Supplementary Information

Synthesis and Analysis of Carvacrol-Derived Morita-Baylis-Hillman Adducts as Potential Anticancer Agents

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Spectra

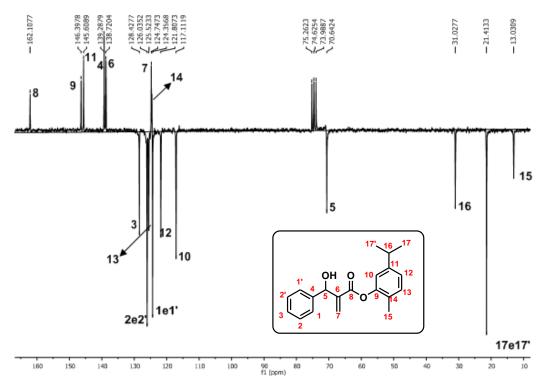


Figure S1. ¹³C NMR spectrum (50 MHz, CDCl₃) of 5-isopropyl-2-methylphenyl 2-(hydroxy(phenyl)methyl)acrylate (1).

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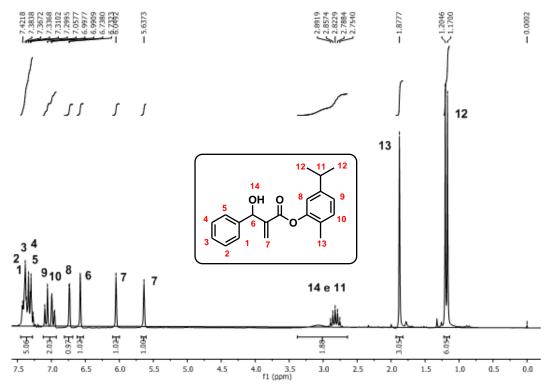


Figure S2. ¹H NMR spectrum (CDCl₃, 200 MHz) of 5-isopropyl-2-methylphenyl 2-(hydroxy(phenyl)methyl)acrylate (1).

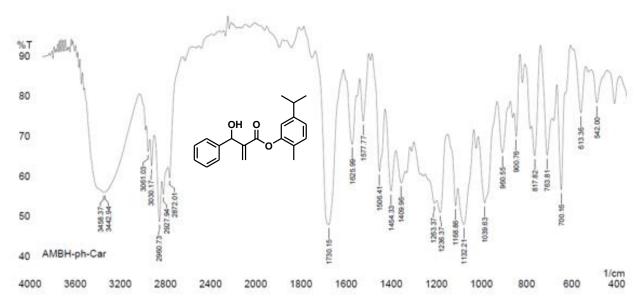


Figure S3. FTIR (KBR) spectrum of 5-isopropyl-2-methylphenyl 2-(hydroxy(phenyl)methyl)acrylate (1).

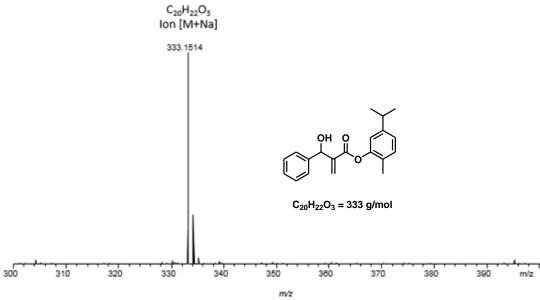


Figure S4. Mass spectrum of 5-isopropyl-2-methylphenyl 2-(hydroxy(phenyl)methyl)acrylate (1).

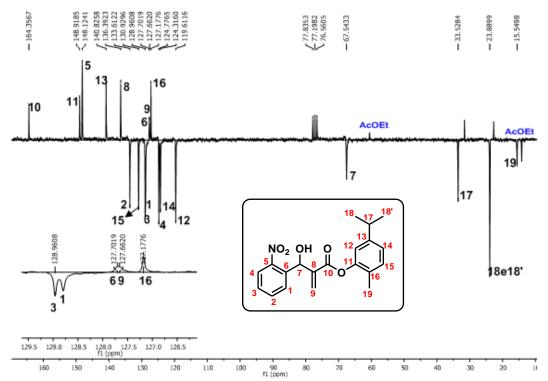
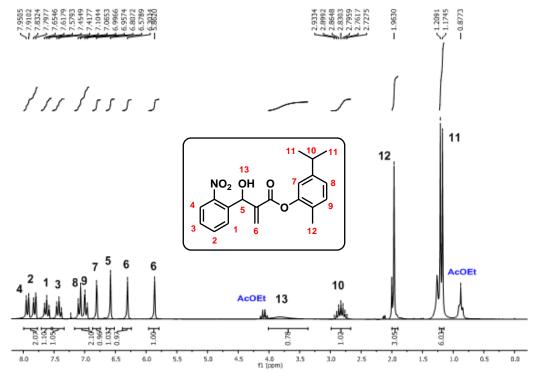


Figure S5. ¹³C NMR spectrum (50 MHz, CDCl₃) of 5-isopropyl-2-methylphenyl 2-(hydroxy(2-nitrophenyl)methyl)acrylate (2).



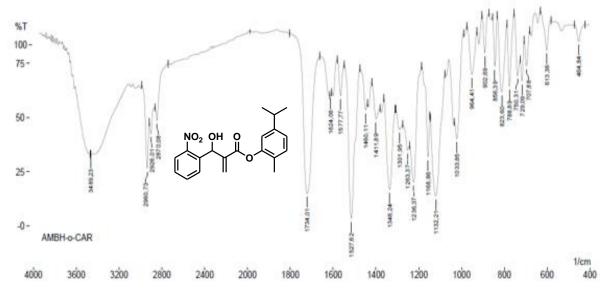
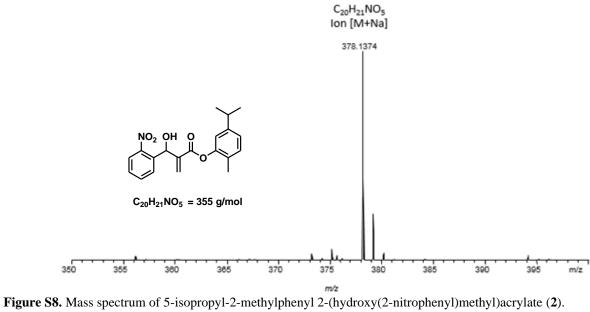
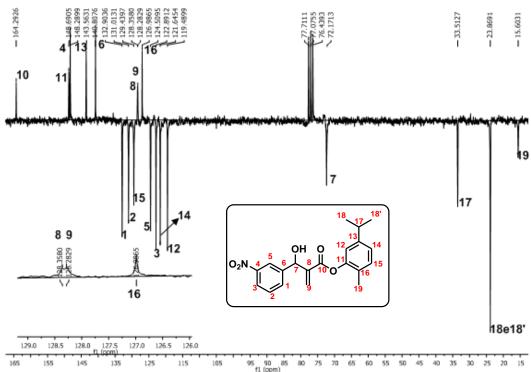


Figure S7. FTIR (KBR) spectrum of 5-isopropyl-2-methylphenyl 2-(hydroxy(2-nitrophenyl)methyl)acrylate (2).





spectrum (50 MHz, CDCl₃) of 5-isopropyl-2-methylphenyl 2-(hydroxy(3-**S9.** ¹³C NMR nitrophenyl)methyl)acrylate (3).

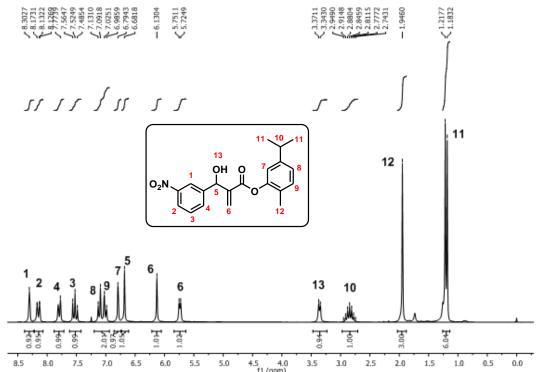


Figure S10. ¹H NMR spectrum (200 MHz, CDCl₃) of 5-isopropyl-2-methylphenyl 2-(hydroxy(3-nitrophenyl)methyl)acrylate (3).

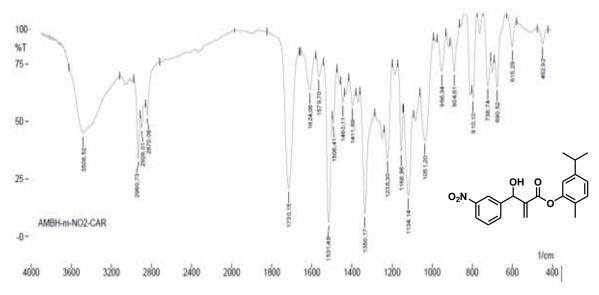


Figure S11. FTIR (KBR) spectrum of 5-isopropyl-2-methylphenyl 2-(hydroxy(3-nitrophenyl)methyl)acrylate (3).

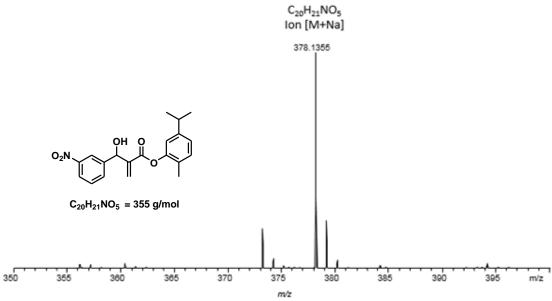


Figure S12. Mass spectrum of 5-isopropyl-2-methylphenyl 2-(hydroxy(3-nitrophenyl)methyl)acrylate (3).

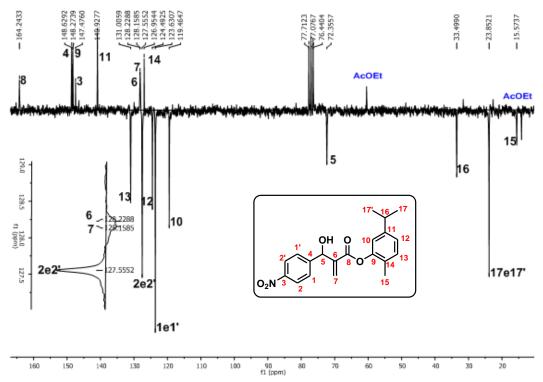


Figure S13. 13 C NMR spectrum 13 C-APT (50 MHz, CDCl₃) of 5-isopropyl-2-methylphenyl 2-(hydroxy(4-nitrophenyl)methyl)acrylate (4).

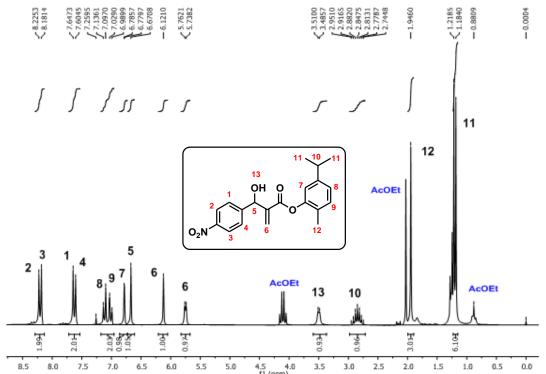


Figure S14. ¹H NMR spectrum (200 MHz, CDCl₃) of 5-isopropyl-2-methylphenyl 2-(hydroxy(4-nitrophenyl)methyl)acrylate (4).

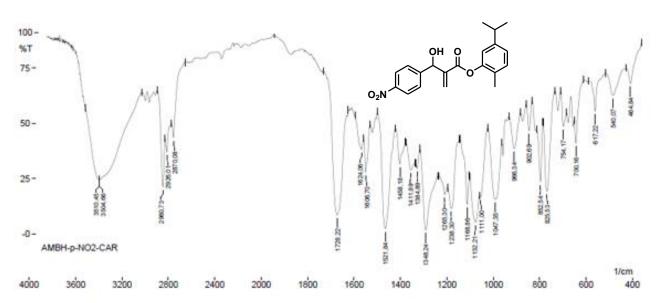


Figure S15. FTIR (KBR) spectrum of 5-isopropyl-2-methylphenyl 2-(hydroxy(4-nitrophenyl)methyl)acrylate (4).

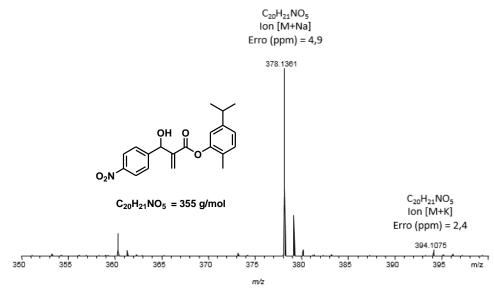
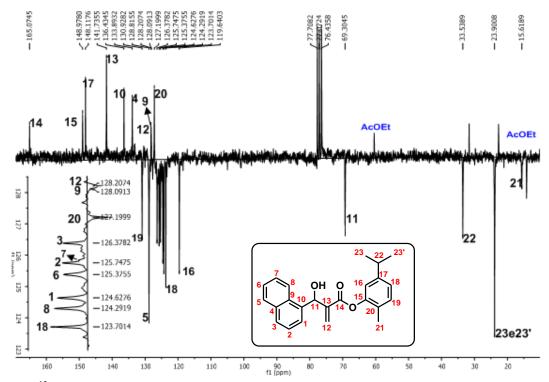
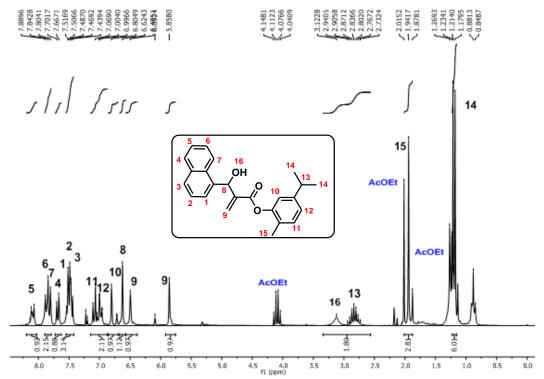


Figure S16. Mass spectrum of 5-isopropyl-2-methylphenyl 2-(hydroxy(4-nitrophenyl)methyl)acrylate (4).



 $\begin{tabular}{ll} \textbf{Figure S17.} & 13C NMR spectrum (50 MHz, CDCl_3) of 5-isopropyl-2-methylphenyl 2-(hydroxy(naphthalen-1-yl)methyl)acrylate (\textbf{5}). \end{tabular}$



 $\begin{tabular}{ll} \textbf{Figure S18.} & \begin{tabular}{ll} 1H NMR spectrum (200 MHz, CDCl_{3}) of 5-isopropyl-2-methylphenyl 2-(hydroxy(naphthalen-1-yl)methyl)acrylate (5). \end{tabular}$

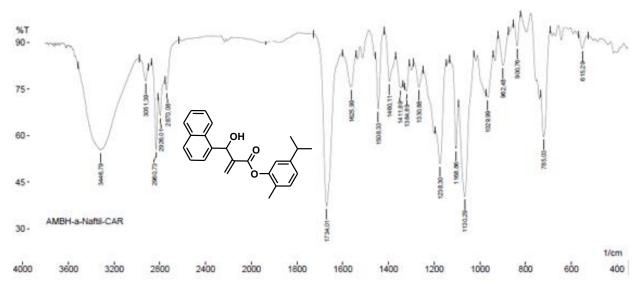


Figure S19. FTIR (KBR) spectrum of 5-isopropyl-2-methylphenyl 2-(hydroxy(naphthalen-1-yl)methyl)acrylate (5).

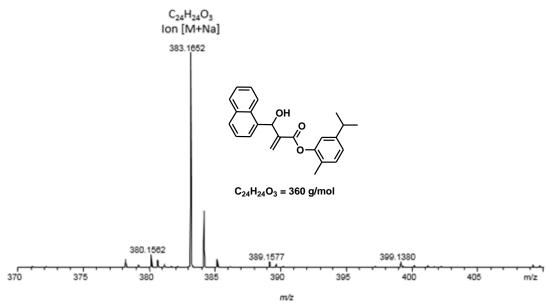


Figure S20. Mass spectrum of 5-isopropyl-2-methylphenyl 2-(hydroxy(naphthalen-1-yl)methyl)acrylate (5).

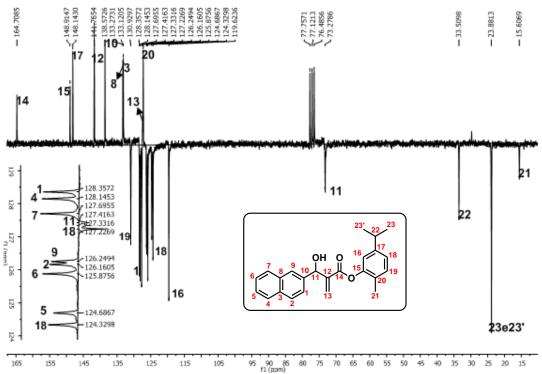
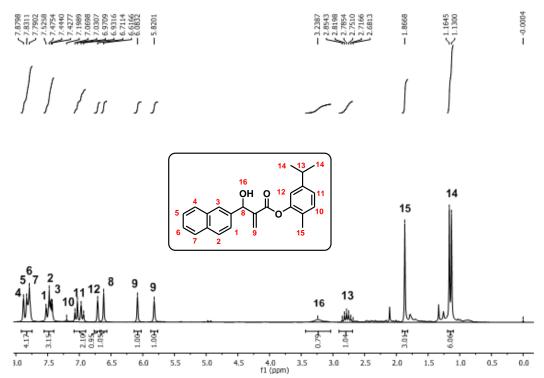


Figure S21. 13 C NMR spectrum (50 MHz, CDCl₃) of 5-isopropyl-2-methylphenyl 2-(hydroxy(naphthalen-2-yl)methyl)acrylate (6).



 $\begin{tabular}{ll} \textbf{Figure S22.} & \begin{tabular}{ll} 1H NMR spectrum (200 MHz, CDCl_{3}) of 5-isopropyl-2-methylphenyl 2-(hydroxy(naphthalen-2-yl)methyl)acrylate (6). \end{tabular}$

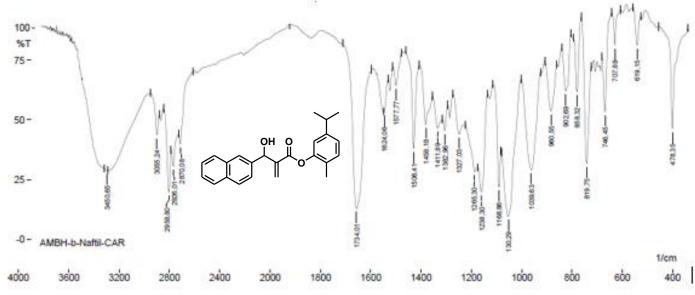


Figure S23. FTIR (KBR) spectrum of 5-isopropyl-2-methylphenyl 2-(hydroxy(naphthalen-2-yl)methyl)acrylate (6).

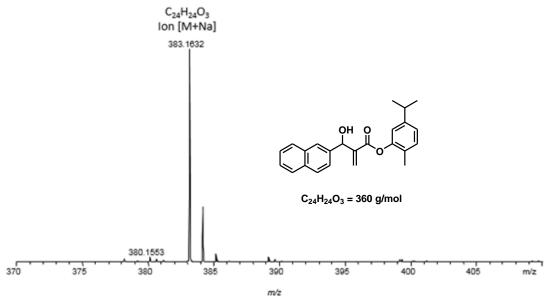


Figure S24. Mass spectrum of 5-isopropyl-2-methylphenyl 2-(hydroxy(naphthalen-2-yl)methyl)acrylate (6).

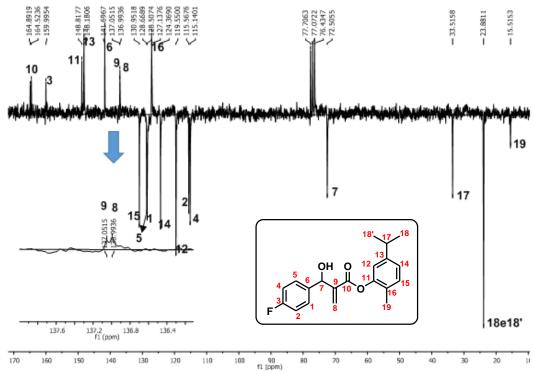
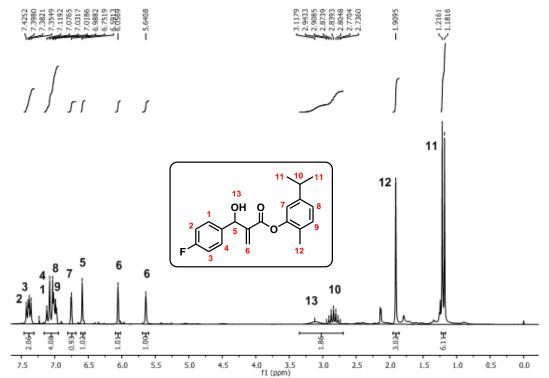


Figure S25. ¹³C NMR spectrum (50 MHz, CDCl₃) of 5-isopropyl-2-methylphenyl 2-((4-fluorophenyl)(hydroxy)methyl)acrylate (7).



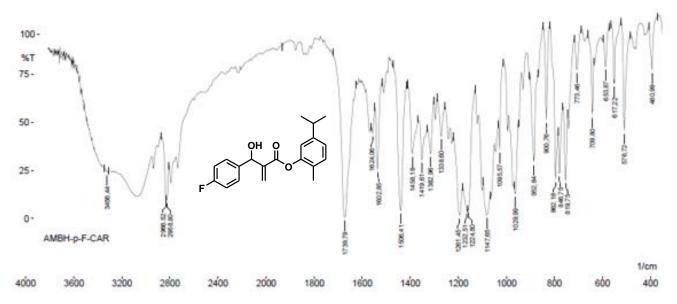


Figure S27. FTIR (KBR) spectrum of 5-isopropyl-2-methylphenyl 2-((4-fluorophenyl)(hydroxy)methyl)acrylate (7).

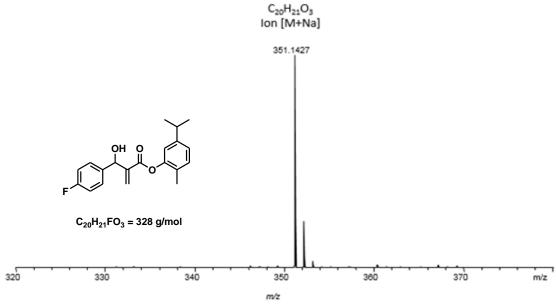


Figure S28. Mass spectrum of 5-isopropyl-2-methylphenyl 2-((4-fluorophenyl)(hydroxy)methyl)acrylate (7).

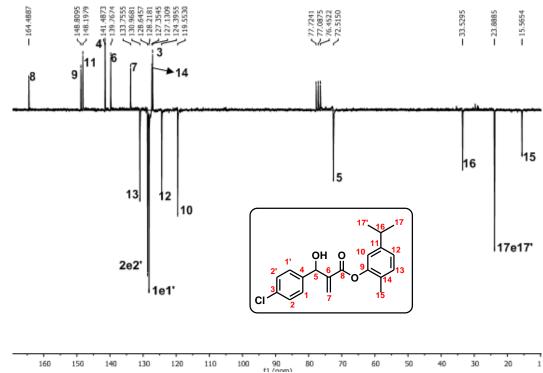


Figure S29. ¹³C NMR spectrum (50 MHz, CDCl₃) of 5-isopropyl-2-methylphenyl 2-((4-chlorophenyl)(hydroxy)methyl)acrylate (8).

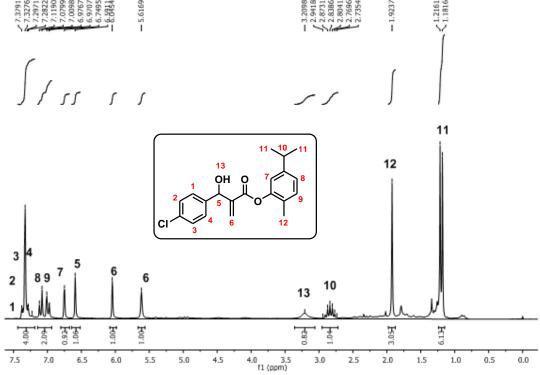


Figure S30. ¹H NMR spectrum (200 MHz, CDCl₃) 5-isopropyl-2-methylphenyl 2-((4-chlorophenyl)(hydroxy)methyl)acrylate (8).

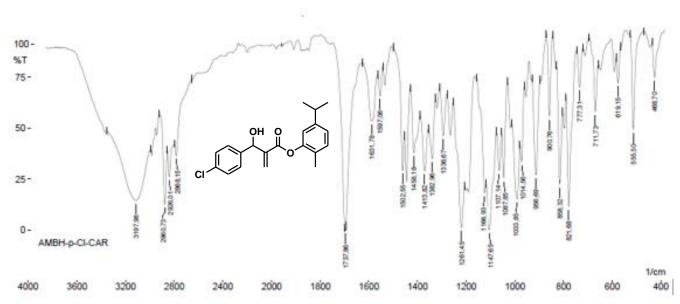


Figure S31. FTIR (KBR) spectrum of 5-isopropyl-2-methylphenyl 2-((4-chlorophenyl)(hydroxy)methyl)acrylate (8).

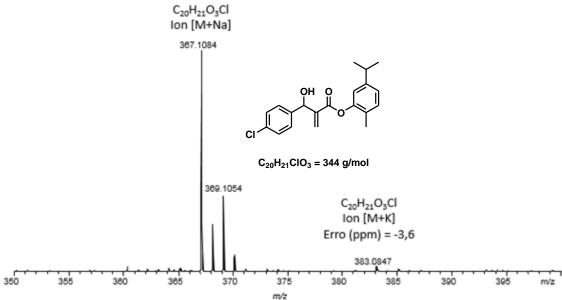


Figure S32. Mass spectrum of 5-isopropyl-2-methylphenyl 2-((4-chlorophenyl)(hydroxy)methyl)acrylate (8).

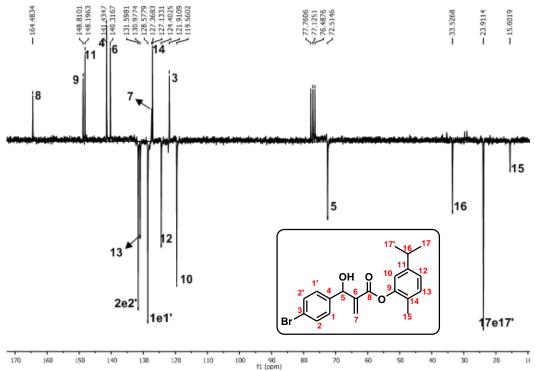


Figure S33. ¹³C NMR spectrum (50 MHz, CDCl₃) of 5-isopropyl-2-methylphenyl 2-((4-bromophenyl)(hydroxy)methyl)acrylate (9).

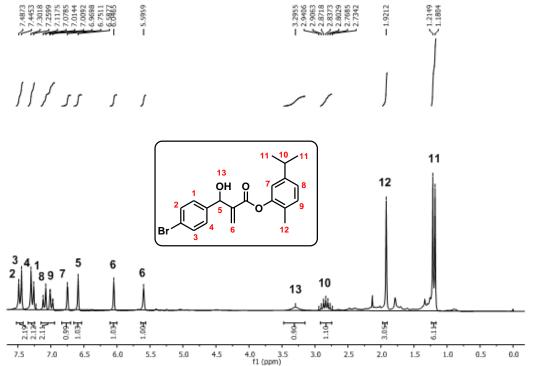


Figure S34. ¹H NMR spectrum (200 MHz, CDCl₃) of 5-isopropyl-2-methylphenyl 2-((4-bromophenyl)(hydroxy)methyl)acrylate (9).

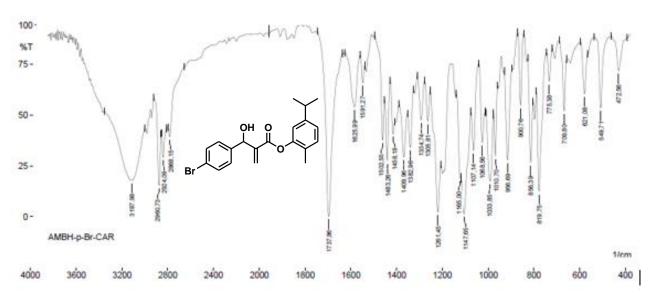


Figure S35. FTIR (KBR) spectrum of 5-isopropyl-2-methylphenyl 2-((4-bromophenyl)(hydroxy)methyl)acrylate (9).

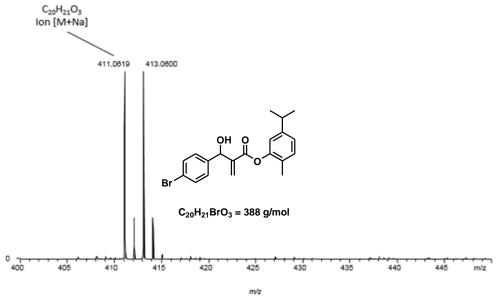
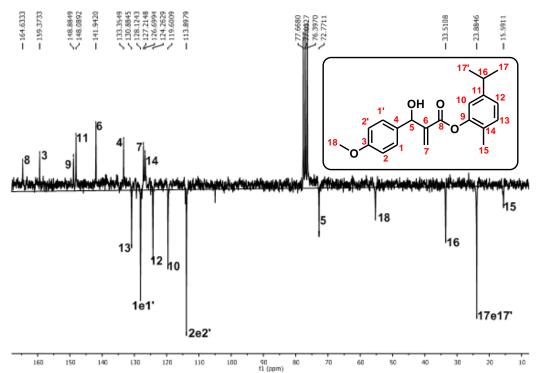
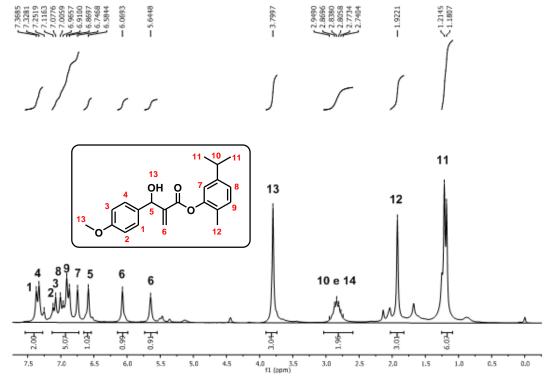


Figure S36. Mass spectrum of 5-isopropyl-2-methylphenyl 2-((4-bromophenyl)(hydroxy)methyl)acrylate (9).





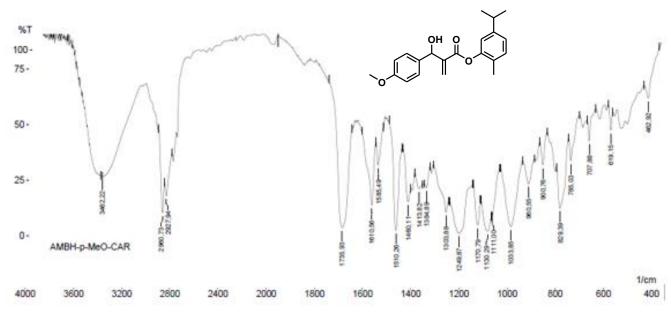


Figure S39. FTIR (KBR) spectrum of 5-isopropyl-2-methylphenyl 2-(hydroxy(4-methoxyphenyl)methyl)acrylate (10).

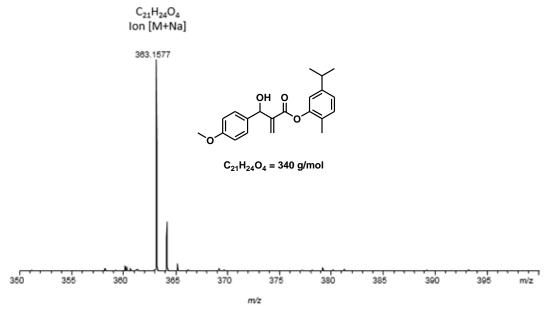
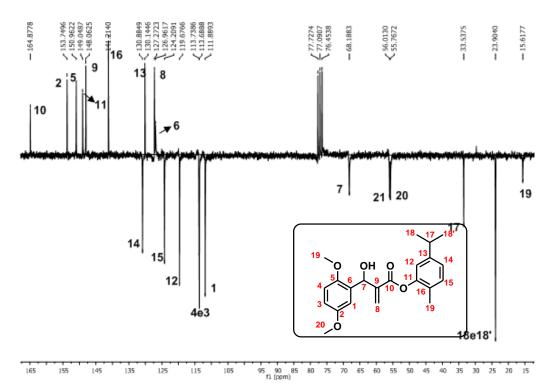


Figure S40. Mass spectrum of 5-isopropyl-2-methylphenyl 2-(hydroxy(4-methoxyphenyl)methyl)acrylate (10).



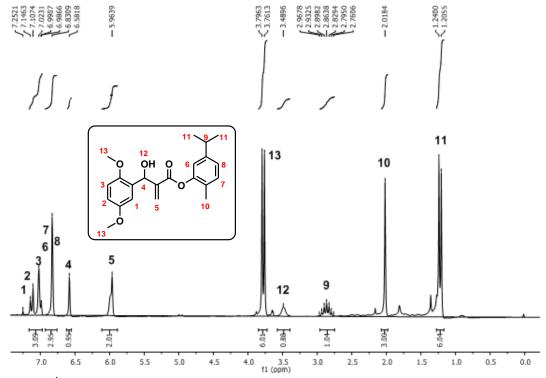
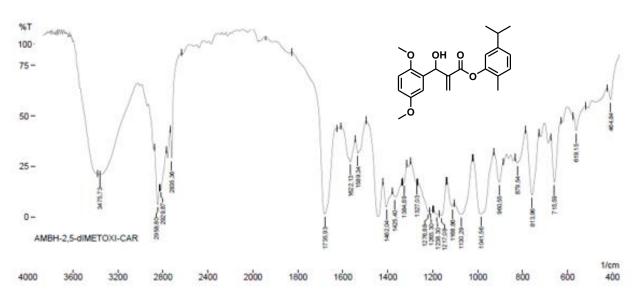
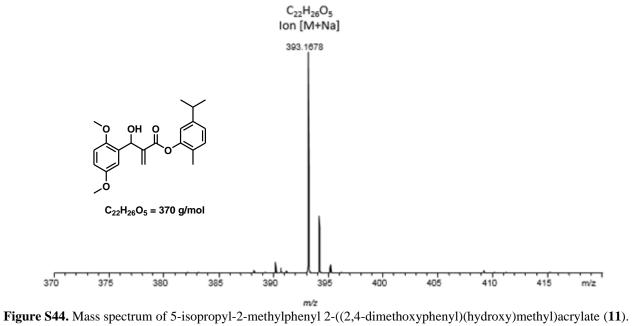


Figure S42. ¹H NMR spectrum (200 MHz, CDCl₃) of 5-isopropyl-2-methylphenyl 2-((2,4-dimethoxyphenyl)(hydroxy)methyl)acrylate (11).



 $\textbf{Figure S43.} \ \ \textbf{FTIR} \ \ (KBR) \ \ spectrum \ \ of \ 5-isopropyl-2-methylphenyl \ 2-((2,4-dimethoxyphenyl)(hydroxy)methyl)acrylate \ \ \textbf{(11)}.$



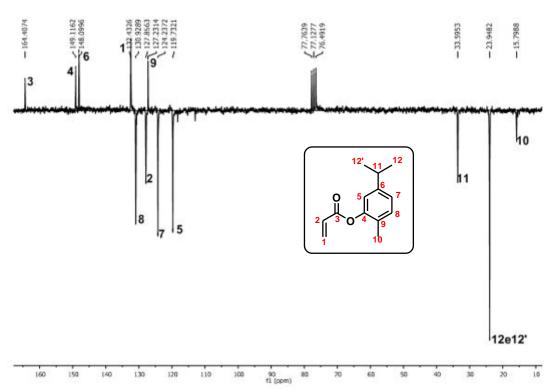


Figure S45. ¹³C NMR spectrum (50 MHz, CDCl₃) of 5-isopropyl-2-methylphenyl acrylate (12).

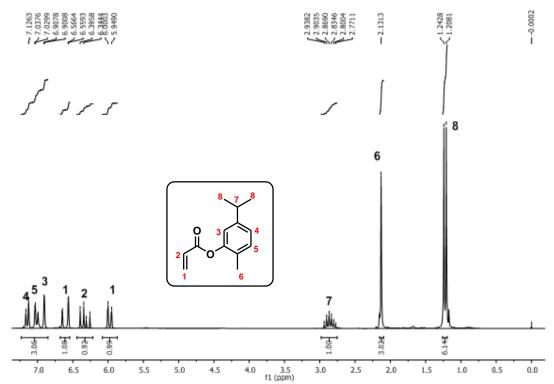


Figure S46. ¹H NMR spectrum (200 MHz, CDCl₃) of 5-isopropyl-2-methylphenyl acrylate (**12**).

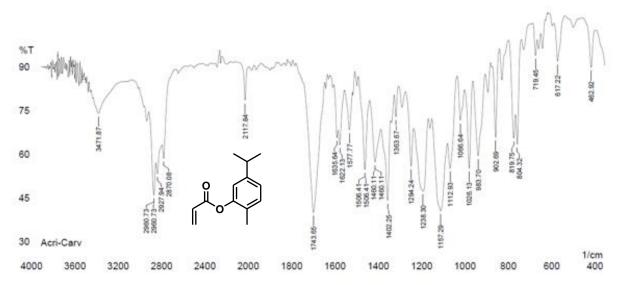


Figure S47. FTIR (KBR) spectrum of 5-isopropyl-2-methylphenyl acrylate (12).

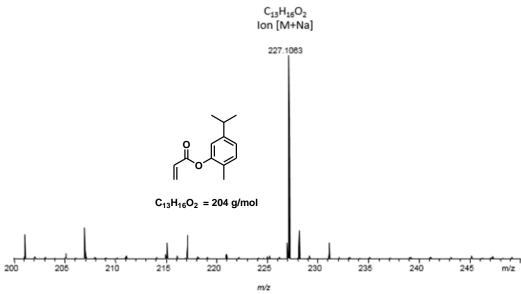


Figure S48. Mass spectrum of 5-isopropyl-2-methylphenyl acrylate (12).