

# Supplementary Information

## Synthesis, *in vitro* Antimalarial Activity and *in silico* Studies of Hybrid Kauranoid 1,2,3-Triazoles Derived from Naturally Occurring Diterpenes

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Copies of IR, <sup>1</sup>H, <sup>13</sup>C NMR and HRMS spectra of compounds

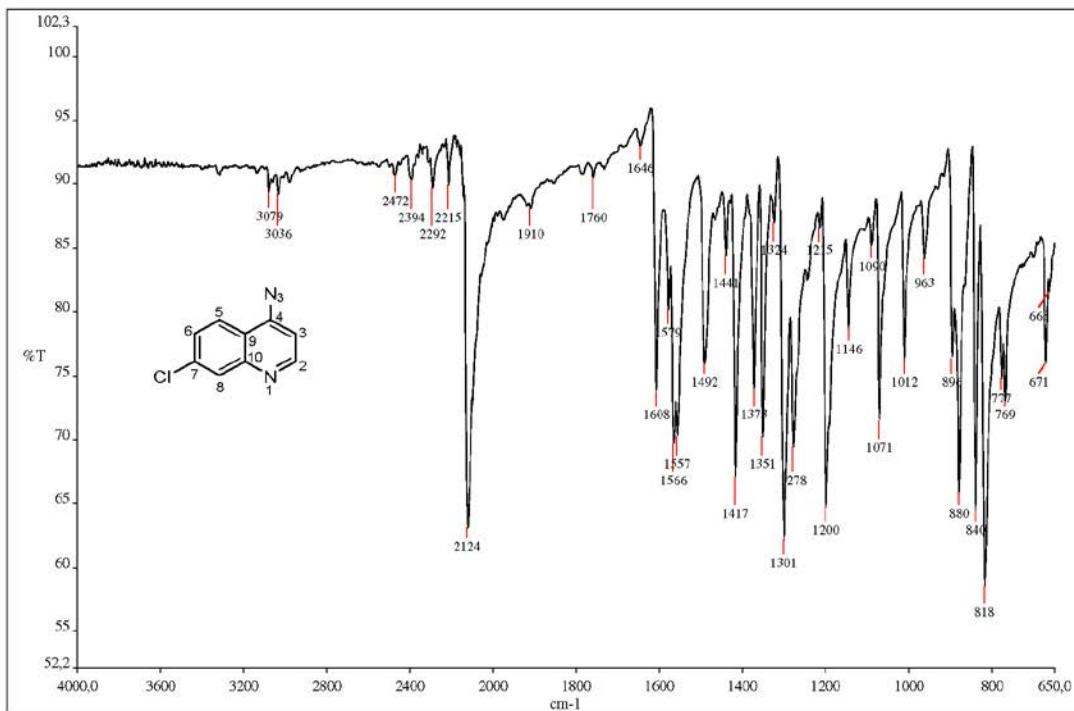
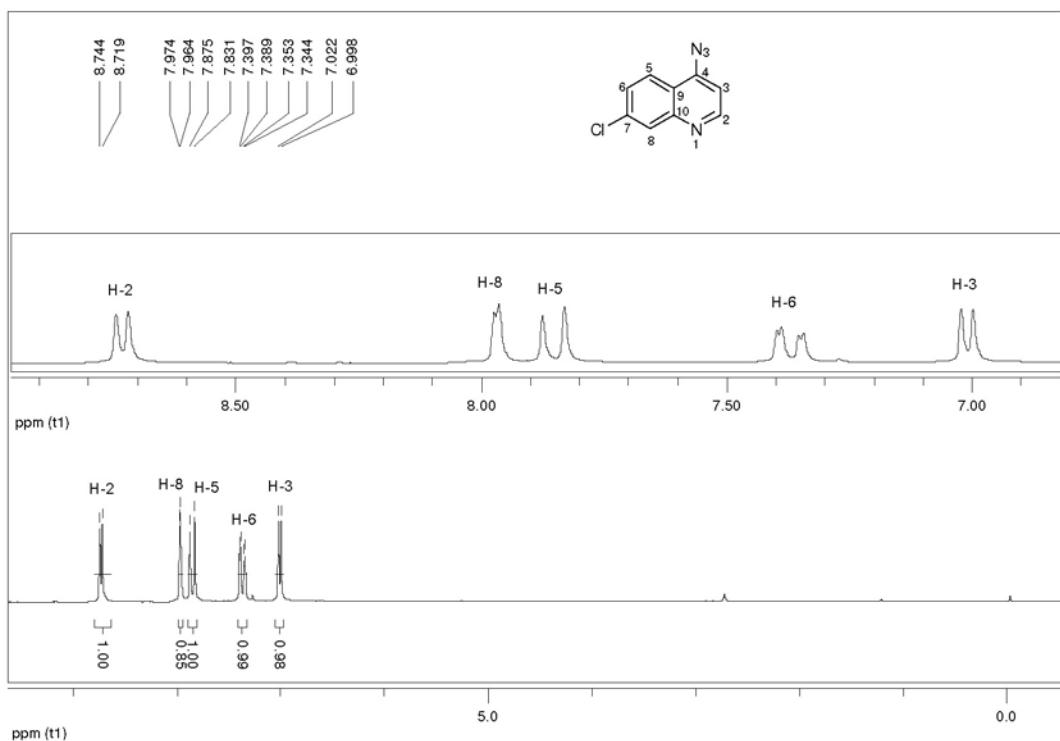
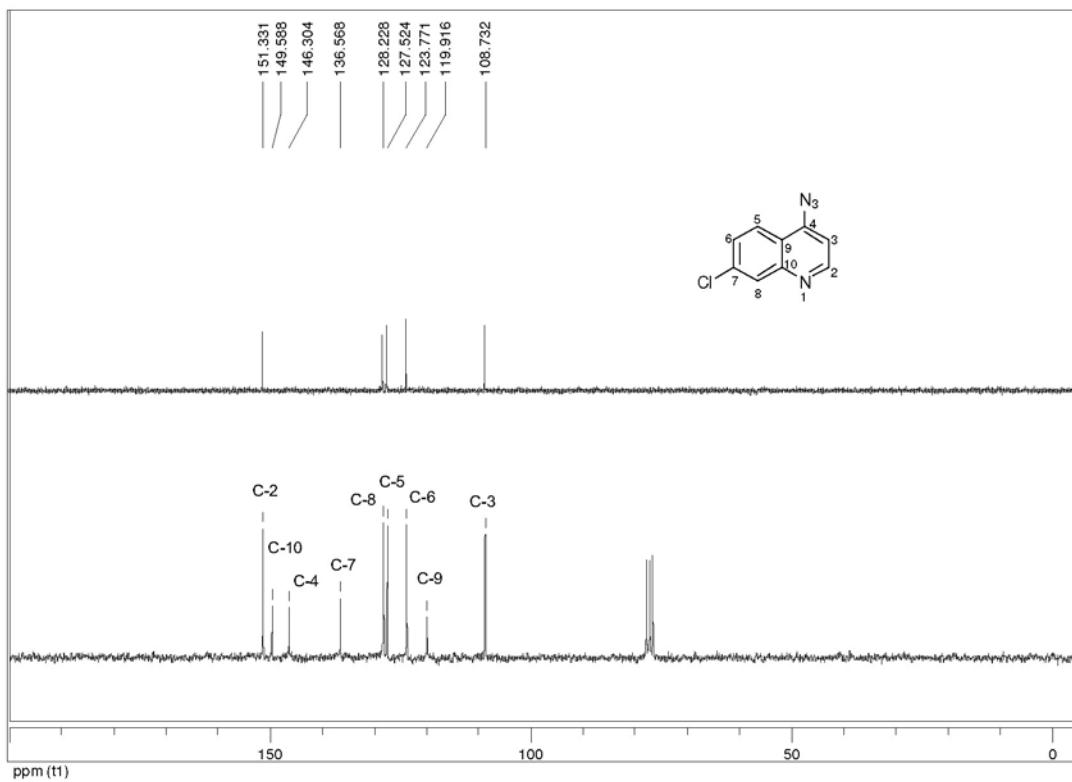


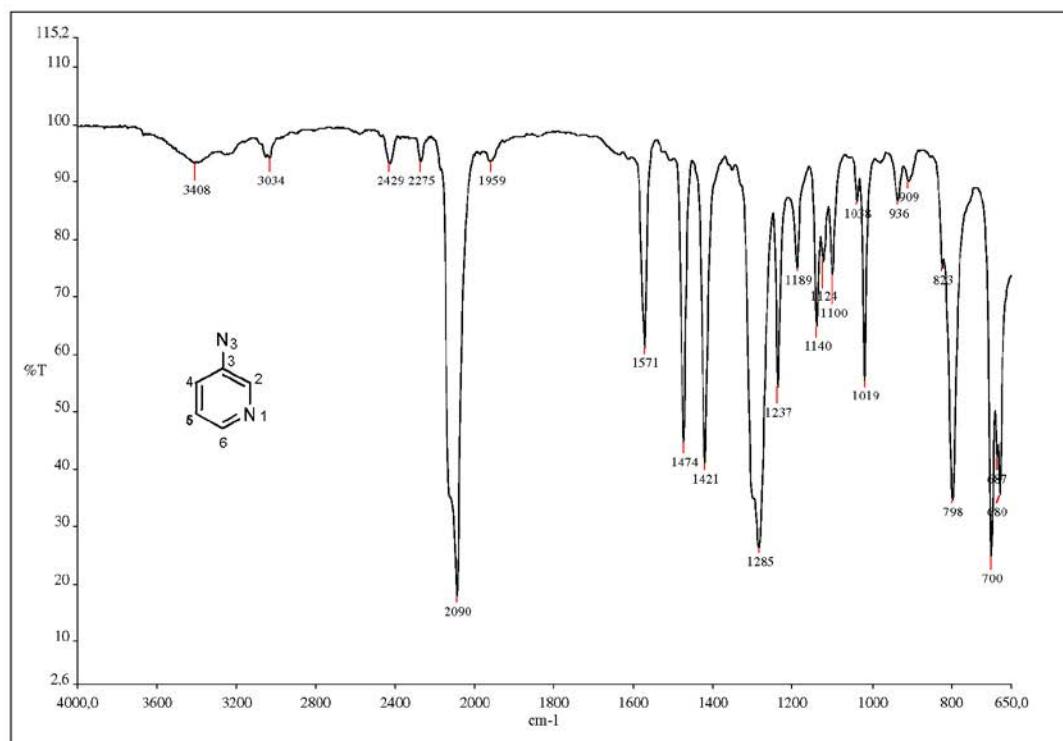
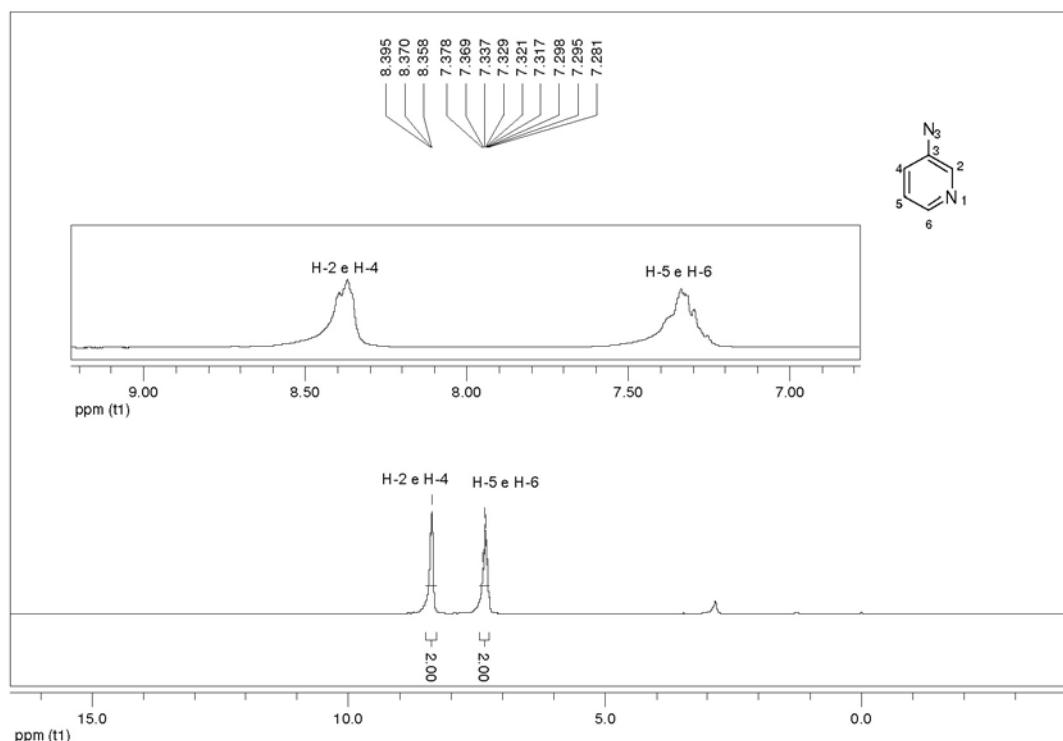
Figure S1. Infrared spectrum (ATR) of compound 14.

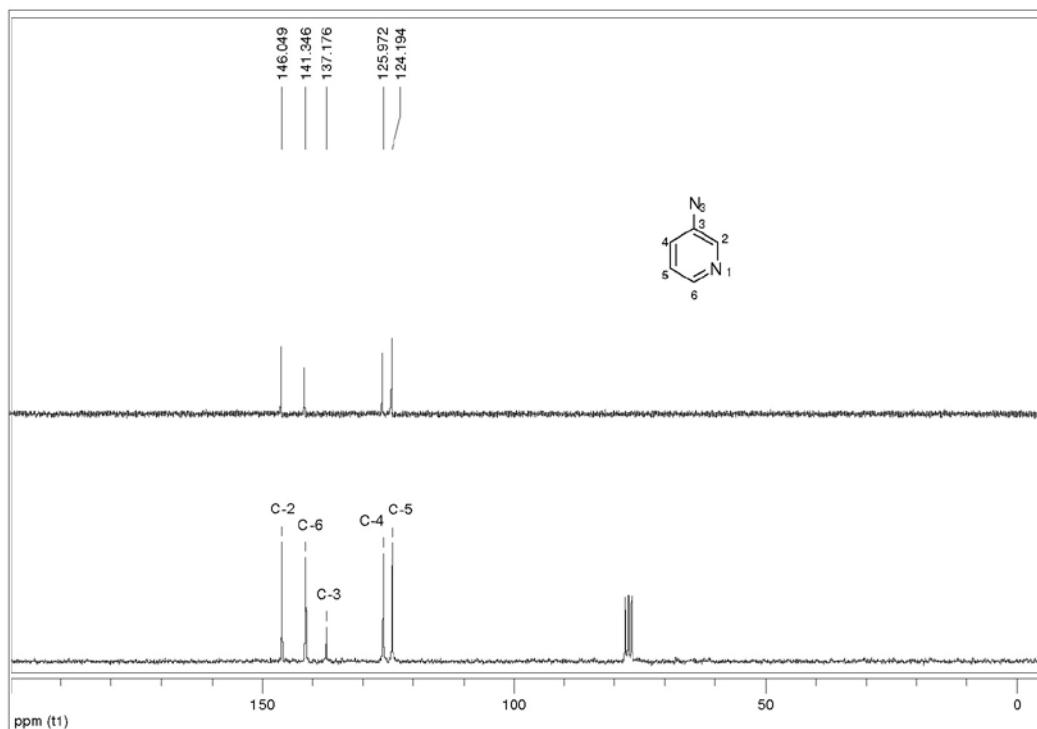


**Figure S2.** <sup>1</sup>H NMR spectrum (200 MHz, CDCl<sub>3</sub>) of compound 14.

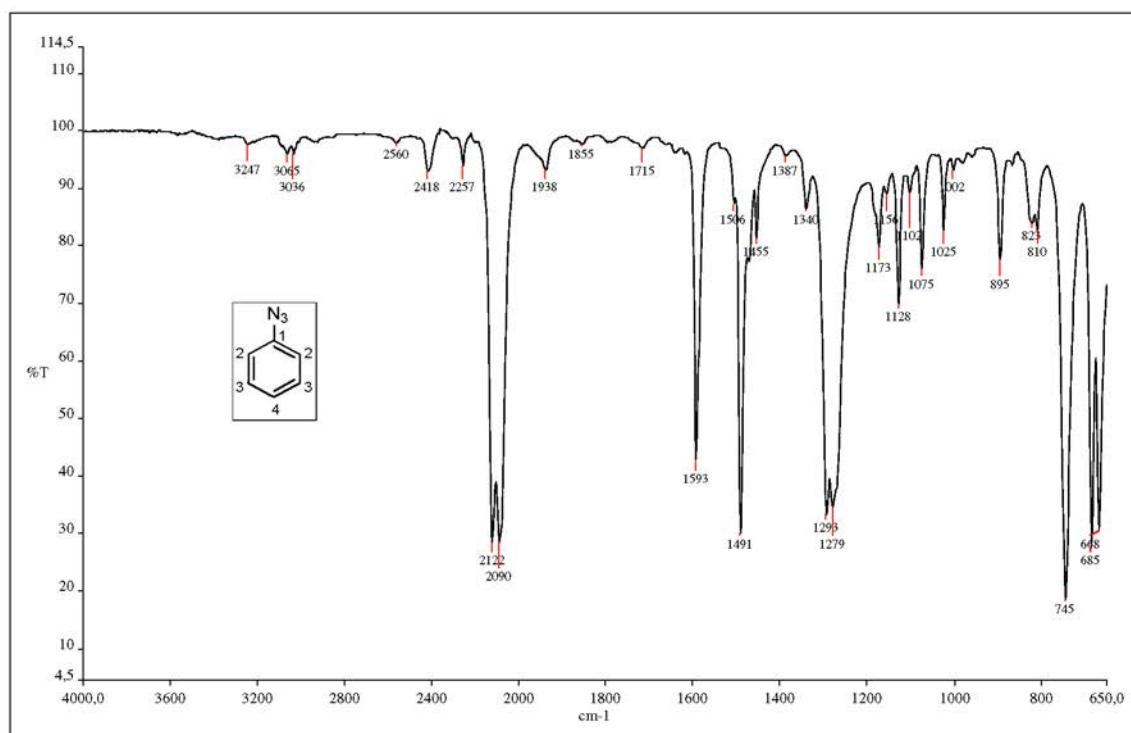


**Figure S3.** <sup>13</sup>C NMR spectrum and DEPT 135 (50 MHz, CDCl<sub>3</sub>) of compound 14.

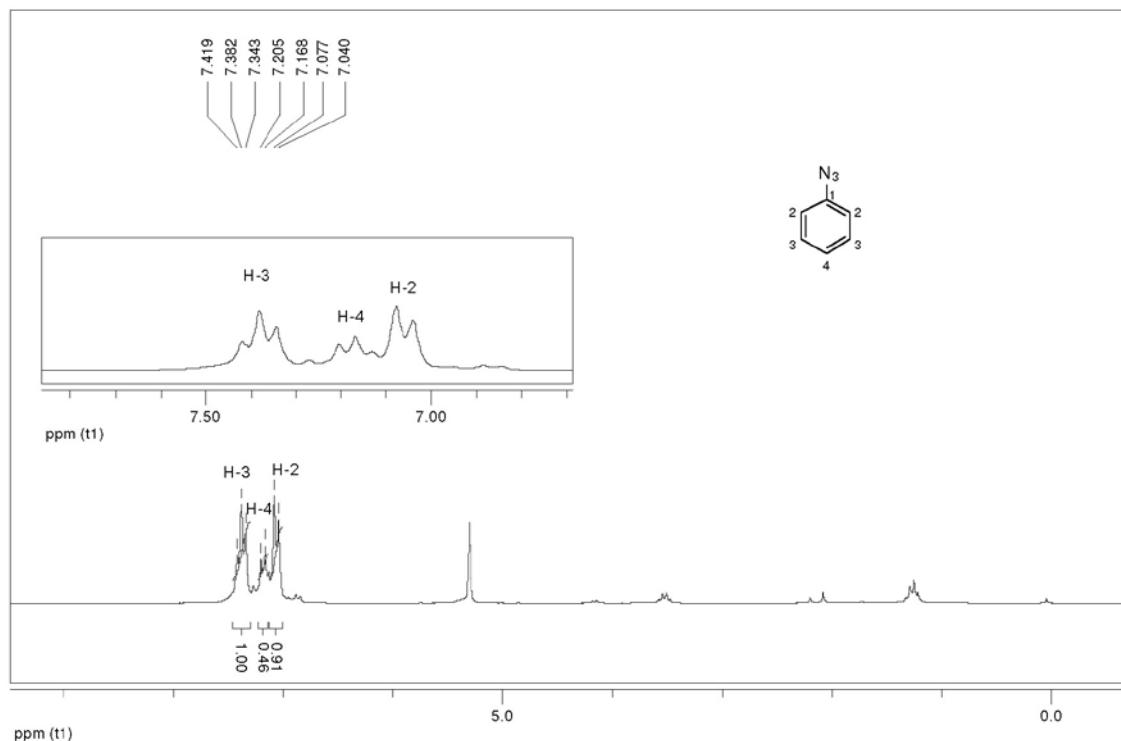
**Figure S4.** Infrared spectrum (ATR) of compound **15**.**Figure S5.**  $^1\text{H}$  NMR spectrum (200 MHz,  $\text{CDCl}_3$ ) of compound **15**.



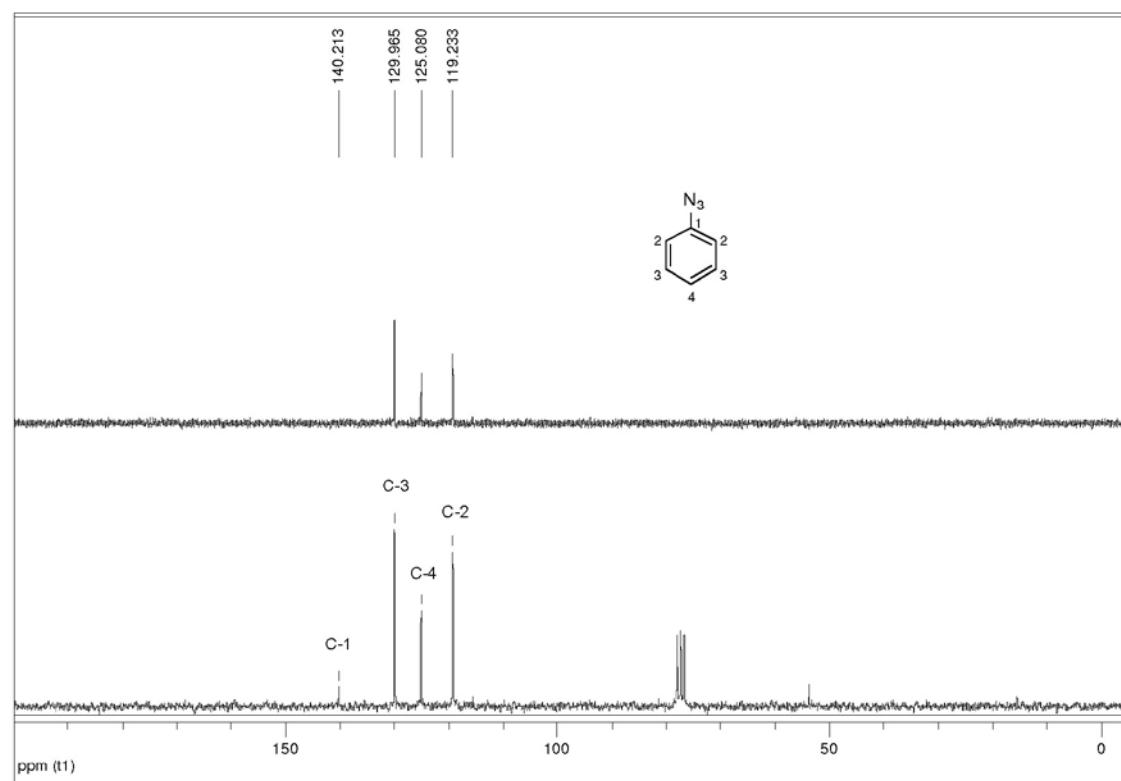
**Figure S6.**  $^{13}\text{C}$  NMR spectrum and DEPT 135 (50 MHz,  $\text{CDCl}_3$ ) of compound **15**.



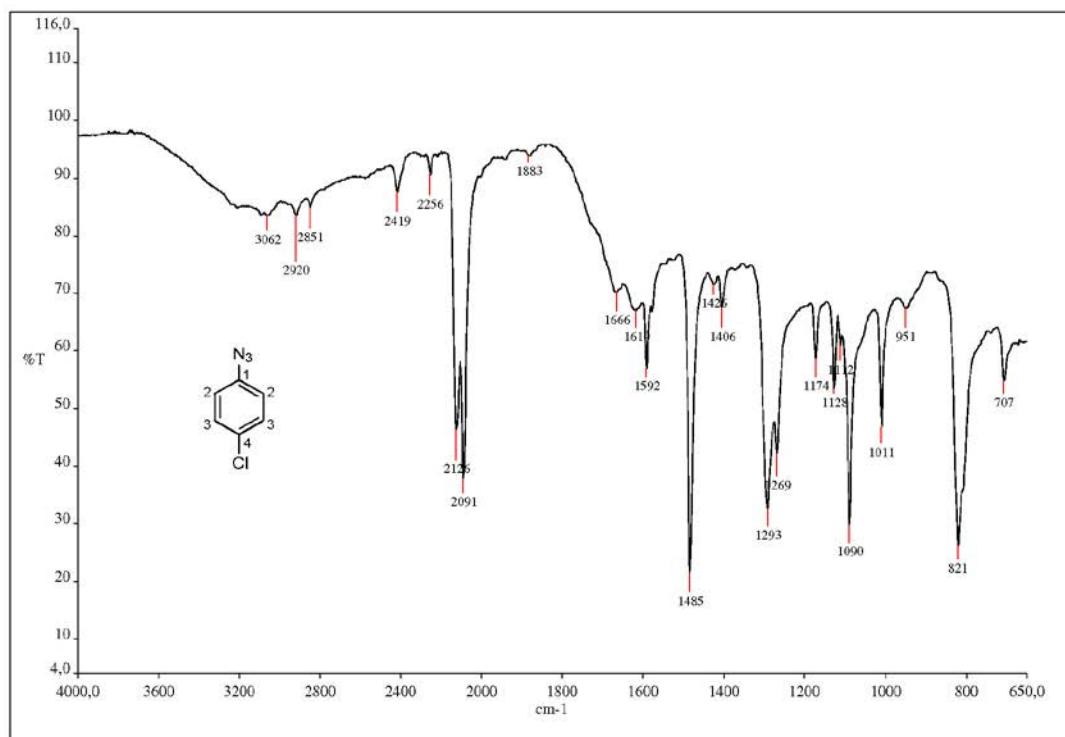
**Figure S7.** Infrared spectrum (ATR) of compound **16**.



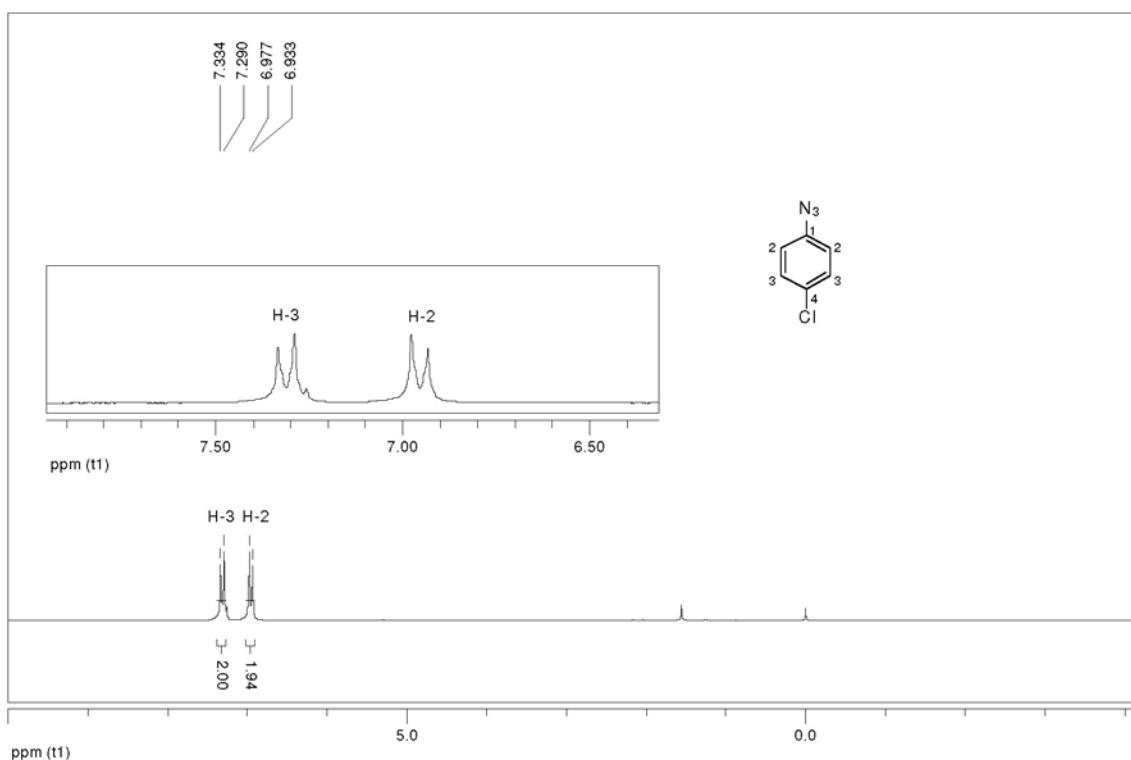
**Figure S8.** <sup>1</sup>H NMR spectrum (200 MHz, CDCl<sub>3</sub>) of compound **16**.



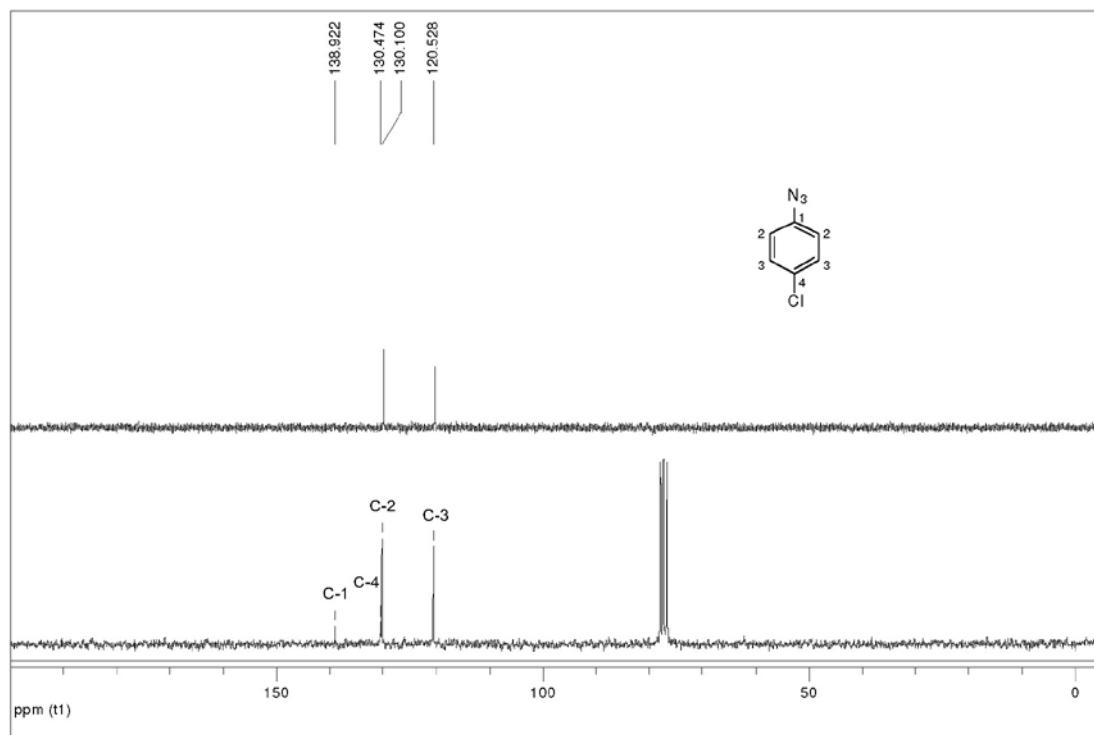
**Figure S9.** <sup>13</sup>C NMR spectrum and DEPT 135 (50 MHz, CDCl<sub>3</sub>) of compound **16**.



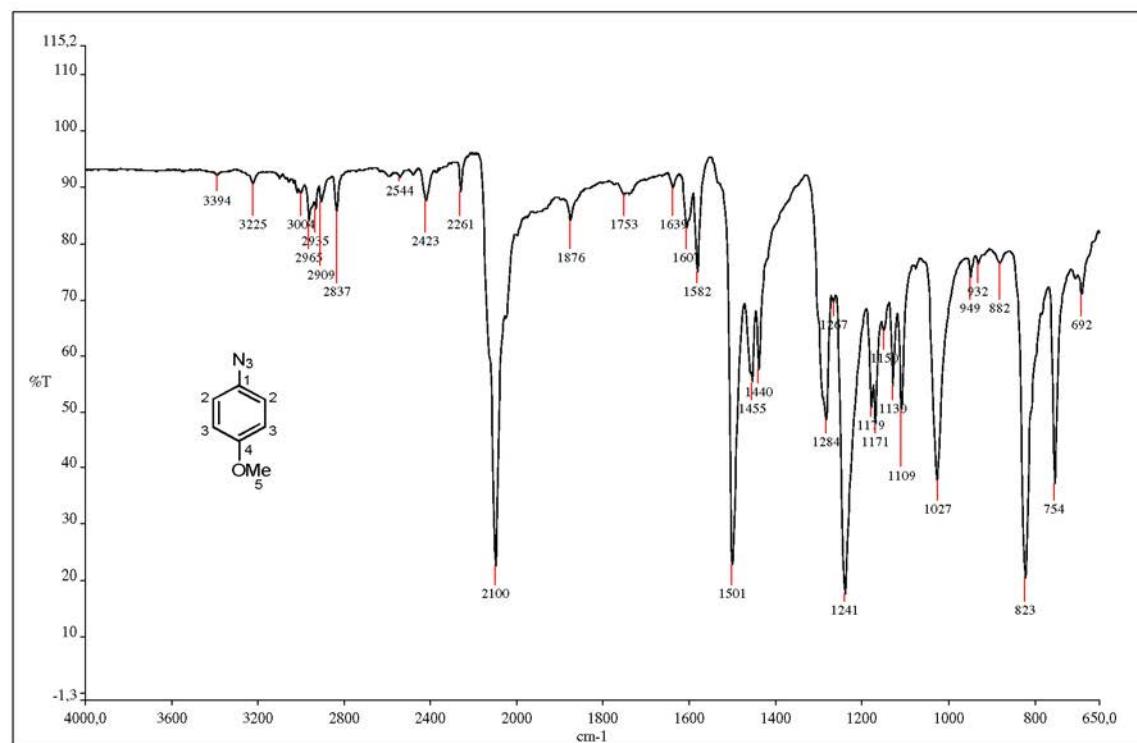
**Figure S10.** Infrared spectrum (ATR) of compound 17.



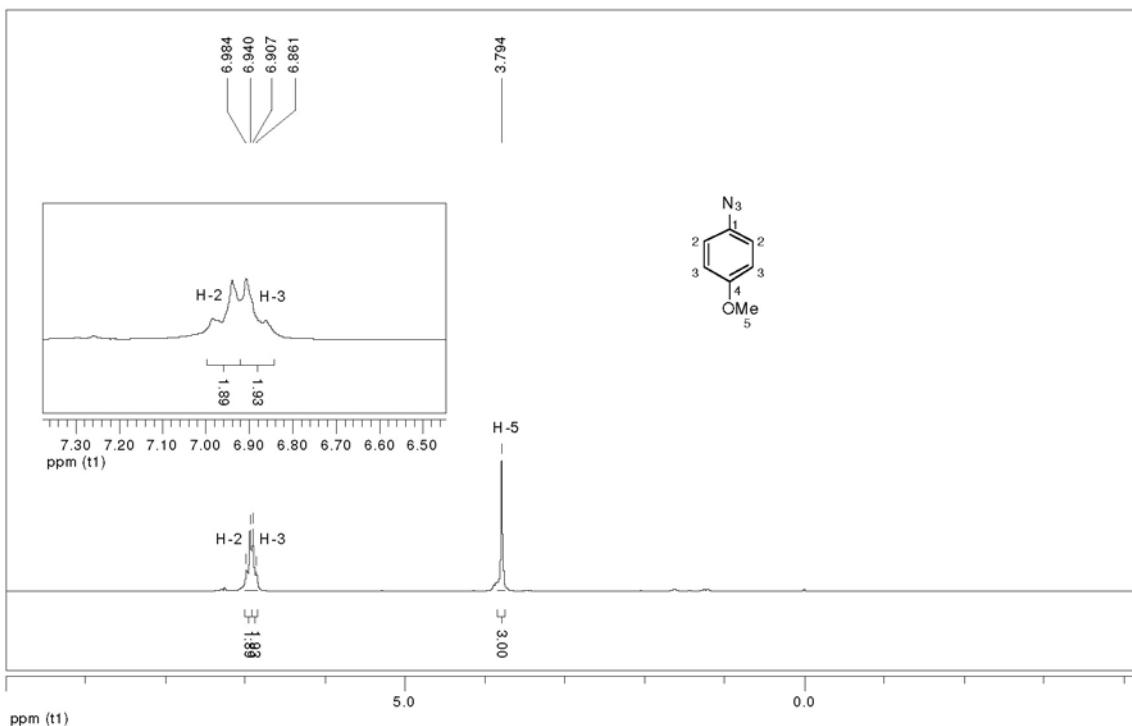
**Figure S11.**  $^1\text{H}$  NMR spectrum (200 MHz,  $\text{CDCl}_3$ ) of compound 17.



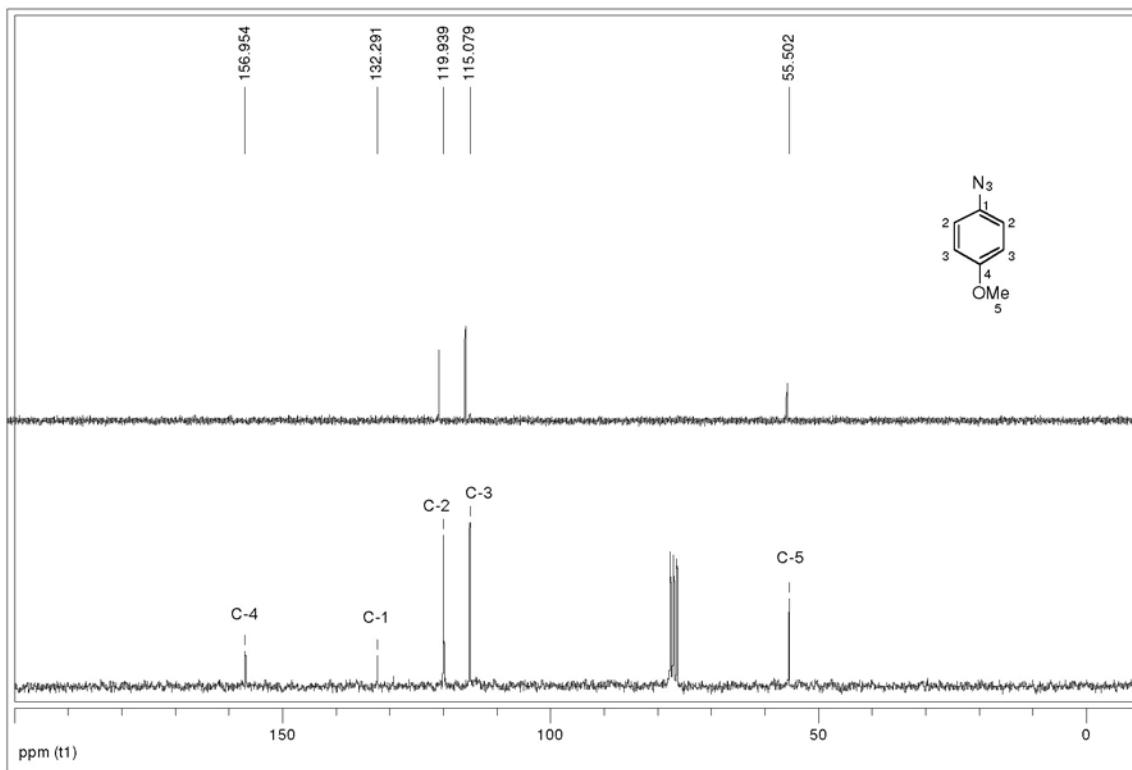
**Figure S12.**  $^{13}\text{C}$  NMR spectrum and DEPT 135 (50 MHz,  $\text{CDCl}_3$ ) of compound **17**.



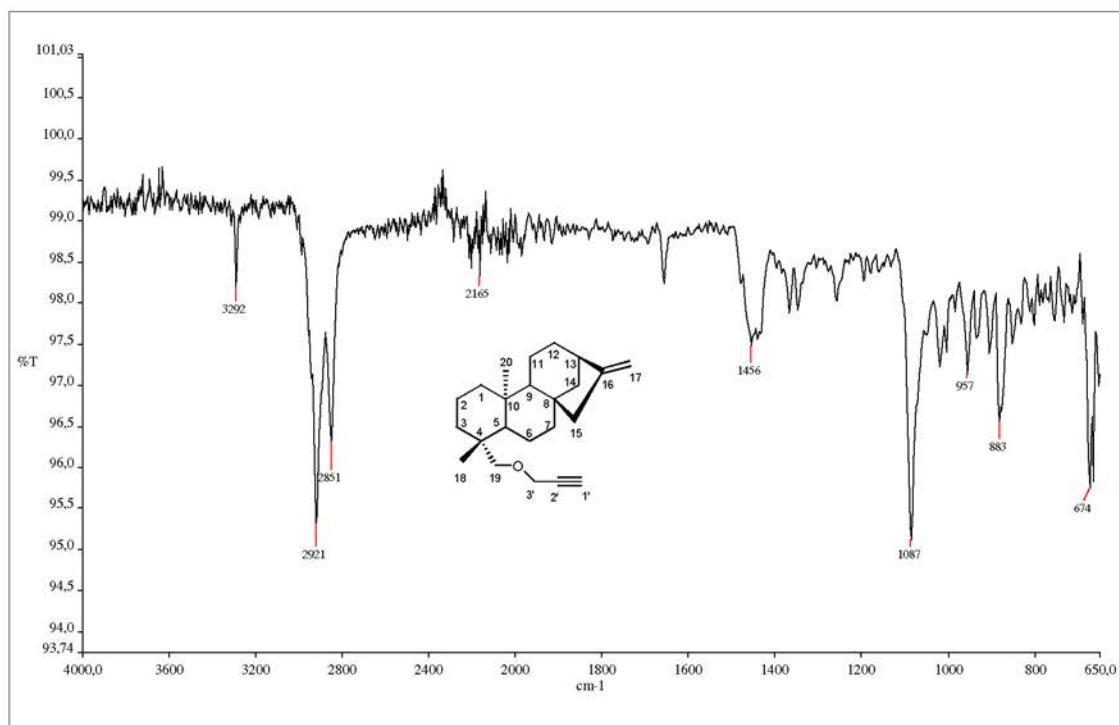
**Figure S13.** Infrared spectrum (ATR) of compound **18**.



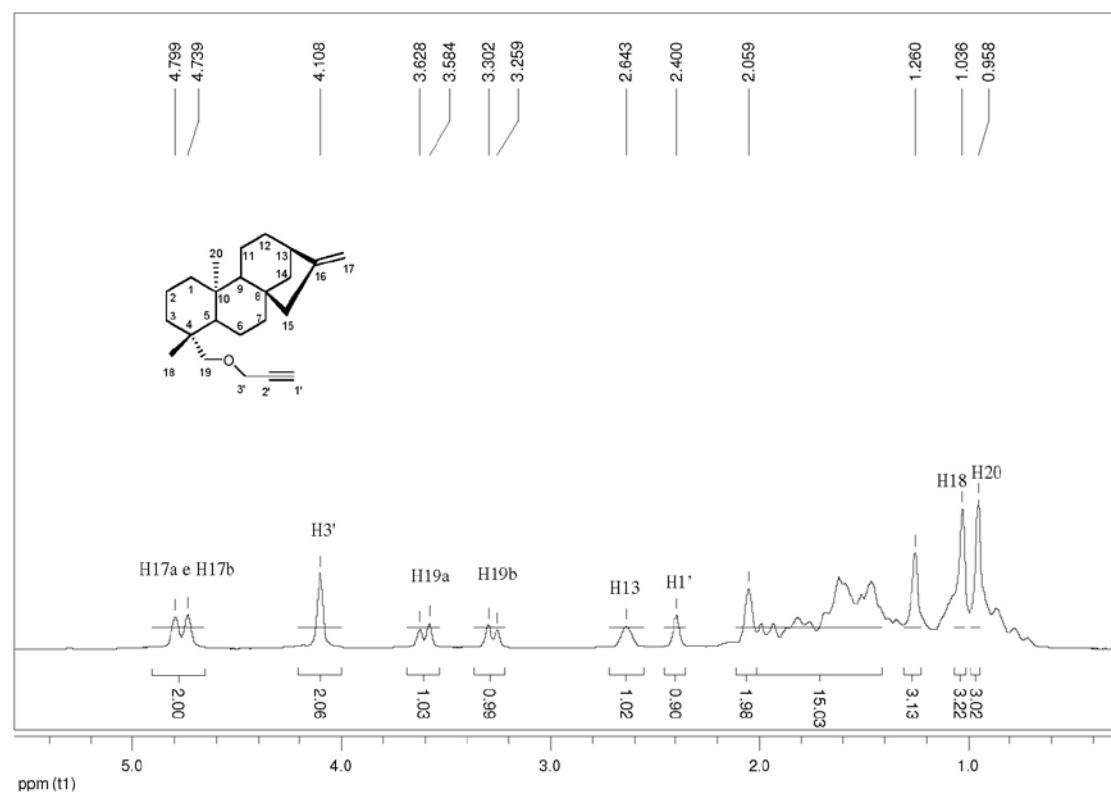
**Figure S14.** <sup>1</sup>H NMR spectrum (200 MHz, CDCl<sub>3</sub>) of compound 18.



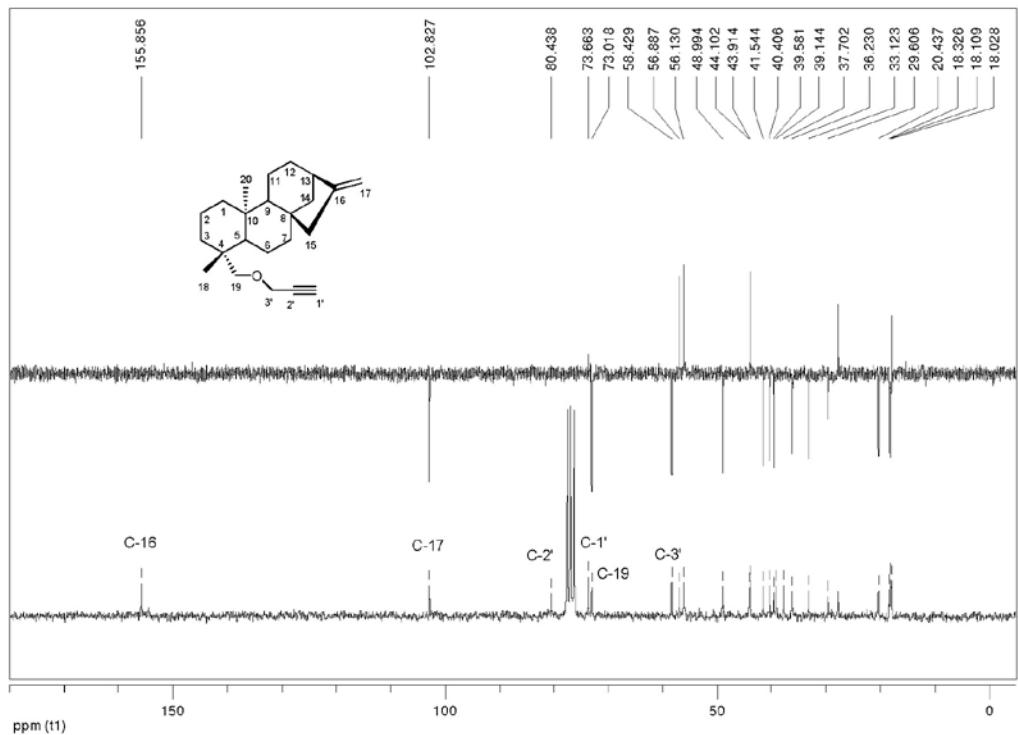
**Figure S15.** <sup>13</sup>C NMR spectrum and DEPT 135 (50 MHz, CDCl<sub>3</sub>) of compound 18.



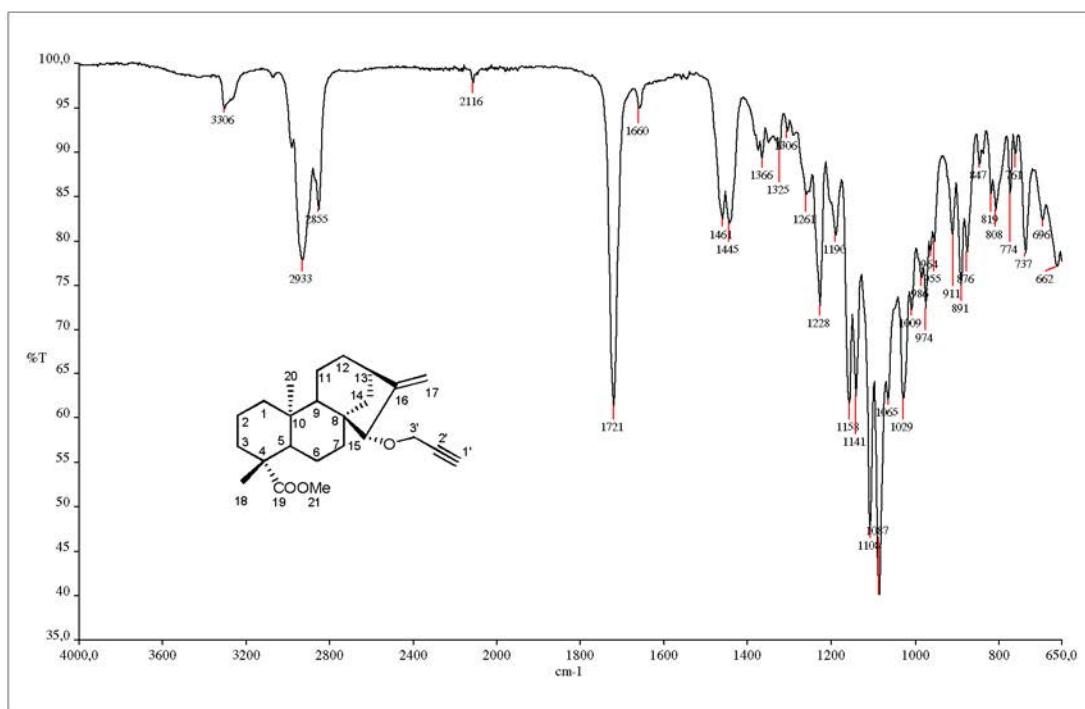
**Figure S16.** Infrared spectrum (ATR) of compound 10.



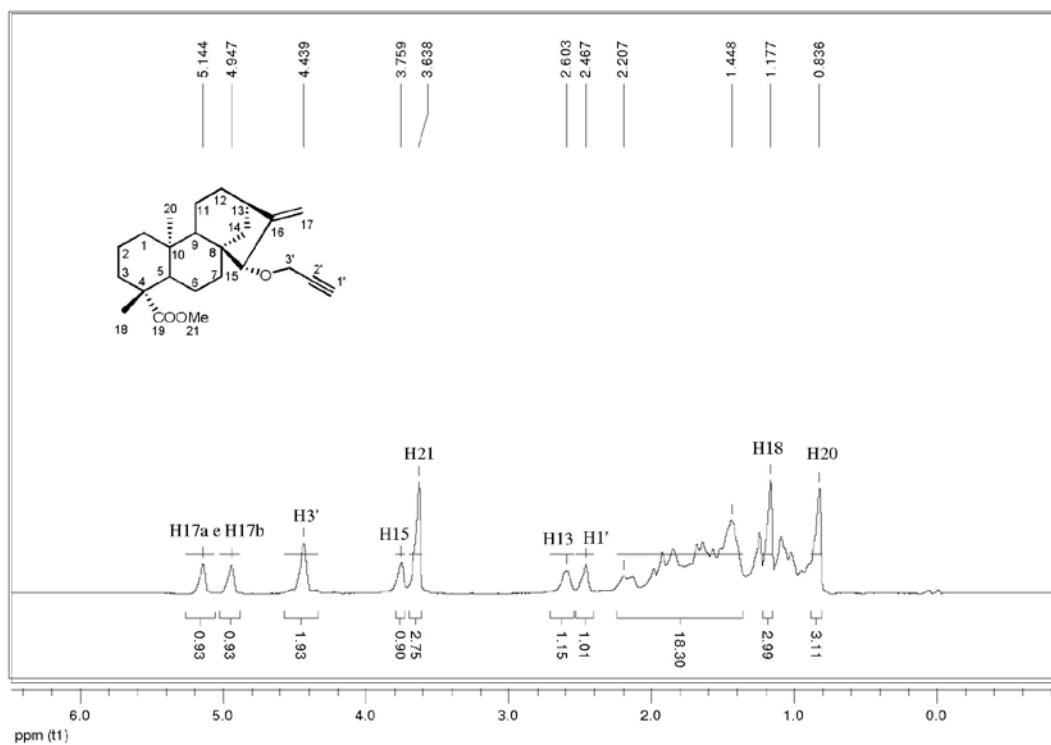
**Figure S17.**  $^1\text{H}$  NMR spectrum (200 MHz,  $\text{CDCl}_3$ ) of compound 10.



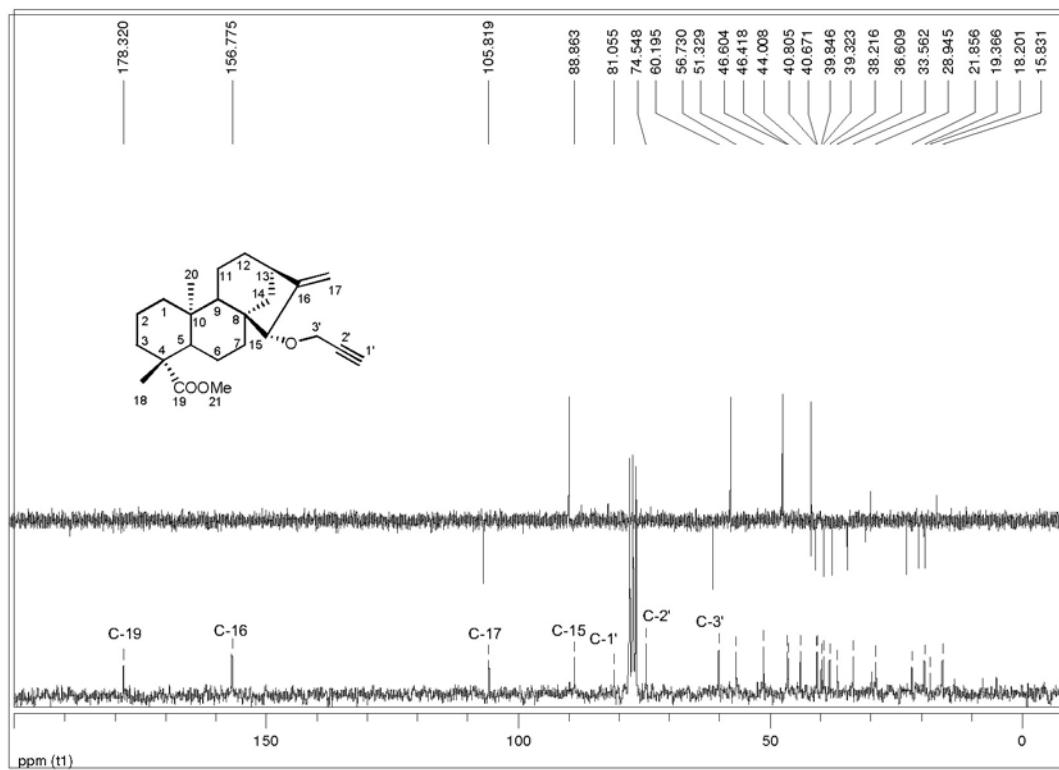
**Figure S18.**  $^{13}\text{C}$  NMR spectrum and DEPT 135 (50 MHz,  $\text{CDCl}_3$ ) of compound **10**.



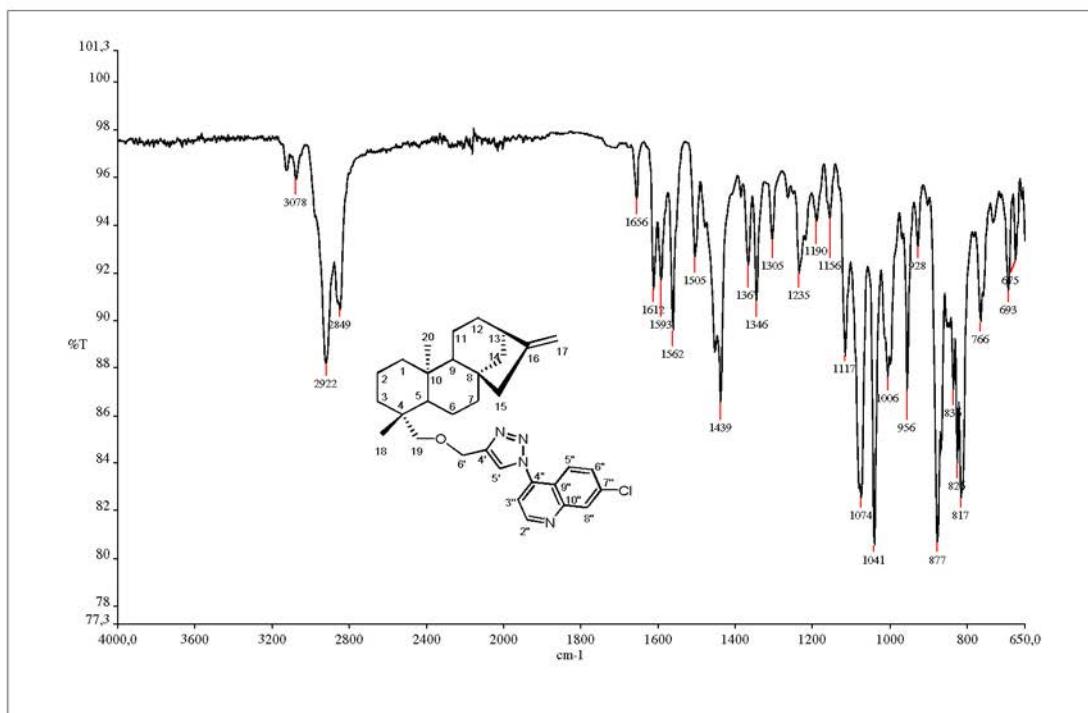
**Figure S19.** Infrared spectrum (ATR) of compound **13**.



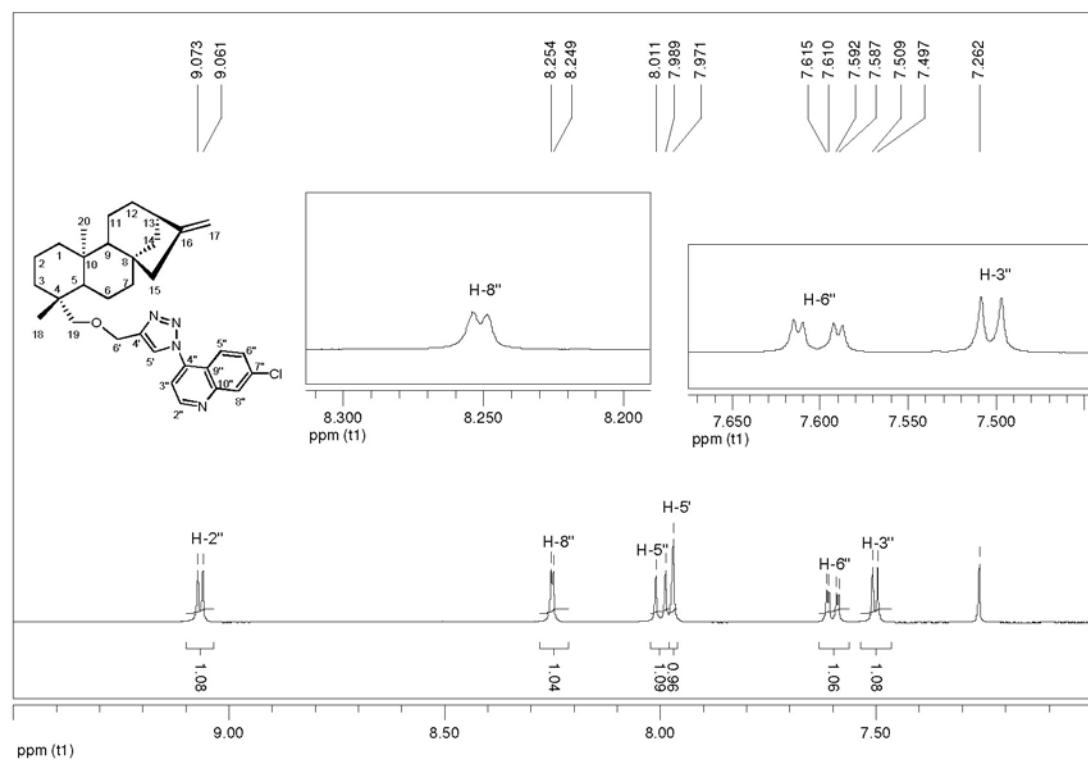
**Figure S20.** <sup>1</sup>H NMR spectrum (200 MHz, CDCl<sub>3</sub>) of compound 13.



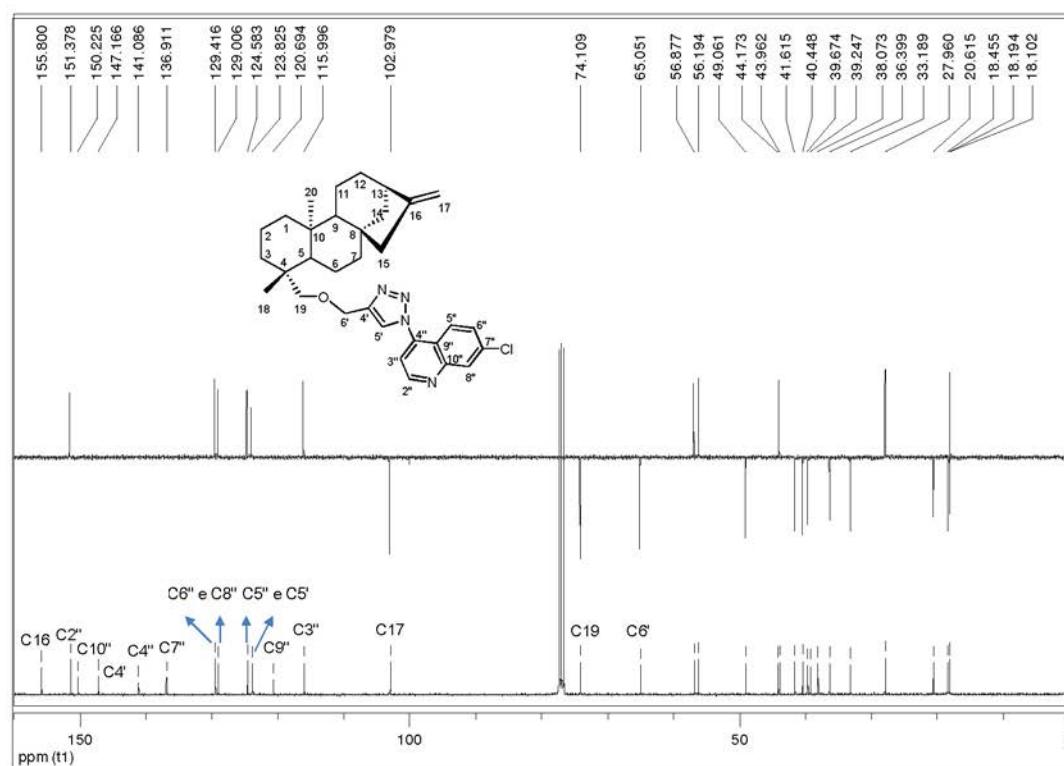
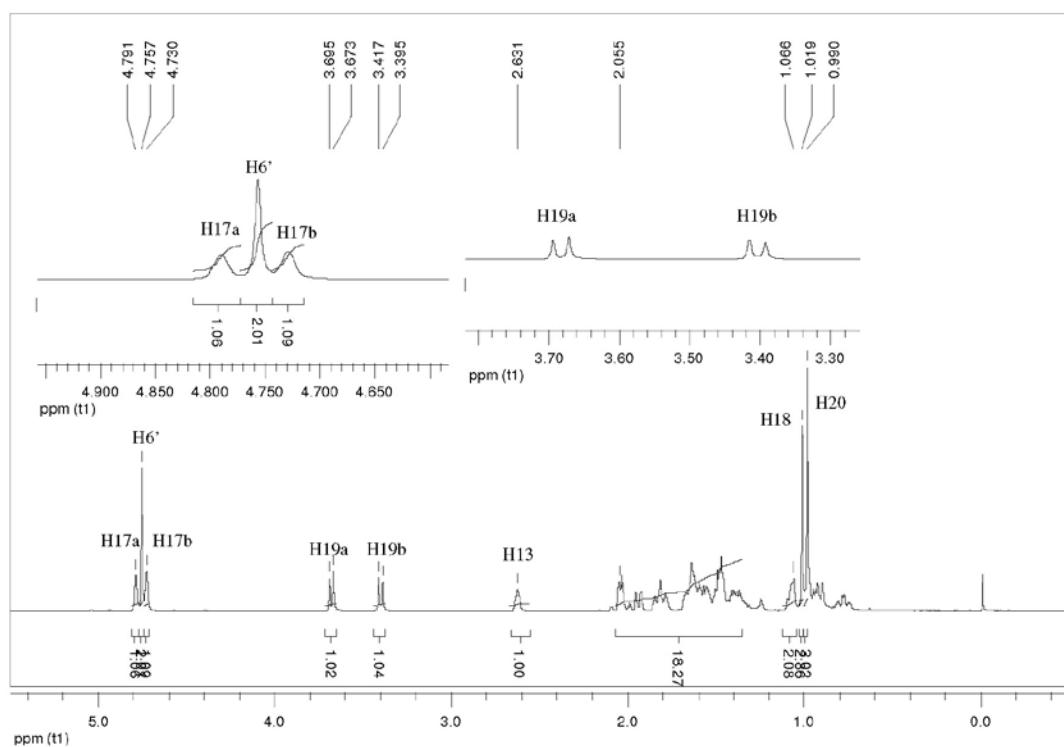
**Figure S21.** <sup>13</sup>C NMR spectrum and DEPT 135 (50 MHz, CDCl<sub>3</sub>) of compound 13.

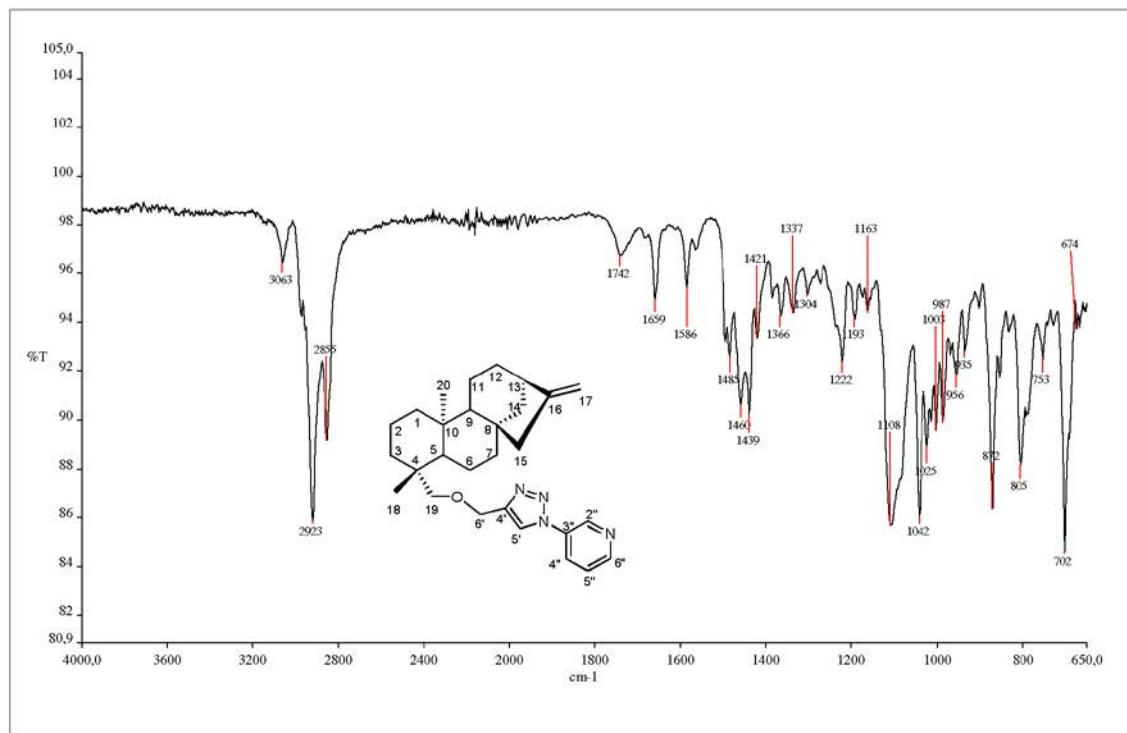


**Figure S22.** Infrared spectrum (ATR) of compound **19**.

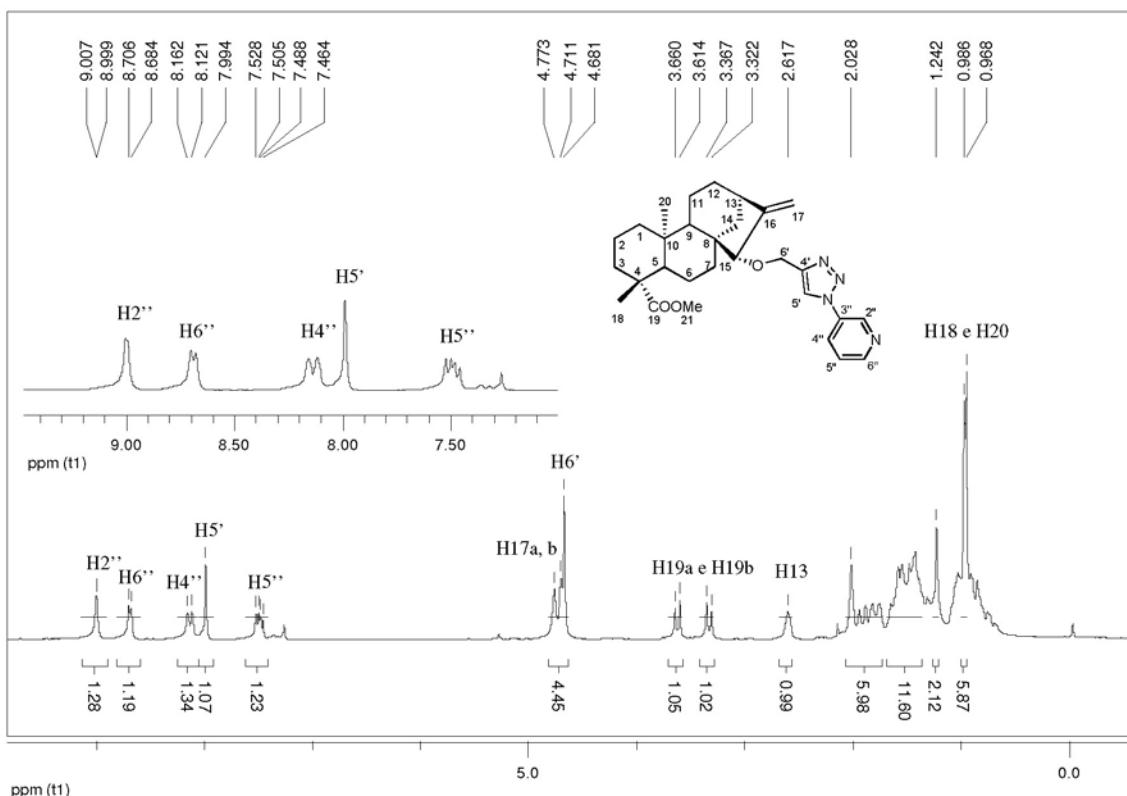


**Figure S23.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ ) of compound **19**. Expansion of the region between 7.0 and 9.5 ppm.

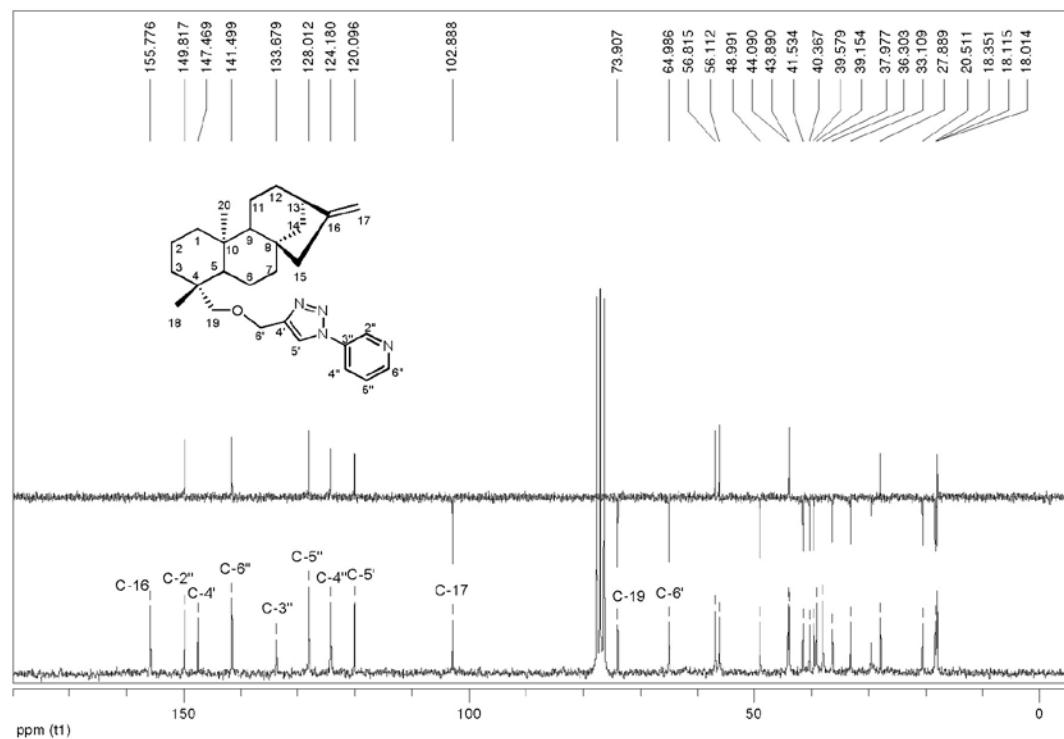




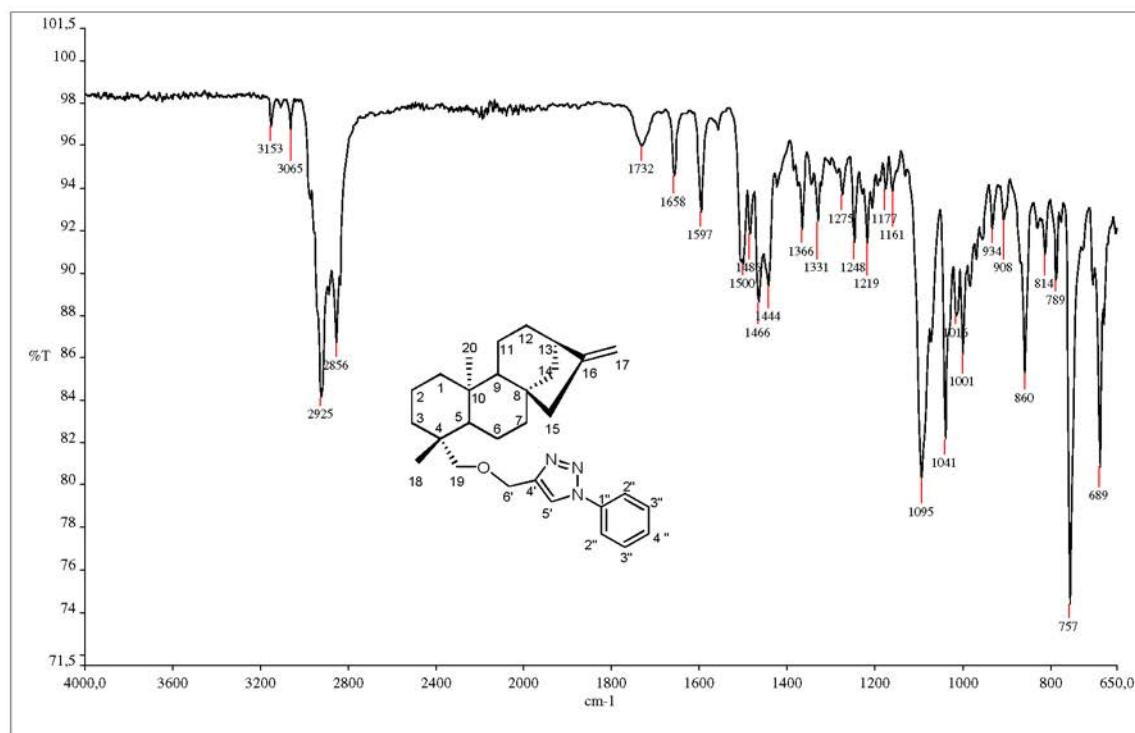
**Figure S26.** Infrared spectrum (ATR) of compound 20.



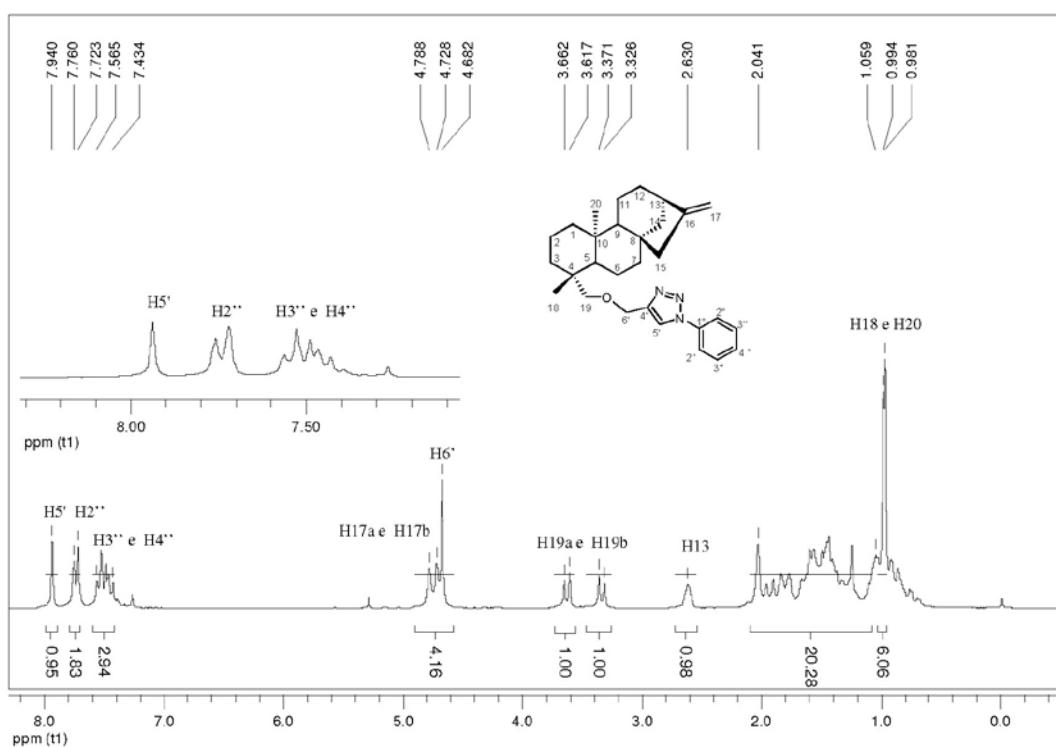
**Figure S27.**  $^1\text{H}$  NMR spectrum (200 MHz,  $\text{CDCl}_3$ ) of compound 20.



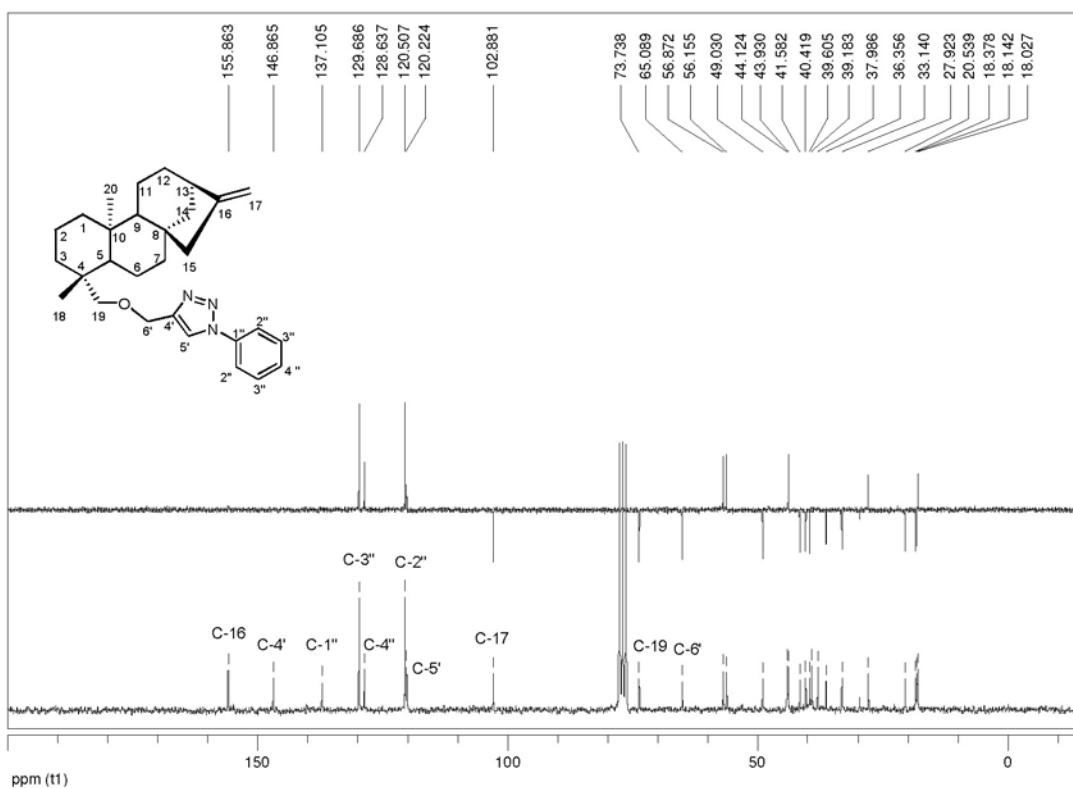
**Figure S28.** <sup>13</sup>C NMR spectrum and DEPT 135 (50 MHz, CDCl<sub>3</sub>) of compound **20**.



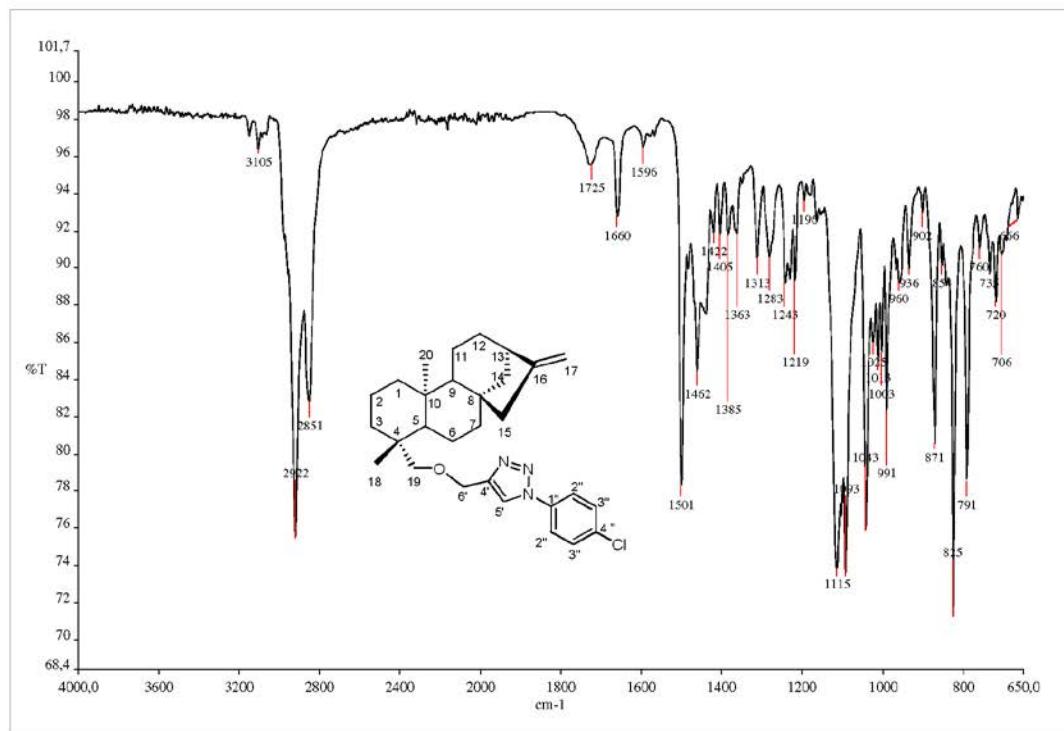
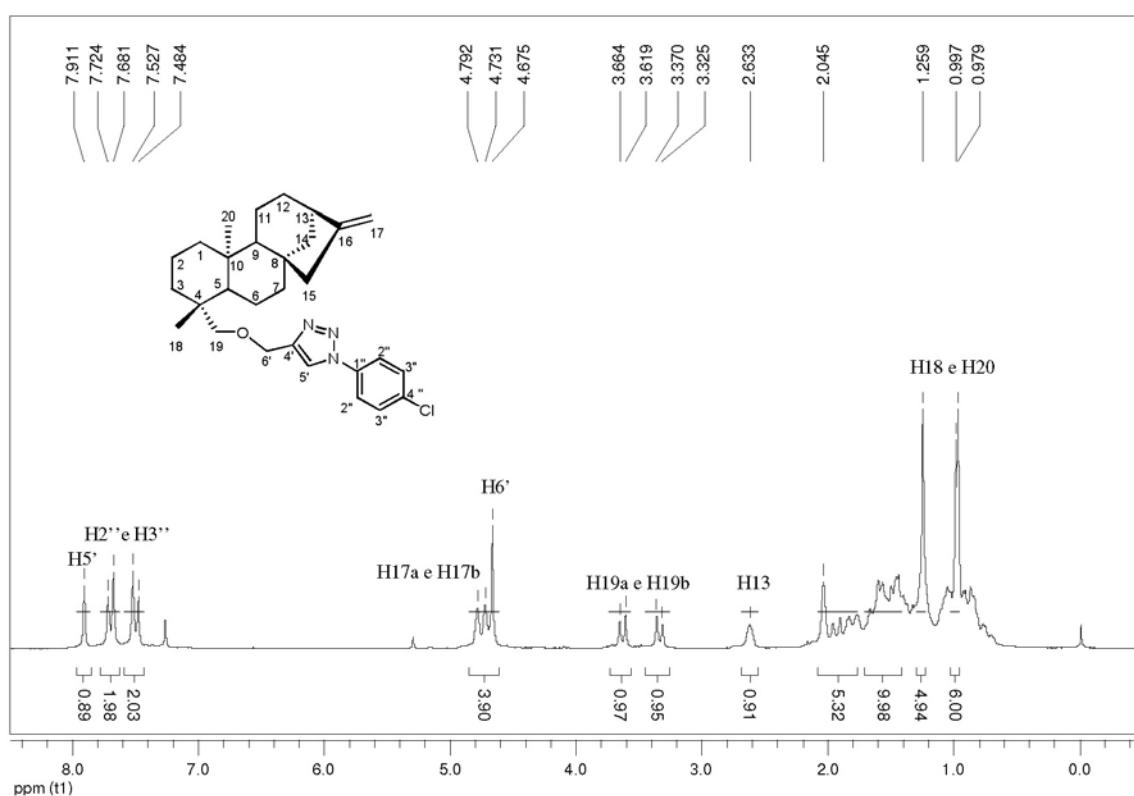
**Figure S29.** Infrared spectrum (ATR) of compound **21**.



**Figure S30.**  $^1\text{H}$  NMR spectrum (200 MHz,  $\text{CDCl}_3$ ) of compound 21.



**Figure S31.**  $^{13}\text{C}$  NMR spectrum and DEPT 135 (50 MHz,  $\text{CDCl}_3$ ) of compound 21.

**Figure S32.** Infrared spectrum (ATR) of compound 22.**Figure S33.** <sup>1</sup>H NMR spectrum (200 MHz, CDCl<sub>3</sub>) of compound 22.

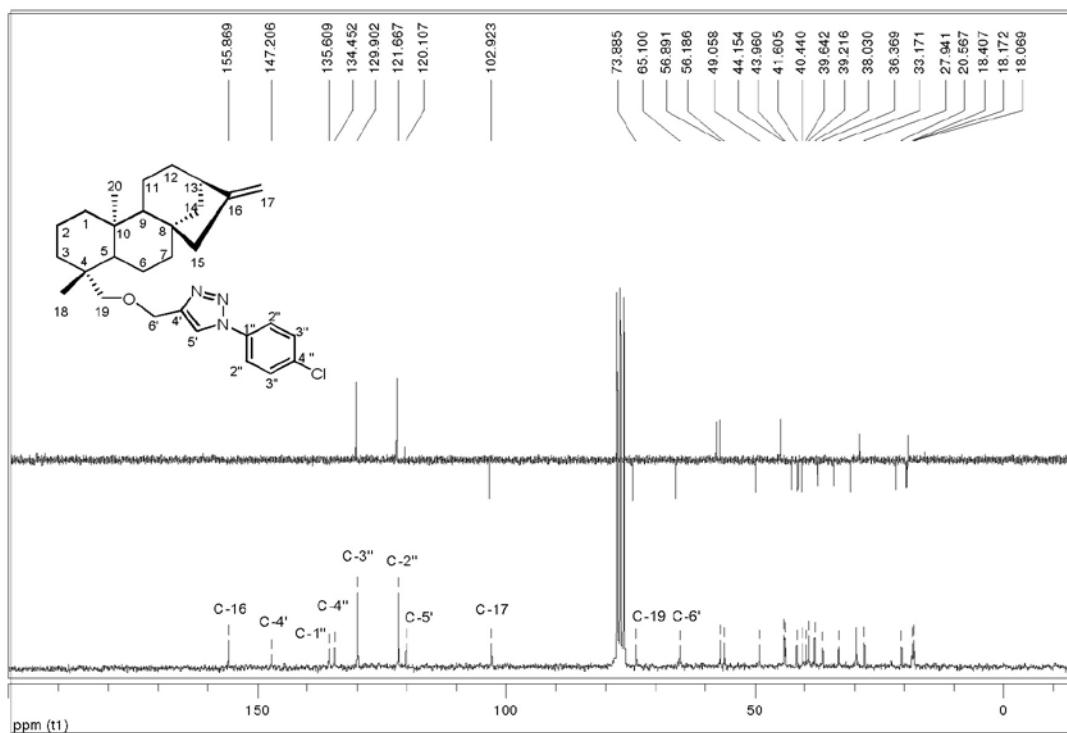


Figure S34. <sup>13</sup>C NMR spectrum and DEPT 135(50 MHz, CDCl<sub>3</sub>) of compound 22.

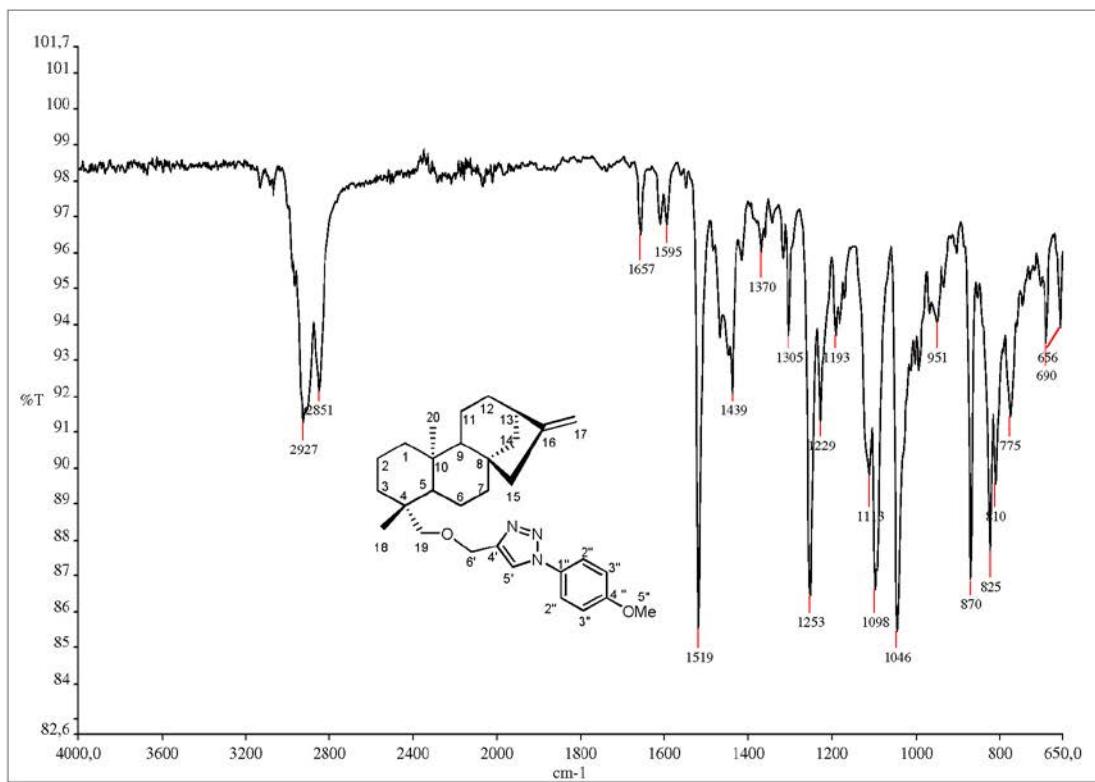
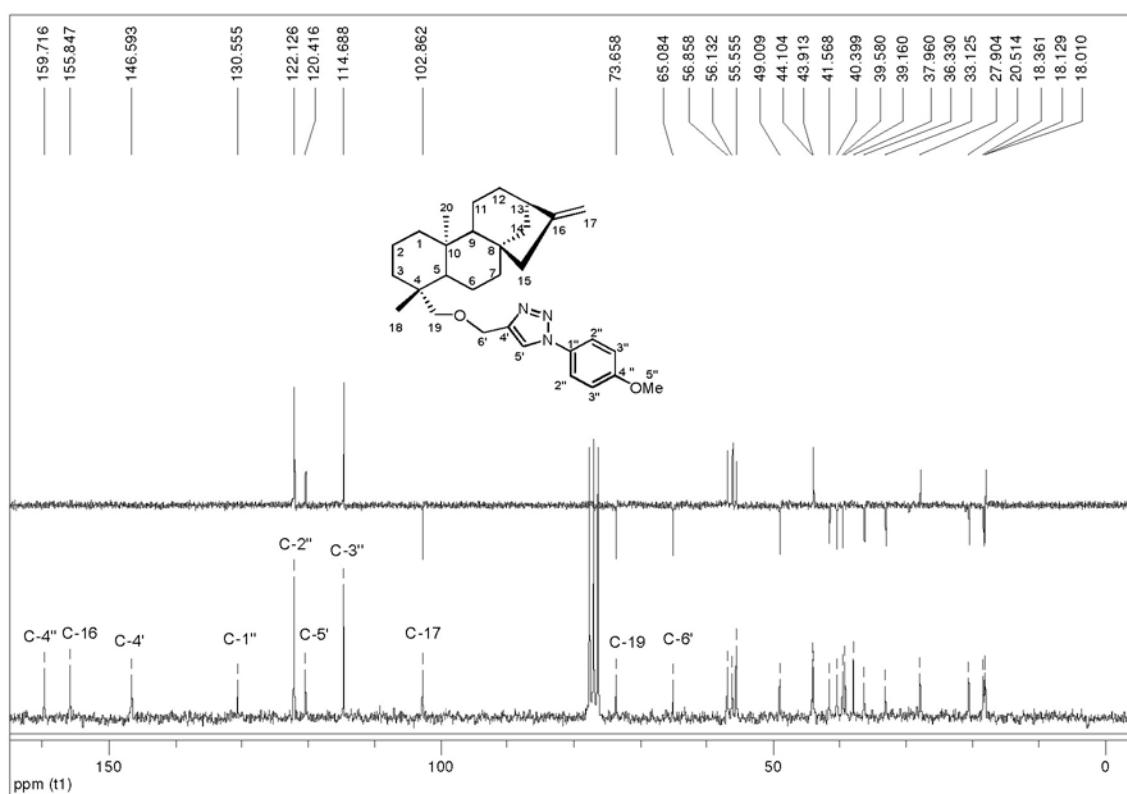
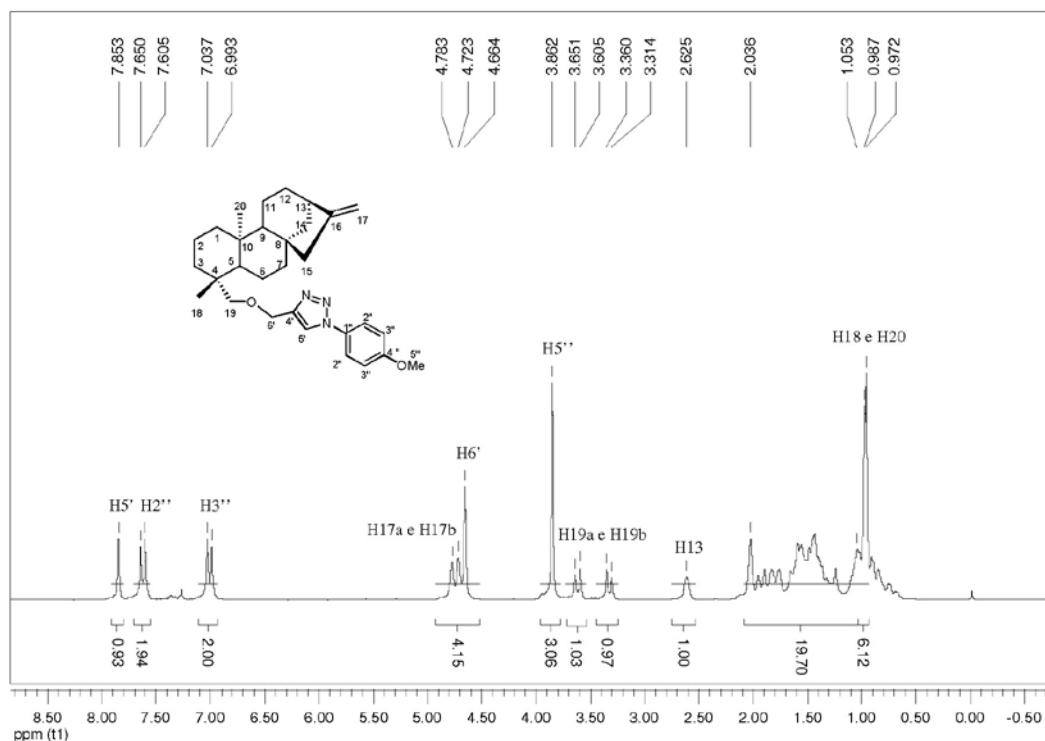
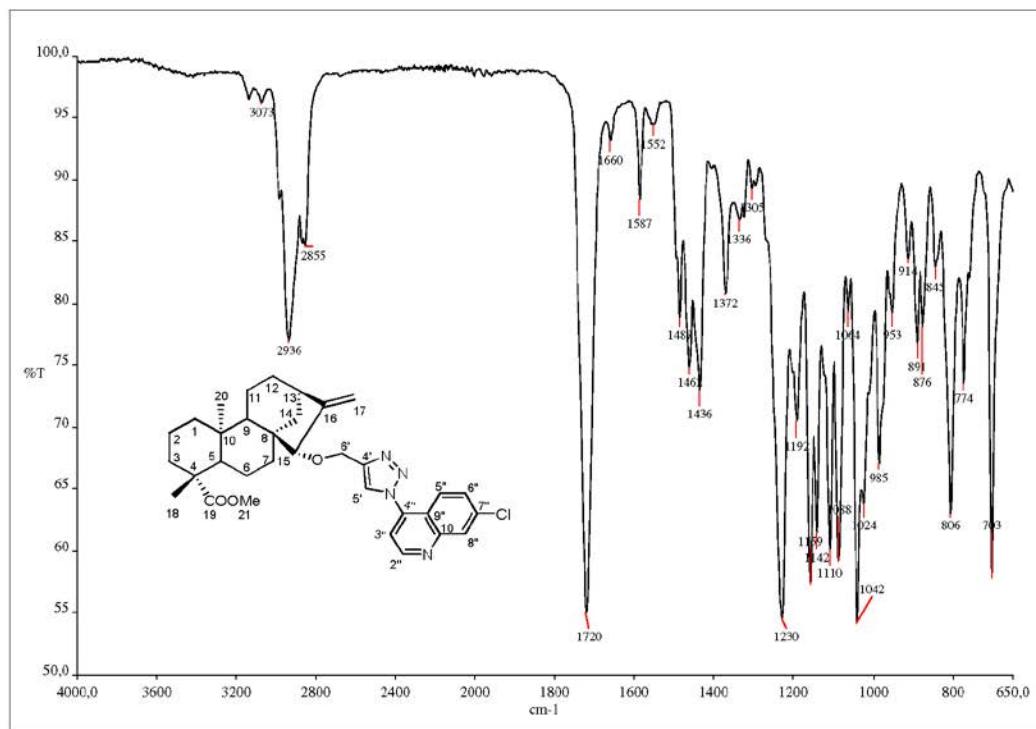
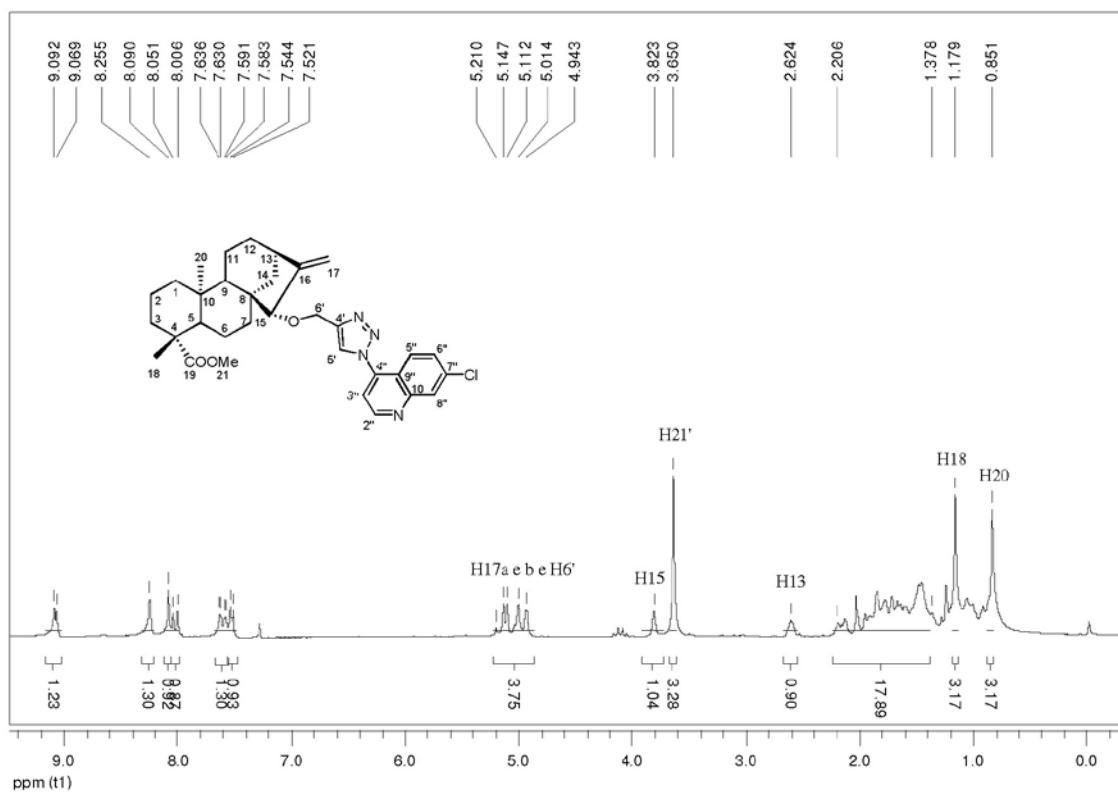


Figure S35. Infrared spectrum (ATR) of compound 23.

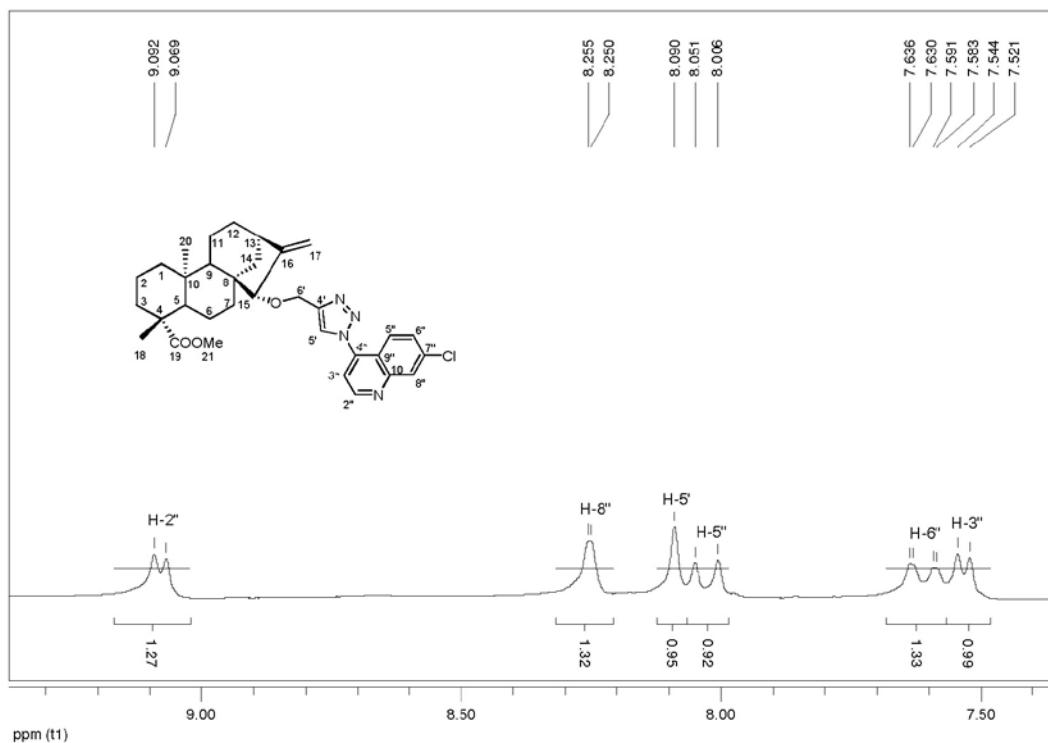




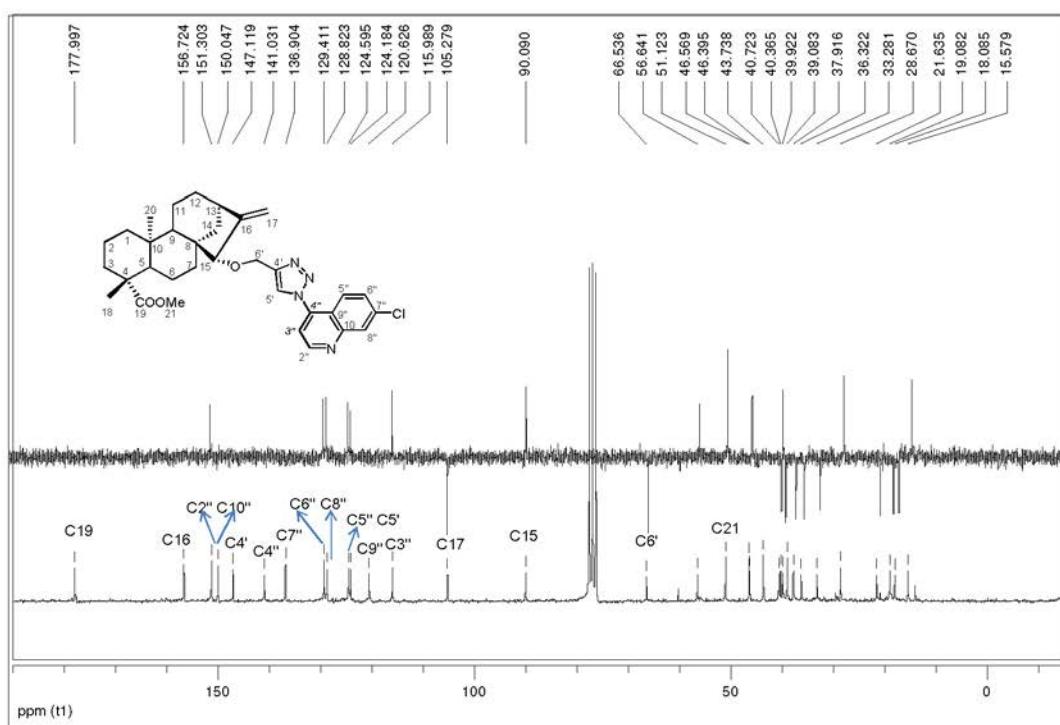
**Figure S38.** Infrared spectrum (ATR) of compound 24.



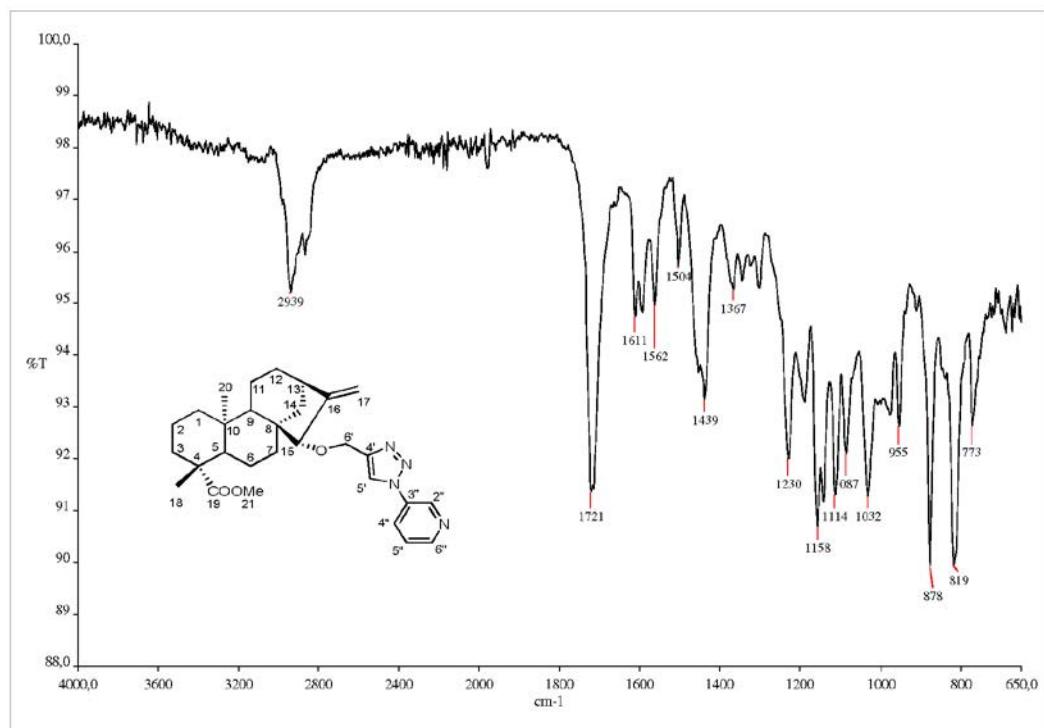
**Figure S39.**  $^1\text{H}$  NMR spectrum (200 MHz,  $\text{CDCl}_3$ ) of compound 24.



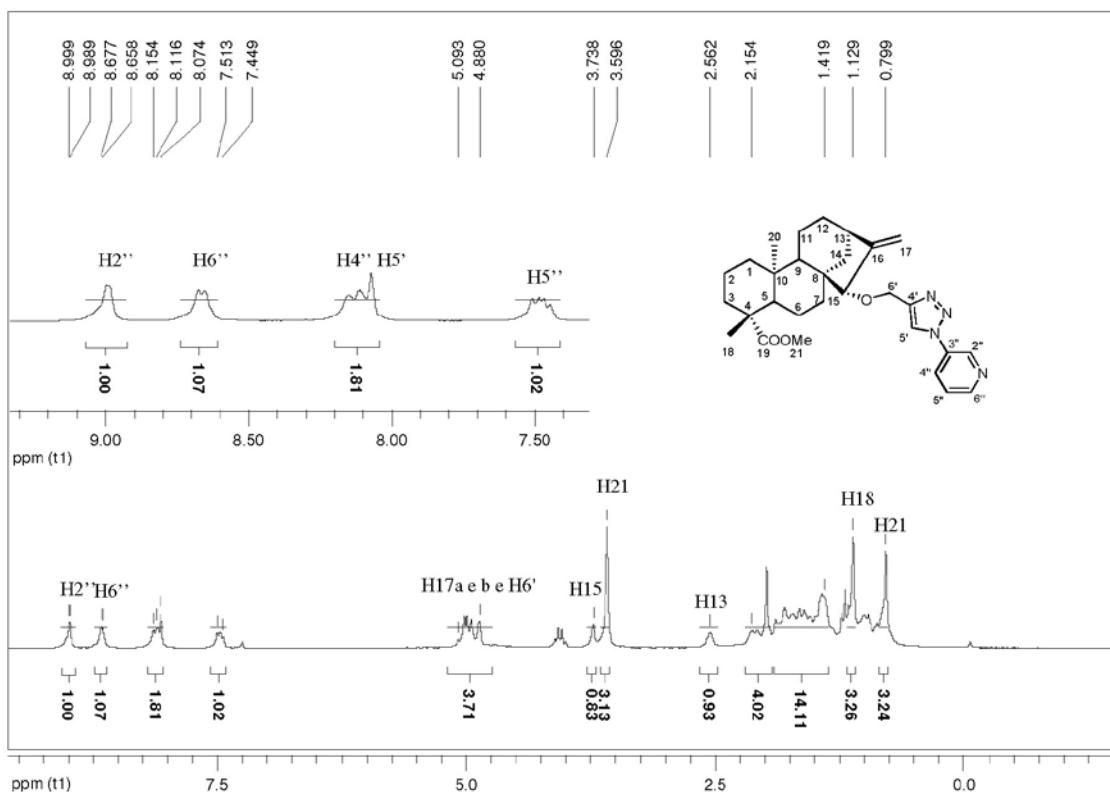
**Figure S40.**  $^1\text{H}$  NMR spectrum (200 MHz,  $\text{CDCl}_3$ ) of compound **24**. Expansion of the region between 7.4 and 9.3 ppm.



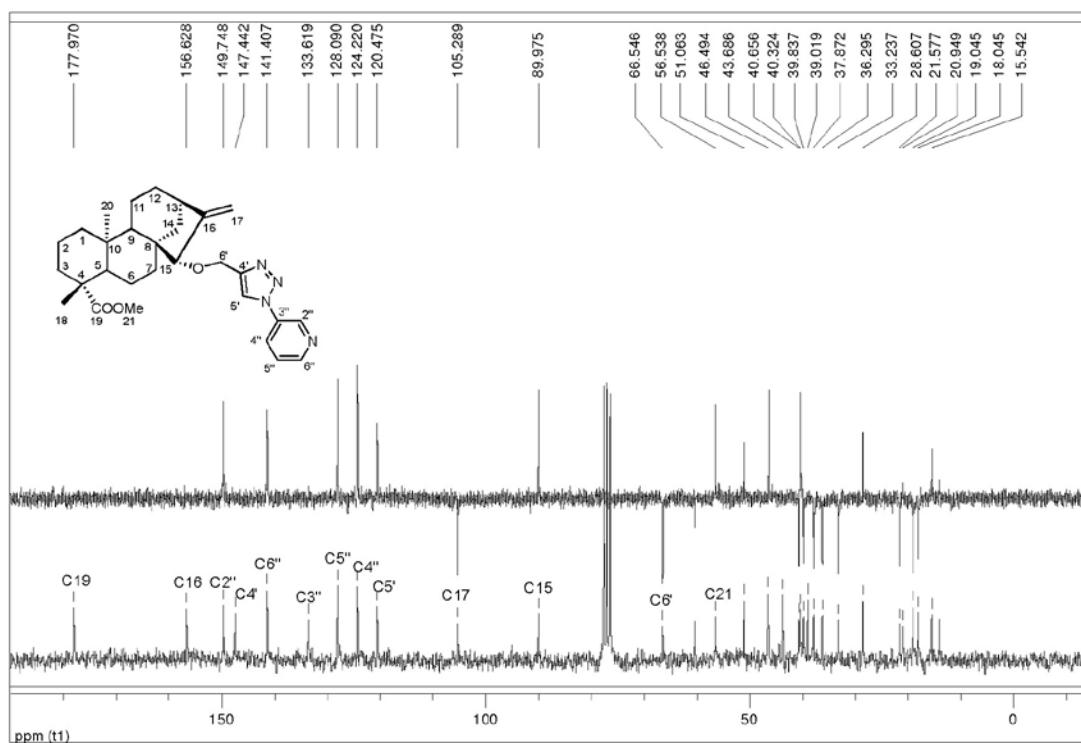
**Figure S41.**  $^{13}\text{C}$  NMR spectrum and DEPT 135 (50 MHz,  $\text{CDCl}_3$ ) of compound **24**.



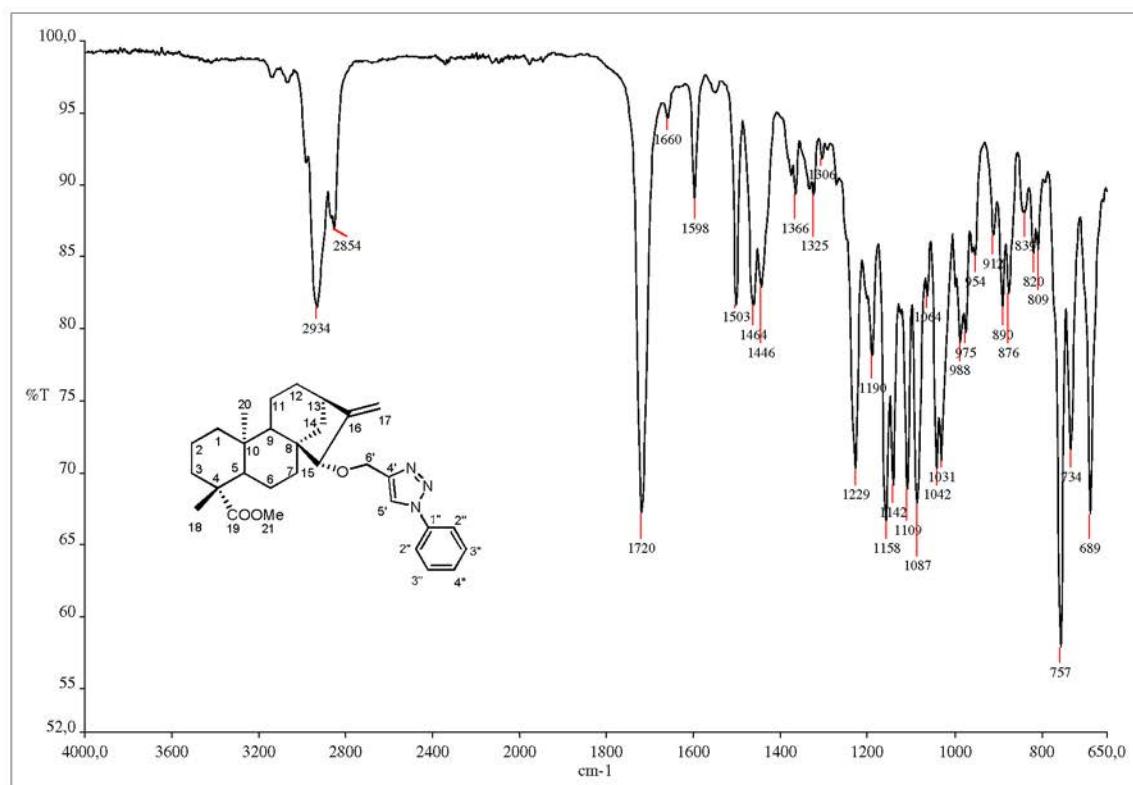
**Figure S42.** Infrared spectrum (ATR) of compound 25.



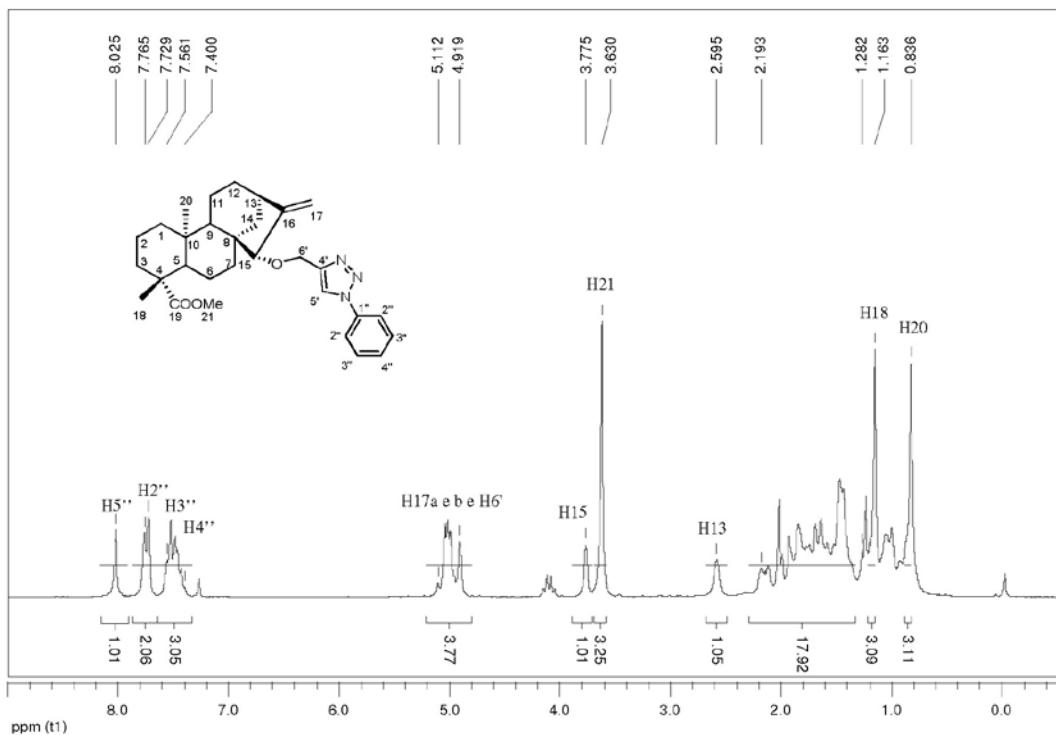
**Figure S43.** <sup>1</sup>H NMR spectrum (200 MHz, CDCl<sub>3</sub>) of compound 25.



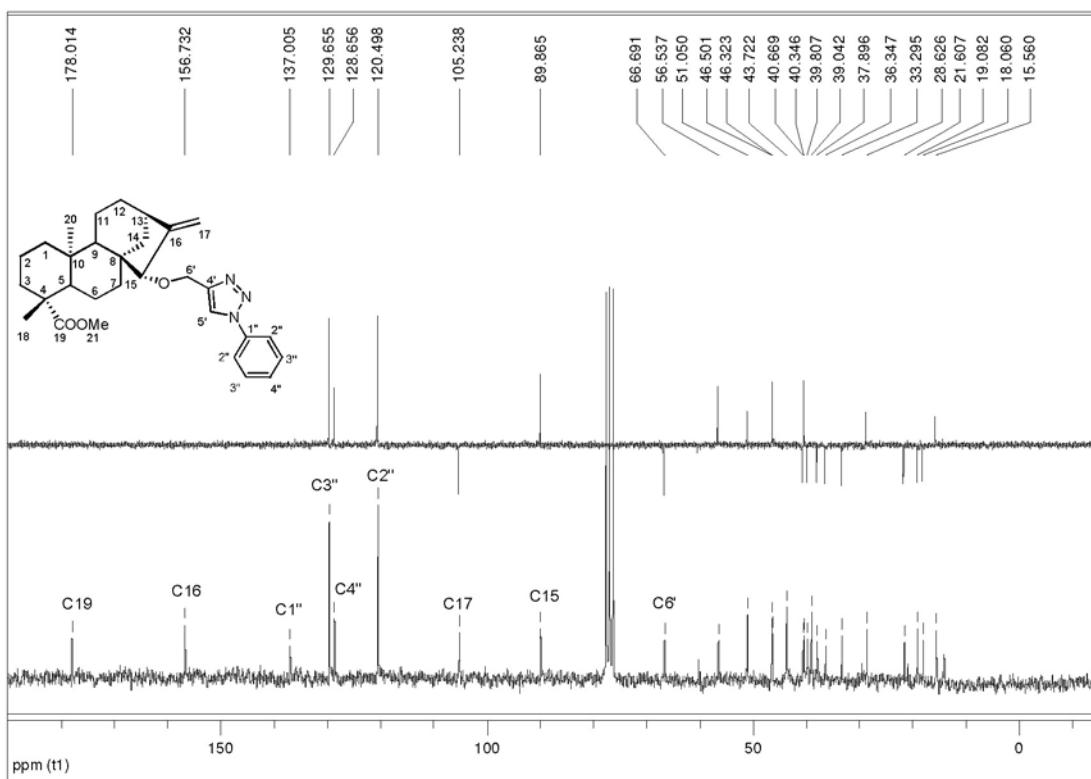
**Figure S44.**  $^{13}\text{C}$  NMR spectrum and DEPT 135 (50 MHz,  $\text{CDCl}_3$ ) of compound **25**.



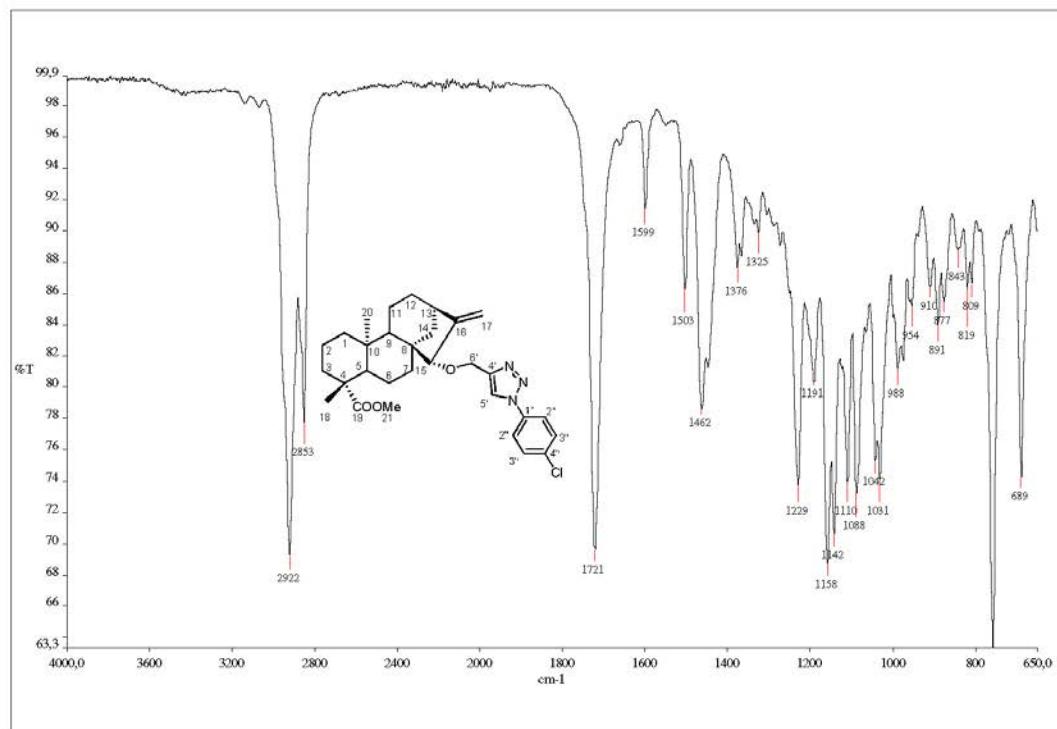
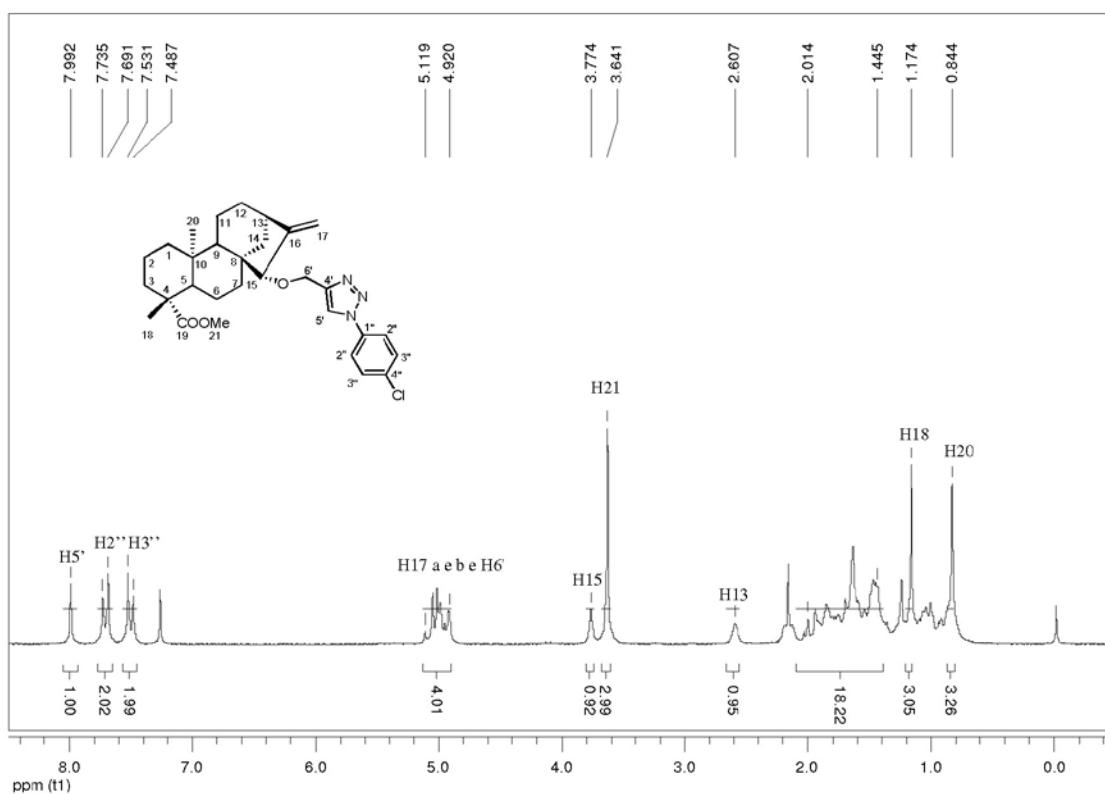
**Figure S45.** Infrared spectrum (ATR) of compound **26**.

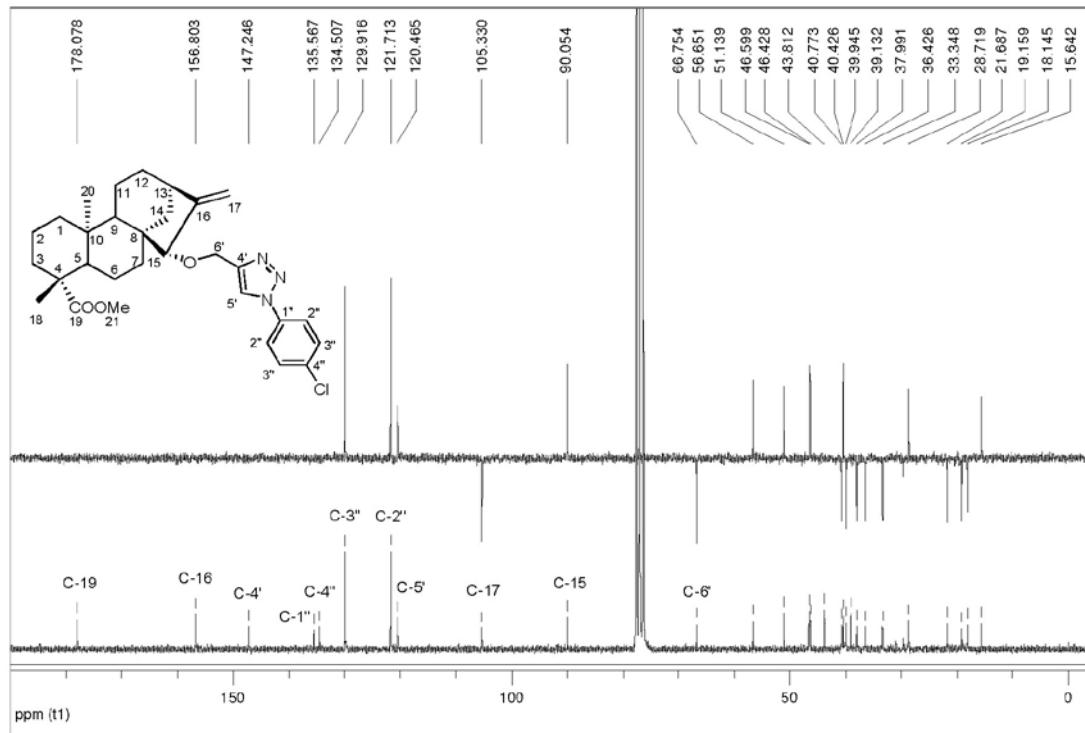


**Figure S46.**  $^1\text{H}$  NMR spectrum (200 MHz,  $\text{CDCl}_3$ ) of compound 26.

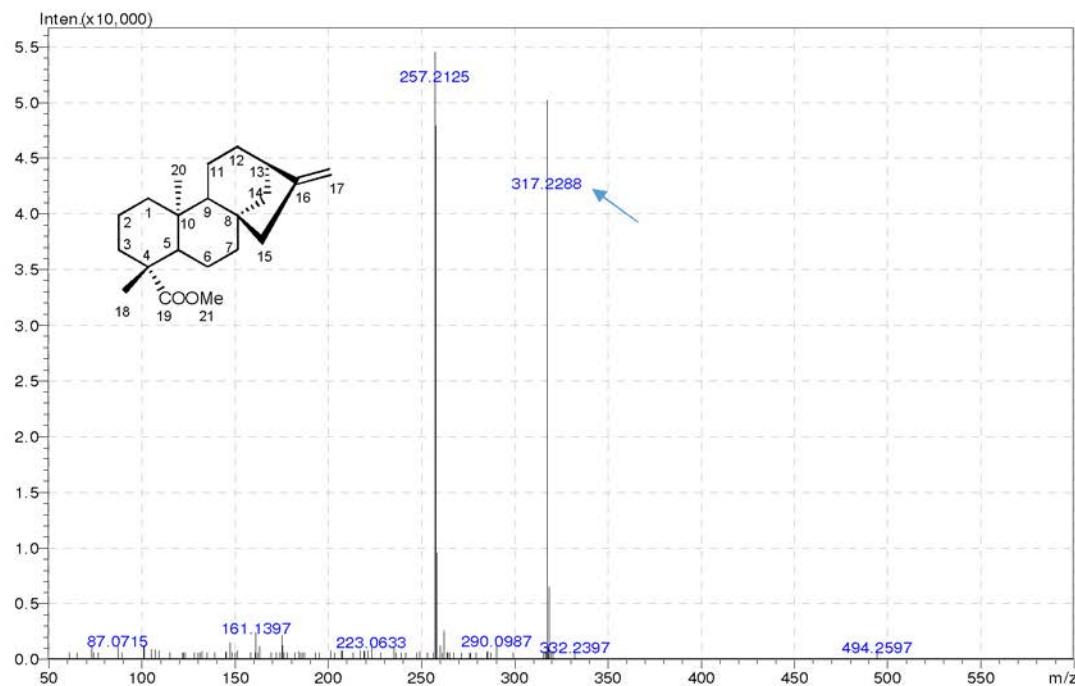


**Figure S47.**  $^{13}\text{C}$  NMR spectrum and DEPT 135 (50 MHz,  $\text{CDCl}_3$ ) of compound 26.

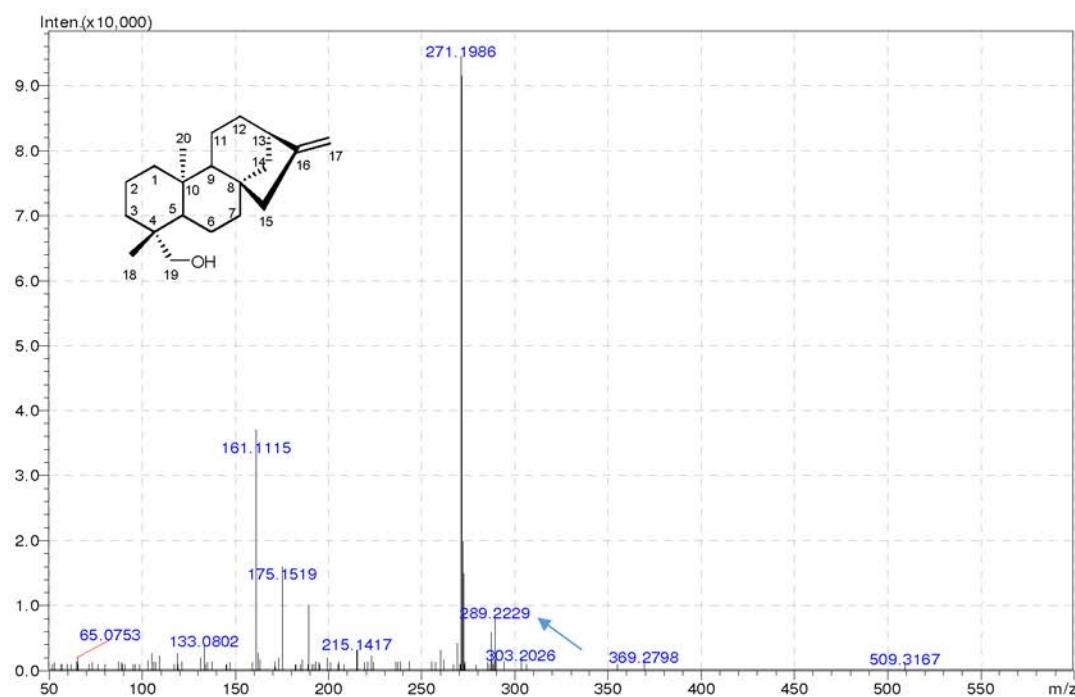
**Figure S48.** Infrared spectrum (ATR) of compound 27.**Figure S49.** <sup>1</sup>H NMR spectrum (200 MHz, CDCl<sub>3</sub>) of compound 27.



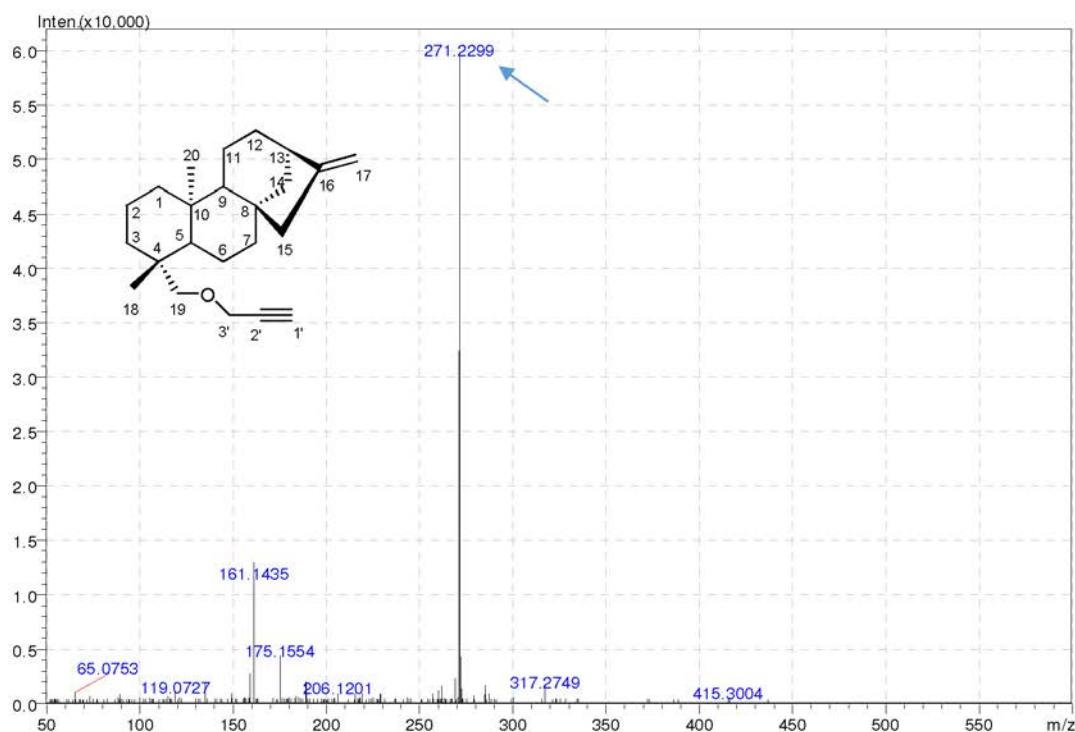
**Figure S50.**  $^{13}\text{C}$  NMR spectrum and DEPT 135 (50 MHz,  $\text{CDCl}_3$ ) of compound 27.



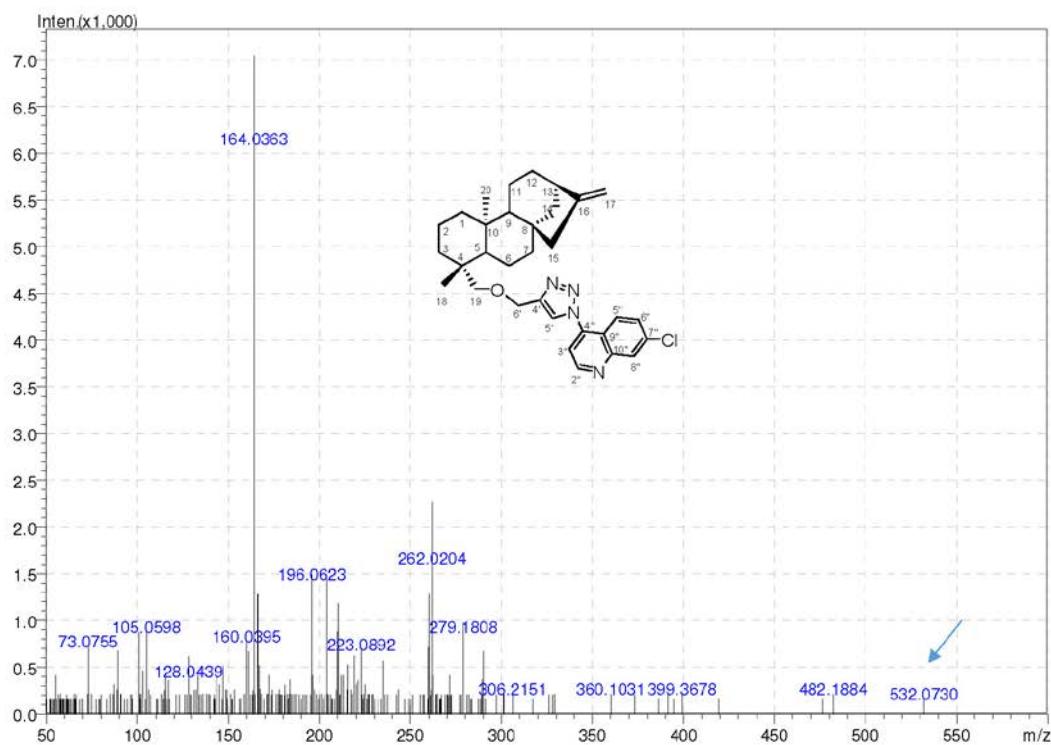
**Figure S51.** HRMS spectrum of compound 8.



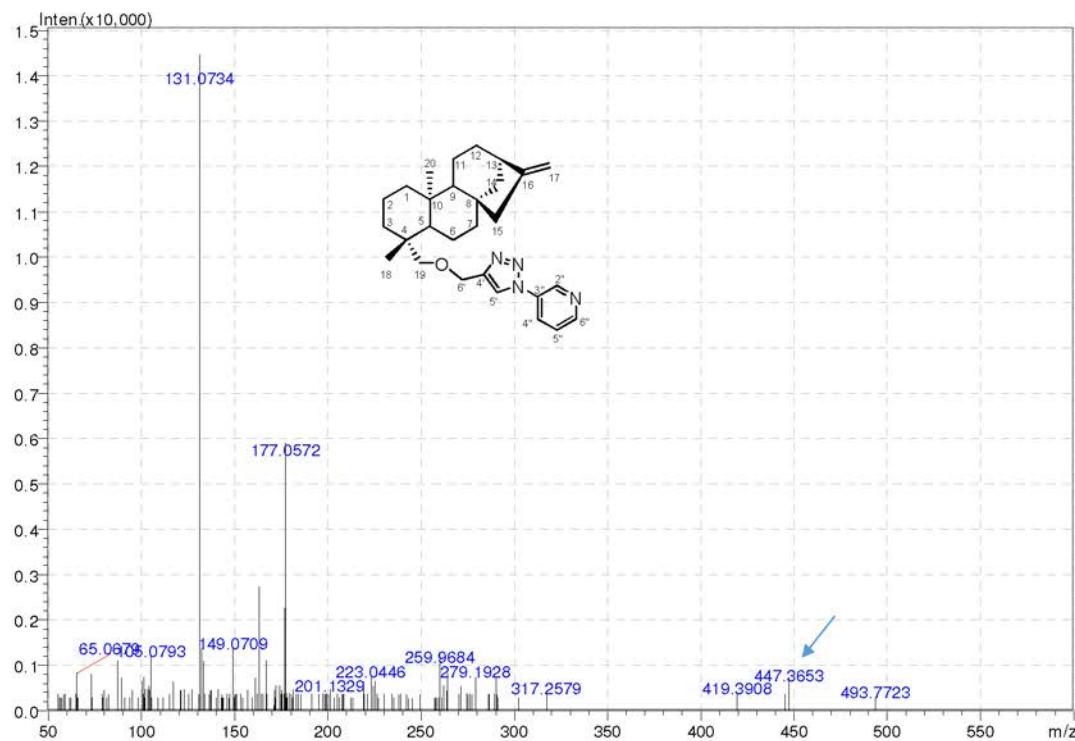
**Figure S52.** HRMS spectrum of compound 9.



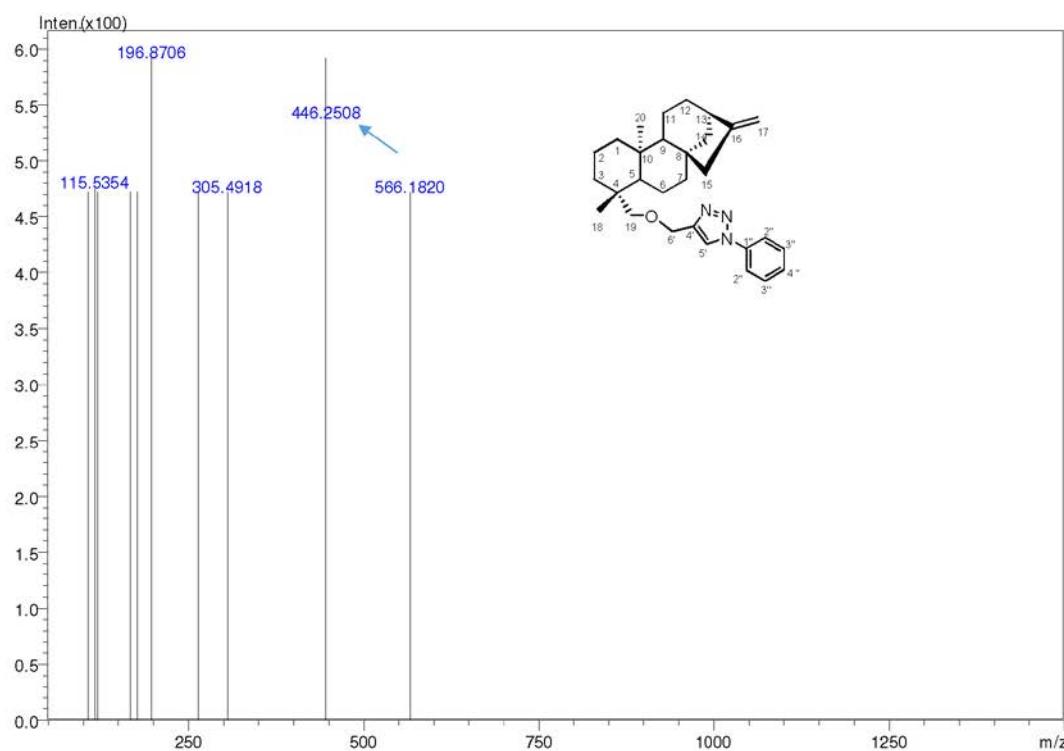
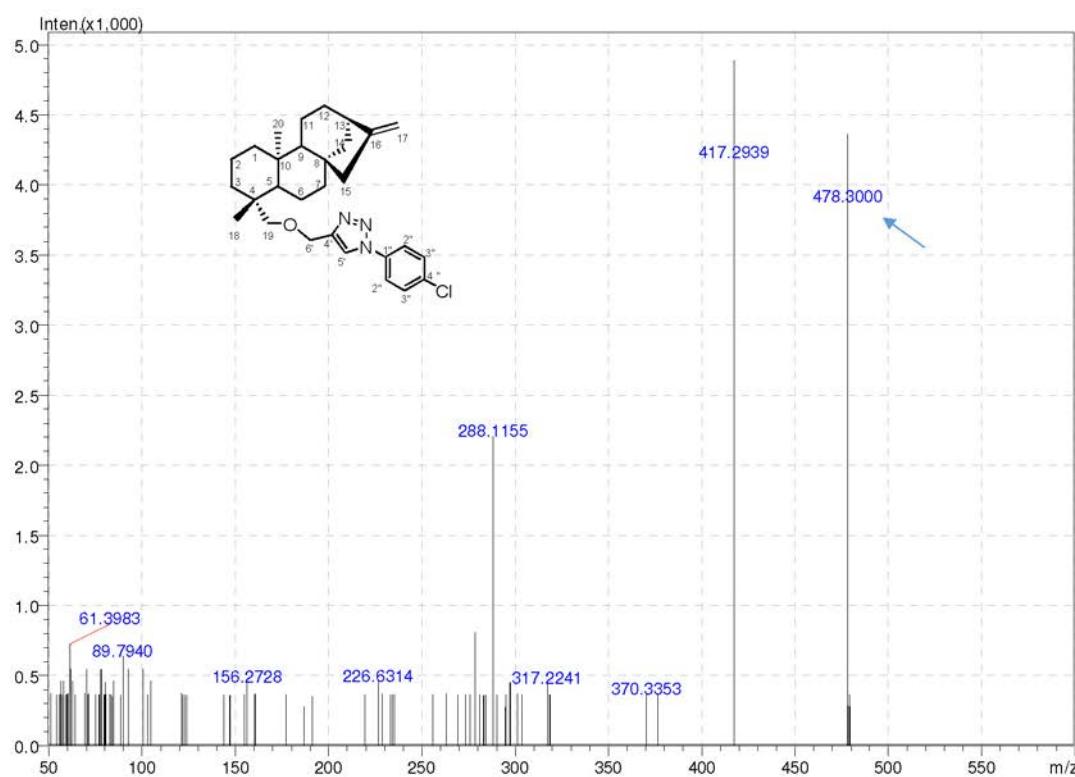
**Figure S53.** HRMS spectrum of compound 10.

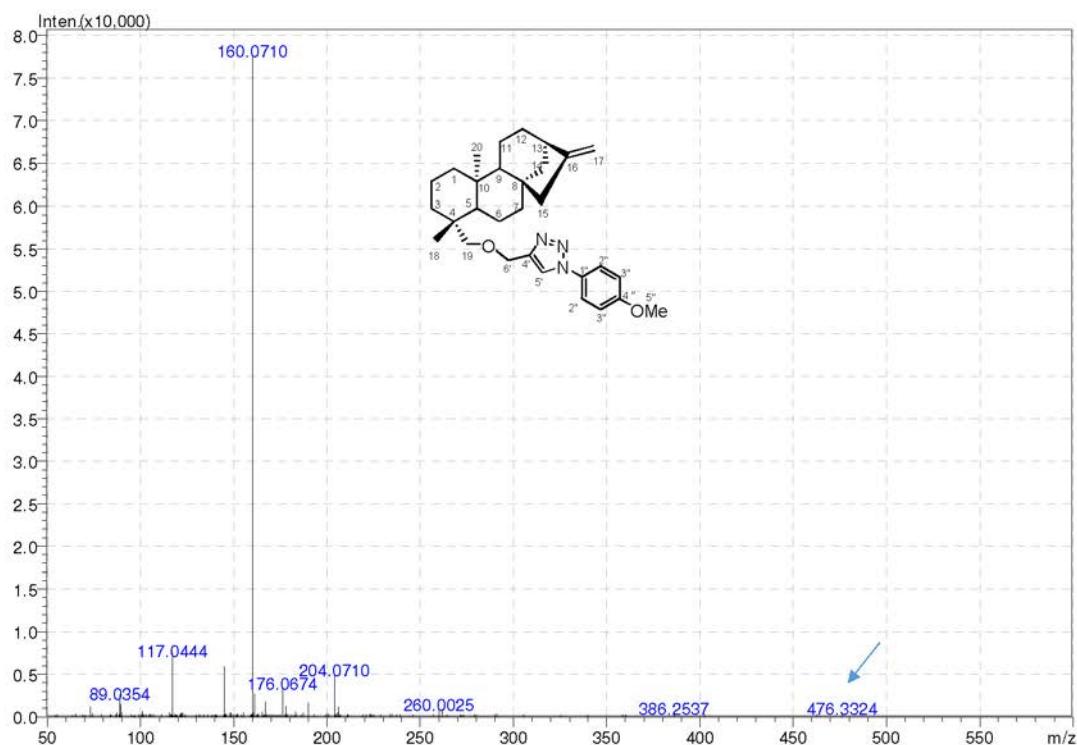


**Figure S54.** HRMS spectrum of compound 19.

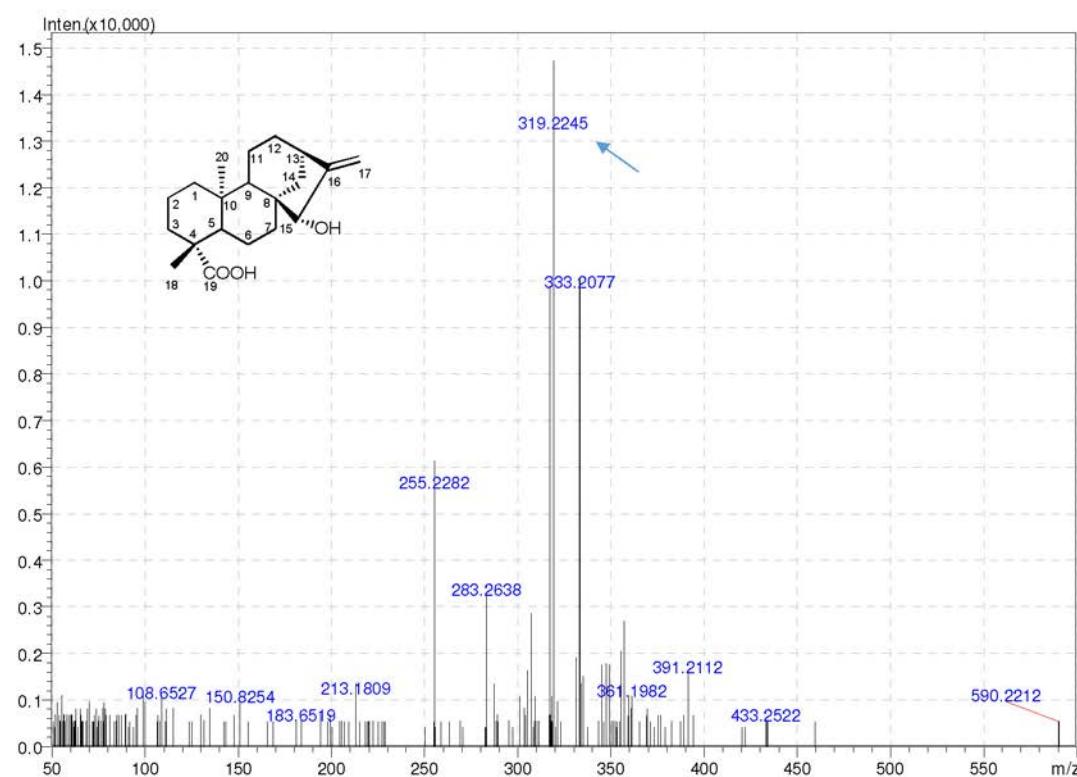


**Figure S55.** HRMS spectrum of compound 20.

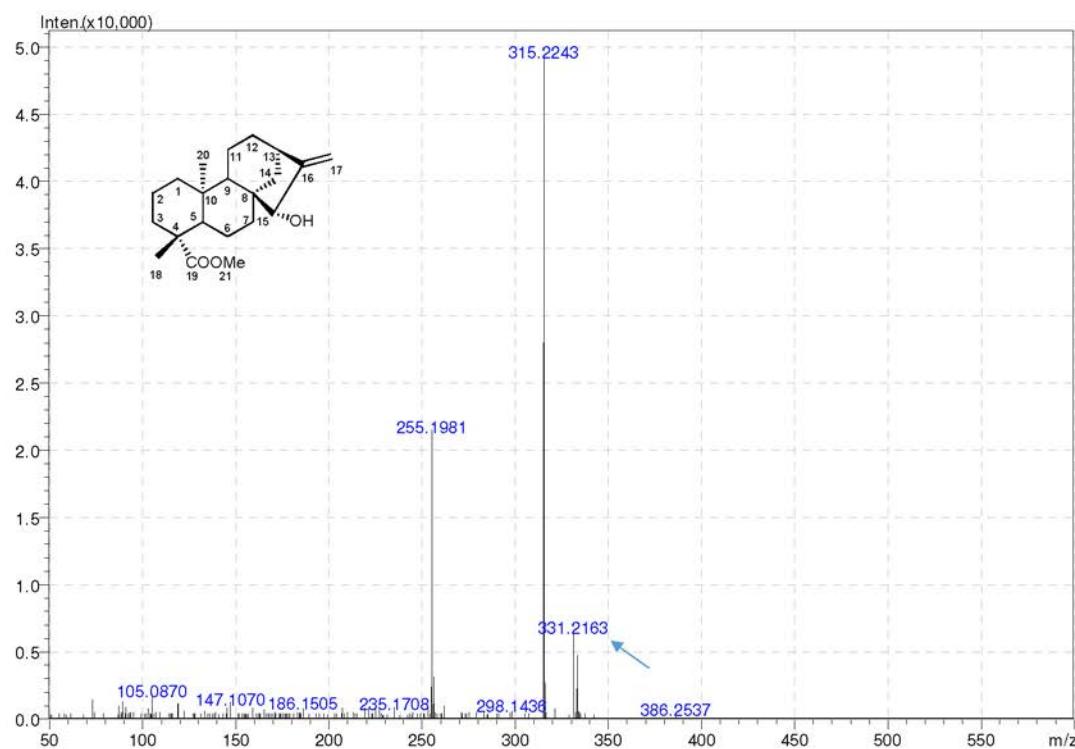
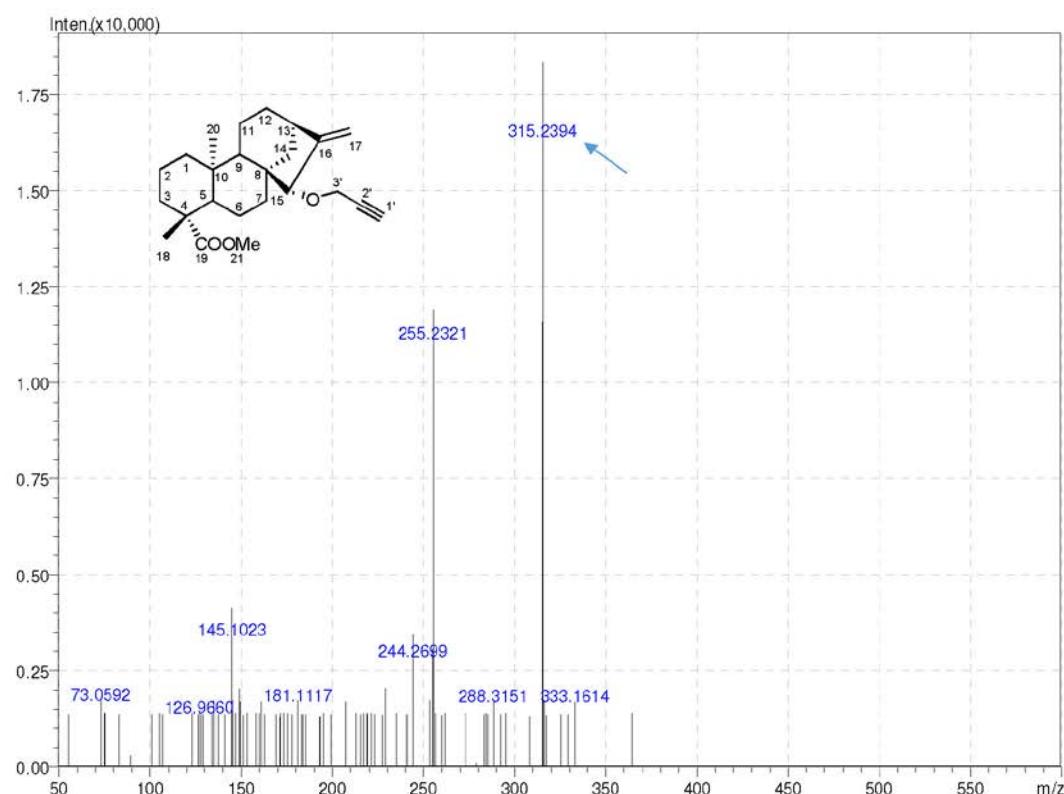
**Figure S56.** HRMS spectrum of compound 21.**Figure S57.** HRMS spectrum of compound 22.

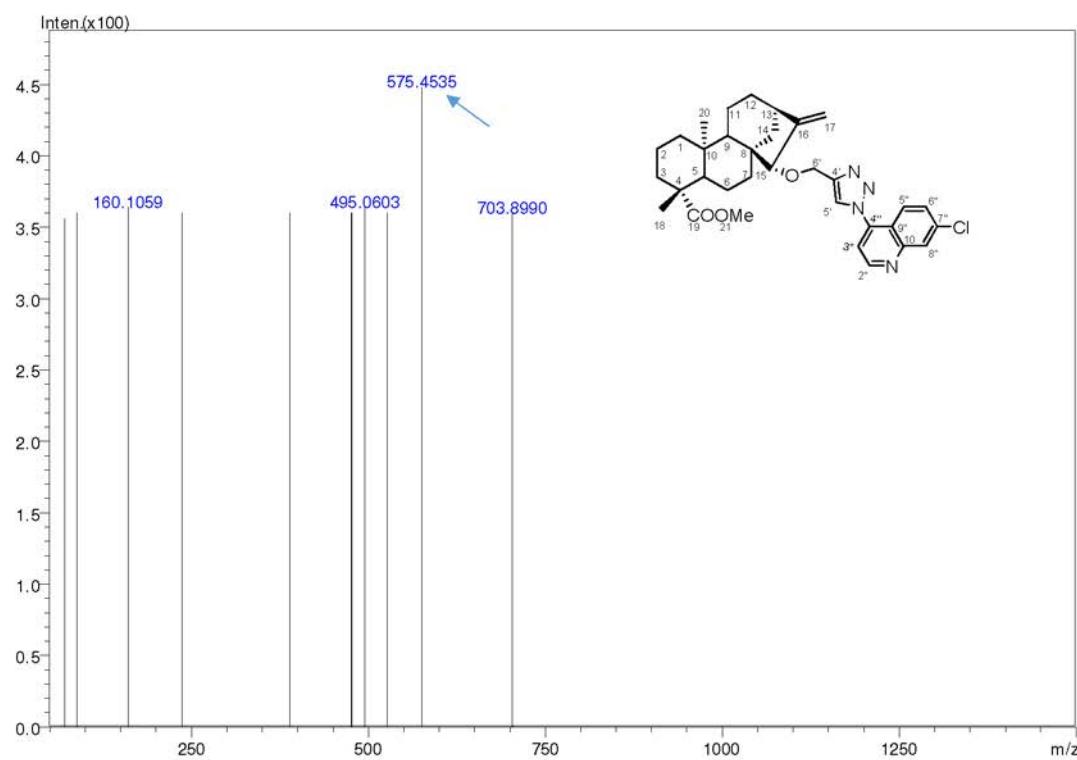


**Figure S58.** HRMS spectrum of compound 23.

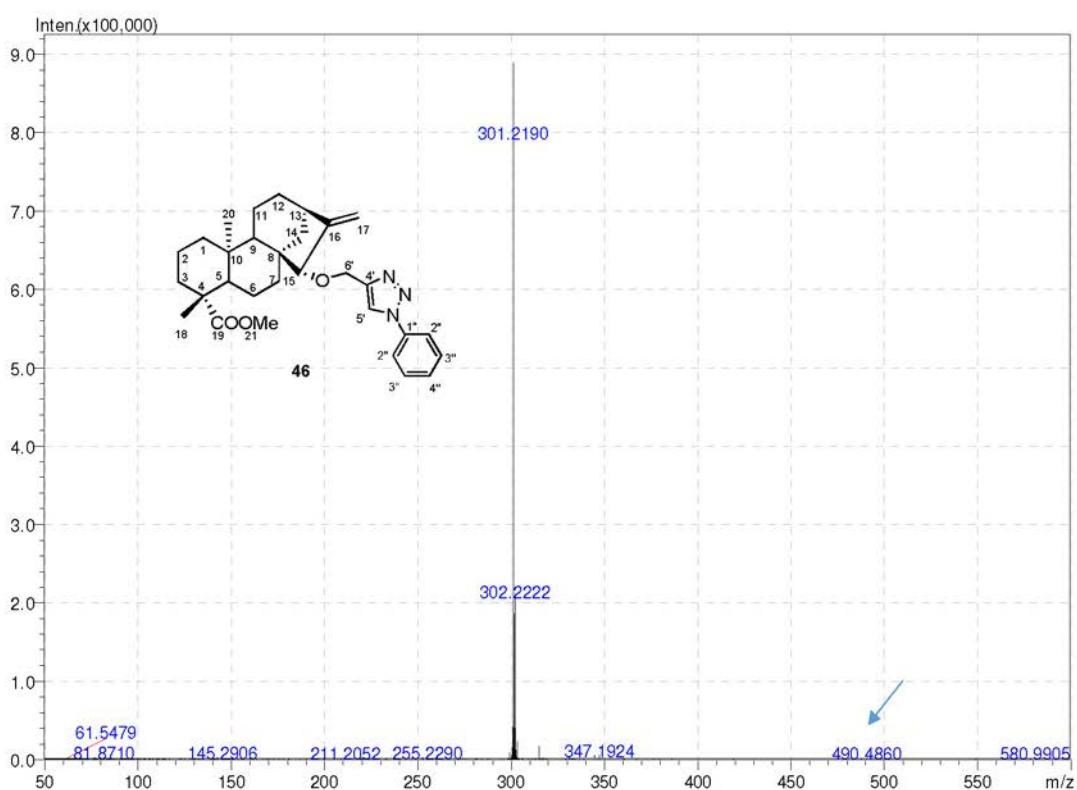


**Figure S59.** HRMS spectrum of compound 11.

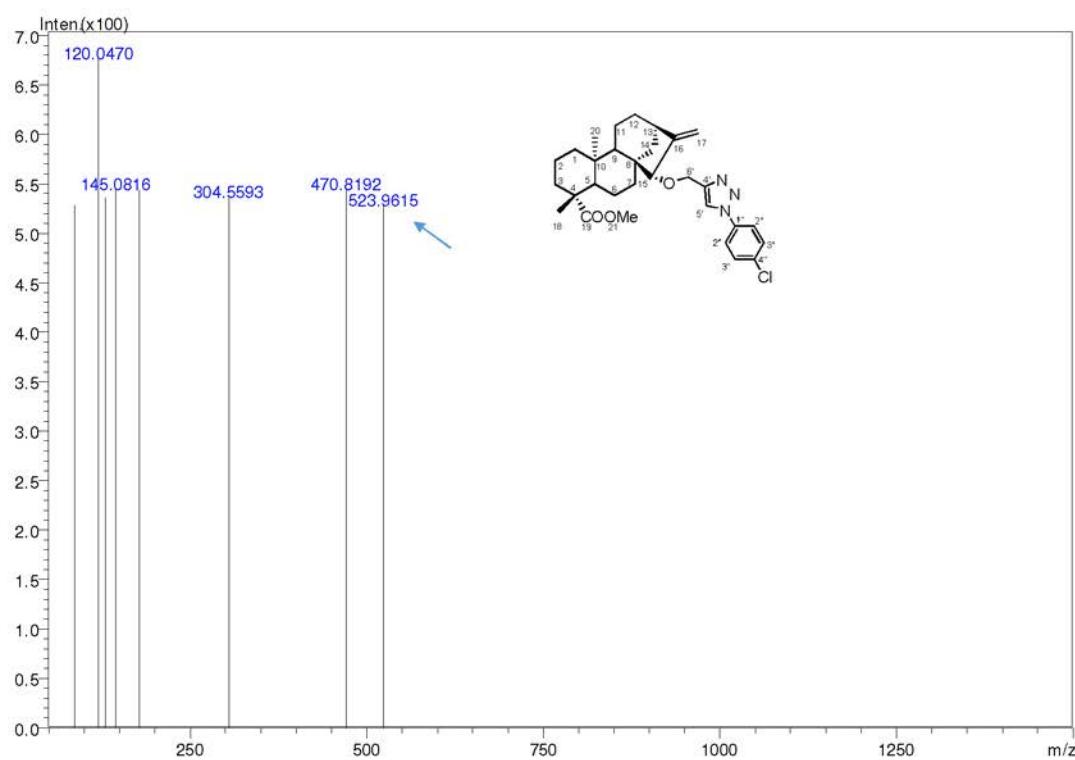
**Figure S60.** HRMS spectrum of compound 12.**Figure S61.** HRMS spectrum of compound 13.



**Figure S62.** HRMS spectrum of compound 24.



**Figure S63.** HRMS spectrum of compound 26.



**Figure S64.** HRMS spectrum of compound 27.