

Supporting Information

L. Kersten, K. Harms and G. Hilt*

“Synthesis of Tri-, Tetra- and Pentacarbonyl Derivatives via Ozonolysis of 1,4-Dienes and Cyclization to Polyaromatic Systems”

Content:

X-ray crystal structures of compounds 45 and 47	S 2
^1H / $^{13}\text{C}\{^1\text{H}\}$ NMR spectra	S 3 – S 42

Corresponding author:

Prof. Dr. Gerhard Hilt

Fachbereich Chemie

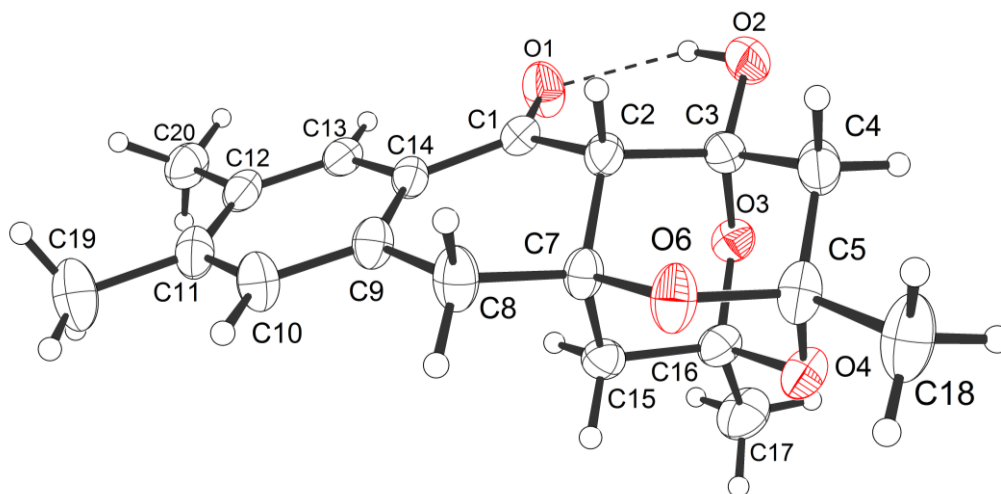
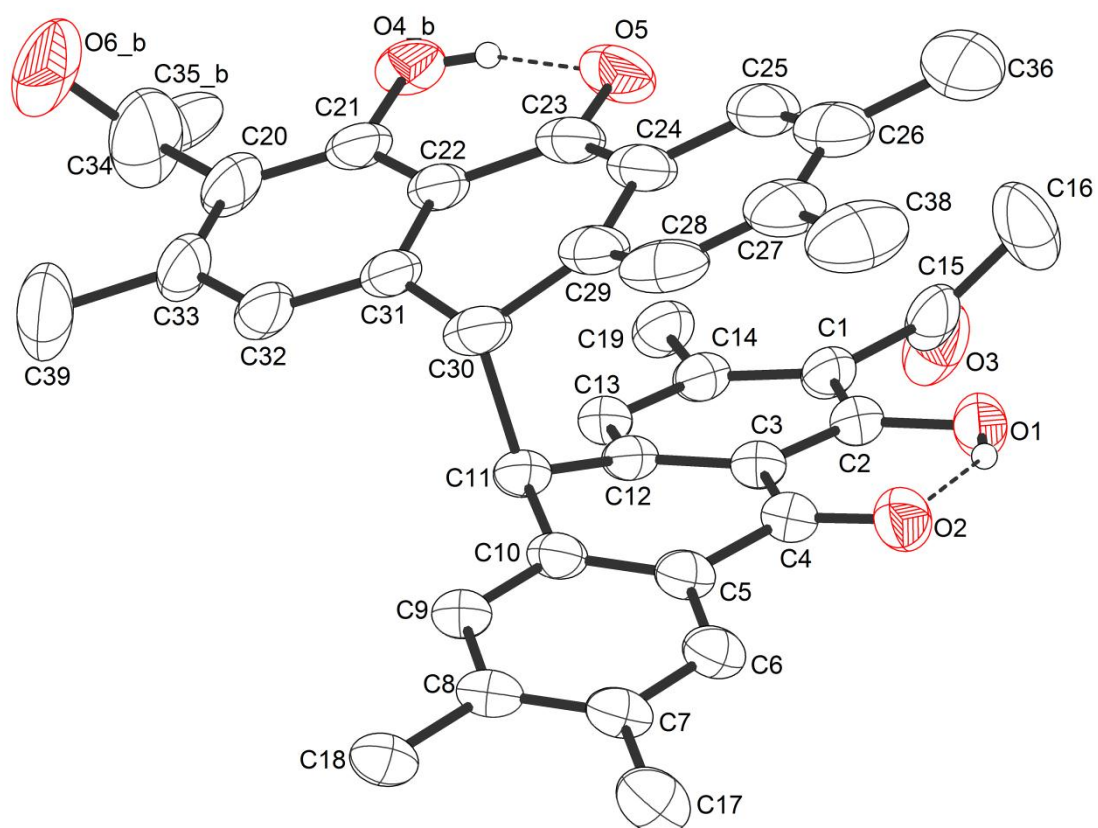
Philipps-Universität Marburg

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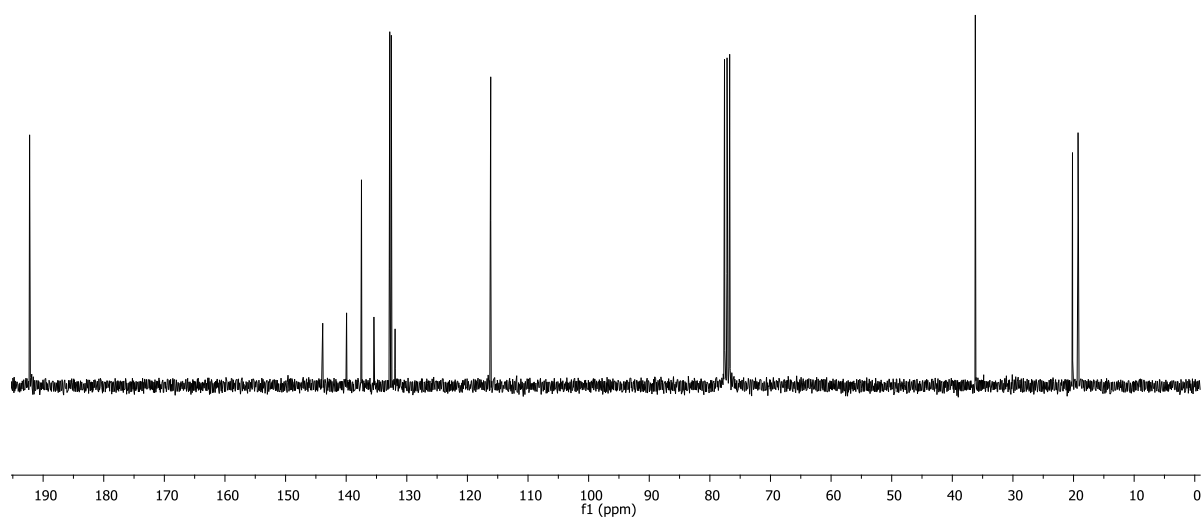
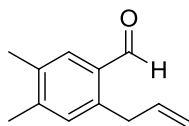
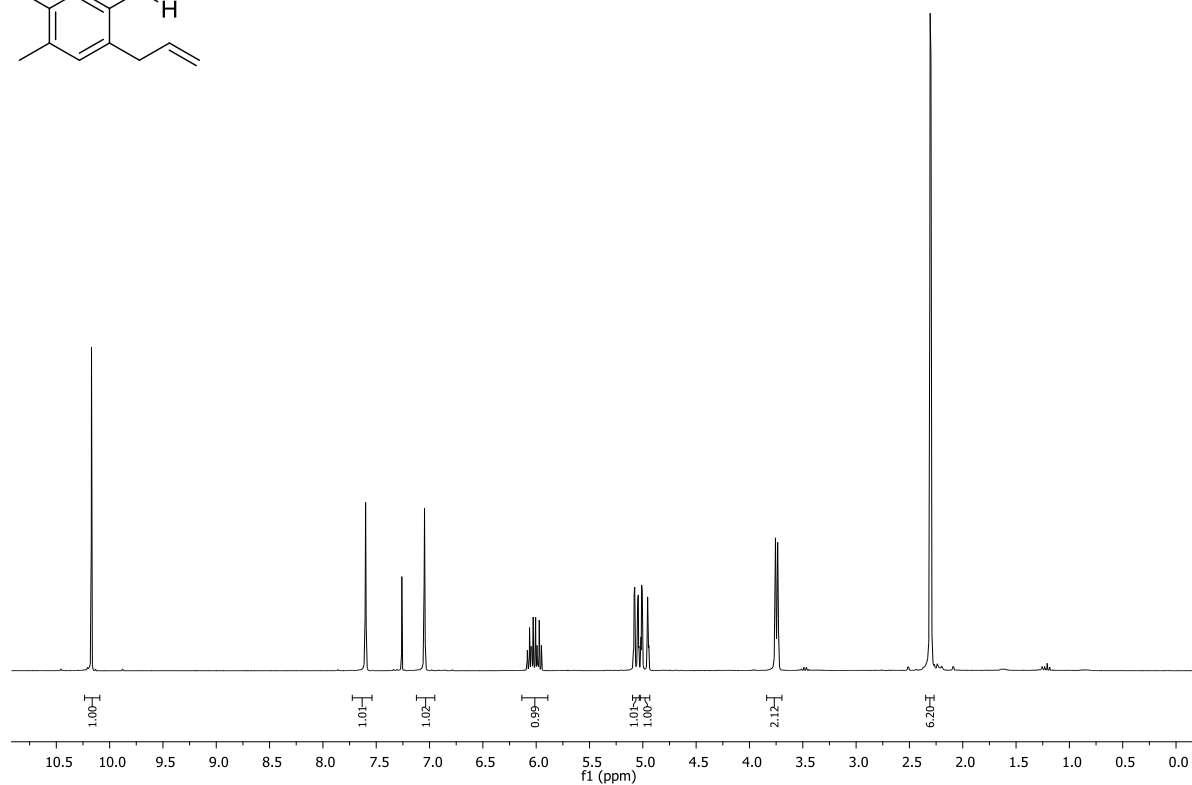
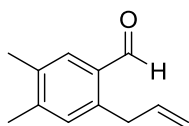
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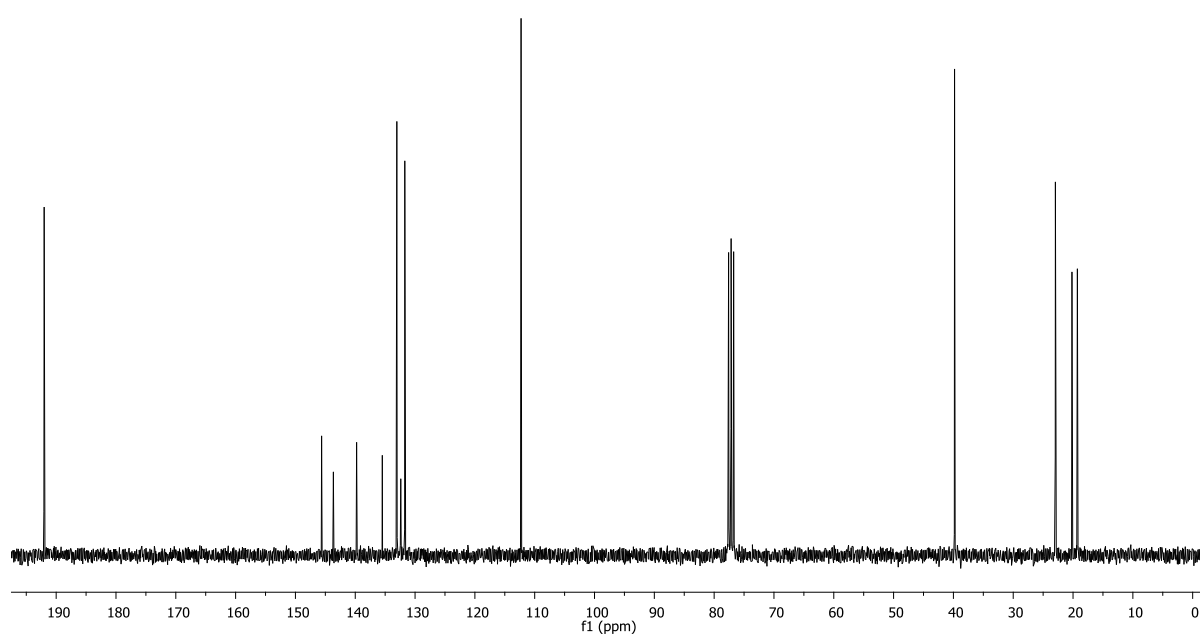
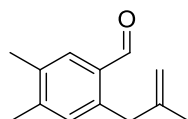
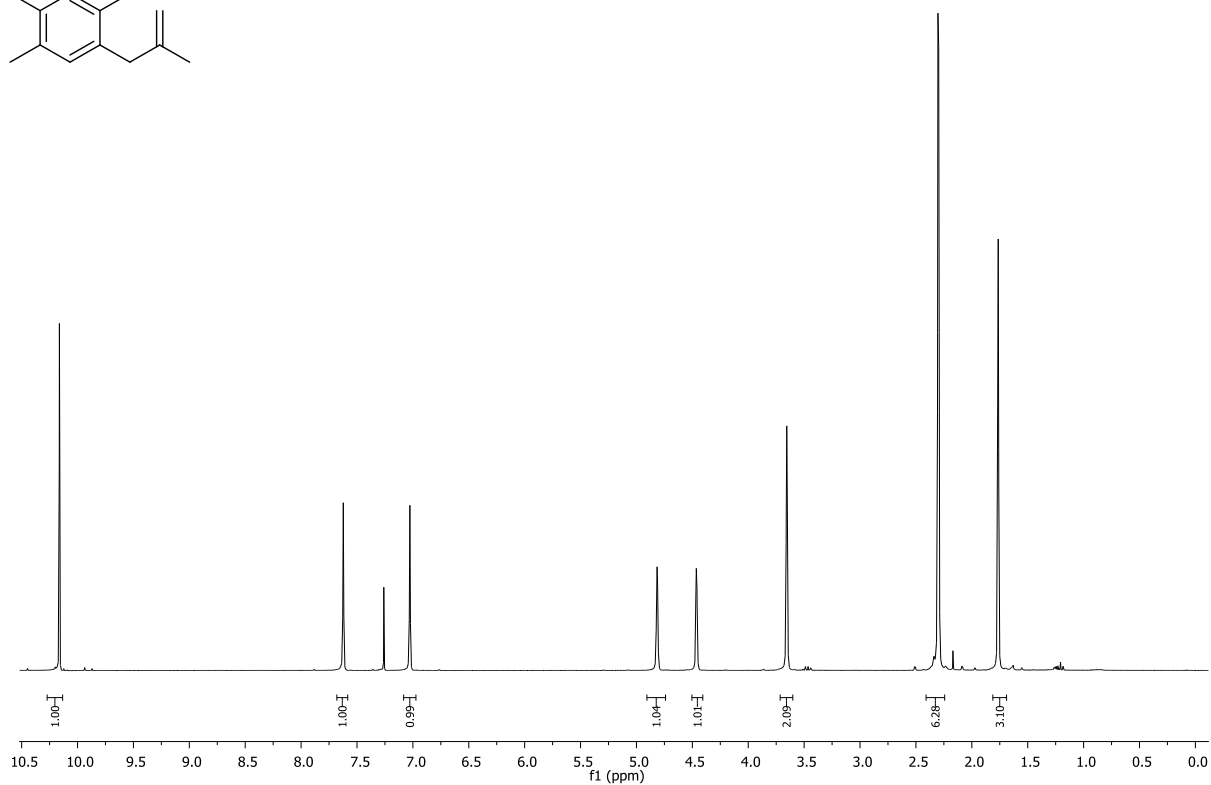
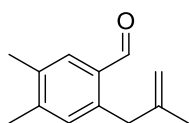
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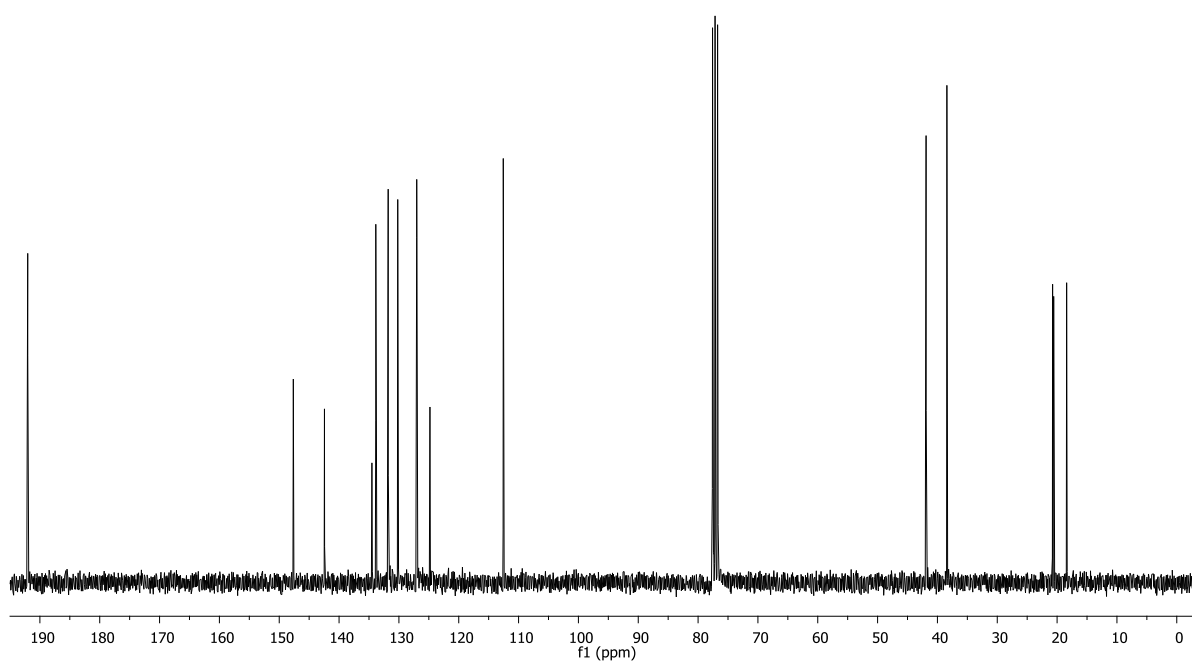
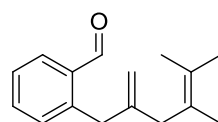
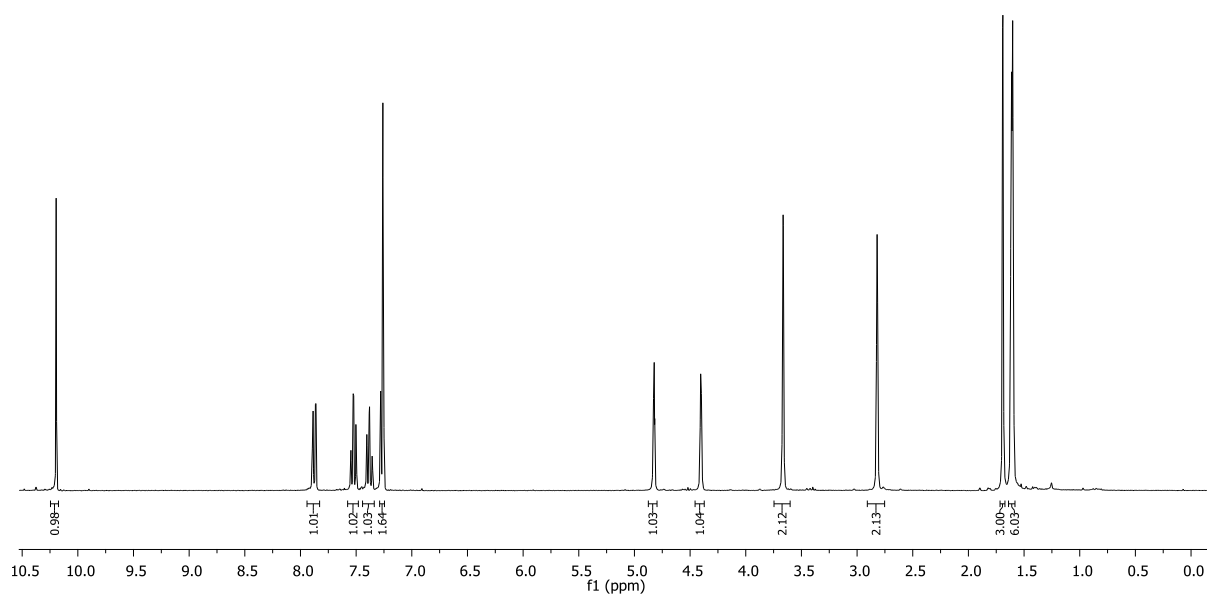
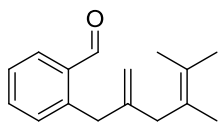
Hilt@chemie.uni-marburg.de

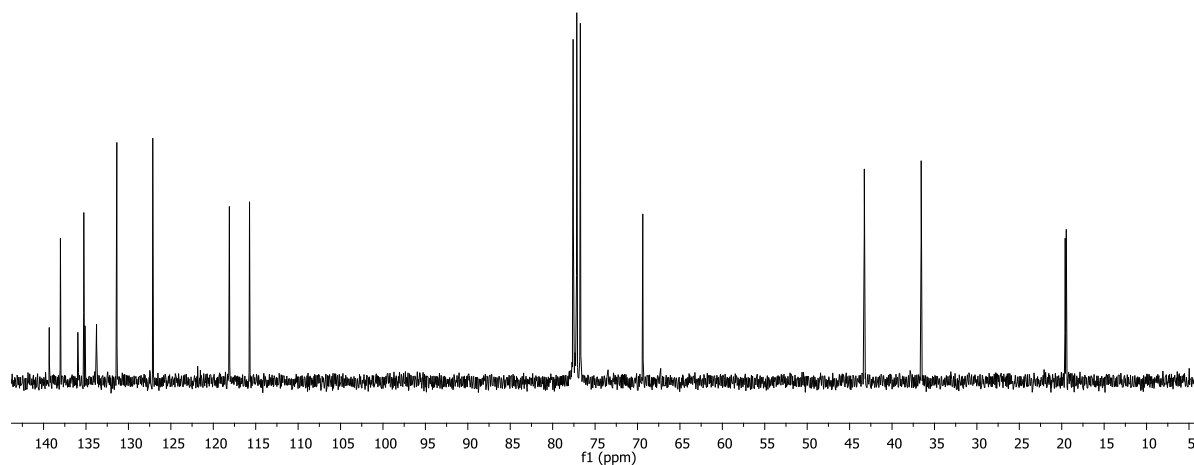
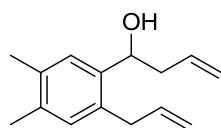
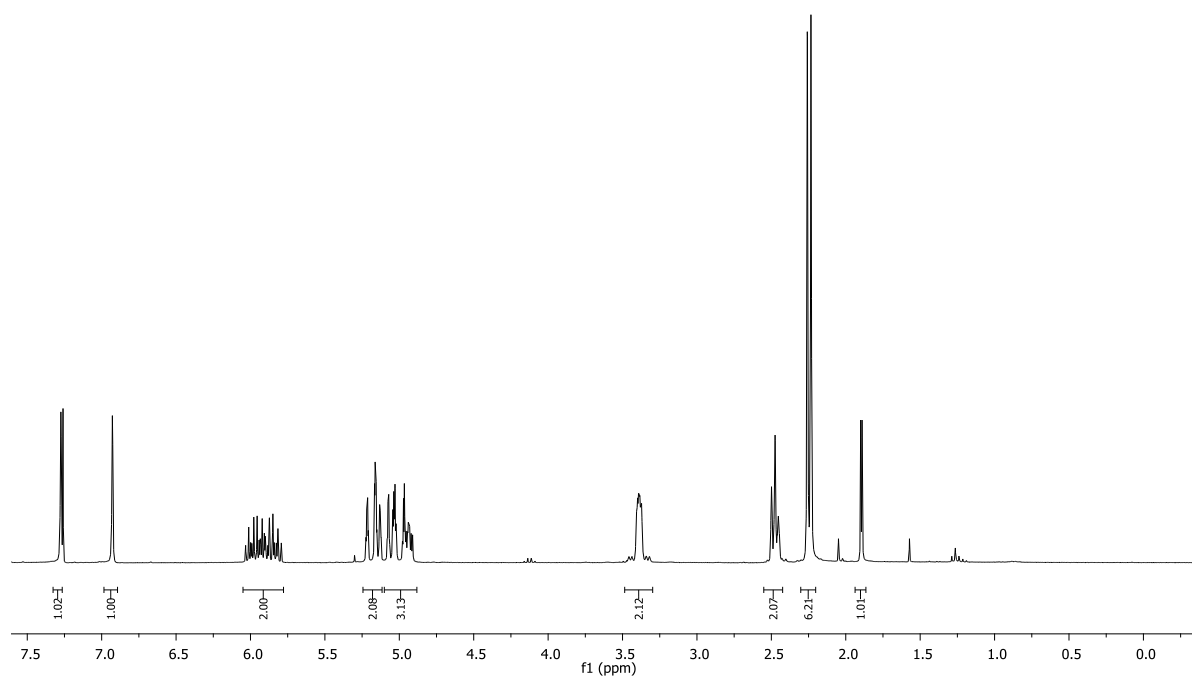
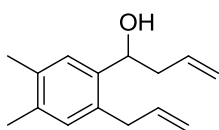
X-ray crystal structure of compound **45**X-ray crystal structure of compound **47**

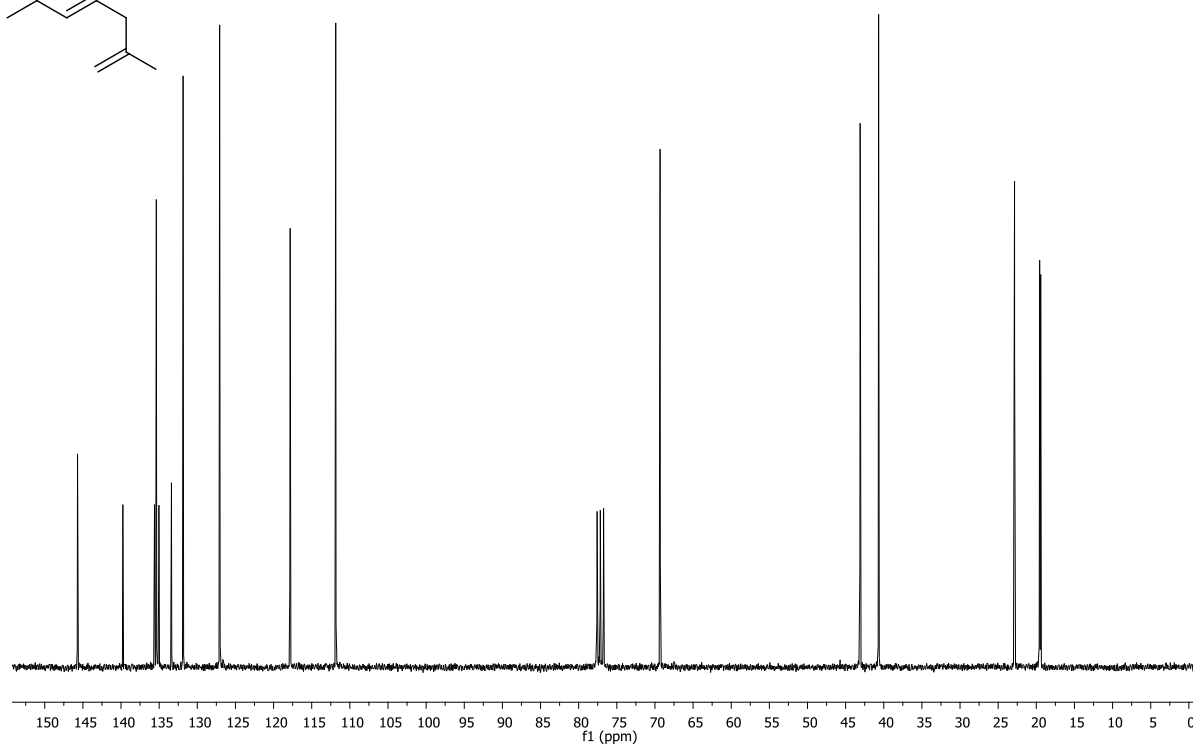
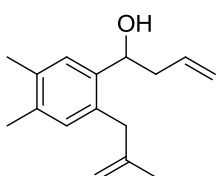
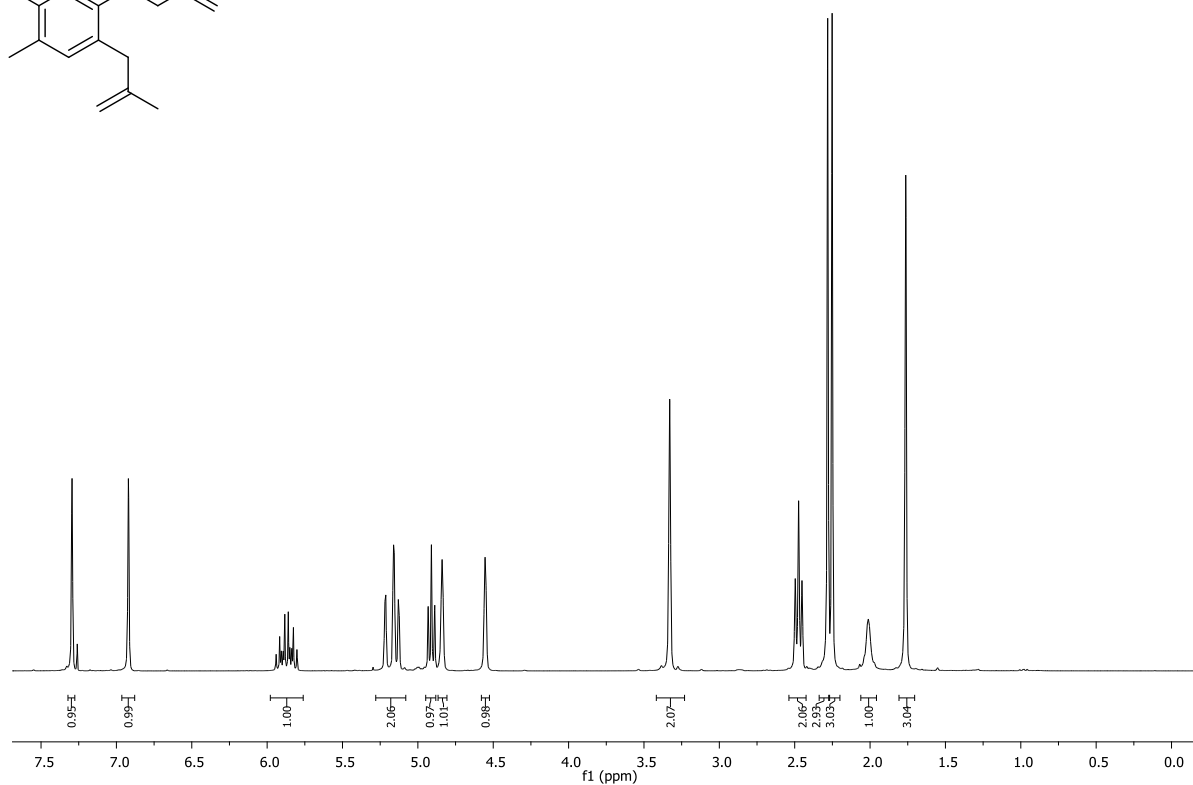
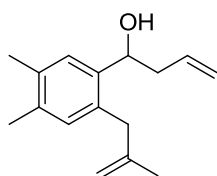
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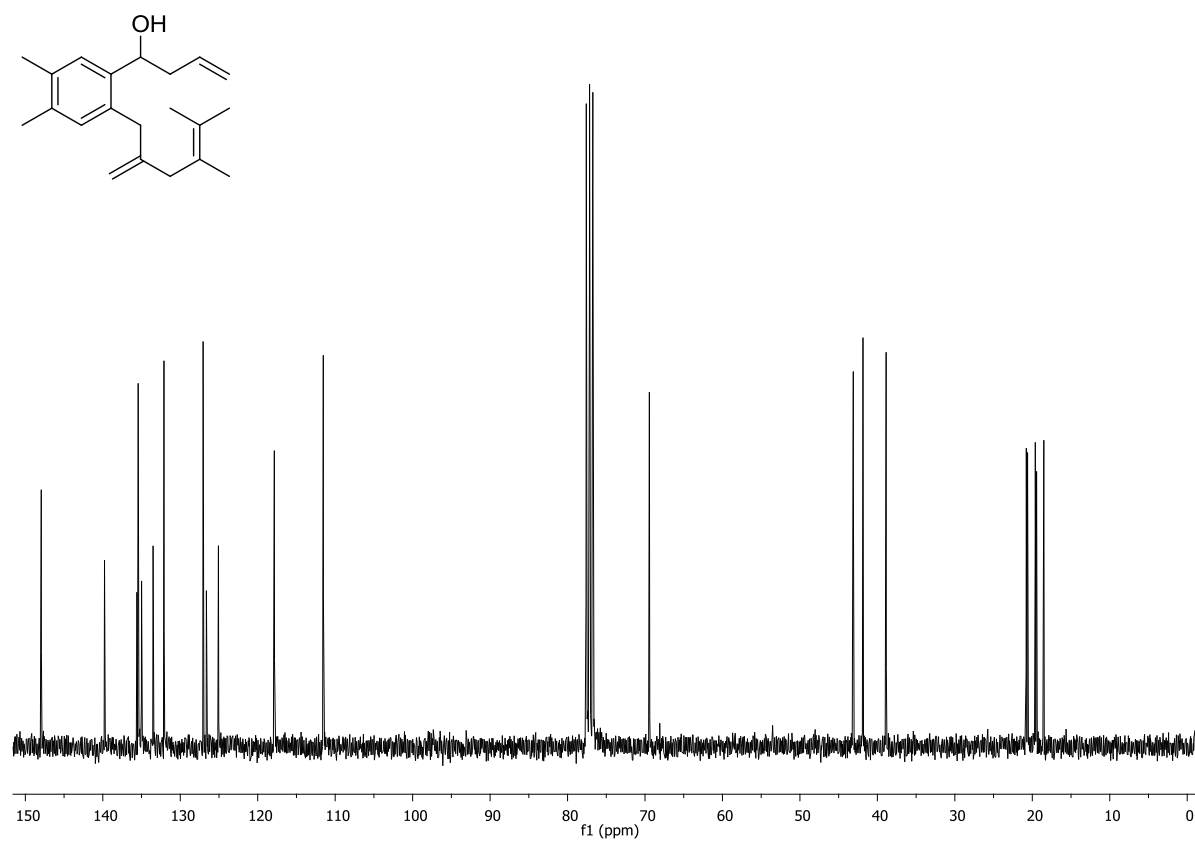
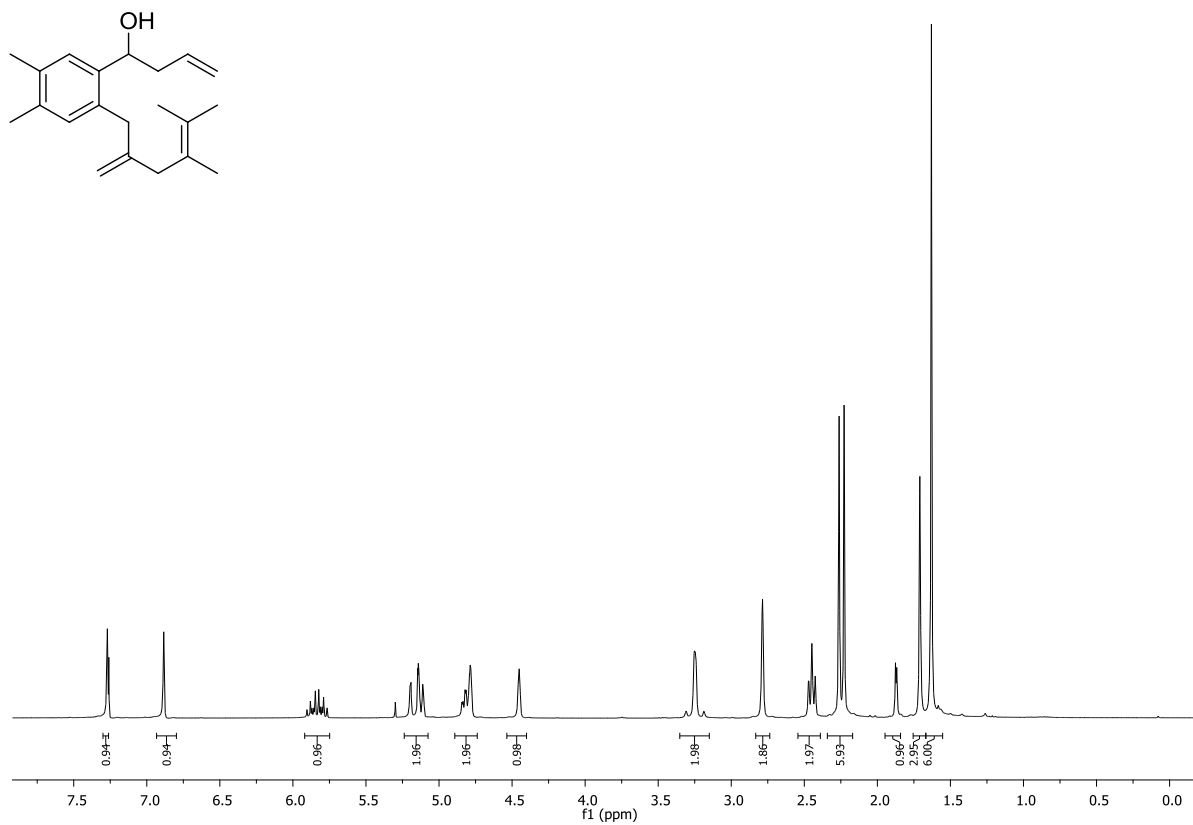
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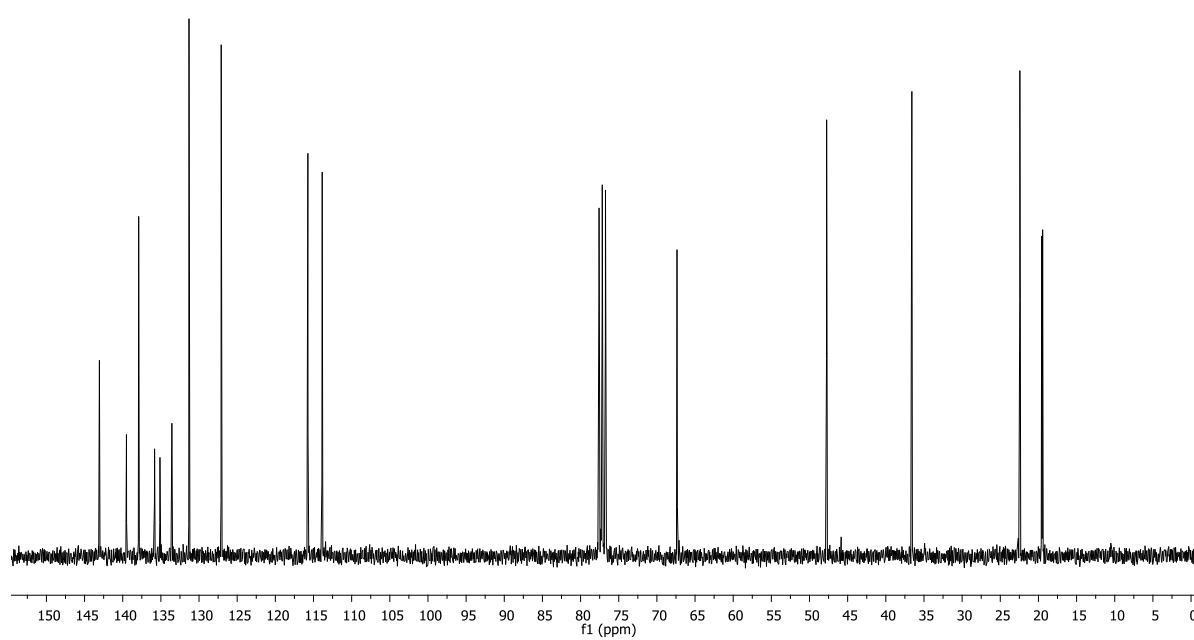
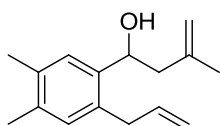
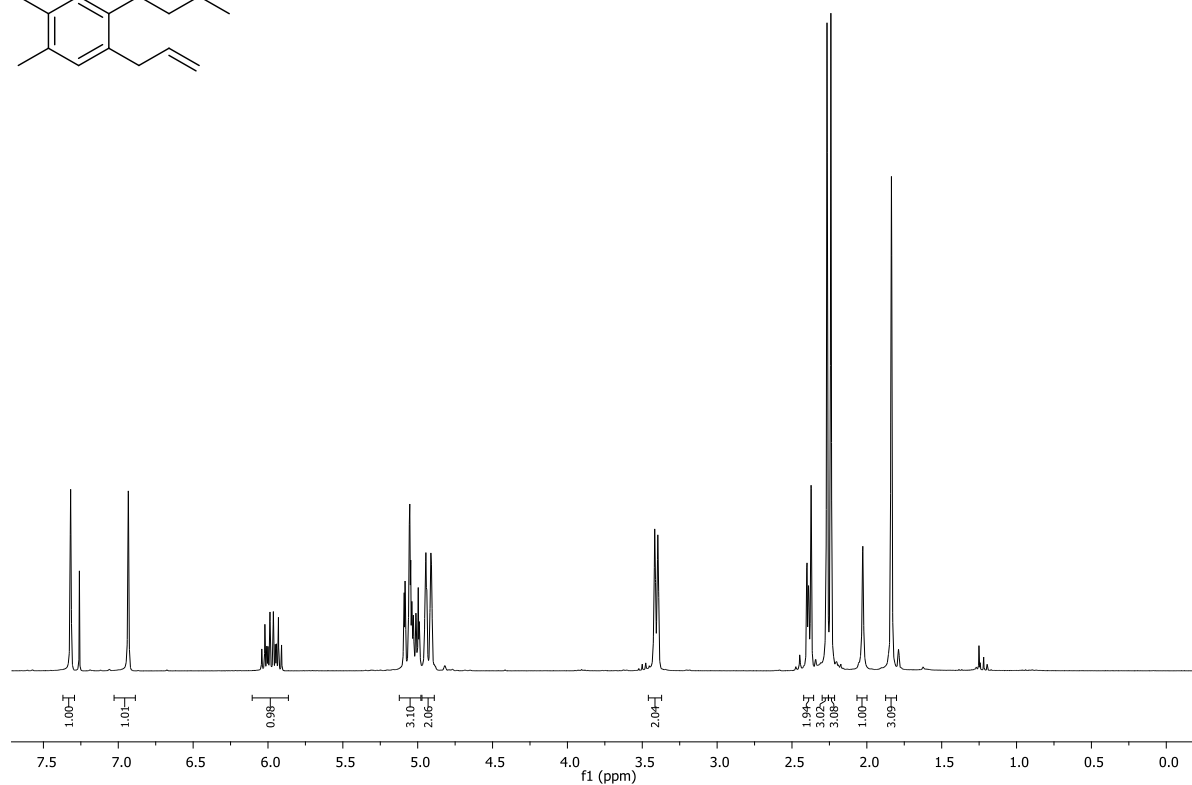
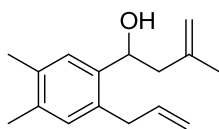
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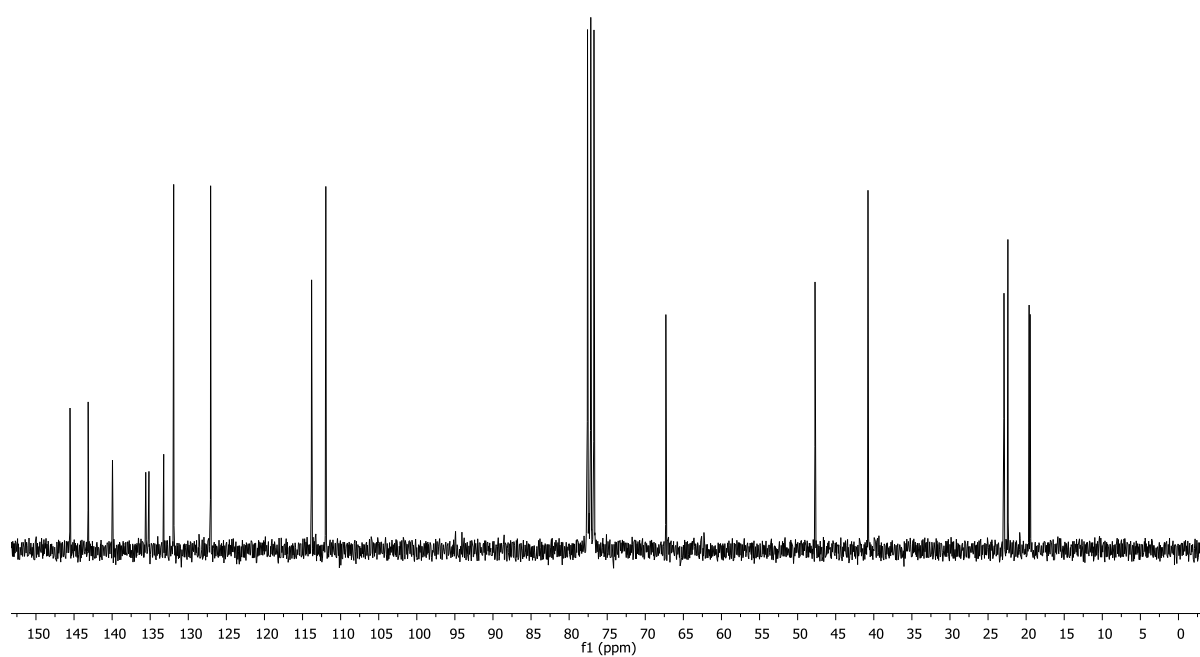
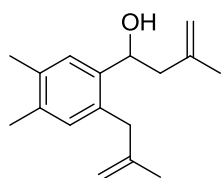
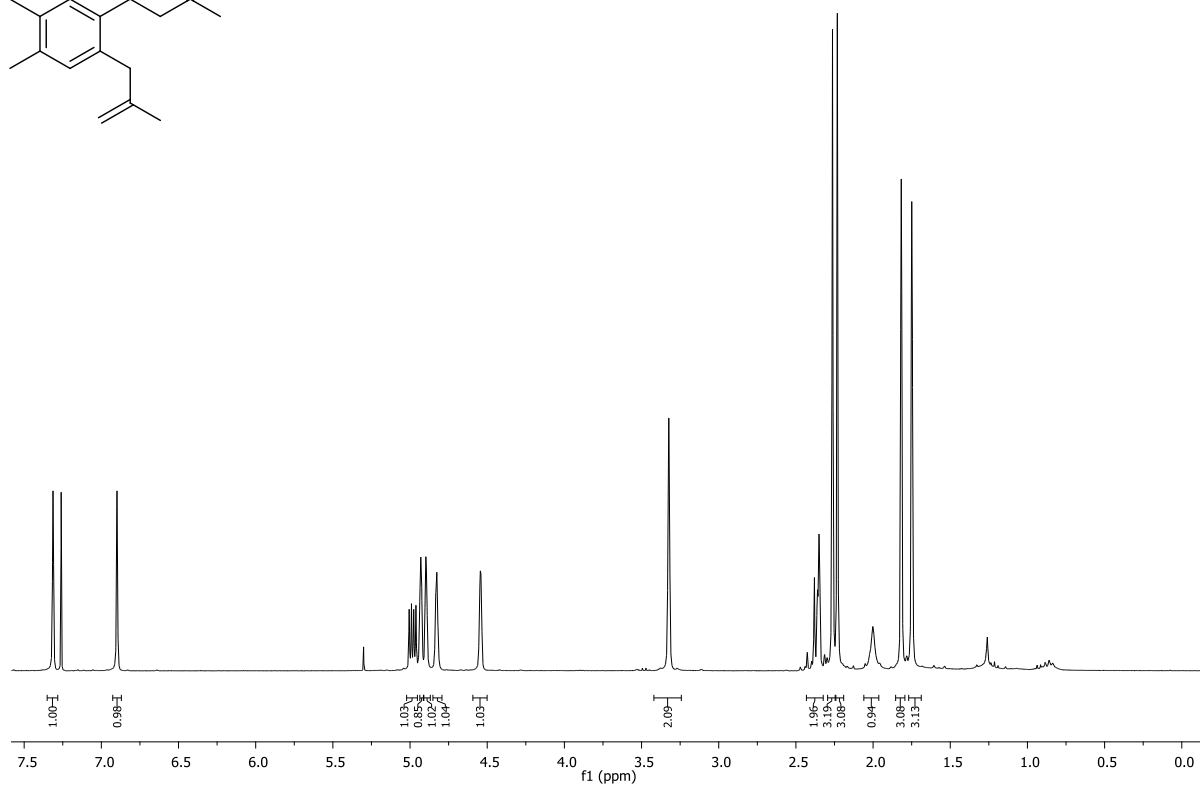
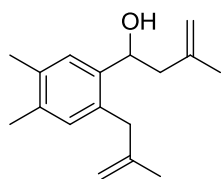
2-(4,5-Dimethyl-2-methylenhex-4-enyl)benzaldehyde (25)

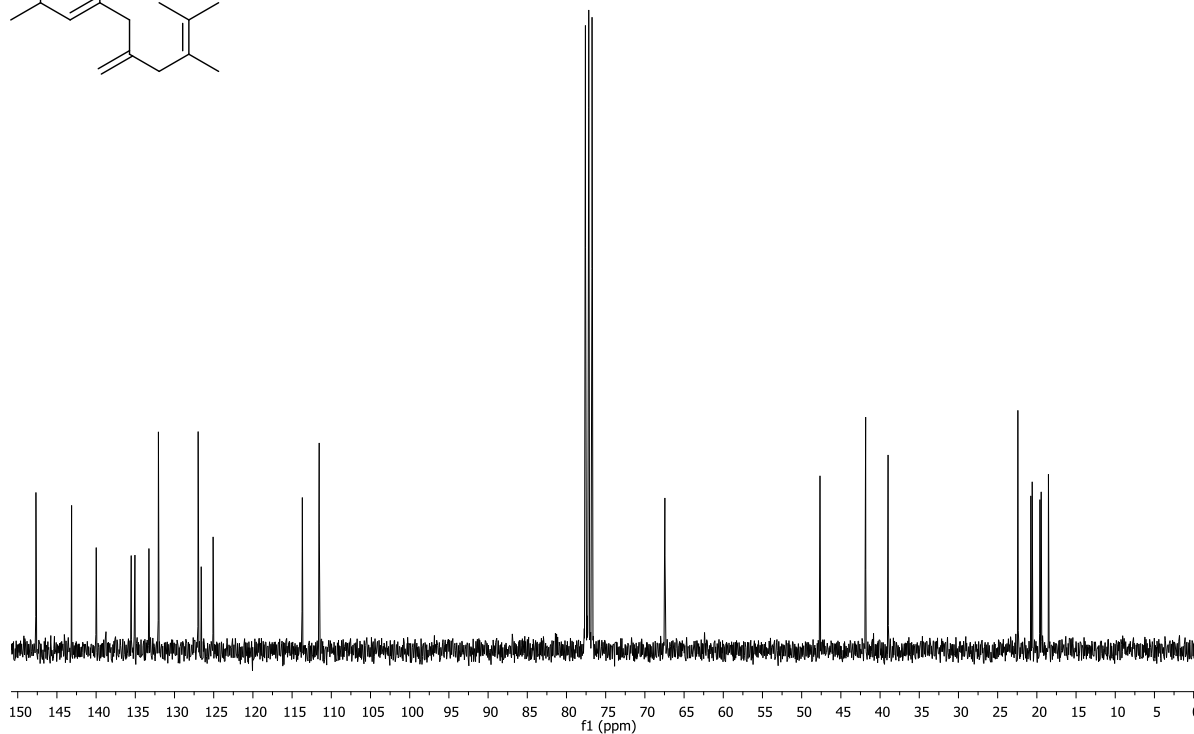
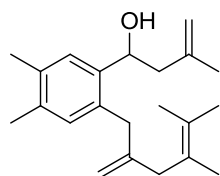
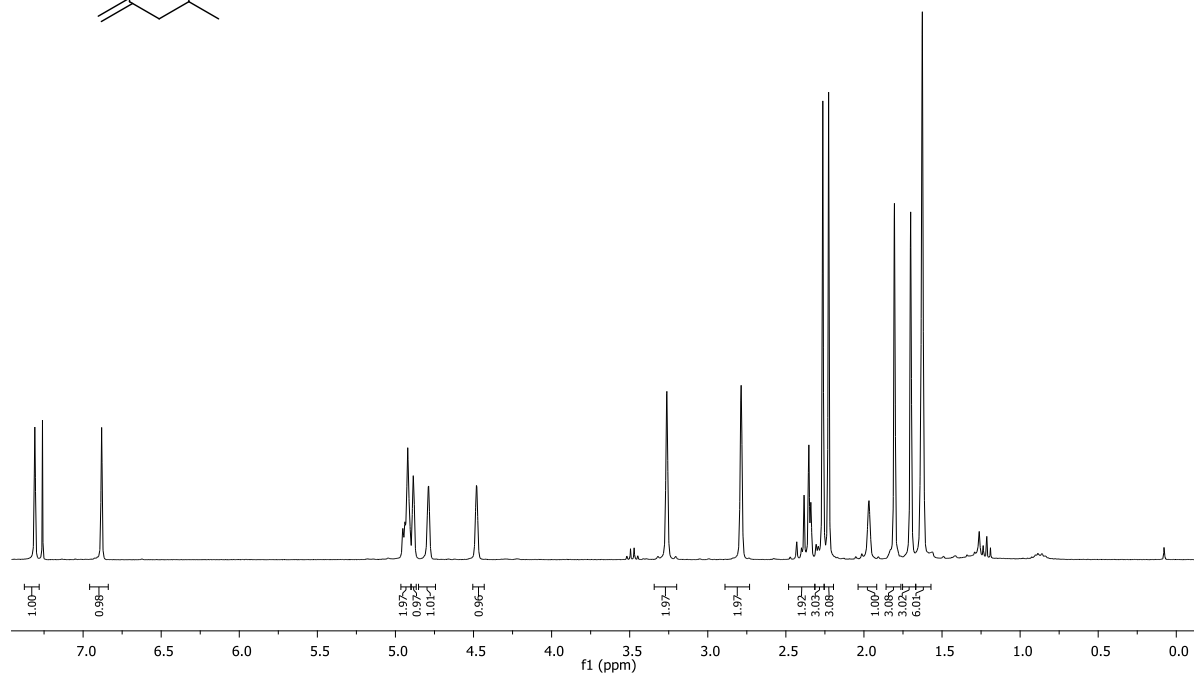
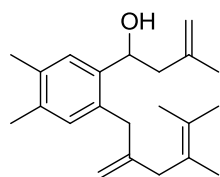
Intermediate: 1-(2-Allyl-4,5-dimethylphenyl)but-3-en-1-ol

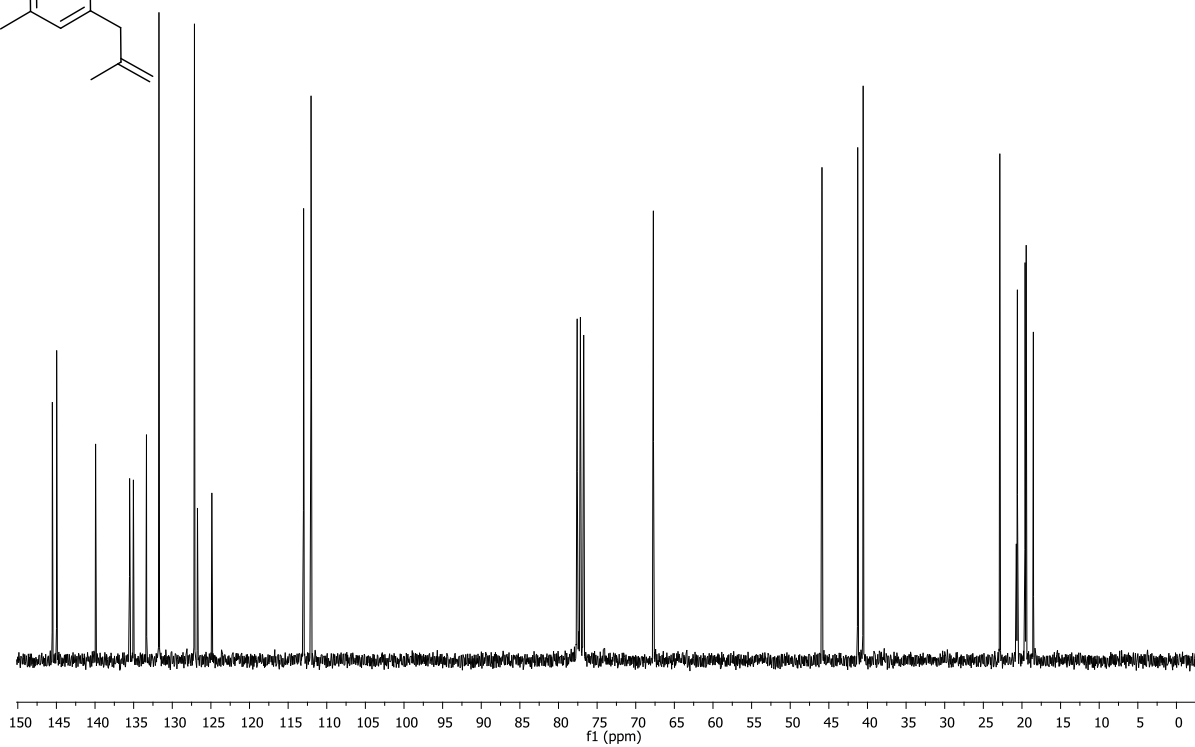
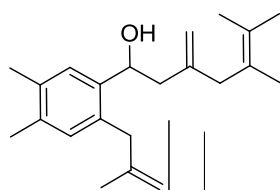
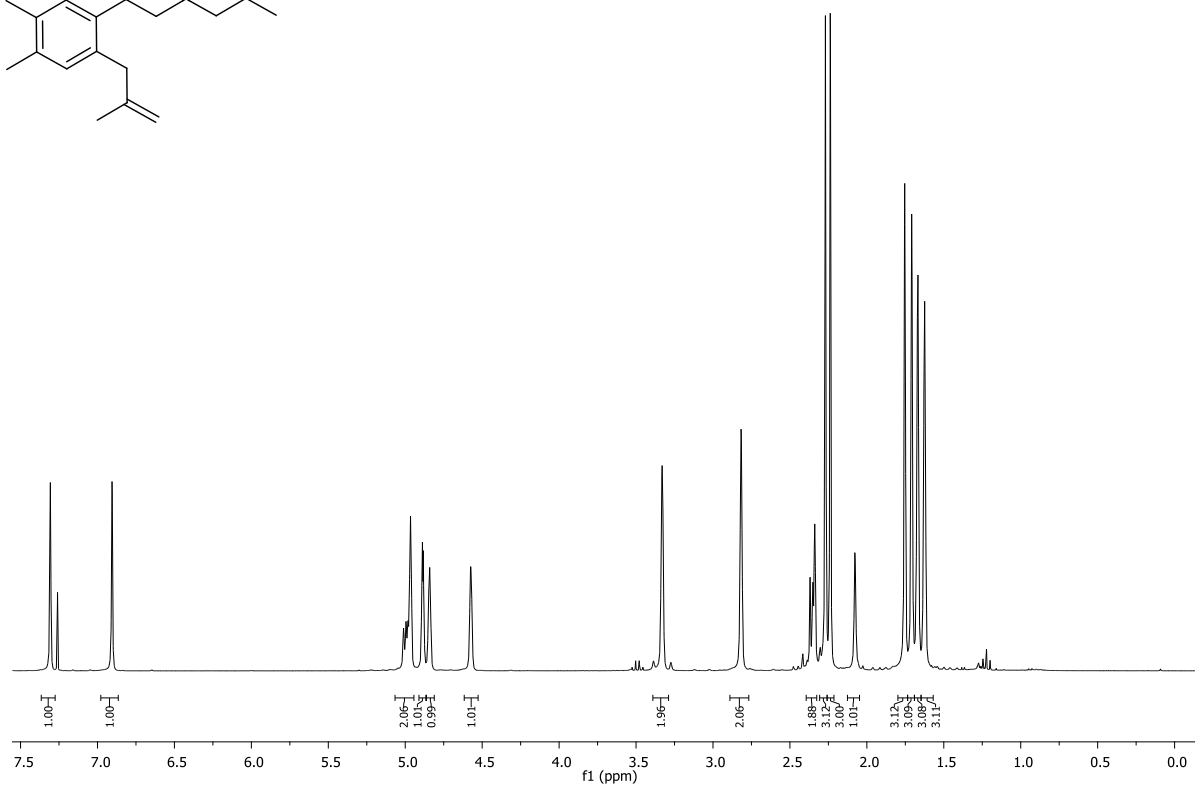
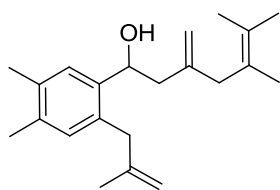
Intermediate: 1-(4,5-Dimethyl-2-(2-methylallyl)phenyl)but-3-en-1-ol

Intermediate: 1-(2-(4,5-Dimethyl-2-methylenhex-4-enyl)-4,5-dimethylphenyl)but-3-en-1-ol

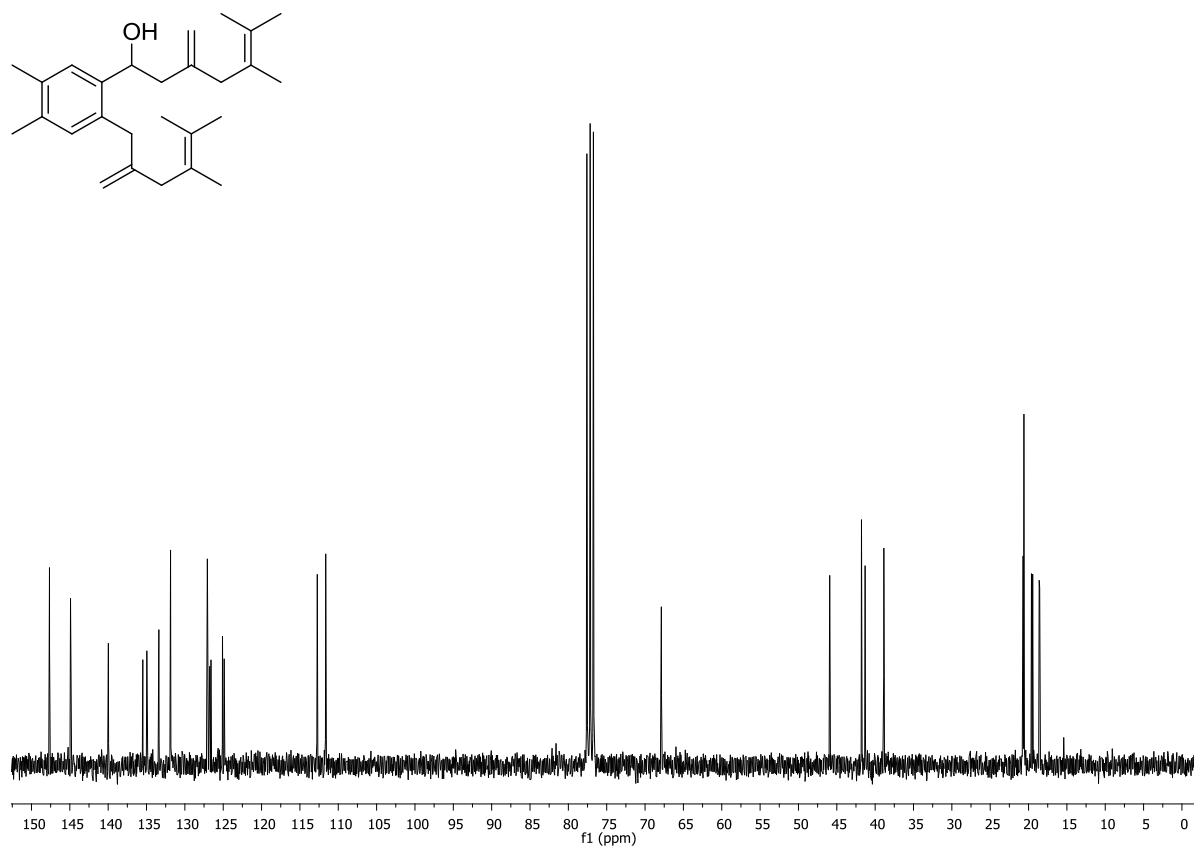
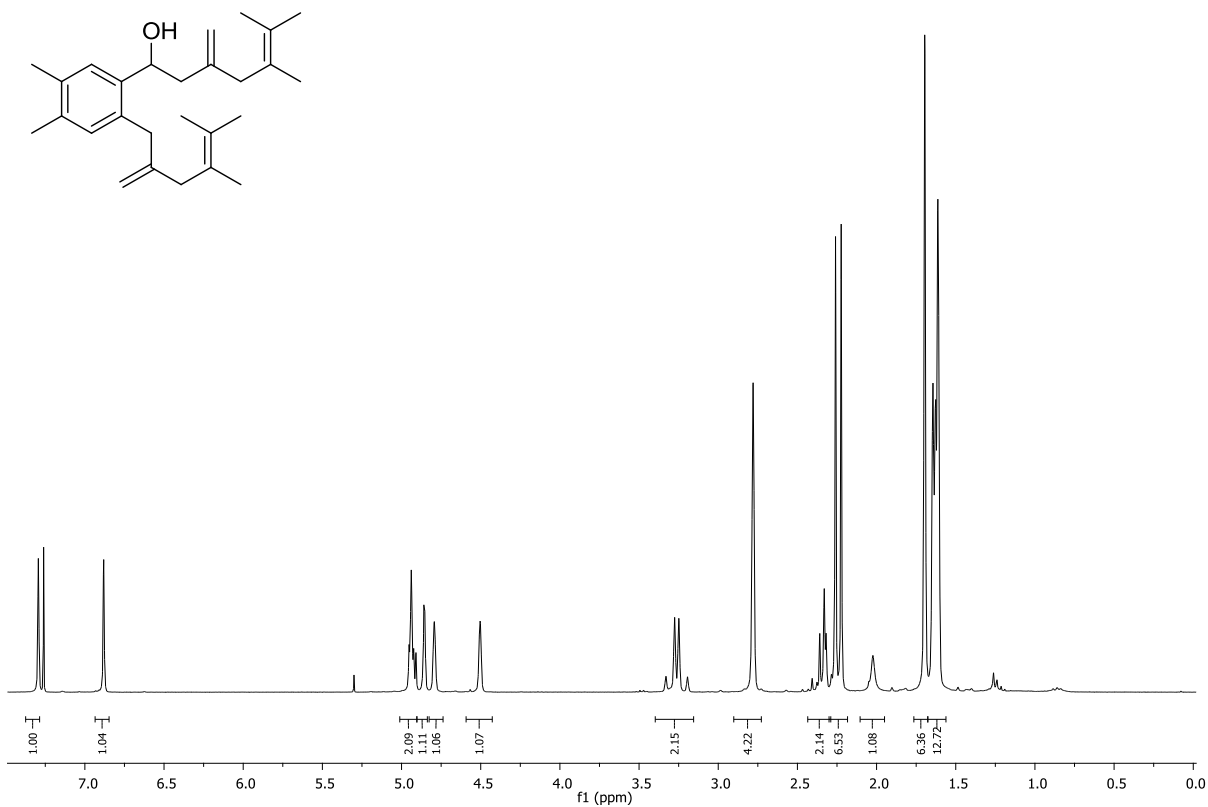
Intermediate: 1-(2-Allyl-4,5-dimethylphenyl)-3-methylbut-3-en-1-ol

Intermediate: 1-(4,5-Dimethyl-2-(2-methylallyl)phenyl)-3-methylbut-3-en-1-ol

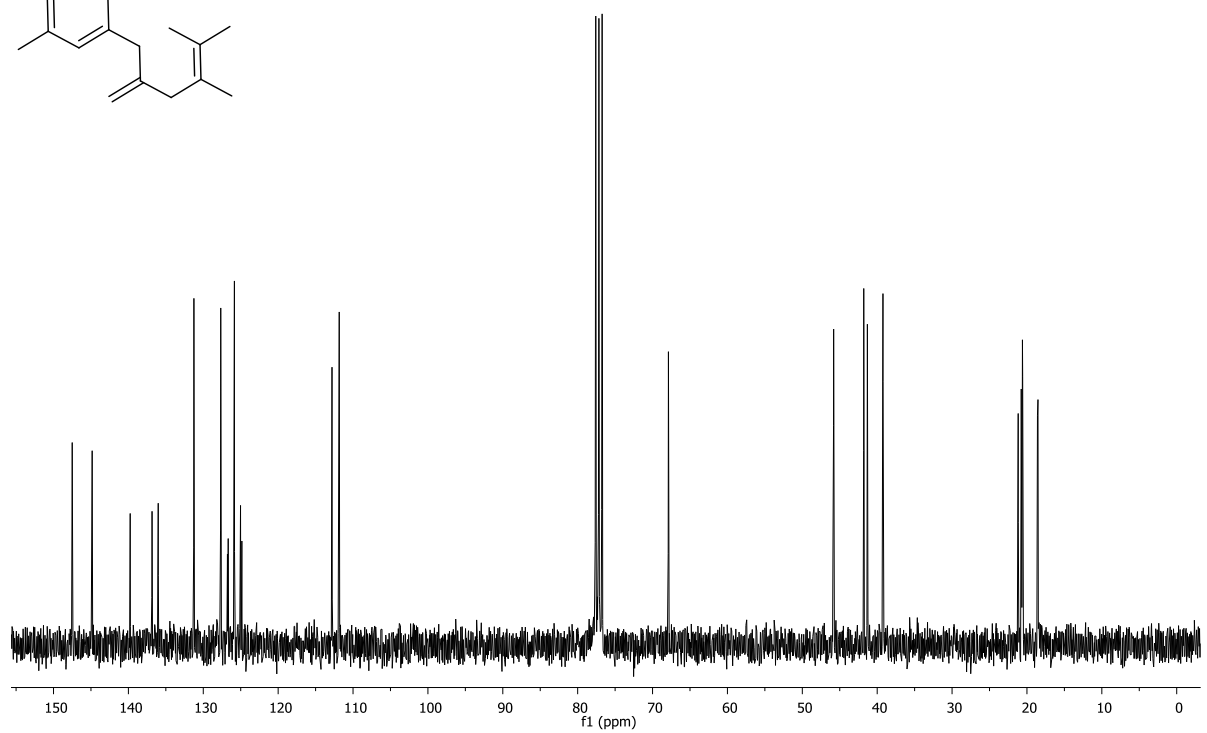
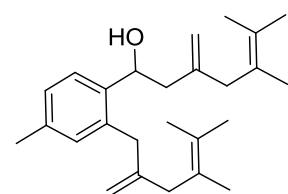
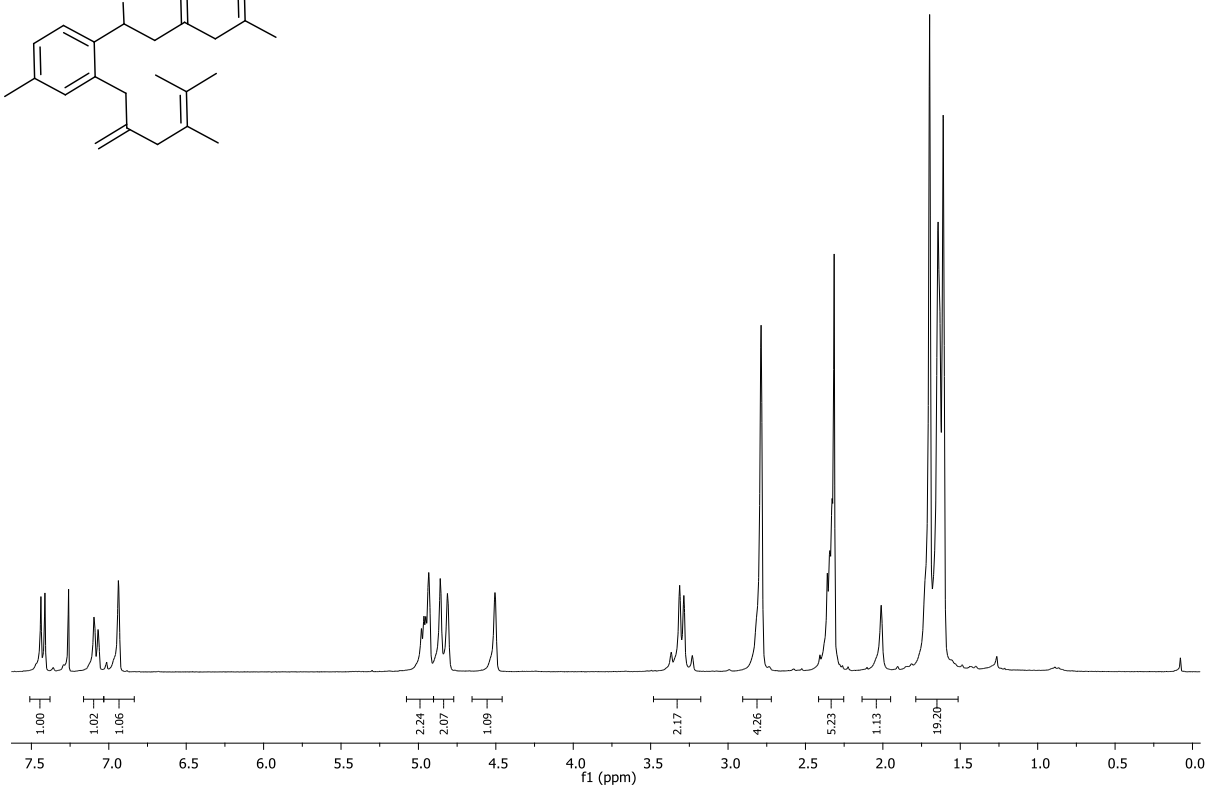
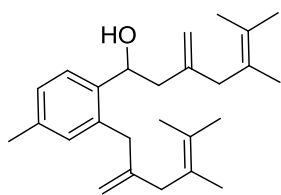
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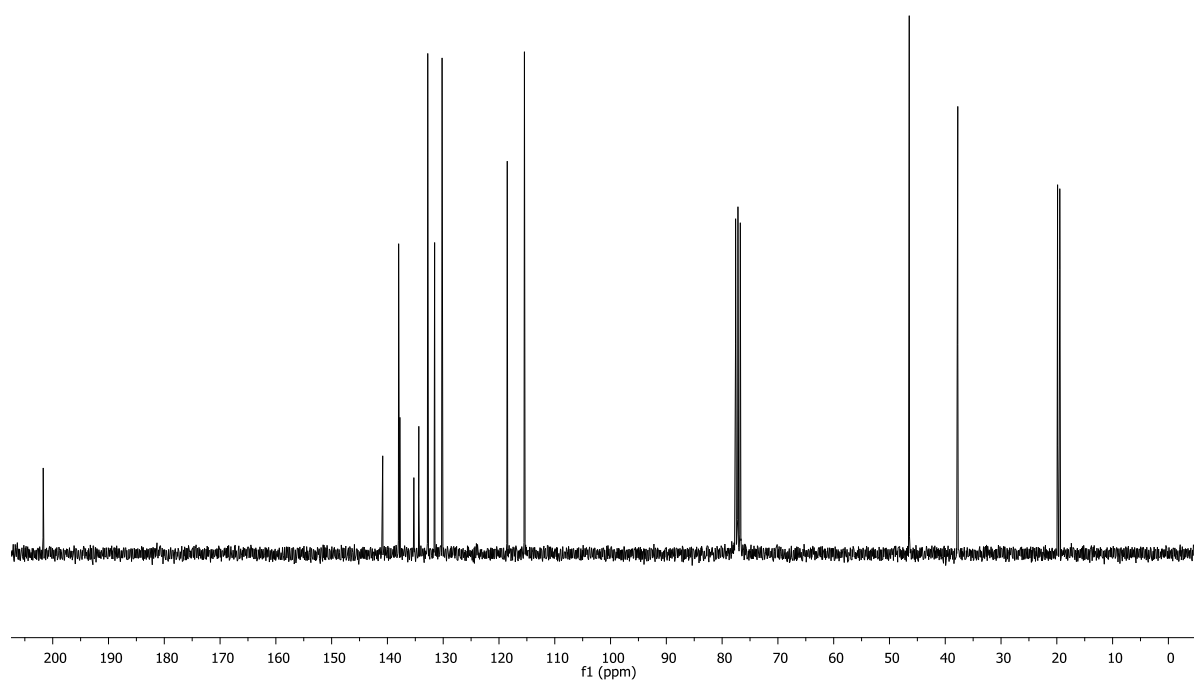
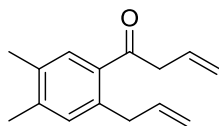
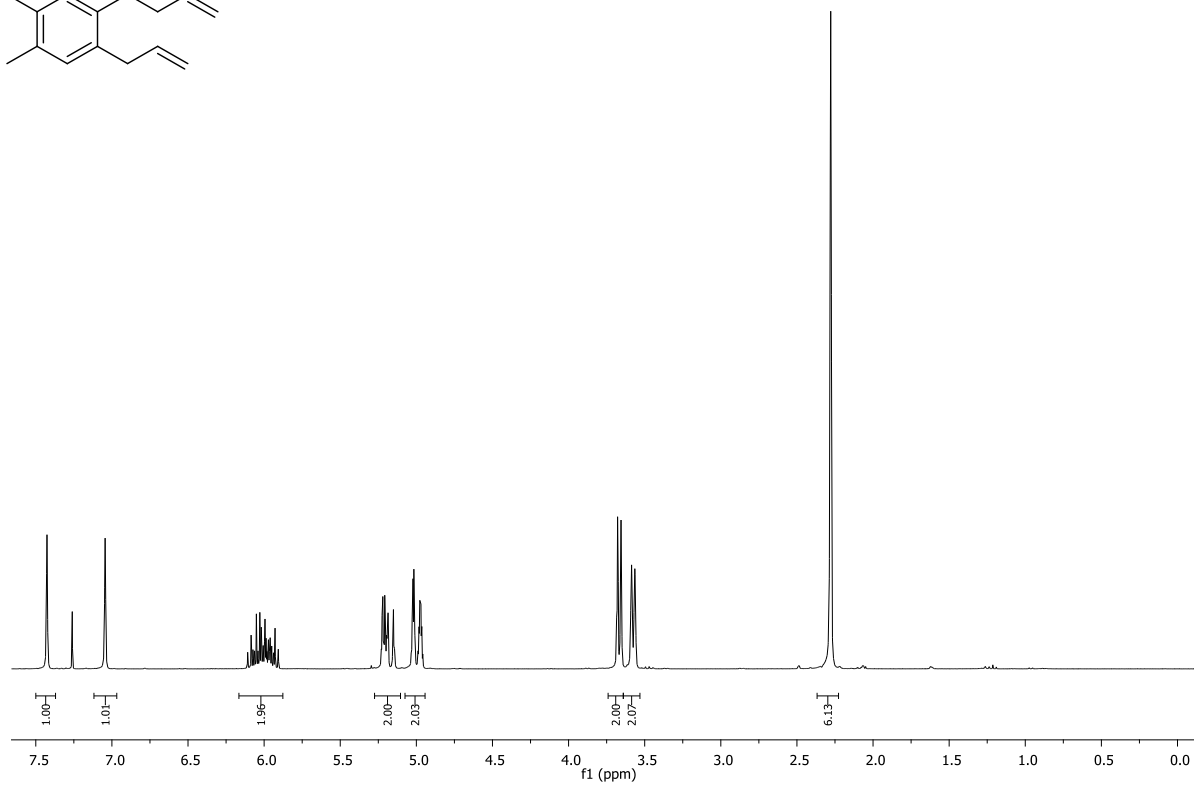
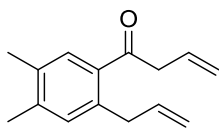
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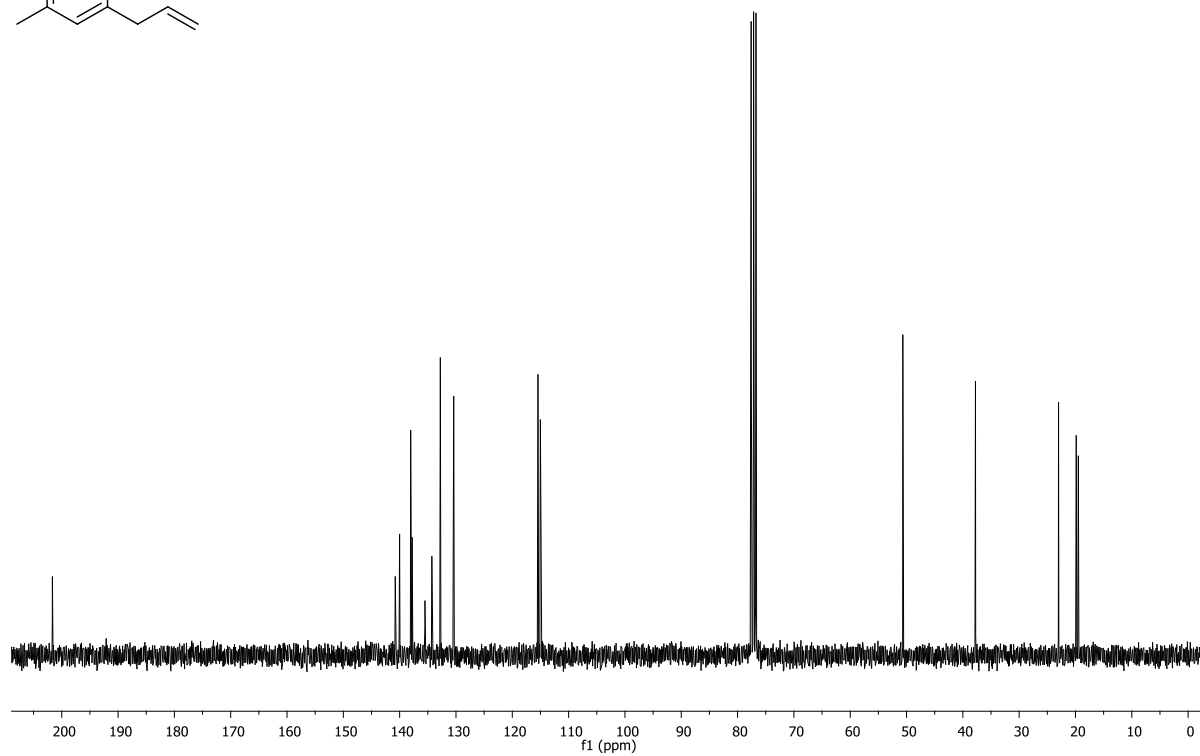
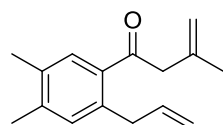
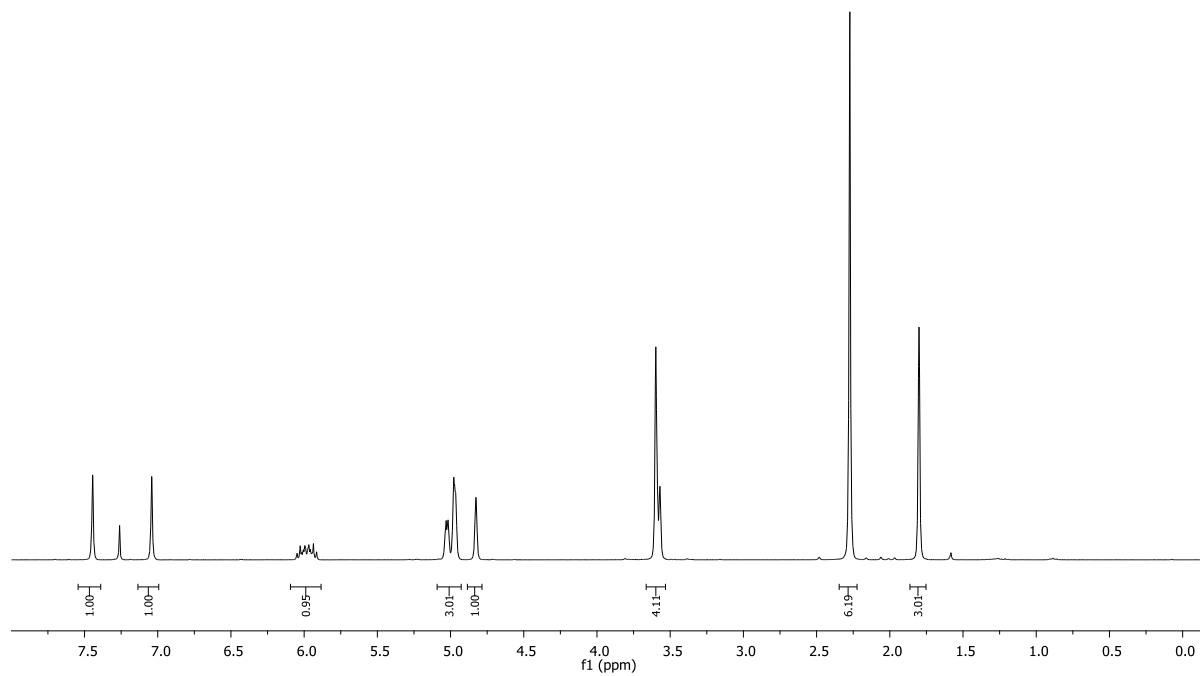
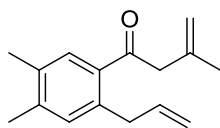
Intermediate: 1-(2-(4,5-Dimethyl-2-methylenhex-4-enyl)-4,5-dimethylphenyl)-5,6-dimethyl-3-methylenhept-5-en-1-ol

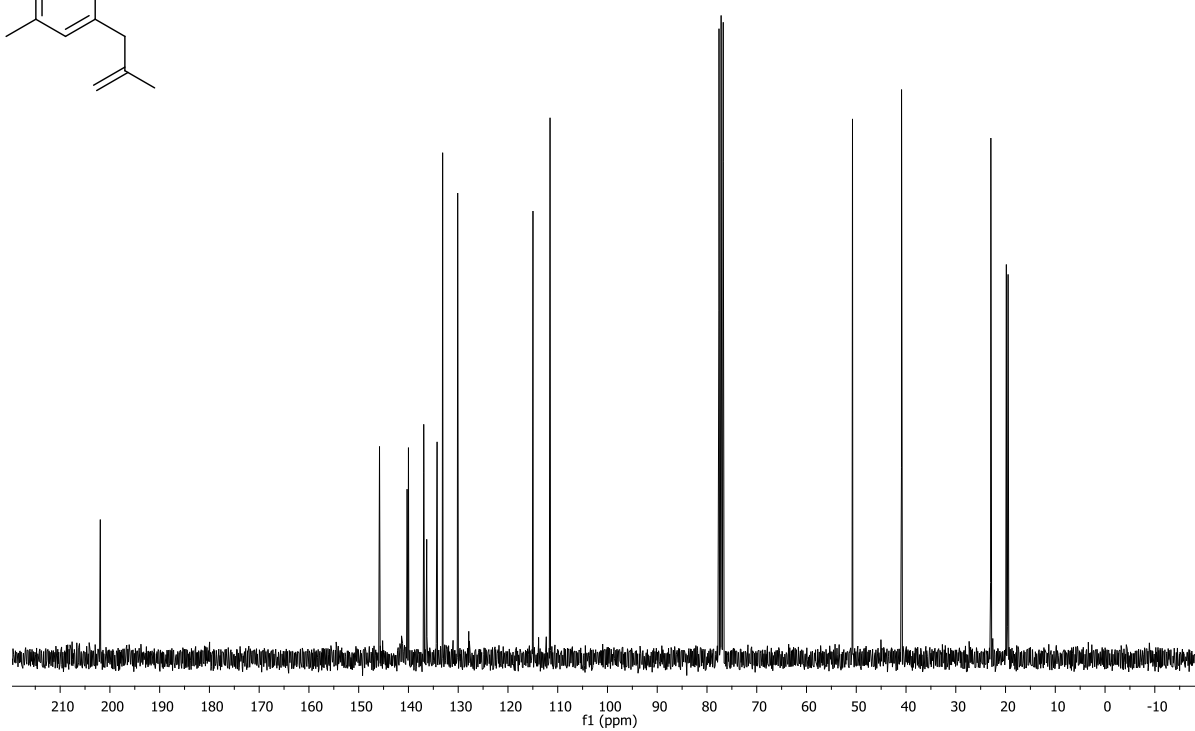
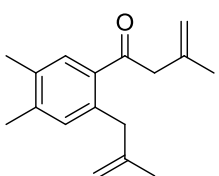
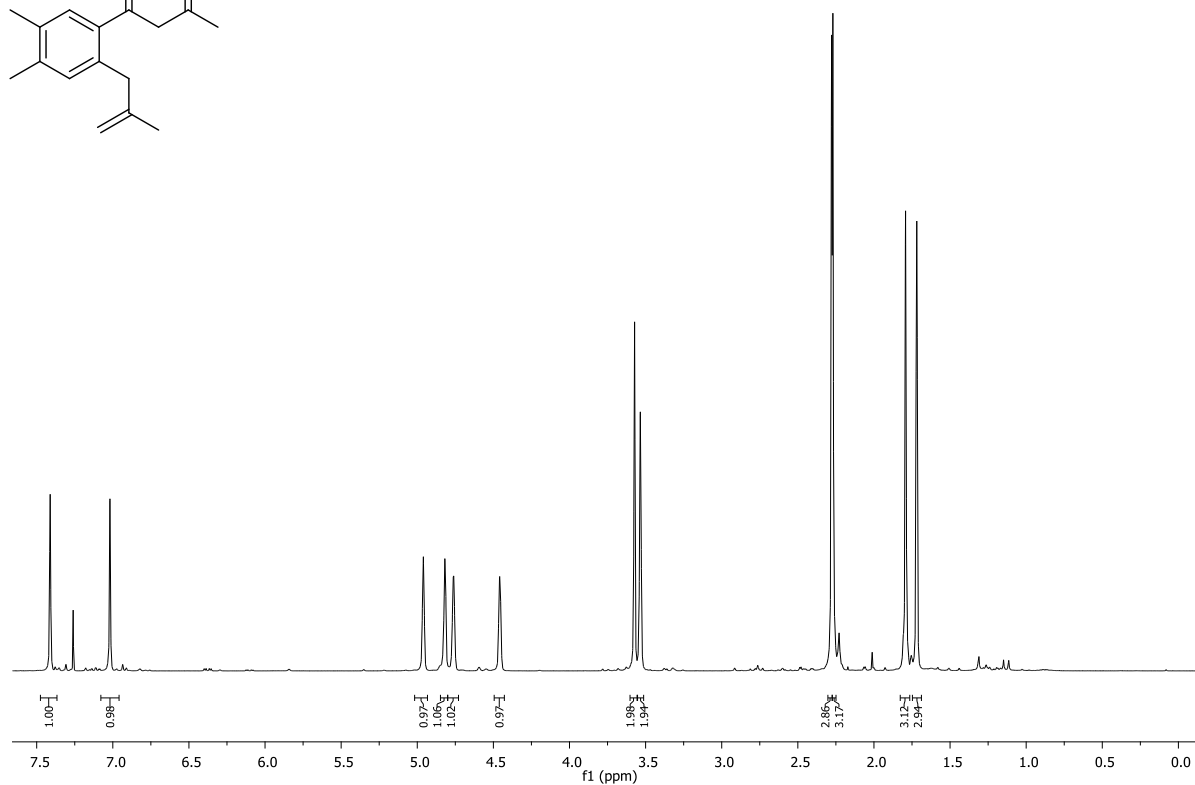
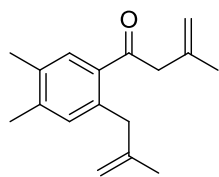


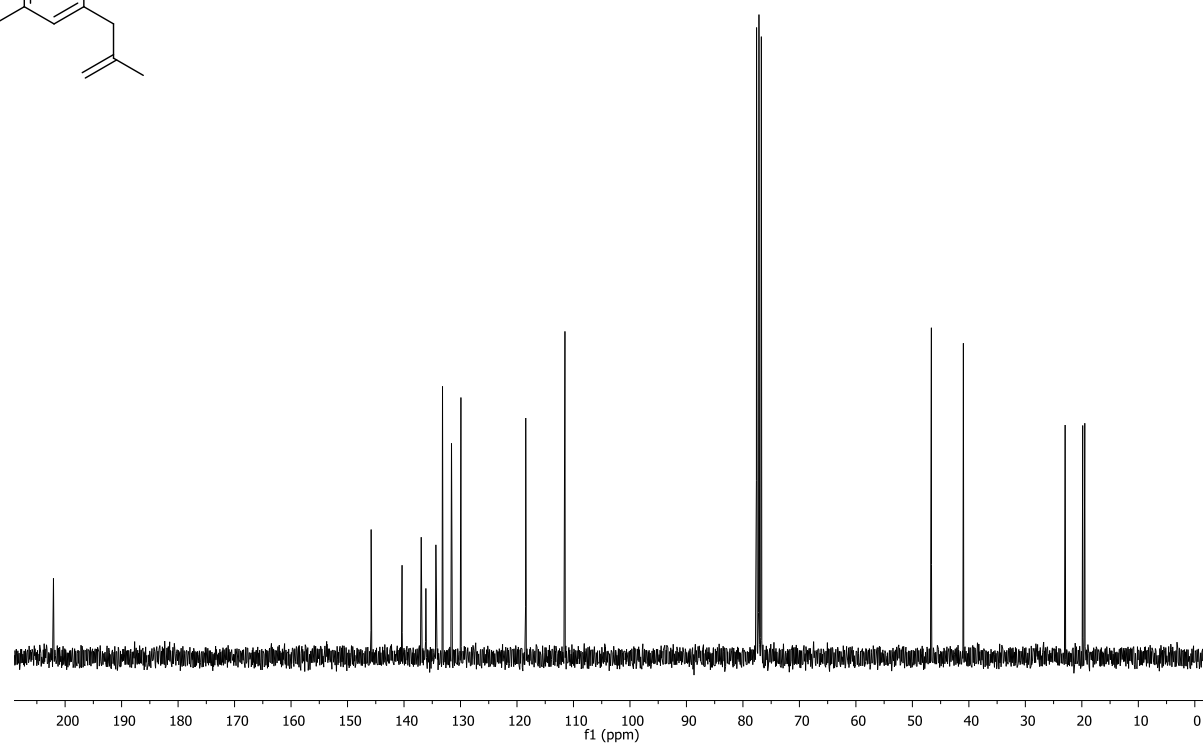
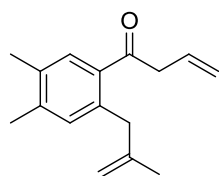
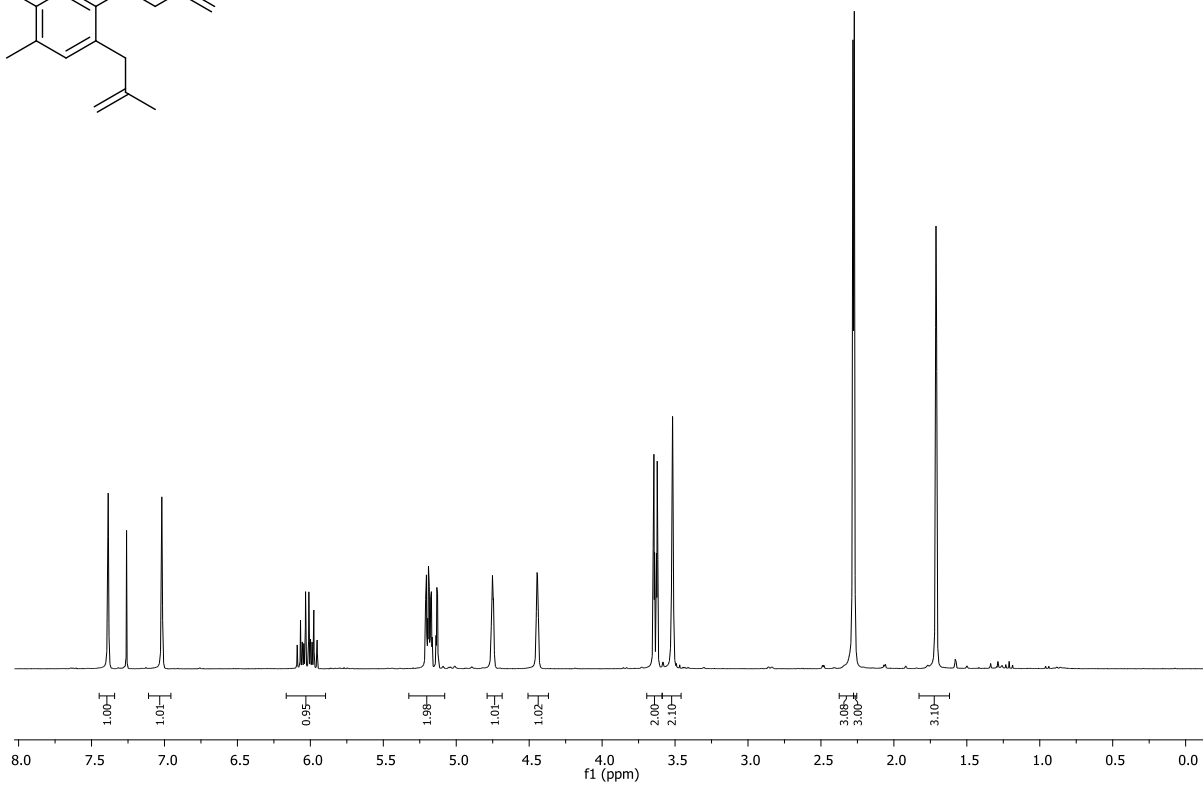
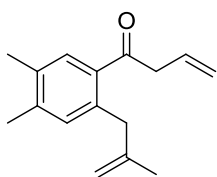
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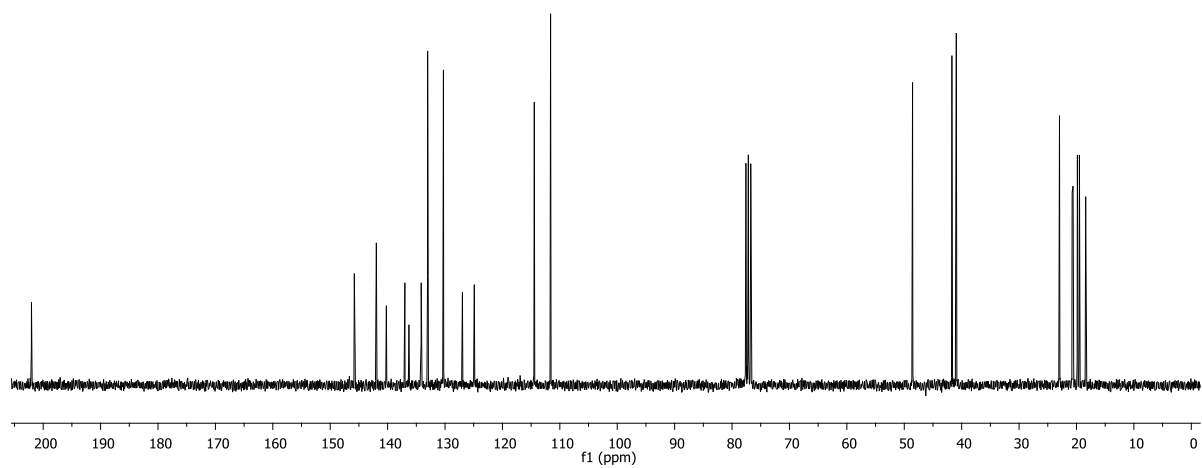
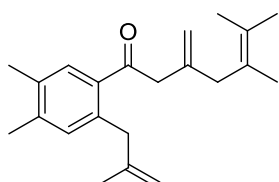
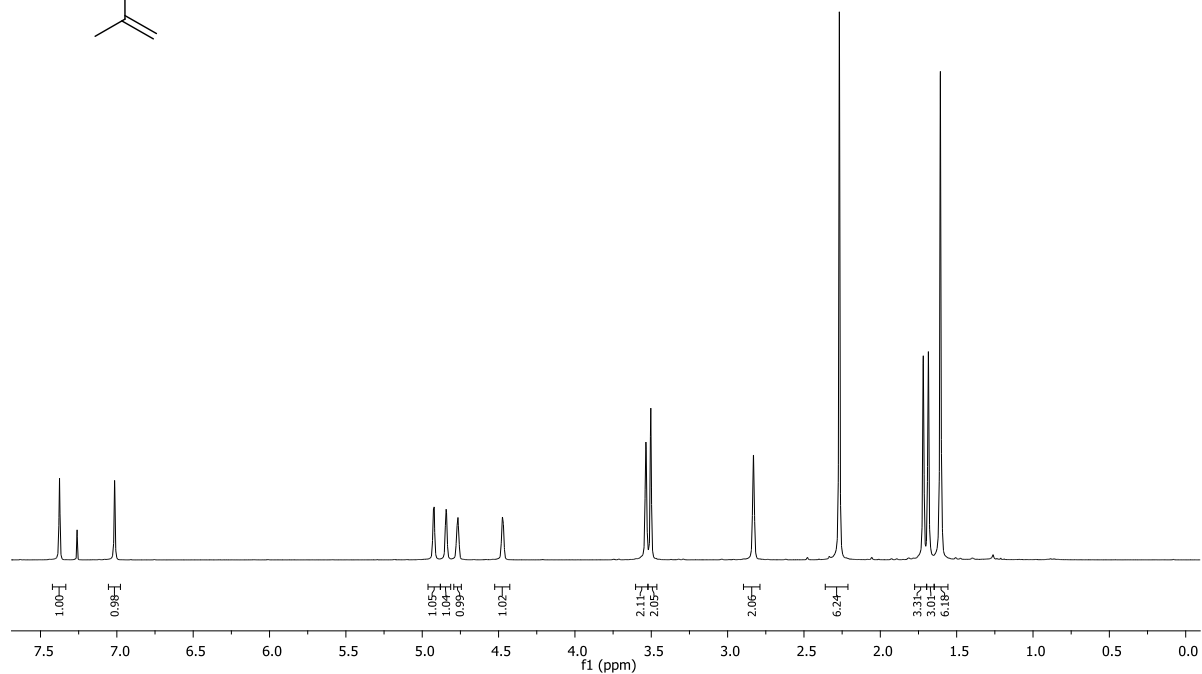
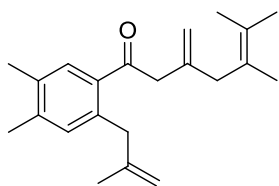


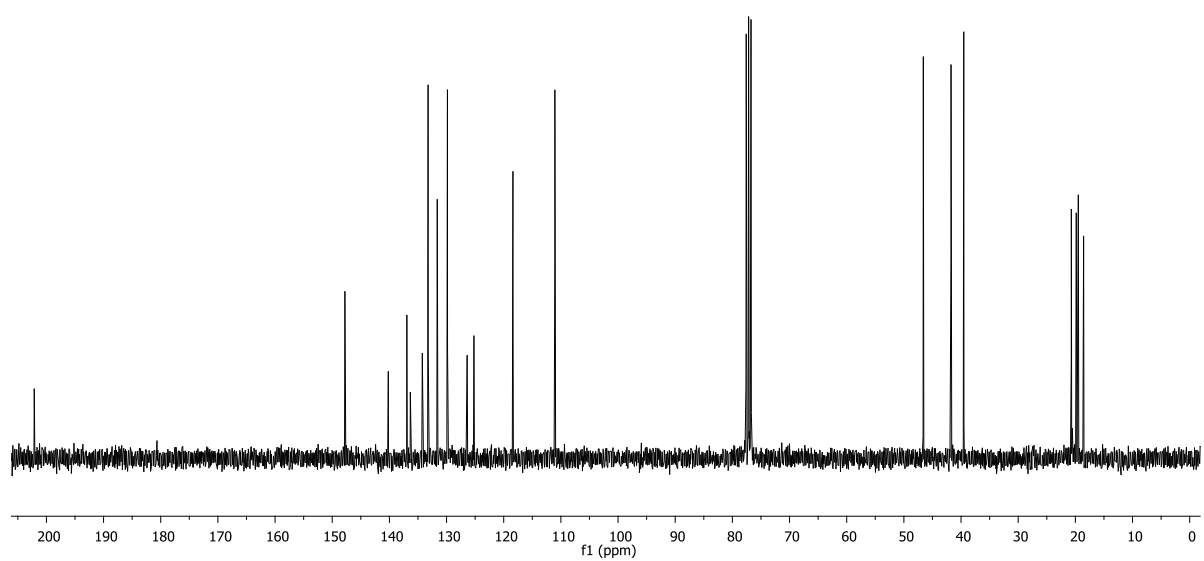
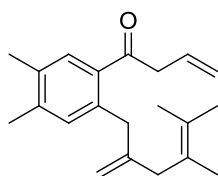
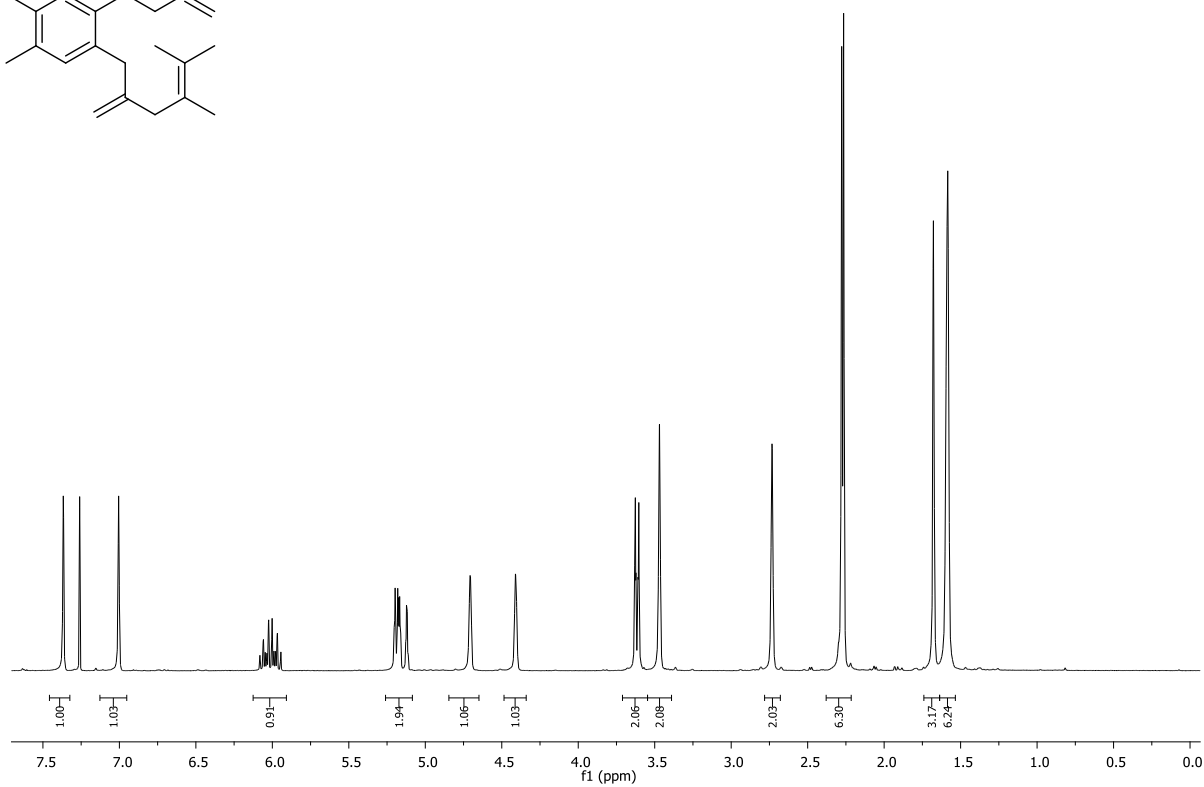
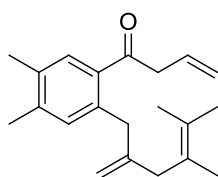
1-(2-Allyl-4,5-dimethylphenyl)but-3-en-1-one (16)

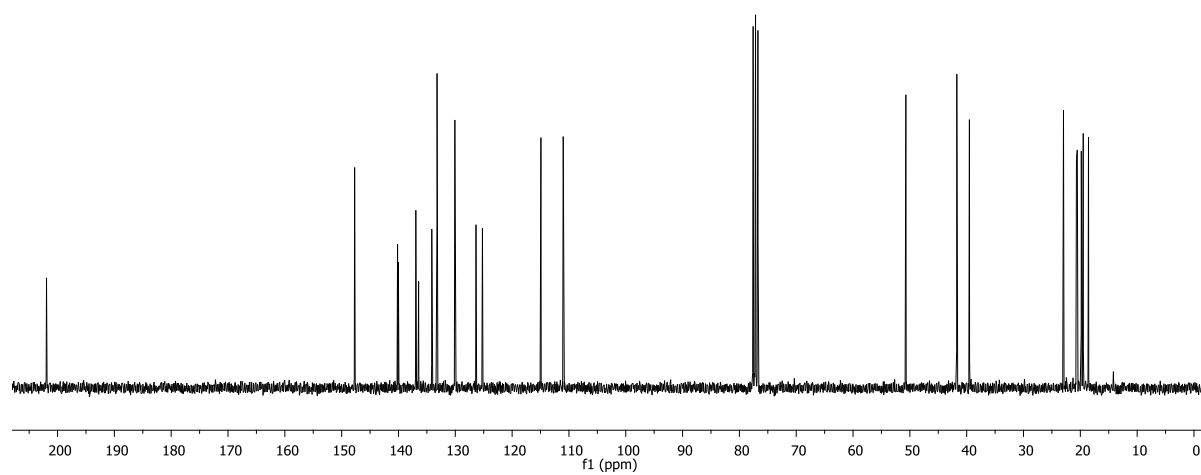
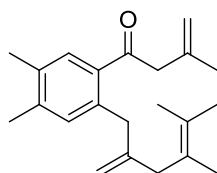
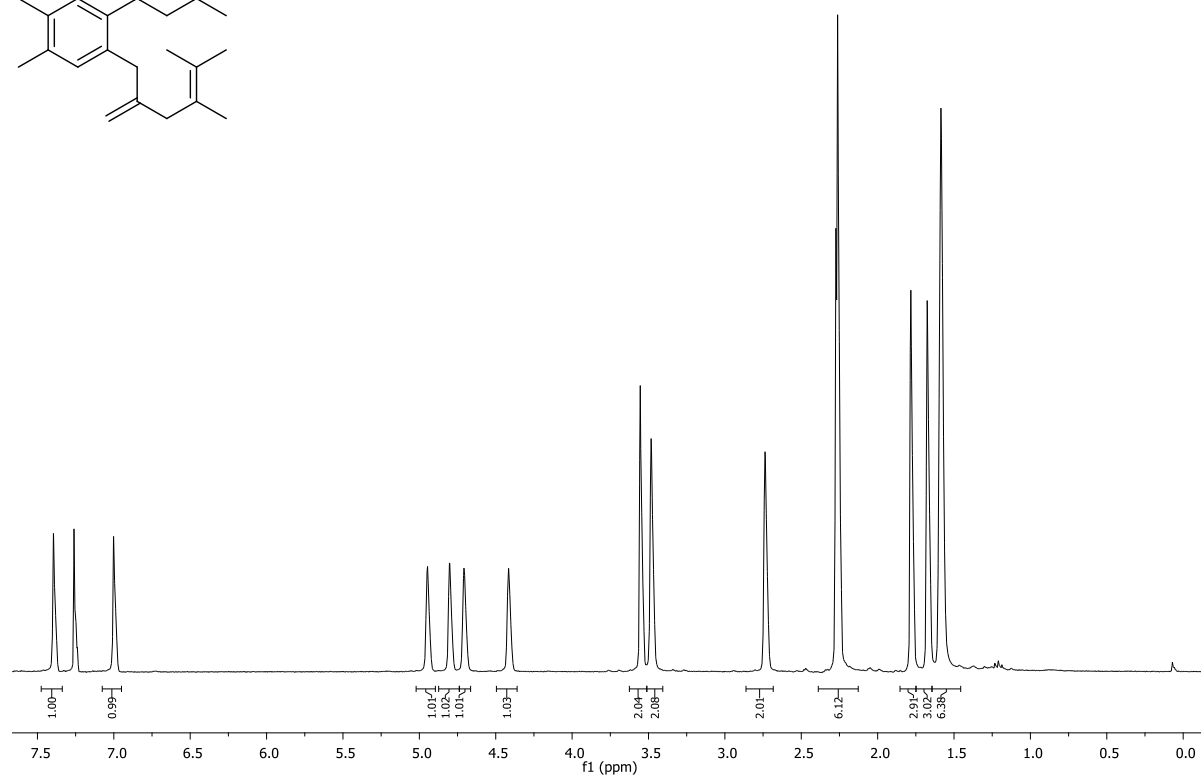
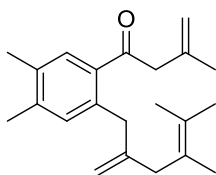
1-(2-Allyl-4,5-dimethylphenyl)-3-methylbut-3-en-1-one (19)

1-(4,5-Dimethyl-2-(2-methylallyl)phenyl)-3-methylbut-3-en-1-one (20)

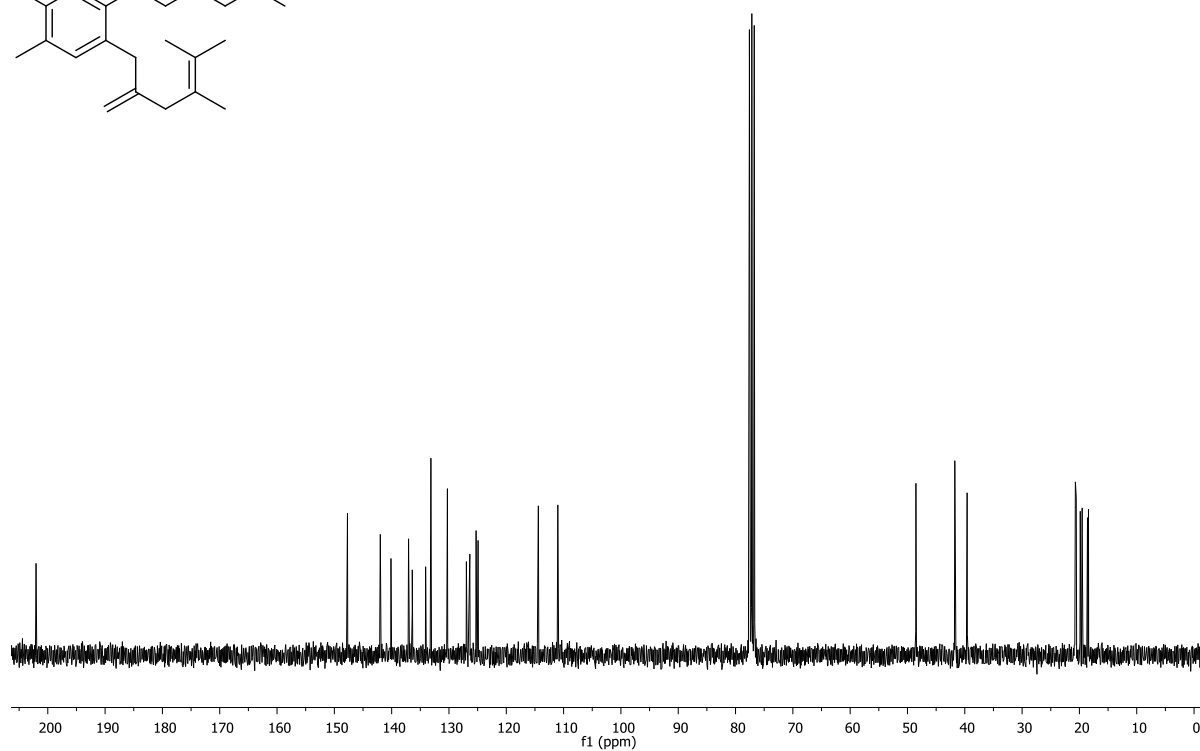
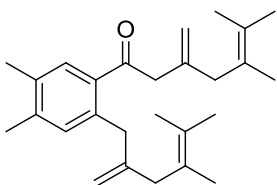
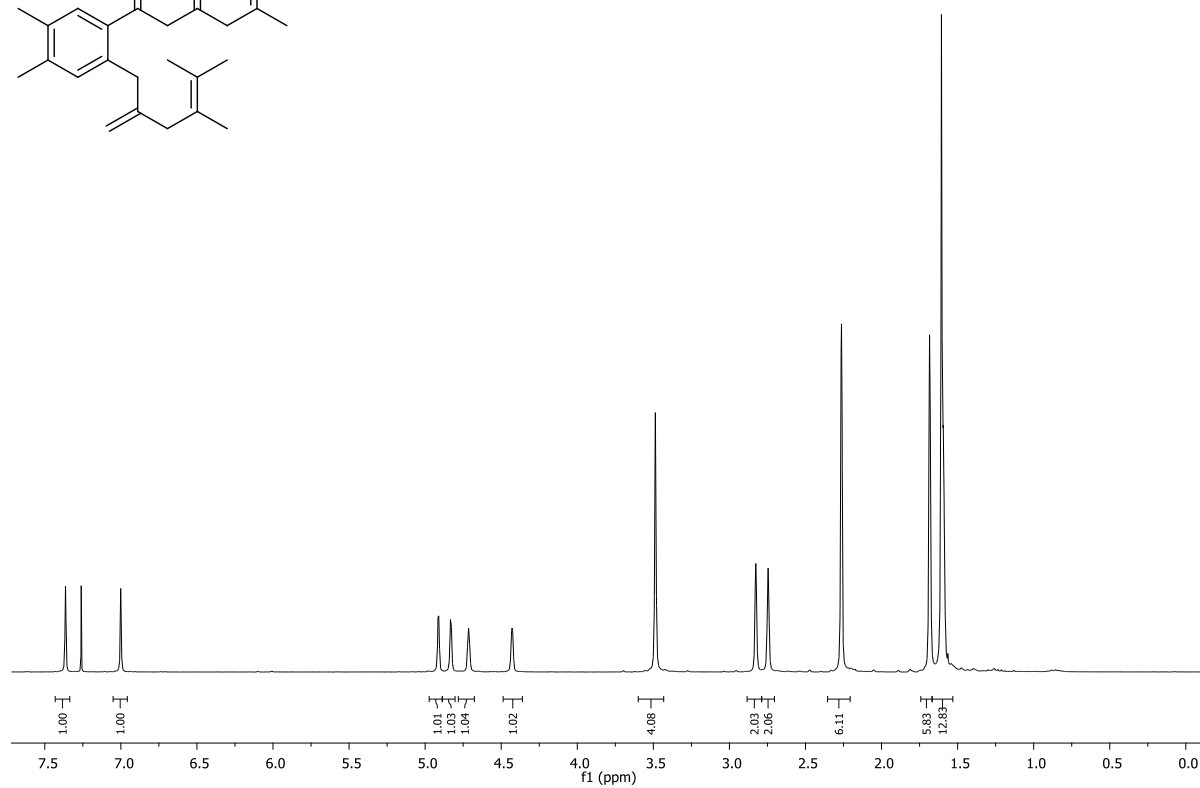
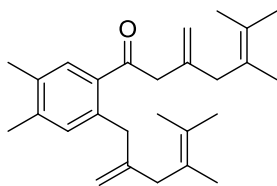
1-(4,5-Dimethyl-2-(2-methylallyl)phenyl)but-3-en-1-one (17)

1-(4,5-Dimethyl-2-(2-methylallyl)phenyl)-5,6-dimethyl-3-methylenehept-5-en-1-one (22)

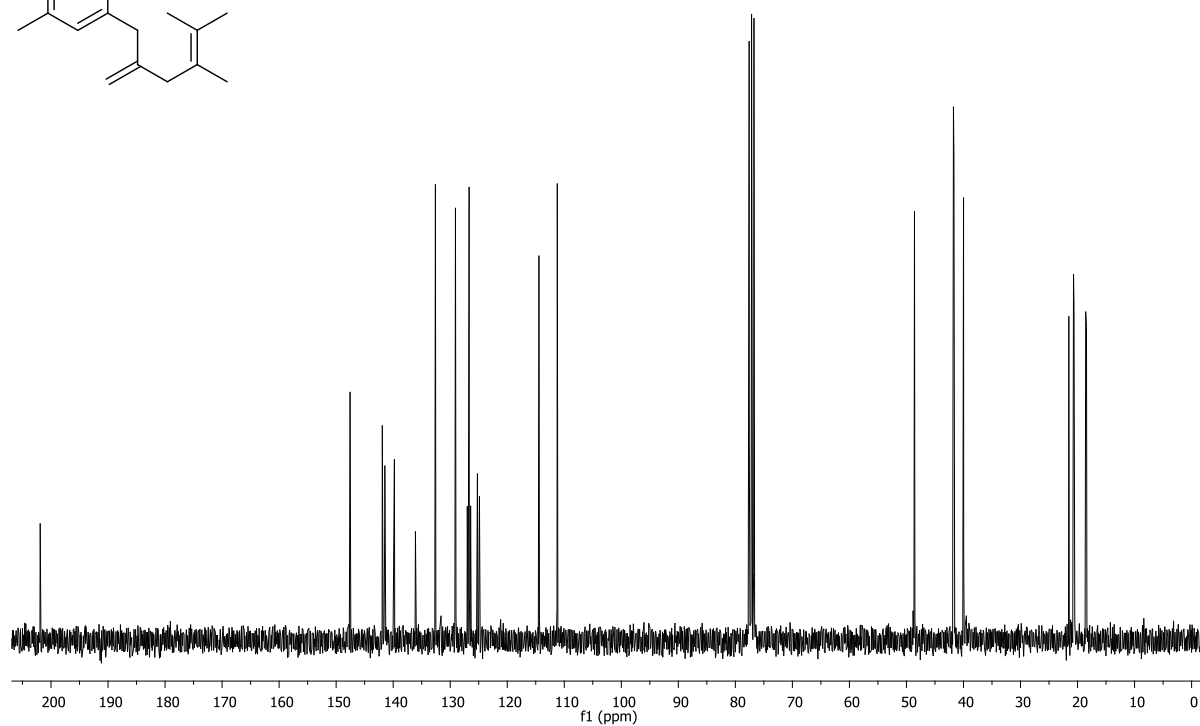
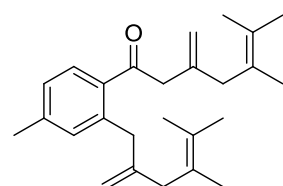
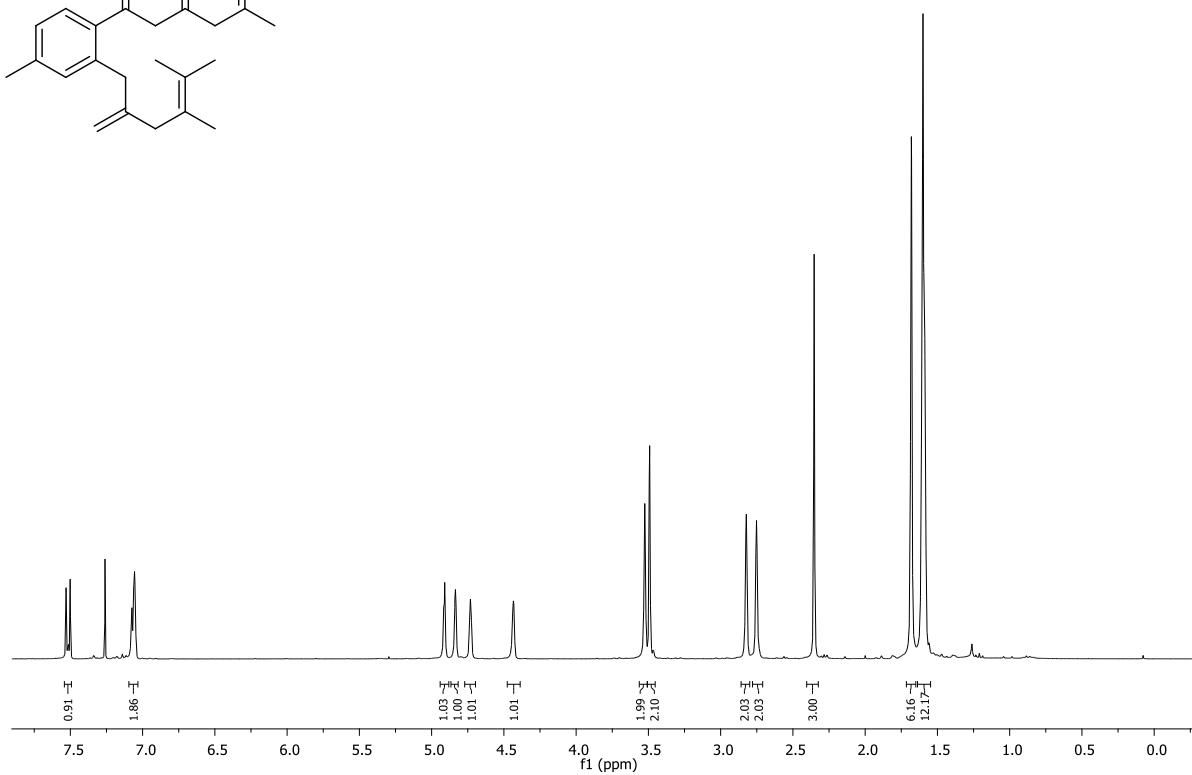
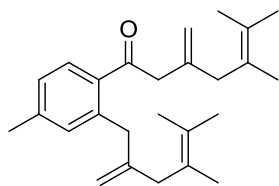
1-(2-(4,5-Dimethyl-2-methylenhex-4-enyl)-4,5-dimethylphenyl)but-3-en-1-one (18)

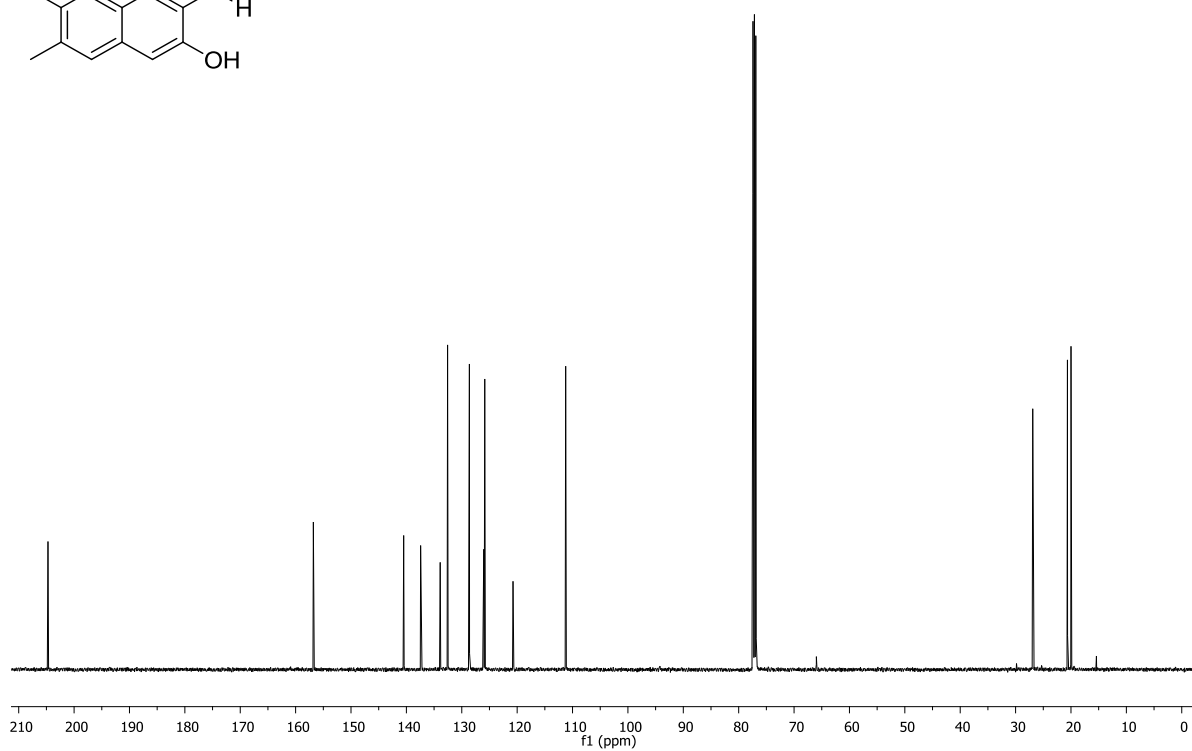
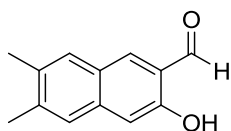
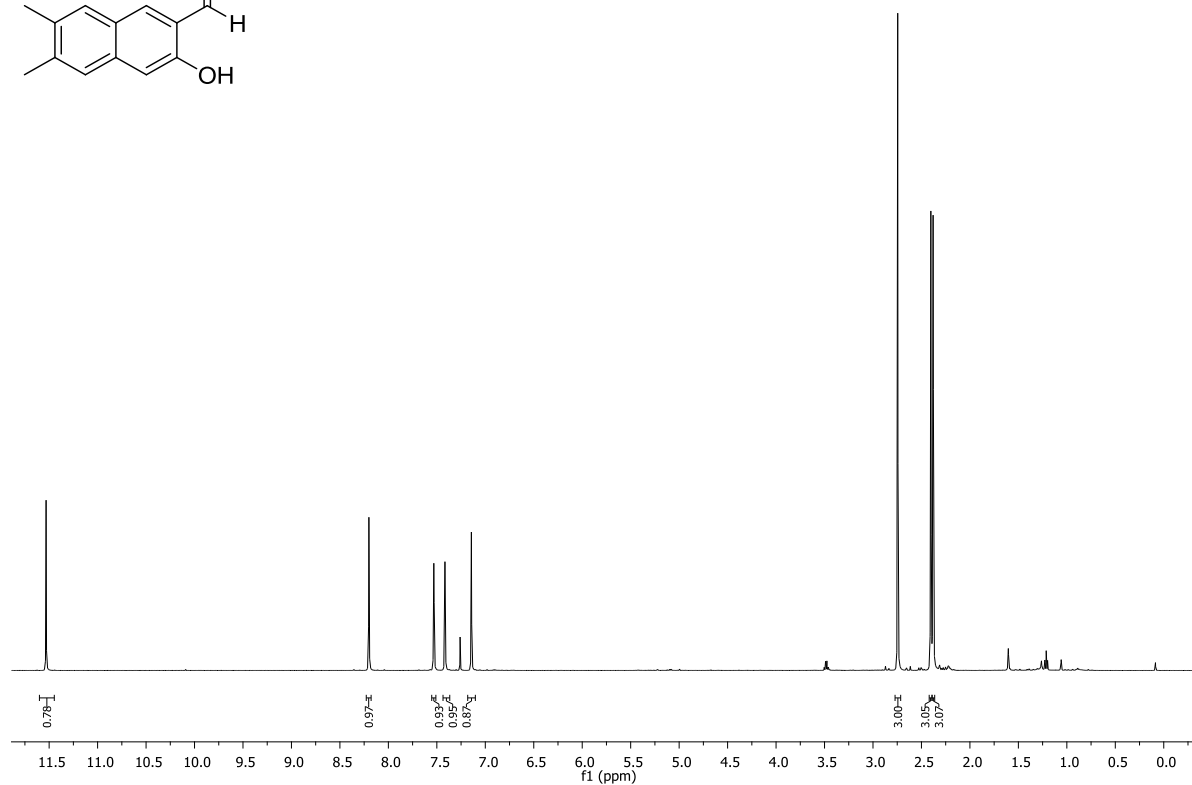
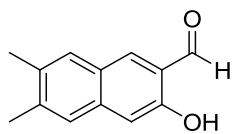
1-(2-(4,5-Dimethyl-2-methylenhex-4-enyl)-4,5-dimethylphenyl)-3-methylbut-3-en-1-one (21)

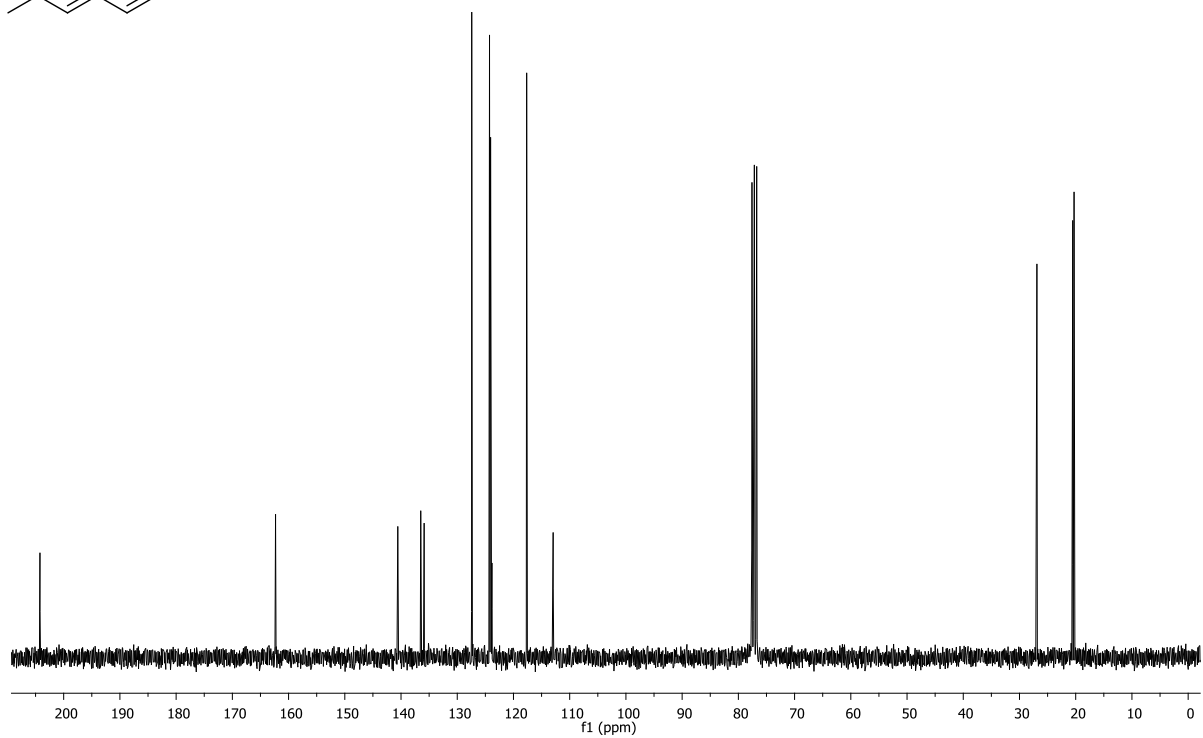
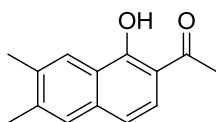
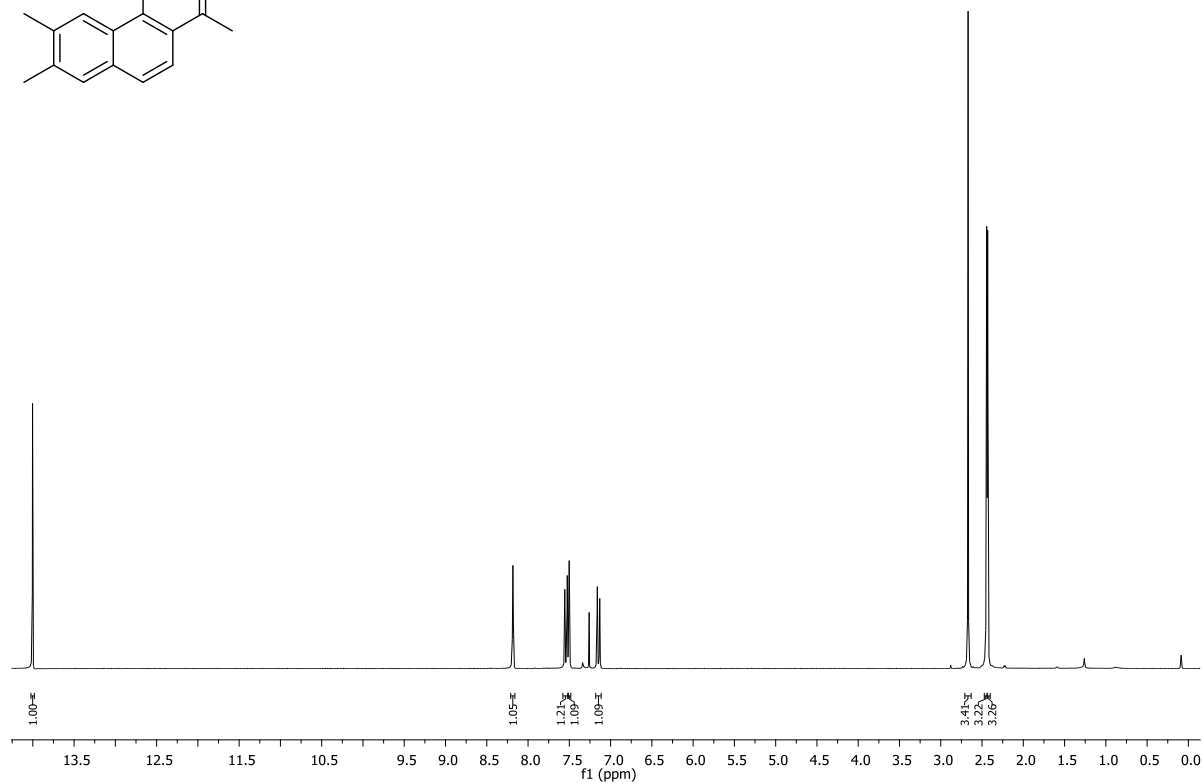
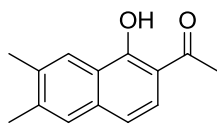
1-(2-(4,5-Dimethyl-2-methylenhex-4-enyl)-4,5-dimethylphenyl)-5,6-dimethyl-3-methylenhept-5-en-1-one (7)



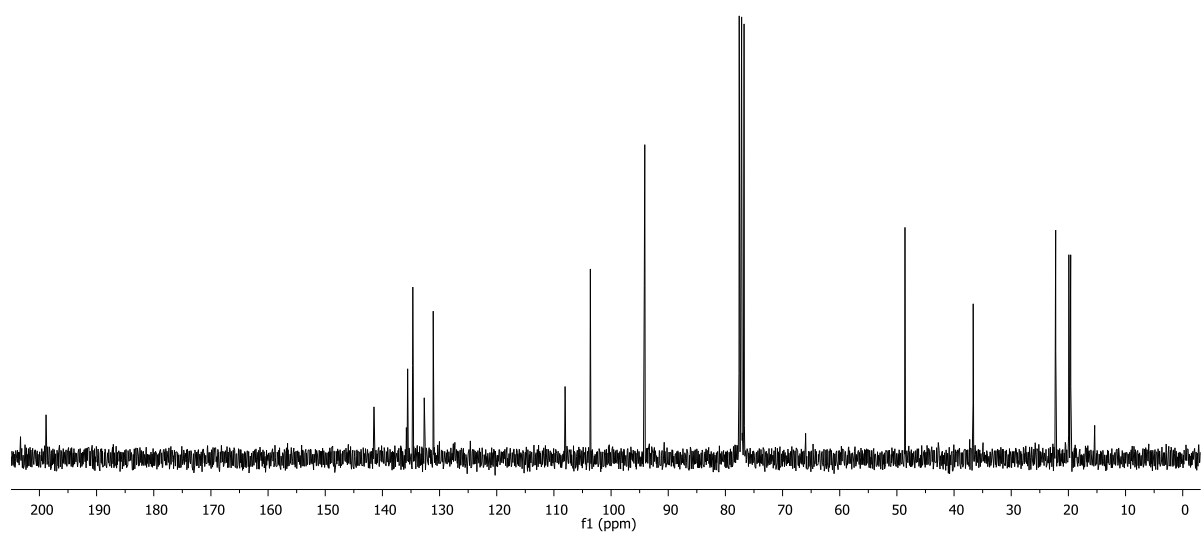
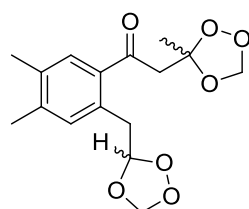
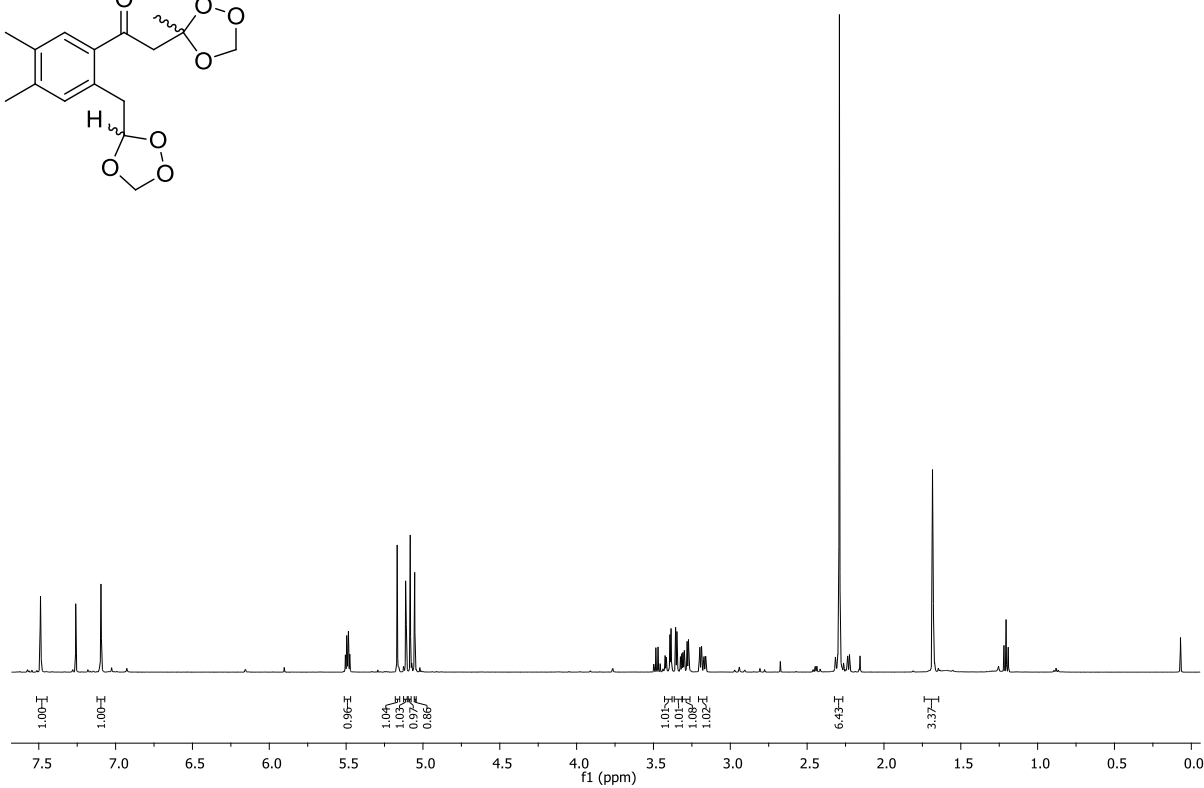
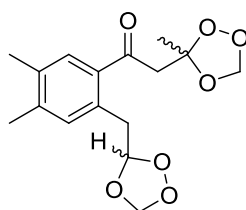
1-(2-(4,5-Dimethyl-2-methylenehex-4-enyl)-4-methylphenyl)-5,6-dimethyl-3-methylenehept-5-en-1-one (51)

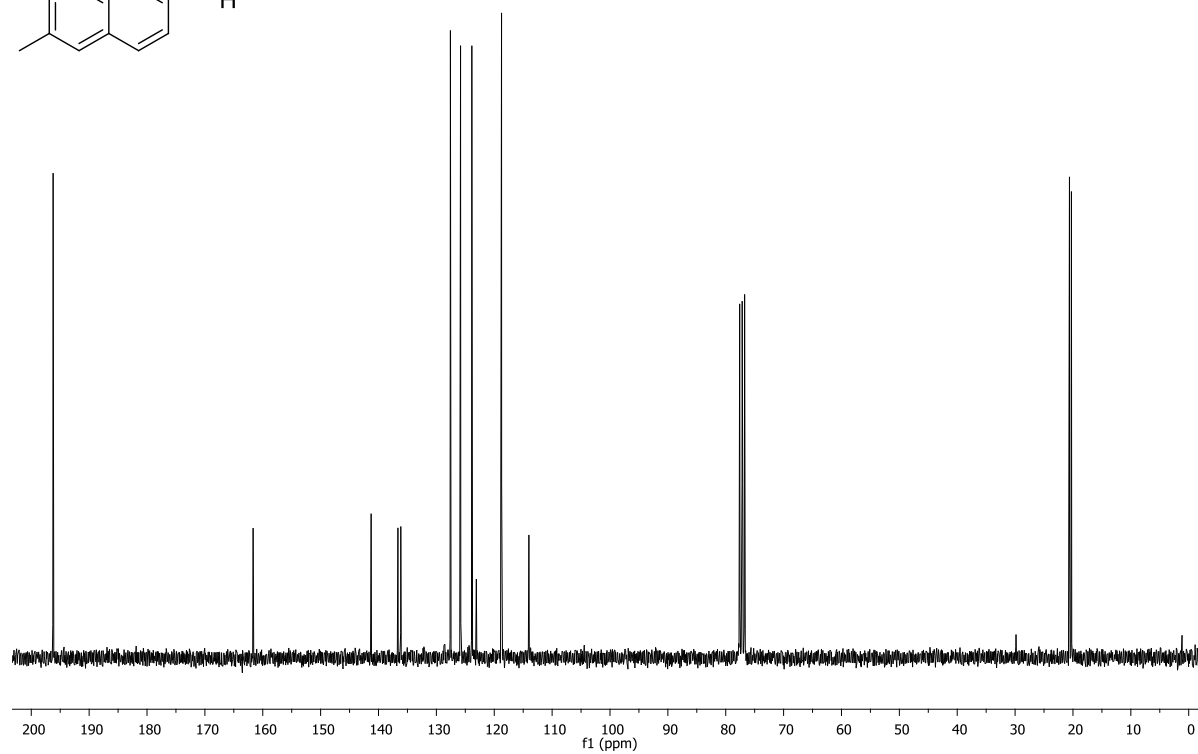
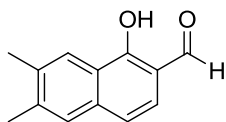
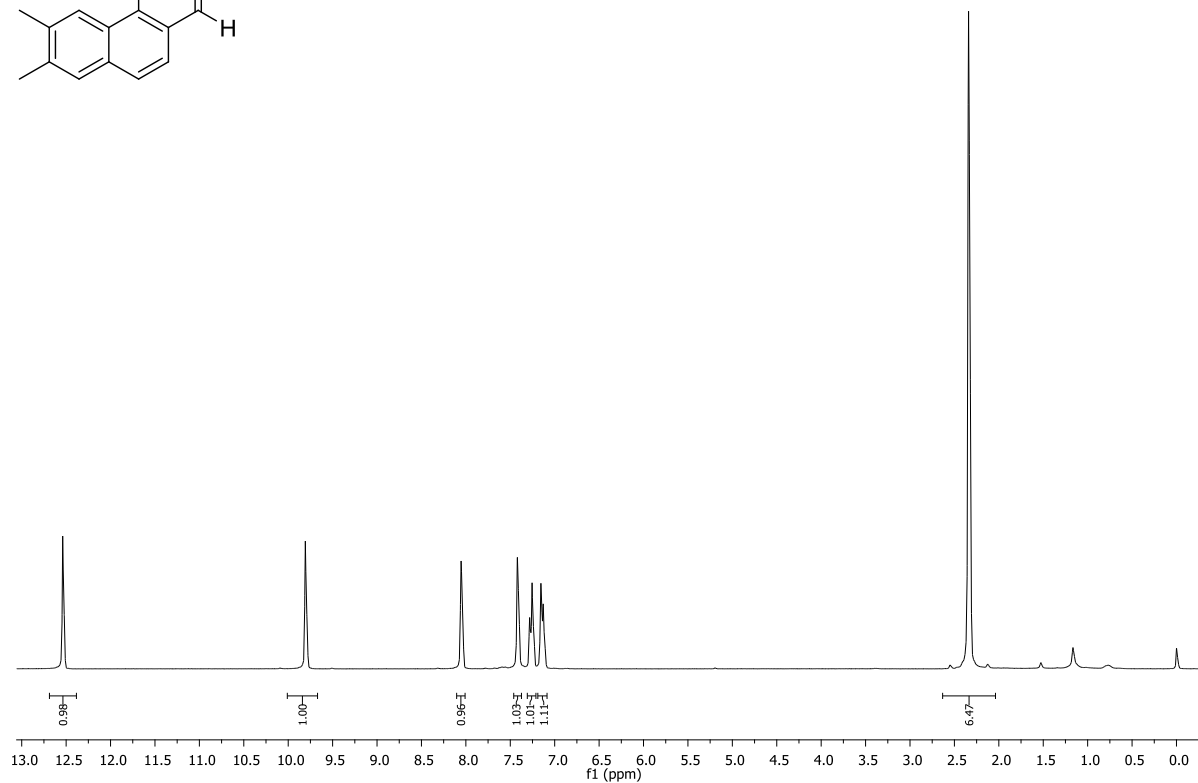
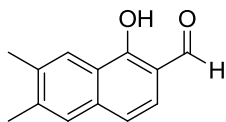


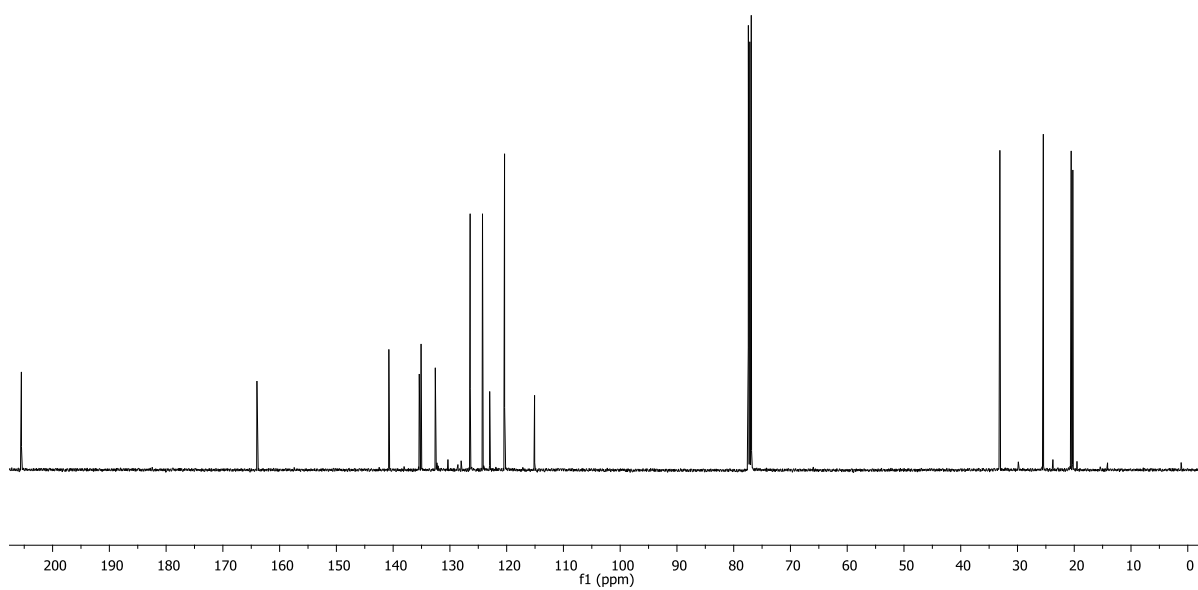
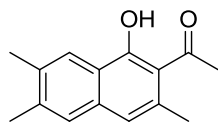
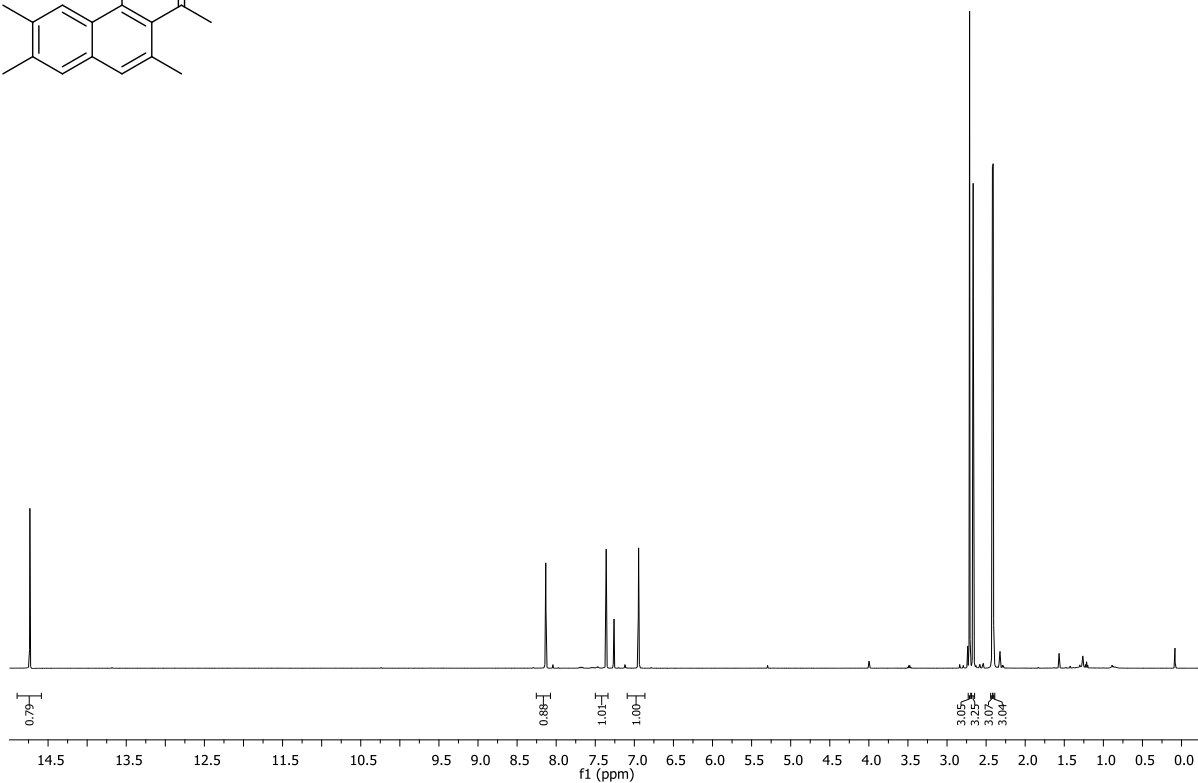
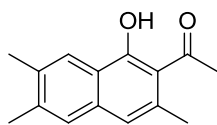
1-(3-Hydroxy-6,7-dimethylnaphthalene-2-yl)ethanone (27)

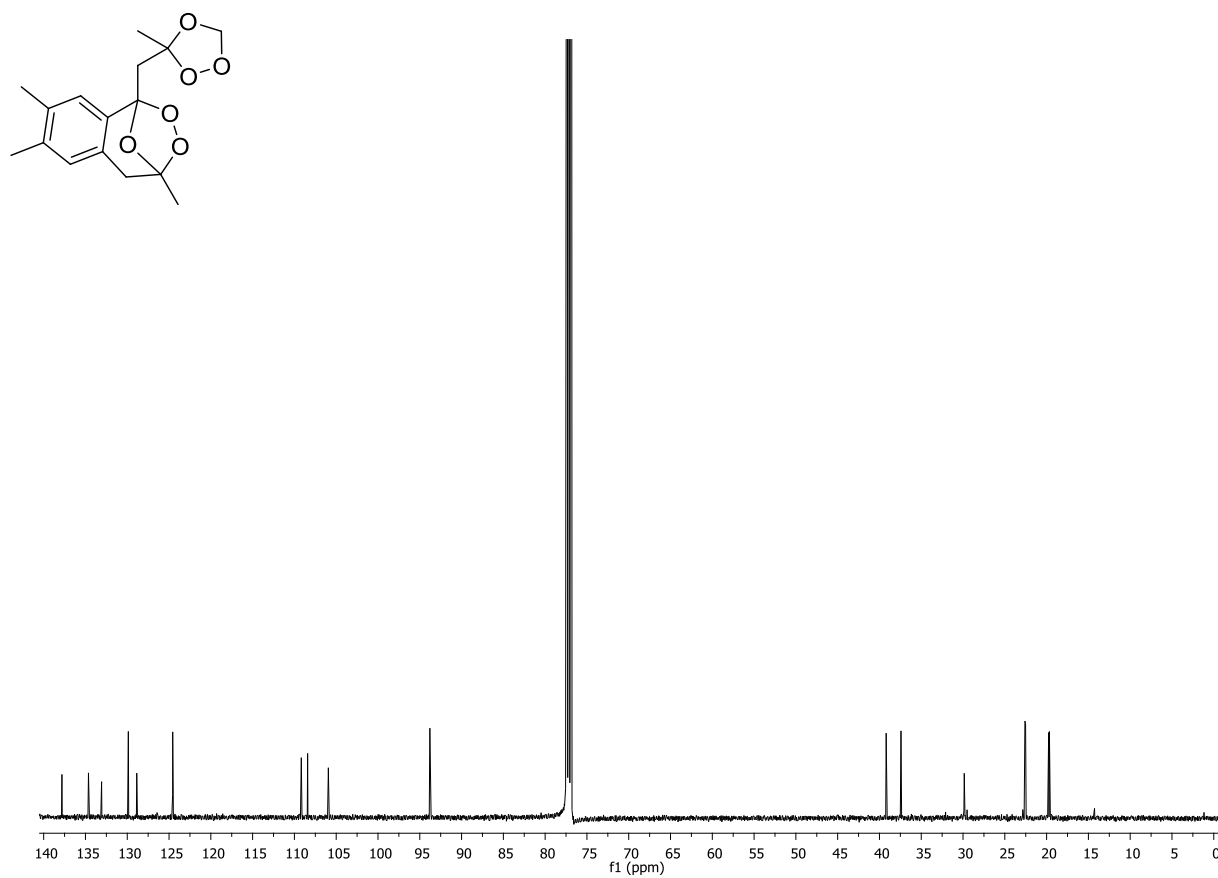
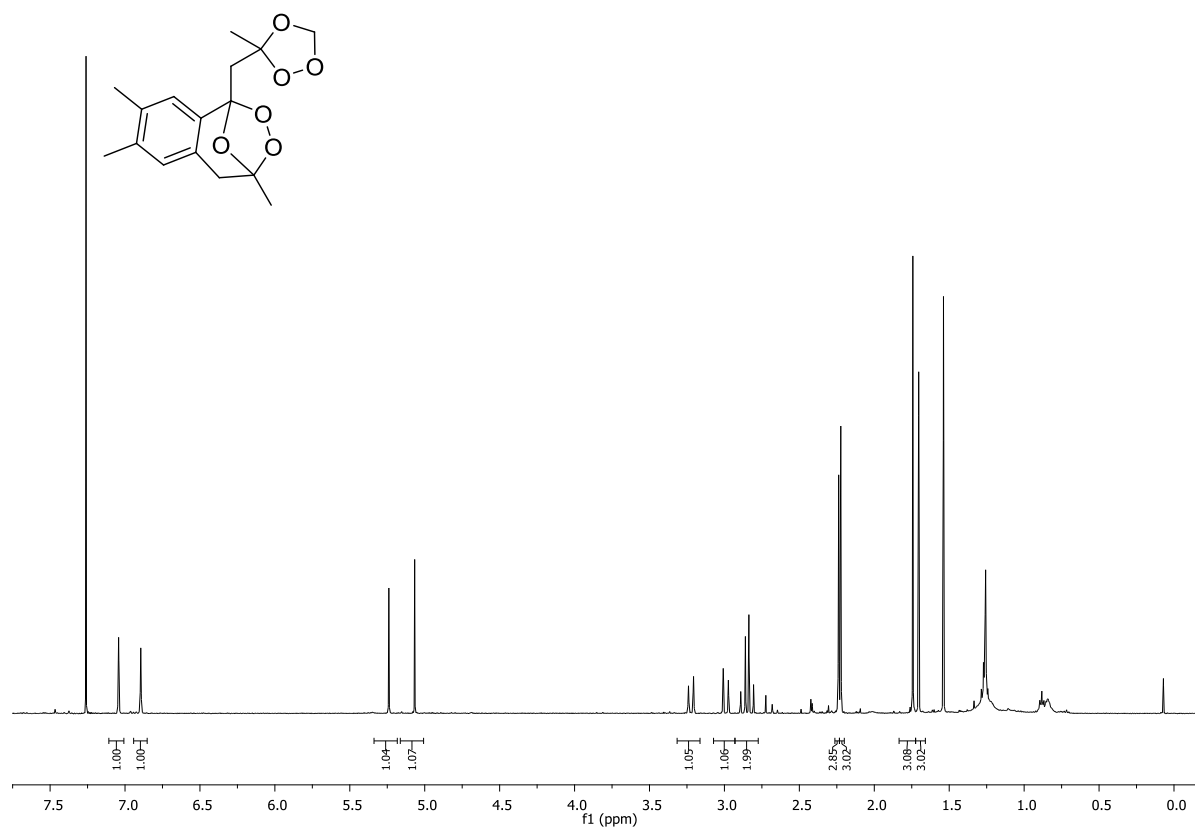
1-(1-Hydroxy-6,7-dimethylnaphthalen-2-yl)ethanon (29)

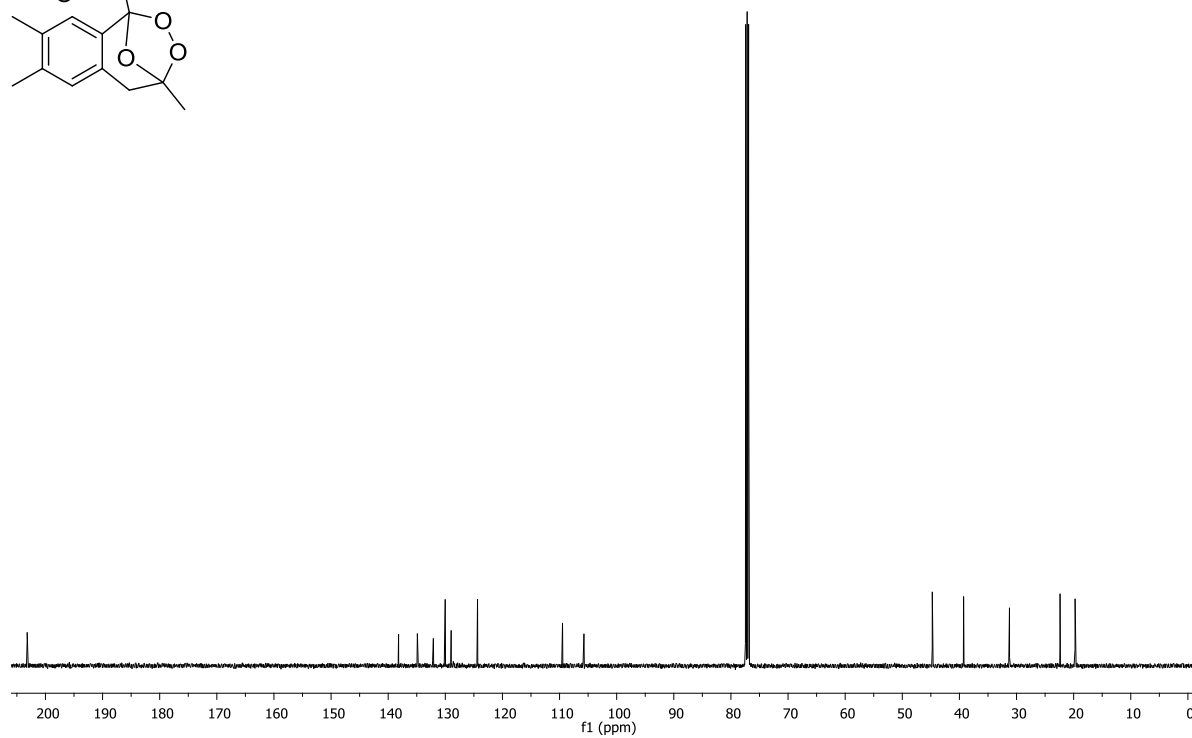
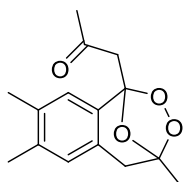
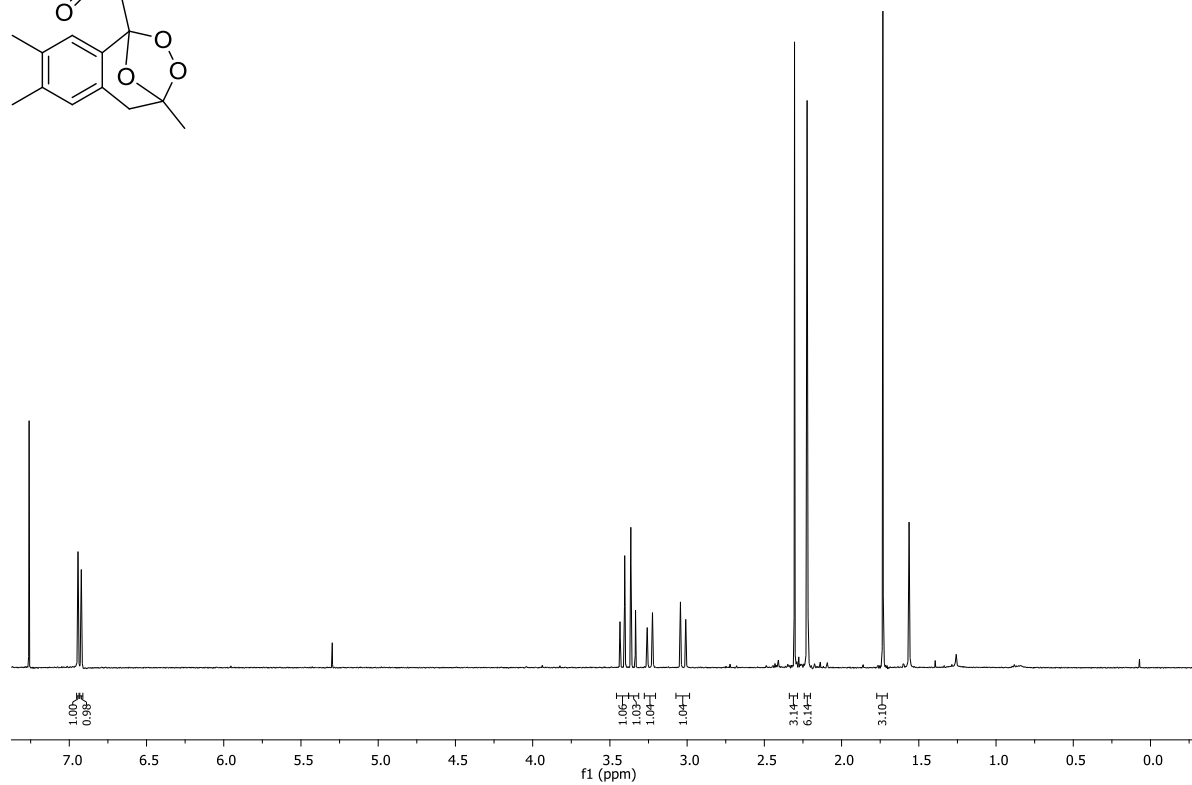
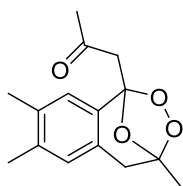
**1-(2-((1,2,4-Trioxolan-3-yl)methyl)-4,5-dimethylphenyl)-2-(3-methyl-1,2,4-trioxolan-3-yl)ethanon
(28)**



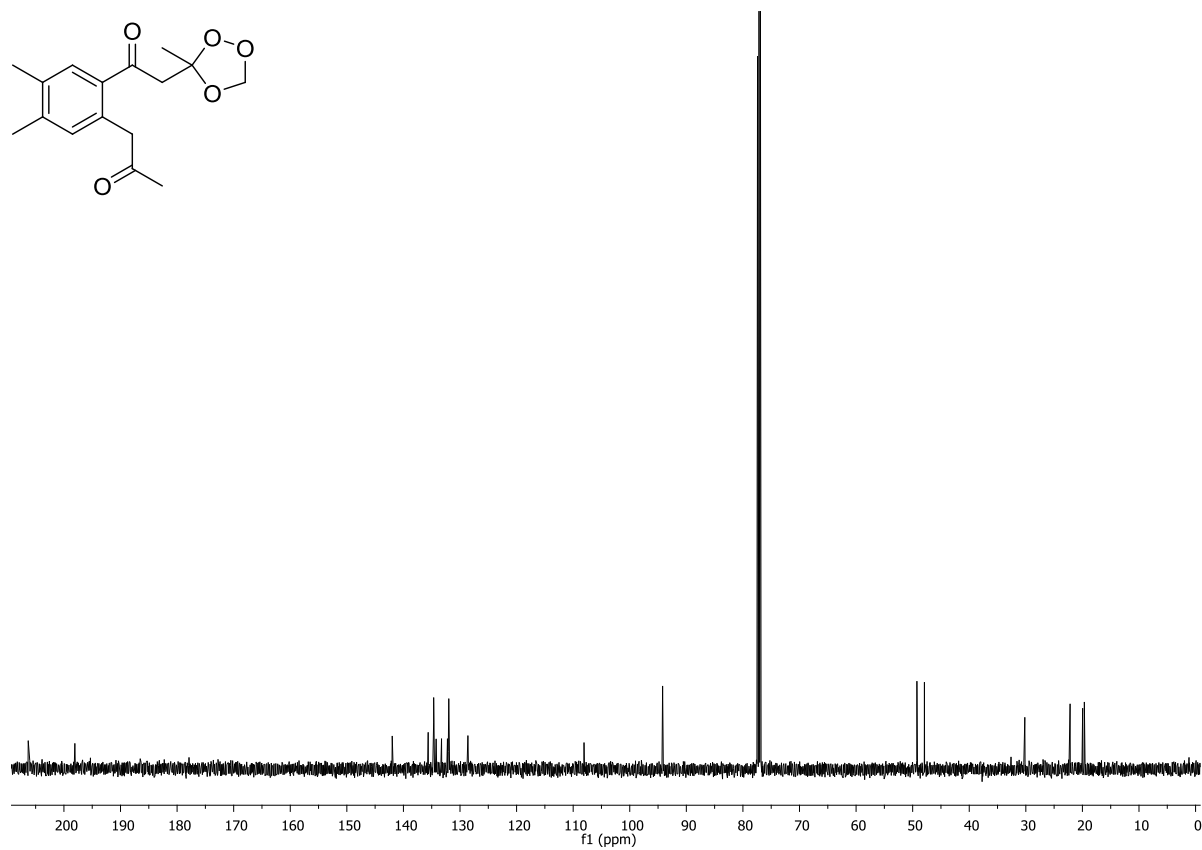
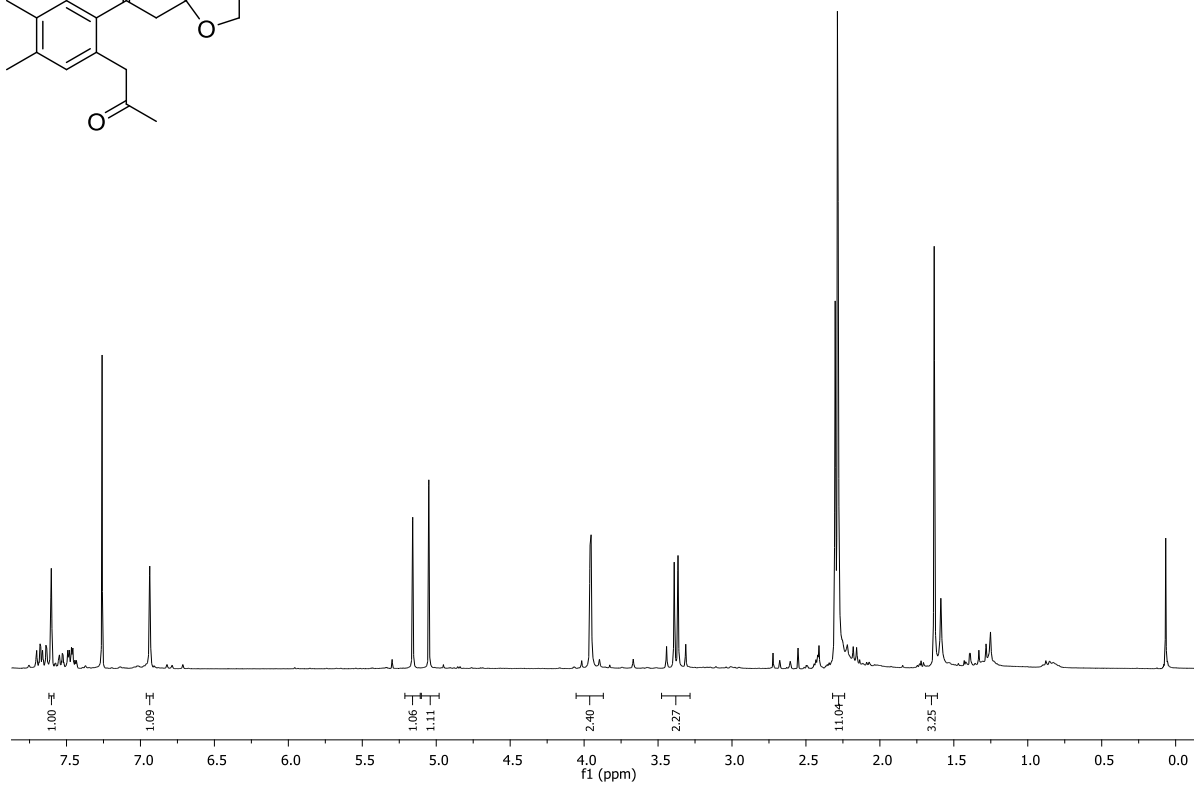
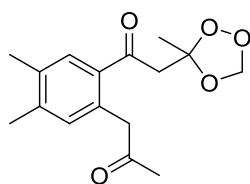
1-Hydroxy-6,7-dimethyl-2-naphthaldehyde (31)

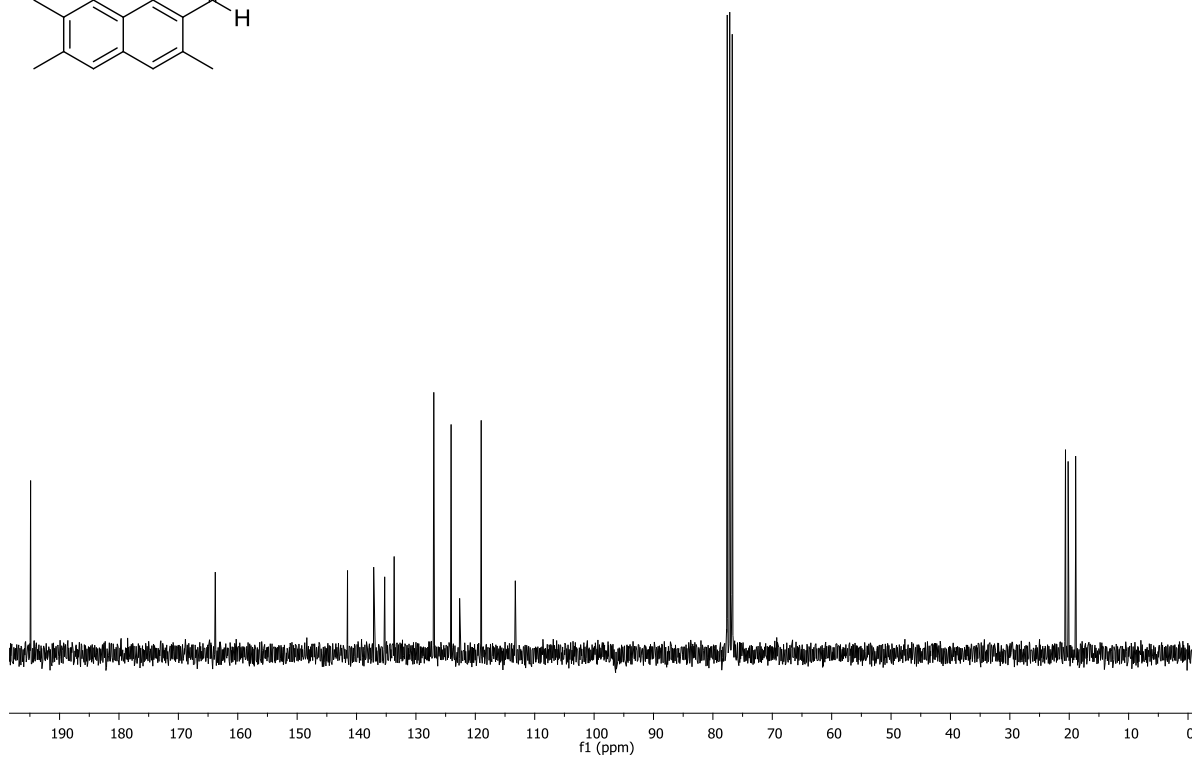
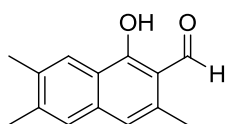
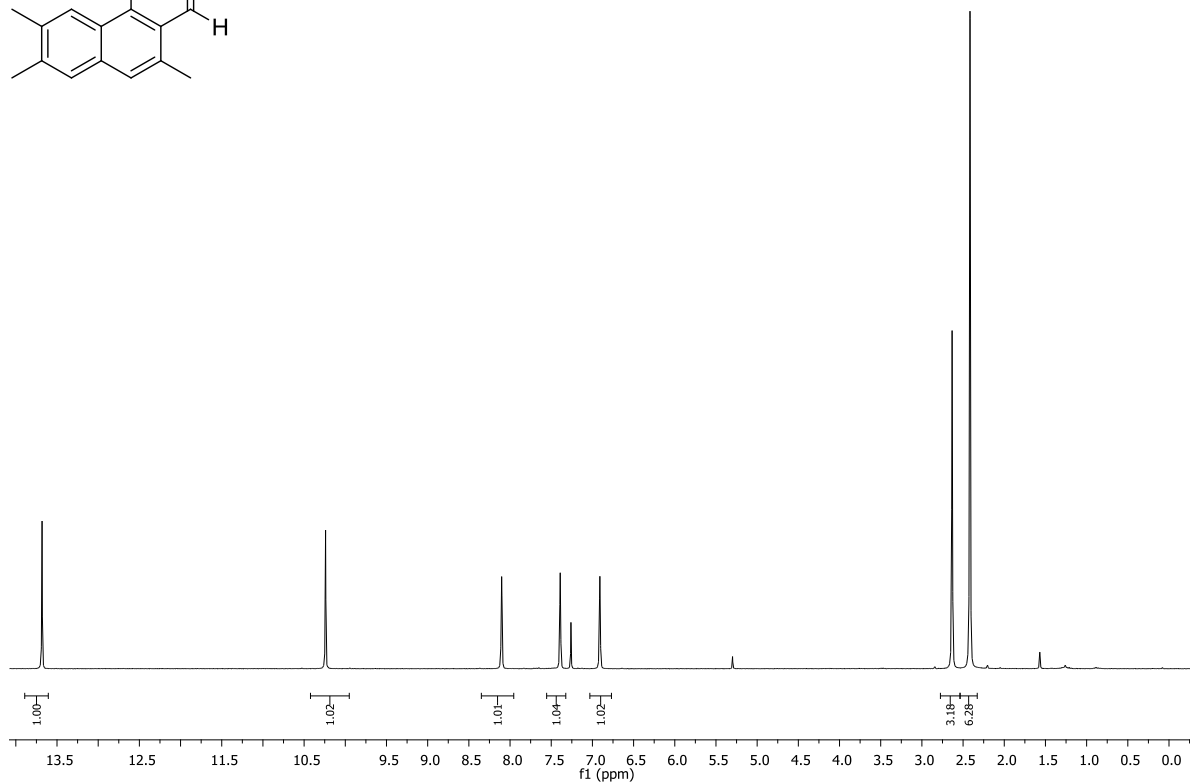
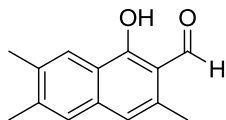
1-(1-Hydroxy-3,6,7-trimethylnaphthalene-2-yl)ethanone (35)

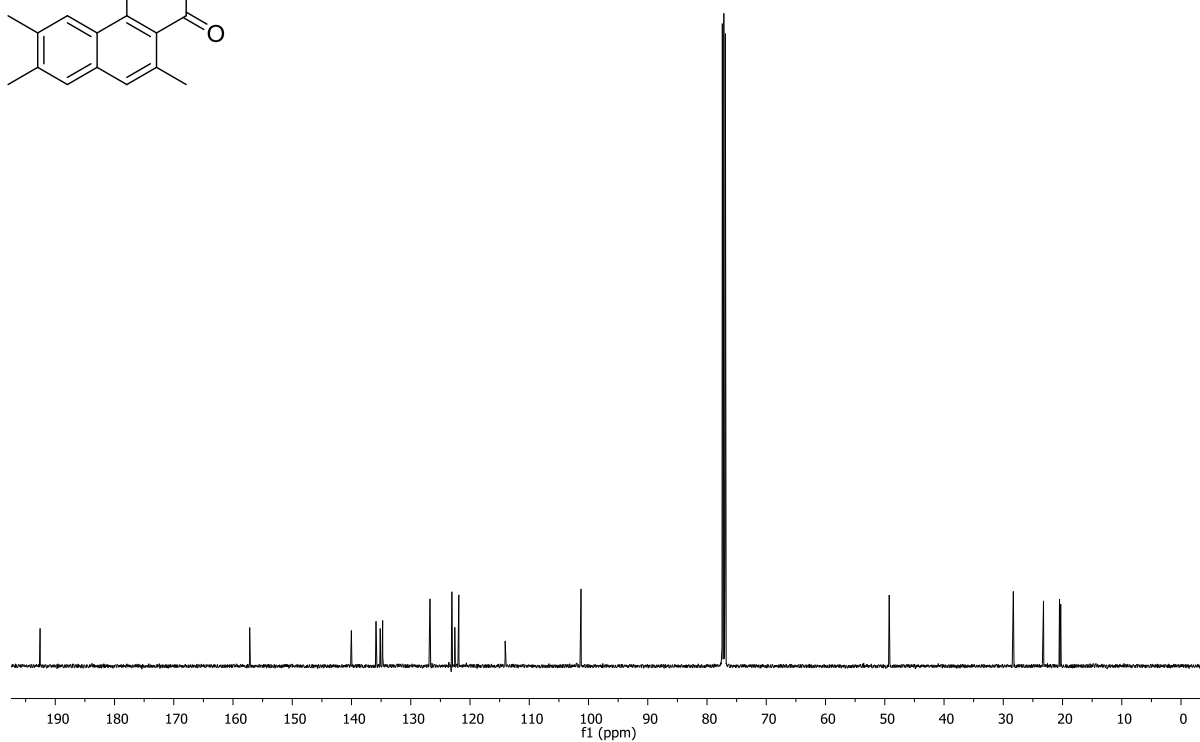
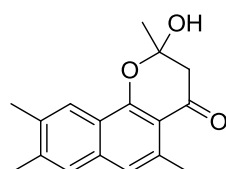
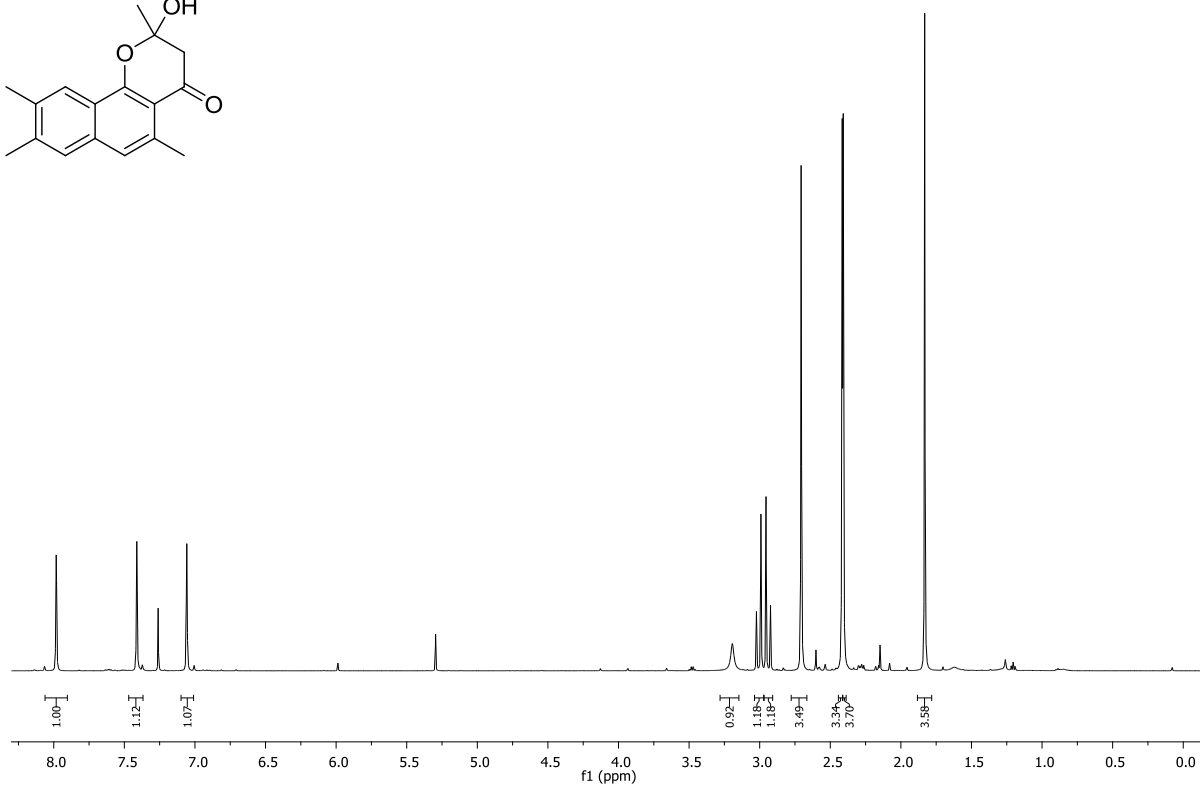
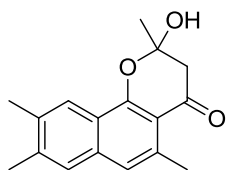
Compound 32

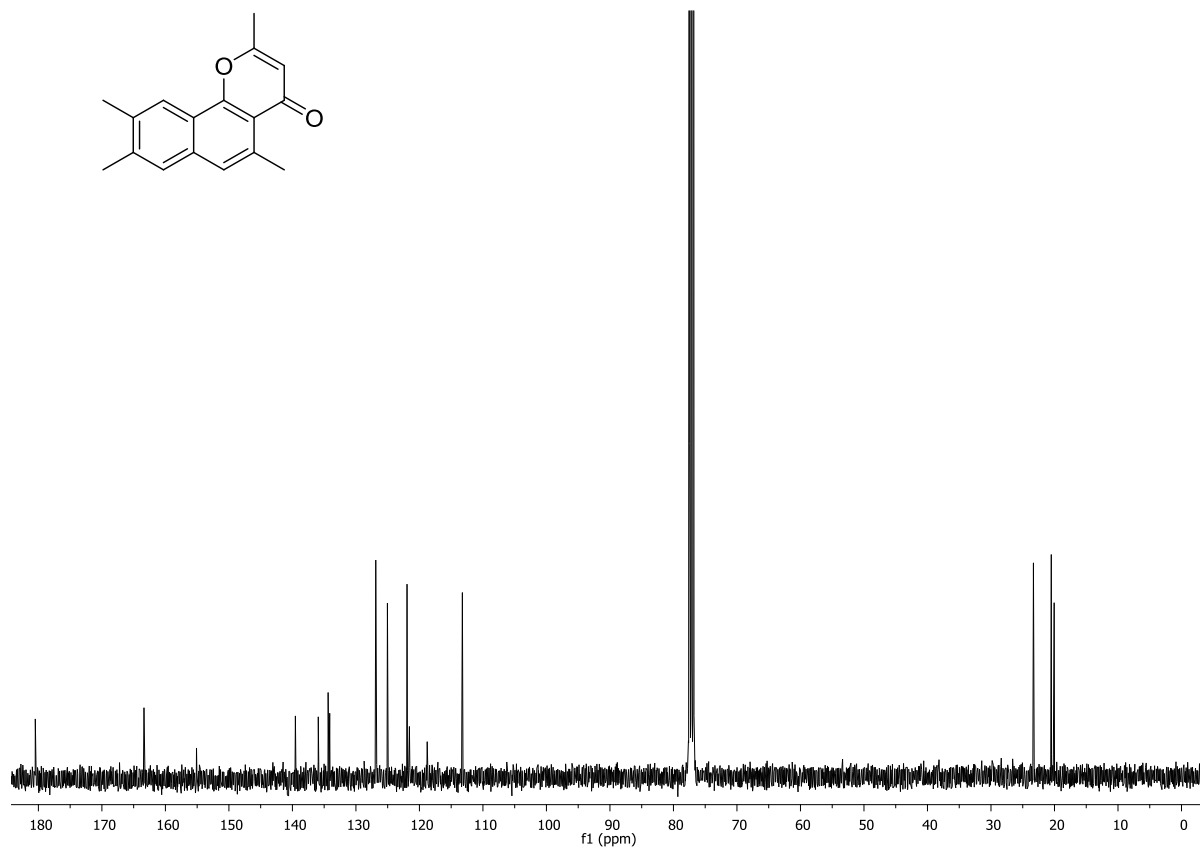
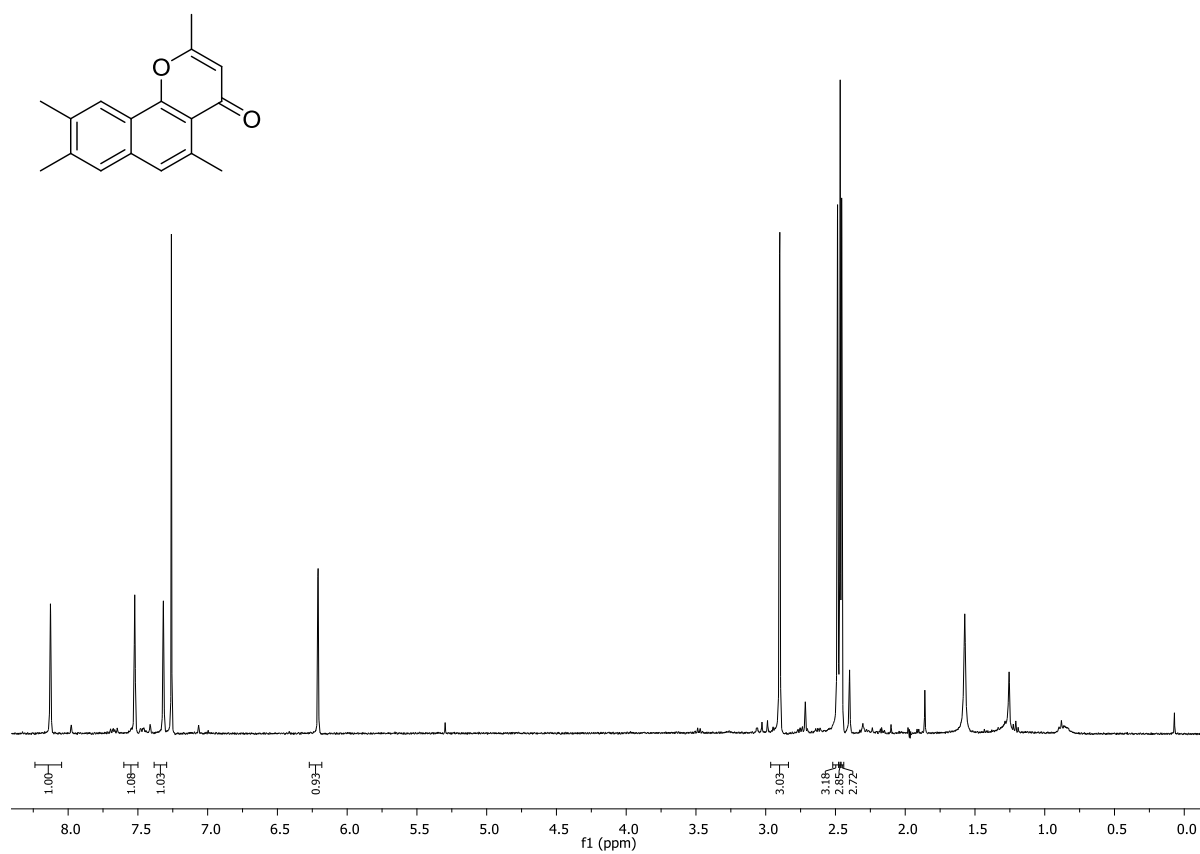
Compound 33

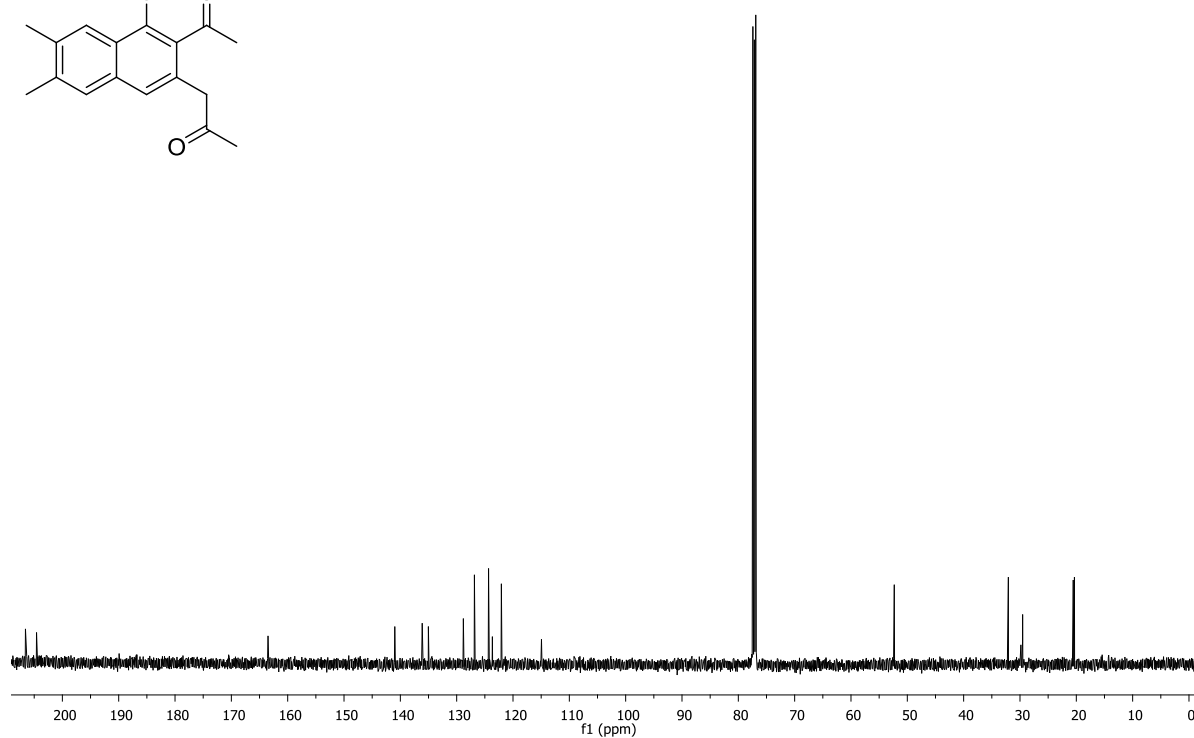
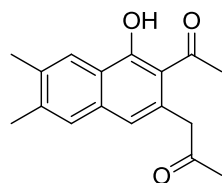
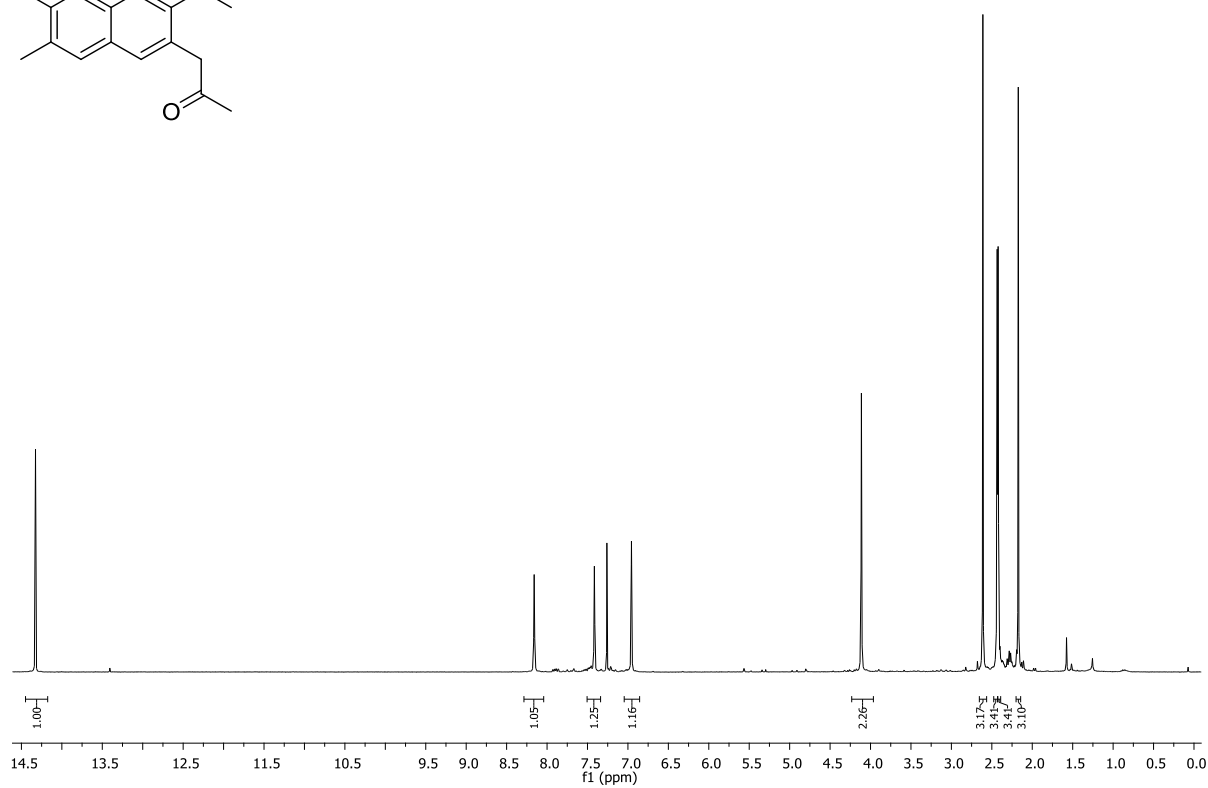
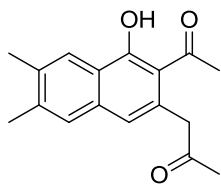
Compound 34

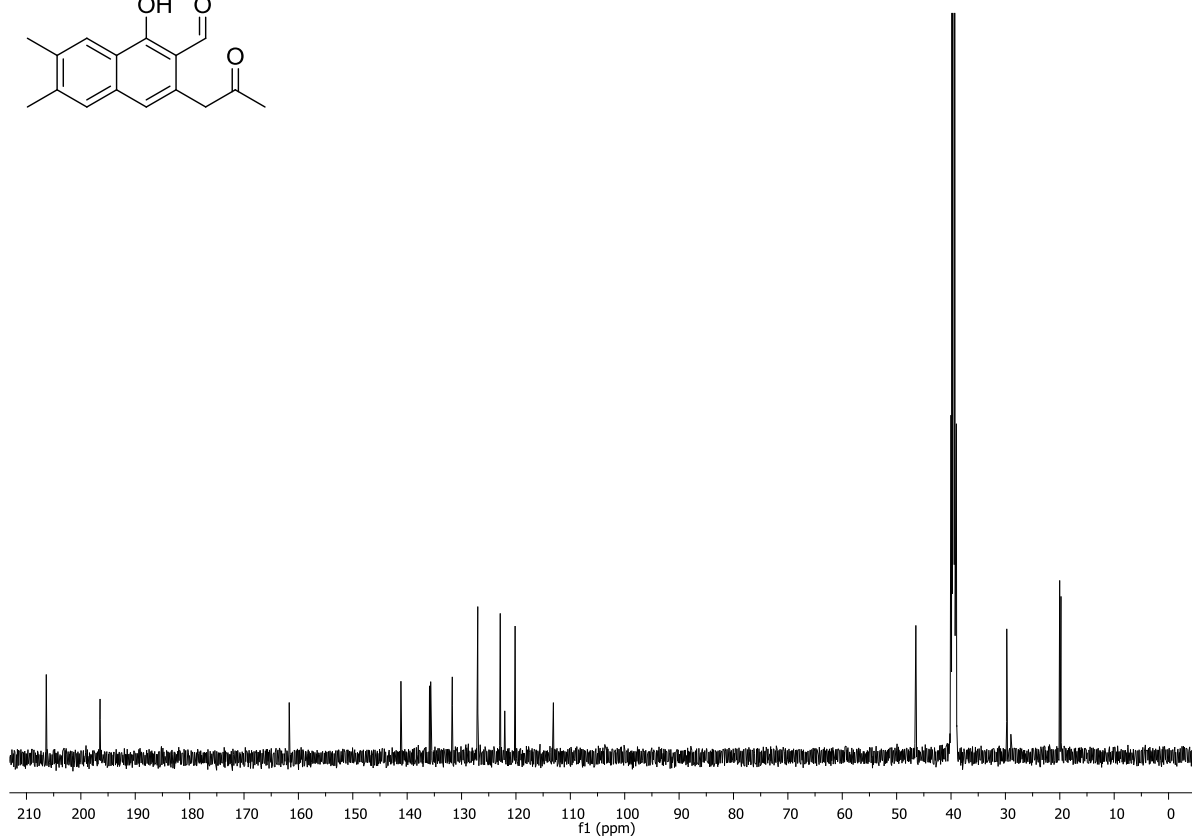
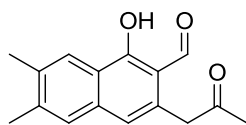
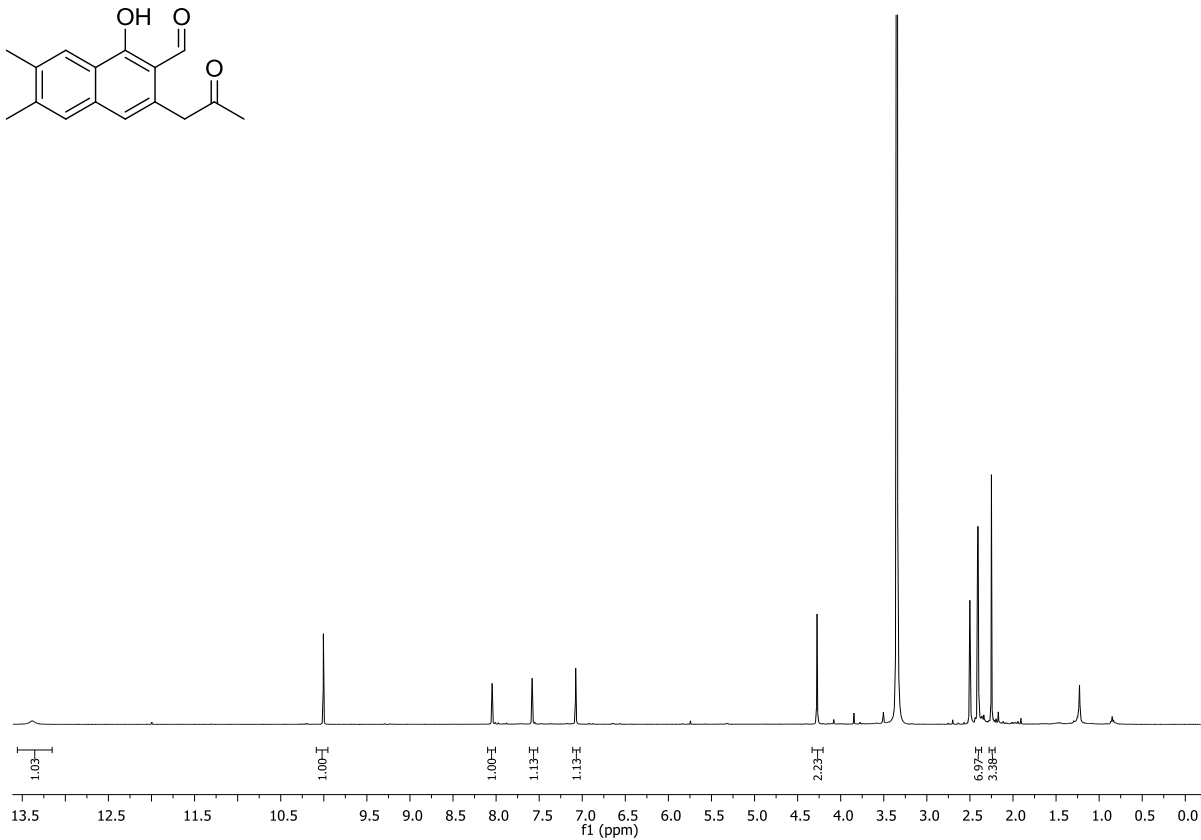
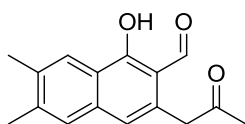


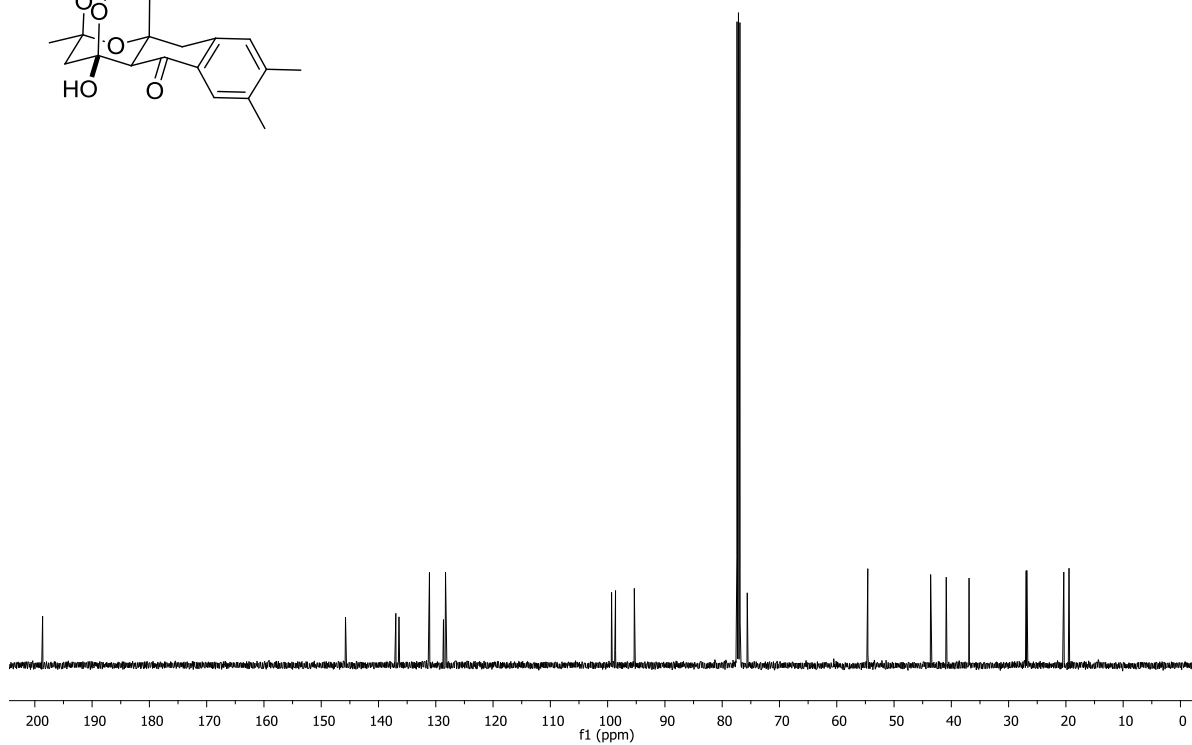
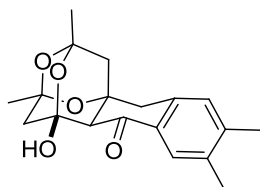
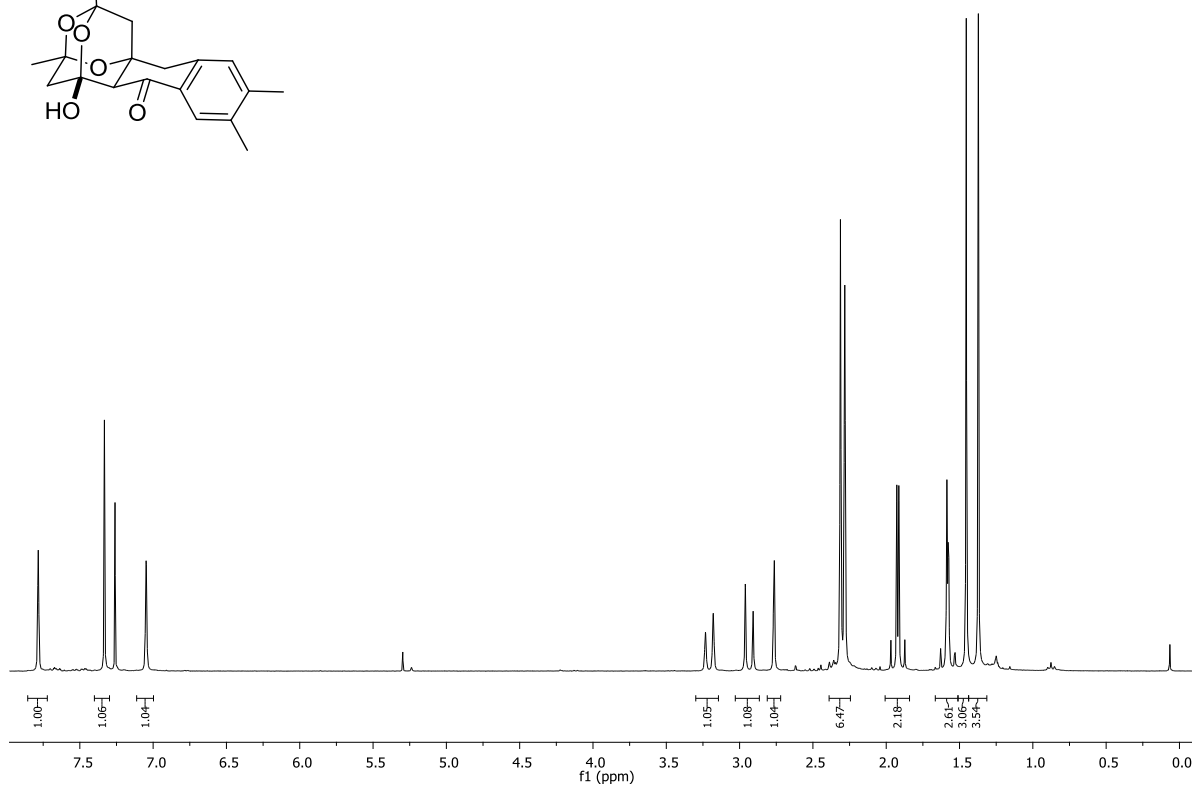
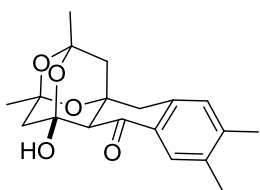
1-Hydroxy-3,6,7-trimethyl-2-naphthaldehyde (37)

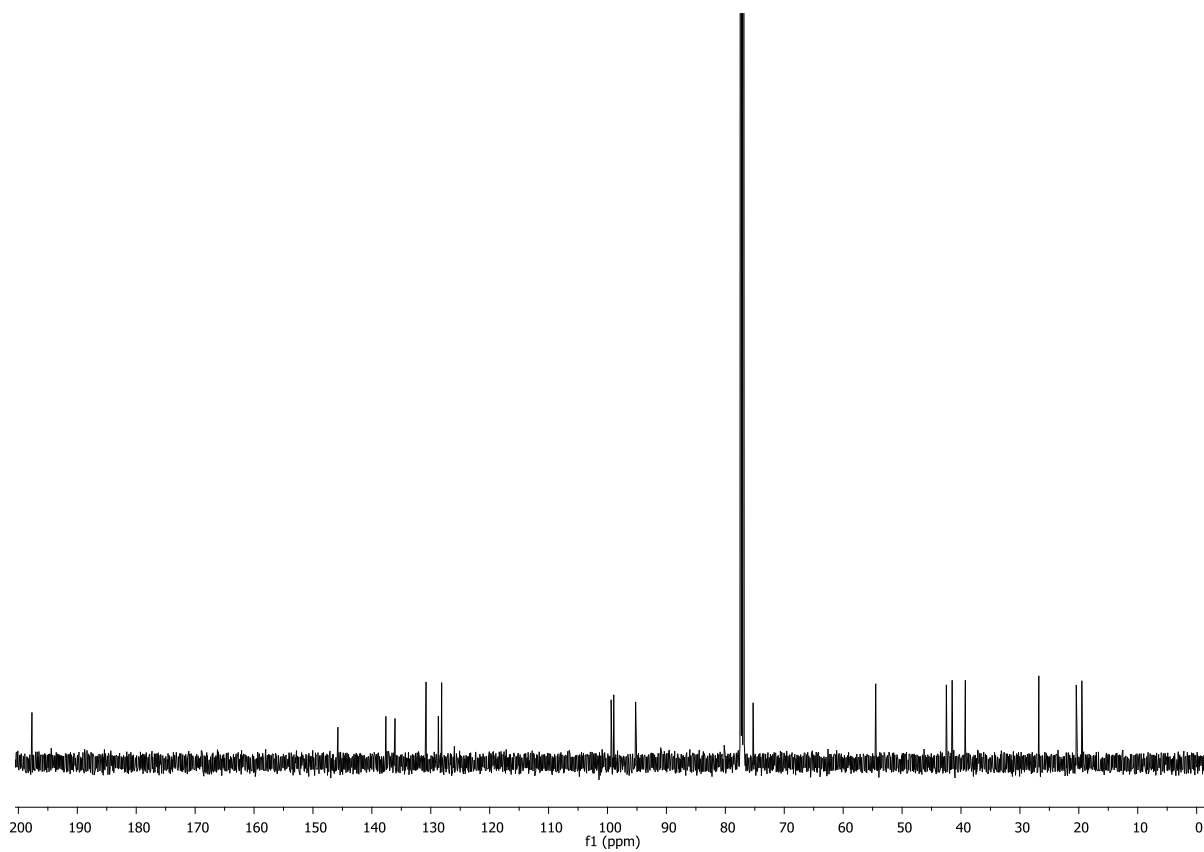
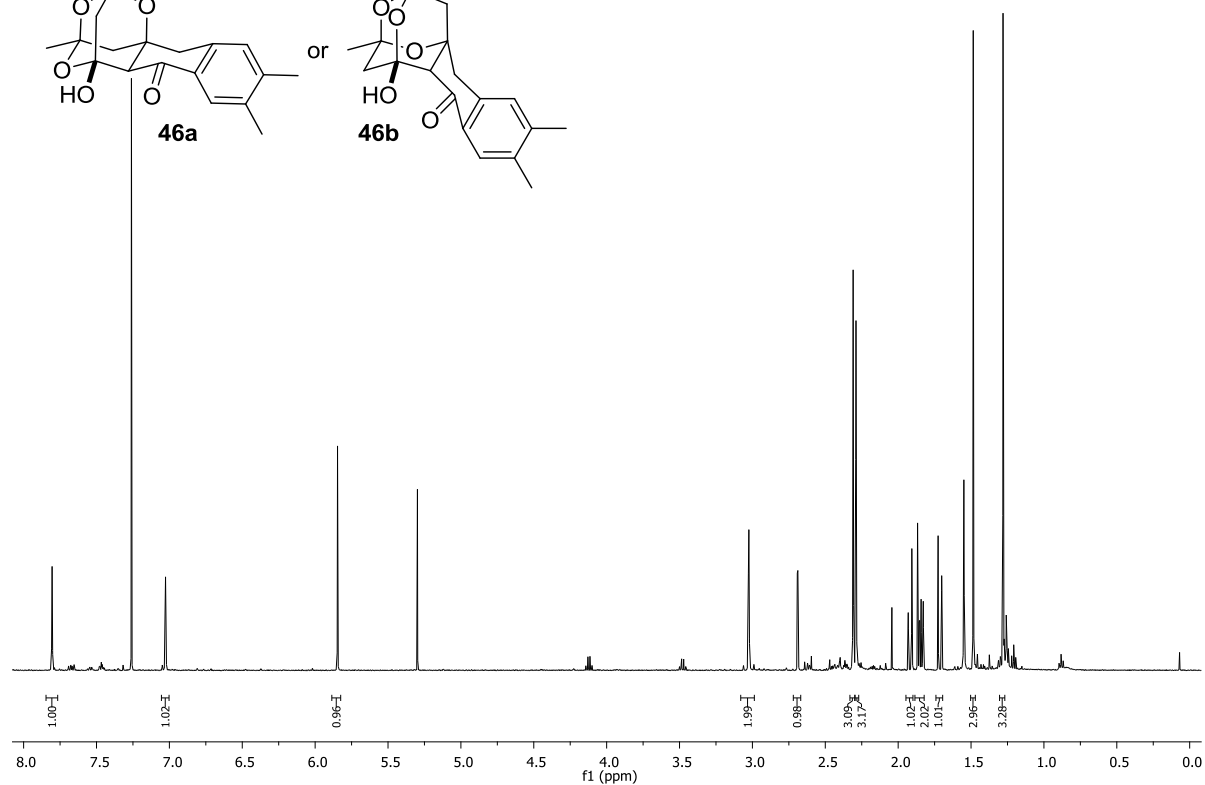
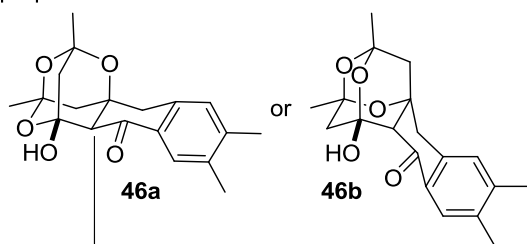
2-Hydroxy-2,5,8,9-tetramethyl-2H-benzo[*h*]chromen-4(3*H*)one (39)

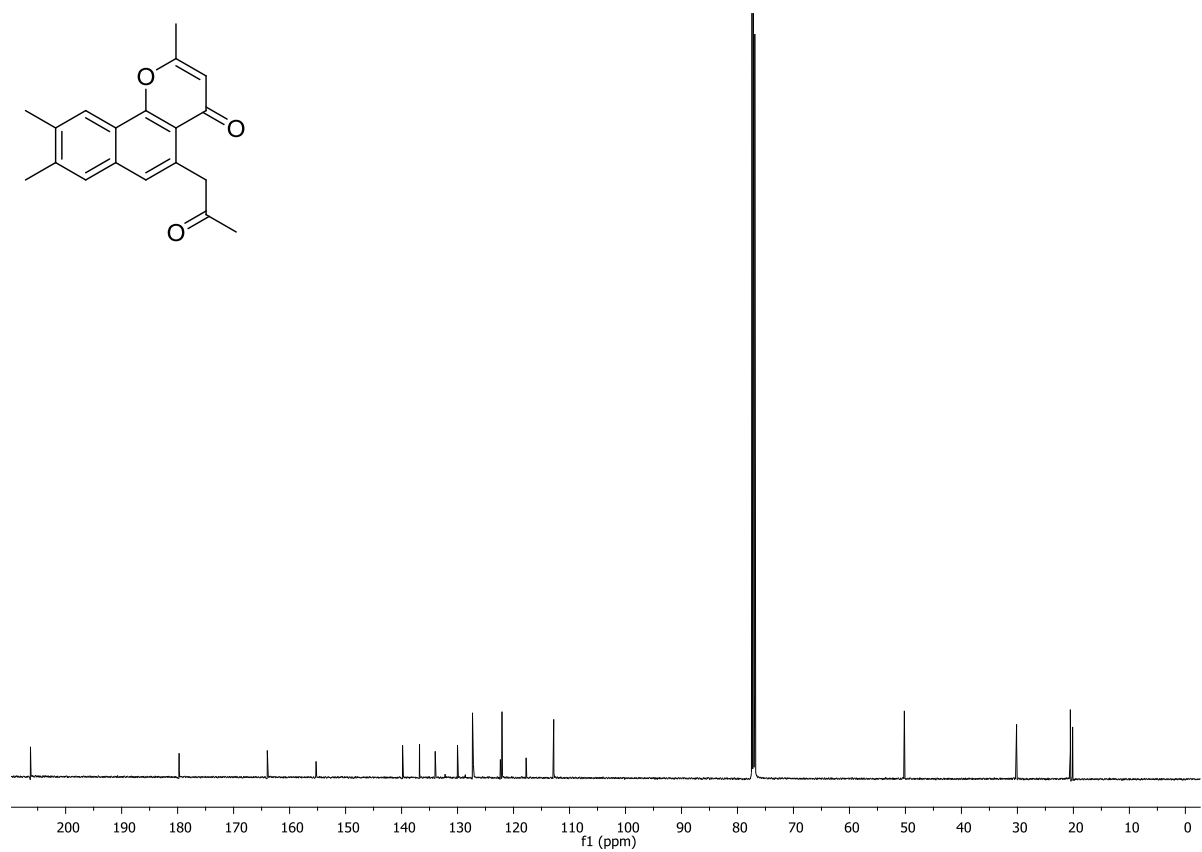
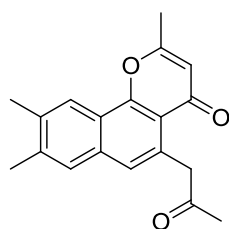
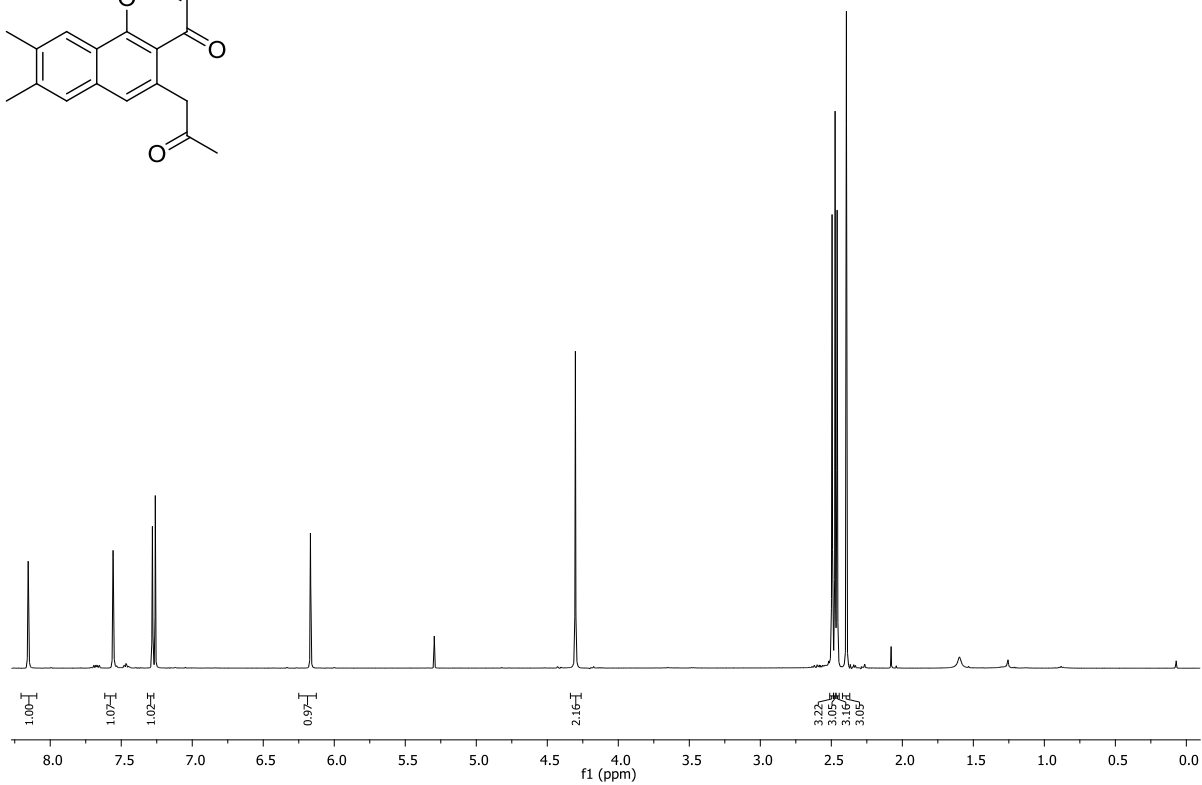
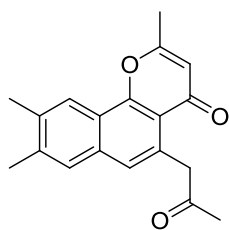
2,5,8,9-Tetramethyl-4H-benzo[*h*]chromen-4-one (40)

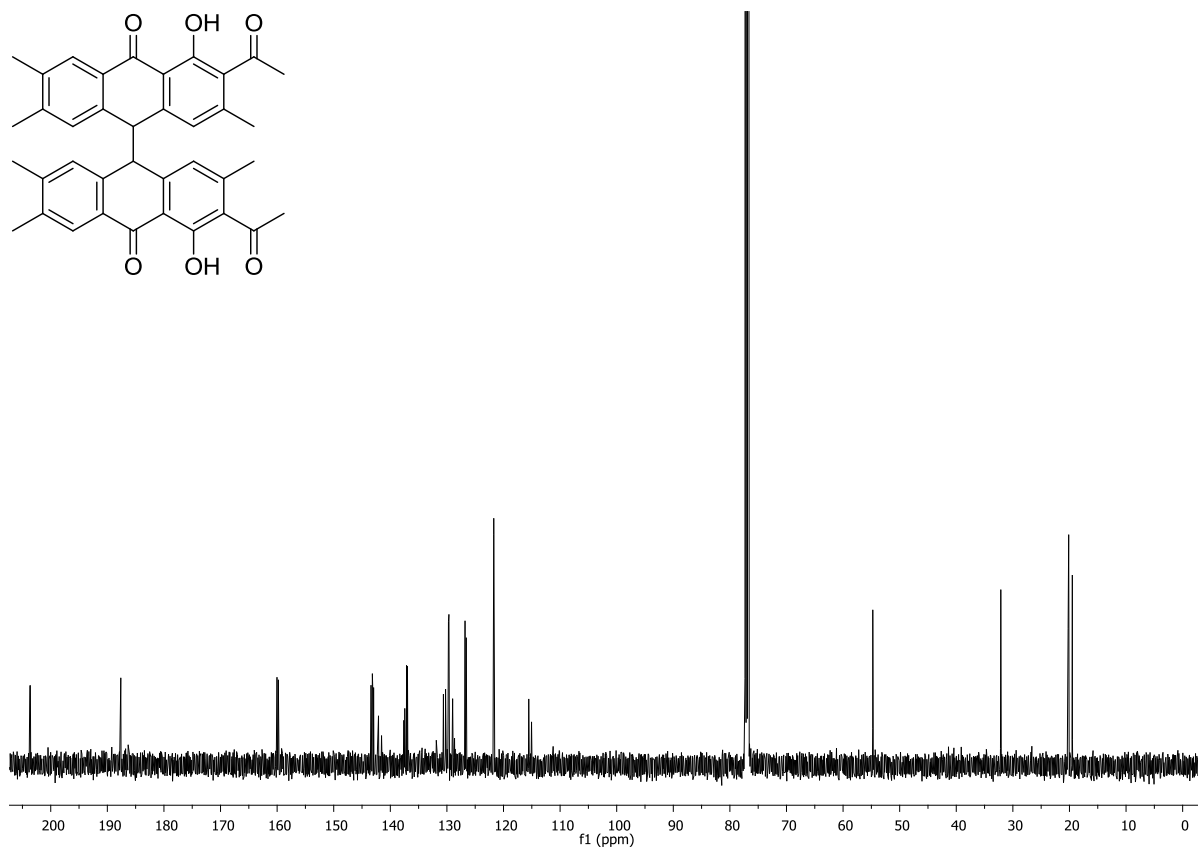
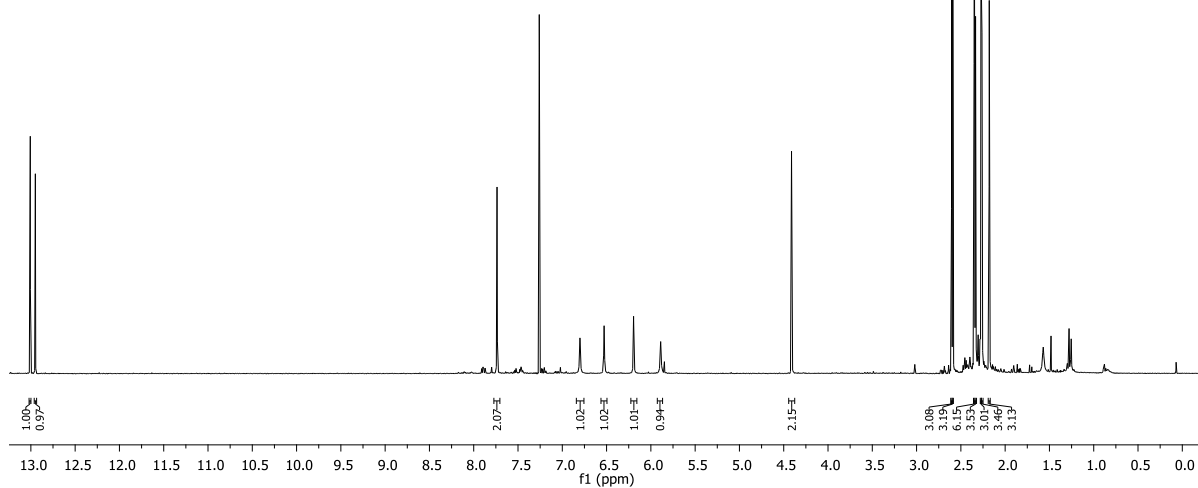
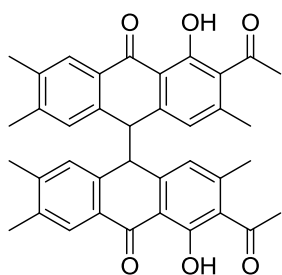
1-(3-Acetyl-4-hydroxy-6,7-dimethylnaphthalene-2-yl)propan-2-one (41)

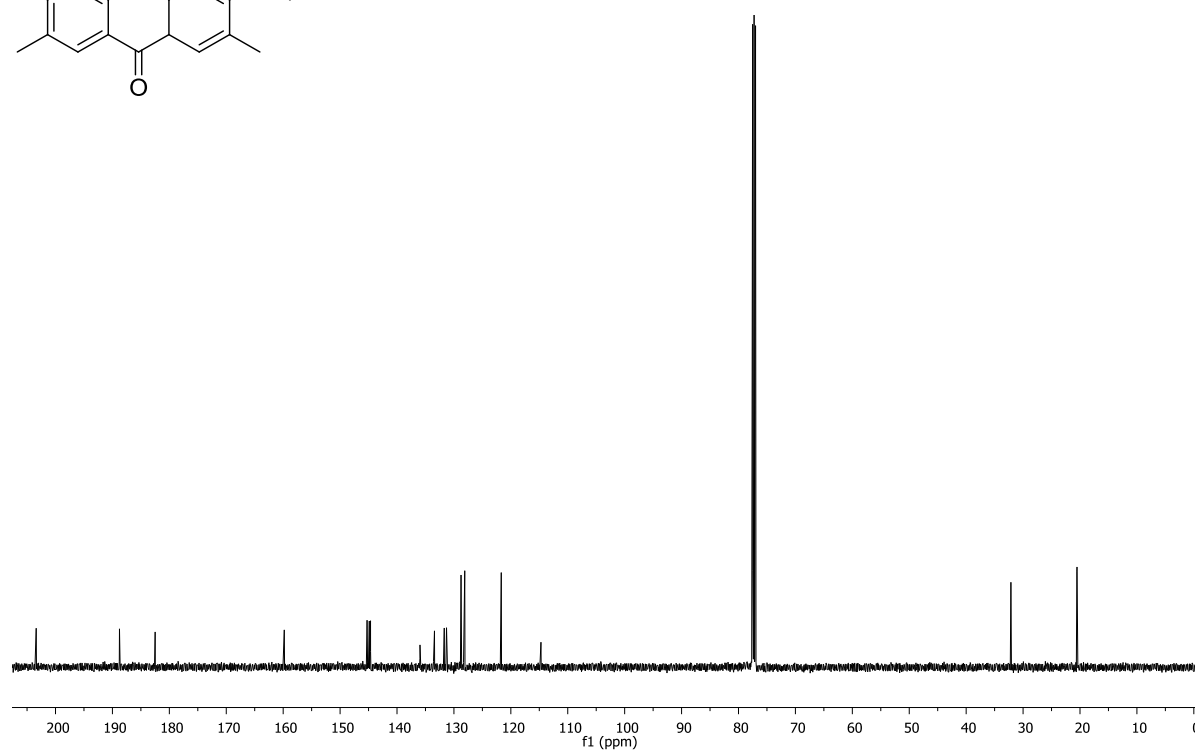
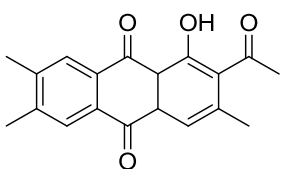
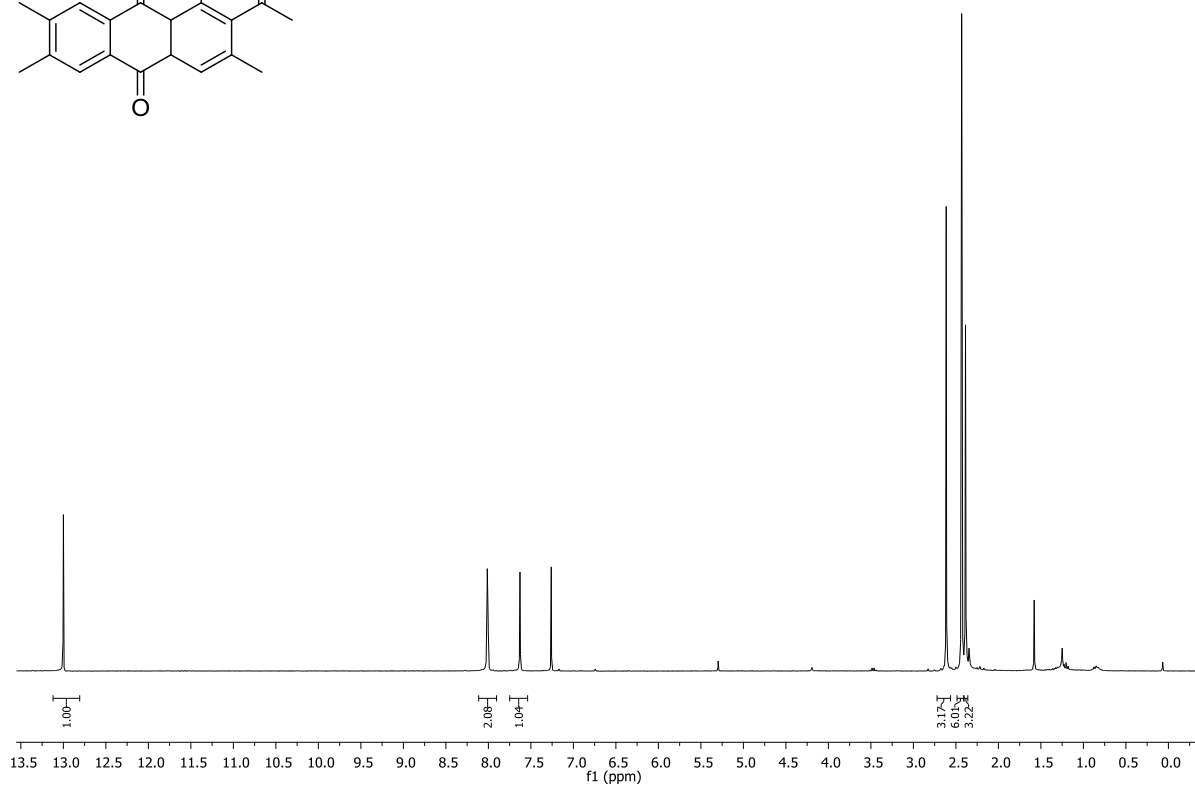
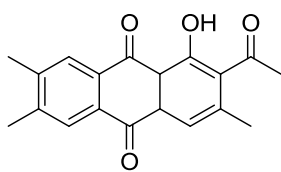
1-Hydroxy-6,7-dimethyl-3-(2-oxopropyl)-2-naphthaldehyde (42)

Trioxadamantane 45 (main isomer)

Trioxaadamantane 46 (minor isomer)proposed structures for trioxaadamantane **46**:

2,8,9-Trimethyl-5-(2-oxopropyl)-4H-benzo[h]chromene-4-one (48)

3,3'-Diacetyl-4,4'-dihydroxy-2,2',6,6',7,7'-hexamethyl-9,9'-bianthracene-10,10'(9*H*,9'*H*)-dione (47)

2-Acetyl-1-hydroxy-3,6,7-trimethylantracene-9,10-dione (9)

KWANZOQUINONE A (44)