

Supporting Information

Synthesis and Anti-Tumor Activities Evaluation of Compounds Based on Toluquinol

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³ IBIMA (Biomedical Research Institute of Málaga), 29071, Málaga (SPAIN)

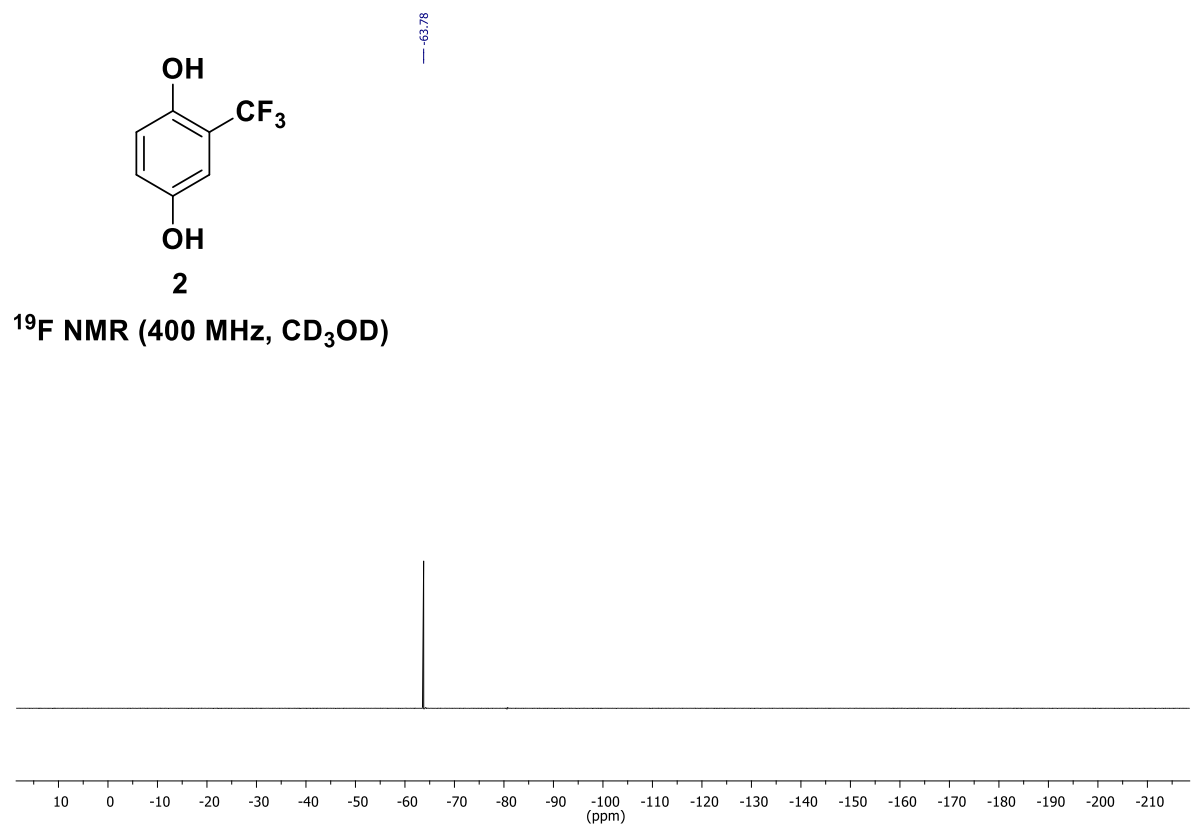
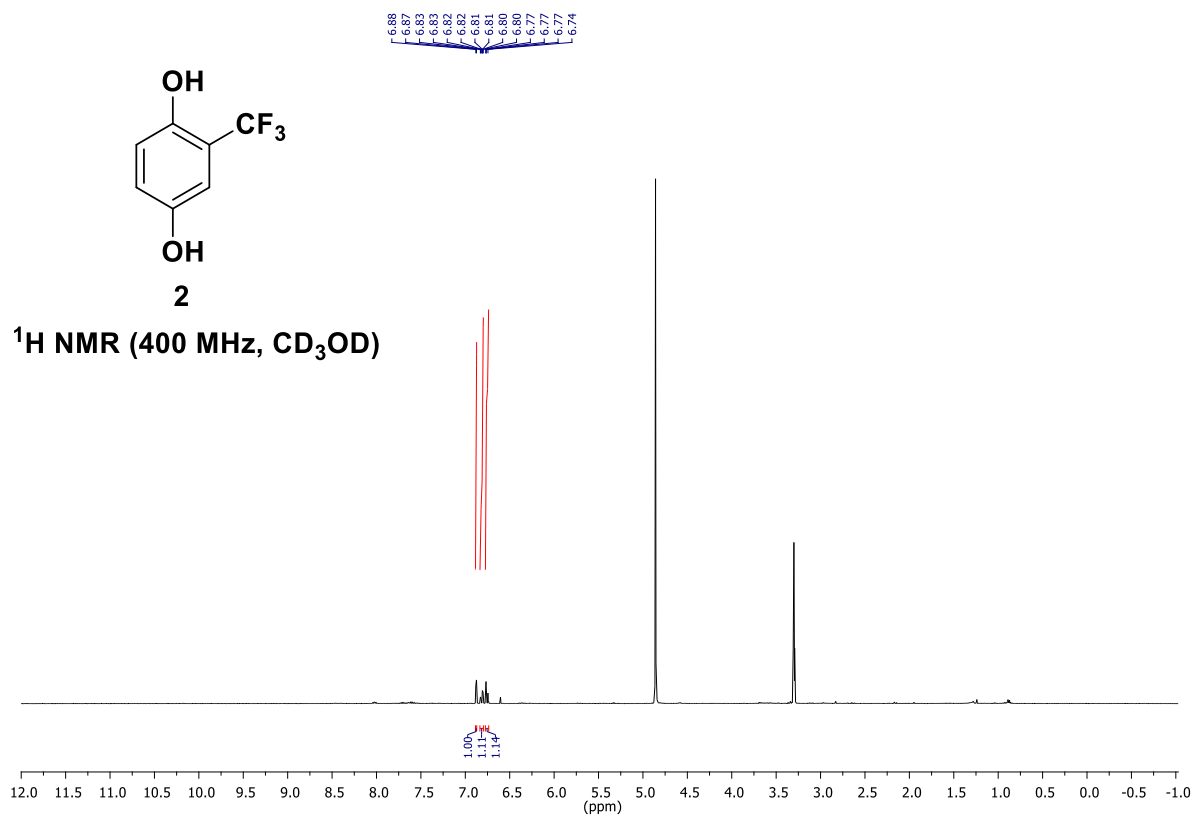
⁴ CIBER of Rare Diseases; Group U741 (CB06/07/0046), 29071 Málaga (SPAIN)

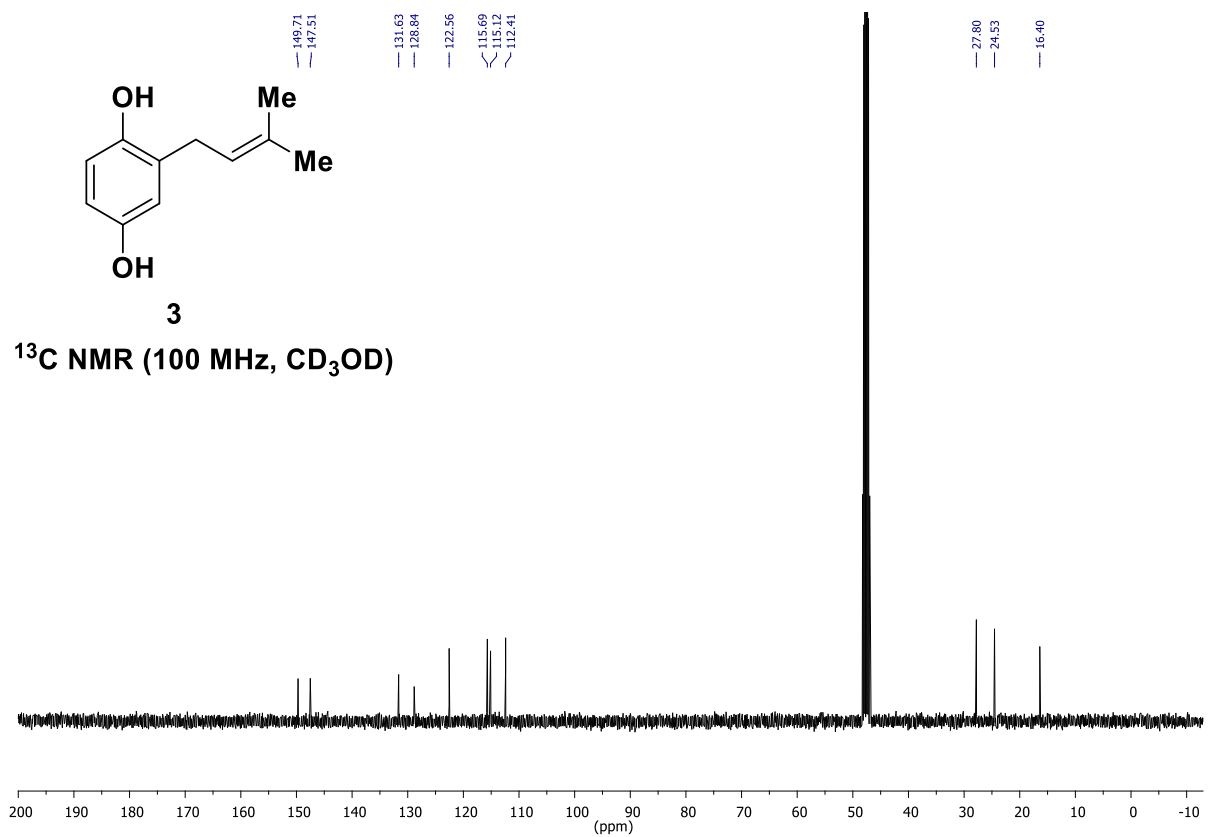
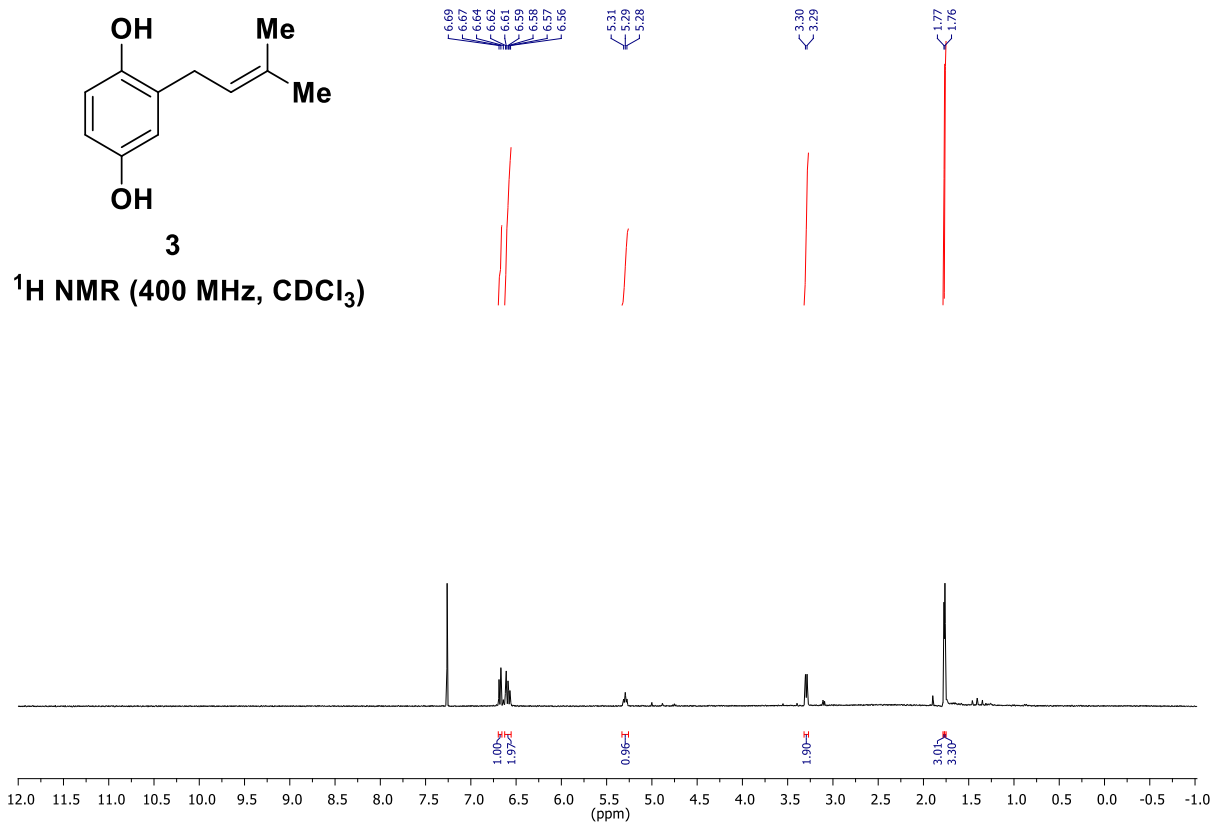
* Correspondence: quesada@uma.es; frsarabia@uma.es; Tel.: +34-952-134-258. Francisco Sarabia and Ana R. Quesada contributed equally to the direction of this work.

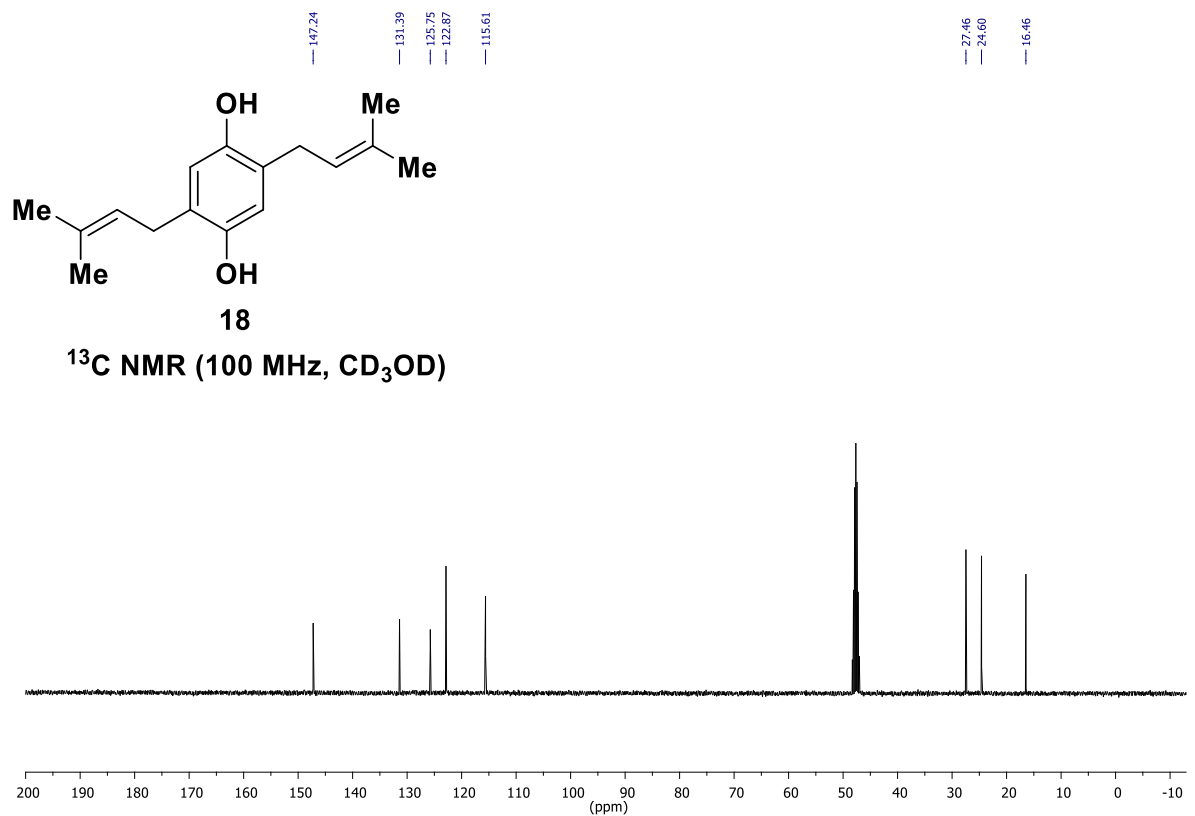
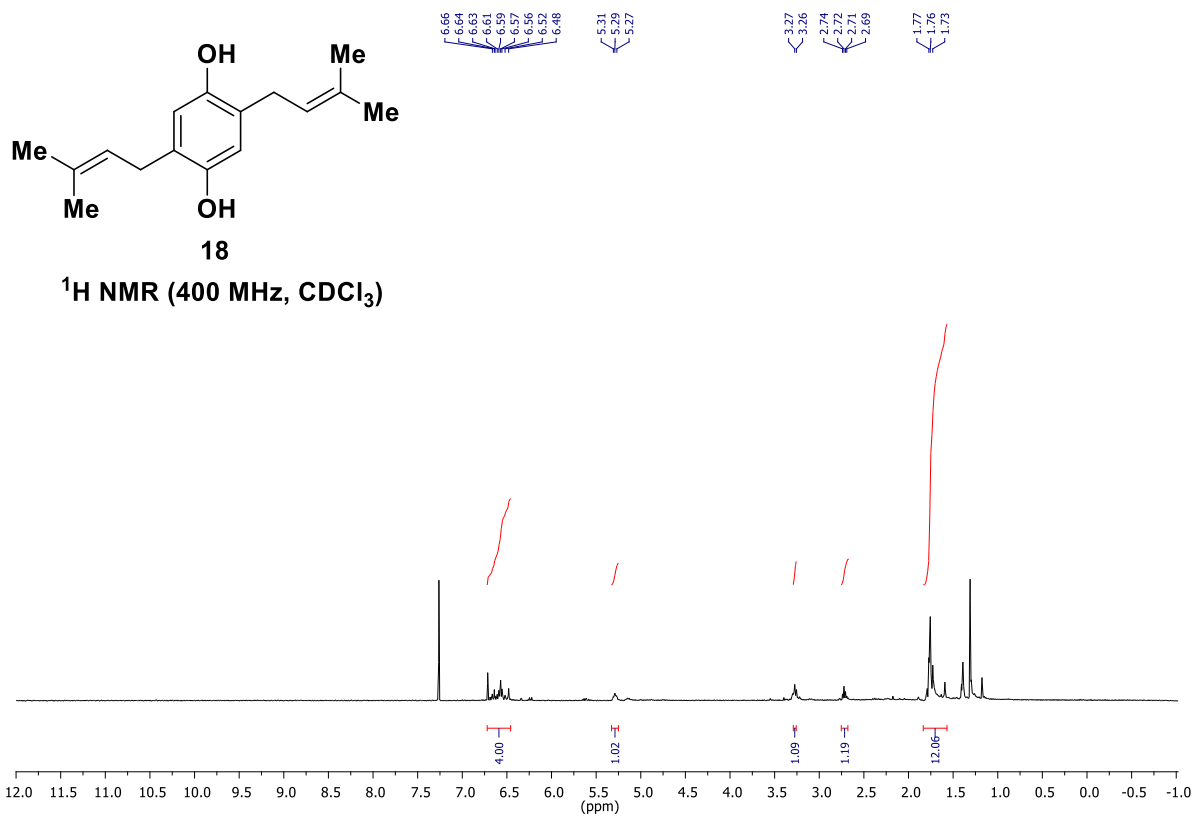
‡ Iván Cheng-Sánchez and José A. Torres-Vargas contributed equally to the execution of this work.

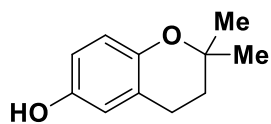
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| Representative dose-response curves | S22-S30 |

¹H and ¹³C NMR Spectra



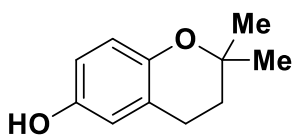
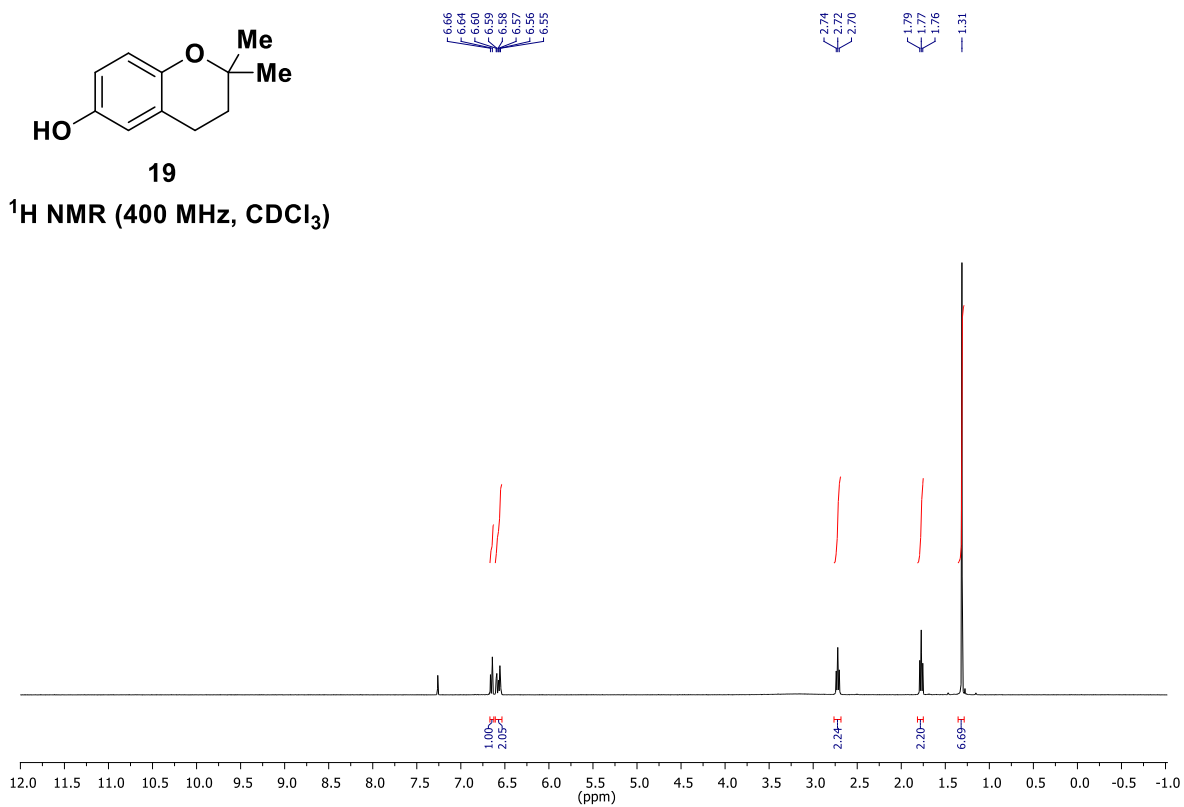






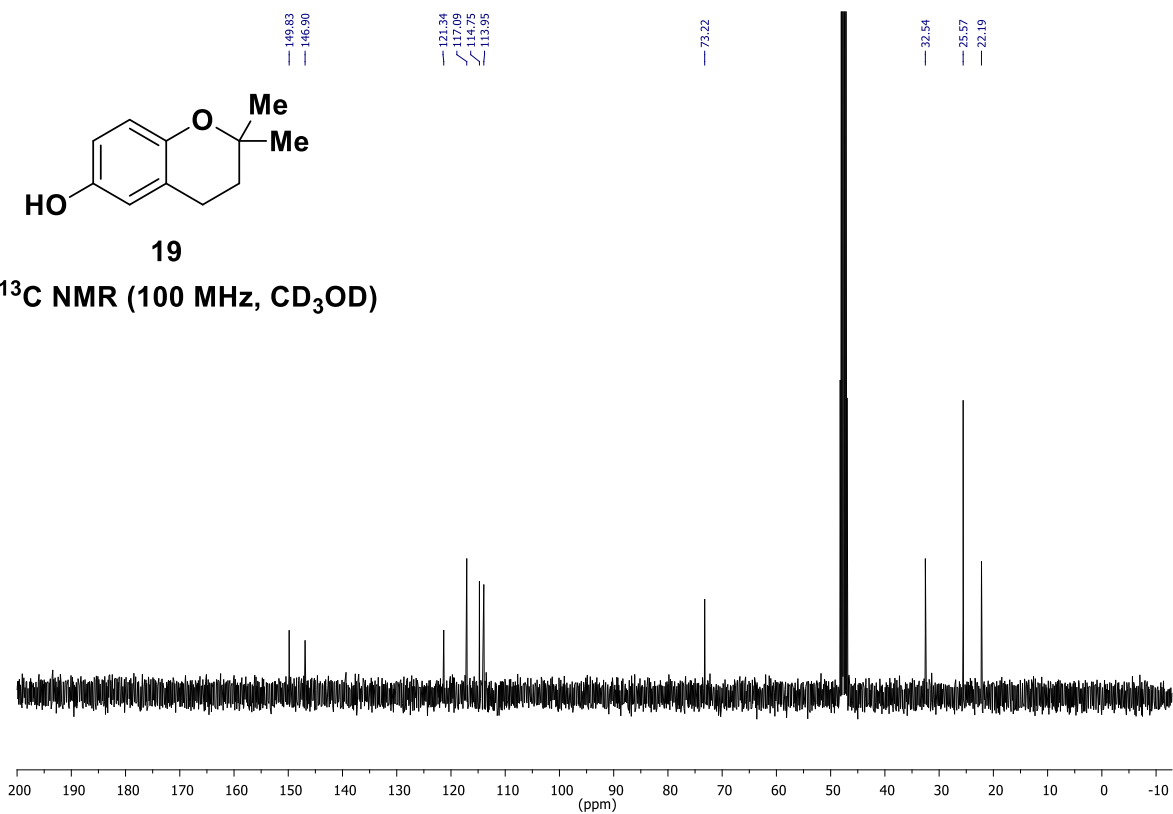
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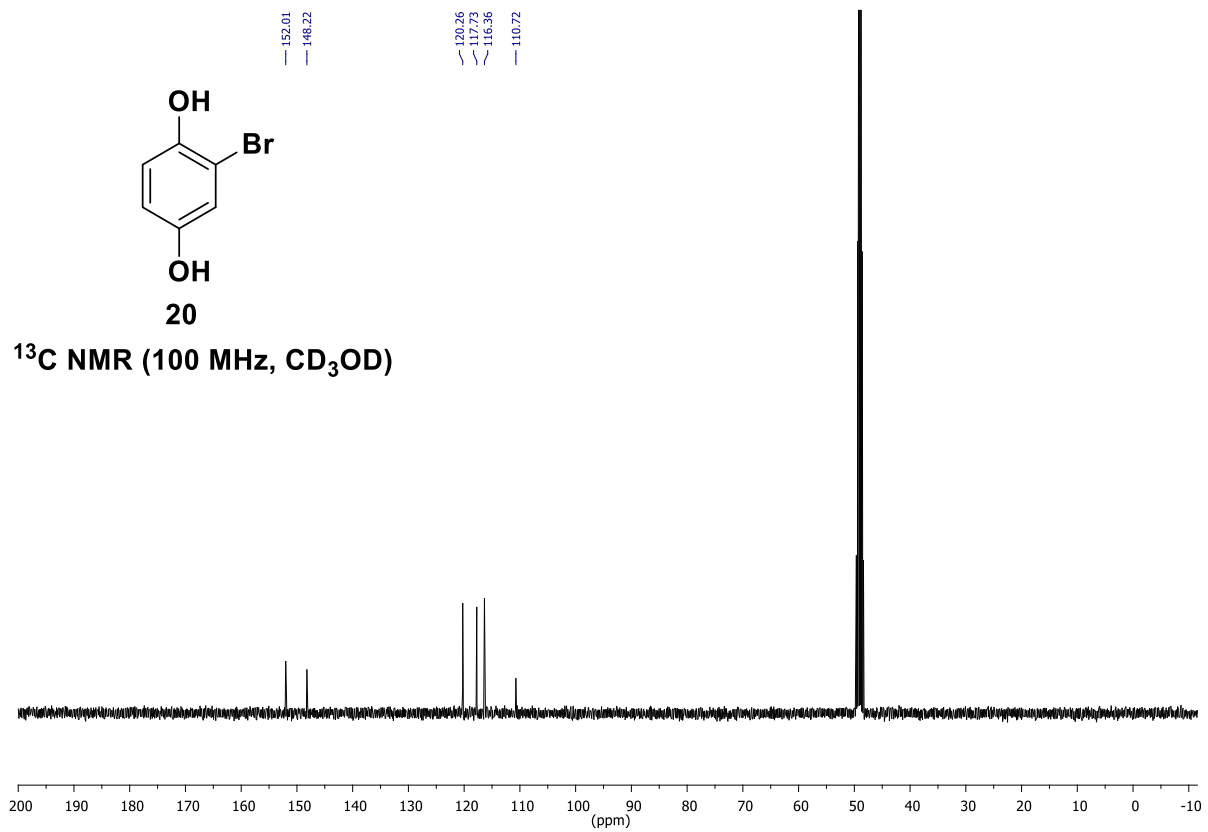
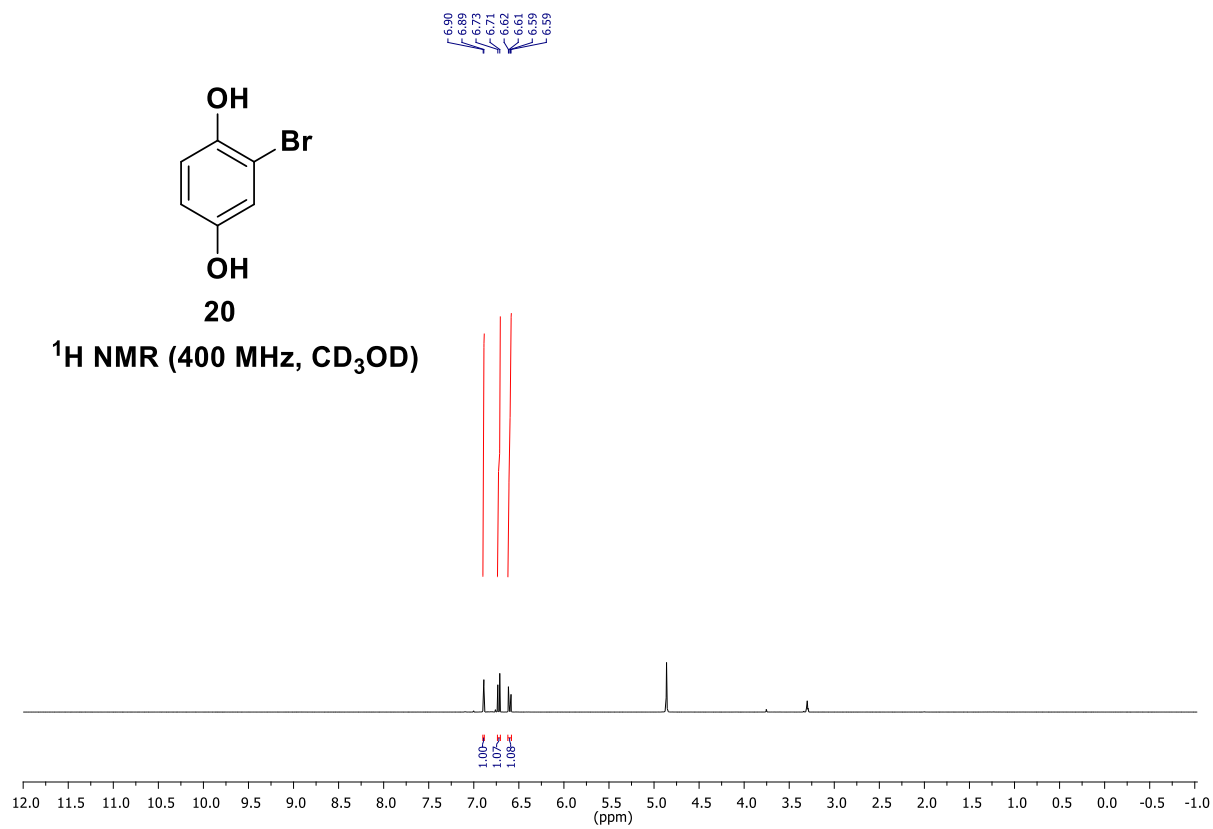
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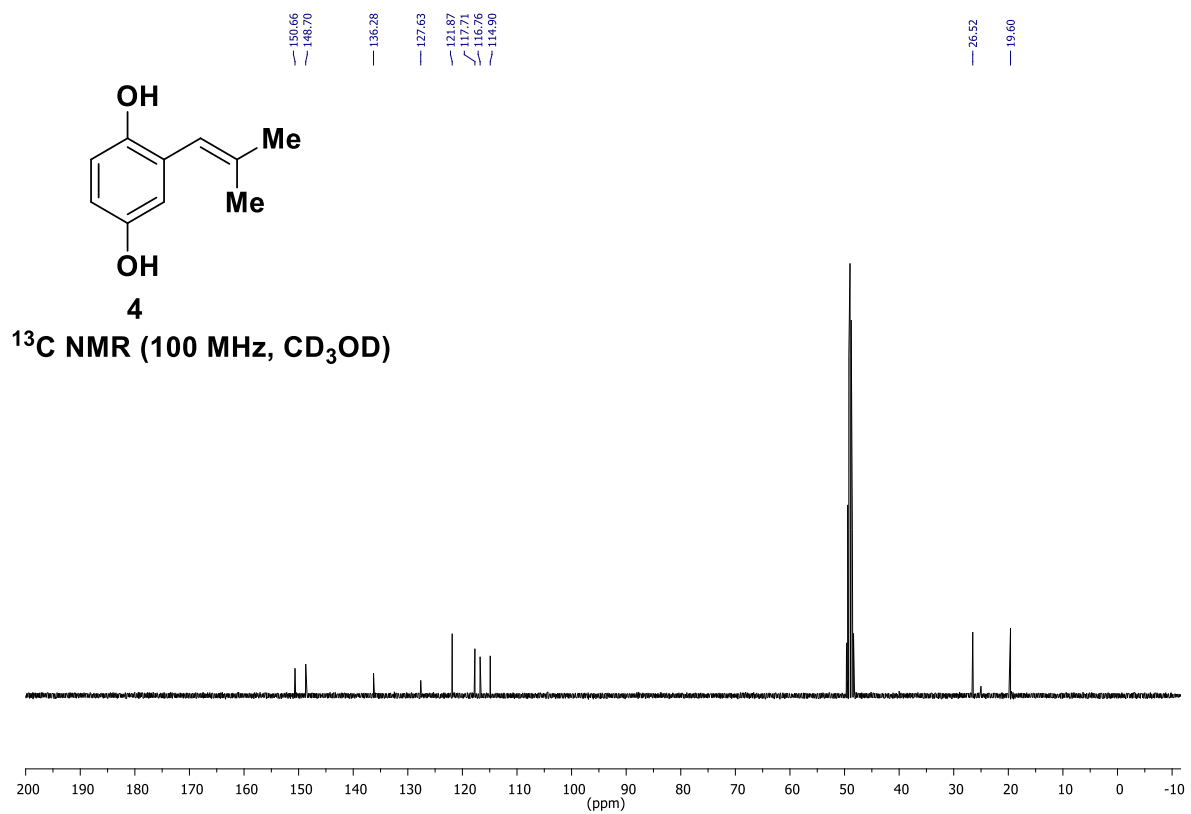
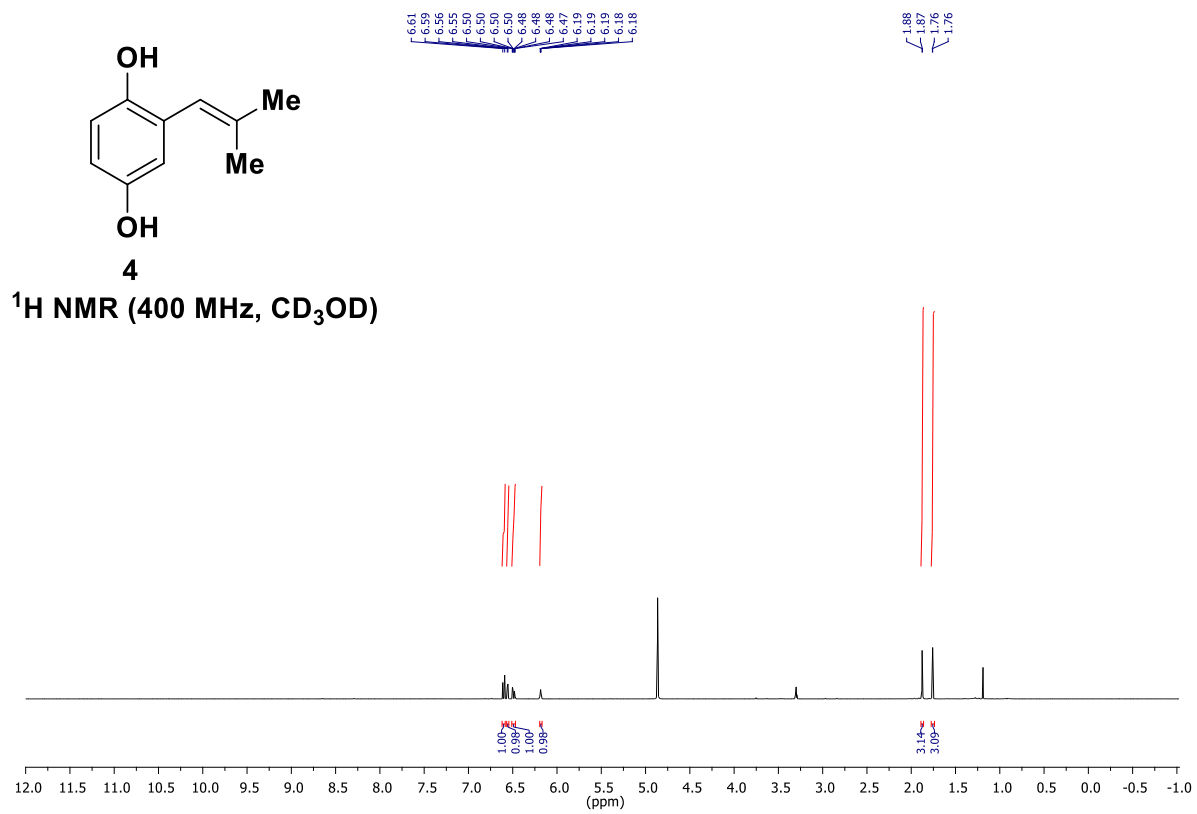


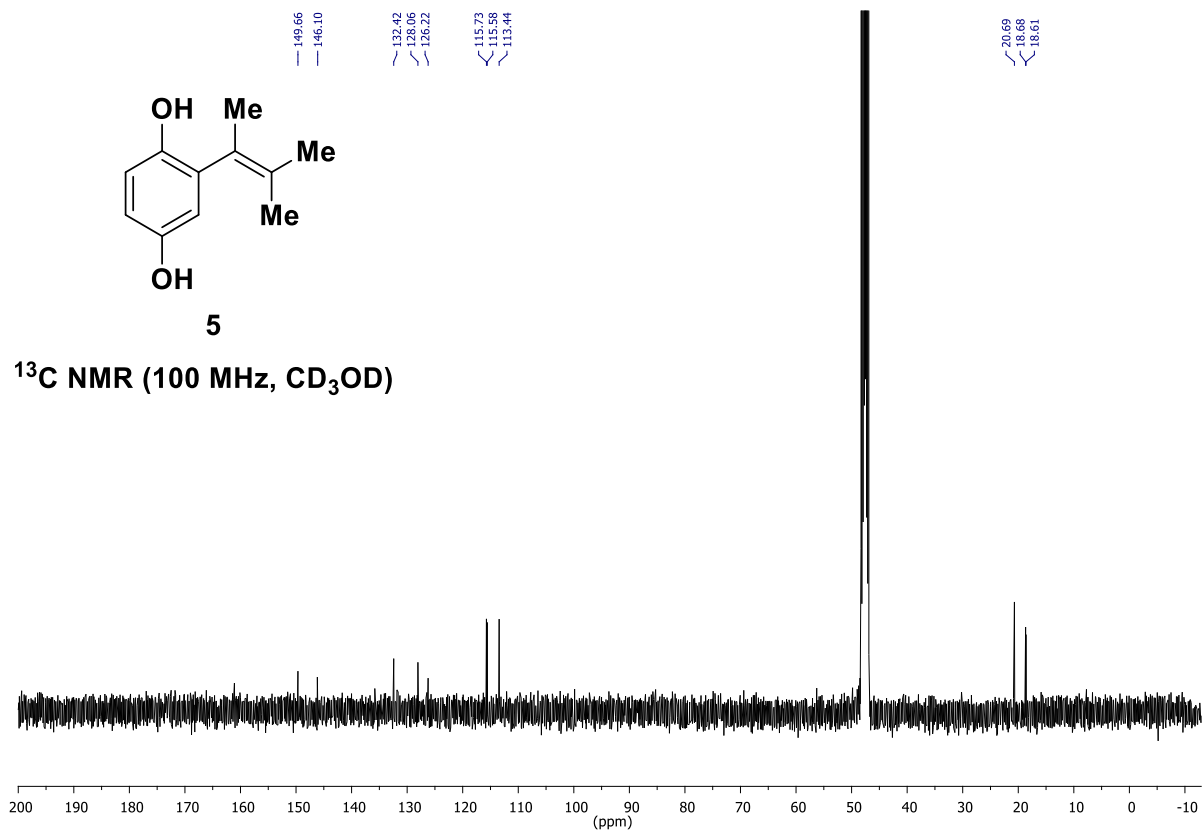
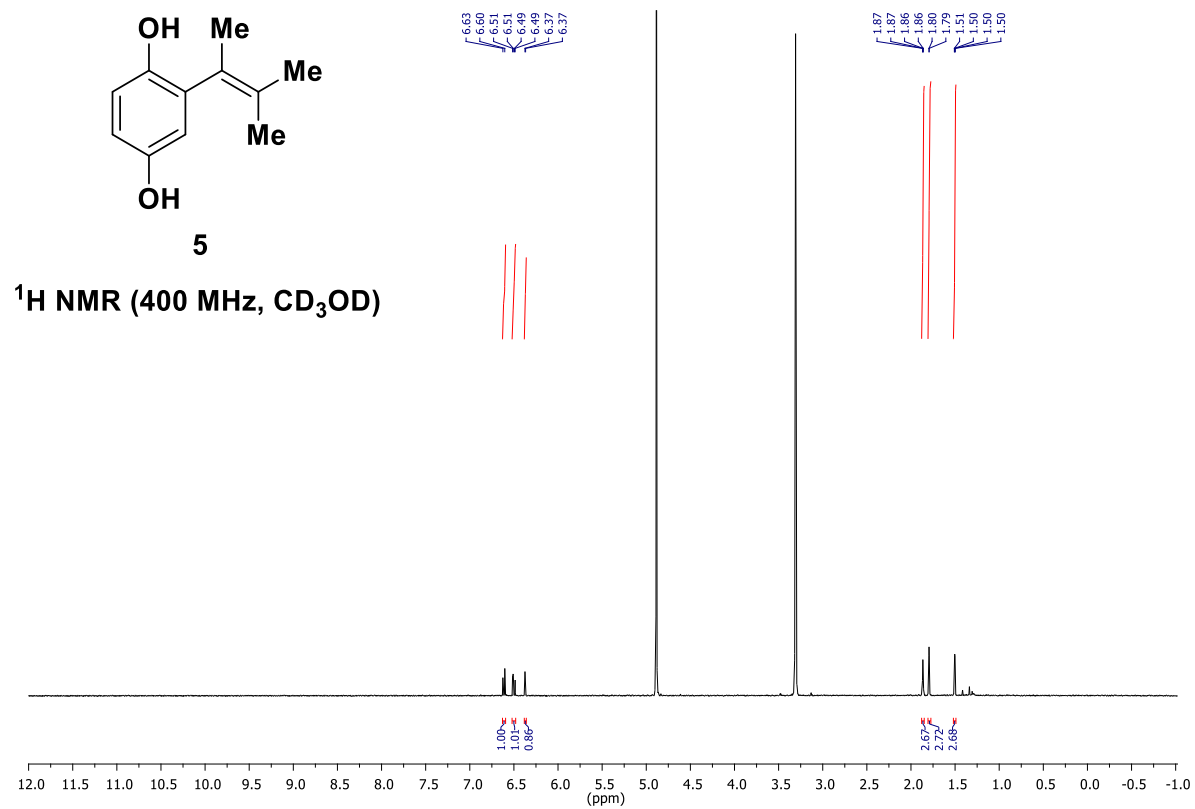
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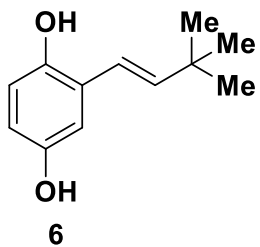
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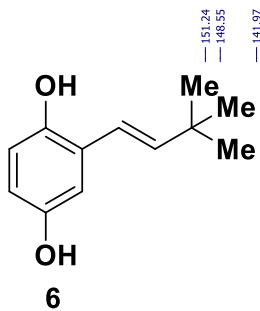
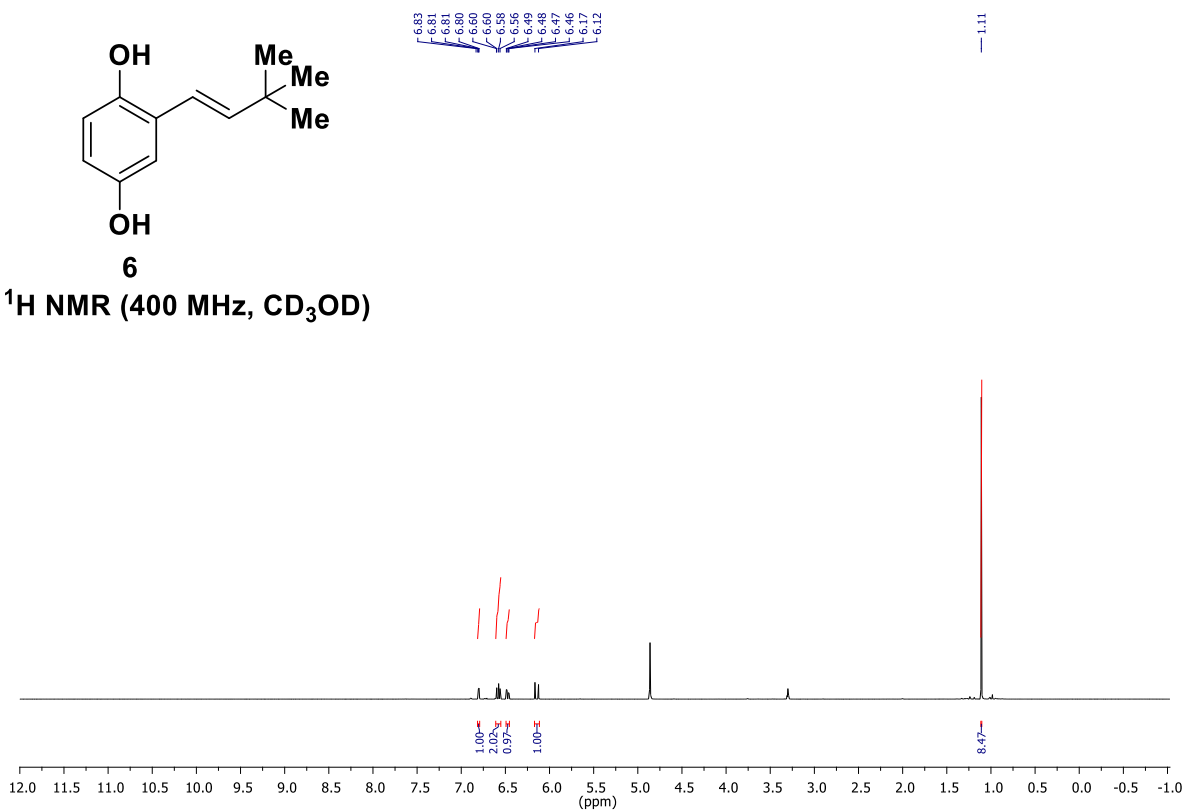




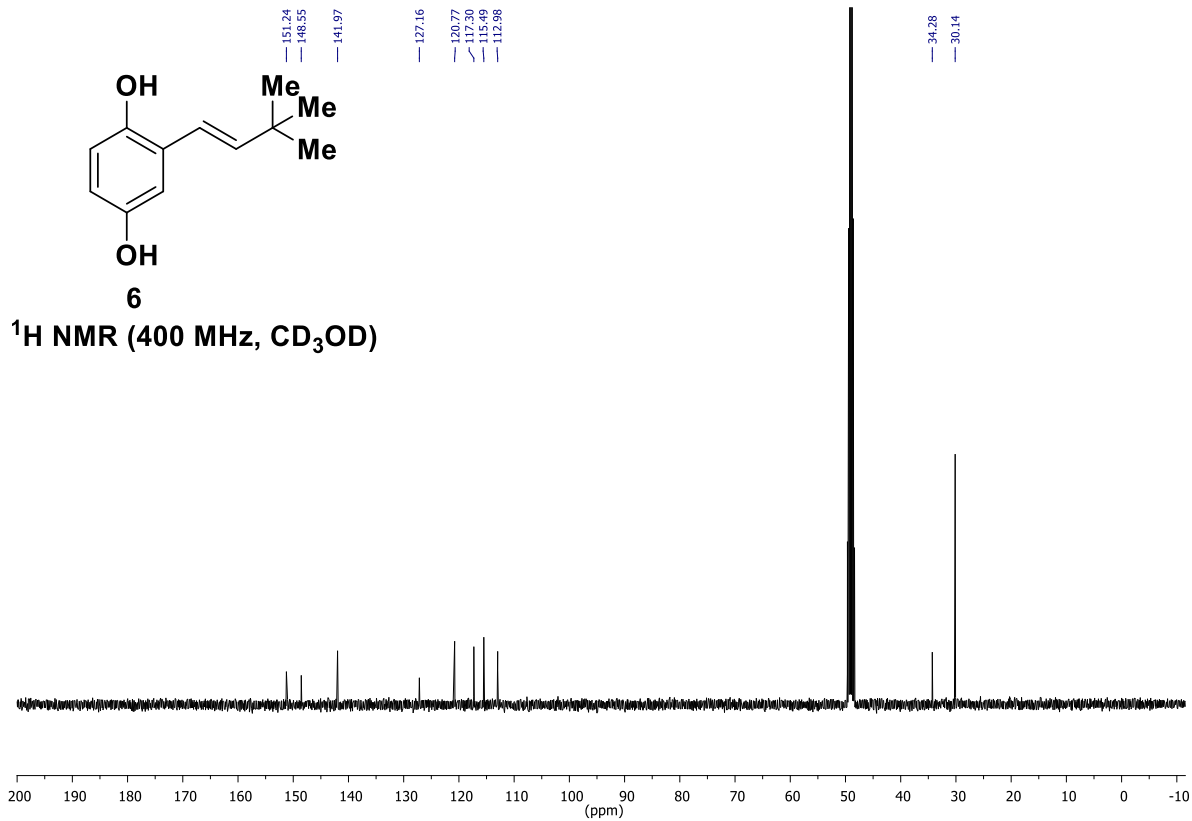


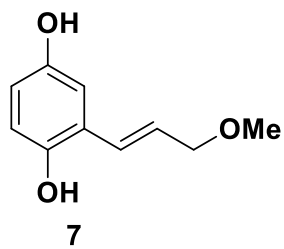


¹H NMR (400 MHz, CD₃OD)

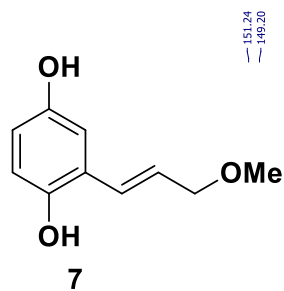
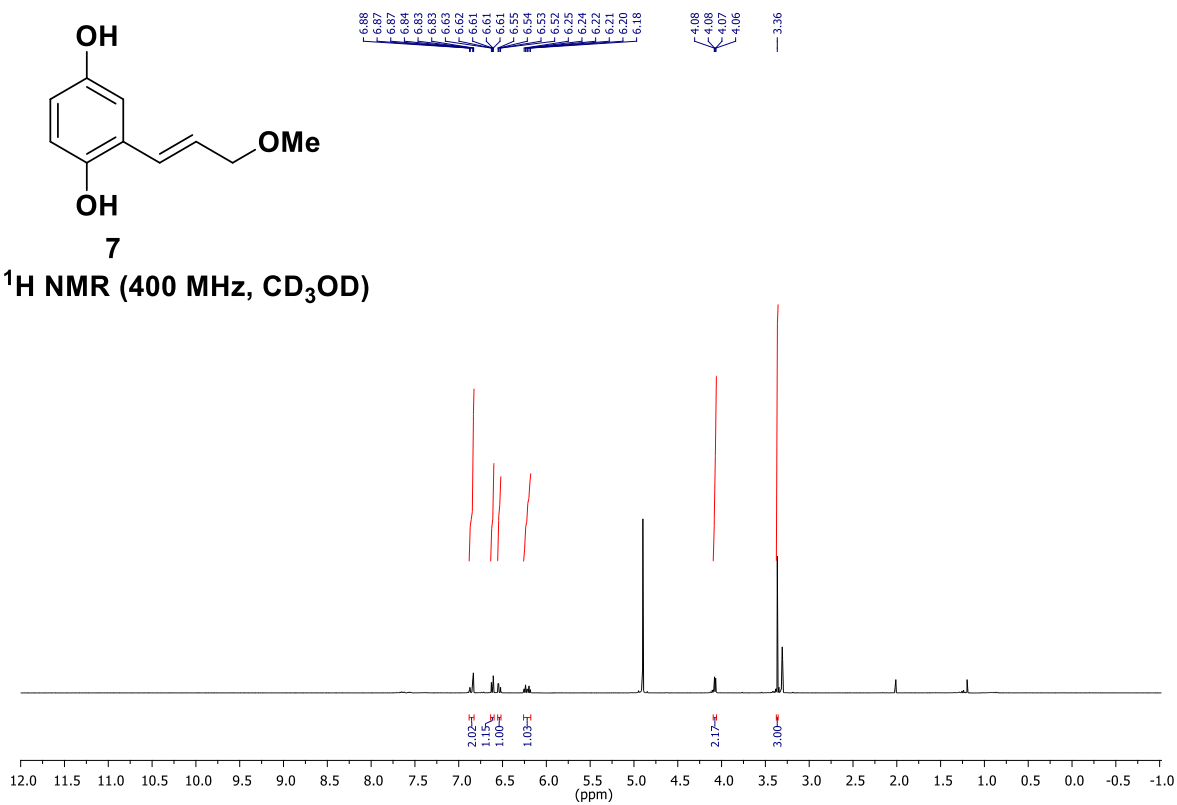


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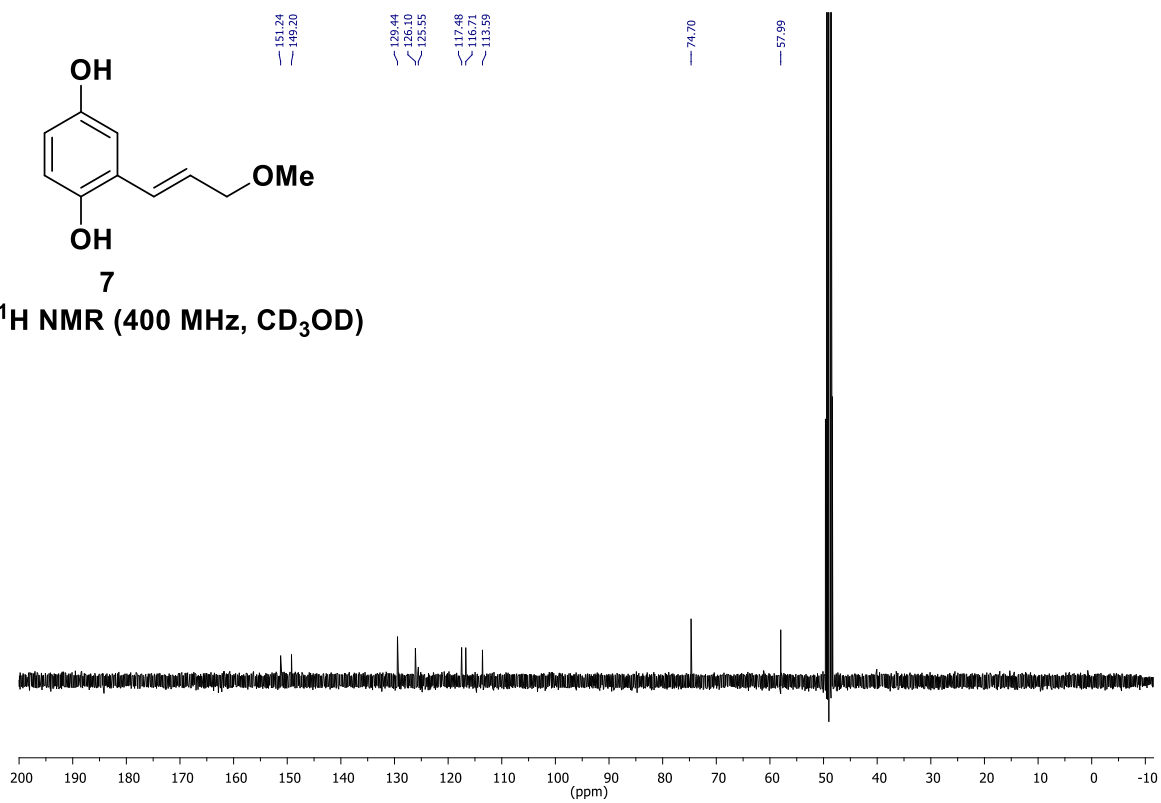


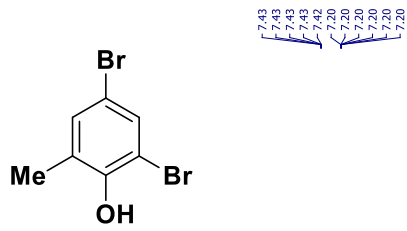


¹H NMR (400 MHz, CD₃OD)



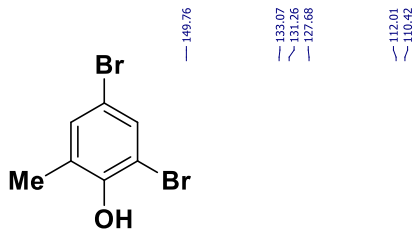
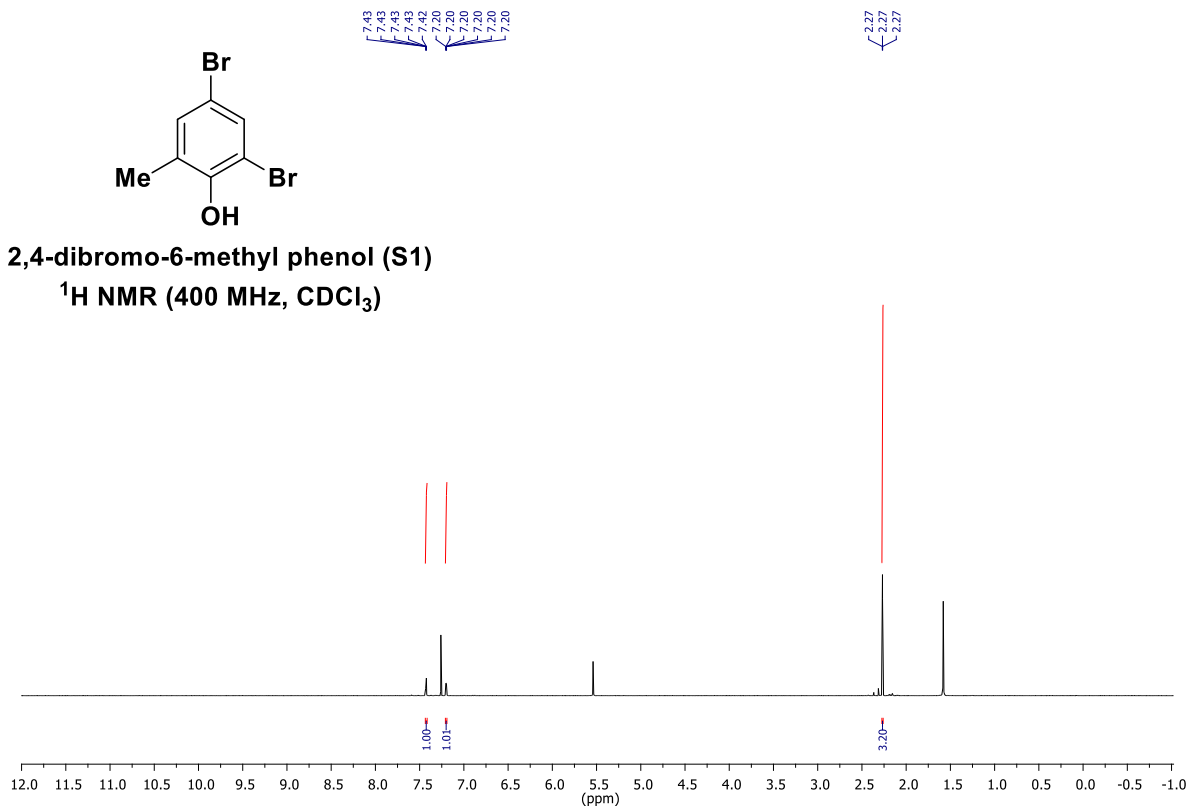
¹H NMR (400 MHz, CD₃OD)





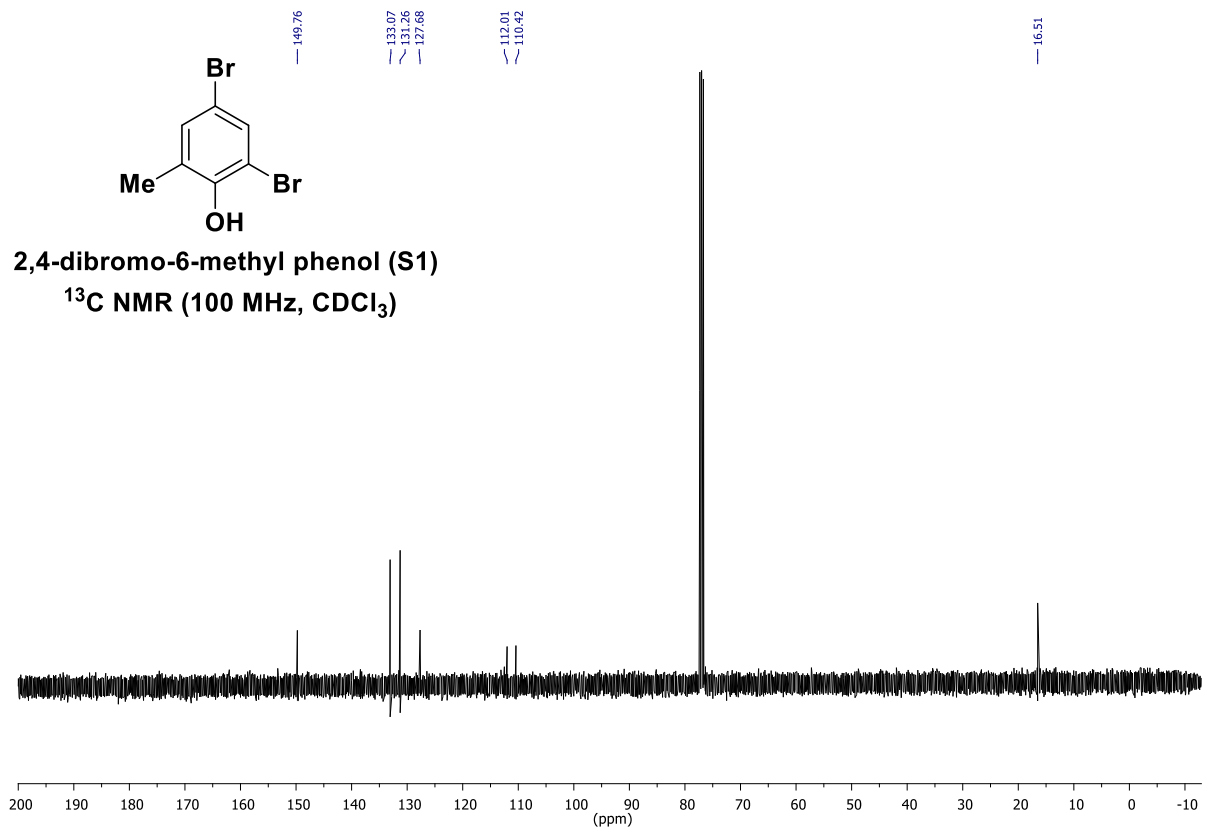
2,4-dibromo-6-methyl phenol (S1)

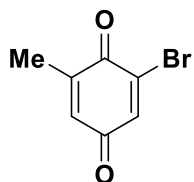
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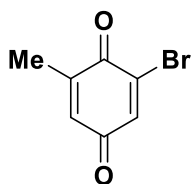
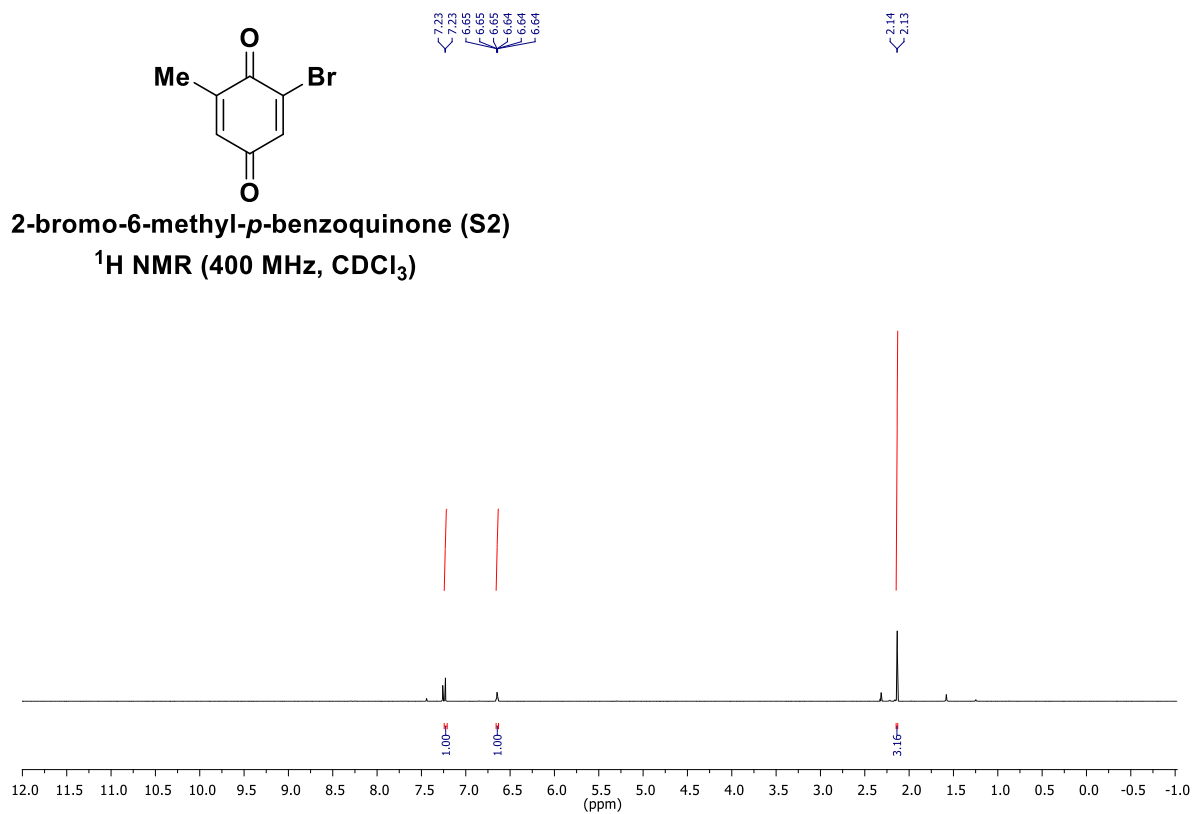
2,4-dibromo-6-methyl phenol (S1)

^{13}C NMR (100 MHz, CDCl_3)

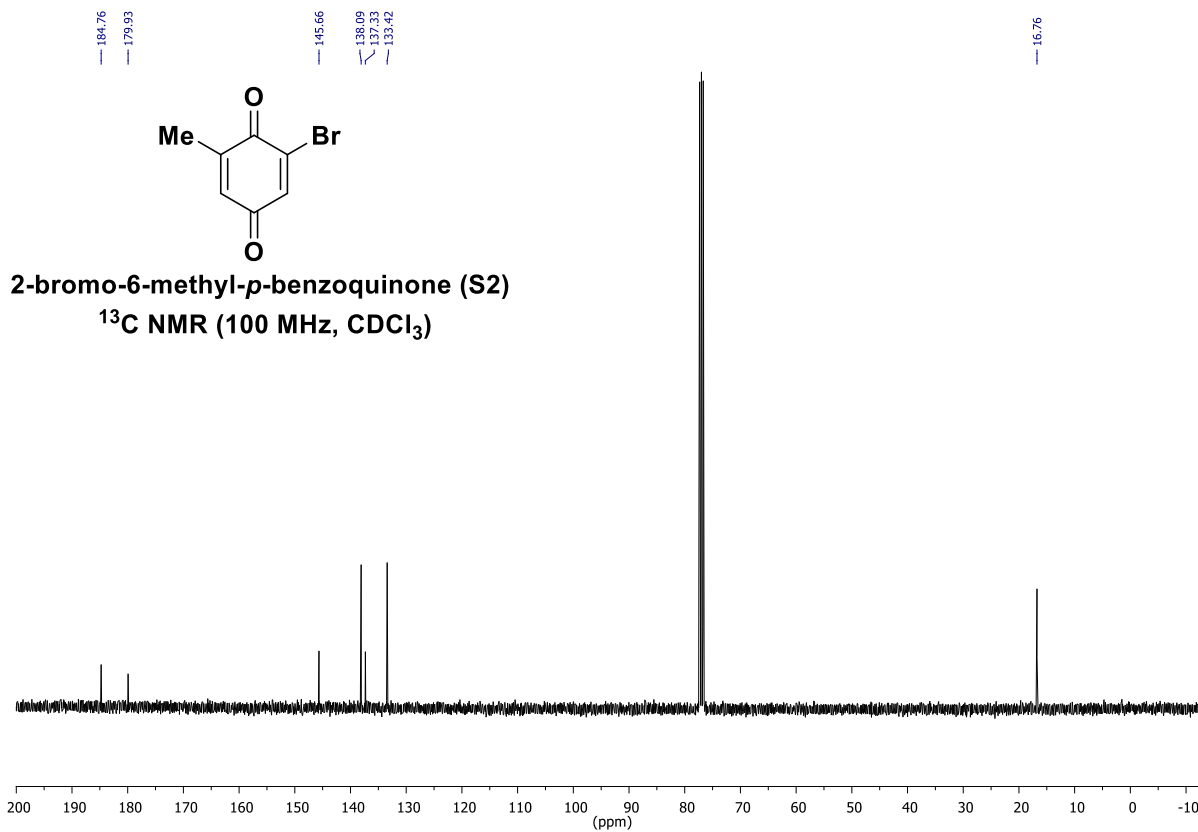


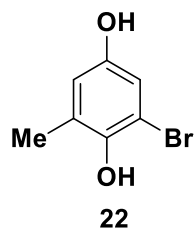


2-bromo-6-methyl-*p*-benzoquinone (S2)
 ^1H NMR (400 MHz, CDCl_3)

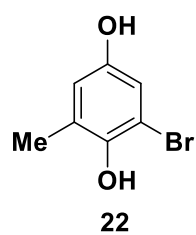
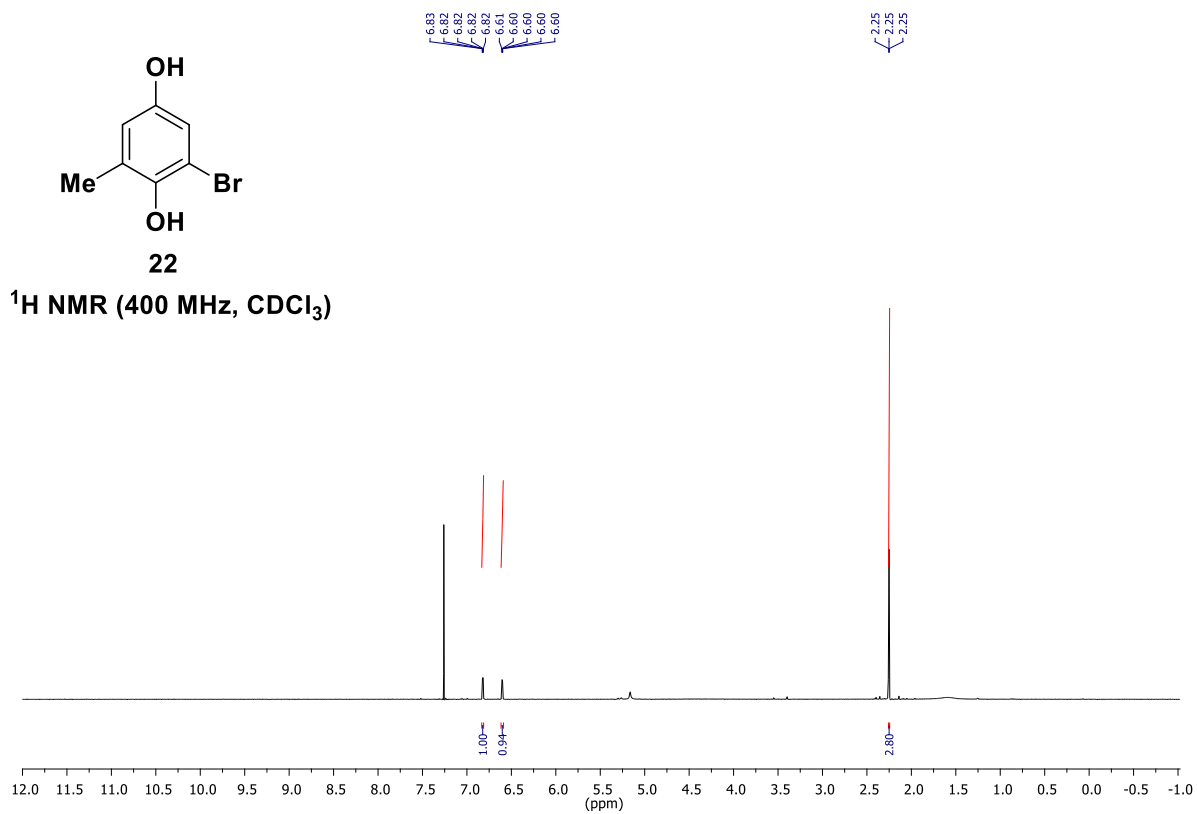


2-bromo-6-methyl-*p*-benzoquinone (S2)
 ^{13}C NMR (100 MHz, CDCl_3)

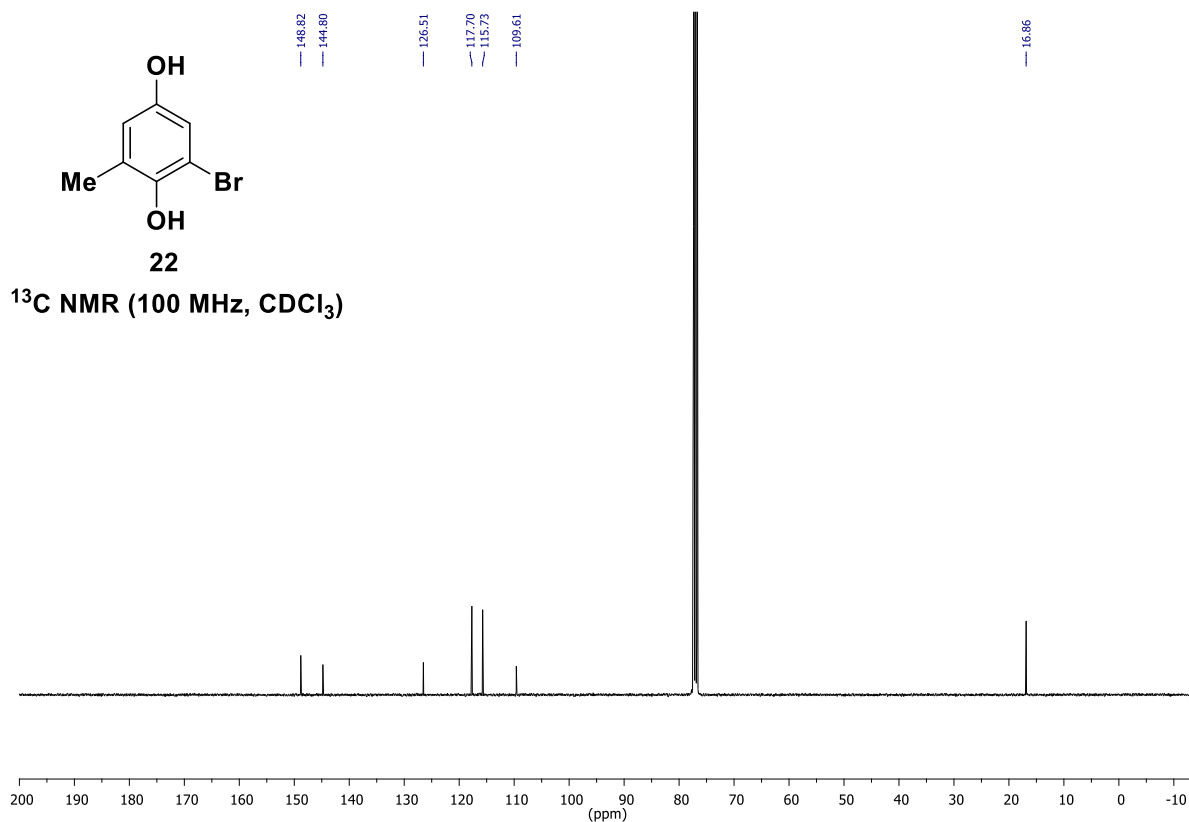


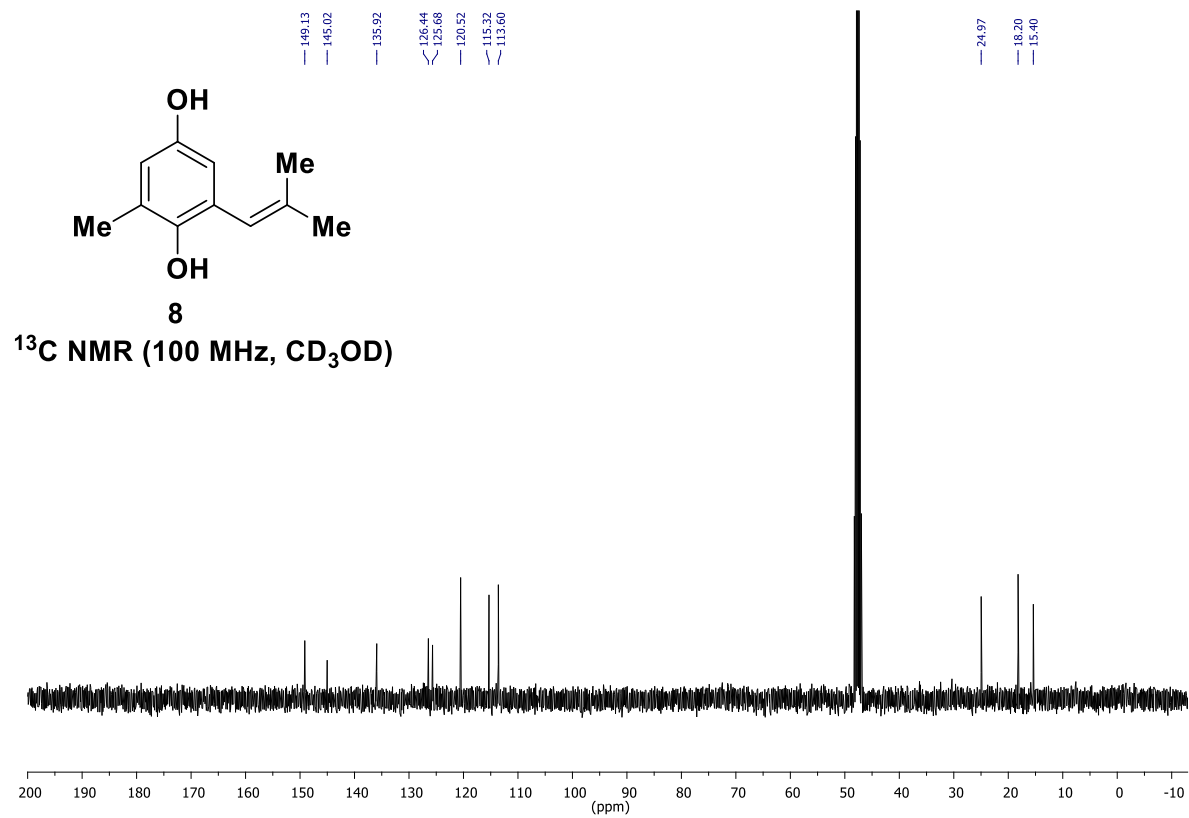
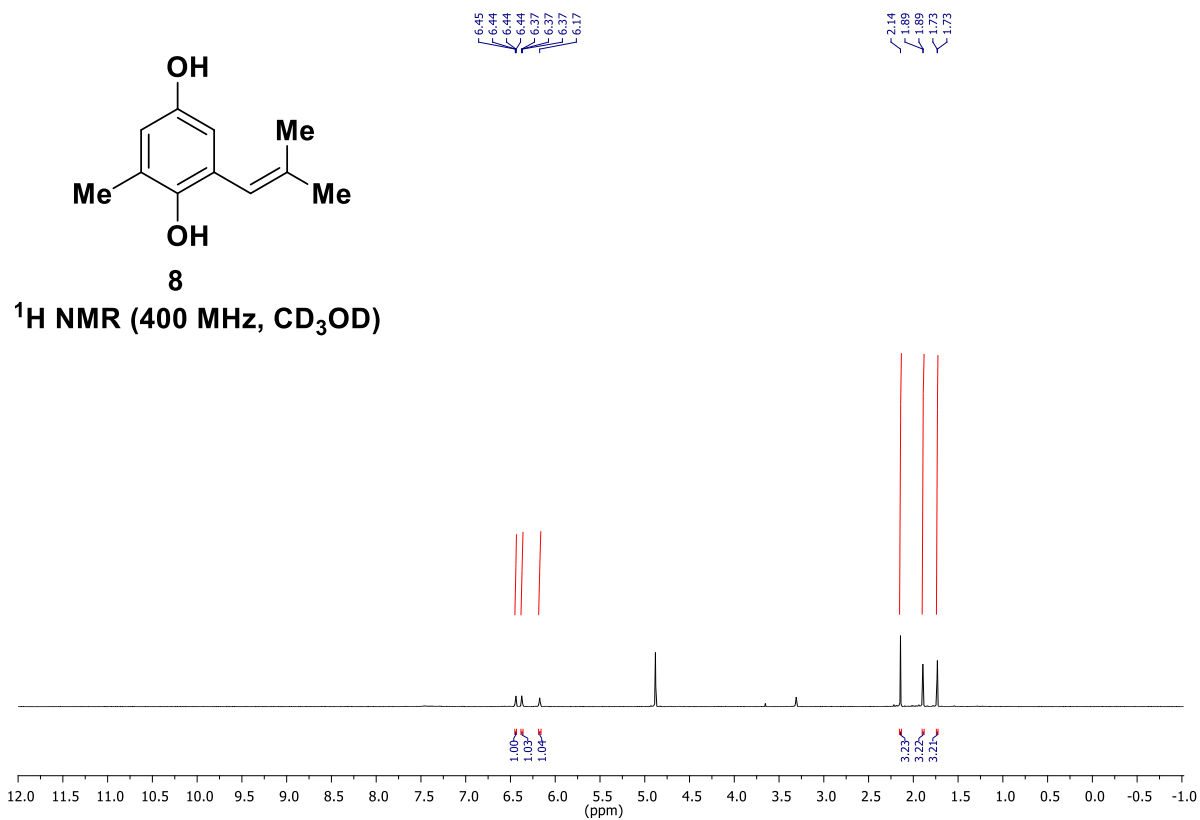


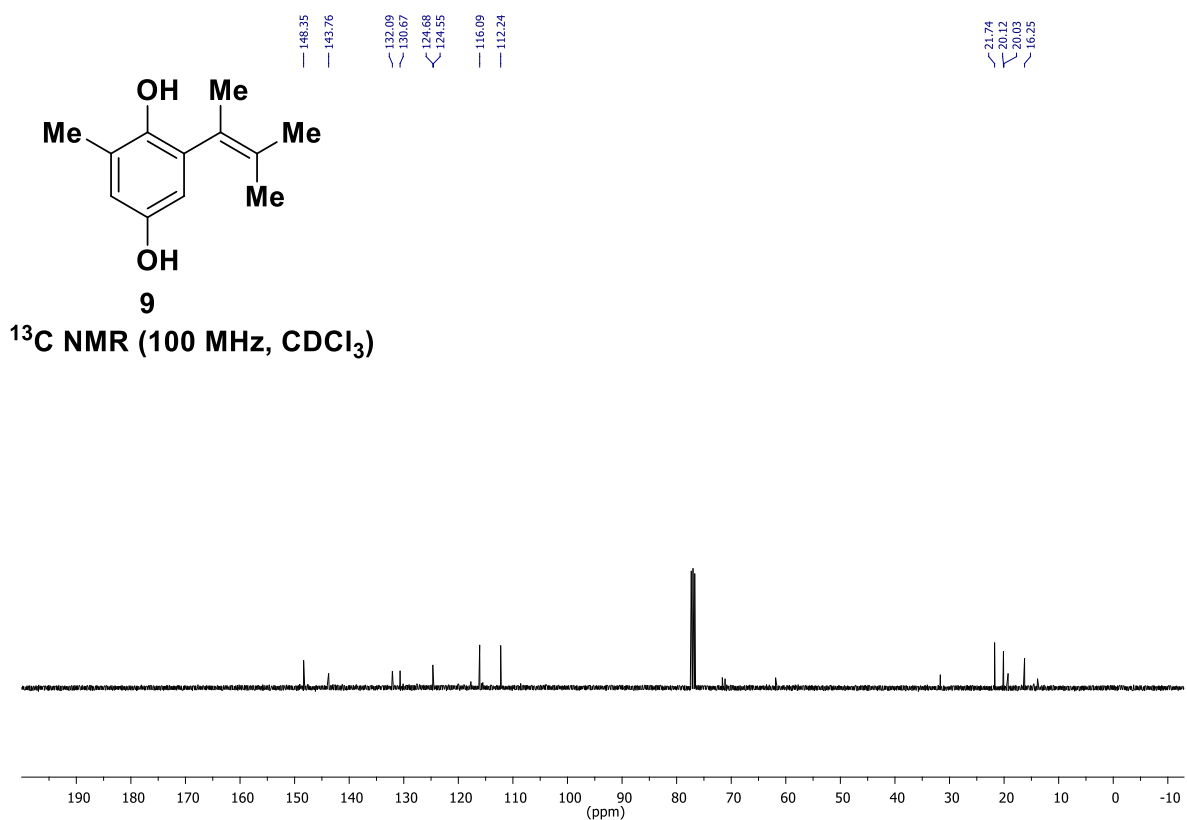
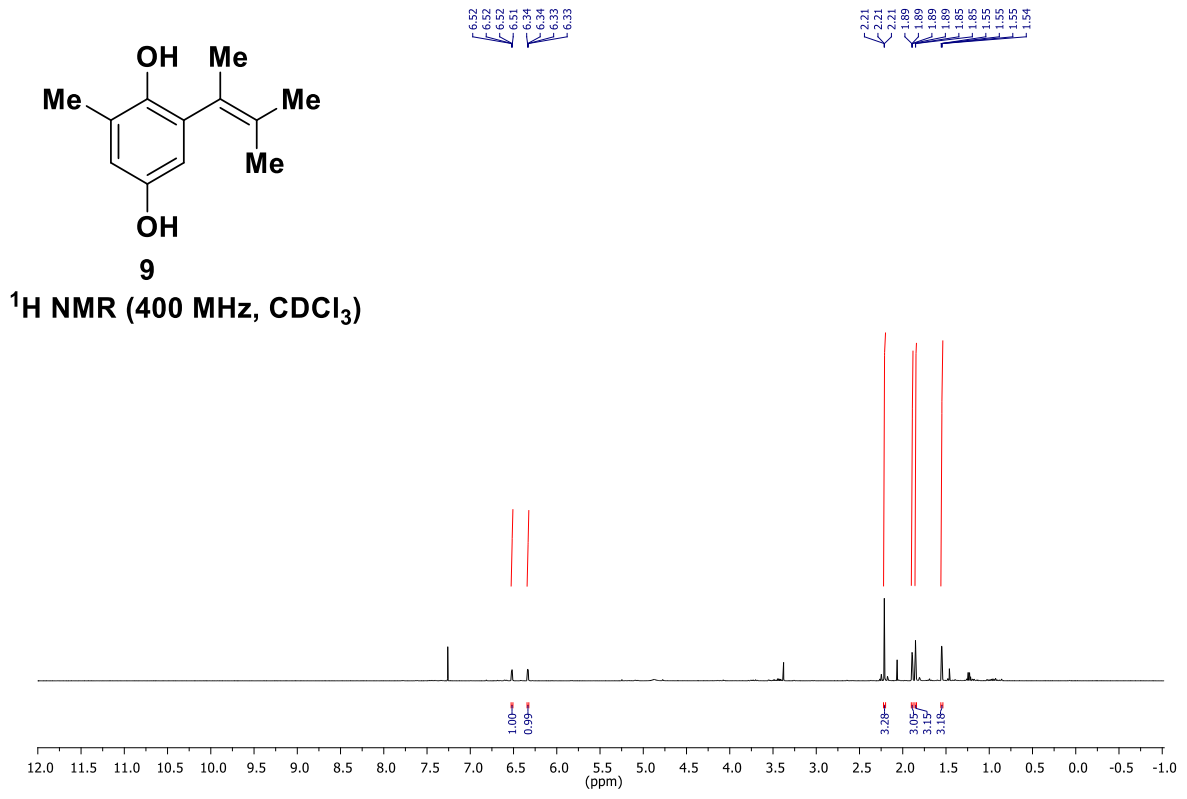
¹H NMR (400 MHz, CDCl₃)

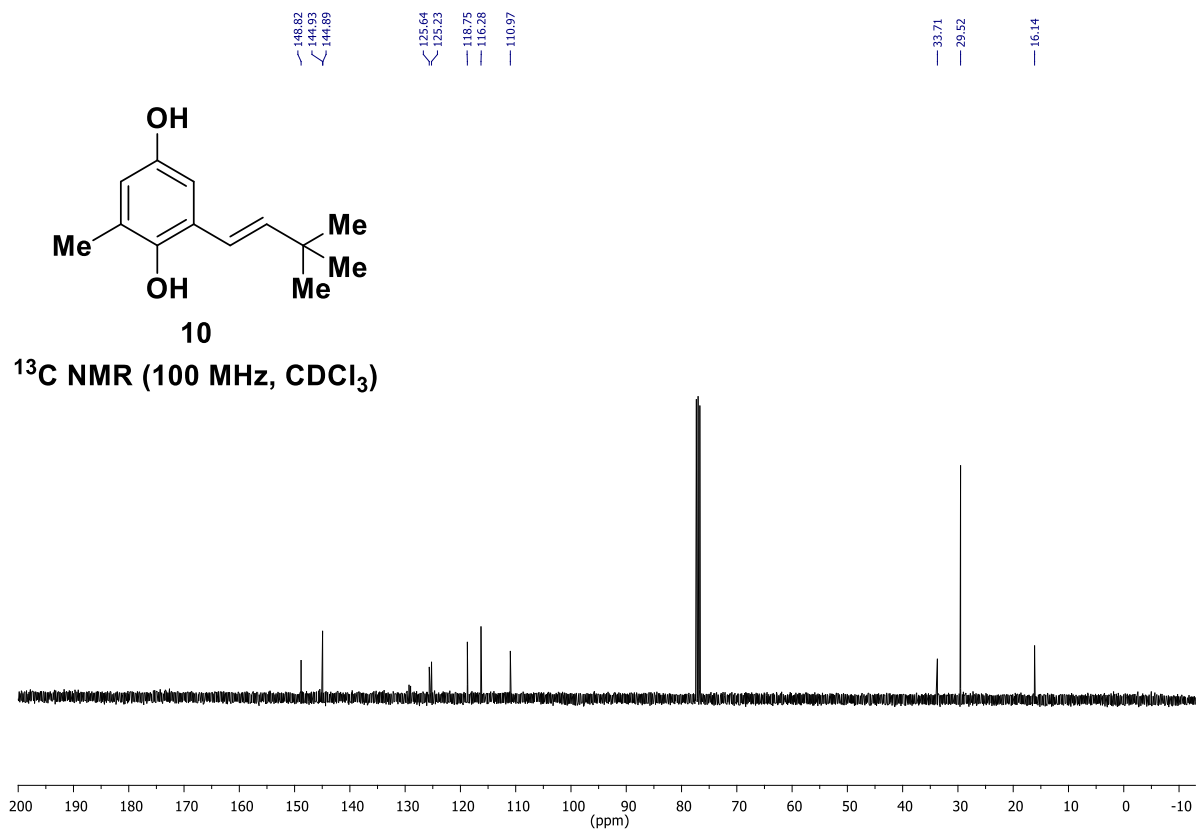
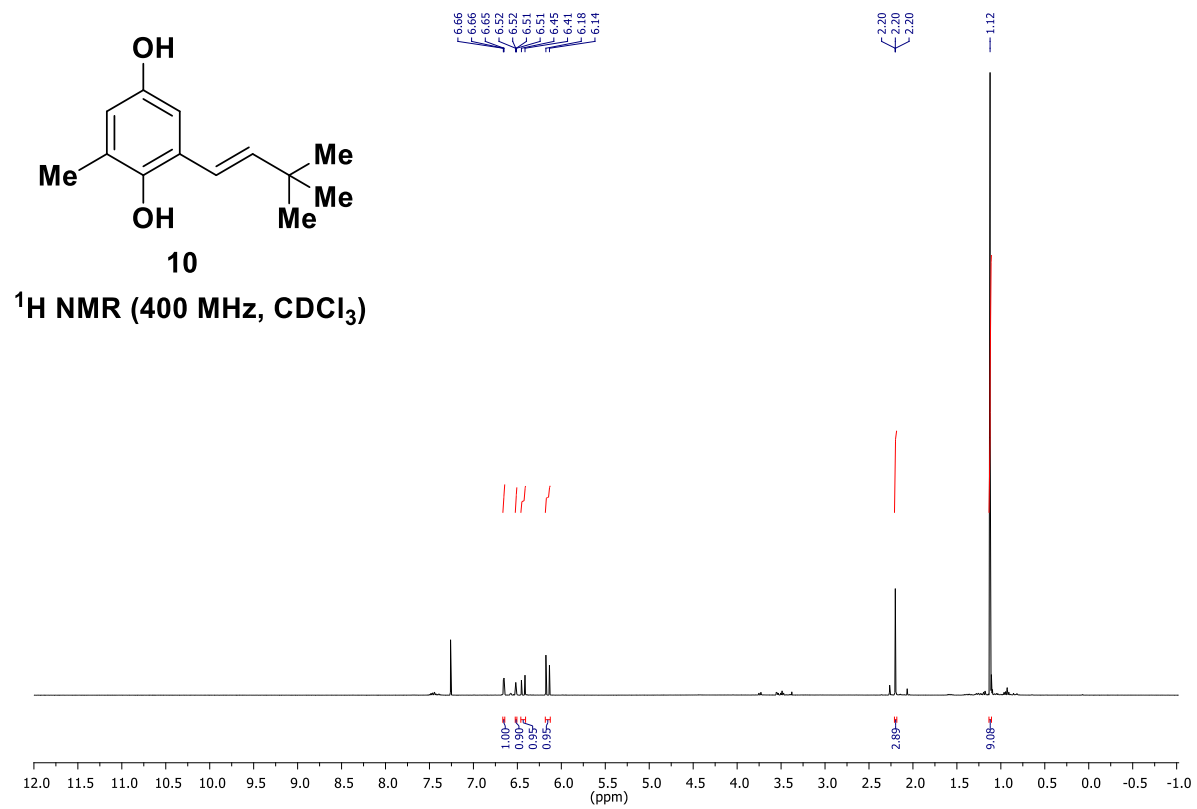


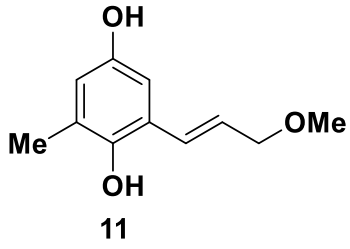
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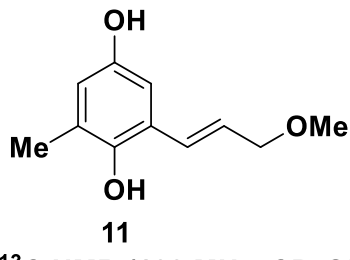
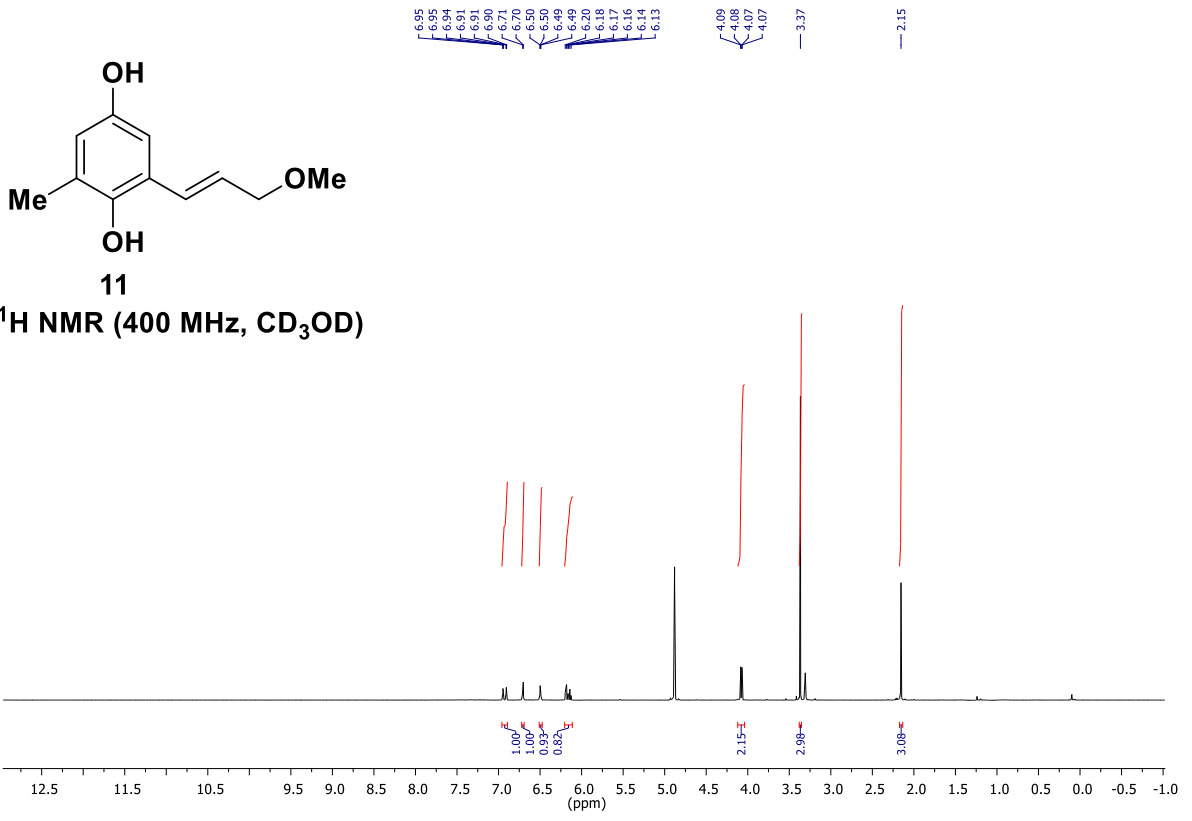




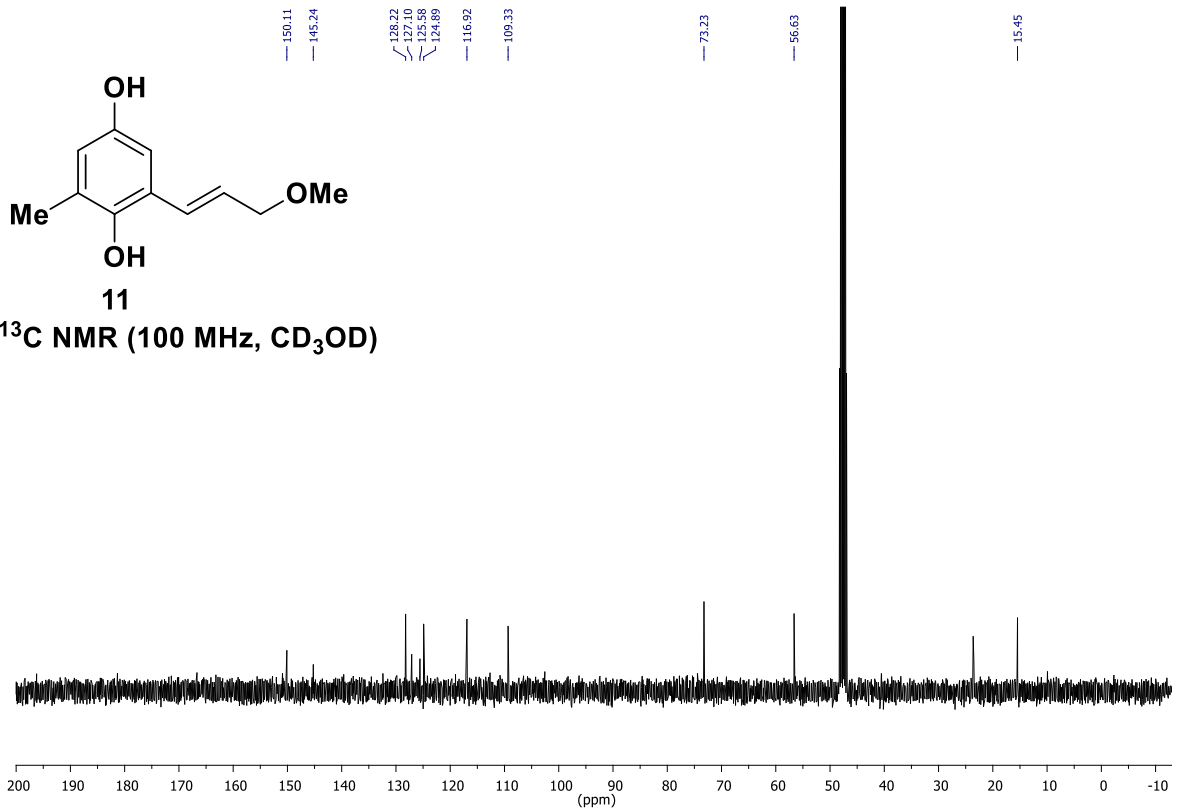


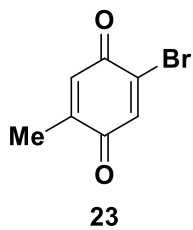


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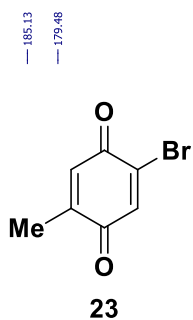
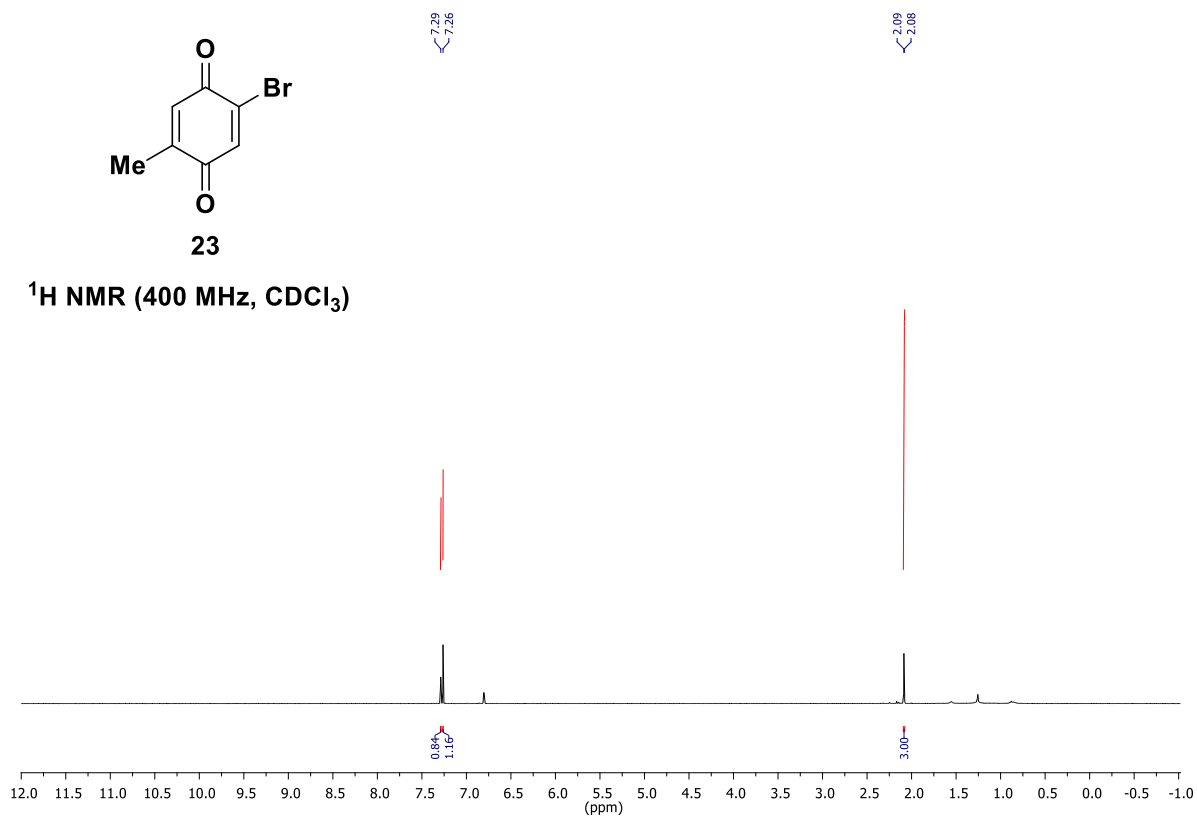


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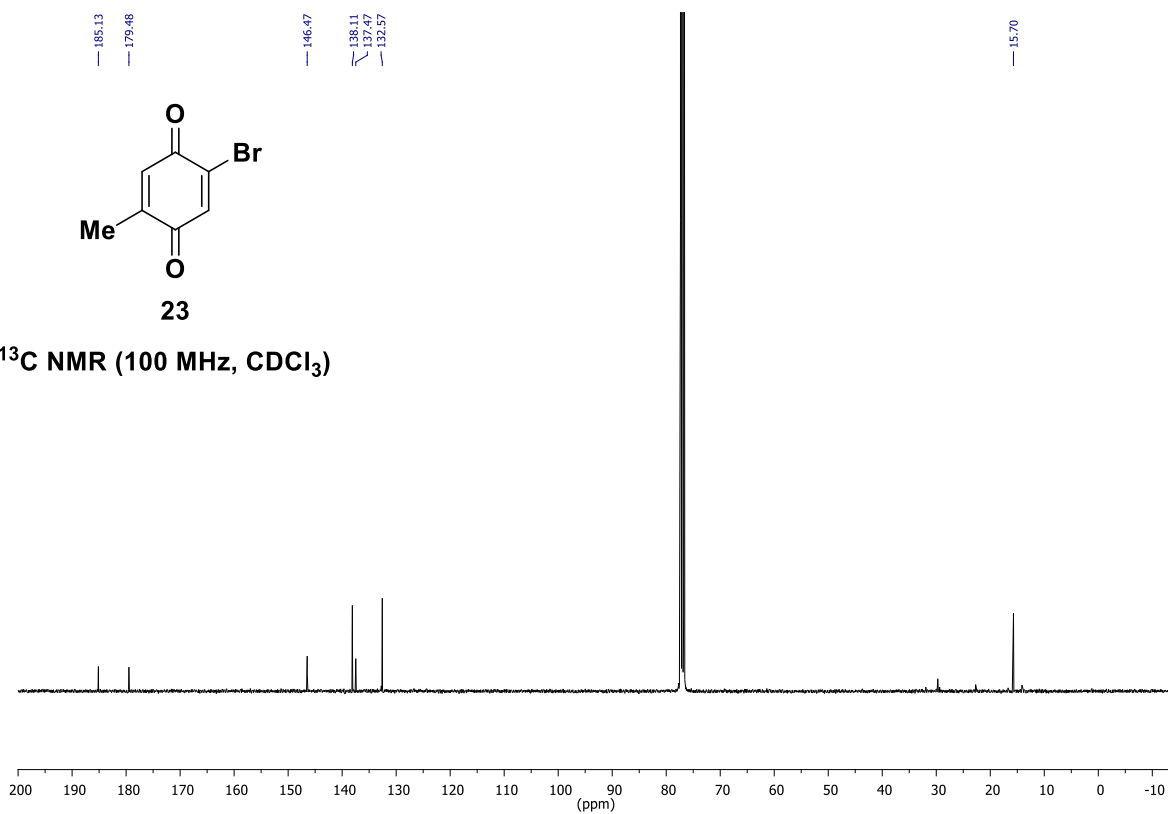


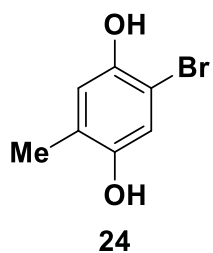


¹H NMR (400 MHz, CDCl₃)

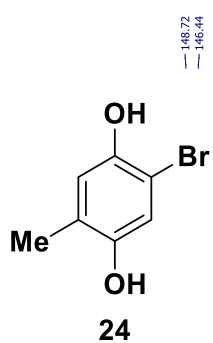
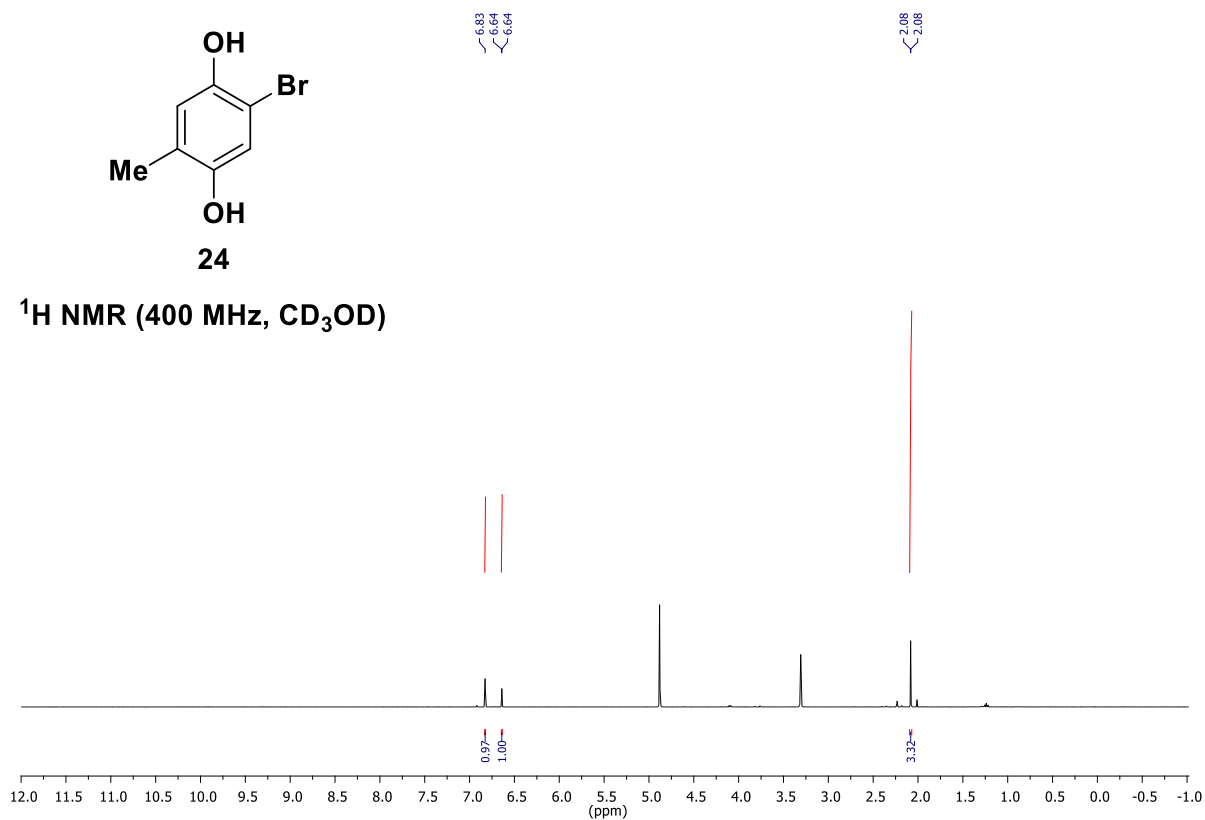


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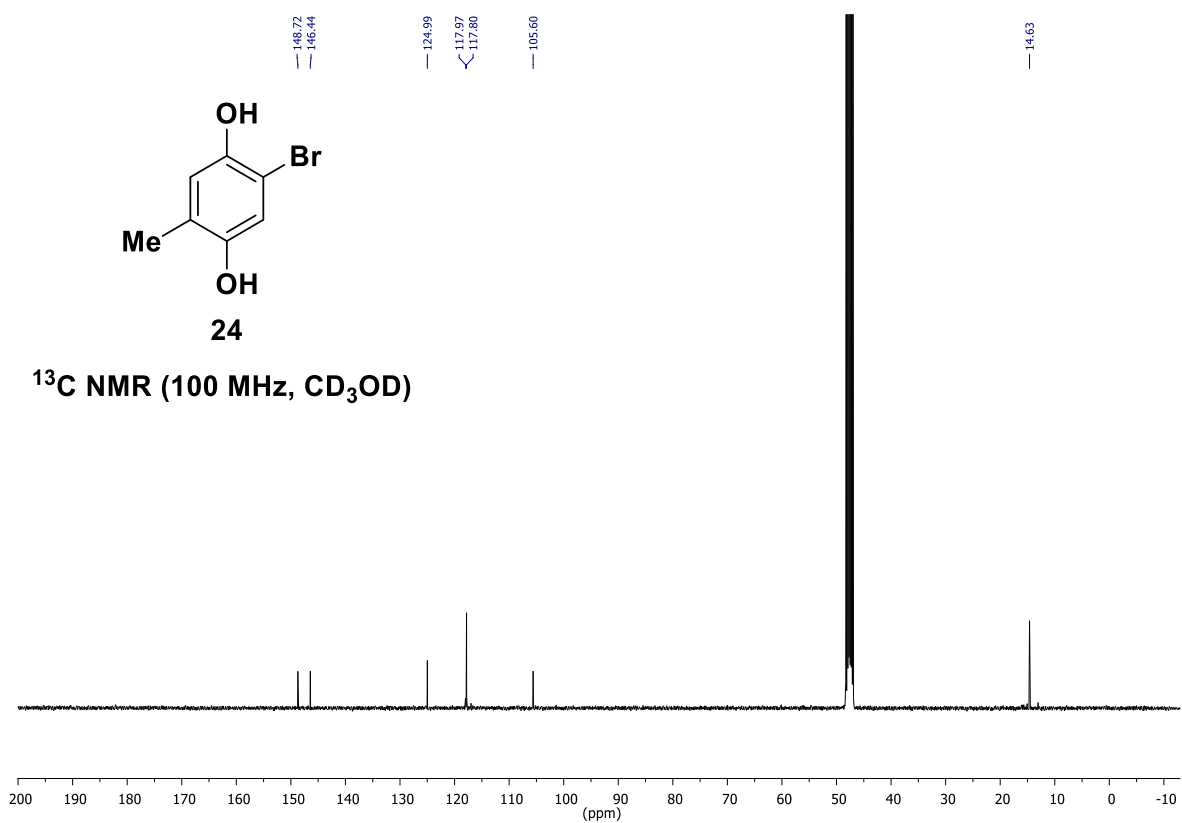


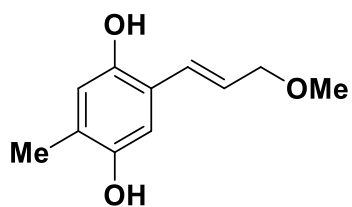


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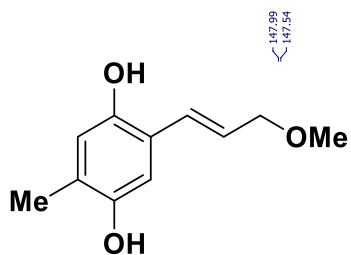
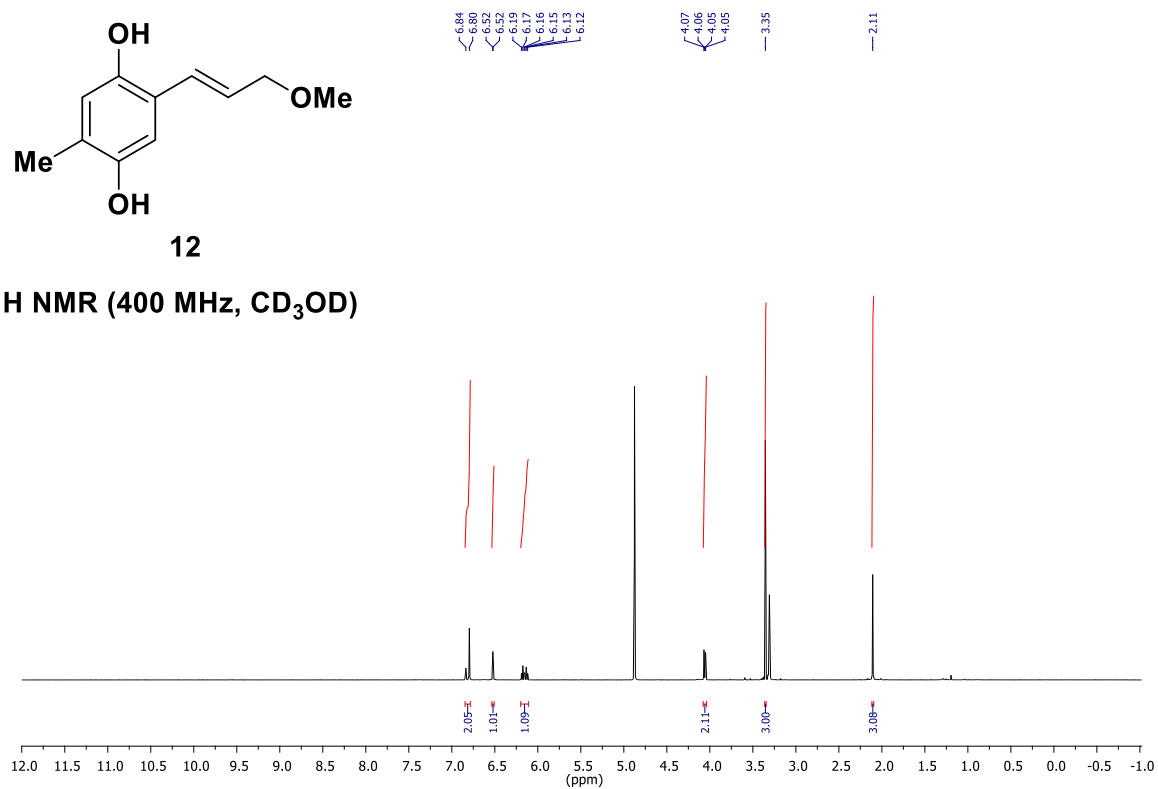
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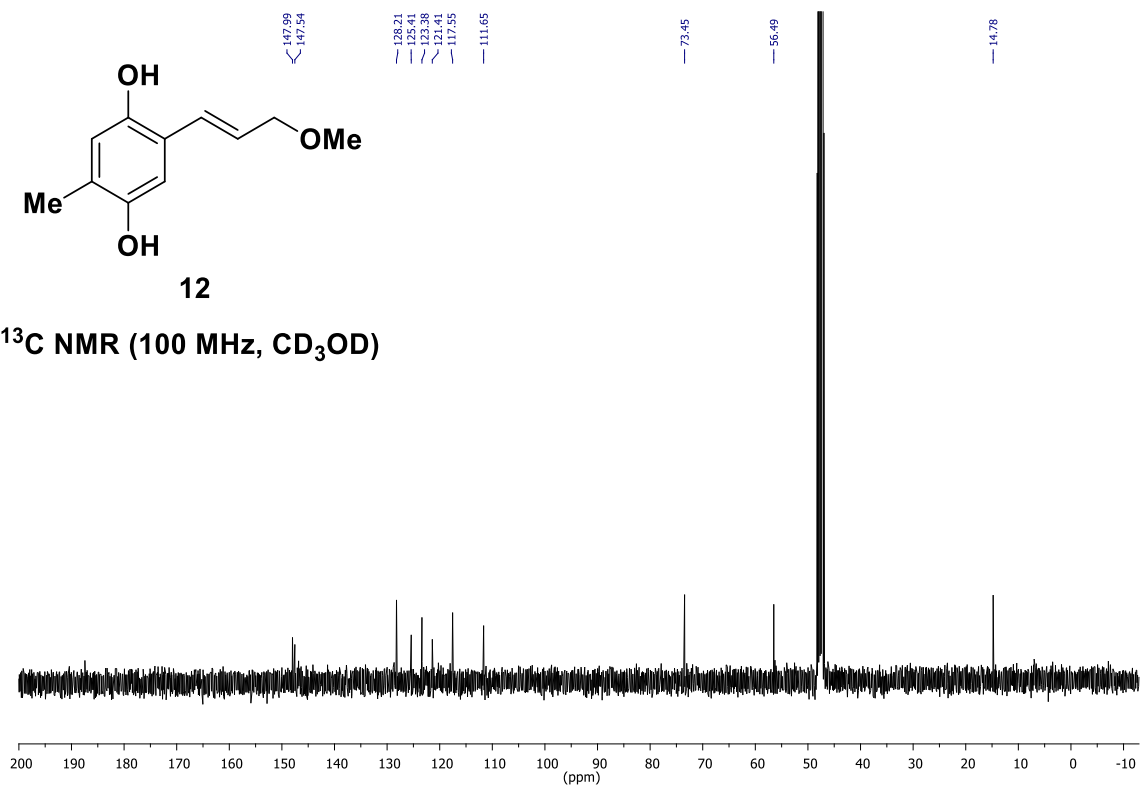
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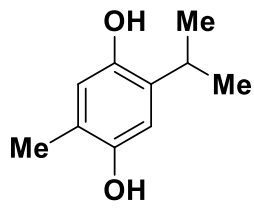
^1H NMR (400 MHz, CD_3OD)



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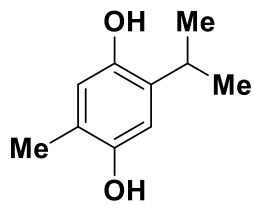
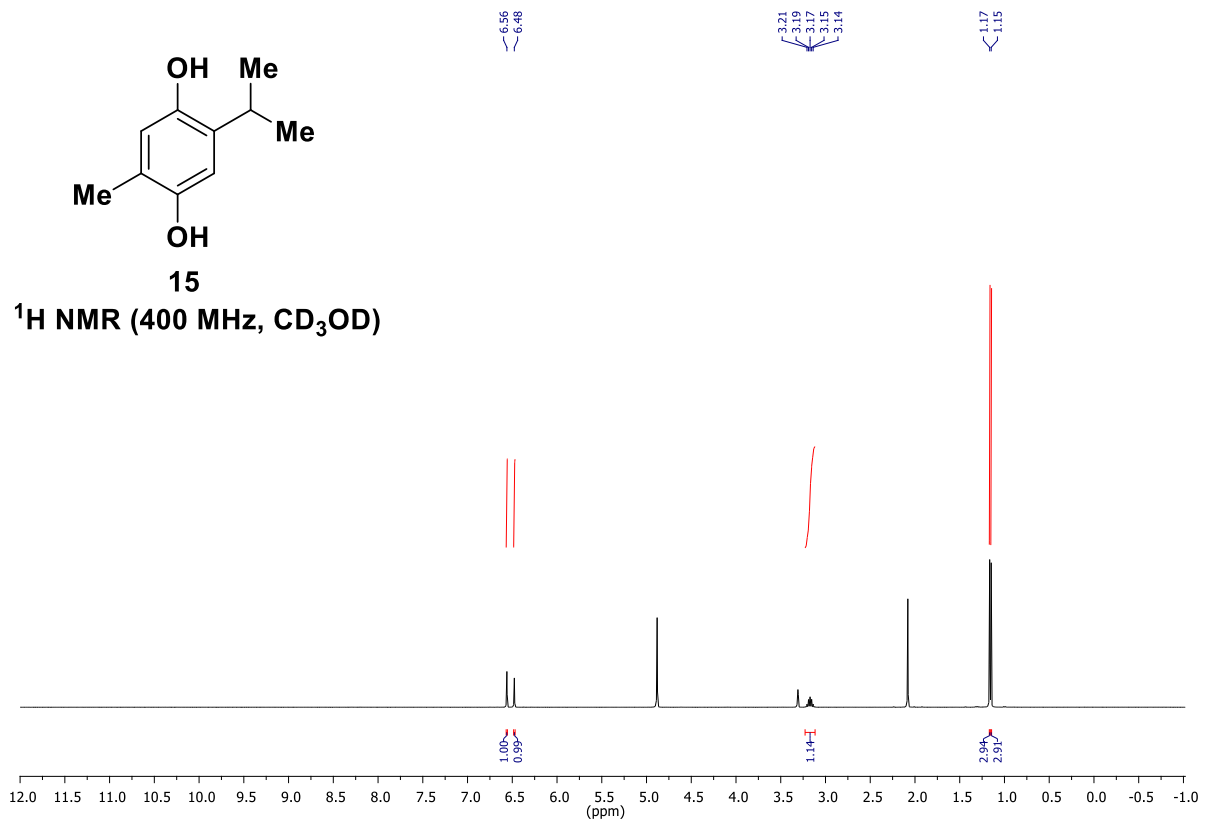
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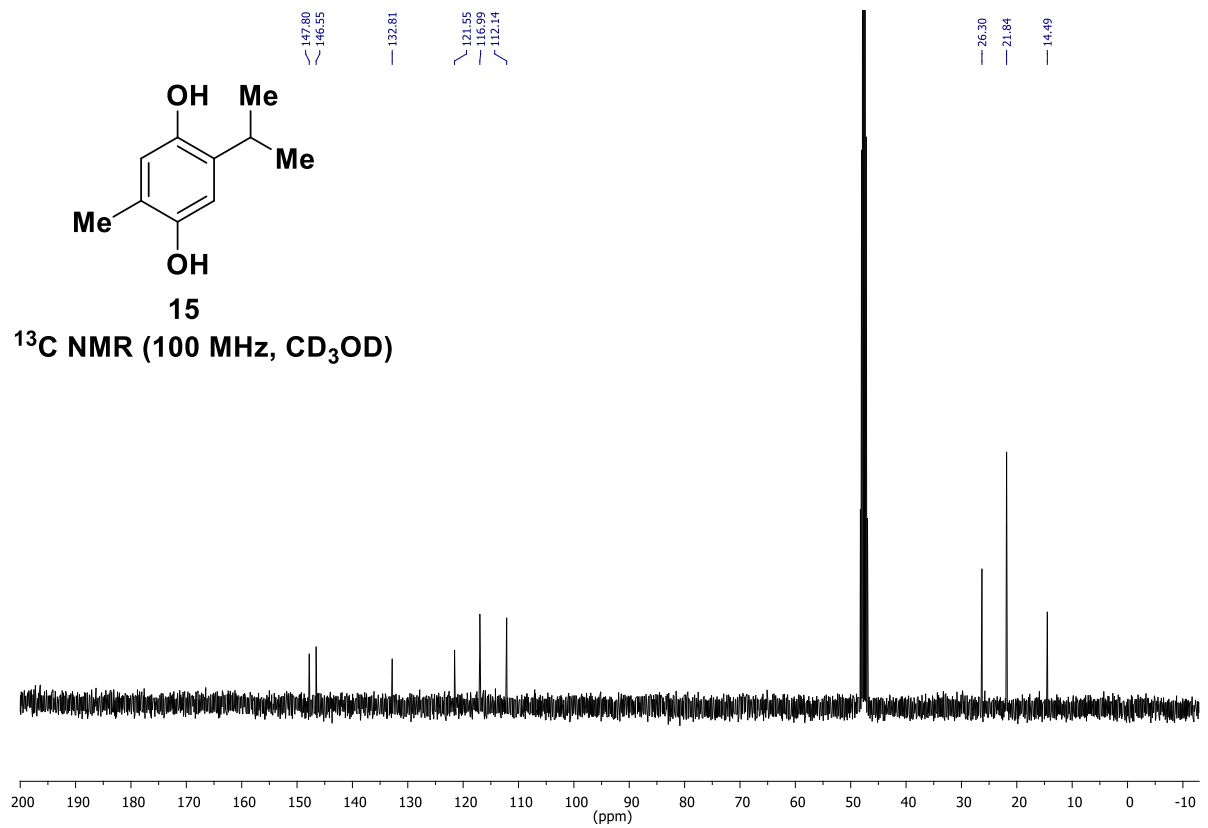
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¹H NMR (400 MHz, CD₃OD)



15

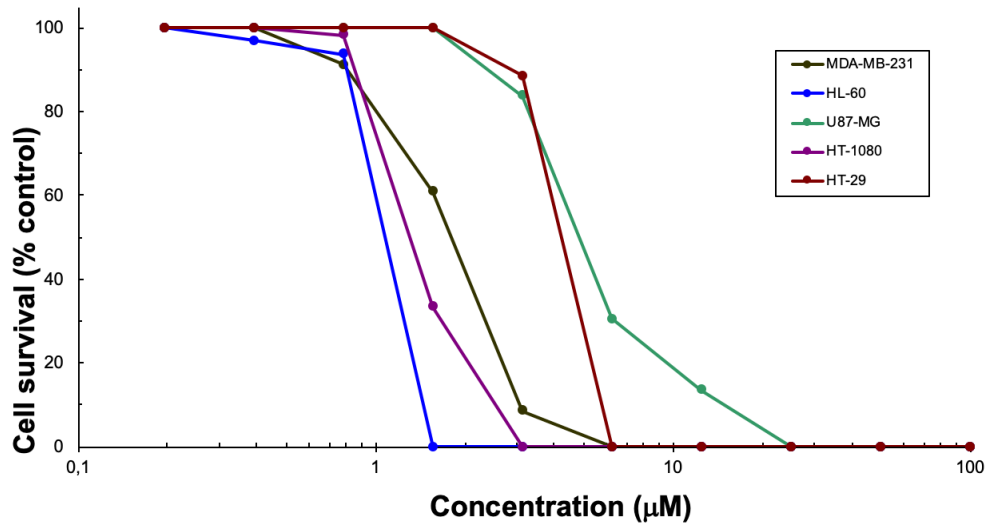
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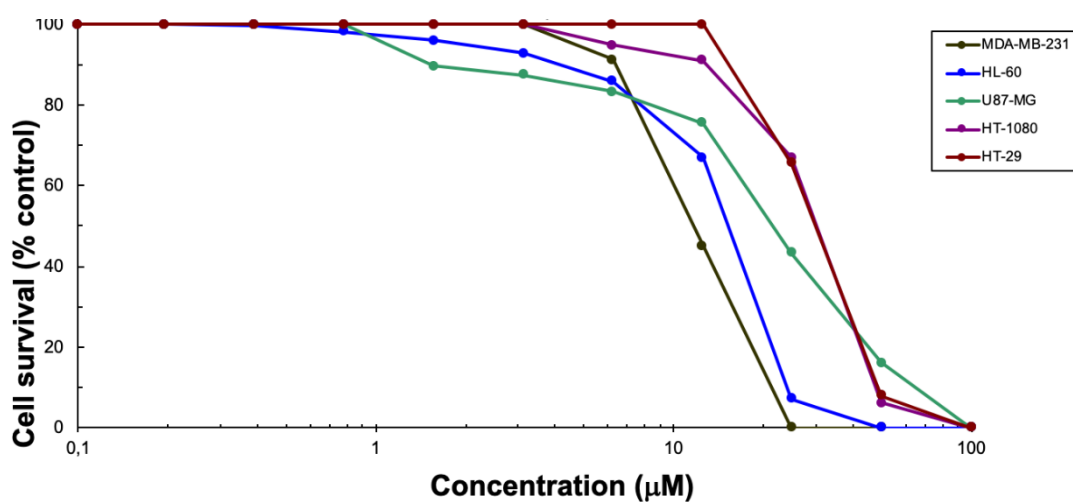
Representative dose-response curves

Each point represents the mean of quadruplicates. SD values, typically lower than 10% of the mean values, have been omitted for clarity.

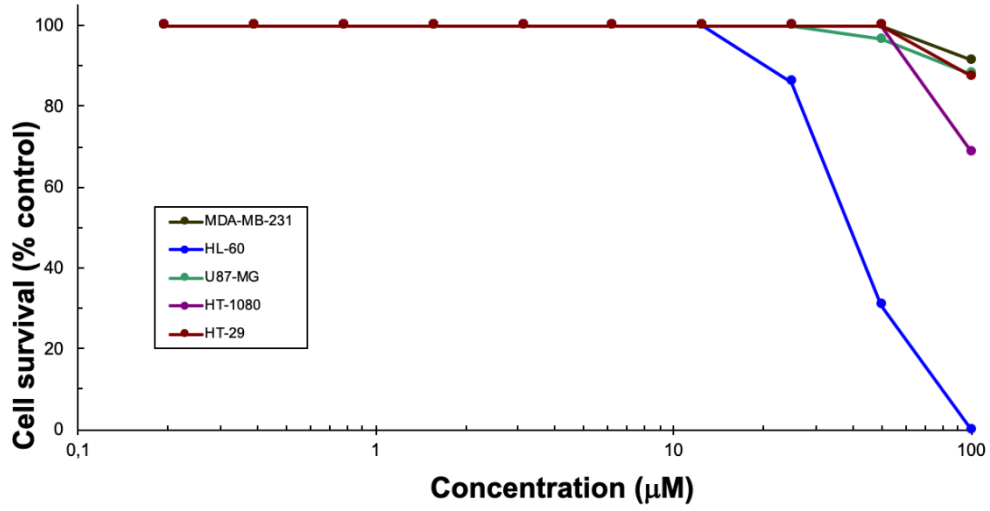
Toluquinol (compound 1)



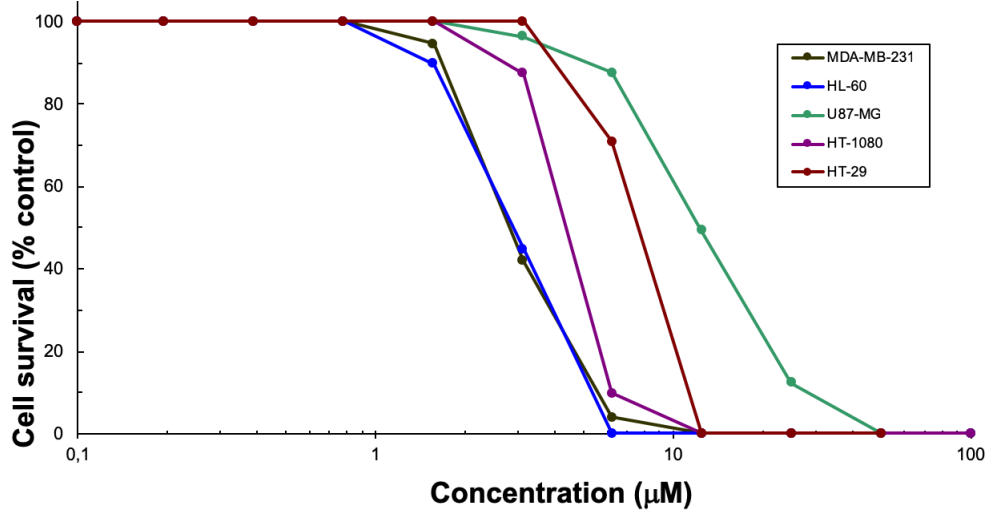
Compound 2



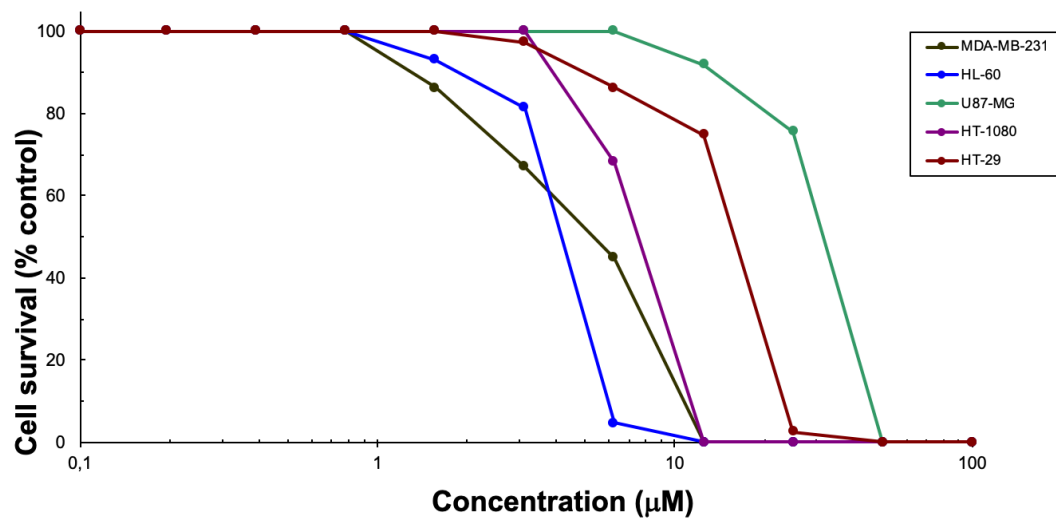
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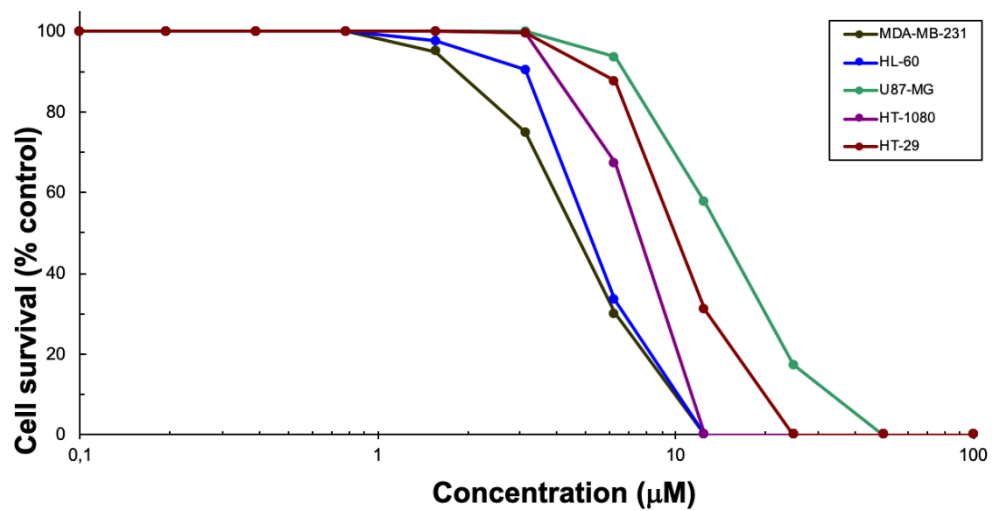
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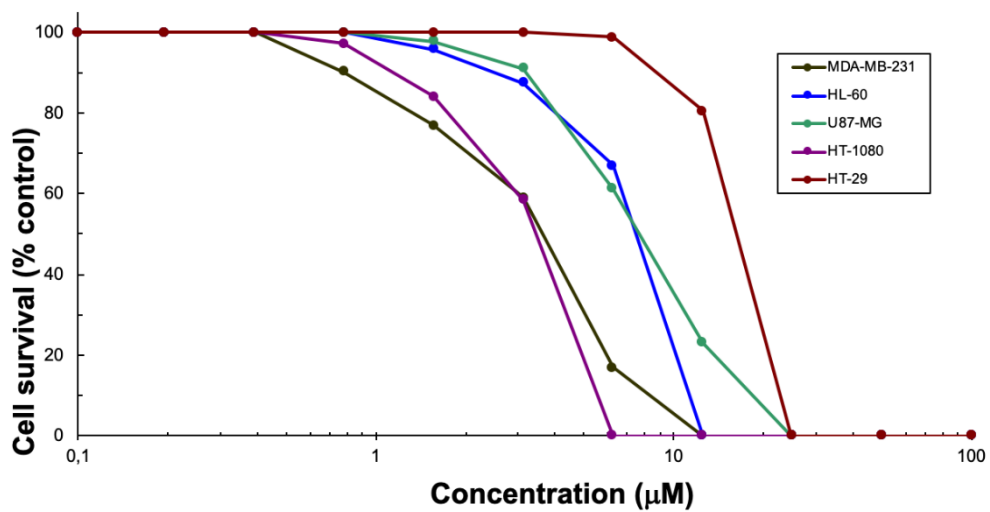
Compound 5



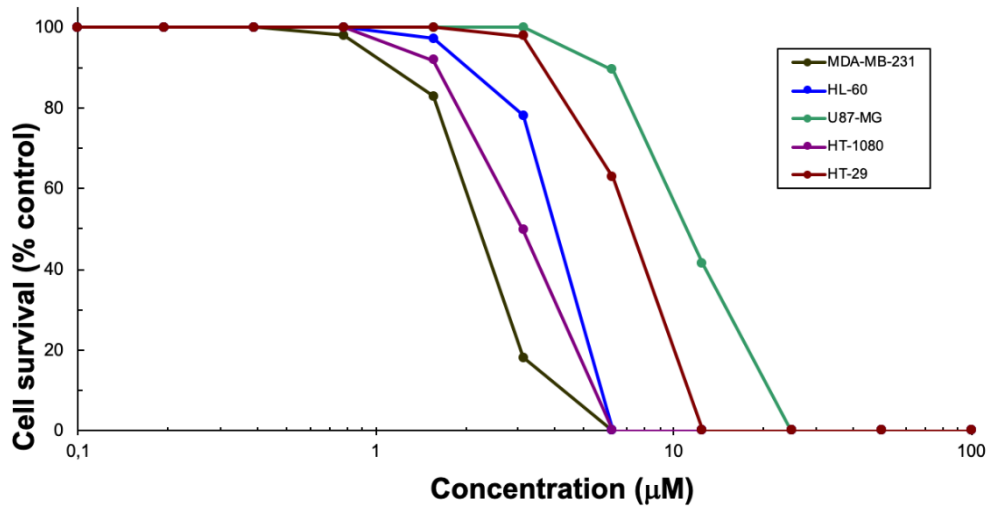
Compound 6



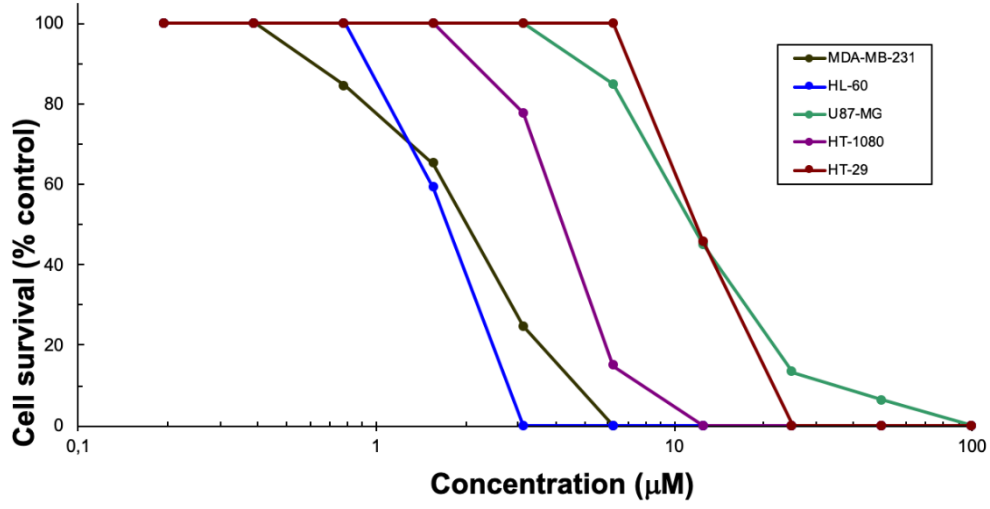
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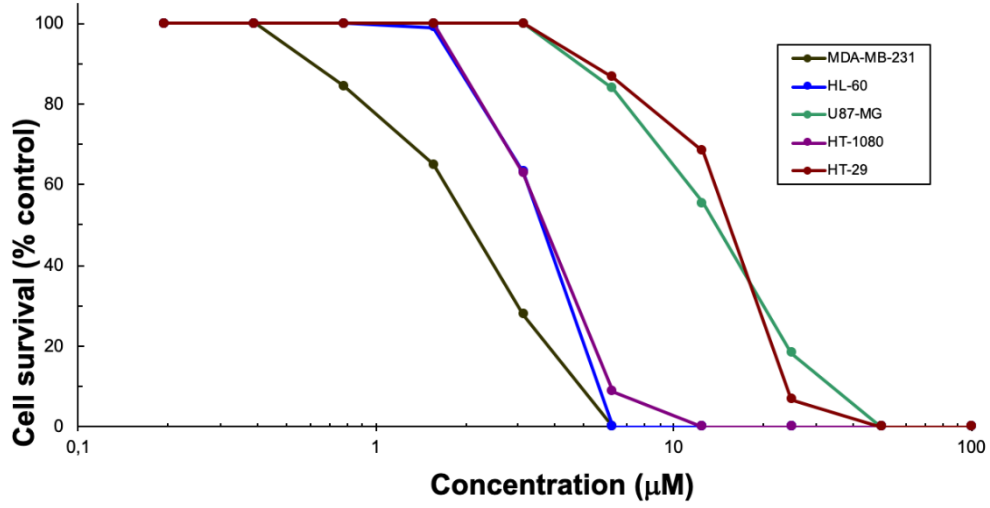
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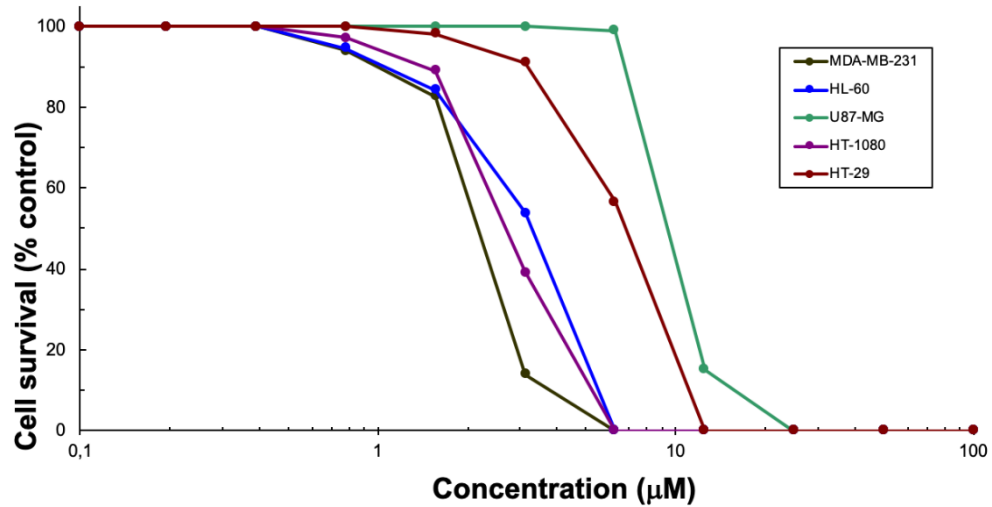
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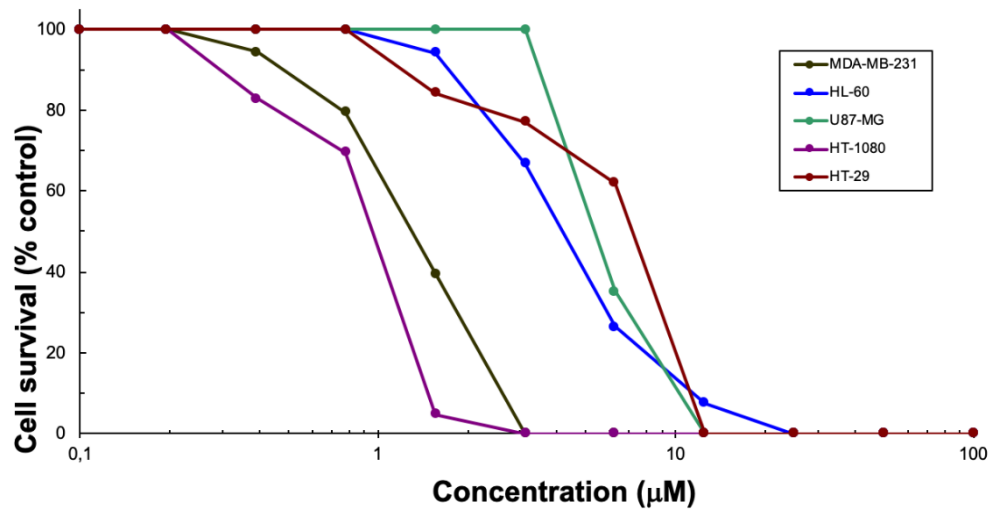
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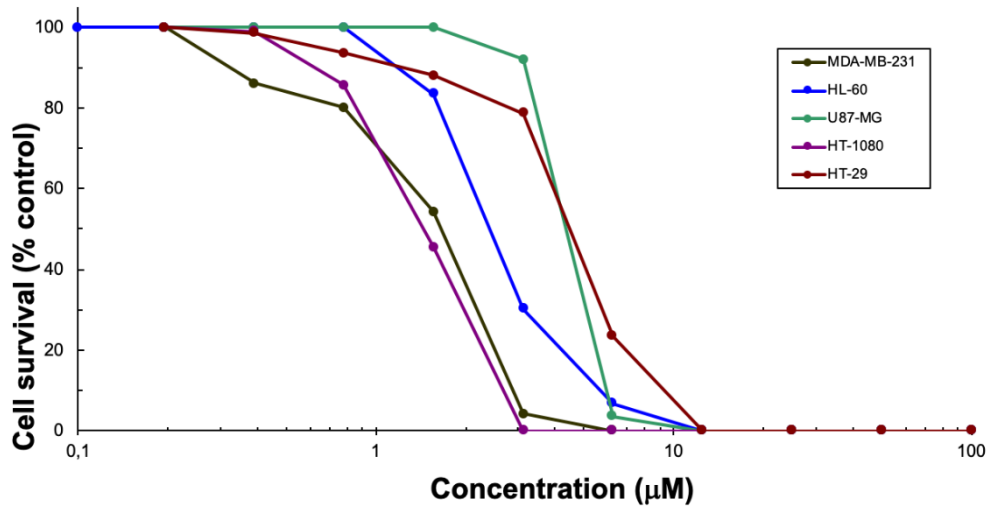
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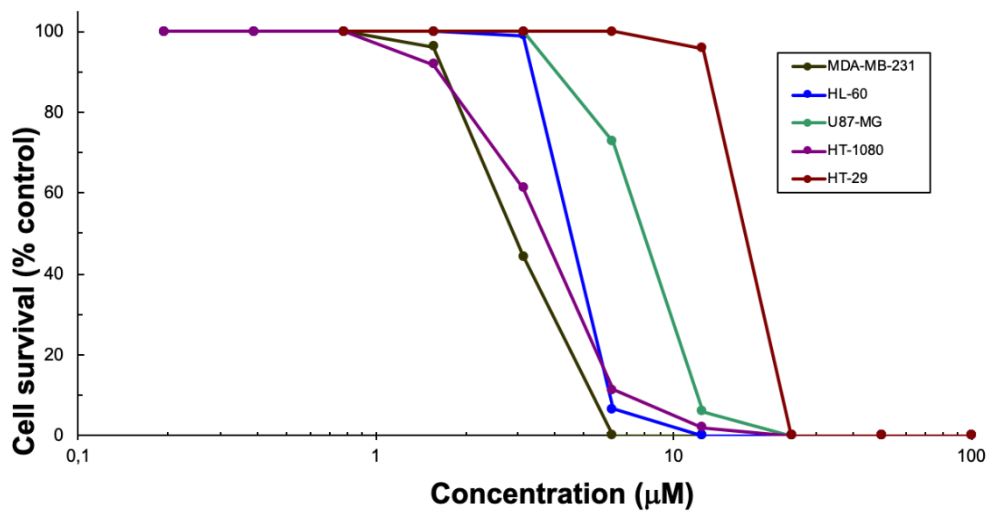
Compound 12



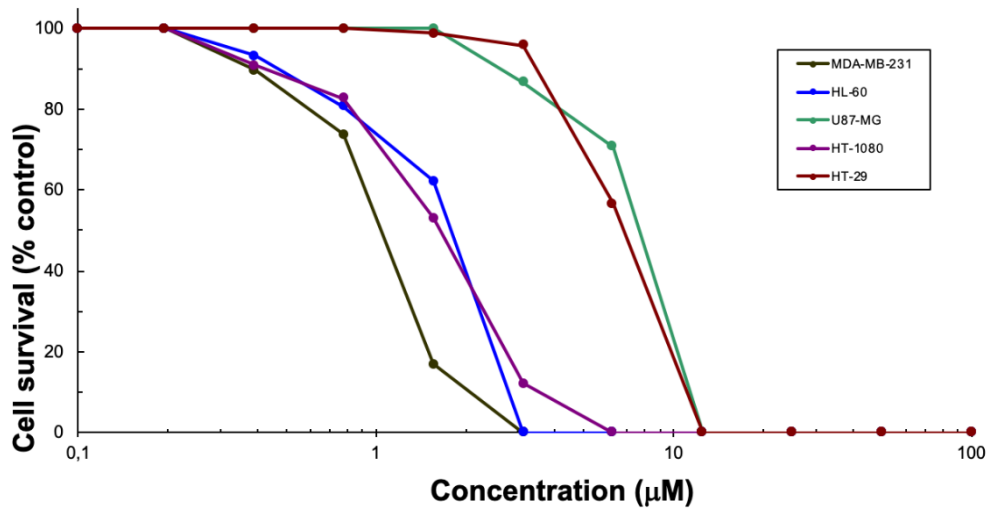
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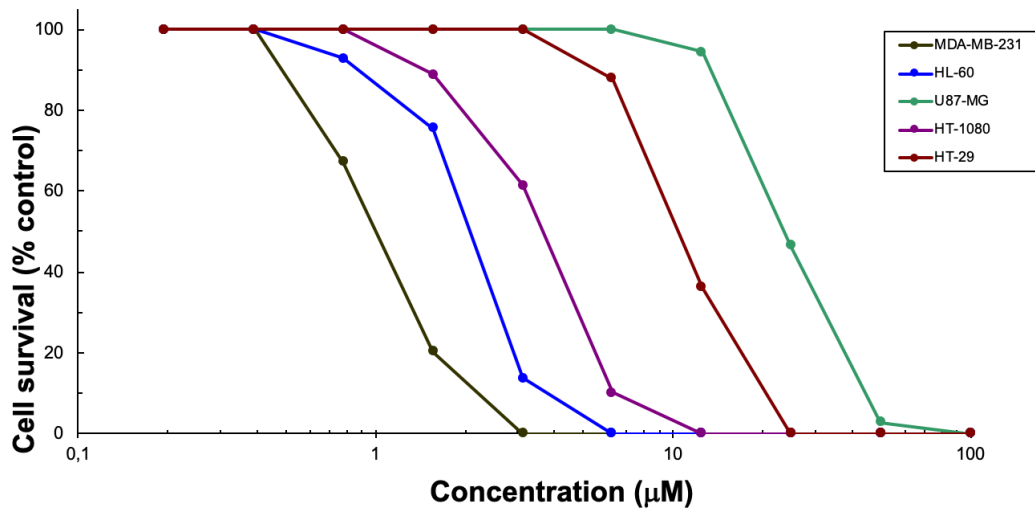
Toluquinone (Compound 14)



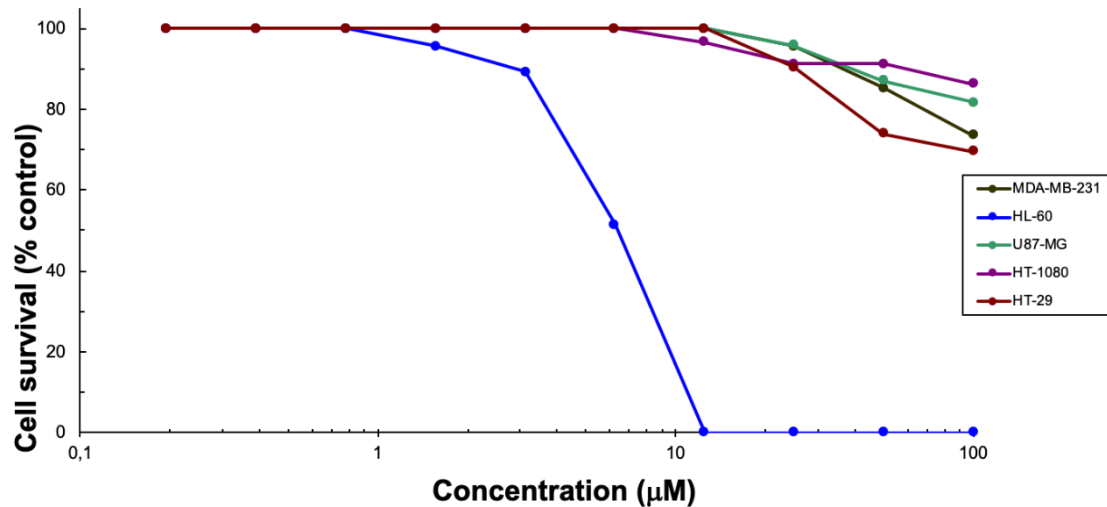
Thymoquinol (Compound 15)



Thymoquinone (compound 16)



Compound 18



Compound 19

