

# Supplementary Information

## Chemical Constituents from Branches of *Maytenus gonoclada* (Celastraceae) and Evaluation of Antimicrobial Activity

*Fernando C. Silva,<sup>a,c</sup> Lucienir P. Duarte,<sup>\*a</sup> Grácia D. F. Silva,<sup>a</sup> Sidney A. V. Filho,<sup>a,b</sup>  
Ivana S. Lula,<sup>a</sup> Jacqueline A. Takahashi<sup>c</sup> and William S. T. Sallum<sup>c</sup>*

<sup>a</sup>Núcleo de Estudos de Plantas Medicinais and <sup>c</sup>Laboratório de Biotecnologia e Bioensaios,  
Departamento de Química, Universidade Federal de Minas Gerais,  
Av. Antônio Carlos, 6627, Pampulha, 31270-901 Belo Horizonte-MG, Brazil

<sup>b</sup>Escola de Farmácia, Universidade Federal de Ouro Preto, Rua Costa Sena, 171,  
35400-000 Ouro Preto-MG, Brazil

**Table S1.** Antimicrobial activities of hexane extract and compounds **1**, **3**, **5** and **6** (each concentration at 100 µg/mL)

Samples	Inhibition zone diameter (mm)			
	<i>E. coli</i>	<i>C. freundii</i>	<i>B. cereus</i>	<i>C. albicans</i>
Hexane extract	ND	ND	ND	8
Compound <b>1</b>	ND	ND	ND	ND
Compound <b>3</b>	ND	ND	ND	ND
Compound <b>5</b>	ND	ND	ND	ND
Compound <b>6</b>	ND	ND	ND	ND
Chloroform <sup>a</sup>	ND	ND	ND	ND
Cloranfenicol <sup>b</sup>	22	29	20	-
Miconazole <sup>c</sup>	-	-	-	17

<sup>a</sup>Negative control; <sup>b</sup>Positive control (bacteria); <sup>c</sup>Positive control (fungus); ND (Not Detected).

**Table S2.** Antimicrobial activities of hexane extract and compounds **3**

Samples	Minimum Inhibitory Concentration (µg/mL)			
	<i>E. coli</i>	<i>C. freundii</i>	<i>B. cereus</i>	<i>C. albicans</i>
Hexane extract	ND	ND	ND	512
Compound <b>3</b>	ND	ND	ND	512
DMSO <sup>a</sup>	ND	ND	ND	ND
Cloranfenicol <sup>b</sup>	8	4	8	-
Miconazole <sup>c</sup>	-	-	-	16

<sup>a</sup>Negative control; <sup>b</sup>Positive control (bacteria); <sup>c</sup>Positive control (fungus); ND (Not Detected).

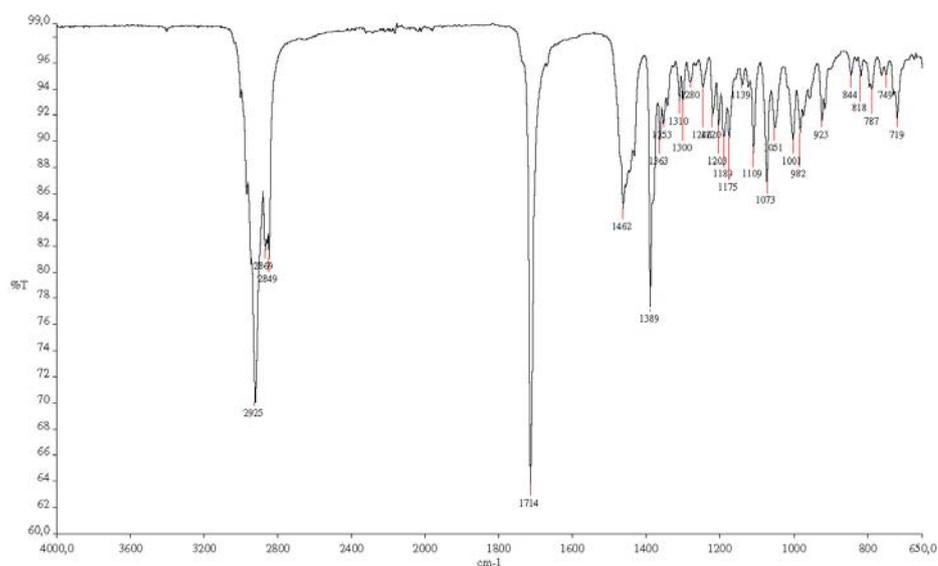


Figure S1. IR spectrum of compound 1 (ATR).

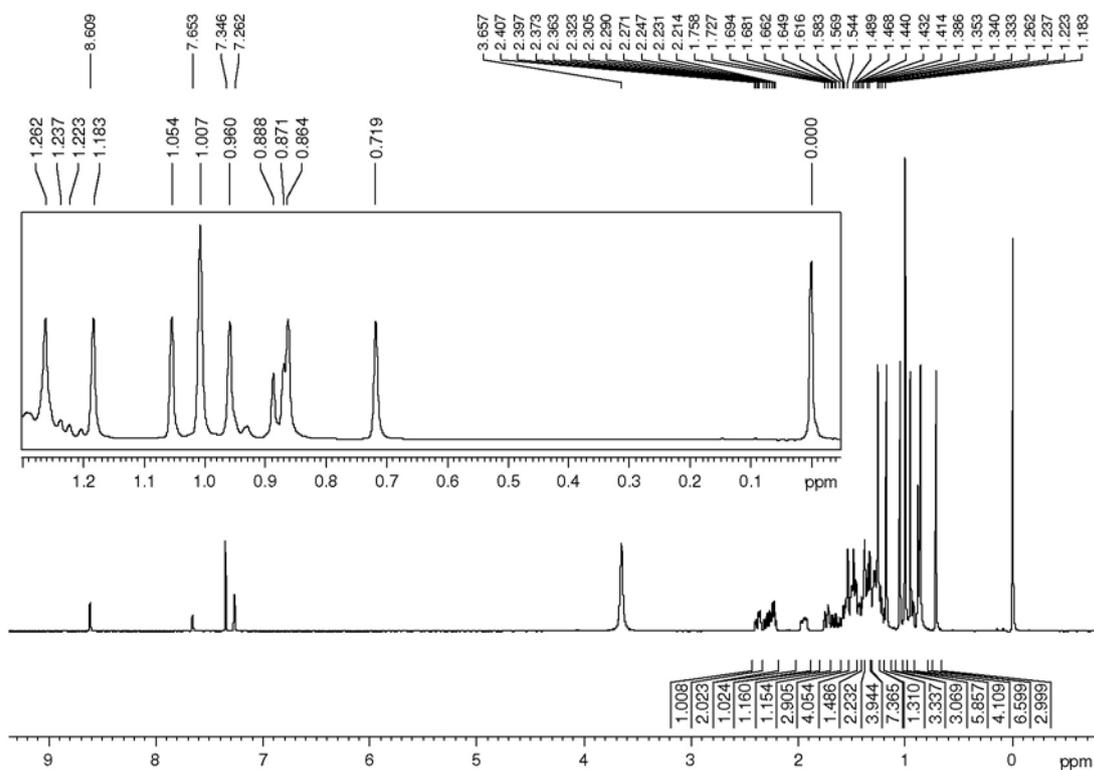
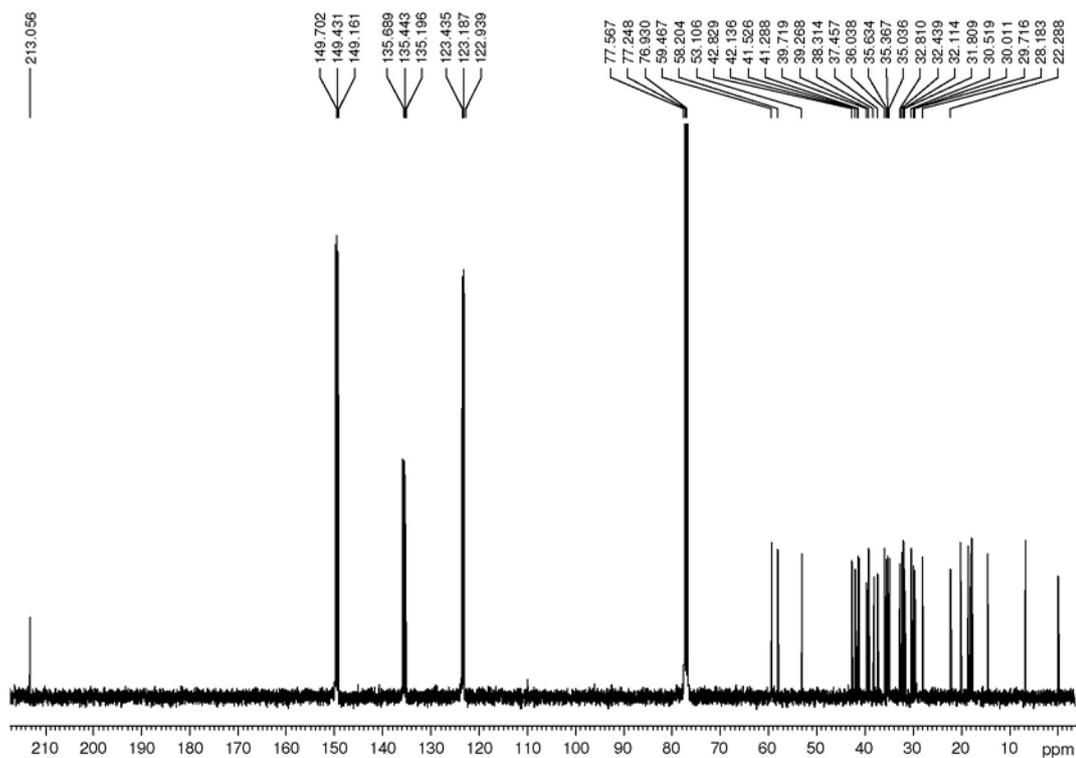
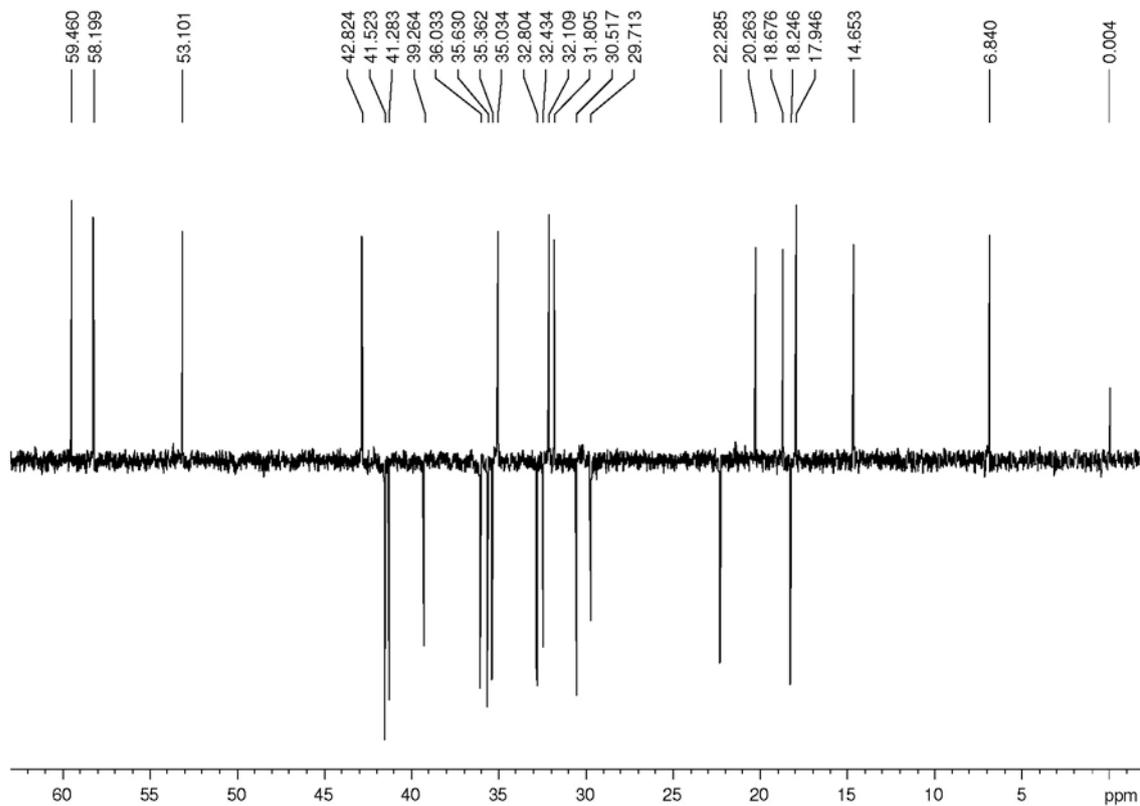


Figure S2.  $^1\text{H}$  NMR spectrum of compound 1 ( $\text{CDCl}_3$  + pyridine- $d_3$ , 400 MHz).



**Figure S3.** <sup>13</sup>C NMR spectrum of compound **1** (CDCl<sub>3</sub> + pyridine-*d*<sub>5</sub>, 100 MHz).



**Figure S4.** <sup>13</sup>C NMR-DEPT spectrum of compound **1** (CDCl<sub>3</sub> + pyridine-*d*<sub>5</sub>, 100 MHz).

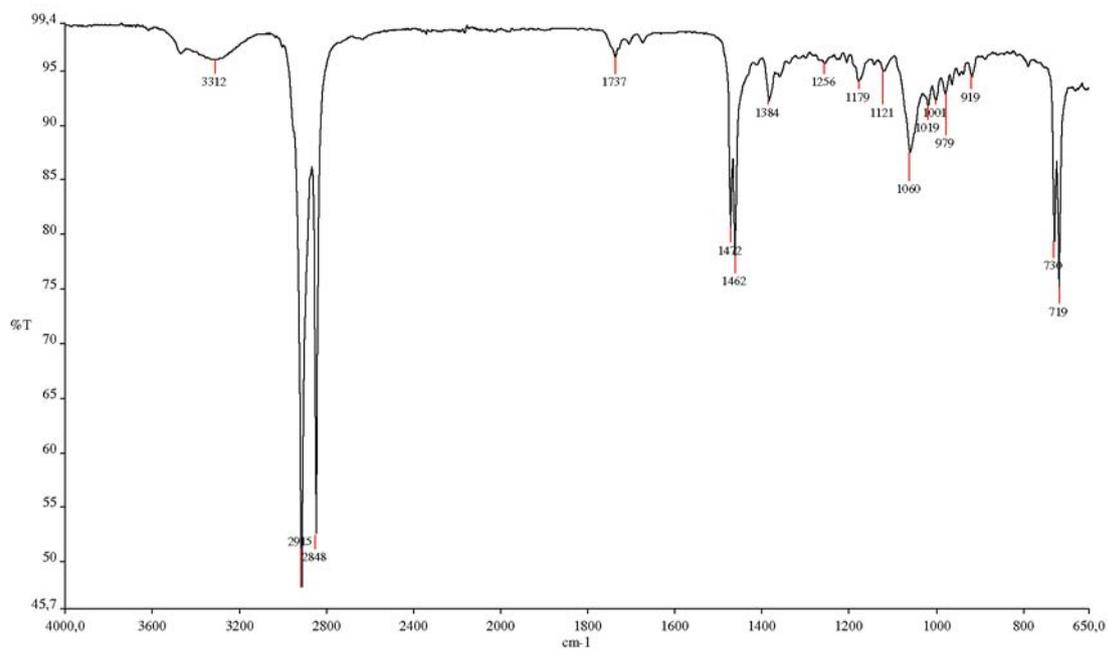


Figure S5. IR spectrum of compound 2 (ATR).

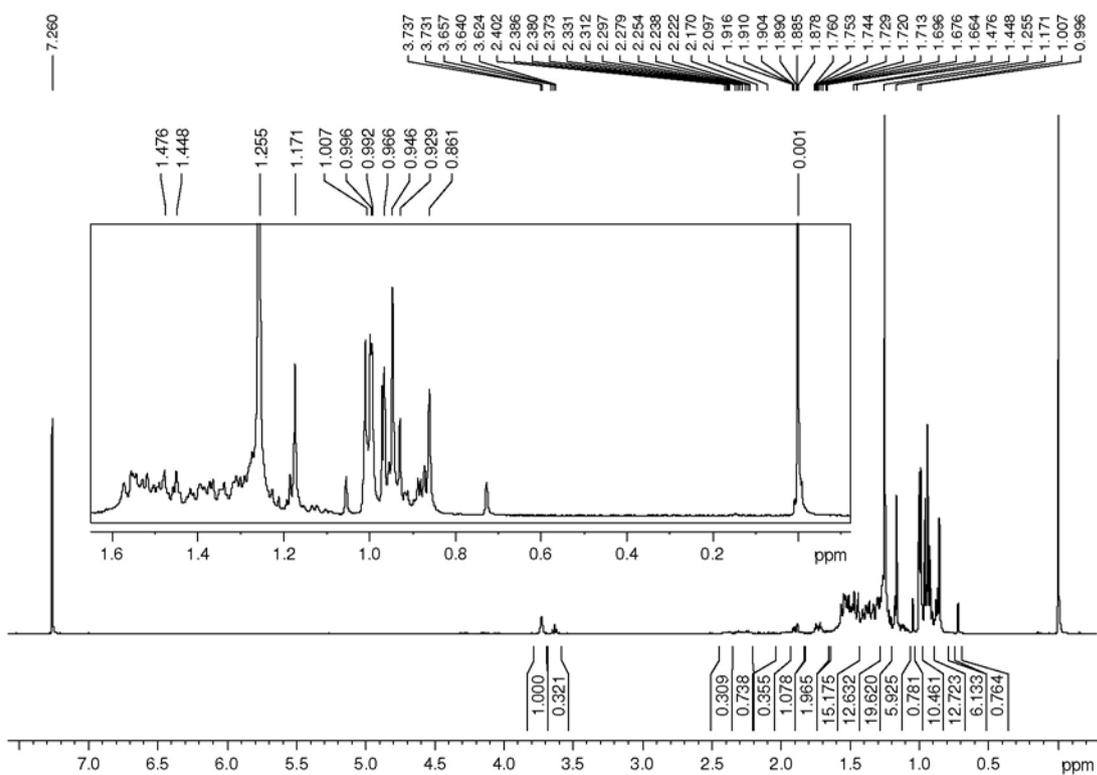


Figure S6.  $^1\text{H}$  NMR spectrum of compound 2 ( $\text{CDCl}_3$ , 400 MHz).

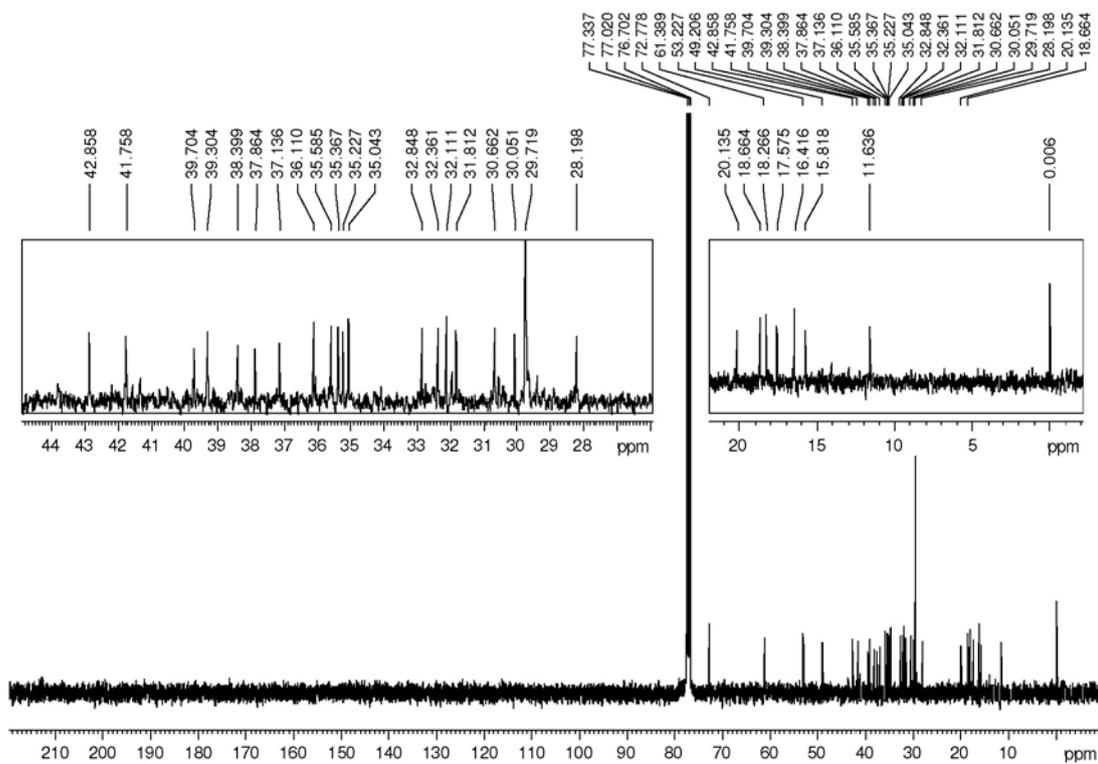


Figure S7.  $^{13}\text{C}$  NMR spectrum of compound **2** ( $\text{CDCl}_3$ , 100 MHz).

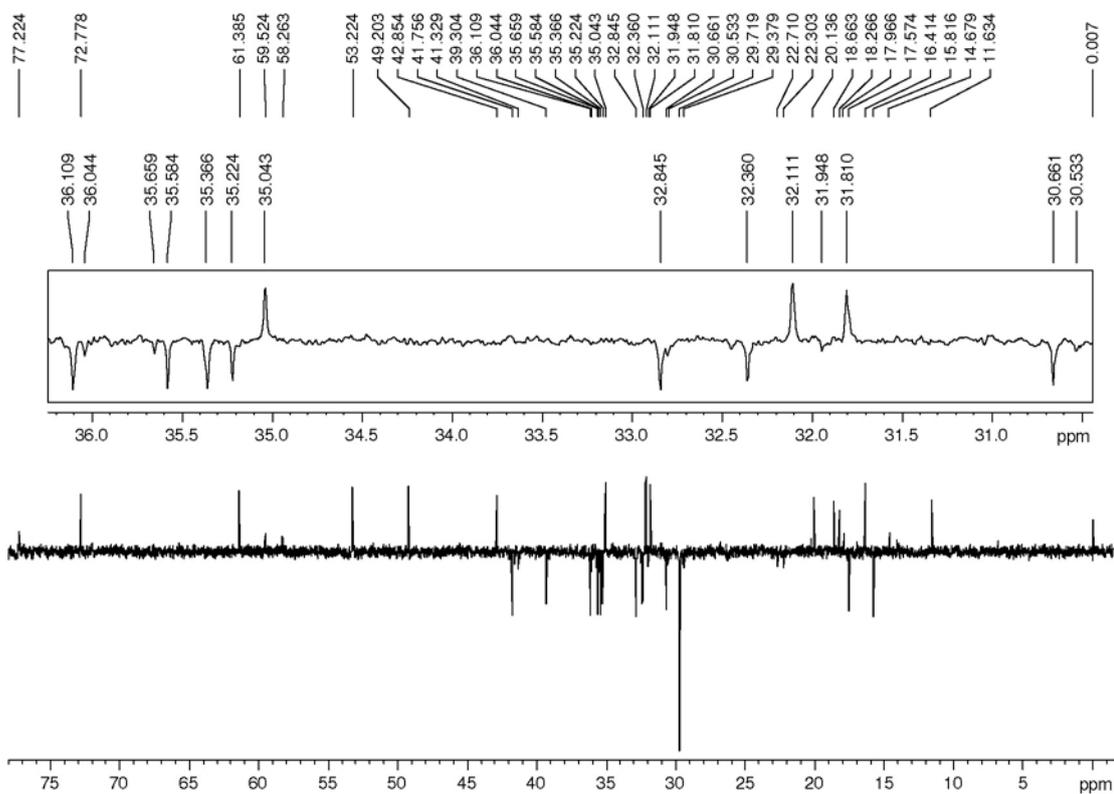


Figure S8.  $^{13}\text{C}$  NMR-DEPT spectrum of compound **2** ( $\text{CDCl}_3$ , 100 MHz).

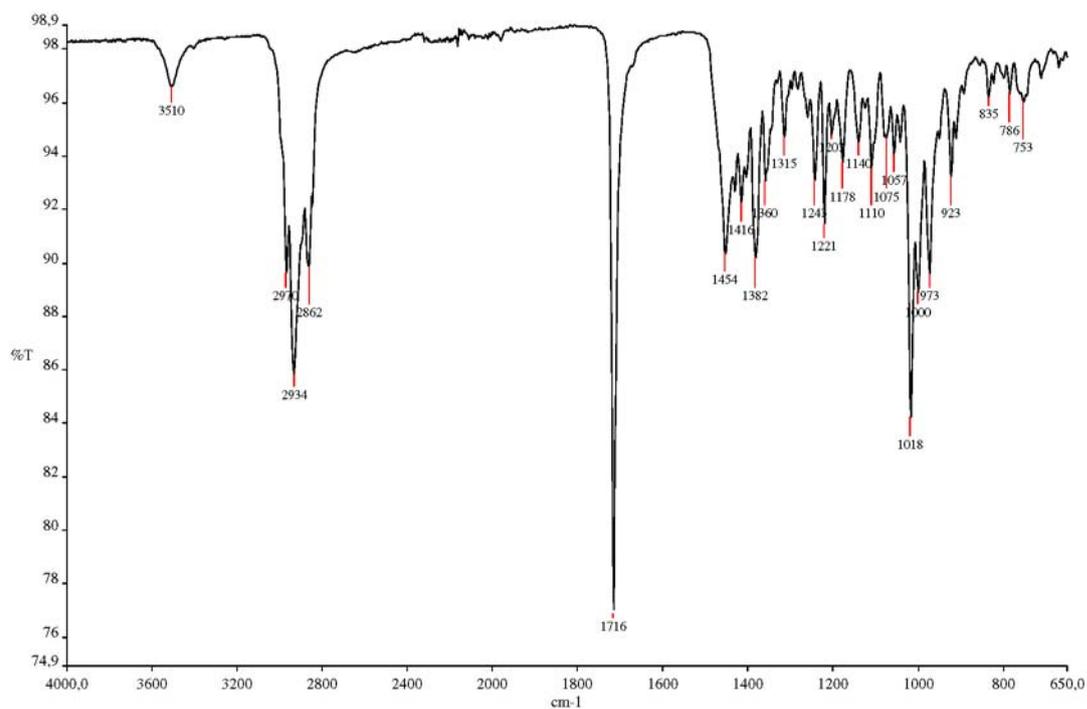


Figure S9. IR spectrum of compound 3 (ATR).

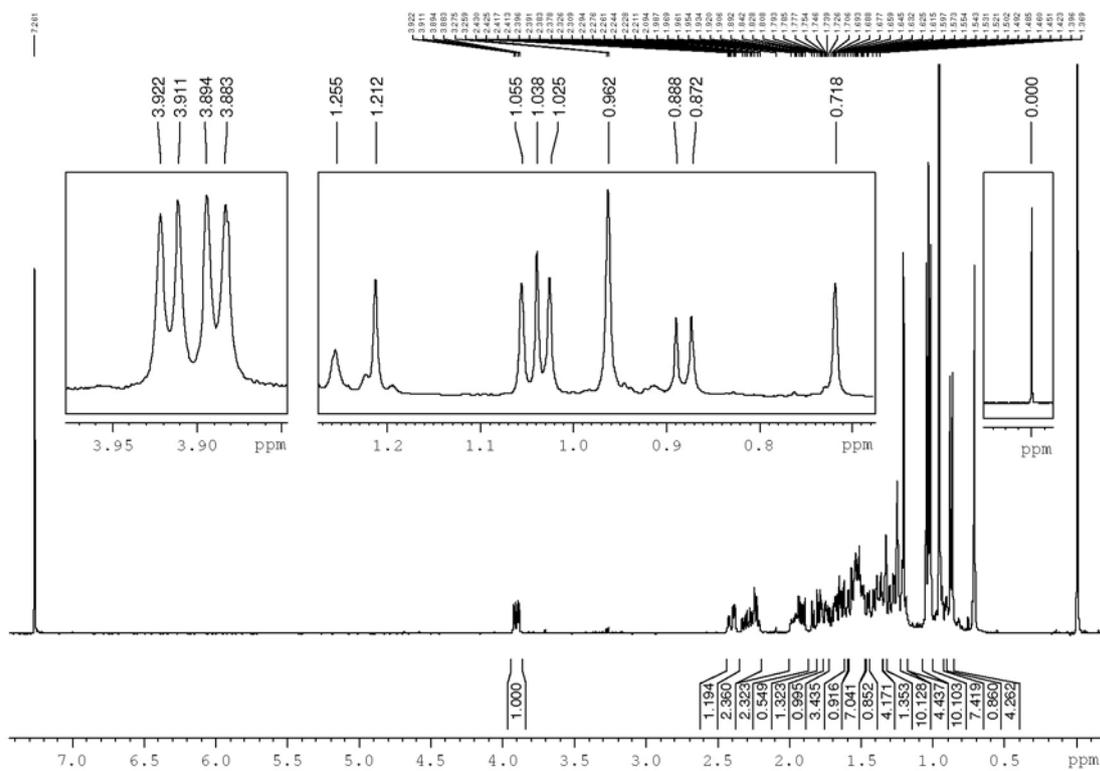


Figure S10. <sup>1</sup>H NMR spectrum of compound 3 (CDCl<sub>3</sub>, 400 MHz).

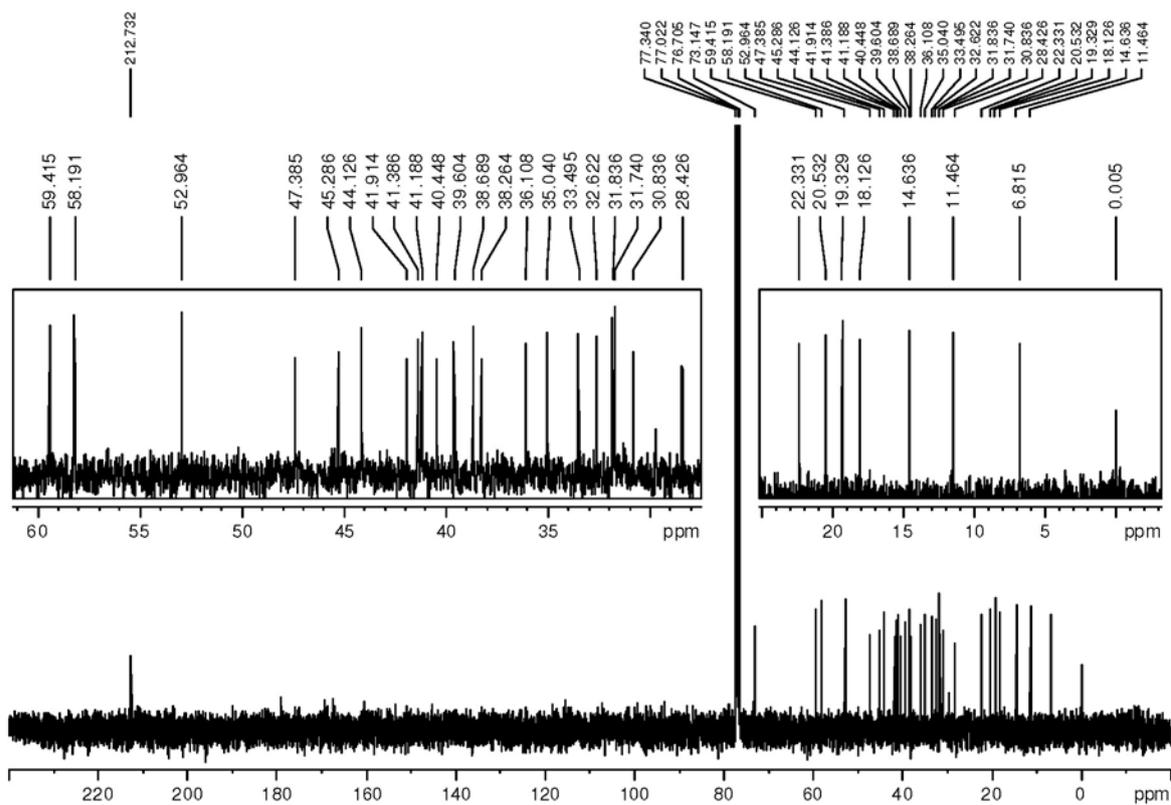


Figure S11.  $^{13}\text{C}$  NMR spectrum of compound **3** ( $\text{CDCl}_3$ , 100 MHz).

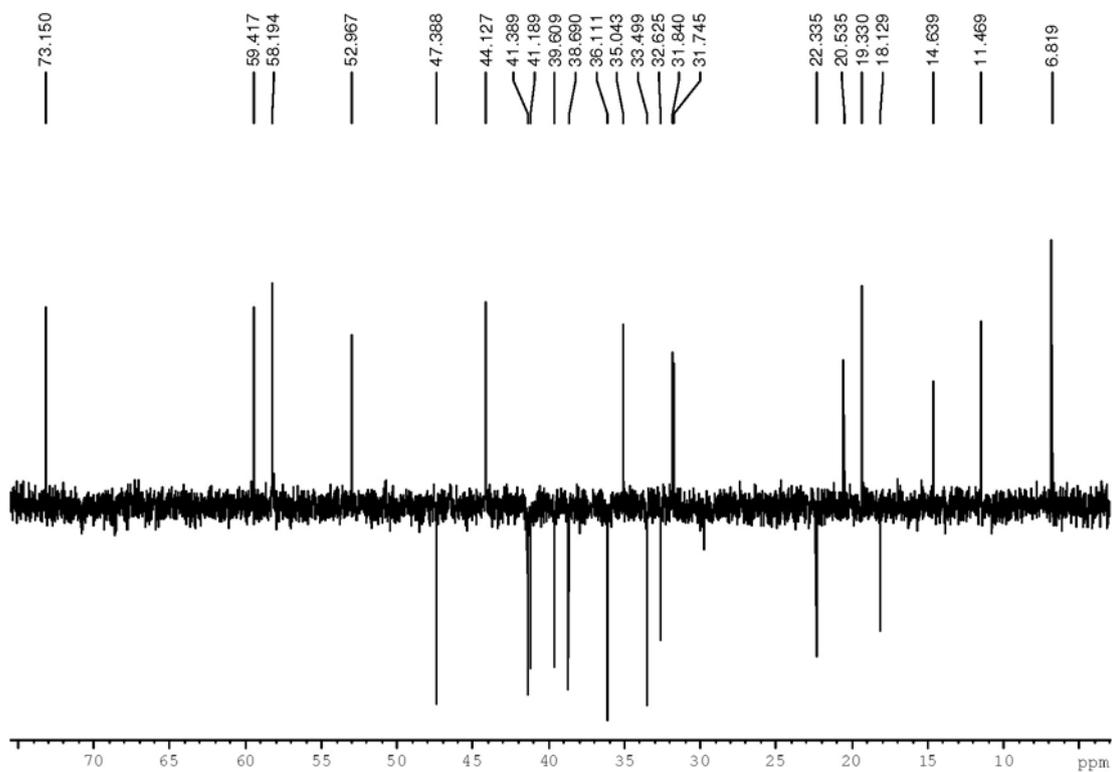


Figure S12.  $^{13}\text{C}$  NMR-DEPT spectrum of compound **3** ( $\text{CDCl}_3$ , 100 MHz).

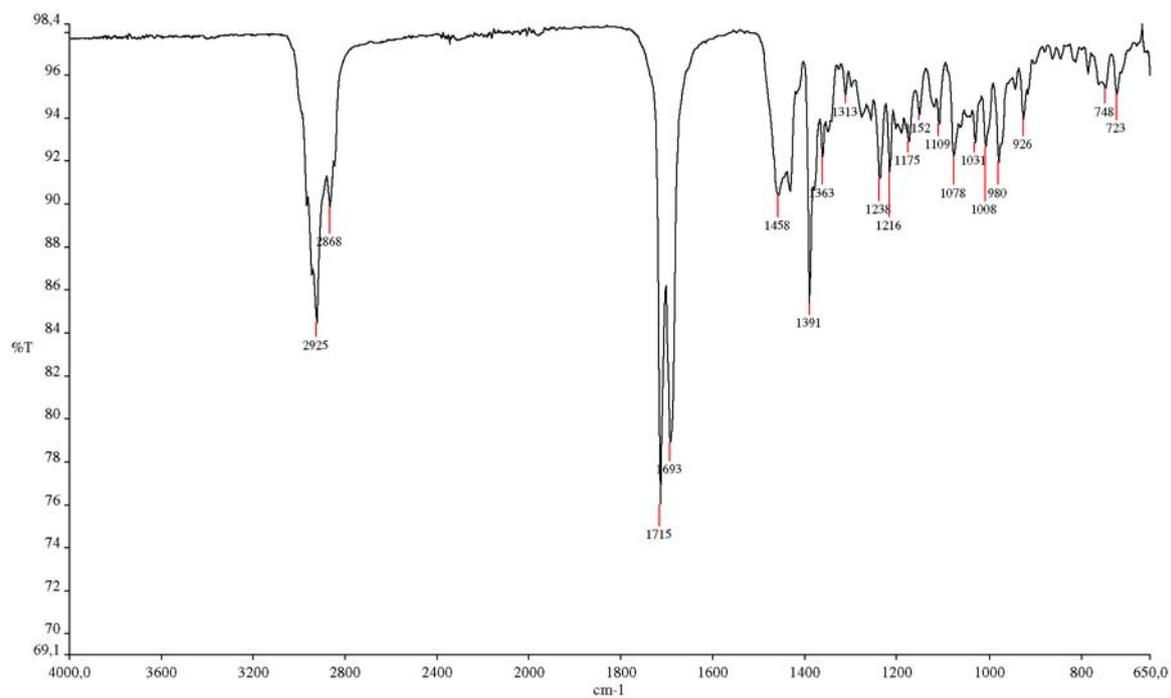


Figure S13. IR spectrum of compound **4** and **5** (ATR).

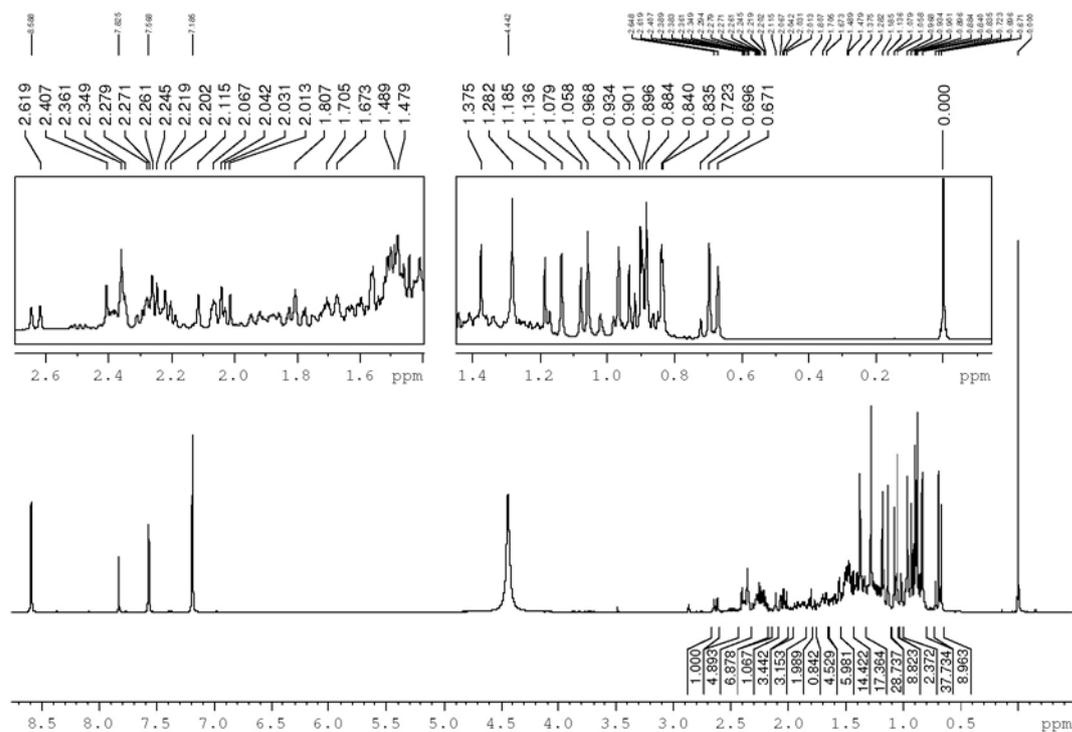


Figure S14.  $^1\text{H}$  NMR spectrum of compound **4** and **5** ( $\text{CDCl}_3 + \text{pyridine-}d_5$ , 400 MHz).



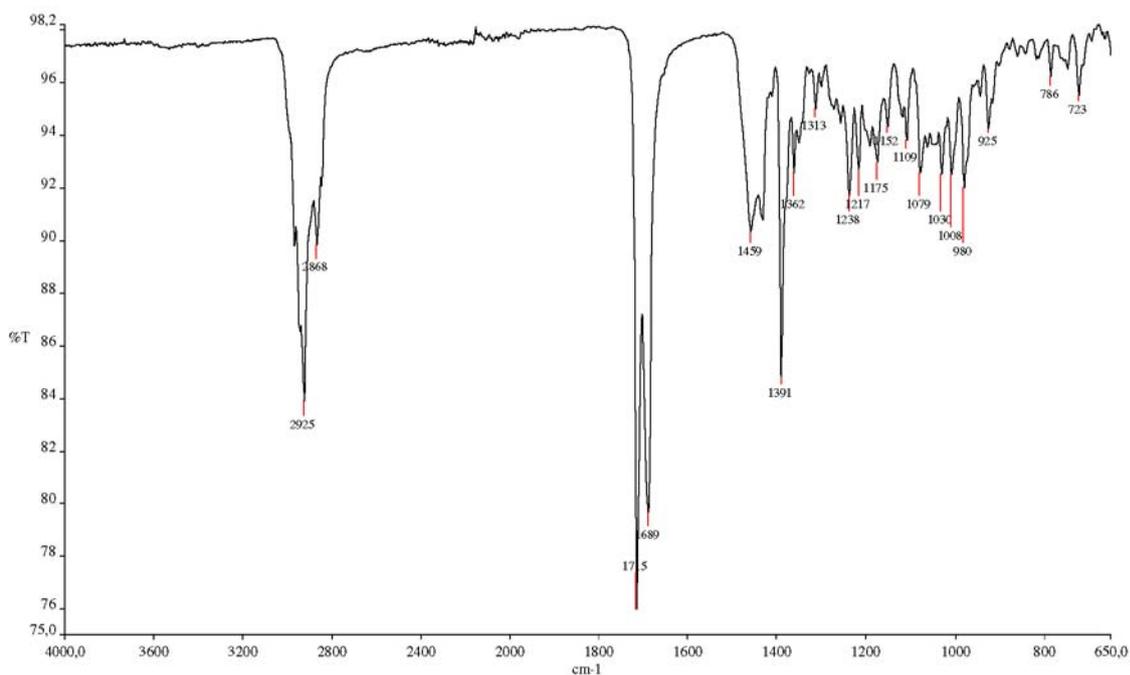


Figure S17. IR spectrum of compound **5** (ATR).

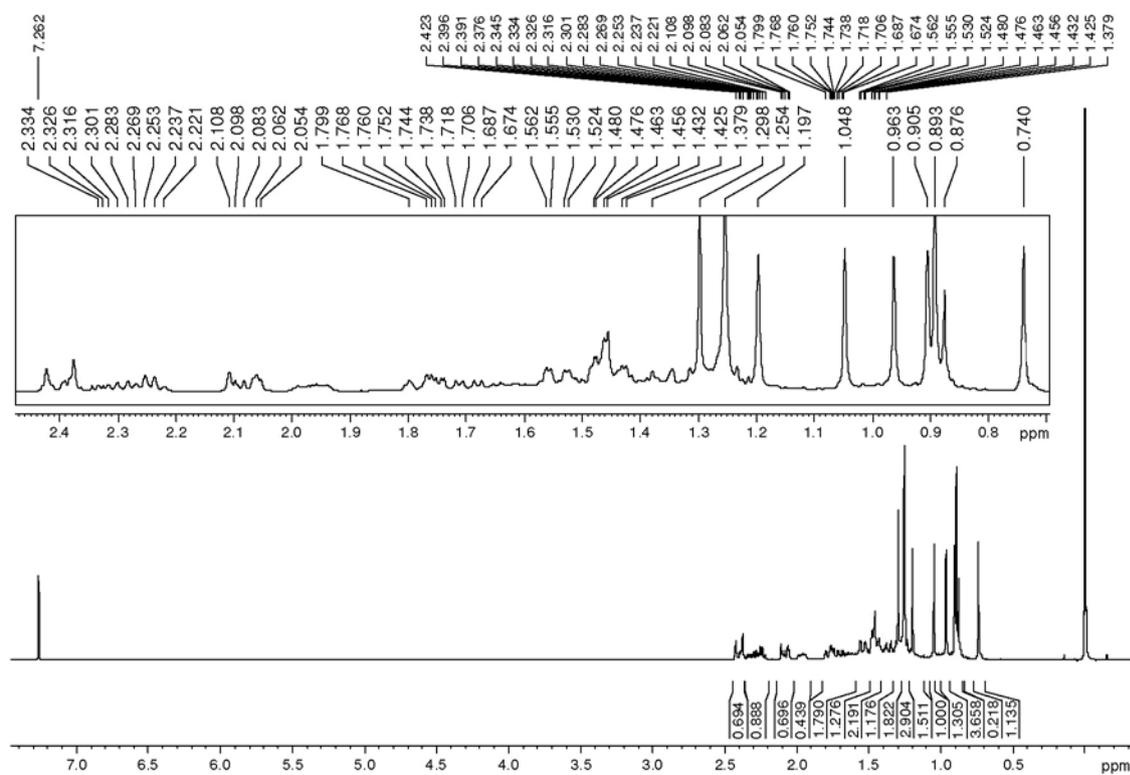


Figure S18.  $^1\text{H}$  NMR spectrum of compound **5** ( $\text{CDCl}_3$ , 400 MHz).

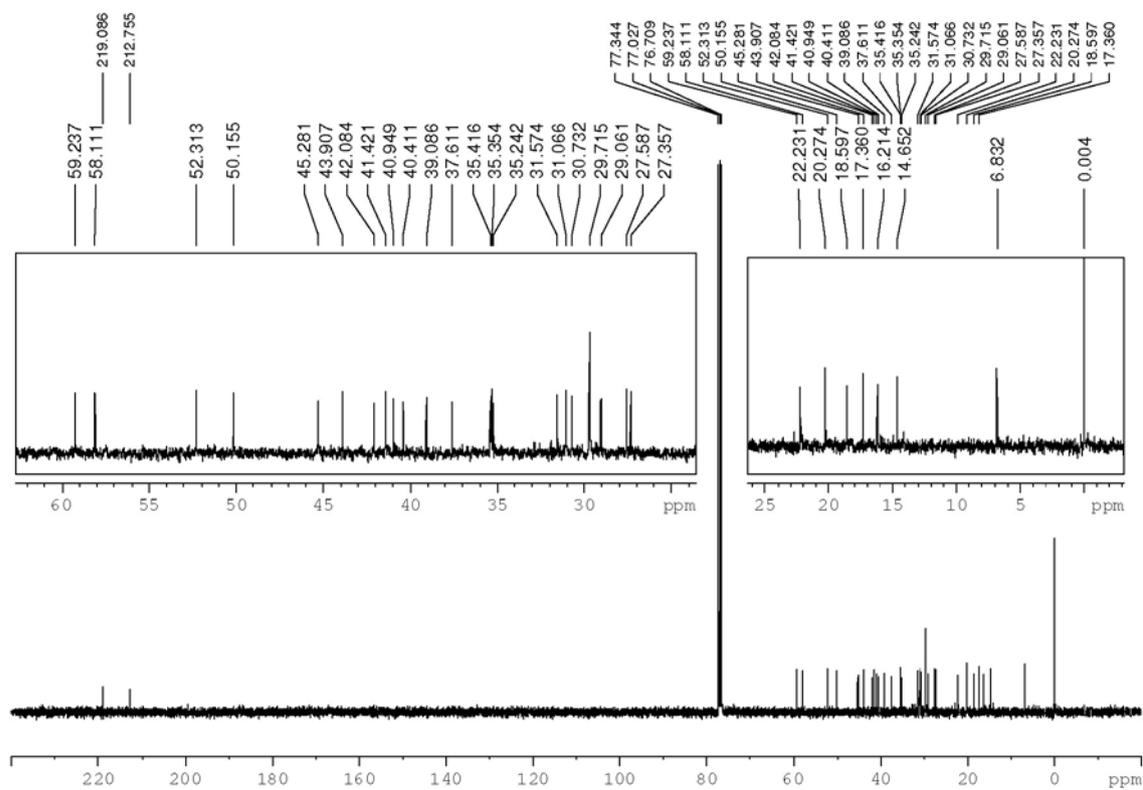


Figure S19.  $^{13}\text{C}$  NMR spectrum of compound **5** ( $\text{CDCl}_3$ , 100 MHz).

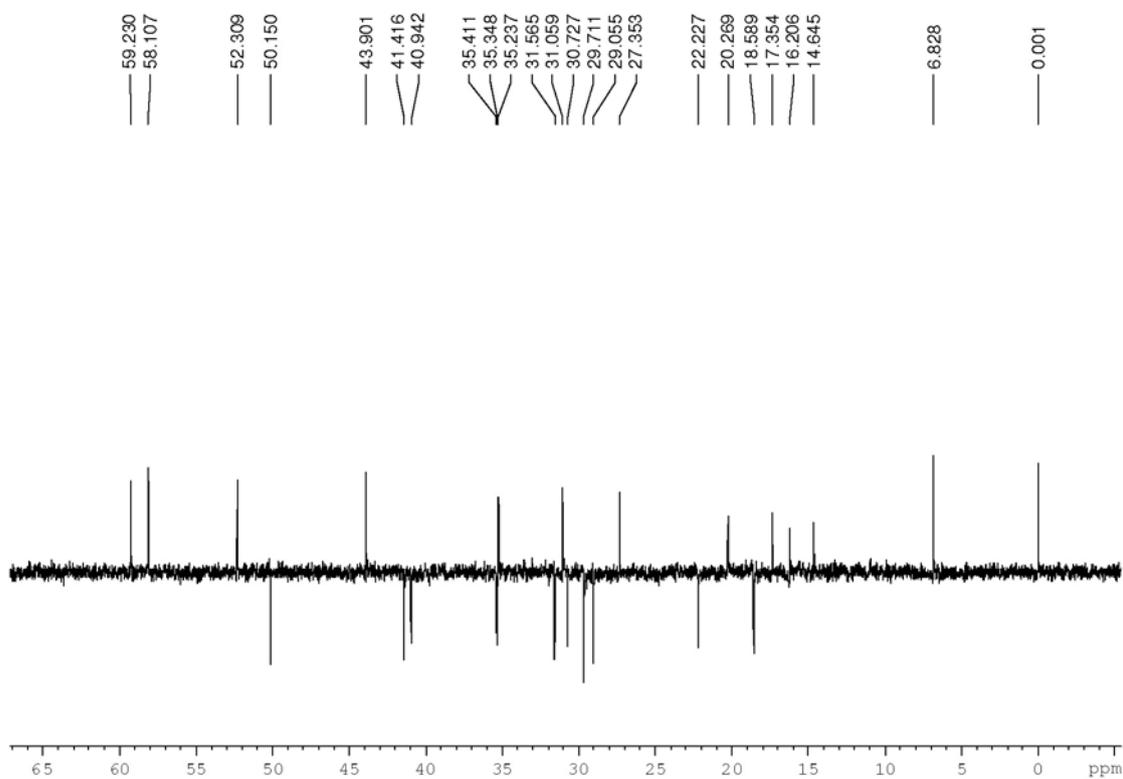


Figure S20.  $^{13}\text{C}$  NMR-DEPT spectrum of compound **5** ( $\text{CDCl}_3$ , 100 MHz).

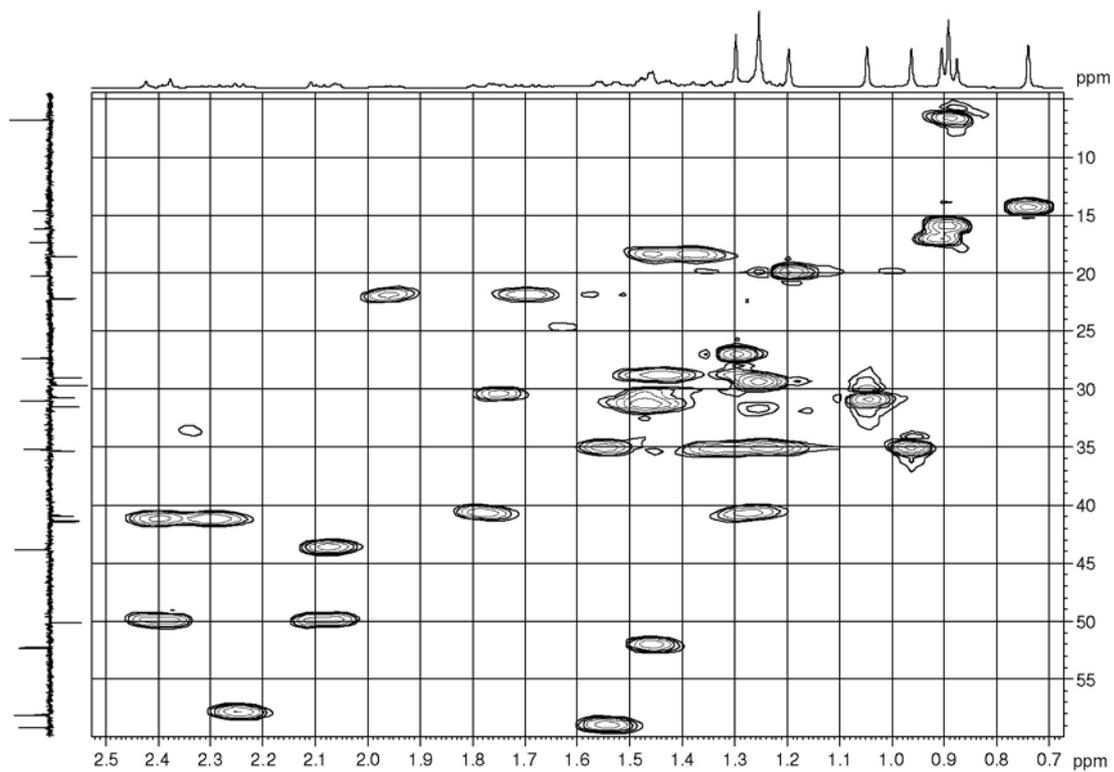


Figure S21. HSQC spectrum of compound **5** (CDCl<sub>3</sub>, 400 MHz).

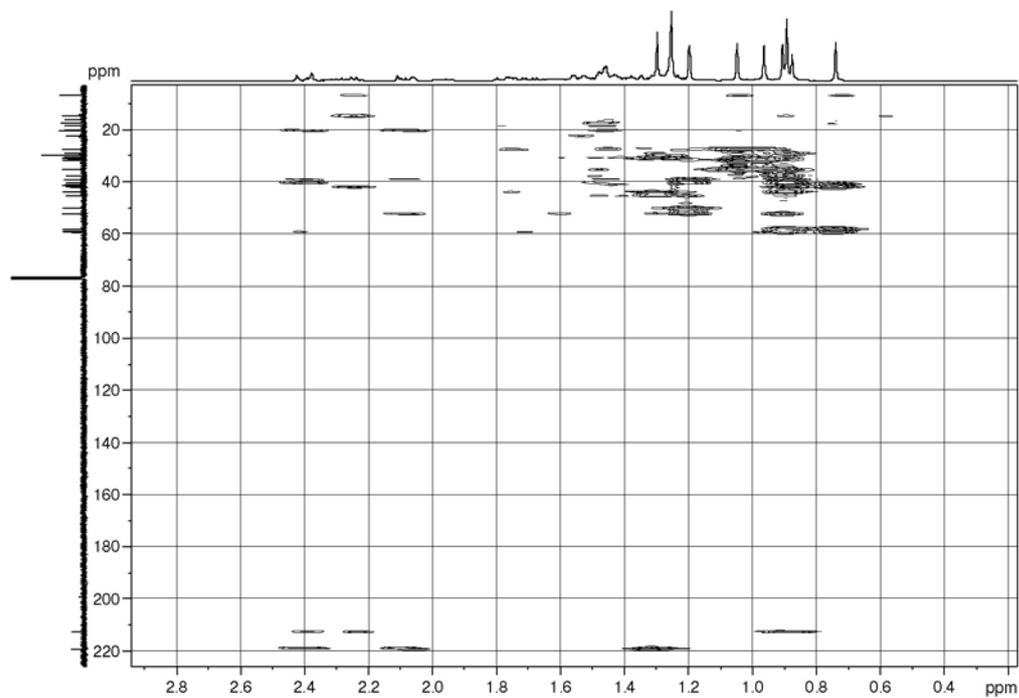
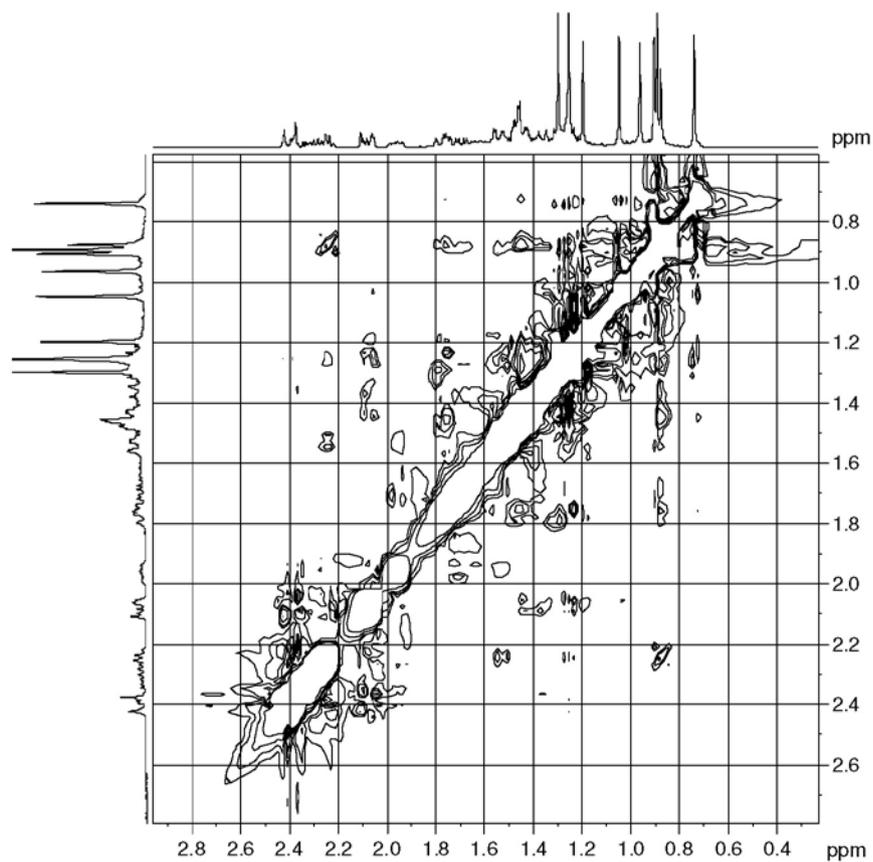
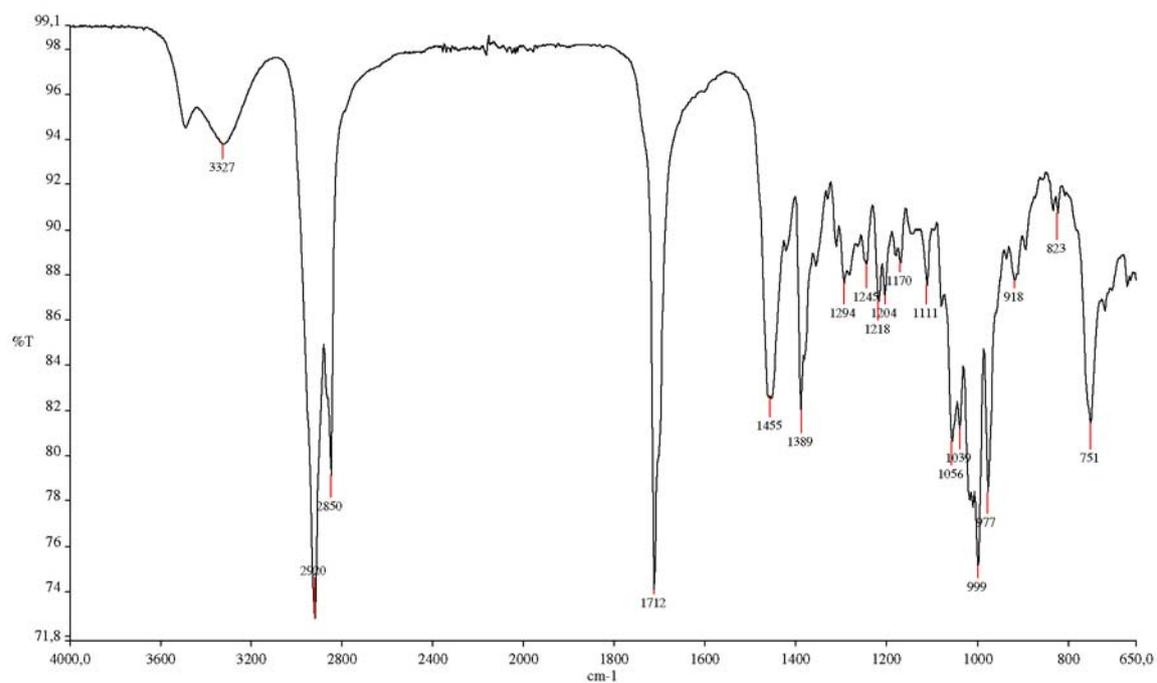


Figure S22. HMBC spectrum of compound **5** (CDCl<sub>3</sub>, 400 MHz).



**Figure S23.** <sup>1</sup>H, <sup>1</sup>H NOESY spectrum of compound 5 (CDCl<sub>3</sub>, 400 MHz).



**Figure S24.** IR spectrum of compound 6 (ATR).



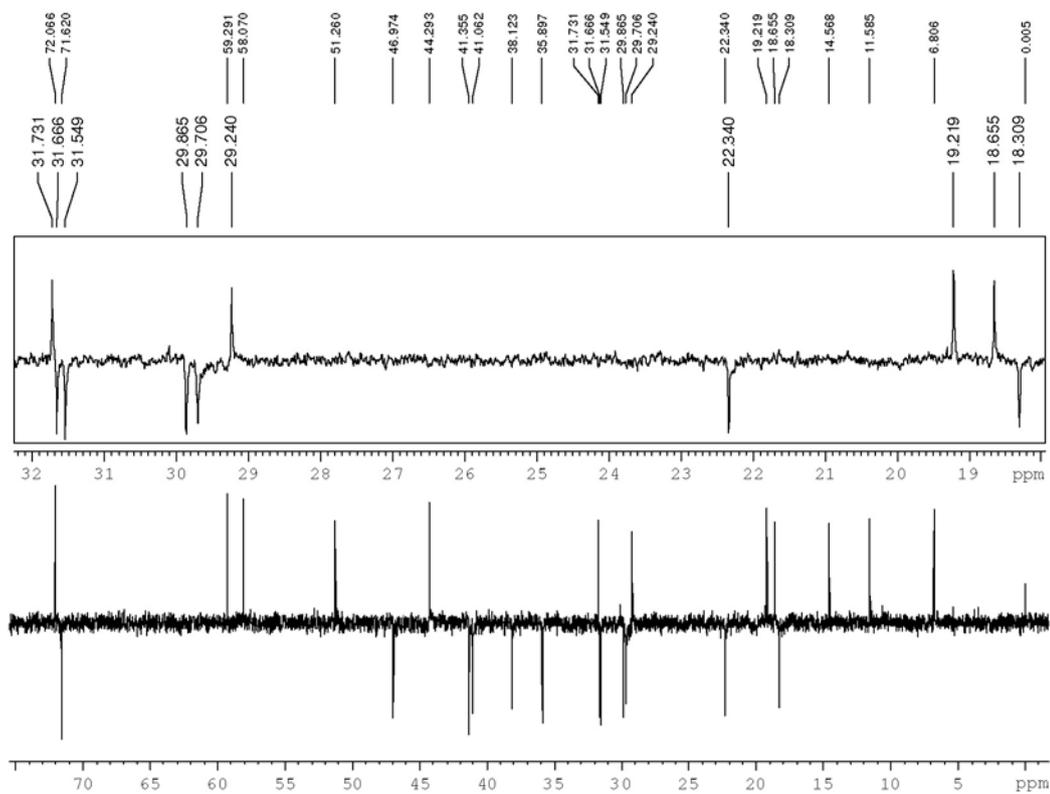


Figure S27. <sup>13</sup>C NMR-DEPT spectrum of compound 6 (CDCl<sub>3</sub> + pyridine-*d*<sub>5</sub>, 100 MHz).

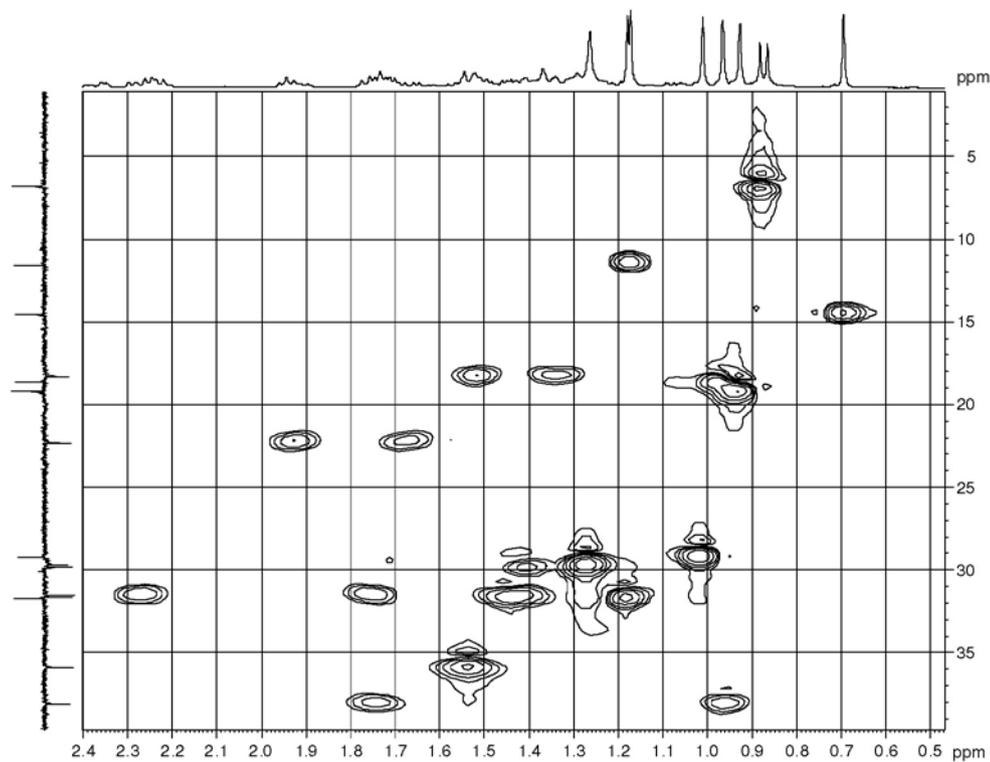


Figure S28. First expansion of HSQC spectrum of compound 6 (CDCl<sub>3</sub> + pyridine-*d*<sub>5</sub>, 400 MHz).

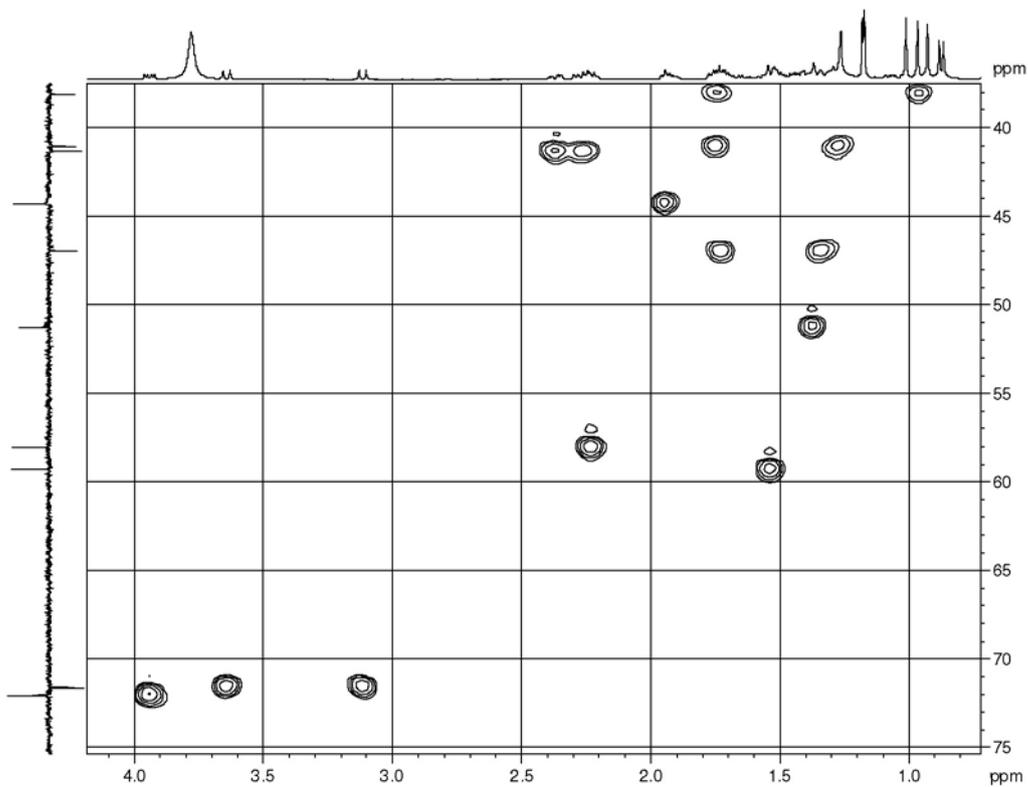


Figure S29. Second expansion of HSQC spectrum of compound **6** (CDCl<sub>3</sub> + pyridine-*d*<sub>5</sub>, 400 MHz).

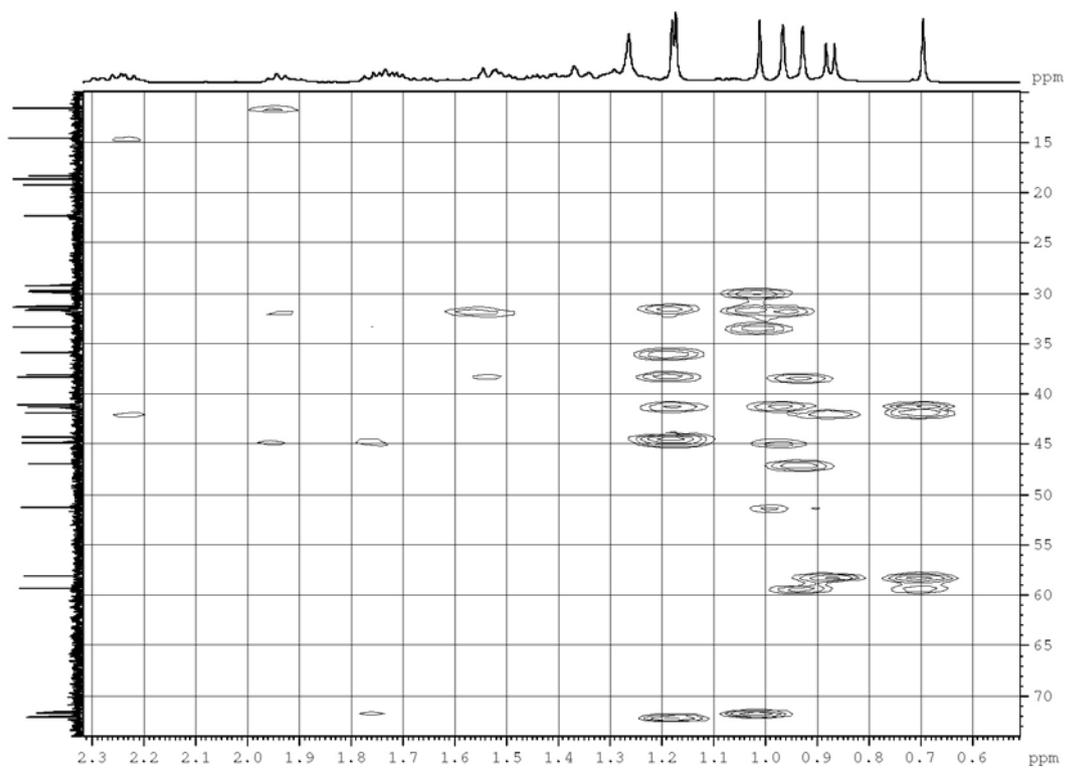
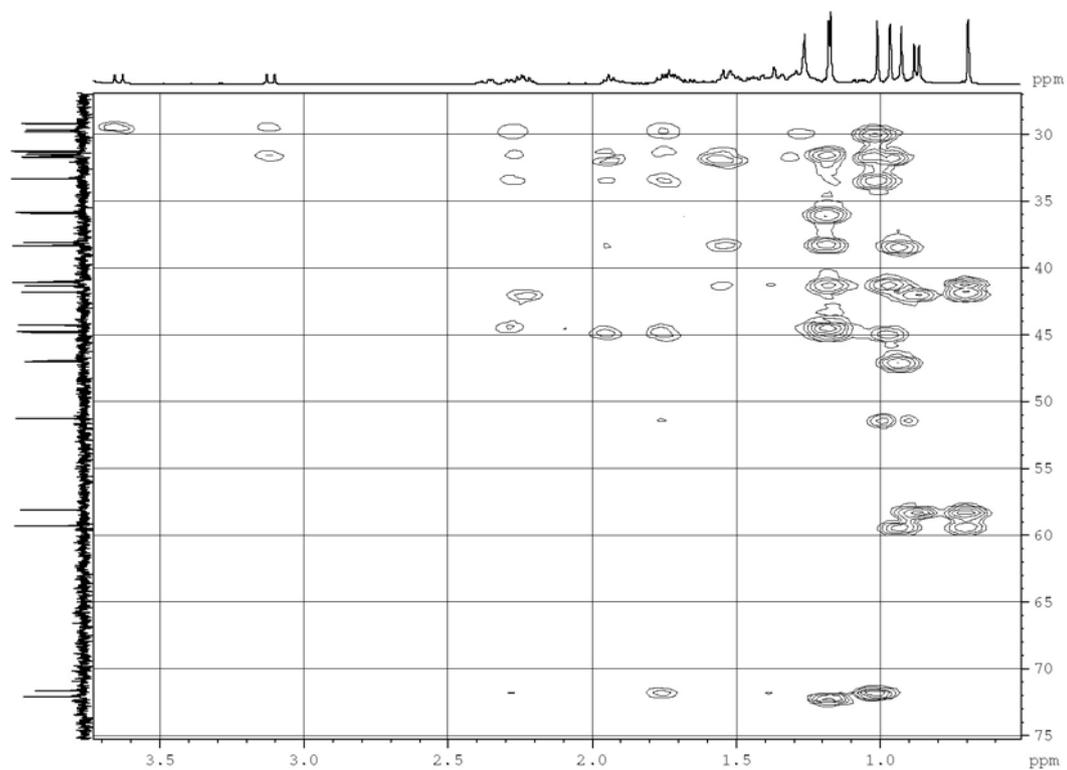
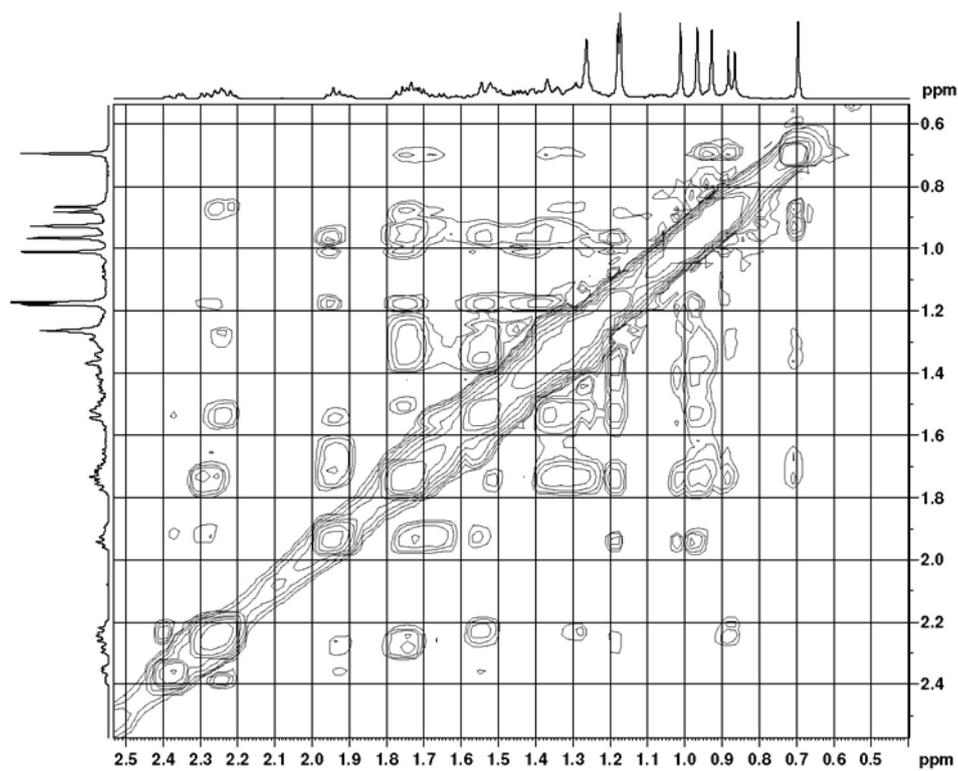


Figure S30. First expansion of HMBC spectrum of compound **6** (CDCl<sub>3</sub> + pyridine-*d*<sub>5</sub>, 400 MHz).



**Figure S31.** Second expansion of HMBC spectrum of compound **6** ( $\text{CDCl}_3$  + pyridine- $d_5$ , 400 MHz).



**Figure S32.** First expansion <sup>1</sup>H, <sup>1</sup>H NOESY spectrum of compound **6** ( $\text{CDCl}_3$  + pyridine- $d_5$ , 400 MHz).

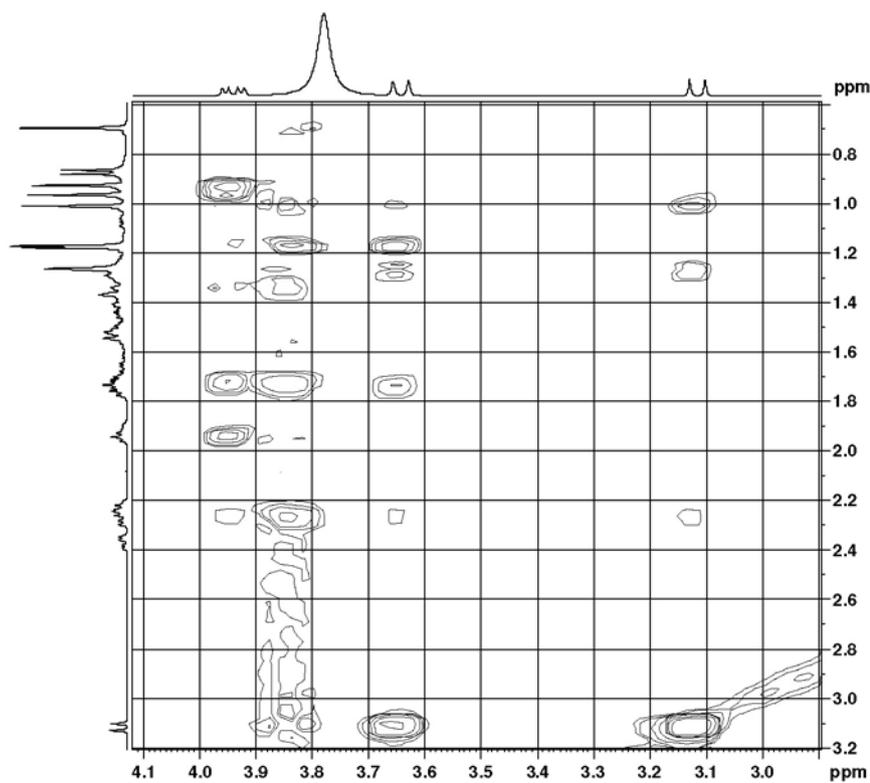


Figure S33. Second expansion  $^1\text{H}$ ,  $^1\text{H}$  NOESY spectrum of compound **6** ( $\text{CDCl}_3$  + pyridine- $d_5$ , 400 MHz).

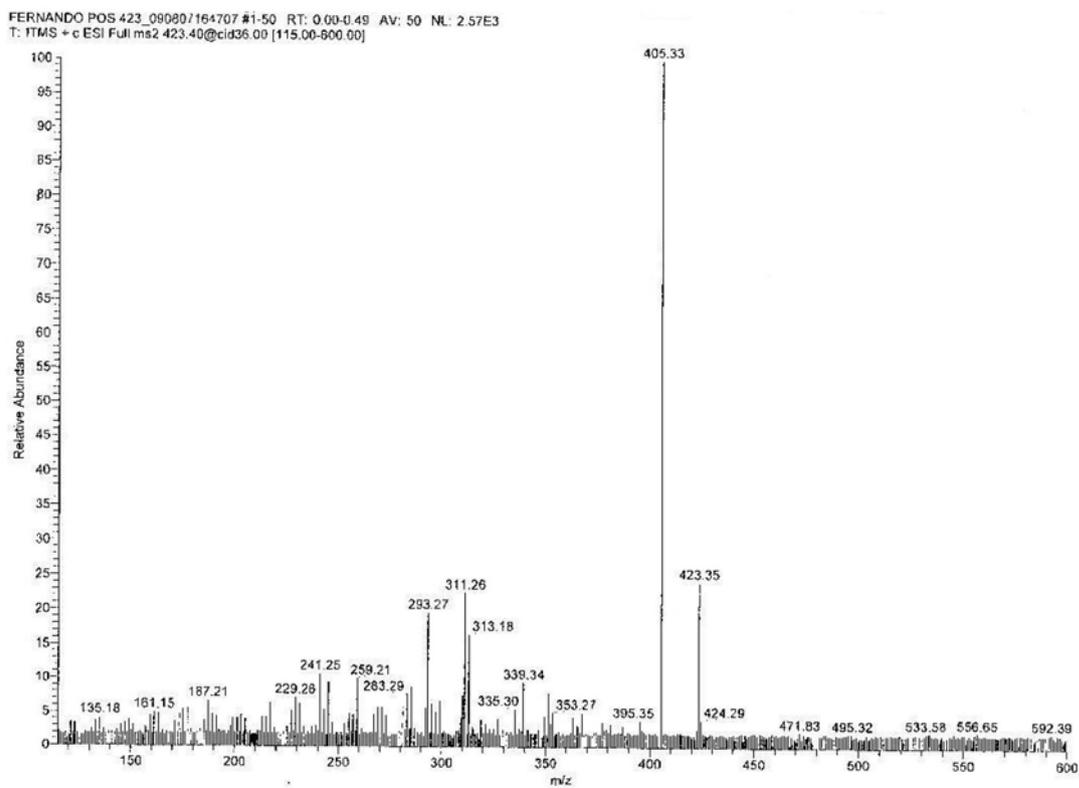


Figure S34. ESI-mass spectrum of compound **6**.