


MATERIAL SUPLEMENTAR

Iridoides, triterpenos e outros constituintes das cascas do caule e flores de *Tabebuia caraiba* Bignoniaceae

Aloízio de O. Soares^a, Caroline Tieppo^b, Luzinátia Ramos Soares^c, Joaquim Corsino^b, Alex Fonseca Souza^b, Fernanda R. Garcez^b e Walmir S. Garcez^{b,*}, 

^aColégio Militar de Campo Grande, 79115-810 Campo Grande – MS, Brasil

^bInstituto de Química, Universidade Federal de Mato Grosso do Sul, 79070-900 Campo Grande – MS, Brasil

^cUniversidade Estadual de Mato Grosso do Sul, Unidade Universitária de Campo Grande, 79400-000 Campo Grande – MS, Brasil

*e-mail: walmir.garcez@ufms.br

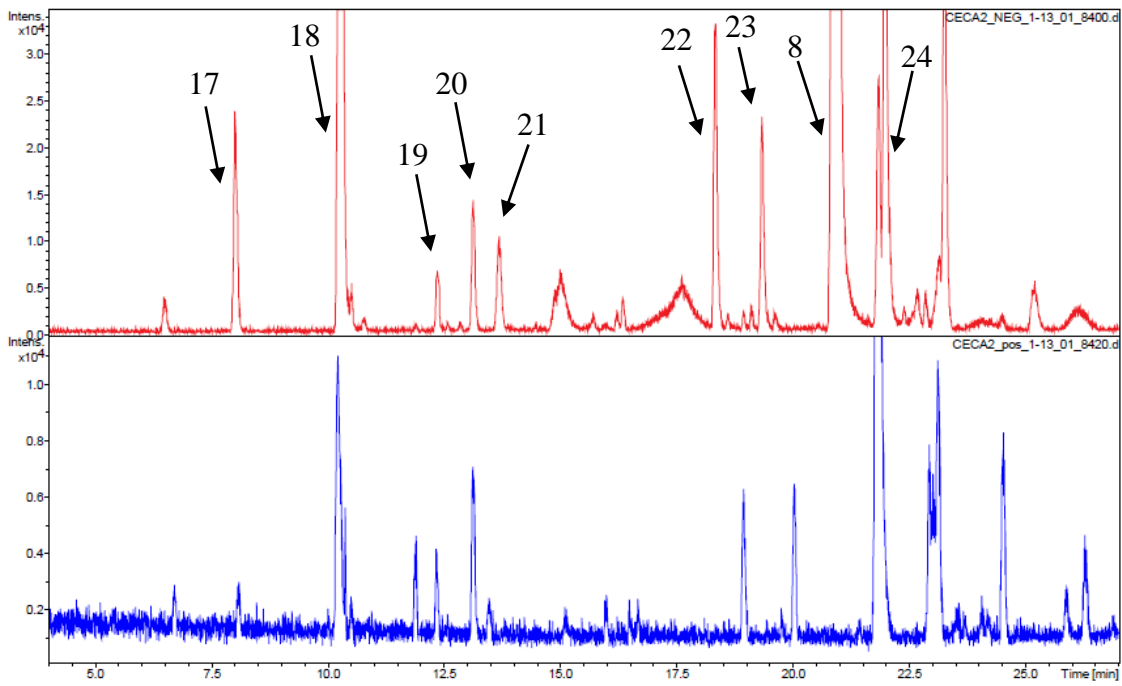
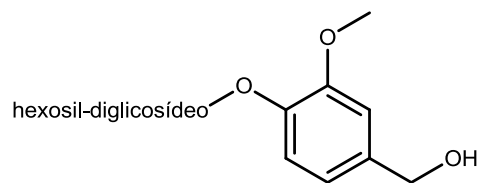
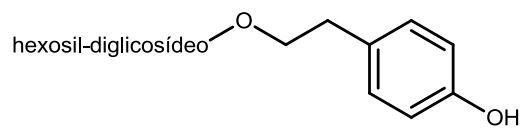


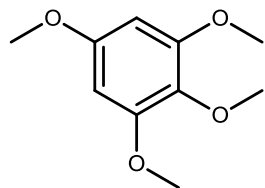
Figura 1S. Cromatograma de íons totais do extrato da casca de *Tabebuia caraíba*: a) modo negativo b) modo positivo



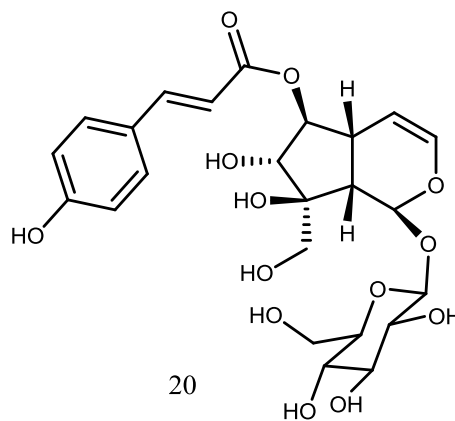
17



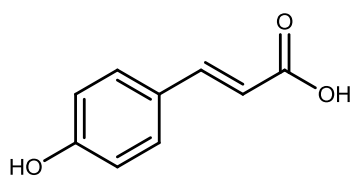
18



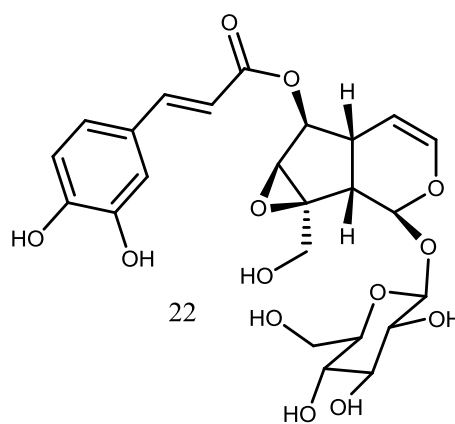
19



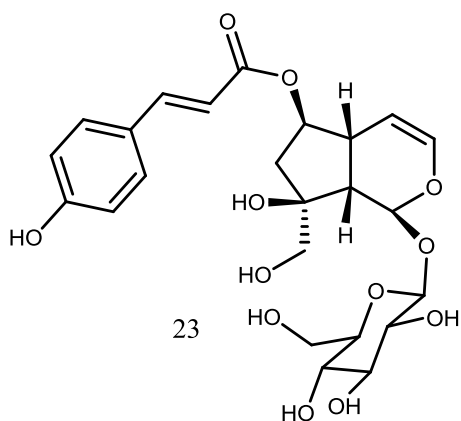
20



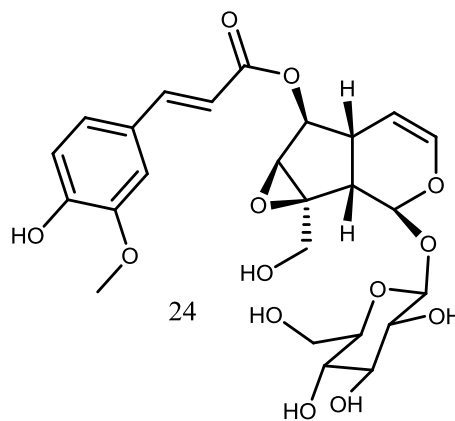
21



22



23



24

Figura 2S. Estruturas das substâncias identificadas por HPLC/DAD/MS na casca do caule de *Tabebuia caraiba*

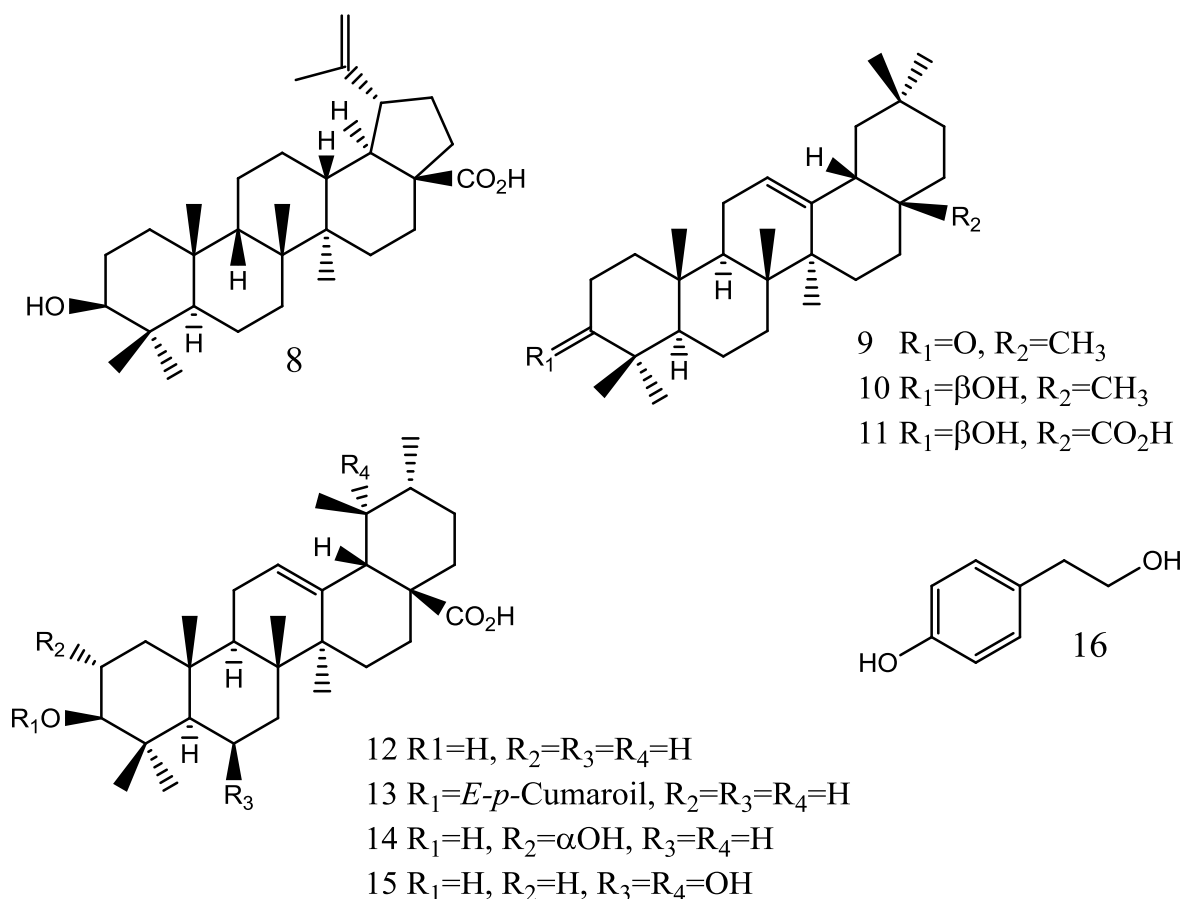


Figura 3S. Estruturas dos triterpenos e do feniletanoide tirosol isolados de *Tabebuia caraiba*

Dados de RMN dos triterpenos e do feniletanoide tirosol isolados de *Tabebuia caraiba*.

Olean-12-en-3-ona (**9**) Sólido branco. RMN ^{13}C ($CDCl_3$, 75 MHz) δc : 39,3 (C-1), 34,2 (C-2), 217,9 (C-3), 47,5 (C-4), 55,3 (C-5), 19,6 (C-6), 32,1 (C-7), 39,8 (C-8), 46,8 (C-9), 36,6 (C-10), 23,6 (C-11), 121,5 (C-12), 145,3 (C-13), 41,8 (C-14), 26,1 (C-15), 26,9 (C-16), 32,5 (C-17), 47,3 (C-18), 46,8 (C-19), 31,1 (C-20), 34,7 (C-21), 37,1 (C-22), 26,5 (C-23), 21,5 (C-24), 15,2 (C-25), 16,7 (C-26), 25,9 (C-27), 28,4 (C-28), 33,3 (C-29), 23,6 (C-30).

Ácido 3-O-E-p-cumaroilursólico (**13**) Sólido branco. RMN ^{13}C ($CDCl_3$, 75 MHz) δc : 38,5 (C-1), 23,3 (C-2), 81,1 (C-3), 37,7 (C-4), 54,4 (C-5), 18,9 (C-6), 33,8 (C-7), 39,7 (C-8), 48,3 (C-9), 37,5 (C-10), 24,0 (C-11), 126,1 (C-12), 139,2 (C-13), 42,1 (C-14), 29,2 (C-15), 25,0 (C-16), 48,2 (C-17), 51,5 (C-18), 39,9 (C-19), 39,8 (C-20), 30,3 (C-21), 37,6 (C-22), 28,4 (C-23), 17,0 (C-24), 15,6 (C-25), 16,6 (C-26), 23,9 (C-27), 179,1 (C-28), 17,1 (C-29), 21,1 (C-30), 126,1 (C-1'), 130,9 (C-2' e C-6'), 116,6 (C-3' e C-5'), 160,7 (C-4'), 115,7 (C- α), 145,4 (C- β), 167,7 (COO).

Ácido 2 α -hidróxi-ursólico (14) (14) Sólido branco. RMN ^{13}C (Pyr- d_5 , 75 MHz) δ_c : 47,8 (C-1), 68,5 (C-2), 83,6 (C-3), 39,7 (C-4), 55,7 (C-5), 18,7 (C-6), 33,1 (C-7), 39,9 (C-8), 47,9 (C-9), 38,3 (C-10), 23,6 (C-11), 125,4 (C-12), 139,1 (C-13), 42,4 (C-14), 28,5 (C-15), 24,8 (C-16), 46,5 (C-17), 53,4 (C-18), 37,3 (C-19), 38,3 (C-20), 30,9 (C-21), 37,3 (C-22), 28,5 (C-23), 16,8 (C-24), 17,3 (C-25), 17,4 (C-26), 23,8 (C-27), 177,9 (C-28), 17,6 (C-29), 21,3 (C-30).

Ácido 6 β ,19 α -di-hidróxi-ursólico (15) Sólido branco. RMN ^{13}C (CD_3OD , 75 MHz) δ_c : 41,9 (C-1), 28,0 (C-2), 80,2 (C-3), 37,6 (C-4), 57,2 (C-5), 68,9 (C-6), 42,0 (C-7), 40,2 (C-8), 49,0 (C-9), 37,6 (C-10), 24,6 (C-11), 129,7 (C-12), 139,3 (C-13), 42,1 (C-14), 29,6 (C-15), 26,6 (C-16), 48,1 (C-17), 55,1 (C-18), 73,6 (C-19), 43,1 (C-20), 27,3 (C-21), 39,0 (C-22), 17,3 (C-23), 28,4 (C-24), 17,3 (C-25), 18,5 (C-26), 24,8 (C-27), 182,4 (C-28), 27,1 (C-29), 16,6 (C-30).

2-(4-hidroxifenil)-Etanol (Tirosol) (16) Sólido branco. RMN ^1H (CDCl_3 , 300 MHz) δ_H : 3,66 (2H, t, $J=7,1$ Hz, H-1), 2,69 (2H, t, $J=7,1$ Hz, H-2), 7,03 (1H, d, $J=8,6$ Hz, H-2' e H-6'), 6,71 (1H, d, $J=8,6$ Hz, H-3' e H-5'). RMN ^{13}C (CDCl_3 , 75 MHz) δ_c : 64,2 (C-1), 39,5 (C-2), 130,7 (C-1'), 130,5 (C-2' e C-6'), 115,8 (C-3' e C-5'), 156,5 (C-4').

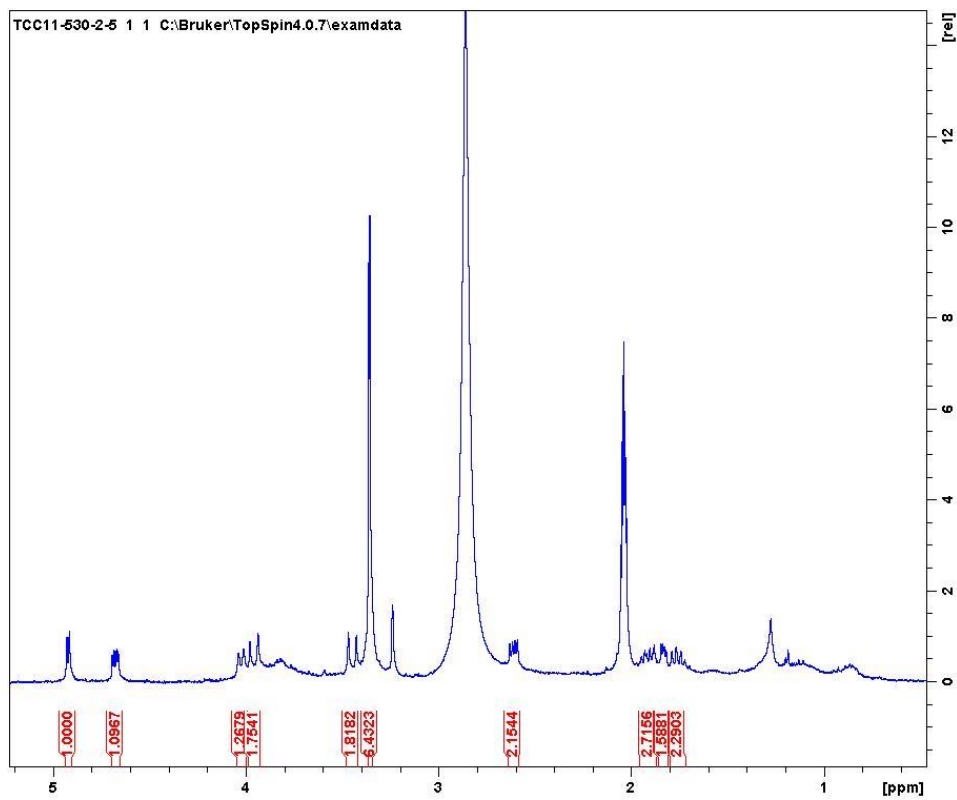


Figura 4S. Espectro RMN ^1H de jioglutina D (**1**) (Acetona- d_6 , 300 MHz)

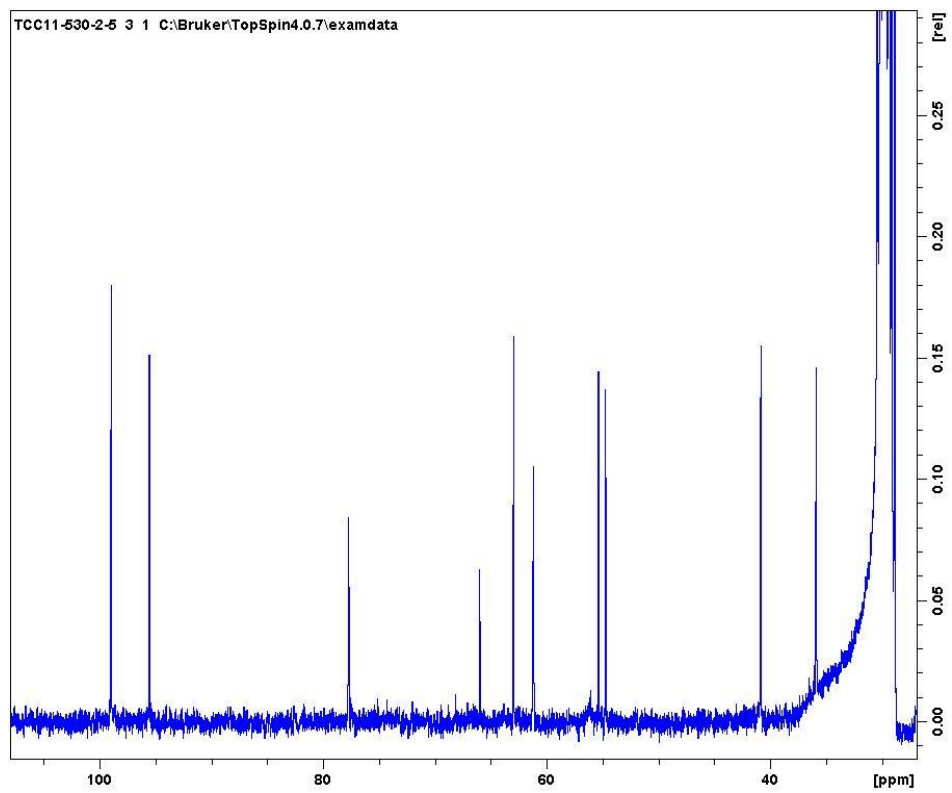


Figura 5S. Espectro RMN ^{13}C de jioglutina D (**1**) (Acetona- d_6 , 75 MHz)

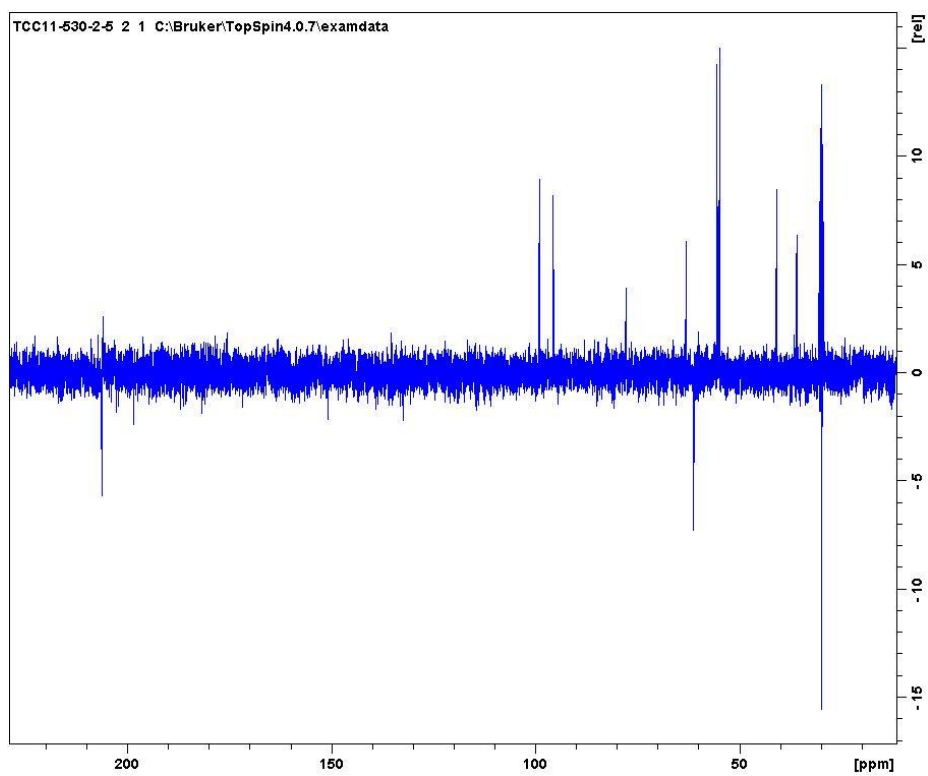


Figura 6S. Espectro RMN ^{13}C DEPT 135° de jioglutina D (1) (Acetona- d_6 , 75 MHz)

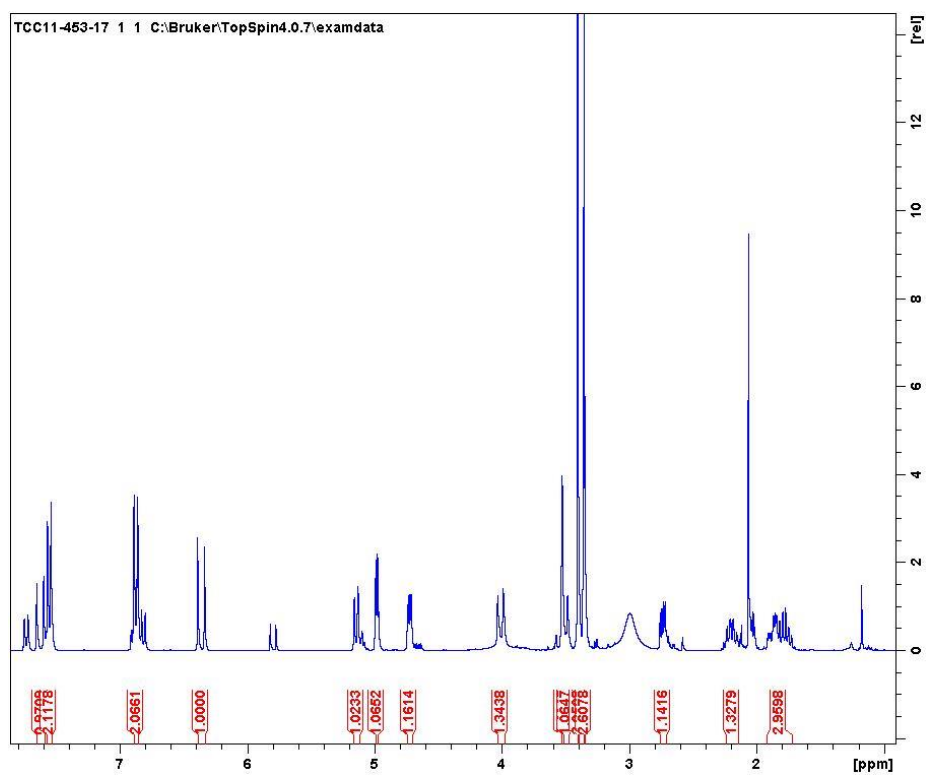


Figura 7S. Espectro RMN ^1H de 6-O-E-p-cumaroiljioglutina D (2) (Acetona- d_6 , 300 MHz)

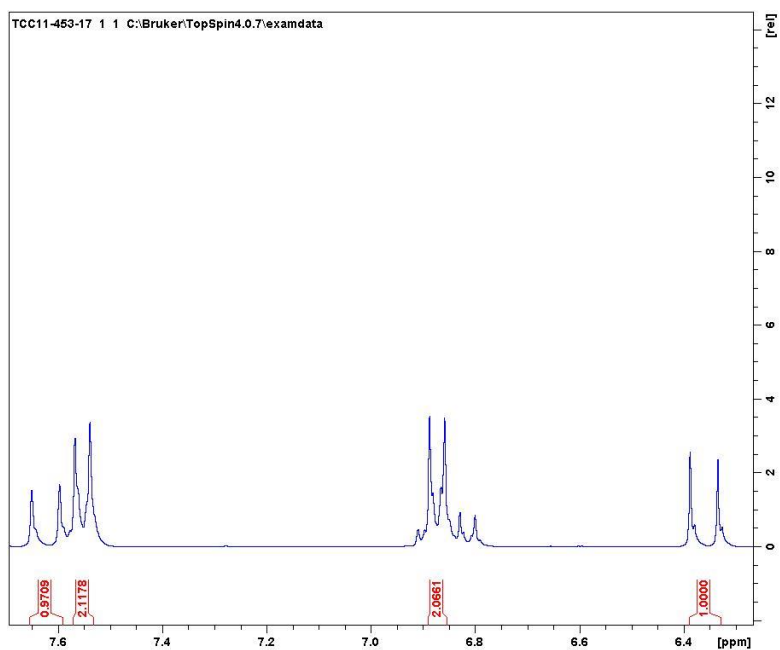


Figura 8S. Expansão do espectro RMN ^1H de 6-O-E-p-cumaroiljioglutina D (2) (Acetona- d_6 , 300 MHz)

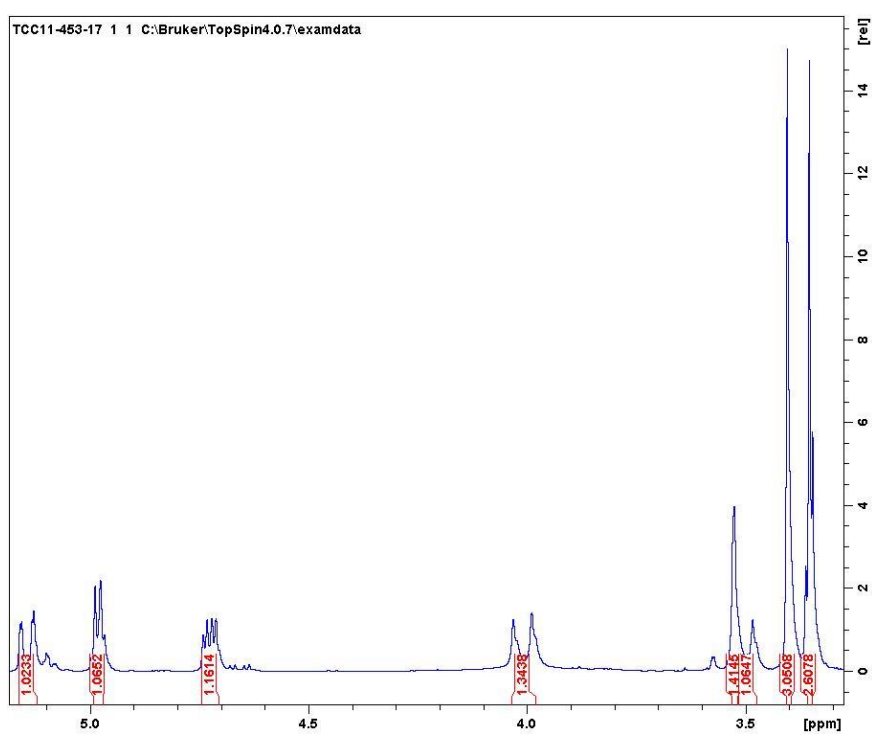


Figura 9S. Expansão do espectro RMN ^1H de 6-O-E-p-cumaroiljioglutina D (2) (Acetona- d_6 , 300 MHz)

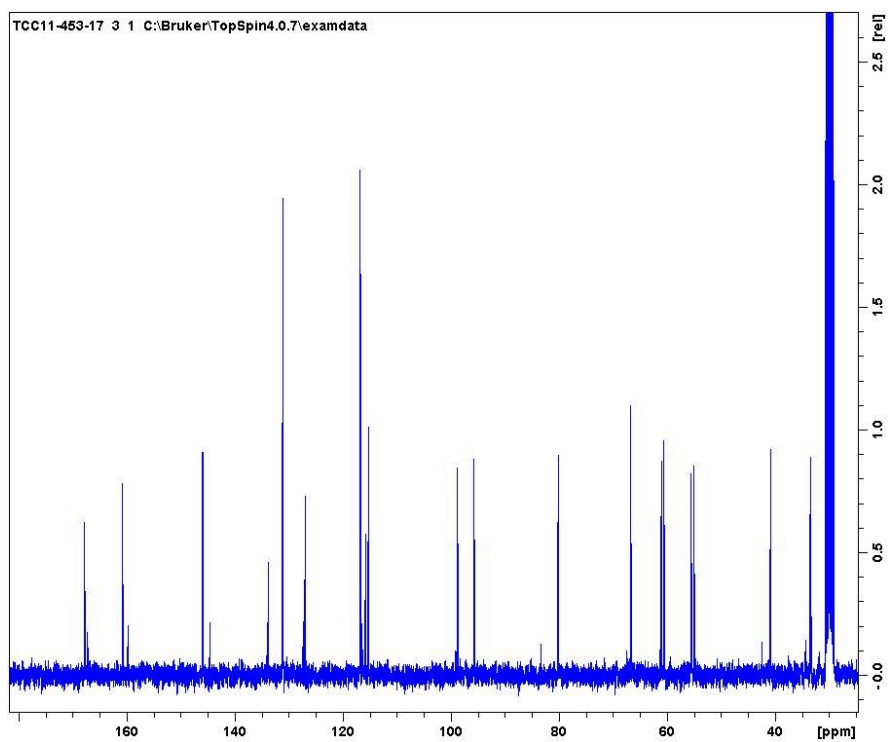


Figura 10S. Espectro RMN ^{13}C de 6-O-E-p-cumaroiljioglutina D (2) (Acetona- d_6 , 75 MHz)

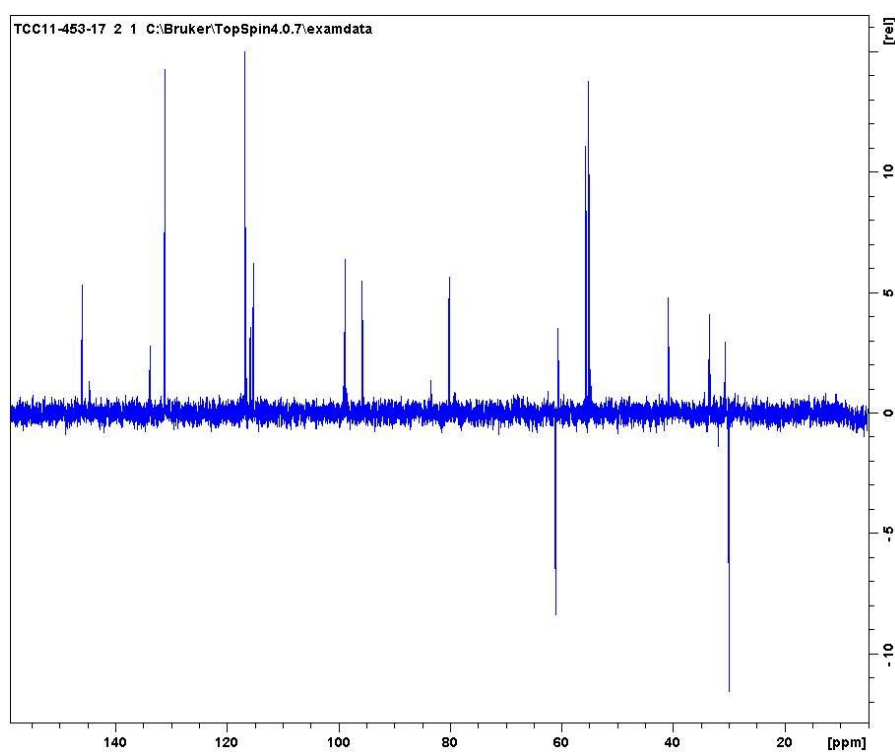


Figura 11S. Espectro RMN ^{13}C DEPT 135° de 6-O-E-p-cumaroiljioglutina D (2) (Acetona- d_6 , 75 MHz)

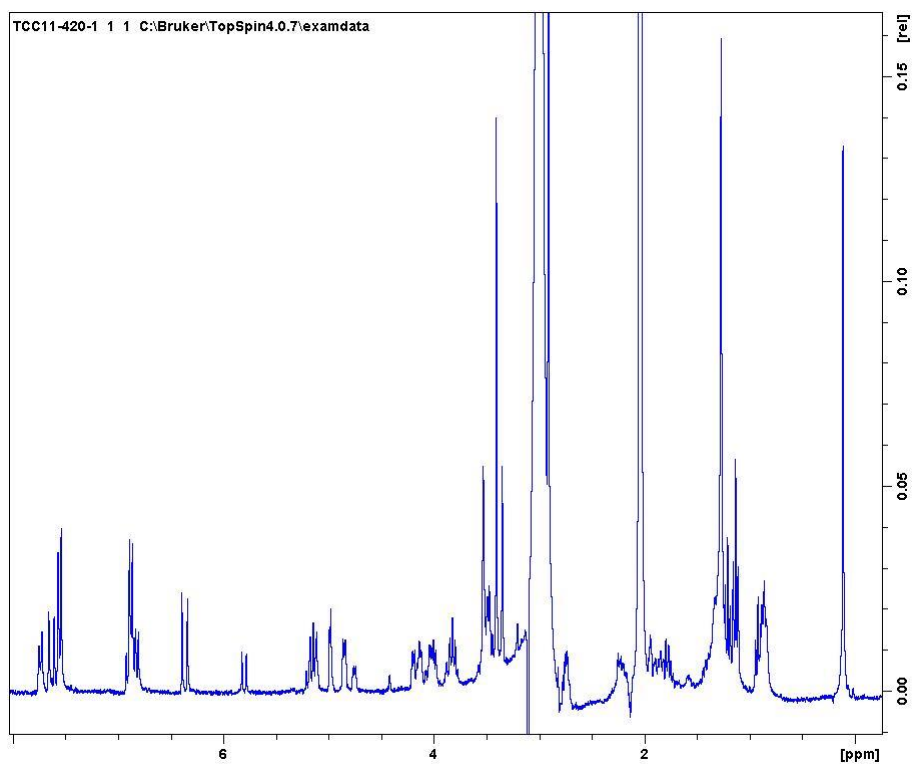


Figura 12S. Espectro RMN ^1H de 6-*O-E-p*-cumaroil-3-desmetil-3-*O*-etiljioglutina D (3) e 6-*O-E-p*-cumaroil-1-desmetil-1-*O*-etiljioglutina D (4) (Acetona- d_6 , 300 MHz)

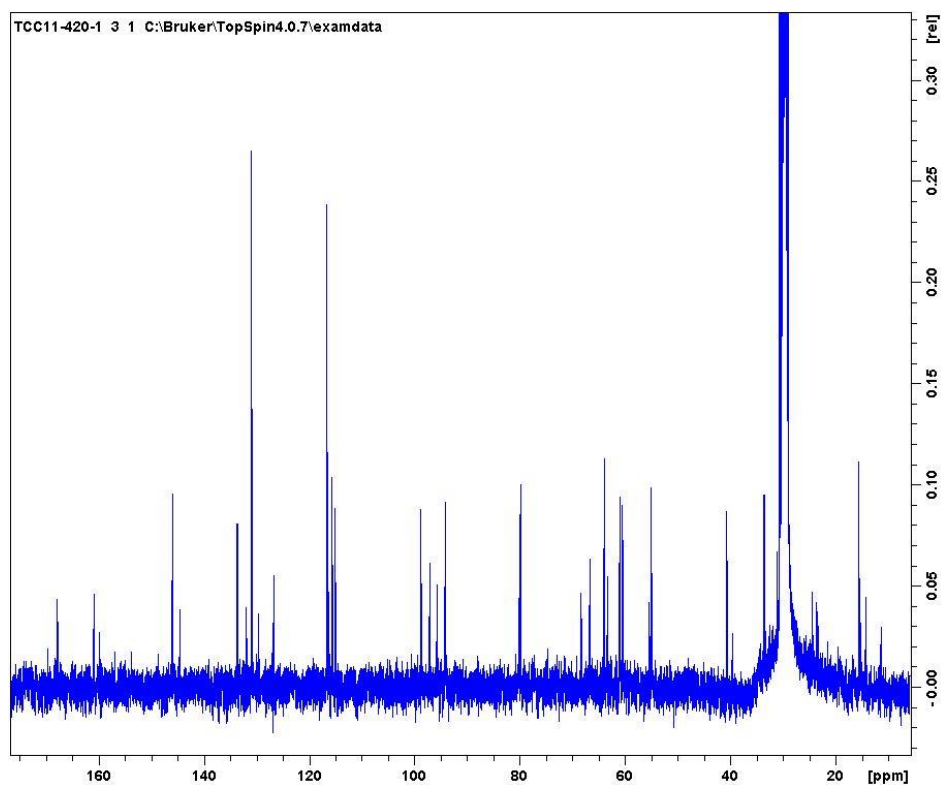


Figura 13S. Espectro RMN ^{13}C de 6-*O-E-p*-cumaroil-3-desmetil-3-*O*-etiljioglutina D (3) e 6-*O-E-p*-cumaroil-1-desmetil-1-*O*-etiljioglutina D (4) (Acetona- d_6 , 75 MHz)

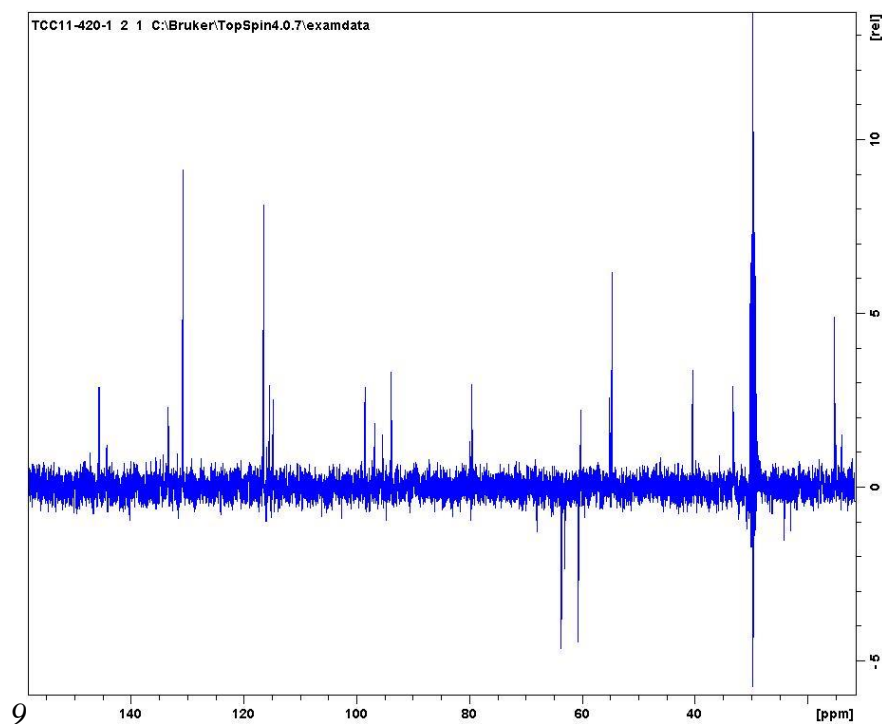


Figura 14S. Espectro RMN ^{13}C DEPT 135° de 6-O-E-p-cumaroil-3-desmetil-3-O-etiljioglutina D (3) e 6-O-E-p-cumaroil-1-desmetil-1-O-etiljioglutina D (4) (Acetona- d_6 , 75 MHz)

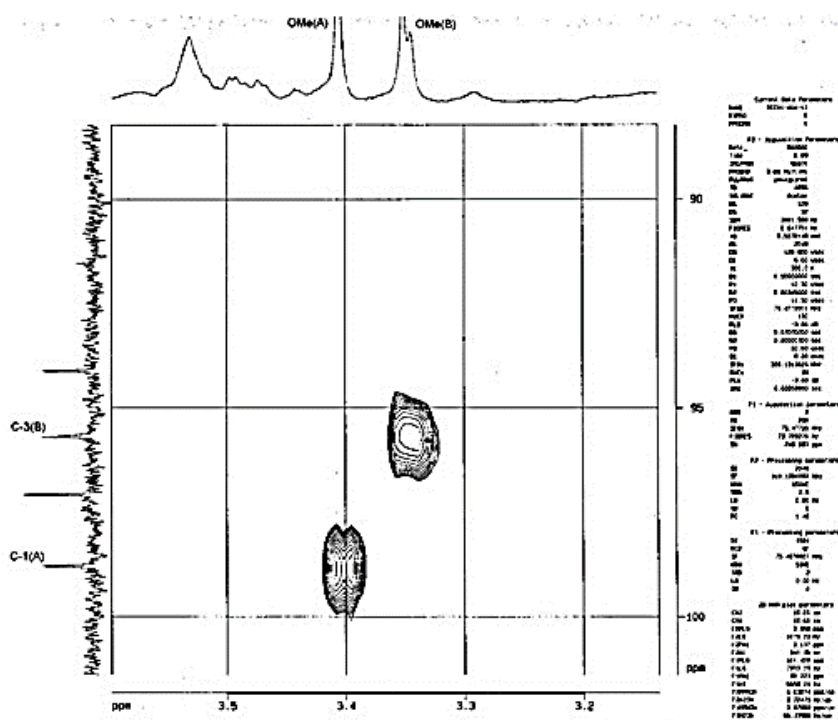


Figura 15S. Experimento HMBC (expansão) de 6-O-E-p-cumaroil-3-desmetil-3-O-etiljioglutina D (3) e 6-O-E-p-cumaroil-1-desmetil-1-O-etiljioglutina D (4) (Acetona- d_6 , 300MHz/75 MHz)

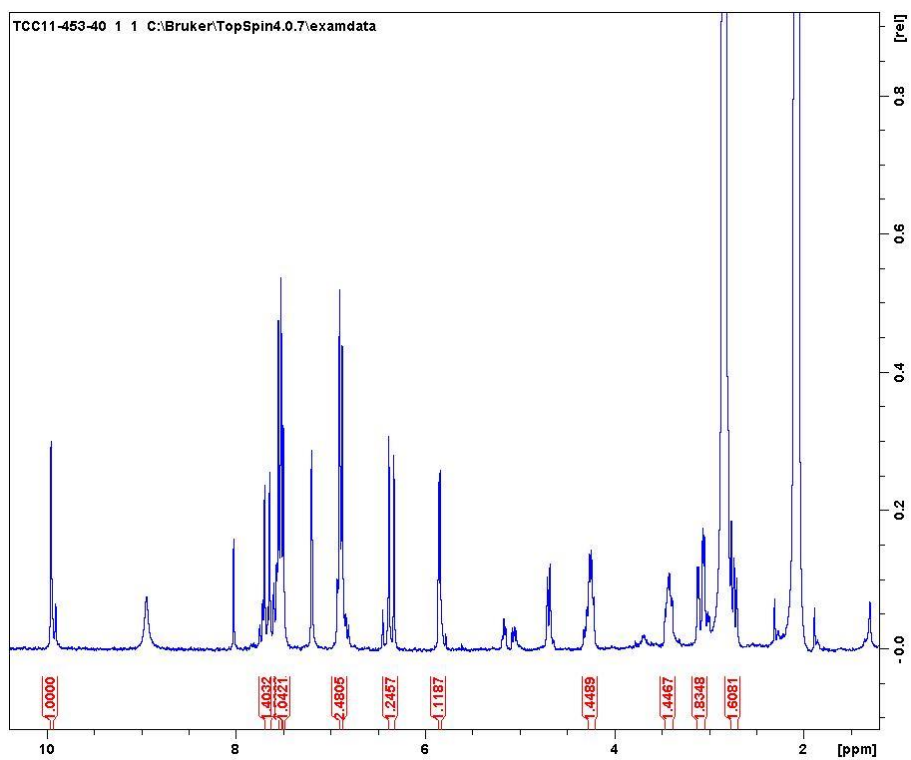


Figura 16S. Espectro RMN ^1H de 7-O-E-p-cumaroiljiofuranaldeído (5) (Acetona- d_6 , 300 MHz)

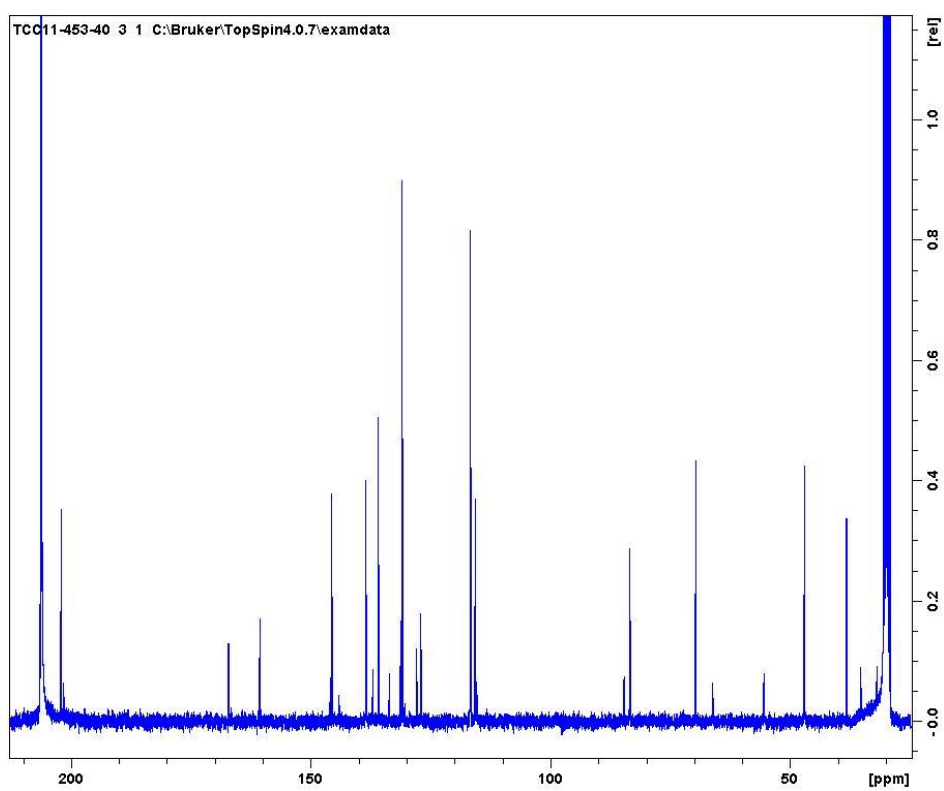


Figura 17S. Espectro RMN ^{13}C de 7-O-E-p-cumaroiljiofuranaldeído (5) (Acetona- d_6 , 75 MHz)

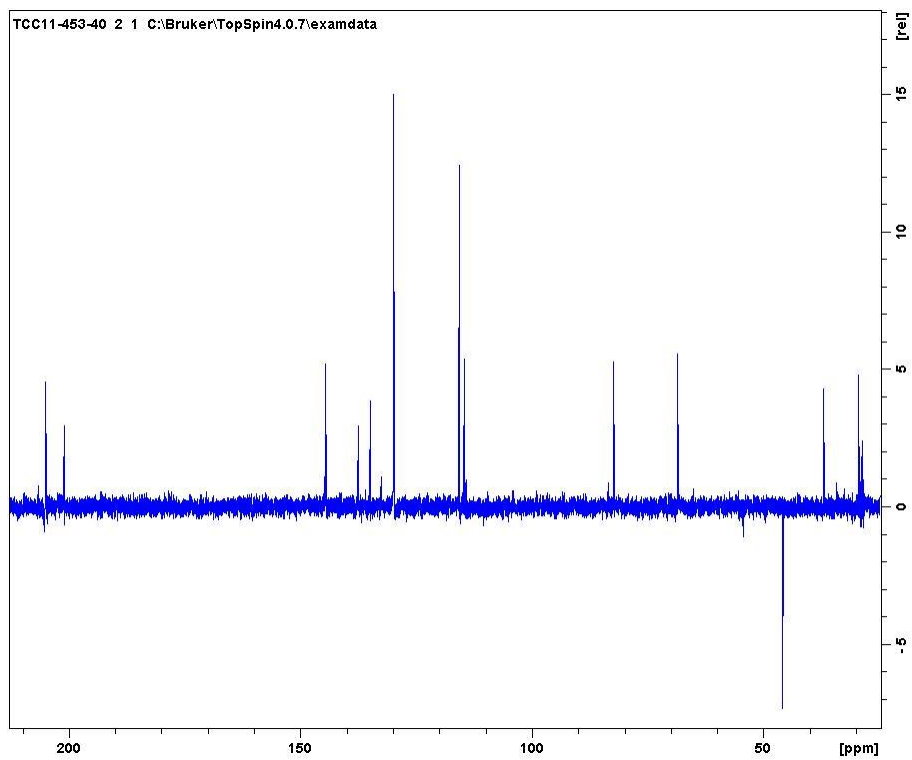


Figura 18S. Espectro RMN ^{13}C DEPT 135° de 7-O-E-p-cumaroiljiofuranaldeído (**5**) (Acetona- d_6 , 75 MHz)

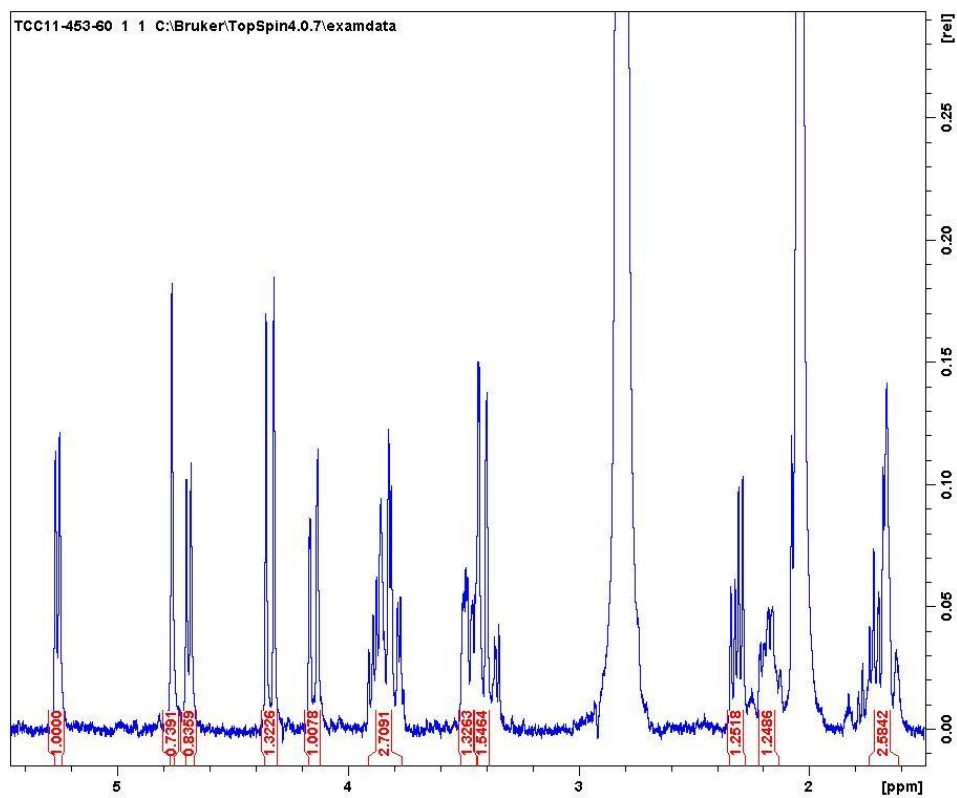


Figura 19S. Espectro RMN ^1H de remaglutina D (**6**) (Acetona- d_6 , 300 MHz)

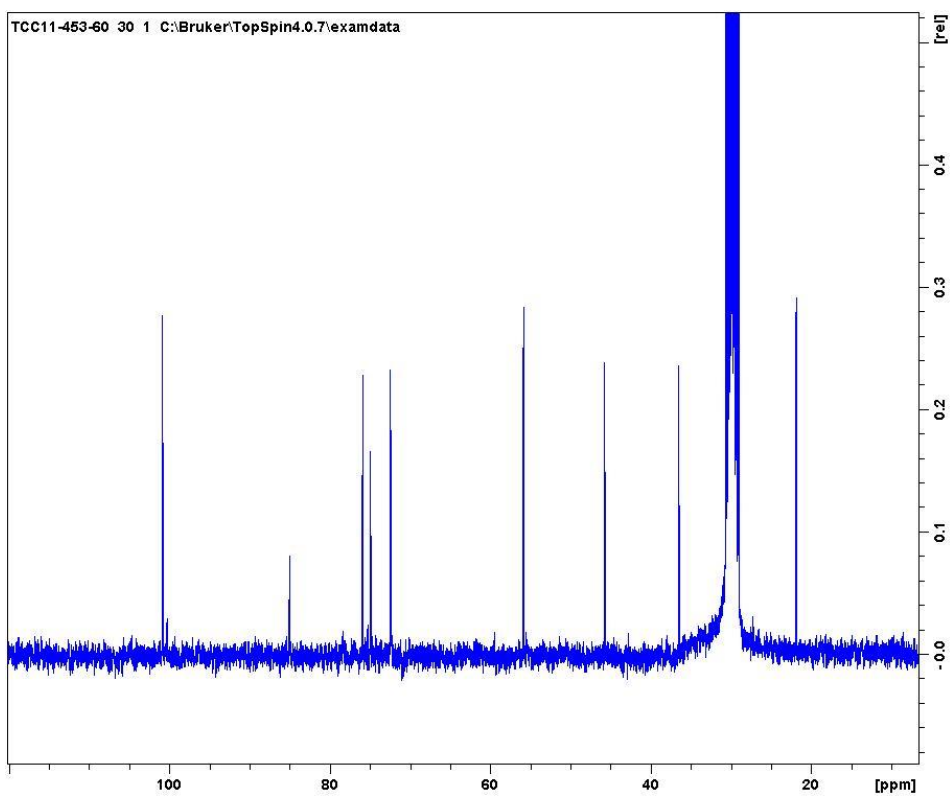


Figura 20S. Espectro RMN ^{13}C DEPT 135° de remaglutina D (6) (Acetona- d_6 , 75 MHz)

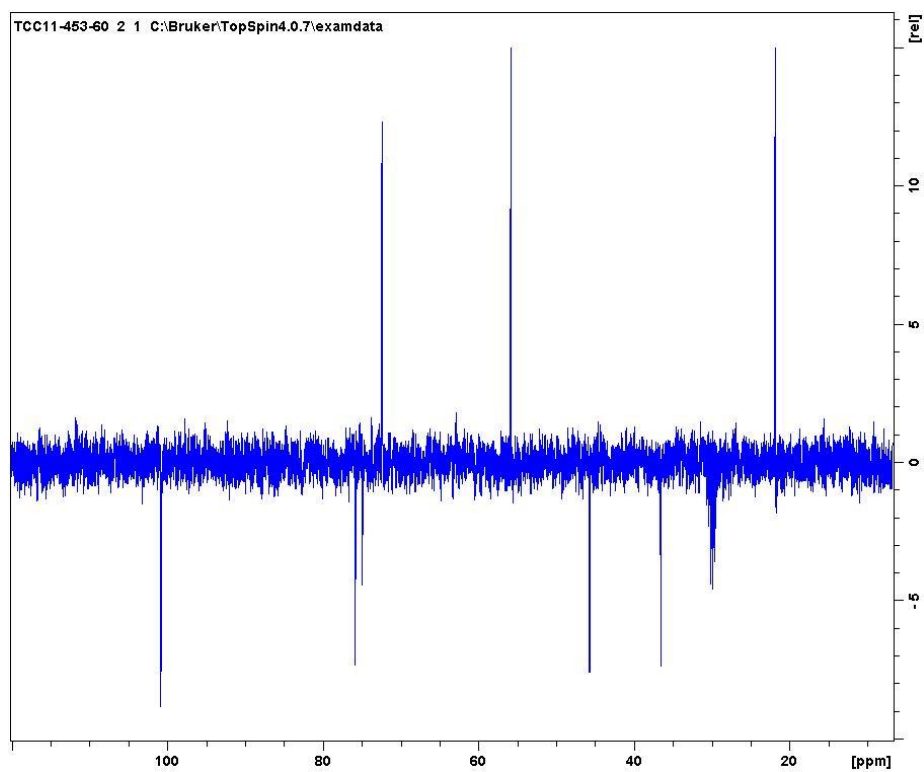


Figura 21S. Espectro RMN ^{13}C DEPT 135° de remaglutina D (6) (Acetona- d_6 , 75 MHz)

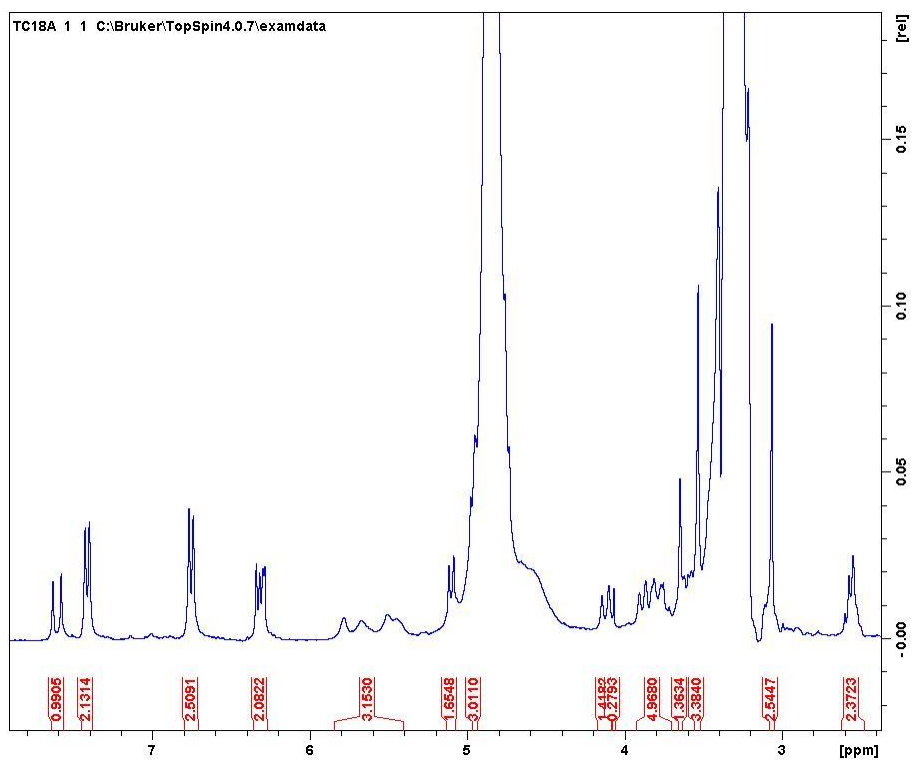


Figura 22S. Espectro RMN ^1H de 6-O- E-p-cumaroilcatalpol (7) (MeOH/D $_2$ O, 300MHz)

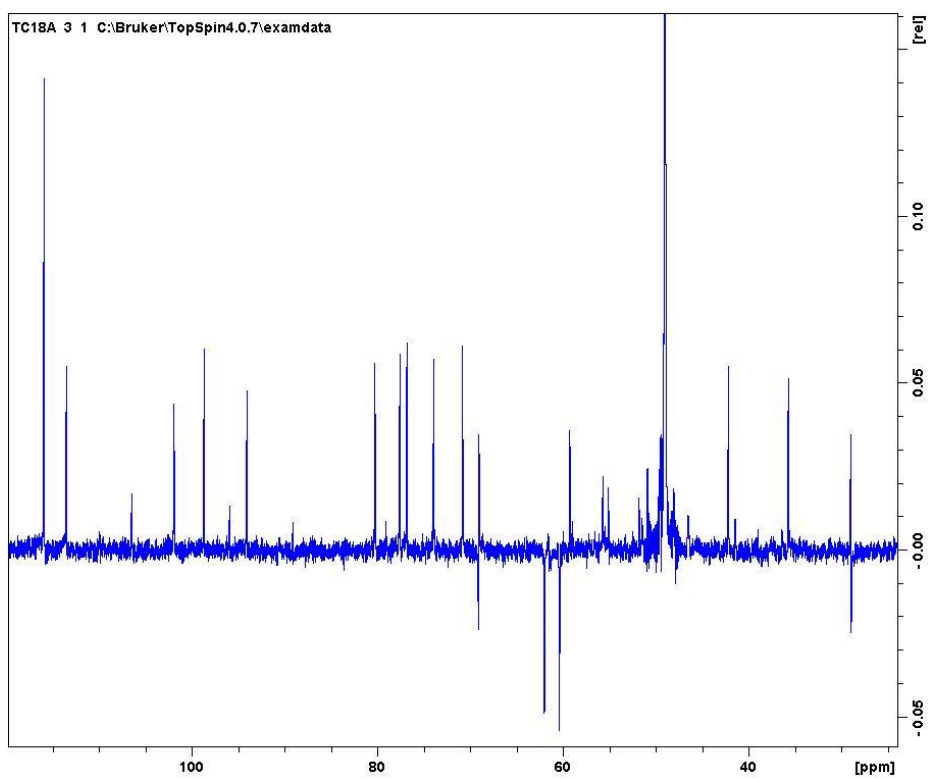


Figura 23S. Espectro RMN ^{13}C de 6-O- E-p-cumaroilcatalpol (7) (MeOH/D $_2$ O, 75MHz)

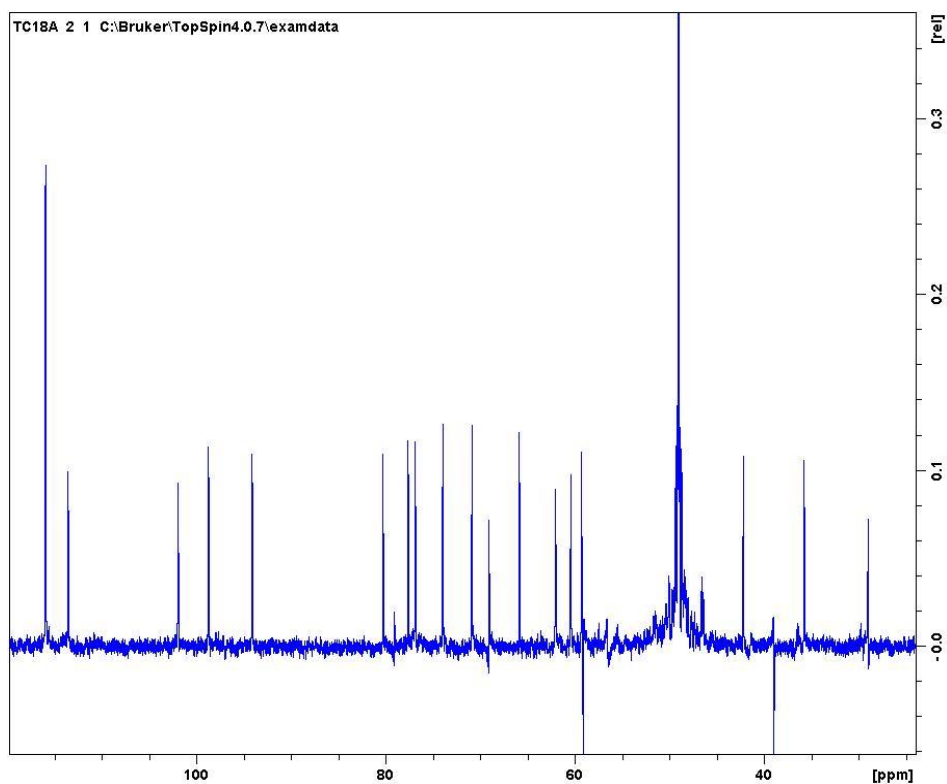


Figura 24S. Espectro RMN ^{13}C DEPT 135° de 6-O- E-p-cumaroilcatalpol (**7**) (MeOH/D $_2$ O, 75MHz)

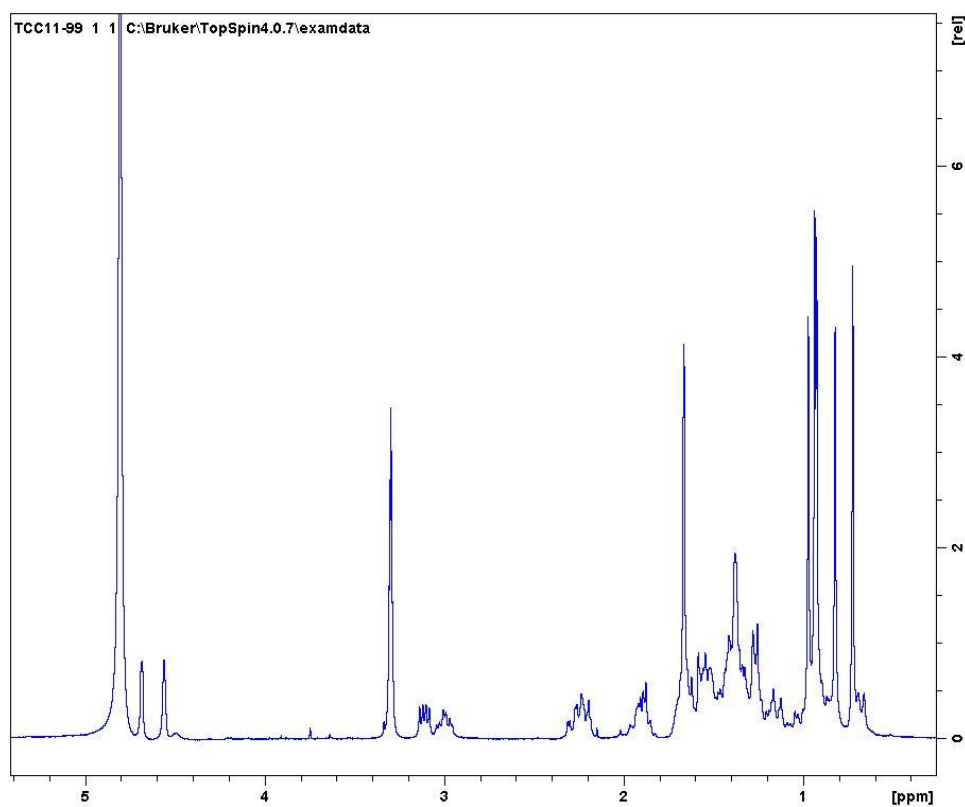


Figura 25S. Espectro RMN ^1H do ácido betulínico (**8**) (CDCl $_3$ /CD $_3$ OD, 300MHz)

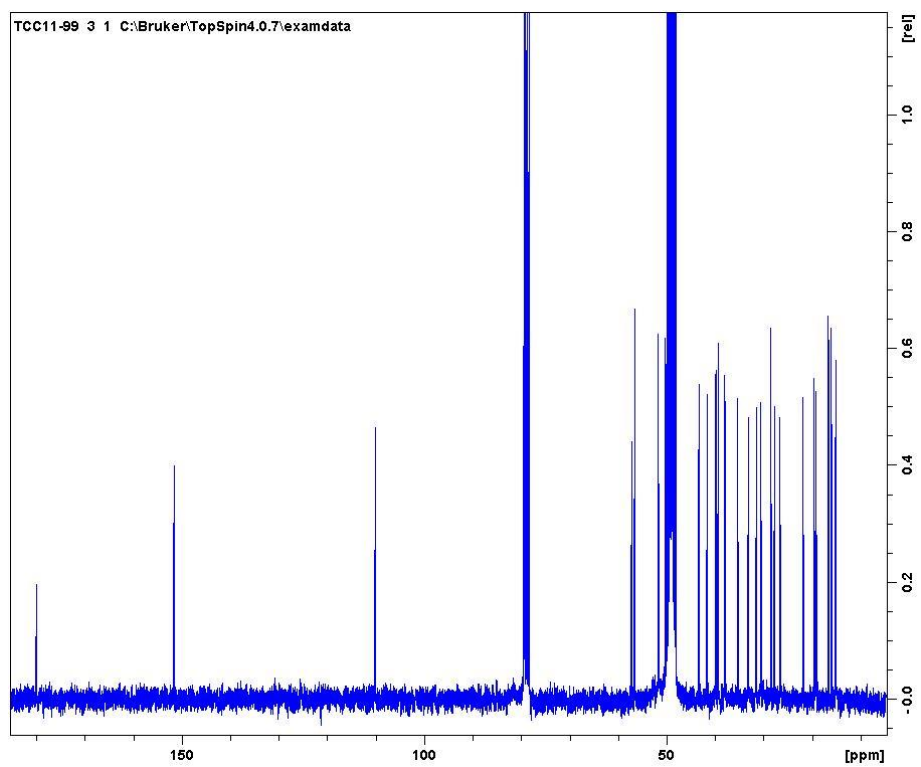


Figura 26S. Espectro RMN ^{13}C do ácido betulínico (8) (($\text{CDCl}_3/\text{CD}_3\text{OD}$, 75 MHz)

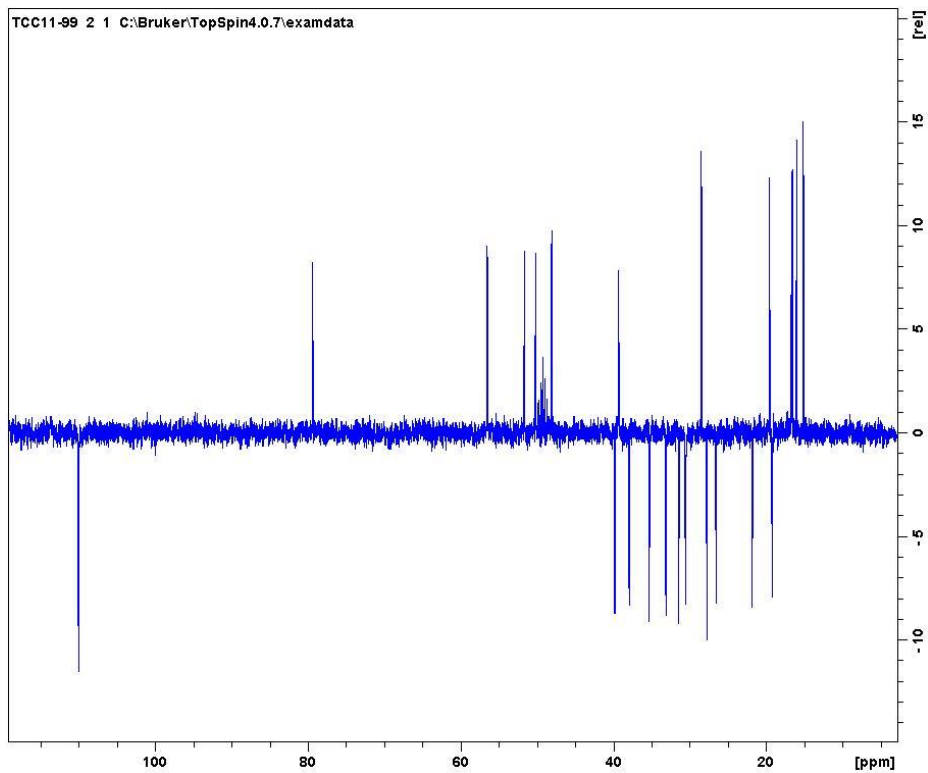


Figura 27S. Espectro RMN ^{13}C DEPT 135° do ácido betulínico (8) (($\text{CDCl}_3/\text{CD}_3\text{OD}$, 75 MHz)

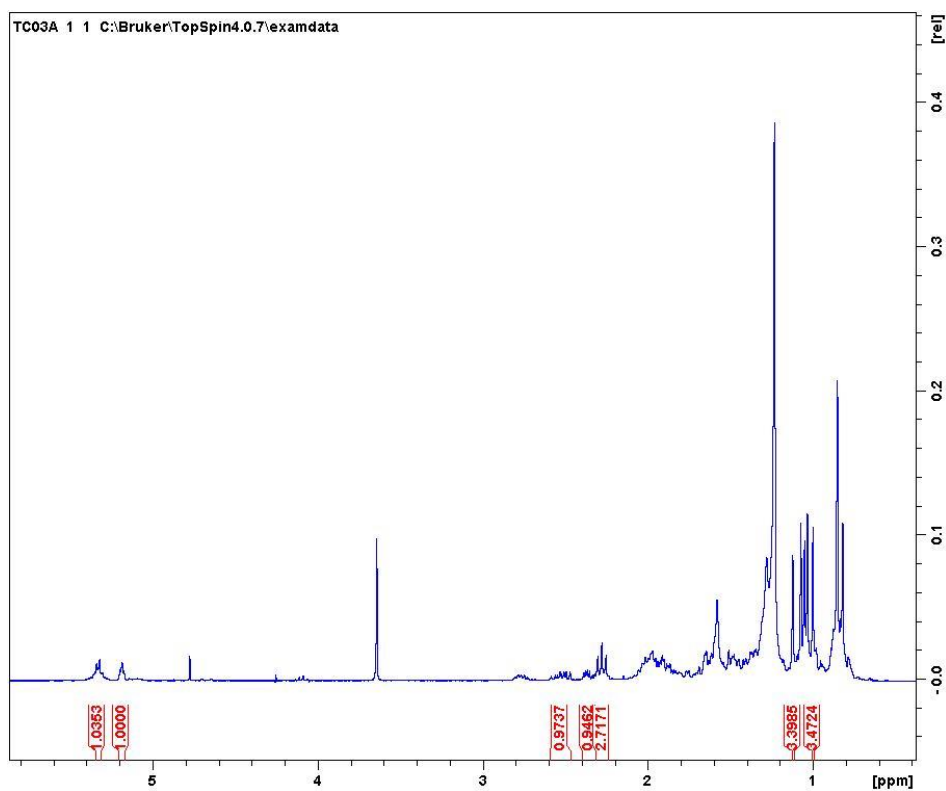


Figura 28S. Espectro RMN ^1H de olean-12-en-3-ona (**9**) (CDCl_3 , 300MHz)

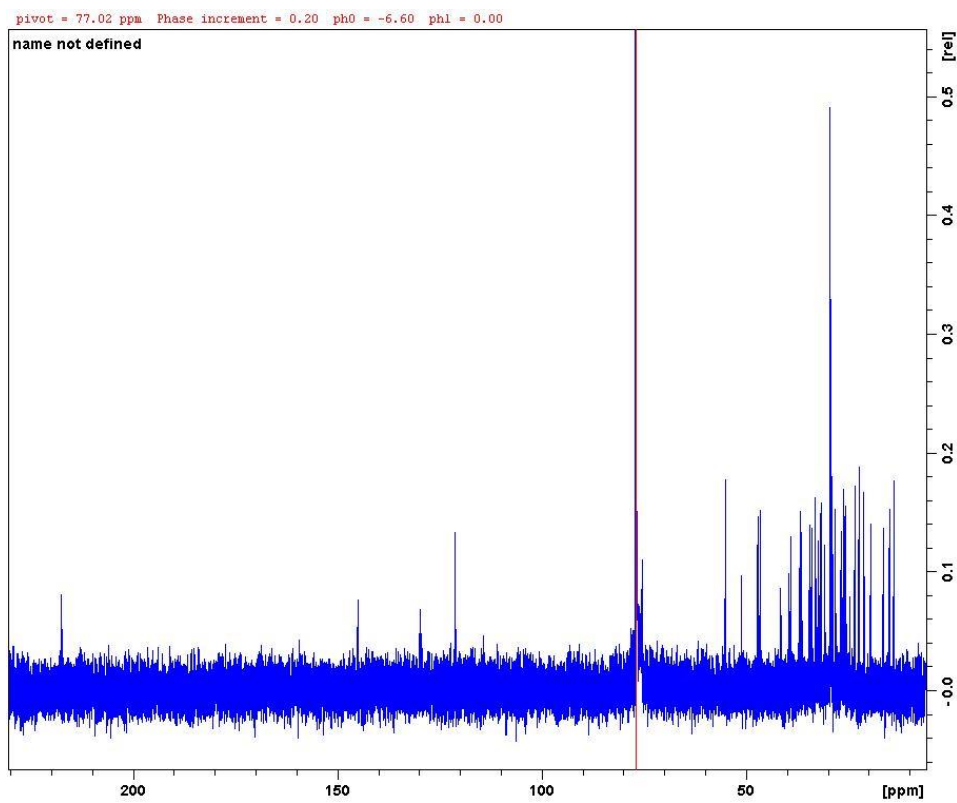


Figura 29S. Espectro RMN ^{13}C de olean-12-en-3-ona (**9**) (CDCl_3 , 75MHz)

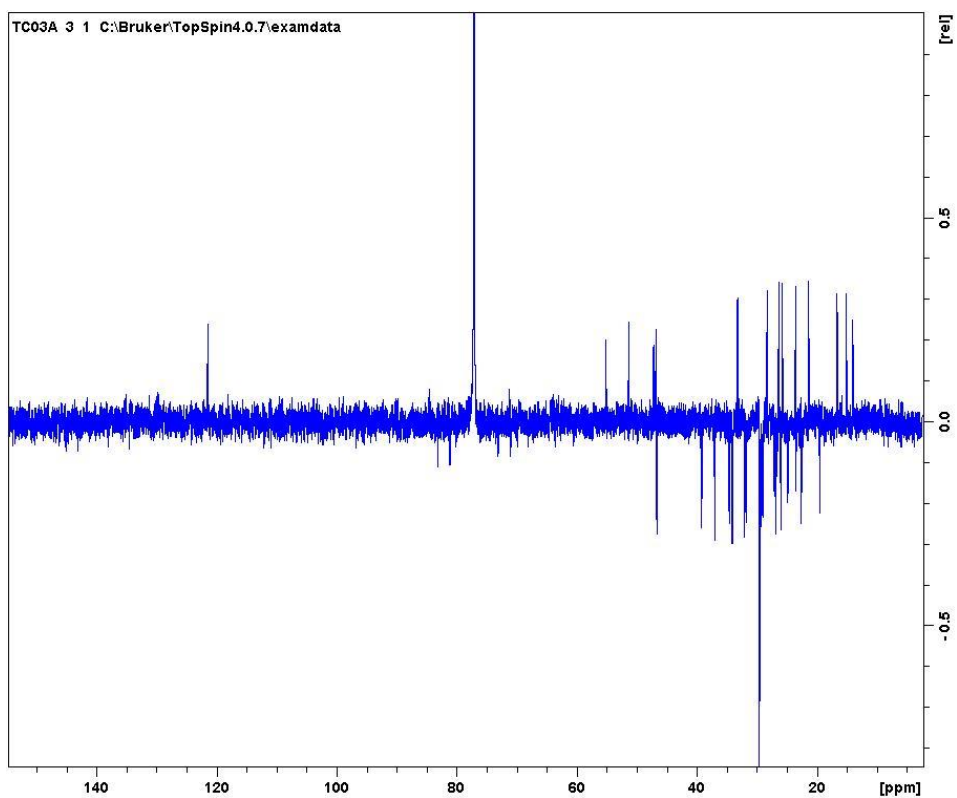


Figura 30S. Espectro RMN ^{13}C DEPT 135° de olean-12-en-3-ona (**9**) (CDCl_3 , 75MHz)

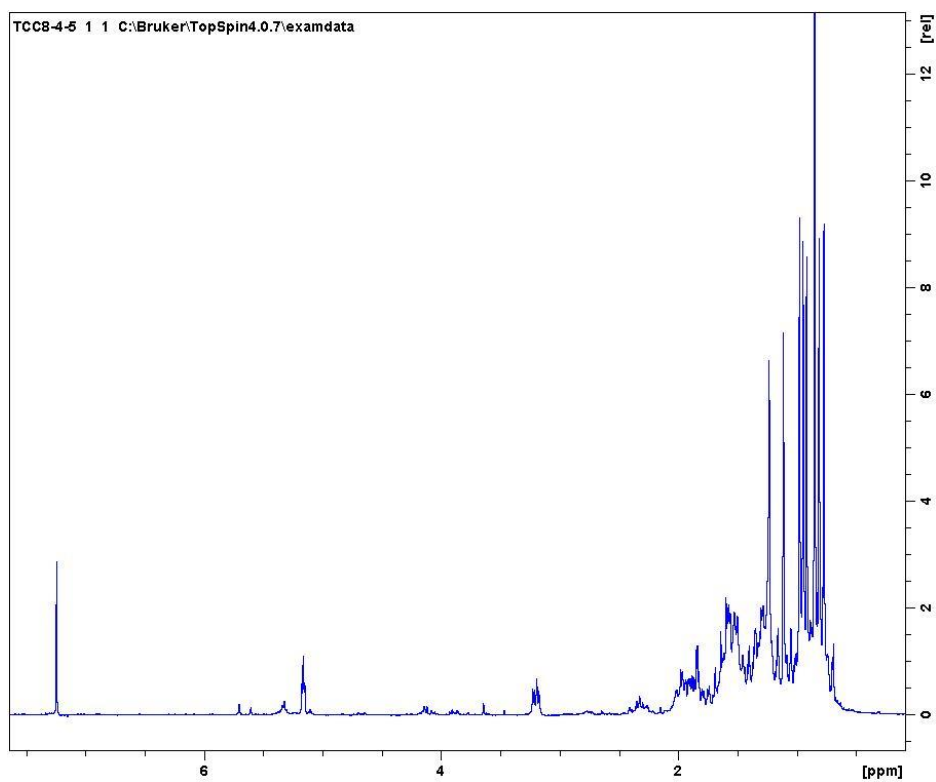


Figura 31S. Espectro RMN ^1H da β -amirina (**10**) (CDCl_3 , 300MHz)

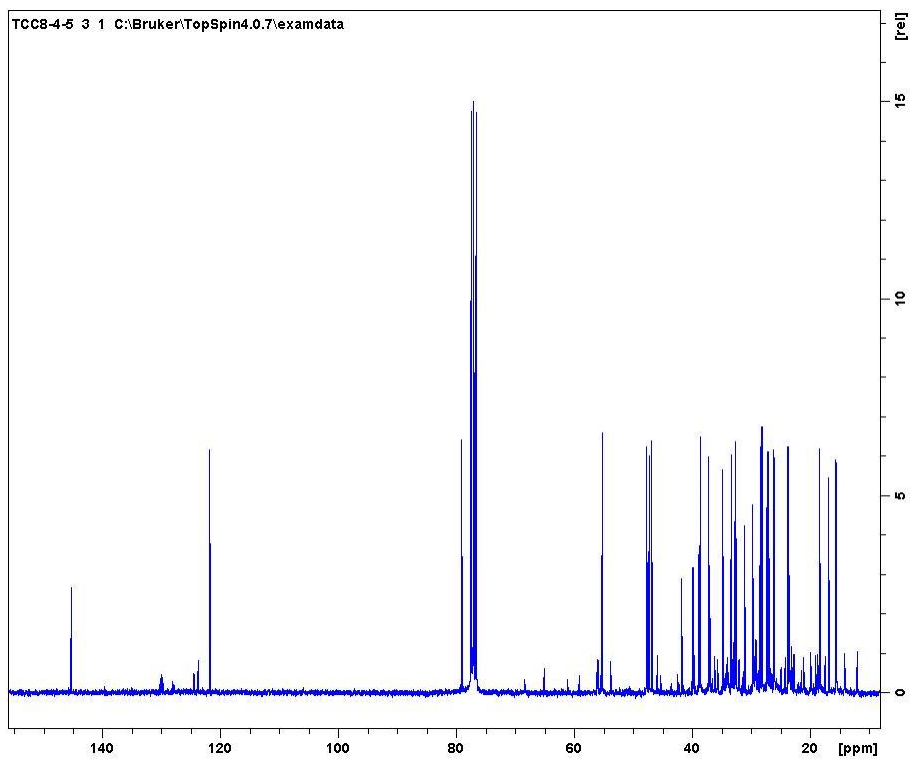


Figura 32S. Espectro RMN ^{13}C da β -amirina (**10**) (CDCl_3 , 75MHz)

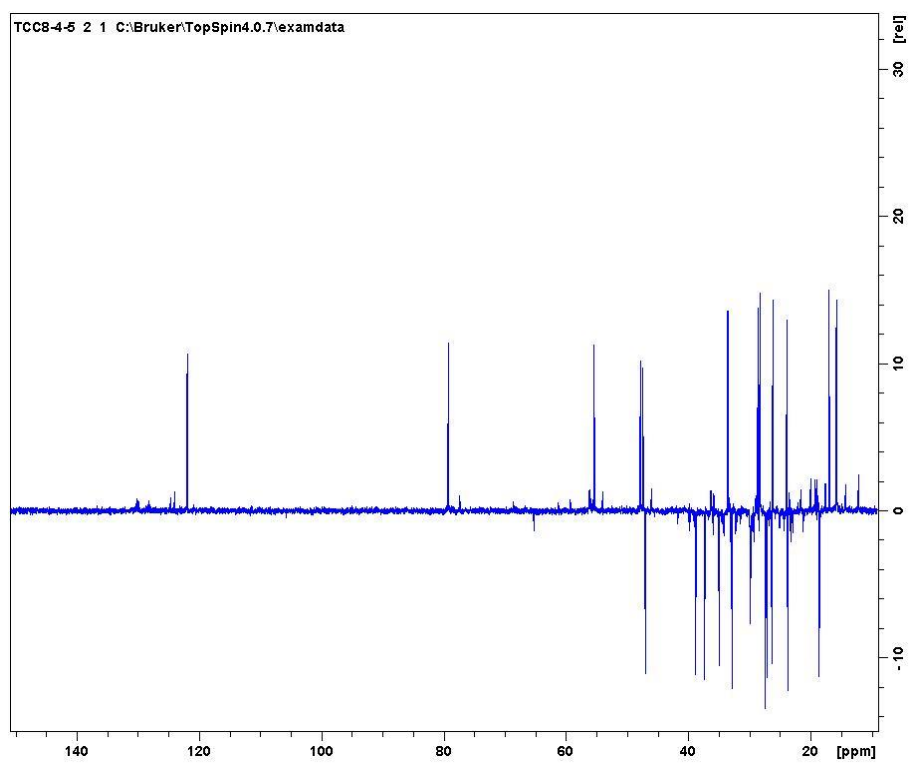


Figura 33S. Espectro RMN ^{13}C DEPT 135° da β -amirina (**10**) (CDCl_3 , 75MHz)

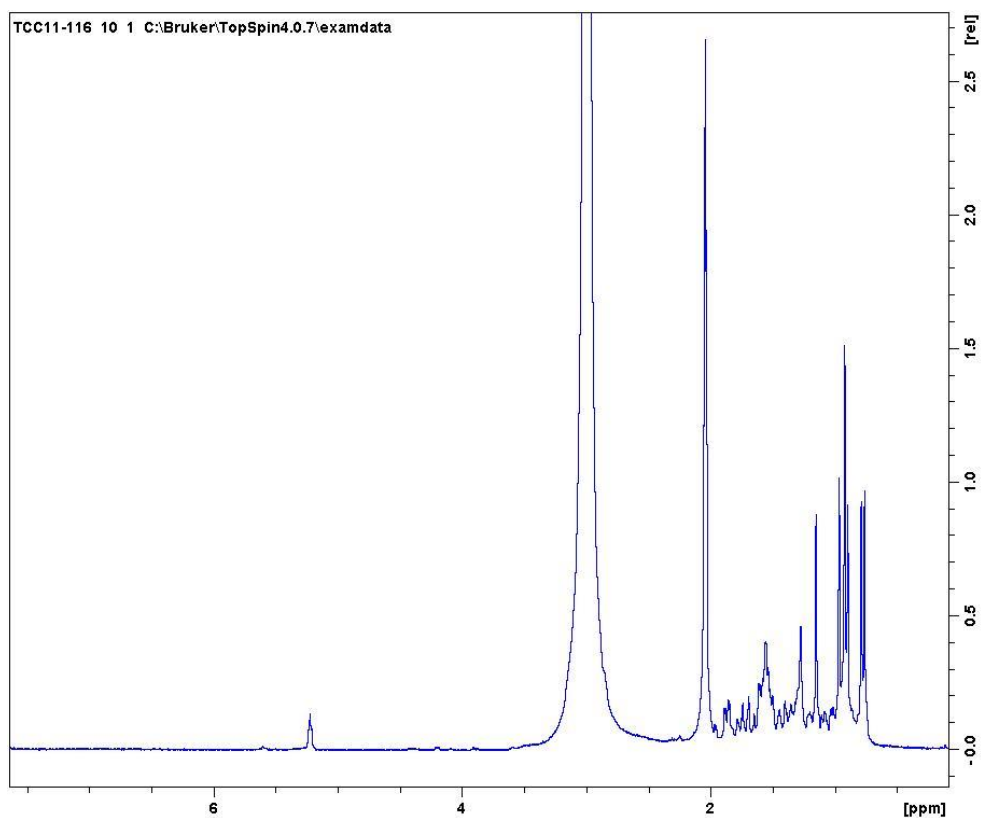


Figura 34S. Espectro RMN ^1H do ácido oleanólico (**11**) (Acetona- d_6 , 300 MHz)

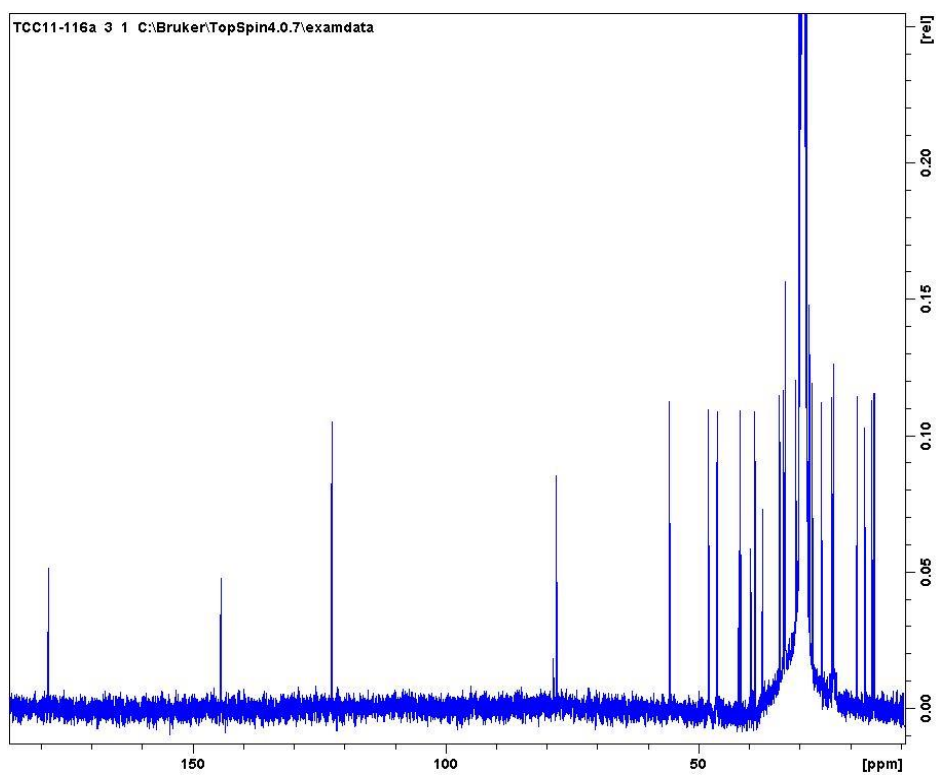


Figura 35S. Espectro RMN ^{13}C do ácido oleanólico (**11**) (Acetona- d_6 , 75 MHz)

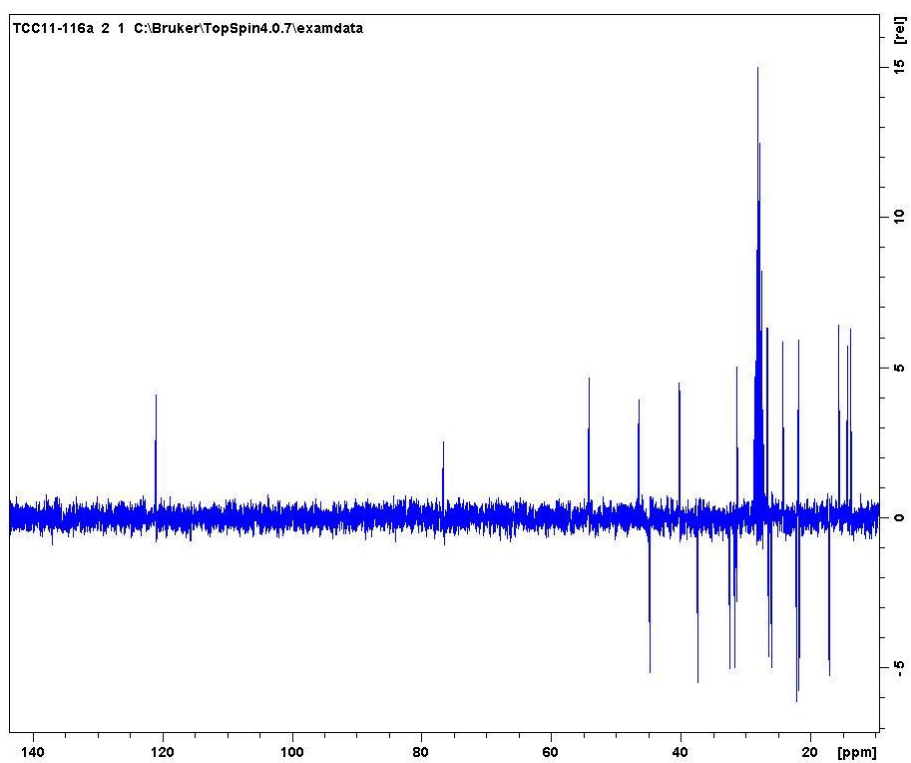


Figura 36S. Espectro RMN ^{13}C DEPT 135° do ácido oleanólico (**11**) (Acetona- d_6 , 75 MHz)

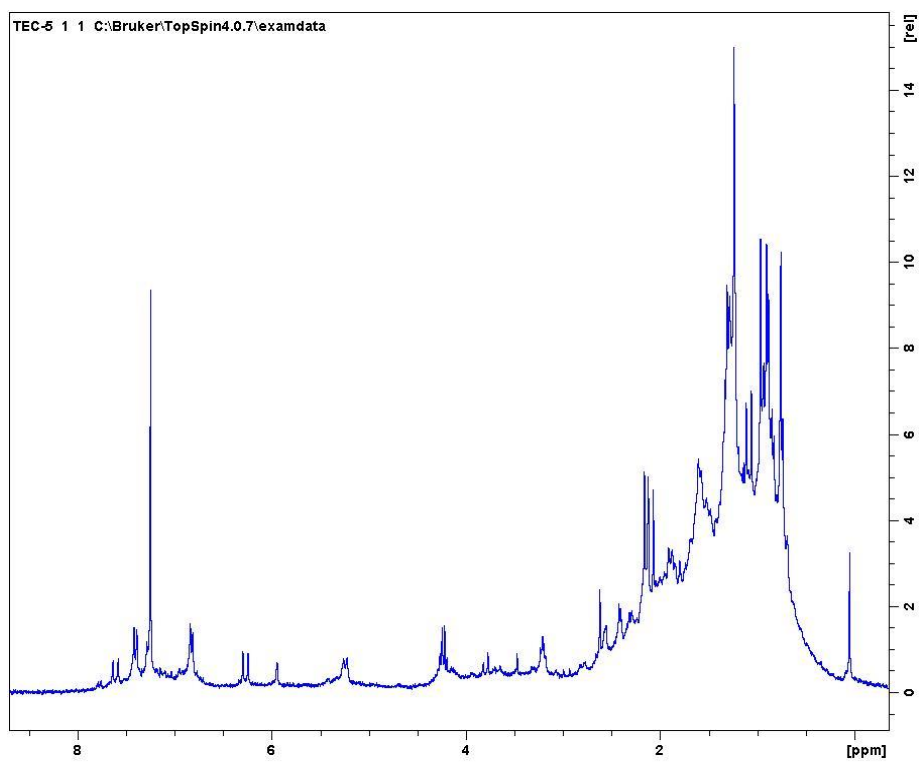


Figura 37S. Espectro RMN ^1H do ácido ursólico (**12**) (CDCl_3 , 300MHz)

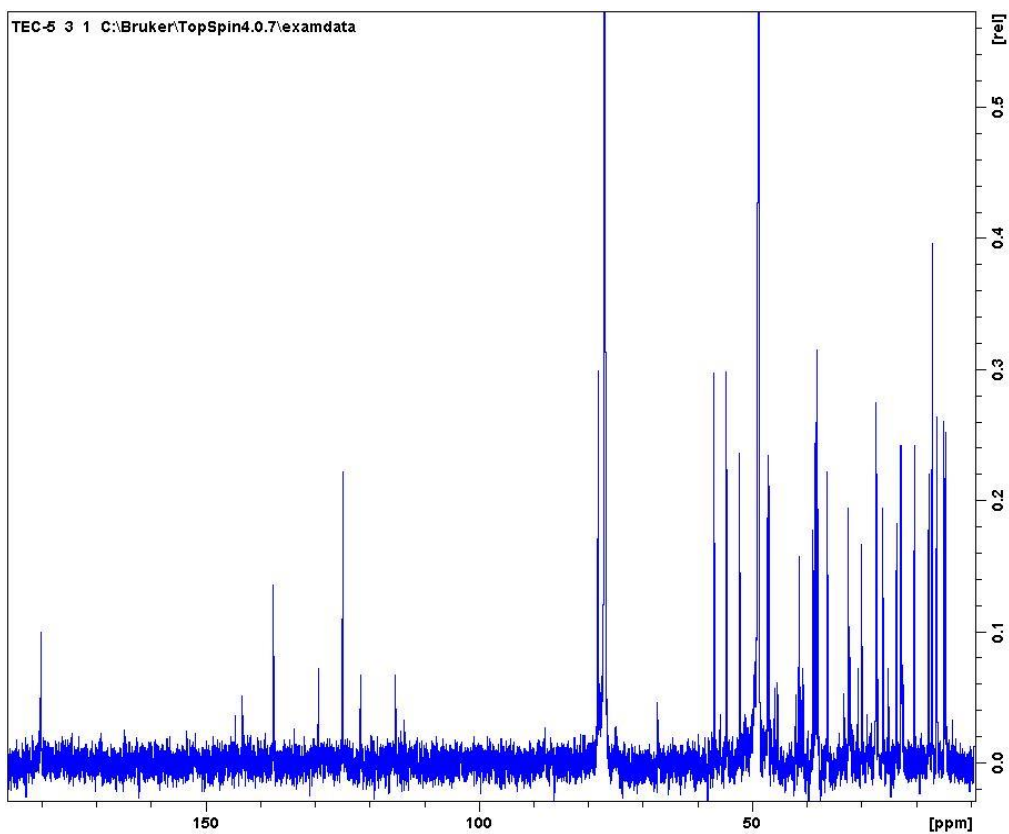


Figura 38S. Espectro RMN ^{13}C do ácido ursólico (12) (CDCl_3 , 75MHz)

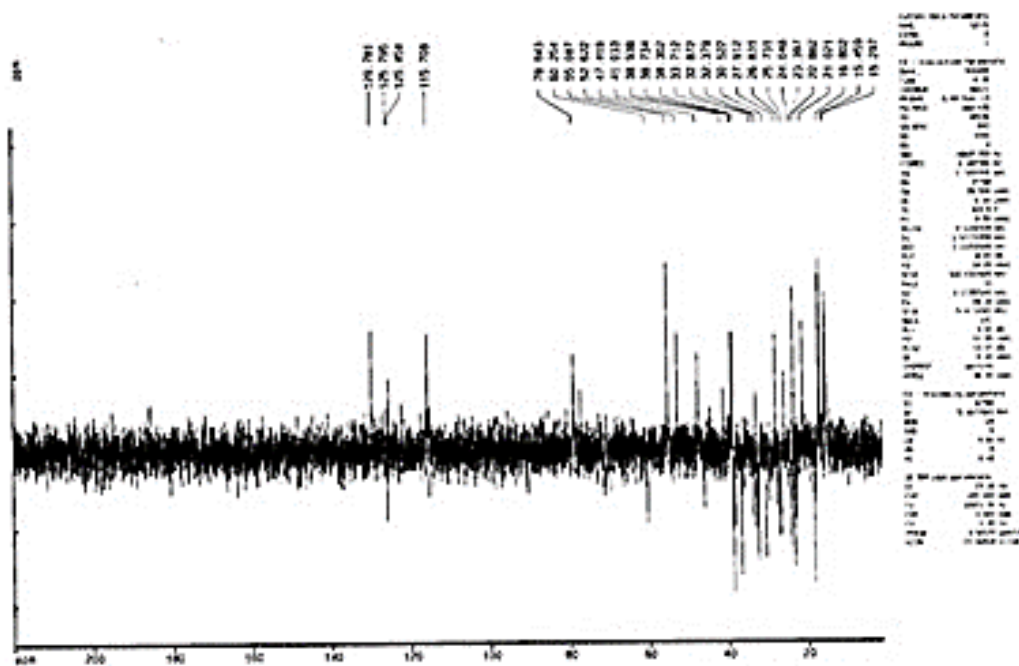


Figura 39S. Espectro RMN ^{13}C DEPT 135° do ácido ursólico (12) (CDCl_3 , 75MHz)

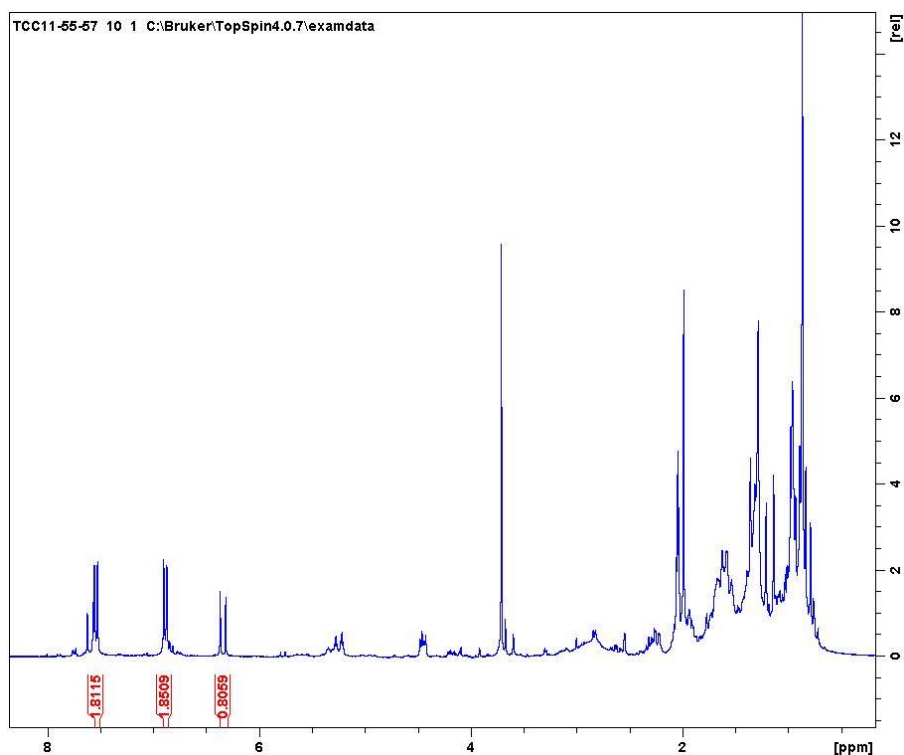


Figura 40S. Espectro RMN ^1H do ácido 3-O-E-p-cumaroil-ursólico (**13**) (Acetona- d_6 , 300 MHz)

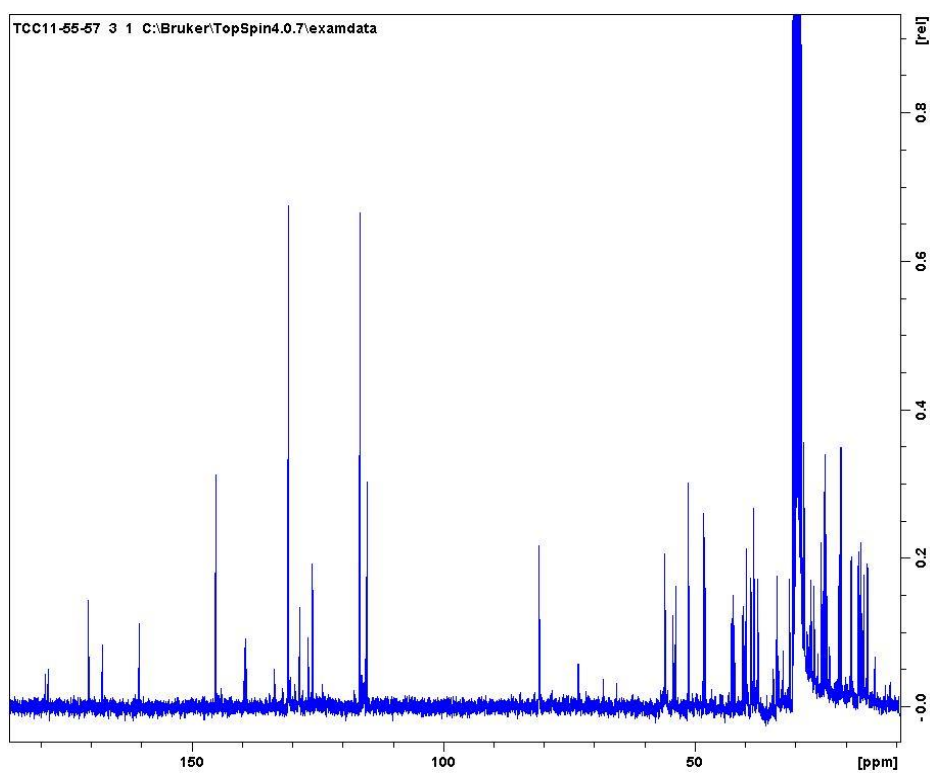


Figura 41S. Espectro RMN ^{13}C do ácido 3-O-E-p-cumaroil-ursólico (**13**) (Acetona- d_6 , 75 MHz)

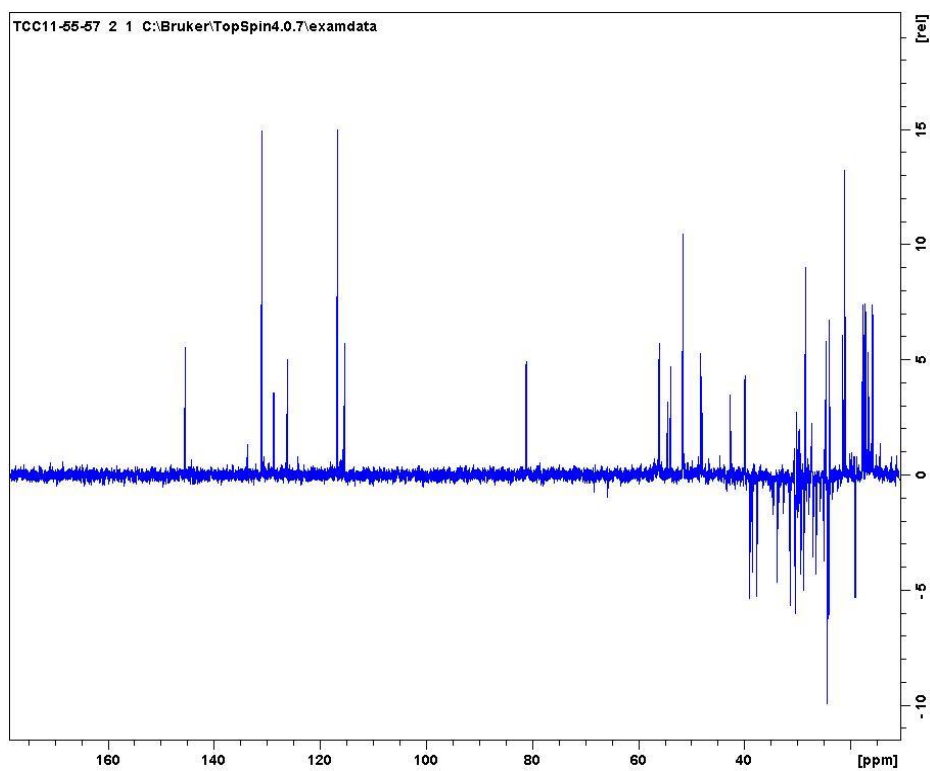


Figura 42S. Espectro RMN ^{13}C DEPT 135° do ácido 3-O-E-p-cumaroil-ursólico (**13**) (Acetona- d_6 , 75 MHz)

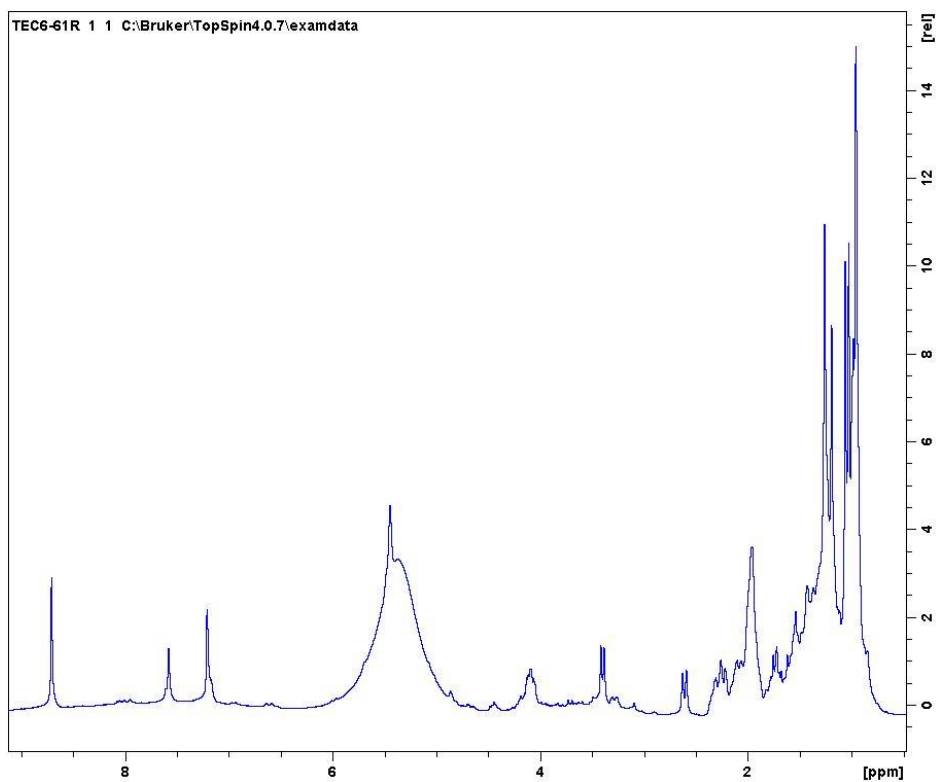


Figura 43S. Espectro RMN ^1H do ácido 2 α -hidroxiursólico (**14**) (Pyr d_5 , 300 MHz)

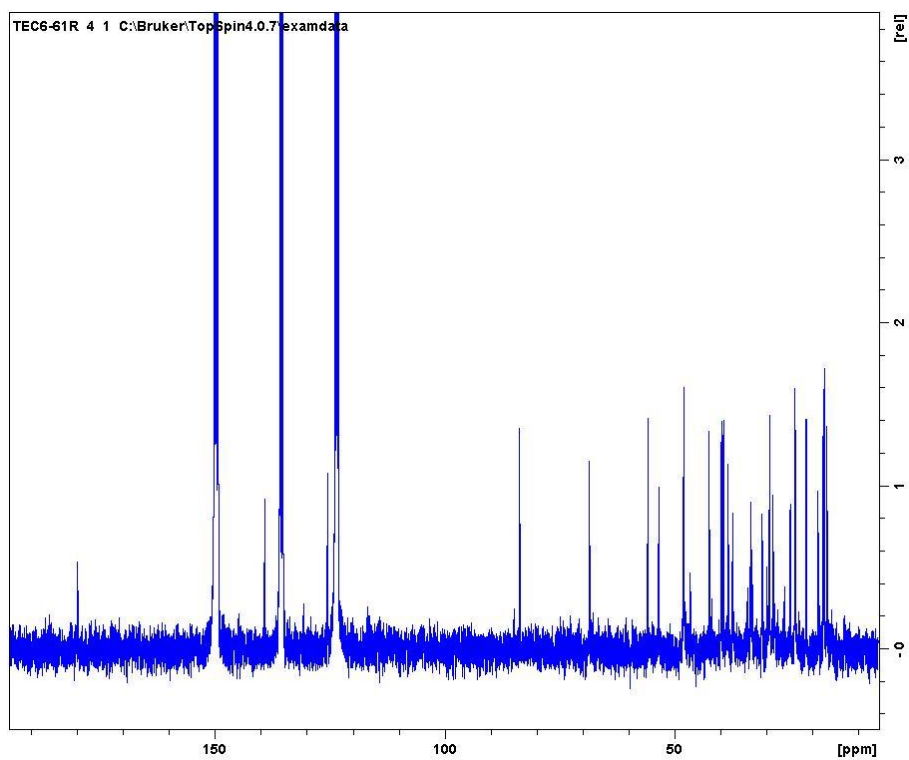


Figura 44S. Espectro RMN ^{13}C do ácido 2 α -hidroxiursólico (**14**) (Pyr d_5 , 75 MHz)

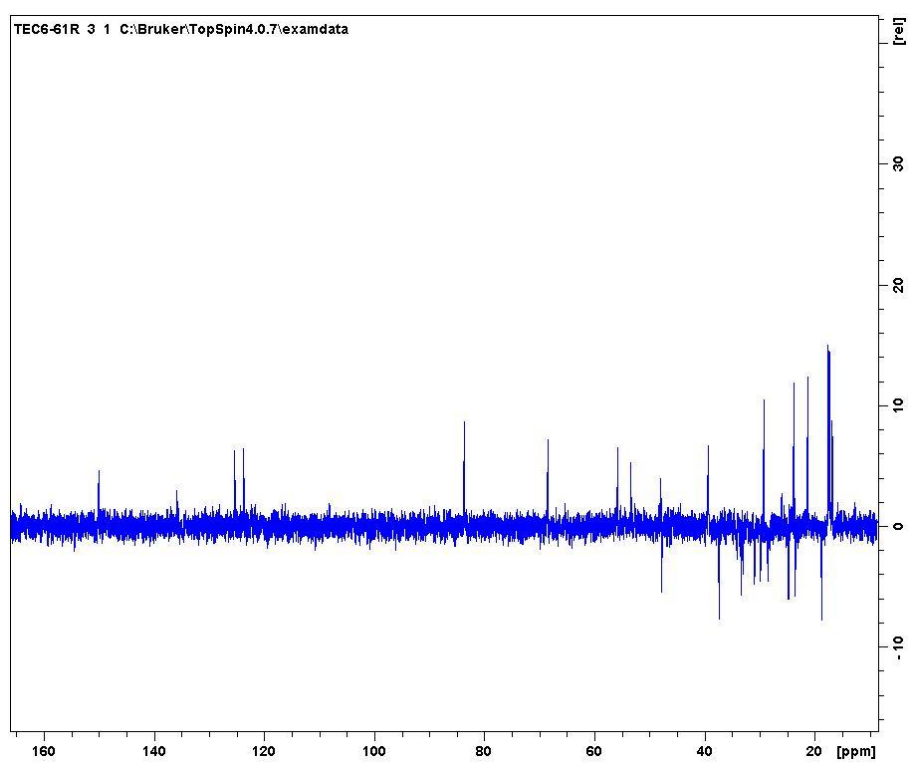


Figura 45S. Espectro RMN ^{13}C DEPT 135° do ácido 2 α -hidroxiursólico (**14**) (Pyr d_5 , 75 MHz)

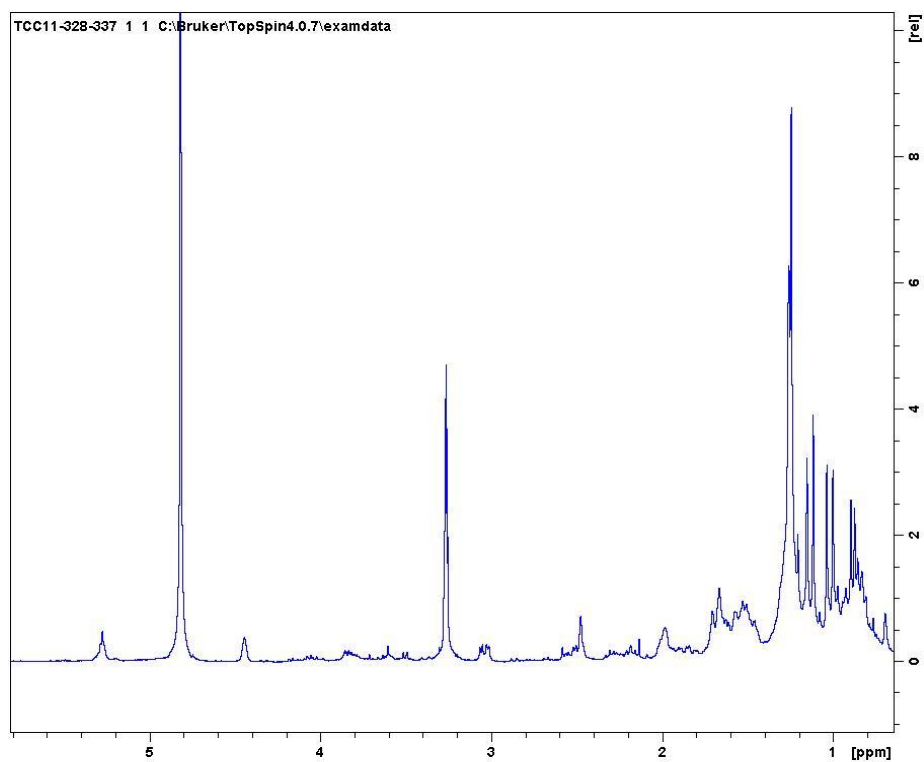


Figura 46S. Espectro RMN ^1H do ácido $6\beta,19\alpha$ -di-hidroxiursólico (**15**) (CD_3OD , 300 MHz)

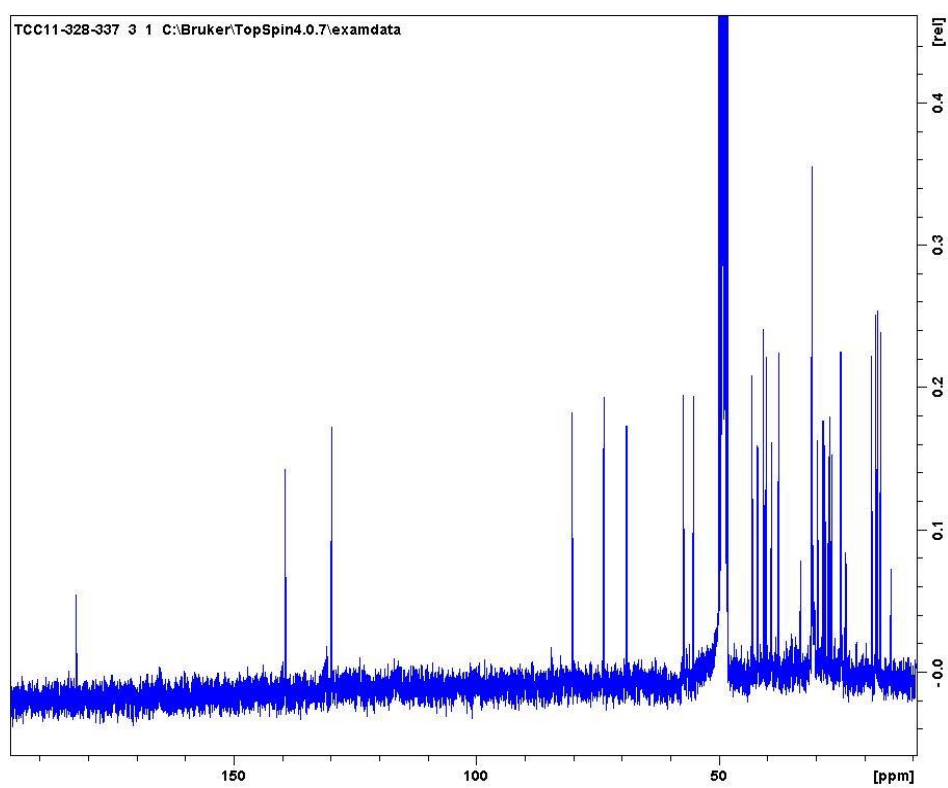


Figura 47S. Espectro RMN ^{13}C do ácido $6\beta,19\alpha$ -di-hidroxiursólico (**15**) (CD_3OD , 75 MHz)

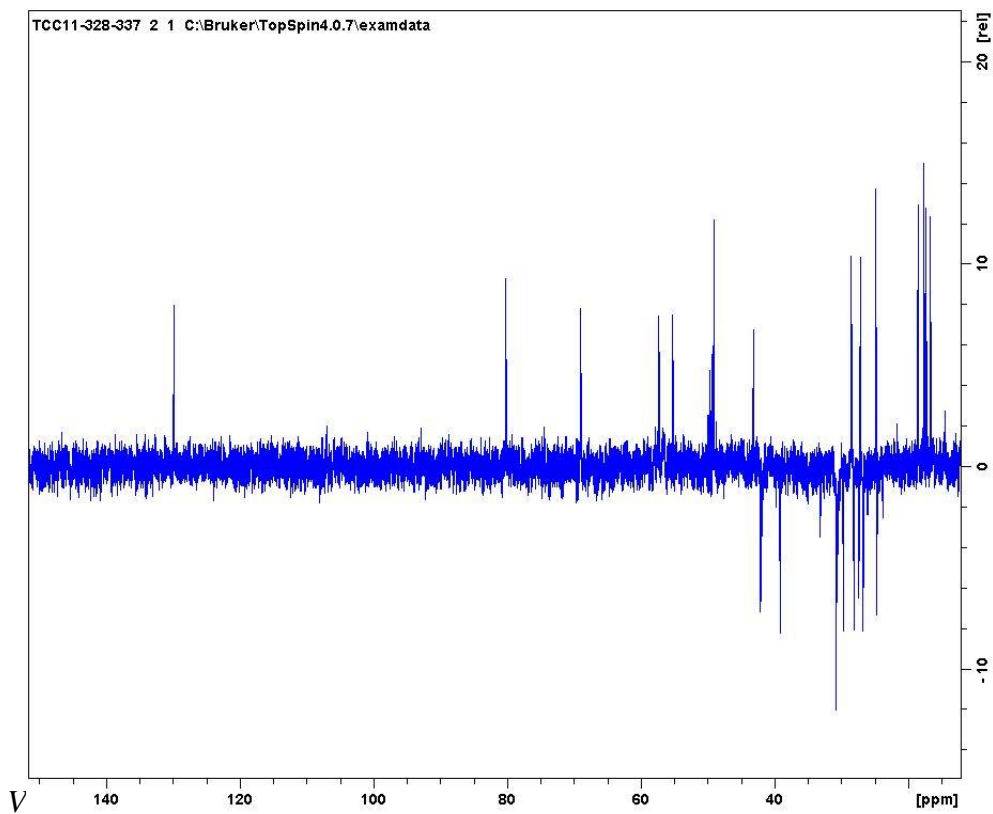


Figura 48S. Espectro RMN ^{13}C DEPT 135° do ácido $6\beta,19\alpha$ -di-hidroxiursólico (**15**) (CD_3OD , 75 MHz)

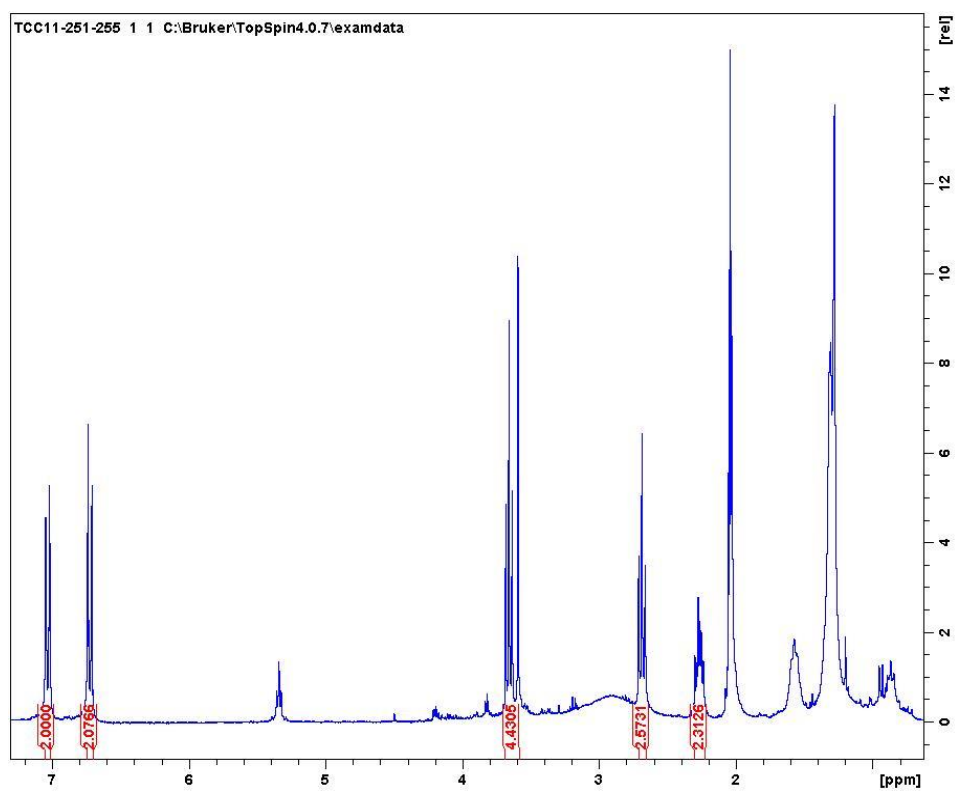


Figura 49S. Espectro RMN ^1H do tirosol (**16**) (Acetona-d_6 , 300 MHz)

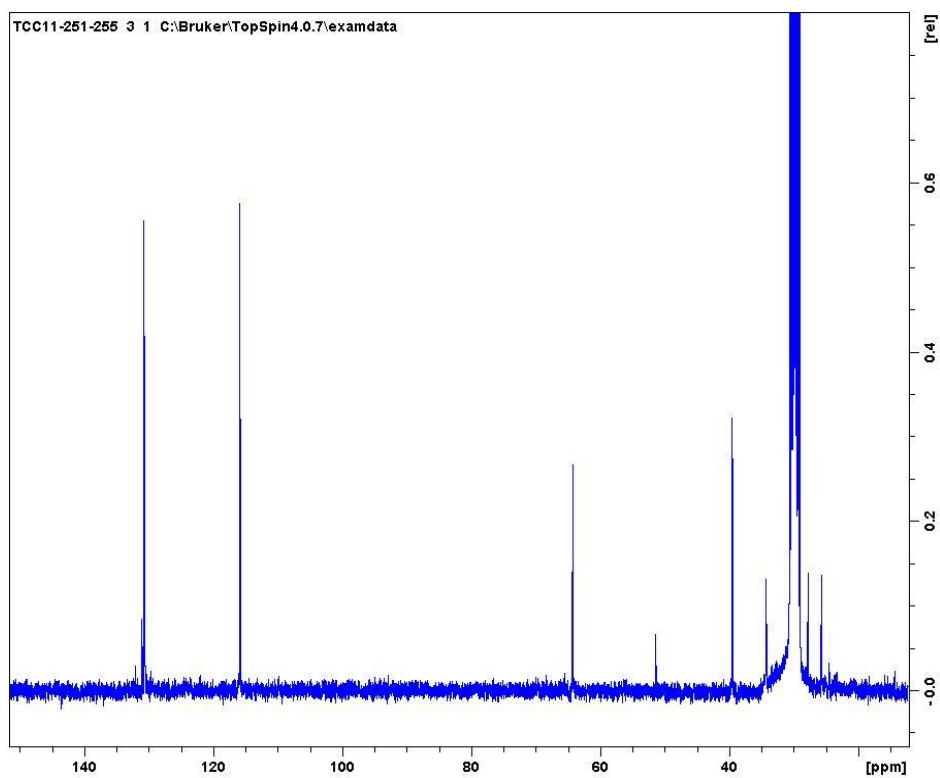


Figura 50S. Espectro RMN ^{13}C do tirosol (**16**) (Acetona- d_6 , 75 MHz)

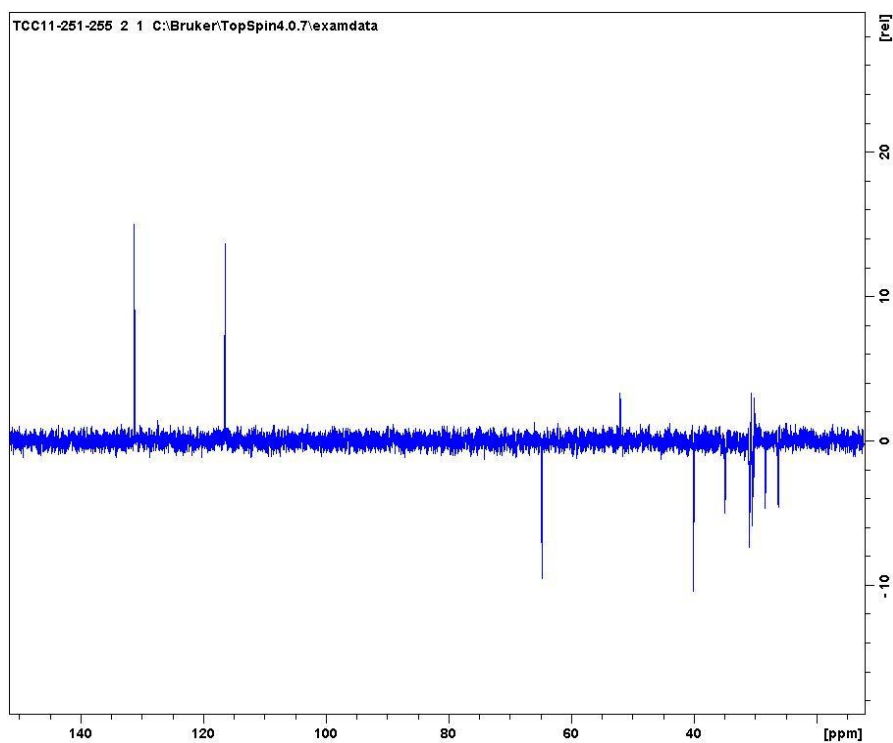


Figura 51S. Espectro RMN ^{13}C DEPT 135° do tirosol (**16**) (Acetona- d_6 , 75 MHz)