

Figura 50 – Espectro de infravermelho do composto **2g** (filme).

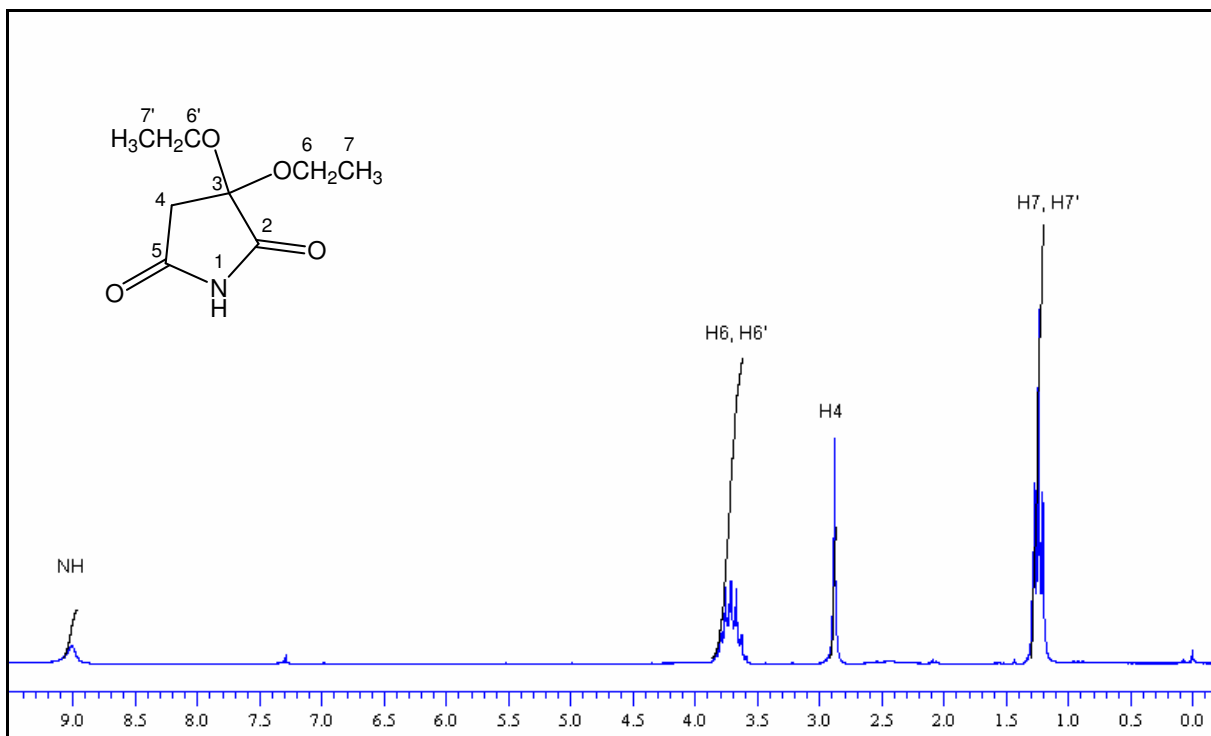


Figura 51 – Espectro de ¹H do composto 3 a 200 MHz em CDCl₃.

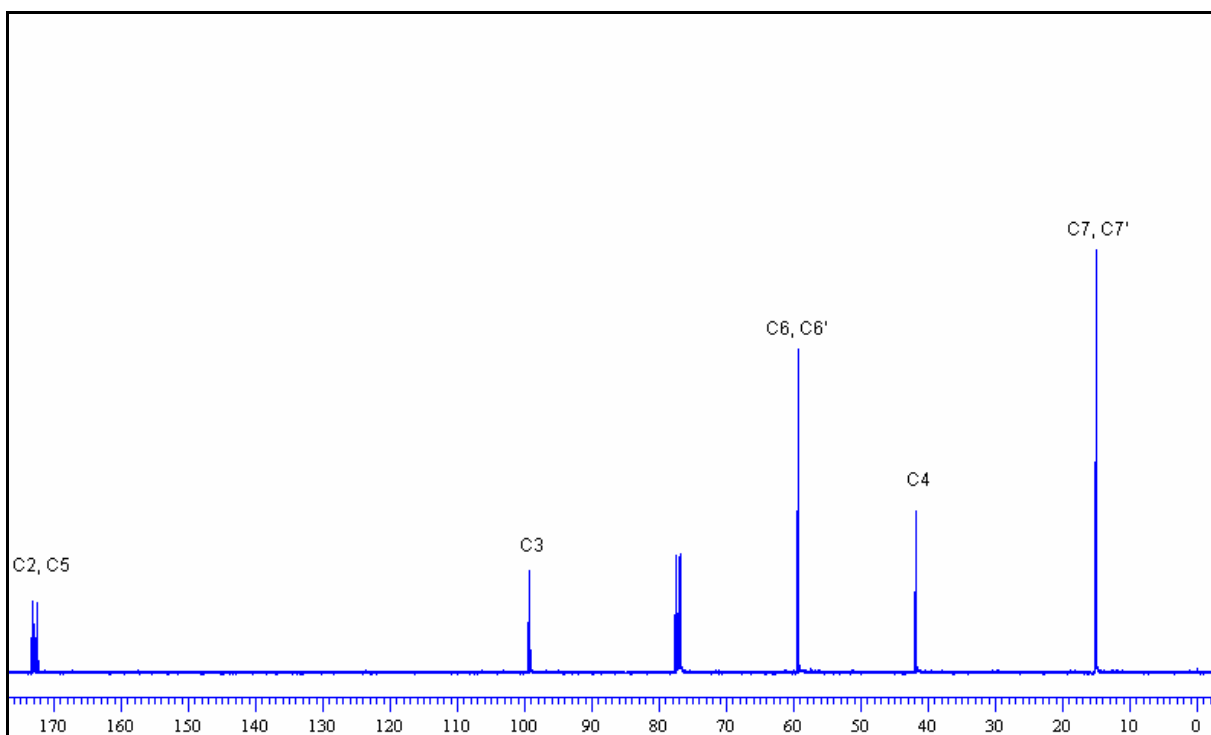


Figura 52 – Espectro de ¹³C do composto 3 a 100 MHz em CDCl₃.

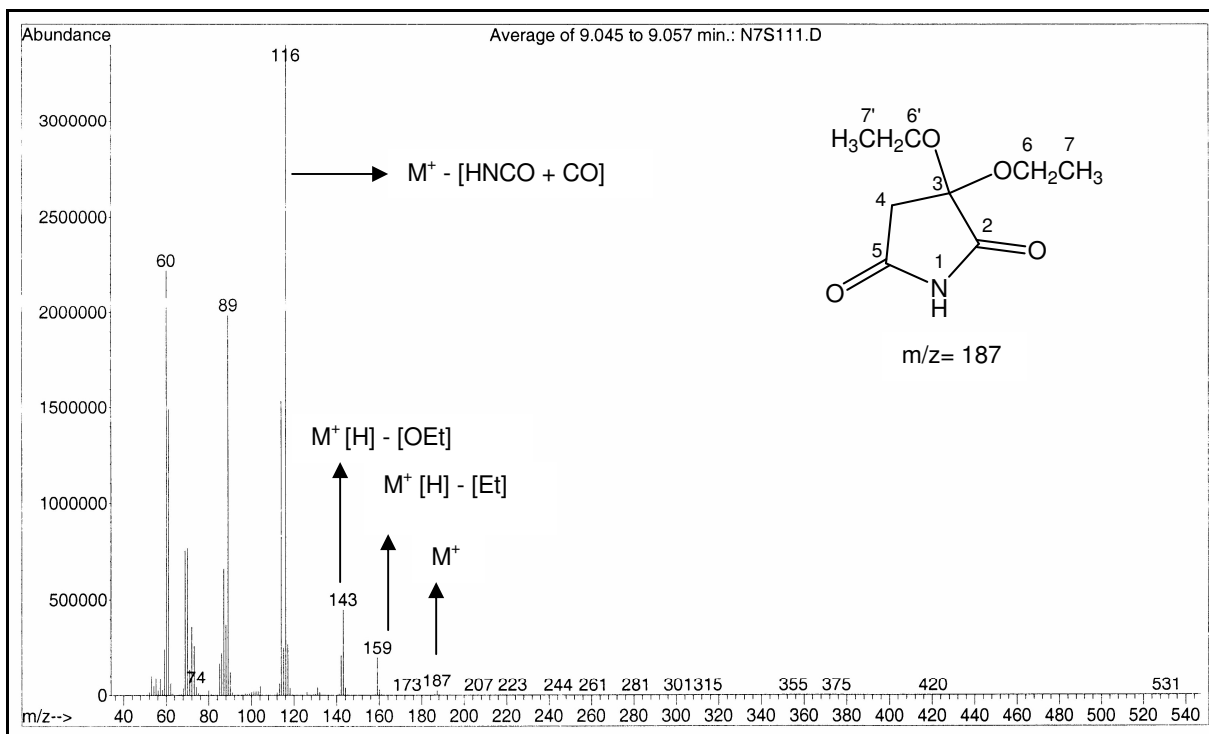


Figura 53 – Espectro de massas do composto 3.

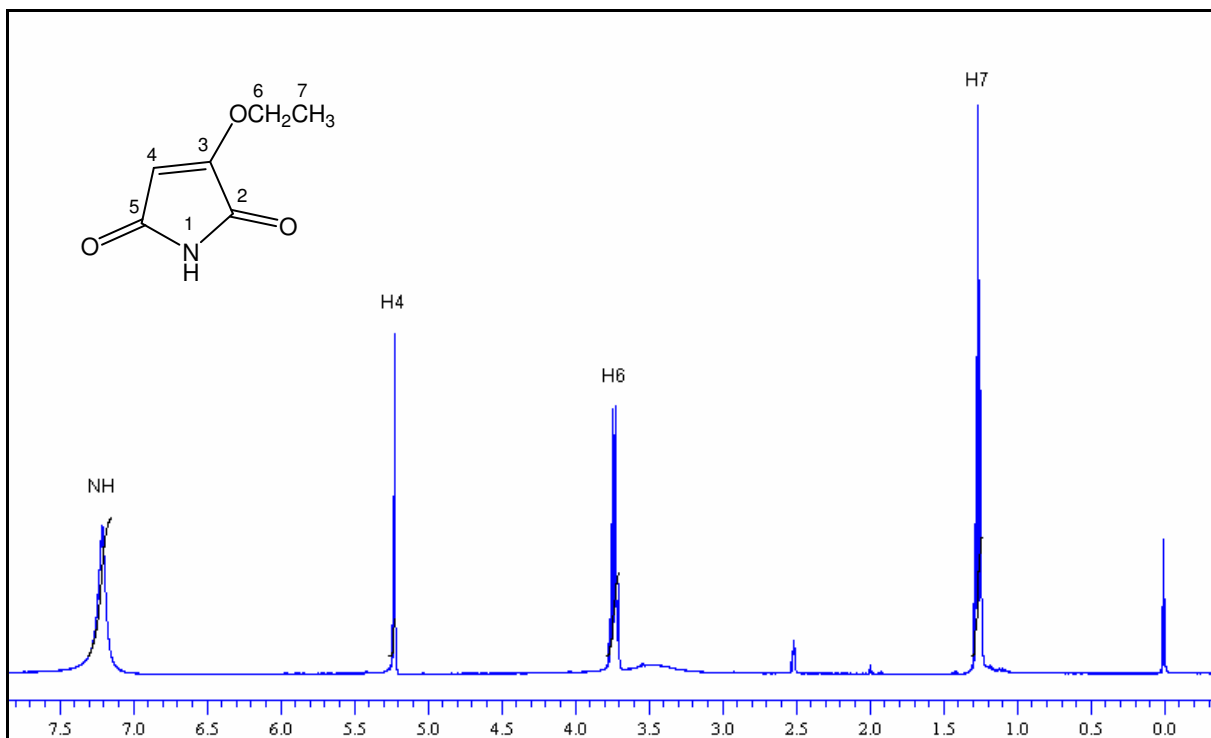


Figura 54 – Espectro de ^1H do composto 4 a 400 MHz em $\text{DMSO-}d_6$.

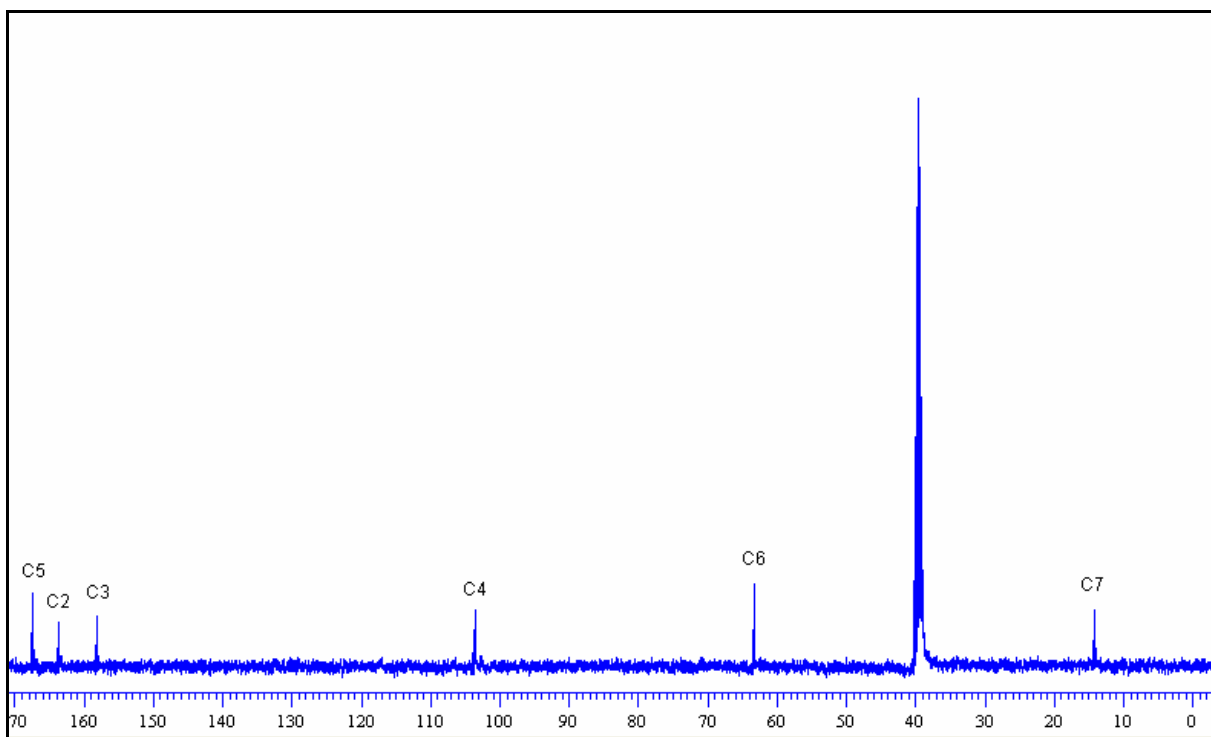


Figura 55 – Espectro de ^{13}C do composto 4 a 100 MHz em $\text{DMSO-}d_6$.

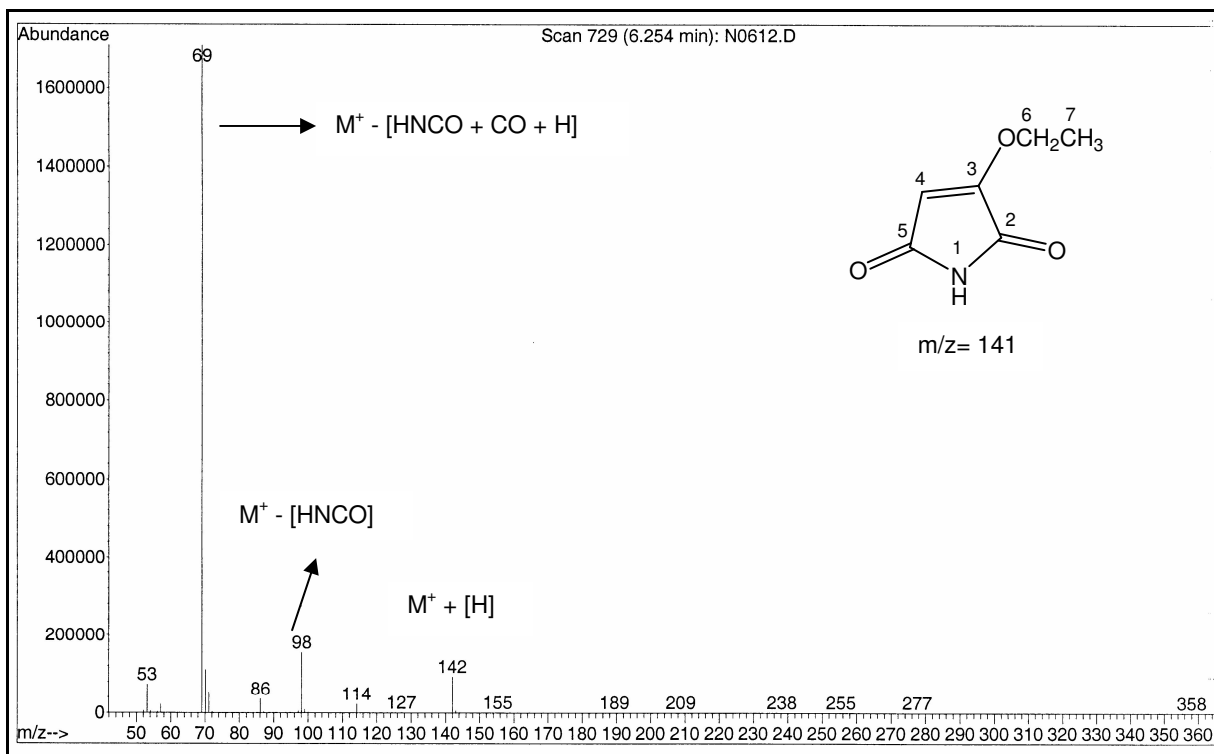


Figura 56 – Espectro de massas do composto 4.

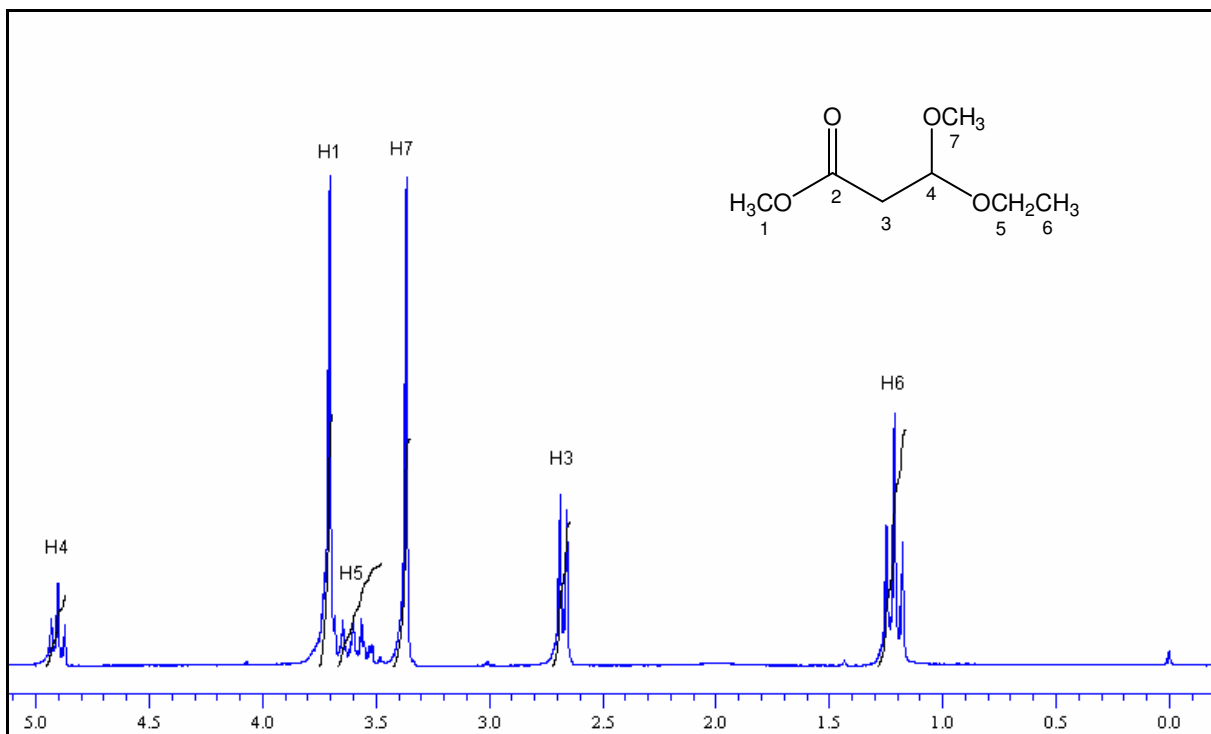


Figura 57 – Espectro de ^1H do composto **5** a 200 MHz em CDCl_3 .

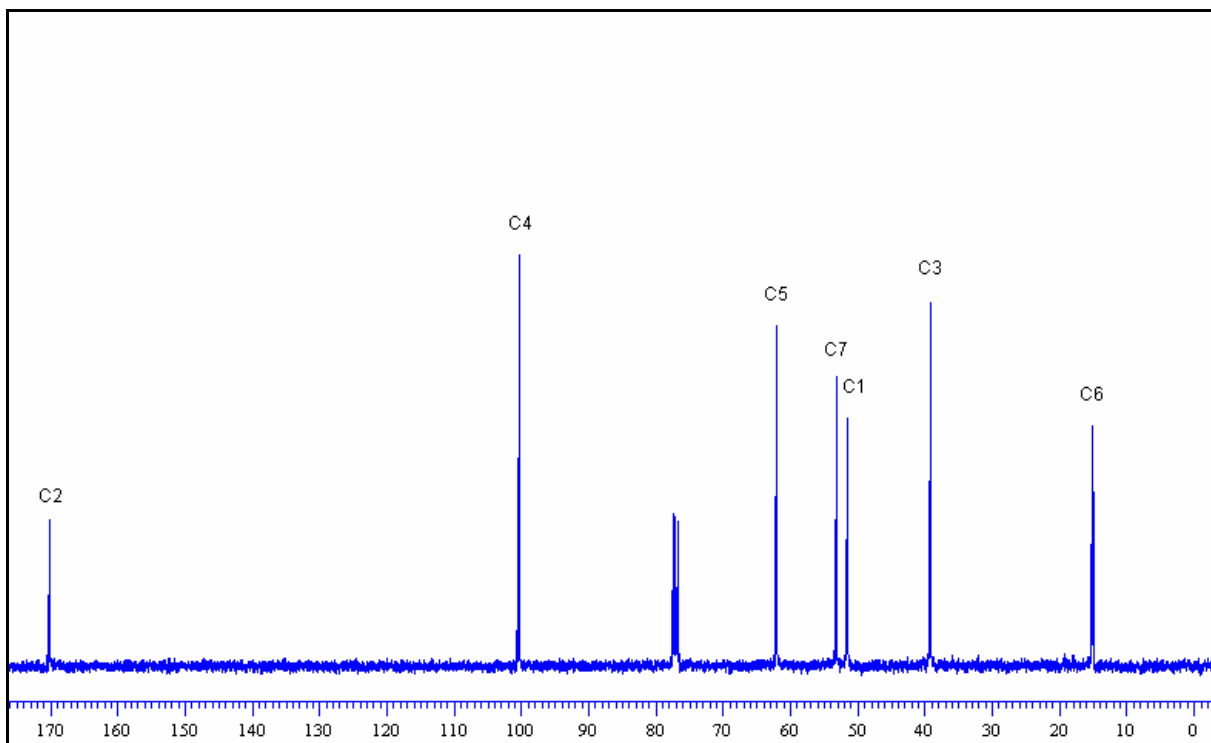


Figura 58 – Espectro de ^{13}C do composto **5** a 100 MHz em CDCl_3 .

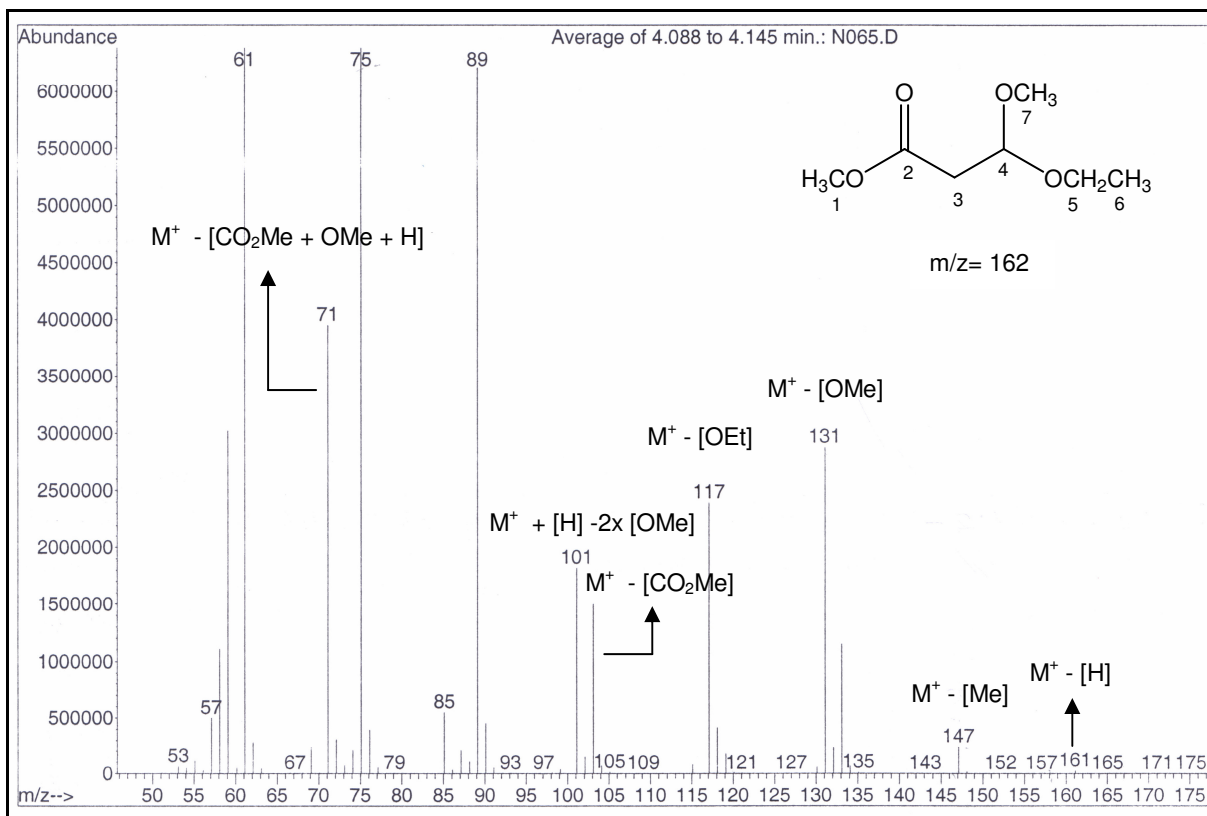


Figura 59 – Espectro de massas do composto 5.

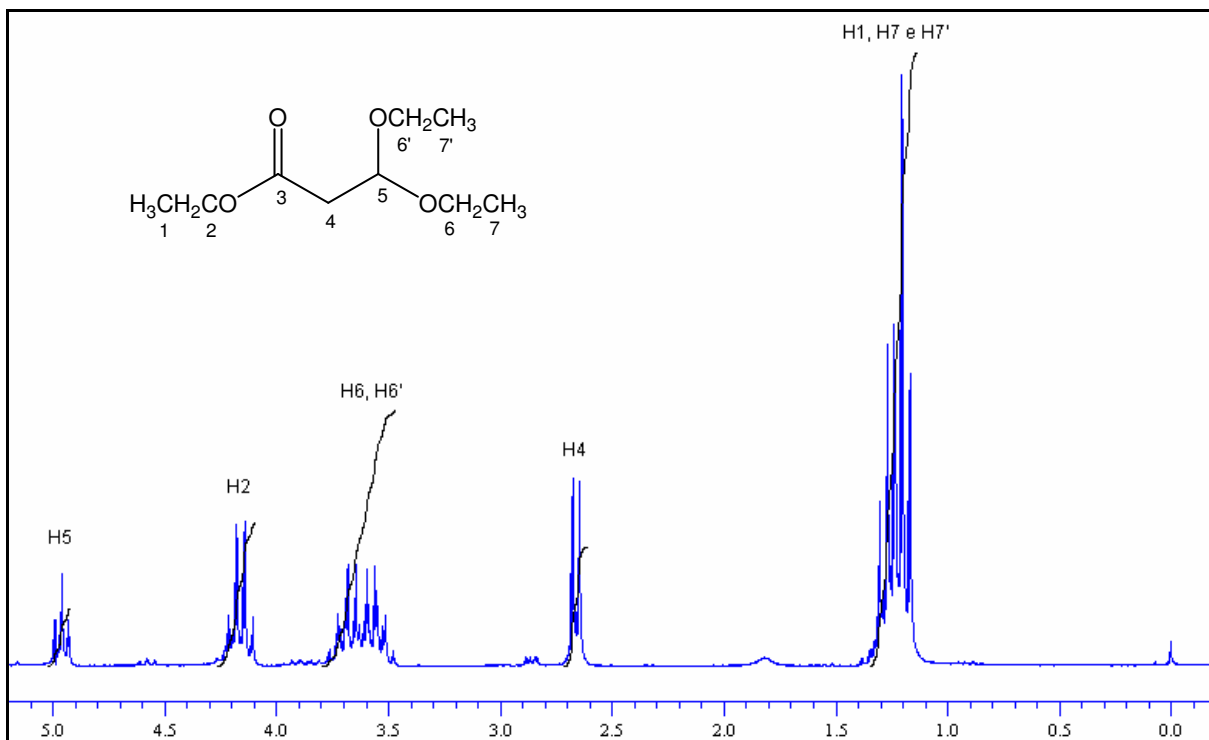


Figura 60 – Espectro de ¹H do composto 6 a 200 MHz em CDCl₃.

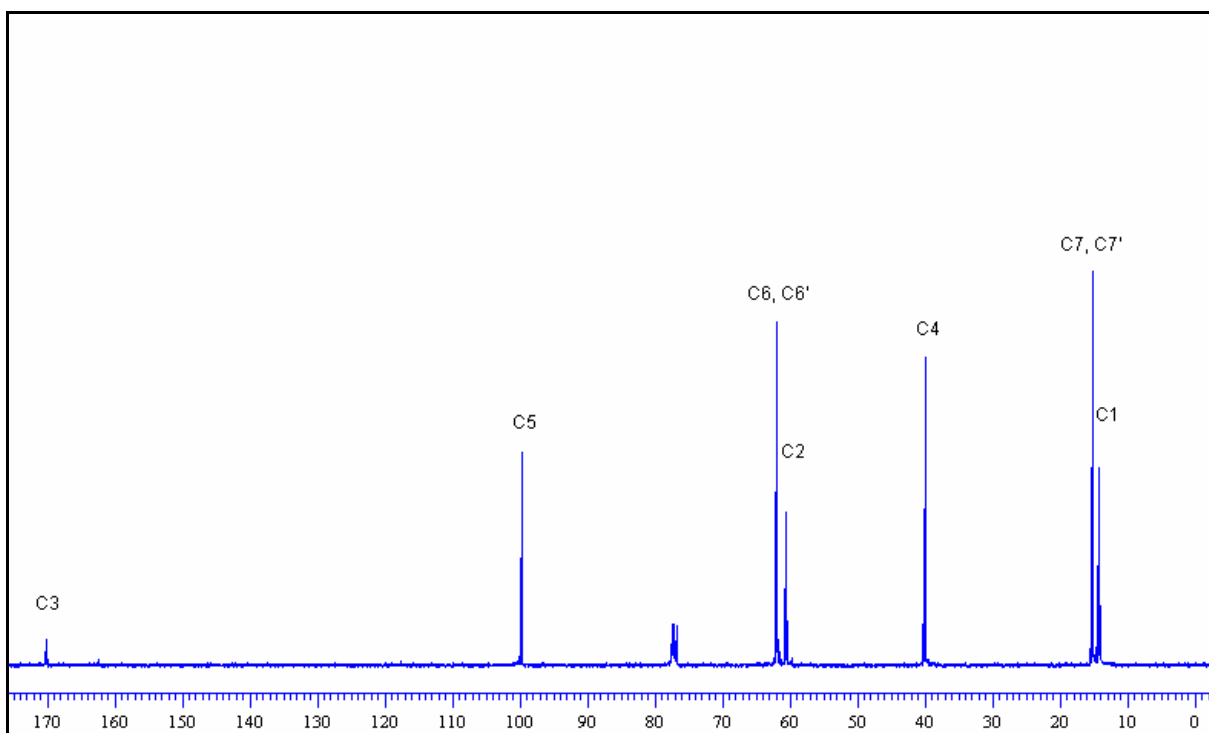


Figura 61 – Espectro de ¹³C do composto 6 a 100 MHz em CDCl₃.

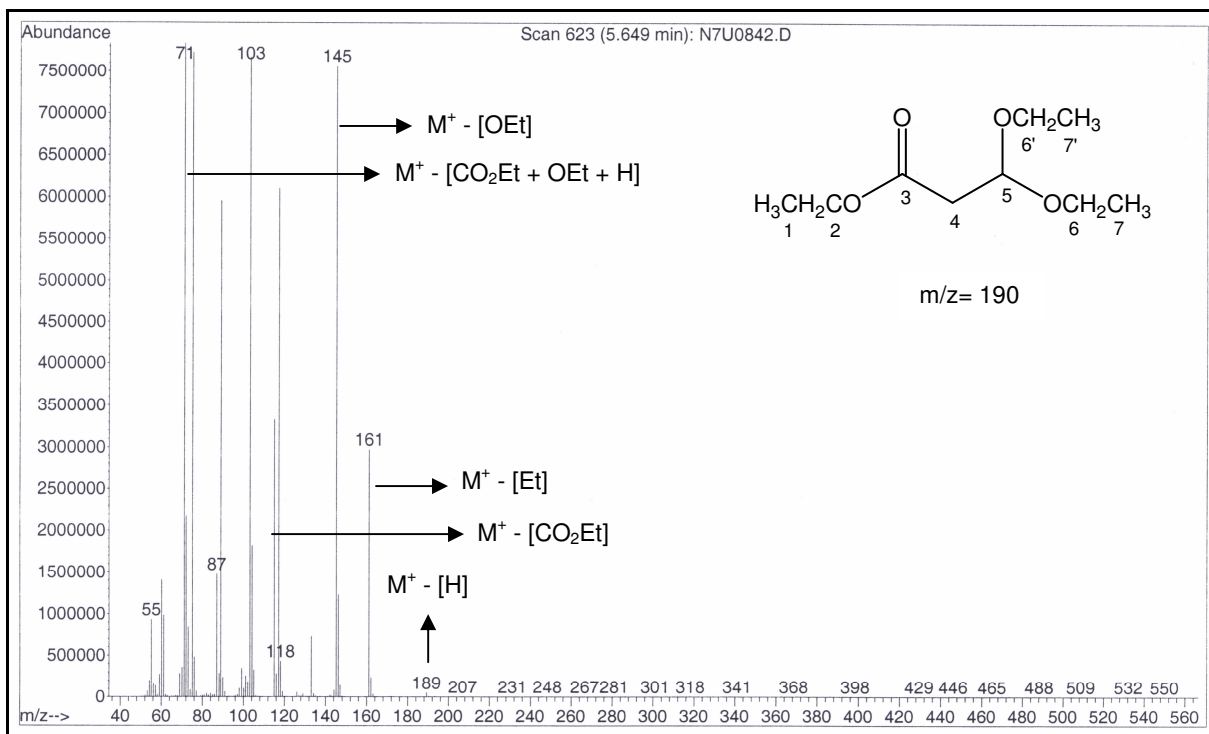


Figura 62 – Espectro de massas do composto 6.

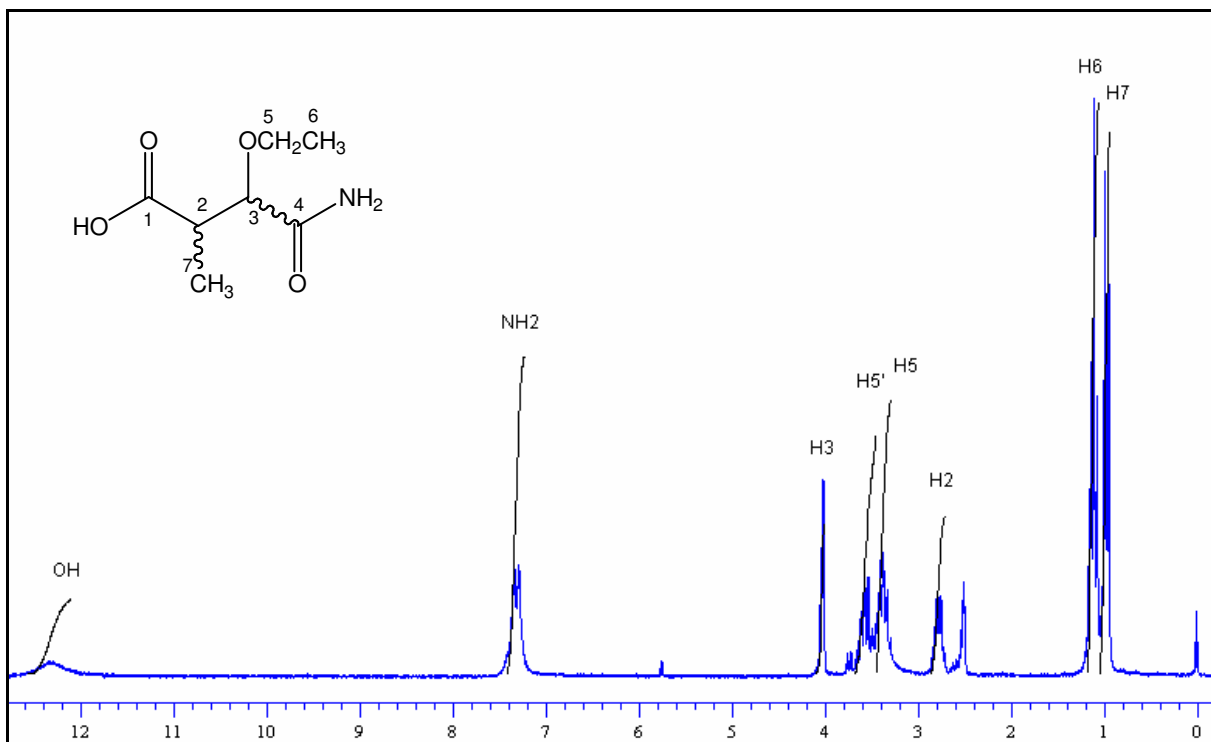


Figura 63 – Espectro de ^1H do composto **7b** a 200 MHz em $\text{DMSO-}d_6$.

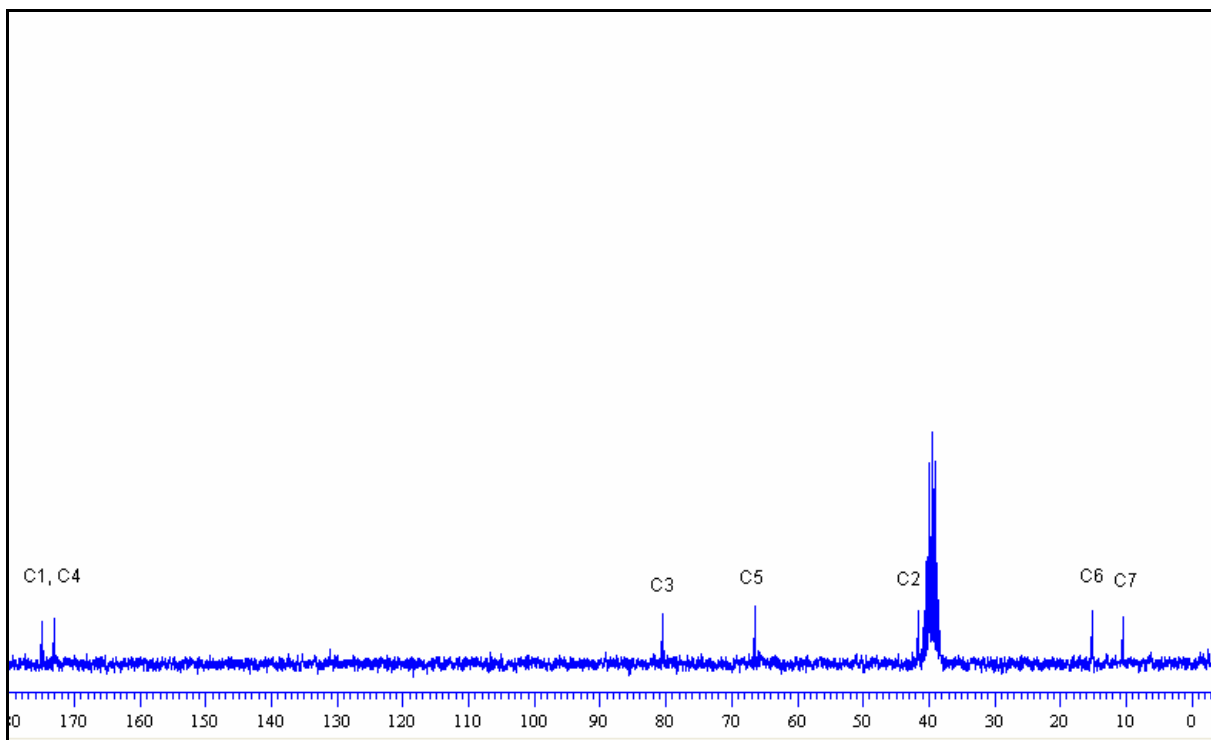


Figura 64 – Espectro de ^{13}C do composto **7b** a 50 MHz em $\text{DMSO-}d_6$.

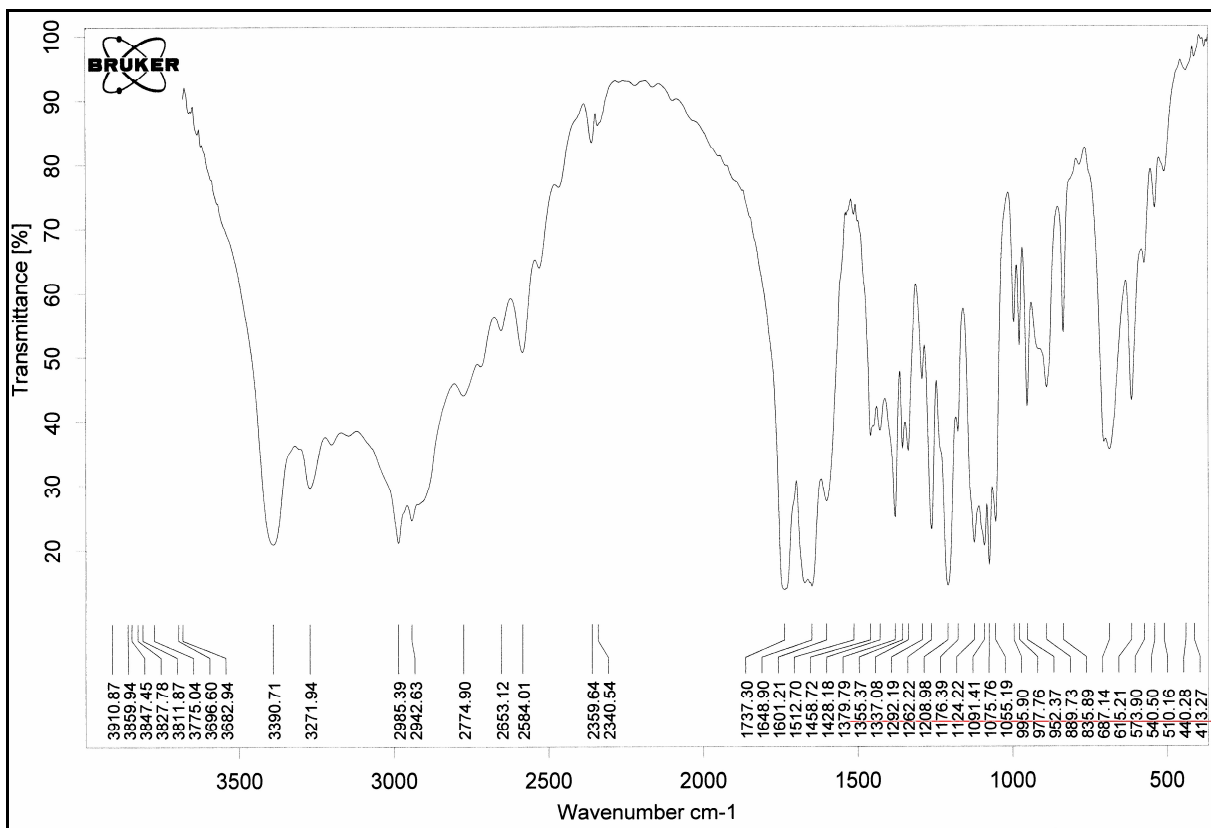


Figura 65 – Espectro de infravermelho do composto **7b** (pastilha de KBr).

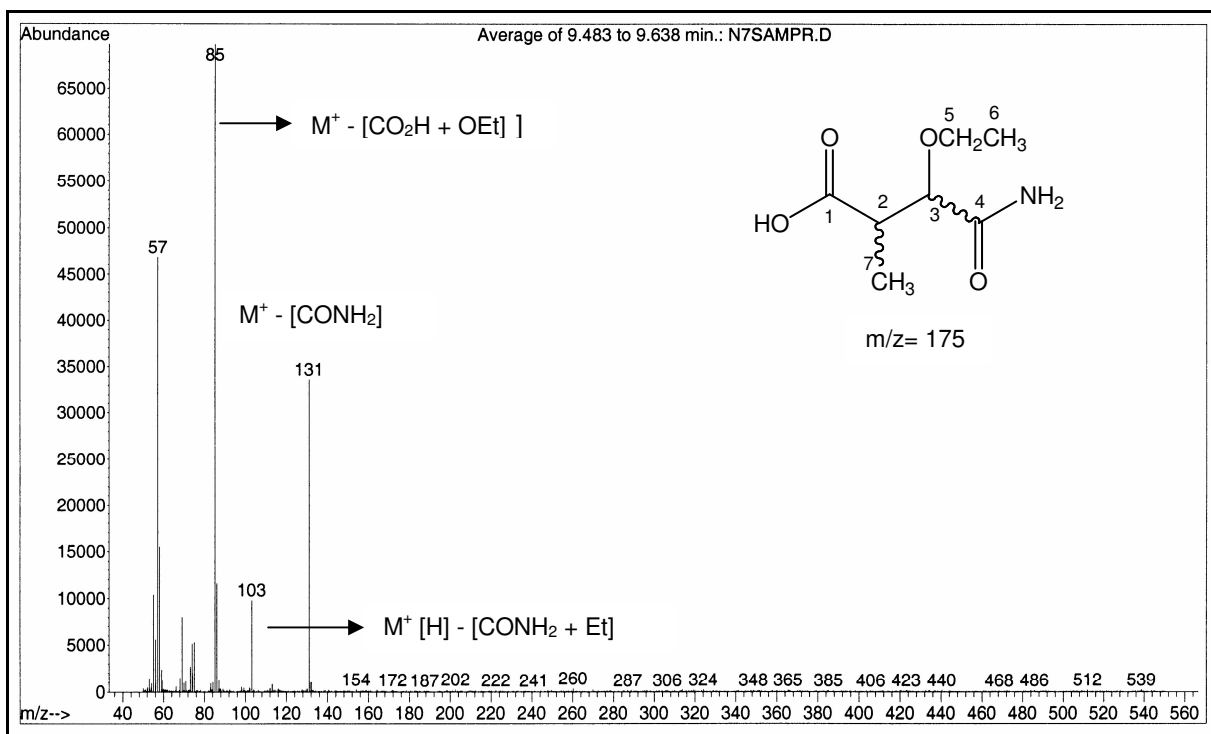


Figura 66 – Espectro de massas do composto **7b**.

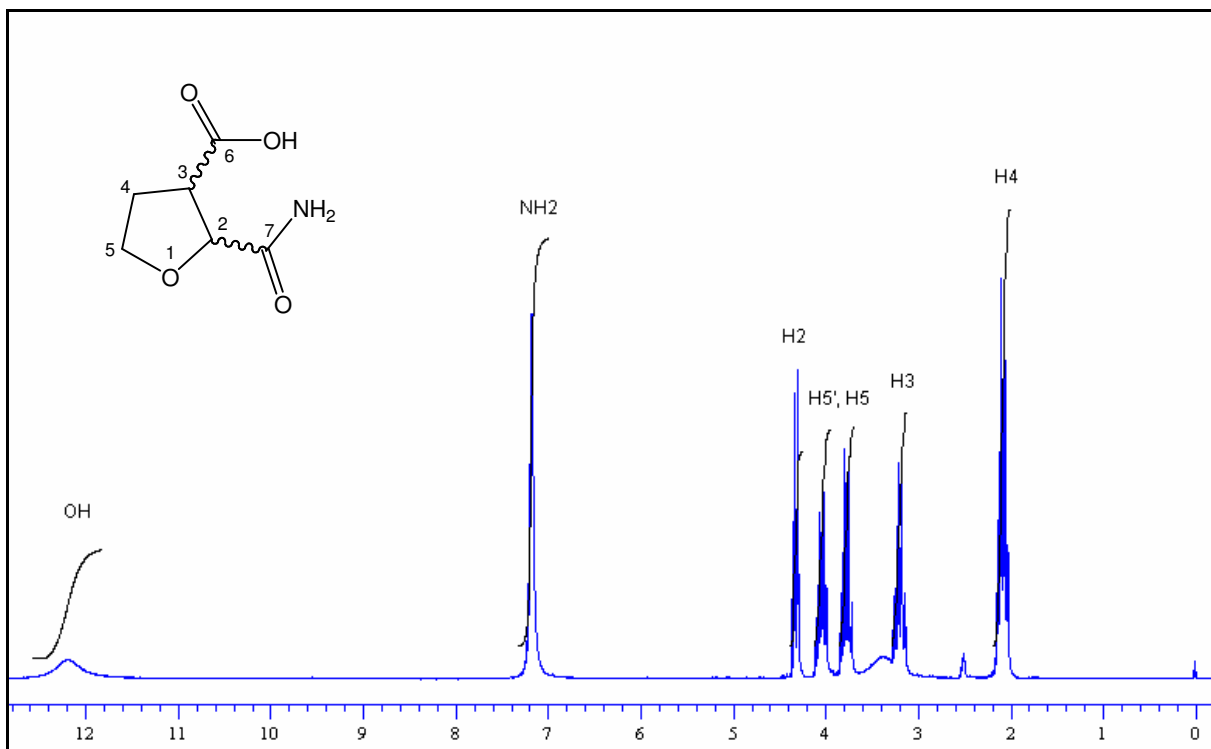


Figura 67 – Espectro de ^1H do composto **7c** a 200 MHz em $\text{DMSO-}d_6$.

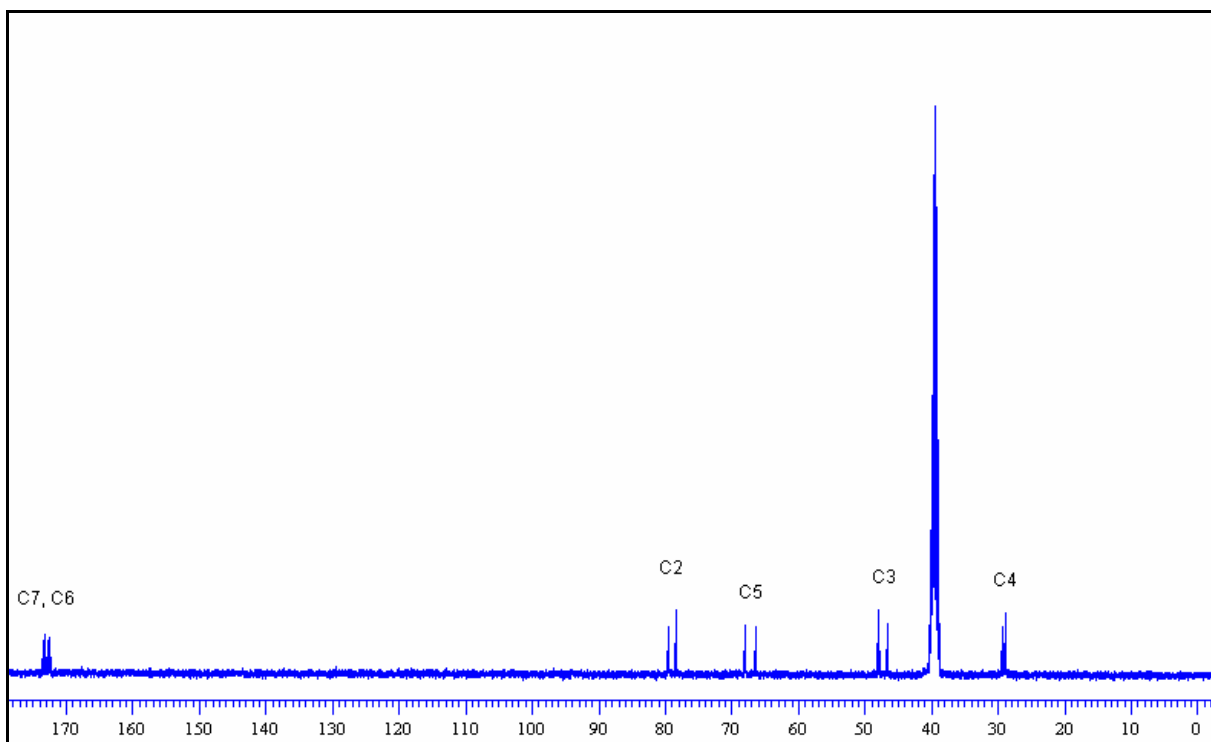


Figura 68 – Espectro de ^{13}C do composto **7c** a 50 MHz em $\text{DMSO-}d_6$.

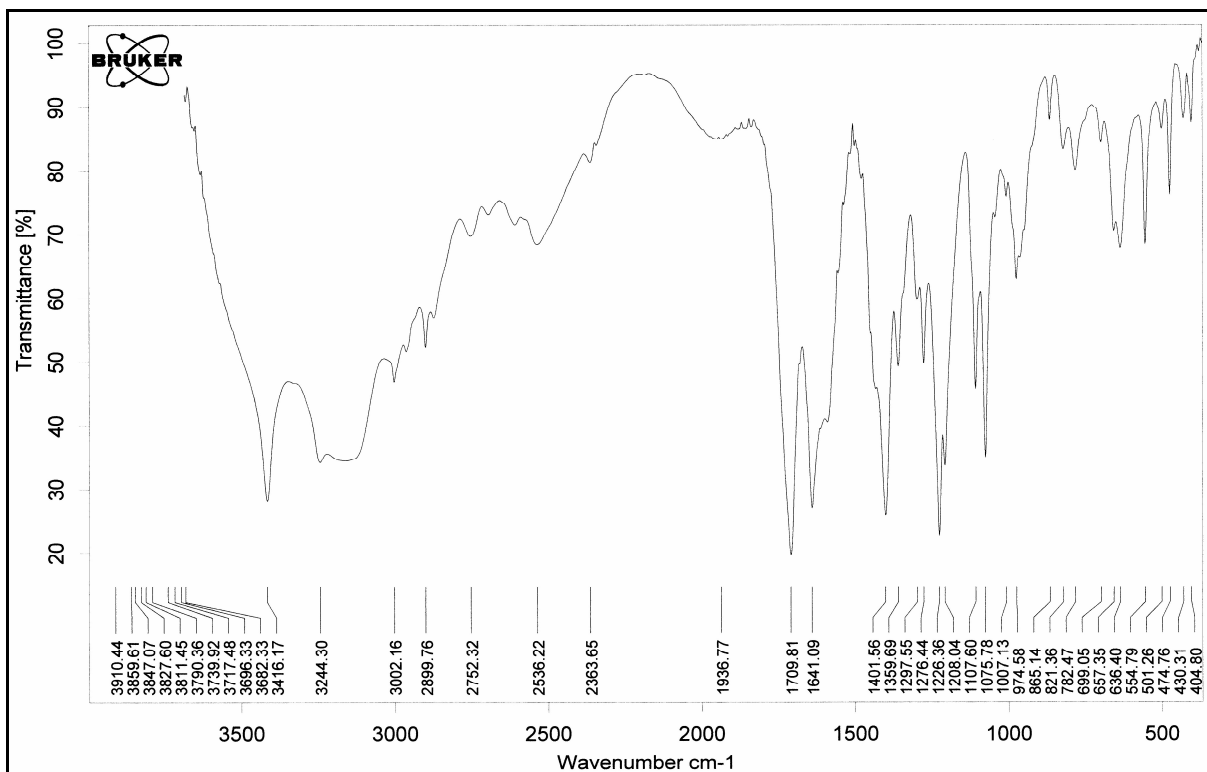


Figura 69 – Espectro de infravermelho do composto **7c** (pastilha de KBr).

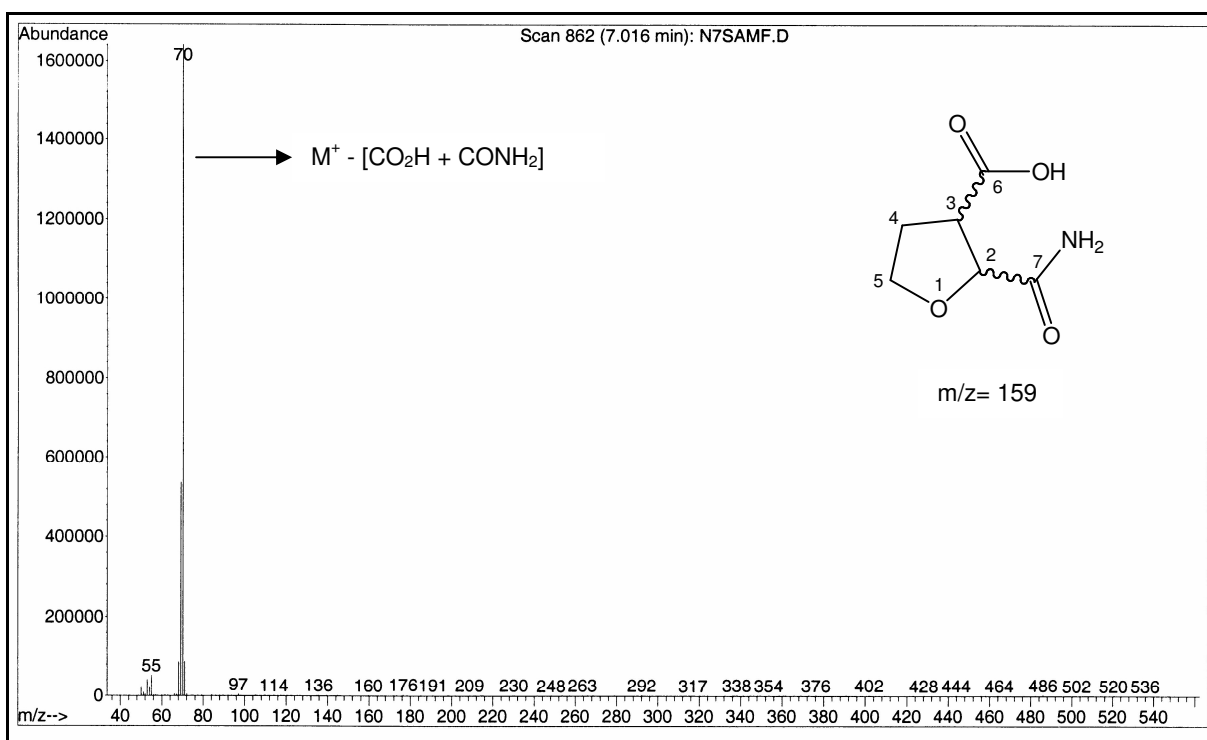


Figura 70 – Espectro de massas do composto **7c**.

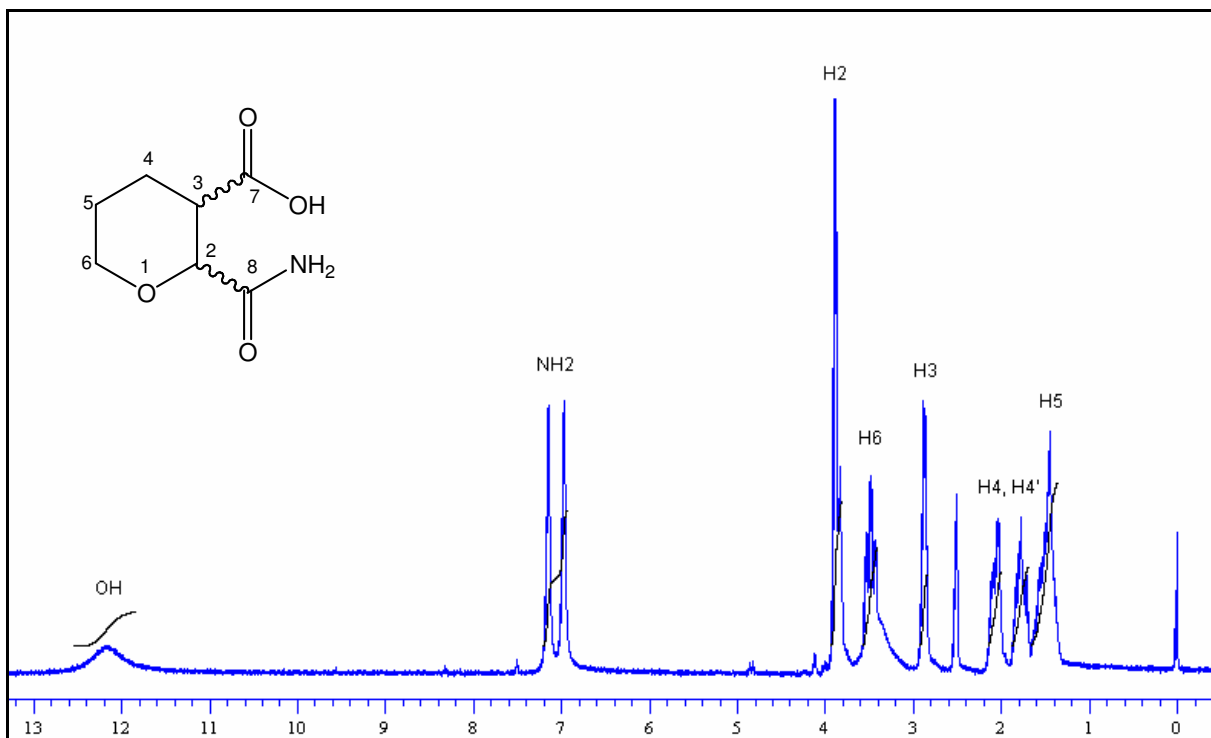


Figura 71 – Espectro de ^1H do composto **7d** a 200 MHz em $\text{DMSO-}d_6$.

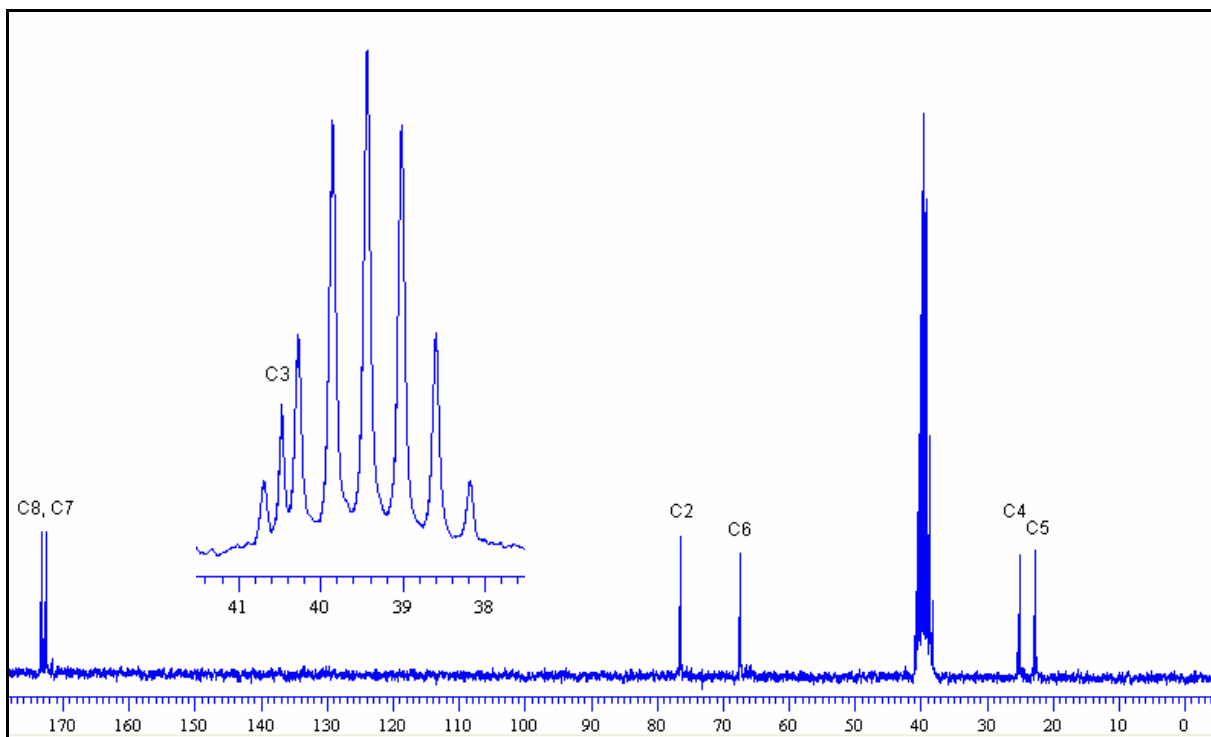


Figura 72 – Espectro de ^{13}C do composto **7d** a 50 MHz em $\text{DMSO-}d_6$.

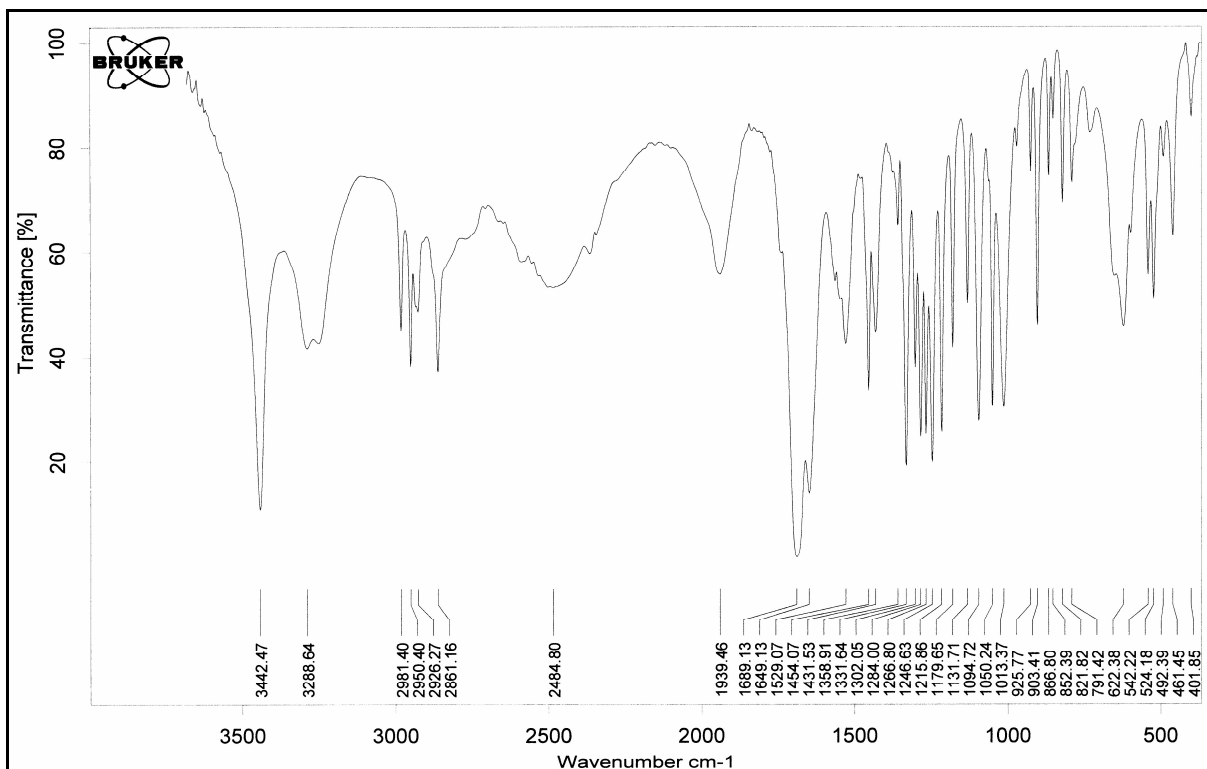


Figura 73 – Espectro de infravermelho do composto 7d (pastilha de KBr).

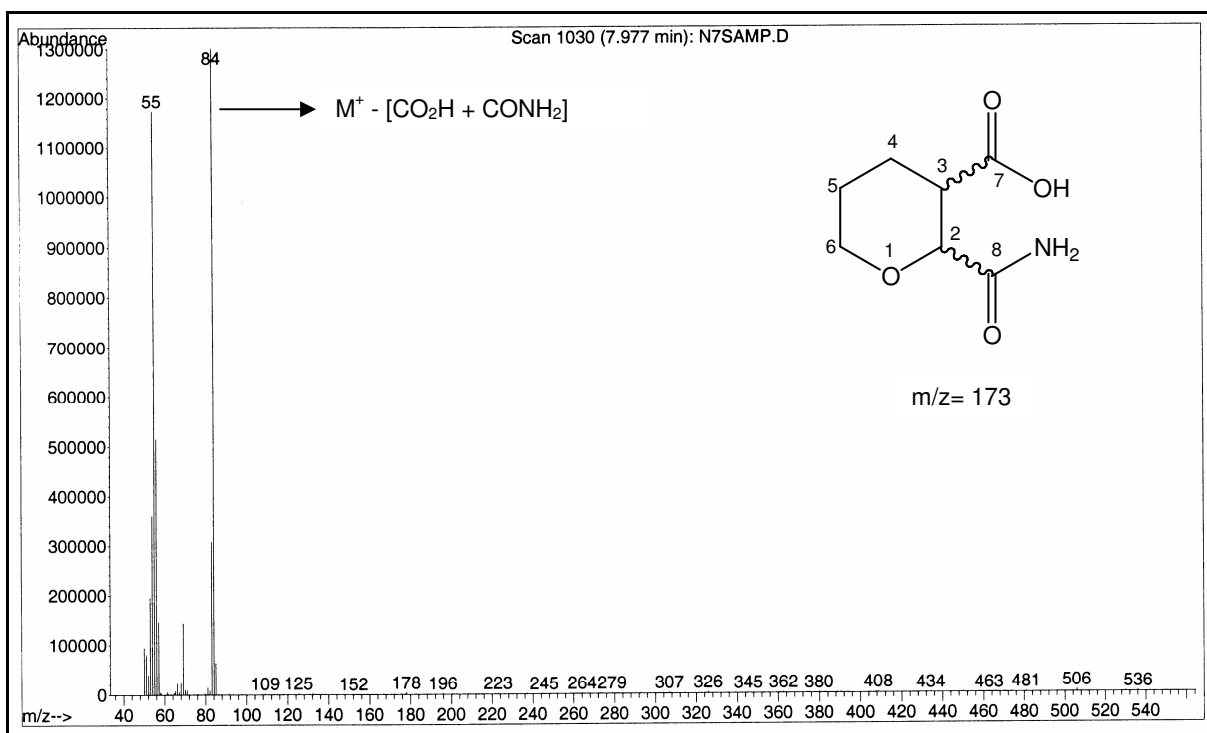


Figura 74 – Espectro de massas do composto 7d.

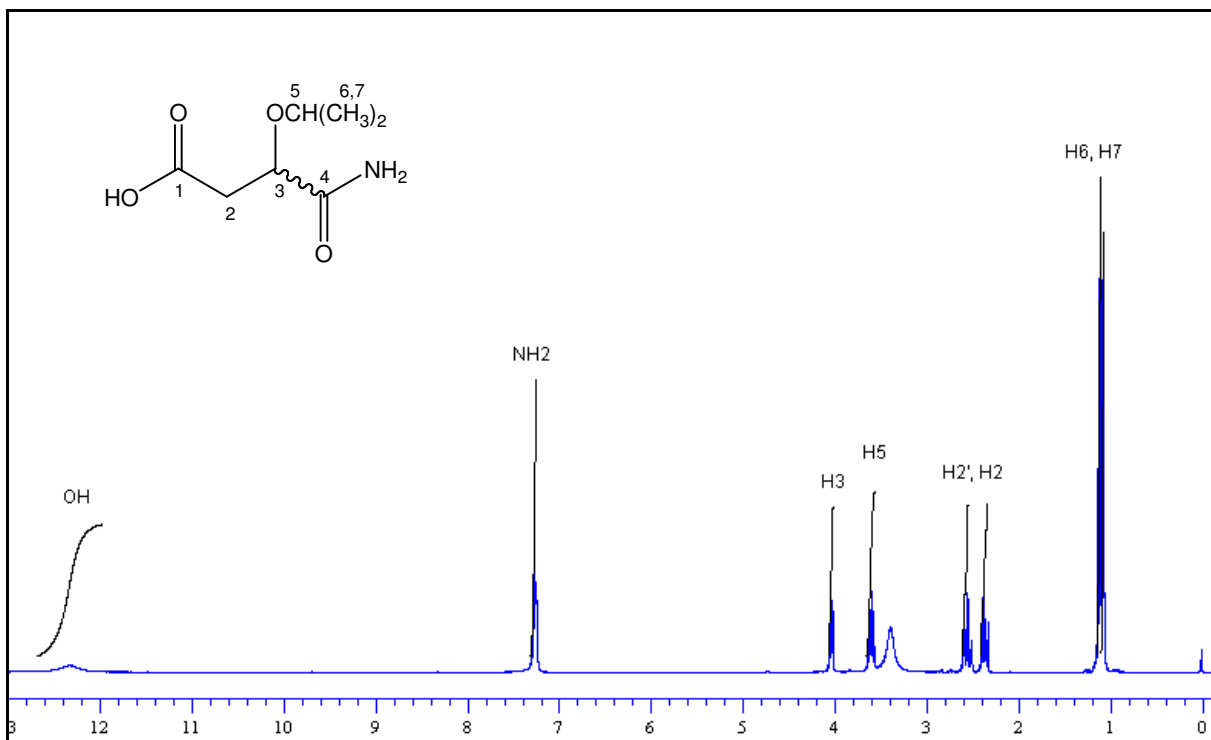


Figura 75 – Espectro de ^1H do composto **7e** a 400 MHz em $\text{DMSO-}d_6$.

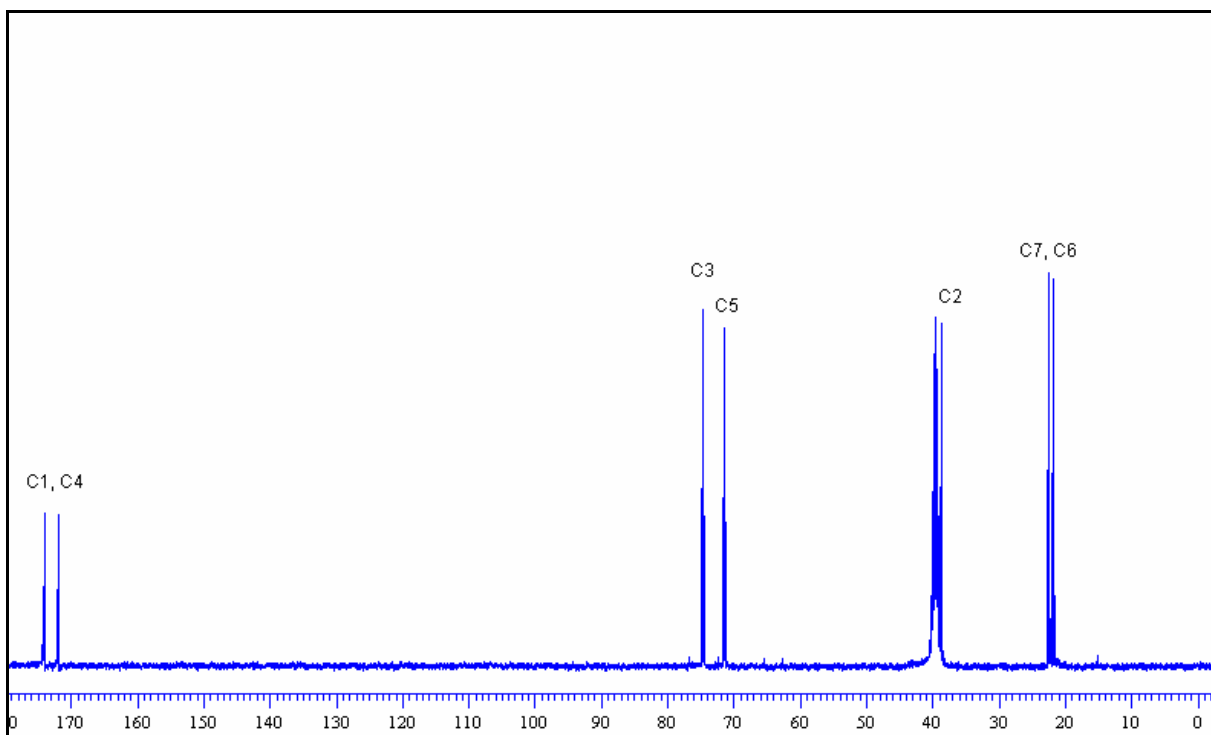


Figura 76 – Espectro de ^{13}C do composto **7e** a 100 MHz em $\text{DMSO-}d_6$.

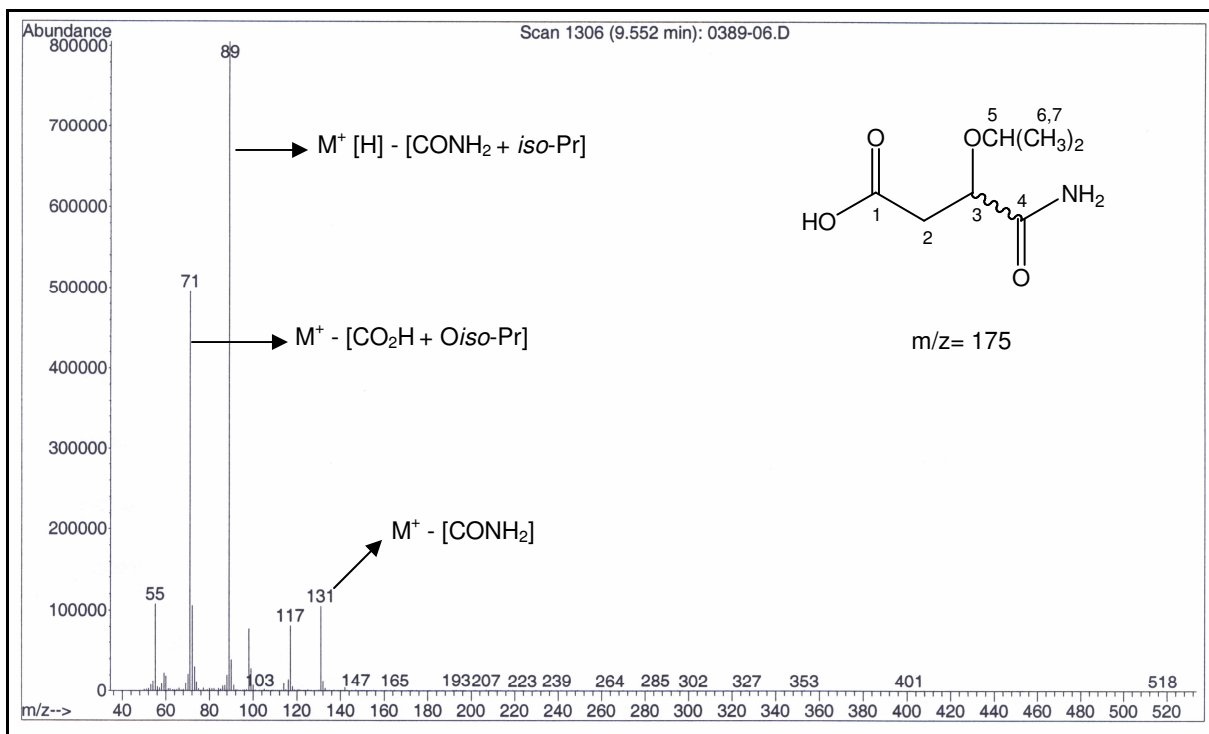


Figura 77 – Espectro de massas do composto 7e.

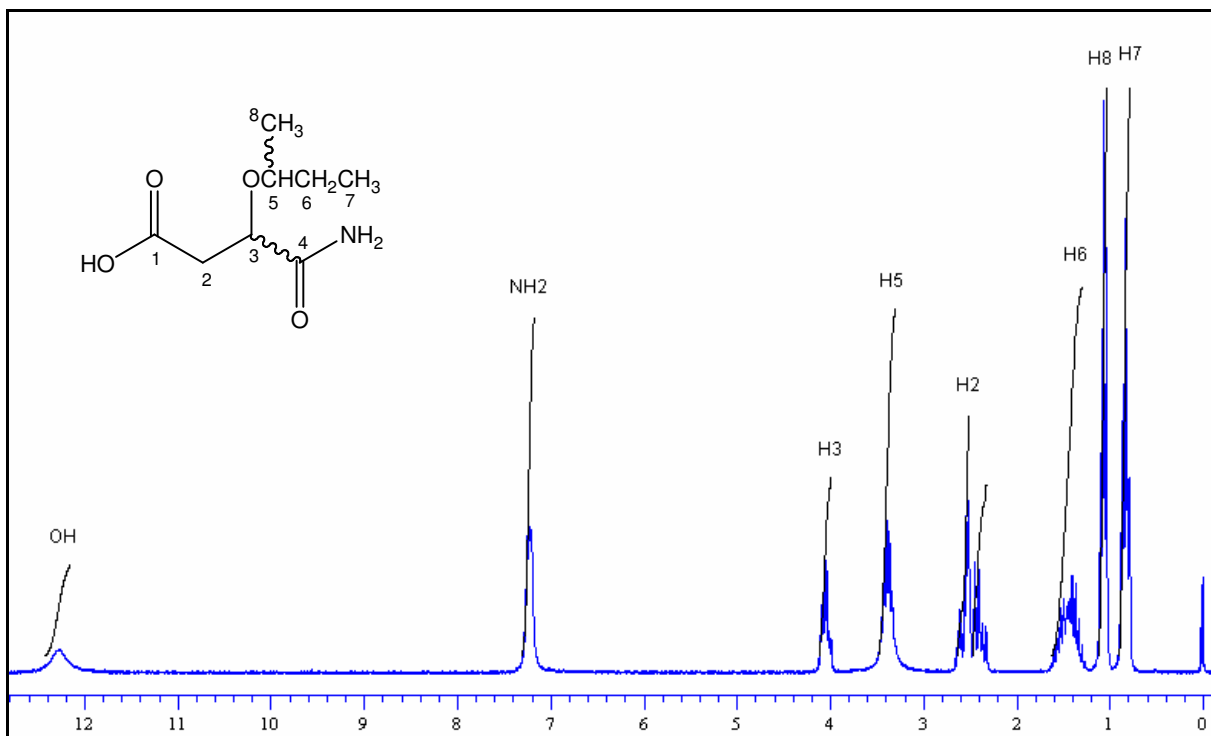


Figura 78 – Espectro de ^1H do composto **7f** a 200 MHz em $\text{DMSO-}d_6$.

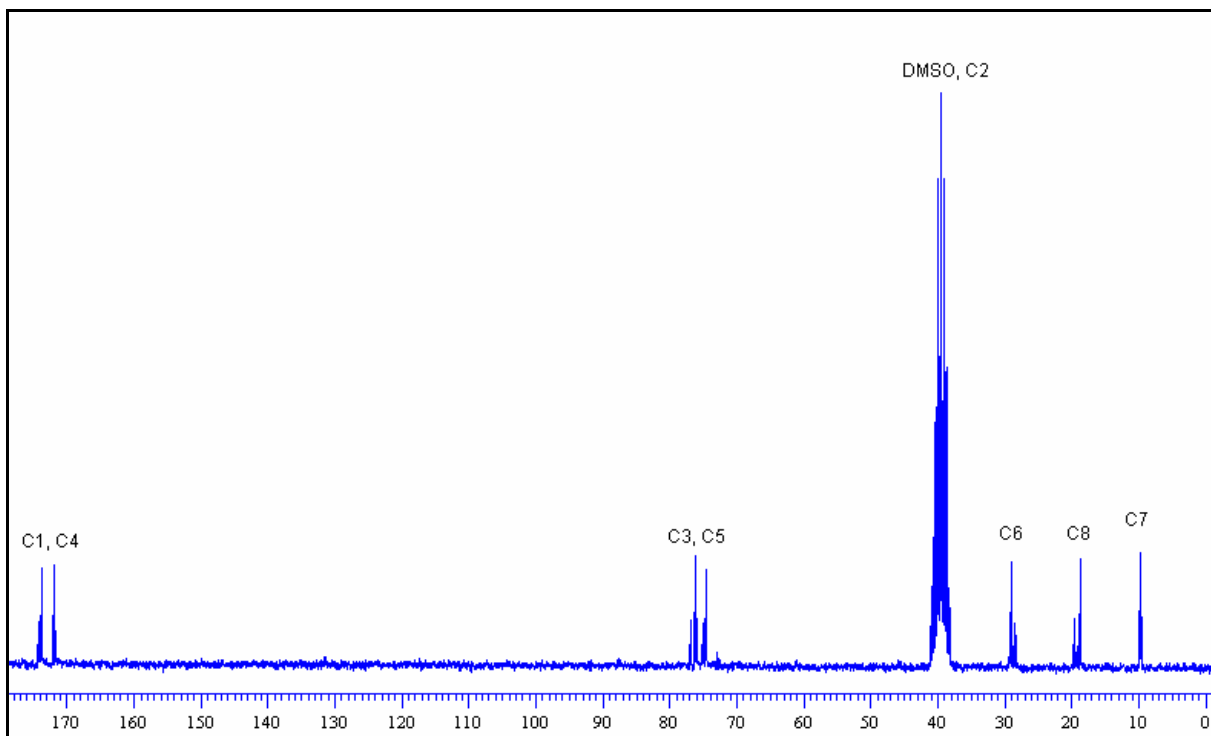


Figura 79 – Espectro de ^{13}C do composto **7f** a 100 MHz em $\text{DMSO-}d_6$.

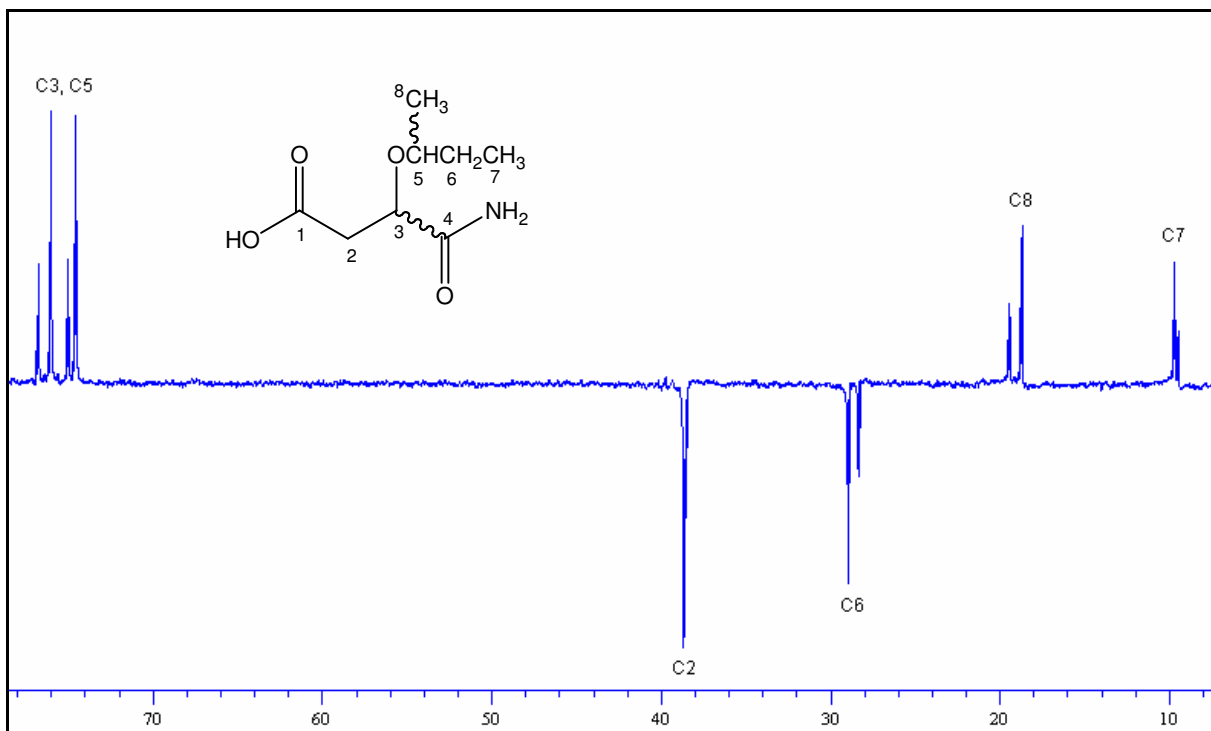


Figura 80 – Espectro de DEPT-135 do composto 7f a 100 MHz em DMSO-*d*₆.

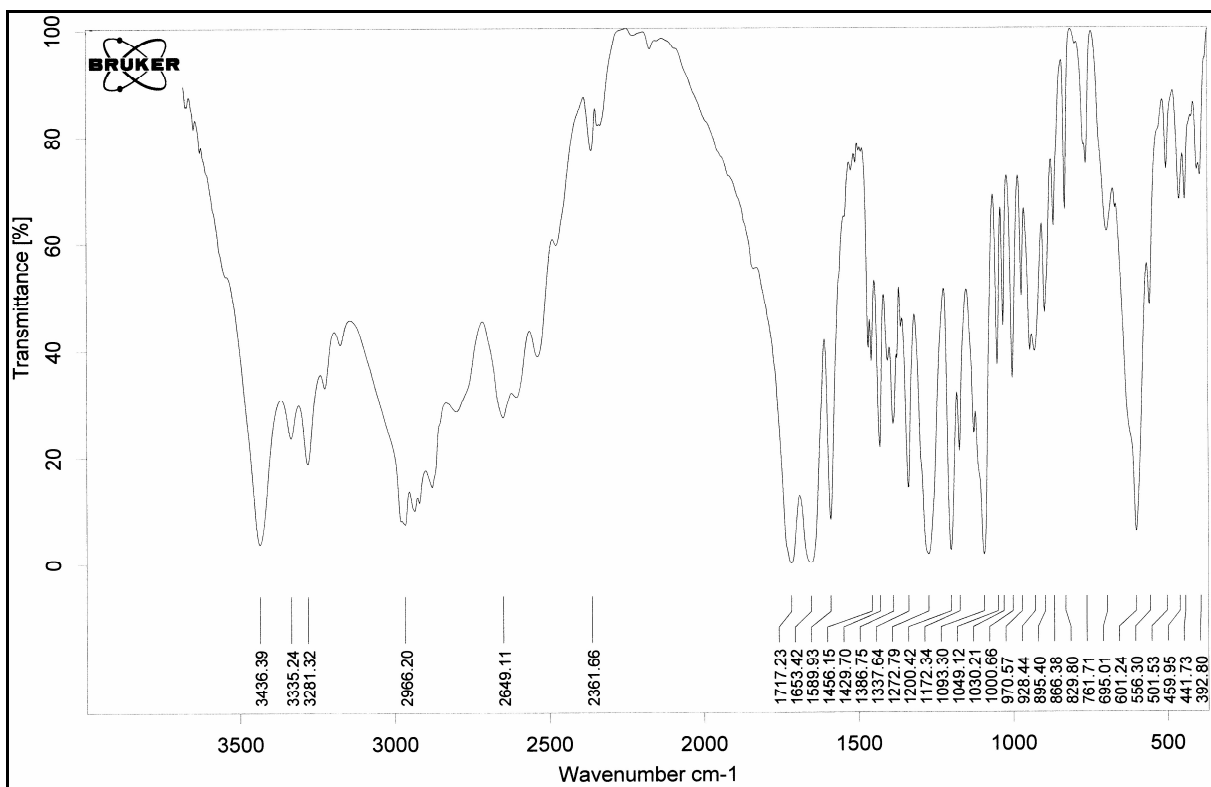


Figura 81 – Espectro de infravermelho do composto 7f (pastilha de KBr).

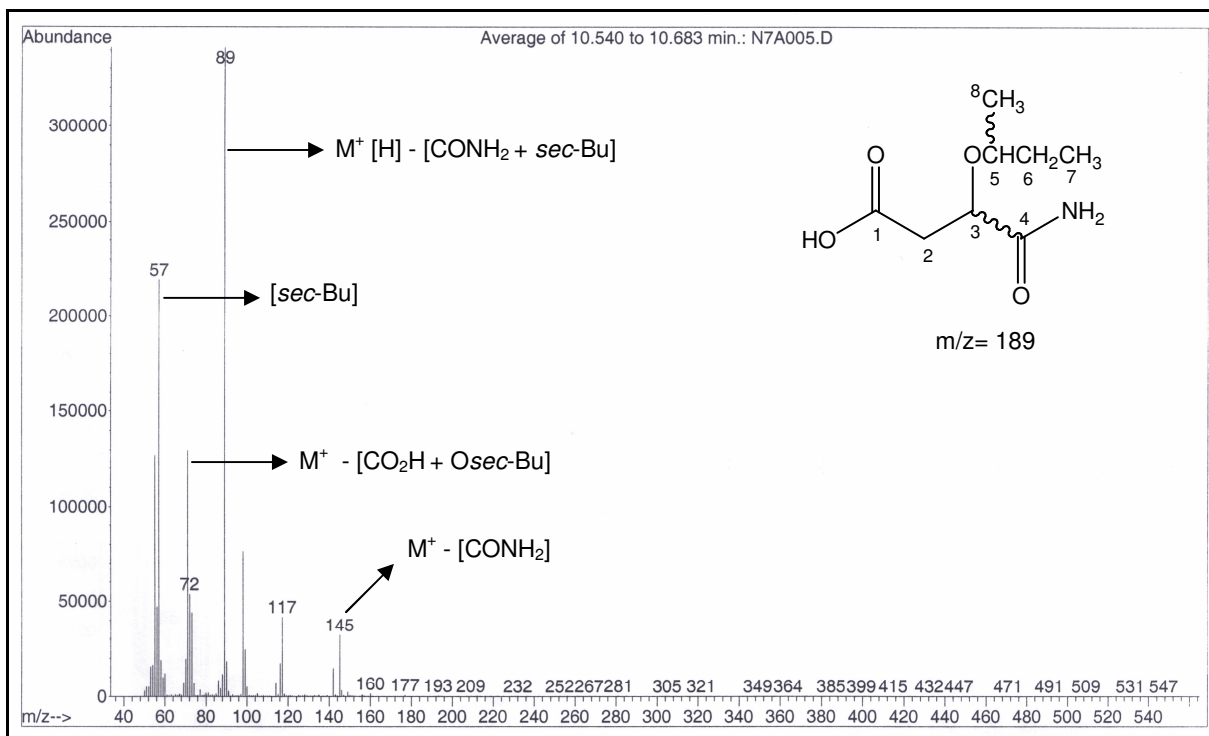


Figura 82 – Espectro massas do composto 7f.

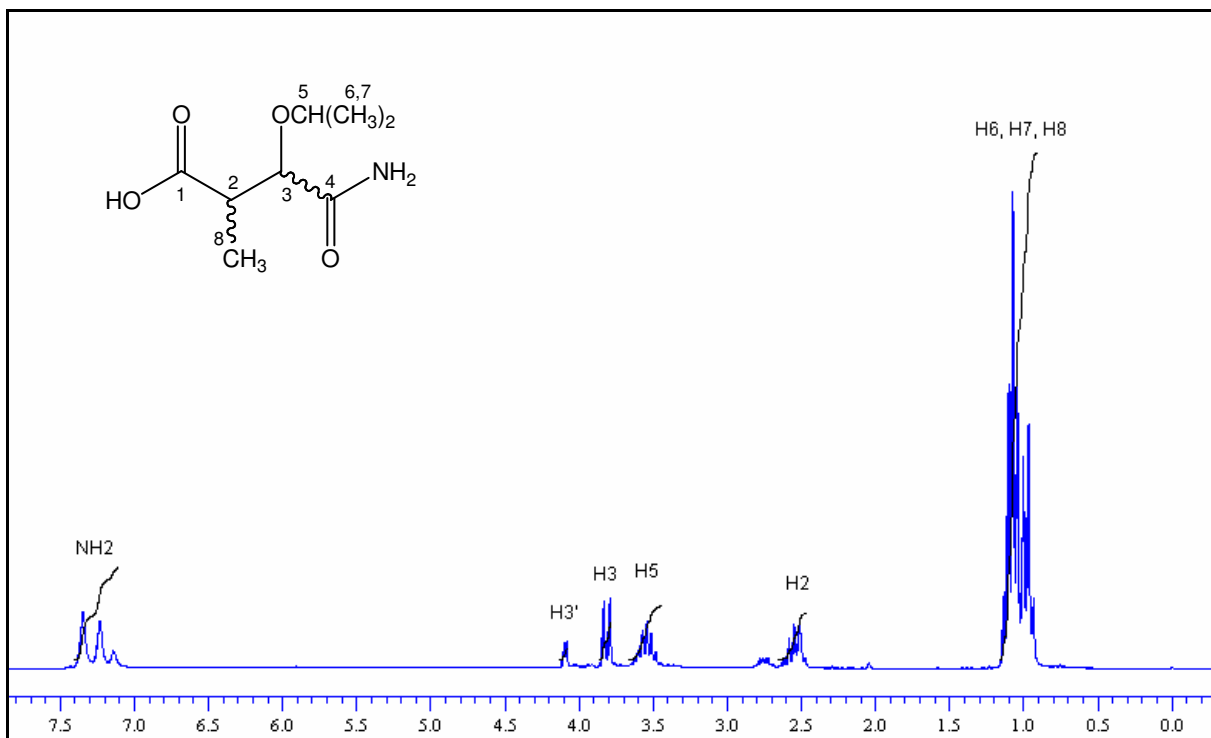


Figura 83 – Espectro de ^1H do composto **7g** a 200 MHz em $\text{DMSO-}d_6$.

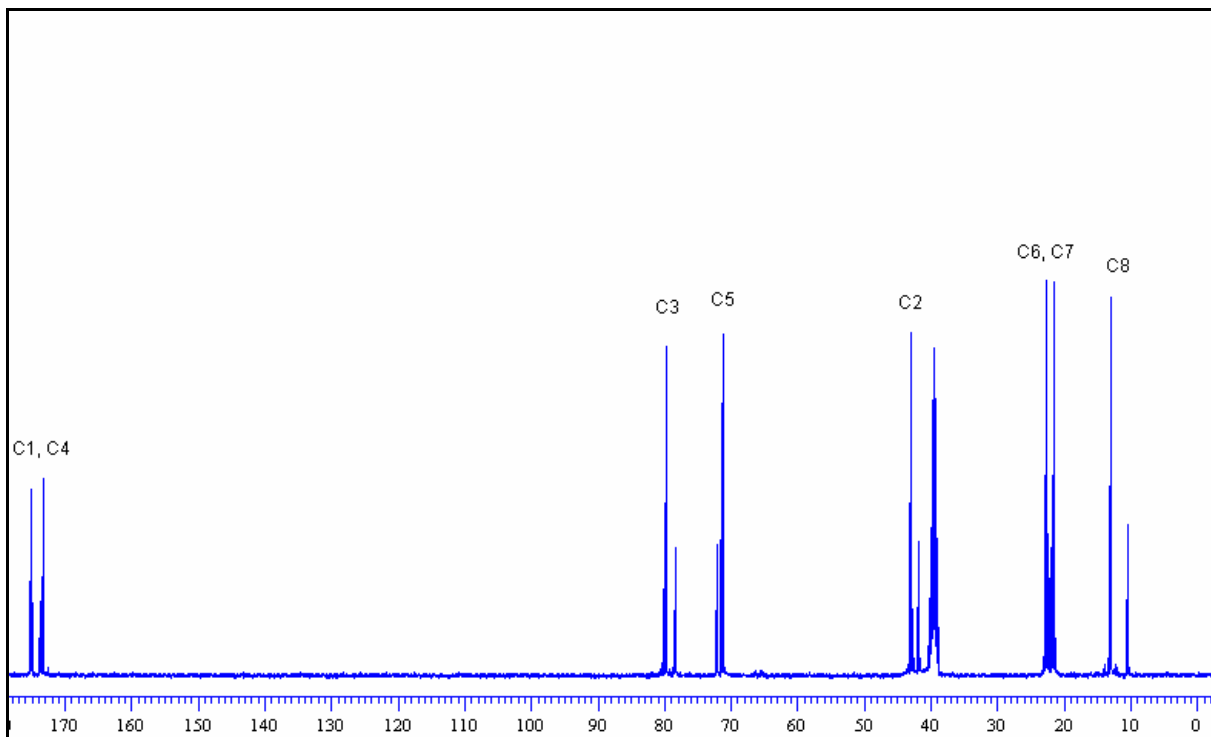


Figura 84 – Espectro de ^{13}C do composto **7g** a 50 MHz em $\text{DMSO-}d_6$.

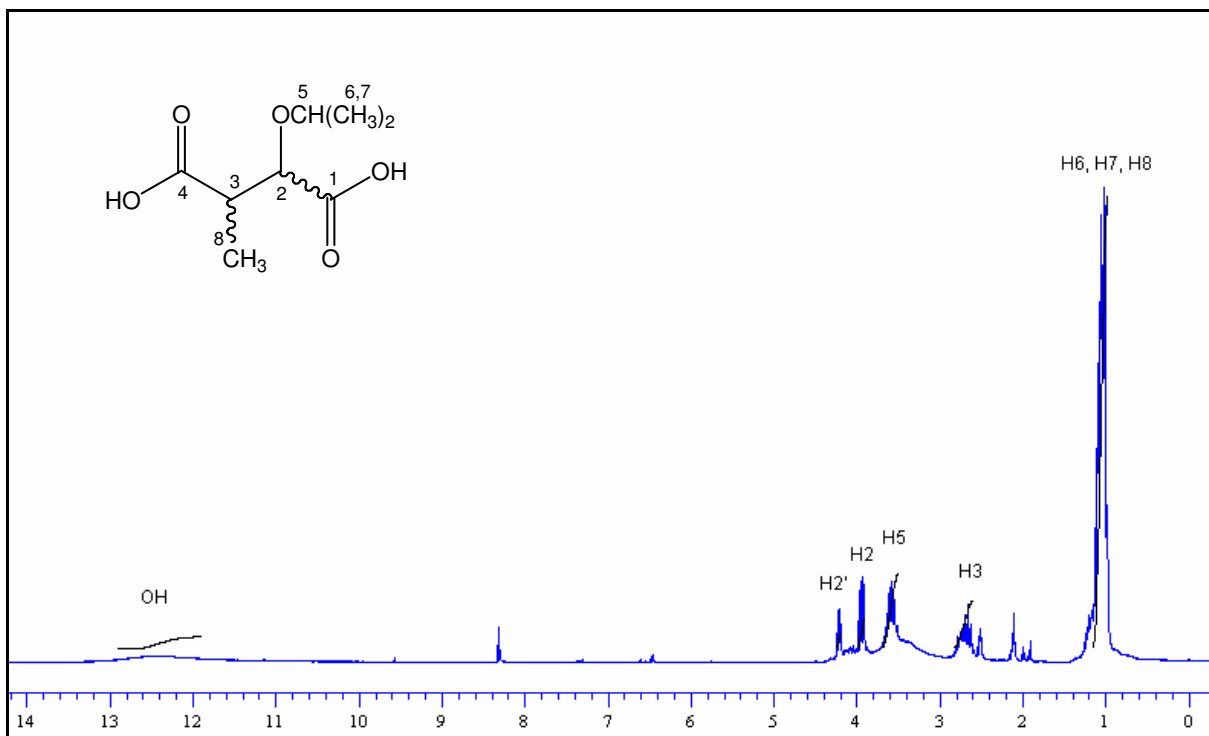


Figura 107 – Espectro de ^1H do composto **8g** a 200 MHz em DMSO- d_6 .

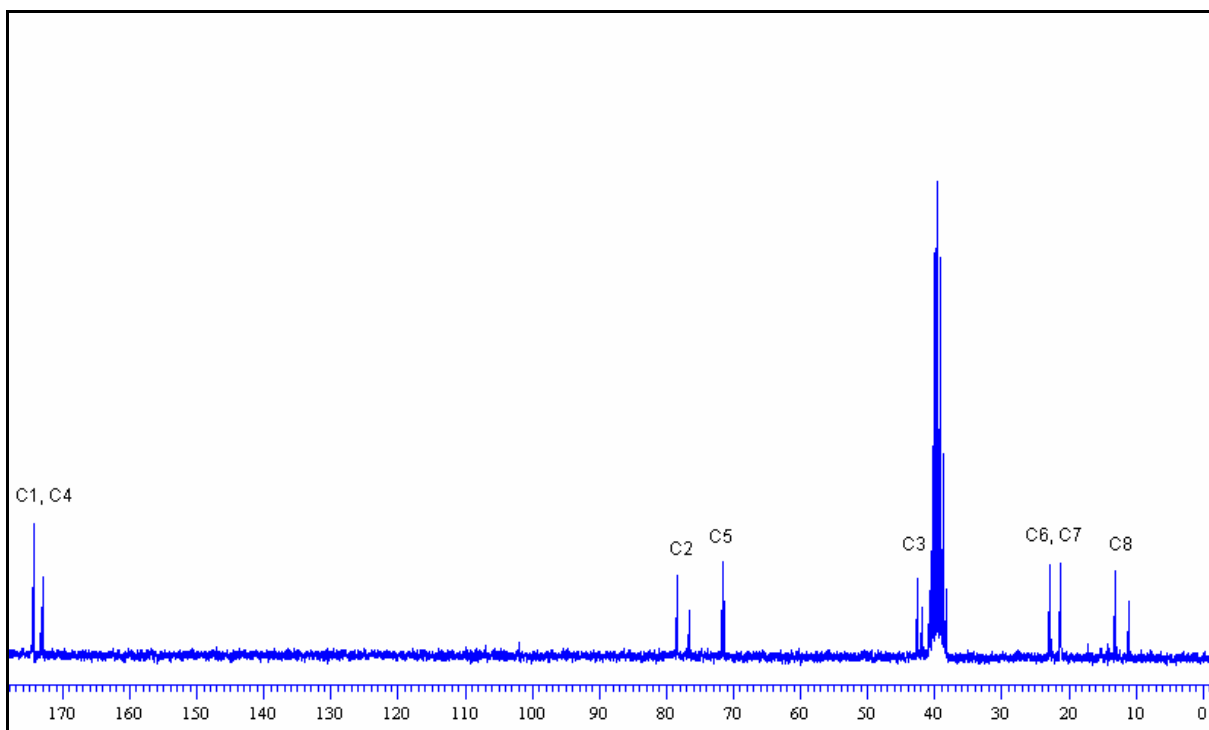


Figura 108 – Espectro de ^{13}C do composto **8g** a 50 MHz em DMSO- d_6 .

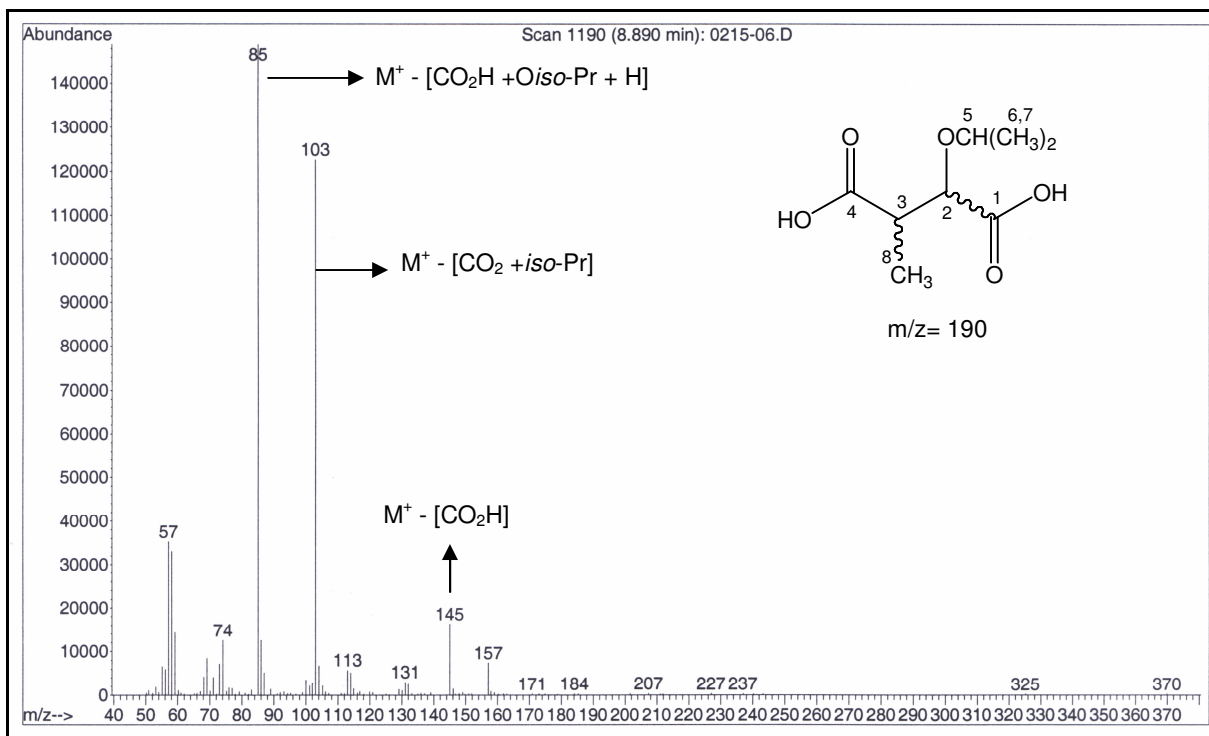


Figura 109 – Espectro de massas do composto 8g.

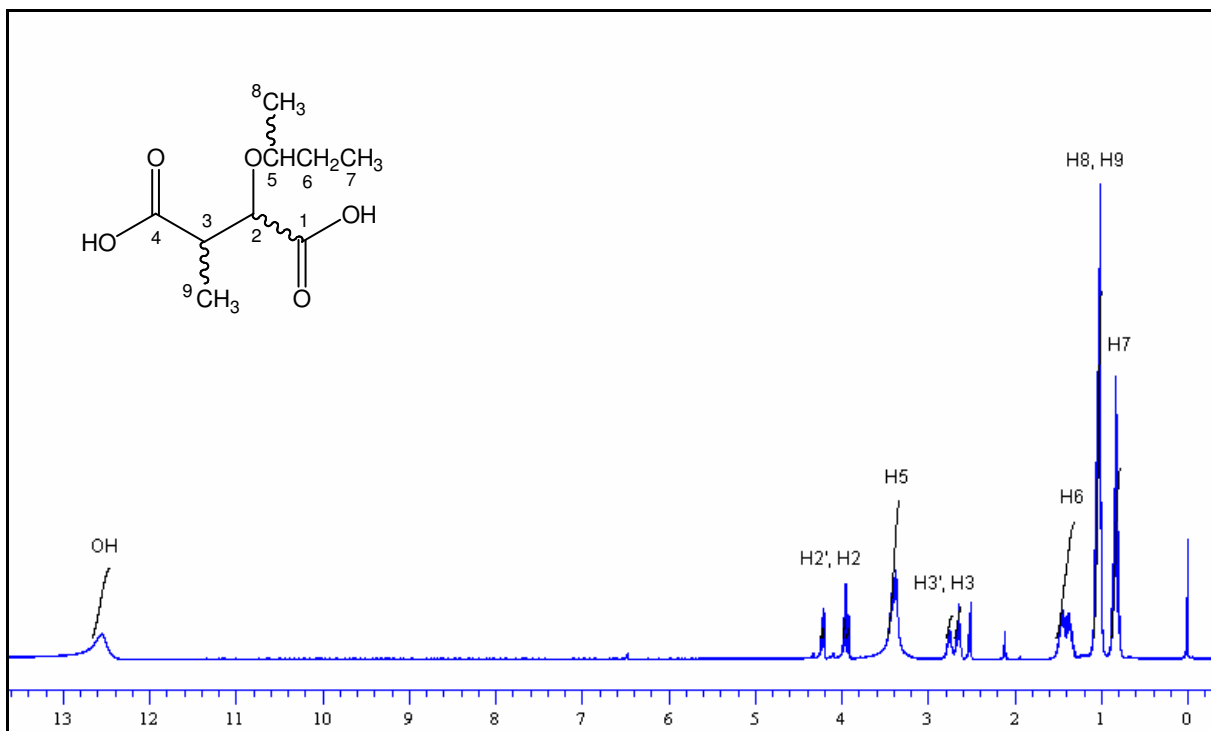


Figura 110 – Espectro de ^1H do composto **8h** a 400 MHz em $\text{DMSO-}d_6$.

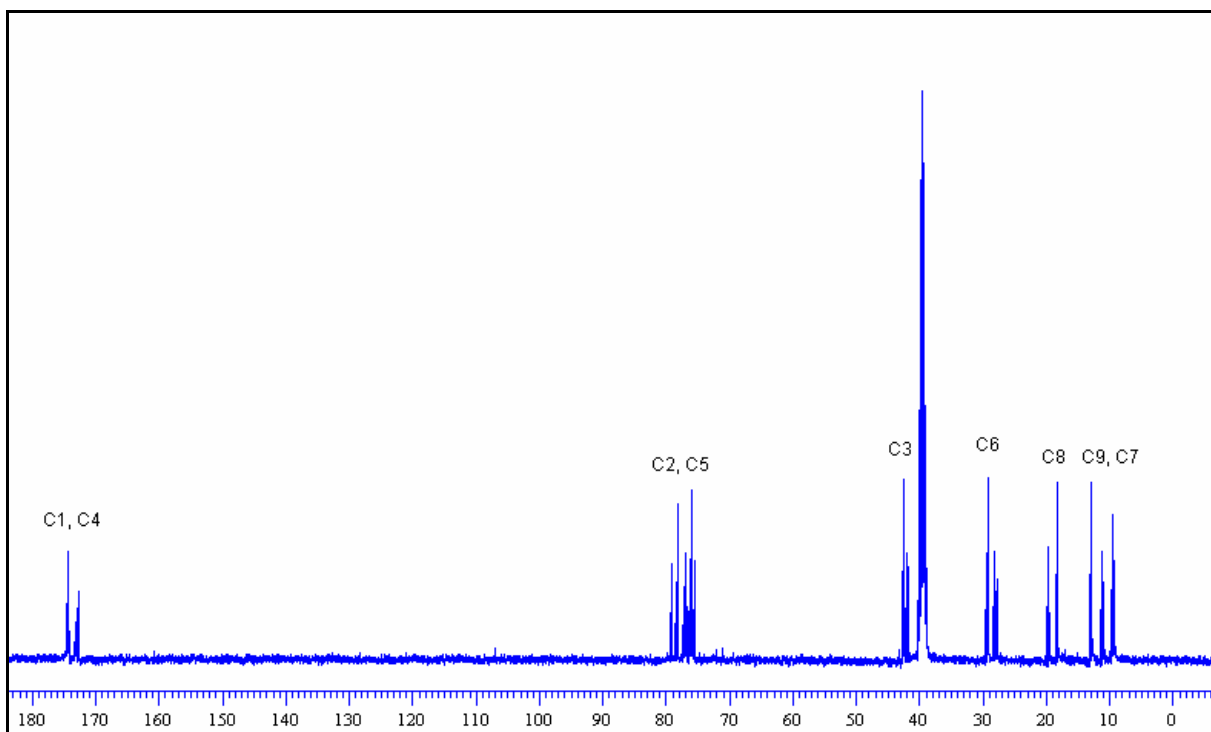


Figura 111 – Espectro de ^{13}C do composto **8h** a 100 MHz em $\text{DMSO-}d_6$.

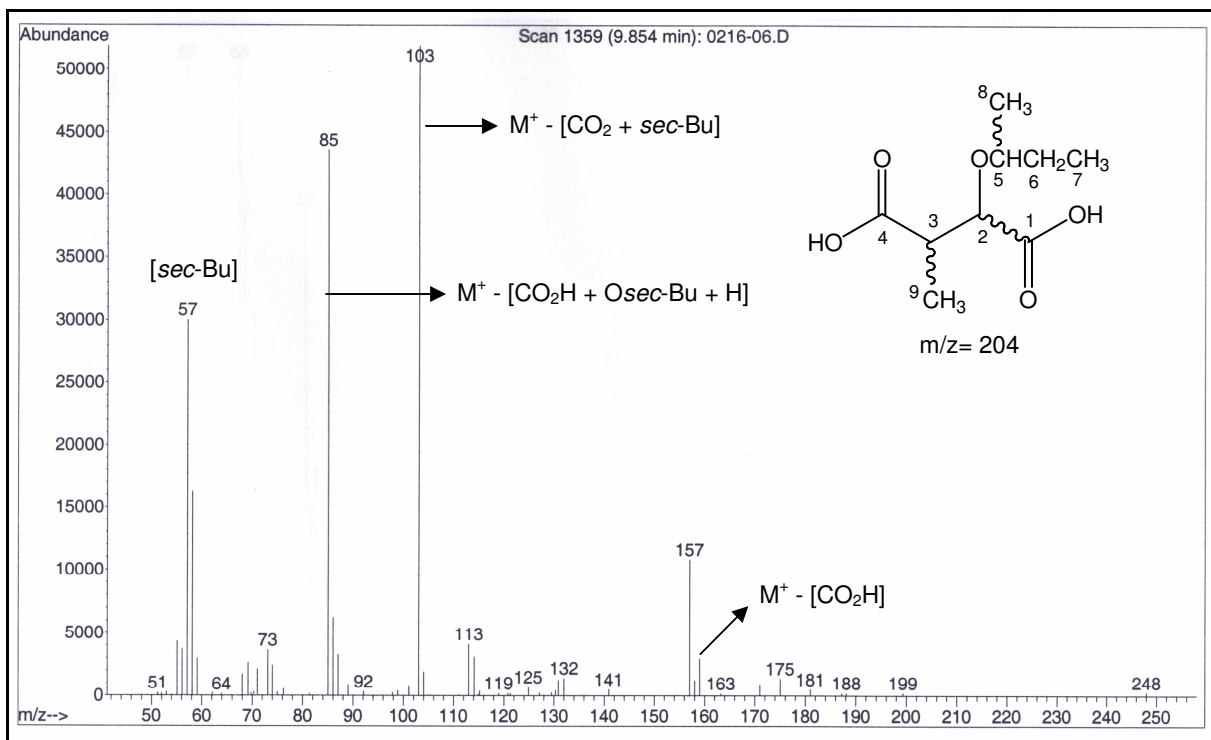


Figura 112 – Espectro de massas do composto 8h.

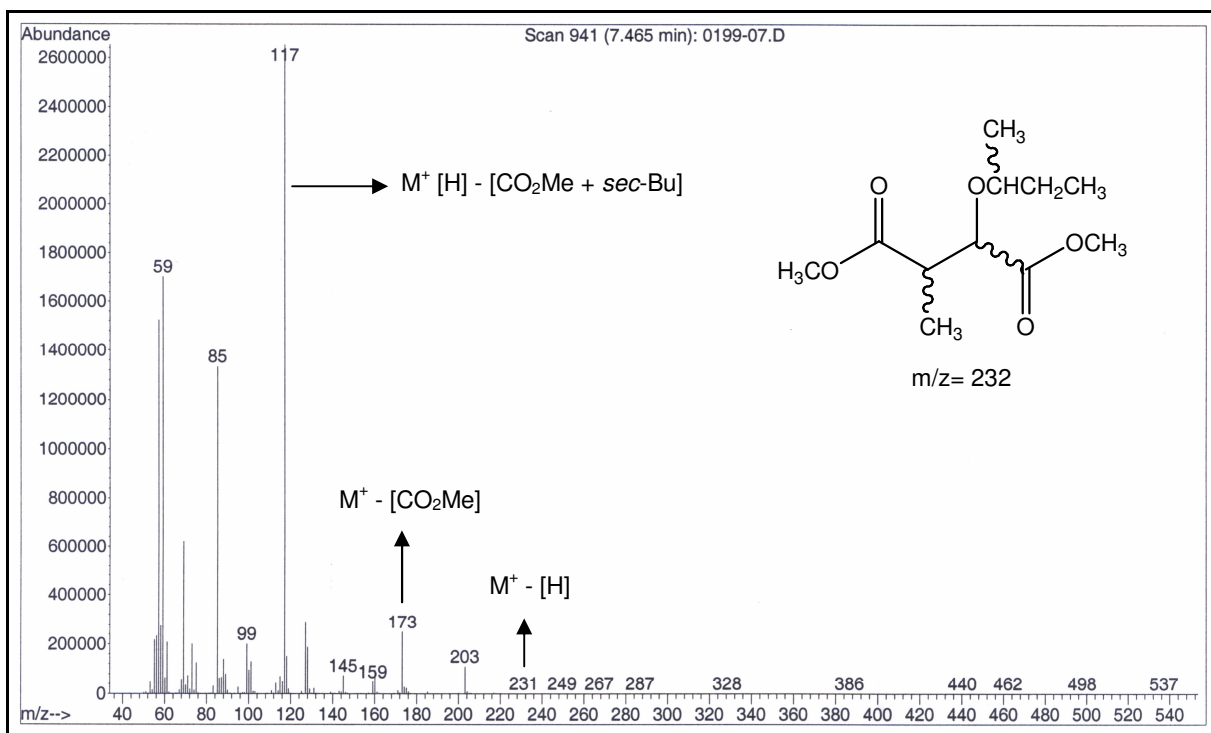


Figura 113 – Espectro de massas do diéster obtido por derivatização do composto 8h com diazometano.

***APÊNDICE B – DADOS DE DIFRAÇÃO
DE RAIOS-X PARA O COMPOSTO 7f***

Tabelas de dados de Difração de Raios-X para do composto 7f

Tabela 16 – Dados cristalográficos e de refinamento estrutural.

Identification code	p-1	
Empirical formula	C ₈ H ₁₅ NO ₄	
Formula weight	189.21	
Temperature	295(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P(-1)	
Unit cell dimensions	a = 7.501(4) Å	α = 90°
	b = 9.024(7) Å	β = 103.59(3)°
	c = 15.550(15) Å	γ = 90°
Volume	1023.1(14) Å ³	
Z	4	
Density (calculated)	1.228 Mg/m ³	
Absorption coefficient	0.098 mm ⁻¹	
F(000)	408	
Crystal size	0.47 x 0.27 x 0.14 mm ³	
Theta range for data collection	3.38 to 25.50°.	
Index ranges	-9 ≤ h ≤ 9, -10 ≤ k ≤ 10, -18 ≤ l ≤ 18	
Reflections collected	15625	
Independent reflections	1896 [R(int) = 0.0402]	
Completeness to theta = 25.50°	99.8 %	
Max. and min. transmission	0.9864 and 0.9553	
Refinement method	Full-matrix least-squares on F ²	

Tabela 16 – Dados cristalográficos e de refinamento estrutural (continuação).

Data / restraints / parameters	1896 / 0 / 124
Goodness-of-fit on F^2	1.134
Final R indices [$I > 2\sigma(I)$]	R1 = 0.0561, wR2 = 0.1772
R indices (all data)	R1 = 0.0746, wR2 = 0.1871
Largest diff. peak and hole	0.315 and -0.311 e.Å ⁻³

Tabela 17 – Coordenadas atômicas ($\times 10^4$) e parâmetros de substituição de equivalência isotrópica (Å² $\times 10^3$).

	x	y	z	U (eq) ^a
C(1)	6406(3)	3201(2)	1778(1)	45(1)
C(2)	4968(3)	4296(2)	1884(2)	48(1)
C(3)	5166(2)	4671(2)	2854(1)	42(1)
C(4)	3696(3)	5788(2)	2941(1)	44(1)
C(5)	5850(5)	3312(3)	4221(2)	77(1)
C(6)	5116(7)	2015(4)	4625(2)	105(1)
C(7)	3210(6)	2163(5)	4601(3)	113(1)
C(8)	8024(5)	3166(6)	4353(3)	131(2)
N(1)	2088(2)	5253(2)	2966(2)	70(1)
O(1)	6088(2)	1929(2)	1560(1)	61(1)
O(2)	8065(2)	3773(2)	1964(1)	63(1)
O(3)	4982(2)	3318(1)	3286(1)	47(1)
O(4)	4027(2)	7135(2)	2959(1)	55(1)

^aU(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Tabela 18 – Comprimentos de ligação [Å] e ângulos [°].

C(1)-O(1)	1.205(3)
C(1)-O(2)	1.315(3)
C(1)-C(2)	1.500(3)
C(2)-C(3)	1.518(3)
C(2)-H(2A)	0.9700
C(2)-H(2B)	0.9700
C(3)-O(3)	1.416(2)
C(3)-C(4)	1.523(3)
C(3)-H(3)	0.9800
C(4)-O(4)	1.239(3)
C(4)-N(1)	1.309(3)
C(5)-O(3)	1.447(3)
C(5)-C(6)	1.493(5)
C(5)-C(8)	1.601(5)
C(5)-H(5)	0.9800
C(6)-C(7)	1.428(6)
C(6)-H(6A)	0.9700
C(6)-H(6B)	0.9700
C(7)-H(7A)	0.9600
C(7)-H(7B)	0.9600
C(7)-H(7C)	0.9600
C(8)-H(8A)	0.9600
C(8)-H(8B)	0.9600
C(8)-H(8C)	0.9600
N(1)-H(1A)	0.8600
N(1)-H(1B)	0.8600
O(2)-H(1)	0.82(4)
O(1)-C(1)-O(2)	123.4(2)
O(1)-C(1)-C(2)	123.9(2)
O(2)-C(1)-C(2)	112.6(2)
C(1)-C(2)-C(3)	110.55(17)

Tabela 18 – Comprimentos de ligação [Å] e ângulos [°] (continuação).

C(1)-C(2)-H(2A)	109.5
C(3)-C(2)-H(2A)	109.5
C(1)-C(2)-H(2B)	109.5
C(3)-C(2)-H(2B)	109.5
H(2A)-C(2)-H(2B)	108.1
O(3)-C(3)-C(2)	106.36(17)
O(3)-C(3)-C(4)	112.04(16)
C(2)-C(3)-C(4)	109.37(16)
O(3)-C(3)-H(3)	109.7
C(2)-C(3)-H(3)	109.7
C(4)-C(3)-H(3)	109.7
O(4)-C(4)-N(1)	122.82(19)
O(4)-C(4)-C(3)	120.42(17)
N(1)-C(4)-C(3)	116.72(18)
O(3)-C(5)-C(6)	107.6(3)
O(3)-C(5)-C(8)	109.5(3)
C(6)-C(5)-C(8)	110.3(3)
O(3)-C(5)-H(5)	109.8
C(6)-C(5)-H(5)	109.8
C(8)-C(5)-H(5)	109.8
C(7)-C(6)-C(5)	112.5(3)
C(7)-C(6)-H(6A)	109.1
C(5)-C(6)-H(6A)	109.1
C(7)-C(6)-H(6B)	109.1
C(5)-C(6)-H(6B)	109.1
H(6A)-C(6)-H(6B)	107.8
C(6)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(6)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5

Tabela 18 – Comprimentos de ligação [Å] e ângulos [°] (continuação).

H(7B)-C(7)-H(7C)	109.5
C(5)-C(8)-H(8A)	109.5
C(5)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(5)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(4)-N(1)-H(1A)	120.0
C(4)-N(1)-H(1B)	120.0
H(1A)-N(1)-H(1B)	120.0
C(1)-O(2)-H(1)	110(3)
C(3)-O(3)-C(5)	114.14(18)

Tabela 19 – Parâmetros de substituição anisotrópica^a (Å² x 10³).

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(1)	41(1)	43(1)	52(1)	4(1)	15(1)	2(1)
C(2)	41(1)	43(1)	61(1)	10(1)	15(1)	7(1)
C(3)	33(1)	30(1)	63(1)	3(1)	10(1)	2(1)
C(4)	33(1)	35(1)	65(1)	0(1)	11(1)	0(1)
C(5)	112(2)	58(2)	57(2)	0(1)	16(2)	9(2)
C(6)	158(4)	84(2)	76(2)	14(2)	34(2)	8(2)
C(7)	123(3)	113(3)	104(3)	6(2)	31(2)	-21(3)
C(8)	95(3)	174(4)	100(3)	31(3)	-27(2)	8(3)
N(1)	39(1)	40(1)	140(2)	-4(1)	35(1)	0(1)
O(1)	47(1)	48(1)	89(1)	-12(1)	17(1)	-1(1)
O(2)	41(1)	45(1)	108(2)	-10(1)	26(1)	-2(1)
O(3)	55(1)	33(1)	53(1)	2(1)	10(1)	3(1)
O(4)	38(1)	32(1)	96(1)	-3(1)	17(1)	1(1)

^aThe anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$.