

# 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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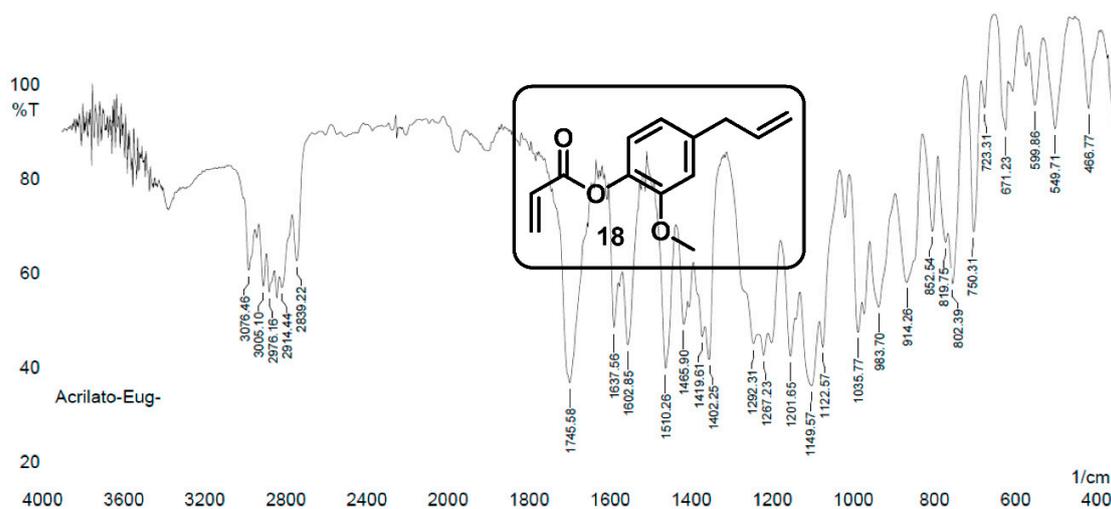


Figure S1. FTIR (KBr) spectrum of 4-allyl-2-methoxyphenyl acrylate 18.

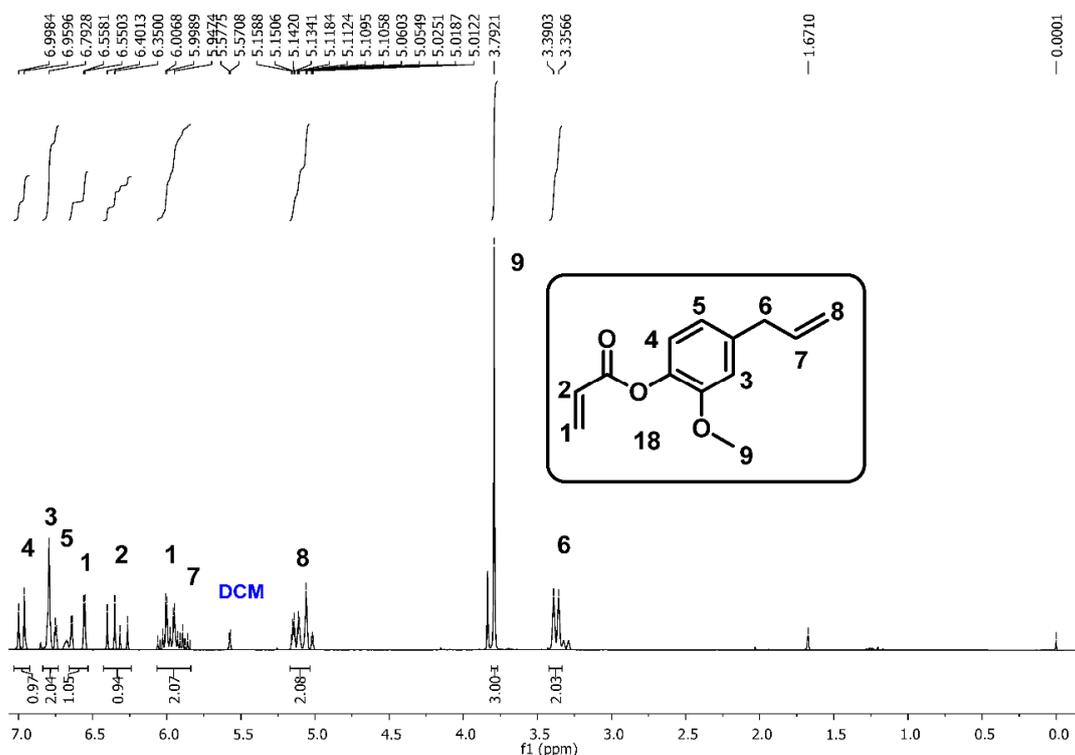


Figure S2. <sup>1</sup>H-NMR spectrum (200 MHz, CDCl<sub>3</sub>) of 4-allyl-2-methoxyphenyl acrylate 18.

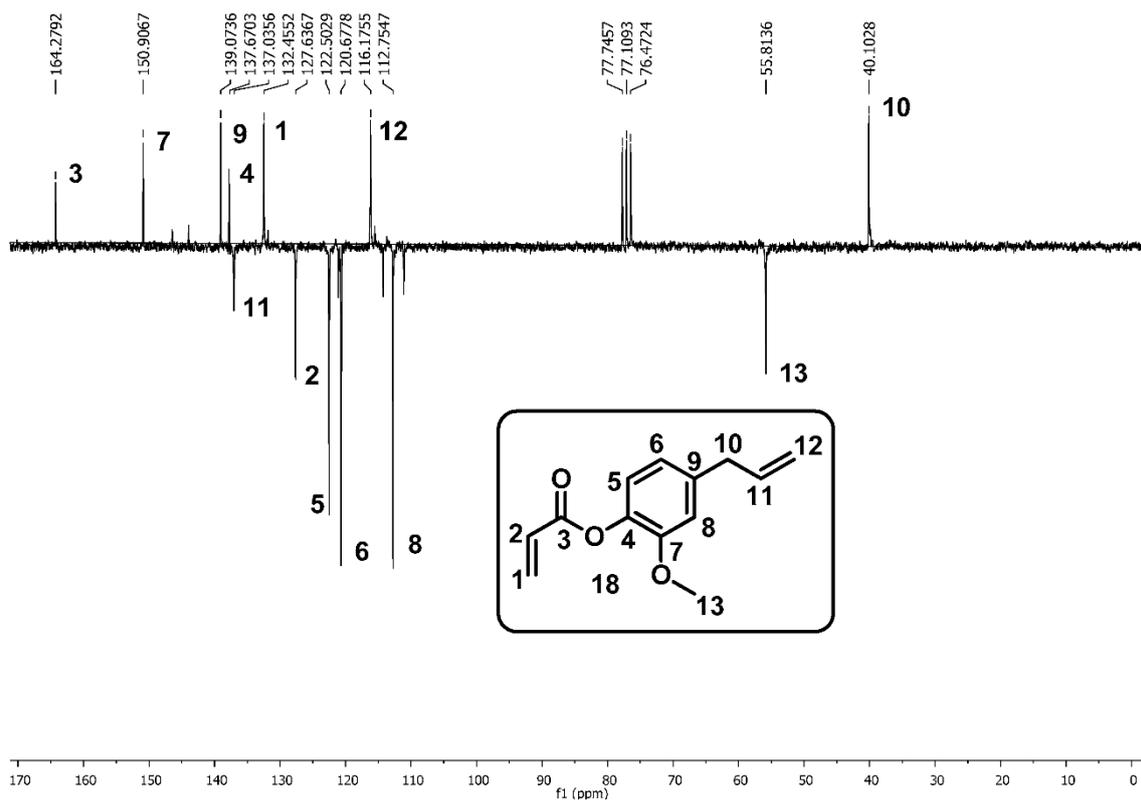


Figure S3. <sup>13</sup>C-NMR spectrum (50 MHz, CDCl<sub>3</sub>) of 4-allyl-2-methoxyphenyl acrylate 18.

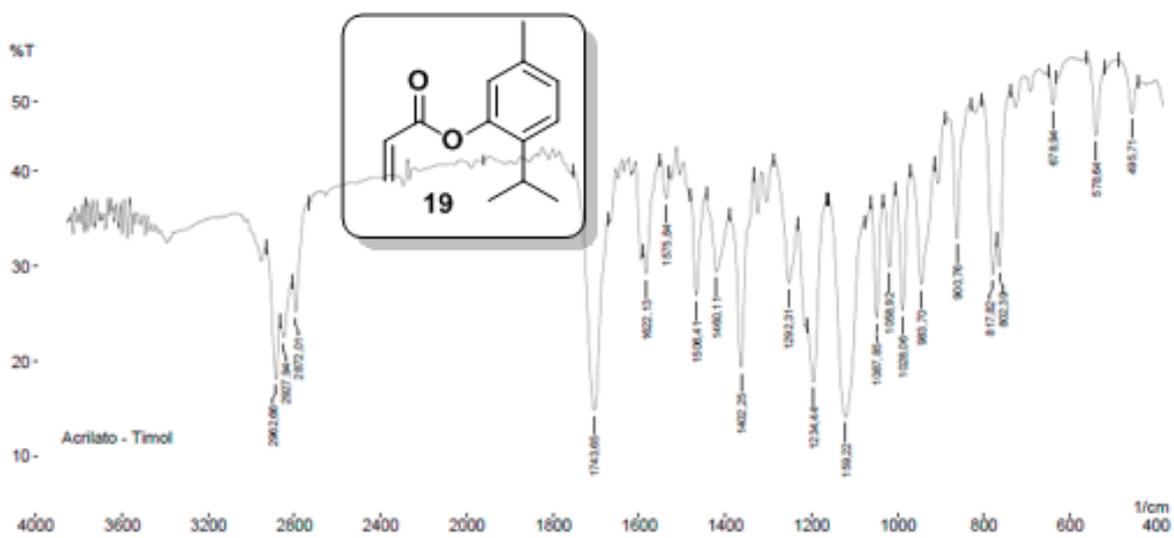
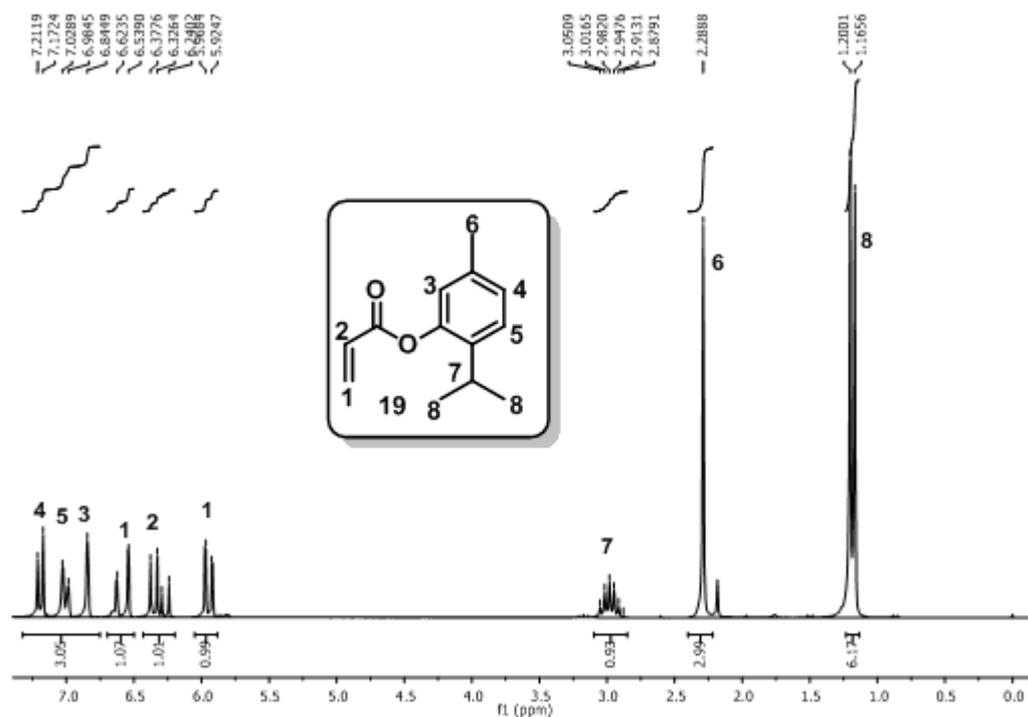
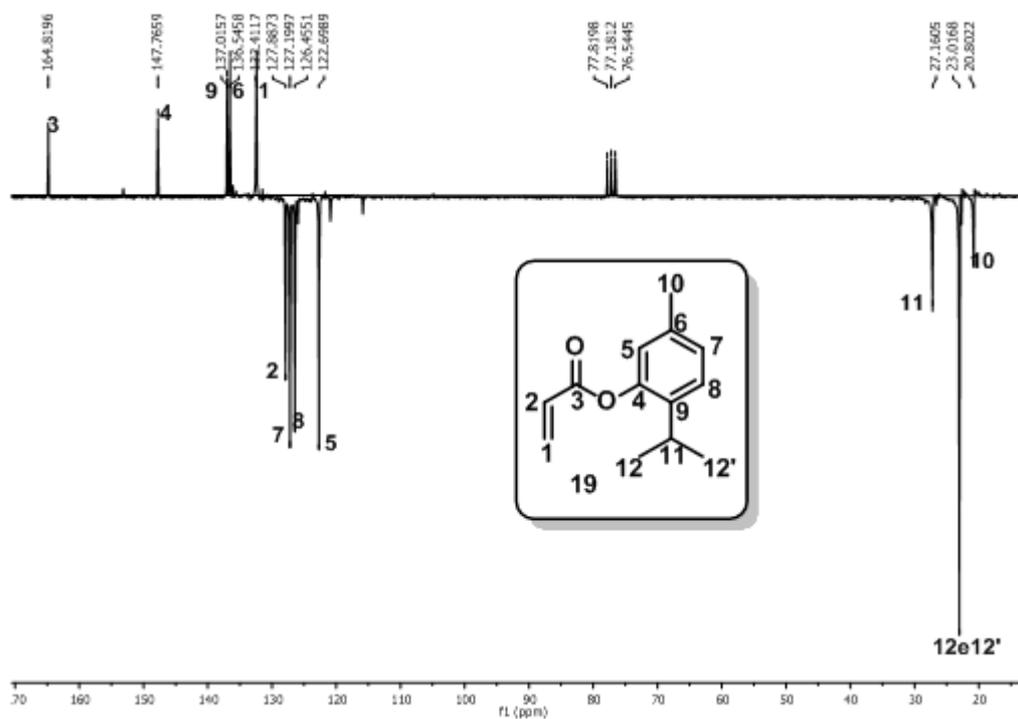


Figure S4. FTIR (KBr) spectrum of 2-isopropyl-5-methylphenyl acrylate 19.



**Figure S5.**  $^1\text{H-NMR}$  spectrum (200 MHz,  $\text{CDCl}_3$ ) of 2-isopropyl-5-methylphenyl acrylate **19**.



**Figure S6.**  $^{13}\text{C-NMR}$  spectrum (50 MHz,  $\text{CDCl}_3$ ) of 2-isopropyl-5-methylphenyl acrylate **19**.

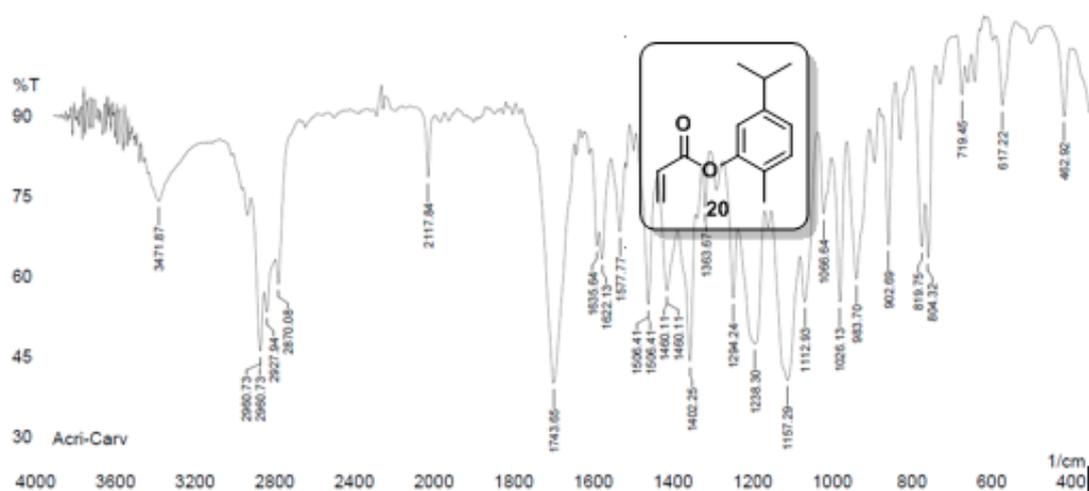


Figure S7. FTIR (KBr) spectrum of 5-isopropyl-2-methylphenyl acrylate 20.

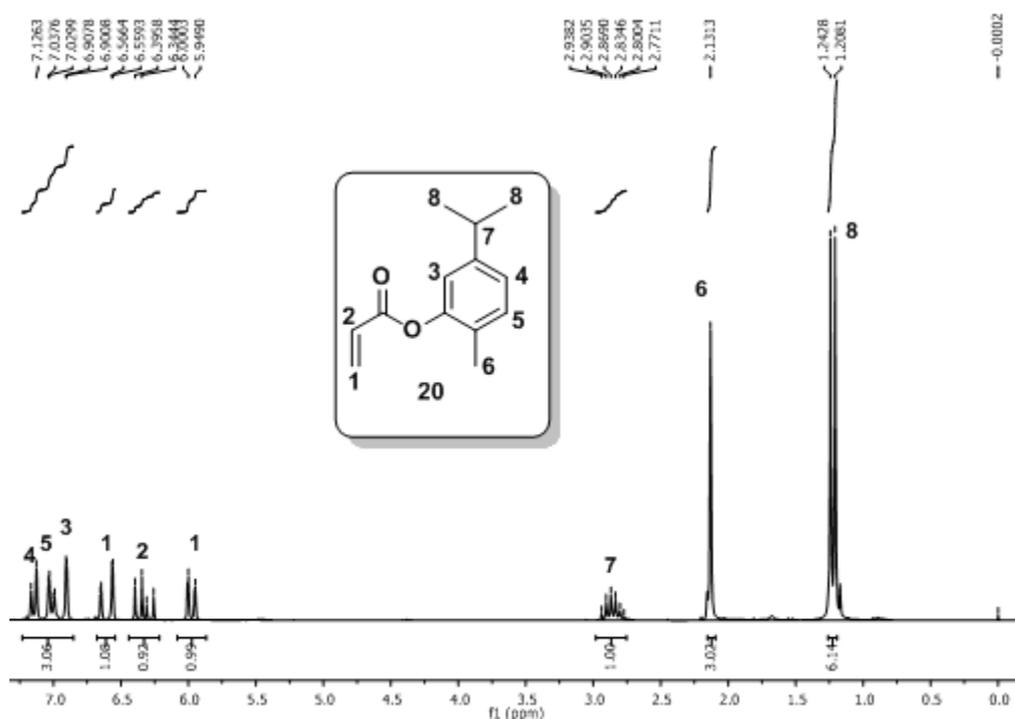


Figure S8. <sup>1</sup>H-NMR spectrum (200 MHz, CDCl<sub>3</sub>) of 5-isopropyl-2-methylphenyl acrylate 20.

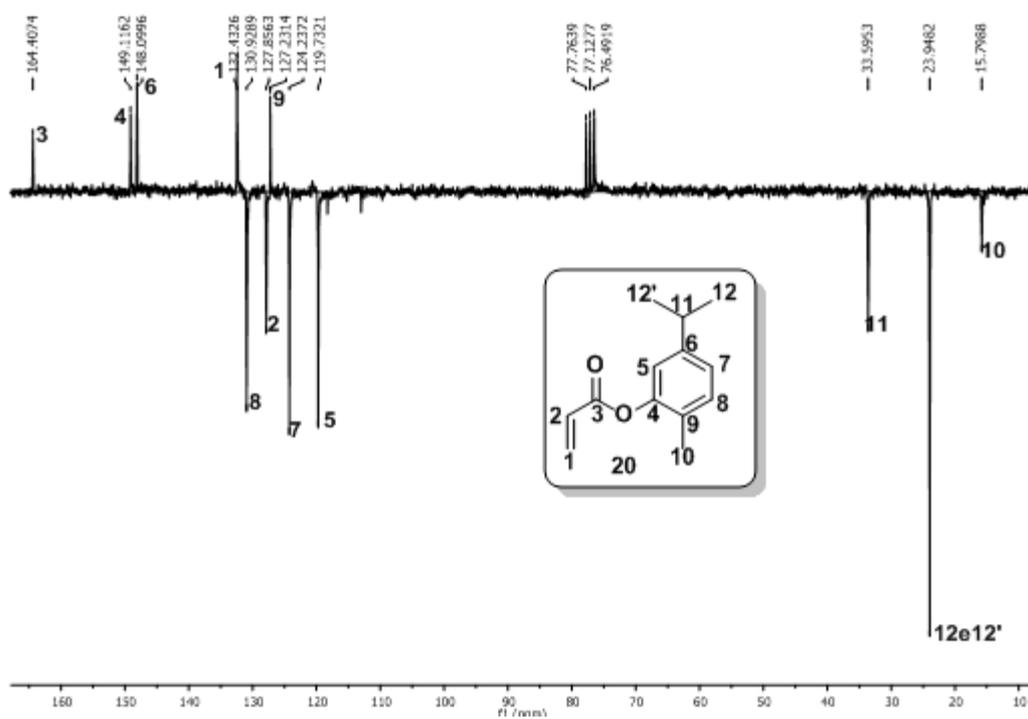


Figure S9.  $^{13}\text{C}$ -NMR spectrum (50 MHz,  $\text{CDCl}_3$ ) of 5-isopropyl-2-methylphenyl acrylate **20**.

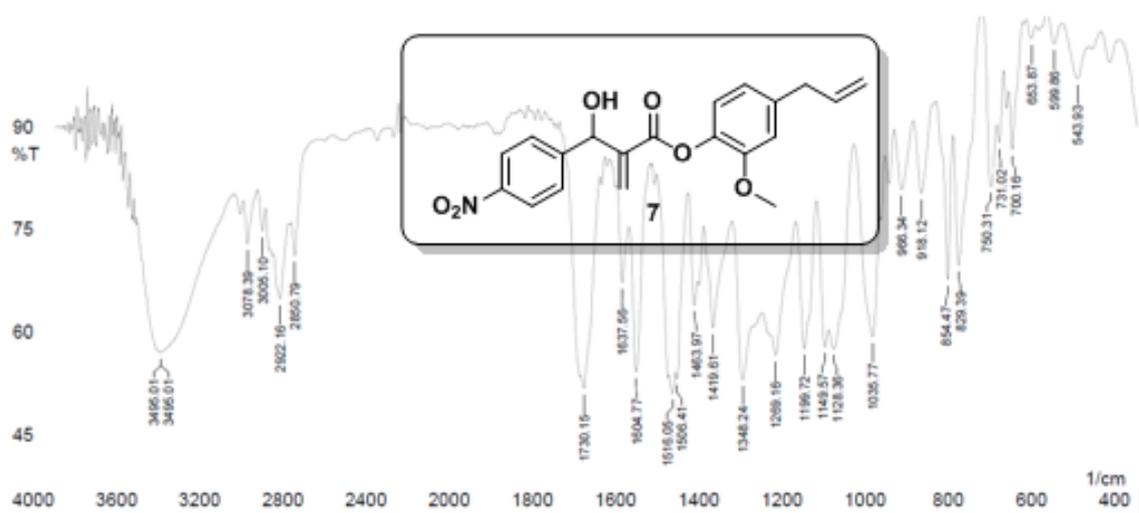
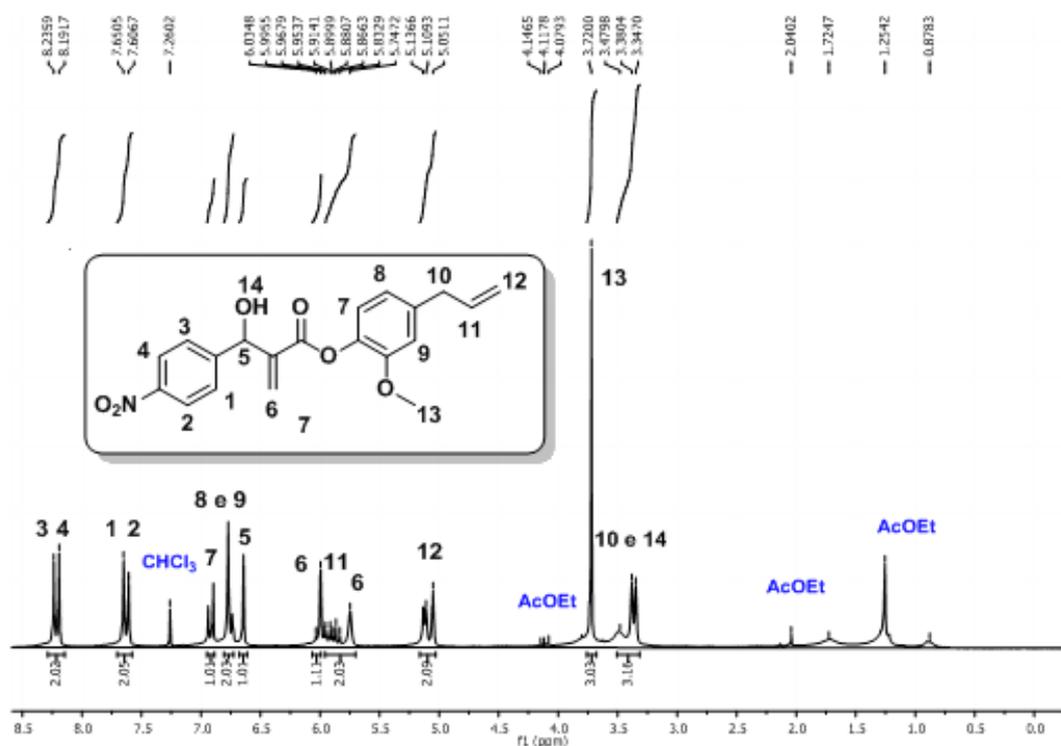
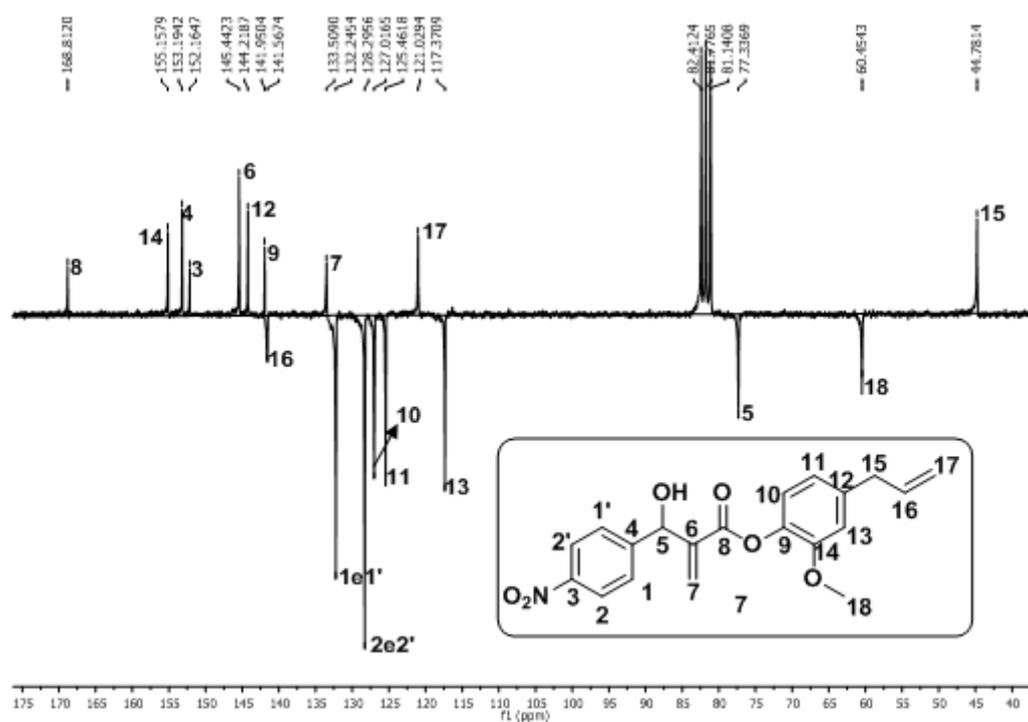


Figure S10. FTIR (KBr) spectrum of 4-allyl-2-methoxyphenyl 2-(hydroxy(4-nitrophenyl)methyl)acrylate **7**.



**Figure S11.**  $^1\text{H-NMR}$  spectrum (200 MHz,  $\text{CDCl}_3$ ) of 4-allyl-2-methoxyphenyl 2-(hydroxy(4-nitrophenyl)methyl)acrylate 7.



**Figure S12.**  $^{13}\text{C-NMR}$  spectrum (50 MHz,  $\text{CDCl}_3$ ) of 4-allyl-2-methoxyphenyl 2-(hydroxy(4-nitrophenyl)methyl)acrylate 7.

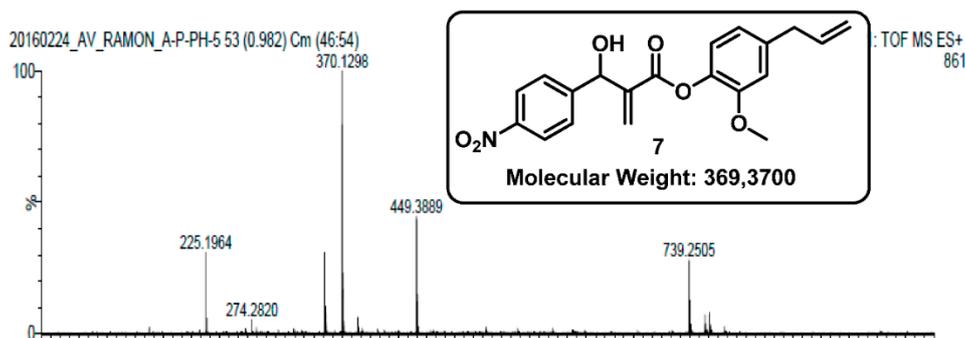


Figure S13. HRMS spectrum of compound 4-allyl-2-methoxyphenyl 2-(hydroxy(4-nitrophenyl)methyl)acrylate 7.

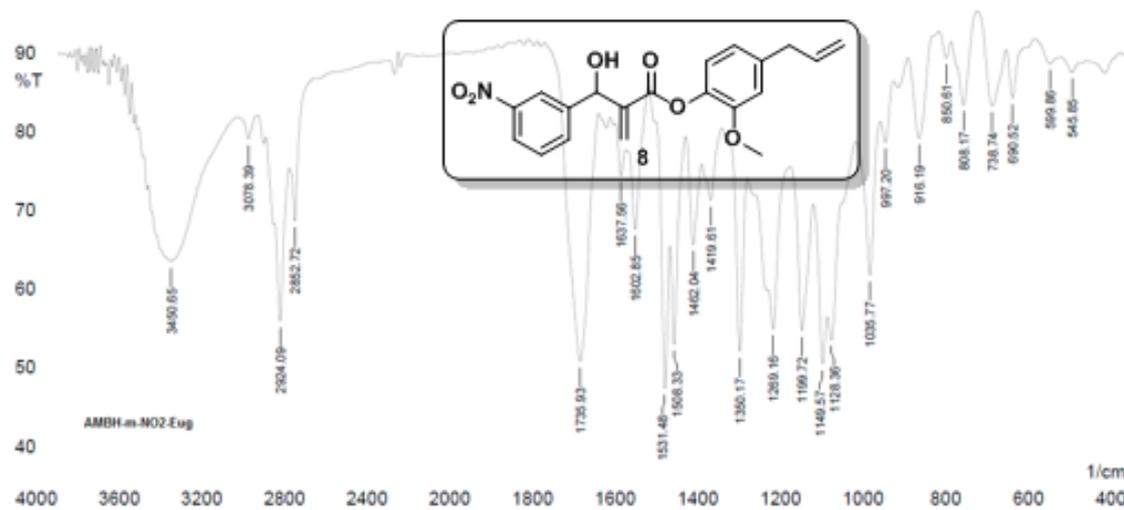


Figure S14. FTIR (KBr) spectrum of 4-allyl-2-methoxyphenyl 2-(hydroxy(3-nitrophenyl)methyl)acrylate 8.

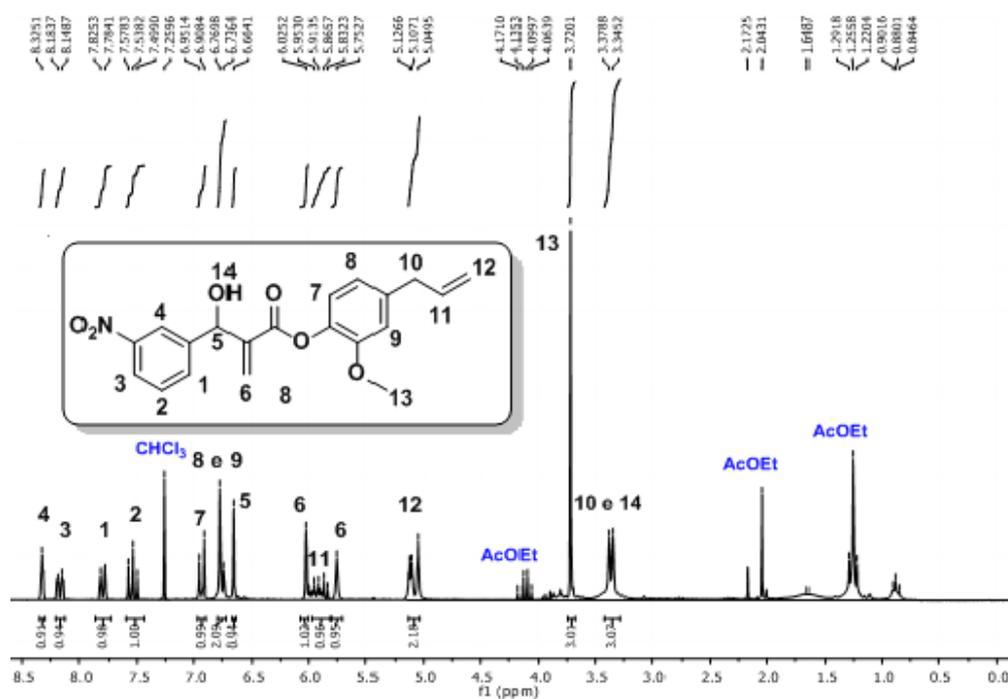
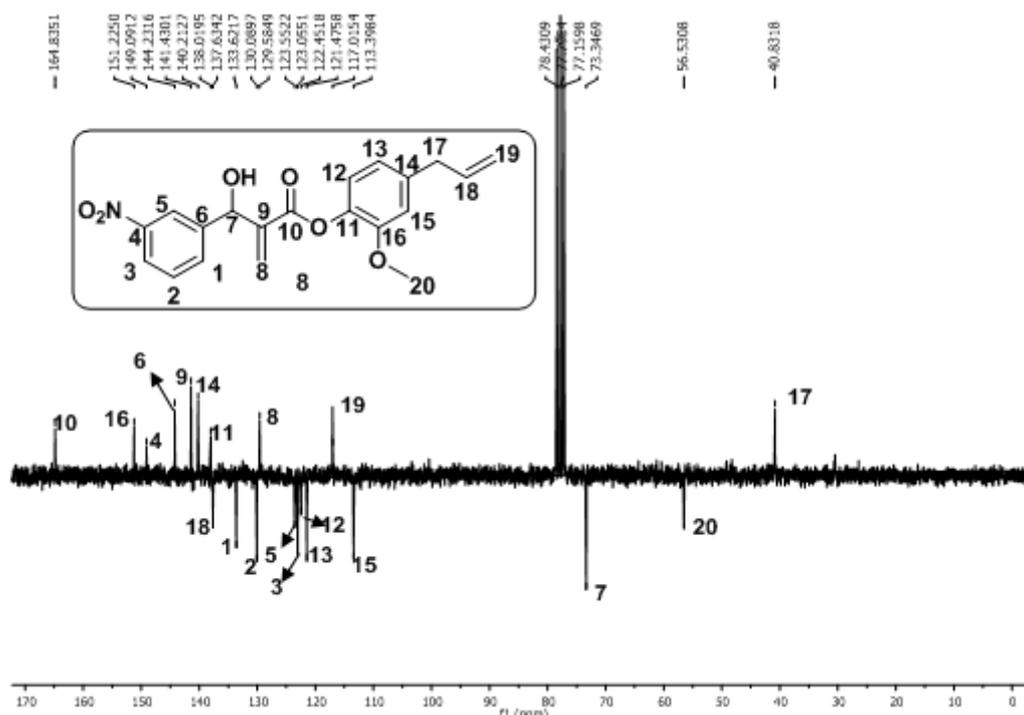
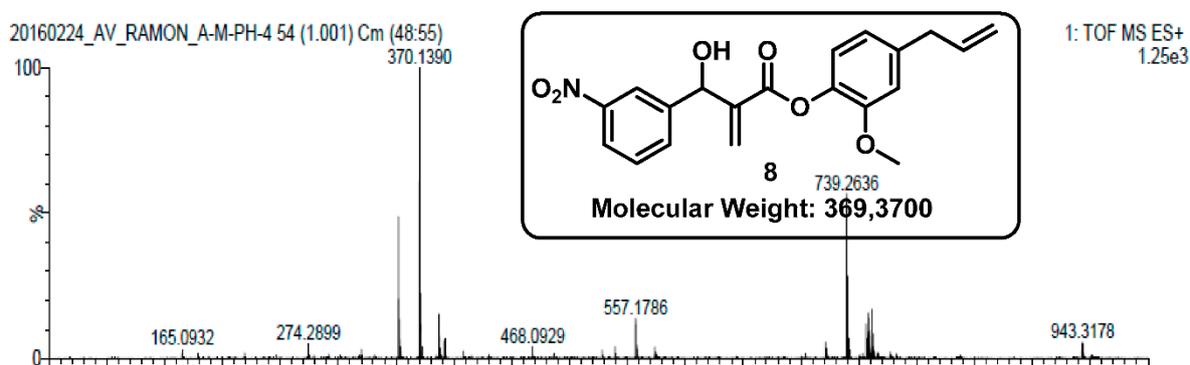


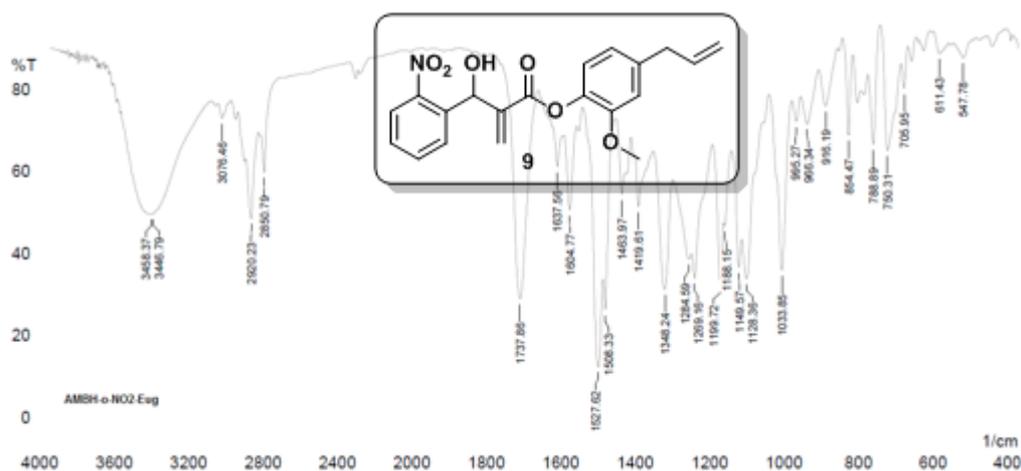
Figure S15.  $^1\text{H-NMR}$  spectrum (200 MHz,  $\text{CDCl}_3$ ) of 4-allyl-2-methoxyphenyl 2-(hydroxy(3-nitrophenyl)methyl)acrylate 8.



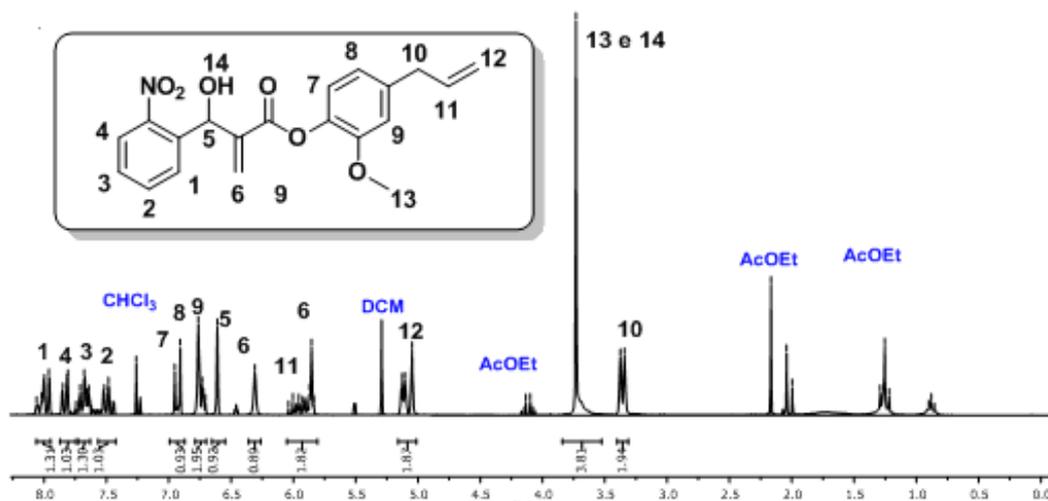
**Figure S16.**  $^{13}\text{C}$ -NMR spectrum (50 MHz,  $\text{CDCl}_3$ ) of 4-allyl-2-methoxyphenyl 2-(hydroxy(3-nitrophenyl)methyl)acrylate 8.



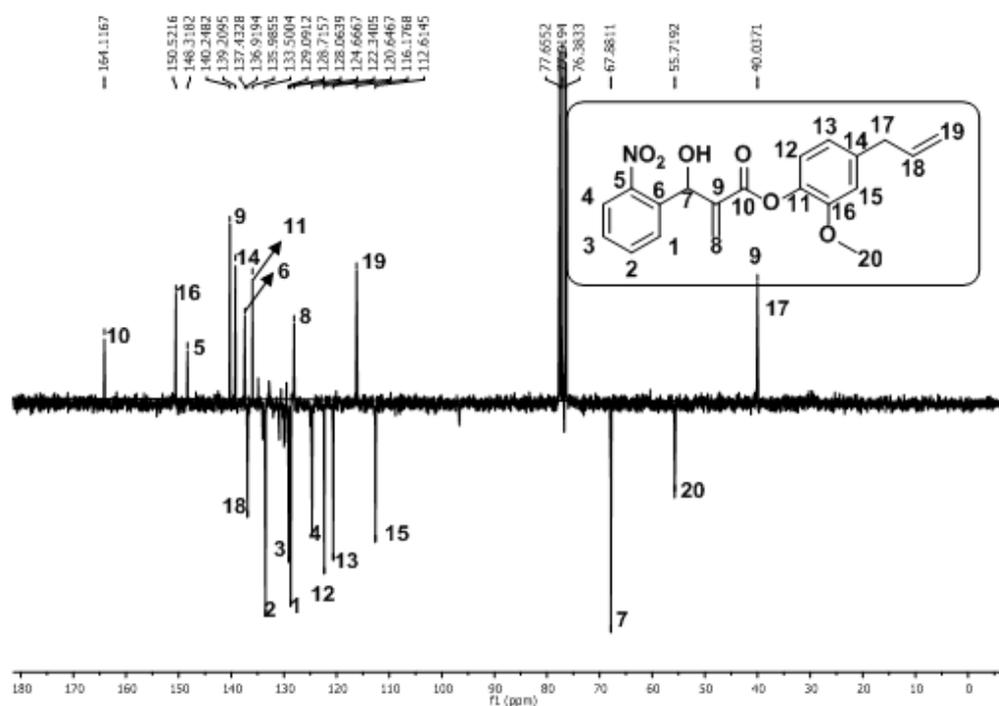
**Figure S17.** HRMS spectrum of compound 4-allyl-2-methoxyphenyl 2-(hydroxy(3-nitrophenyl)methyl)acrylate 8.



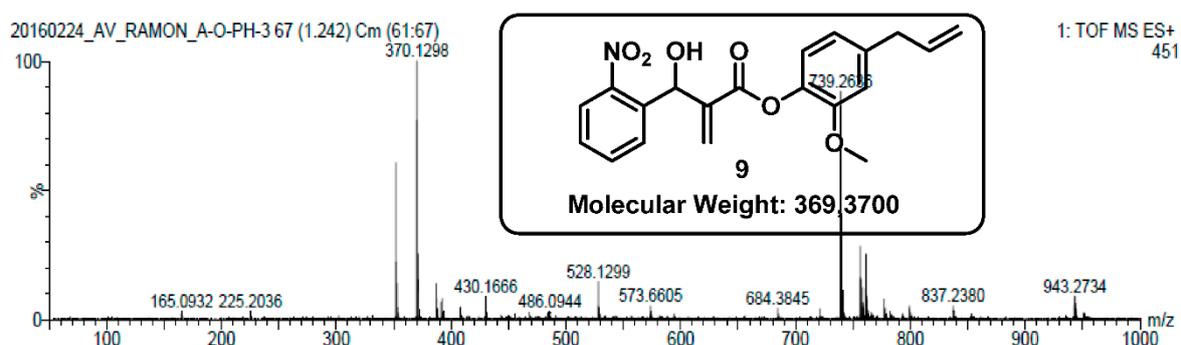
**Figure S18.** FTIR (KBr) spectrum of 4-allyl-2-methoxyphenyl 2-(hydroxy(2-nitrophenyl)methyl)acrylate 9.



**Figure S19.**  $^1\text{H-NMR}$  spectrum (200 MHz,  $\text{CDCl}_3$ ) of 4-allyl-2-methoxyphenyl 2-(hydroxy(2-nitrophenyl)methyl)acrylate 9.



**Figure S20.**  $^{13}\text{C-NMR}$  spectrum (50 MHz,  $\text{CDCl}_3$ ) 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.

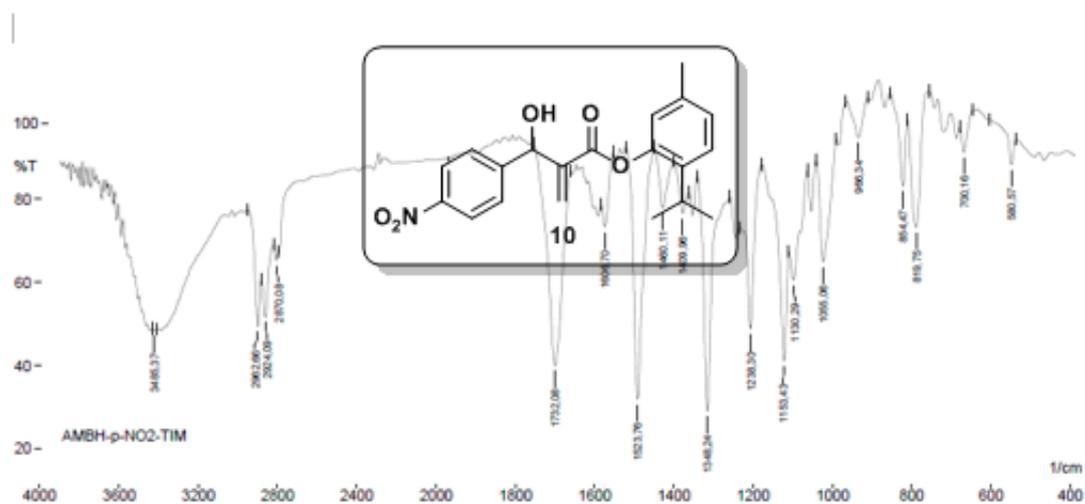


Figure S22. FTIR (KBr) spectrum of 2-isopropyl-5-methylphenyl 2-(hydroxy(4-nitrophenyl)methyl)acrylate 10.

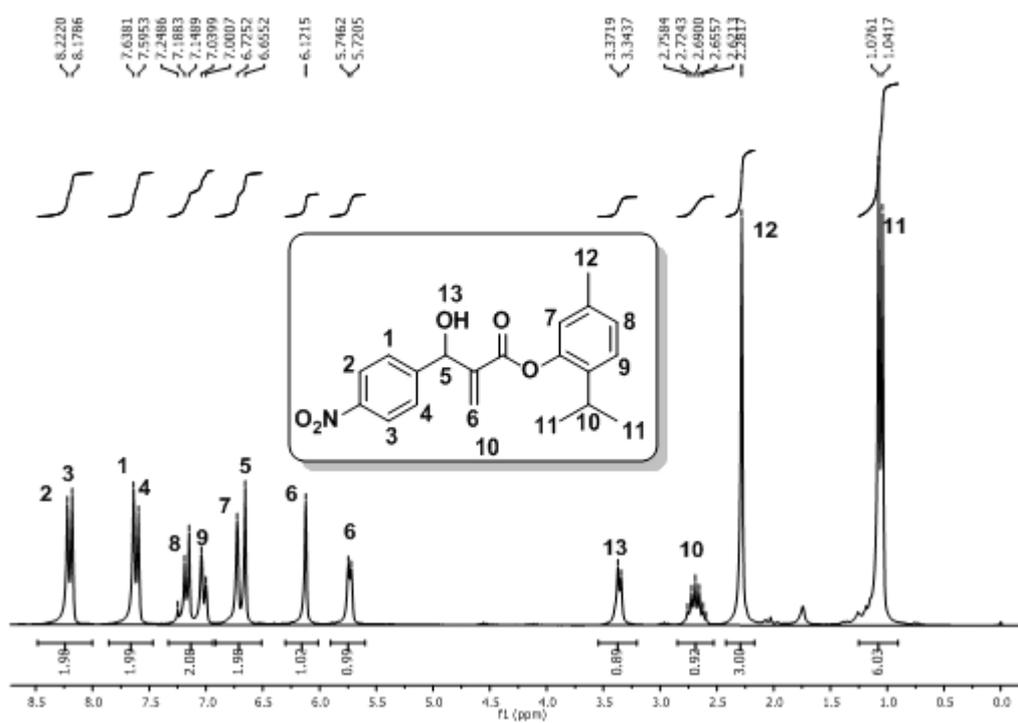
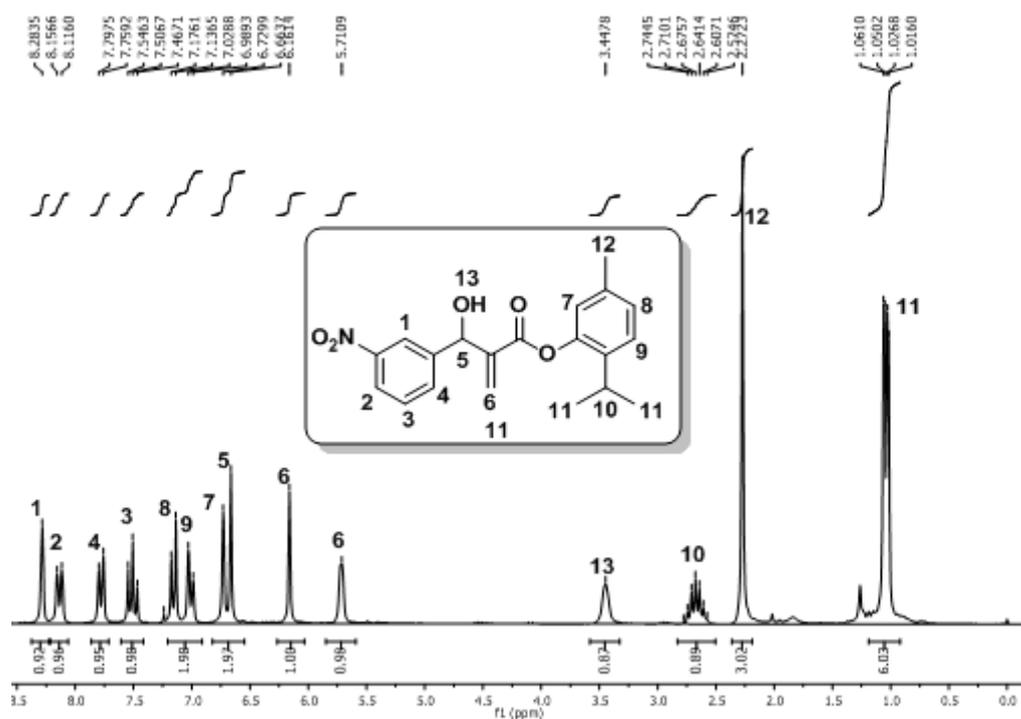
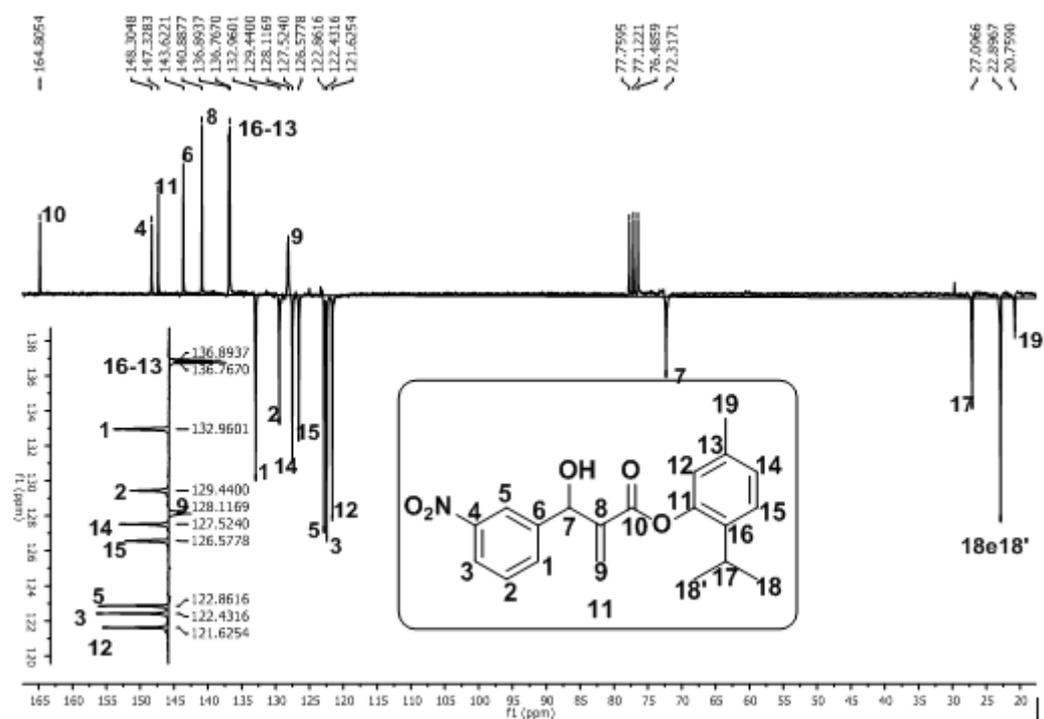


Figure S23.  $^1\text{H-NMR}$  spectrum (200 MHz,  $\text{CDCl}_3$ ) of 2-(hydroxy(4-nitrophenyl)methyl)acrylate 10.





**Figure S27.**  $^1\text{H-NMR}$  spectrum (200 MHz,  $\text{CDCl}_3$ ) of 2-(hydroxy(3-nitrophenyl)methyl)acrylate **11**.



**Figure S28.**  $^{13}\text{C-NMR}$  spectrum (50 MHz,  $\text{CDCl}_3$ ) of 2-(hydroxy(3-nitrophenyl)methyl)acrylate **11**.

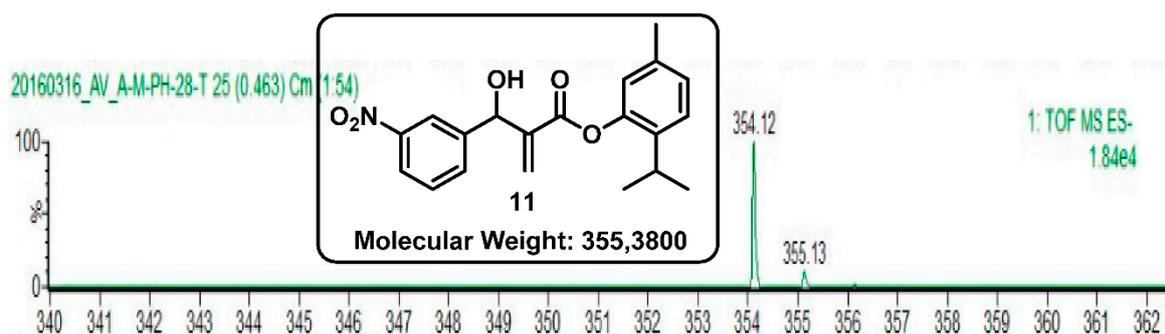


Figure S29. HRMS spectrum of compound 2-(hydroxy(3-nitrophenyl)methyl)acrylate 11.

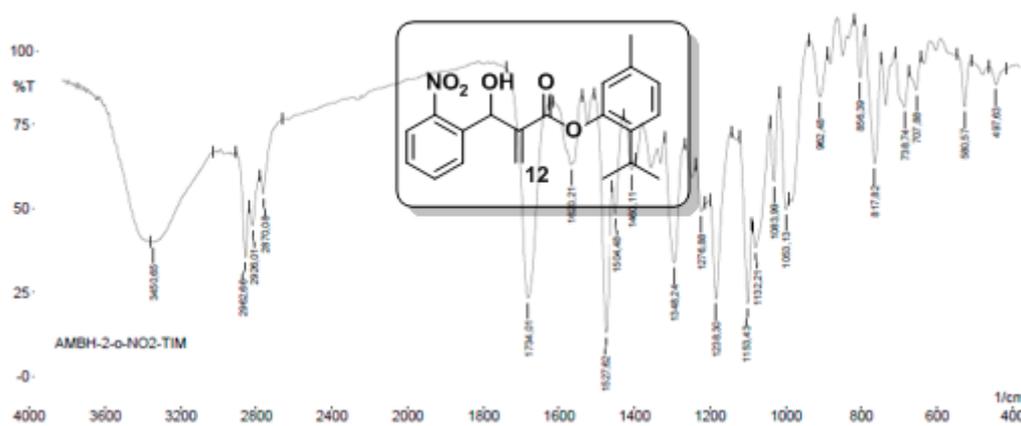


Figure S30. FTIR (KBr) spectrum of 2-isopropyl-5-methylphenyl 2-(hydroxy(2-nitrophenyl)methyl)acrylate 12.

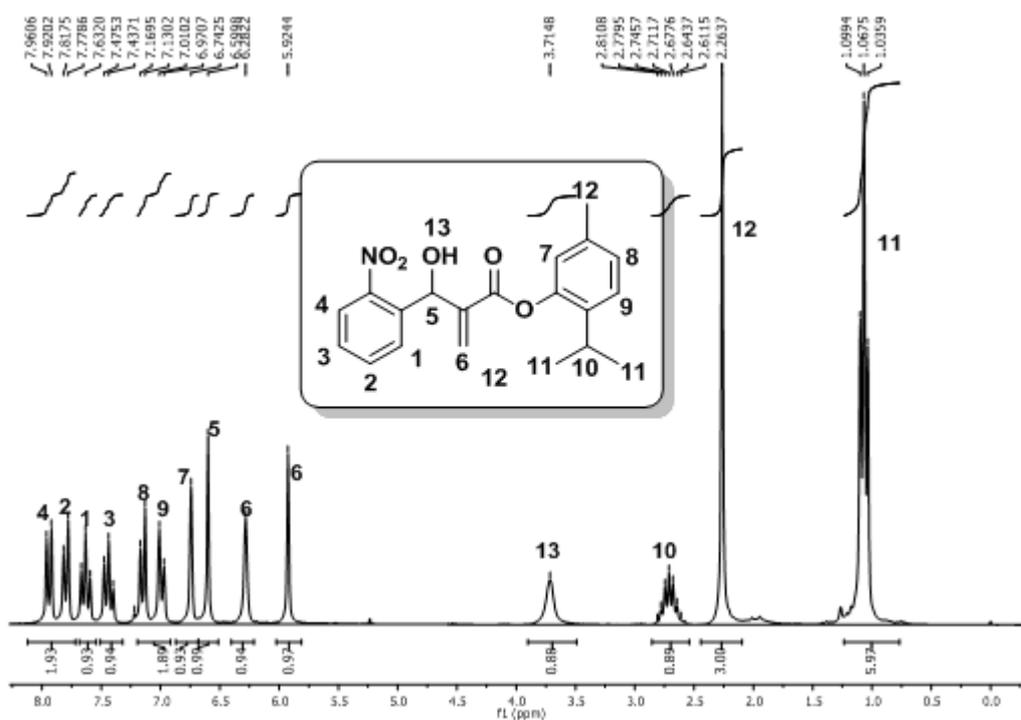


Figure S31.  $^1\text{H-NMR}$  spectrum (200 MHz,  $\text{CDCl}_3$ ) of 2-(hydroxy(2-nitrophenyl)methyl)acrylate 12.

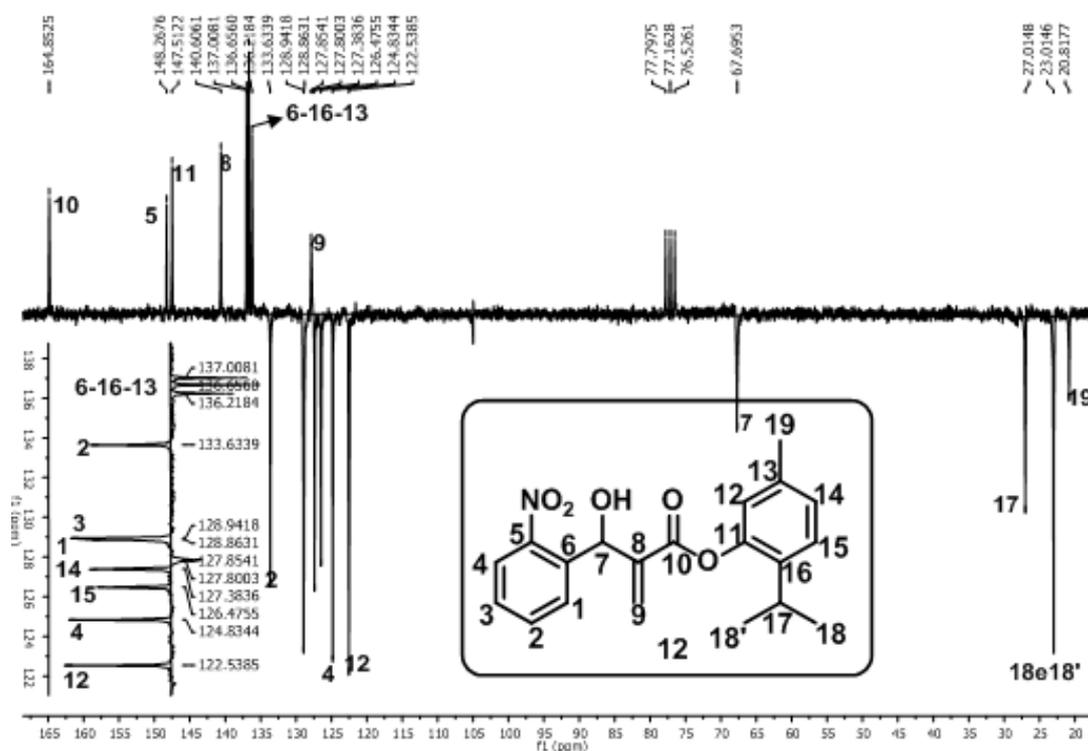


Figure S32.  $^{13}\text{C}$ -NMR spectrum (50 MHz,  $\text{CDCl}_3$ ) of 2-(hydroxy(2-nitrophenyl)methyl)acrylate **12**.

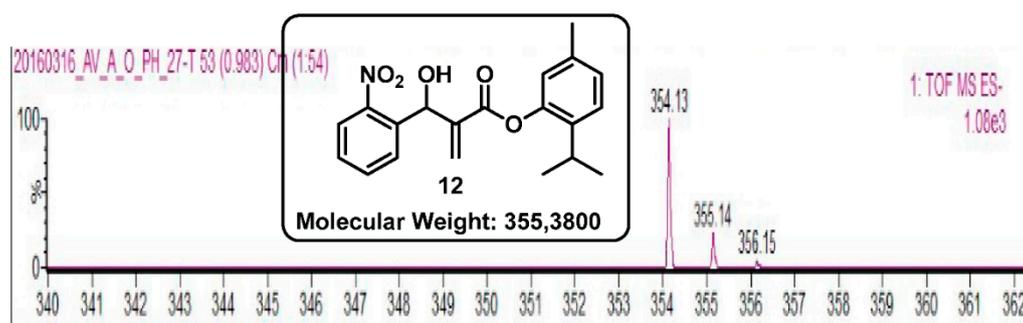


Figure S33. HRMS spectrum of compound 2-(hydroxy(2-nitrophenyl)methyl)acrylate **12**.

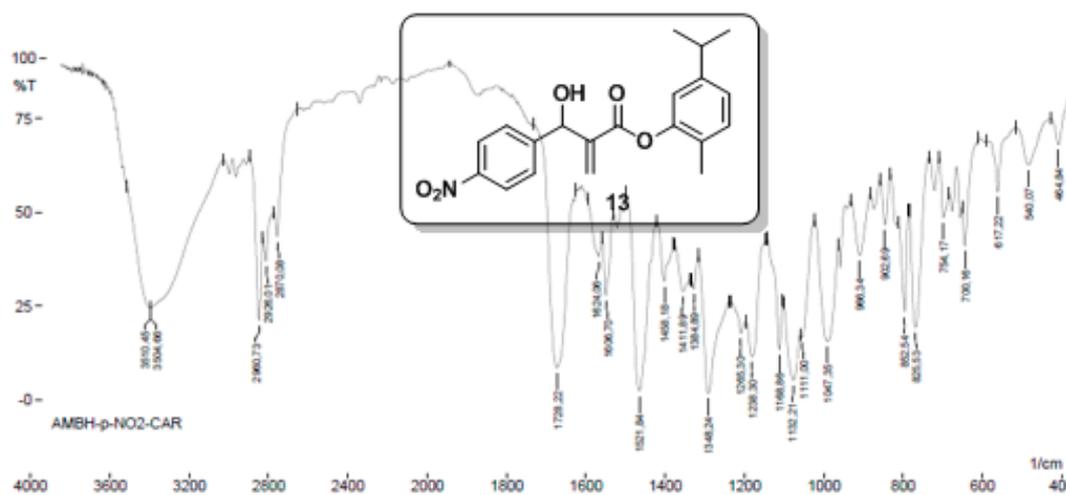
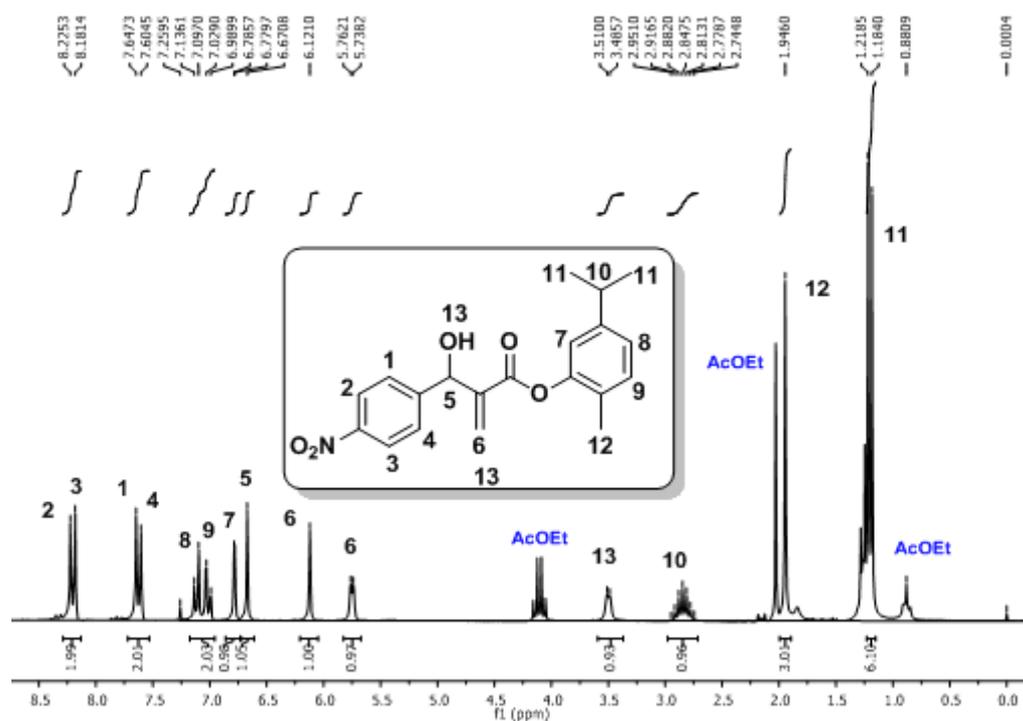
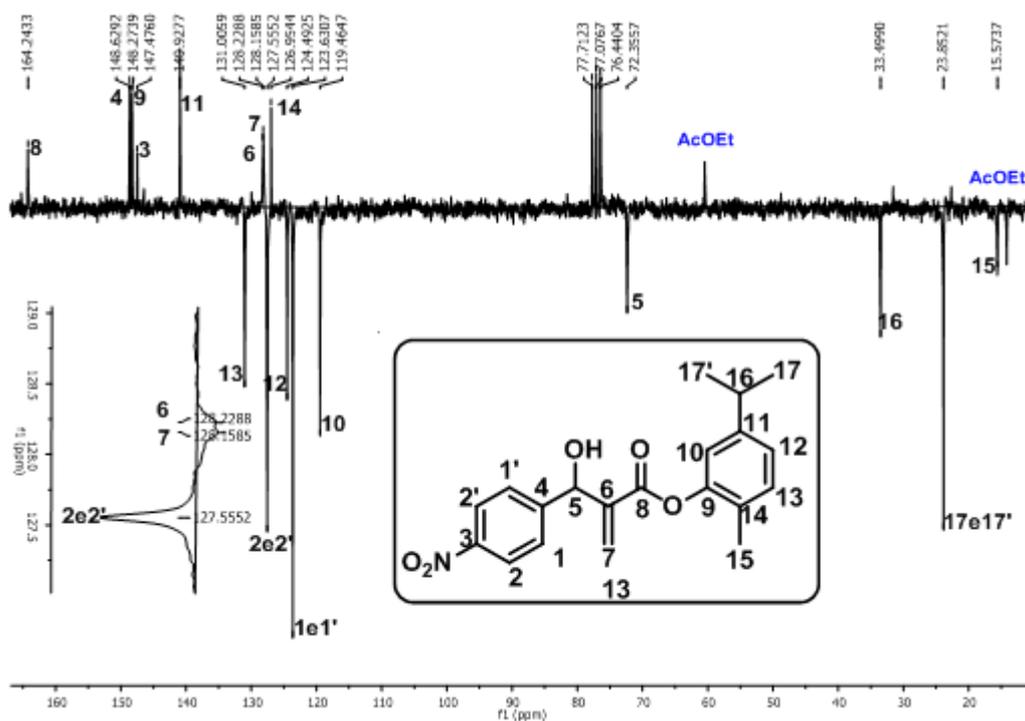


Figure S34. FTIR (KBr) spectrum of 5-isopropyl-2-methylphenyl 2-(hydroxy(4-nitrophenyl)methyl)acrylate **13**.



**Figure S35.**  $^1\text{H-NMR}$  spectrum (200 MHz,  $\text{CDCl}_3$ ) of 5-isopropyl-2-methylphenyl 2-(hydroxy(4-nitrophenyl)methyl)acrylate 13.



**Figure S36.**  $^{13}\text{C-NMR}$  spectrum (50 MHz,  $\text{CDCl}_3$ ) of 5-isopropyl-2-methylphenyl 2-(hydroxy(4-nitrophenyl)methyl)acrylate 13.

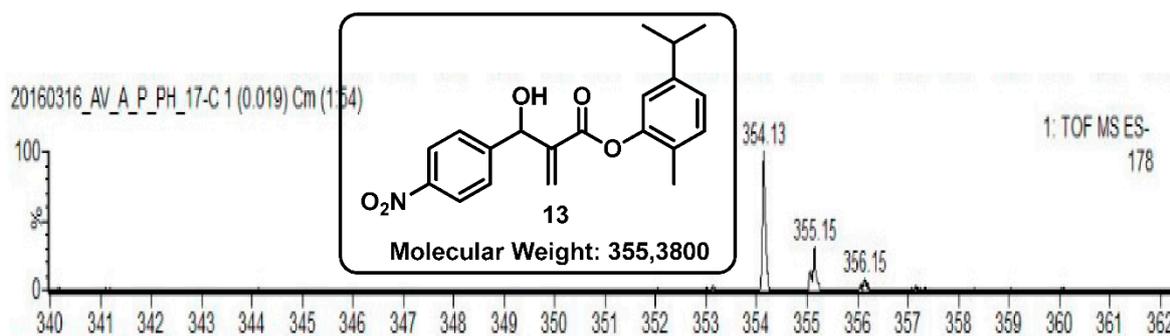


Figure S37. HRMS spectrum of of 5-isopropyl-2-methylphenyl 2-(hydroxy(4-nitrophenyl)methyl)acrylate 13.

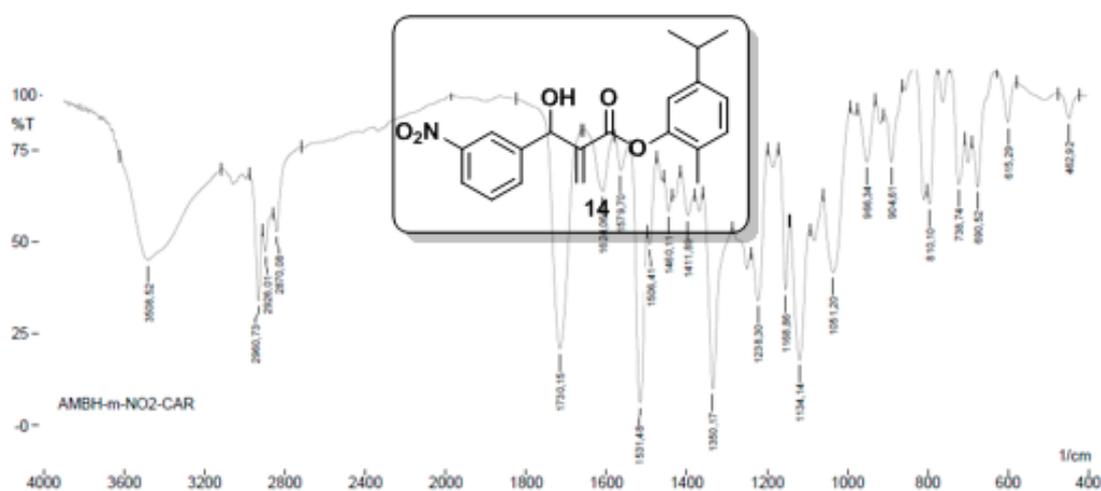


Figure S38. FTIR (KBr) spectrum of 5-isopropyl-2-methylphenyl 2-(hydroxy(3-nitrophenyl)methyl)acrylate 14.

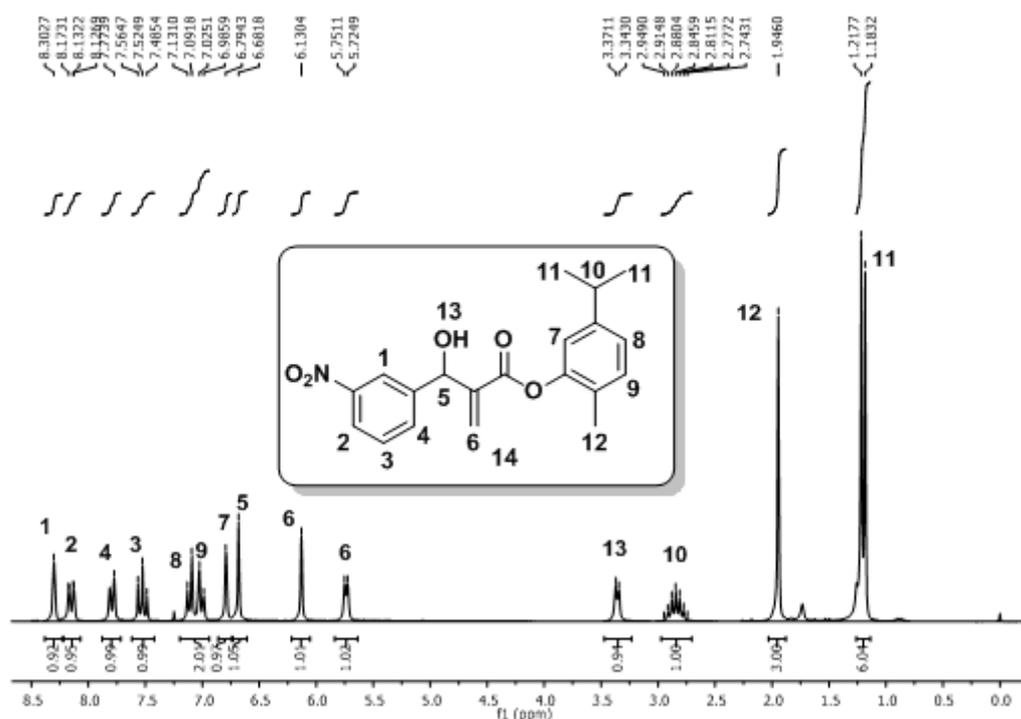
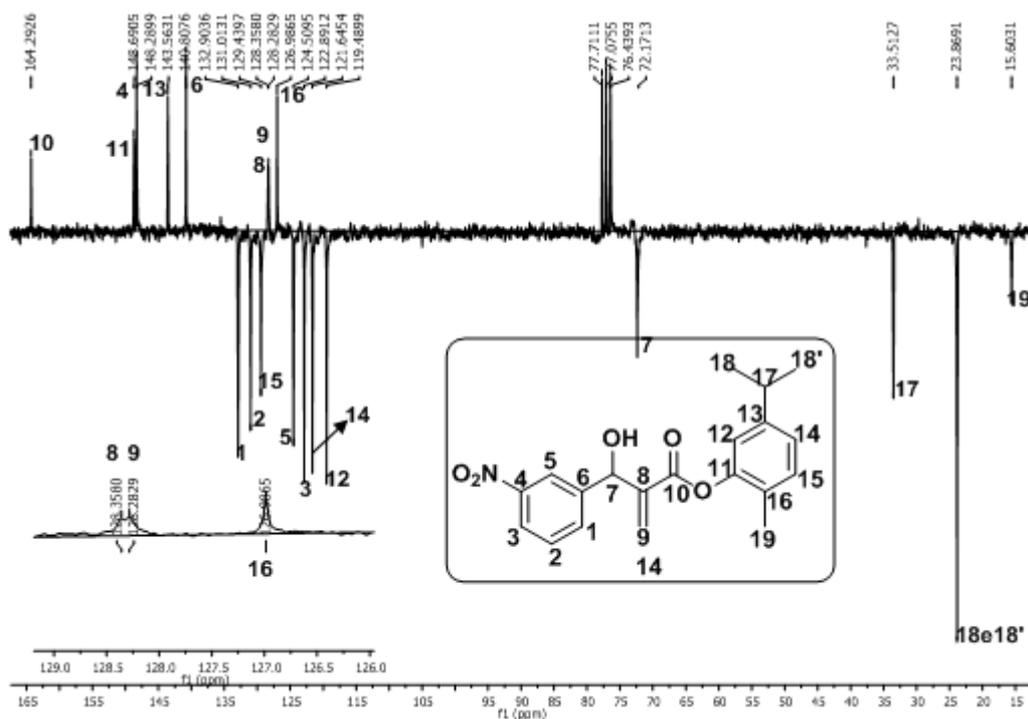
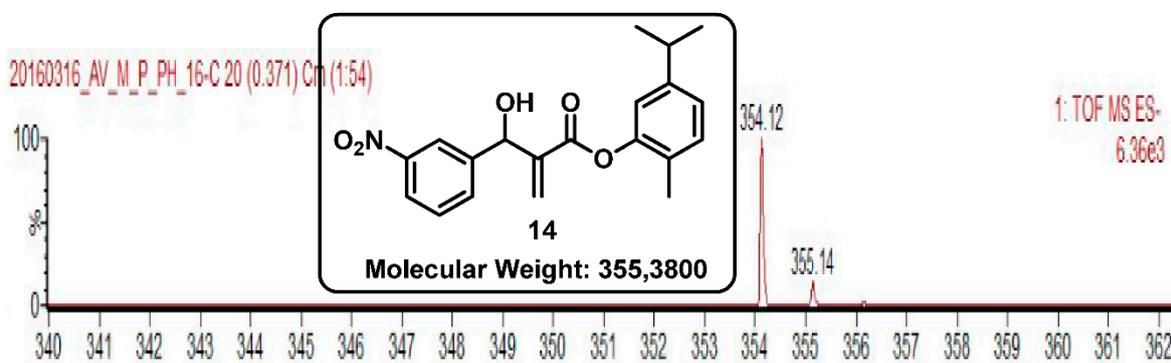


Figure S39.  $^1\text{H-NMR}$  spectrum (200 MHz,  $\text{CDCl}_3$ ) of 5-isopropyl-2-methylphenyl 2-(hydroxy(3-nitrophenyl)methyl)acrylate 14.



**Figure S40.**  $^{13}\text{C}$ -NMR spectrum (50 MHz,  $\text{CDCl}_3$ ) 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.

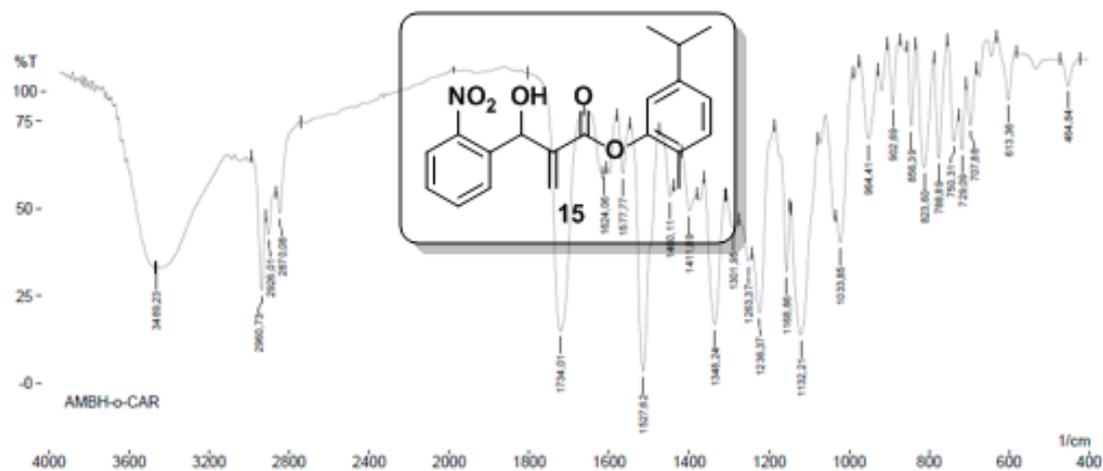


Figure S42. FTIR (KBr) spectrum of 5-isopropyl-2-methylphenyl 2-(hydroxy(2-nitrophenyl)methyl)acrylate 15.

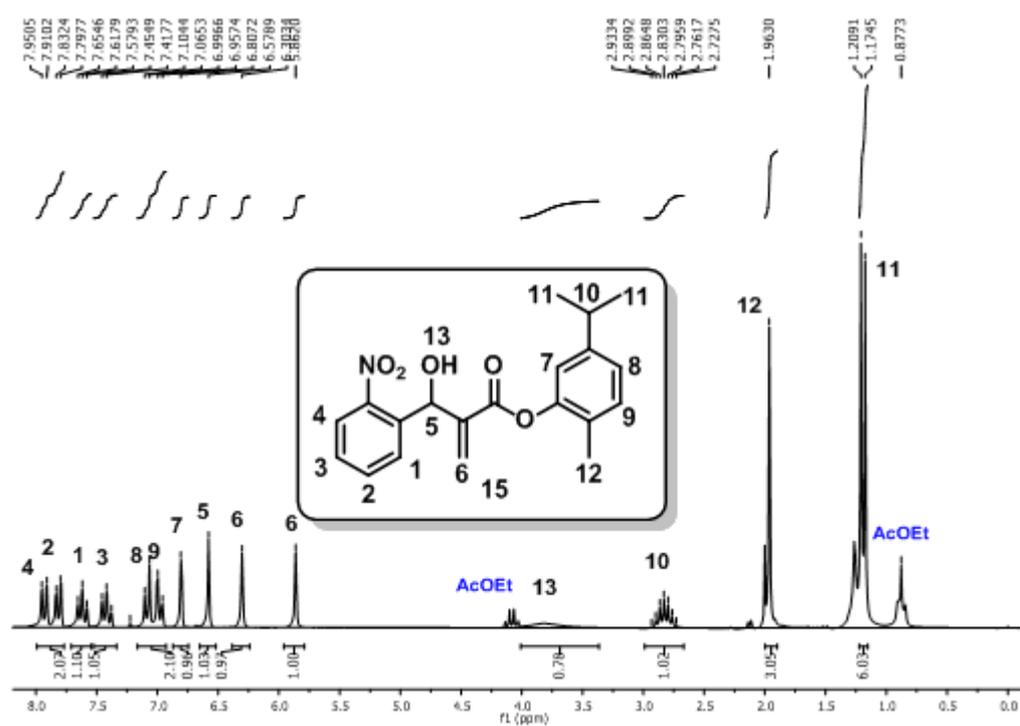
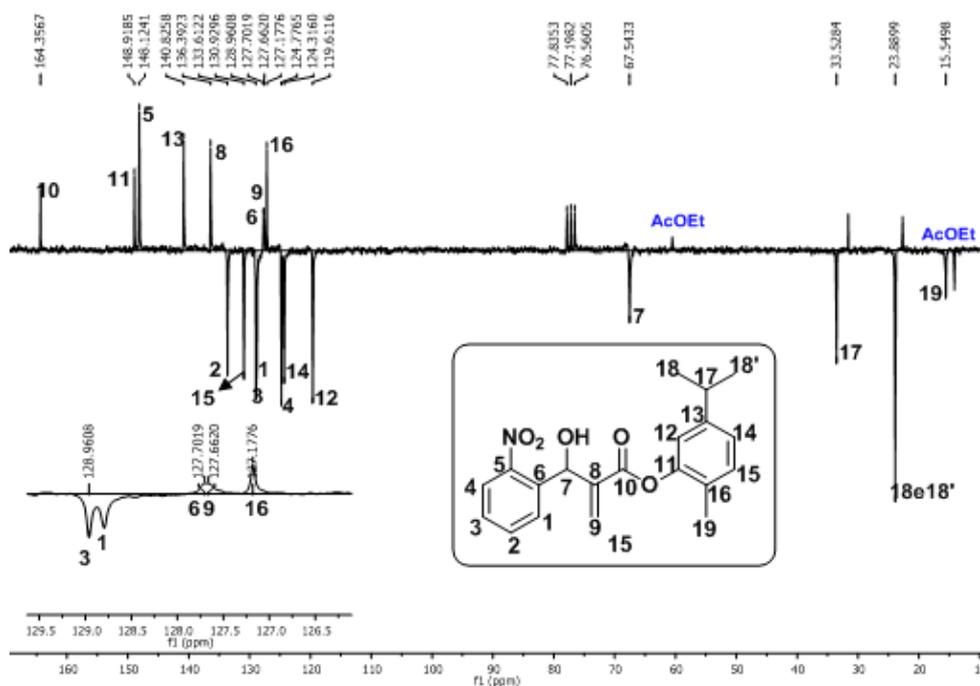
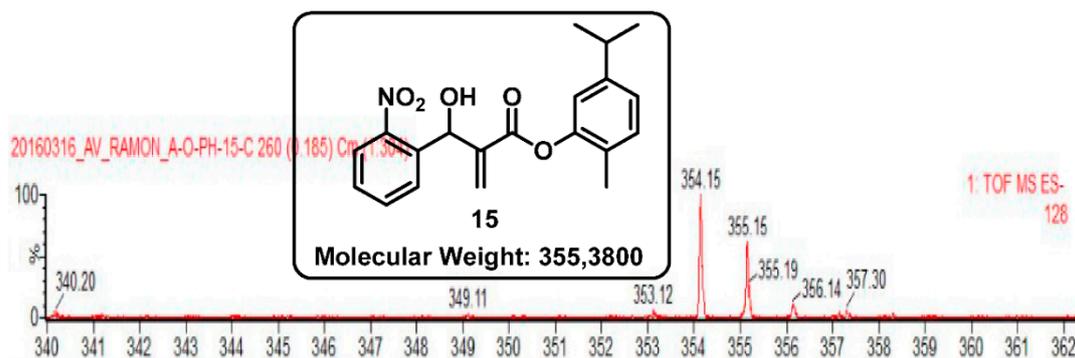


Figure S43.  $^1\text{H-NMR}$  spectrum (200 MHz,  $\text{CDCl}_3$ ) of 5-isopropyl-2-methylphenyl 2-(hydroxy(2-nitrophenyl)methyl)acrylate 15.



**Figure S44.**  $^{13}\text{C}$ -NMR spectrum (50 MHz,  $\text{CDCl}_3$ ) 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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**m062x\_water\_ortho (9)**

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0.6169 3.0861 -2.0749 H 0 0 0 0 0 0 0 0 0 0 0 0  
3.7799 2.1551 -0.1635 O 0 0 0 0 0 0 0 0 0 0 0 0  
4.4657 1.9319 0.4901 H 0 0 0 0 0 0 0 0 0 0 0 0

```
0.2794 0.9296 -0.4802 C 0 0 0 0 0 0 0 0 0 0 0 0
0.1940 0.0754 0.3787 O 0 0 0 0 0 0 0 0 0 0 0 0
4.1545 -0.6609 1.8523 N 0 0 0 0 0 0 0 0 0 0 0 0
4.1674 -1.5051 2.7332 O 0 0 0 0 0 0 0 0 0 0 0 0
4.4707 0.5081 2.0391 O 0 0 0 0 0 0 0 0 0 0 0 0
-1.9608 0.5988 -1.0667 C 0 0 0 0 0 0 0 0 0 0 0 0
-2.3984 -0.3817 -1.9330 C 0 0 0 0 0 0 0 0 0 0 0 0
-2.7336 1.0071 0.0305 C 0 0 0 0 0 0 0 0 0 0 0 0
-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
-2.1954 1.9839 0.8071 O 0 0 0 0 0 0 0 0 0 0 0 0
-2.9713 2.4384 1.9139 C 0 0 0 0 0 0 0 0 0 0 0 0
-3.1479 1.6236 2.6229 H 0 0 0 0 0 0 0 0 0 0 0 0
-2.3782 3.2194 2.3885 H 0 0 0 0 0 0 0 0 0 0 0 0
-3.9248 2.8527 1.5715 H 0 0 0 0 0 0 0 0 0 0 0 0
1 2 4 0 0 0 0
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1 7 1 0 0 0 0
2 3 4 0 0 0 0
2 8 1 0 0 0 0
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
6 10 1 0 0 0 0
11 12 1 0 0 0 0
11 13 1 0 0 0 0
11 17 1 0 0 0 0
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
```

24 25 2 0 0 0 0  
24 26 4 0 0 0 0  
24 33 1 0 0 0 0  
25 27 4 0 0 0 0  
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27 30 4 0 0 0 0  
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37 38 1 0 0 0 0  
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39 41 1 0 0 0 0  
42 43 1 0 0 0 0  
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43 45 1 0 0 0 0  
43 46 1 0 0 0 0