

An unprecedented reactivity of D-A cyclopropane derivatives: decyanation reaction

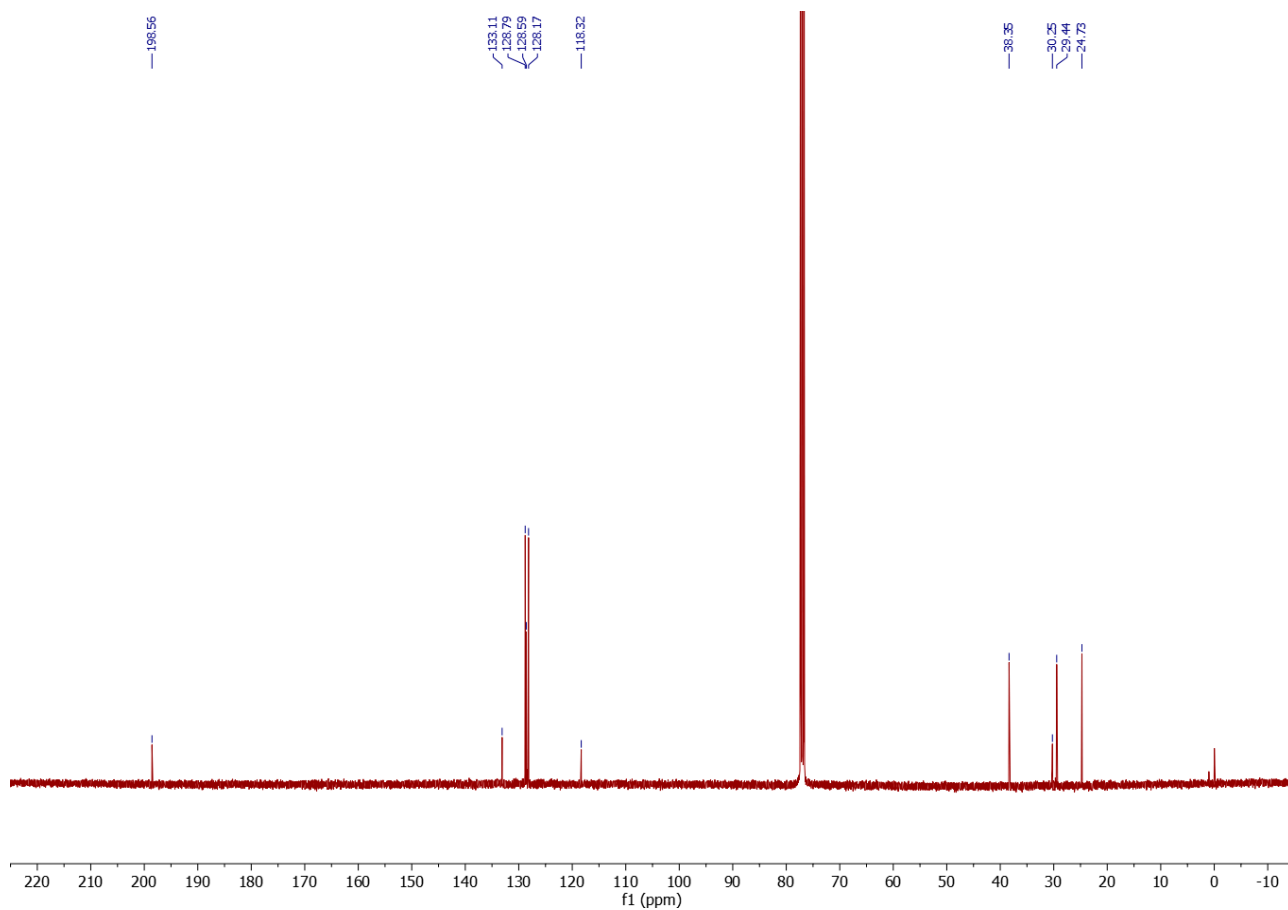
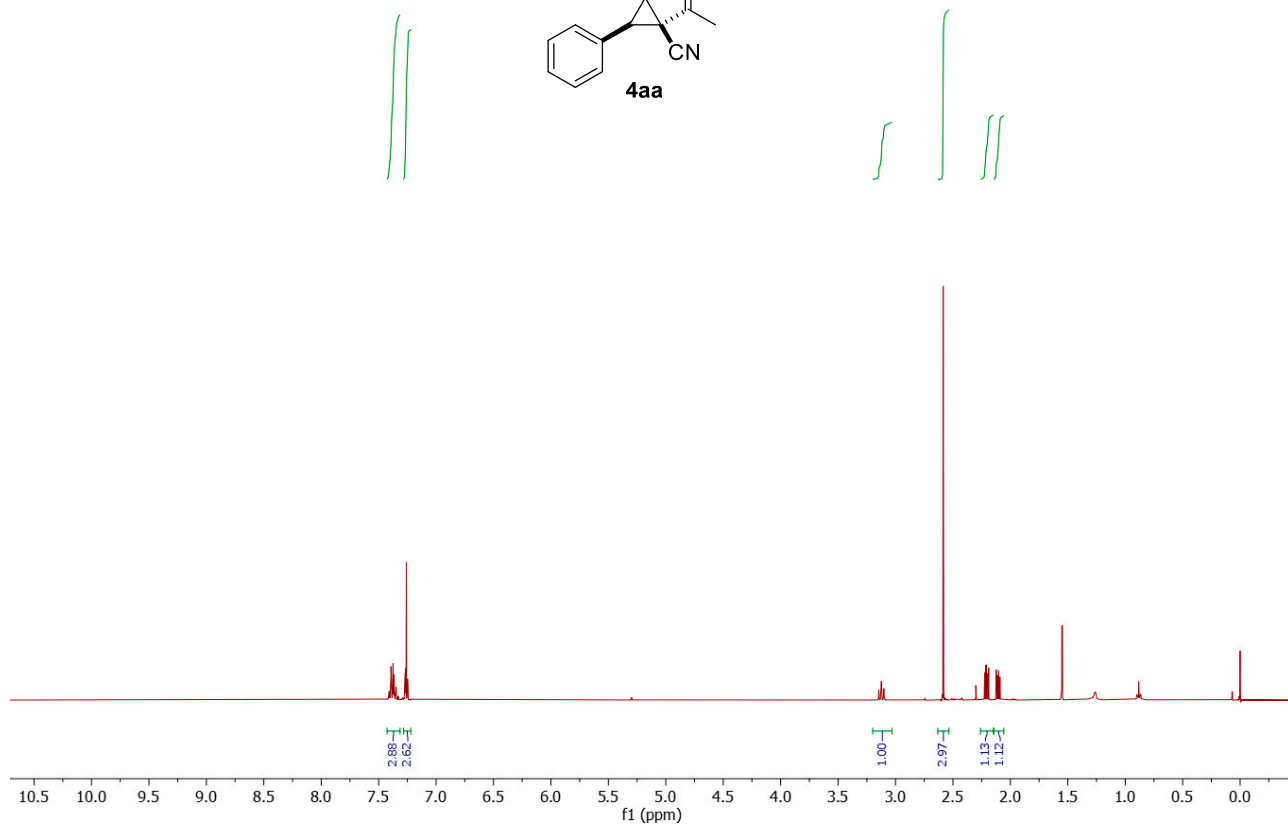
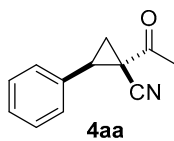
Giorgiana Denisa Bisag,¹ Pietro Viola,¹ Luca Bernardi,^{1,*} Mariafrancesca Fochi^{1,*}

Supporting information

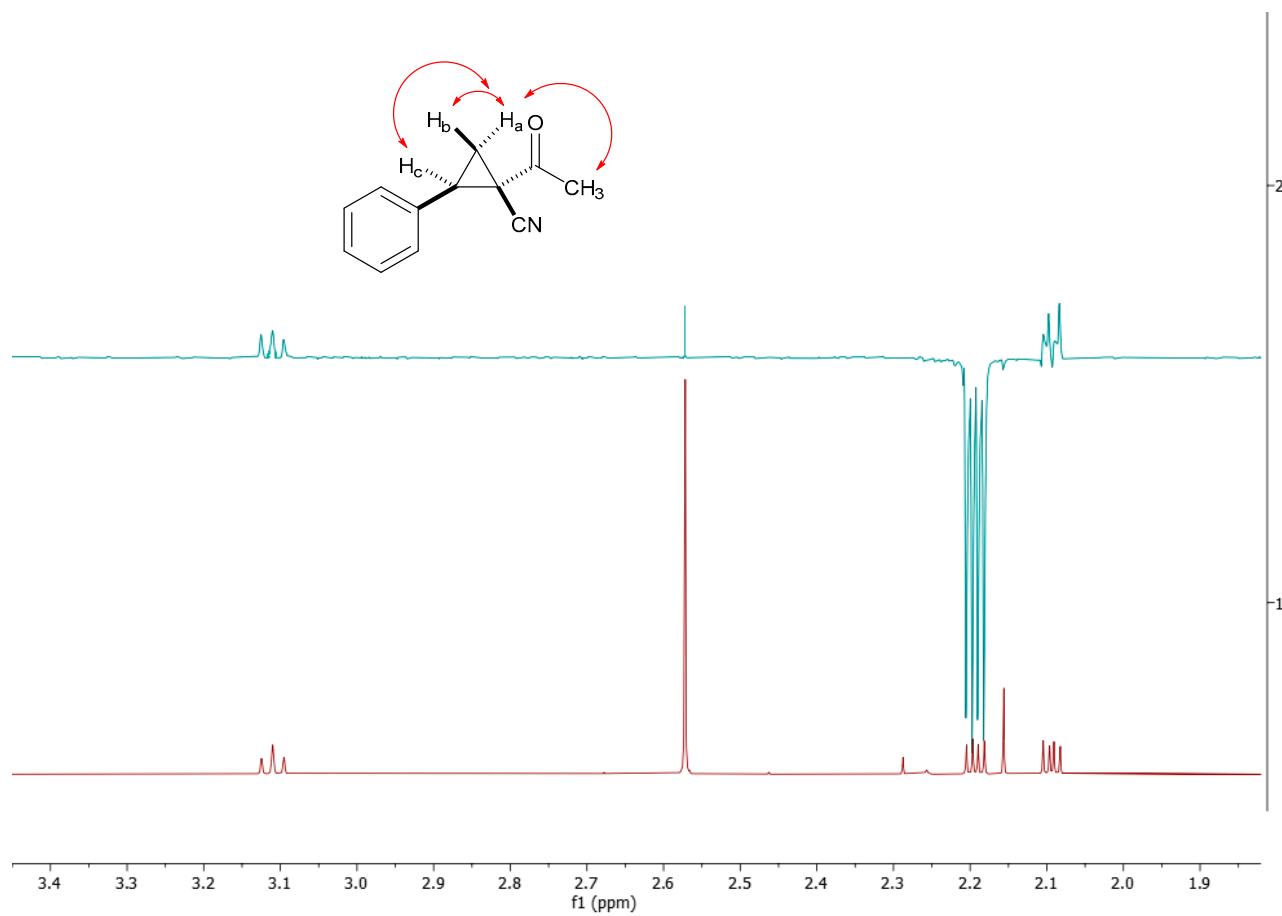
Selected NMR spectra

1-acetyl-2-phenylcyclopropane-1-carbonitrile 4aa (¹ H, ¹³ C, Cosy, HSQC, NOE)	S1
1-acetyl-2-(4-bromophenyl)cyclopropane-1-carbonitrile 4ba (¹ H, ¹³ C)	S6
1-acetyl-2-(2-bromophenyl)cyclopropane-1-carbonitrile 4ca (¹ H, ¹³ C)	S7
1-acetyl-2-(3-chlorophenyl)cyclopropane-1-carbonitrile 4da (¹ H, ¹³ C)	S8
1-acetyl-2-(2-chlorophenyl)cyclopropane-1-carbonitrile 4ea (¹ H, ¹³ C)	S9
1-acetyl-2-(4-chlorophenyl)cyclopropane-1-carbonitrile 4fa (¹ H, ¹³ C)	S10
1-acetyl-2-(3-nitrophenyl)cyclopropane-1-carbonitrile 4ga (¹ H, ¹³ C)	S11
1-acetyl-2-(p-tolyl)cyclopropane-1-carbonitrile 4ha (¹ H, ¹³ C)	S12
1-acetyl-2-(4-isopropylphenyl)cyclopropane-1-carbonitrile 4ia (¹ H, ¹³ C)	S13
1-acetyl-2-(4-methoxyphenyl)cyclopropane-1-carbonitrile 4ja (¹ H, ¹³ C)	S14
1-acetyl-2-(naphthalen-2-yl)cyclopropane-1-carbonitrile 4ka (¹ H, ¹³ C)	S15
S-(3,3-dicyano-1-phenylpropyl) ethanethioate 3aa (¹ H, ¹³ C)	S16
S-(1-(4-bromophenyl)-3,3-dicyanopropyl) ethanethioate 3ba (¹ H, ¹³ C)	S17
S-(1-(3-chlorophenyl)-3,3-dicyanopropyl) ethanethioate 3da (¹ H, ¹³ C)	S18
S-(1-(4-chlorophenyl)-3,3-dicyanopropyl) ethanethioate 3fa (¹ H, ¹³ C)	S19
S-(3,3-dicyano-1-(3-nitrophenyl)propyl) ethanethioate 3ga (¹ H, ¹³ C)	S20
S-(3,3-dicyano-1-(p-tolyl)propyl) ethanethioate 3ha (¹ H, ¹³ C)	S21
S-(3,3-dicyano-1-(4-isopropylphenyl)propyl) ethanethioate 3ia (¹ H, ¹³ C)	S22
S-(3,3-dicyano-1-(4-methoxyphenyl)propyl) ethanethioate 3ja (¹ H, ¹³ C)	S23
S-(3,3-dicyano-1-phenylpropyl) benzothioate 3ab (¹ H, ¹³ C)	S24
S-(3,3-dicyano-1-(4-methoxyphenyl)propyl) benzothioate 3jb (¹ H, ¹³ C)	S25

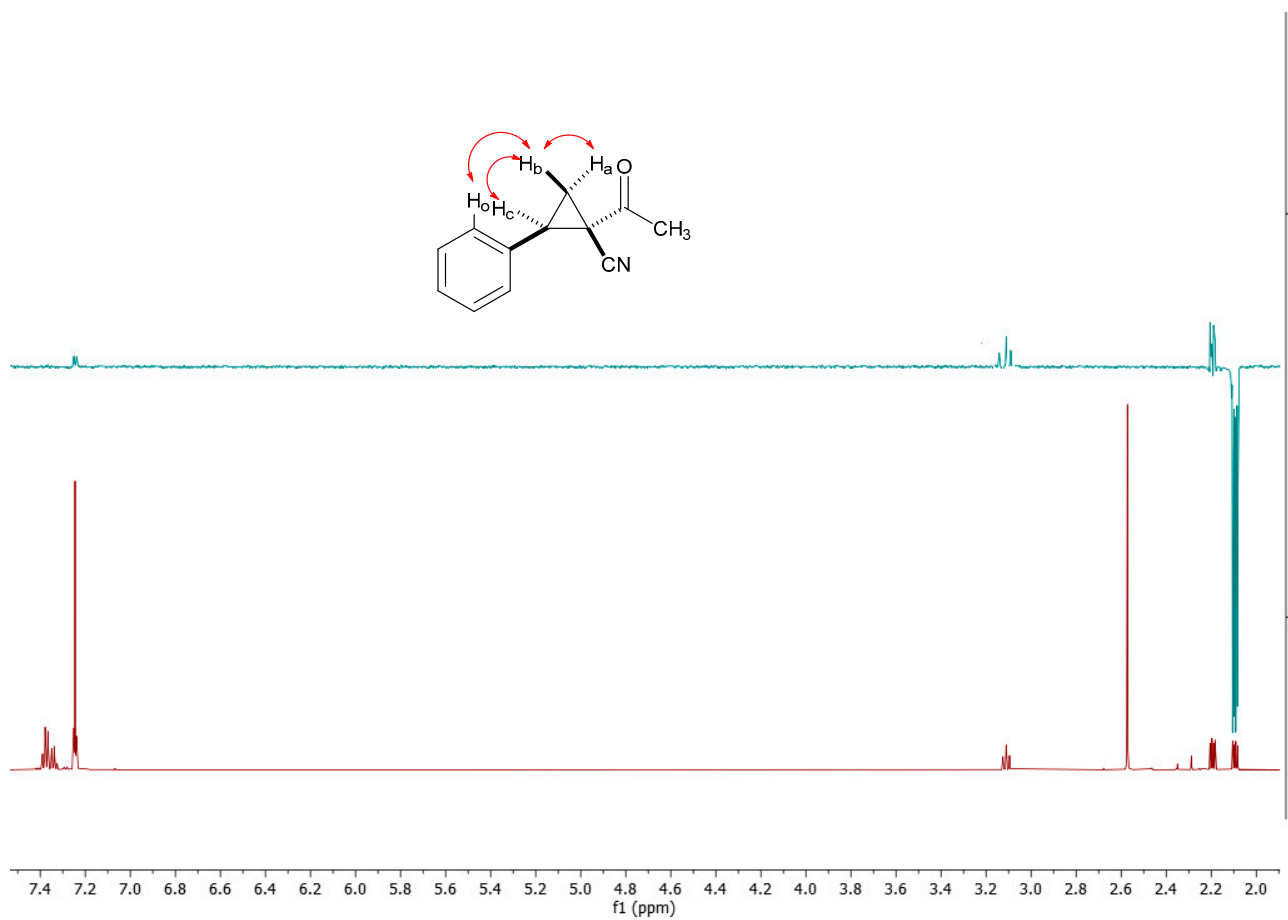
1-acetyl-2-phenylcyclopropane-1-carbonitrile 4aa



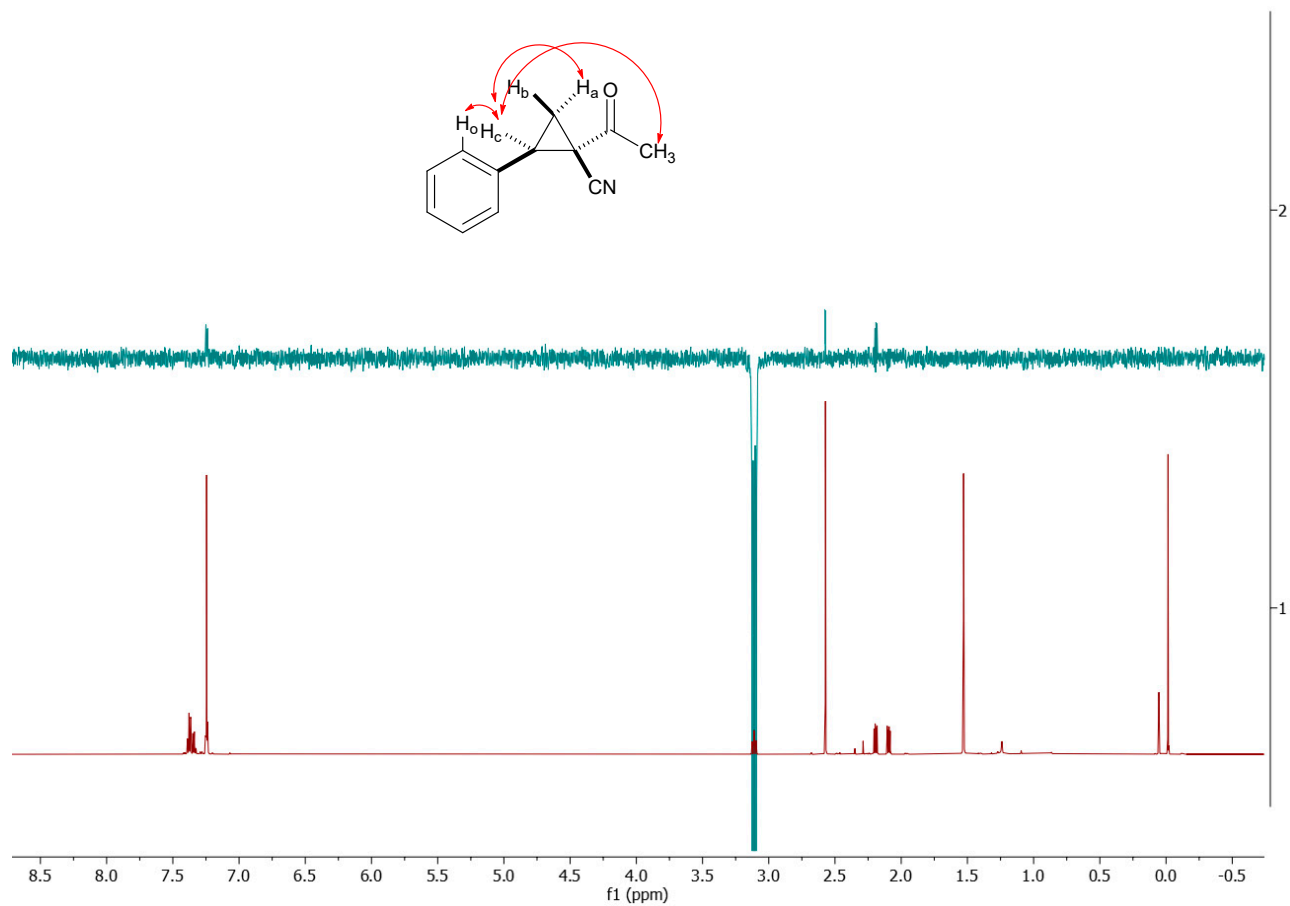
Irradiation of the H_a at 2.21 ppm gave NOE effect on the signal at 2.58 ppm assigned to CH₃, on the signal at 2.11 assigned to H_b and on the signal at 3.12 ppm assigned to H_c.



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.

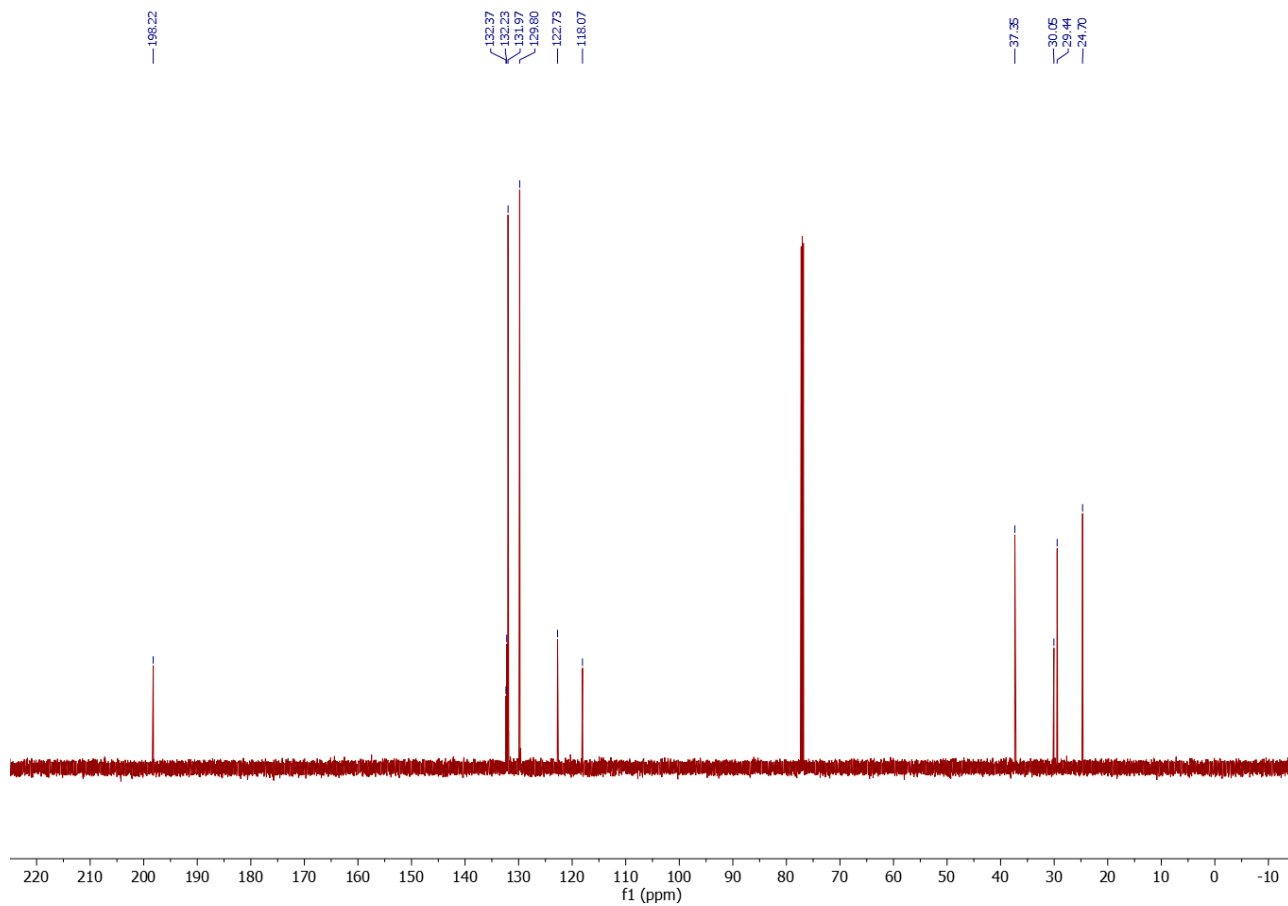
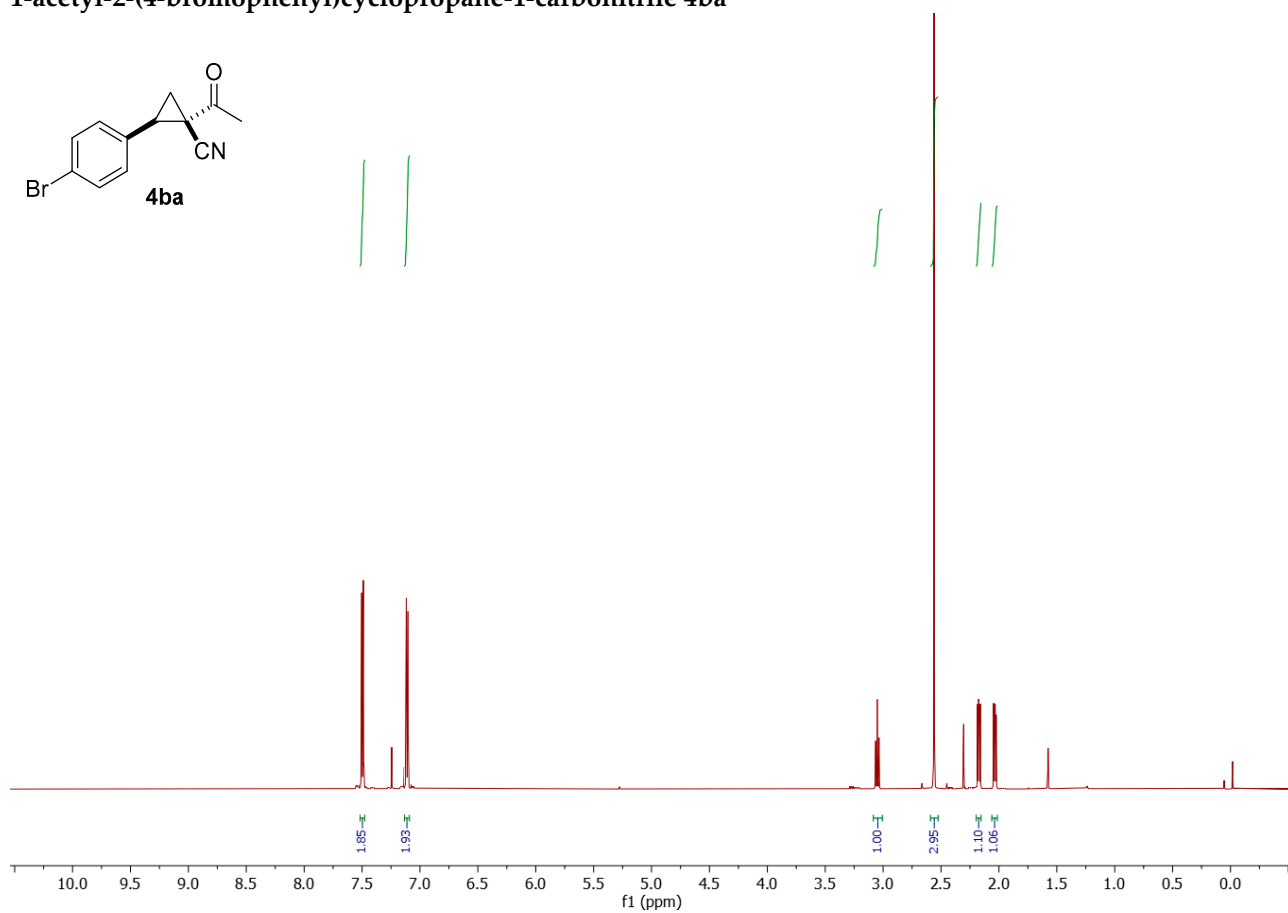
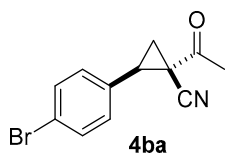


Irradiation of the H_c at 3.12 ppm gave NOE effect on the signal at 2.58 ppm assigned to CH₃, on the signal at 2.21 assigned to H_a and on the signal at 7.20 ppm of the *ortho*-aromatic protons.

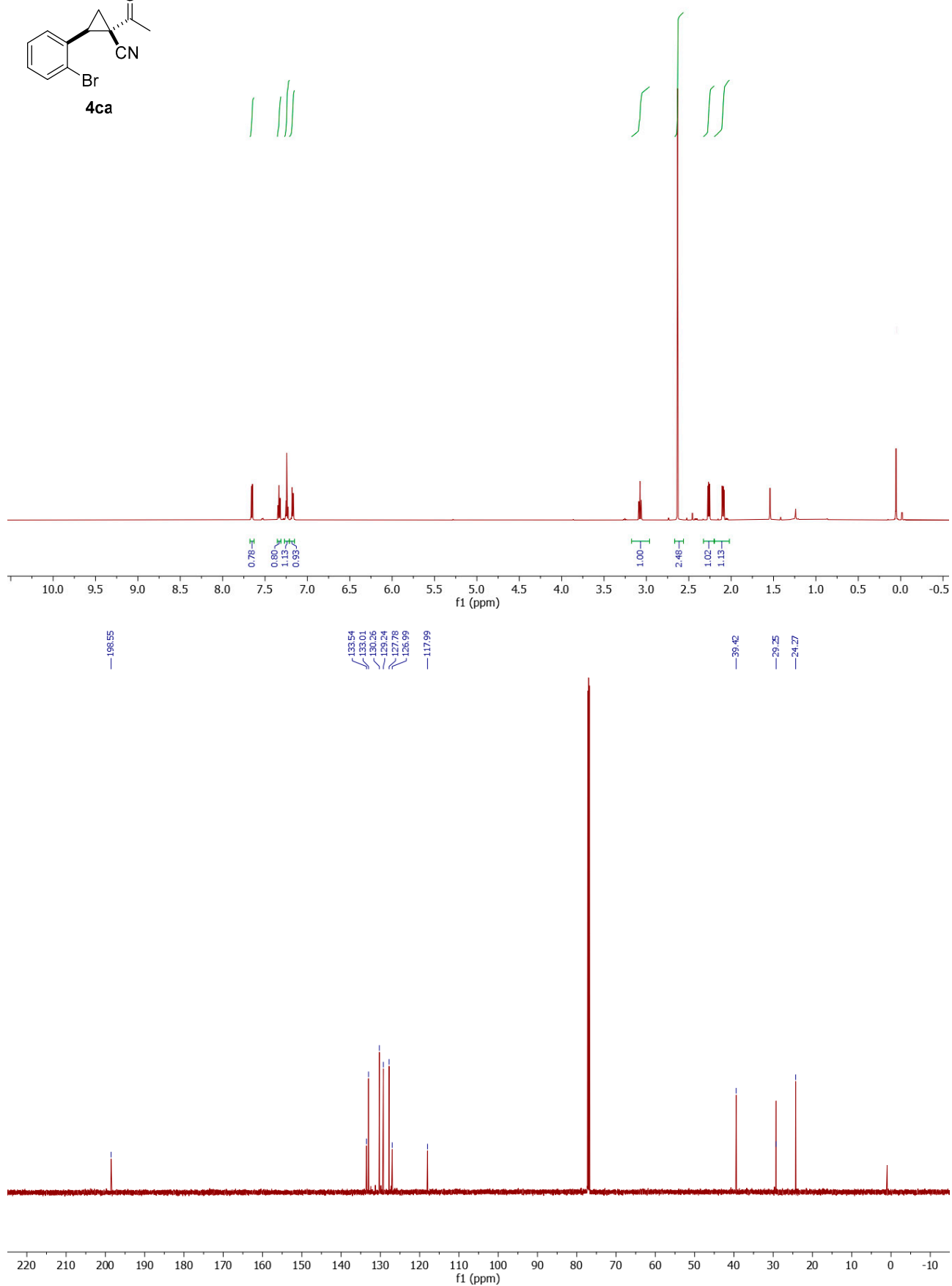
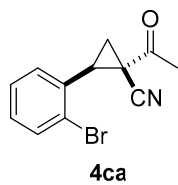


These results indicate a *cis*-relationship between H_c and CH₃ and thus, ultimately, a *trans* configuration of product **4aa**.

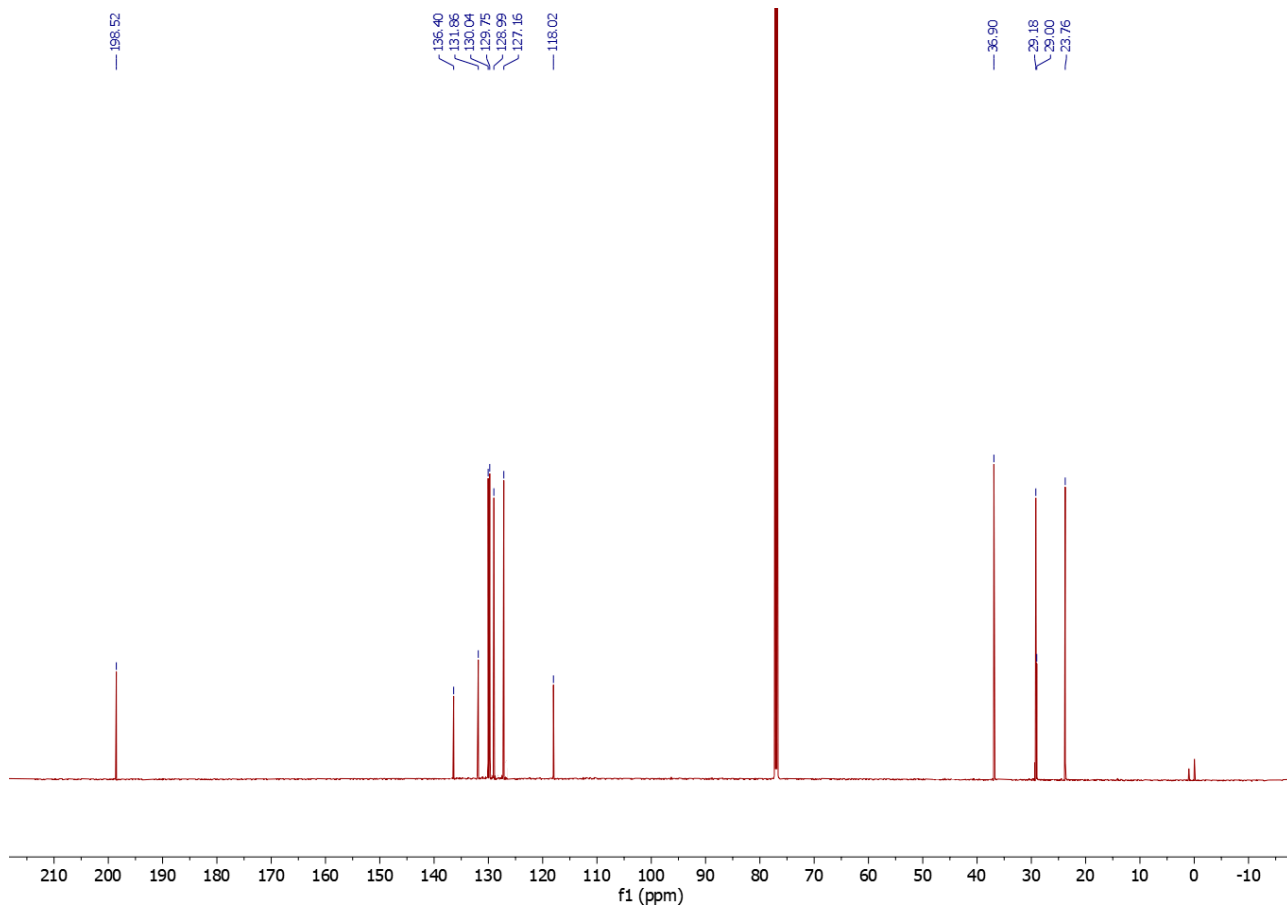
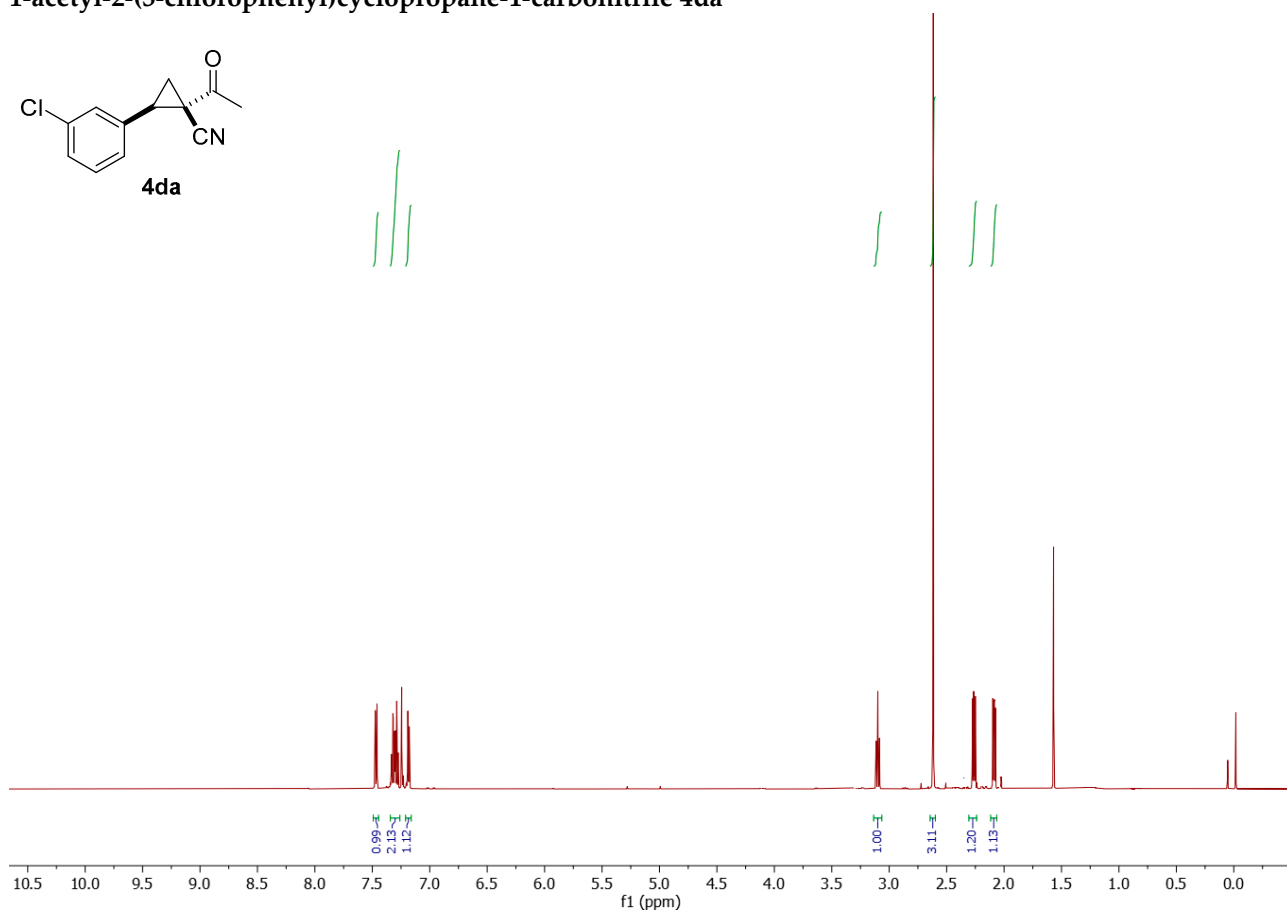
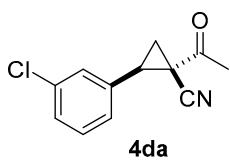
1-acetyl-2-(4-bromophenyl)cyclopropane-1-carbonitrile 4ba



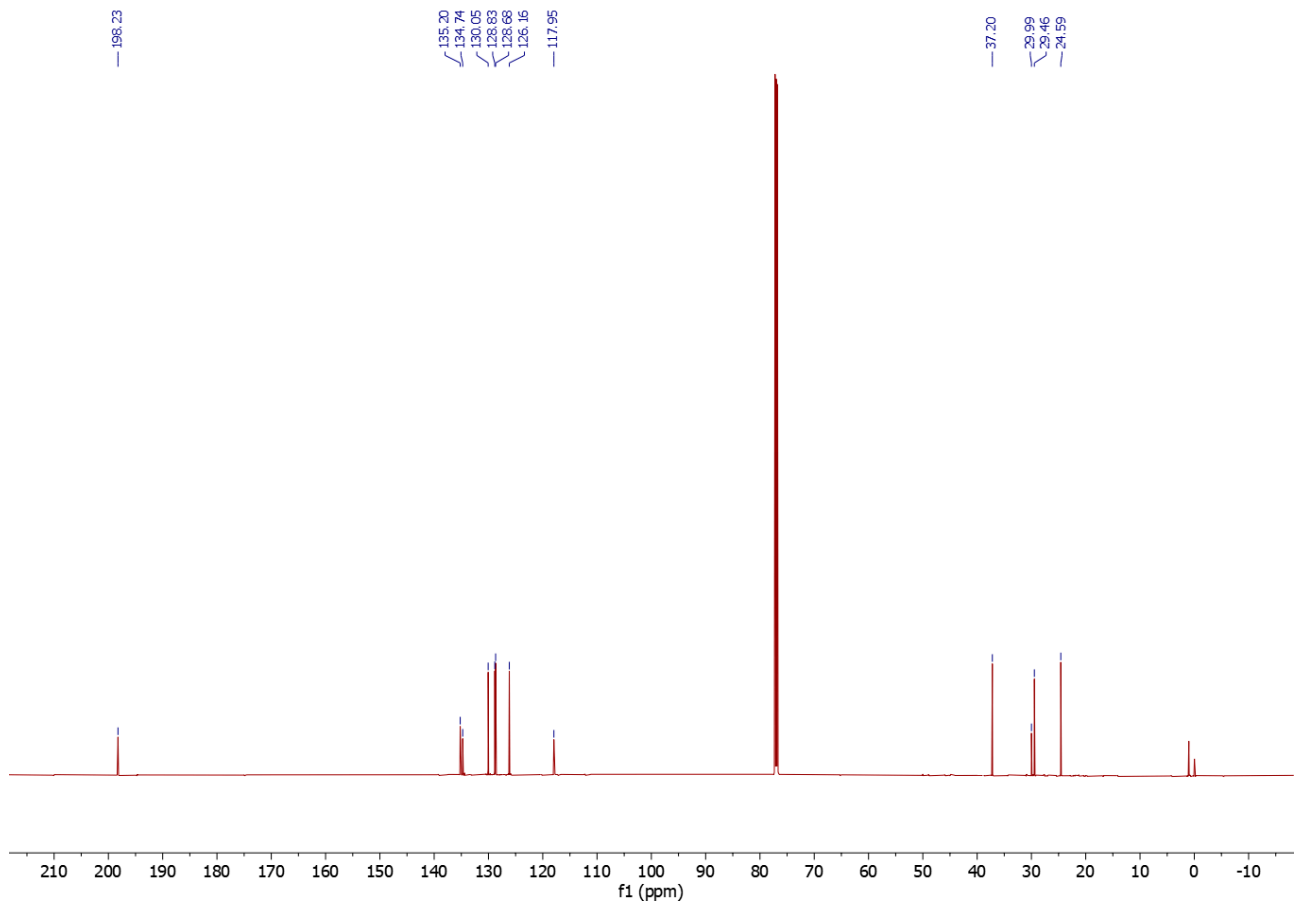
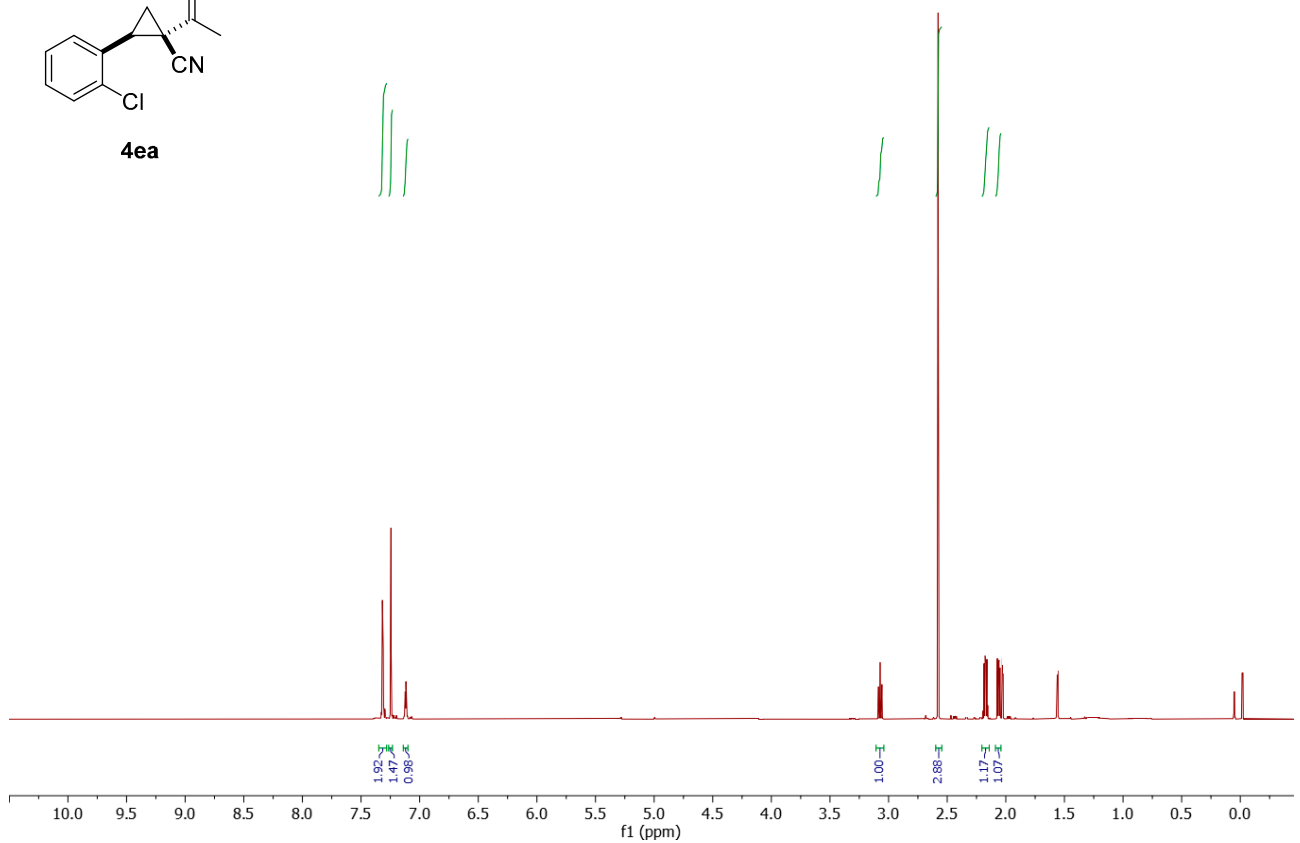
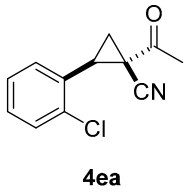
1-acetyl-2-(2-bromophenyl)cyclopropane-1-carbonitrile 4ca



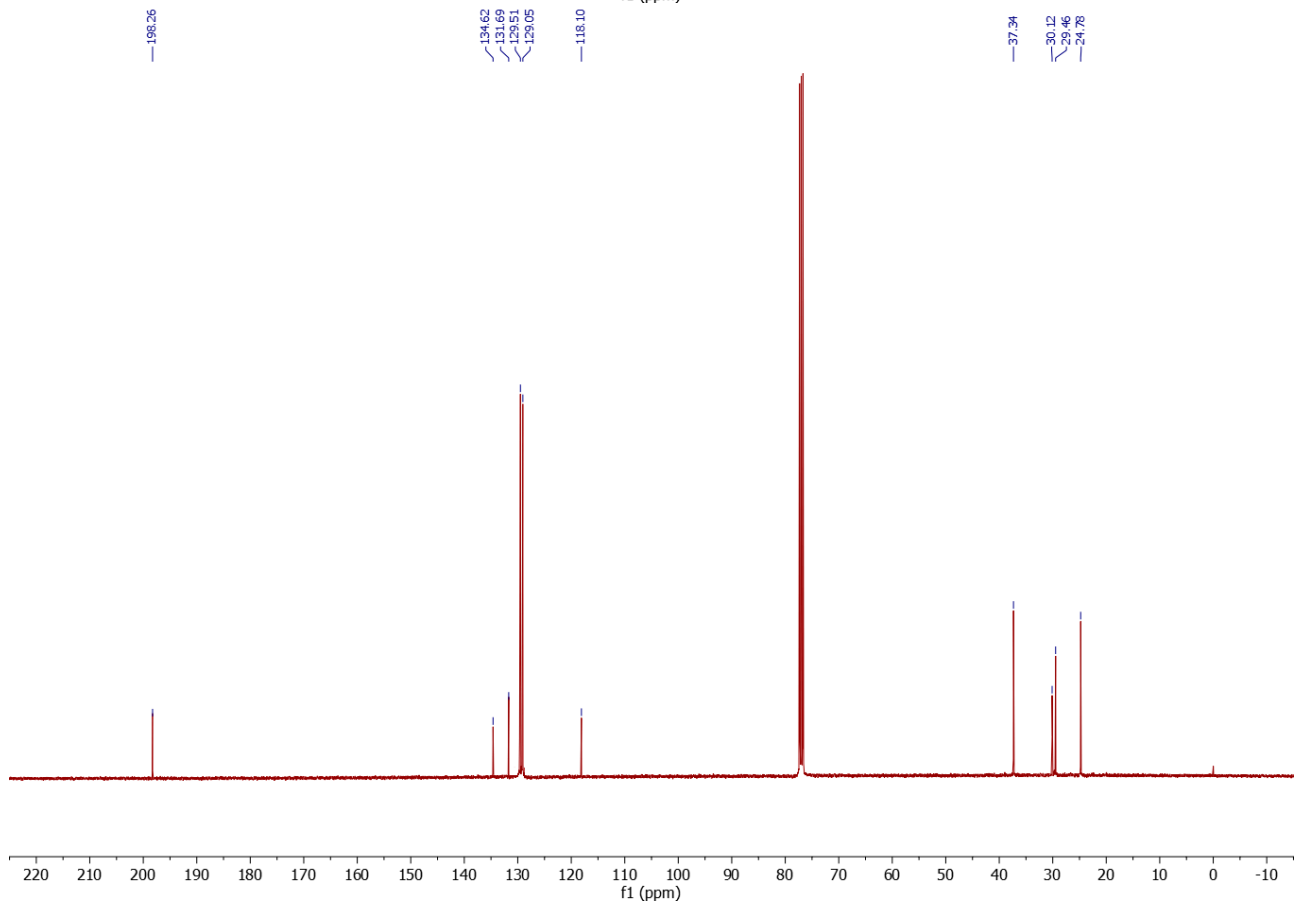
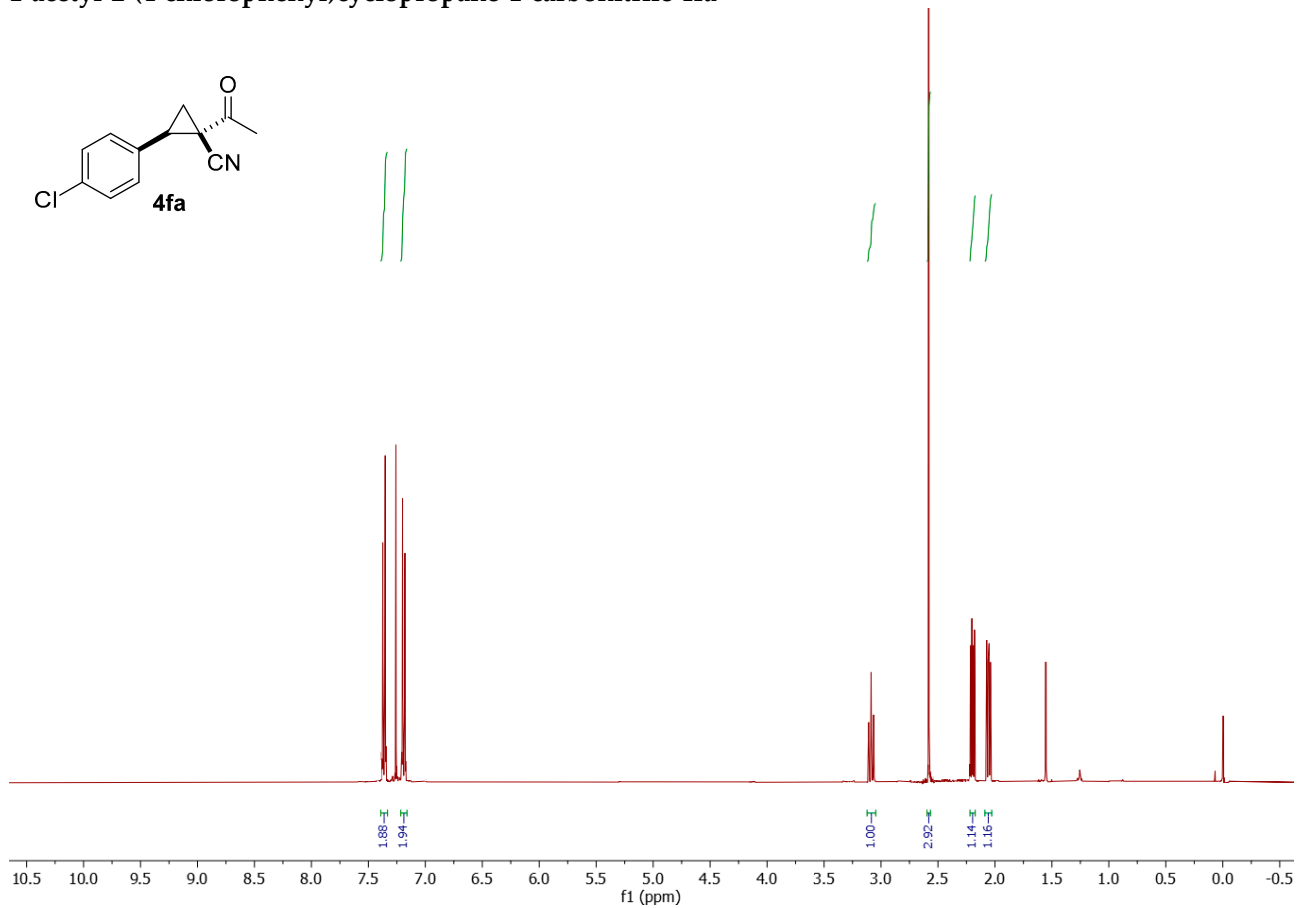
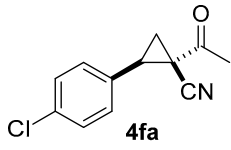
1-acetyl-2-(3-chlorophenyl)cyclopropane-1-carbonitrile 4da



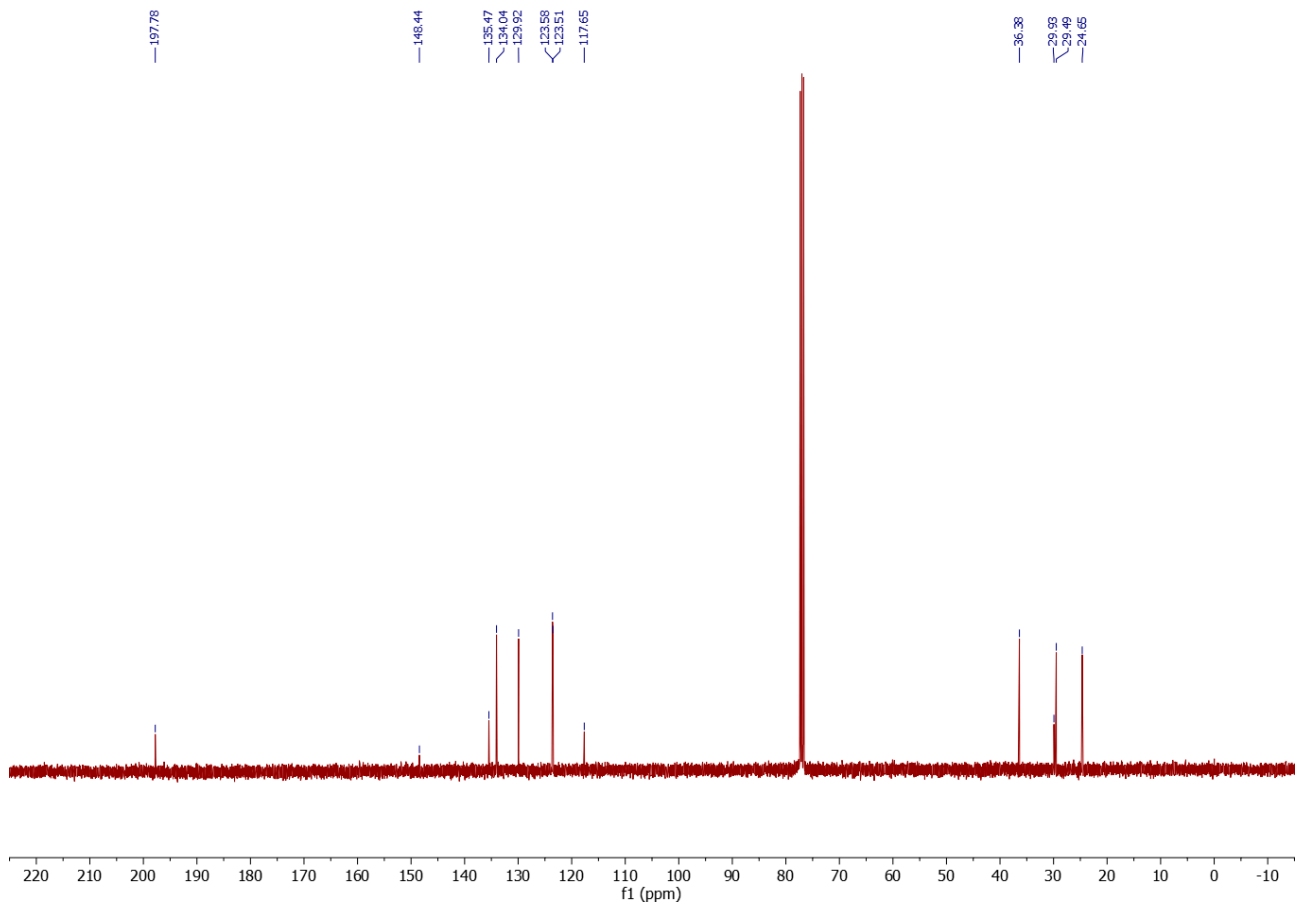
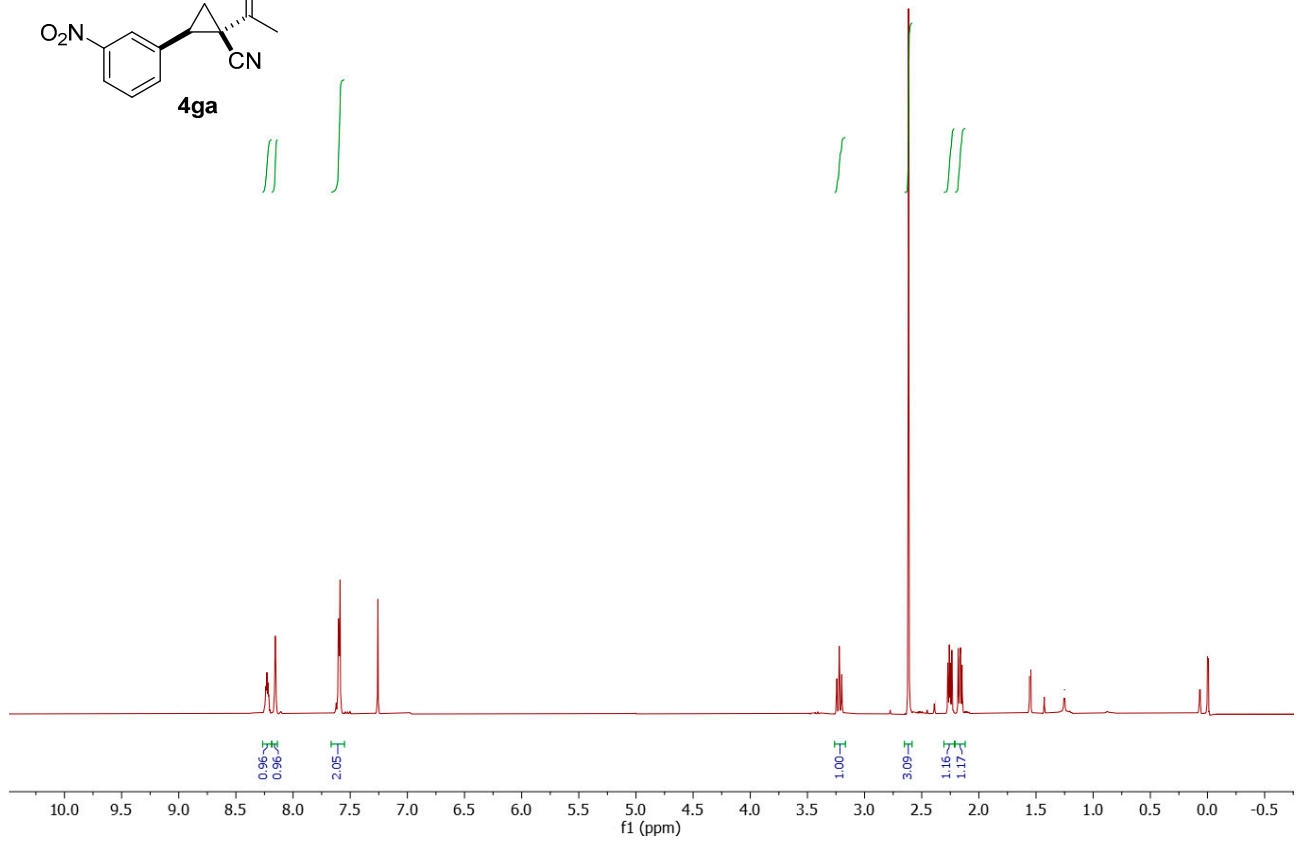
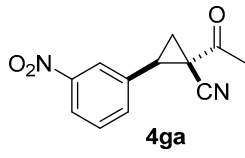
1-acetyl-2-(2-chlorophenyl)cyclopropane-1-carbonitrile 4ea



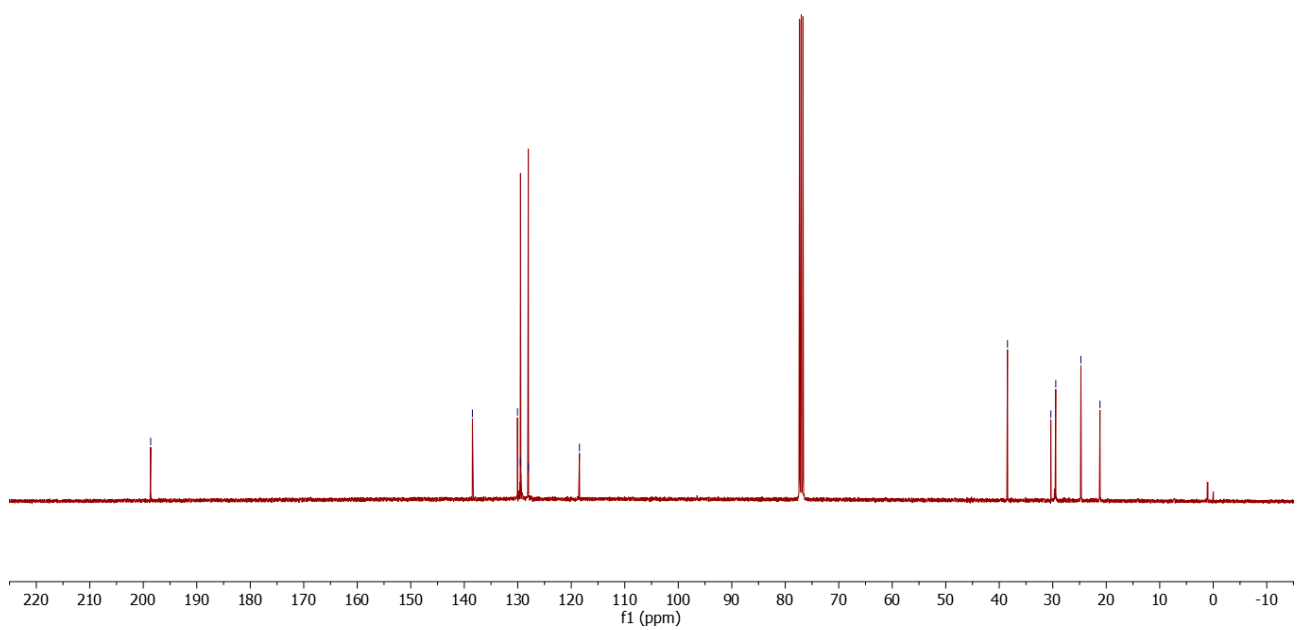
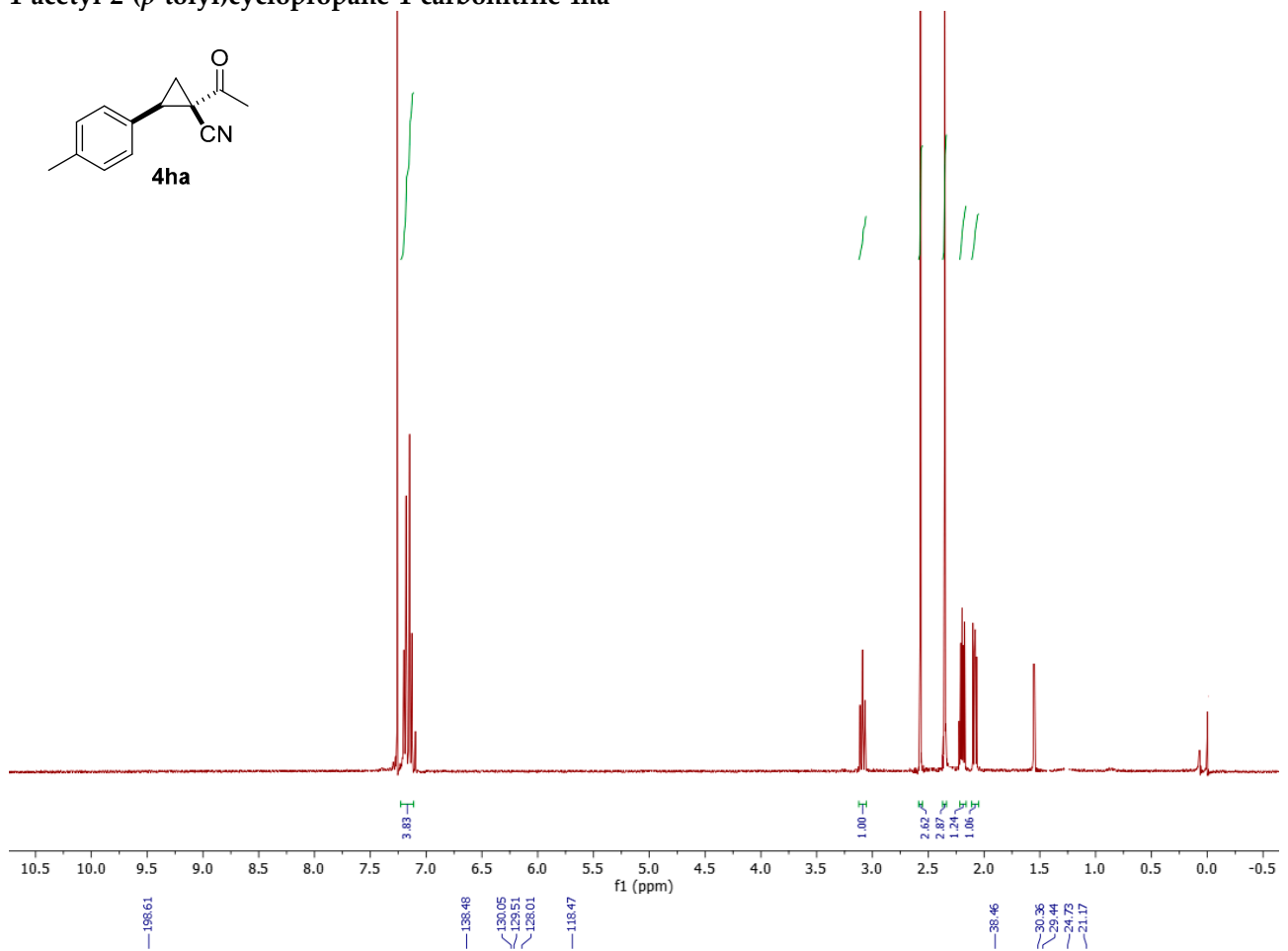
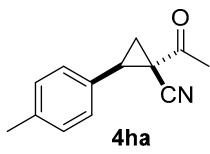
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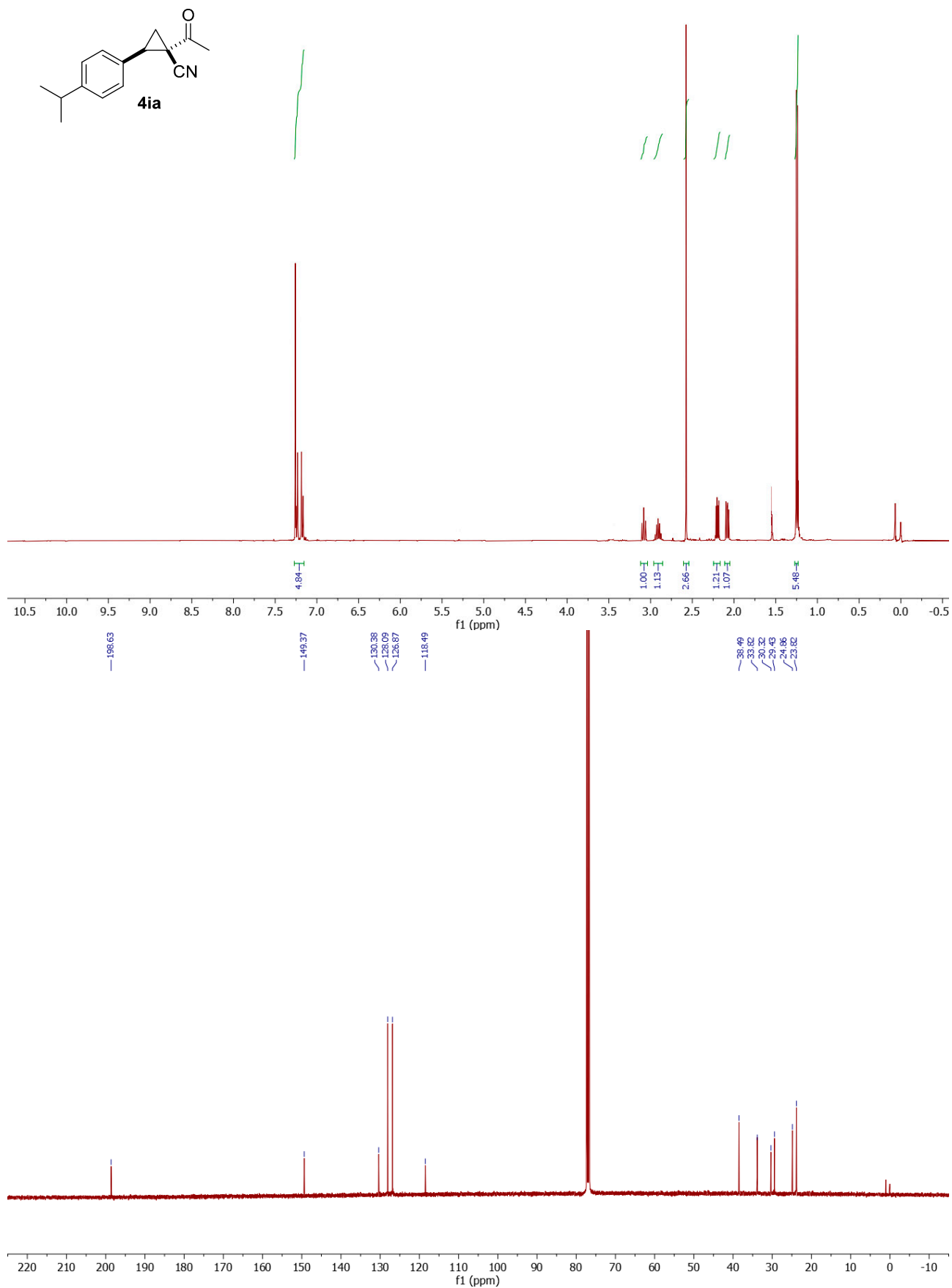
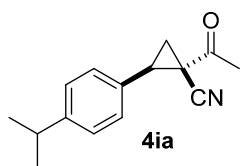
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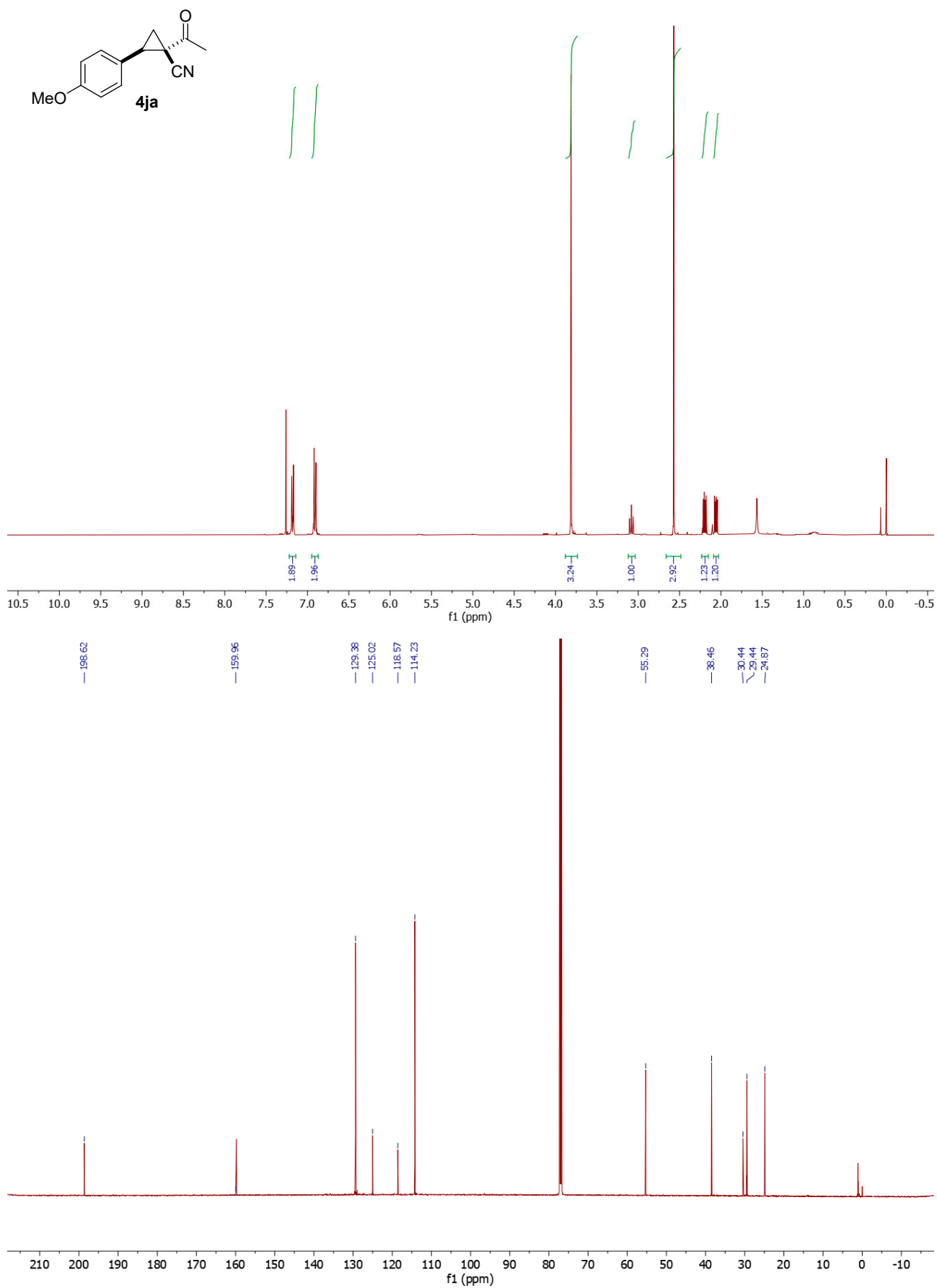
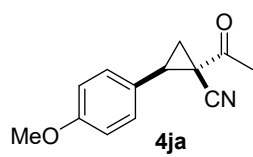
1-acetyl-2-(*p*-tolyl)cyclopropane-1-carbonitrile 4ha



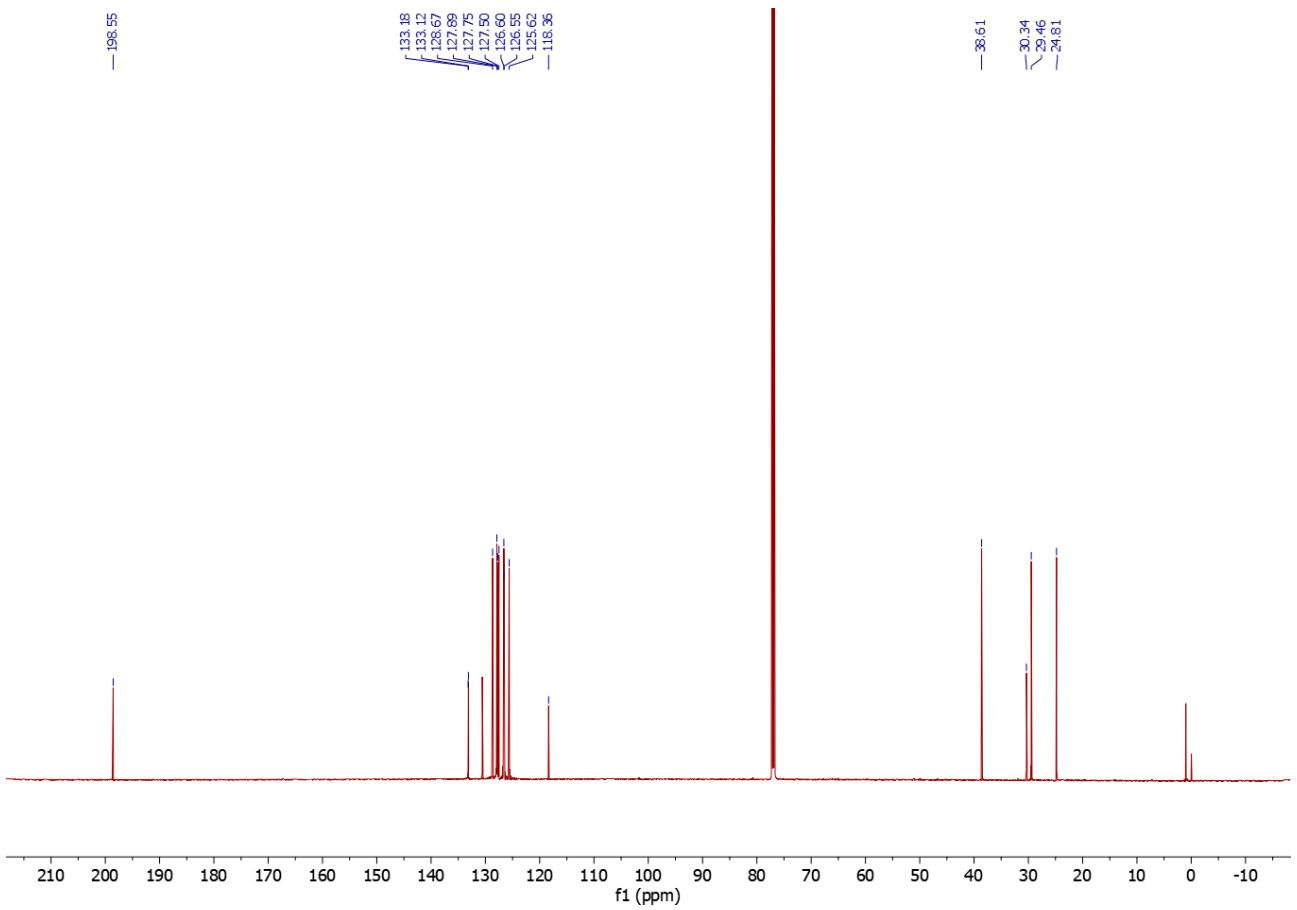
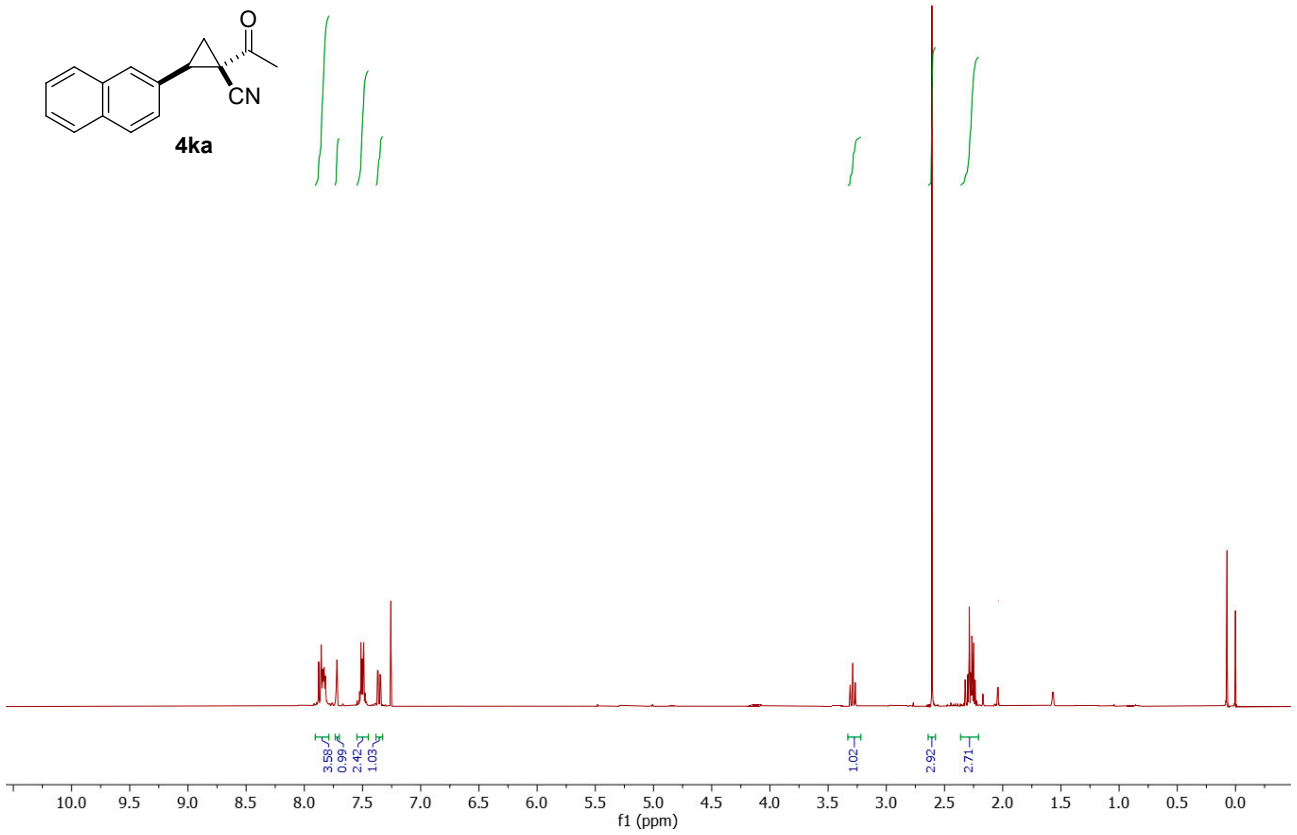
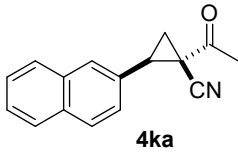
1-acetyl-2-(4-isopropylphenyl)cyclopropane-1-carbonitrile 4ia



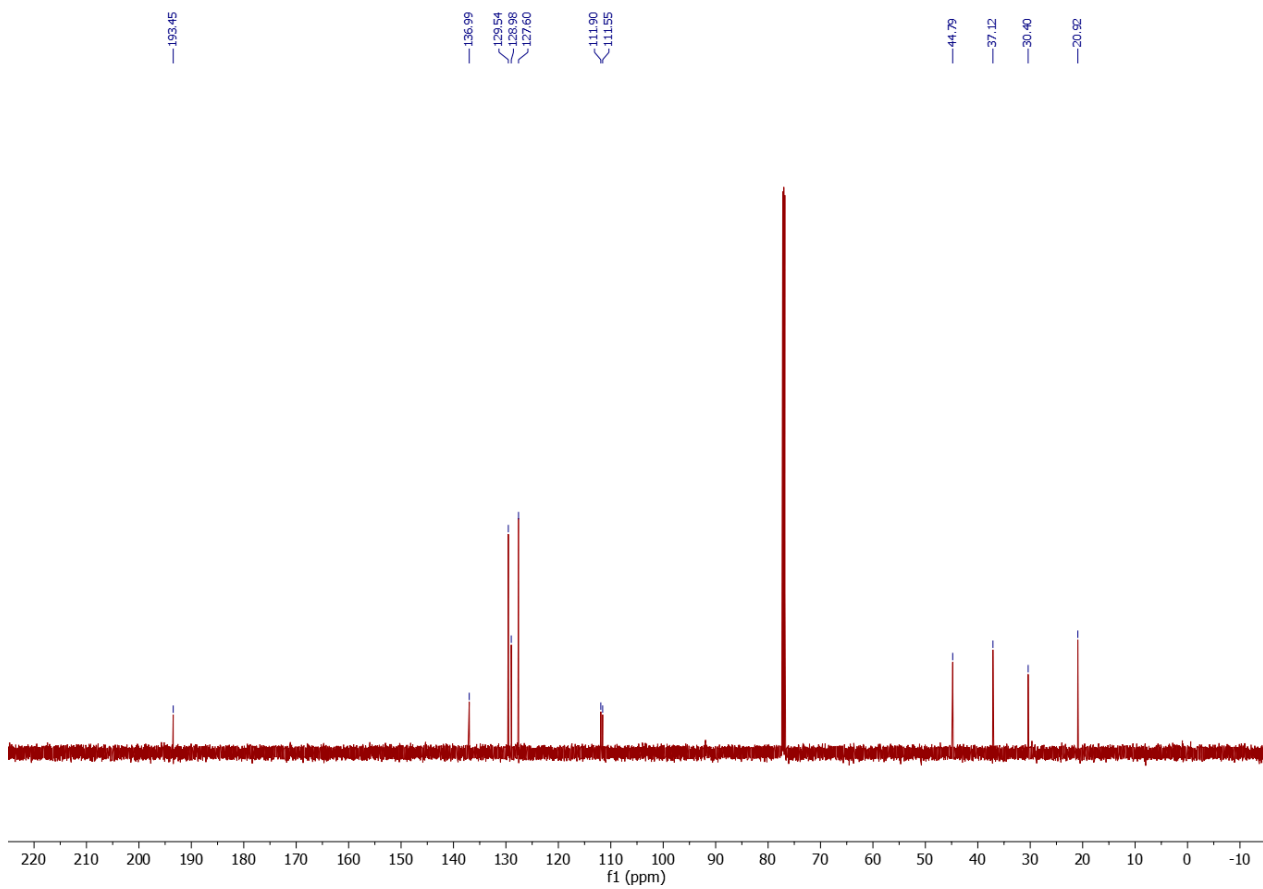
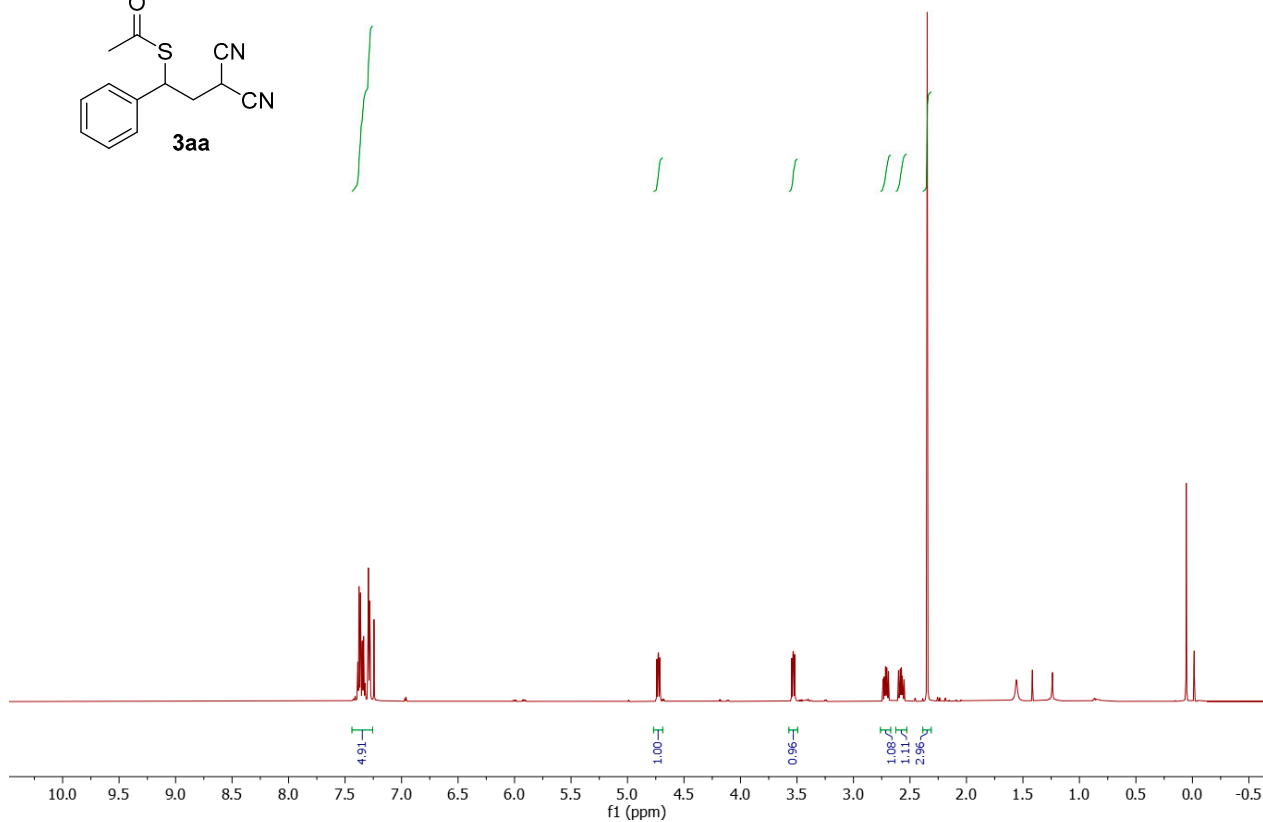
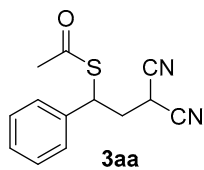
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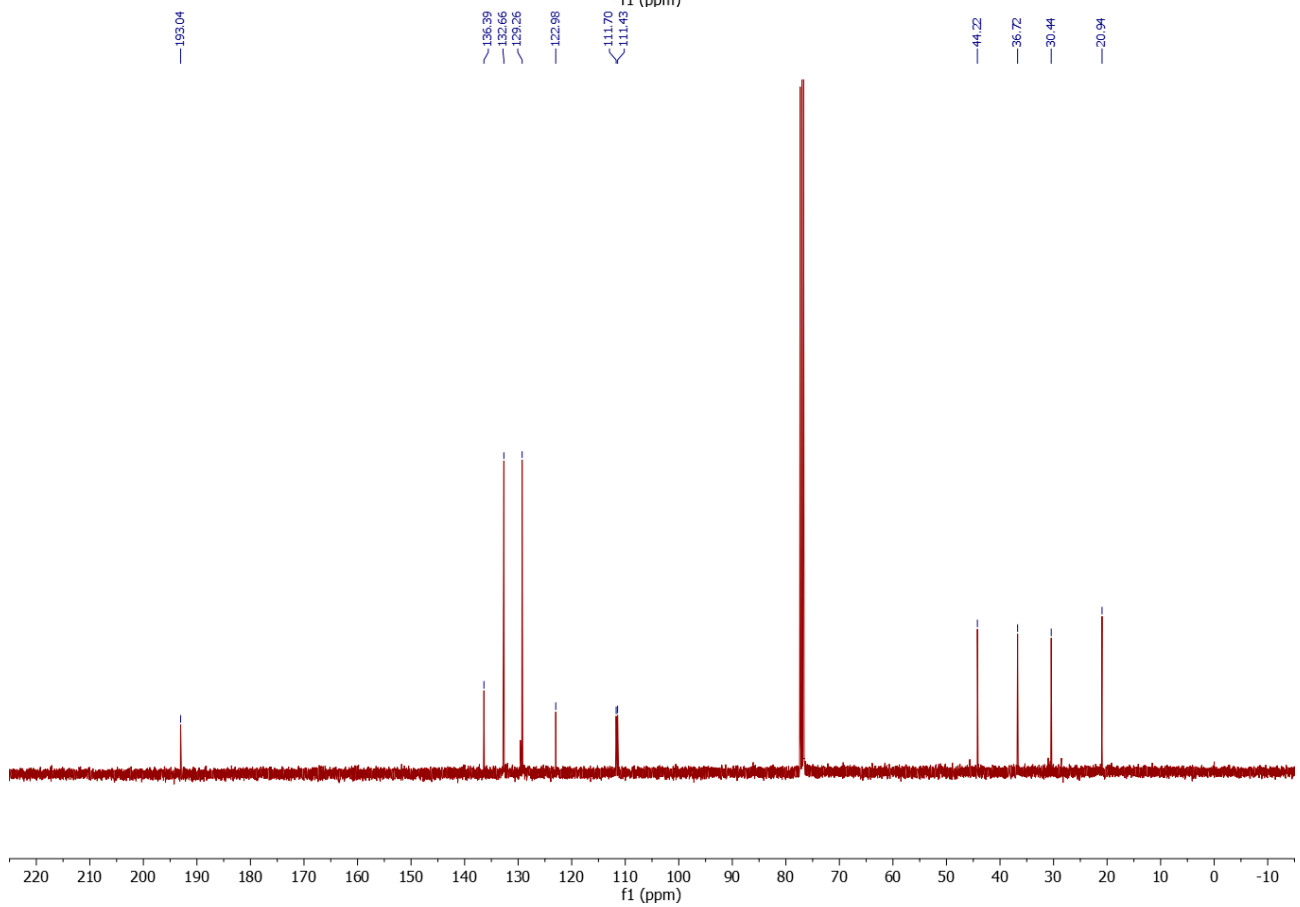
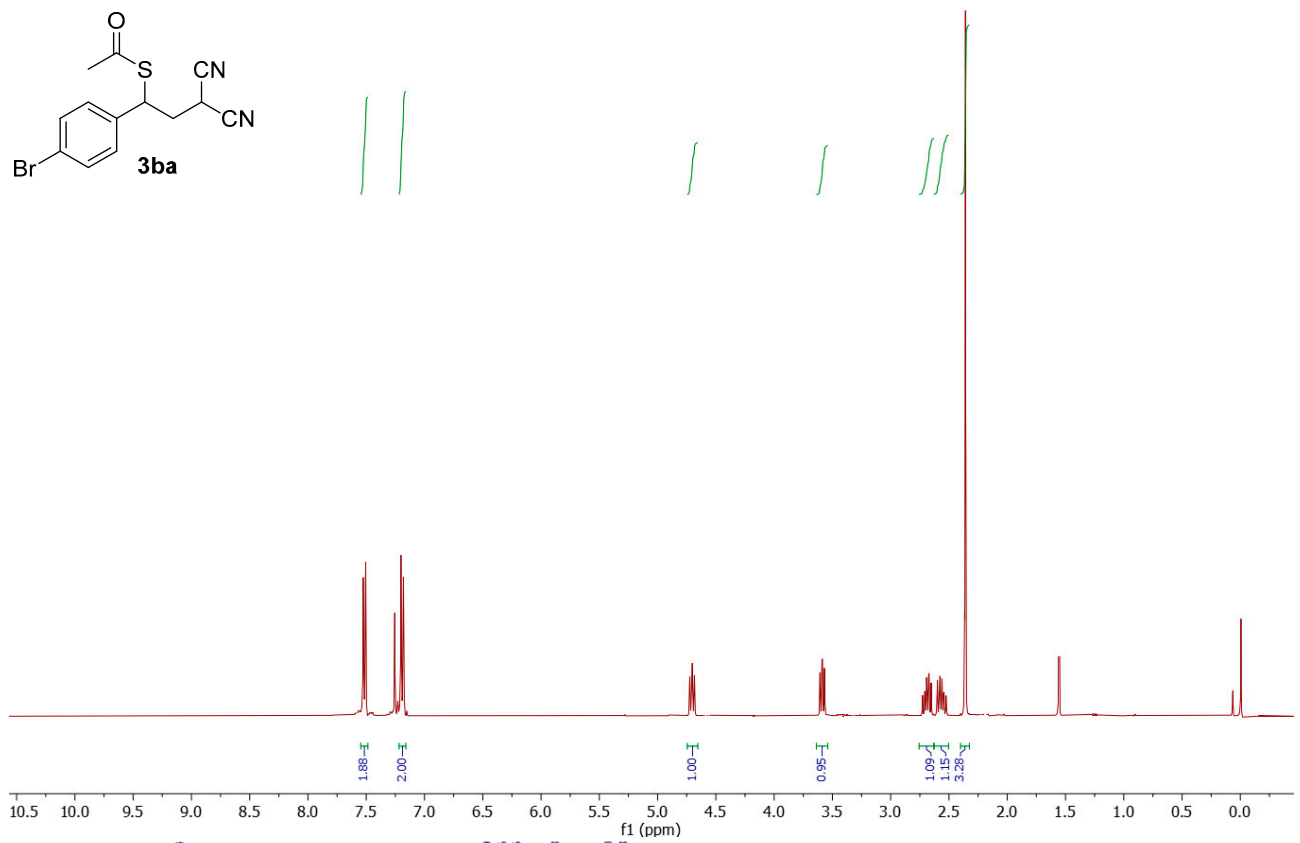
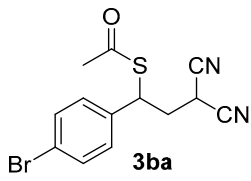
1-acetyl-2-(naphthalen-2-yl)cyclopropane-1-carbonitrile 4ka



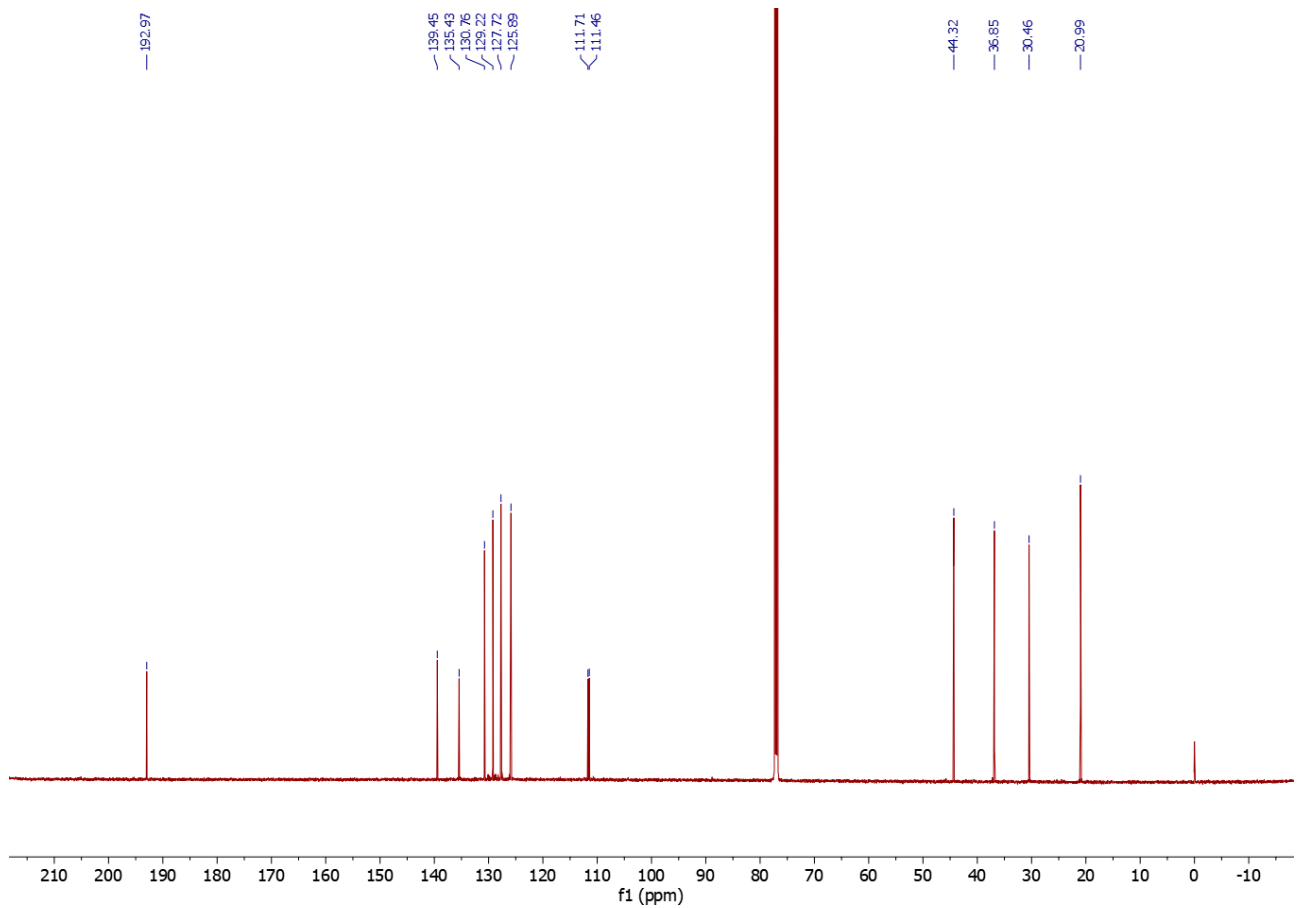
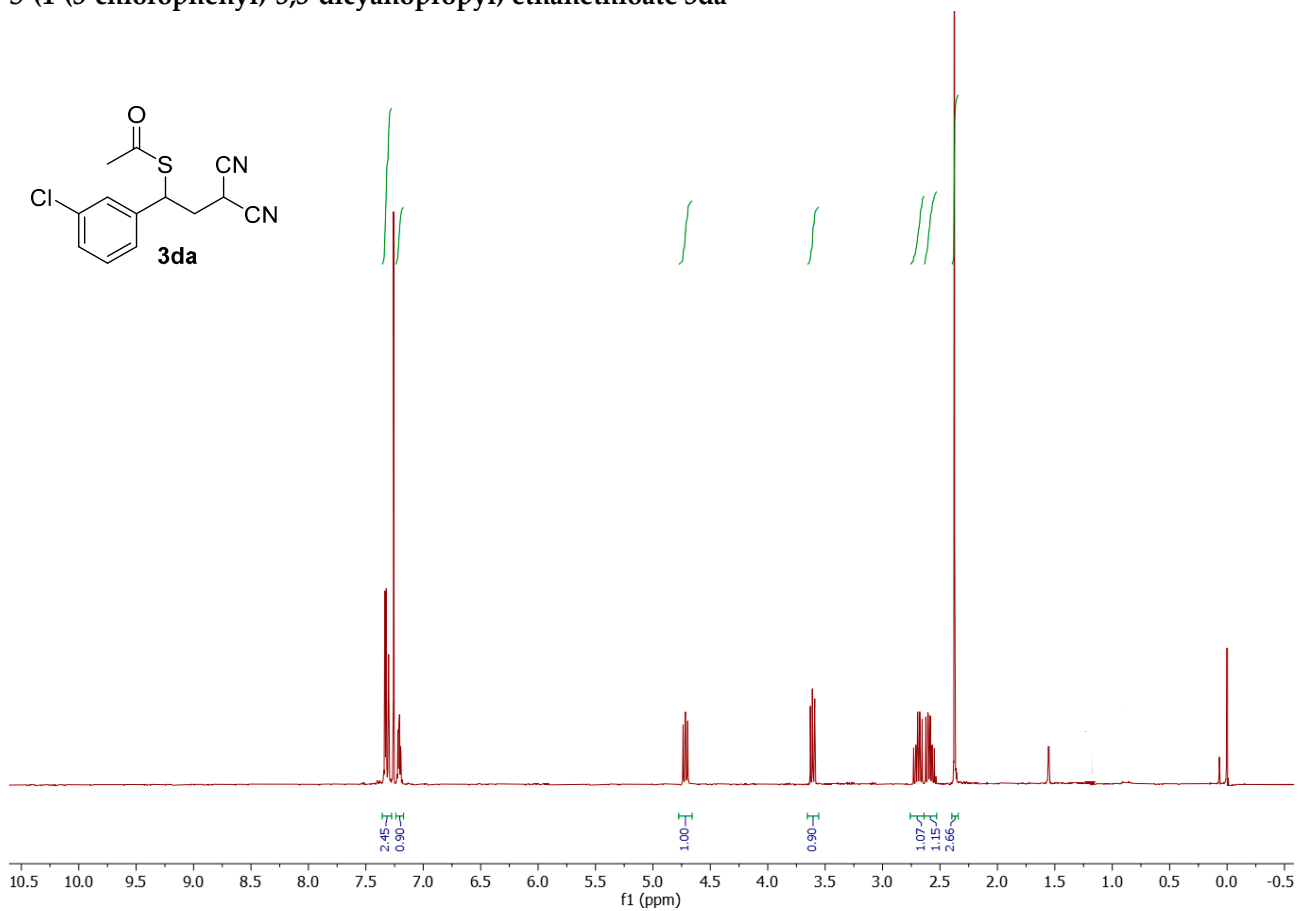
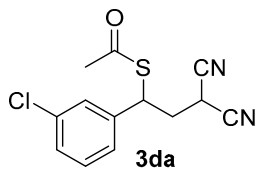
S-(3,3-dicyano-1-phenylpropyl) ethanethioate 3aa



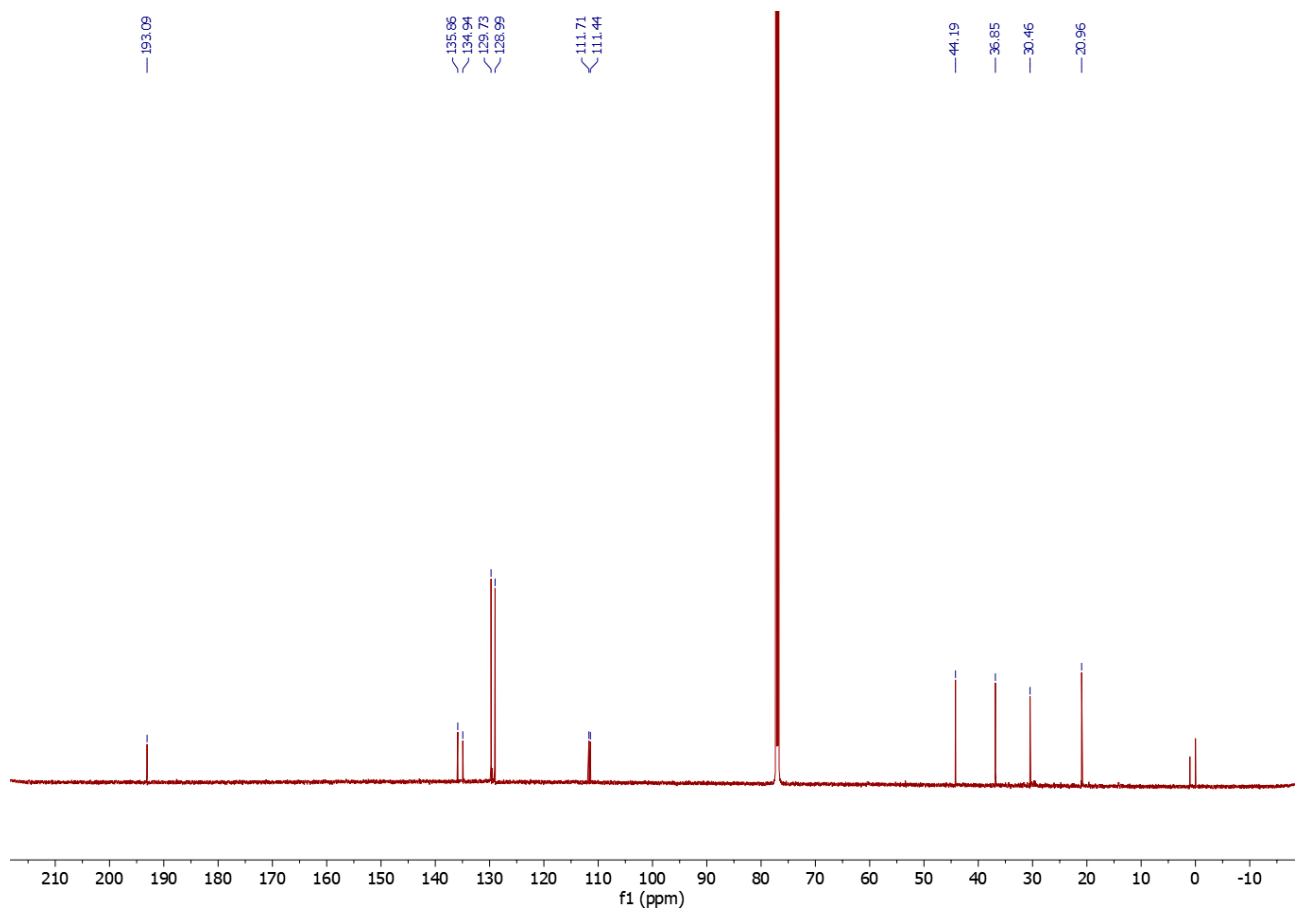
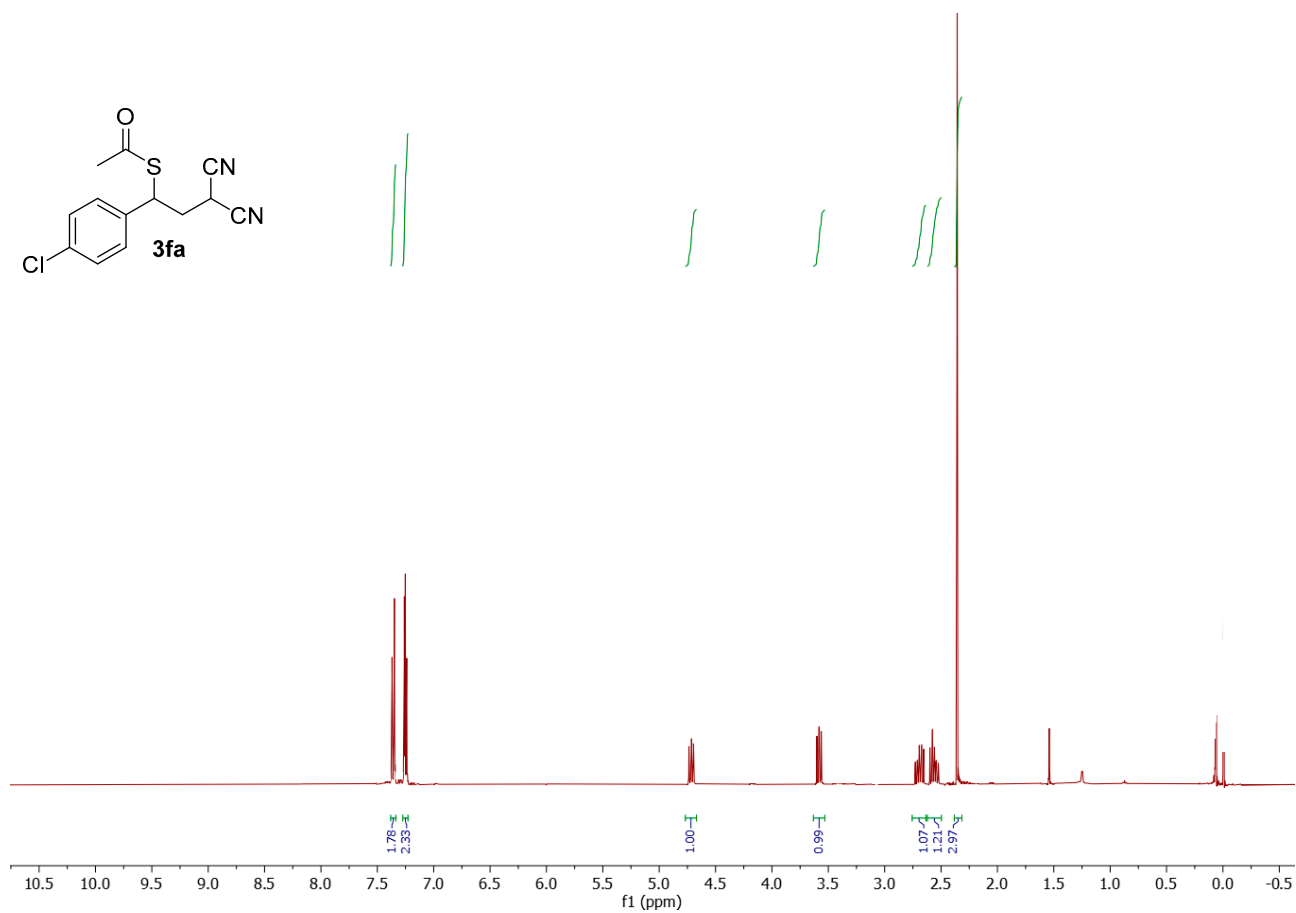
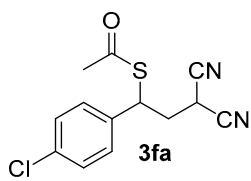
S-(1-(4-bromophenyl)-3,3-dicyanopropyl) ethanethioate 3ba



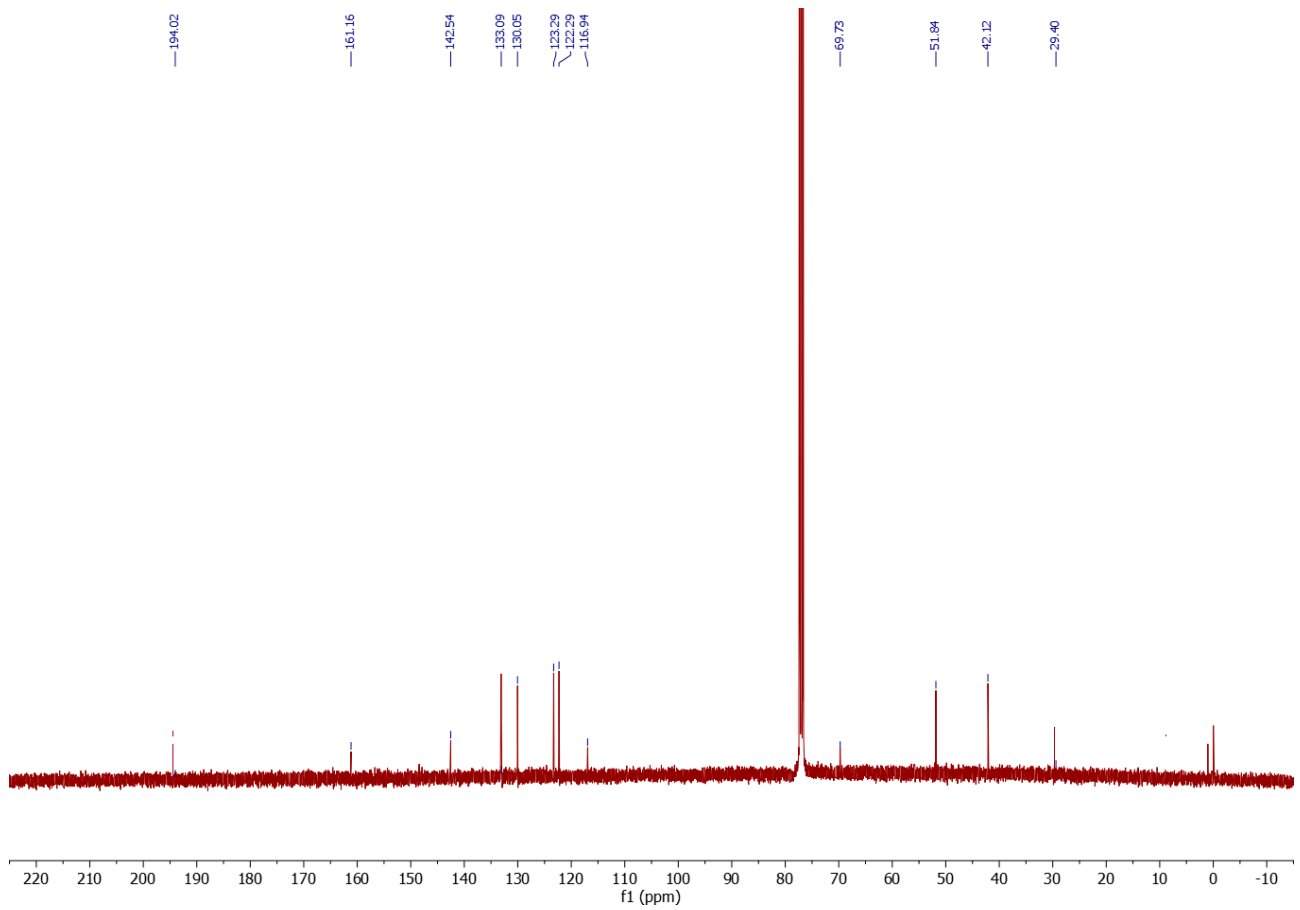
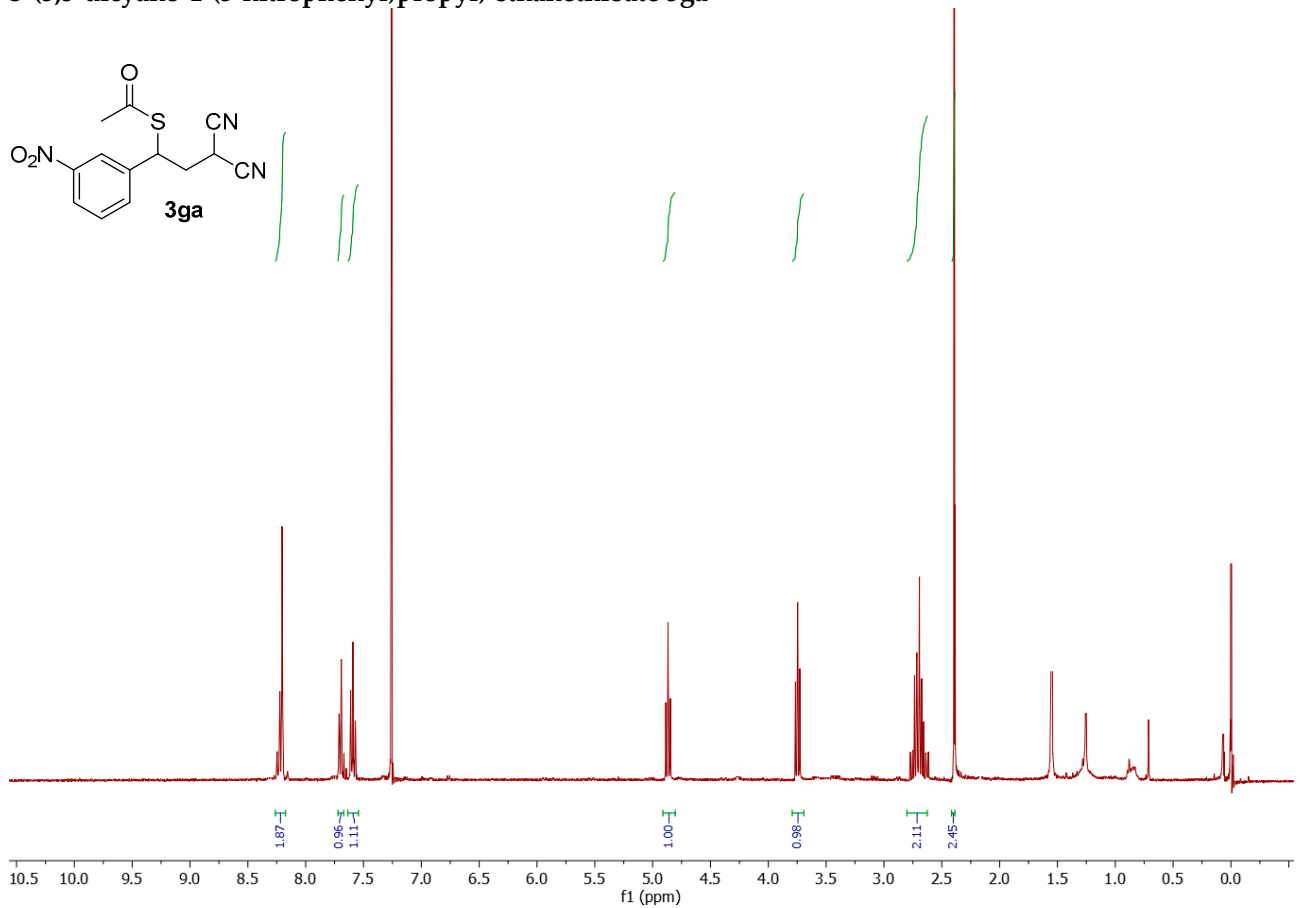
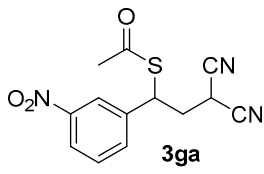
S-(1-(3-chlorophenyl)-3,3-dicyanopropyl) ethanethioate 3da



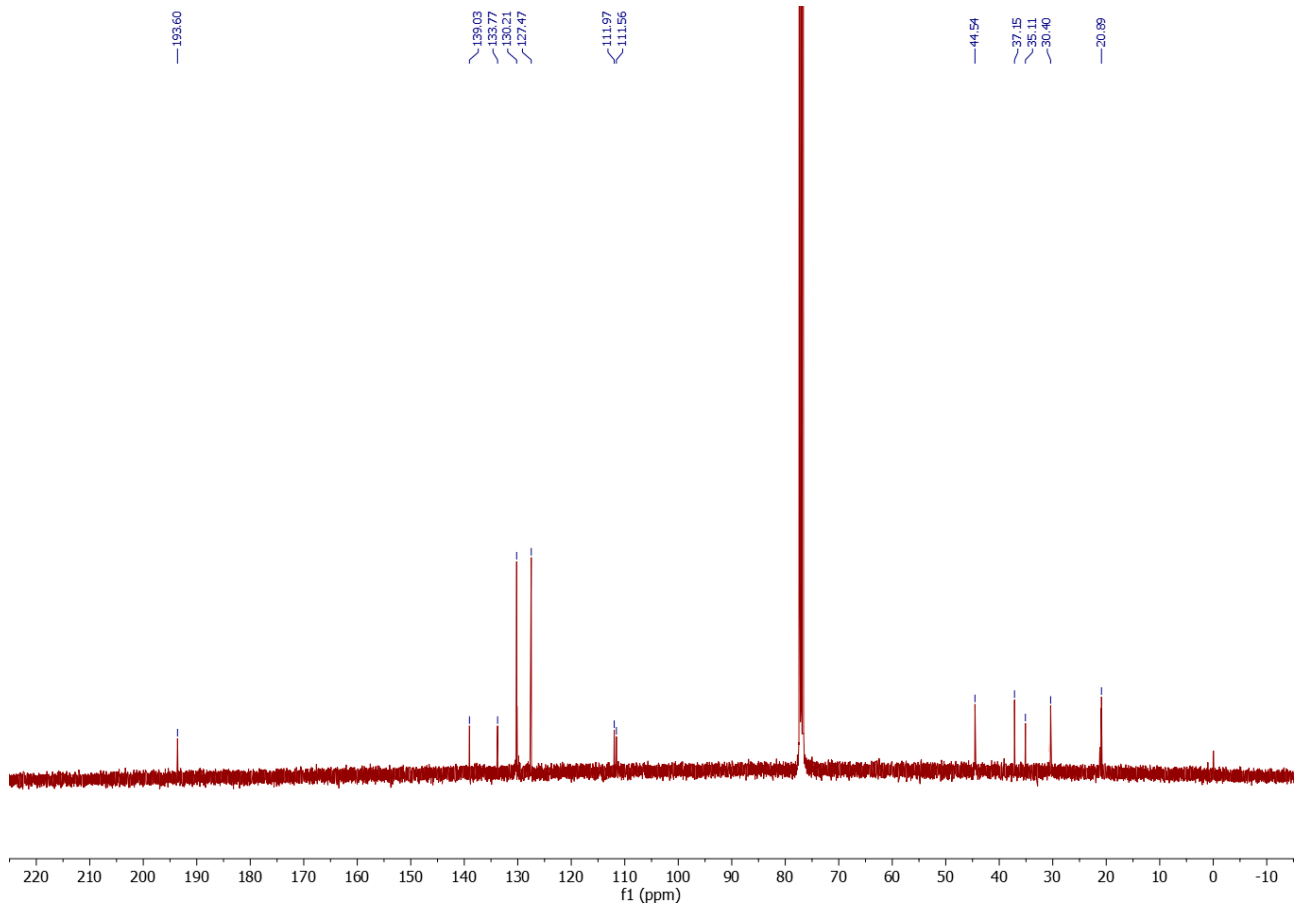
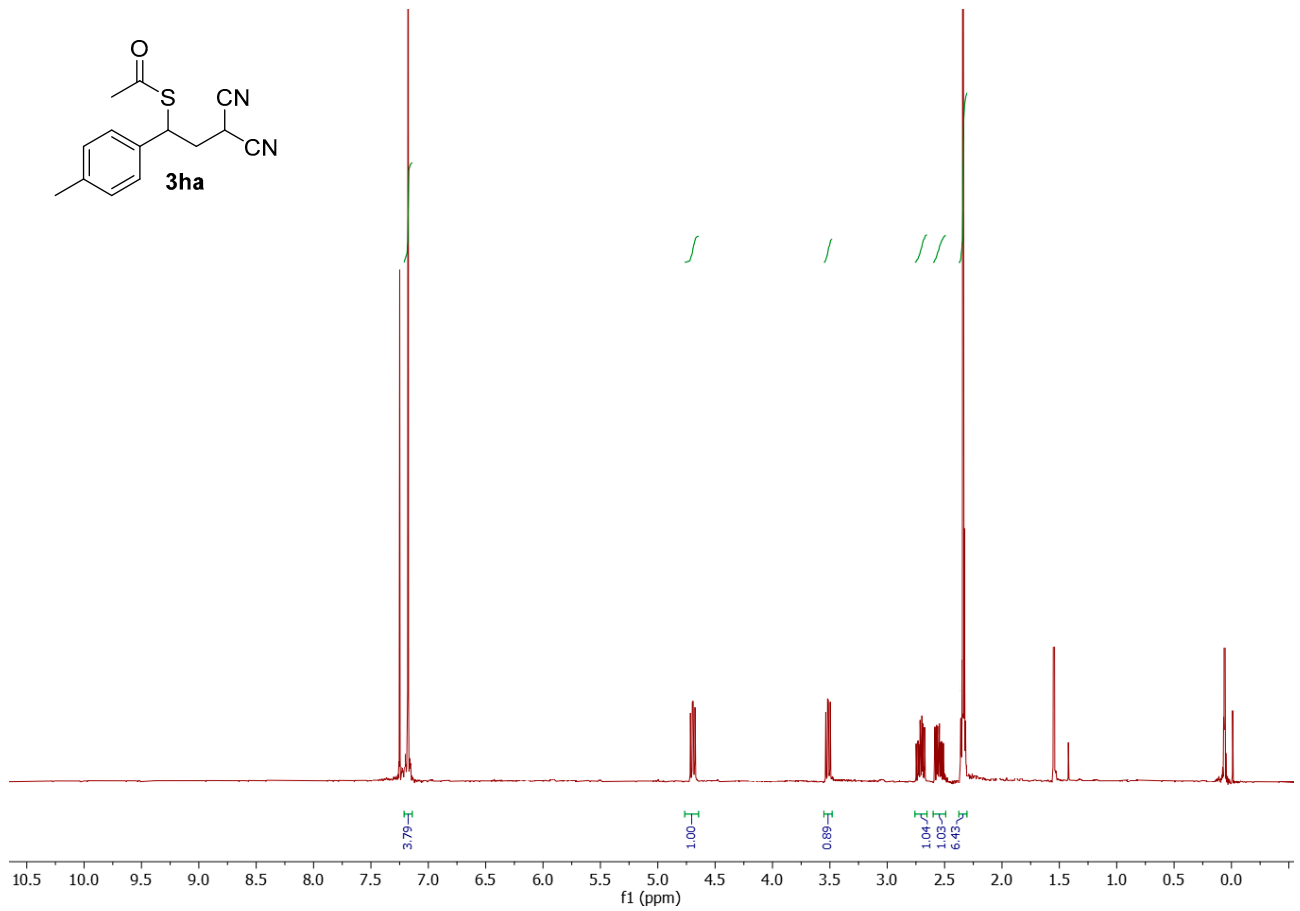
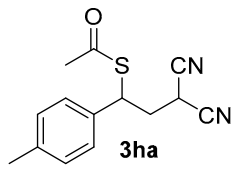
S-(1-(4-chlorophenyl)-3,3-dicyanopropyl) ethanethioate 3fa



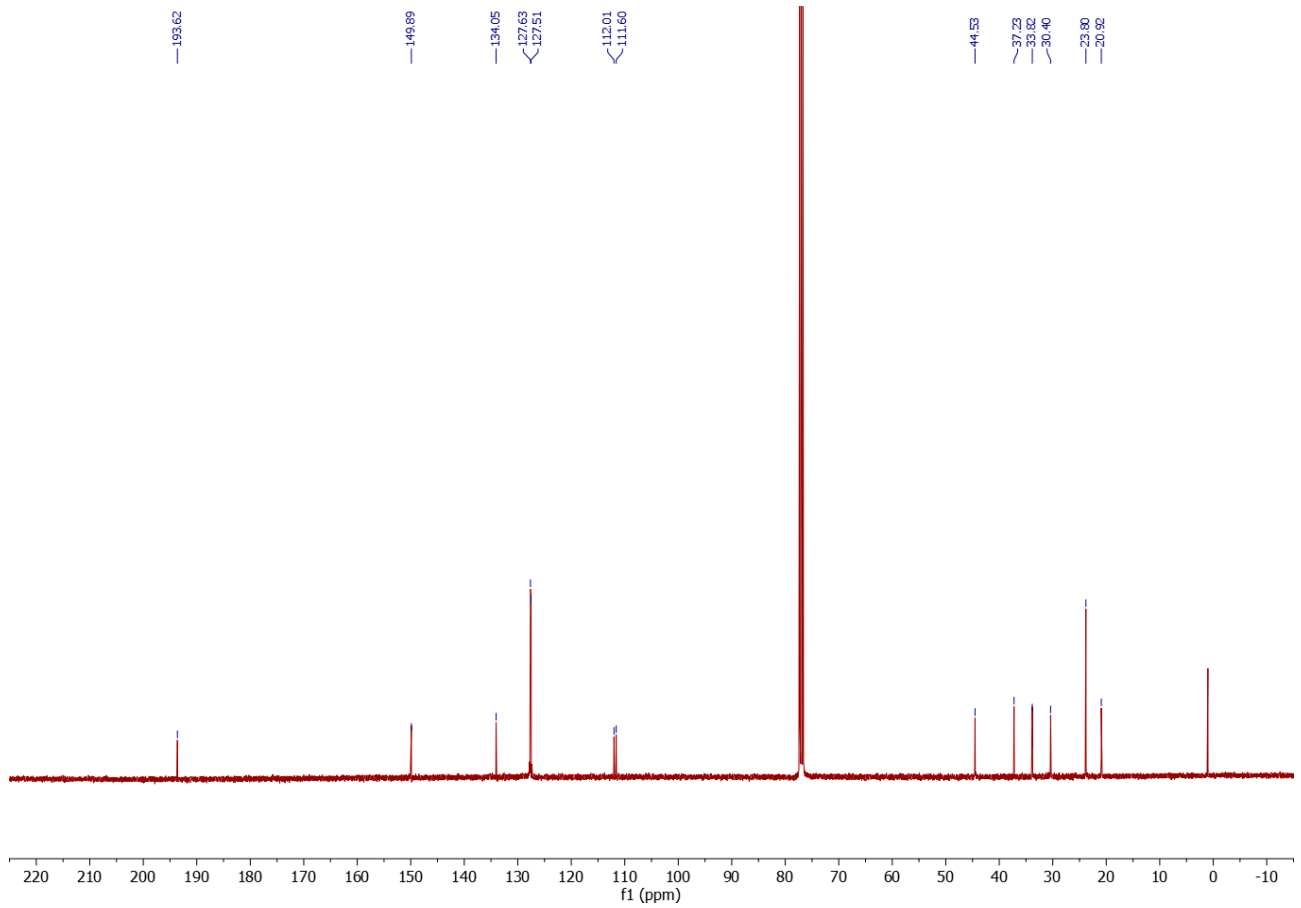
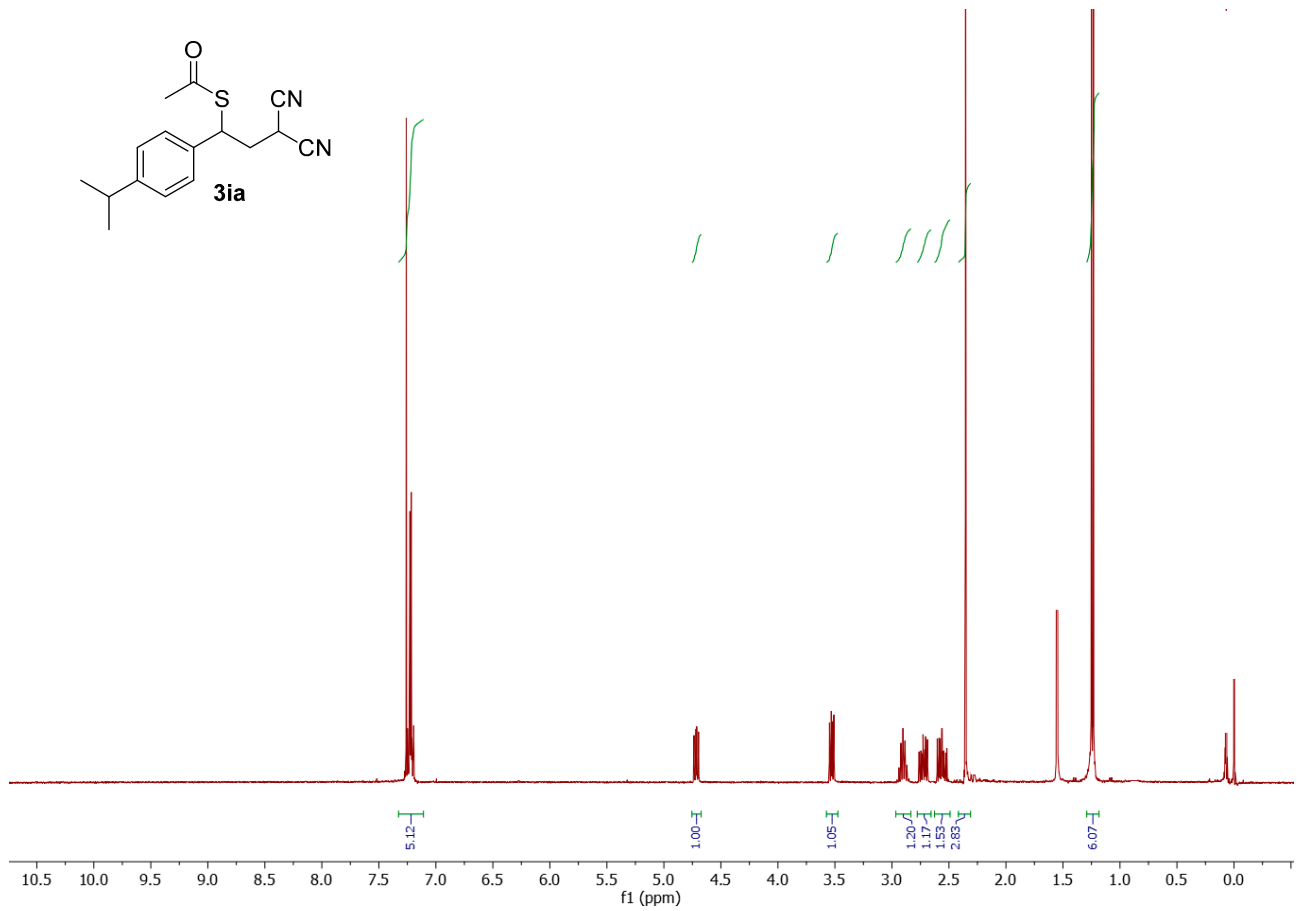
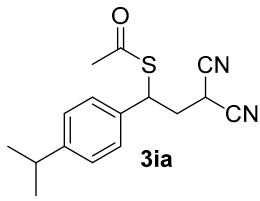
S-(3,3-dicyano-1-(3-nitrophenyl)propyl) ethanethioate 3ga



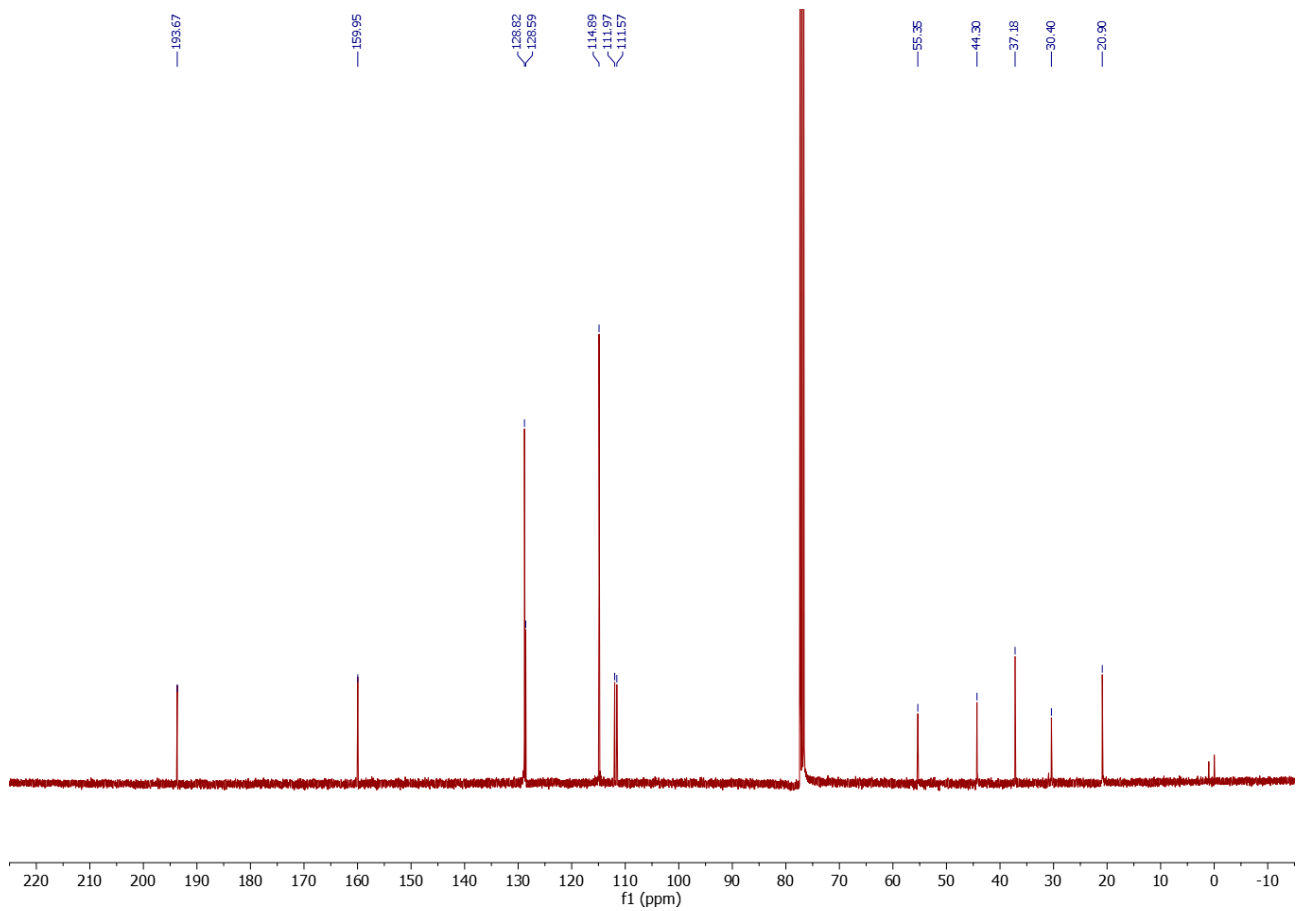
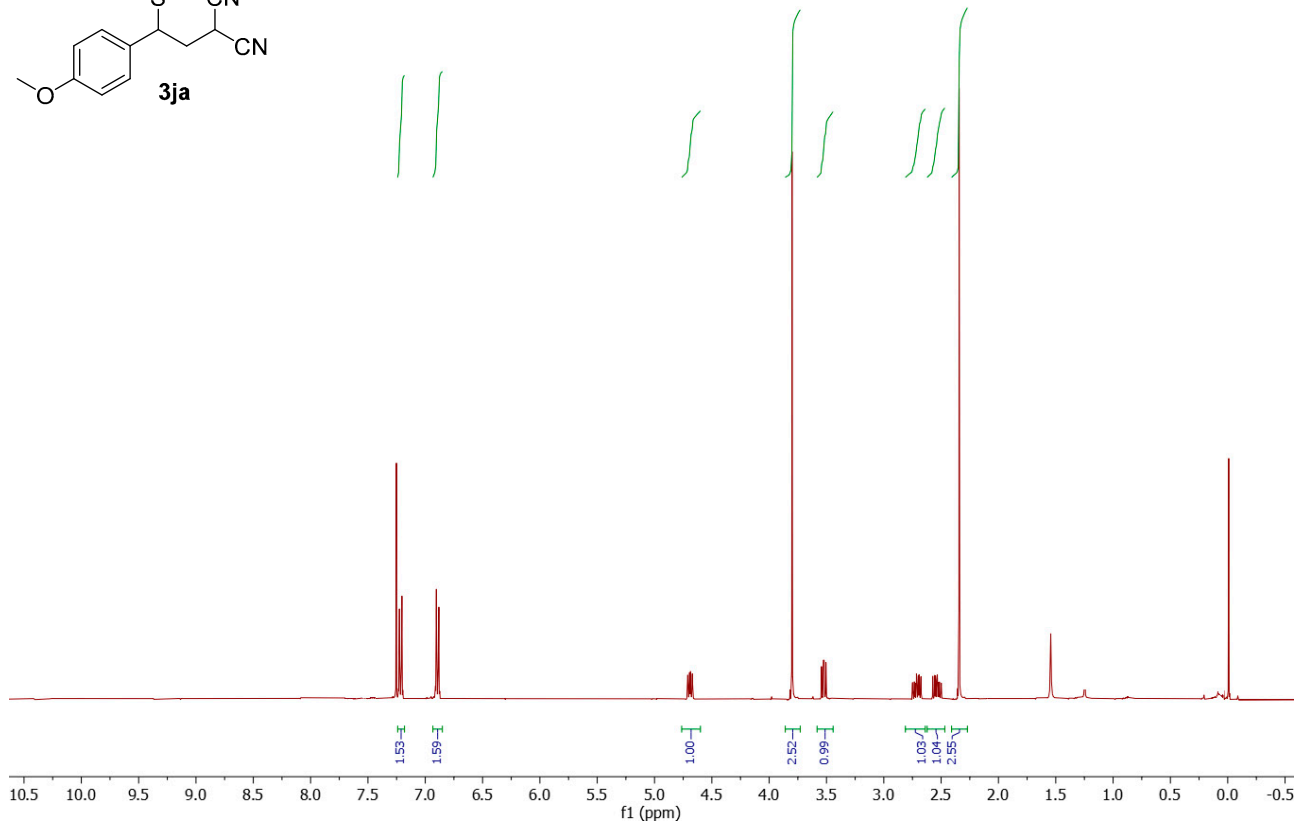
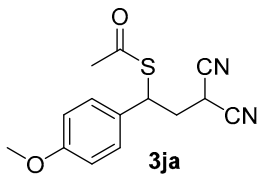
S-(3,3-dicyano-1-(p-tolyl)propyl) ethanethioate 3ha



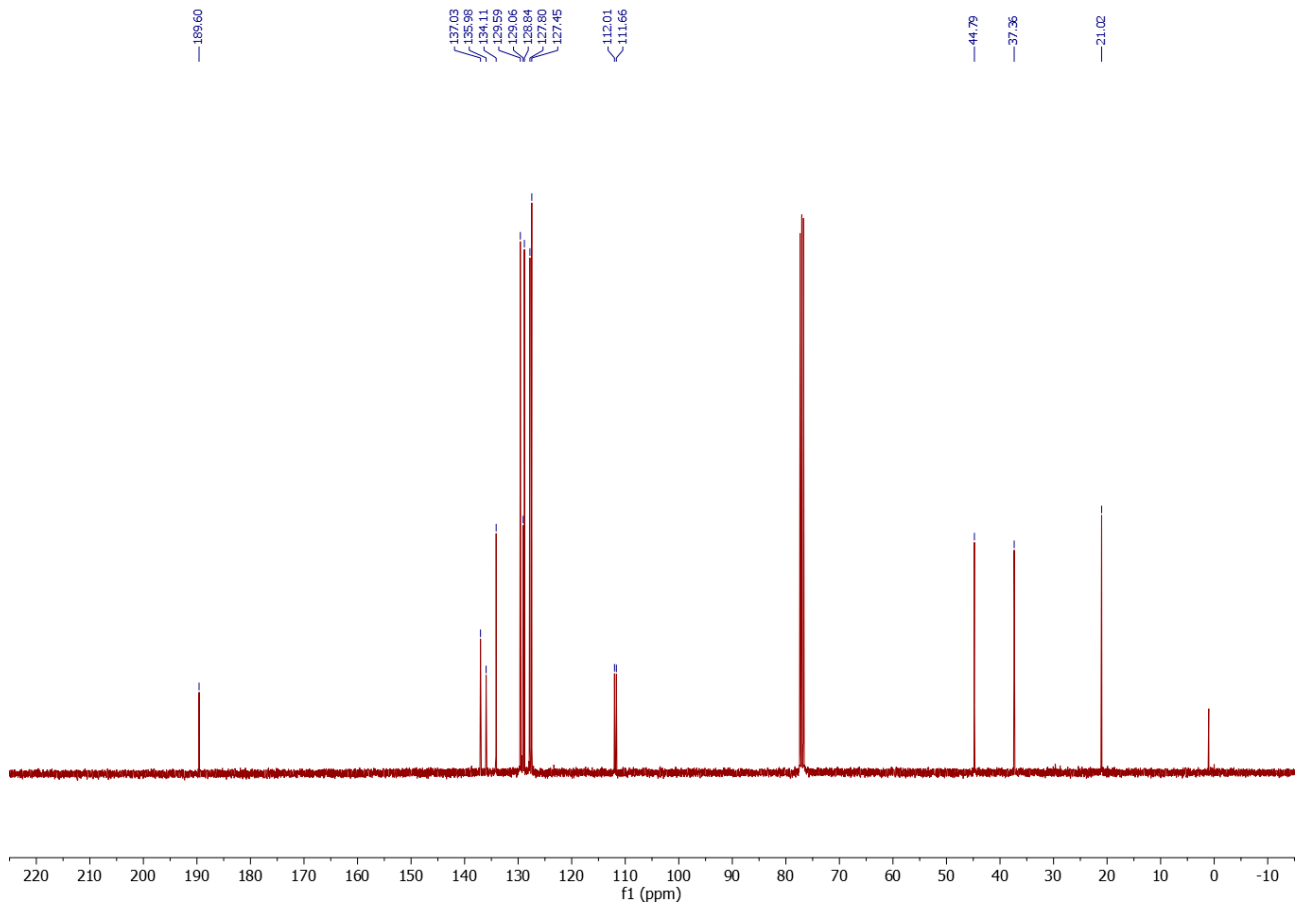
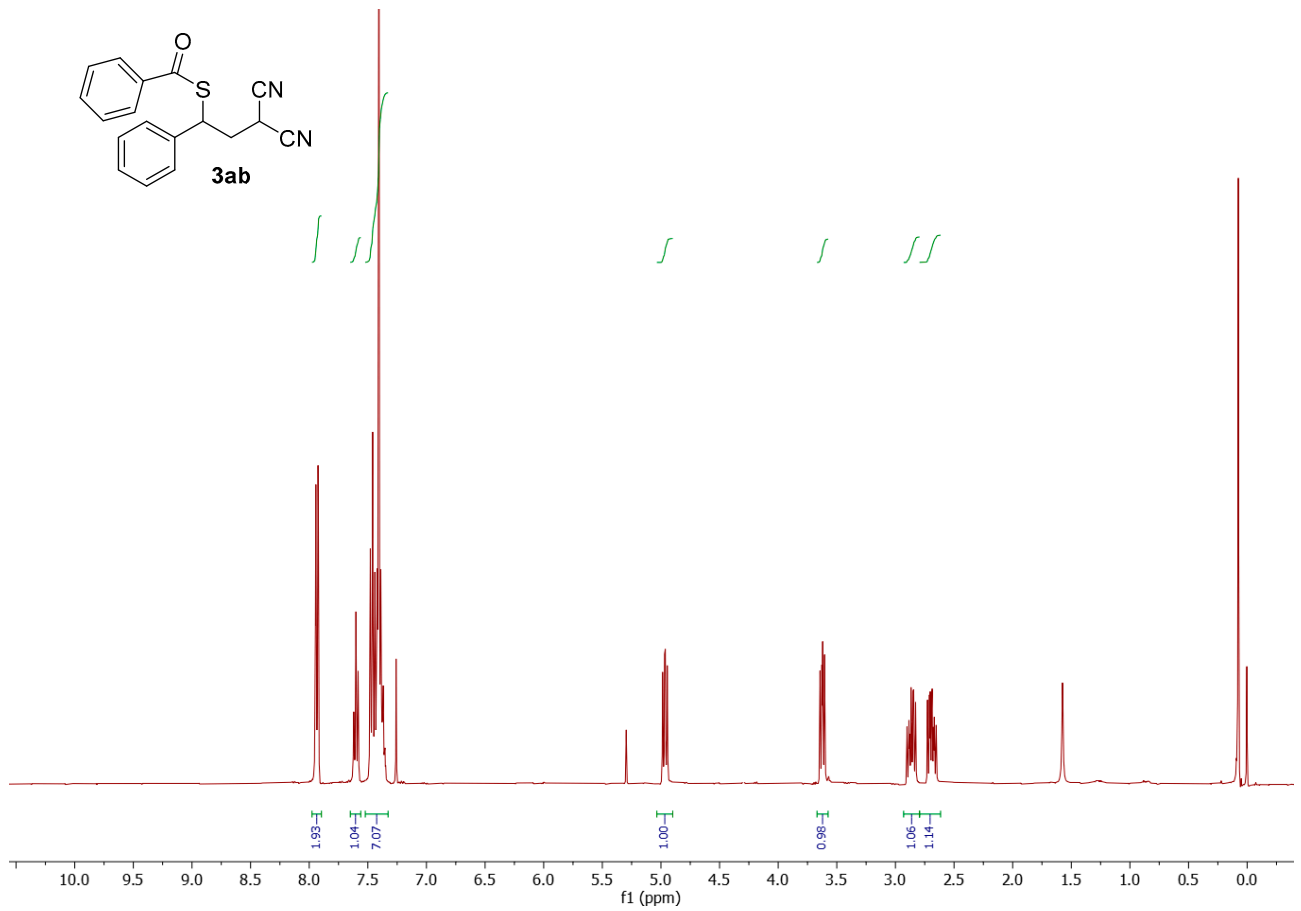
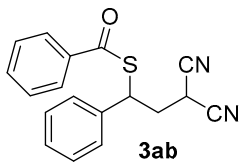
S-(3,3-dicyano-1-(4-isopropylphenyl)propyl) ethanethioate 3ia



S-(3,3-dicyano-1-(4-methoxyphenyl)propyl) ethanethioate 3ja



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



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

