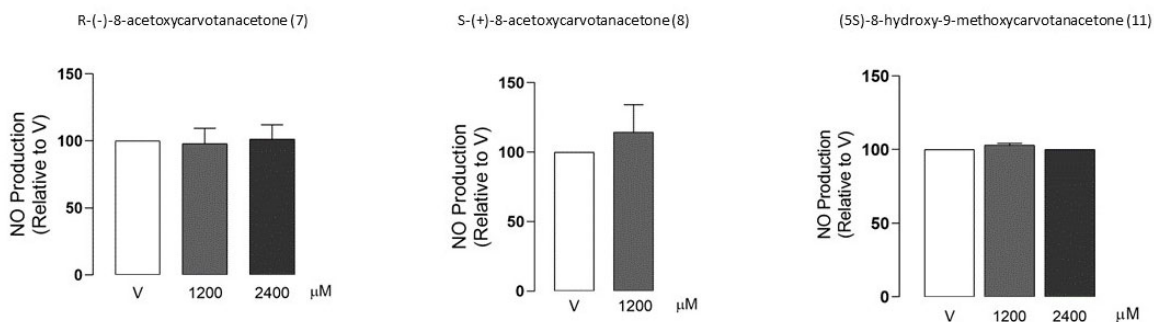


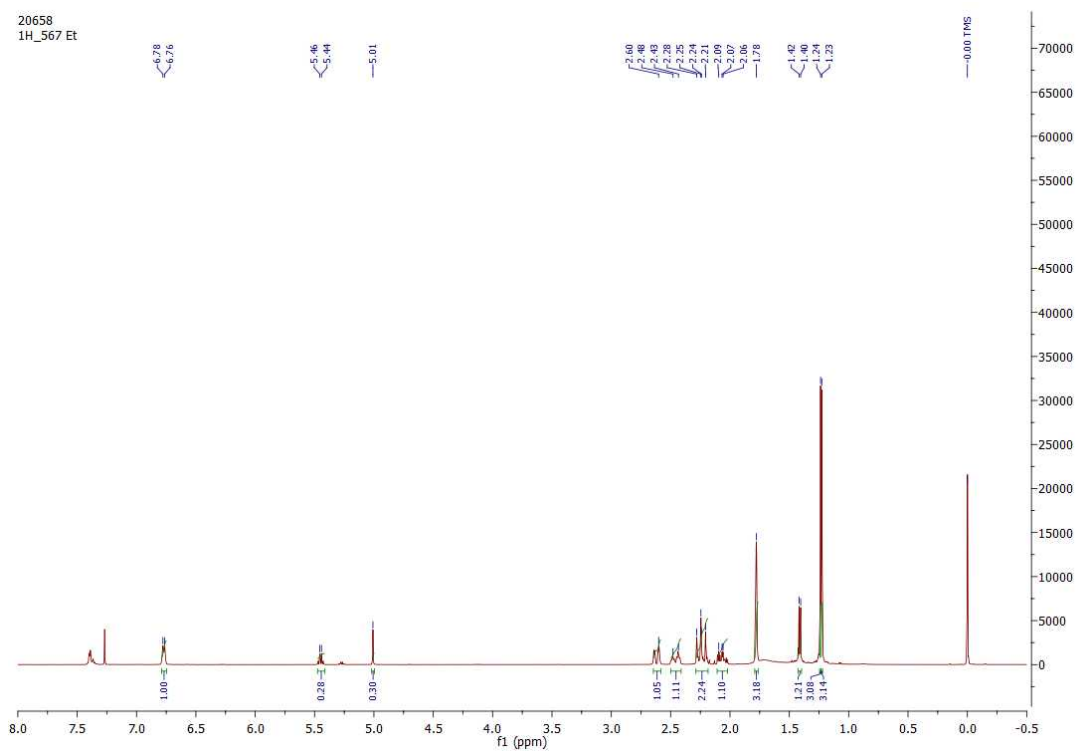
Supplementary Materials to “Synthesis of Carvone Derivatives and *In Silico*  
and *In Vitro* Screening of Anti-Inflammatory Activity in Murine  
Macrophages” by Gabriela Moço, Cátia Sousa, Ana Capitão, Stephen Scott  
MacKinnon, Alcino Leitão and Alexandrina Ferreira Mendes

*NO Production*

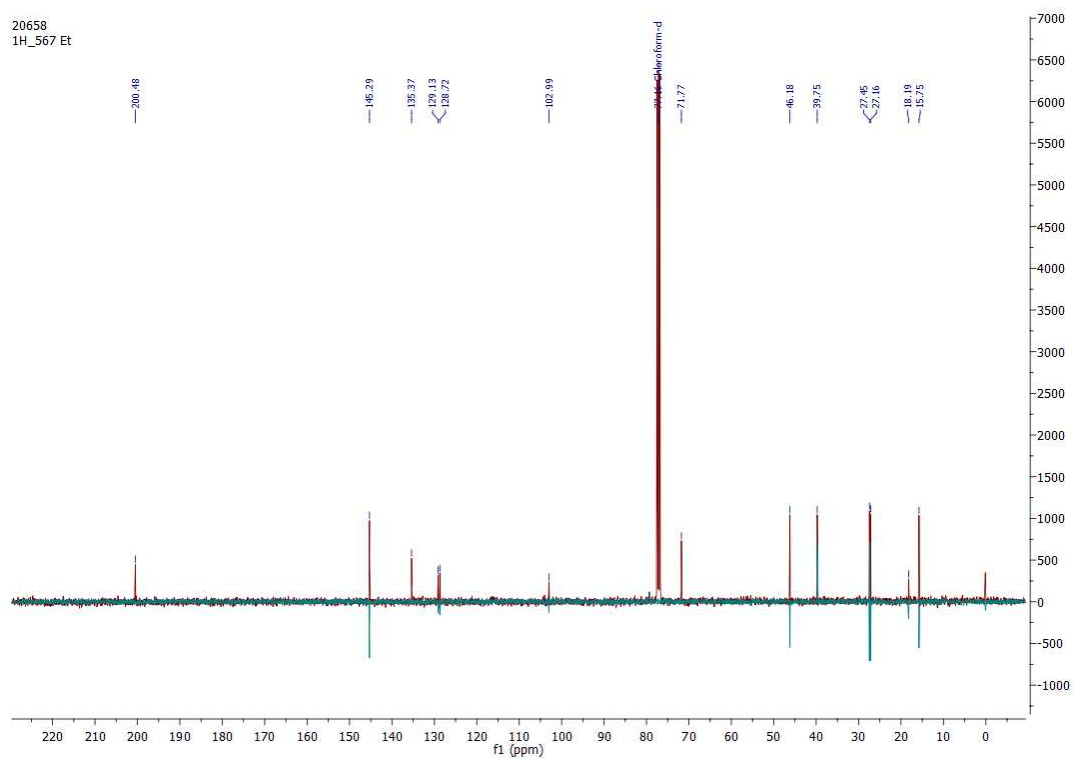


**Figure S1.** Effect of the test compounds on NO production. Raw 264.7 cells were treated with 1200 or 2400  $\mu$ M of the test compounds for 18 h in the absence of LPS; control cells (V) were treated with the vehicle alone (0,1% DMSO) for 18 h. Each column represents the mean  $\pm$  SEM of three independent experiments.

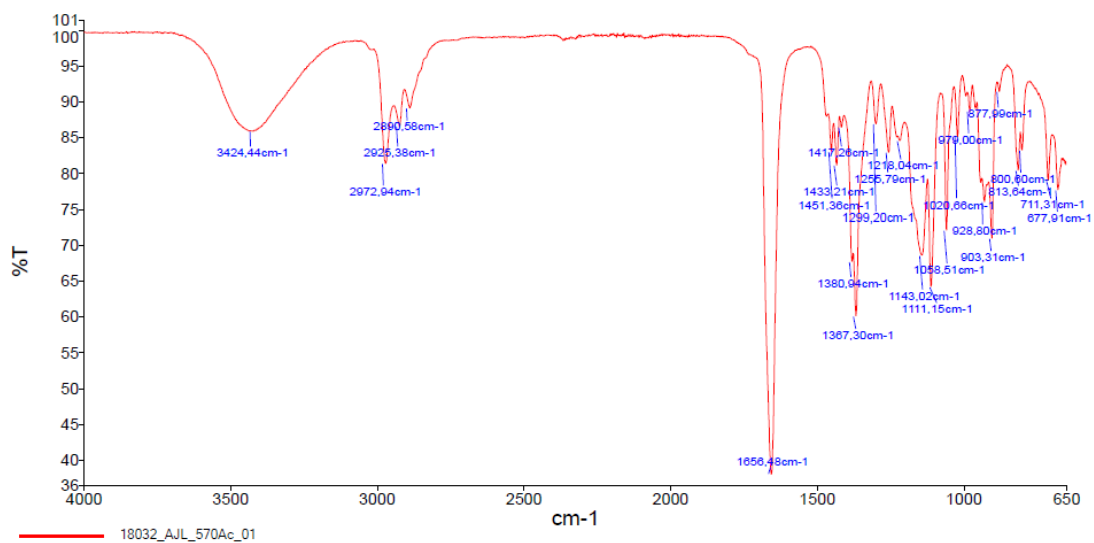
*NMR ( $^1$ H and  $^{13}$ C) and FT-IR Spectroscopy*



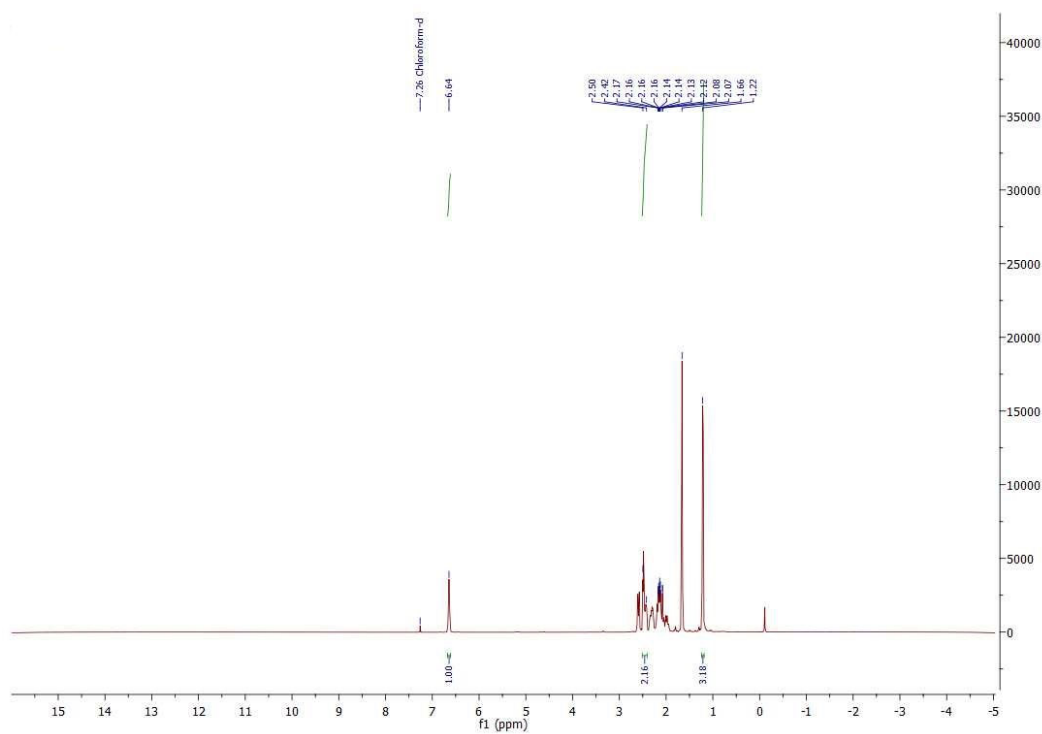
**Figure S2.**  $^1\text{H}$  NMR spectrum of **3**.



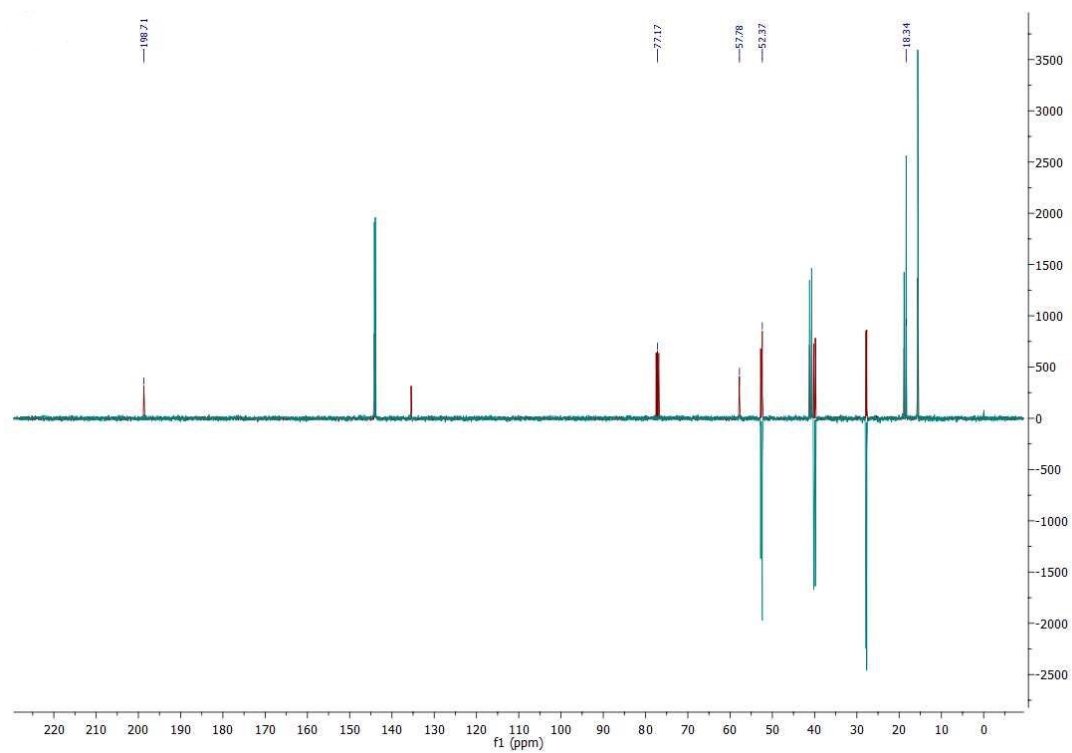
**Figure S3.**  $^{13}\text{C}$  NMR and DEPT-135 spectra of **3**.



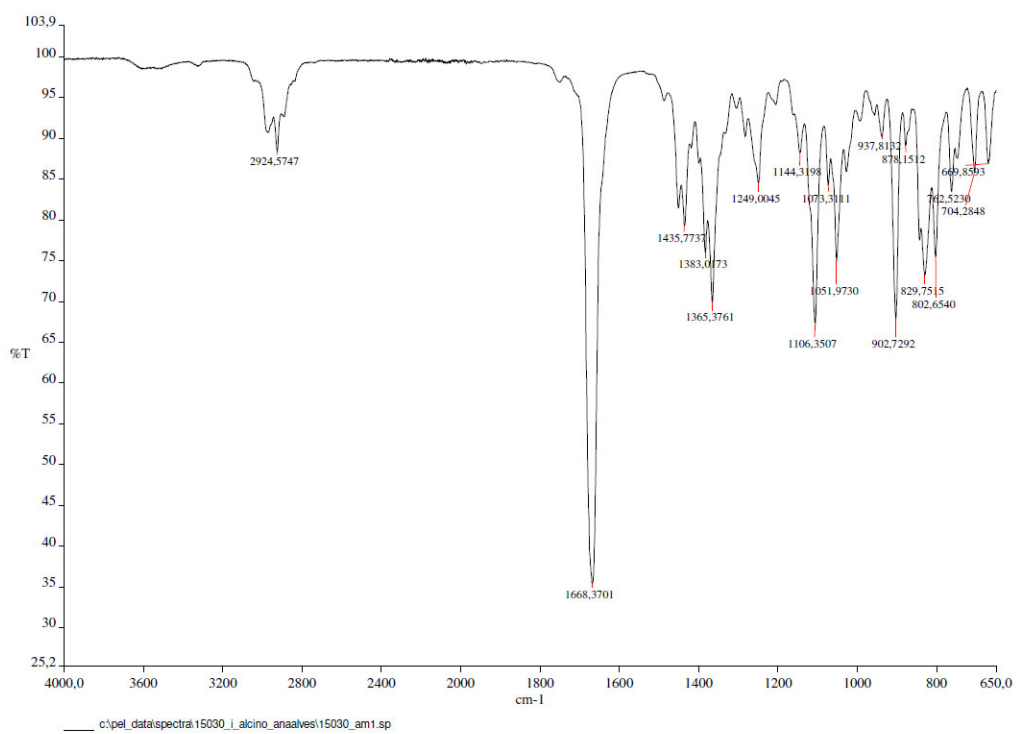
**Figure S4.** FT-IR spectrum of **3**.



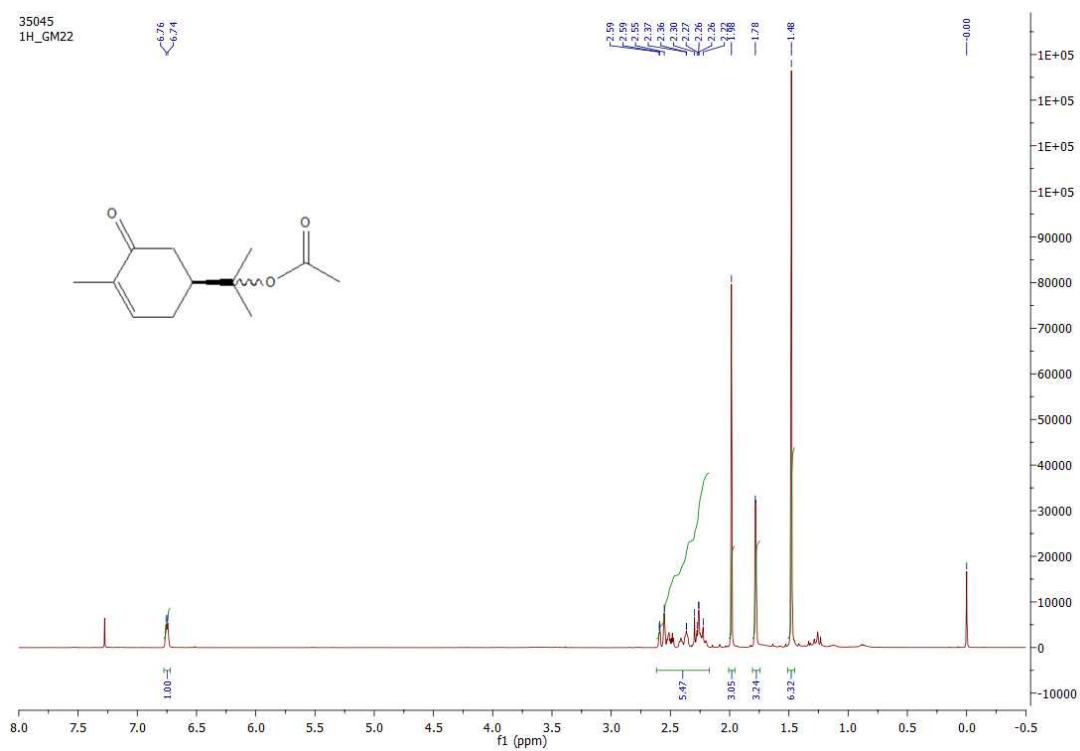
**Figure S5.**  $^1\text{H}$  NMR spectrum of **5**.



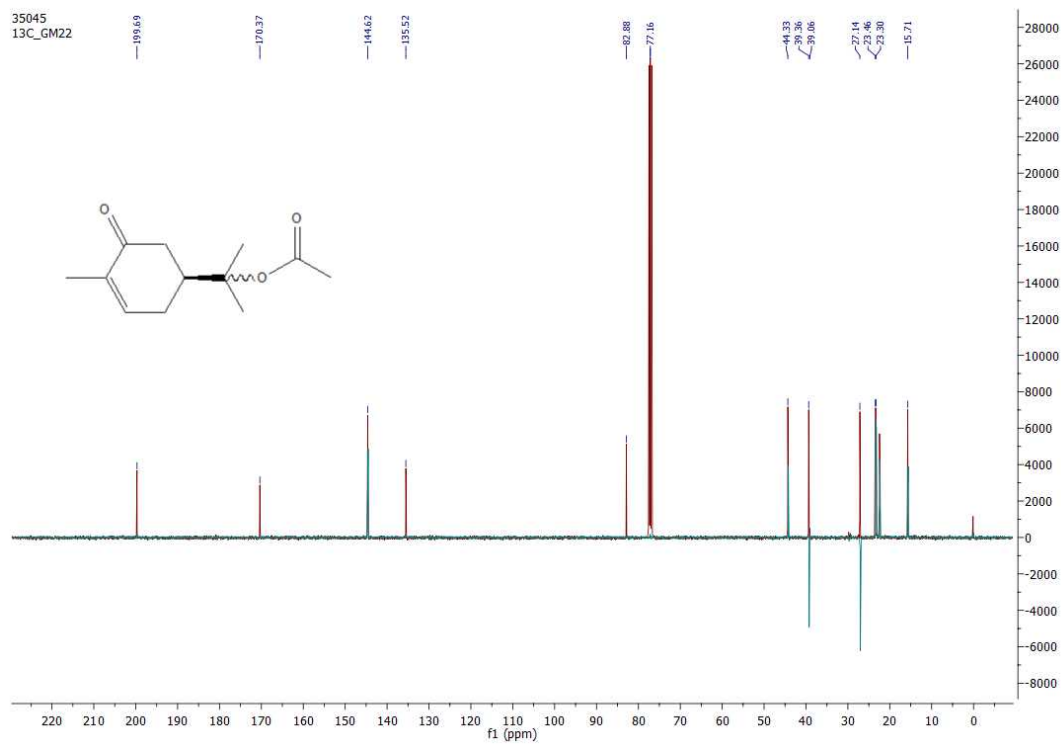
**Figure S6.**  $^{13}\text{C}$  NMR and DEPT-135 spectra of 5.



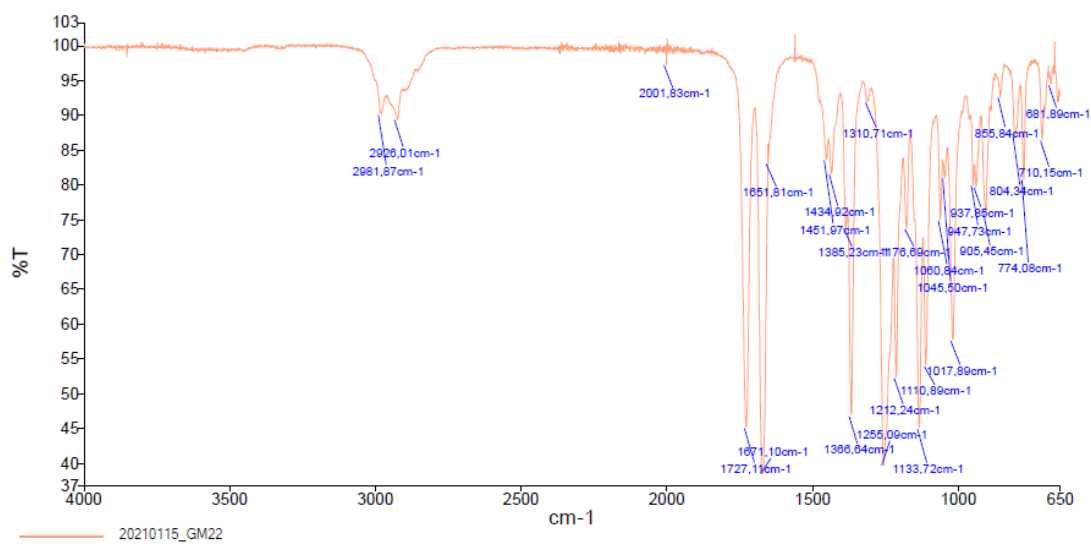
**Figure S7.** FT-IR spectrum of 5.



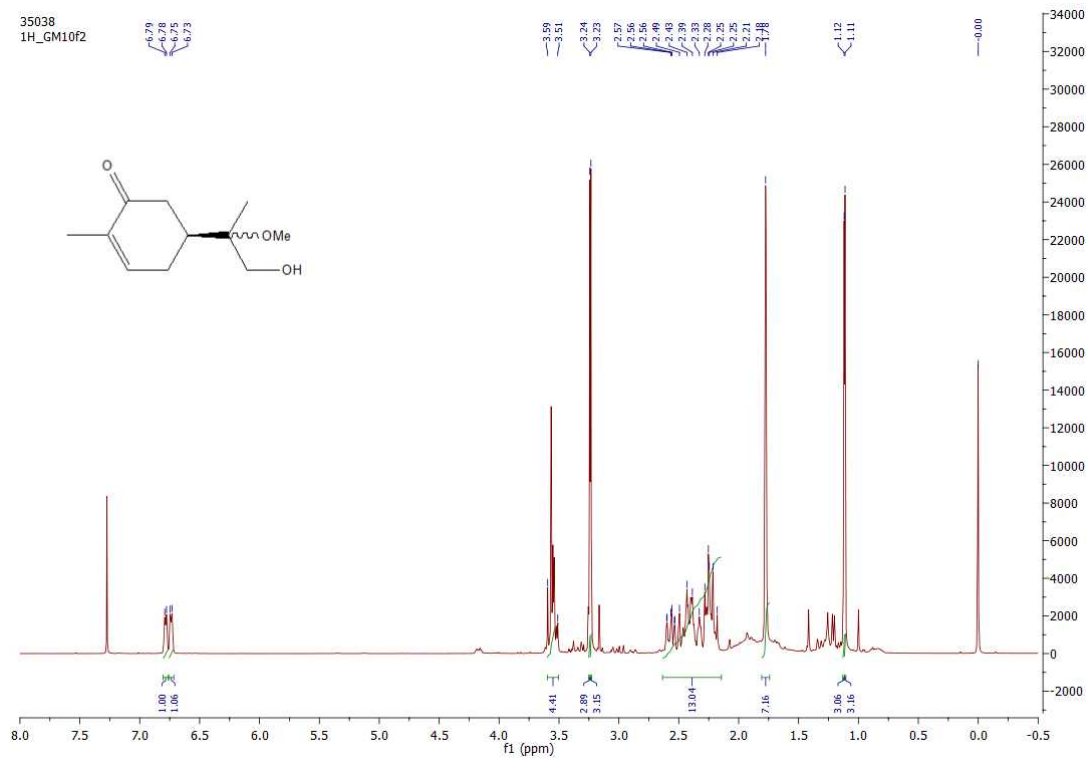
**Figure S8.**  $^1\text{H}$  NMR spectrum of **8**.



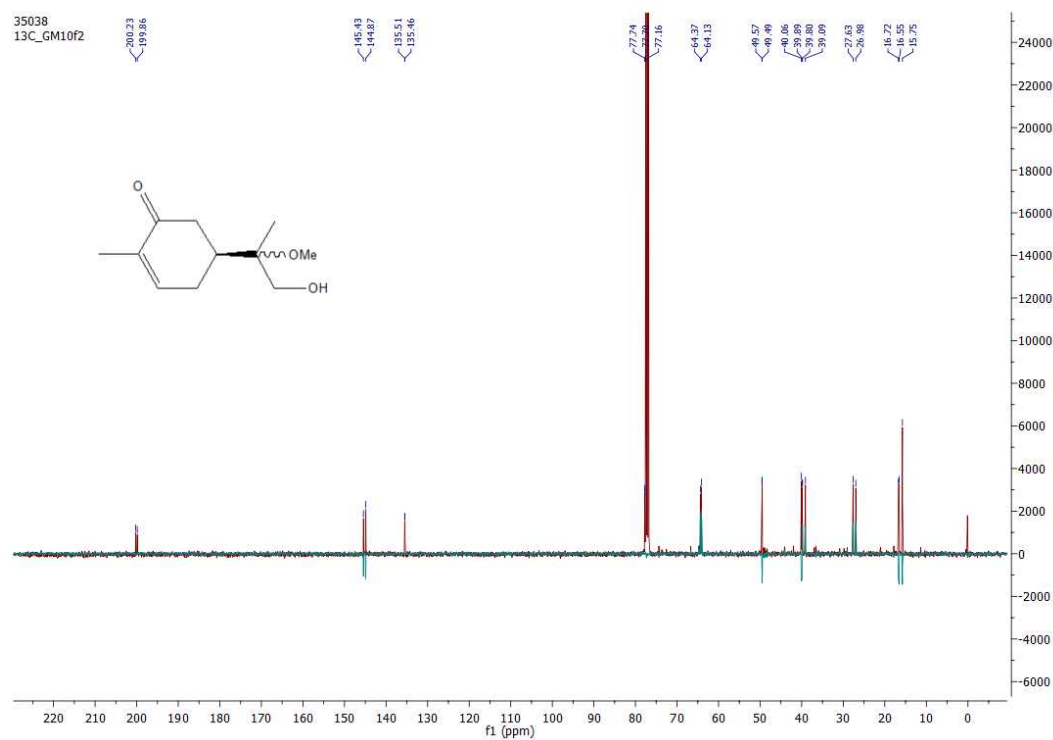
**Figure S9.**  $^{13}\text{C}$  NMR and DEPT-135 spectra of **8**.



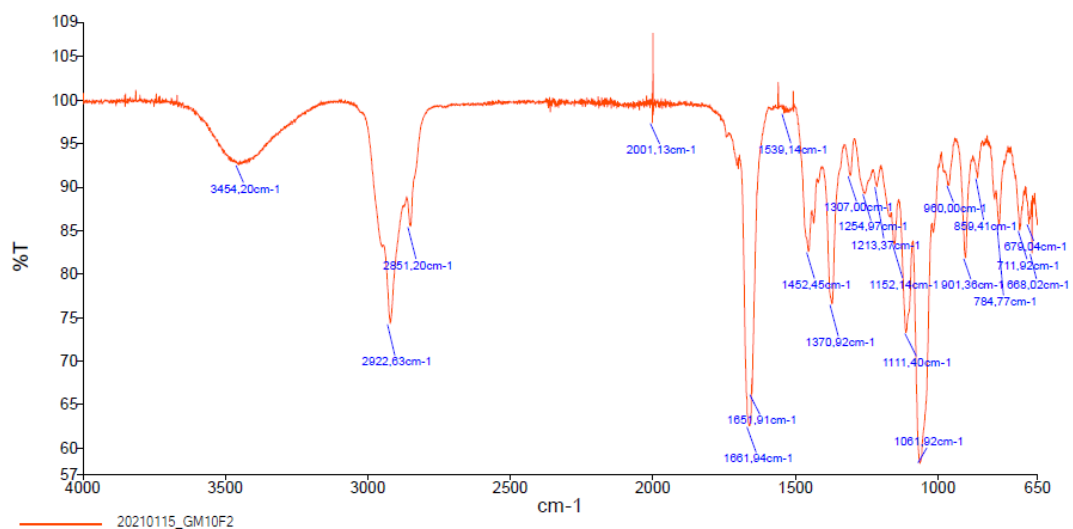
**Figure S10.** FT-IR spectrum of **8**.



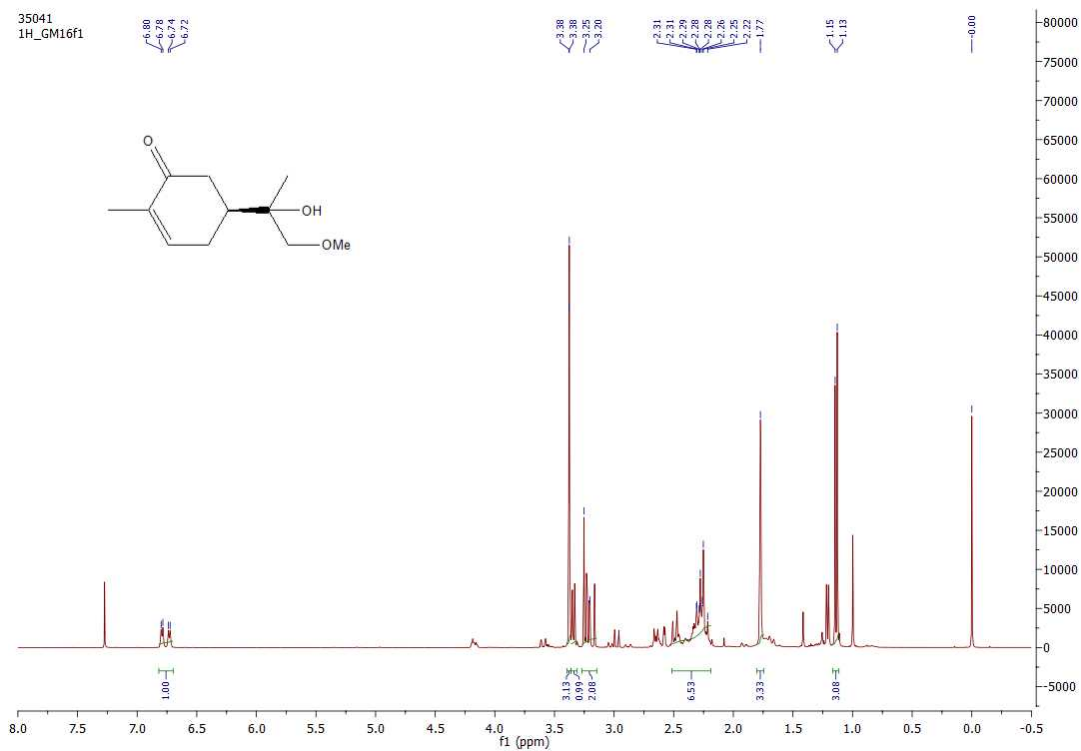
**Figure S11.**  $^1\text{H}$  NMR spectrum of 10.



**Figure S12.**  $^{13}\text{C}$  NMR and DEPT-135 spectra of 10.

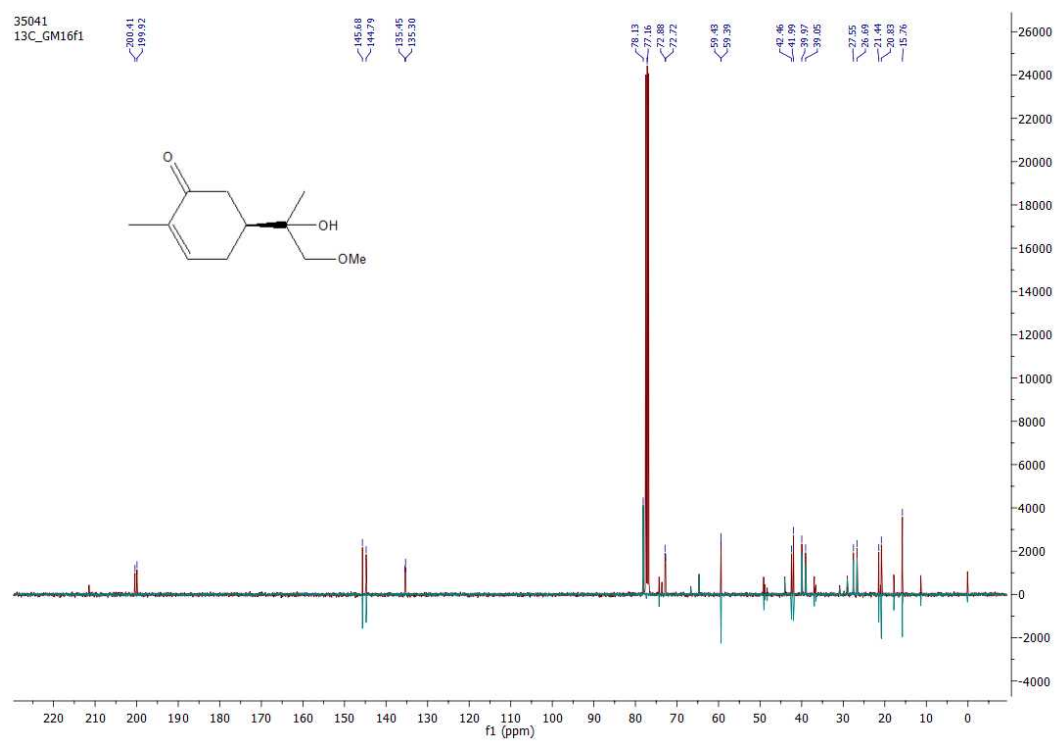


**Figure S13.** FT-IR spectrum of 10.

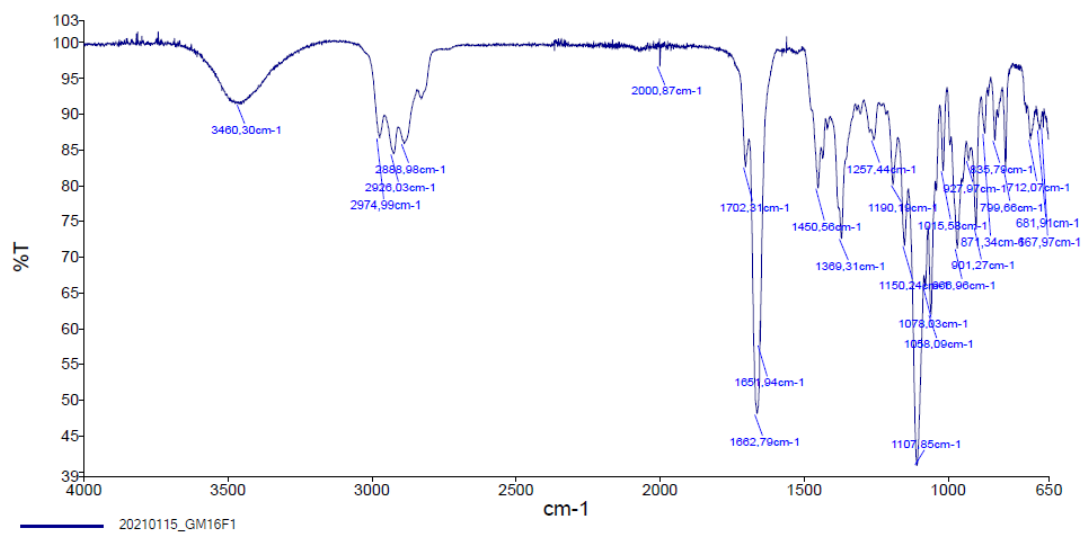


**Figure S14.** <sup>1</sup>H NMR spectrum of 11.





**Figure S15.**  $^{13}\text{C}$  NMR and DEPT-135 spectra of **11**.



**Figure S16.** FT-IR spectrum of **11**.

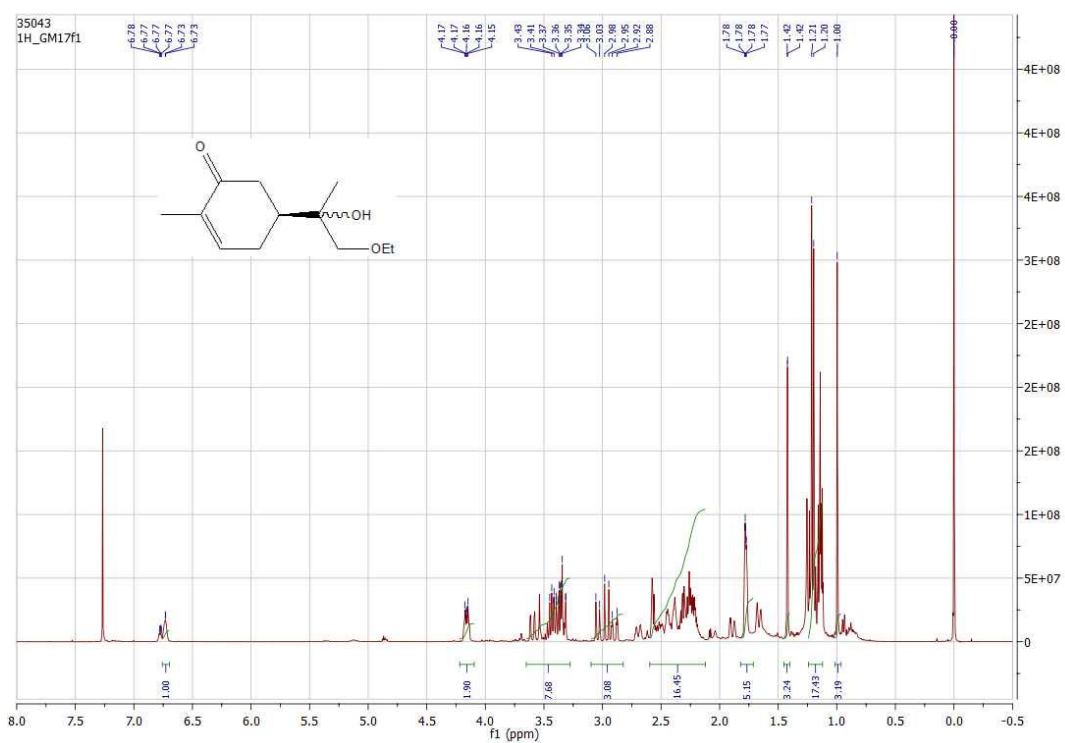


Figure S17.  $^1\text{H}$  NMR spectrum of 15.

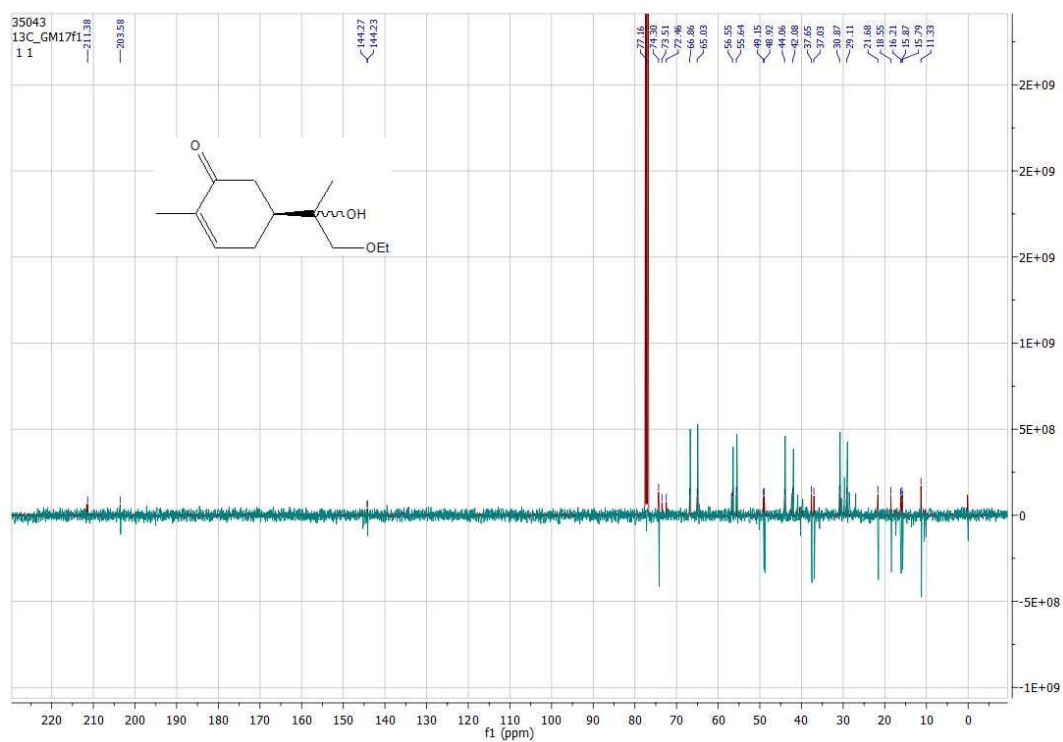


Figure S18.  $^{13}\text{C}$  NMR and DEPT spectra of 15.

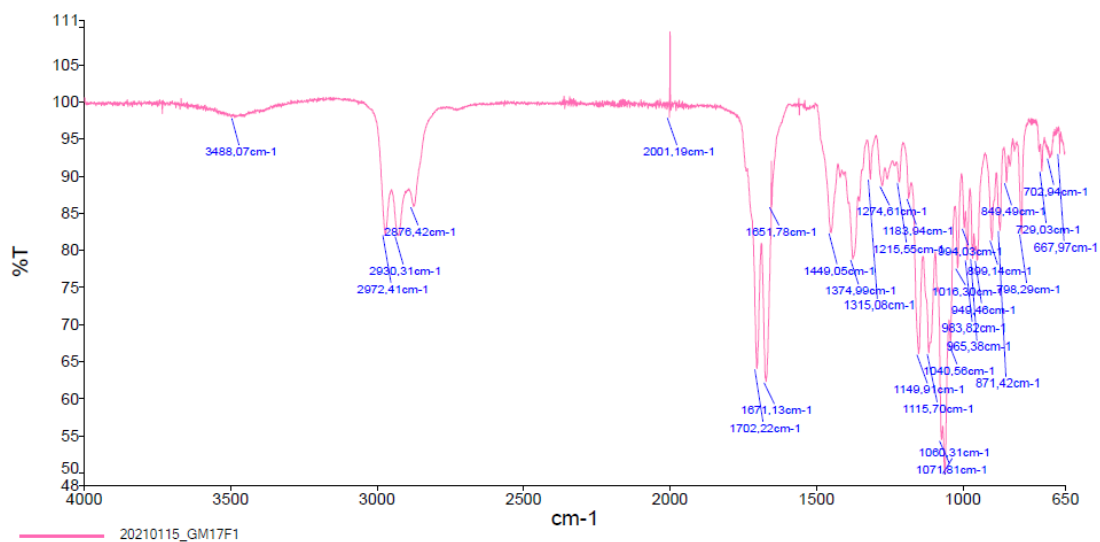


Figure S19. FT-IR spectrum of 15.

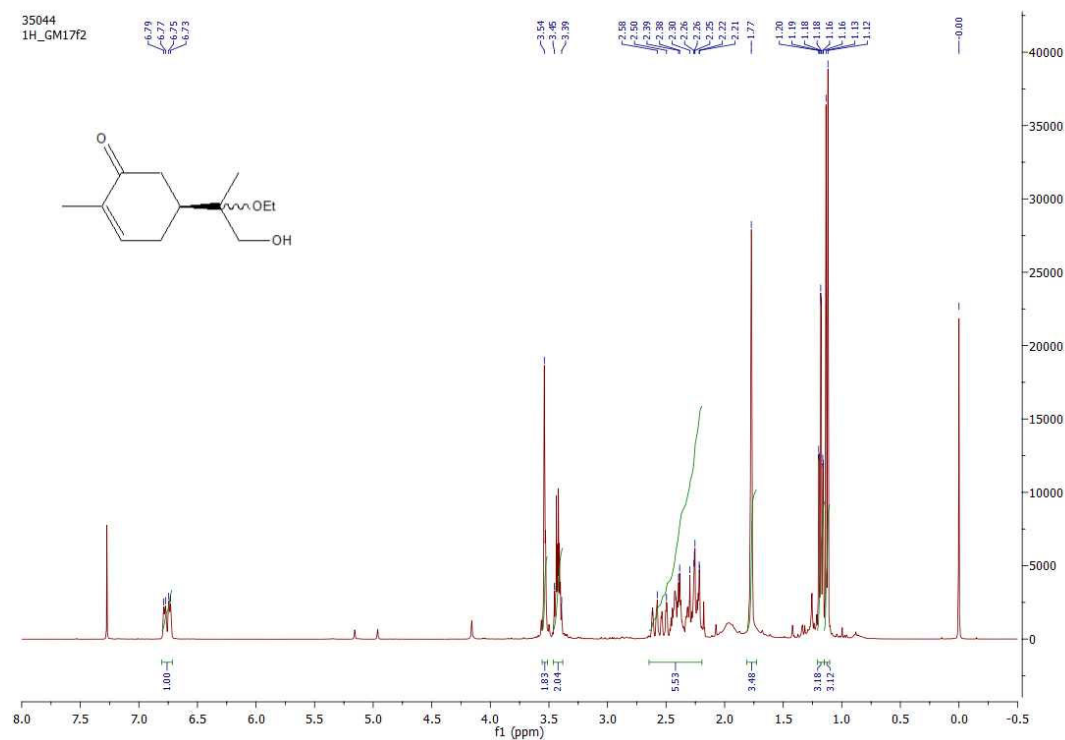


Figure S20. <sup>1</sup>H NMR spectrum of 16.

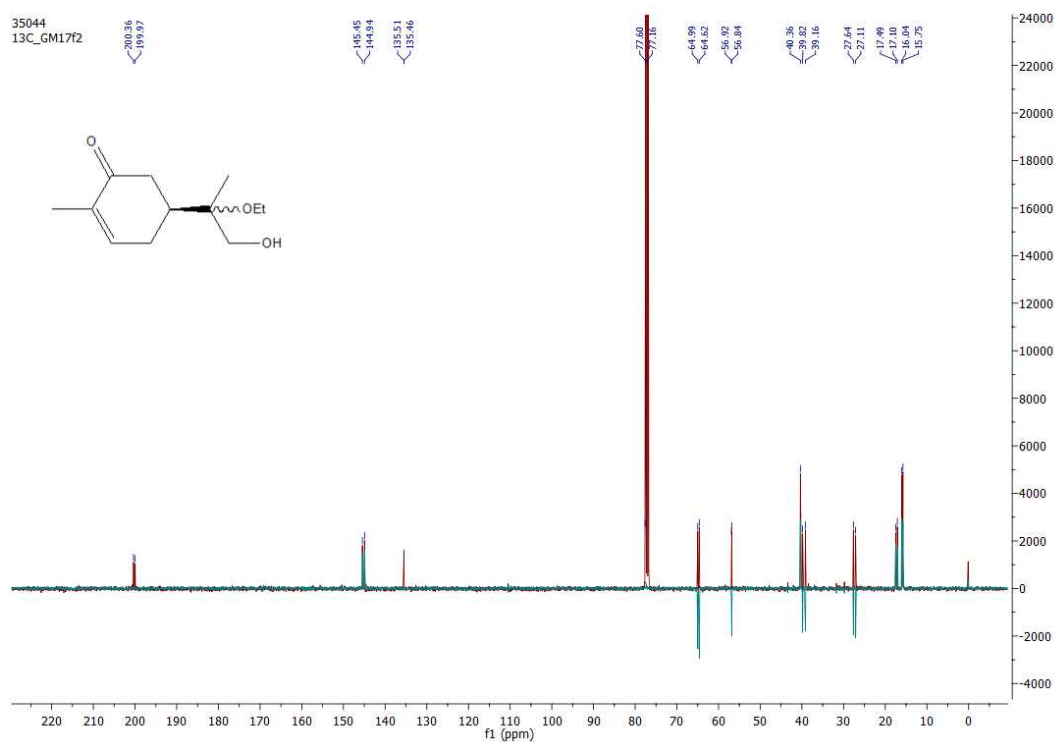


Figure S21.  $^{13}\text{C}$  NMR and DEPT-135 spectra of 16.

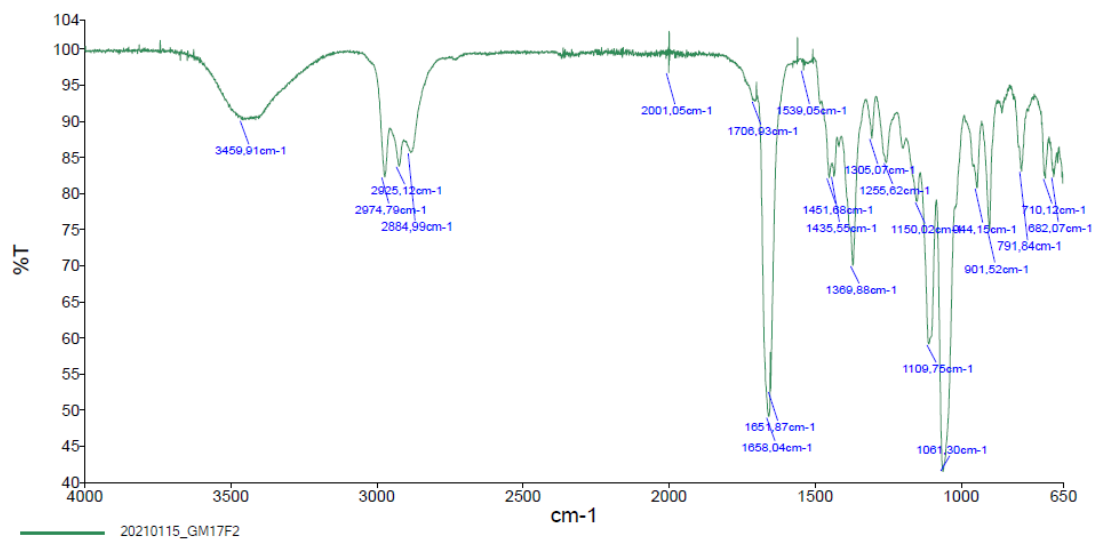


Figure S22. FT-IR spectrum of 16.

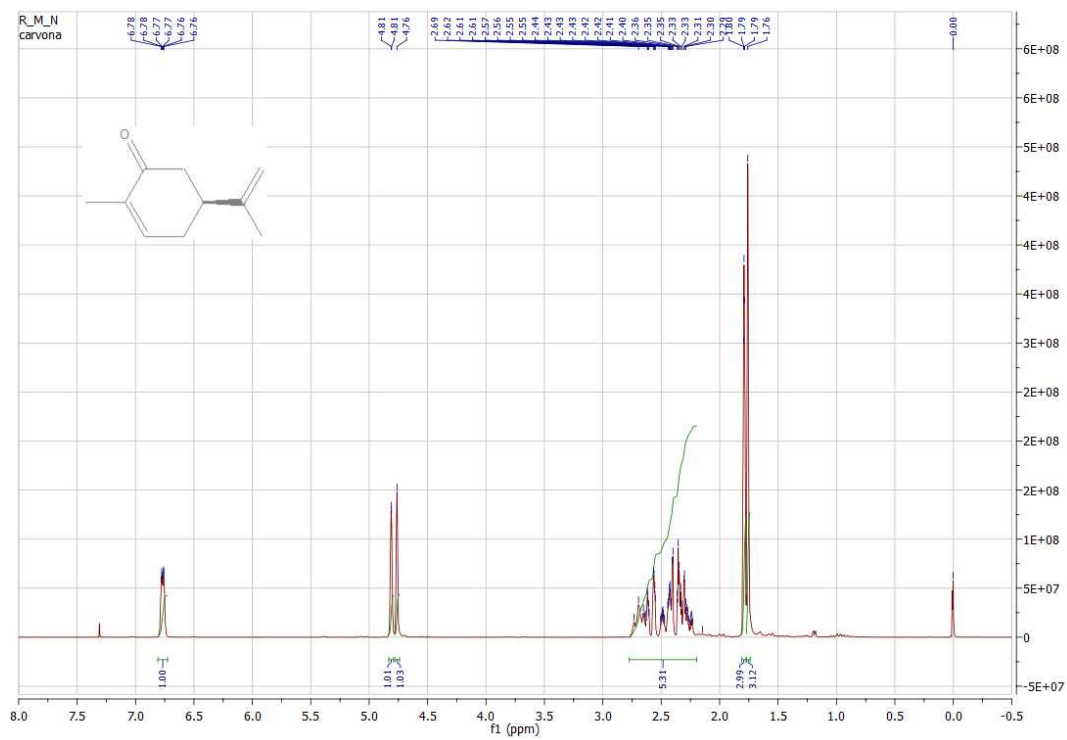


Figure S23.  $^1\text{H}$  NMR spectrum of Carvone.

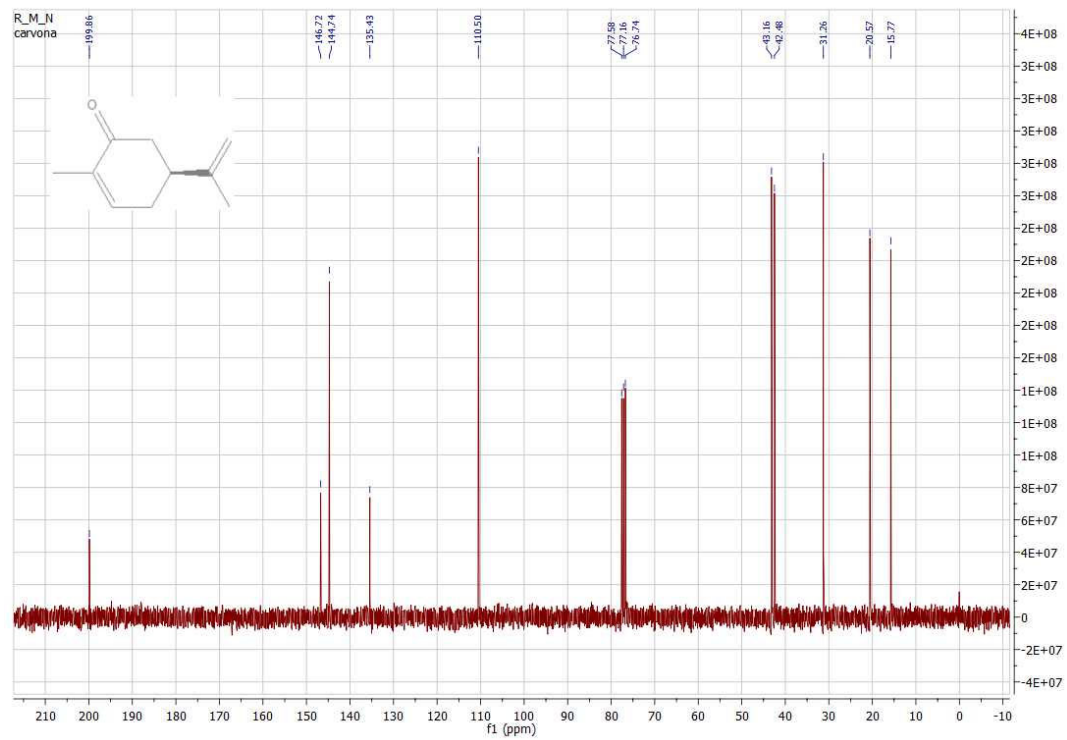


Figure S24.  $^{13}\text{C}$  NMR spectrum of Carvone.

Uncropped Blots

Figure S25. Uncropped Blots from Fig. 4A



Figure S26. Uncropped Blots from Fig. 4B

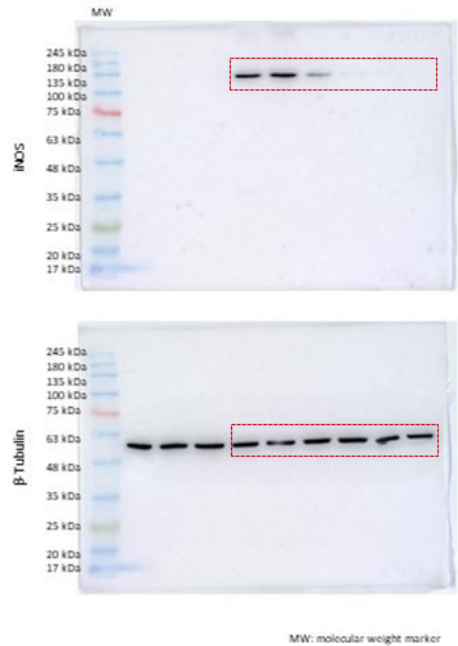
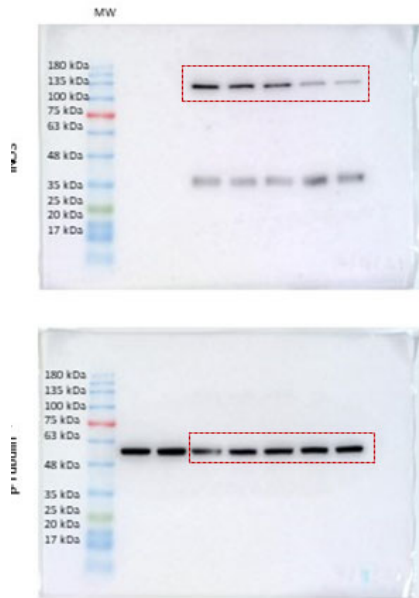
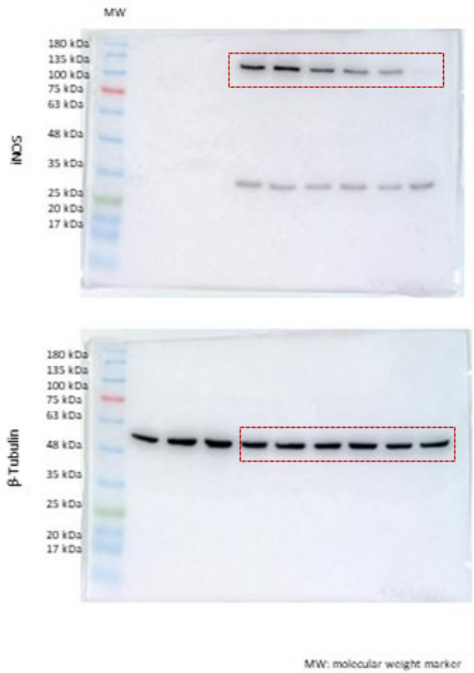


Figure S27. Uncropped Blots from Fig. 4C



\* This membrane is the same shown on Fig. 5C

Figure S28. Uncropped Blots from Fig. 4D



The membrane from Fig. 4A was cut at  $\approx 68$  kDa so that the upper piece was incubated with anti-iNOS antibody and the lower one with the anti- $\beta$ -tubulin I antibody. The membranes from Figs. 4C and 4D were probed with the anti-iNOS antibody without stripping the anti-pro-IL-1 $\beta$  antibody.

Figure S29. Uncropped Blots from Fig. 5A

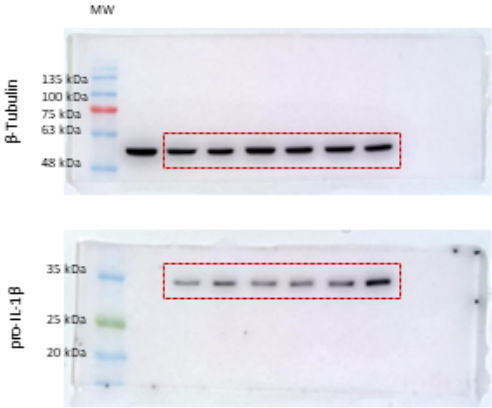
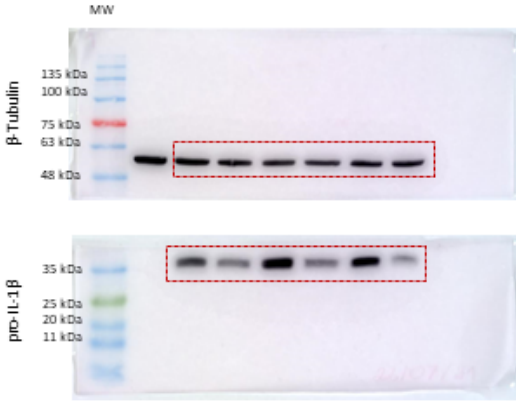


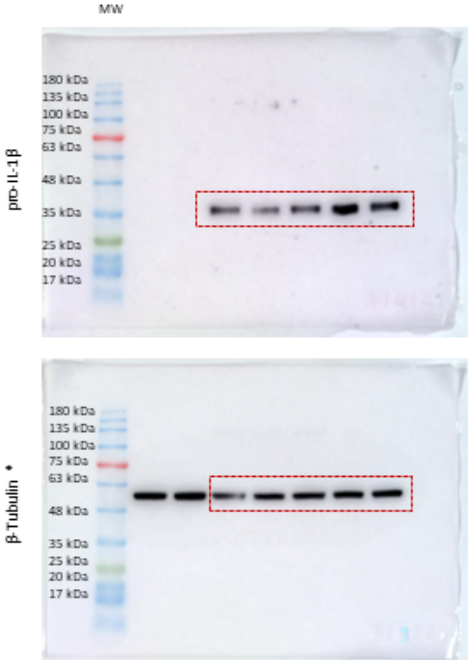
Figure S30. Uncropped Blots from Fig. 5B



MW: molecular weight marker

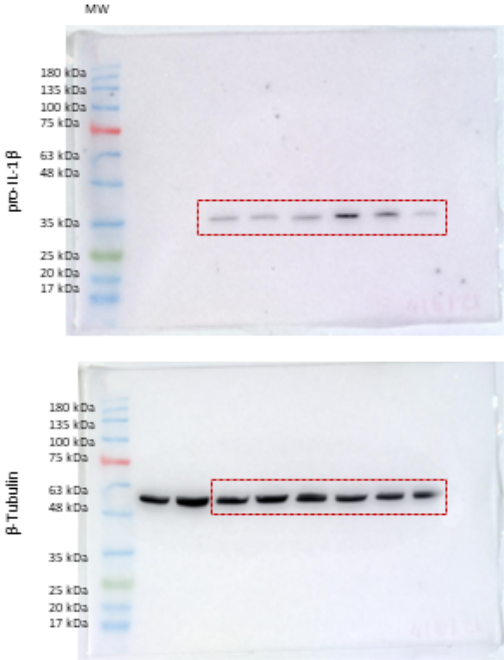
The membranes from Fig. 5A and 5B were cut at  $\approx 43$  kDa so that the upper pieces were incubated with the anti- $\beta$ -tubulin I antibody and the lower ones with the anti-pro-IL-1 $\beta$  antibody.

Figure S31. Uncropped Blots from Fig. 5C



\* This membrane is the same shown on Fig. 4C

Figure S32. Uncropped Blots from Fig. 5D



MW: molecular weight marker