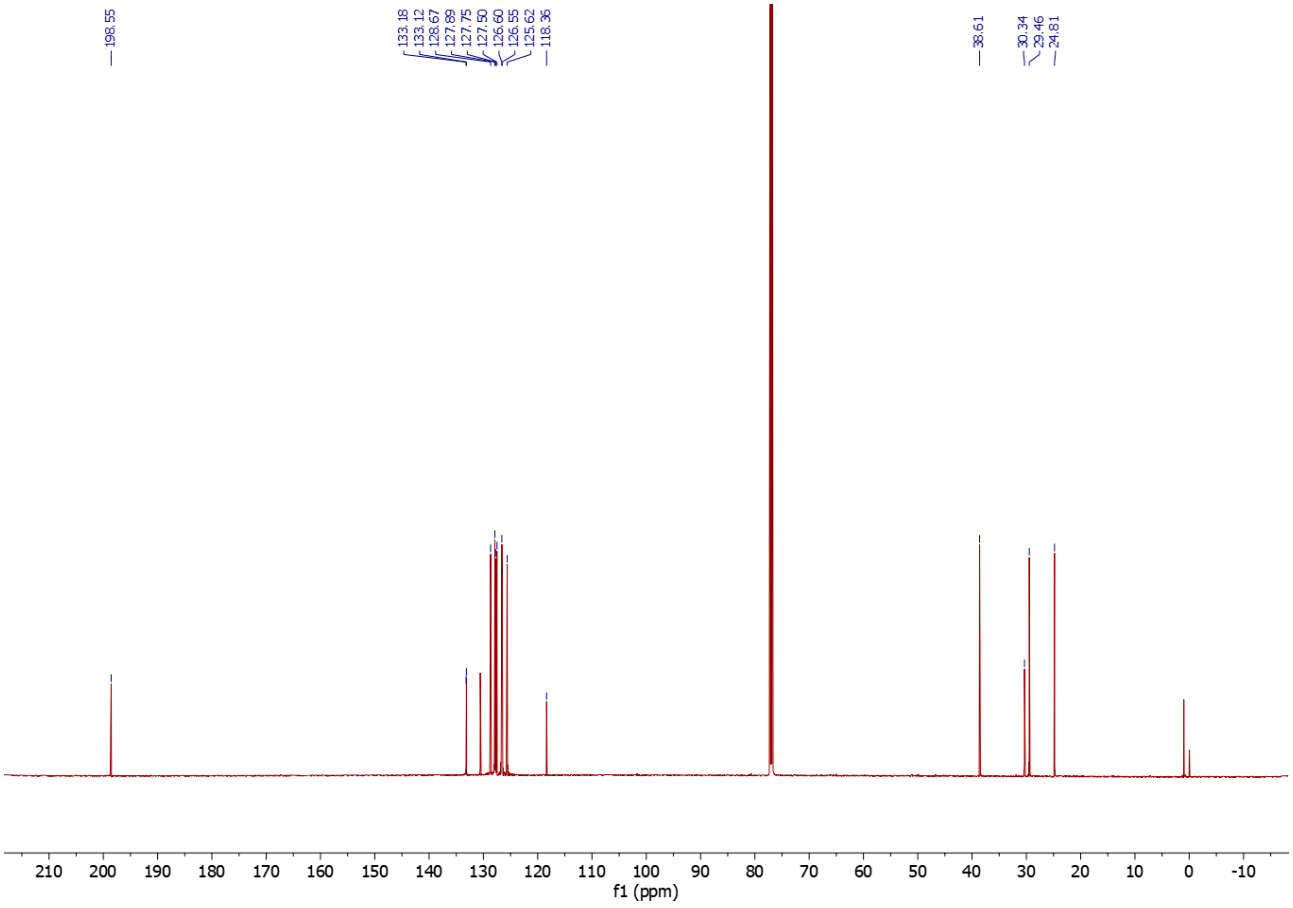




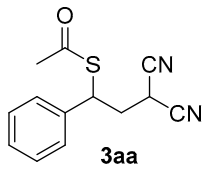
1-acetyl-2-(naphthalen-2-yl)cyclopropane-1-carbonitrile 4ka

4ka

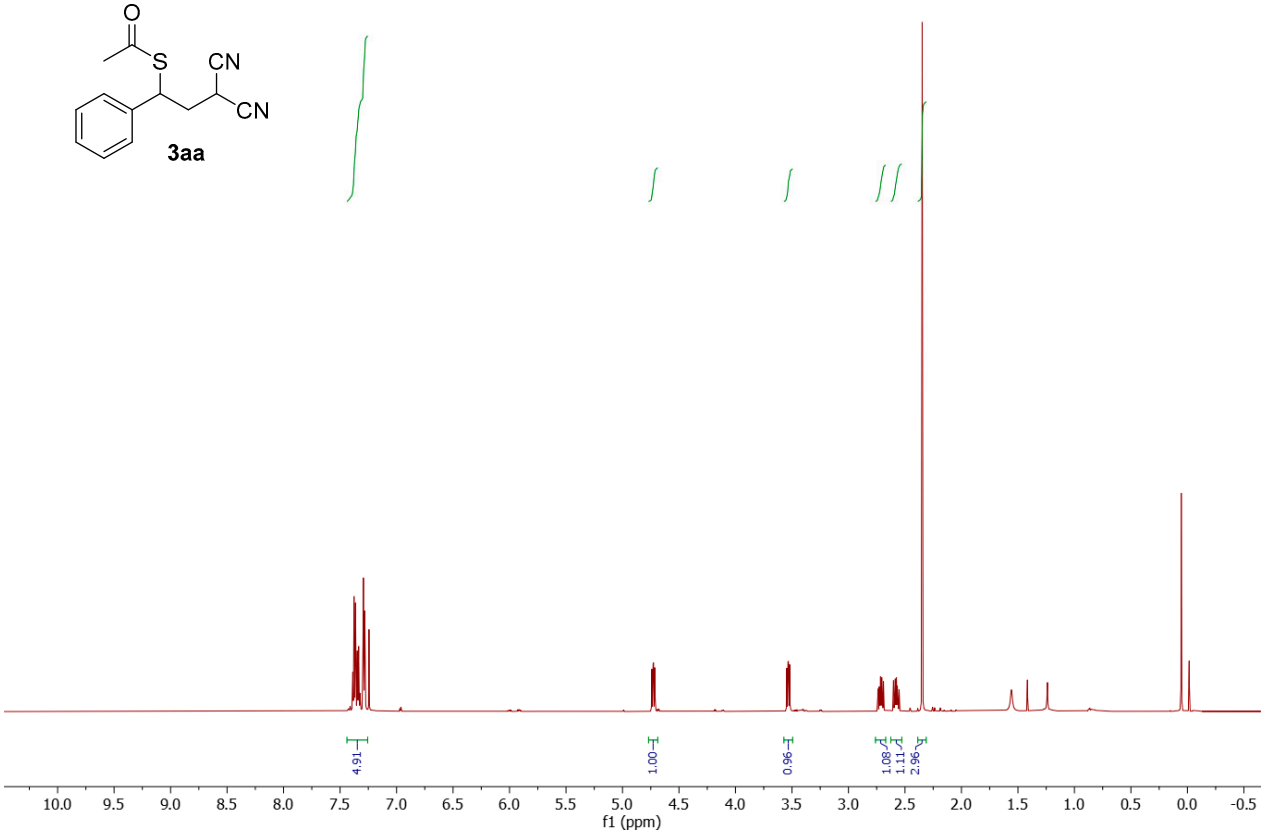


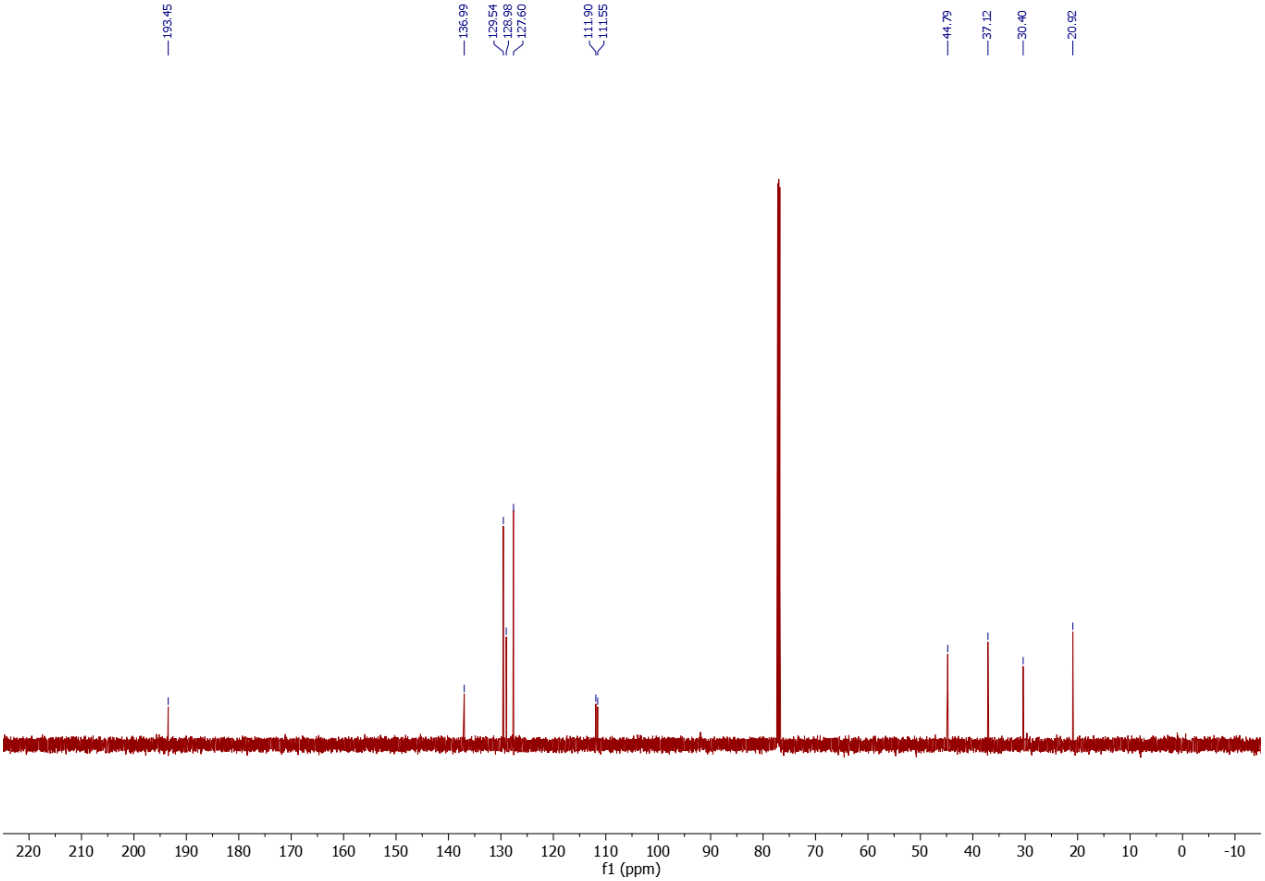


S-(3,3-dicyano-1-phenylpropyl) ethanethioate 3aa

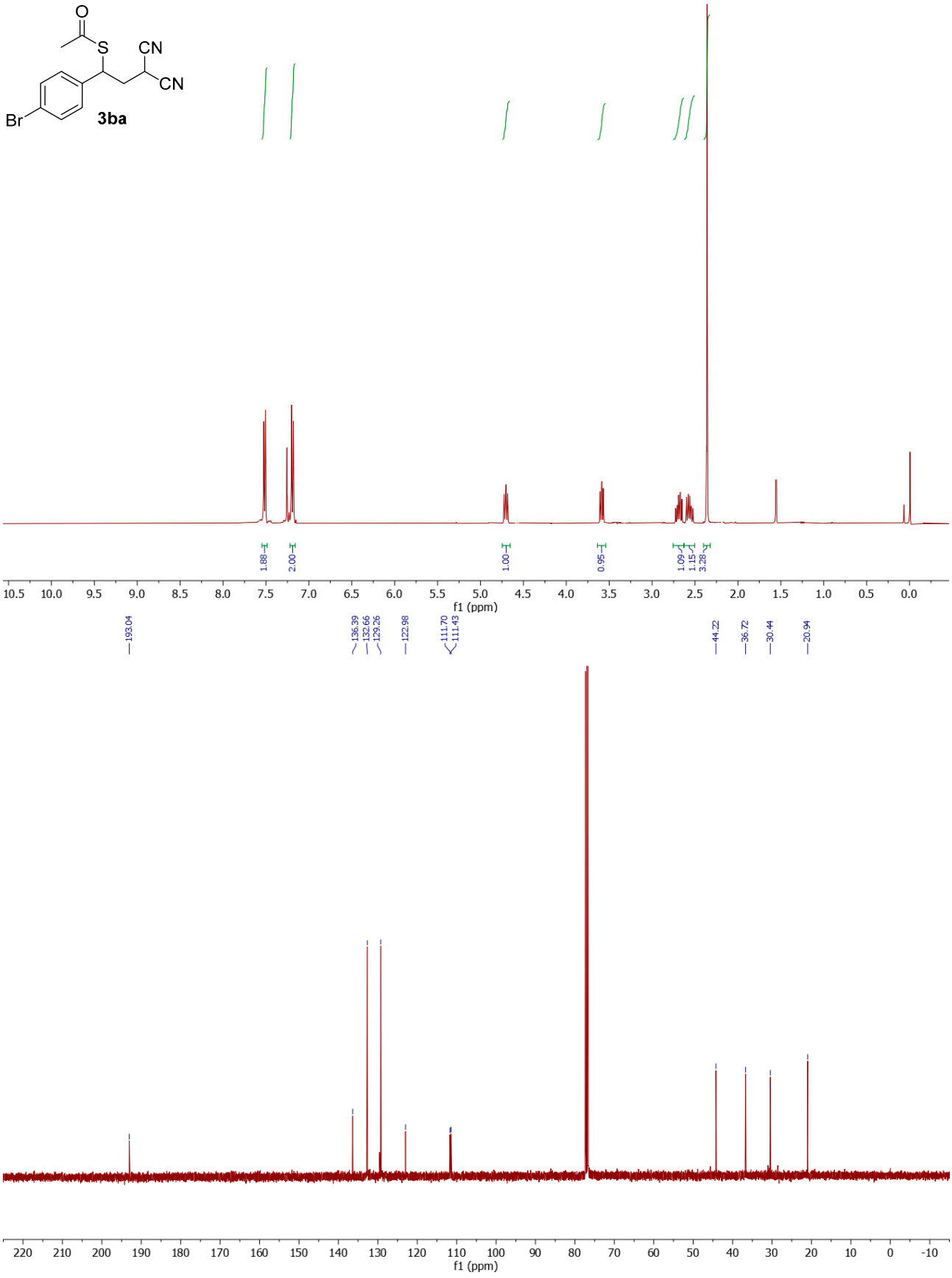


3aa

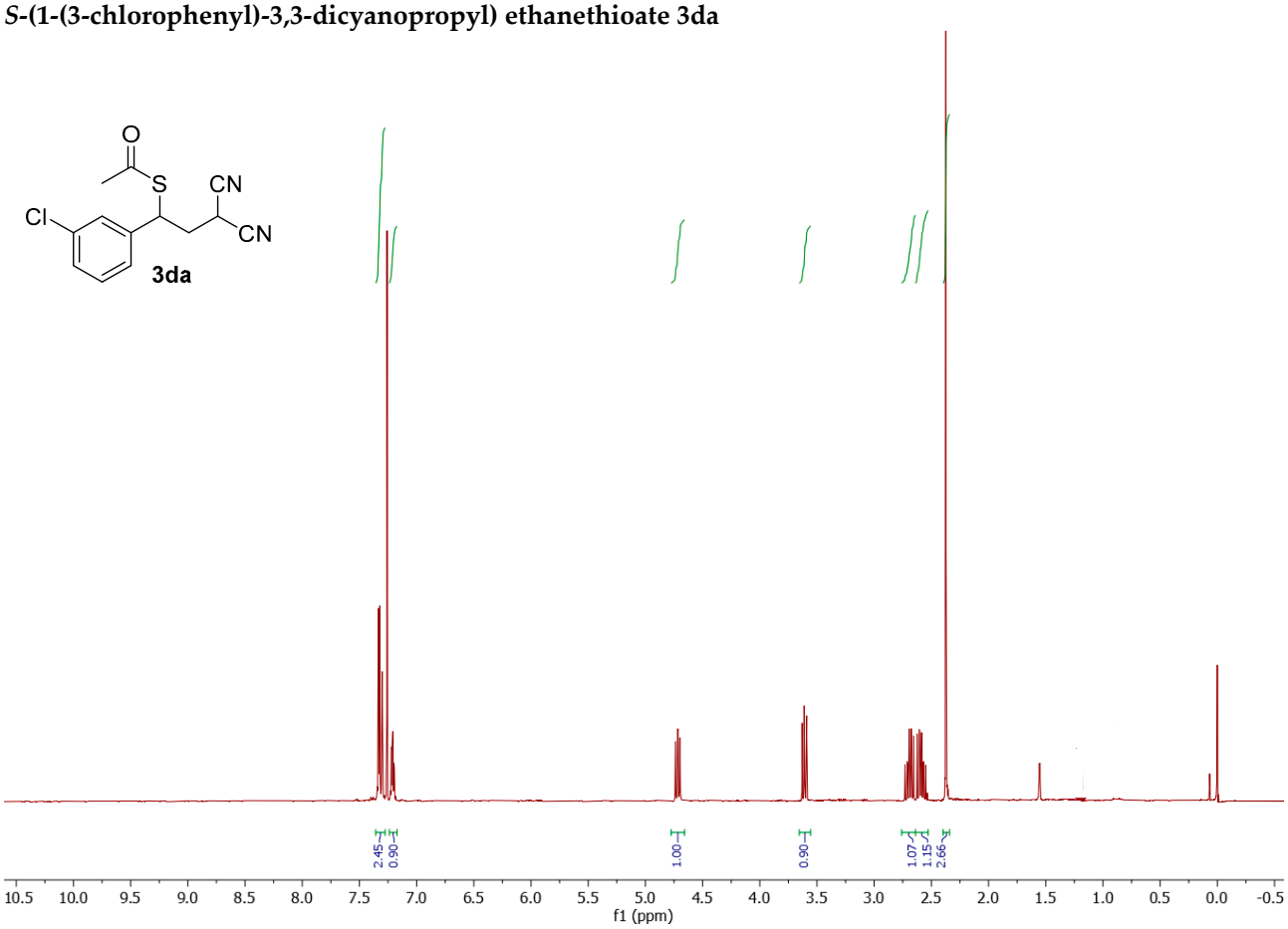


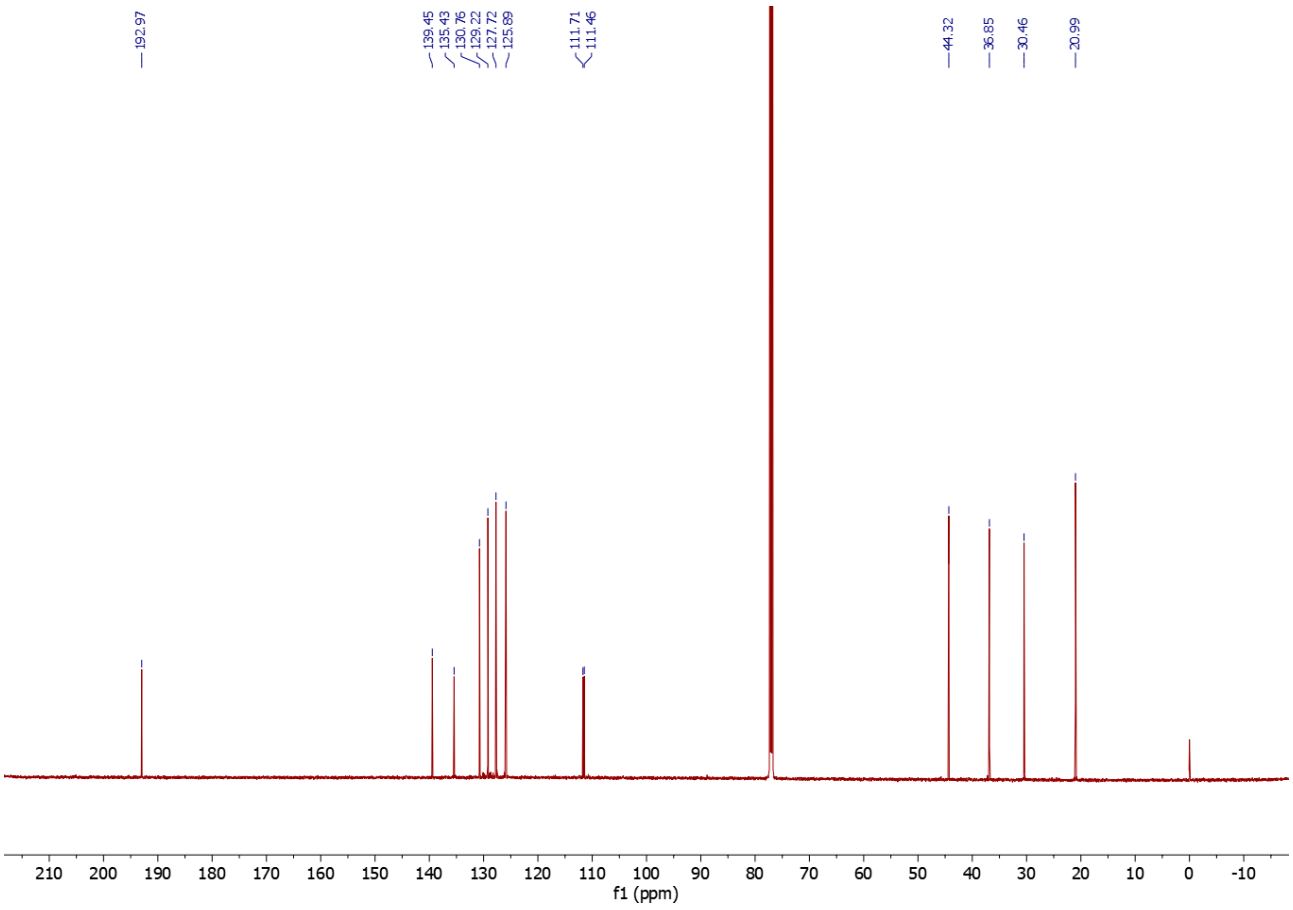


S-(1-(4-bromophenyl)-3,3-dicyanopropyl) ethanethioate 3ba



S-(1-(3-chlorophenyl)-3,3-dicyanopropyl) ethanethioate 3da





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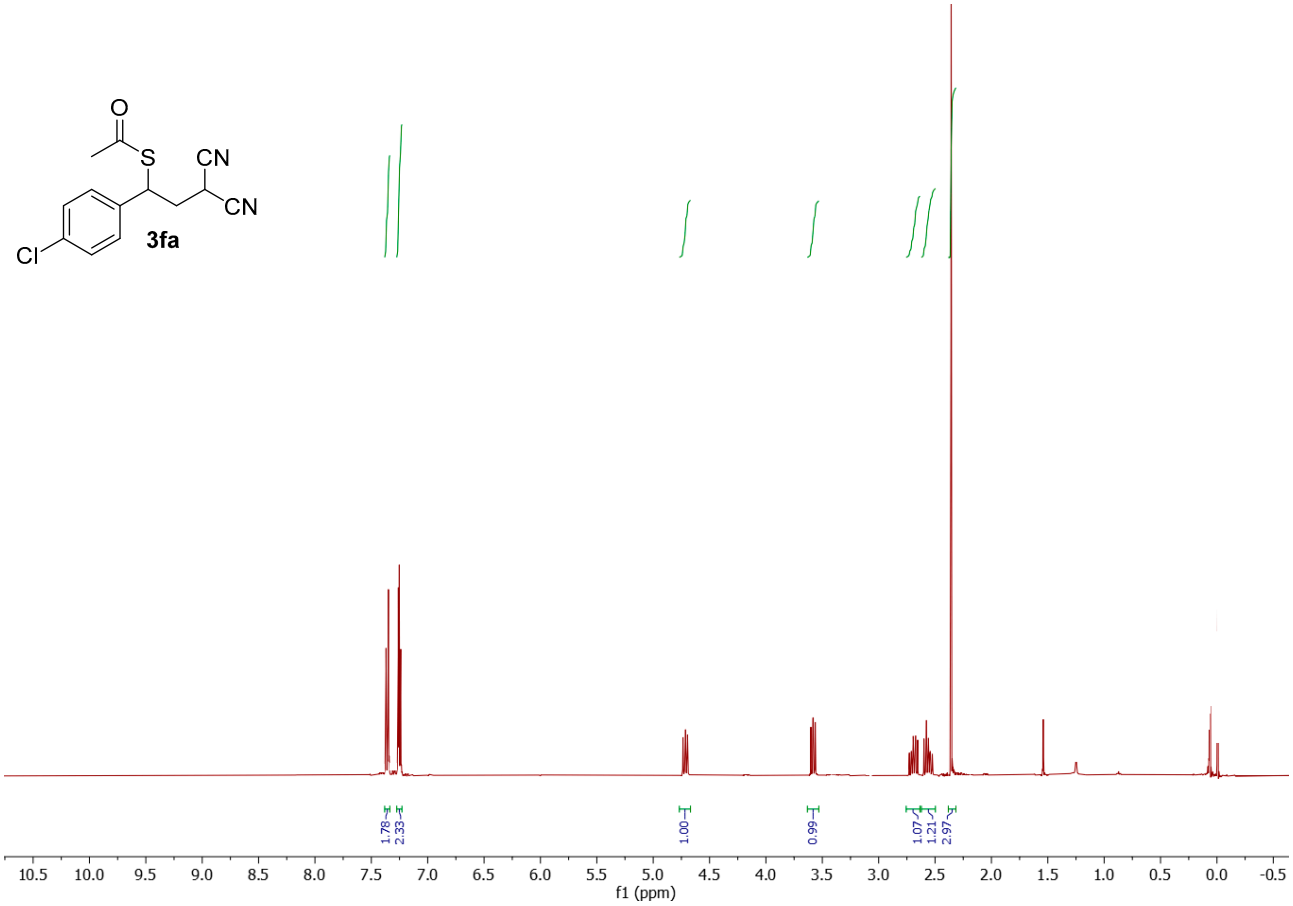
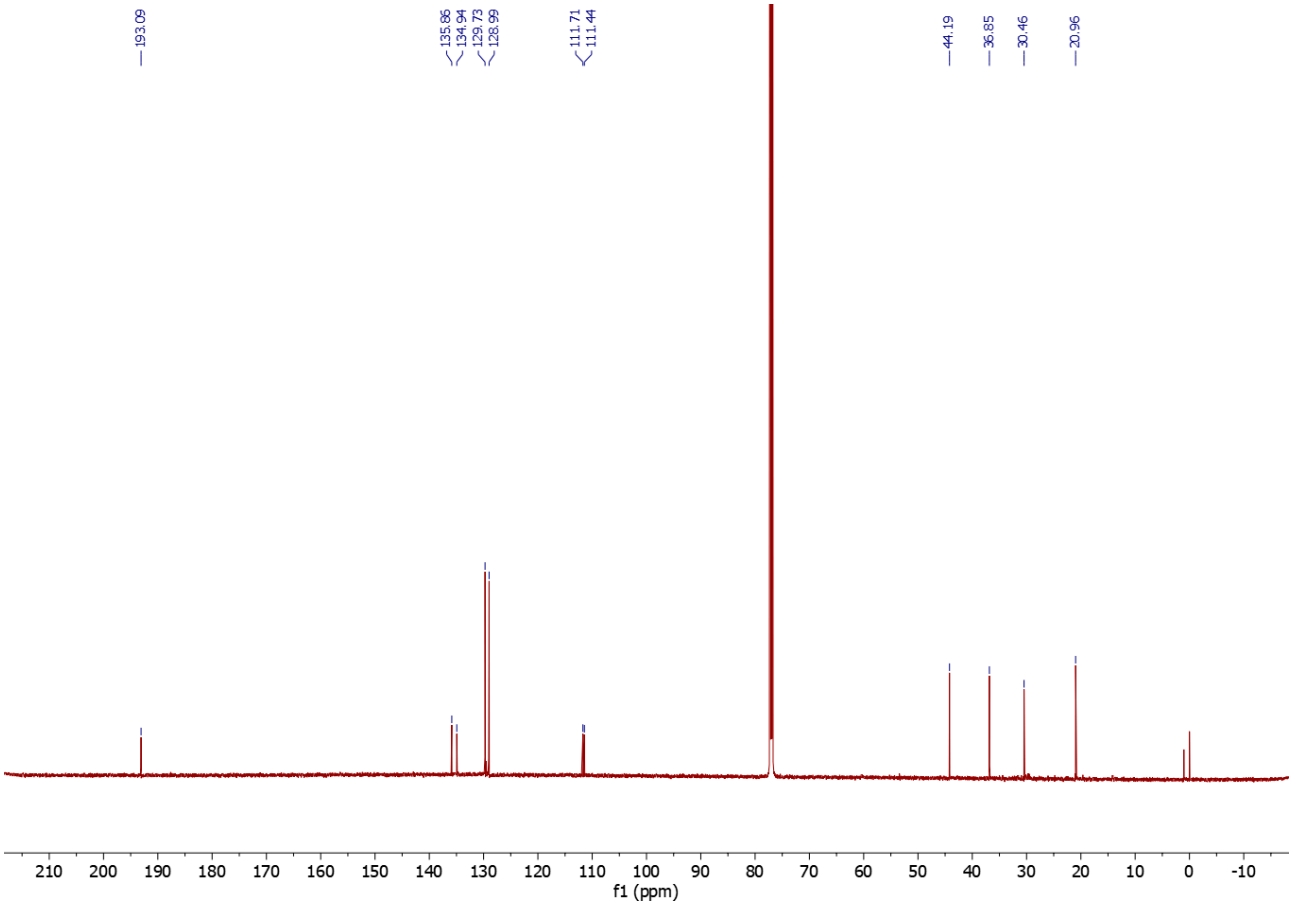
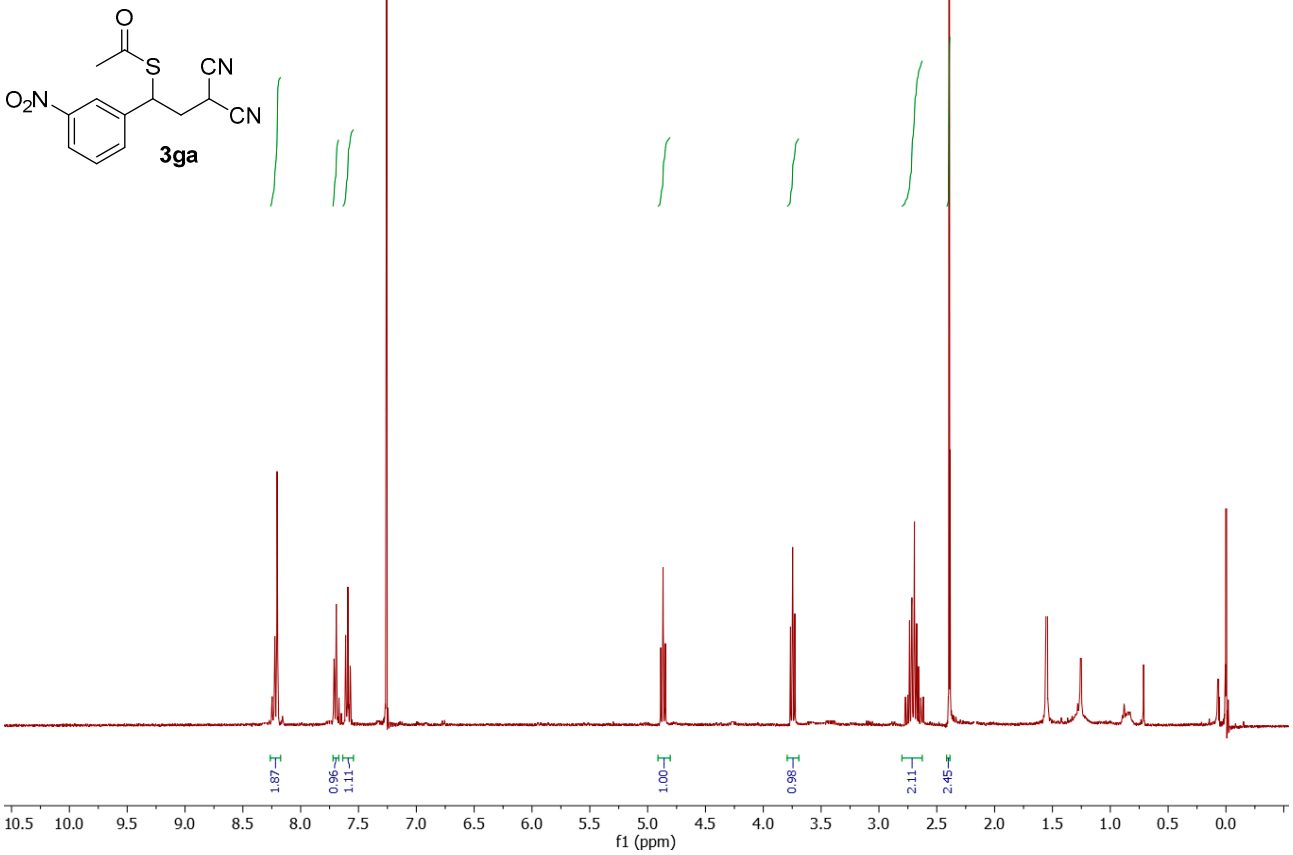
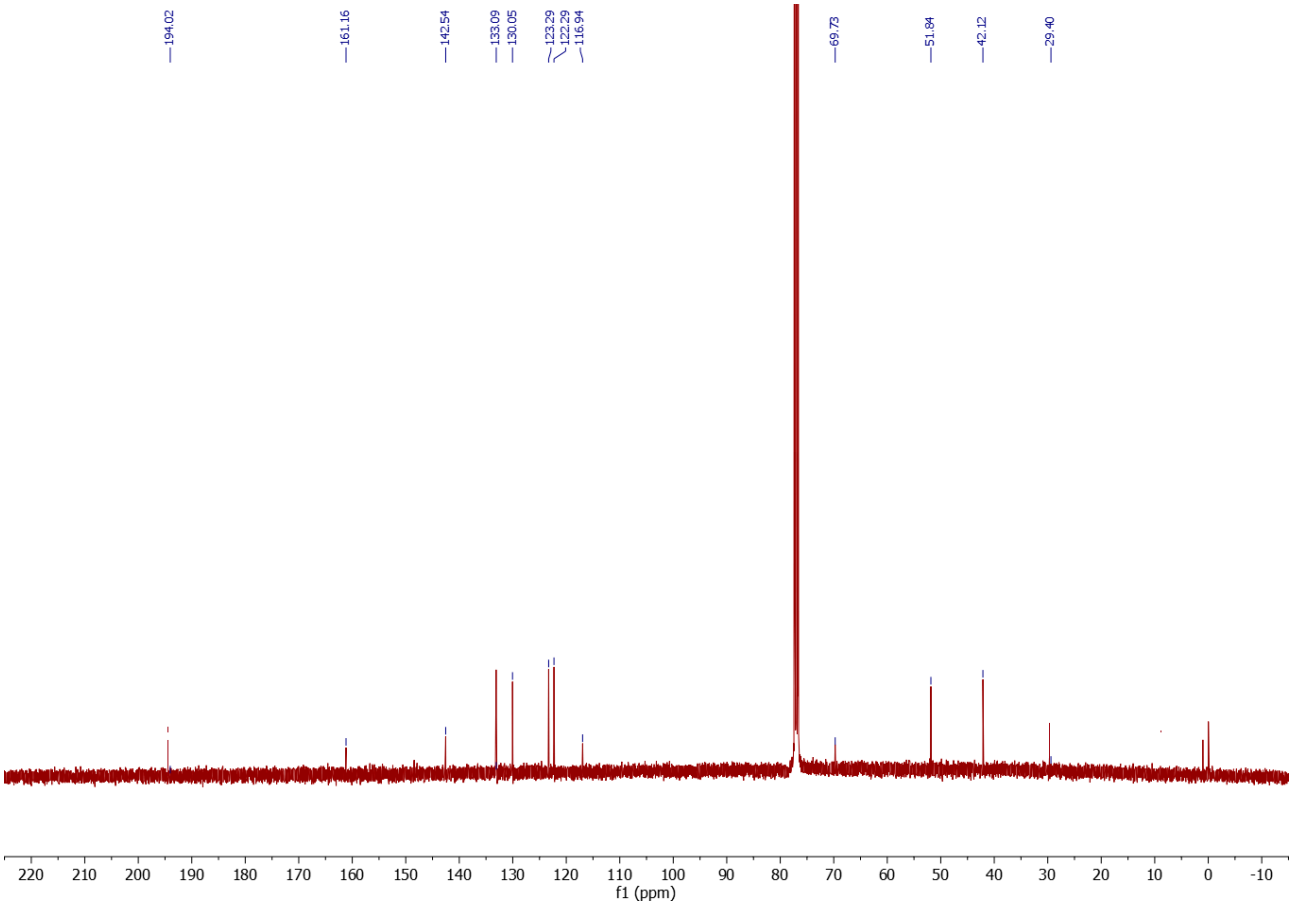




S-(3,3-dicyano-1-(3-nitrophenyl)propyl) ethanethioate 3ga





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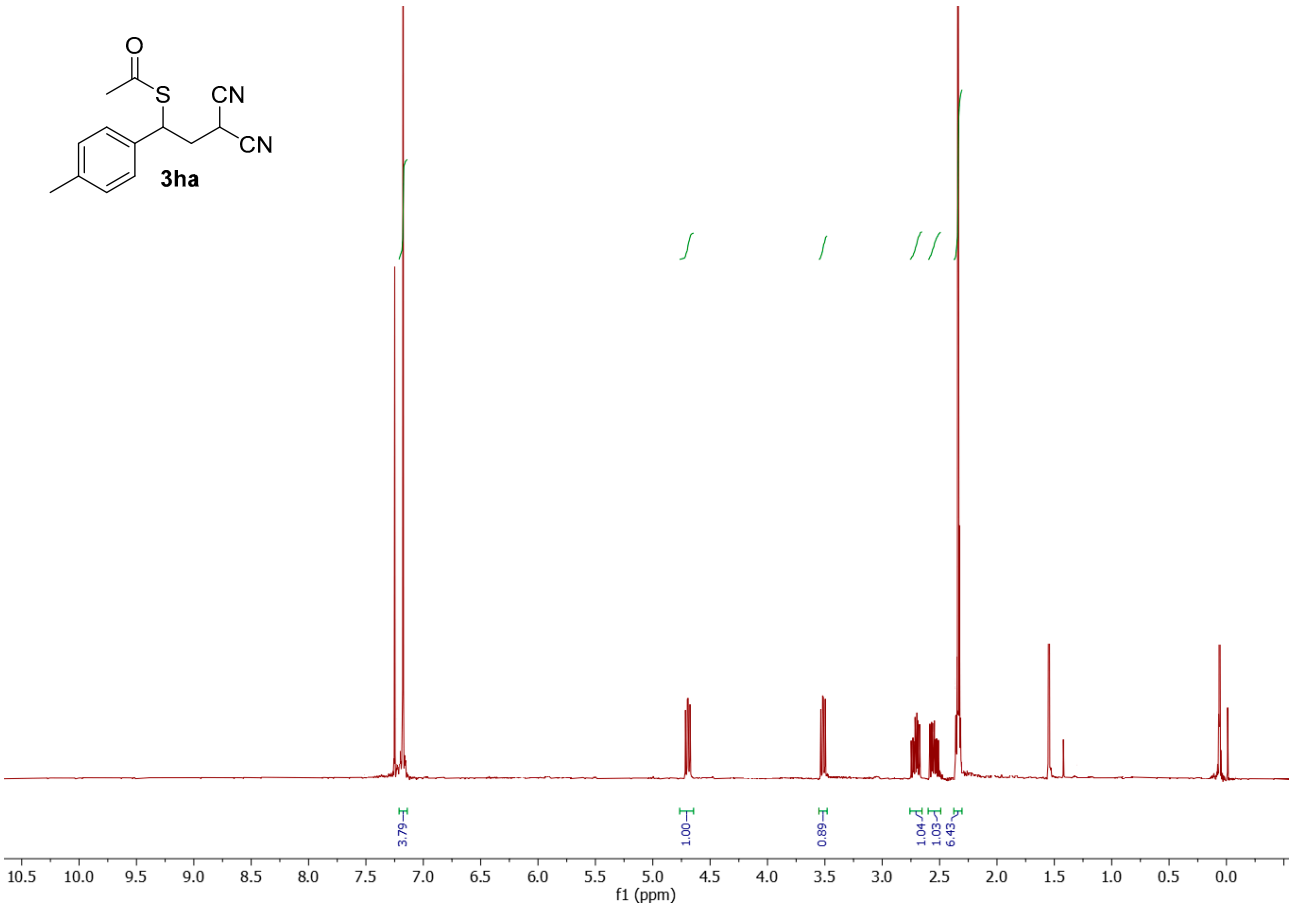

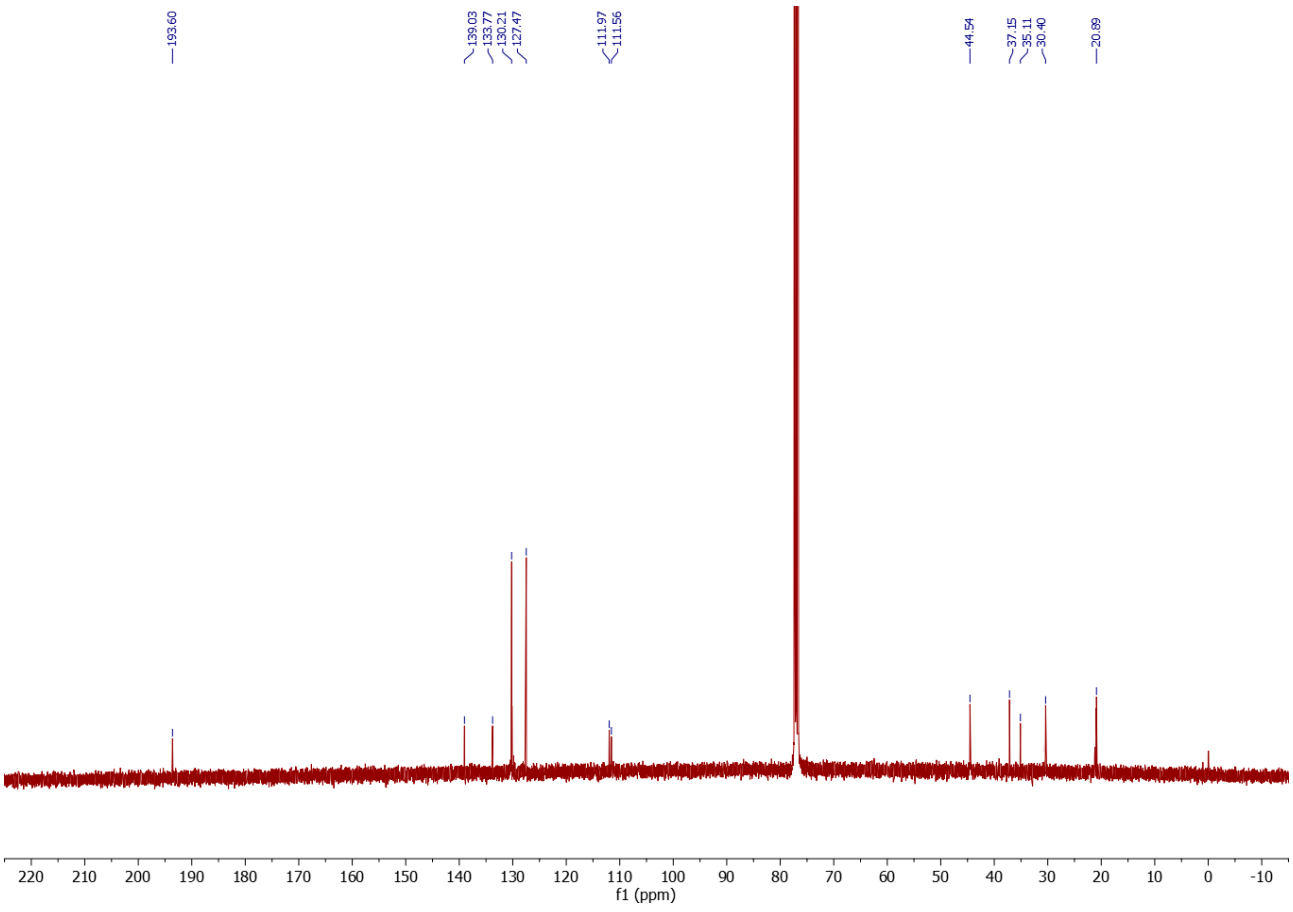

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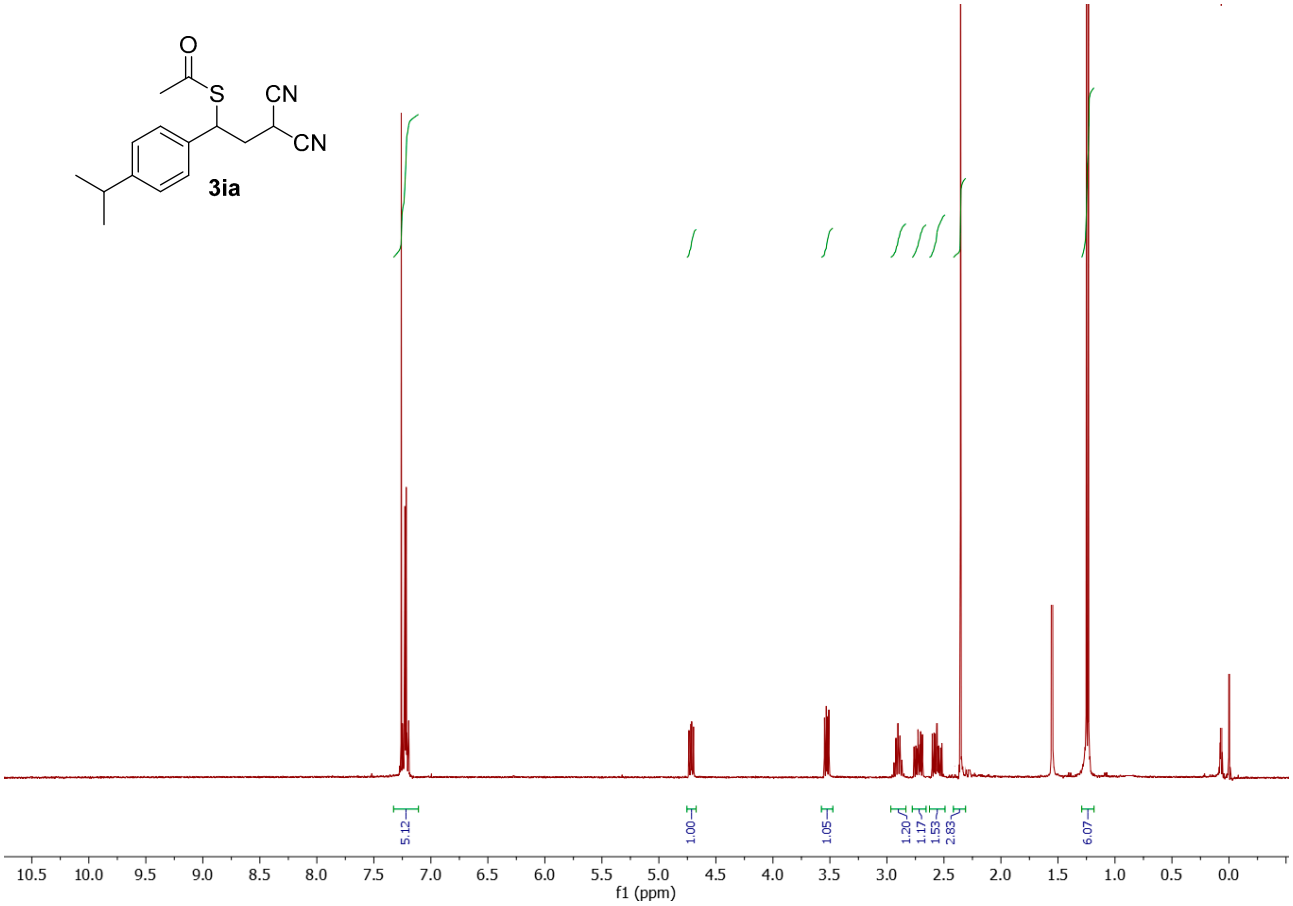

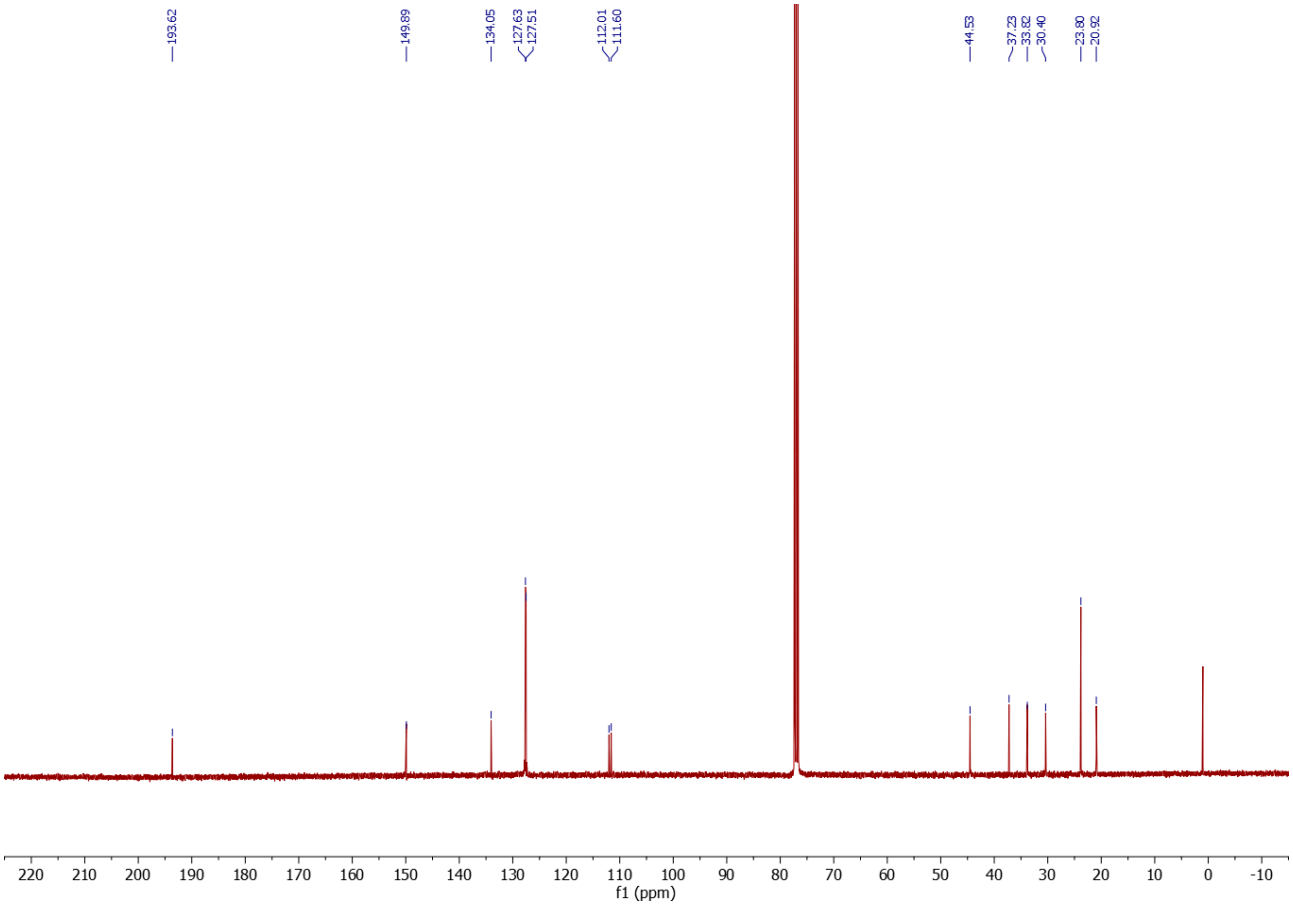

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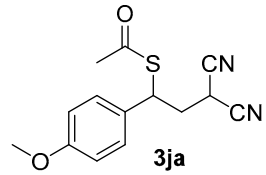
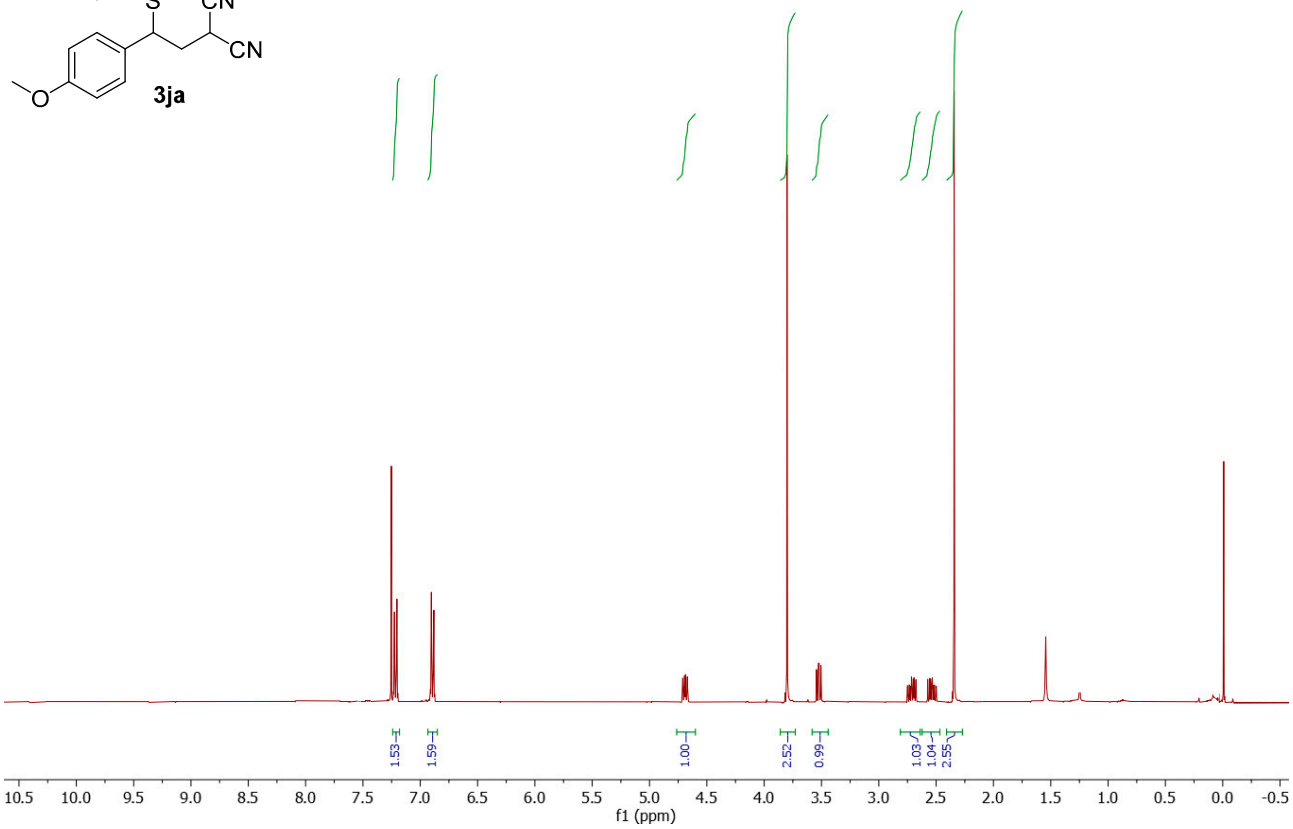
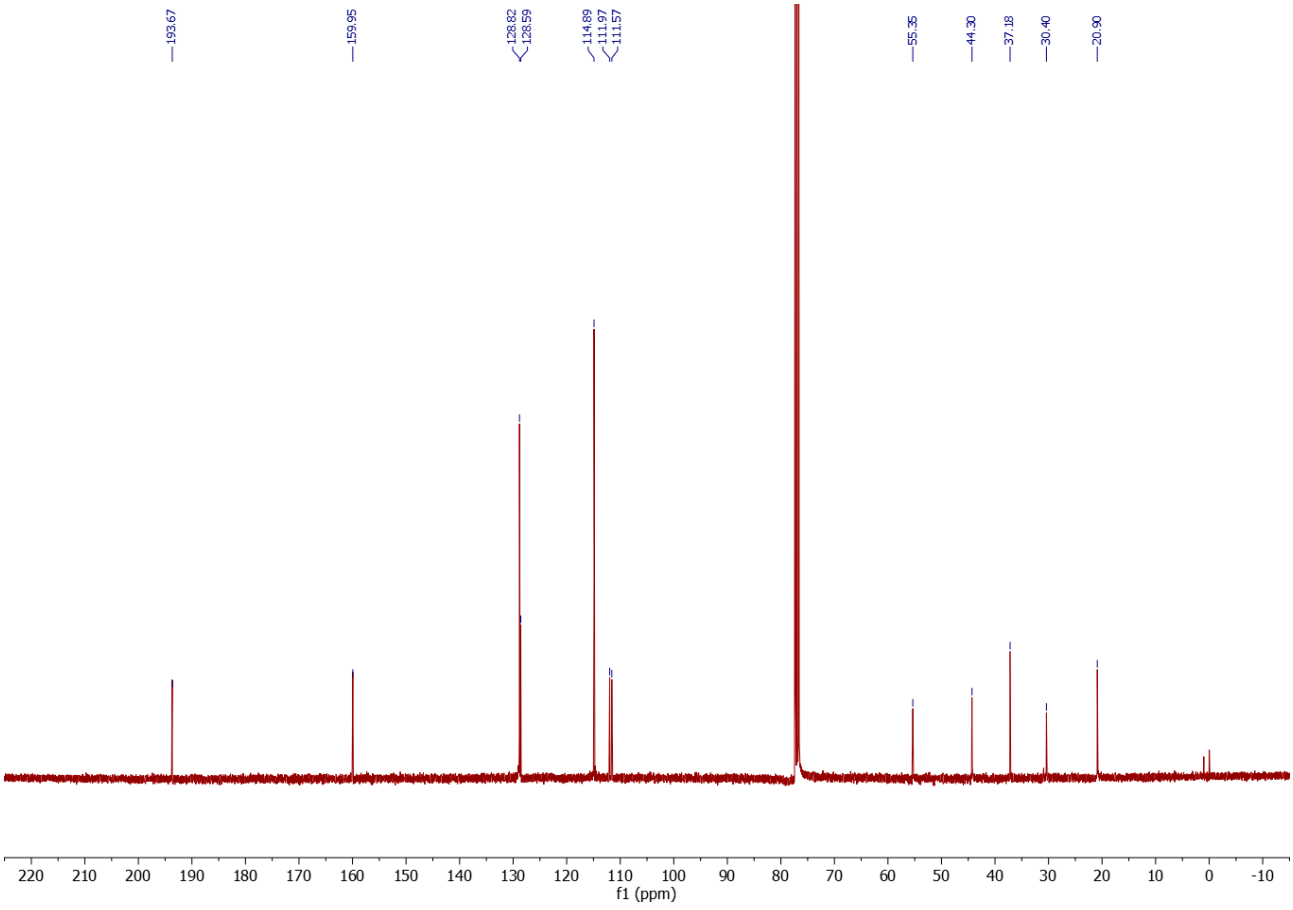
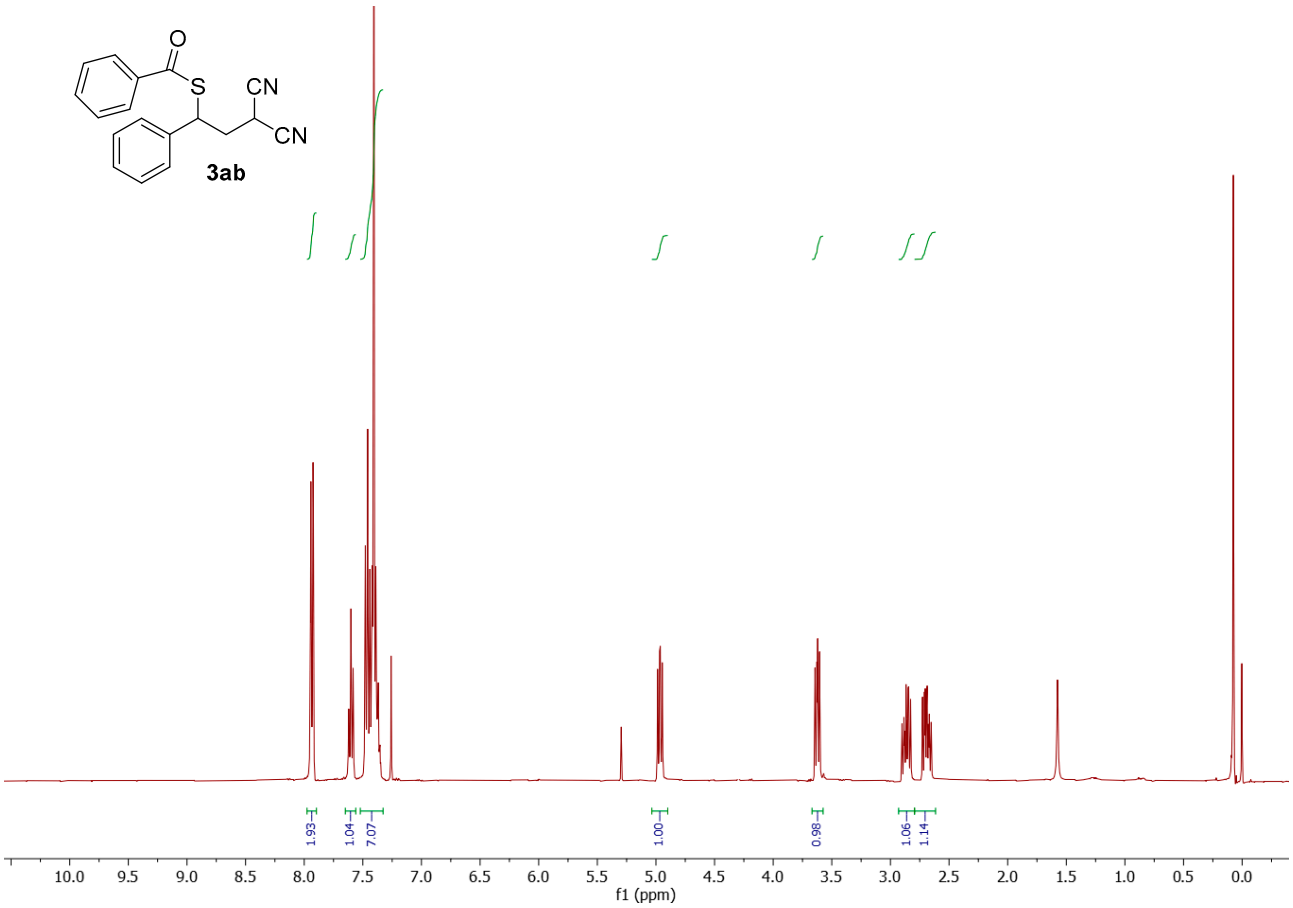
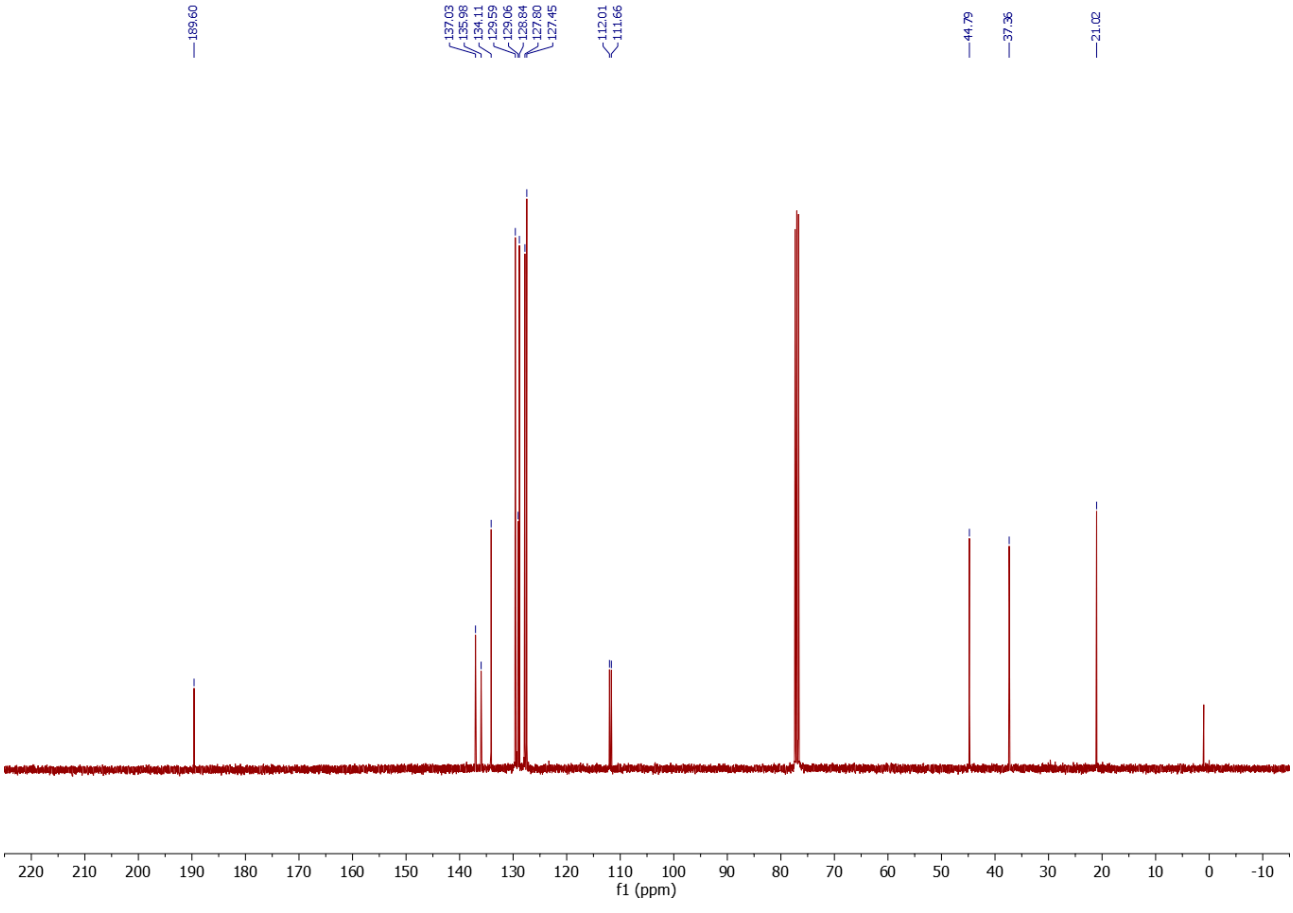






***S*-(3,3-dicyano-1-phenylpropyl) benzothioate 3ab**





S-(3,3-dicyano-1-(4-methoxyphenyl)propyl) benzothioate 3jb