

FLAVONOÏDES E TERPENOÏDES DE *Croton muscicarpa* (Euphorbiaceae)

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**Tabela 1S.** Dados de RMN  $^{13}\text{C}$  dos flavonoides isolados de *C. muscicarpa*

C	$\delta_{\text{C}}$							
	3 <sup>a</sup>	4 <sup>b</sup>	5 <sup>c</sup>	6 <sup>a</sup>	8 <sup>d</sup>	9 <sup>a</sup>	10 <sup>a</sup>	13 <sup>a</sup>
2	156,0	156,2	147,9	156,2	148,2	155,6	156,2	156,1
3	139,2	139,2	138,7	139,1	137,3	139,0	138,9	139,0
4	178,9	179,1	177,6	179,0	177,5	179,0	179,1	179,1
5	162,2	162,3	162,0	162,3	162,7	152,7	153,0	152,5
6	98,0	98,1	98,3	98,1	99,4	132,2	132,5	132,5
7	165,6	165,7	165,9	165,7	165,7	158,8	159,0	159,0
8	92,4	92,4	92,3	92,4	94,6	90,3	90,5	90,5
9	157,0	157,0	157,2	157,0	158,4	152,3	152,5	153,0
10	106,2	106,4	105,6	106,3	104,7	106,6	106,8	106,8
1'	123,1	123,1	125,5	122,7	123,9	123,6	123,0	123,1
2'	111,5	130,4	116,5	111,2	130,9	114,3	130,3	111,5
3'	149,0	114,3	146,2	146,6	115,7	145,6	114,3	149,0
4'	151,6	162,0	150,6	148,6	160,7	148,7	161,9	151,6
5'	111,1	114,3	112,4	114,8	115,7	110,4	114,3	111,1
6'	122,4	130,4	120,8	122,9	130,9	121,6	130,3	122,4
3'-OMe	60,4	60,4		60,0		60,1	60,3	60,4
6'-OMe						60,9	61,0	61,1
7'-OMe	56,0	56,0	56,2	56,1		56,3	56,5	56,2
3'-OMe	56,3			56,4				56,5
4'-OMe	56,2	55,7	56,1			56,0	55,6	56,3

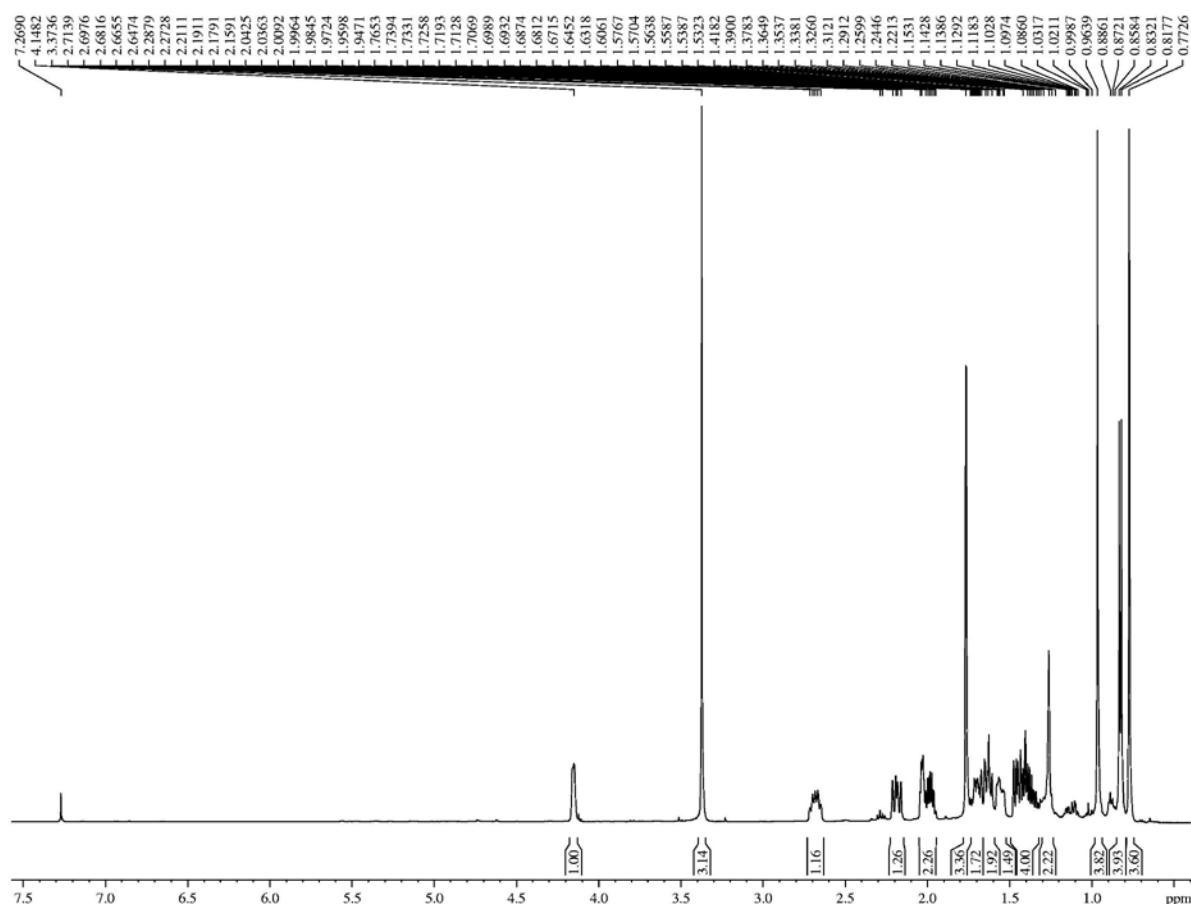
<sup>a</sup> 125 MHz, CDCl<sub>3</sub>; <sup>b</sup> 75 MHz, CDCl<sub>3</sub>; <sup>c</sup> 125 MHz, C<sub>5</sub>D<sub>5</sub>N; <sup>d</sup> 125 MHz, CD<sub>3</sub>OD.

**Tabela 2S.** Dados de RMN <sup>1</sup>H dos flavonoides **3** a **6** isolados de *C. muscicarpa*

C	3 <sup>a</sup>	4 <sup>b</sup>	5 <sup>c</sup>	6 <sup>a</sup>
6	6,34 d (1,9)	6,36 d (2,2)	6,56 d (2,0)	6,37 d (2,1)
8	6,43 d (1,9)	6,45 d (2,2)	6,61 d (2,0)	6,45 d (2,1)
2'	7,68 d (1,6)	8,08 d (9,1)	8,50 d (2,0)	7,71 d (1,8)
3'		7,03 d (9,1)		
5'	6,98 d (8,6)	7,03 d (9,1)	7,17 d (8,6)	7,05 d (8,4)
6'	7,72 dd (8,6; 1,6)	8,08 d (9,1)	8,15 dd (8,6; 2,0)	7,68 dd (8,4; 1,8)
3'-OMe	3,86 s	3,87 s		3,87 s
7-OMe	3,87 s	3,88 s	3,78 s	3,88 s
3'-OMe	3,96 s			3,99 s
4'-OMe	3,97 s	3,91 s	3,85 s	
5-OH		12,67 bl	13,13 bl	12,63 bl

<sup>a</sup> 500 MHz, CDCl<sub>3</sub>; <sup>b</sup> 300 MHz, CDCl<sub>3</sub>; <sup>c</sup> 500 MHz, C<sub>5</sub>D<sub>5</sub>N.**Tabela 3S.** Dados de RMN <sup>1</sup>H dos flavonoides **8** a **10** e **13** isolados de *C. muscicarpa*

C	8 <sup>d</sup>	9 <sup>a</sup>	10 <sup>a</sup>	13 <sup>a</sup>
6	6,17 d (2,0)			
8	6,39 d (2,0)	6,52 s	6,50 s	6,50 s
2'	8,09 d (9,0)	7,69 d (2,0)	8,06 d (9,0)	7,68 d (1,8)
3'	6,90 d (9,0)		7,02 d (9,0)	
5'	6,90 d (9,0)	6,98 d (8,5)	7,02 d (9,0)	6,99 d (8,5)
6'	8,10 d (9,0)	7,74 dd (8,5; 2,0)	8,06 d (9,0)	7,73 dd (8,5; 1,8)
3'-OMe		3,87 s	3,86 s	3,86 s
6-OMe		3,91 s	3,90 s	3,92 s
7-OMe		3,93 s	3,92 s	3,96 s
3'-OMe				3,96 s
4'-OMe		4,00 s	3,96 s	3,96 s
5-OH				12,60 s

<sup>a</sup> 500 MHz, CDCl<sub>3</sub>; <sup>d</sup> 500 MHz, CD<sub>3</sub>OD.**Figura 1S.** Espectro de RMN <sup>1</sup>H do 6α-metoxi-cipereno (**1**) (500 MHz, CDCl<sub>3</sub>)

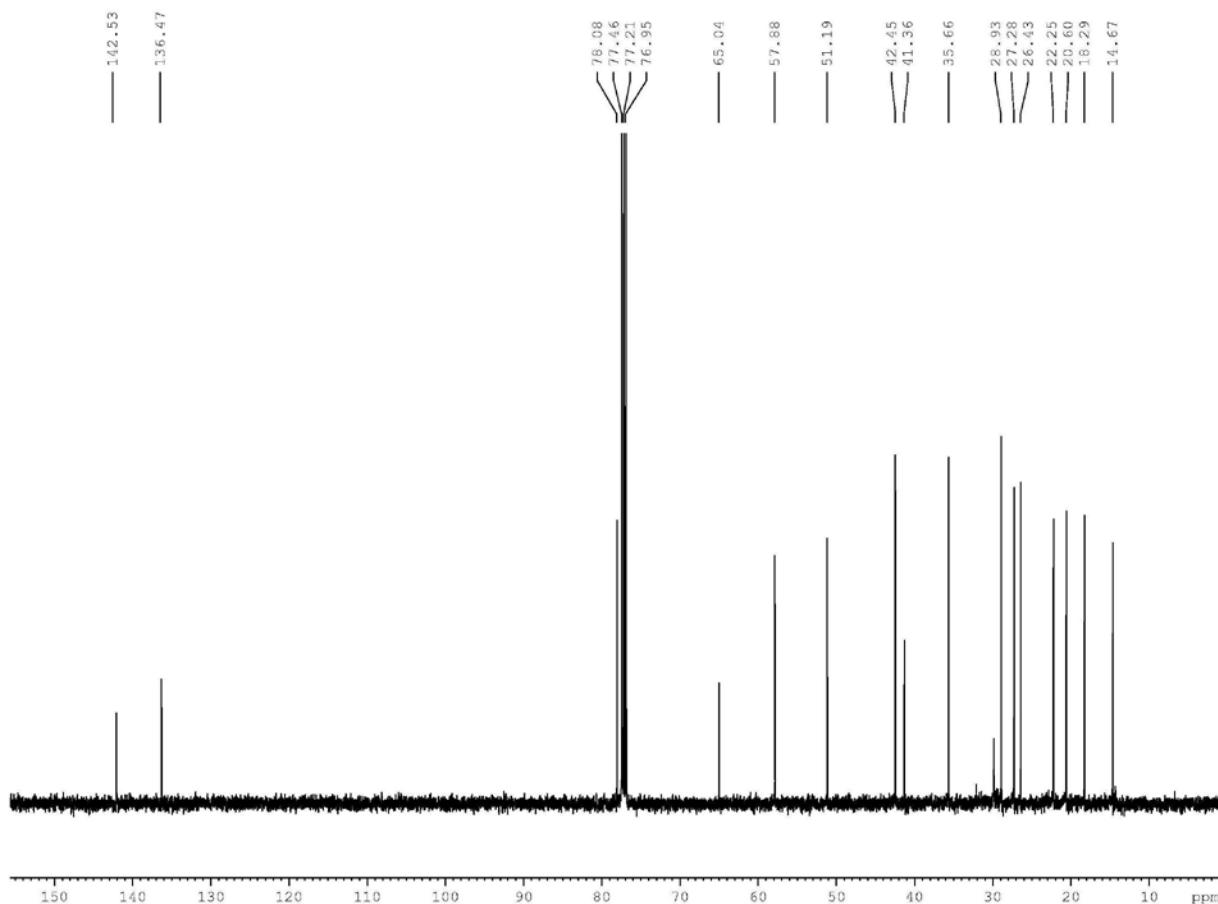


Figura 2S. Espectro de RMN  $^{13}\text{C}$ -CPD do  $6\alpha$ -metoxi-cipereno (**I**) (125 MHz,  $\text{CDCl}_3$ )

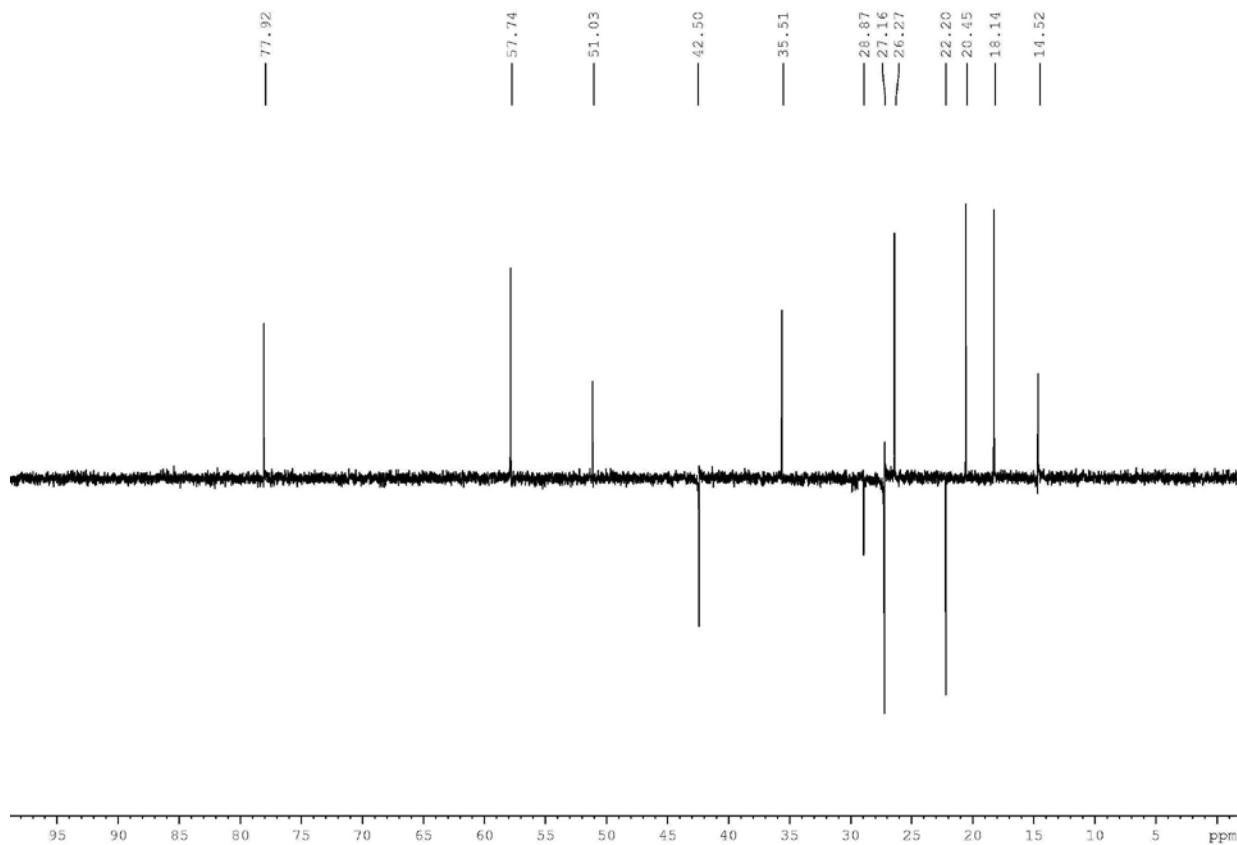


Figura 3S. Espectro de RMN  $^{13}\text{C}$ -DEPT ( $\theta = 135$ ) do  $6\alpha$ -metoxi-cipereno (**I**) (125 MHz,  $\text{CDCl}_3$ )

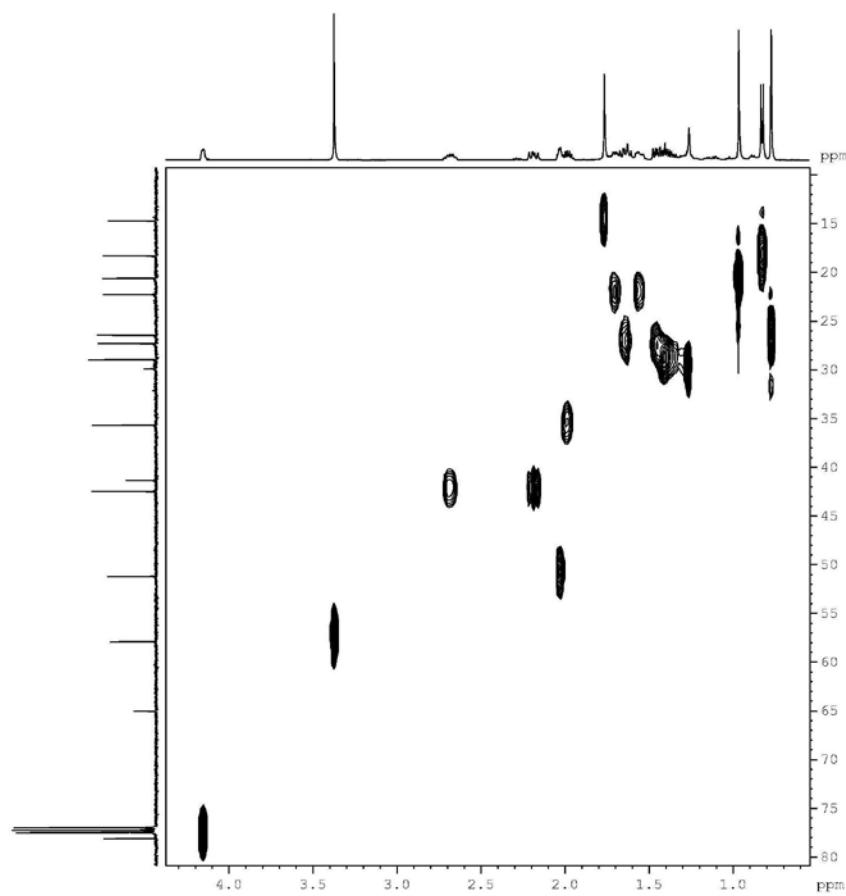


Figura 4S. Mapa de contorno do espectro de RMN HSQC do  $6\alpha$ -metoxi-cipereno (**I**) (500 x 125 MHz,  $\text{CDCl}_3$ )

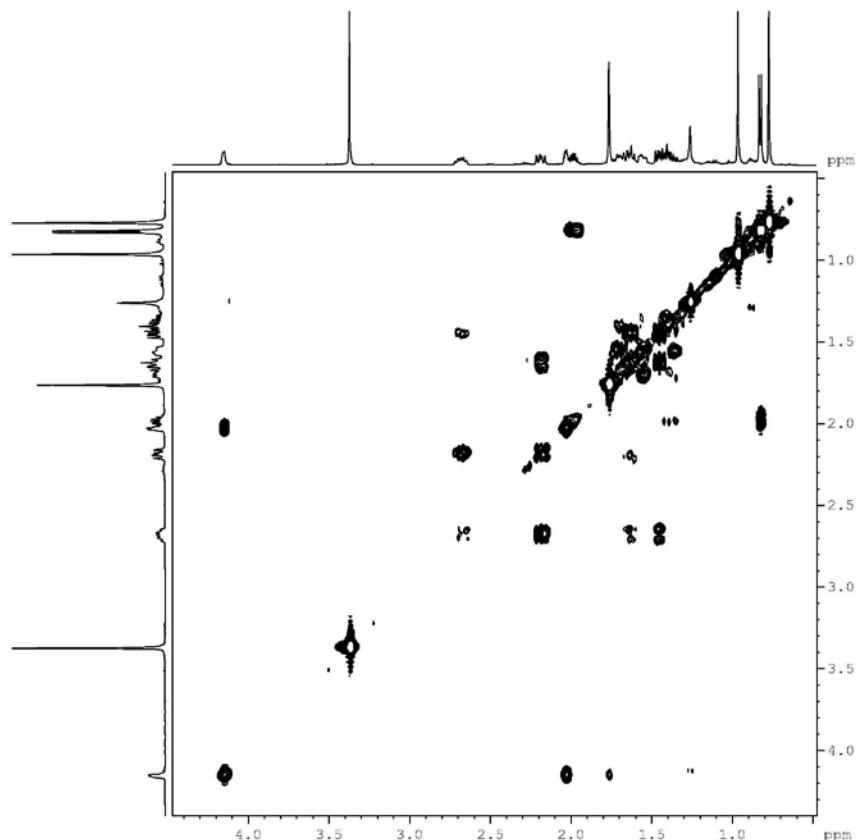


Figura 5S. Mapa de contorno do espectro de RMN  $^1\text{H}$ ,  $^1\text{H}$ -COSY do  $6\alpha$ -metoxi-cipereno (**I**) (500 x 500 MHz,  $\text{CDCl}_3$ )

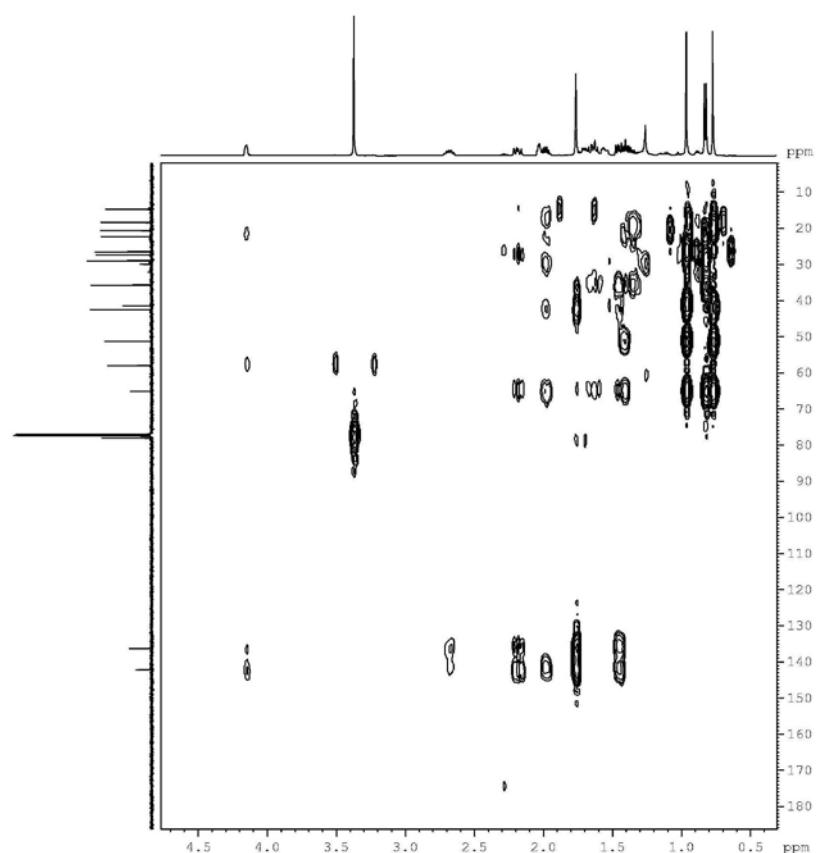


Figura 6S. Mapa de contorno do espectro de RMN HMBC do  $6\alpha$ -metoxi-cipereno (**I**) (500 x 125 MHz,  $\text{CDCl}_3$ )

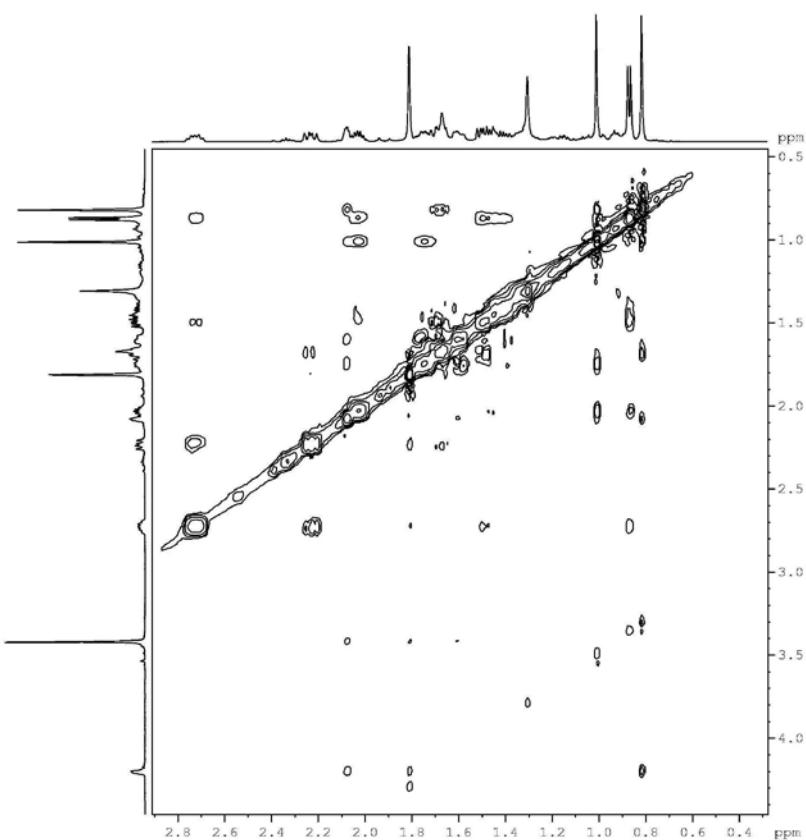
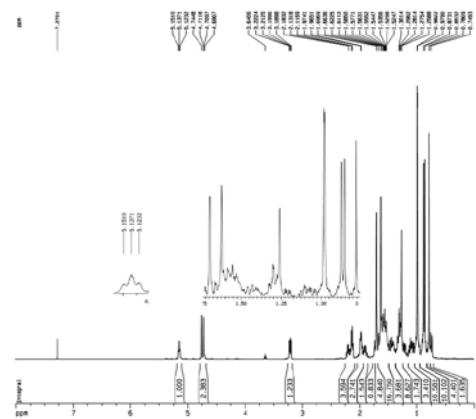
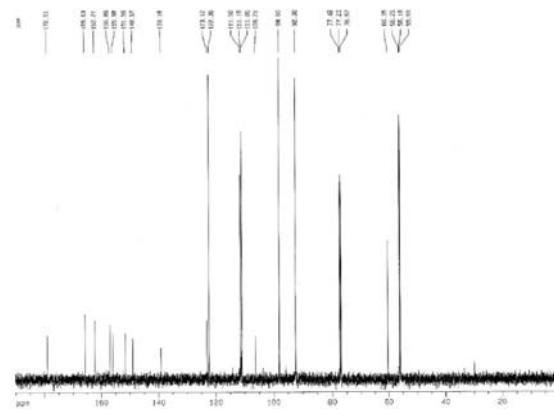


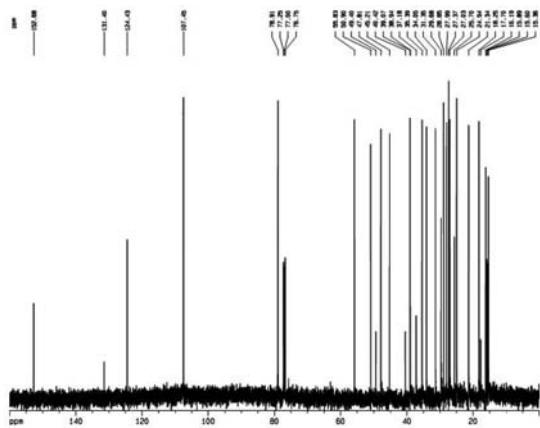
Figura 7S. Mapa de contorno do espectro de RMN do espectro de RMN  $^1\text{H}$ ,  $^1\text{H}$ -NOESY do  $6\alpha$ -metoxi-cipereno (**I**) (500 x 500 MHz,  $\text{CDCl}_3$ )



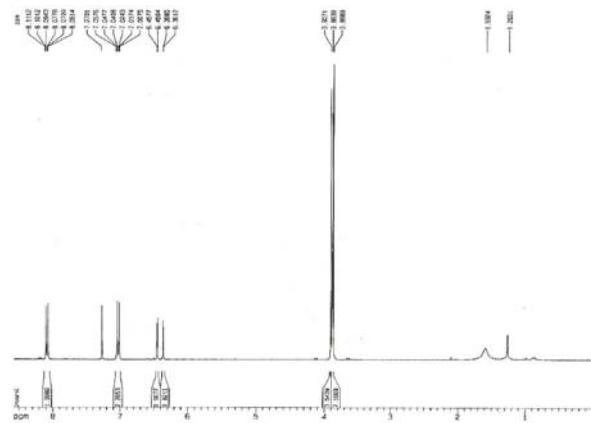
**Figura 8S.** Espectro de RMN  $^1H$  do damaradienol (**2**) ( $CDCl_3$ , 500 MHz)



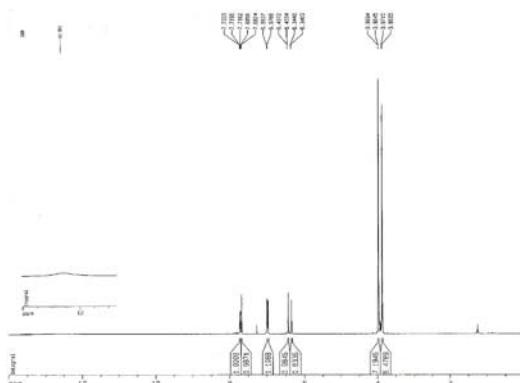
**Figura 11S.** Espectro de RMN  $^{13}\text{C}$ -CPD da retusina (3) (125 MHz,  $\text{CDCl}_3$ )



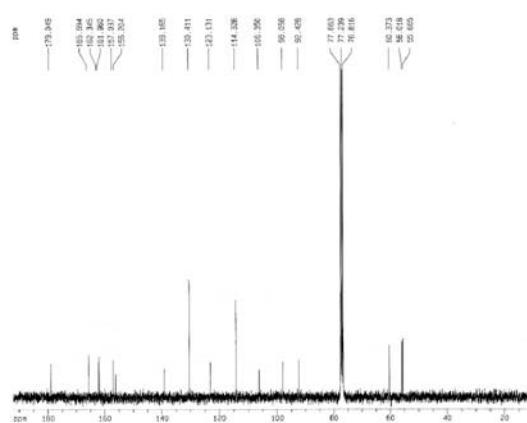
**Figura 9S.** Espectro de RMN  $^{13}\text{C}$ -CPD do damaradienol (**2**) (125 MHz,  $\text{CDCl}_3$ )



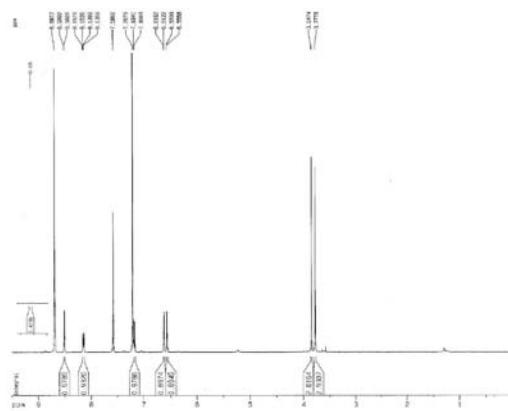
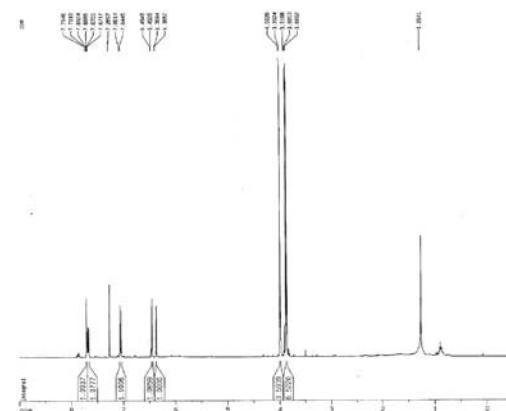
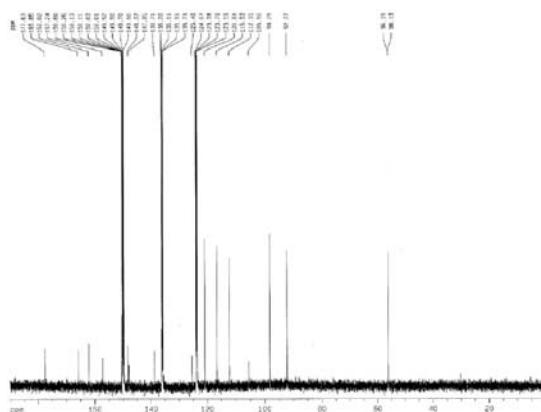
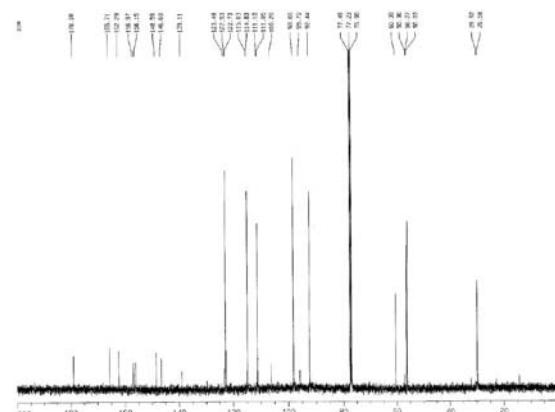
**Figura 12S.** Espectro de RMN  $^1H$  do 3,7,4'-trimetoxicanferol (**4**) (300 MHz,  $CDCl_3$ )

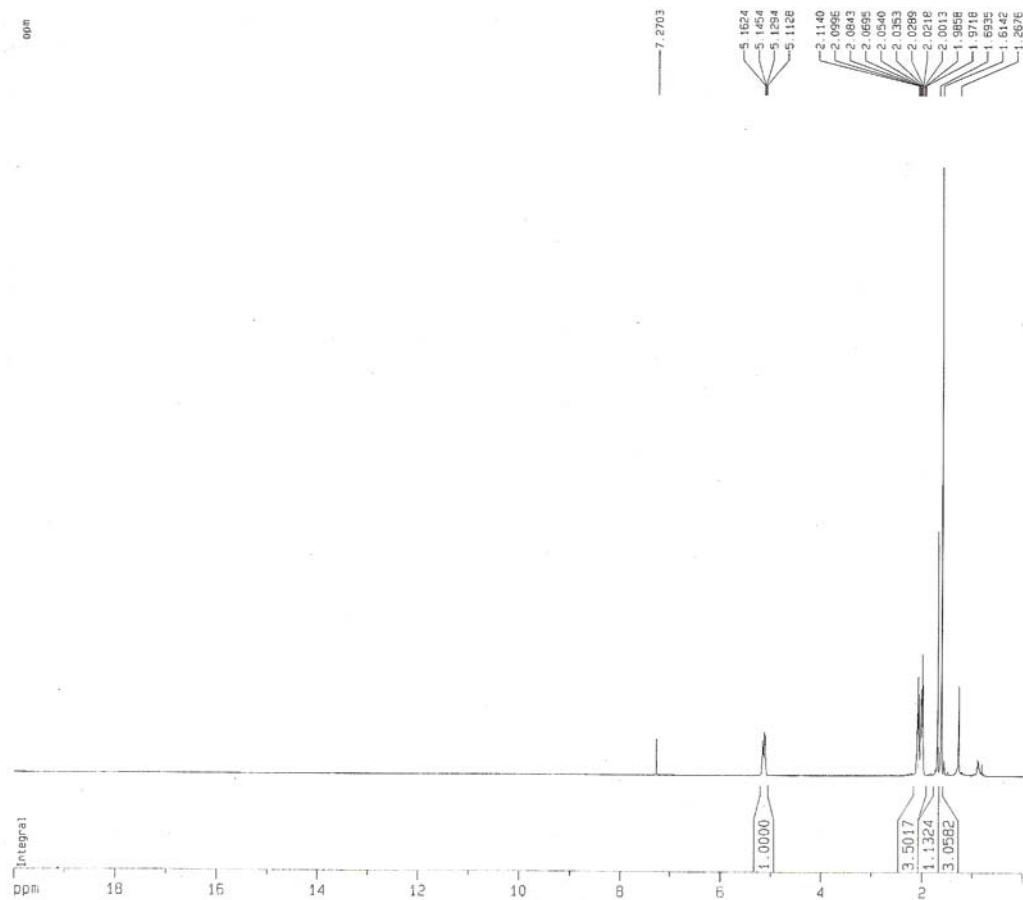


**Figura 10S.** Espectro de RMN  $^1H$  da retusina (3) ( $CDCl_3$ , 500 MHz)

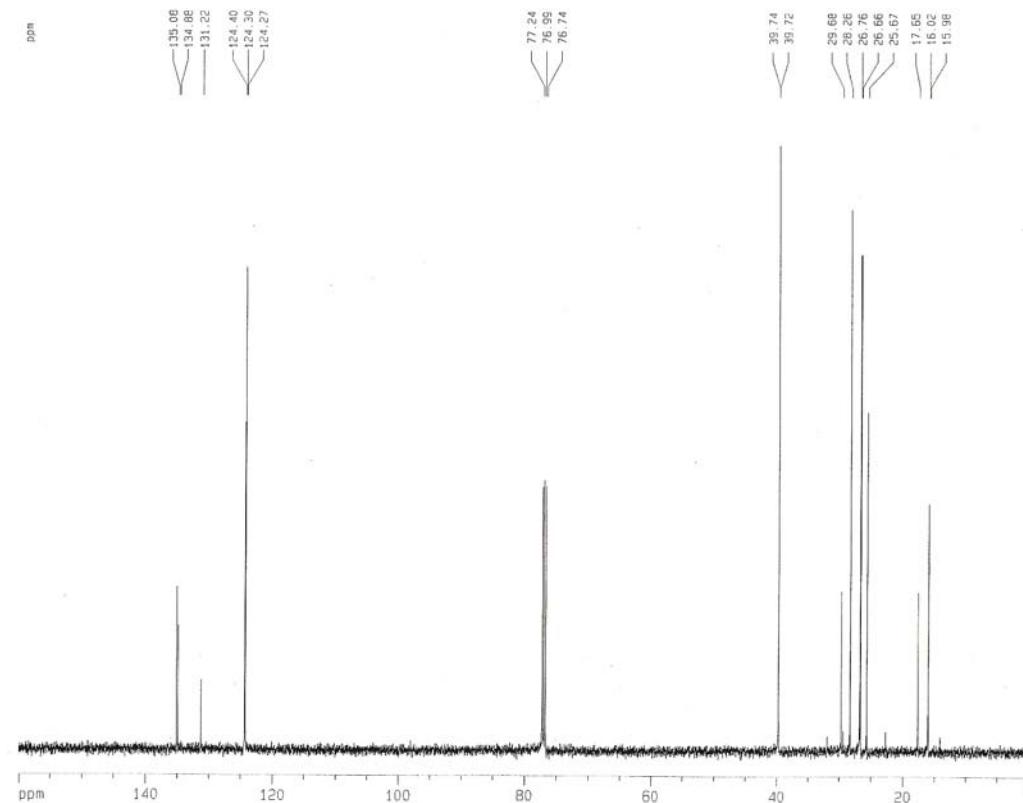


**Figura 13S.** Espectro de RMN  $^{13}\text{C}$ -CPD do 3,7,4'-trimetoxicanferol (**4**) (75 MHz,  $\text{CDCl}_3$ )

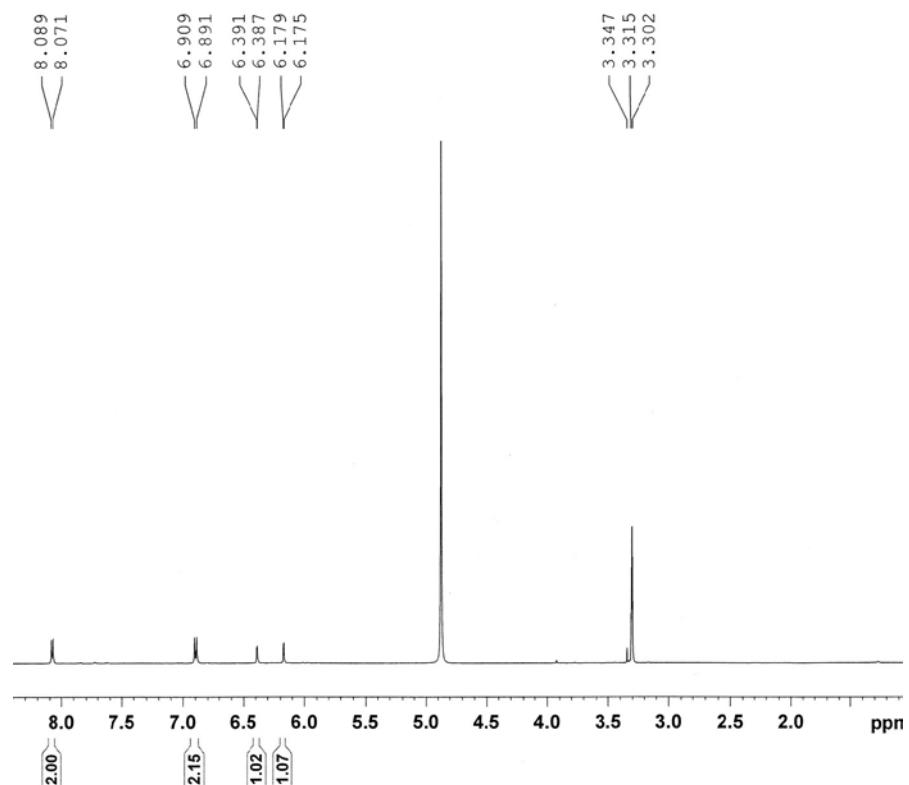
Figura 14S. Espectro de RMN  $^1\text{H}$  da ombuína (**5**) (500 MHz,  $\text{C}_5\text{D}_5\text{N}$ )Figura 16S. Espectro de RMN  $^1\text{H}$  do pachipodol (**6**) (500 MHz,  $\text{CDCl}_3$ )Figura 15S. Espectro de RMN  $^{13}\text{C}$ -CPD da ombuína (**5**) (125 MHz,  $\text{C}_5\text{D}_5\text{N}$ )Figura 17S. Espectro de RMN  $^{13}\text{C}$ -CPD do pachipodol (**6**) (125 MHz,  $\text{CDCl}_3$ )



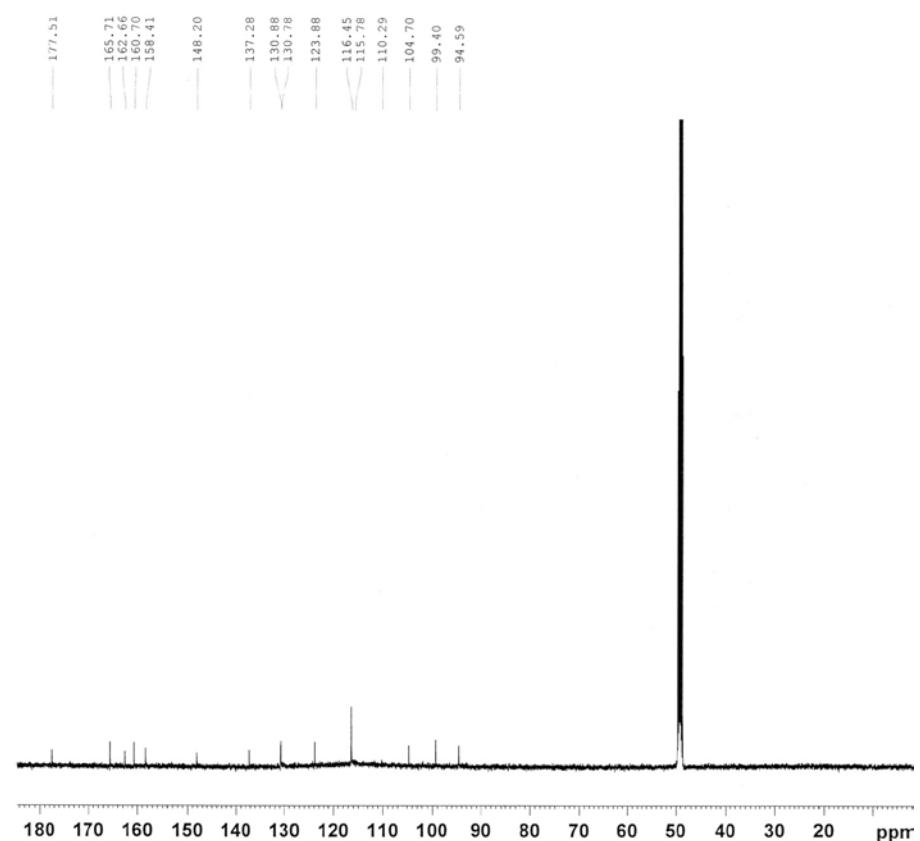
**Figura 18S.** Espectro de RMN  $^1\text{H}$  do esqualeno (7) (500 MHz,  $\text{CDCl}_3$ )



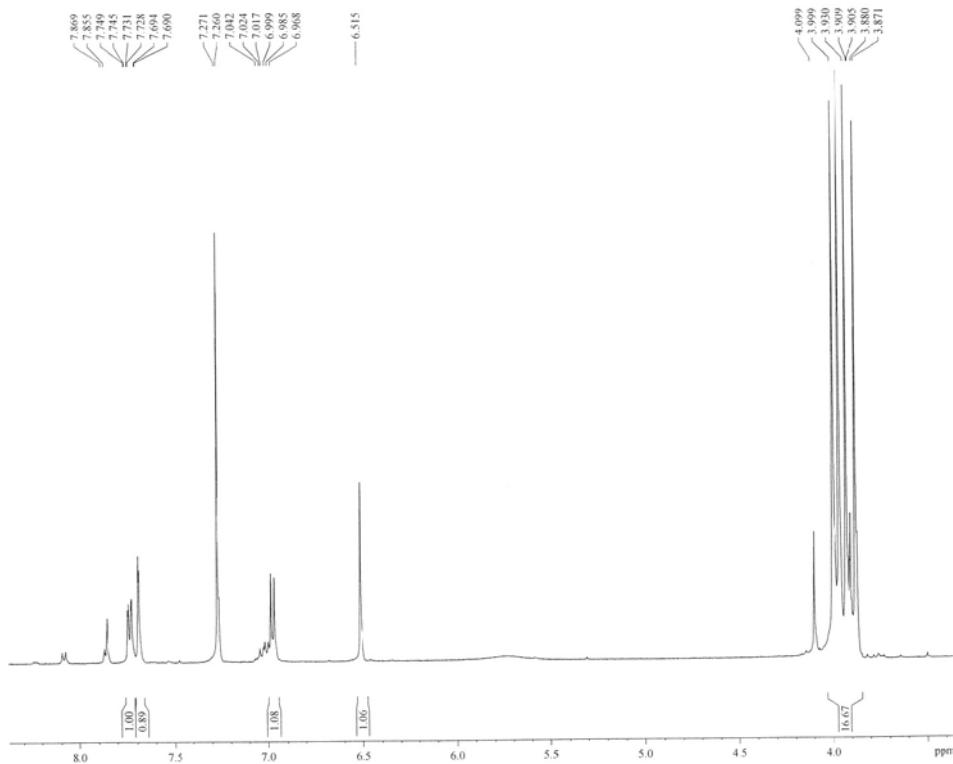
**Figura 19S.** Espectro de RMN  $^{13}\text{C}$ -CPD do esqualeno (7) (125 MHz,  $\text{CDCl}_3$ )



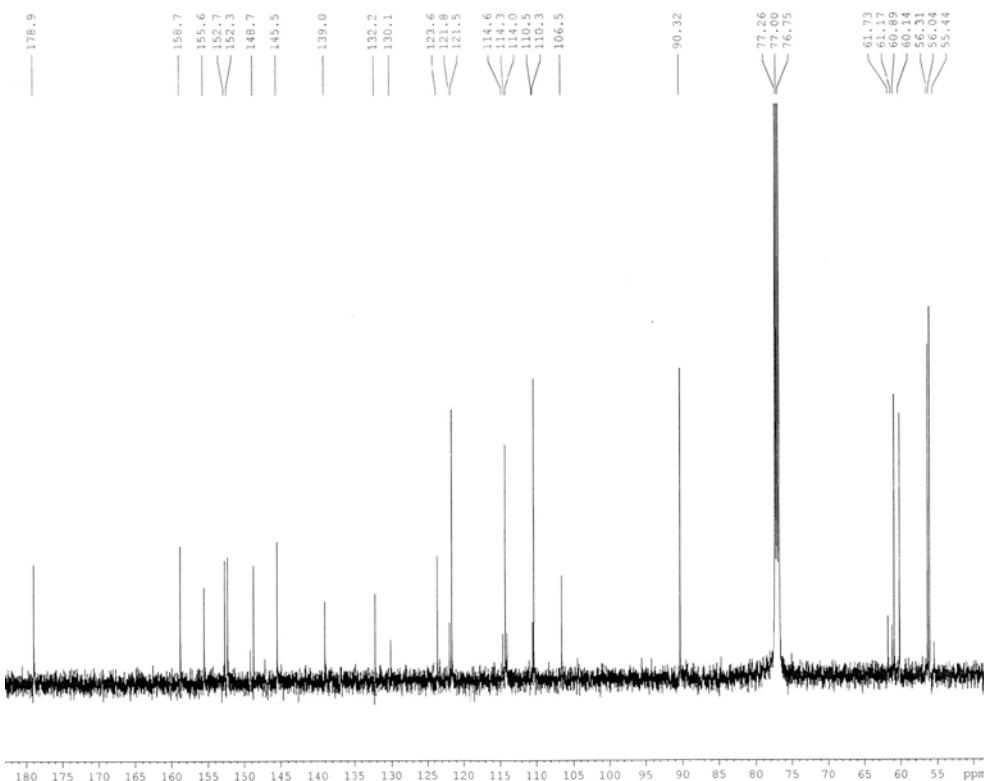
**Figura 20S.** Espectro de RMN  $^1\text{H}$  do canferol (8) (500 MHz,  $\text{CD}_3\text{OD}$ )



**Figura 21S.** Espectro de RMN  $^{13}\text{C}$ -CPD do canferol (8) (125 MHz,  $\text{CD}_3\text{OD}$ )



**Figura 22S.** Espectro de RMN  $^1\text{H}$  da casticina (**9**) (500 MHz,  $\text{CDCl}_3$ )



**Figura 23S.** Espectro de RMN  $^{13}\text{C}$ -CPD da casticina (**9**) (125 MHz,  $\text{CDCl}_3$ )

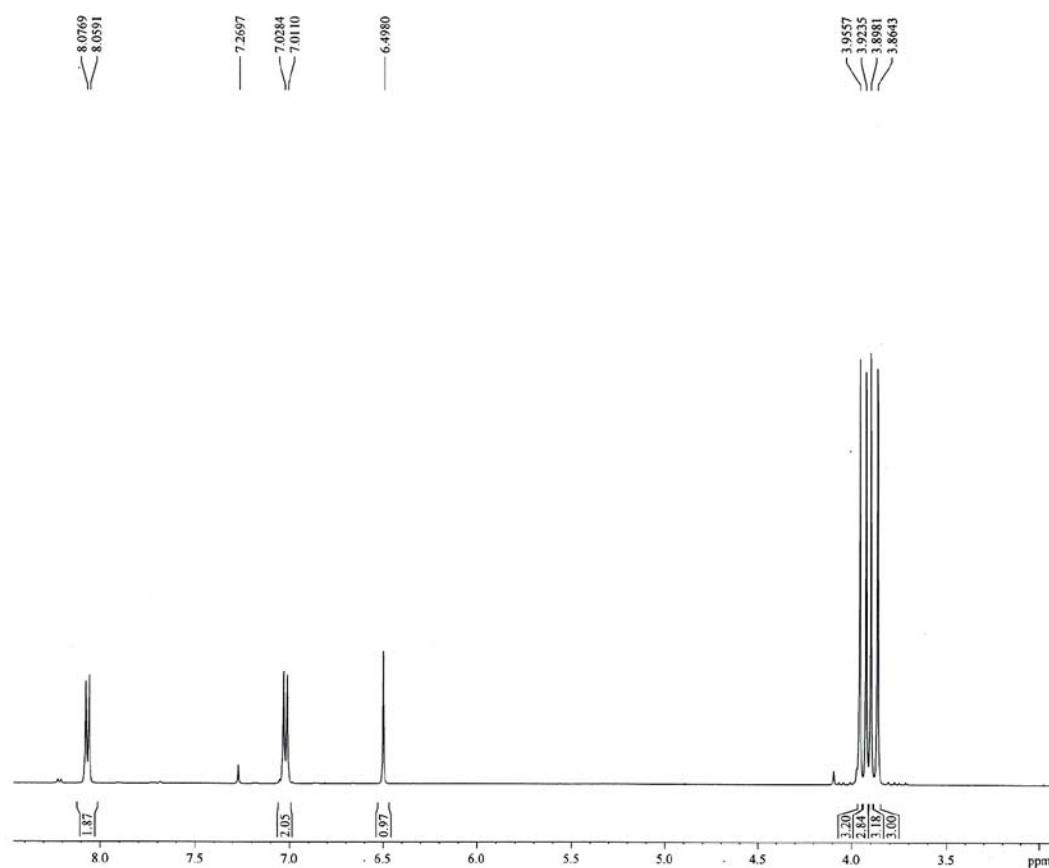


Figura 24S. Espectro de RMN  $^1\text{H}$  do 5-hidroxi-3,6,7,4'-tetrametoxiflavona (**10**) (500 MHz,  $\text{CDCl}_3$ )

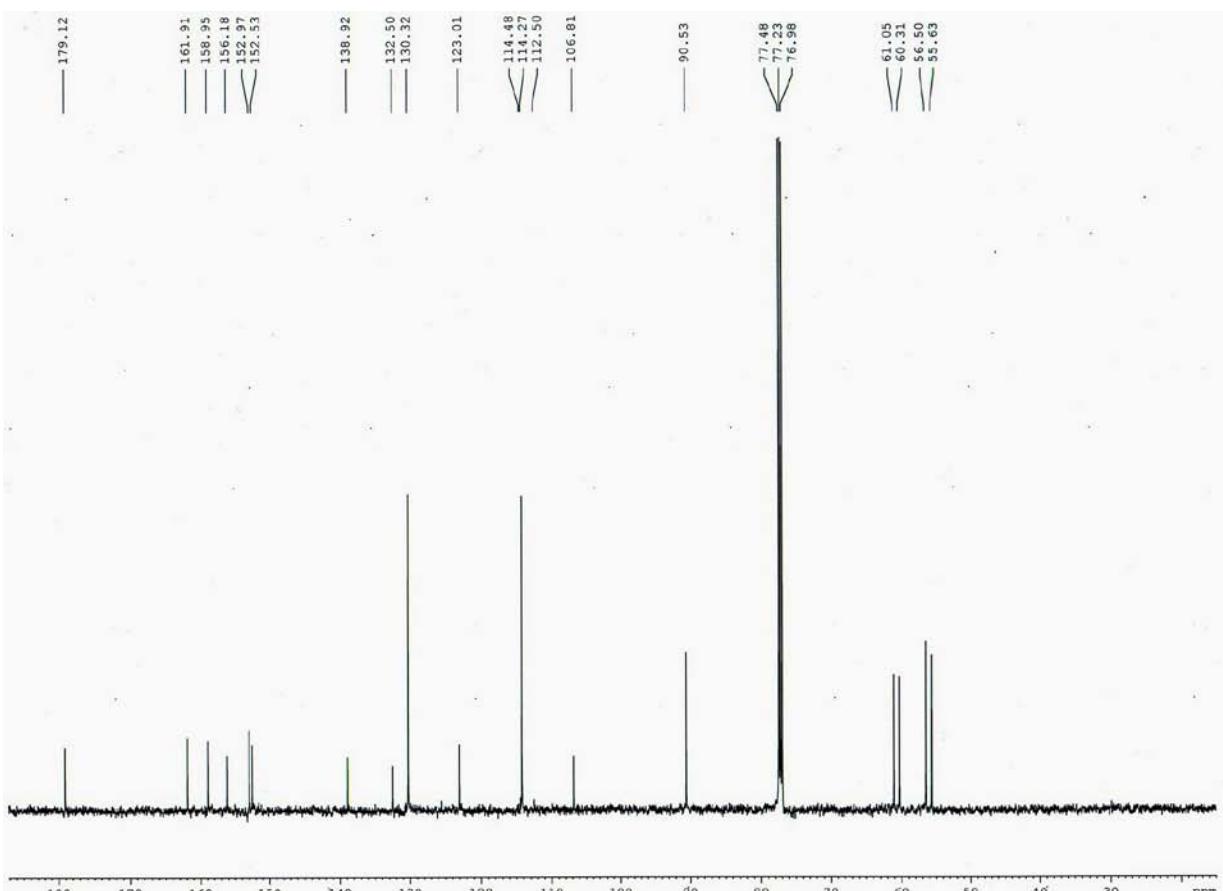
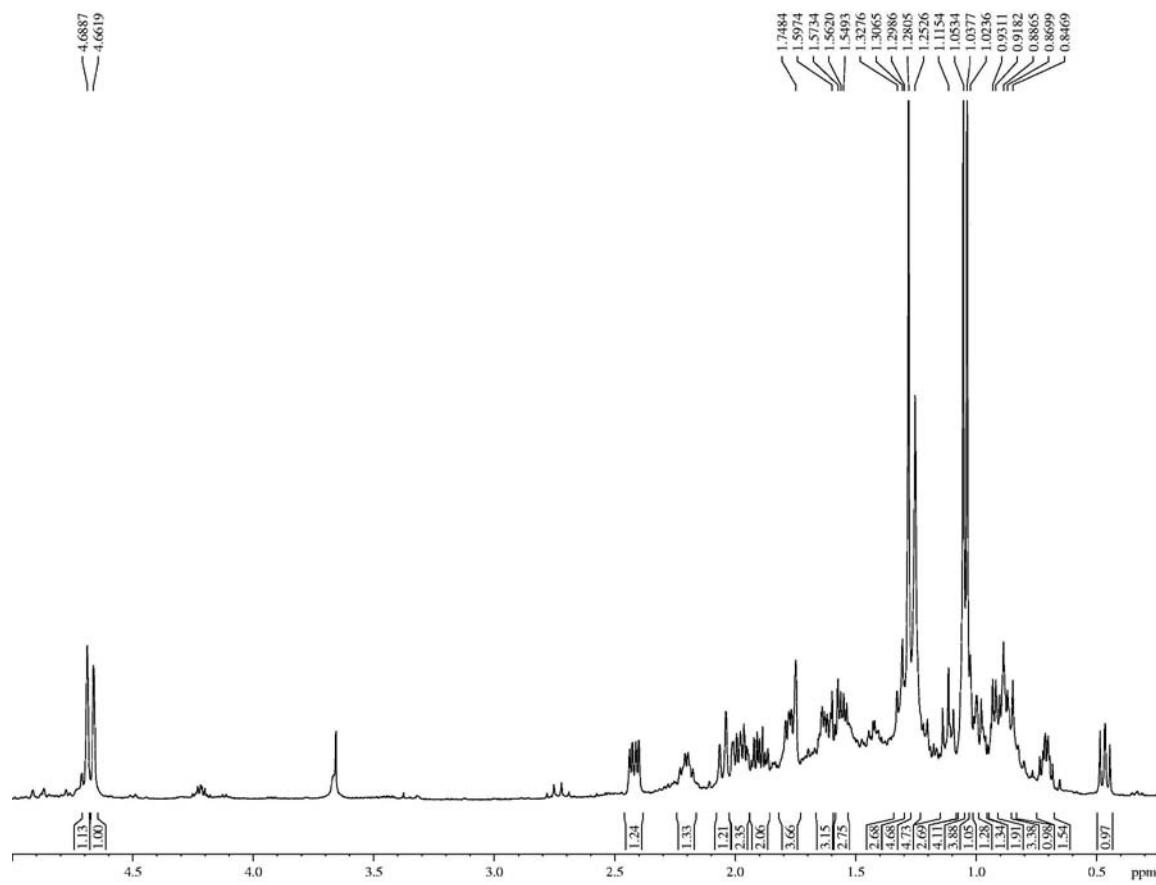
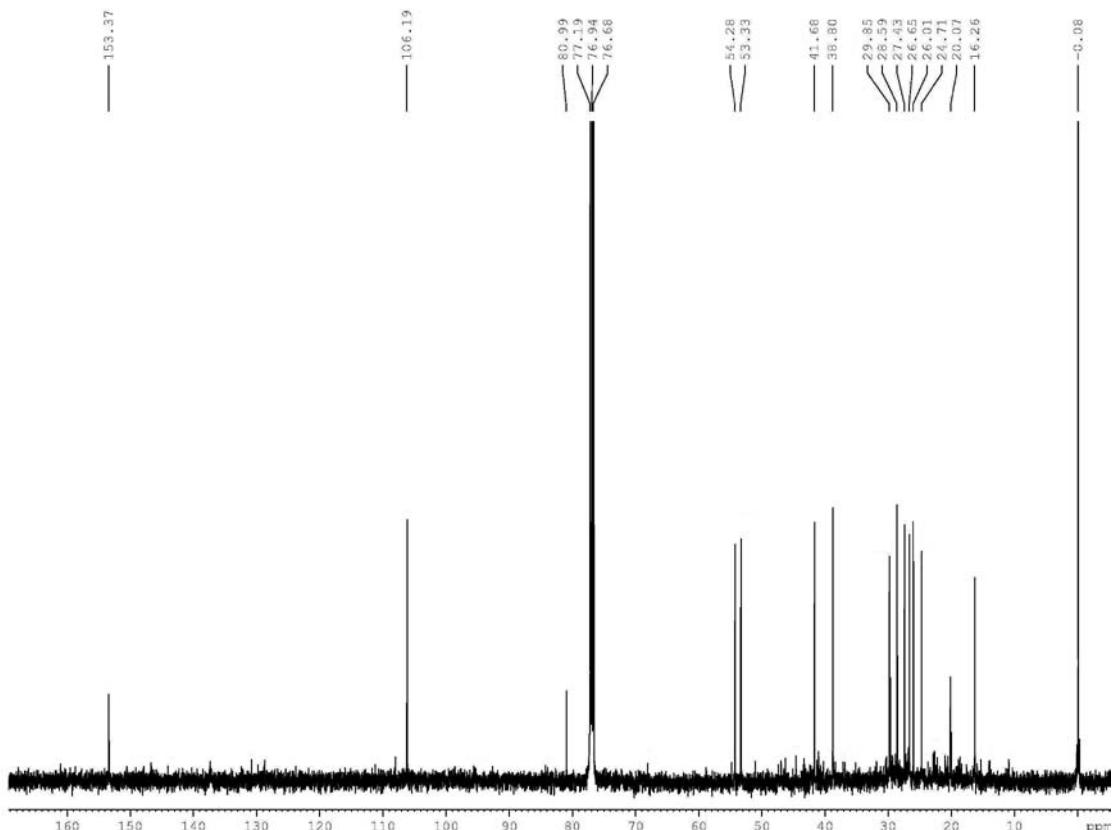


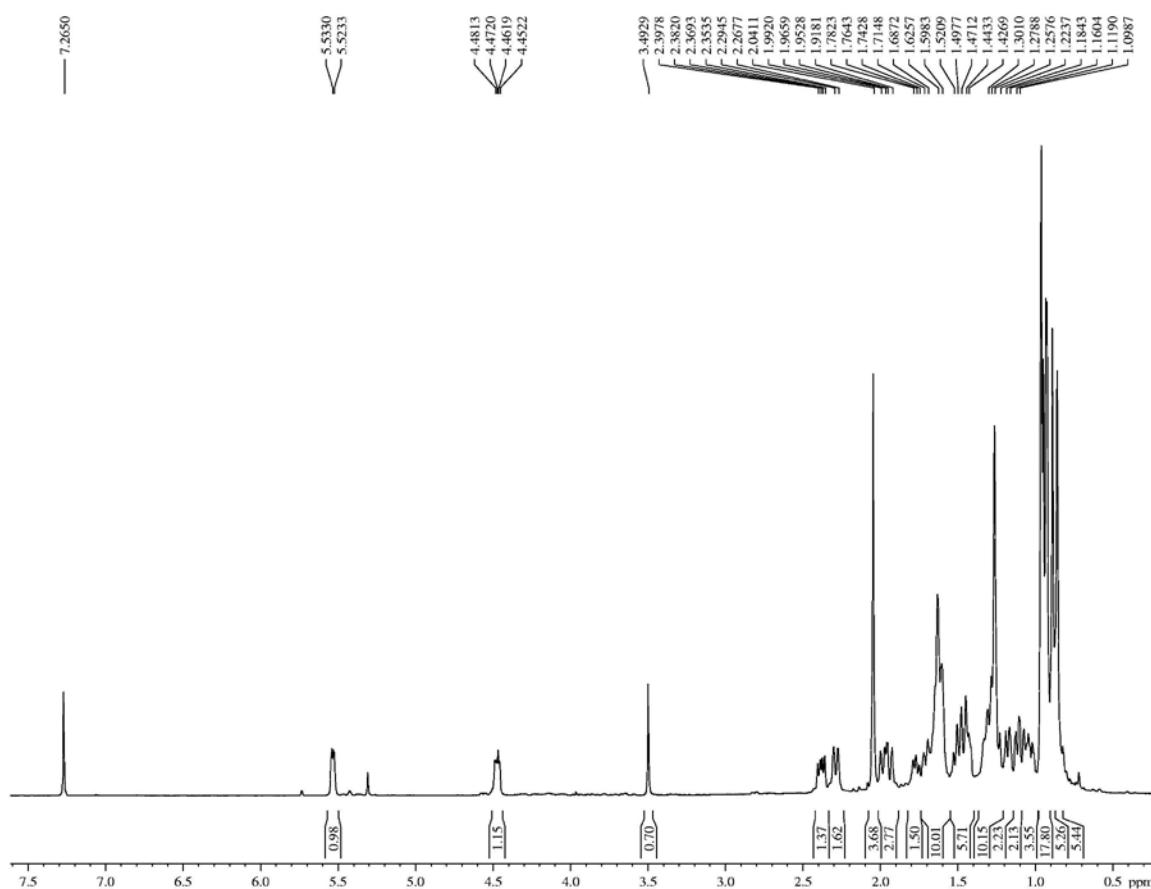
Figura 25S. Espectro de RMN  $^{13}\text{C}$ -CPD do 5-hidroxi-3,6,7,4'-tetrametoxiflavona (**10**) (125 MHz,  $\text{CDCl}_3$ )



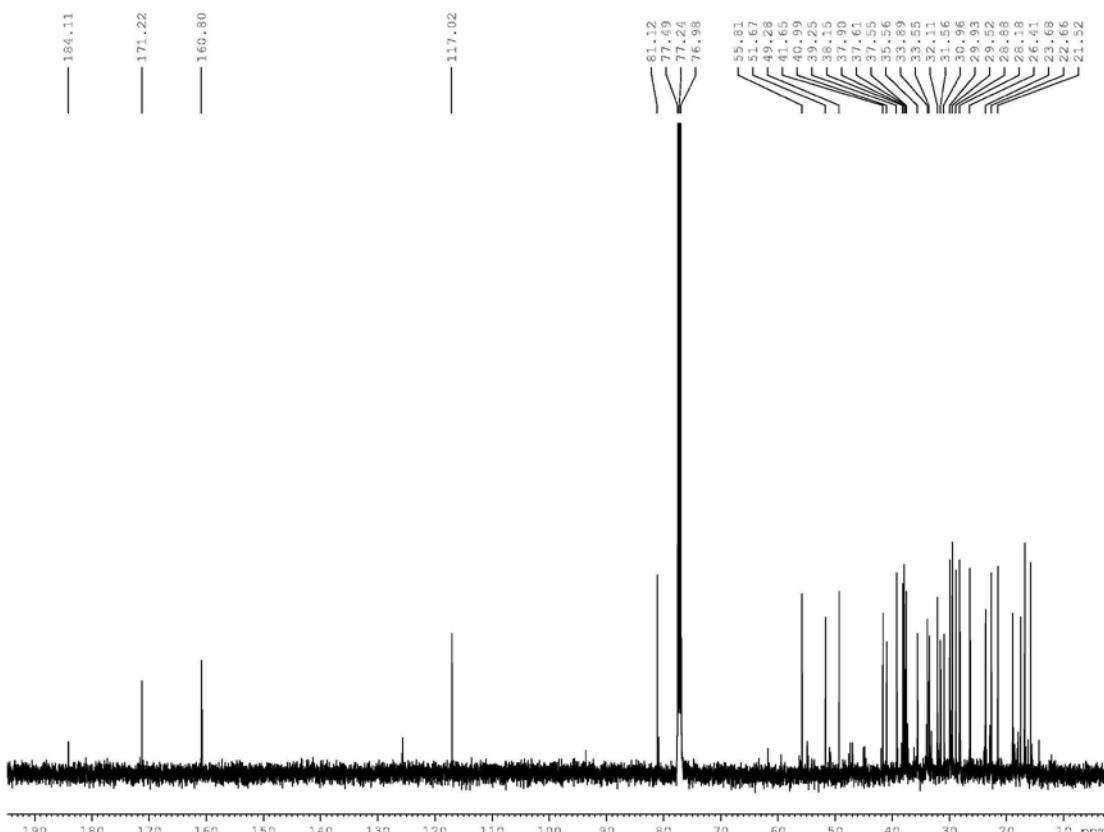
**Figura 26S.** Espectro de RMN  $^1\text{H}$  do espatulenol (II) (500 MHz,  $\text{CDCl}_3$ )



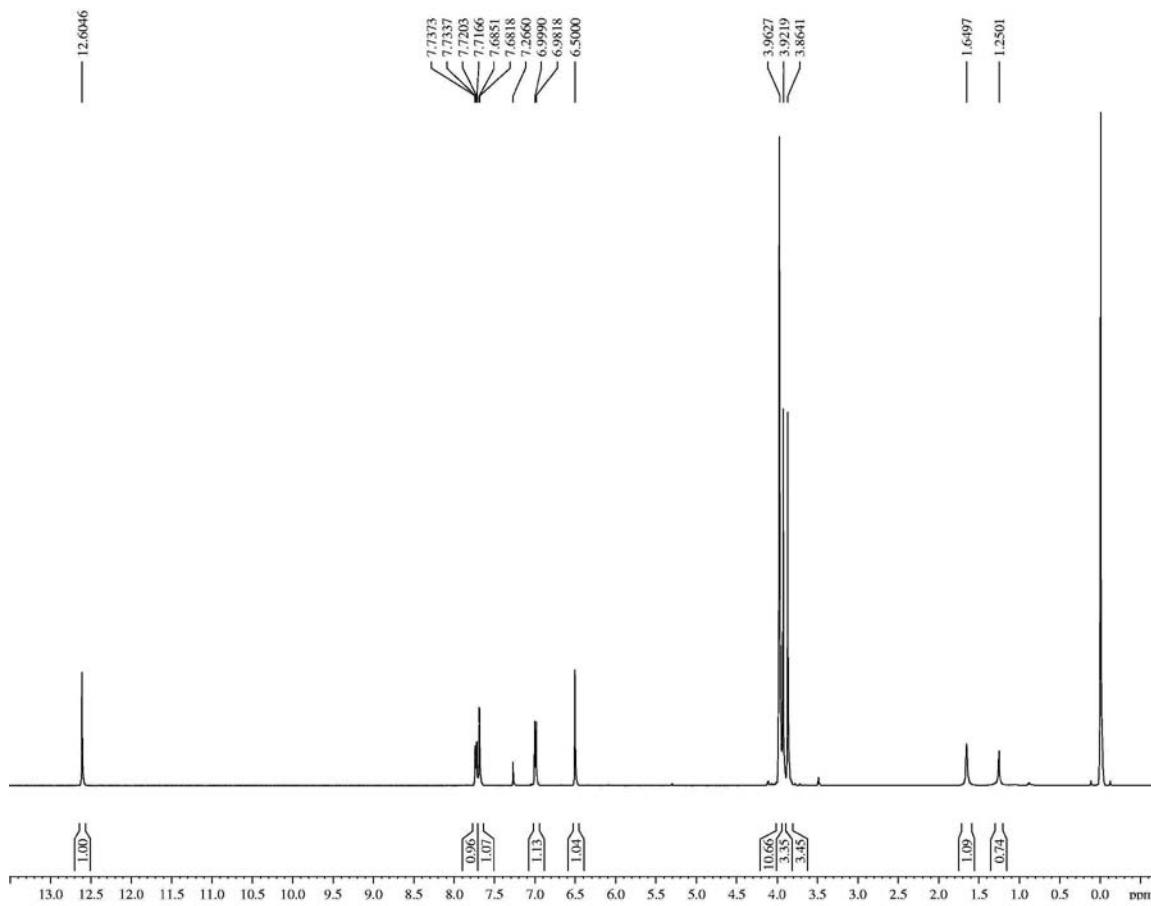
**Figura 27S.** Espectro de RMN  $^{13}\text{C}$ -CPD do espatulenol (II) (125 MHz,  $\text{CDCl}_3$ )



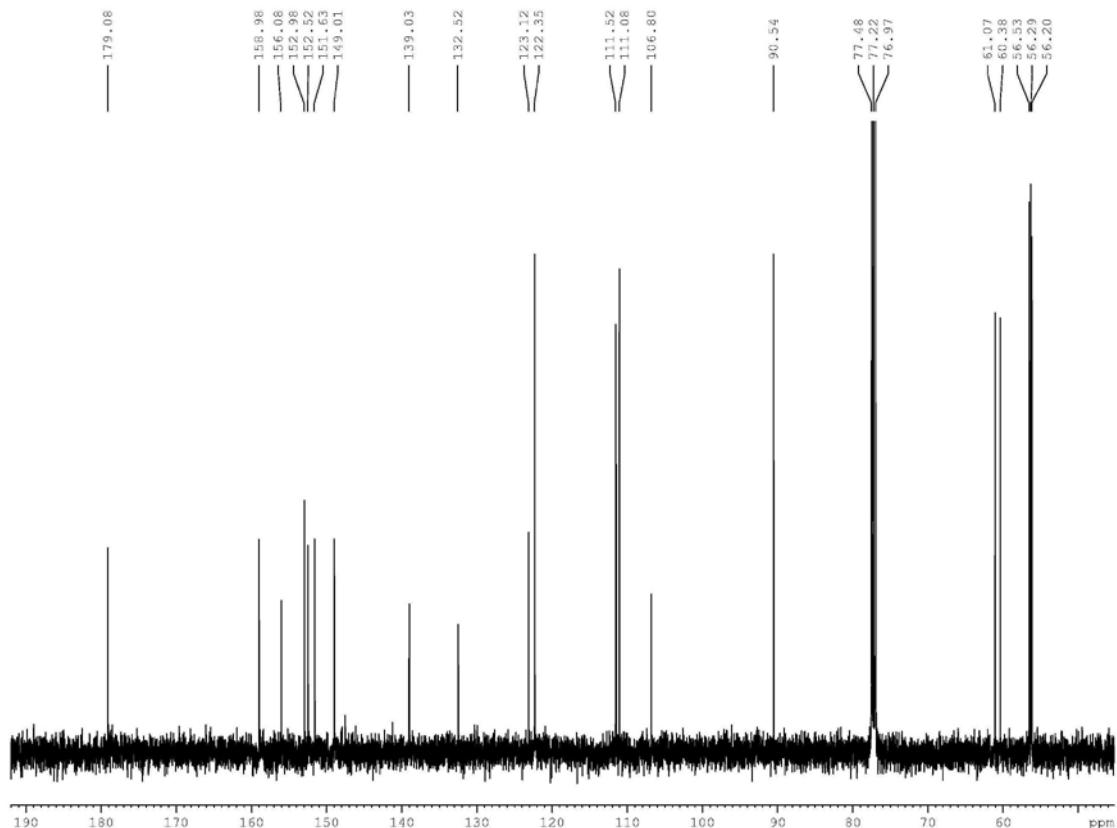
**Figura 28S.** Espectro de RMN  $^1\text{H}$  do ácido acetil aleurítólico (I2) (500 MHz,  $\text{CDCl}_3$ )



**Figura 29S.** Espectro de RMN  $^{13}\text{C}$ -CPD do ácido acetil aleurítólico (I2) (125 MHz,  $\text{CDCl}_3$ )



**Figura 30S.** Espectro de RMN  $^1\text{H}$  da artemetina (**13**) (500 MHz,  $\text{CDCl}_3$ )



**Figura 31S.** Espectro de RMN  $^{13}\text{C}$ -CPD da artemetina (**13**) (125 MHz,  $\text{CDCl}_3$ )