

Supplementary Materials: Synthesis and *In Vitro* Anti *Leishmania amazonensis* Biological Screening of Morita-Baylis-Hillman Adducts Prepared from Eugenol, Thymol and Carvacrol

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Tatjana Souza Lima Keesen, Marcia Rosa de Oliveira, Fábio Pedrosa Lins Silva
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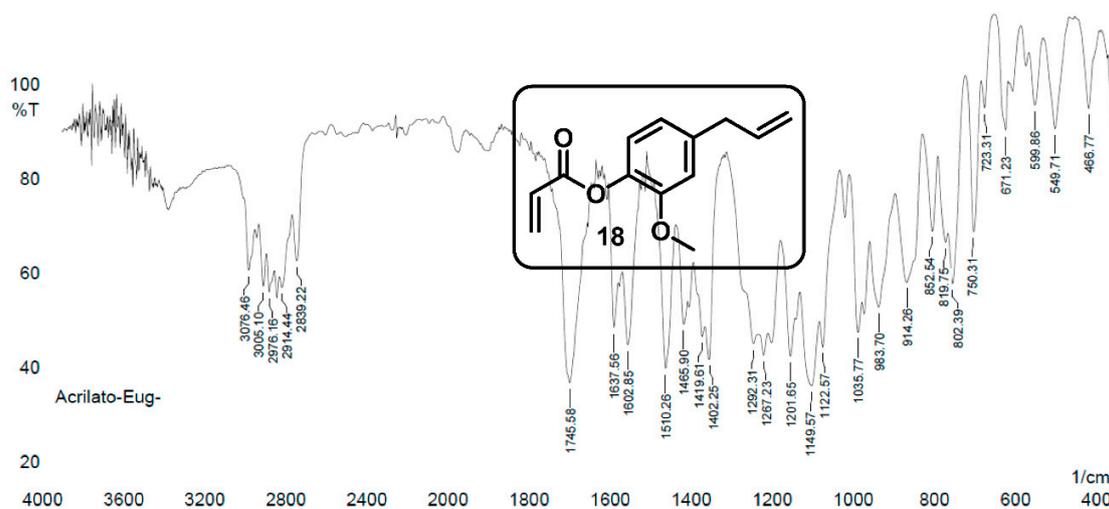


Figure S1. FTIR (KBr) spectrum of 4-allyl-2-methoxyphenyl acrylate 18.

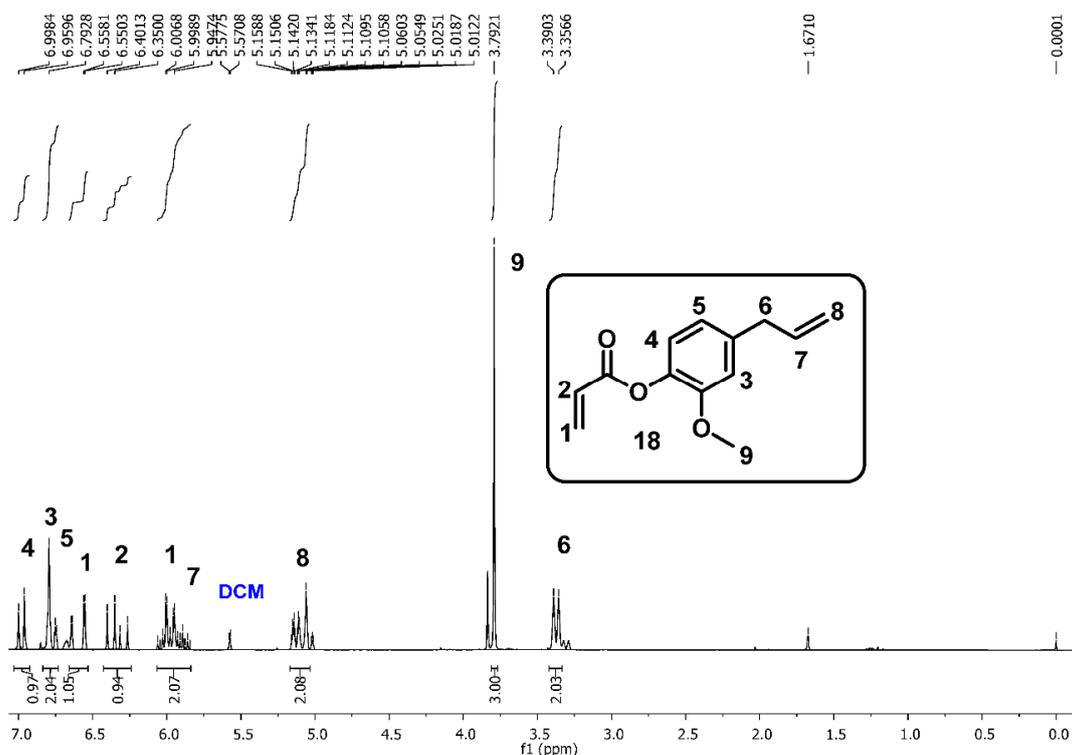


Figure S2. $^1\text{H-NMR}$ spectrum (200 MHz, CDCl_3) of 4-allyl-2-methoxyphenyl acrylate 18.

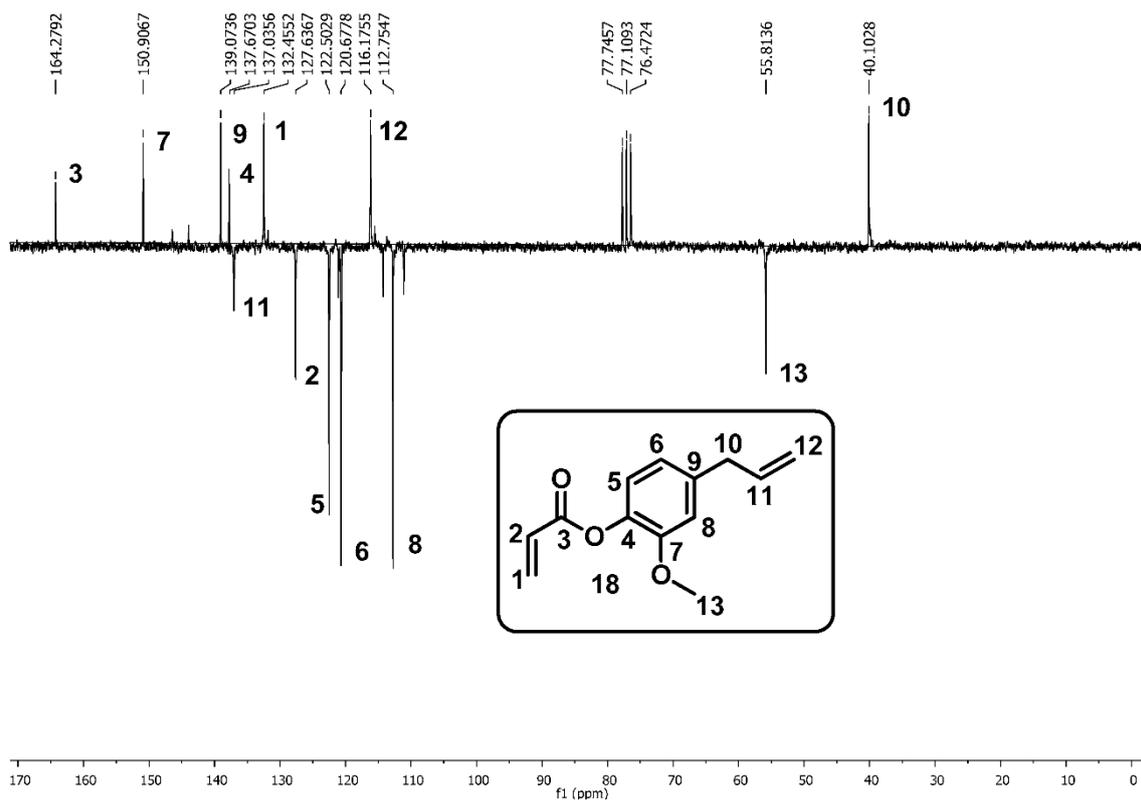


Figure S3. ¹³C-NMR spectrum (50 MHz, CDCl₃) of 4-allyl-2-methoxyphenyl acrylate 18.

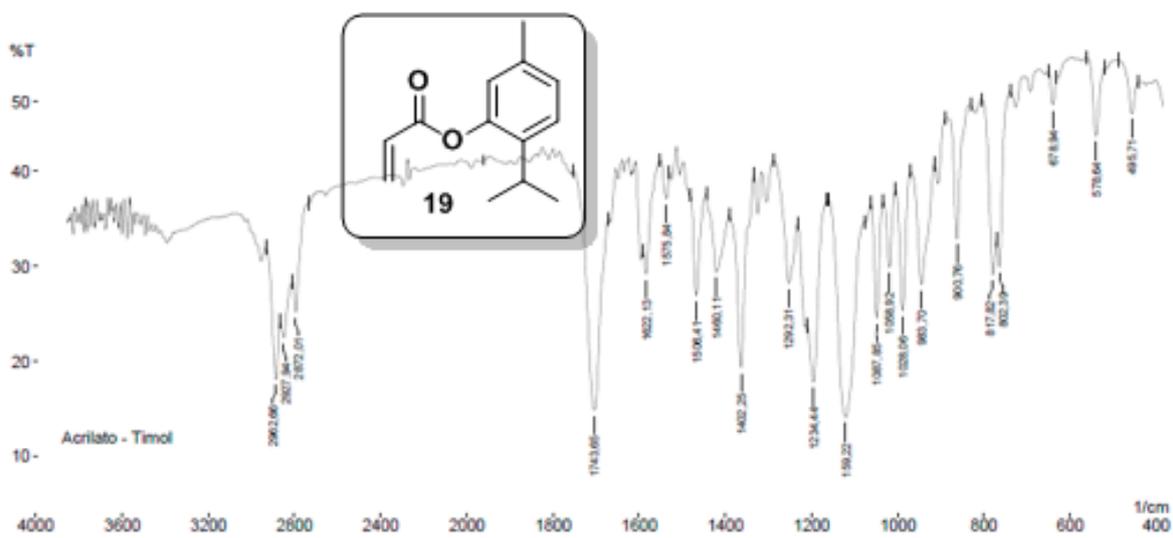


Figure S4. FTIR (KBr) spectrum of 2-isopropyl-5-methylphenyl acrylate 19.

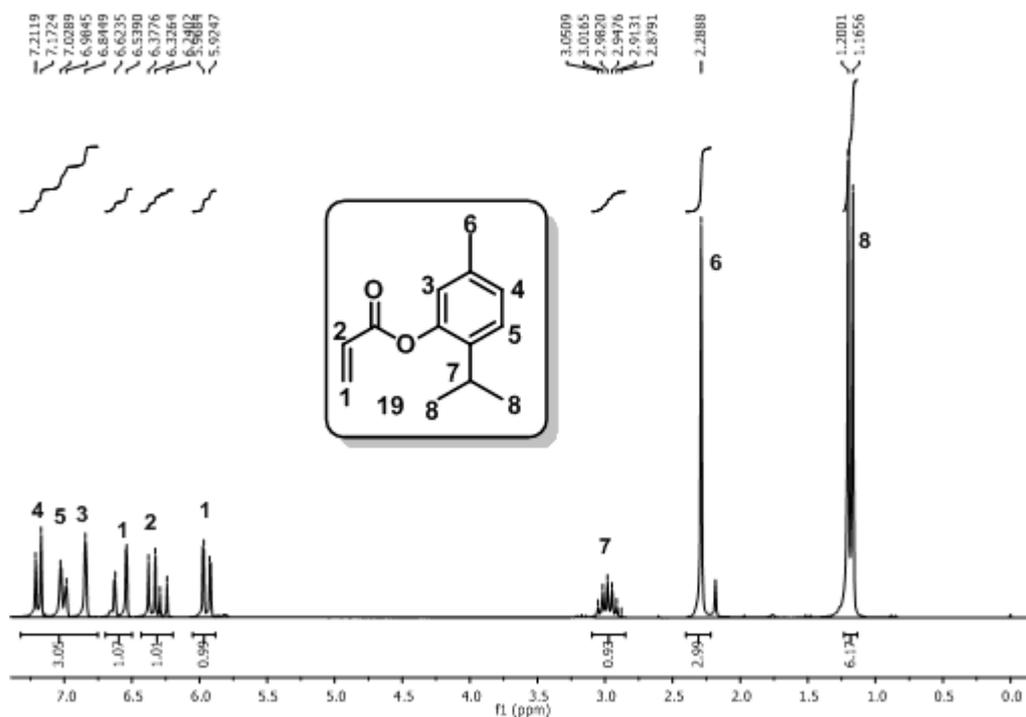


Figure S5. $^1\text{H-NMR}$ spectrum (200 MHz, CDCl_3) of 2-isopropyl-5-methylphenyl acrylate **19**.

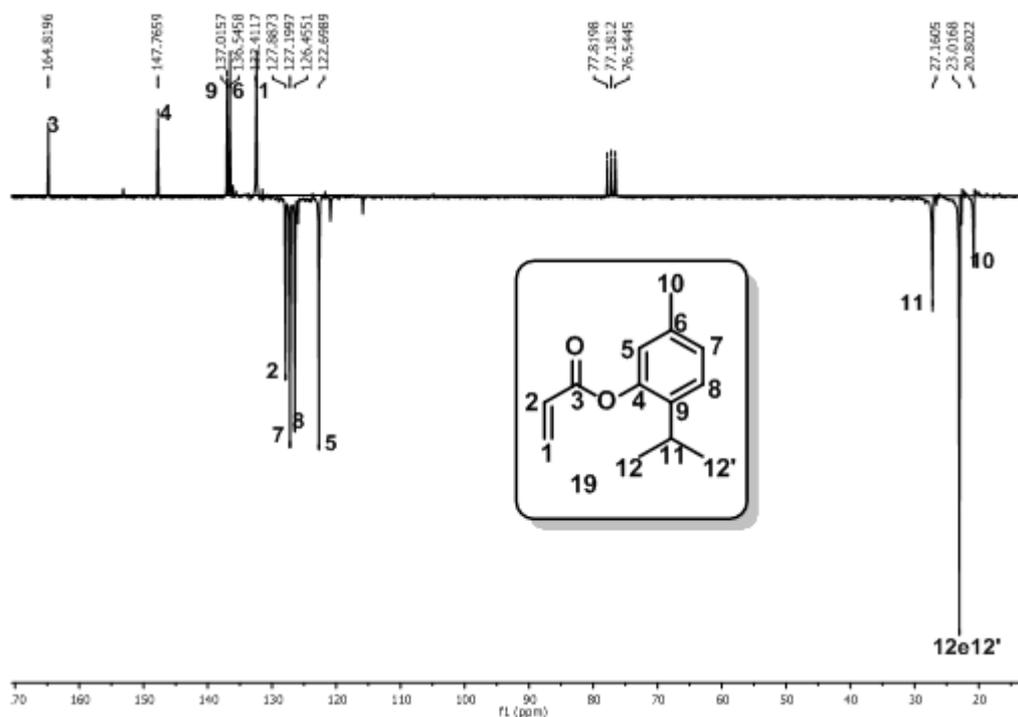


Figure S6. $^{13}\text{C-NMR}$ spectrum (50 MHz, CDCl_3) of 2-isopropyl-5-methylphenyl acrylate **19**.

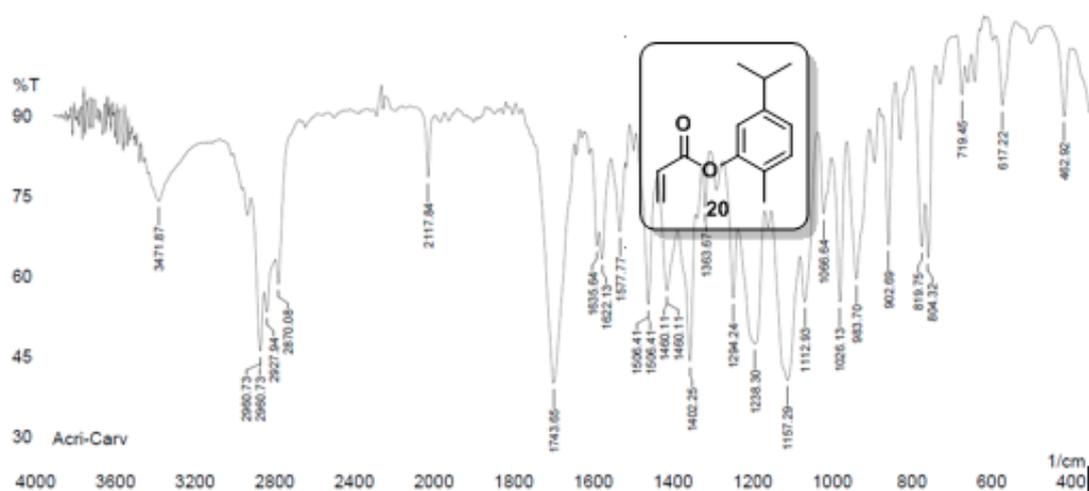


Figure S7. FTIR (KBr) spectrum of 5-isopropyl-2-methylphenyl acrylate 20.

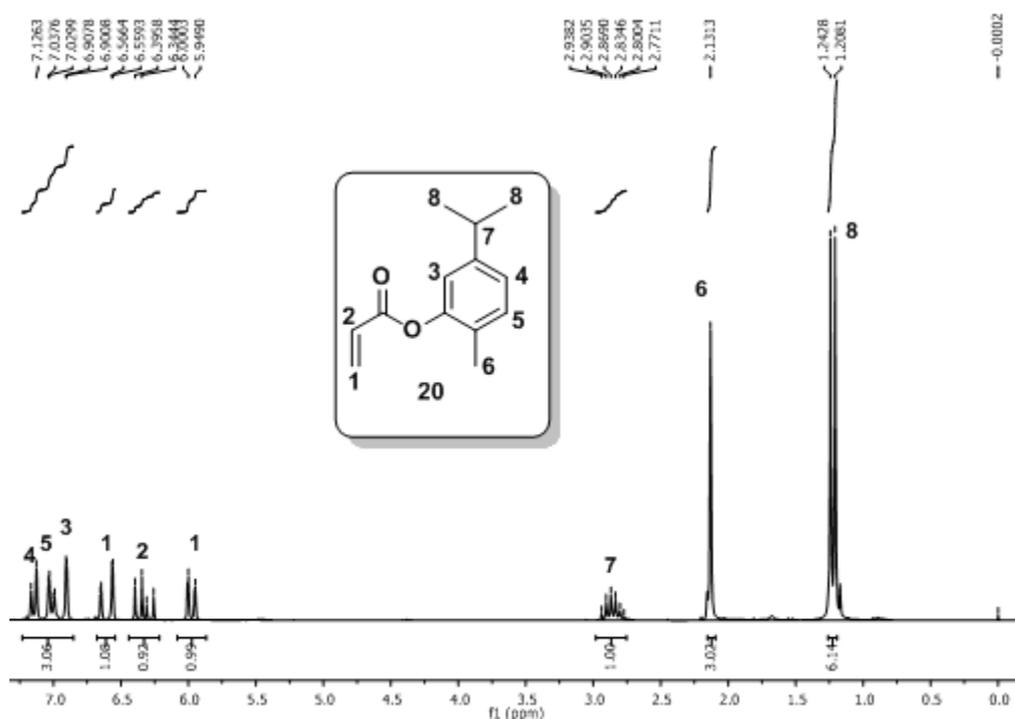


Figure S8. ¹H-NMR spectrum (200 MHz, CDCl₃) of 5-isopropyl-2-methylphenyl acrylate 20.

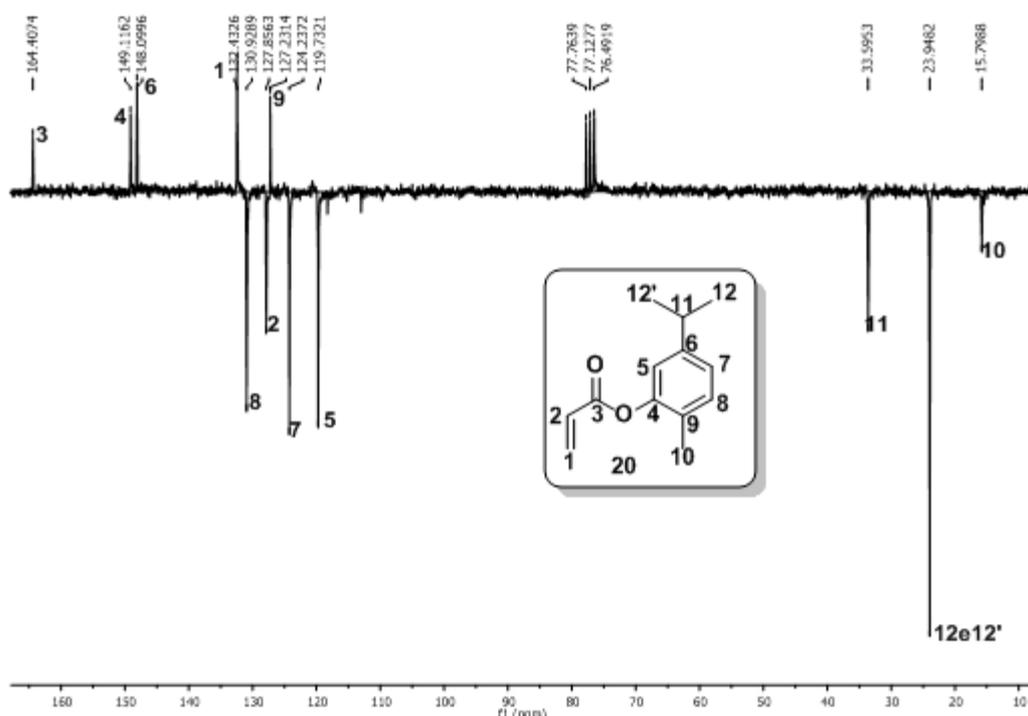


Figure S9. ¹³C-NMR spectrum (50 MHz, CDCl₃) of 5-isopropyl-2-methylphenyl acrylate 20.

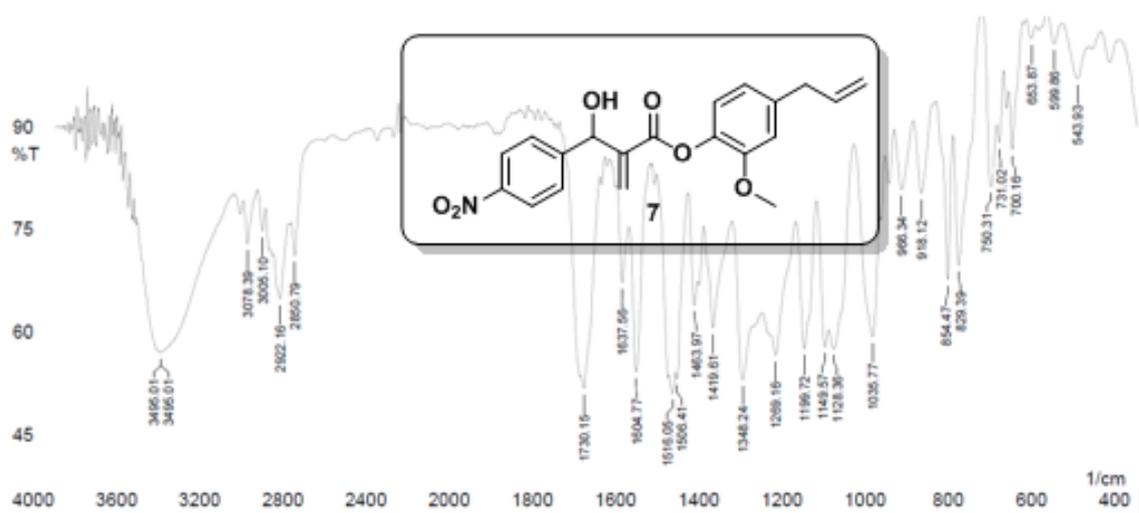


Figure S10. FTIR (KBr) spectrum of 4-allyl-2-methoxyphenyl 2-(hydroxy(4-nitrophenyl)methyl)acrylate 7.

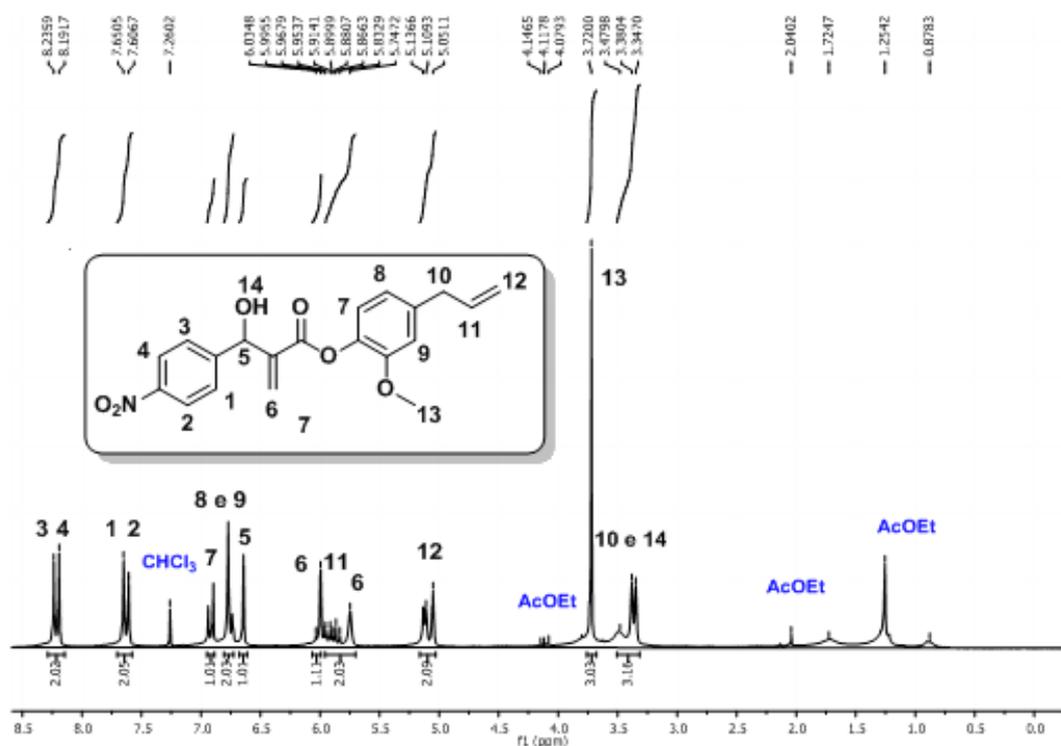


Figure S11. $^1\text{H-NMR}$ spectrum (200 MHz, CDCl_3) of 4-allyl-2-methoxyphenyl 2-(hydroxy(4-nitrophenyl)methyl)acrylate 7.

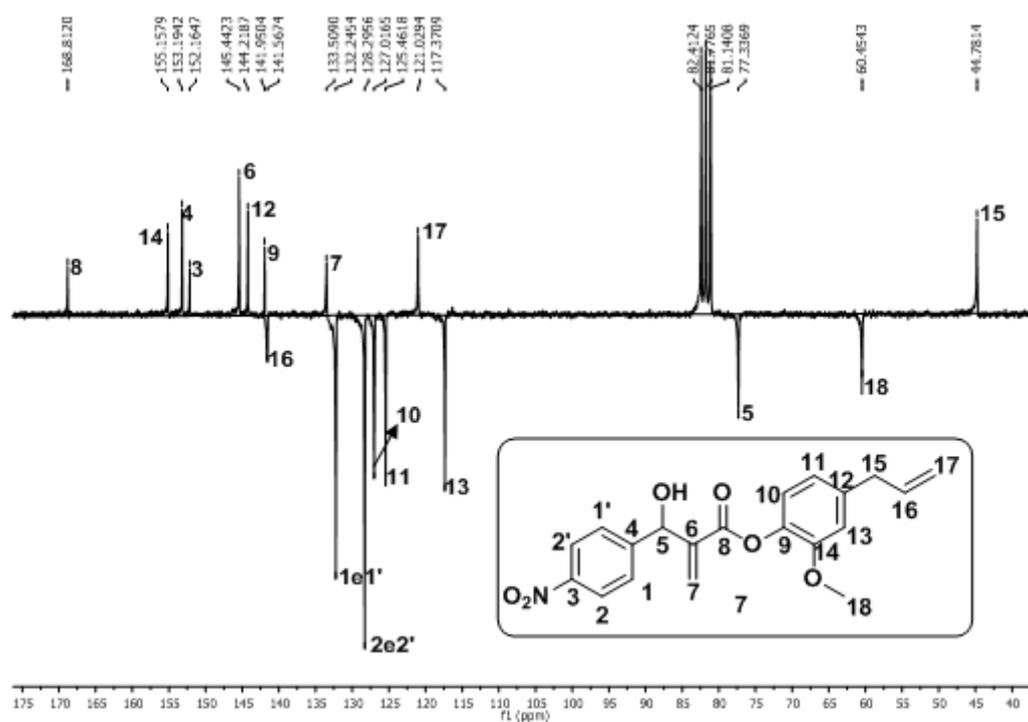


Figure S12. $^{13}\text{C-NMR}$ spectrum (50 MHz, CDCl_3) of 4-allyl-2-methoxyphenyl 2-(hydroxy(4-nitrophenyl)methyl)acrylate 7.

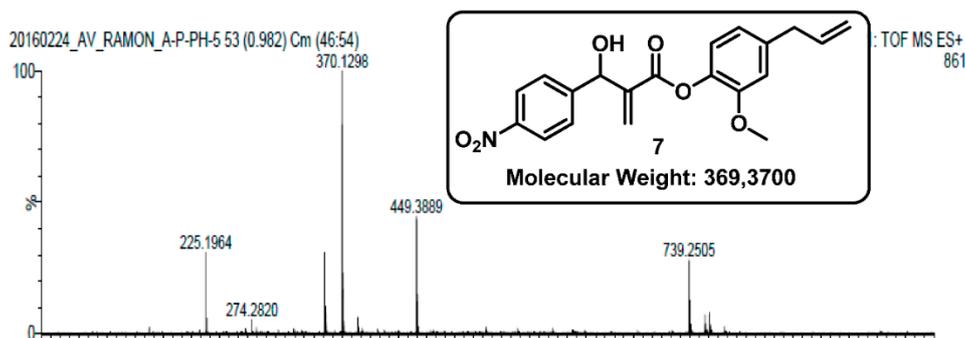


Figure S13. HRMS spectrum of compound 4-allyl-2-methoxyphenyl 2-(hydroxy(4-nitrophenyl)methyl)acrylate 7.

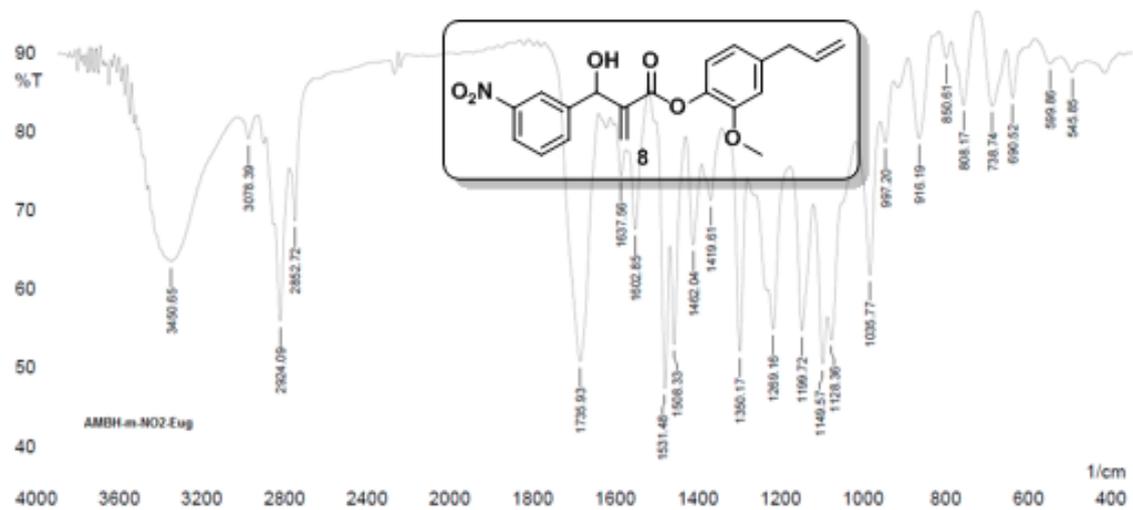


Figure S14. FTIR (KBr) spectrum of 4-allyl-2-methoxyphenyl 2-(hydroxy(3-nitrophenyl)methyl)acrylate 8.

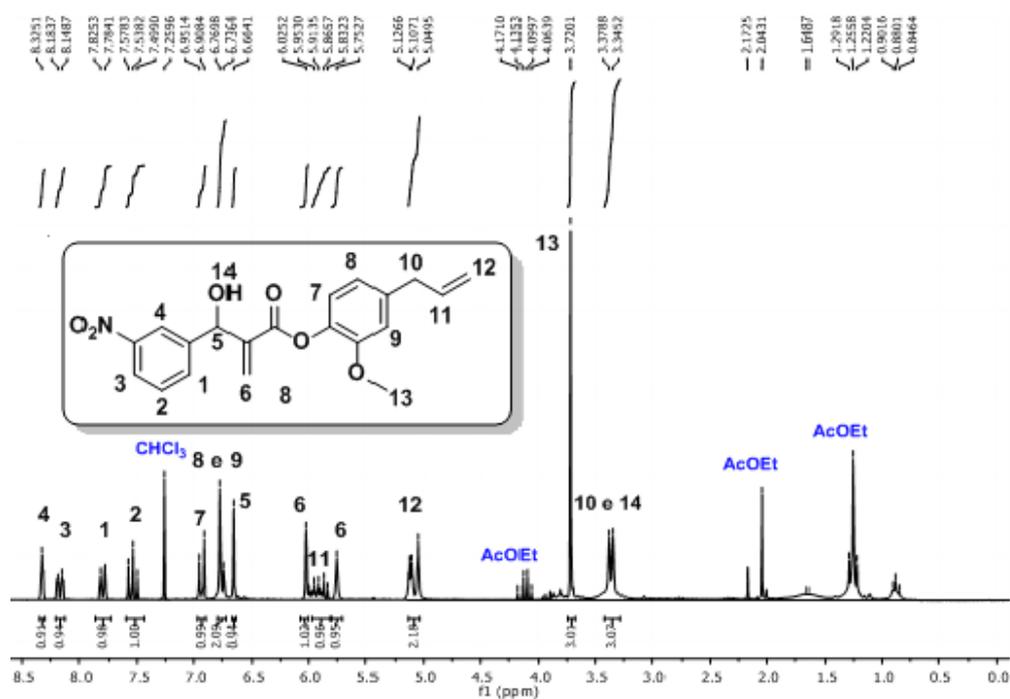


Figure S15. $^1\text{H-NMR}$ spectrum (200 MHz, CDCl_3) of 4-allyl-2-methoxyphenyl 2-(hydroxy(3-nitrophenyl)methyl)acrylate 8.

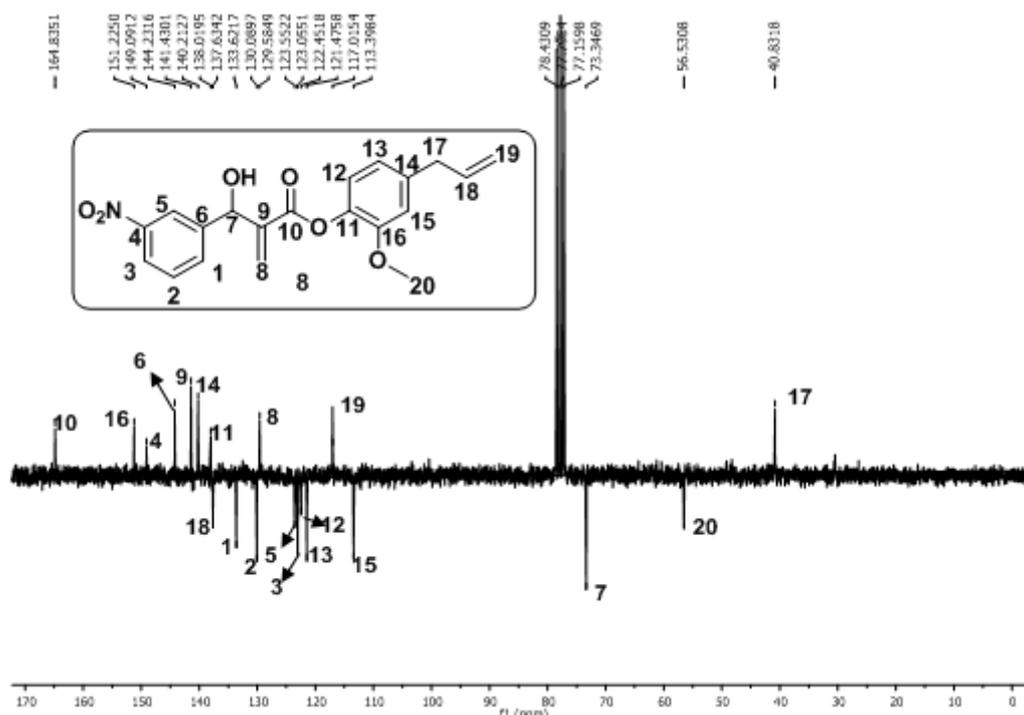


Figure S16. ^{13}C -NMR spectrum (50 MHz, CDCl_3) of 4-allyl-2-methoxyphenyl 2-(hydroxy(3-nitrophenyl)methyl)acrylate **8**.

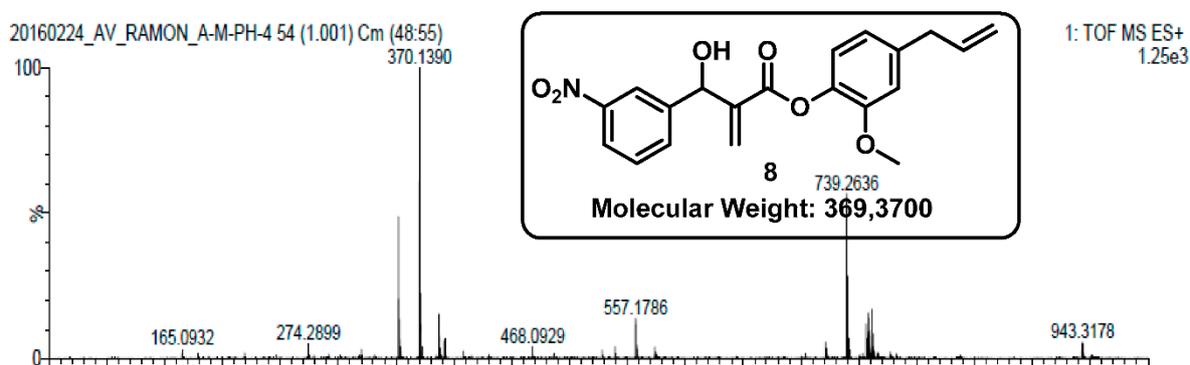


Figure S17. HRMS spectrum of compound 4-allyl-2-methoxyphenyl 2-(hydroxy(3-nitrophenyl)methyl)acrylate **8**.

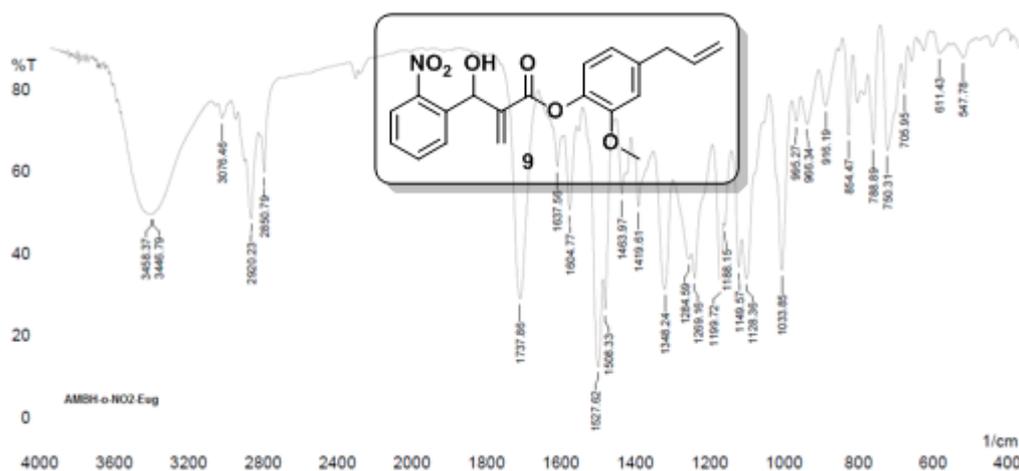


Figure S18. FTIR (KBr) spectrum of 4-allyl-2-methoxyphenyl 2-(hydroxy(2-nitrophenyl)methyl)acrylate **9**.

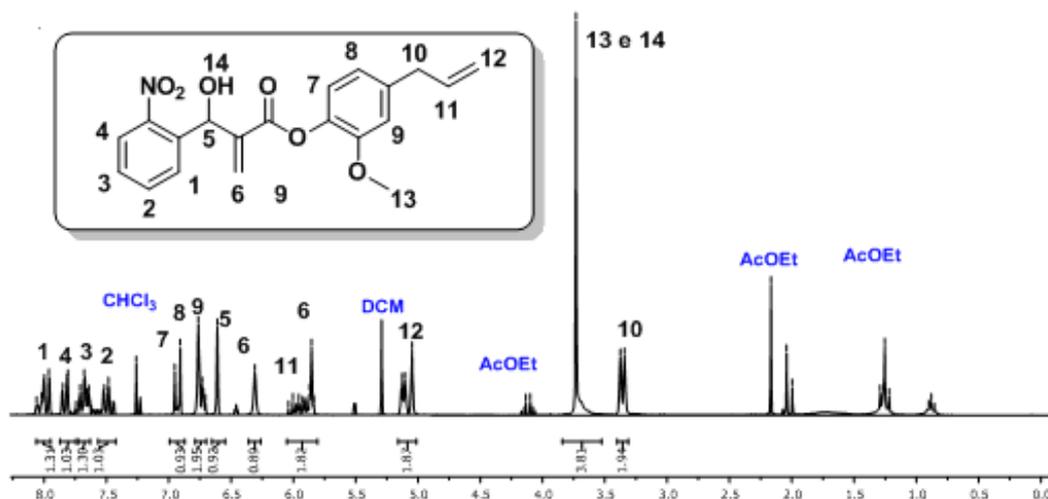


Figure S19. ¹H-NMR spectrum (200 MHz, CDCl₃) of 4-allyl-2-methoxyphenyl 2-(hydroxy(2-nitrophenyl)methyl)acrylate 9.

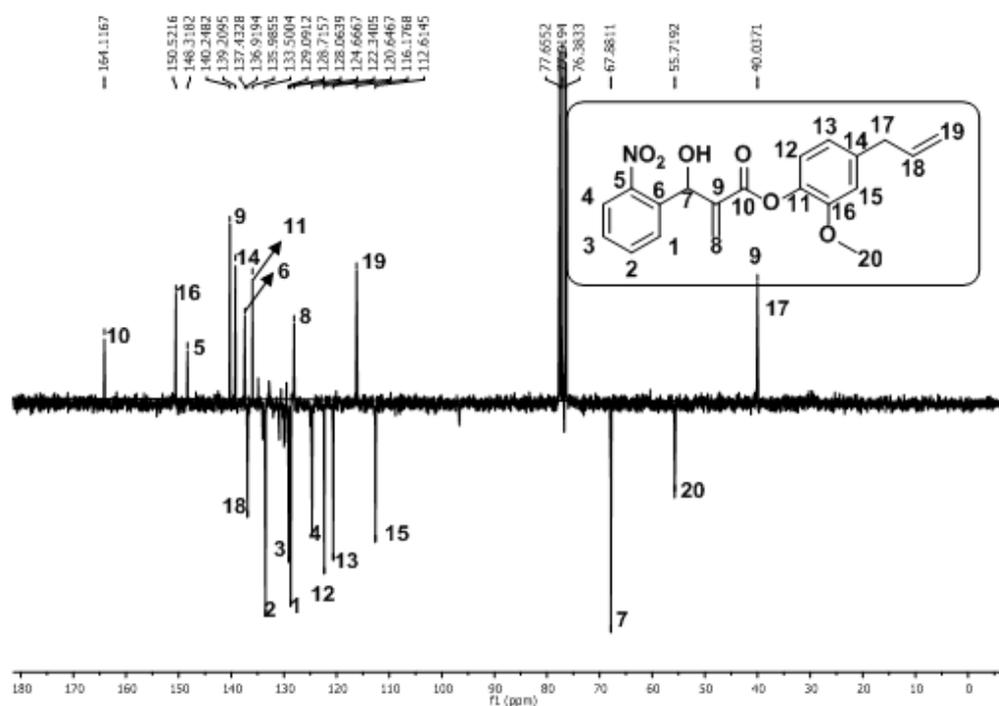


Figure S20. ¹³C-NMR spectrum (50 MHz, CDCl₃) of 4-allyl-2-methoxyphenyl 2-(hydroxy(2-nitrophenyl)methyl)acrylate 9.

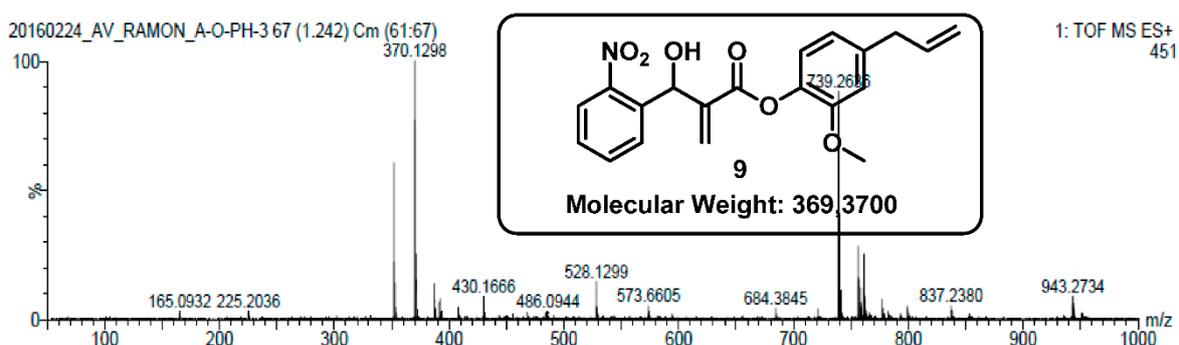


Figure S21. HRMS spectrum of compound 4-allyl-2-methoxyphenyl 2-(hydroxy(2-nitrophenyl)methyl)acrylate 9.

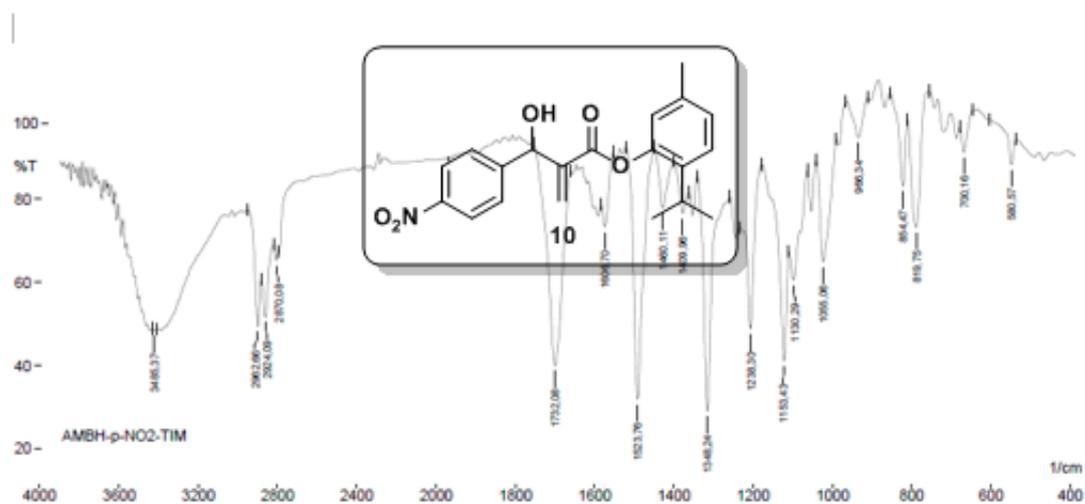


Figure S22. FTIR (KBr) spectrum of 2-isopropyl-5-methylphenyl 2-(hydroxy(4-nitrophenyl)methyl)acrylate 10.

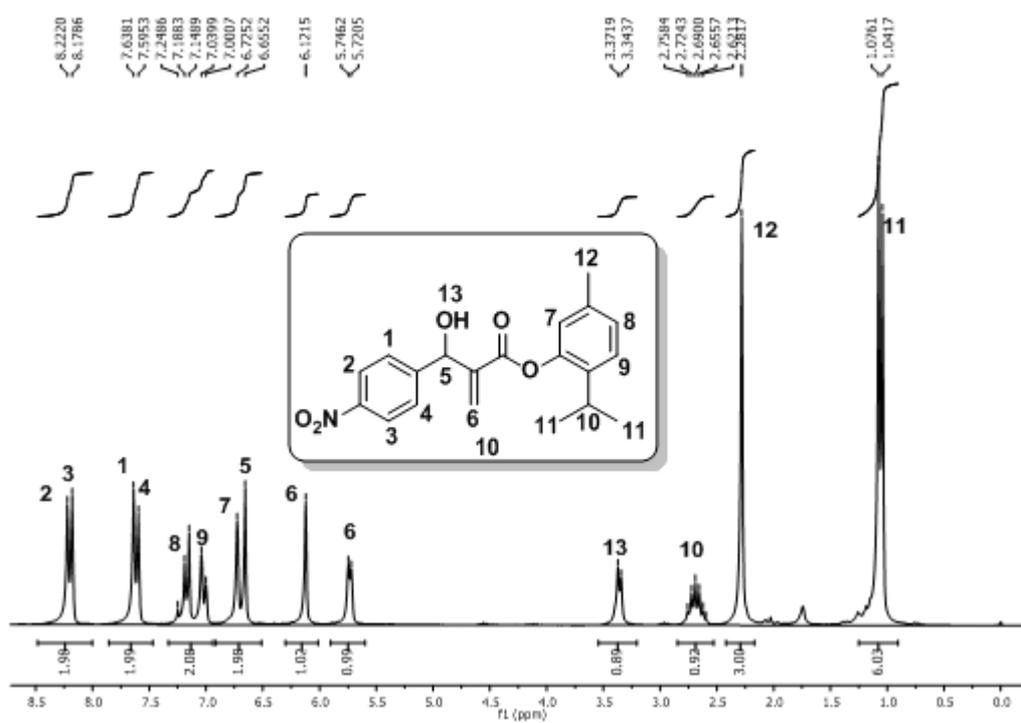


Figure S23. $^1\text{H-NMR}$ spectrum (200 MHz, CDCl_3) of 2-(hydroxy(4-nitrophenyl)methyl)acrylate 10.

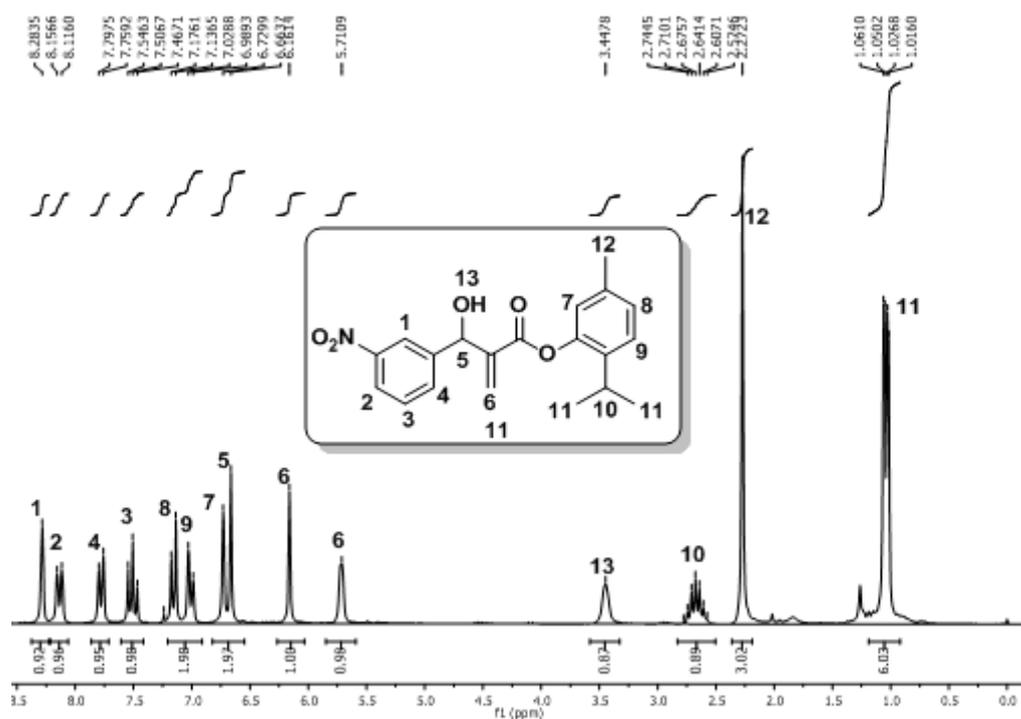


Figure S27. $^1\text{H-NMR}$ spectrum (200 MHz, CDCl_3) of 2-(hydroxy(3-nitrophenyl)methyl)acrylate **11**.

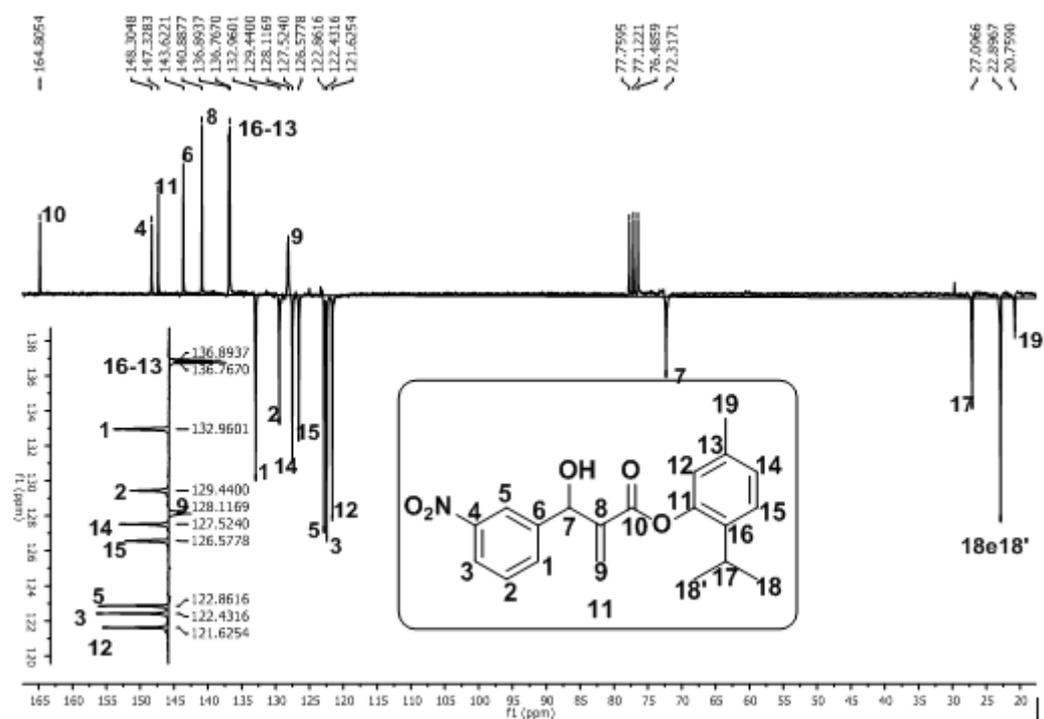


Figure S28. $^{13}\text{C-NMR}$ spectrum (50 MHz, CDCl_3) of 2-(hydroxy(3-nitrophenyl)methyl)acrylate **11**.

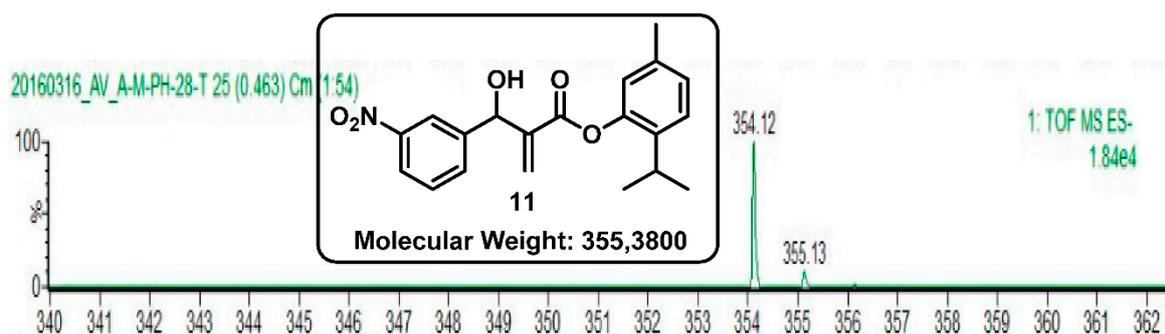


Figure S29. HRMS spectrum of compound 2-(hydroxy(3-nitrophenyl)methyl)acrylate 11.

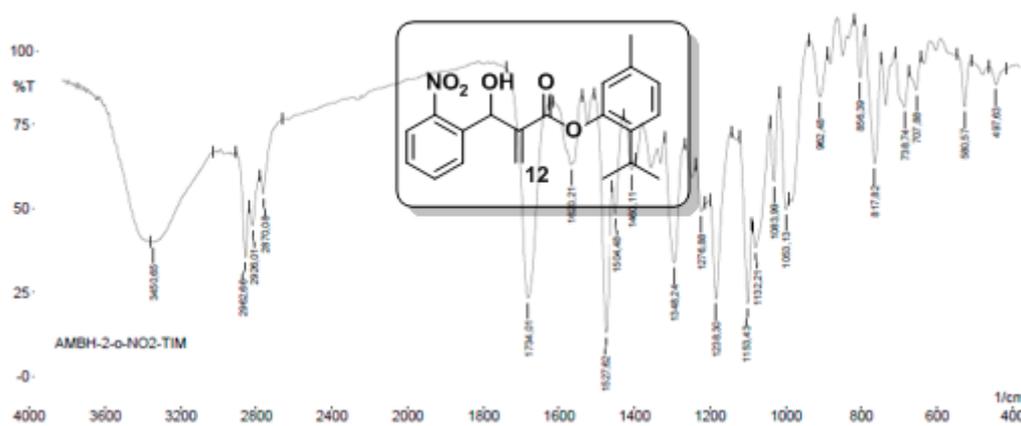


Figure S30. FTIR (KBr) spectrum of 2-isopropyl-5-methylphenyl 2-(hydroxy(2-nitrophenyl)methyl)acrylate 12.

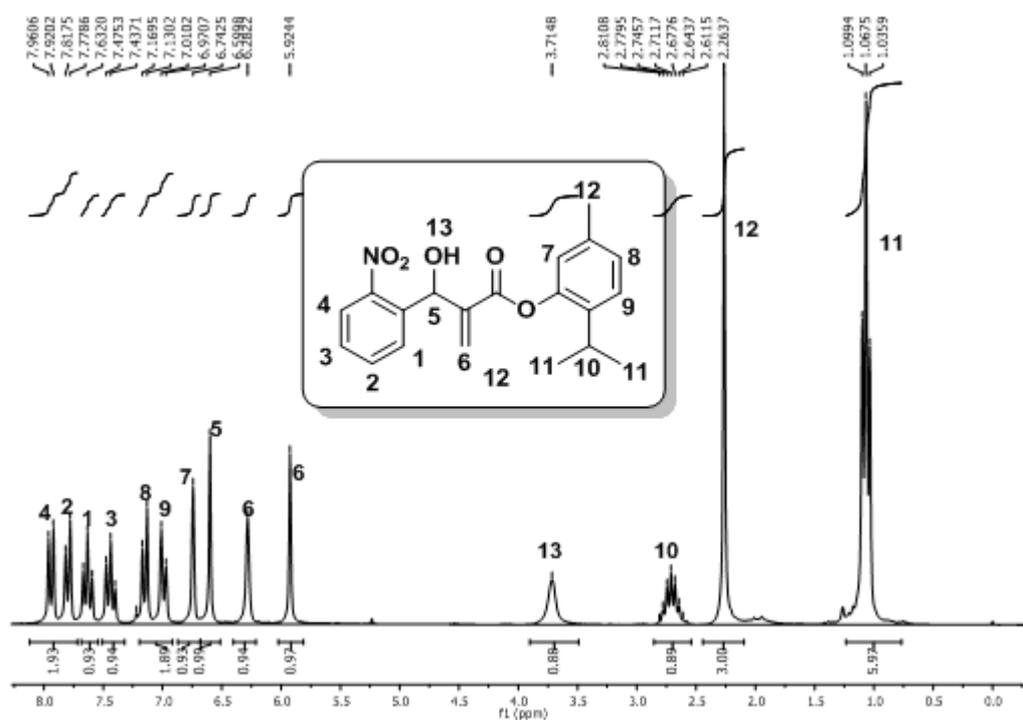


Figure S31. $^1\text{H-NMR}$ spectrum (200 MHz, CDCl_3) of 2-(hydroxy(2-nitrophenyl)methyl)acrylate 12.

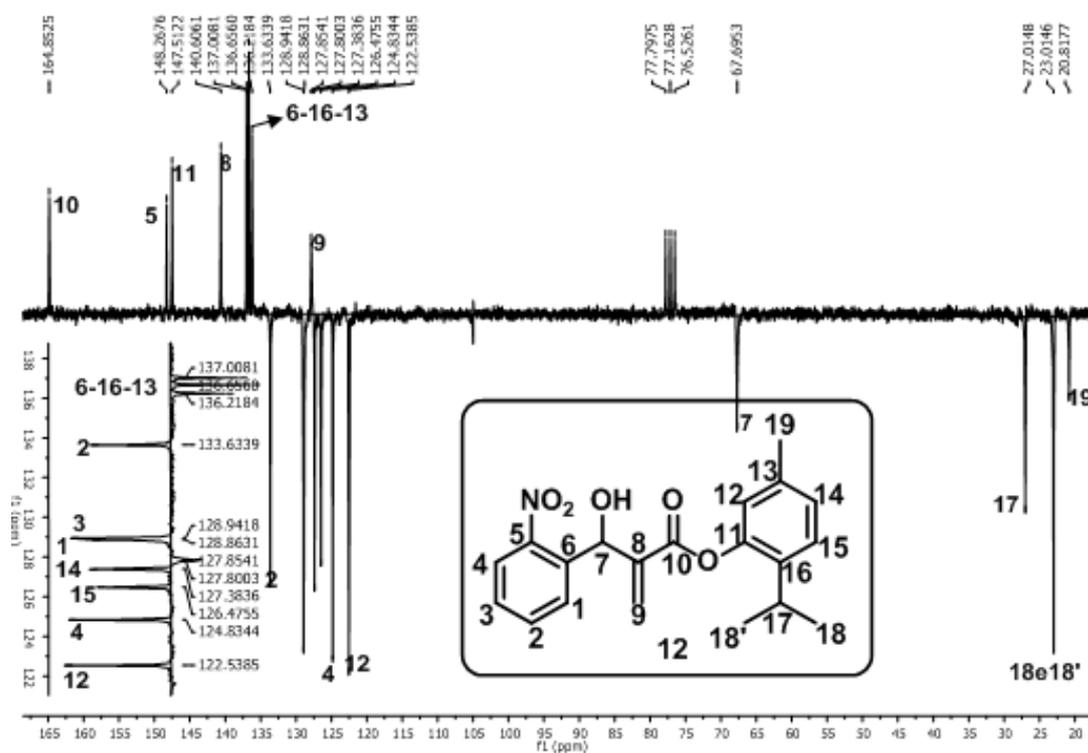


Figure S32. ^{13}C -NMR spectrum (50 MHz, CDCl_3) of 2-(hydroxy(2-nitrophenyl)methyl)acrylate **12**.

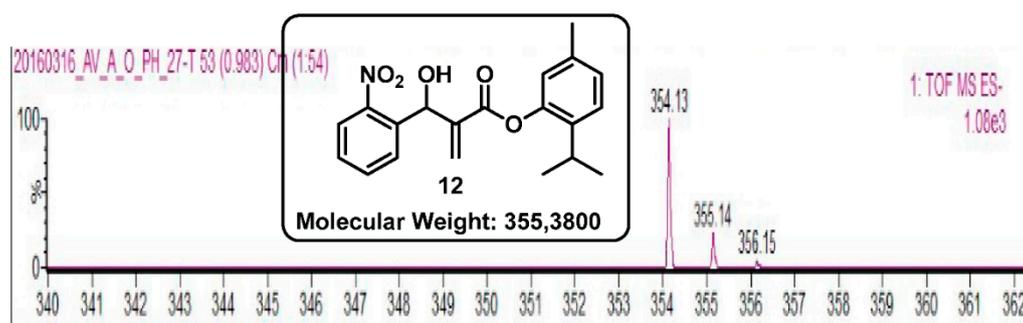


Figure S33. HRMS spectrum of compound 2-(hydroxy(2-nitrophenyl)methyl)acrylate **12**.

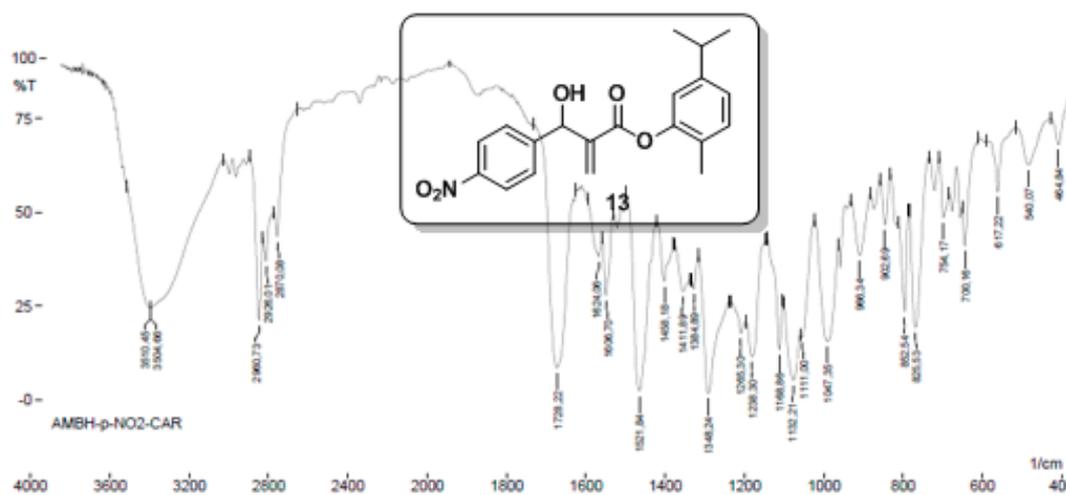


Figure S34. FTIR (KBr) spectrum of 5-isopropyl-2-methylphenyl 2-(hydroxy(4-nitrophenyl)methyl)acrylate **13**.

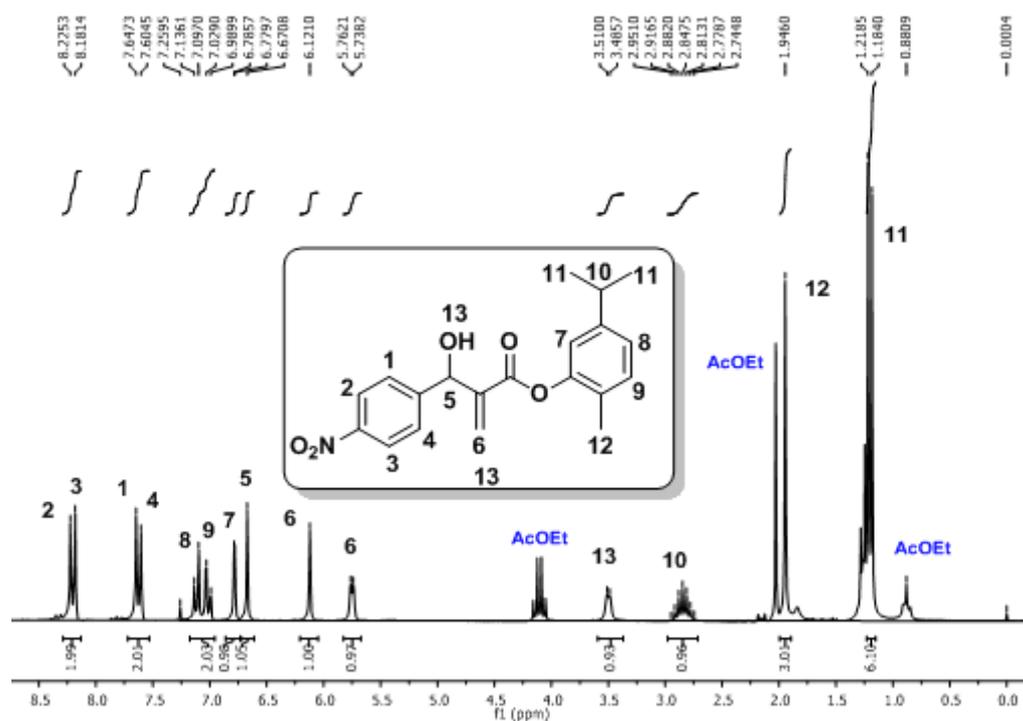


Figure S35. $^1\text{H-NMR}$ spectrum (200 MHz, CDCl_3) of 5-isopropyl-2-methylphenyl 2-(hydroxy(4-nitrophenyl)methyl)acrylate 13.

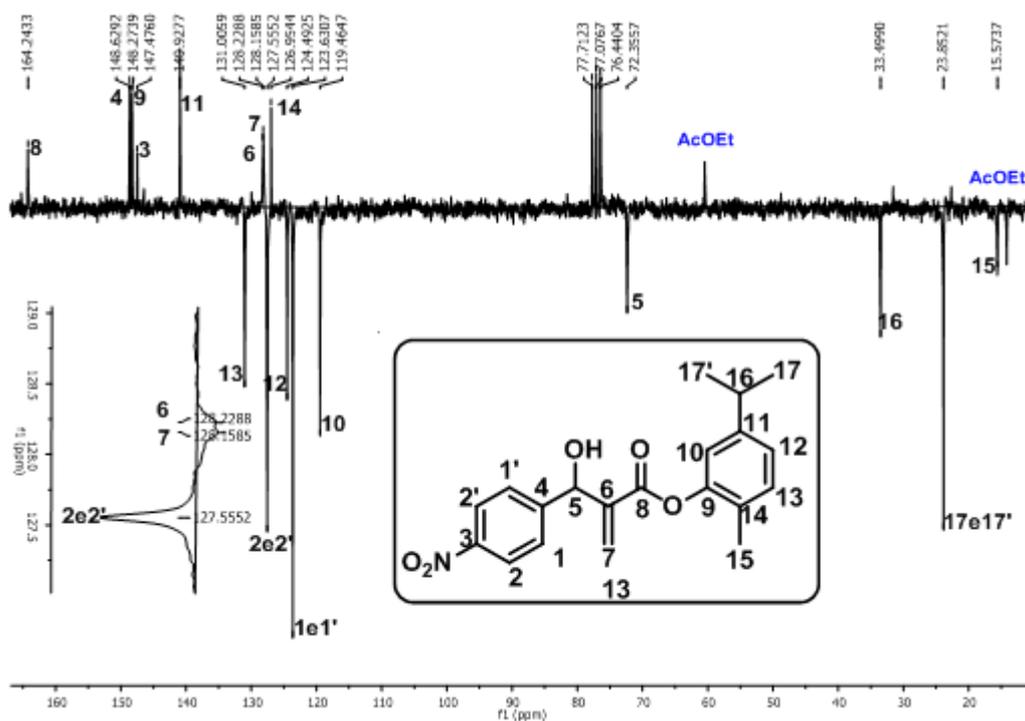


Figure S36. $^{13}\text{C-NMR}$ spectrum (50 MHz, CDCl_3) of 5-isopropyl-2-methylphenyl 2-(hydroxy(4-nitrophenyl)methyl)acrylate 13.

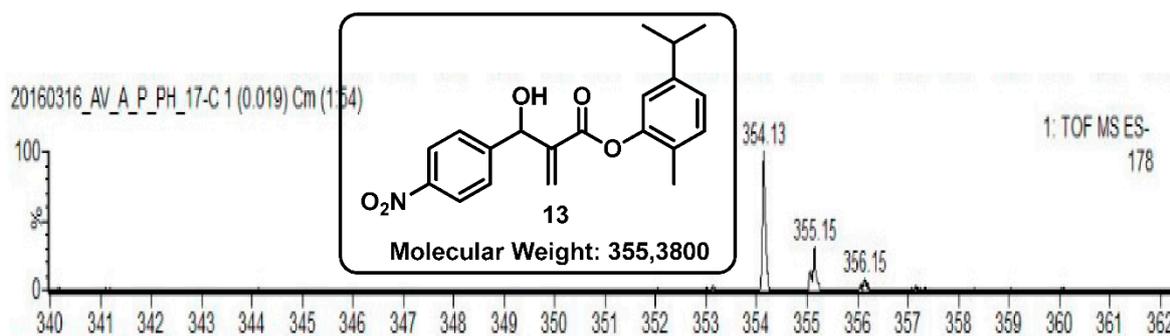


Figure S37. HRMS spectrum of of 5-isopropyl-2-methylphenyl 2-(hydroxy(4-nitrophenyl)methyl)acrylate 13.

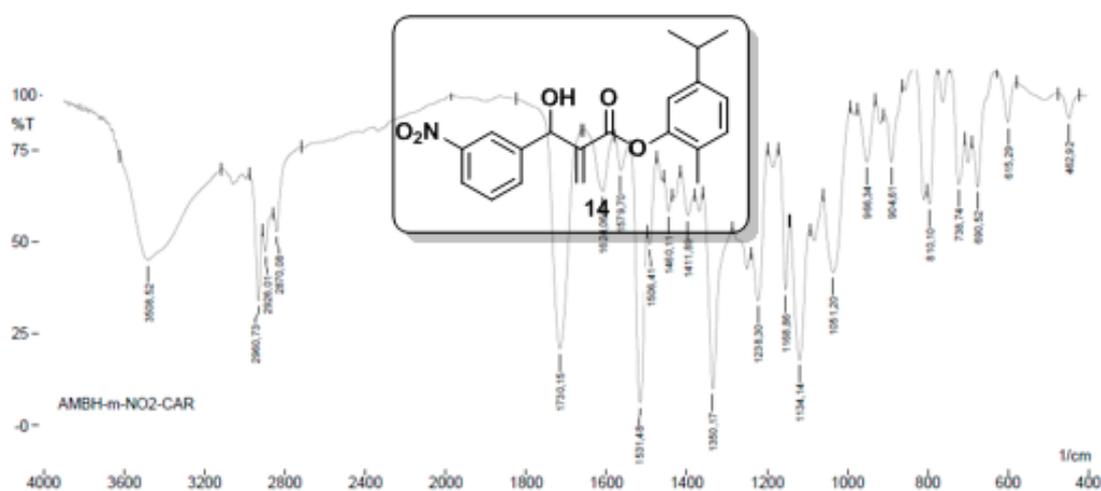


Figure S38. FTIR (KBr) spectrum of 5-isopropyl-2-methylphenyl 2-(hydroxy(3-nitrophenyl)methyl)acrylate 14.

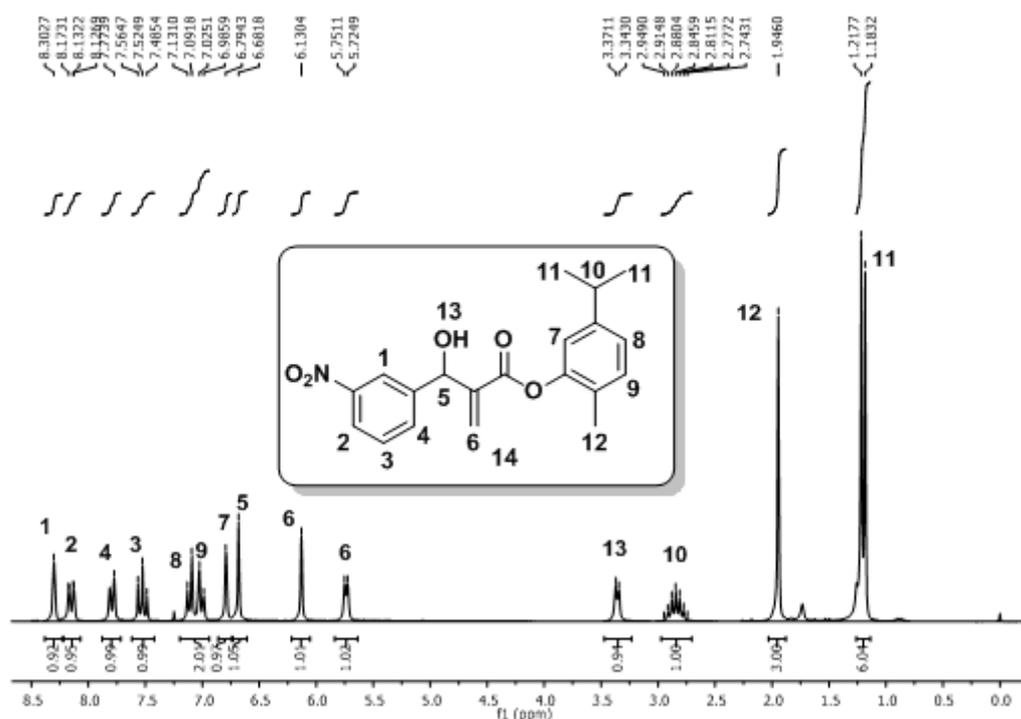


Figure S39. $^1\text{H-NMR}$ spectrum (200 MHz, CDCl_3) of 5-isopropyl-2-methylphenyl 2-(hydroxy(3-nitrophenyl)methyl)acrylate 14.

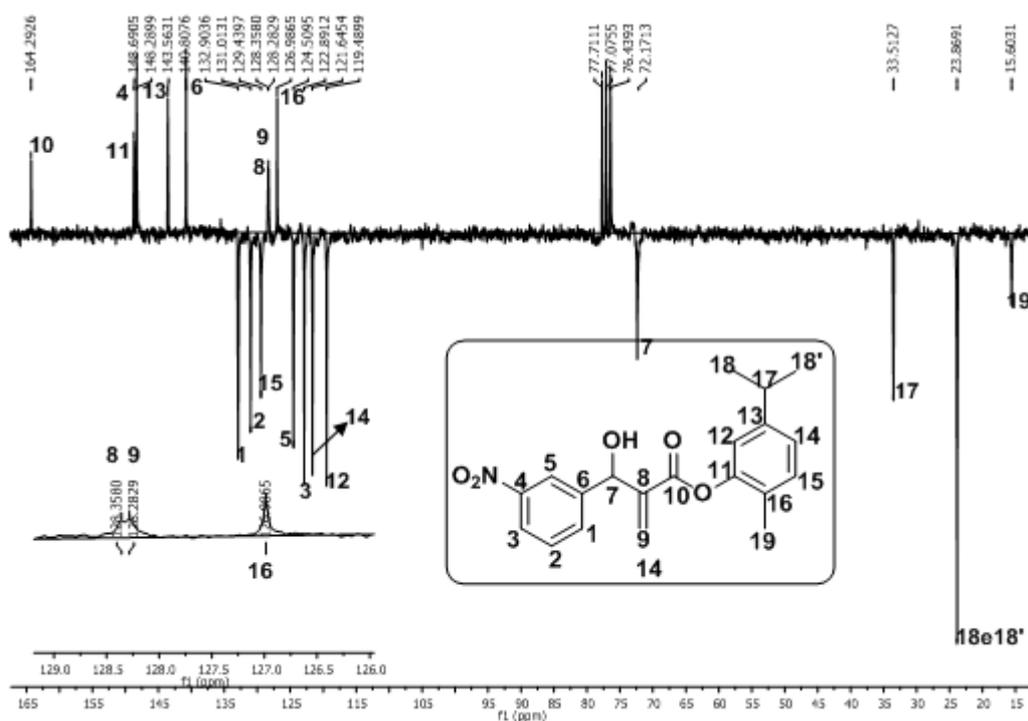


Figure S40. ^{13}C -NMR spectrum (50 MHz, CDCl_3) of 5-isopropyl-2-methylphenyl 2-(hydroxy(3-nitrophenyl)methyl)acrylate **14**.

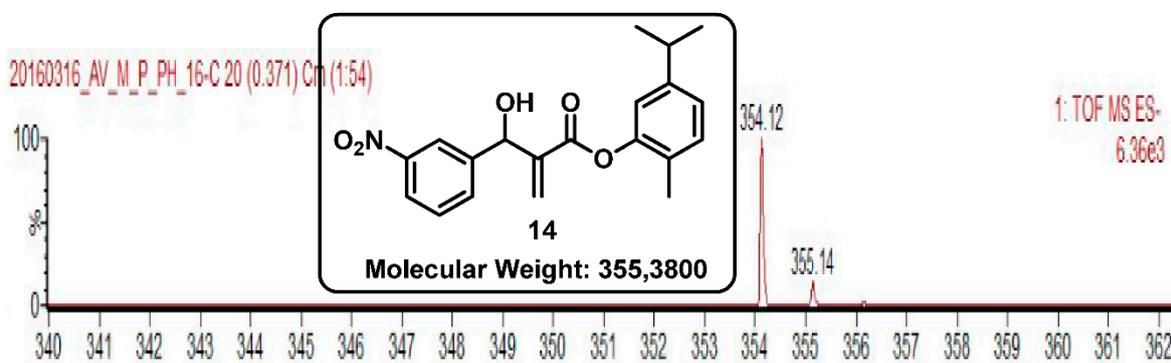


Figure S41. HRMS spectrum of compound 5-isopropyl-2-methylphenyl 2-(hydroxy(3-nitrophenyl)methyl)acrylate **14**.

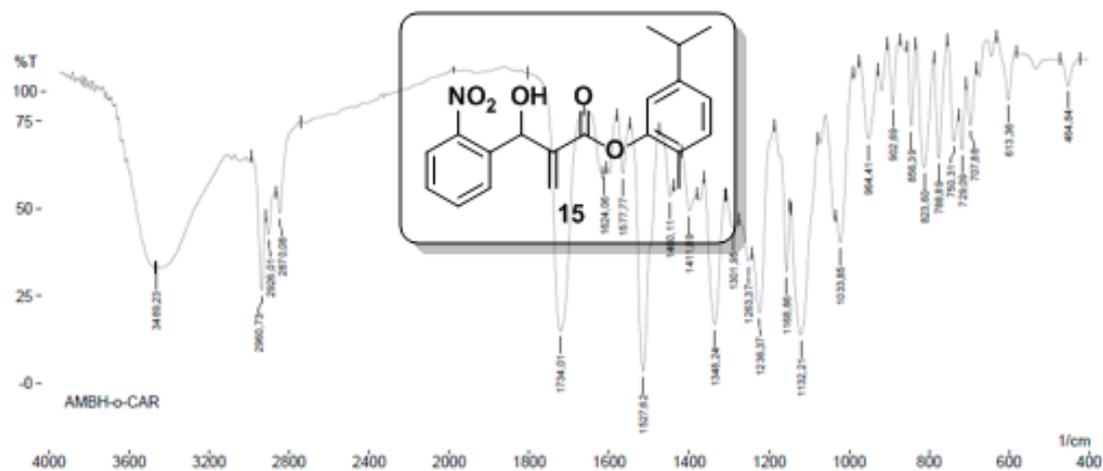


Figure S42. FTIR (KBr) spectrum of 5-isopropyl-2-methylphenyl 2-(hydroxy(2-nitrophenyl)methyl)acrylate 15.

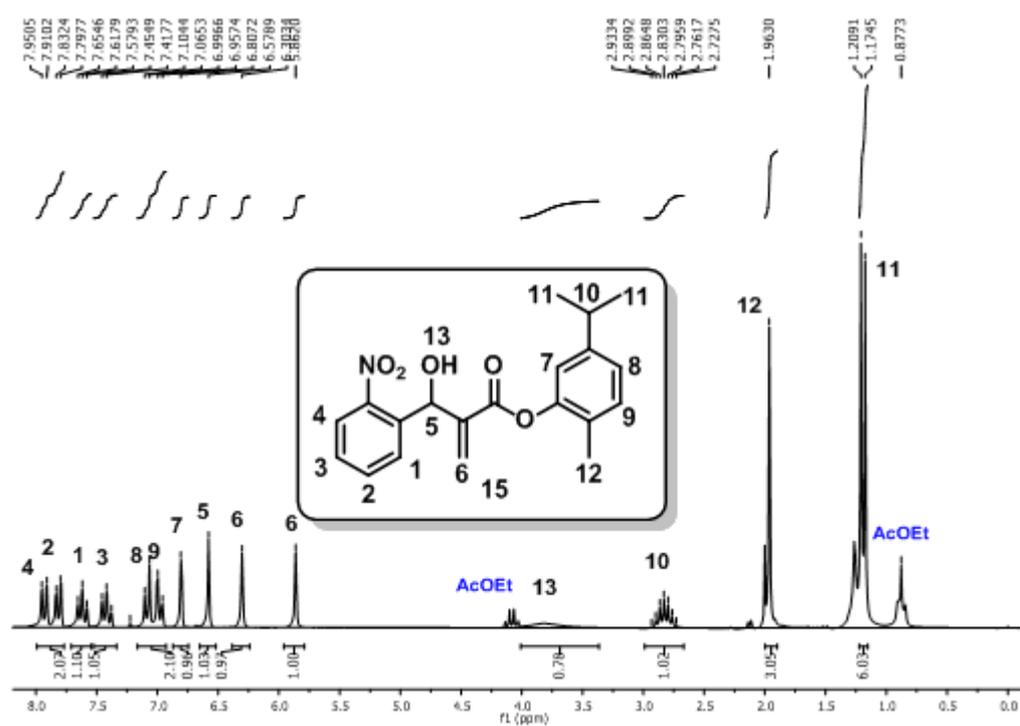


Figure S43. $^1\text{H-NMR}$ spectrum (200 MHz, CDCl_3) of 5-isopropyl-2-methylphenyl 2-(hydroxy(2-nitrophenyl)methyl)acrylate 15.

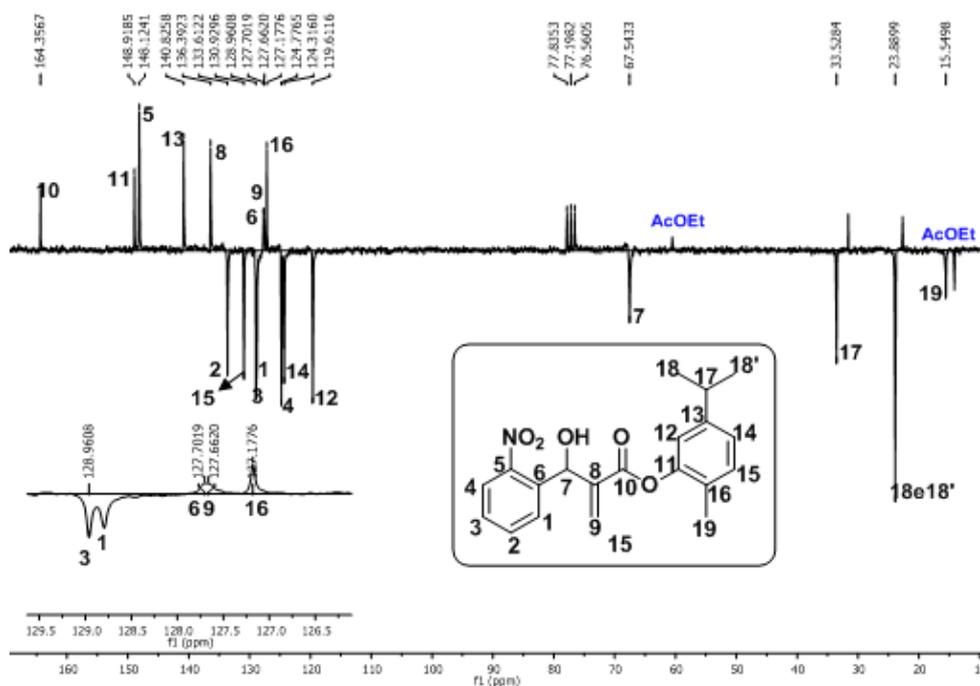


Figure S44. ^{13}C -NMR spectrum (50 MHz, CDCl_3) of 5-isopropyl-2-methylphenyl 2-(hydroxy(2-nitrophenyl)methyl)acrylate 15.

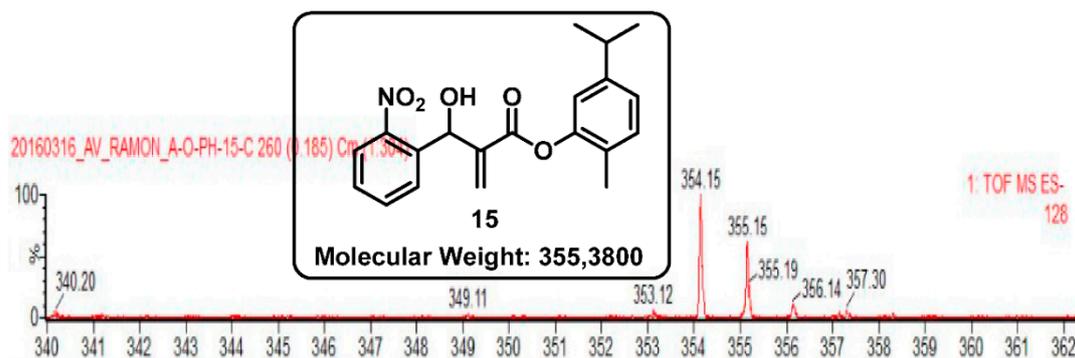


Figure S45. HRMS spectrum of compound 5-isopropyl-2-methylphenyl 2-(hydroxy(2-nitrophenyl)methyl)acrylate 15.

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-3.6417 -0.9842 -1.7160 C 0 0 0 0 0 0 0 0 0 0 0 0
-1.7685 -0.6673 -2.7704 H 0 0 0 0 0 0 0 0 0 0 0 0
-3.9654 0.3952 0.2434 C 0 0 0 0 0 0 0 0 0 0 0 0
-4.4263 -0.6007 -0.6309 C 0 0 0 0 0 0 0 0 0 0 0 0
-3.9948 -1.7534 -2.3970 H 0 0 0 0 0 0 0 0 0 0 0 0
-4.5839 0.6826 1.0887 H 0 0 0 0 0 0 0 0 0 0 0 0
-0.7438 1.2427 -1.3066 O 0 0 0 0 0 0 0 0 0 0 0 0
-5.7701 -1.2490 -0.3633 C 0 0 0 0 0 0 0 0 0 0 0 0
-6.5512 -0.4802 -0.3228 H 0 0 0 0 0 0 0 0 0 0 0 0
-6.0066 -1.9216 -1.1960 H 0 0 0 0 0 0 0 0 0 0 0 0
-5.7691 -2.0202 0.9300 C 0 0 0 0 0 0 0 0 0 0 0 0
-5.0748 -2.8599 0.9859 H 0 0 0 0 0 0 0 0 0 0 0 0
-6.5348 -1.7231 1.9809 C 0 0 0 0 0 0 0 0 0 0 0 0
-7.2322 -0.8873 1.9537 H 0 0 0 0 0 0 0 0 0 0 0 0
-6.4929 -2.3052 2.8979 H 0 0 0 0 0 0 0 0 0 0 0 0
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-2.9713 2.4384 1.9139 C 0 0 0 0 0 0 0 0 0 0 0 0
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-3.9248 2.8527 1.5715 H 0 0 0 0 0 0 0 0 0 0 0 0
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1 7 1 0 0 0 0
2 3 4 0 0 0 0
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3 4 4 0 0 0 0
3 11 1 0 0 0 0
4 5 4 0 0 0 0
4 21 1 0 0 0 0
5 6 4 0 0 0 0
5 9 1 0 0 0 0
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13 14 2 0 0 0 0
13 19 1 0 0 0 0
14 15 1 0 0 0 0
14 16 1 0 0 0 0
17 18 1 0 0 0 0
19 20 2 0 0 0 0
19 33 1 0 0 0 0
21 22 2 0 0 0 0
21 23 4 0 0 0 0
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24 25 2 0 0 0 0
24 26 4 0 0 0 0
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25 28 1 0 0 0 0
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27 31 1 0 0 0 0
29 30 4 0 0 0 0
29 32 1 0 0 0 0
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34 37 1 0 0 0 0
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37 39 2 0 0 0 0
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43 46 1 0 0 0 0