

Mayker Lazaro Dantas Miranda<sup>a</sup>, Fernanda Rodrigues Garcez<sup>a</sup>, Alfredo Raúl Abot<sup>b</sup> e Walimir Silva Garcez<sup>a,\*</sup><sup>a</sup>Instituto de Química, Universidade Federal de Mato Grosso do Sul, CP 549, 79070-900 Campo Grande – MS, Brasil<sup>b</sup>Universidade Estadual de Mato Grosso do Sul, Unidade Universitária de Aquidauana, 79200-000 Aquidauana – MS, Brasil**Dados experimentais dos compostos 3-16 isolados de folhas de *Pterodon pubescens***

*1β,6α-Diidróxi-4(15)-eudesmeno (3)*: Óleo incolor.  $[\alpha]_D^{23} +2,6$  (CHCl<sub>3</sub>; c. 0,16)e Lit.<sup>5</sup>  $[\alpha]_D^{23} +2,6$  (CHCl<sub>3</sub>; c. 0,20). RMN de <sup>13</sup>C (75 MHz, CDCl<sub>3</sub>)  $\delta_c$ : 79,0 (C-1), 31,8 (C-2), 35,1 (C-3), 146,2 (C-4), 55,8 (C-5), 67,0 (C-6), 49,3 (C-7), 18,1 (C-8), 36,3 (C-9), 41,6 (C-10), 26,0 (C-11), 21,3 (C-12), 16,2 (C-13), 11,6 (C-14), 107,8 (C-15).

*Óxido de cariofileno (4)*: Óleo incolor.  $[\alpha]_D^{23} -56,4$  (CHCl<sub>3</sub>; c. 0,20)e Lit.<sup>6</sup>  $[\alpha]_D^{20} -57,7$  (CHCl<sub>3</sub>; c. 0,60). RMN de <sup>13</sup>C (75 MHz, CDCl<sub>3</sub>)  $\delta_c$ : 63,7 (C-1), 30,2 (C-2), 29,7 (C-3), 151,8 (C-4), 48,7 (C-5), 39,7 (C-6), 50,7 (C-7), 27,2 (C-8), 39,2 (C-9), 59,8 (C-10), 34,0 (C-11), 21,6 (C-12), 29,8 (C-13), 112,7 (C-14), 16,9 (C-15).

*α-Cadinol (5)*: Óleo incolor.  $[\alpha]_D^{23} -36,8$  (CHCl<sub>3</sub>; c. 0,17)e Lit.<sup>7</sup>  $[\alpha]_D^{20} -37,1$  (CHCl<sub>3</sub>; c. 0,9). RMN de <sup>13</sup>C (75 MHz, CDCl<sub>3</sub>)  $\delta_c$ : 50,0 (C-1), 22,6 (C-2), 31,0 (C-3), 134,9 (C-4), 122,3 (C-5), 39,8 (C-6), 46,6 (C-7), 22,6 (C-8), 42,1 (C-9), 72,4 (C-10), 26,0 (C-11), 21,5 (C-12), 15,1 (C-13), 20,7 (C-14), 23,8 (C-15).

*Espatulenol (6)*: Óleo incolor.  $[\alpha]_D^{23} +7,2$  (CHCl<sub>3</sub>; c. 0,20) e Lit.<sup>8</sup>  $[\alpha]_D^{20} +7,2$  (CHCl<sub>3</sub>; c. 1,3). RMN de <sup>13</sup>C (75 MHz, CDCl<sub>3</sub>)  $\delta_c$ : 54,3 (C-1), 26,7 (C-2), 41,7 (C-3), 80,9 (C-4), 53,4 (C-5), 29,9 (C-6), 27,5 (C-7), 24,7 (C-8), 38,8 (C-9), 153,4 (C-10), 20,9 (C-11), 28,6 (C-12), 16,3 (C-13), 26,0 (C-14), 106,6 (C-15).

*β-Sitosterol (7)*: Sólido branco amorfo. RMN de <sup>13</sup>C (75 MHz, CDCl<sub>3</sub>)  $\delta_c$ : 37,4 (C-1), 31,6 (C-2), 71,8 (C-3), 42,3 (C-4), 140,7 (C-5), 121,7 (C-6), 31,6 (C-7), 31,9 (C-8), 50,1 (C-9), 36,1 (C-10), 21,0 (C-11), 39,7 (C-12), 42,3 (C-13), 56,7 (C-14), 24,3 (C-15), 28,2 (C-16), 56,0 (C-17), 11,9 (C-18), 19,0 (C-19), 36,1 (C-20), 18,7 (C-21), 33,9 (C-22), 26,0 (C-23), 45,8 (C-24), 29,1 (C-25), 19,8 (C-26), 19,3 (C-27), 23,0 (C-28), 12,0 (C-29).

*Stigmasterol (8)*: Sólido branco amorfo. RMN de <sup>13</sup>C (75 MHz, CDCl<sub>3</sub>)  $\delta_c$ : 37,2 (C-1), 31,6 (C-2), 71,8 (C-3), 42,3 (C-4), 140,7 (C-5), 121,7 (C-6), 31,6 (C-7), 31,9 (C-8), 50,1 (C-9), 36,5 (C-10), 21,0 (C-11), 39,7 (C-12), 56,8 (C-13), 56,7 (C-14), 24,3 (C-15), 28,9 (C-16), 56,0 (C-17), 12,2 (C-18), 19,0 (C-19), 40,4 (C-20), 21,2 (C-21), 138,3 (C-22), 129,2 (C-23), 51,2 (C-24), 29,7 (C-25), 21,2 (C-26), 18,9 (C-27), 25,4 (C-28), 12,2 (C-29).

*Feofitina A (9)*: Sólido esverdeado. RMN de <sup>13</sup>C (75 MHz, CDCl<sub>3</sub>)  $\delta_c$ : 142,2 (C-1), 132,1 (C-2), 12,2 (C-2<sup>1</sup>), 136,6 (C-3), 129,0 (C-3<sup>1</sup>), 123,0 (C-3<sup>2</sup>), 136,4 (C-4), 97,6 (C-5), 155,5 (C-6), 136,1 (C-7), 11,2 (C-7<sup>1</sup>), 145,2 (C-8), 19,5 (C-8<sup>1</sup>), 17,4 (C-8<sup>2</sup>), 149,8 (C-9), 104,5 (C-10), 137,9 (C-11), 128,8 (C-12), 12,1 (C-12<sup>1</sup>), 128,8 (C-13), 189,6 (C-13<sup>1</sup>), 64,7 (C-13<sup>2</sup>), 169,5 (C-13<sup>3</sup>), 52,9 (C-13<sup>4</sup>), 149,8 (C-14),

105,4 (C-15), 161,3 (C-16), 51,2 (C-17), 29,9 (C-17<sup>1</sup>), 31,2 (C-17<sup>2</sup>), 172,9 (C-17<sup>3</sup>), 50,2 (C-18), 23,1 (C-18<sup>1</sup>), 172,4 (C-19), 93,5 (C-20), 60,5 (C-P1), 117,7 (C-P2), 142,3 (C-P3), 38,7 (C-P4), 23,7 (C-P5), 37,1 (C-P6), 31,9 (C-P7), 37,1 (C-P8), 23,1 (C-P9), 37,1 (C-P10), 31,9 (C-P11), 36,6 (C-P12), 23,1 (C-P13), 38,7 (C-P14), 28,9 (C-P15), 22,9 (C-P16), 22,6 (C-P17), 19,5 (C-P11<sup>1</sup>), 19,5 (C-P7<sup>1</sup>), 17,4 (C-P3<sup>1</sup>).

*Luteolina (10)*: Sólido amarelo. RMN de <sup>13</sup>C (75 MHz, CD<sub>3</sub>OD)  $\delta_c$ : 162,9 (C-2), 103,6 (C-3), 183,8 (C-4), 166,6 (C-5), 100,4 (C-6), 166,3 (C-7), 95,3 (C-8), 159,4 (C-9), 105,0 (C-10), 123,5 (C-1<sup>1</sup>), 114,2 (C-2<sup>1</sup>), 146,9 (C-3<sup>1</sup>), 151,0 (C-4<sup>1</sup>), 116,8 (C-5<sup>1</sup>), 120,5 (C-6<sup>1</sup>).

*Kaempferol(11)*: Sólido amarelo. RMN de <sup>13</sup>C (75 MHz, CD<sub>3</sub>OD)  $\delta_c$ : 148,0 (C-2), 137,3 (C-3), 177,5 (C-4), 162,5 (C-5), 99,2 (C-6), 165,6 (C-7), 94,4 (C-8), 158,2 (C-9), 104,6 (C-10), 123,8 (C-1<sup>1</sup>), 130,7 (C-2<sup>1</sup>e 6<sup>1</sup>), 116,3 (C-3<sup>1</sup>e 5<sup>1</sup>), 160,5 (C-4<sup>1</sup>).

*Quercetina (12)*: Sólido amarelo. RMN de <sup>13</sup>C (75 MHz, CD<sub>3</sub>OD)  $\delta_c$ : 148,0 (C-2), 137,2 (C-3), 177,3 (C-4), 162,5 (C-5), 99,2 (C-6), 165,6 (C-7), 94,4 (C-8), 158,2 (C-9), 104,5 (C-10), 124,1 (C-1<sup>1</sup>), 115,9 (C-2<sup>1</sup>), 146,2 (C-3<sup>1</sup>), 148,7 (C-4<sup>1</sup>), 116,2 (C-5<sup>1</sup>), 121,6 (C-6<sup>1</sup>).

*(+)-Catequina (13)*: Sólido amarelo.  $[\alpha]_D^{23} +15$  (CH<sub>3</sub>OH; c. 0,93) e Lit.<sup>9</sup>  $[\alpha]_D^{23} +15$  (CH<sub>3</sub>OH; c. 0,88). RMN de <sup>13</sup>C (75 MHz, CD<sub>3</sub>OD)  $\delta_c$ : 82,7 (C-2), 68,7 (C-3), 28,4 (C-4), 156,8 (C-5), 96,4 (C-6), 157,6 (C-7), 95,5 (C-8), 157,4 (C-9), 100,8 (C-10), 132,1 (C-1<sup>1</sup>), 115,3 (C-2<sup>1</sup>), 146,2 (C-3<sup>1</sup>), 157,6 (C-4<sup>1</sup>), 116,2 (C-5<sup>1</sup>), 120,1 (C-6<sup>1</sup>).

*Quercetina-3-O-α-L-rhamnopiranosídeo (14)*: Sólido amarelo. RMN de <sup>13</sup>C (75 MHz, CD<sub>3</sub>OD)  $\delta_c$ : 159,3 (C-2), 131,8 (C-3), 179,5 (C-4), 162,9 (C-5), 99,8 (C-6), 165,8 (C-7), 94,8 (C-8), 158,4 (C-9), 105,8 (C-10), 122,9 (C-1<sup>1</sup>), 116,4 (C-2<sup>1</sup>), 146,3 (C-3<sup>1</sup>), 149,7 (C-4<sup>1</sup>), 116,9 (C-5<sup>1</sup>), 122,8 (C-6<sup>1</sup>), 103,4 (C-1<sup>11</sup>), 71,8 (C-2<sup>11</sup>), 71,9 (C-3<sup>11</sup>), 73,2 (C-4<sup>11</sup>), 71,9 (C-5<sup>11</sup>), 17,6 (C-6<sup>11</sup>).

*Rutina (15)*: Sólido amarelo. RMN de <sup>13</sup>C (75 MHz, CD<sub>3</sub>OD)  $\delta_c$ : 158,4 (C-2), 135,5 (C-3), 179,3 (C-4), 162,9 (C-5), 99,9 (C-6), 165,9 (C-7), 94,9 (C-8), 159,3 (C-9), 105,5 (C-10), 123,1 (C-1<sup>1</sup>), 117,7 (C-2<sup>1</sup>), 145,7 (C-3<sup>1</sup>), 149,7 (C-4<sup>1</sup>), 116,0 (C-5<sup>1</sup>), 123,5 (C-6<sup>1</sup>), 104,6 (C-1<sup>11</sup>), 75,6 (C-2<sup>11</sup>), 78,1 (C-3<sup>11</sup>), 71,3 (C-4<sup>11</sup>), 77,1 (C-5<sup>11</sup>), 68,5 (C-6<sup>11</sup>), 102,3 (C-1<sup>111</sup>), 72,0 (C-2<sup>111</sup>), 72,2 (C-3<sup>111</sup>), 73,8 (C-4<sup>111</sup>), 69,6 (C-5<sup>111</sup>), 17,8 (C-6<sup>111</sup>).

*Ácido p-hidroxibenzoico (16)*: Sólido branco. RMN de <sup>13</sup>C (75 MHz, CD<sub>3</sub>OD)  $\delta_c$ : 122,5 (C-1), 132,9 (C-2 e C-6), 116,0 (C-3 e C-5), 163,2 (C-4), 170,2 (C-7).

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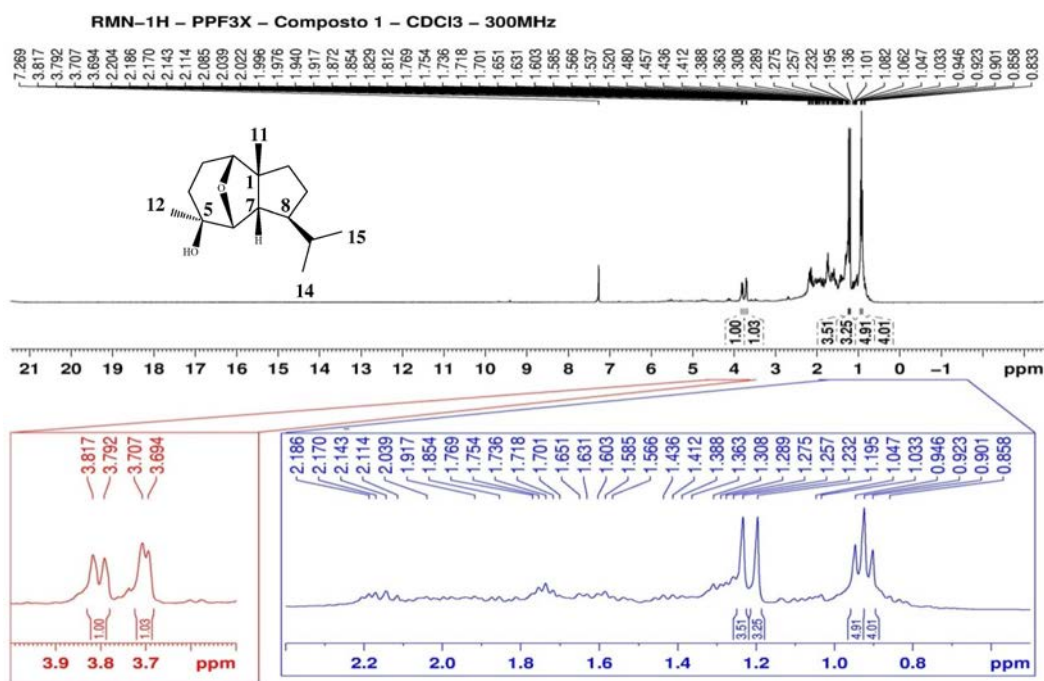
Espectros dos compostos 1-16 isolados de folhas de *Pterodon pubescens*

Figura 1S. Espectro de RMN de <sup>1</sup>H (300 MHz, CDCl<sub>3</sub>) do composto 1 ((rel)-6β,2β-epóxi-5β-hidróxi-isodaucano)

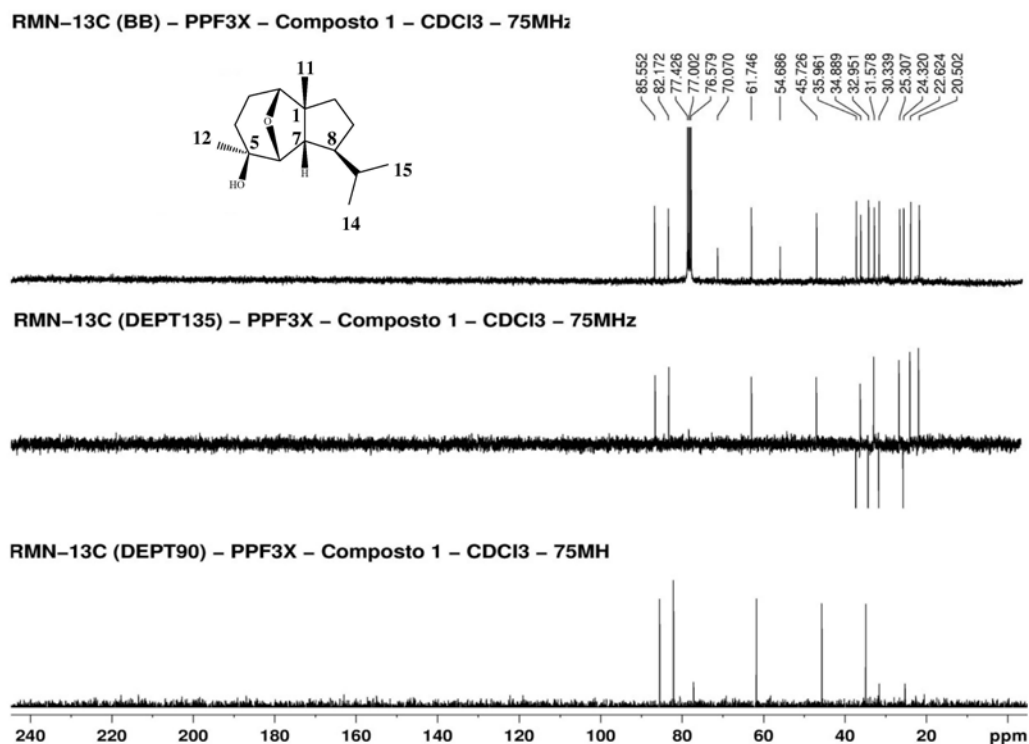


Figura 2S. Espectro de RMN de <sup>13</sup>C e experimentos de DEPT 135° e 90° (75 MHz, CDCl<sub>3</sub>) do composto 1 ((rel)-6β,2β-epóxi-5β-hidróxi-isodaucano)

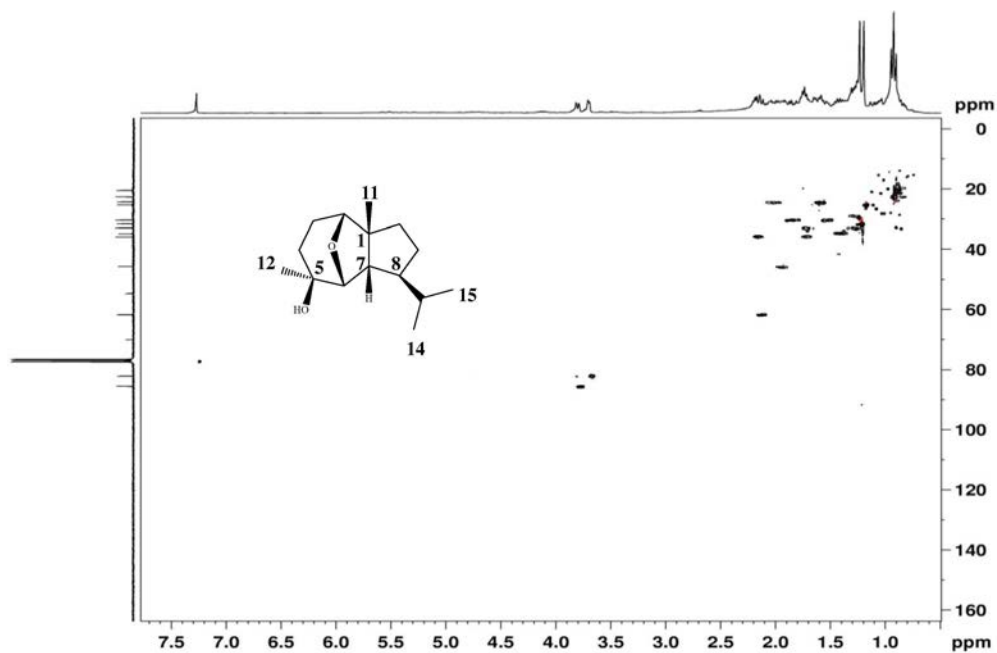


Figura 3S. Experimento HSQC (300/75 MHz, CDCl<sub>3</sub>) do composto 1 ((rel)-6β,2β-epóxi-5β-hidróxi-isodaucano)

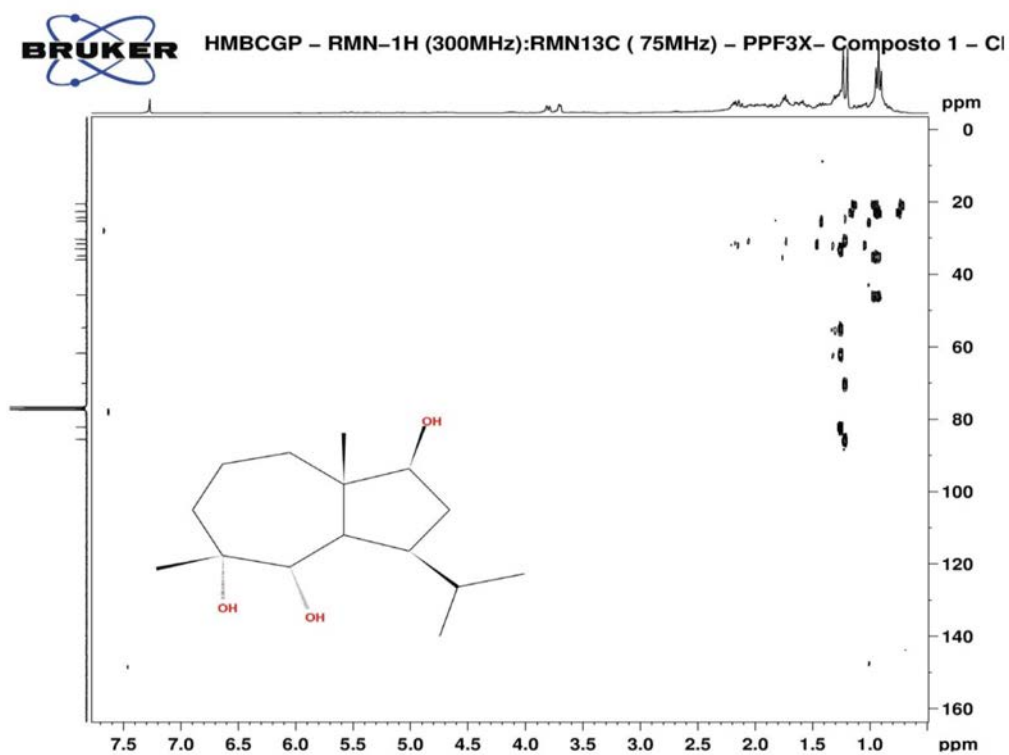


Figura 4S. Experimento HMBC (300/75 MHz, CDCl<sub>3</sub>) do composto 1 ((rel)-6β,2β-epóxi-5β-hidróxi-isodaucano)

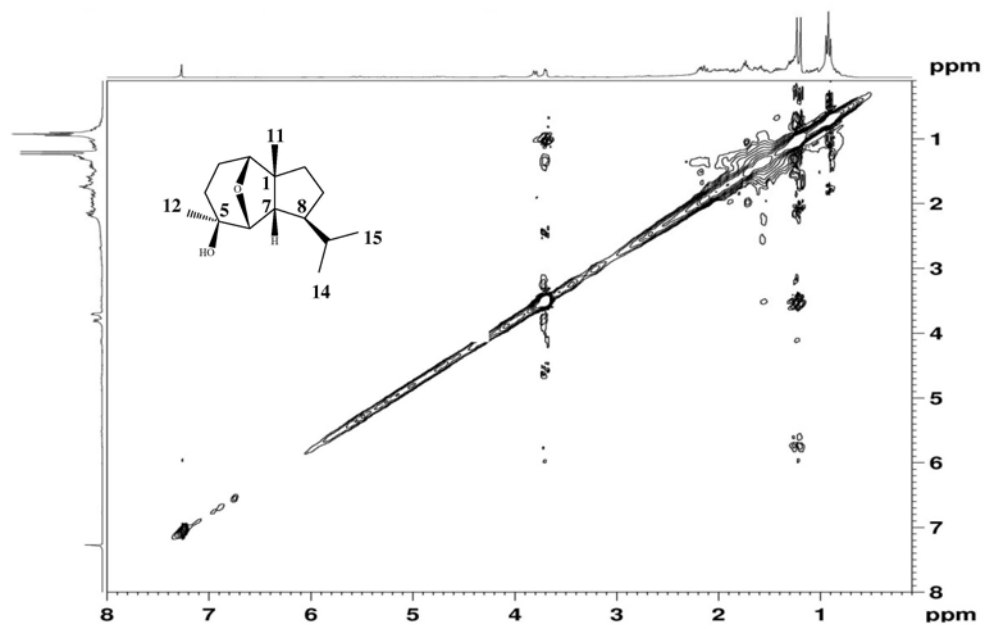


Figura 5S. Experimento NOESY (300 MHz, CDCl<sub>3</sub>) do composto 1 ((rel)-6β,2β-epóxi-5β-hidróxi-isodaucano)

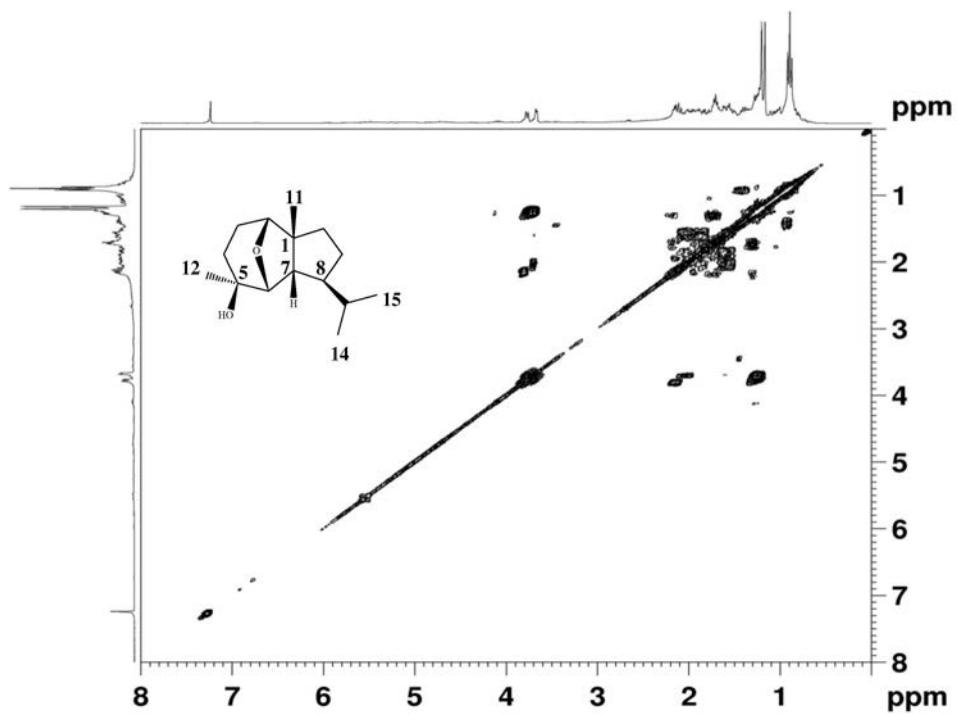


Figura 6S. Experimento COSY (300 MHz, CDCl<sub>3</sub>) do composto 1 ((rel)-6β,2β-epóxi-5β-hidróxi-isodaucano)

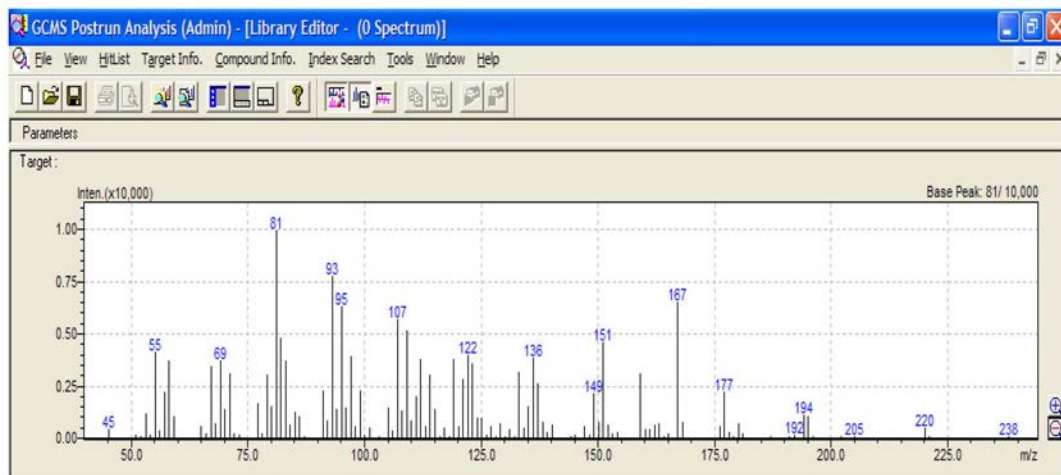


Figura 7S. Espectro de Massas do composto **1** ((rel)-6 $\beta$ ,2 $\beta$ -epóxi-5 $\beta$ -hidróxi-isodaucano)

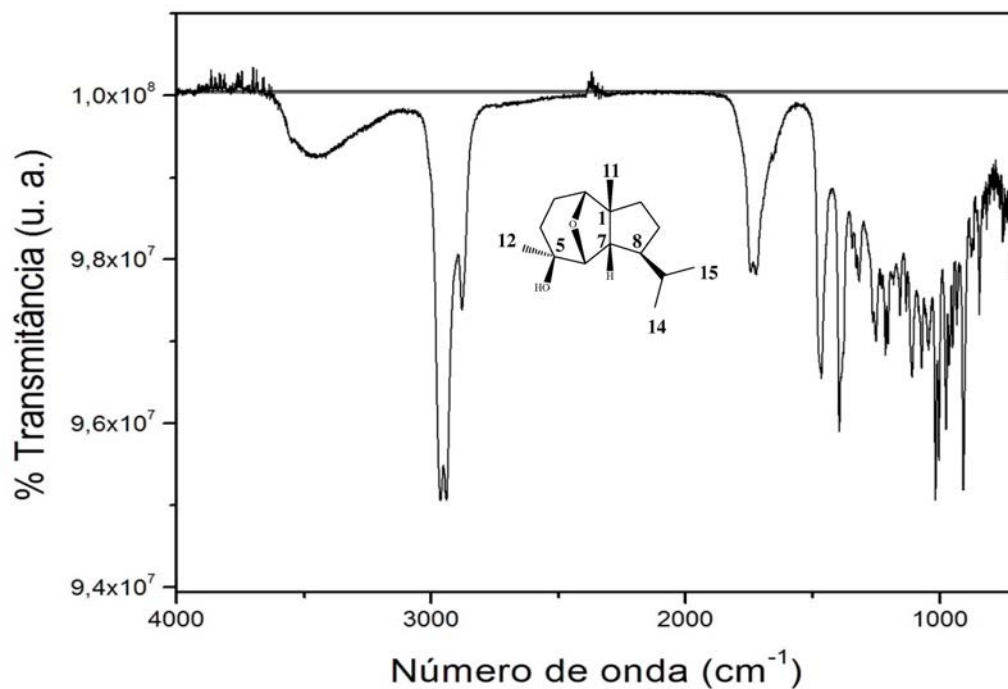


Figura 8S. Espectro de infravermelho do composto **1** ((rel)-6 $\beta$ ,2 $\beta$ -epóxi-5 $\beta$ -hidróxi-isodaucano)

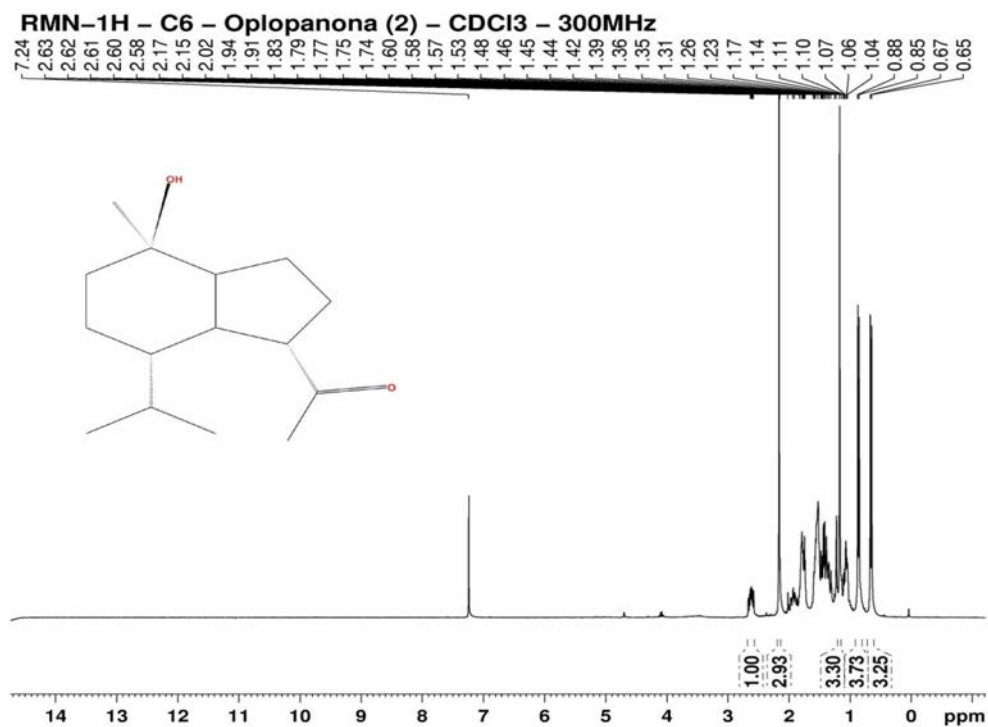


Figura 9S. Espectro de RMN de <sup>1</sup>H (300 MHz, CDCl<sub>3</sub>) do composto 2 (oplopanona)

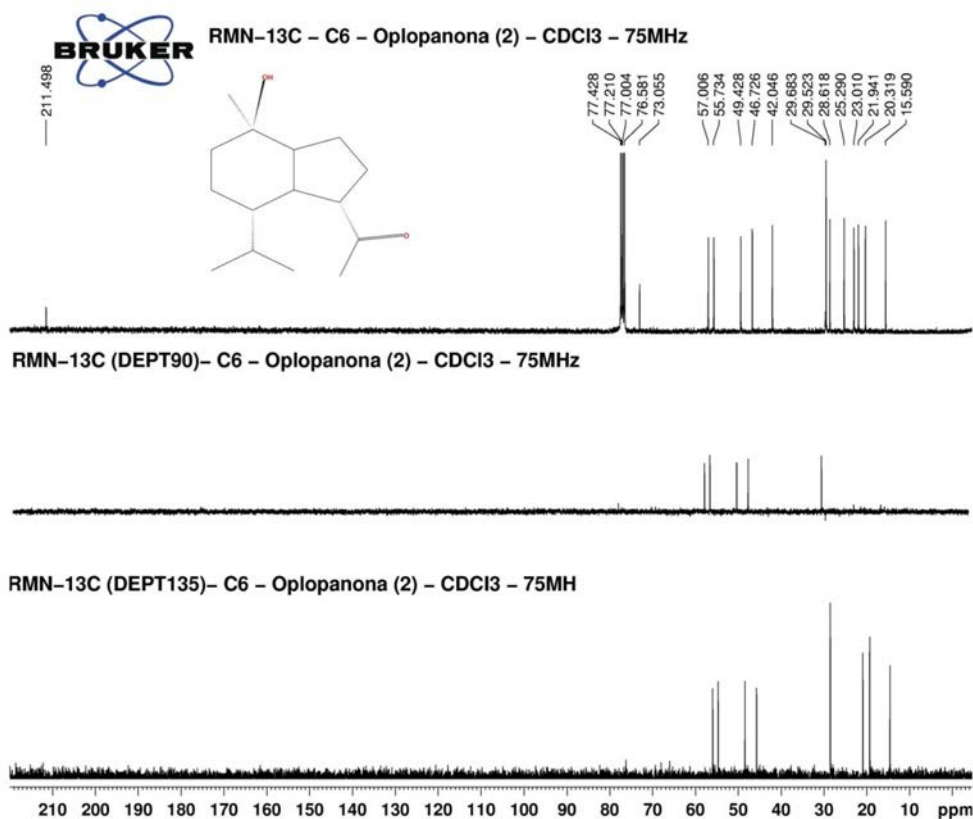


Figura 10S. Espectro de RMN de <sup>13</sup>C e experimentos DEPT 90° e DEPT 135° (75 MHz, CDCl<sub>3</sub>) do composto 2 (oplopanona)

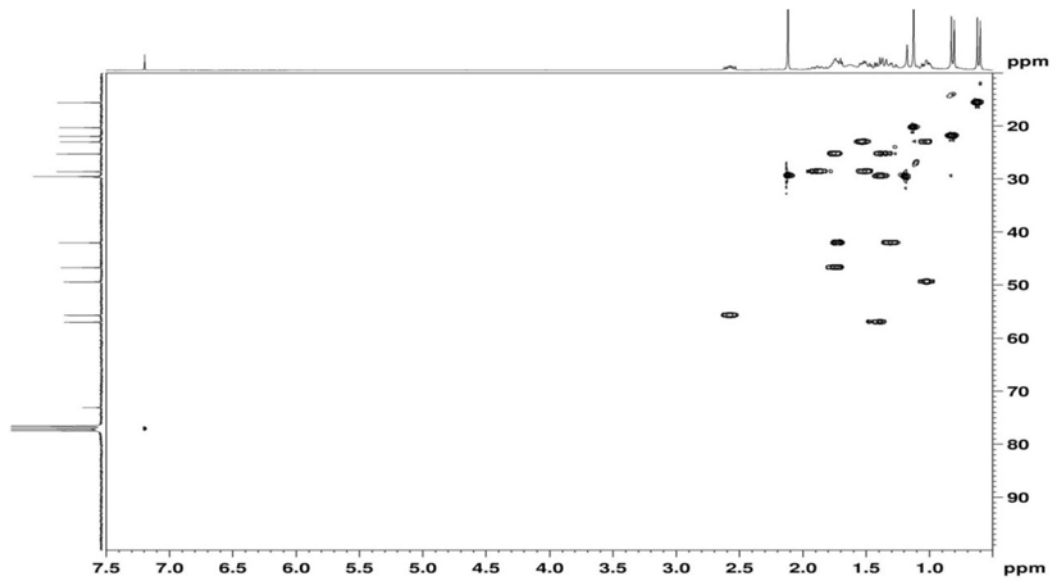


Figura 11S. Experimento HSQC (300/75 MHz,  $CDCl_3$ ) do composto 2 (oplopanona)

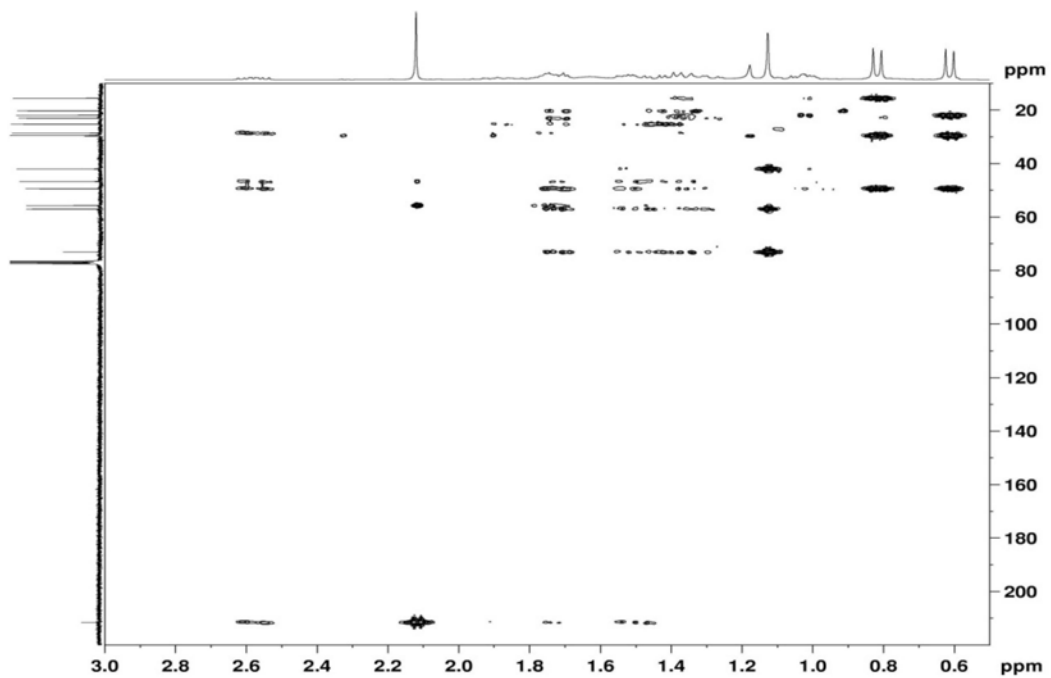


Figura 12S. Experimento HMBC (300/75 MHz,  $CDCl_3$ ) do composto 2 (oplopanona)

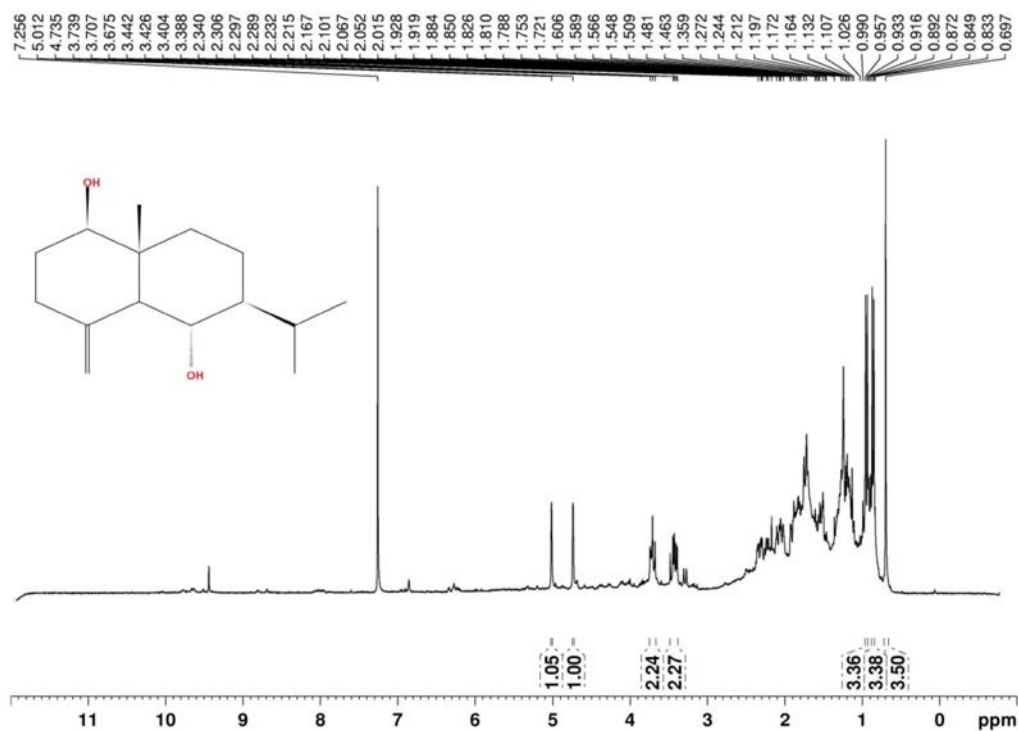


Figura 13S. Espectro de RMN de  $^1\text{H}$  (300 MHz,  $\text{CDCl}_3$ ) do composto 3 (Eudes-4(15)-eno-1 $\beta$ ,6 $\alpha$ -diol)

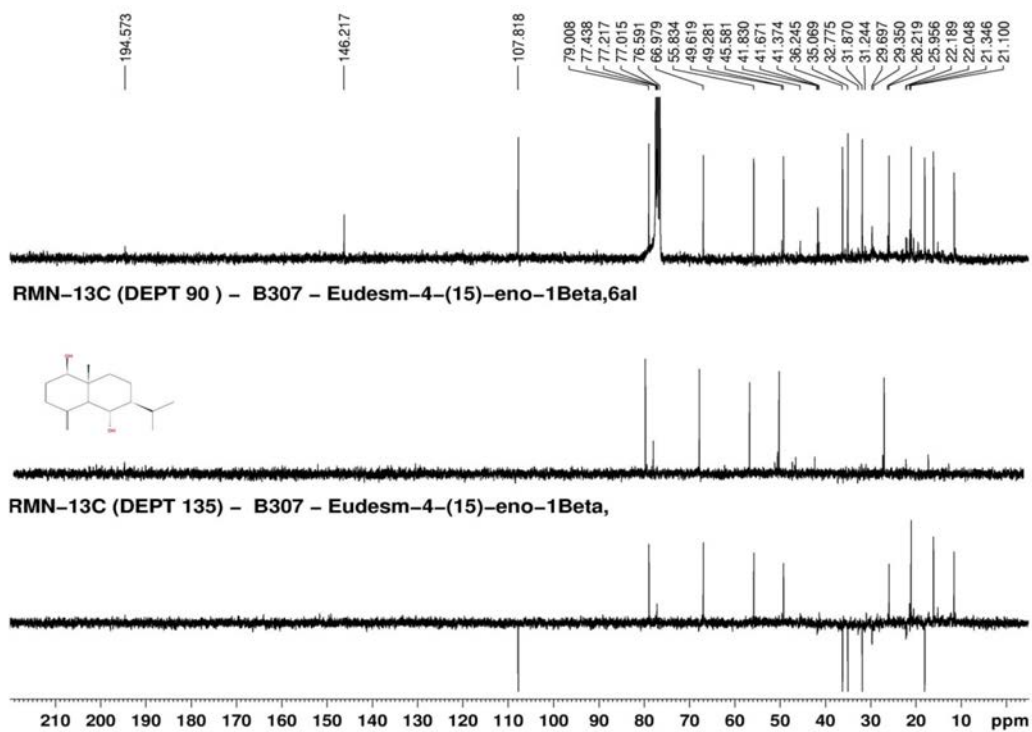


Figura 14S. Espectro de RMN de  $^{13}\text{C}$  e experimentos DEPT 90° e 135° (75 MHz,  $\text{CDCl}_3$ ) do composto 3 (Eudes-4(15)-eno-1 $\beta$ ,6 $\alpha$ -diol)



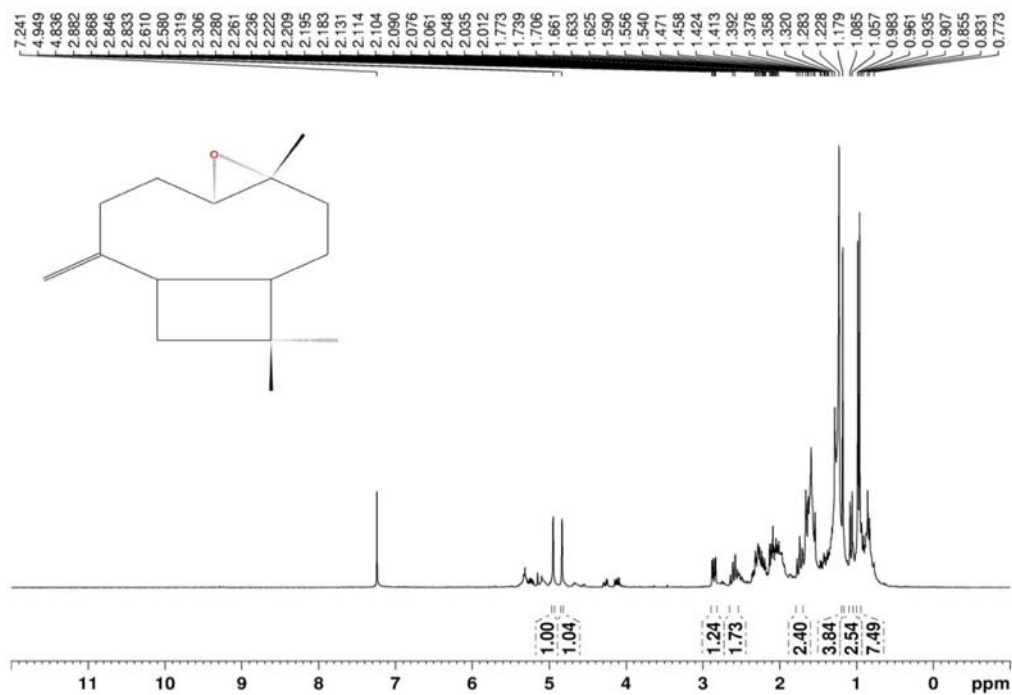


Figura 15S. Espectro de RMN de  $^1\text{H}$  (300 MHz,  $\text{CDCl}_3$ ) do composto 4 (Óxido de Cariofileno)

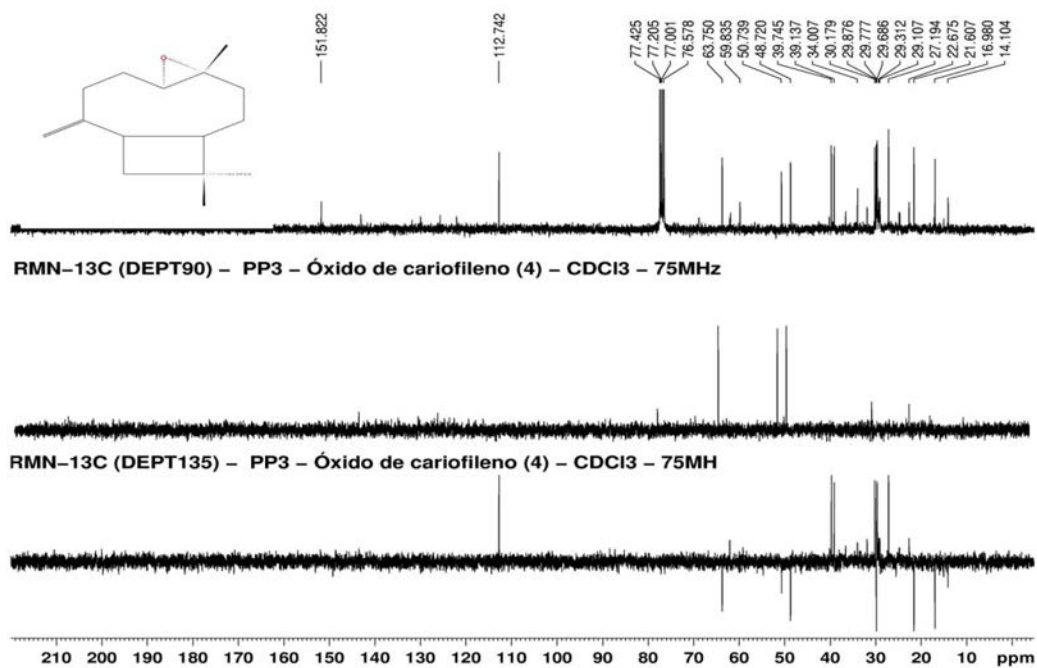


Figura 16S. Espectro de RMN de  $^{13}\text{C}$  e experimentos DEPT 90° e 135° (75 MHz,  $\text{CDCl}_3$ ) do composto 4 (Óxido de Cariofileno)

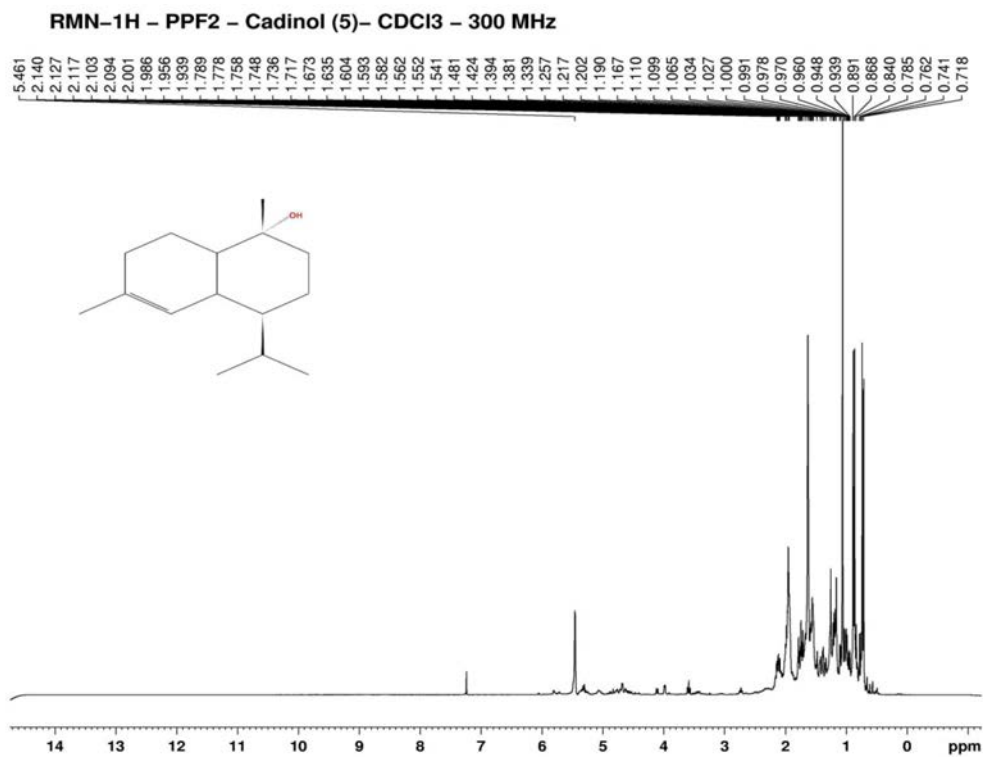


Figura 17S. Espectro de RMN de <sup>1</sup>H (300 MHz, CDCl<sub>3</sub>) do composto 5 (α-Cadinol)

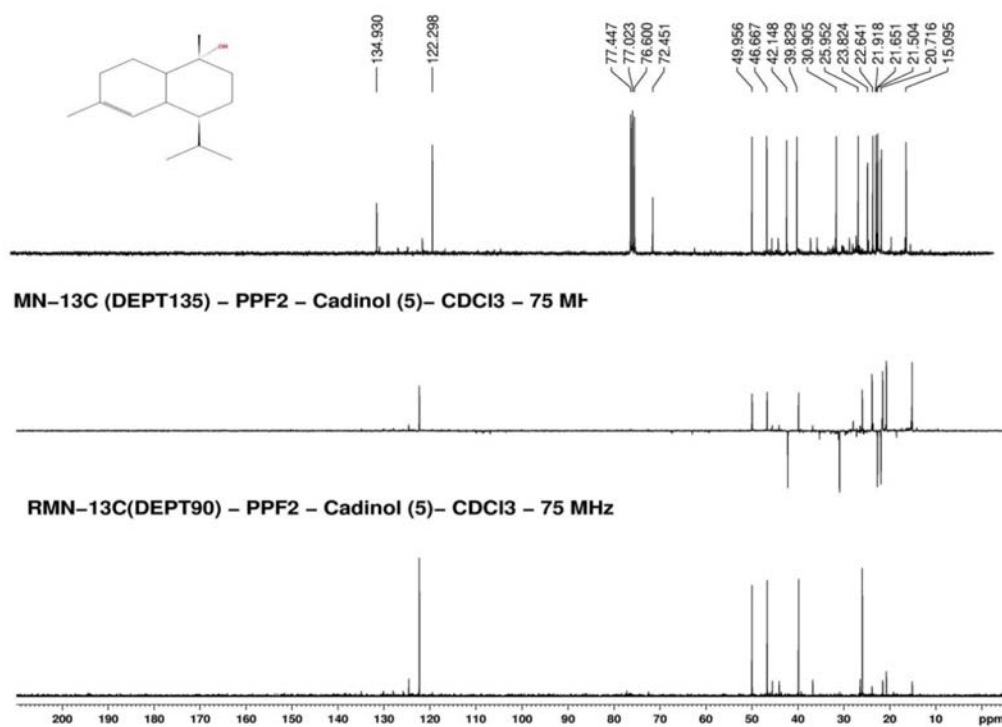


Figura 18S. Espectro de RMN de <sup>13</sup>C e experimentos DEPT 135° e 90° (75 MHz, CDCl<sub>3</sub>) do composto 5 (α-Cadinol)

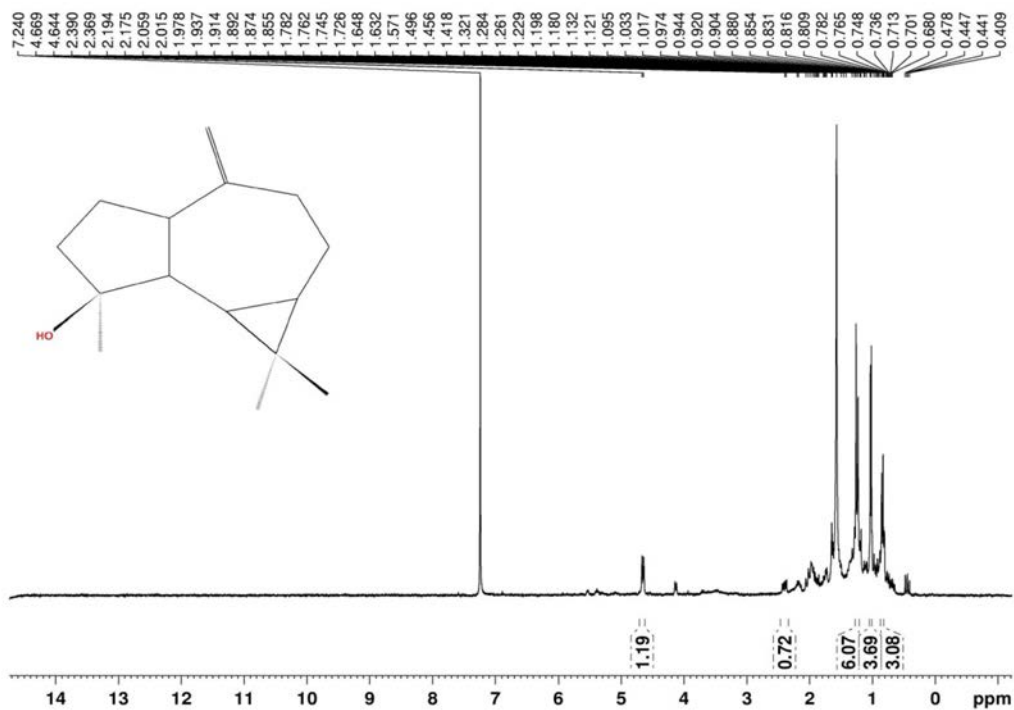


Figura 19S. Espectro de RMN de <sup>1</sup>H (300 MHz, CDCl<sub>3</sub>) do composto 6 (Espatulanol)

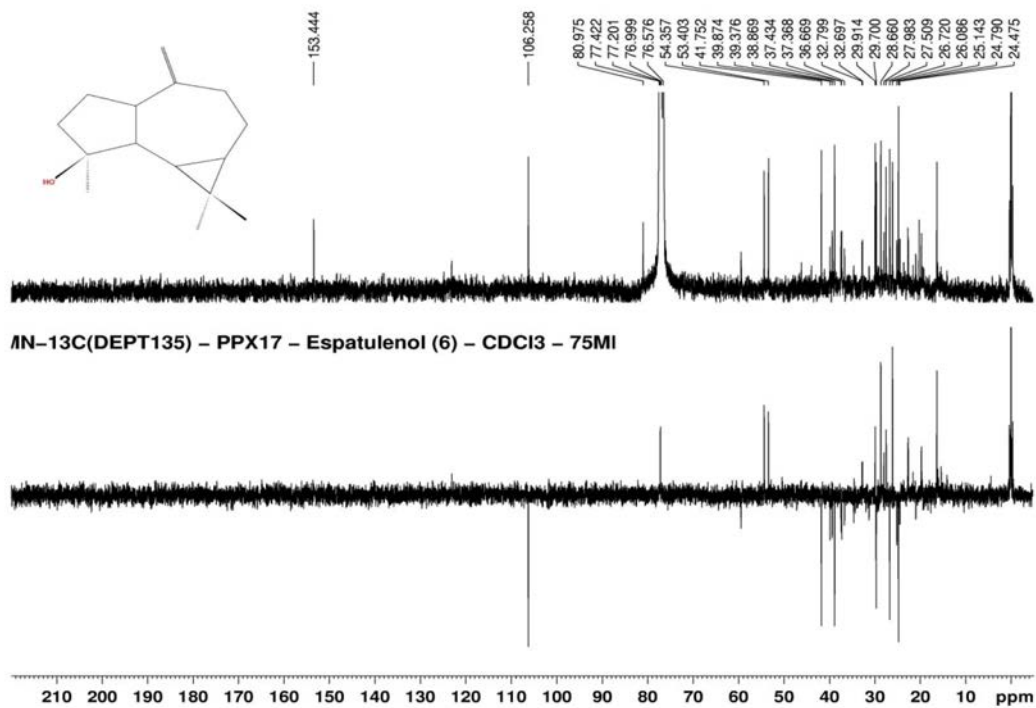


Figura 20S. Espectro de RMN de <sup>13</sup>C e experimento DEPT 135° (75 MHz, CDCl<sub>3</sub>) do composto 6 (Espatulanol)

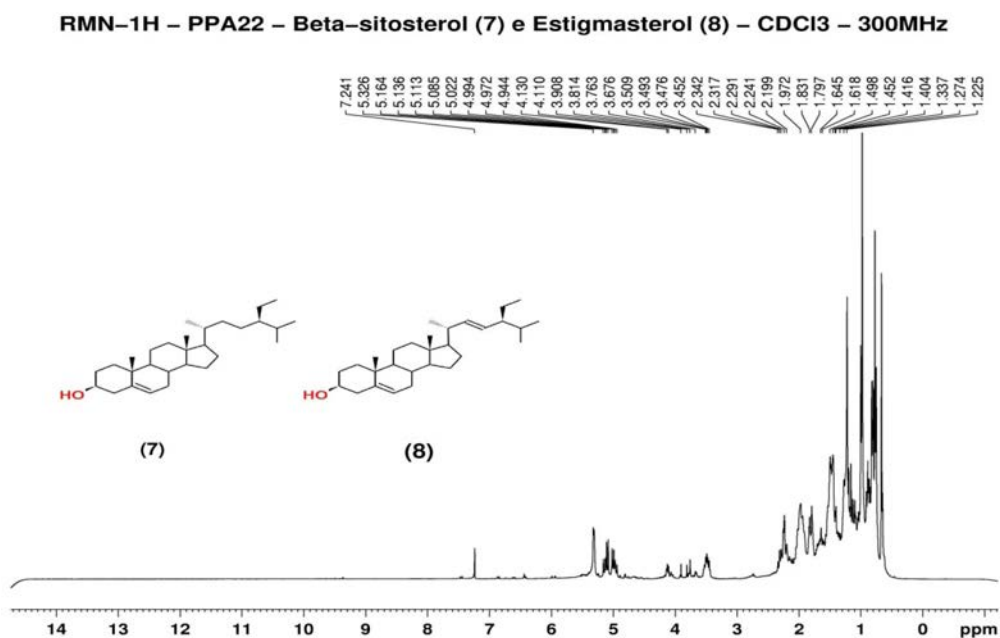


Figura 21S. Espectro de RMN de <sup>1</sup>H (300 MHz, CDCl<sub>3</sub>) do composto 7 e 8 (β-sitosterol e Estigmasterol)

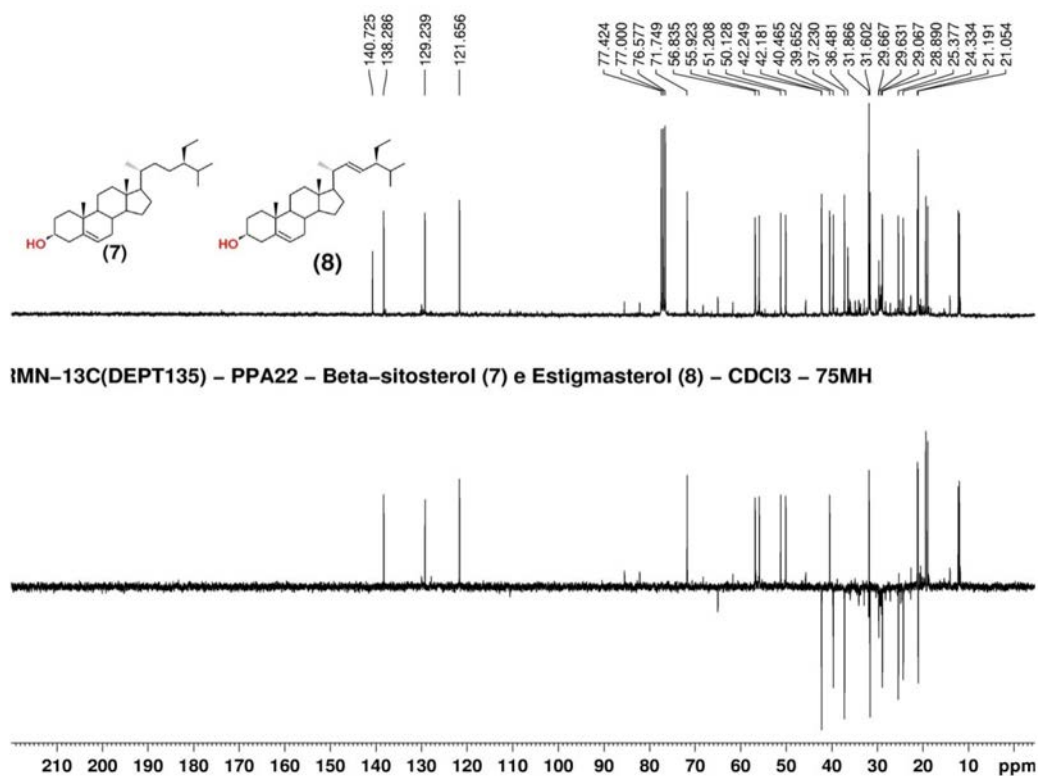


Figura 22S. Espectro de RMN de <sup>13</sup>C e DEPT 135° (75 MHz, CDCl<sub>3</sub>) do composto 7 e 8 (β-sitosterol e Estigmasterol)

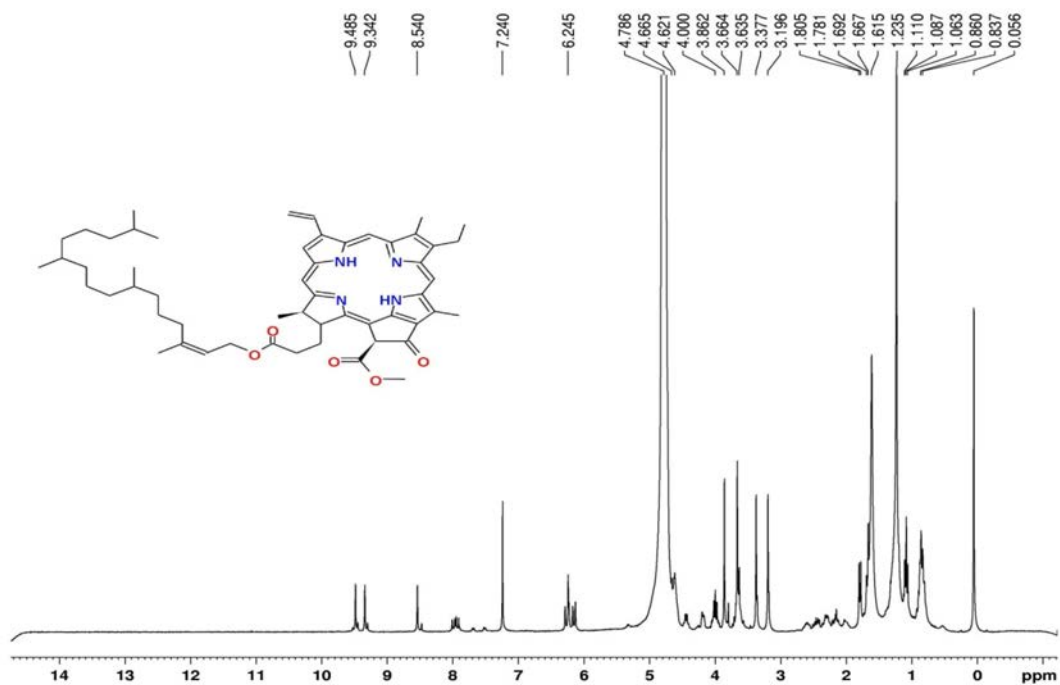


Figura 23S. Espectro de RMN de  $^1\text{H}$  (300 MHz,  $\text{CDCl}_3$ ) do composto **9** (Feofitina A)

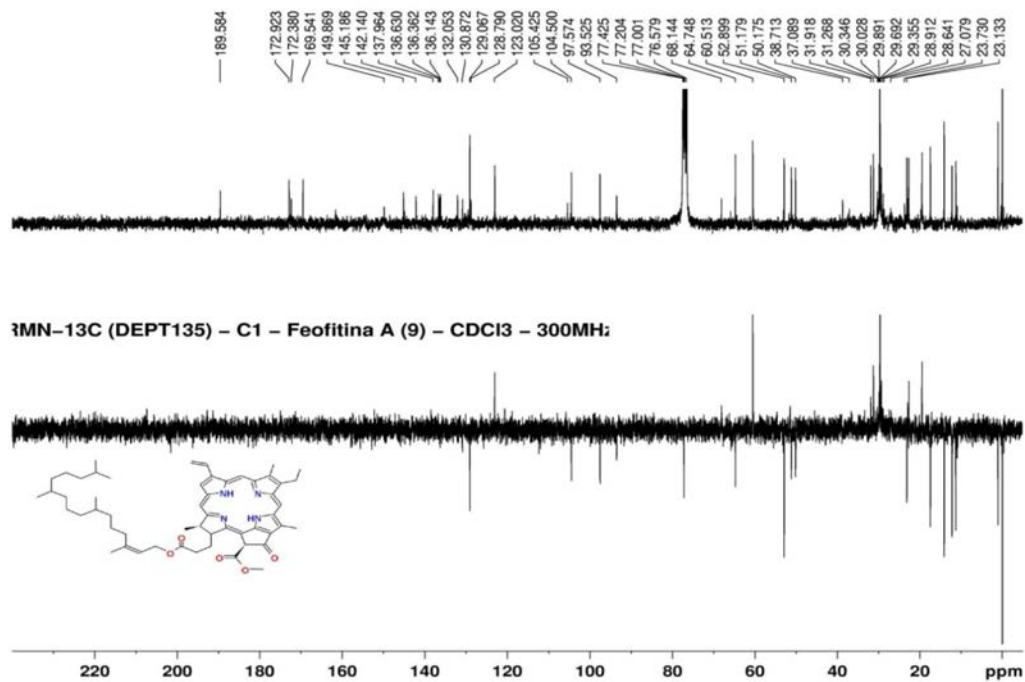


Figura 24S. Espectro de RMN de  $^{13}\text{C}$  e DEPT 135 $^\circ$  (75 MHz,  $\text{CDCl}_3$ ) do composto **9** (Feofitina A)

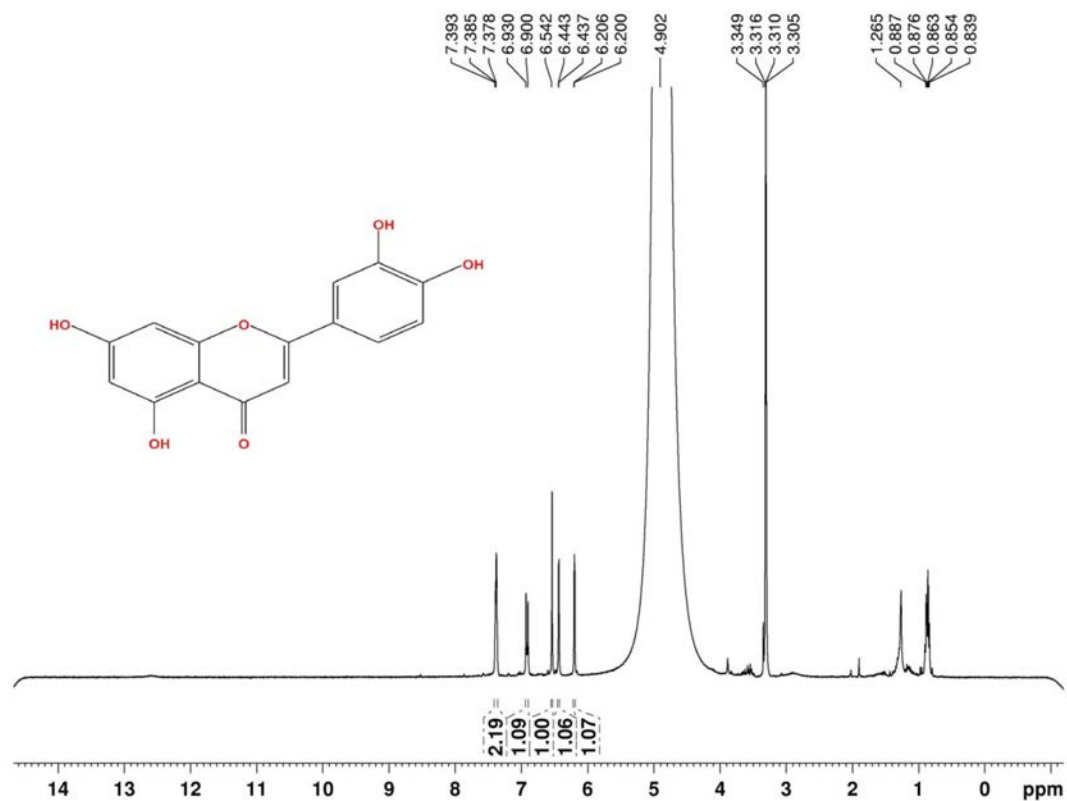


Figura 25S. Espectro de RMN de  $^1\text{H}$  (300 MHz,  $\text{CD}_3\text{OD}$ ) do composto 10 (Luteolina)

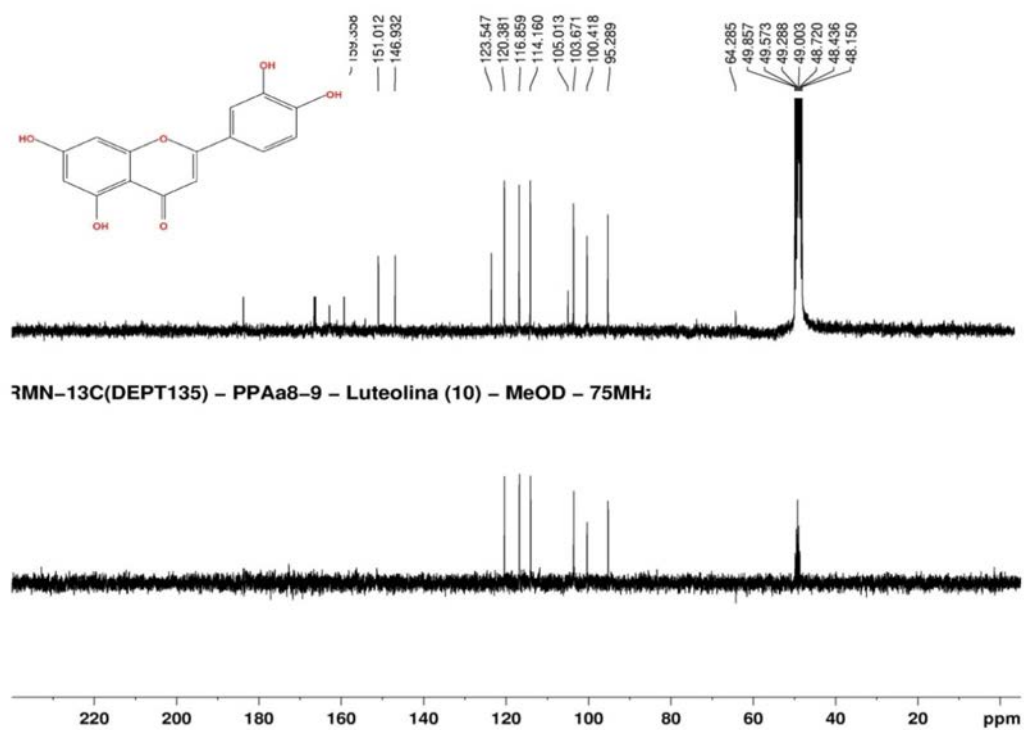


Figura 26S. Espectro de RMN de  $^{13}\text{C}$  e experimento DEPT 135° (75 MHz,  $\text{CD}_3\text{OD}$ ) do composto 10 (Luteolina)

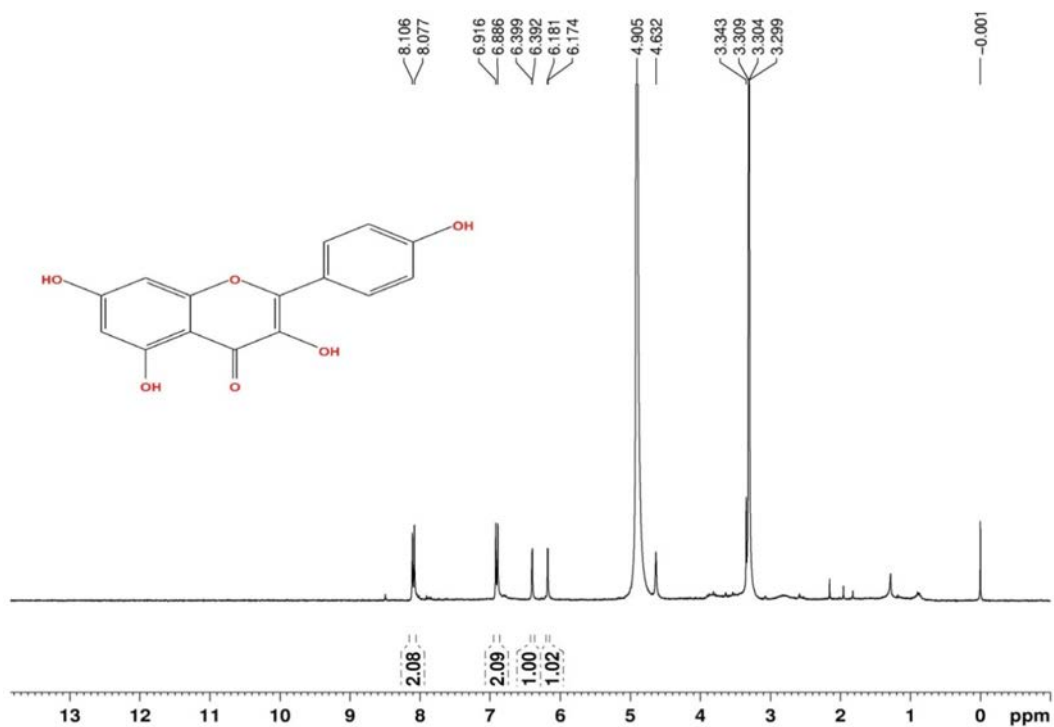


Figura 27S. Espectro de RMN de <sup>1</sup>H (300 MHz, CD<sub>3</sub>OD) do composto II (Kaempferol)

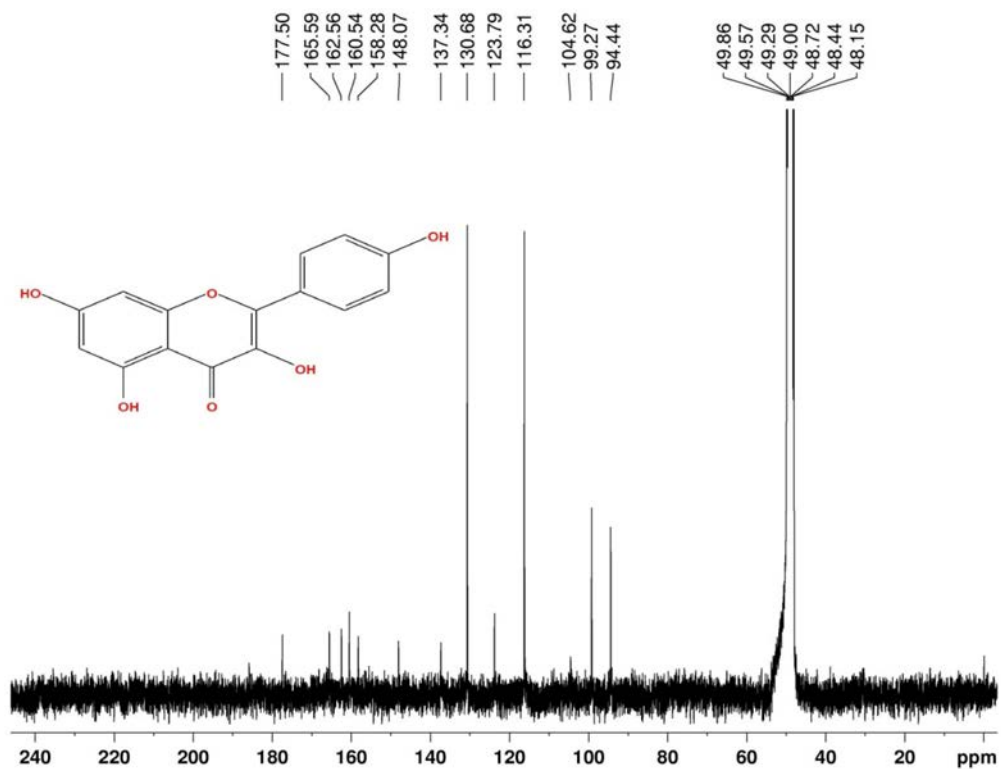


Figura 28S. Espectro de RMN de <sup>13</sup>C (75 MHz, CD<sub>3</sub>OD) do composto II (Kaempferol)

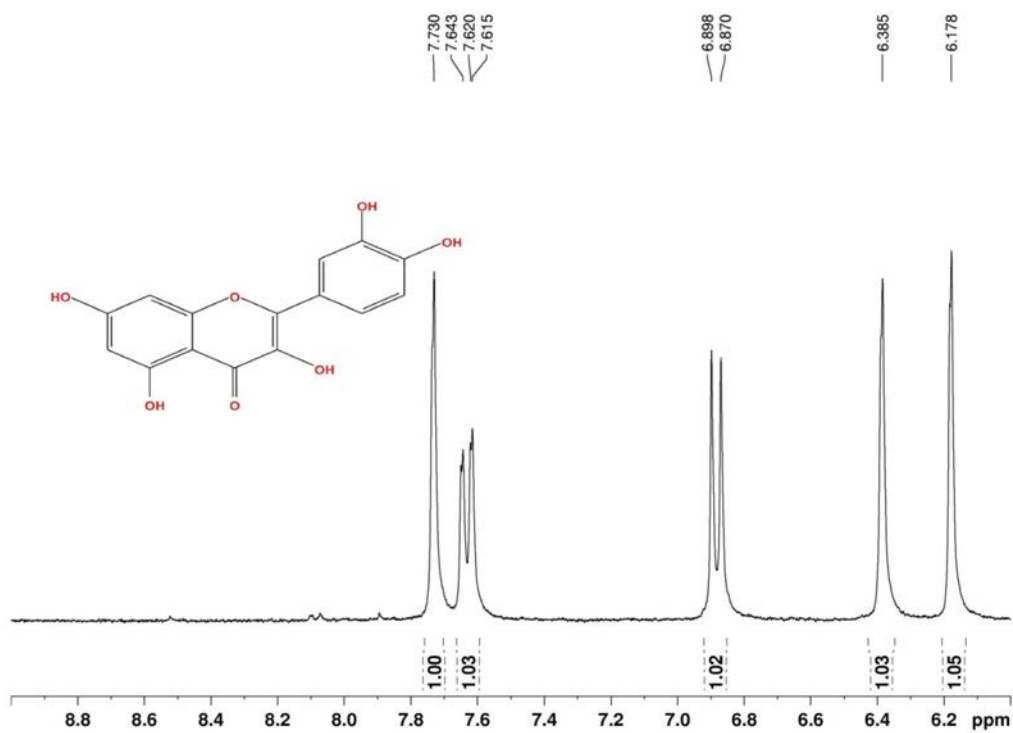


Figura 29S. Espectro de RMN de  $^1\text{H}$  (300 MHz,  $\text{CD}_3\text{OD}$ ) do composto 12 (Quercetina)

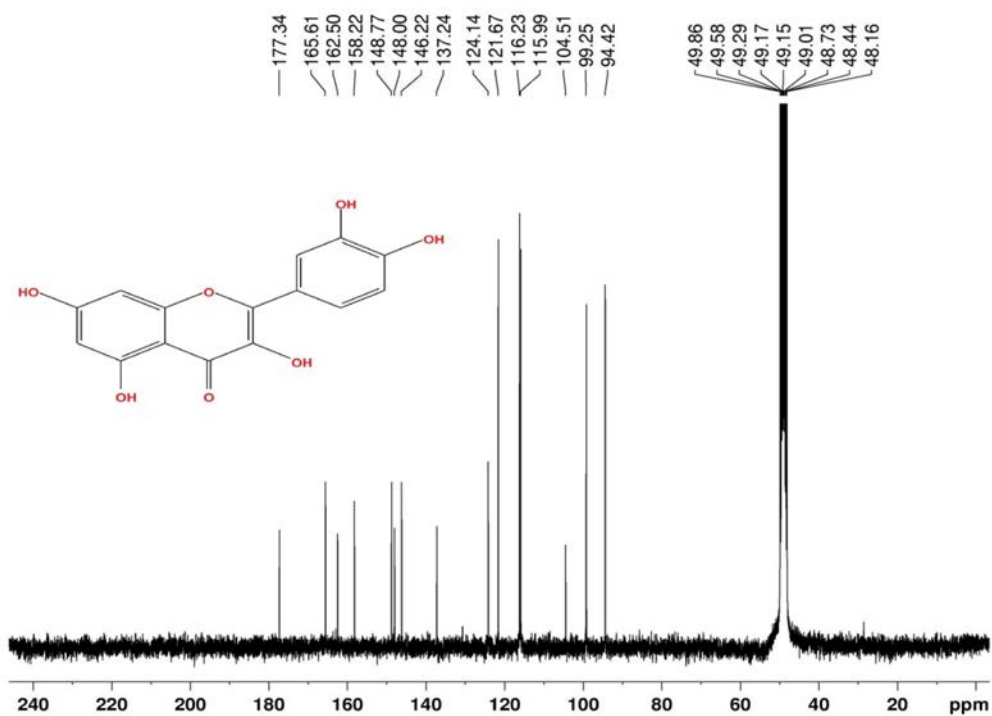


Figura 30S. Espectro de RMN de  $^{13}\text{C}$  (75 MHz,  $\text{CD}_3\text{OD}$ ) do composto 12 (Quercetina)



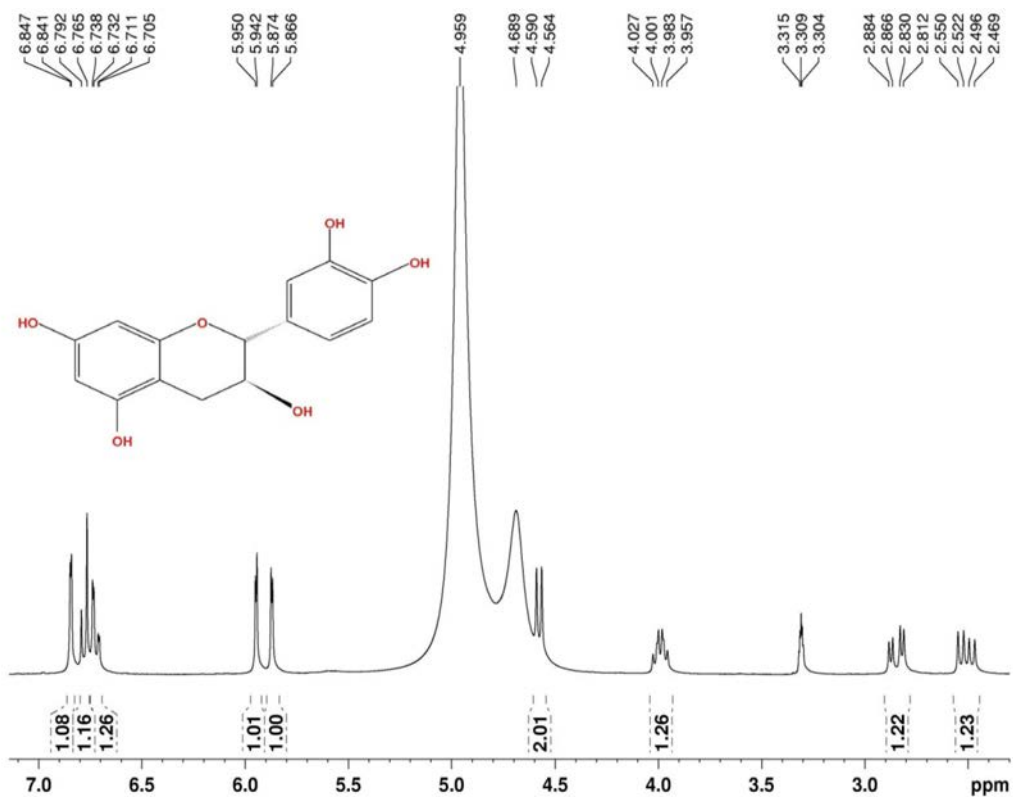


Figura 31S. Espectro de RMN de <sup>1</sup>H (300 MHz, CD<sub>3</sub>OD) do composto 13 ((+)-catequina)

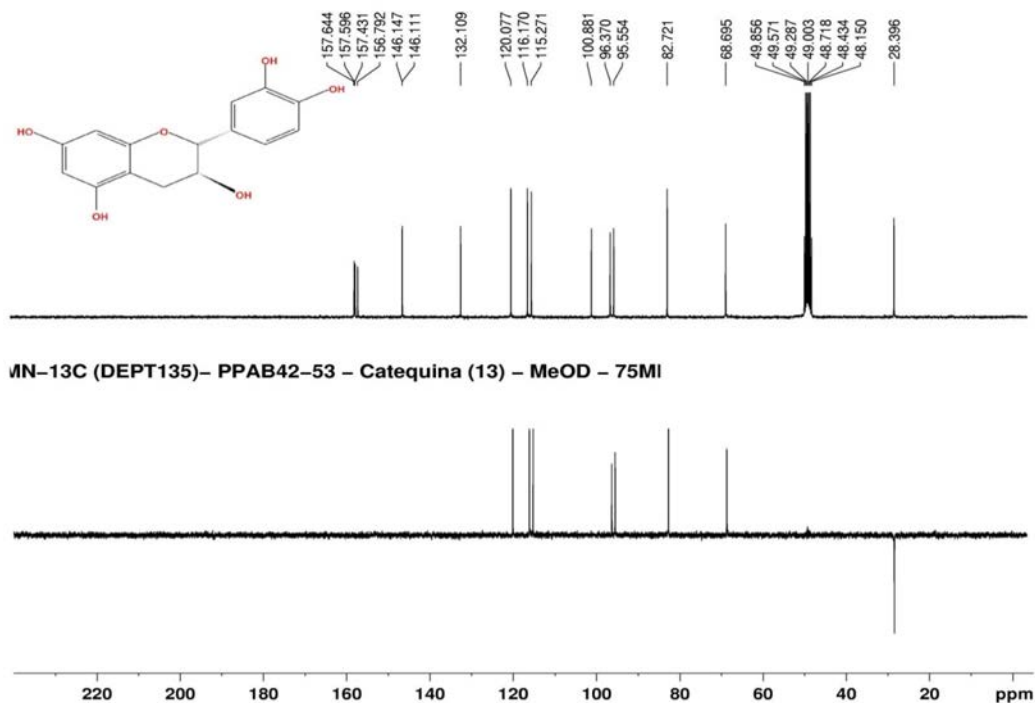


Figura 32S. Espectro de RMN de <sup>13</sup>C (75 MHz, CD<sub>3</sub>OD) do composto 13 ((+)-catequina)

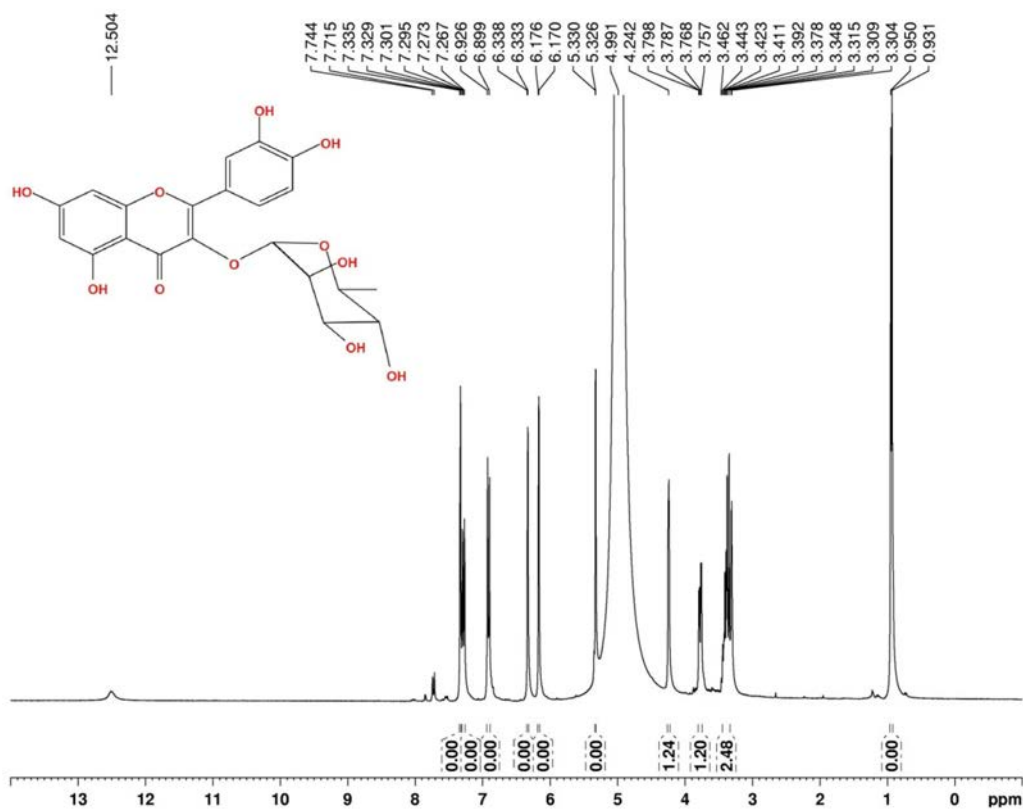


Figura 33S. Espectro de RMN de  $^1\text{H}$  (300 MHz,  $\text{CD}_3\text{OD}$ ) do composto **14** (Quercetina-3-O- $\alpha$ -L-rhamnopyranosídeo)

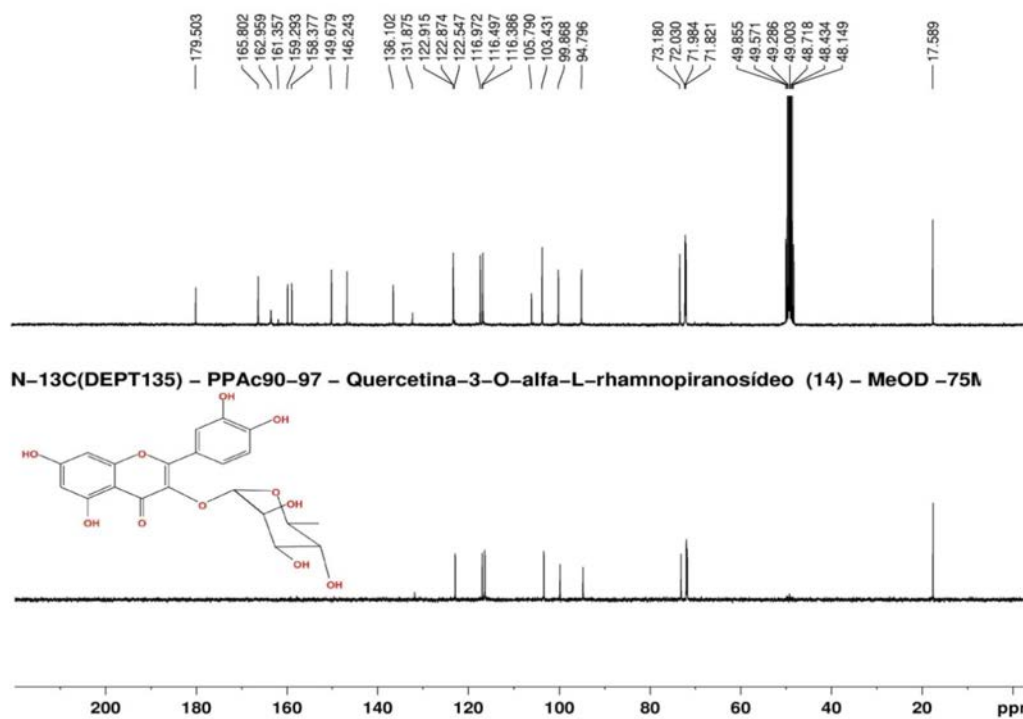


Figura 34S. Espectro de RMN de  $^{13}\text{C}$  e experimento DEPT 135° (75 MHz,  $\text{CD}_3\text{OD}$ ) do composto **14** (Quercetina-3-O- $\alpha$ -L-rhamnopyranosídeo)

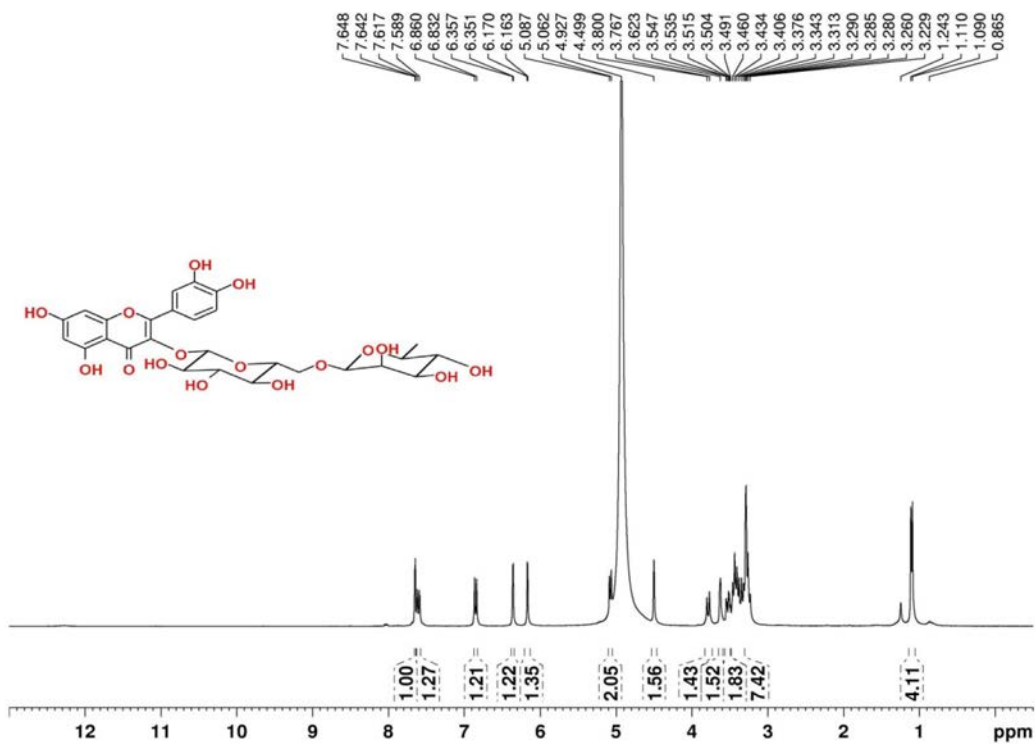


Figura 35S. Espectro de RMN de <sup>1</sup>H (300 MHz, CD<sub>3</sub>OD) do composto 15 (Rutina)

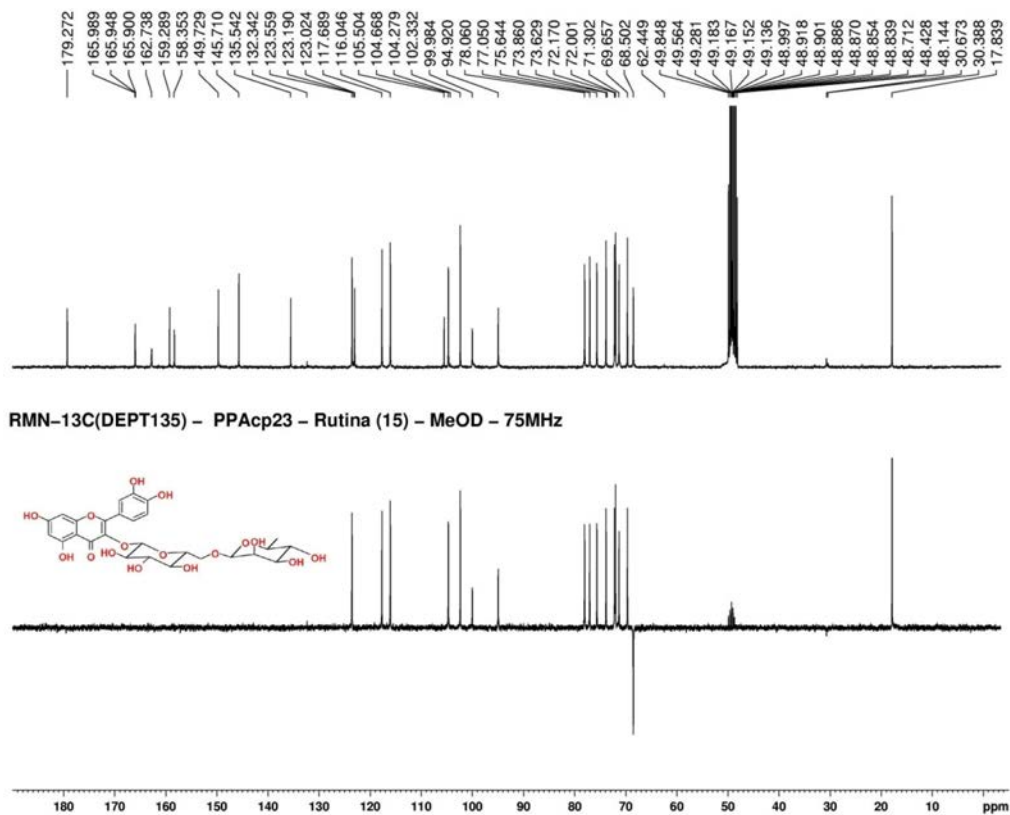


Figura 36S. Espectro de RMN de <sup>13</sup>C e experimento DEPT 135° (75 MHz, CD<sub>3</sub>OD) do composto 15 (Rutina)

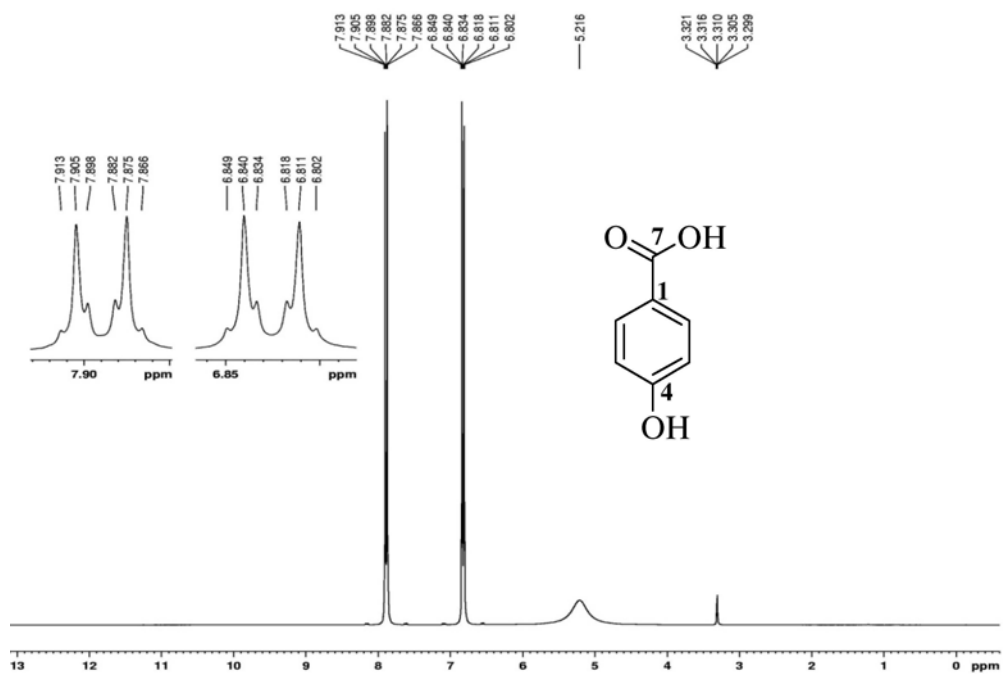


Figura 37S. Espectro de RMN de  $^1\text{H}$  (300 MHz,  $\text{CD}_3\text{OD}$ ) do composto **16** (Ácido p-hidroxibenzoico)

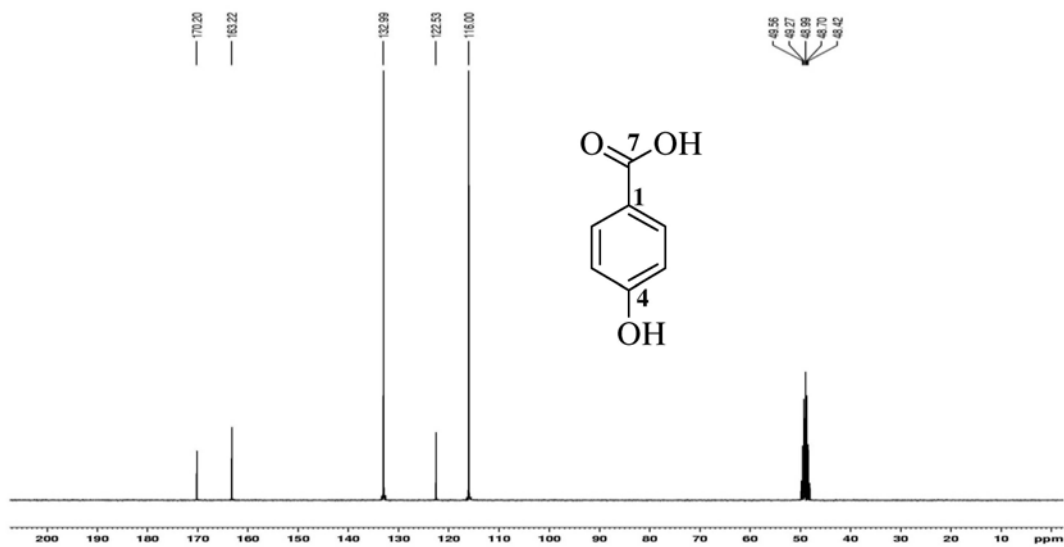
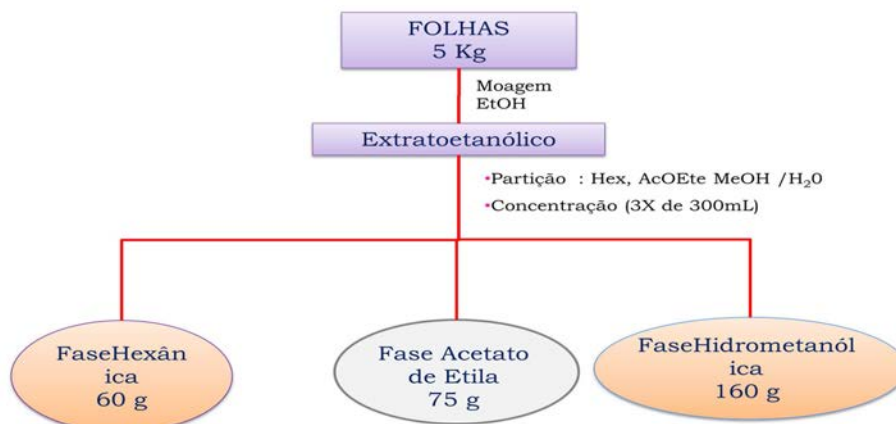


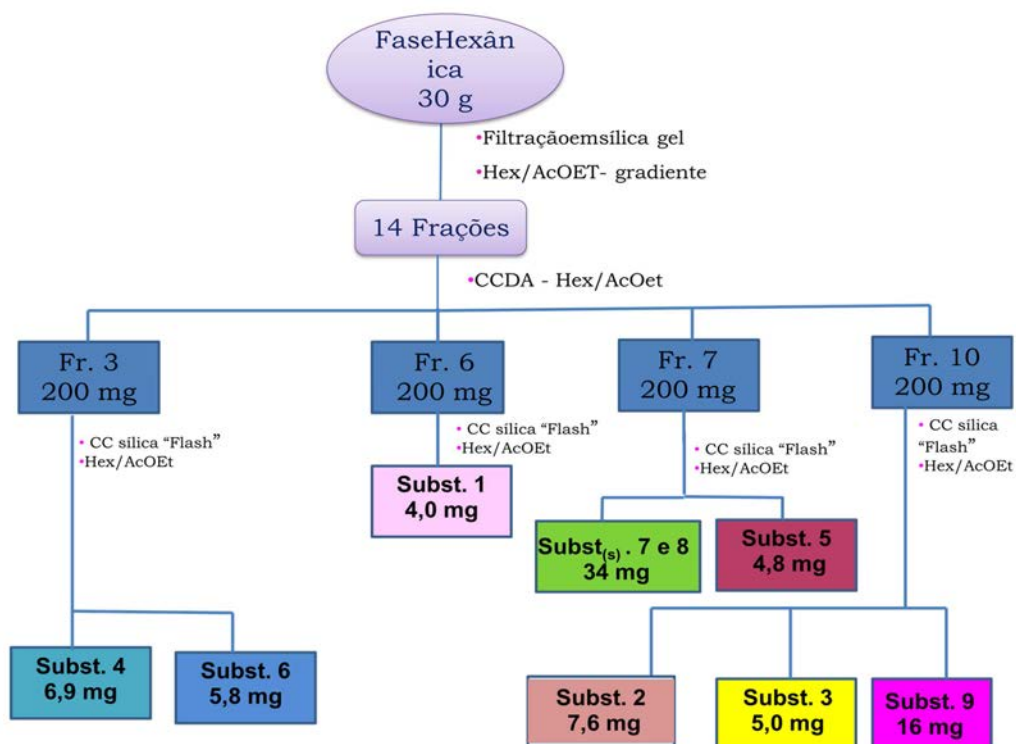
Figura 38S. Espectro de RMN de  $^{13}\text{C}$  (75 MHz,  $\text{CD}_3\text{OD}$ ) do composto **16** (Ácido p-hidroxibenzoico)

**Fracionamento do extrato etanólico das folhas de *Pterodon pubescens*: obtenção dos compostos 1-16**

a) Fluxograma da partição do extrato etanólico e obtenção dos resíduos orgânicos das folhas de *P. pubescens*.



b) Fluxograma do fracionamento cromatográfico realizado com as frações obtidas da fase hexânica do extrato etanólico das folhas de *Pterodon pubescens*.



c) Fluxograma do fracionamento cromatográfico realizado com as frações obtidas da fase acetato de etila do extrato etanólico das folhas de *Pterodon pubescens*.

