

SÍNTESE DE 1-INDANONAS ATRAVÉS DA REAÇÃO DE ACILAÇÃO DE FRIEDEL-CRAFTS INTRAMOLECULAR UTILIZANDO NbCl<sub>5</sub> COMO ÁCIDO DE LEWIS

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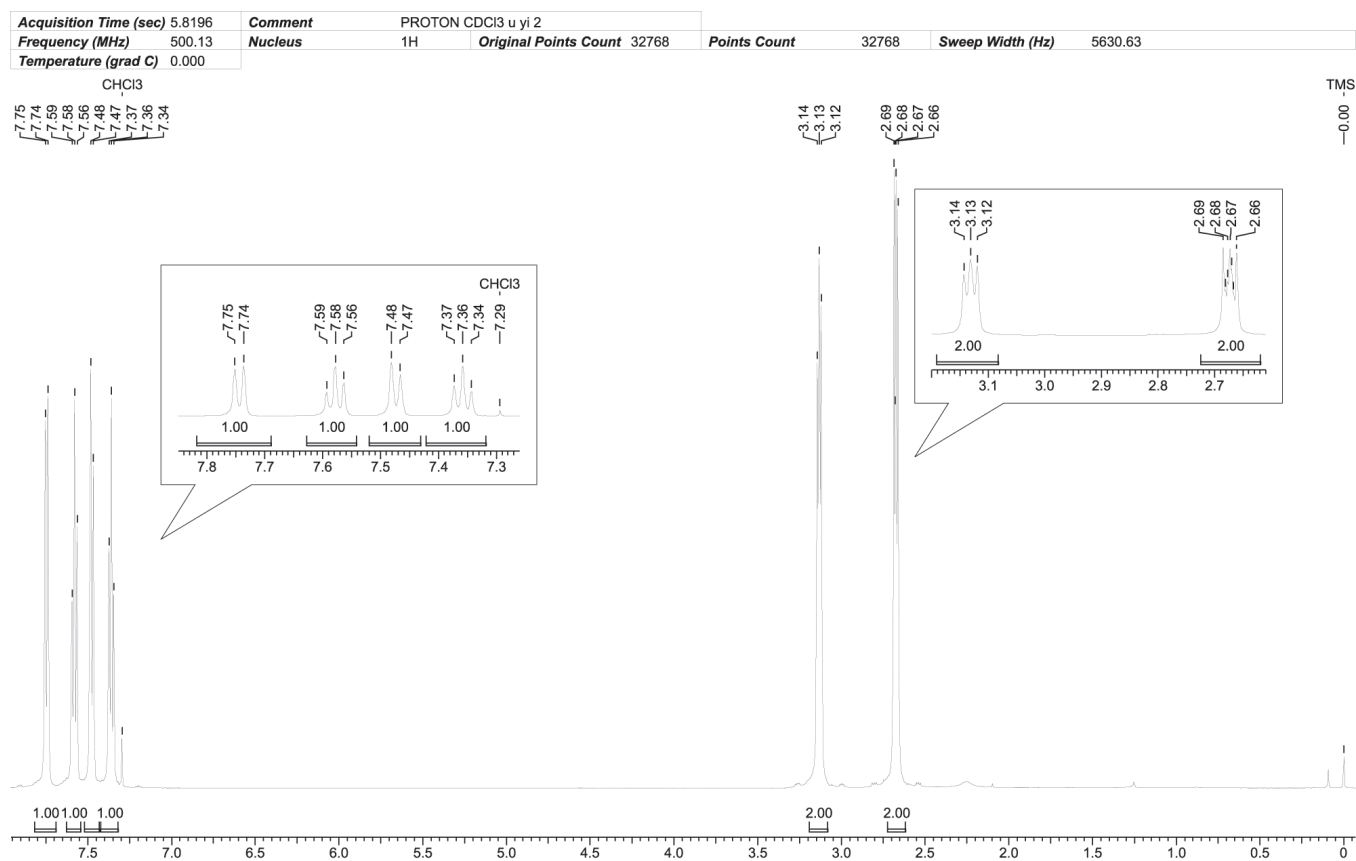


Figura 1S. Espectro de RMN <sup>1</sup>H (500 MHz, CDCl<sub>3</sub>) do composto 5

Acquisition Time (sec)	1.3664	Comment	C13CPD CDCI3 u mgc 2		
Frequency (MHz)	100.61	Nucleus	13C	Original Points Count	32768
Temperature (grad C)	0.000			Points Count	32768
				Sweep Width (Hz)	23980.81

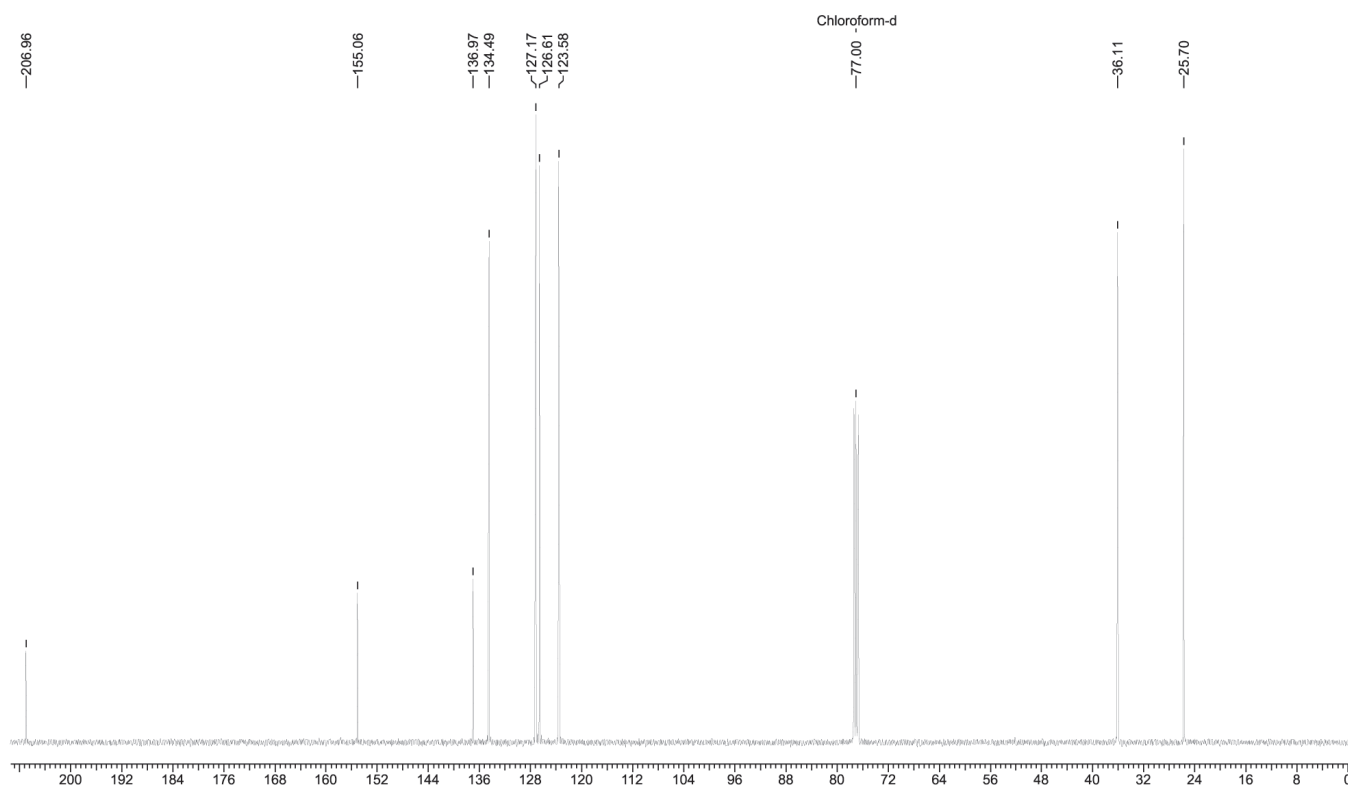


Figura 2S. Espectros de RMN  $^{13}\text{C}$  (100 MHz,  $\text{CDCl}_3$ ) do composto 5

Acquisition Time (sec)	1.3664	Comment	C13DEPT135 CDCI3 u mgc 2		
Frequency (MHz)	100.61	Nucleus	13C	Original Points Count	32768
Temperature (grad C)	0.000			Points Count	32768
				Sweep Width (Hz)	23980.81

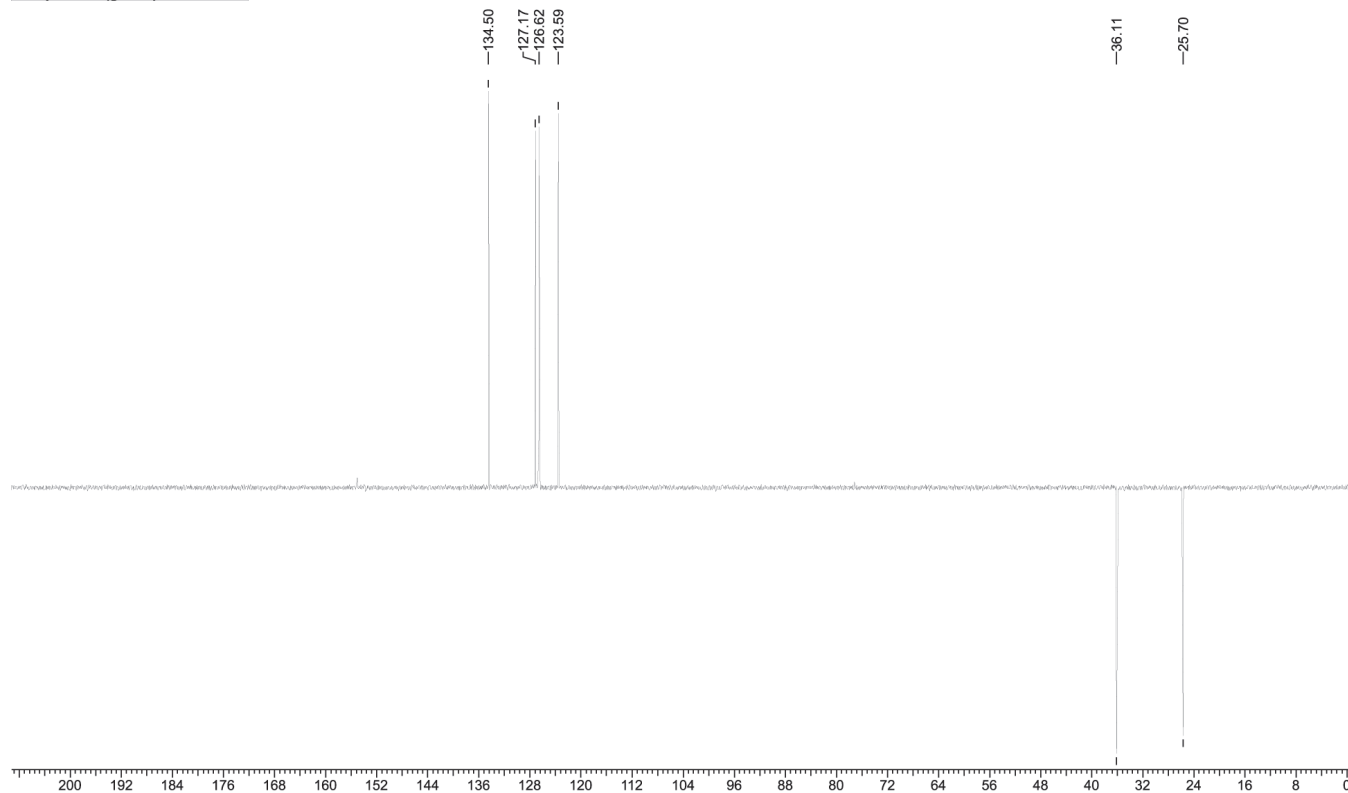


Figura 3S. Espectro de RMN  $^{13}\text{C}$  (100 MHz,  $\text{CDCl}_3$ ) DEPT-135 do composto 5

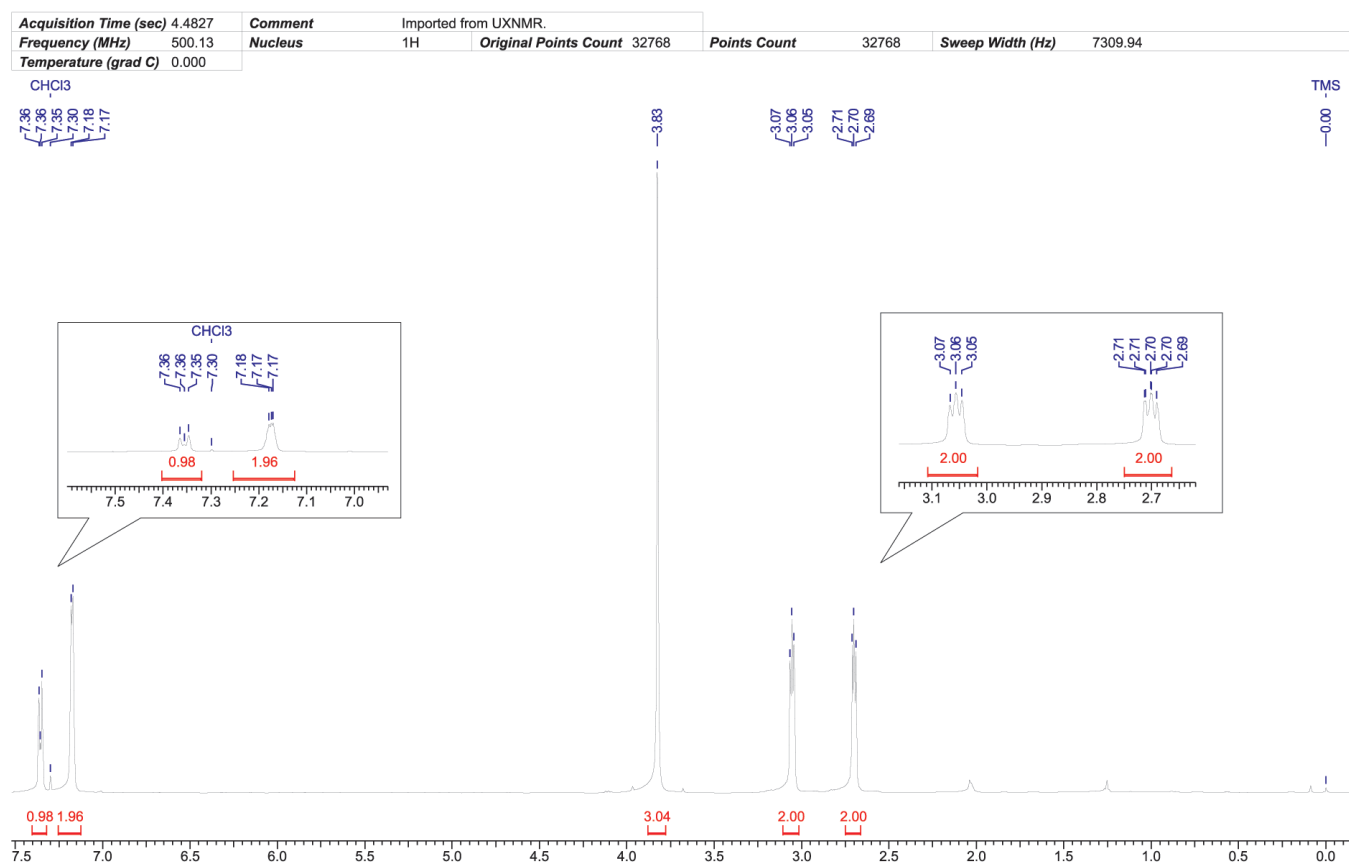


Figura 4S. Espectro de RMN <sup>1</sup>H (500 MHz, CDCl<sub>3</sub>) do composto 6

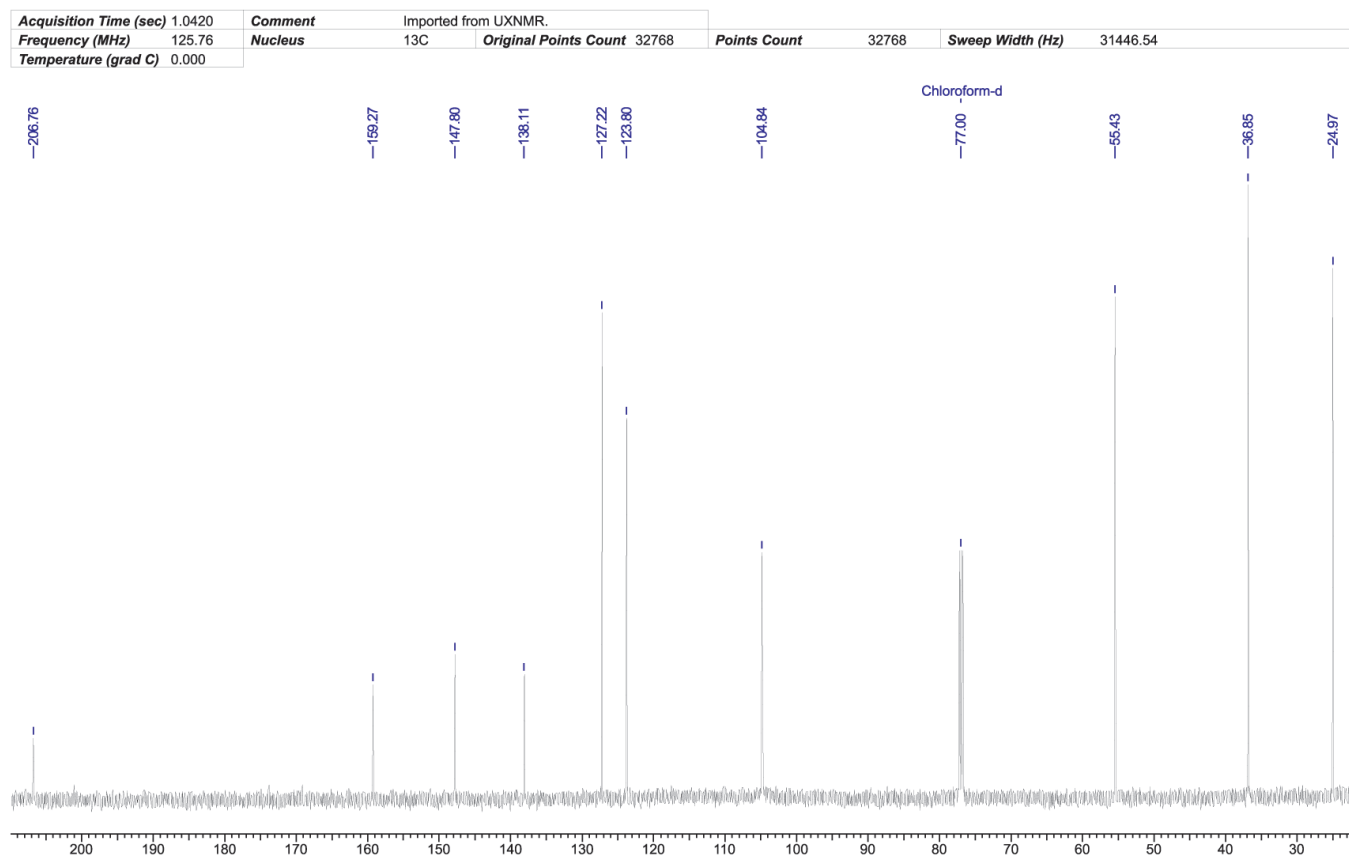


Figura 5S. Espectros de RMN <sup>13</sup>C (100 MHz, CDCl<sub>3</sub>) do composto 6

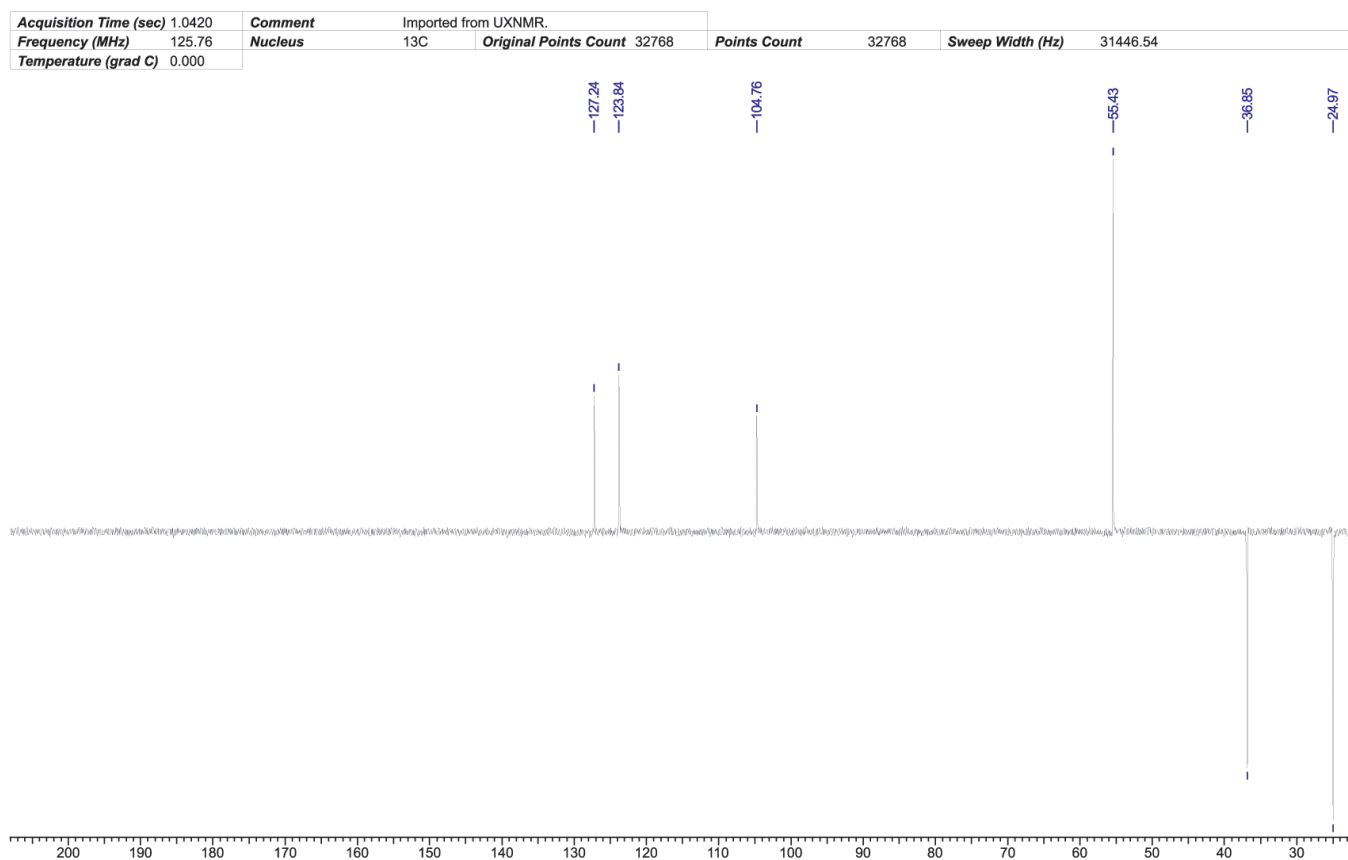


Figura 6S. Espectro de RMN  $^{13}\text{C}$  (100 MHz,  $\text{CDCl}_3$ ) DEPT-135 do composto 6

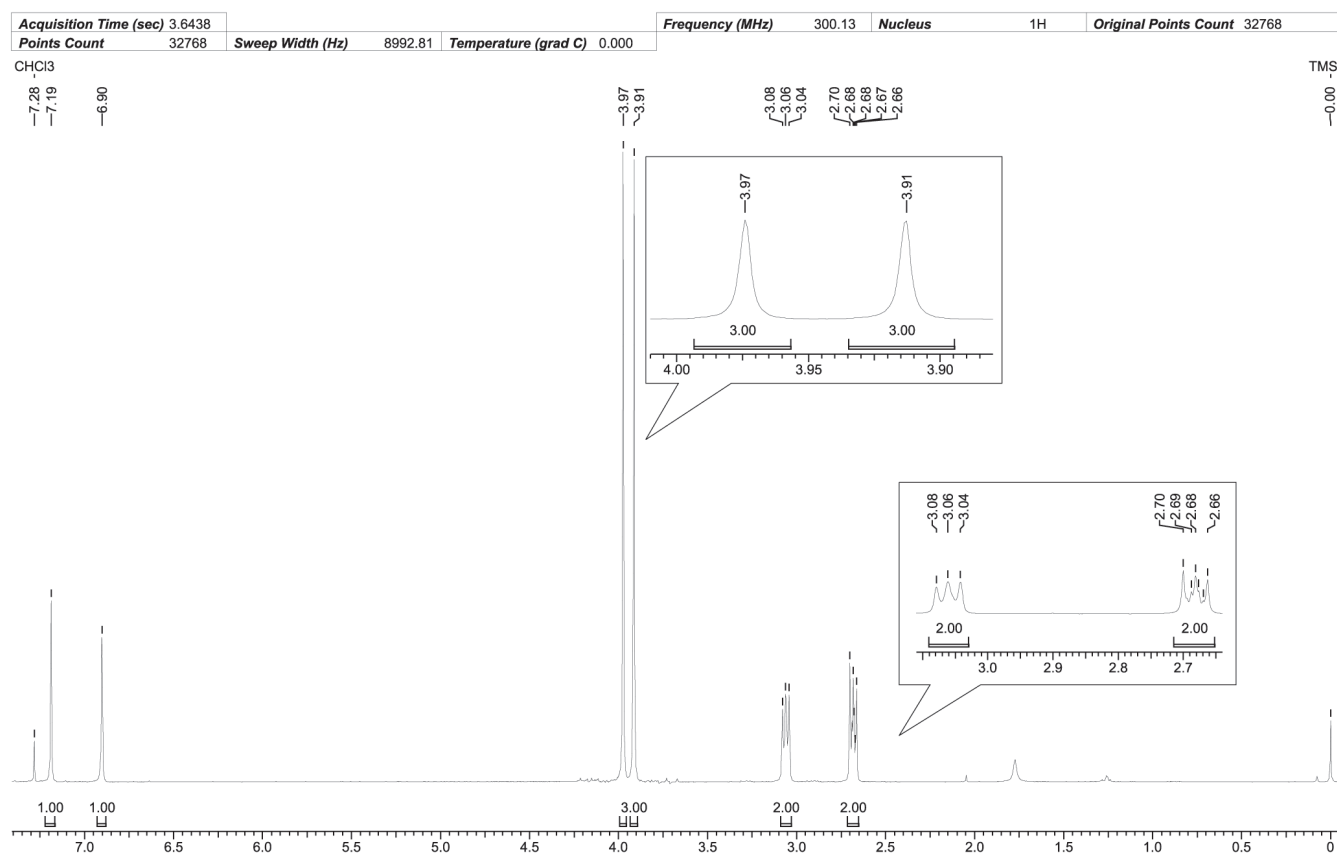


Figura 7S. Espectro de RMN  $^1\text{H}$  (300 MHz,  $\text{CDCl}_3$ ) do composto 7

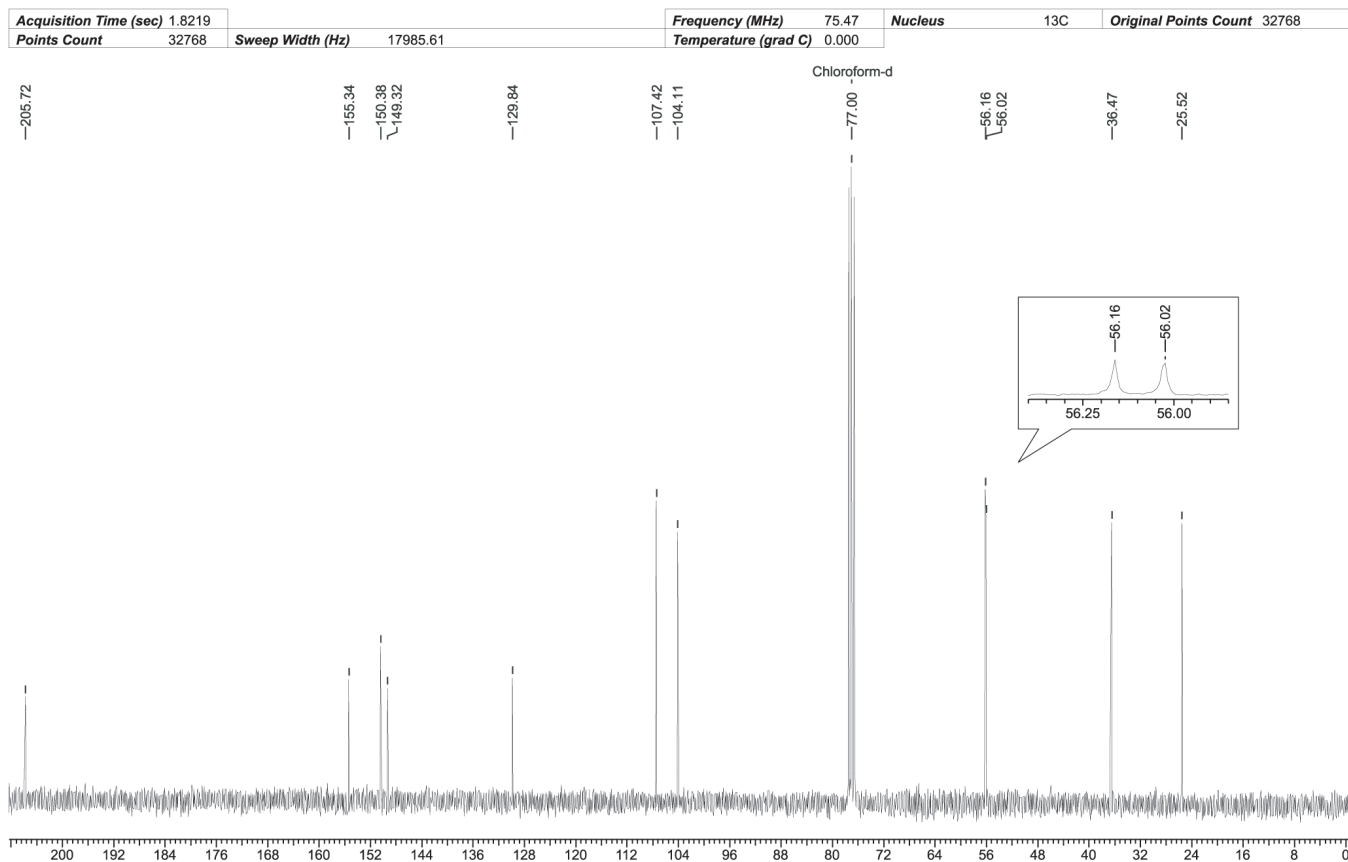


Figura 8S. Espectros de RMN  $^{13}\text{C}$  (75 MHz,  $\text{CDCl}_3$ ) do composto 7

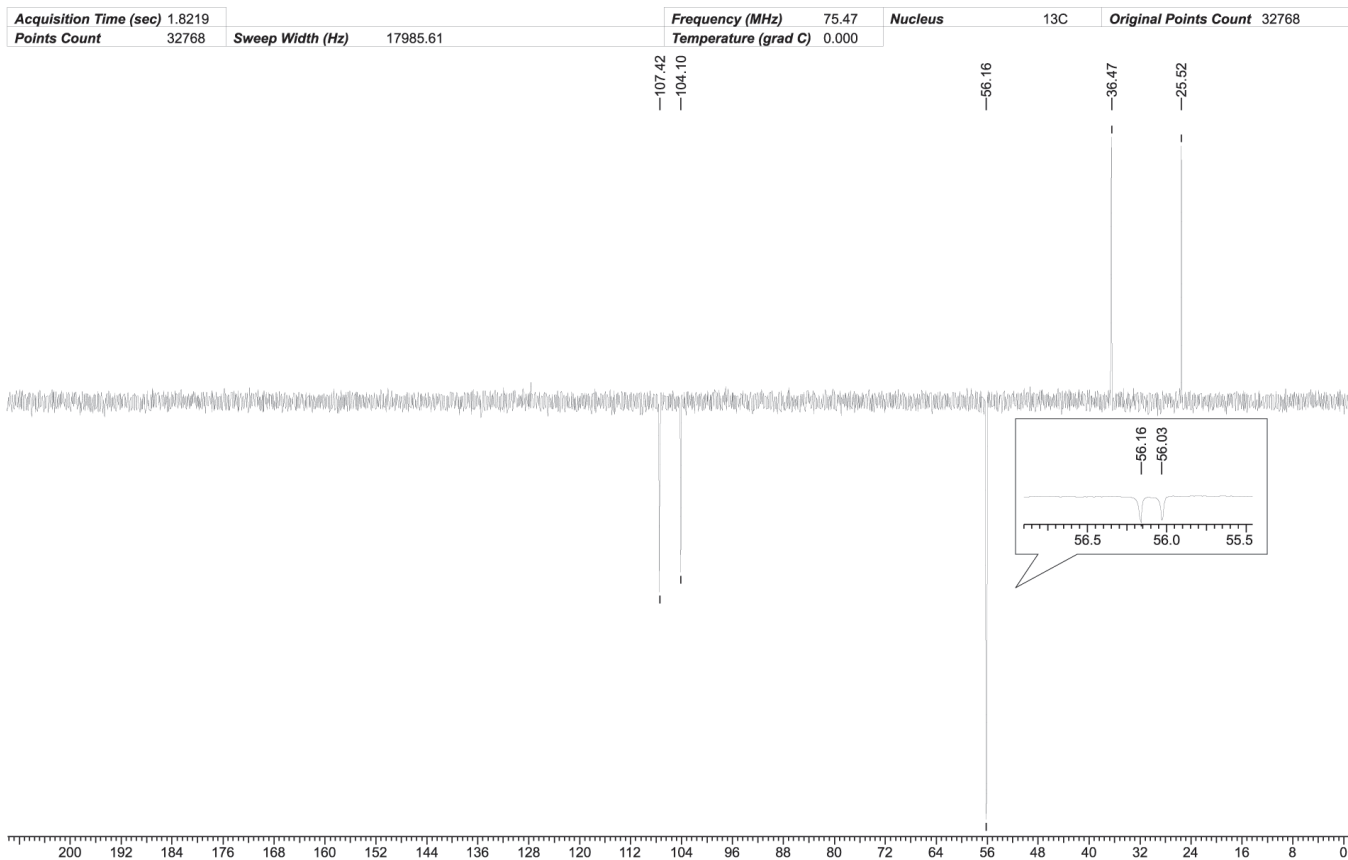


Figura 9S. Espectro de RMN  $^{13}\text{C}$  (75 MHz,  $\text{CDCl}_3$ ) DEPT-135 do composto 7

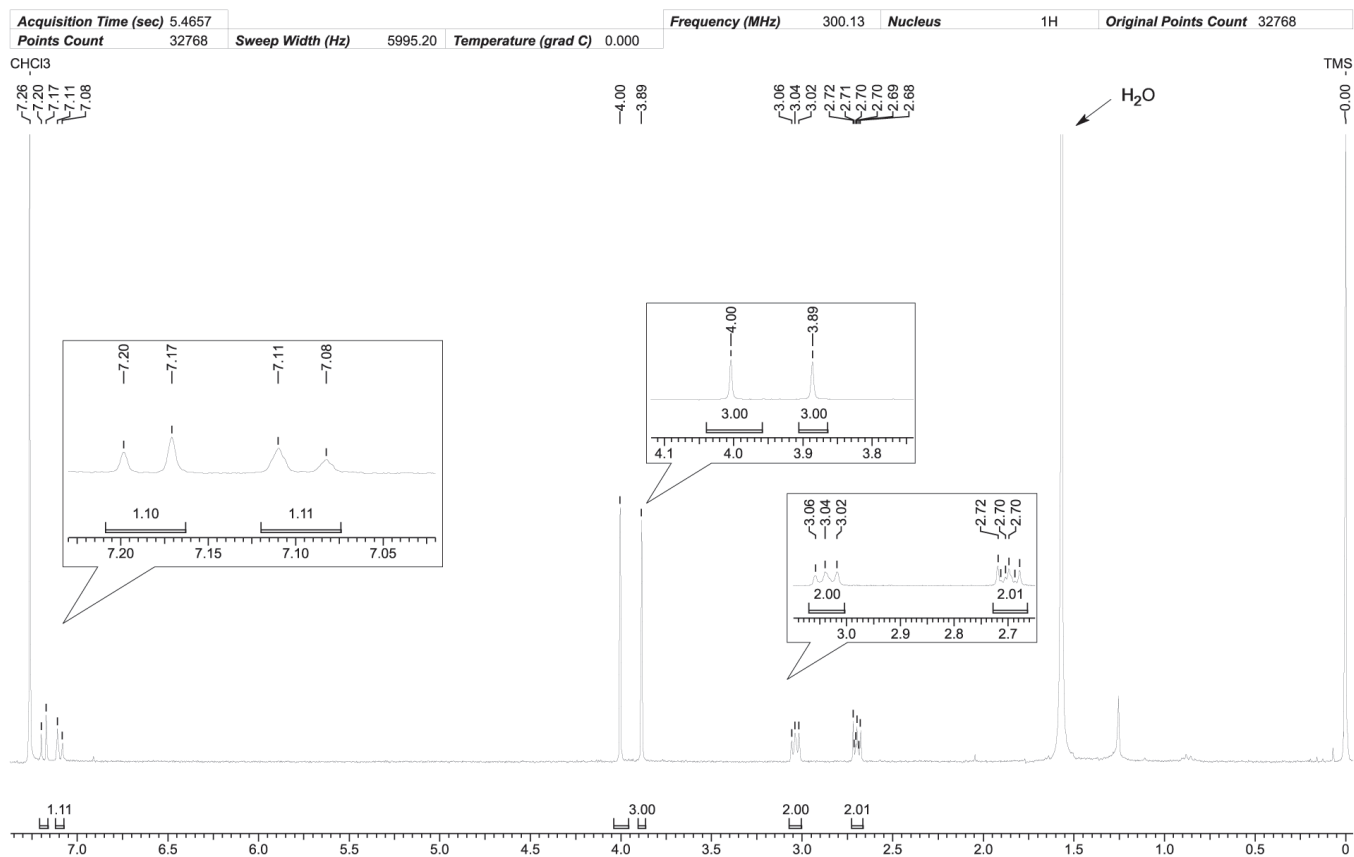


Figura 10S. Espectro de RMN <sup>1</sup>H (300 MHz, CDCl<sub>3</sub>) do composto 8

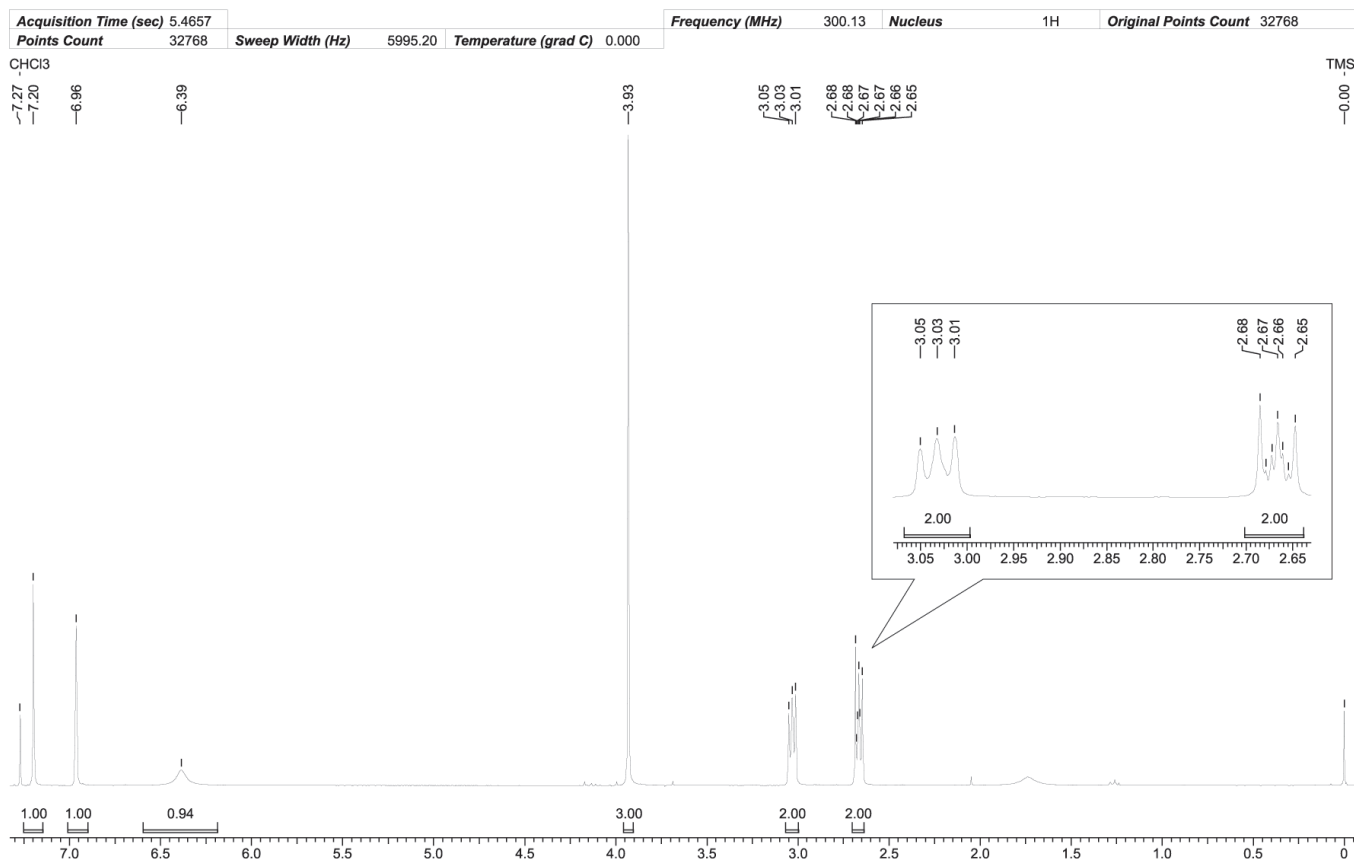


Figura 11S. Espectro de RMN <sup>1</sup>H (300 MHz, CDCl<sub>3</sub>) do composto 9

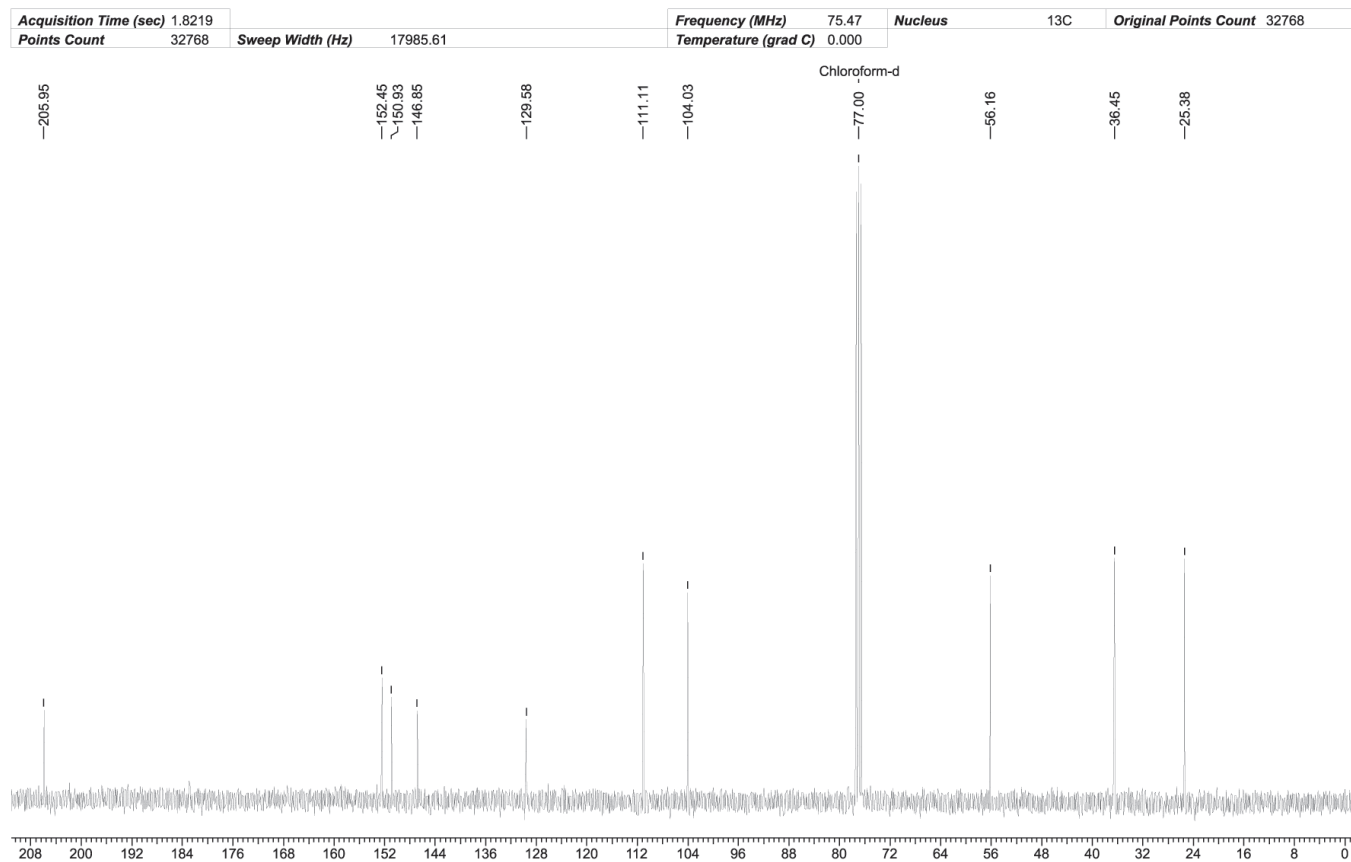


Figura 12S. Espectros de RMN  $^{13}\text{C}$  (75 MHz,  $\text{CDCl}_3$ ) do composto **9**

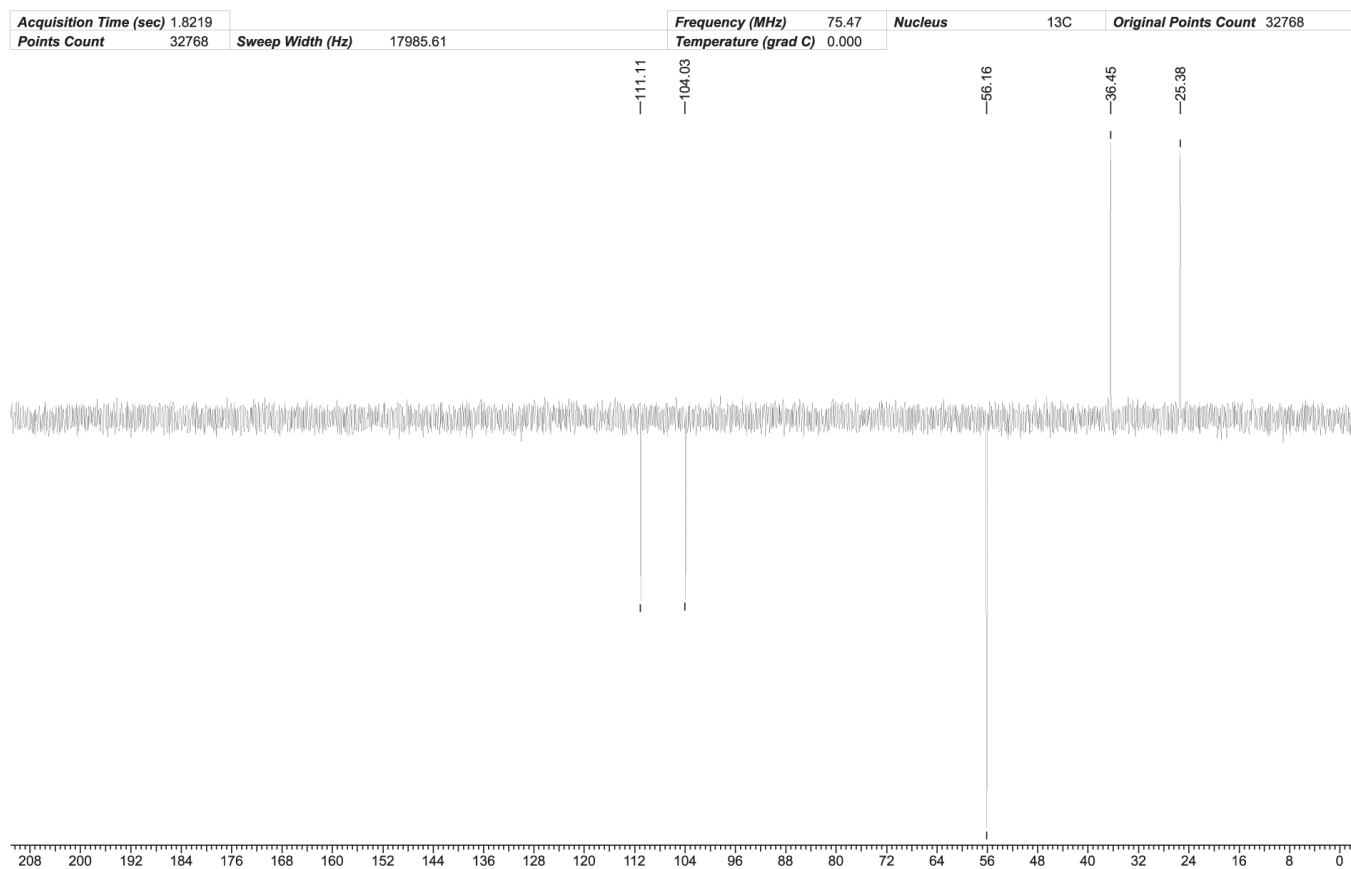


Figura 13S. Espectro de RMN  $^{13}\text{C}$  (75 MHz,  $\text{CDCl}_3$ ) DEPT-135 do composto **9**

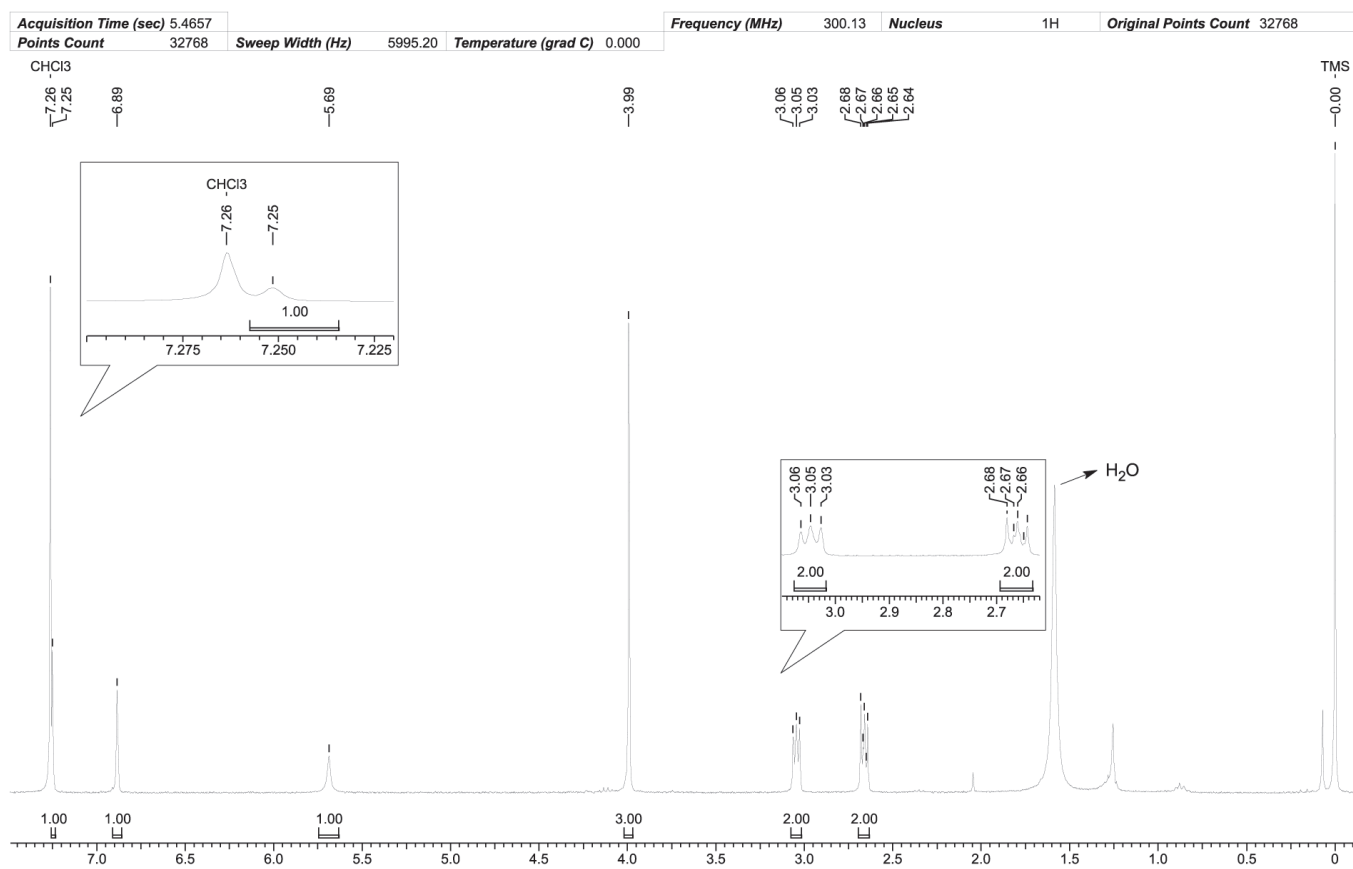


Figura 14S. Espectro de RMN  $^1\text{H}$  (300 MHz,  $\text{CDCl}_3$ ) do composto **10**

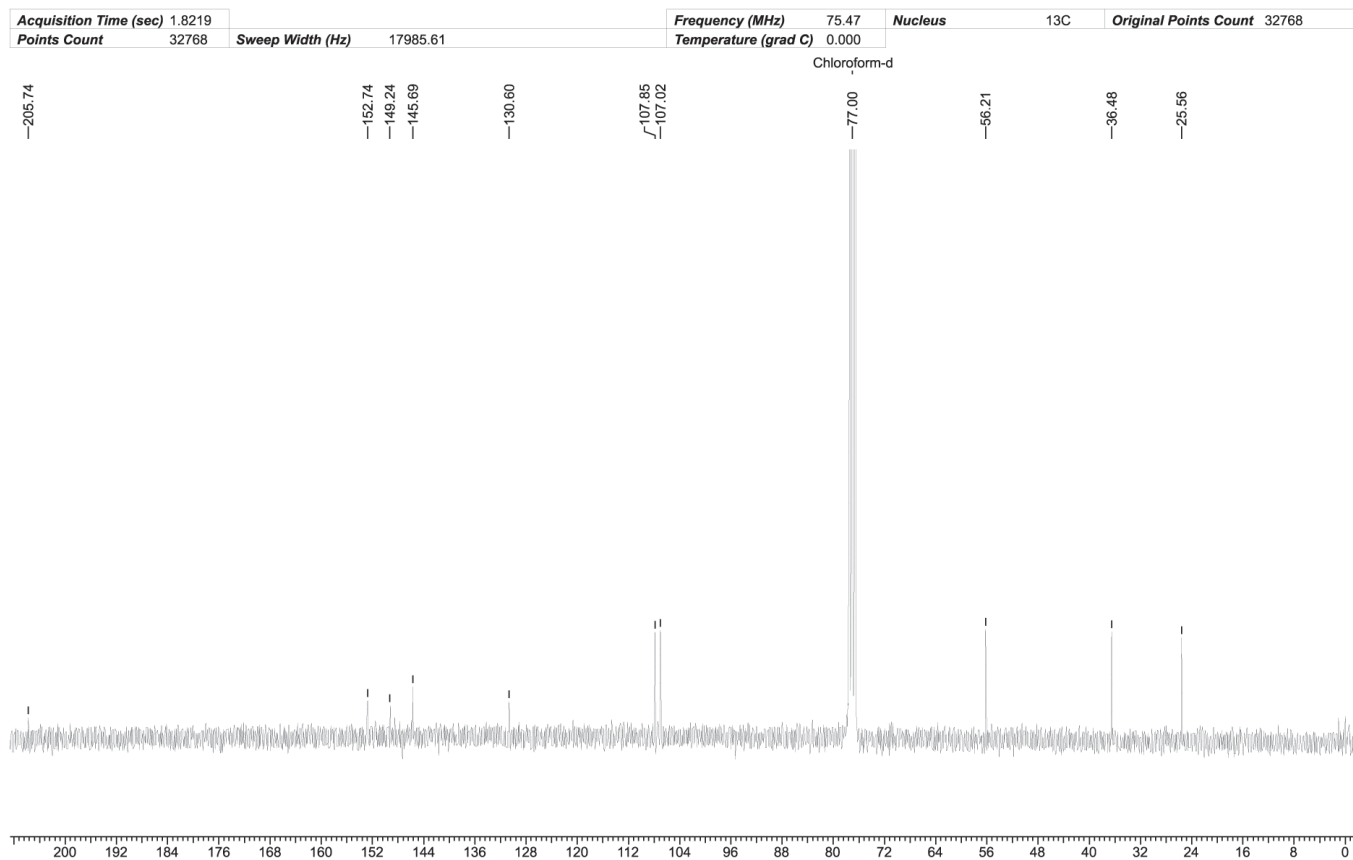


Figura 15S. Espectros de RMN  $^{13}\text{C}$  (75 MHz,  $\text{CDCl}_3$ ) do composto **10**



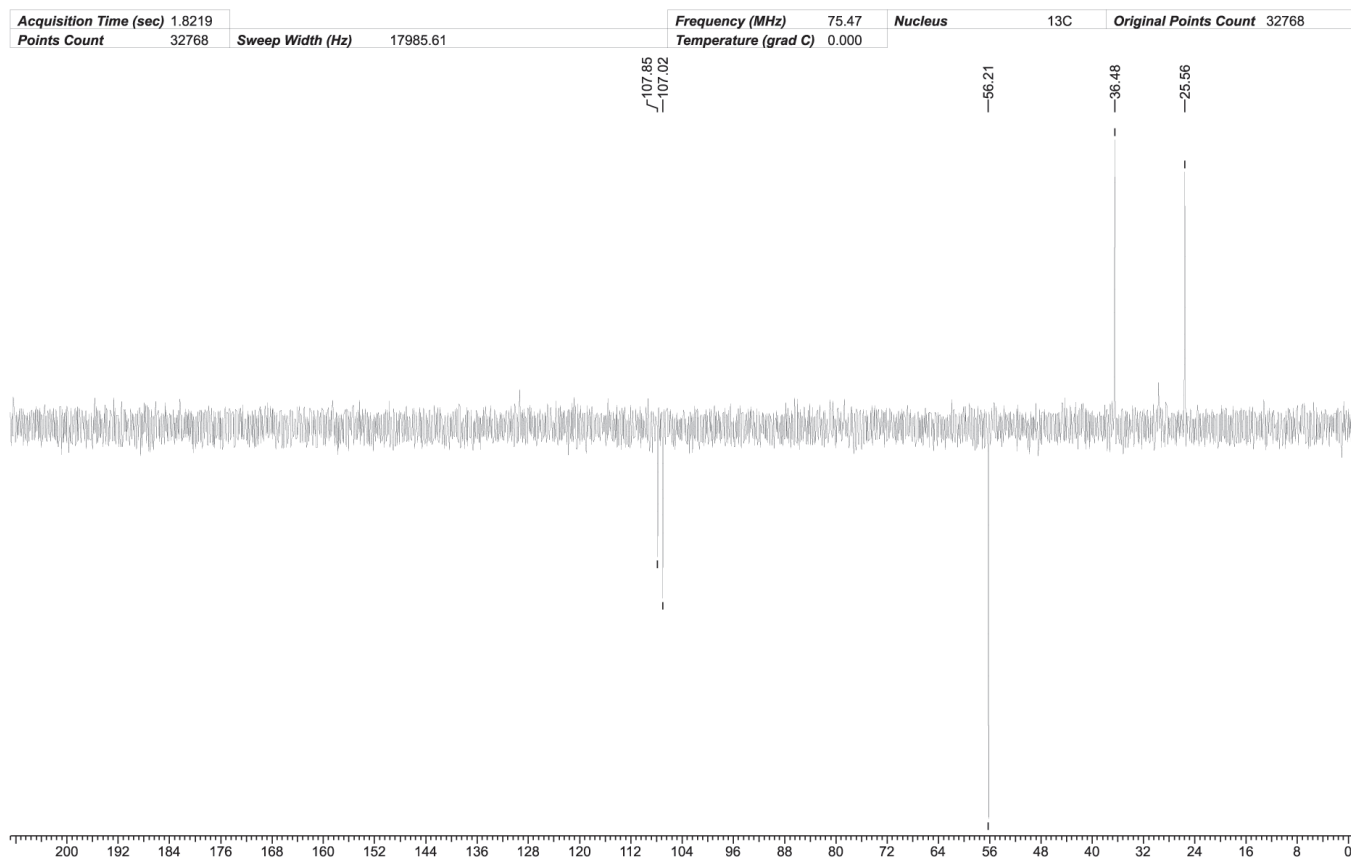


Figura 16S. Espectro de RMN <sup>13</sup>C (75 MHz, CDCl<sub>3</sub>) DEPT-135 do composto 10

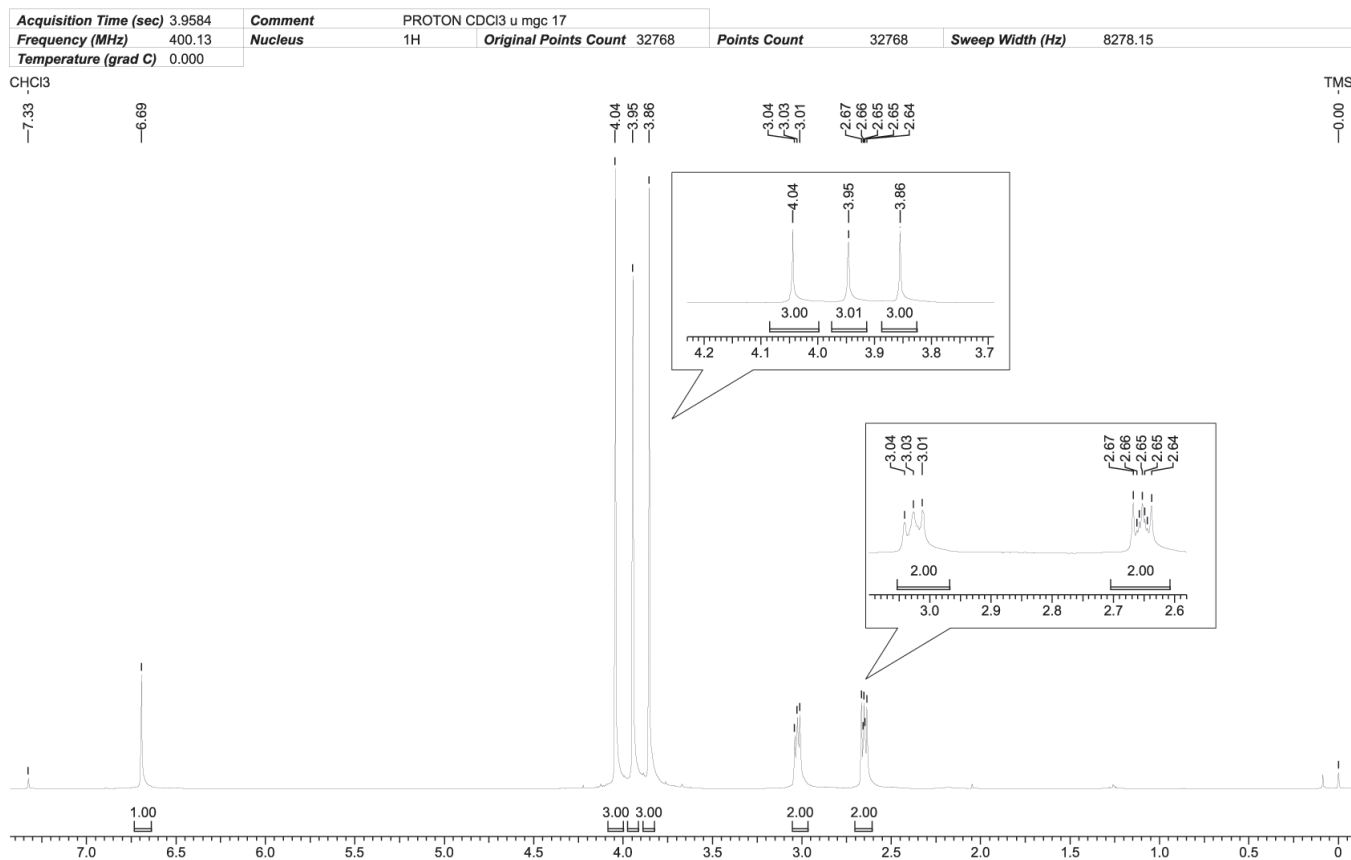


Figura 17S. Espectro de RMN <sup>1</sup>H (400 MHz, CDCl<sub>3</sub>) do composto 11

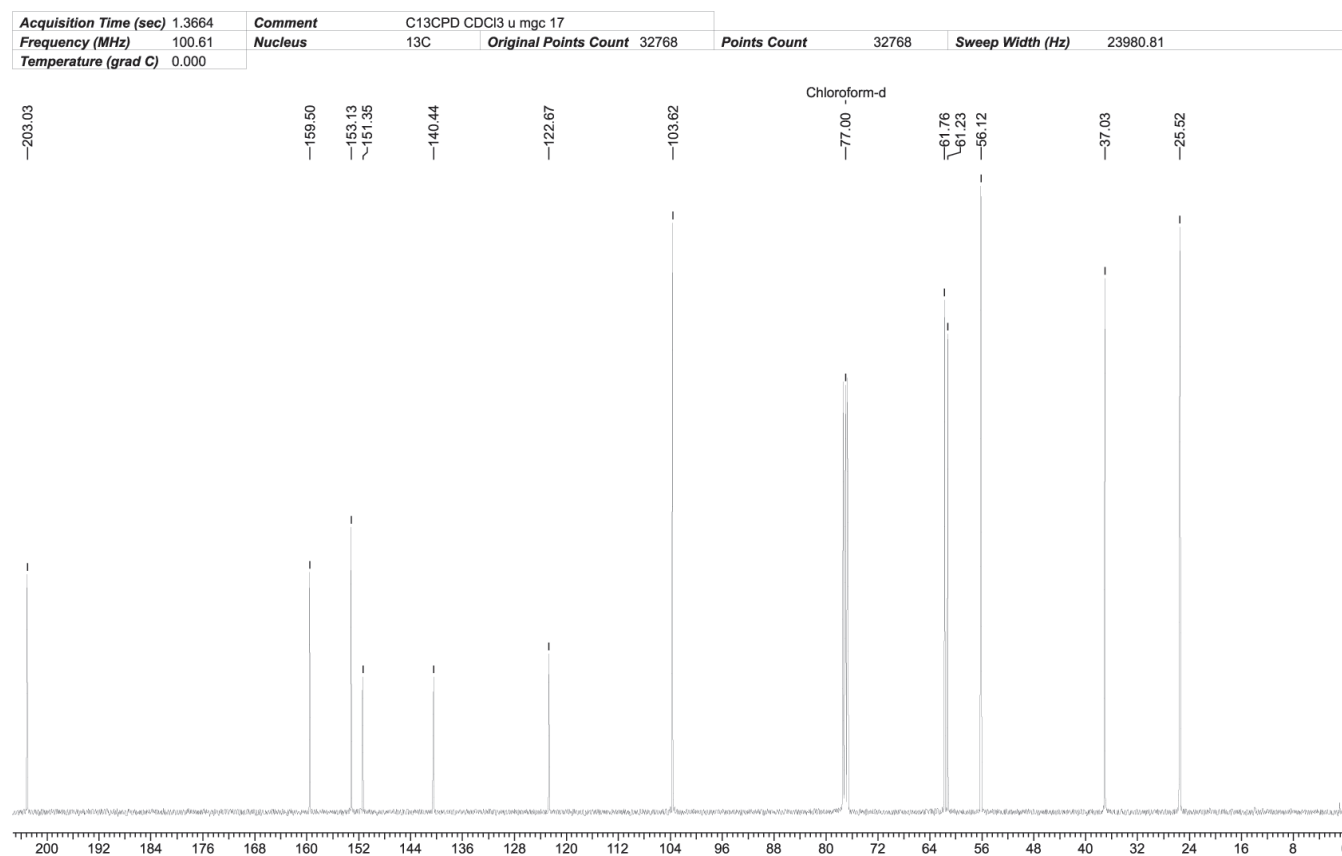


Figura 18S. Espectros de RMN  $^{13}\text{C}$  (100 MHz,  $\text{CDCl}_3$ ) do composto **II**

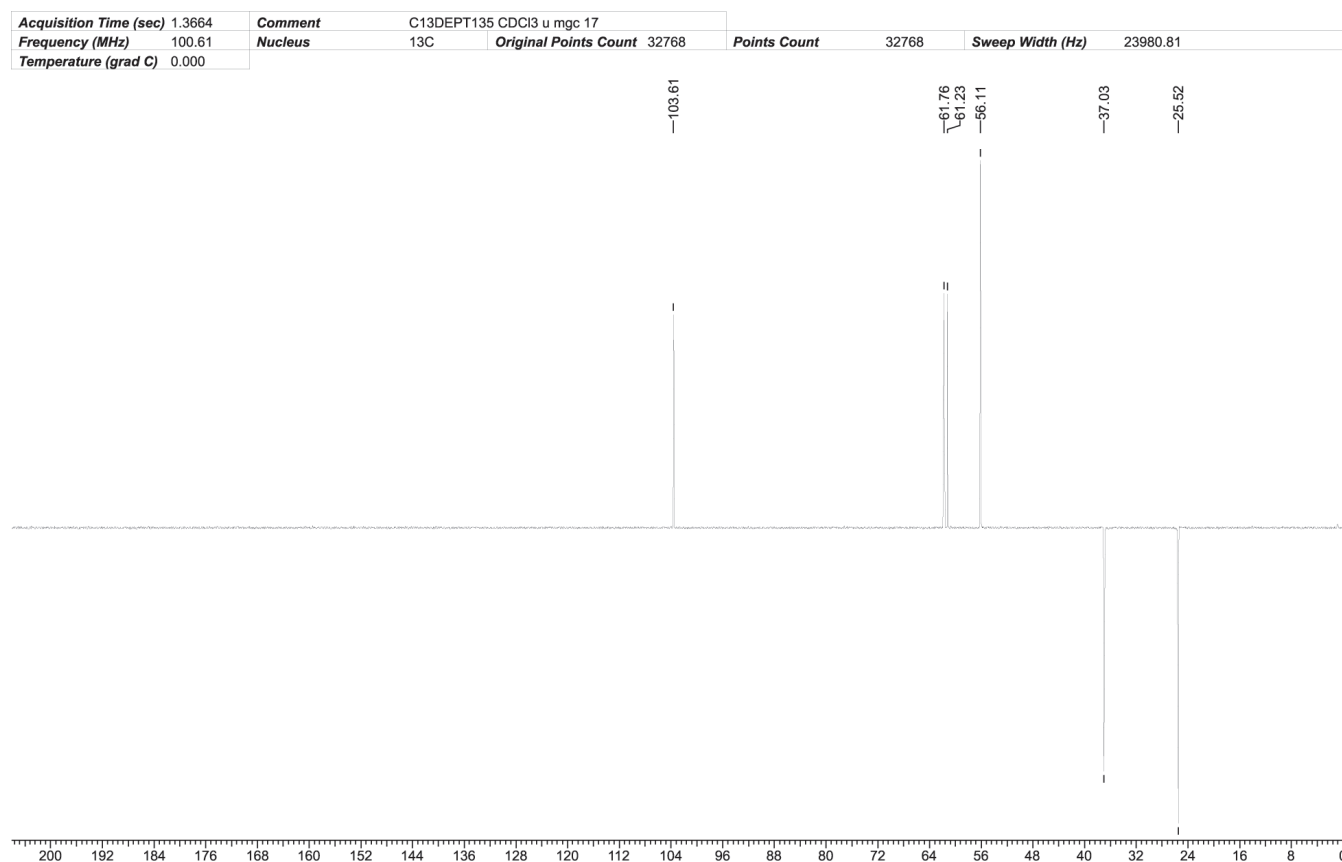


Figura 19S. Espectro de RMN  $^{13}\text{C}$  (100 MHz,  $\text{CDCl}_3$ ) DEPT-135 do composto **II**

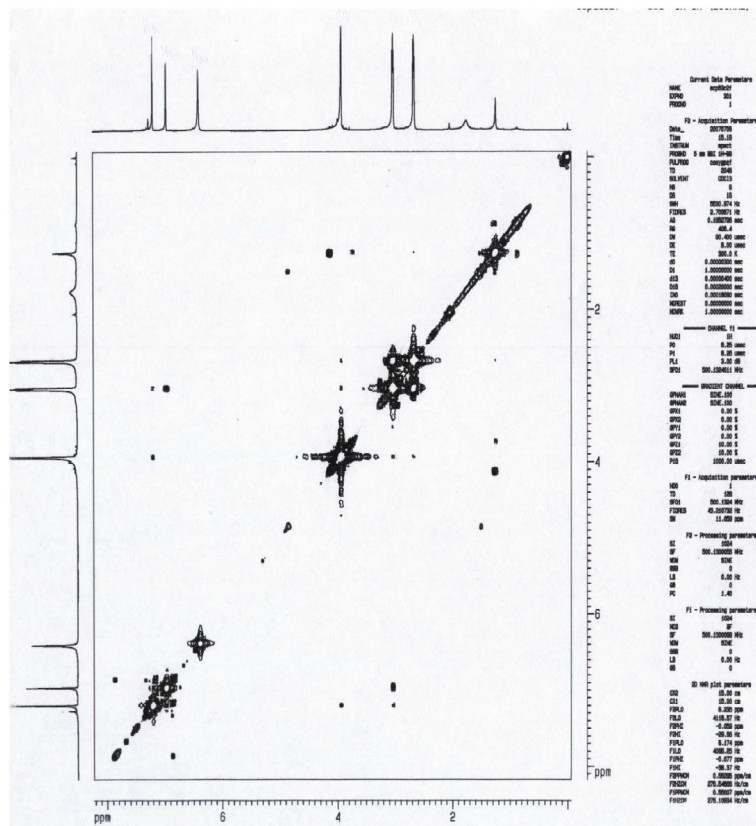


Figura 20S. Espectro COSY do composto 9

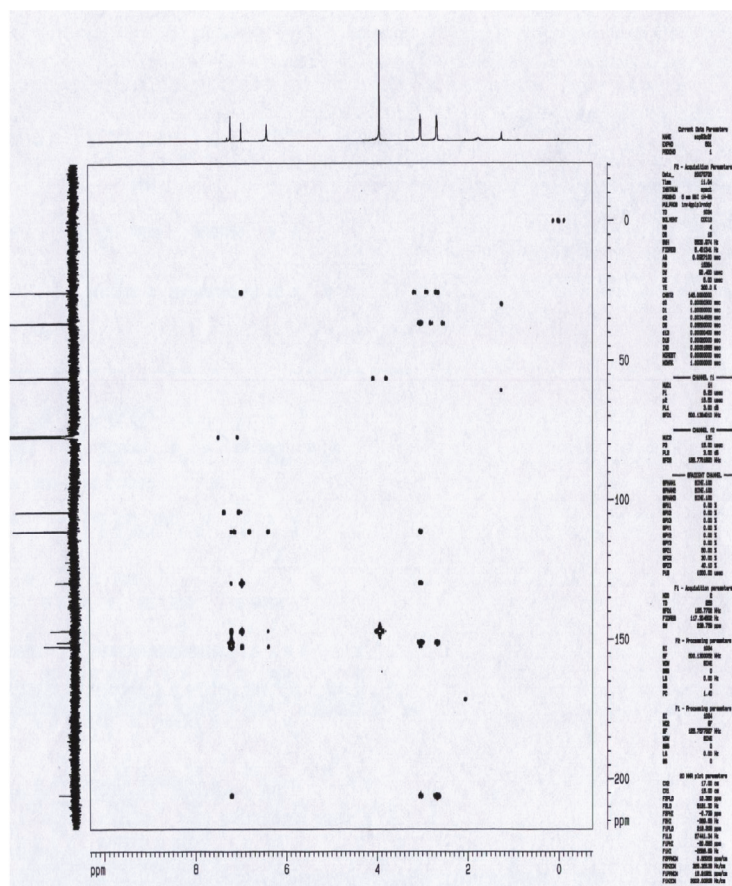


Figura 21S. Espectro gHMBC do composto 9

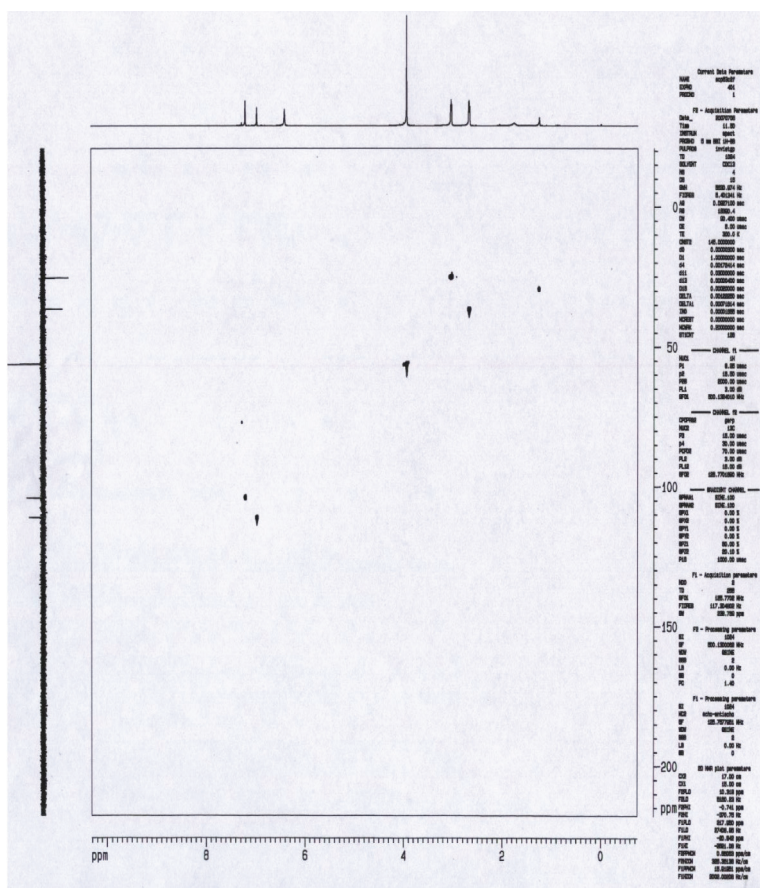


Figura 22S. Espectro gHMOC do composto 9

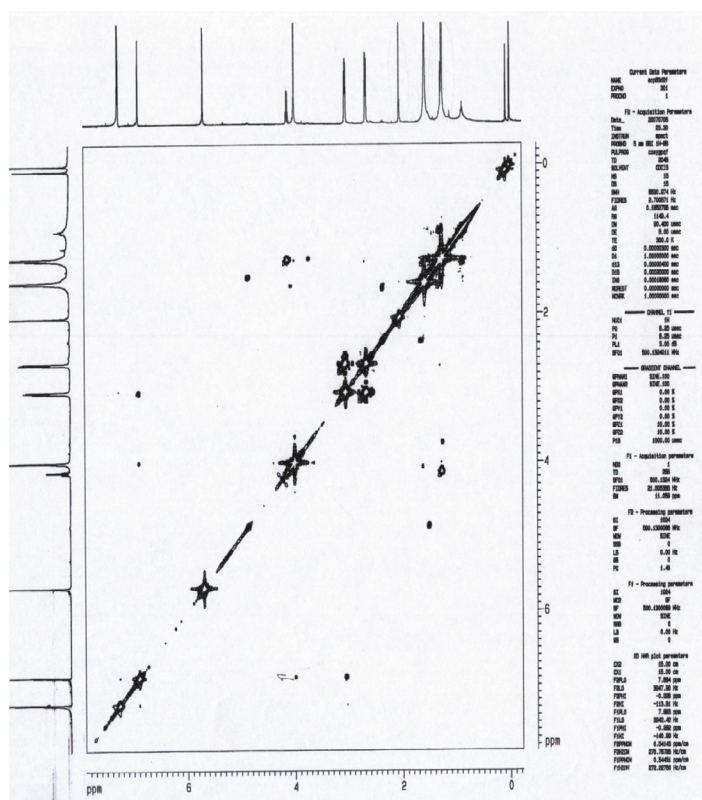


Figura 23S. Espectro COSY do composto 10



**Tabela 1S.** Comparação da reação de Friedel-Crafts intramolecular do ácido 3-fenilpropanóico (**1**) com diferentes ácidos de Lewis\*

ácido de Lewis	% mol do ácido de Lewis	Solvente	Tempo (h)	Temp. (°C)	Rendimento %
NbCl <sub>5</sub>	200	CHCl <sub>2</sub>	2	t. a.	78
	250	CHCl <sub>2</sub>	2	t. a.	82
Bi(NTf <sub>2</sub> ) <sub>3</sub>	5	C <sub>6</sub> H <sub>5</sub> Cl	10	200 <sup>a</sup>	16
Ga(OTf) <sub>3</sub>	5	C <sub>6</sub> H <sub>5</sub> Cl	2	240 <sup>a</sup>	3
In(OTf) <sub>3</sub>	10	C <sub>6</sub> H <sub>5</sub> Cl	3	240 <sup>a</sup>	12
Tb(OTf) <sub>3</sub>	10	C <sub>6</sub> H <sub>5</sub> Cl	1	250 <sup>a</sup>	93

<sup>a</sup> reação realizada em tubo selado.

\* Cui, D. M.; Zhang, C.; Kawamura, M.; Shimada, S.; *Tetrahedron Lett.* **2004**, *45*, 1741.