

Anexo I: Espectrometria de Massa

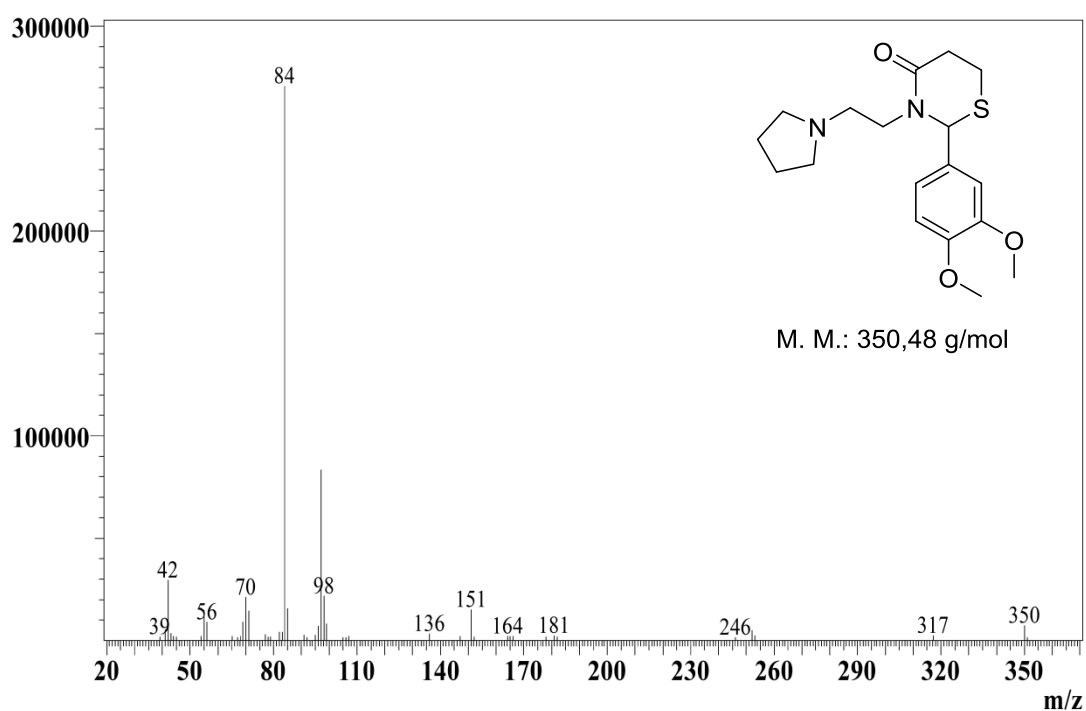
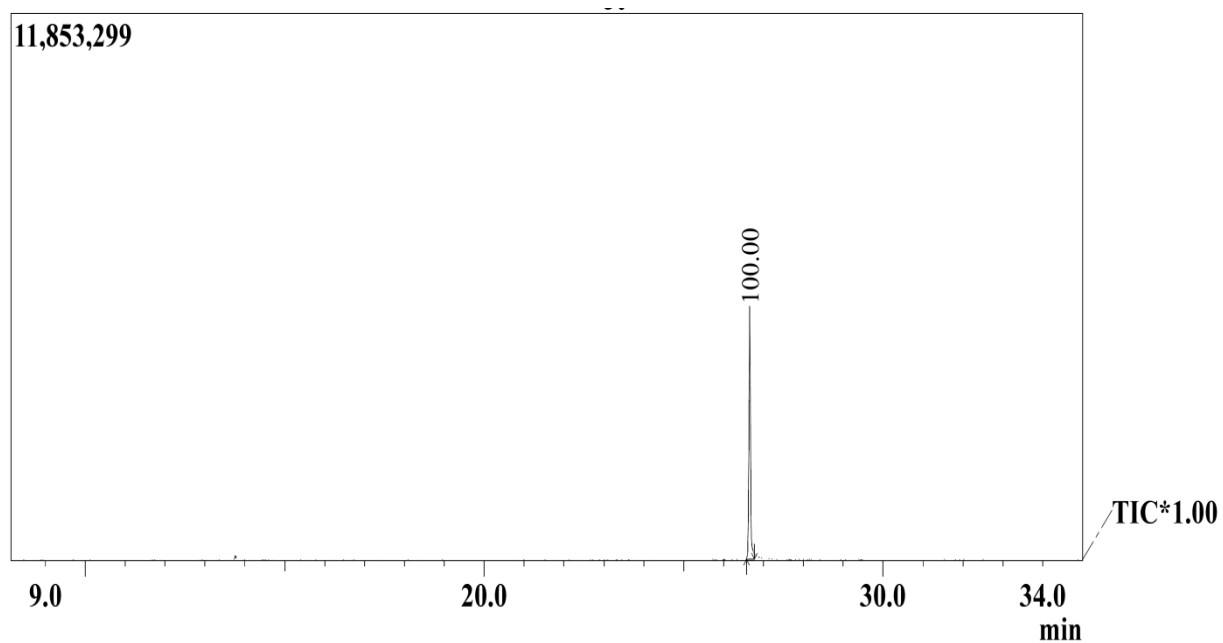


Figura 89: Espectro de massa (CG/EM) tiazinan-4-ona **11u**.

Anexo II: Espectros de EMAR

Anexo II: Espectrometria de EMAR

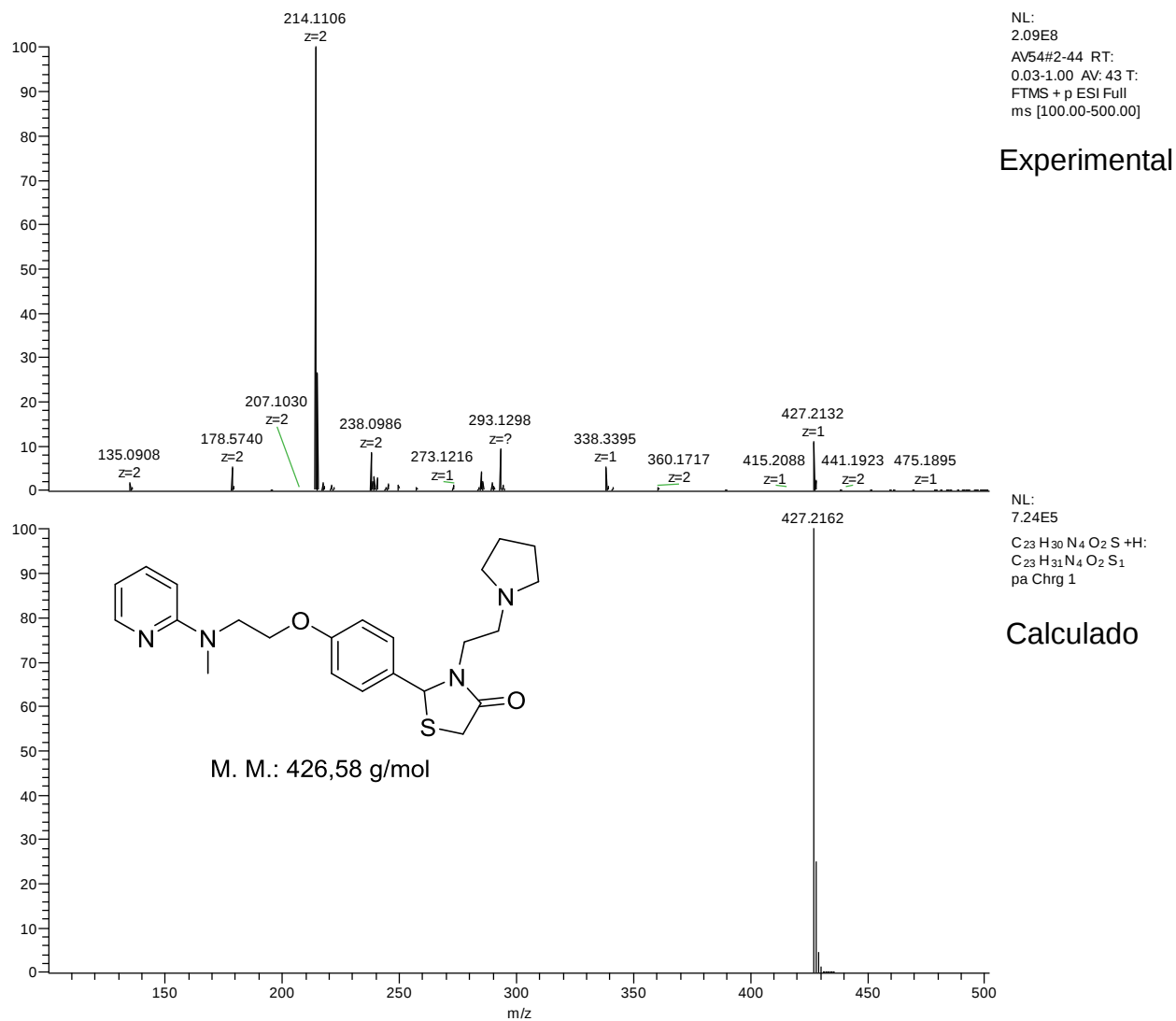


Figura 90: Espectro EMAR da tiazolidin-4-ona **8a**.

Anexo II: Espectrometria de EMAR

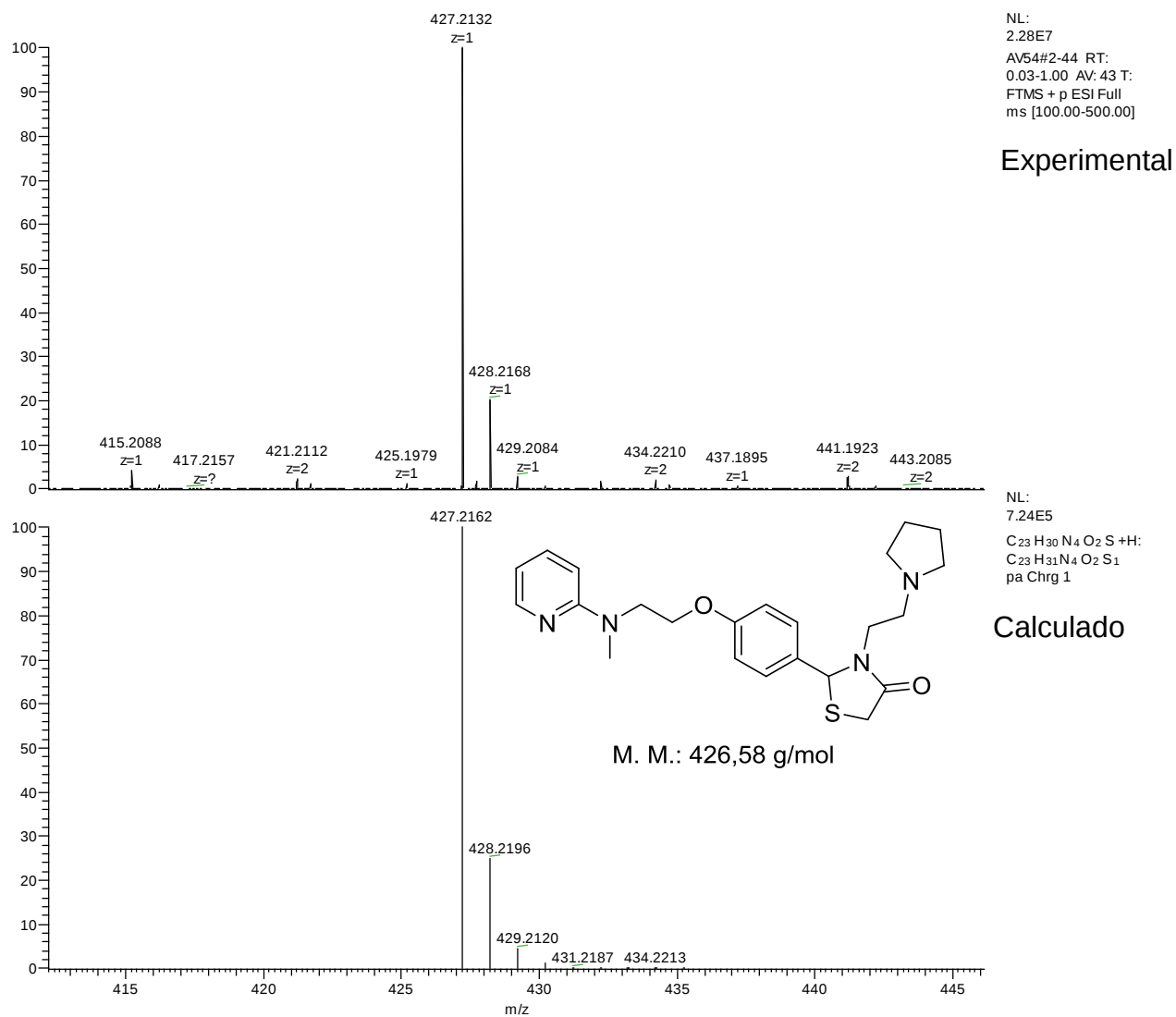


Figura 91: Expansão do espectro EMAR da tiazolidin-4-ona **8a**.

Anexo II: Espectrometria de EMAR

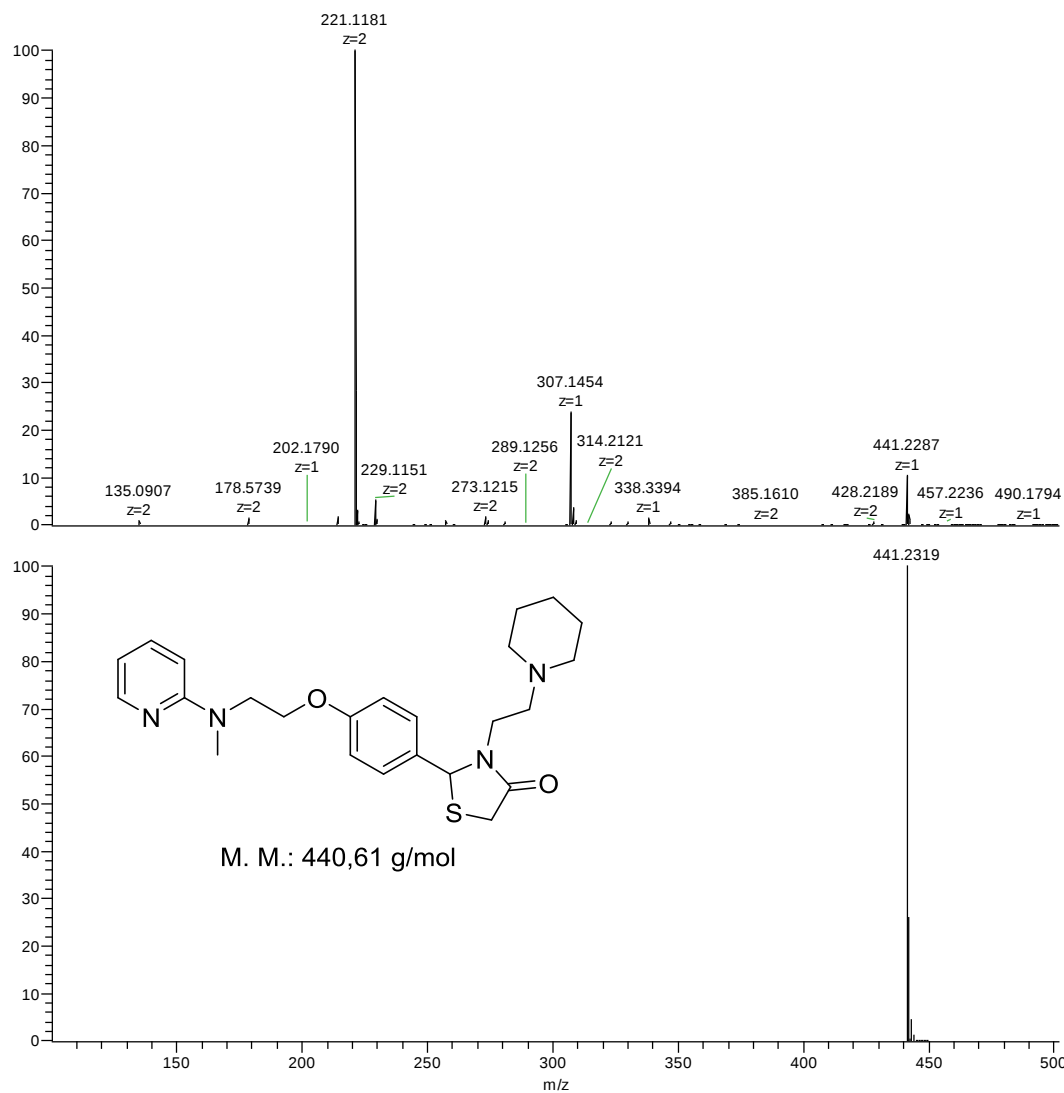


Figura 92: Espectro EMAR da tiazolidin-4-ona **8b**.

Anexo II: Espectrometria de EMAR

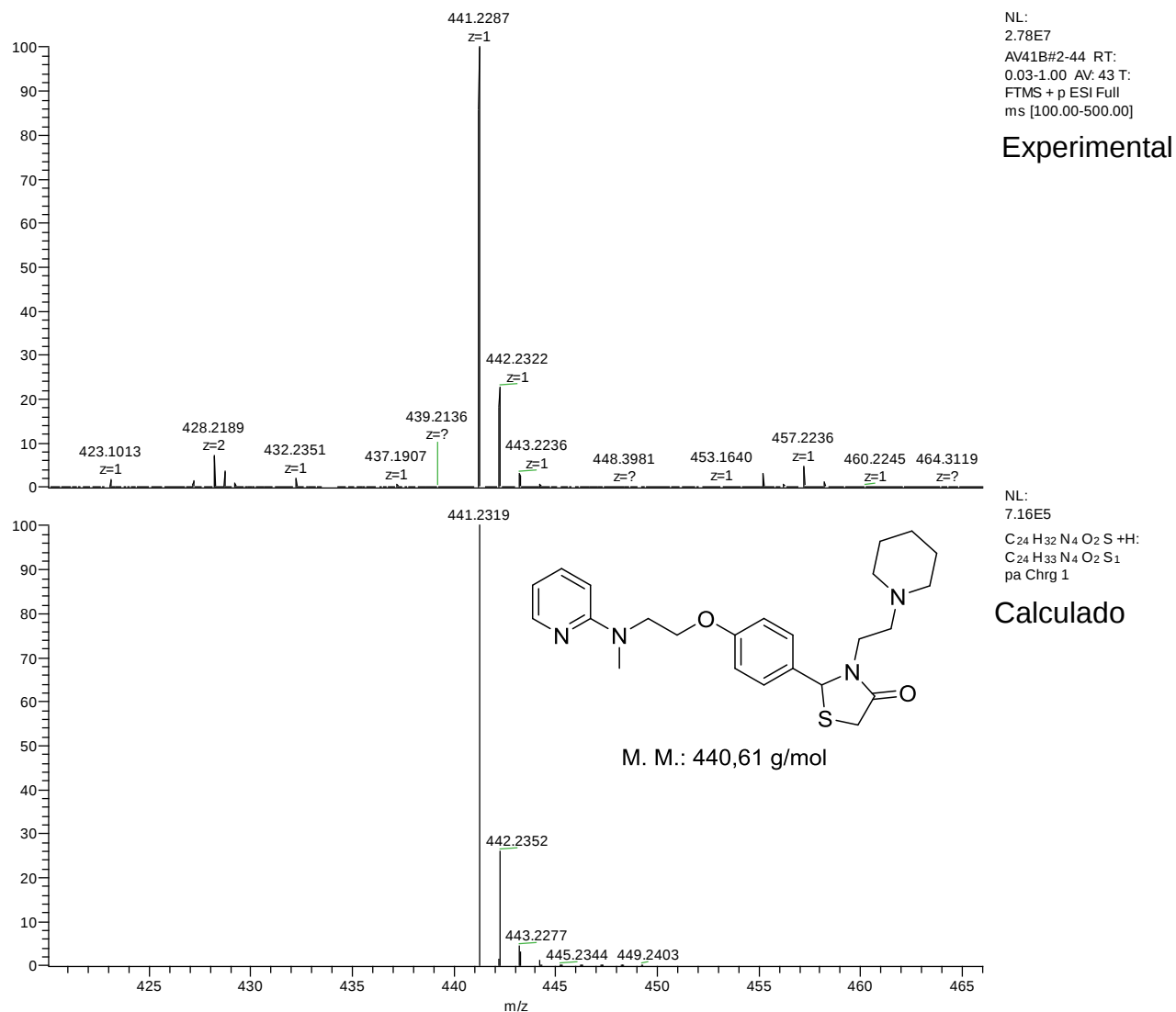


Figura 93: Expansão do espectro EMAR da tiazolidin-4-ona **8b**.

Anexo II: Espectrometria de EMAR

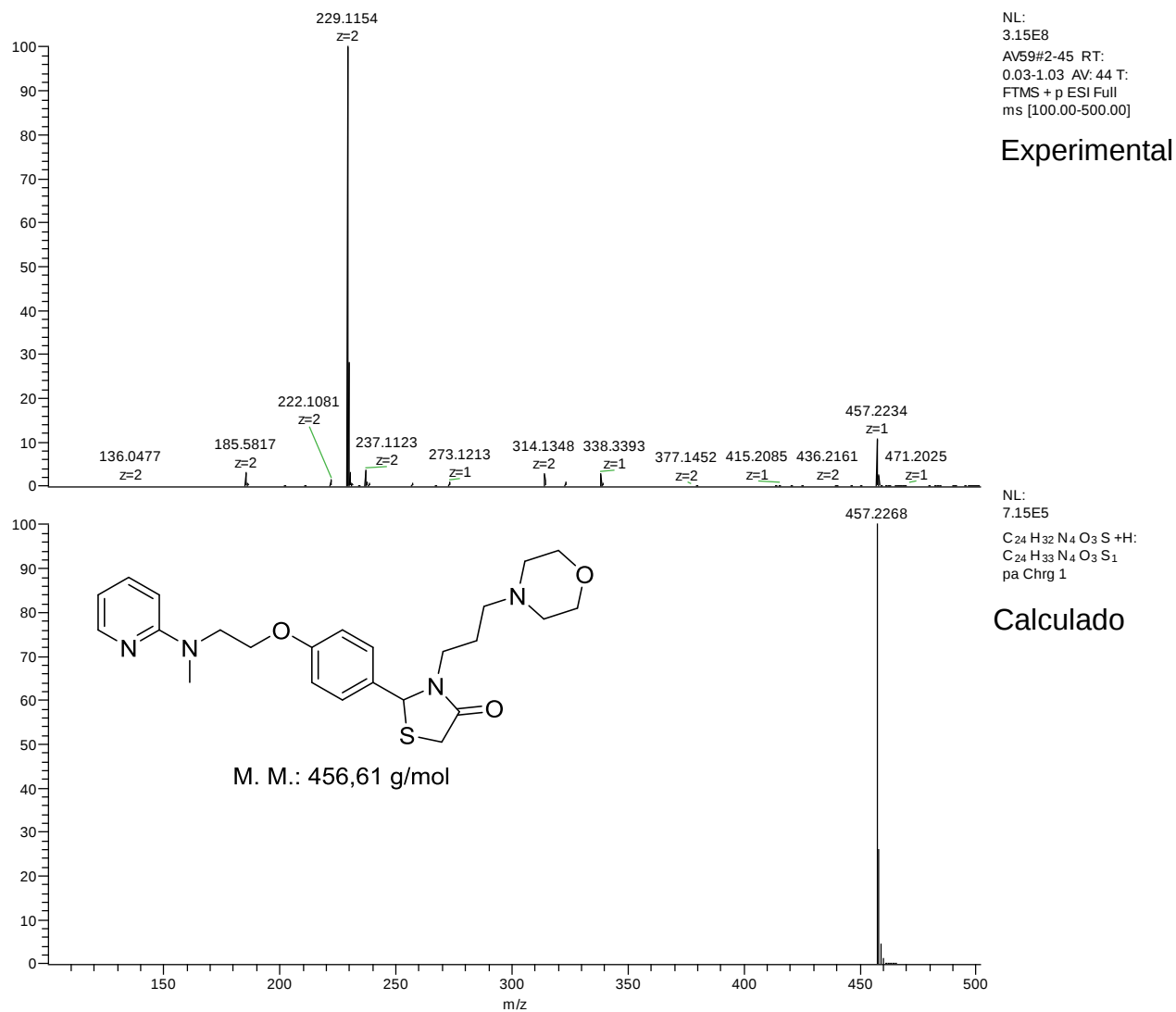
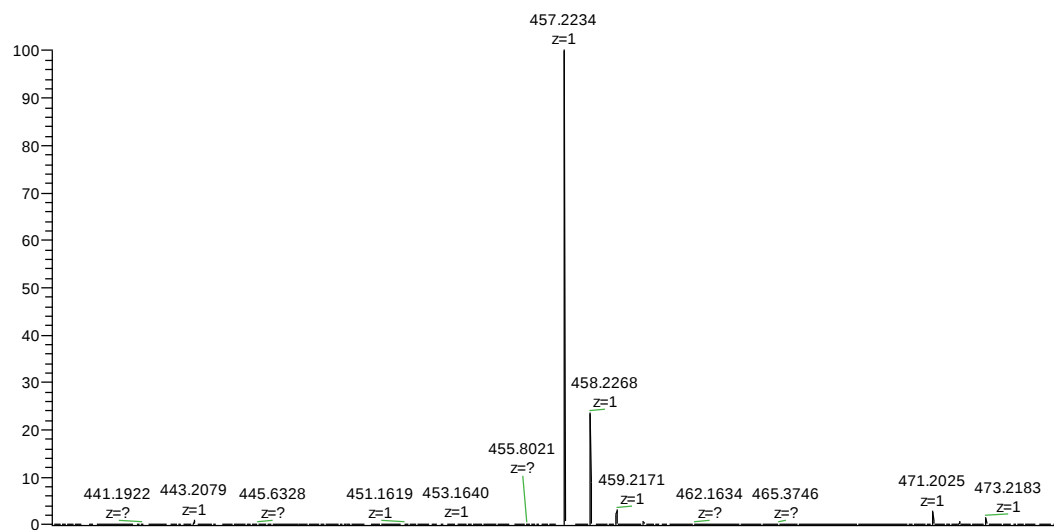


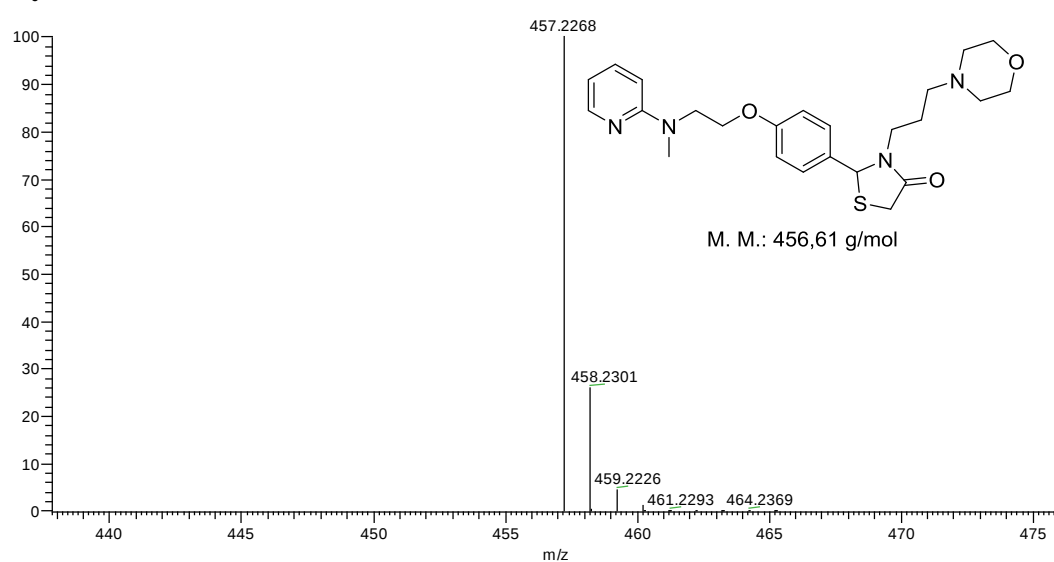
Figura 94: Espectro EMAR da tiazolidin-4-ona **8f**.

Anexo II: Espectrometria de EMAR



NL:
3.38E7
AV59#2-45 RT:
0.03-1.03 AV: 44 T:
FTMS + p ESI Full
ms [100.00-500.00]

Experimental



NL:
7.15E5
C₂₄H₃₂N₄O₃S +H:
C₂₄H₃₃N₄O₃S₁
pa Chrg 1

Calculado

Figura 95: Expansão do espectro EMAR da tiazolidin-4-ona **8f**.

Anexo II: Espectrometria de EMAR

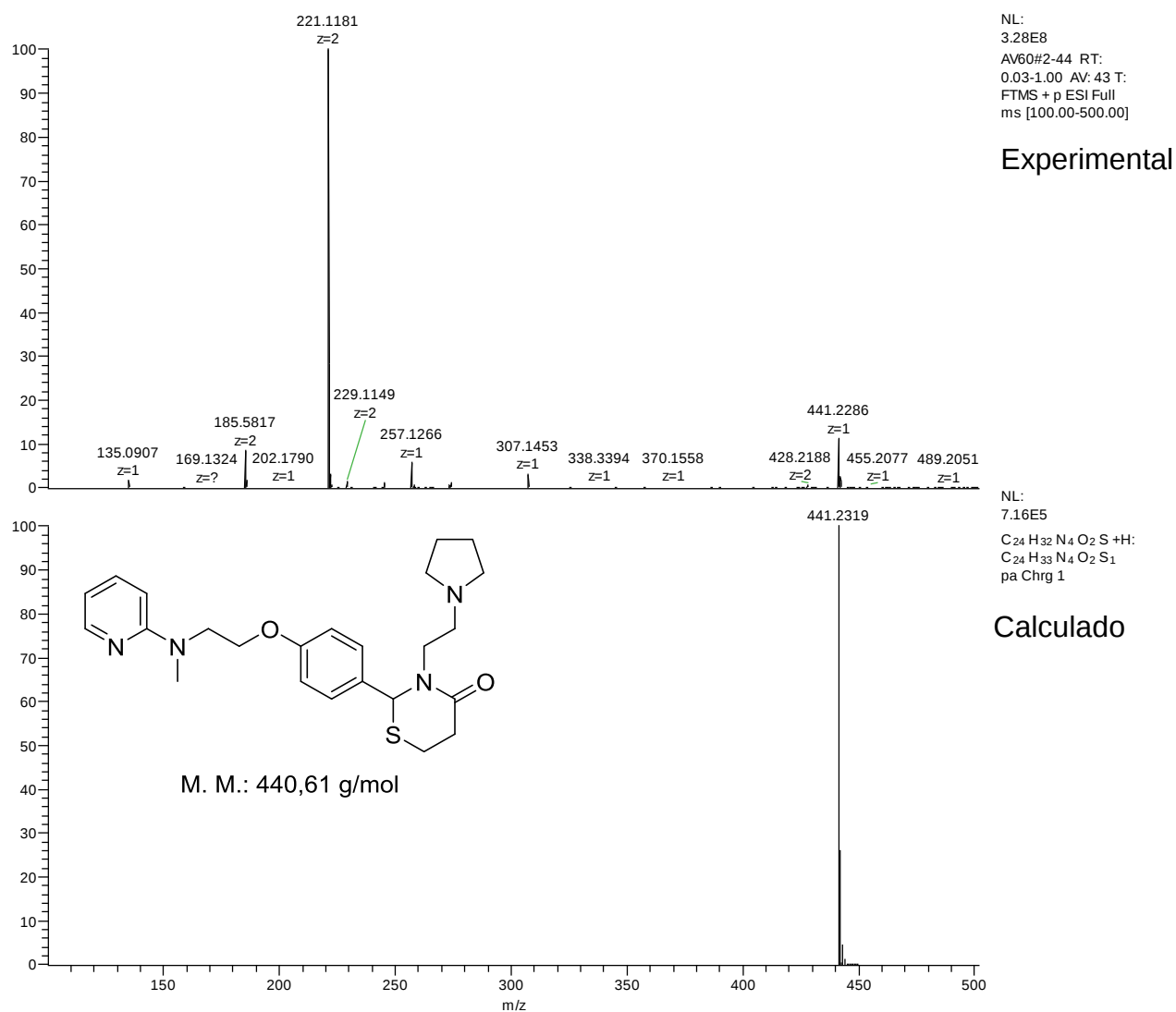
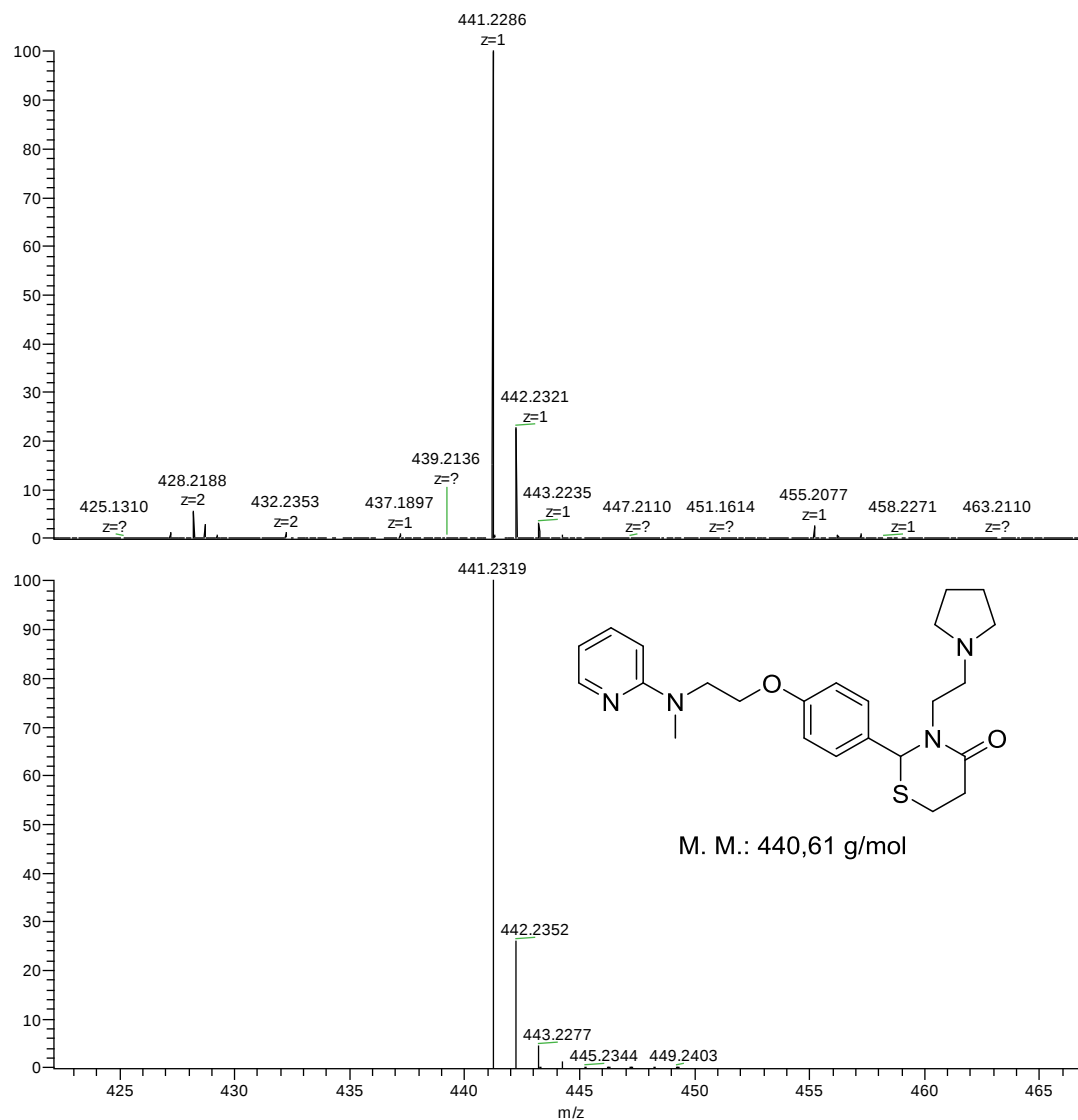


Figura 96: Espectro EMAR da tiazinan-4-ona **9a**.

Anexo II: Espectrometria de EMAR



NL:
3.69E7
AV60#2-44 RT:
0.03-1.00 AV: 43 T:
FTMS + p ESI Full
ms [100.00-500.00]

Experimental

NL:
7.16E5
C₂₄ H₃₂ N₄ O₂ S +H:
C₂₄ H₃₃ N₄ O₂ S₁
pa Chrg 1

Calculado

Figura 97: Expansão do espectro EMAR da tiazinan-4-ona **9a**.

Anexo II: Espectrometria de EMAR

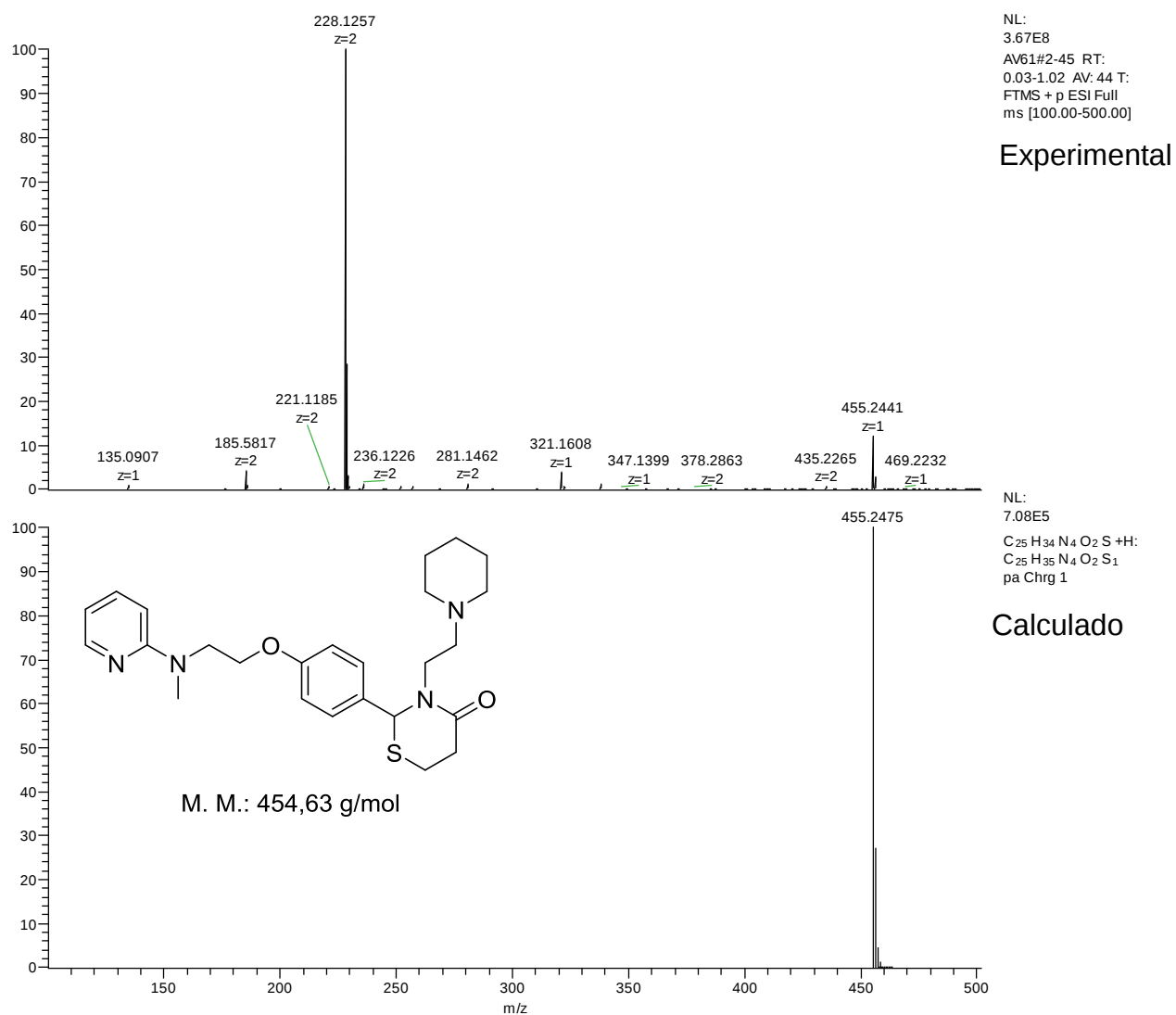


Figura 98: Espectro EMAR da tiazinan-4-ona **9b**.

Anexo II: Espectrometria de EMAR

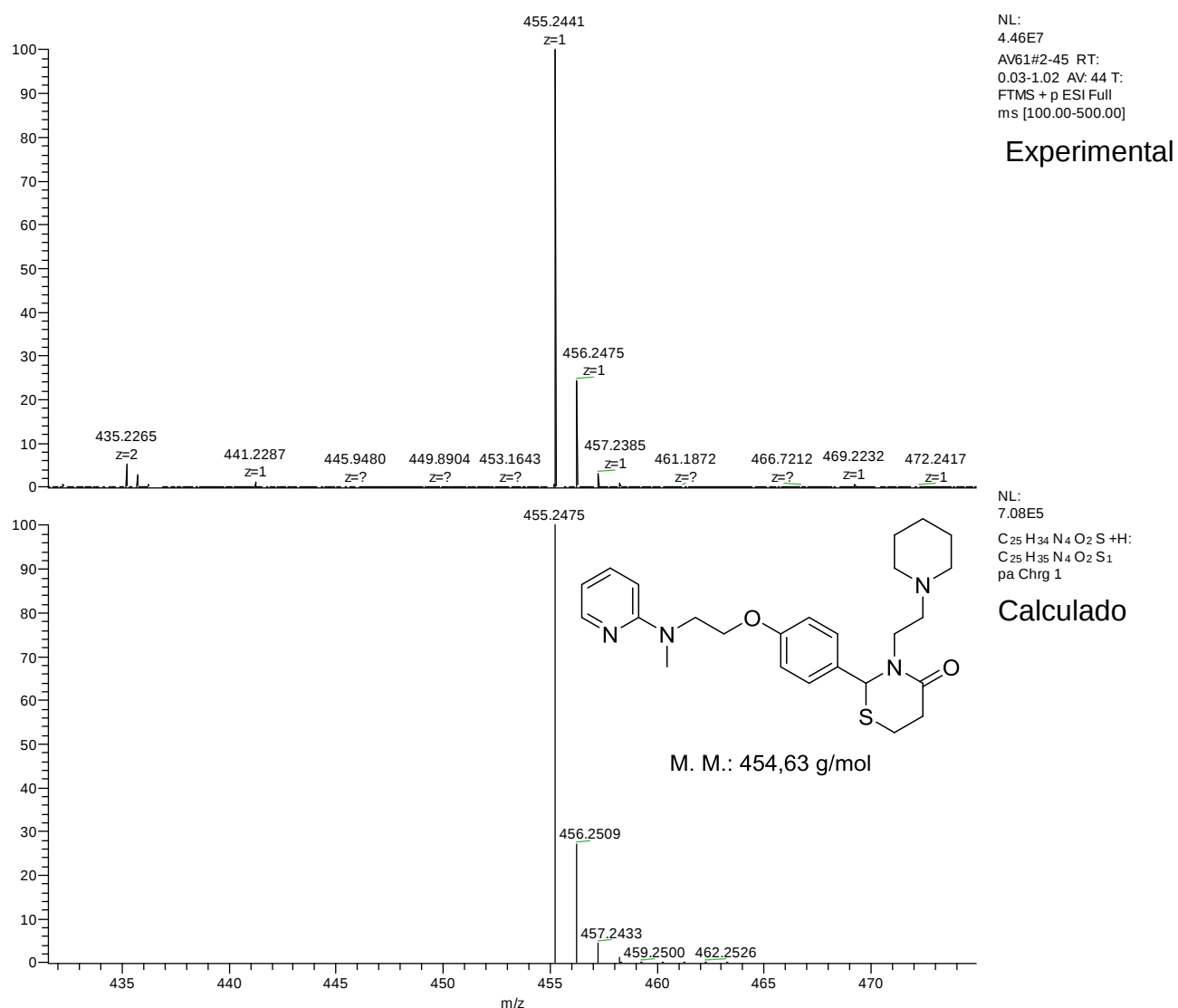


Figura 99: Expansão do espectro EMAR da tiazinan-4-ona **9b**.

Anexo II: Espectrometria de EMAR

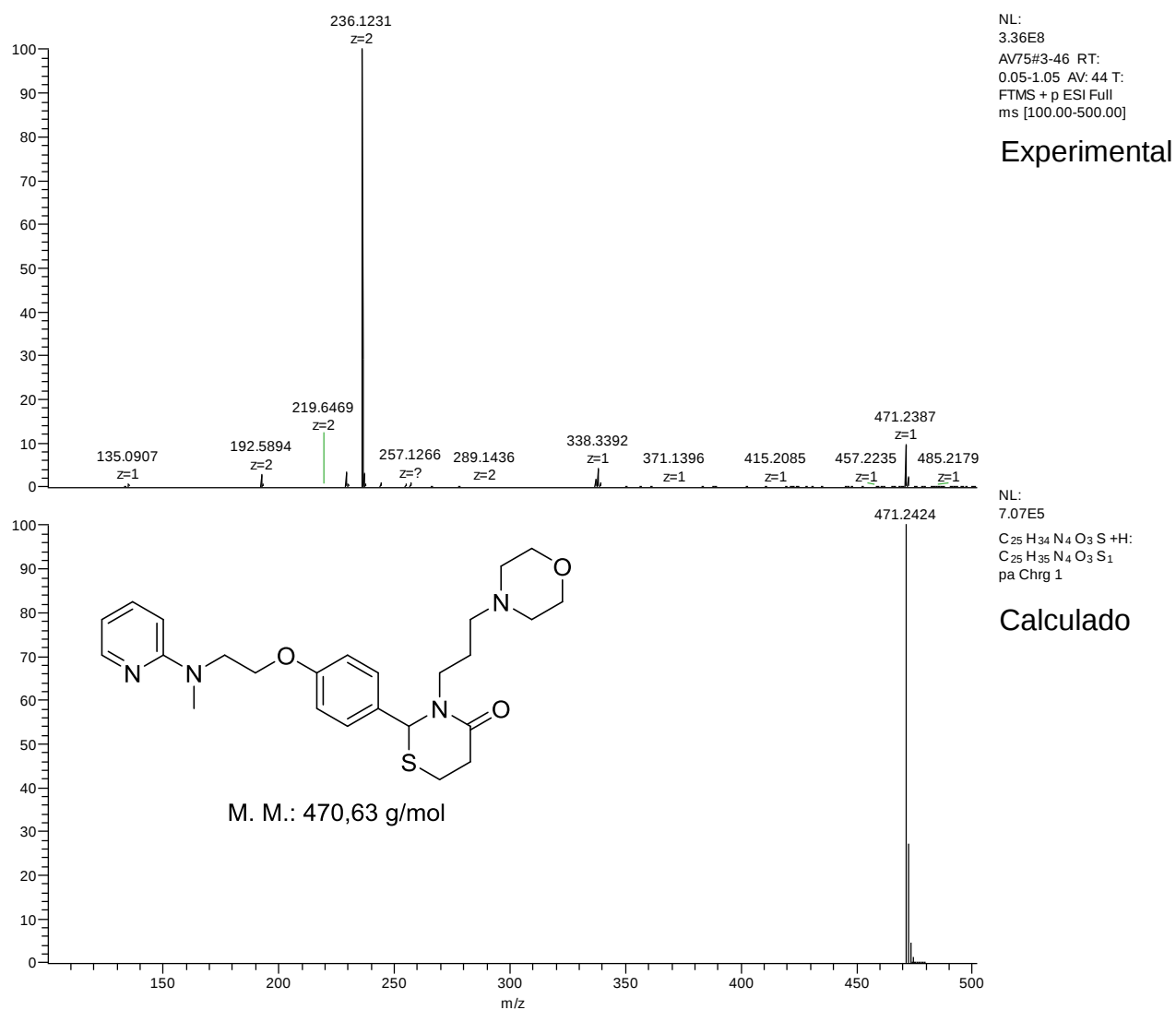


Figura 100: Espectro EMAR da tiazinan-4-ona **9f**.

Anexo II: Espectrometria de EMAR

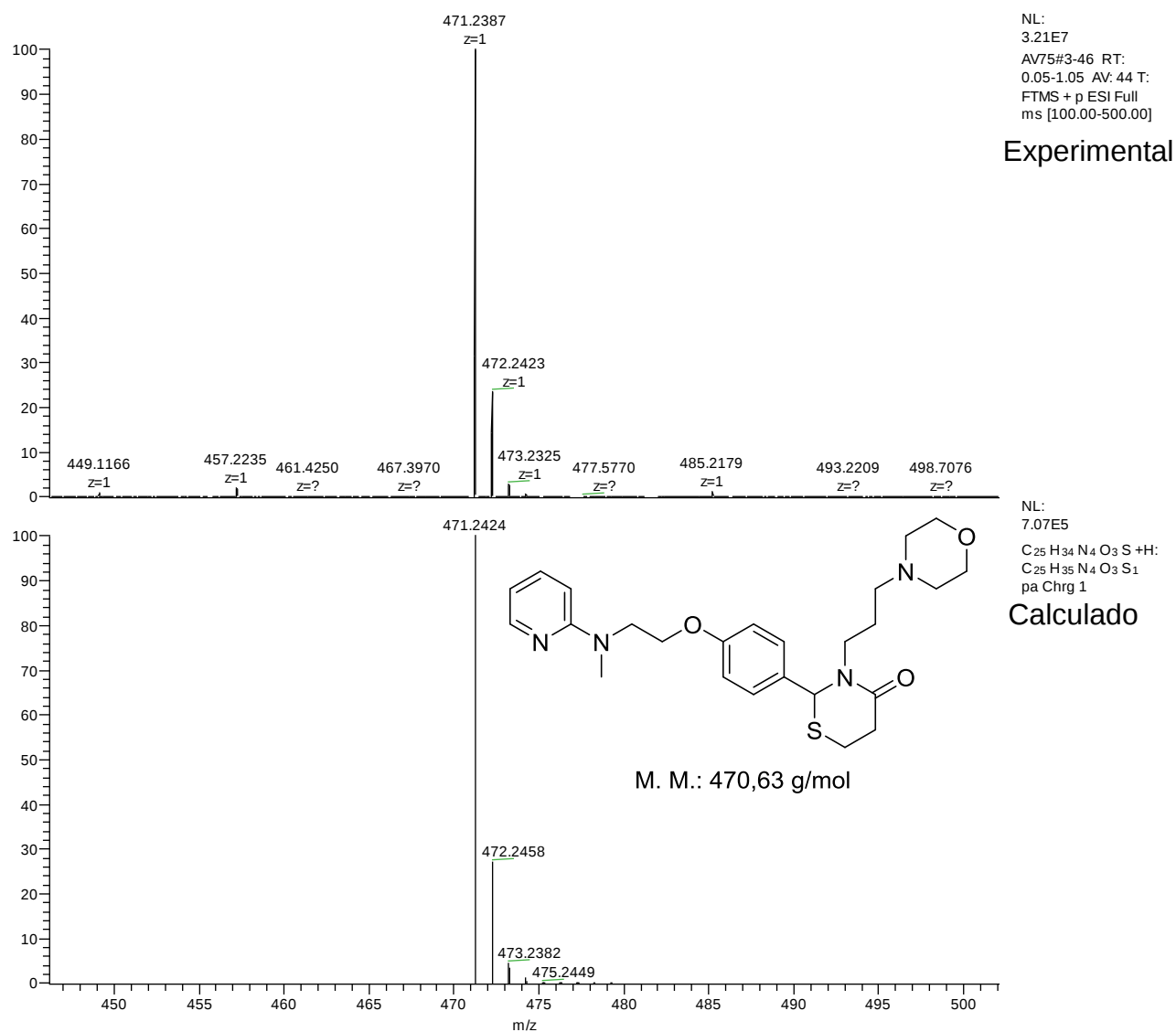


Figura 101: Expansão do espectro EMAR da tiazinan-4-ona **9f**.

Anexo III: Espectros de RMN ^1H e ^{13}C

Anexo III: Espectroscopia de RMN

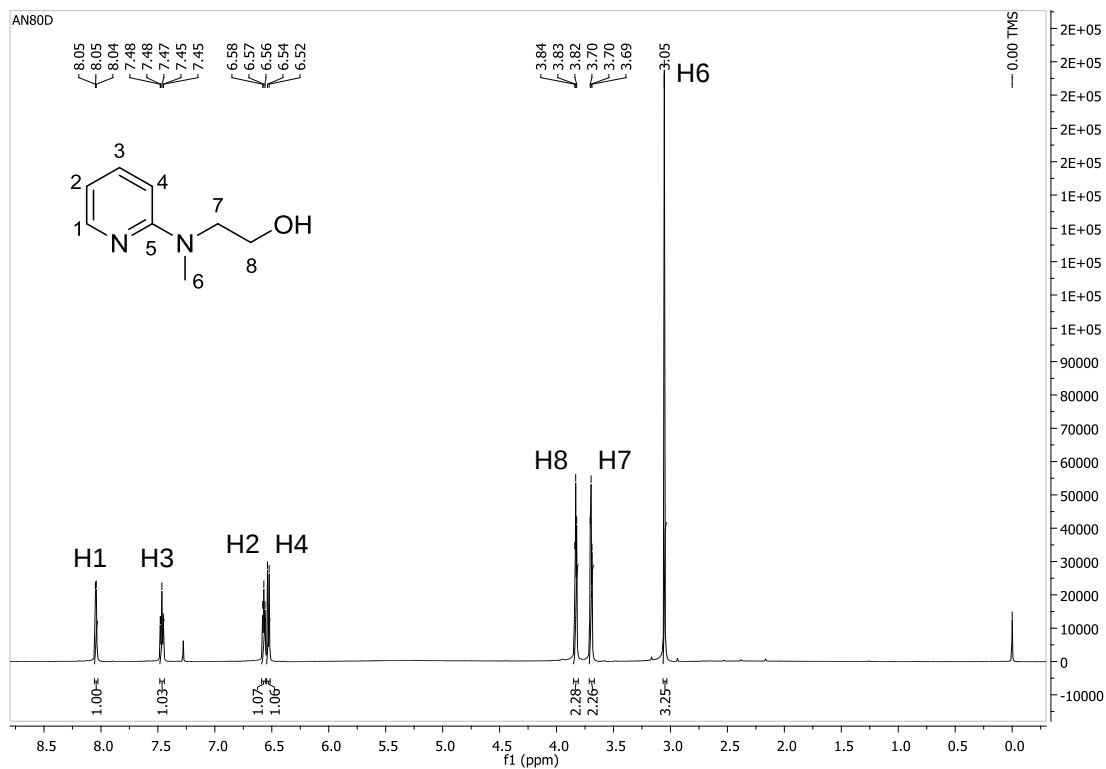


Figura 102: Espectro de RMN de ^1H do 2-(metilpiridin-2-il)aminoetanol **3** (CDCl_3 - 600 MHz).

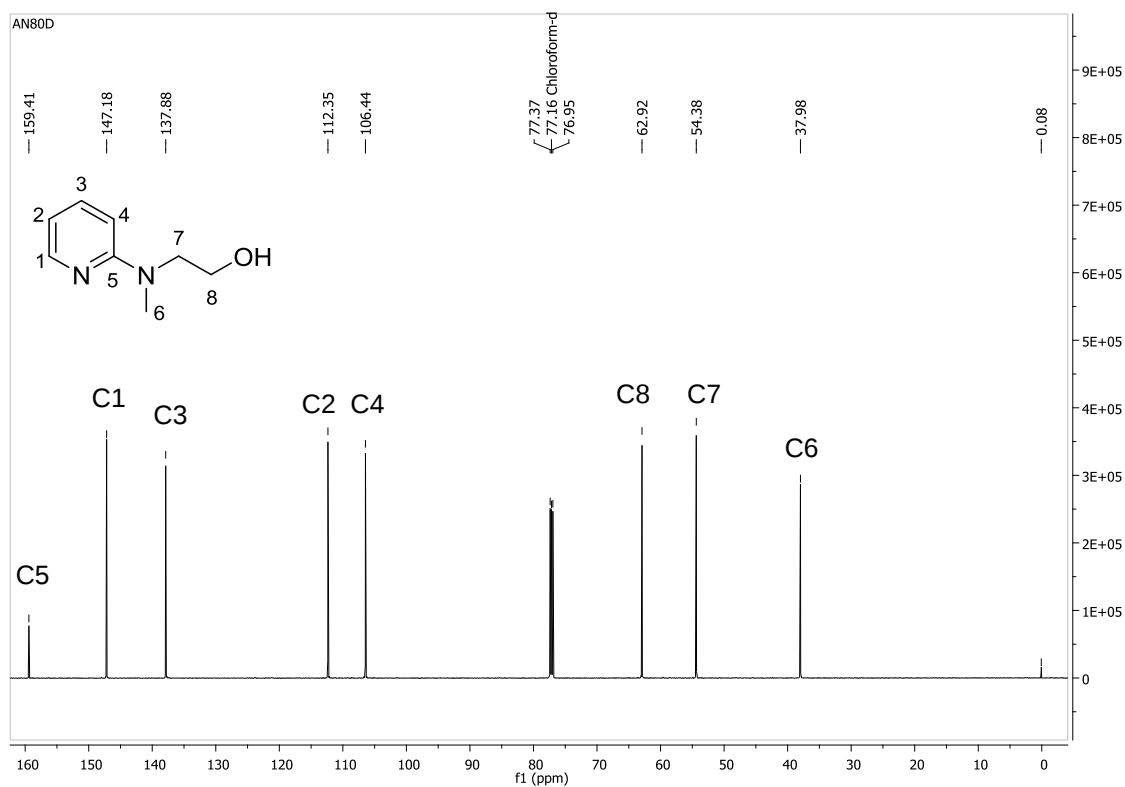


Figura 103: Espectro de RMN de ^{13}C do 2-(metilpiridin-2-il)aminoetanol **3** (CDCl_3 - 150 MHz).

Anexo III: Espectroscopia de RMN

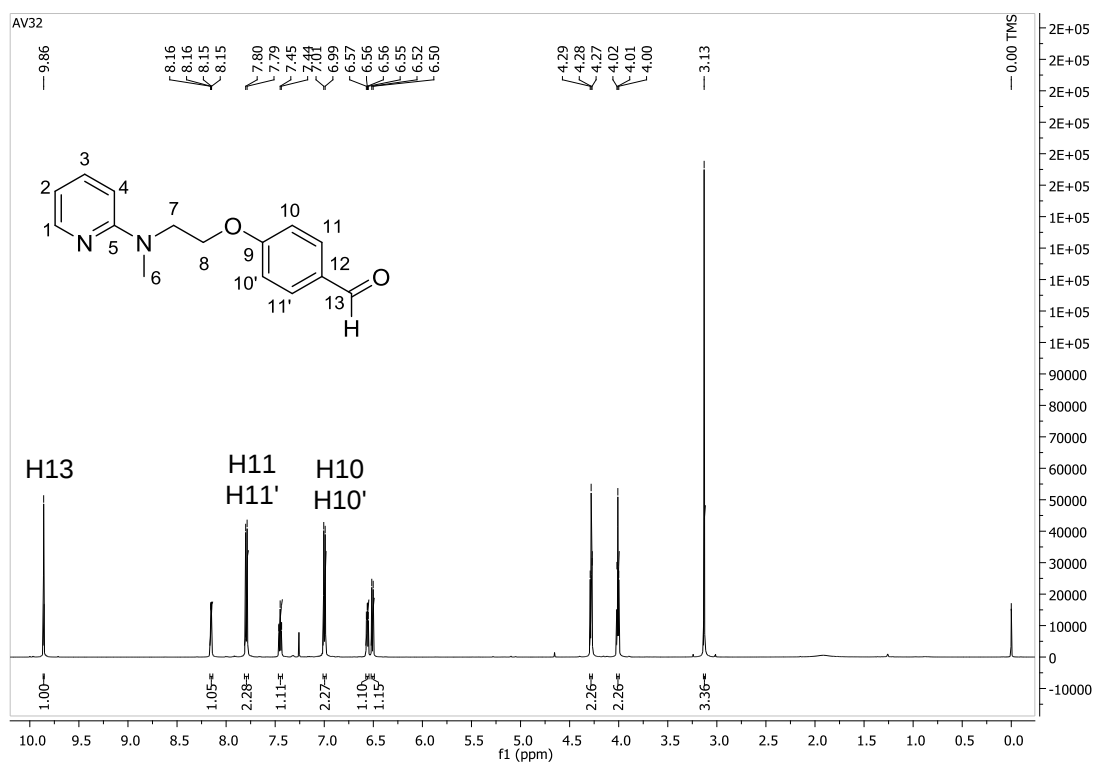


Figura 104: Espectro de RMN de ^1H do 4-(2-(metil(piridin-2-il)amino)etoxi) benzaldeído **5** (CDCl_3 - 600 MHz).

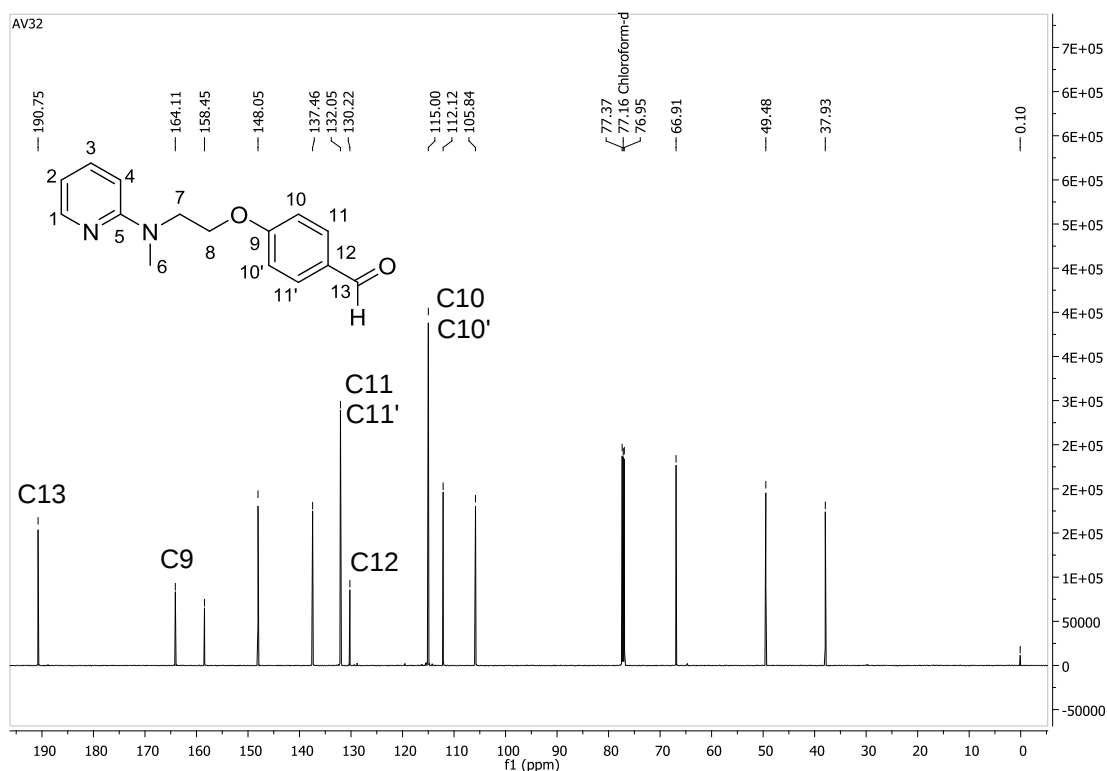


Figura 105: Espectro de RMN de ^{13}C do 4-(2-(metil(piridin-2-il)amino)etoxi) benzaldeído **5** (CDCl_3 - 150 MHz).

Anexo III: Espectroscopia de RMN

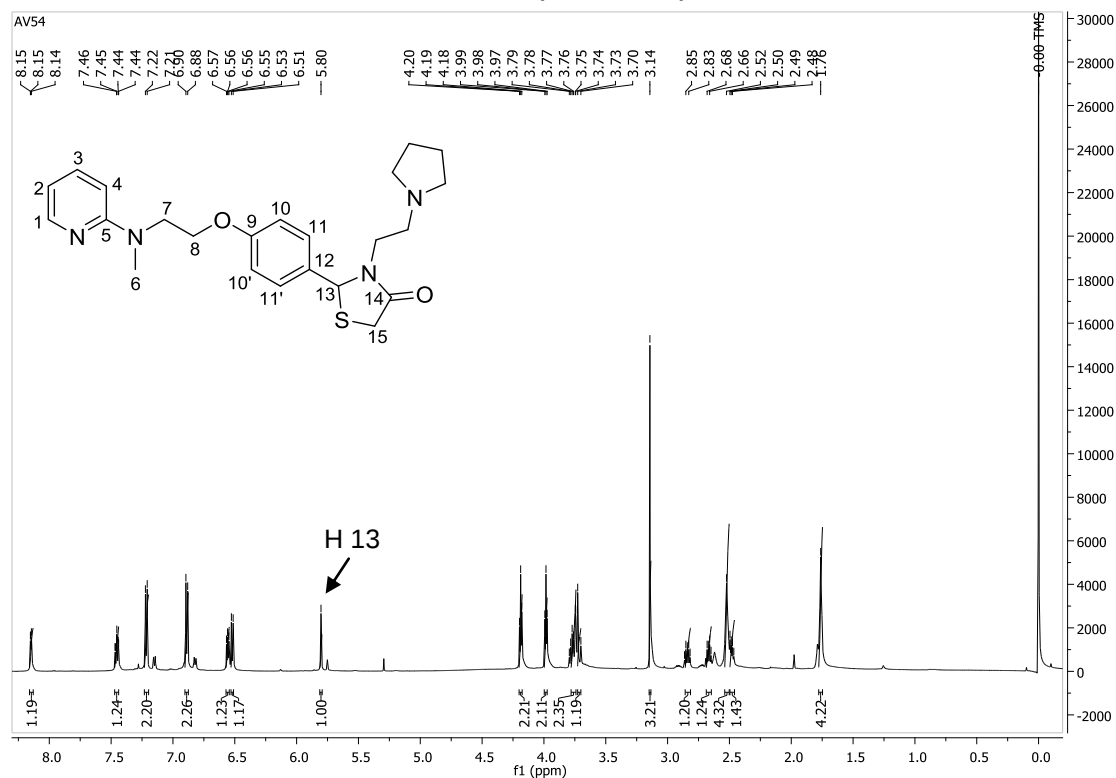


Figura 106: Espectro de RMN ¹H da tiazolidin-4-ona **8a** (CDCl₃ - 600 MHZ).

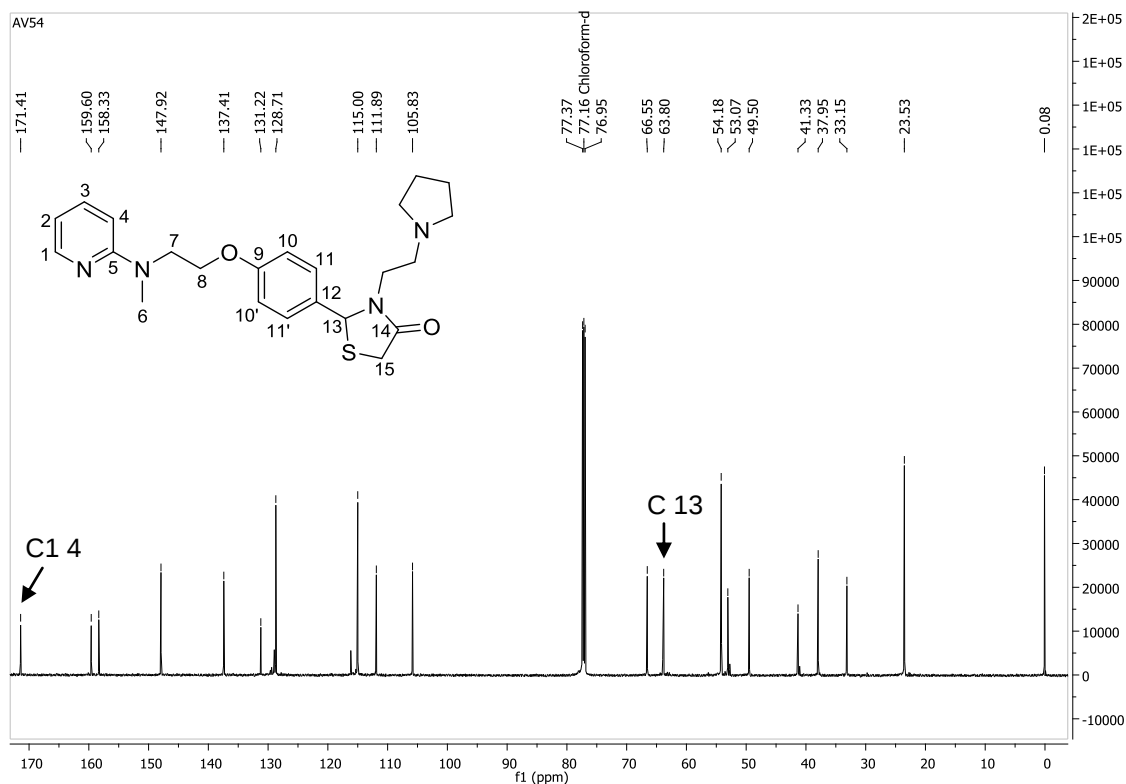


Figura 107: Espectro de ¹³C da tiazolidin-4-ona **8a** (CDCl₃ - 150 MHZ).

Anexo III: Espectroscopia de RMN

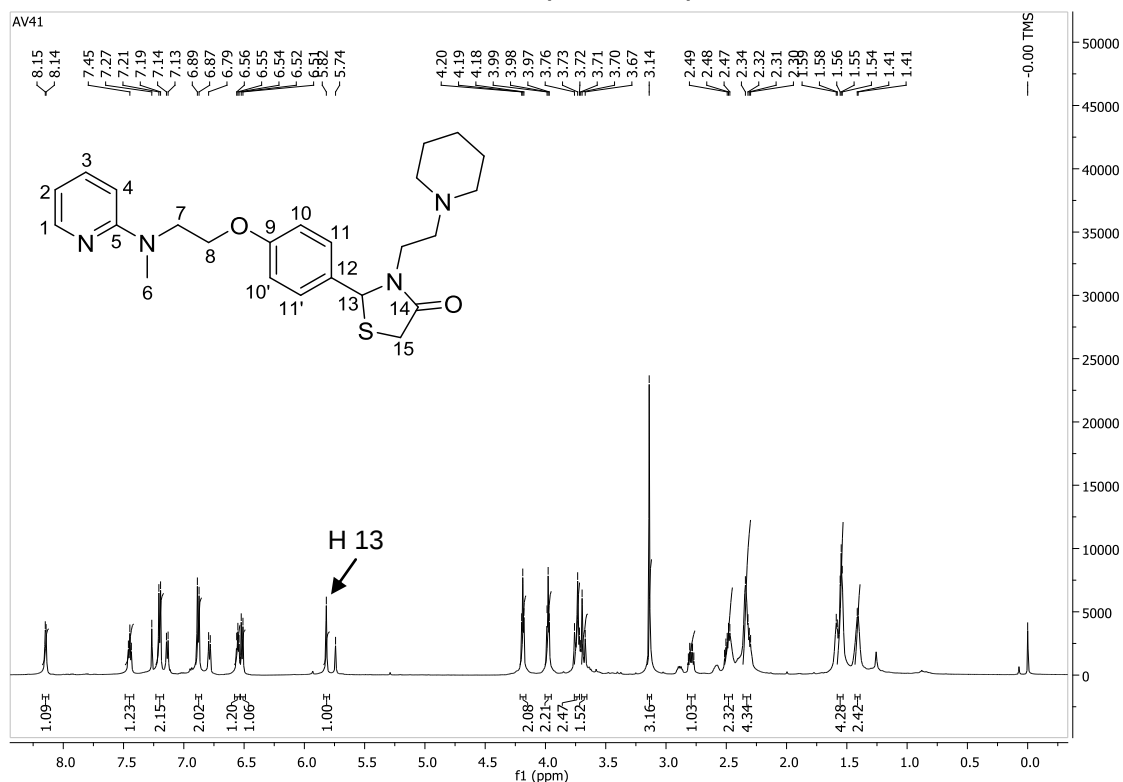


Figura 108: Espectro de RMN ¹H da tiazolidin-4-ona **8b** (CDCl₃ - 600 MHZ).

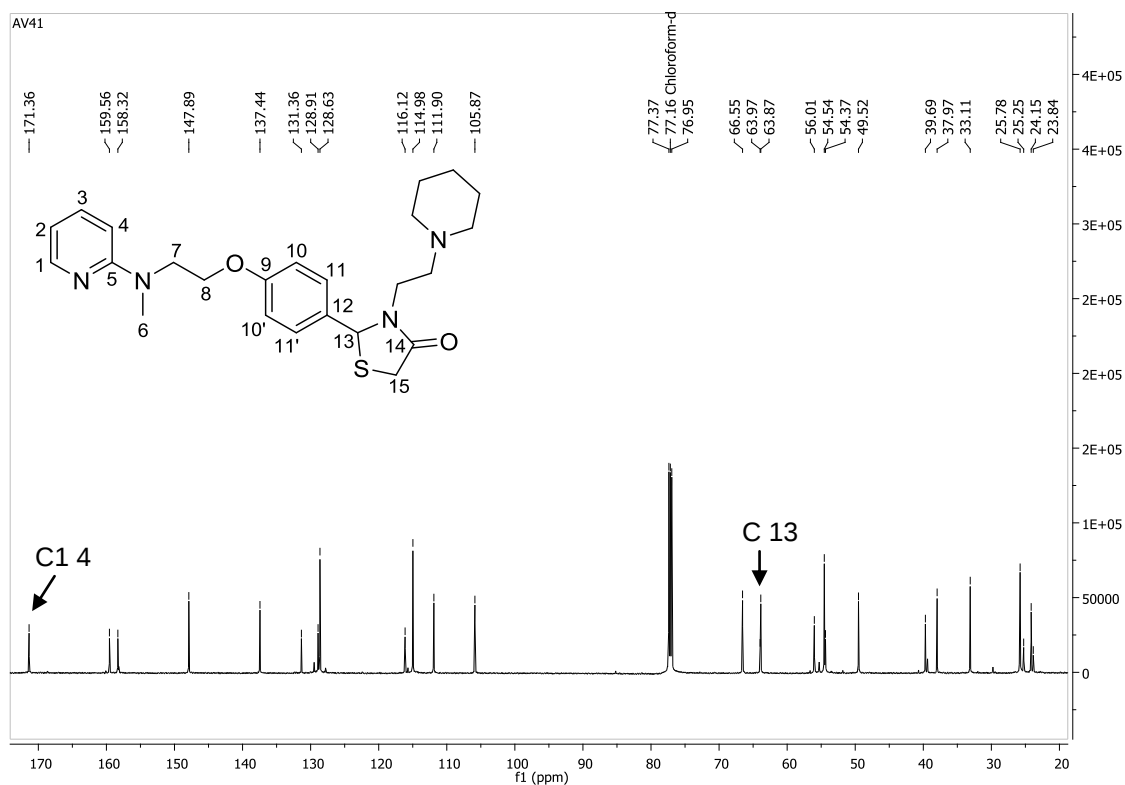


Figura 109: Espectro de ¹³C da tiazolidin-4-ona **8b** (CDCl₃ - 150 MHZ).

Anexo III: Espectroscopia de RMN

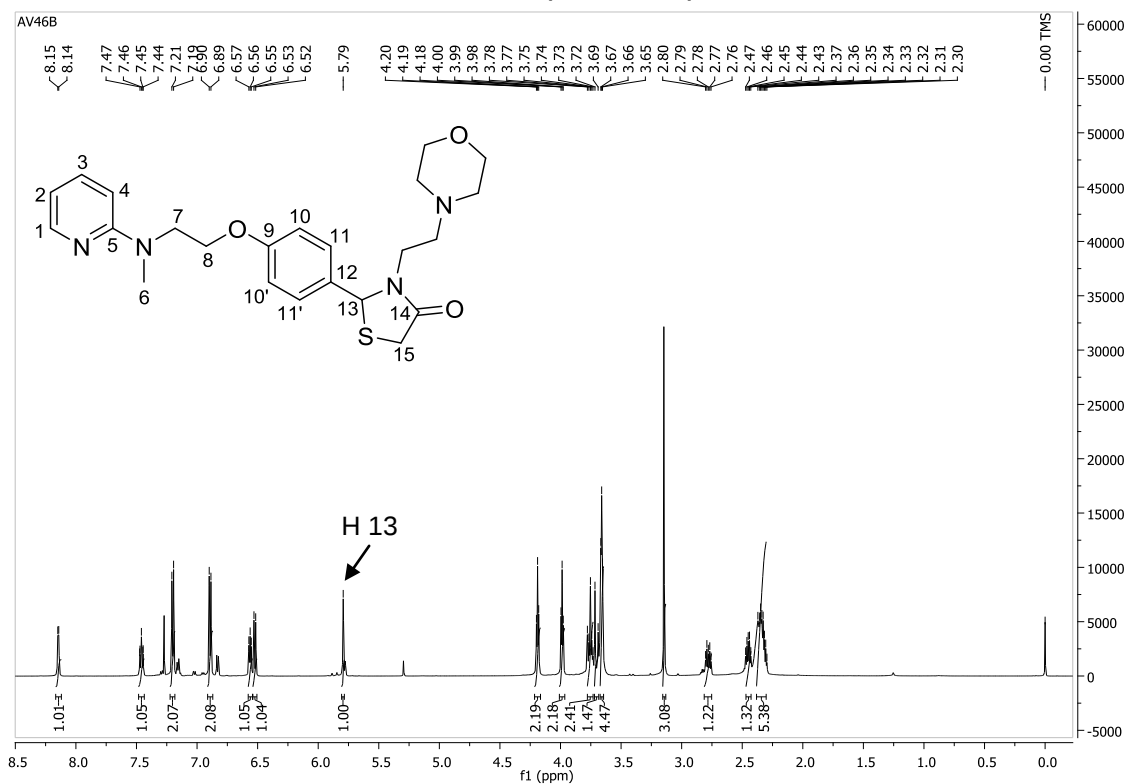


Figura 110: Espectro de RMN ^1H da tiazolidin-4-ona **8c** (CDCl_3 - 600 MHz).

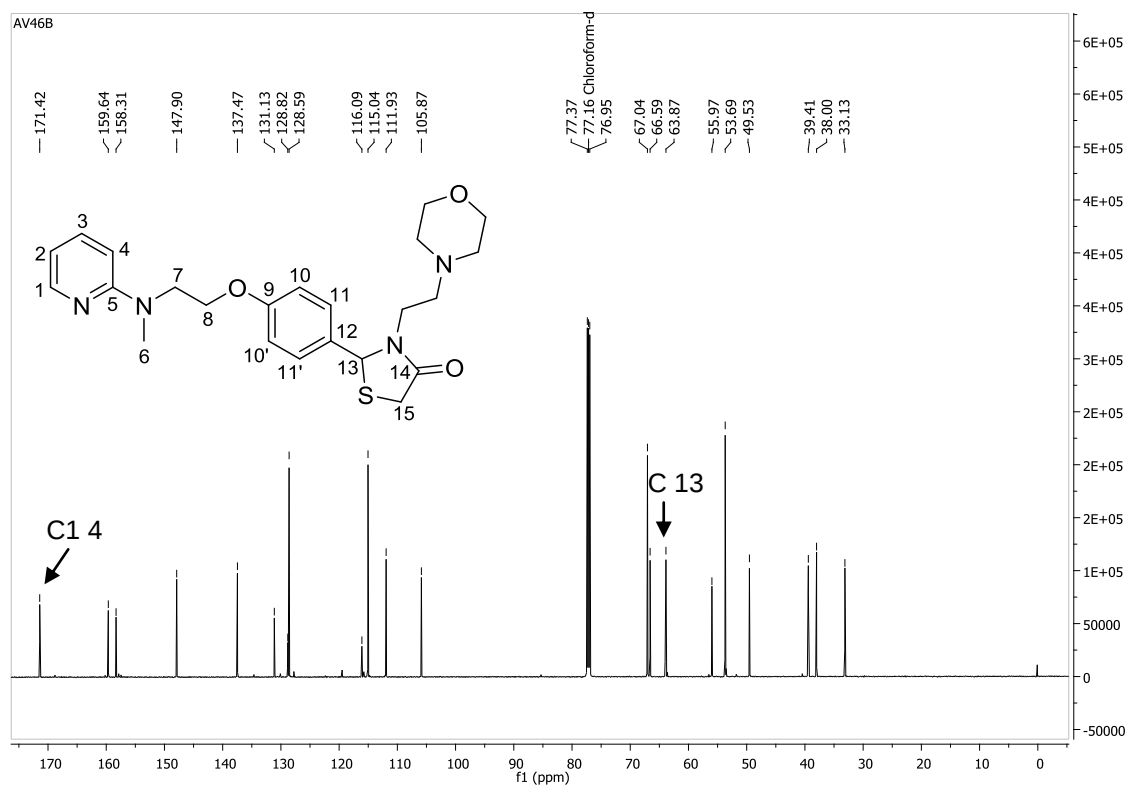


Figura 111: Espectro de ^{13}C da tiazolidin-4-ona **8c** (CDCl_3 - 150 MHz).

Anexo III: Espectroscopia de RMN

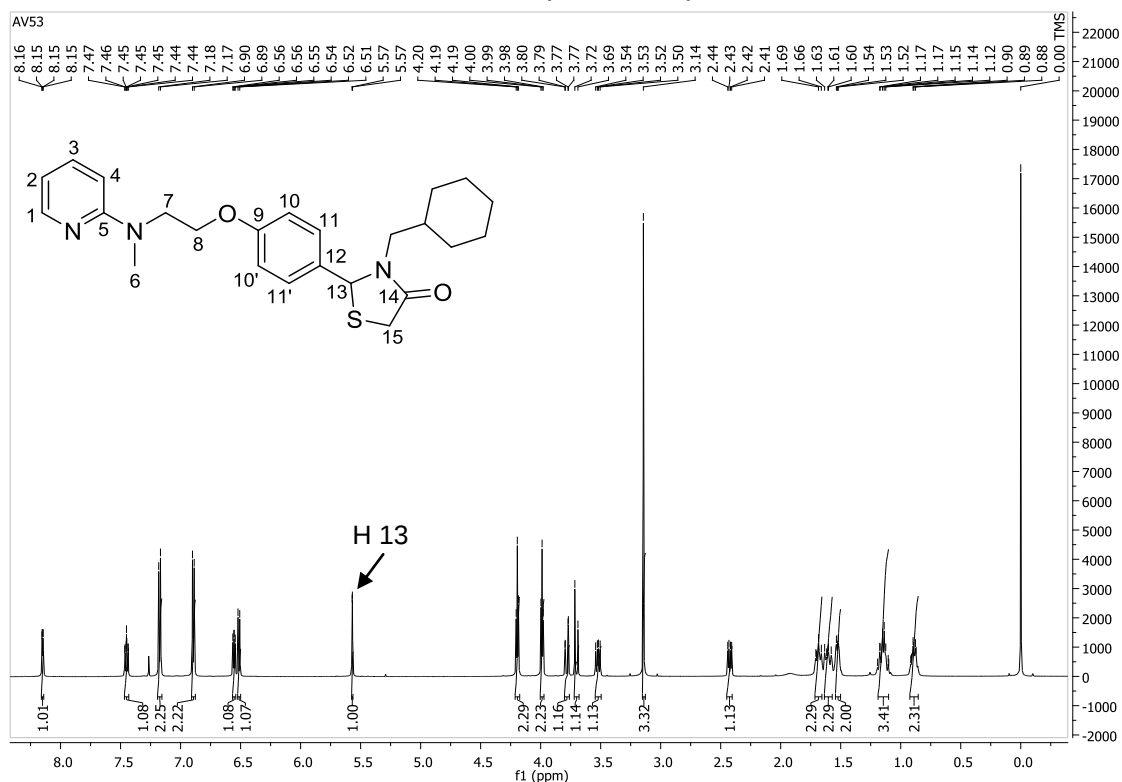


Figura 112: Espectro de RMN ^1H da tiazolidin-4-ona **8d** (CDCl_3 - 600 MHz).

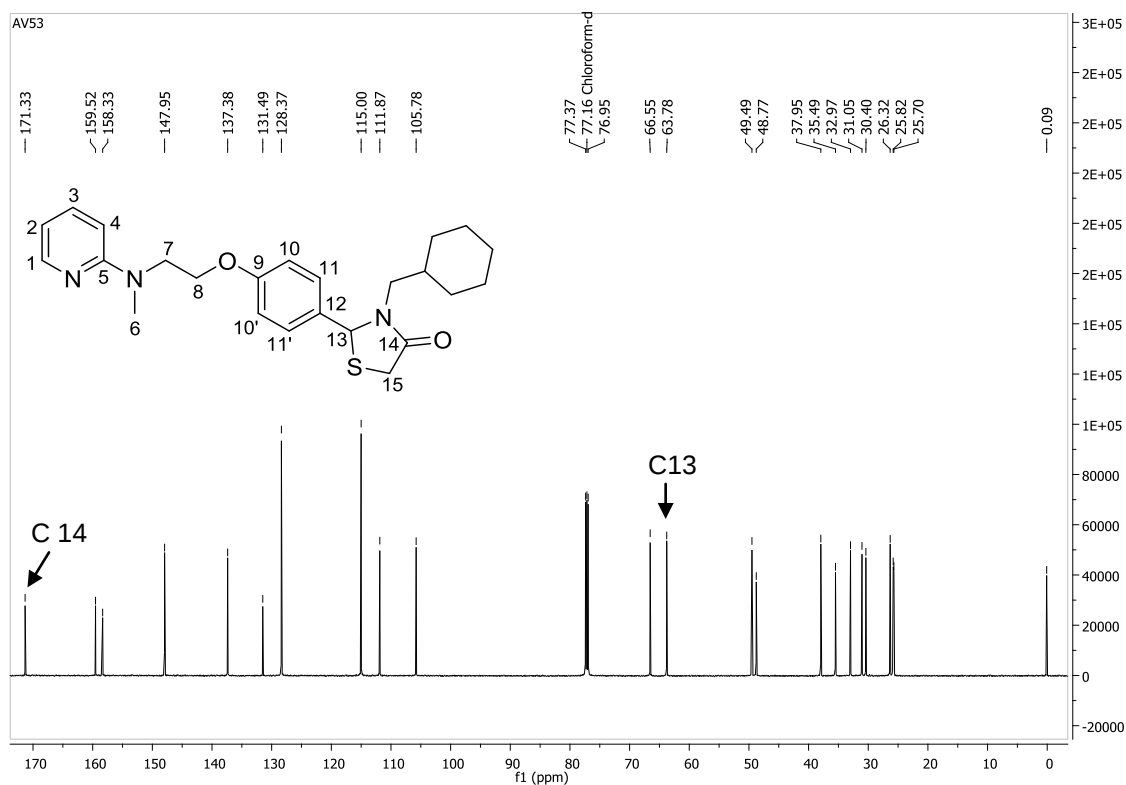


Figura 113: Espectro de ^{13}C da tiazolidin-4-ona **8d** (CDCl_3 - 150 MHz).

Anexo III: Espectroscopia de RMN

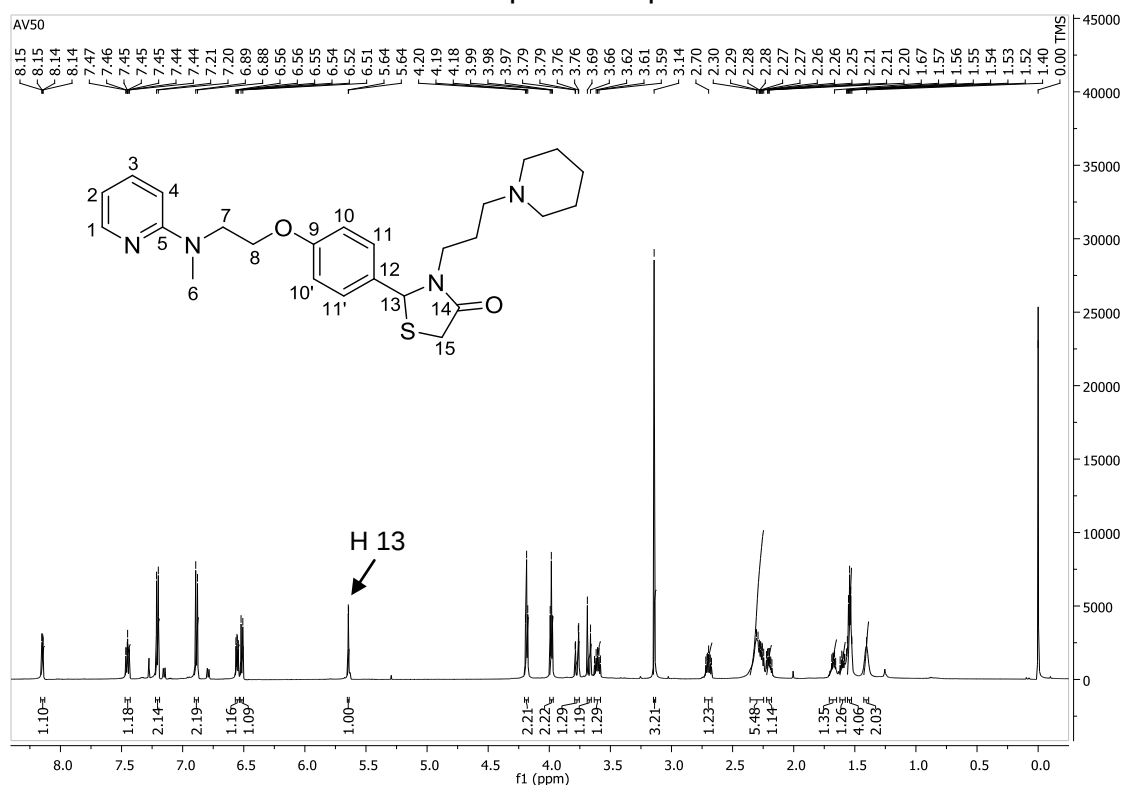


Figura 114: Espectro de RMN ¹H da tiazolidin-4-ona **8e** (CDCl₃ - 600 MHz).

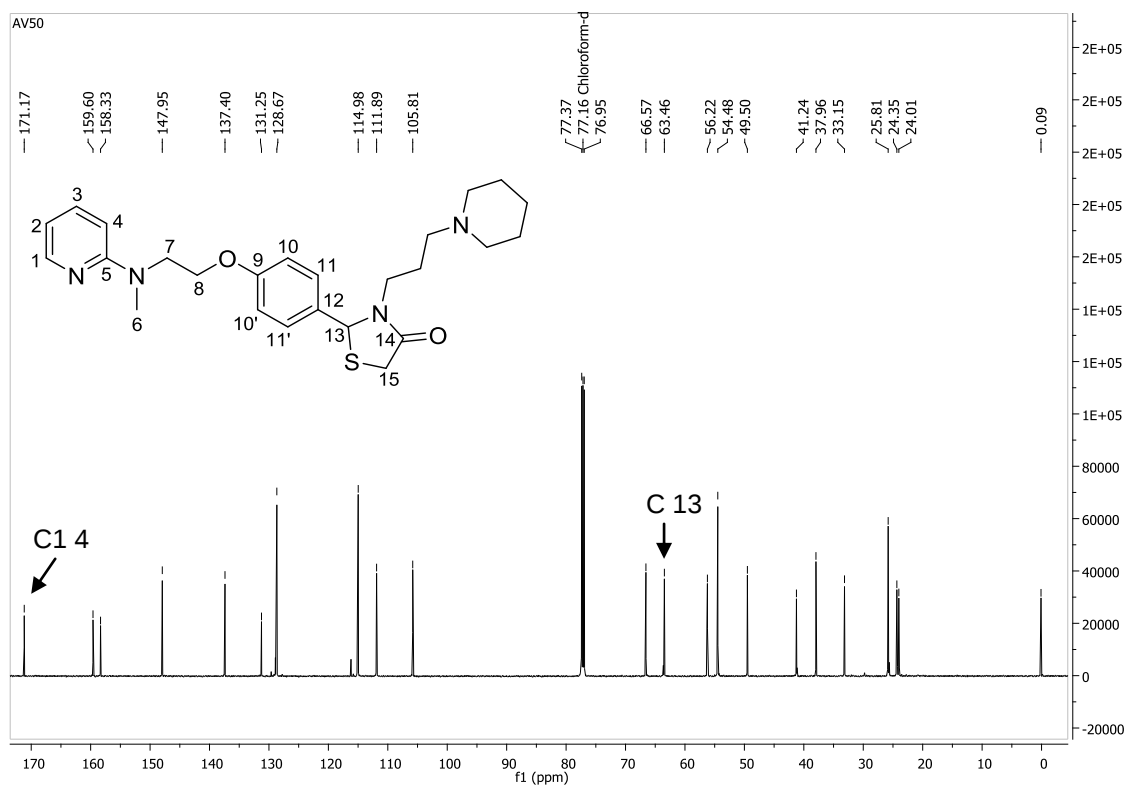


Figura 115: Espectro de ¹³C da tiazolidin-4-ona **8e** (CDCl₃ - 150 MHz).

Anexo III: Espectroscopia de RMN

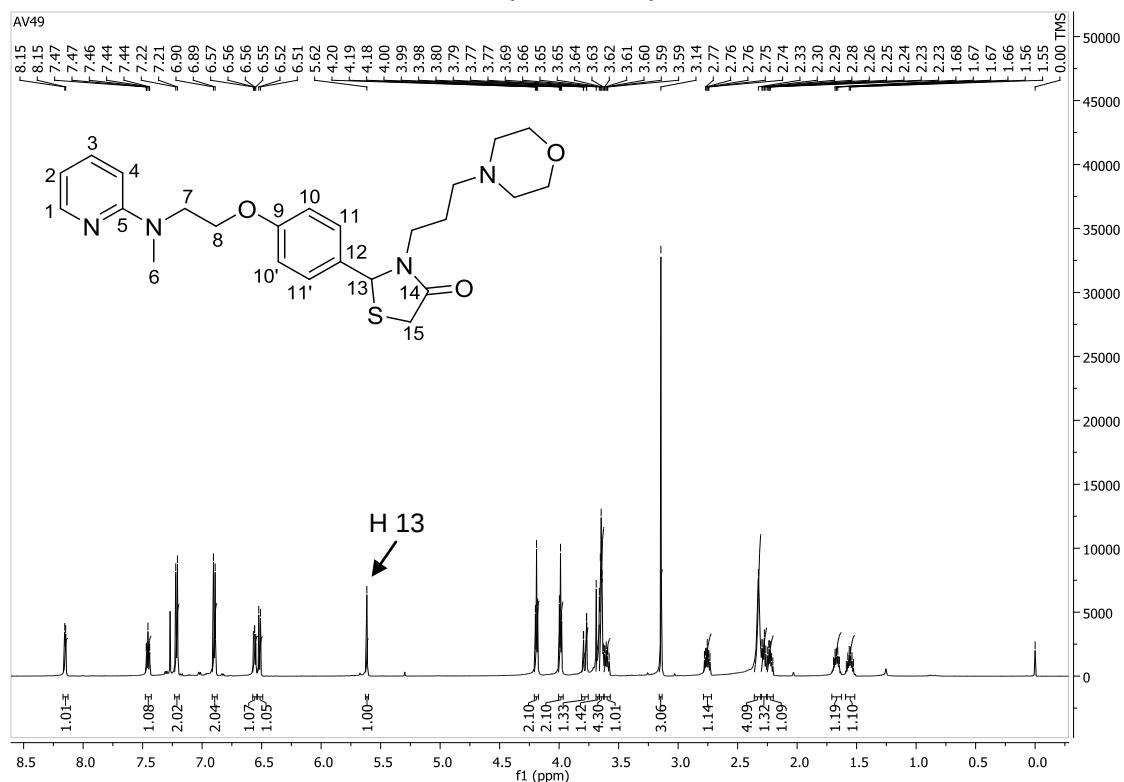


Figura 116: Espectro de RMN ¹H da tiazolidin-4-ona **8f** (CDCl₃ - 600 MHz).

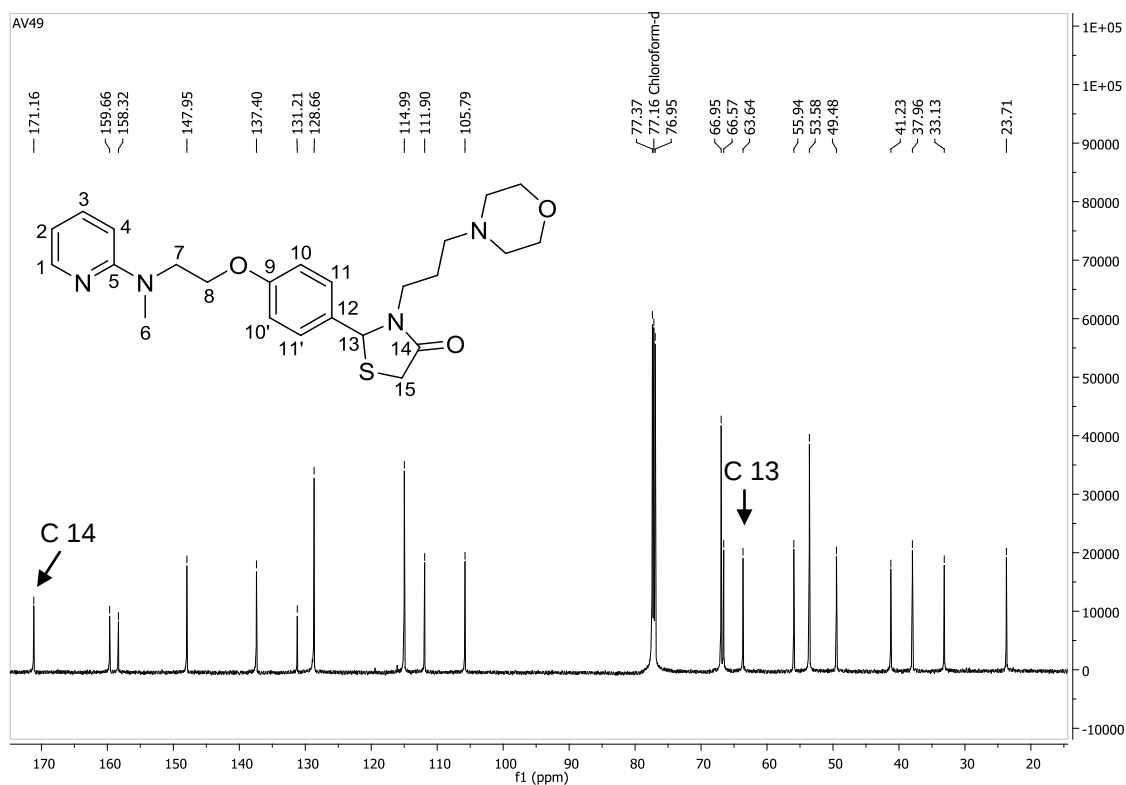


Figura 117: Espectro de ¹³C da tiazolidin-4-ona **8f** (CDCl₃ - 150 MHz).

Anexo III: Espectroscopia de RMN

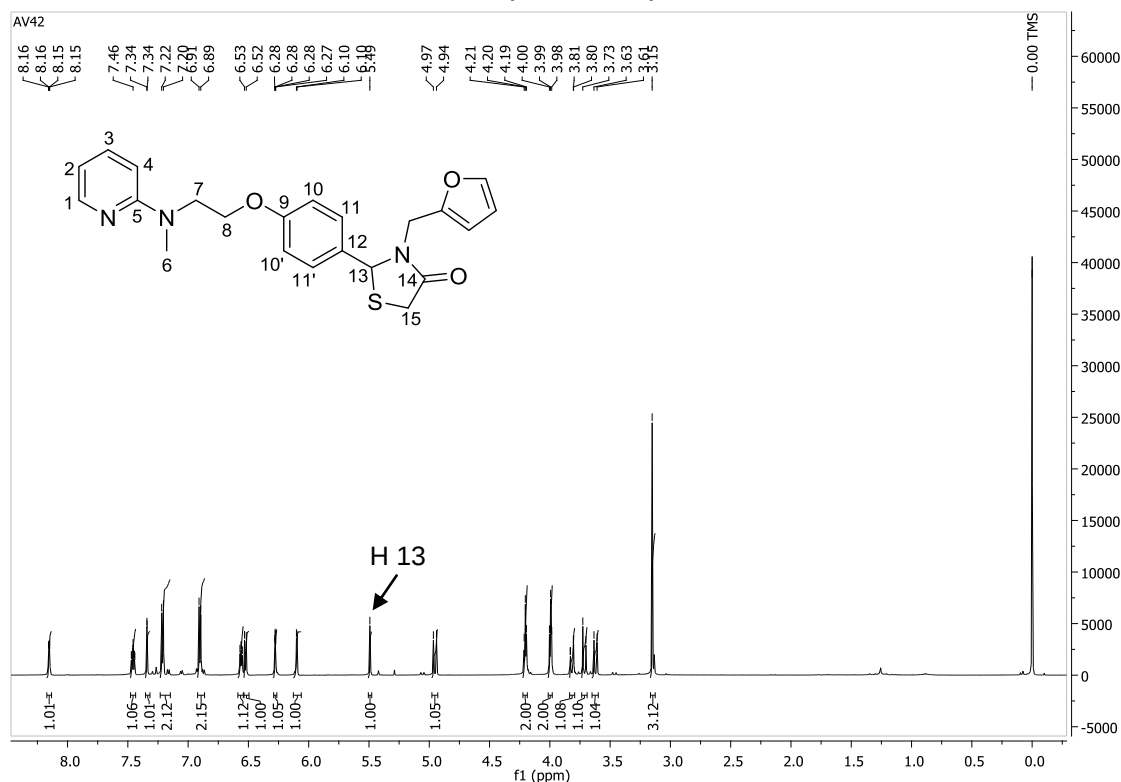


Figura 118: Espectro de RMN ¹H da tiazolidin-4-ona **8g** (CDCl₃ - 600 MHz).

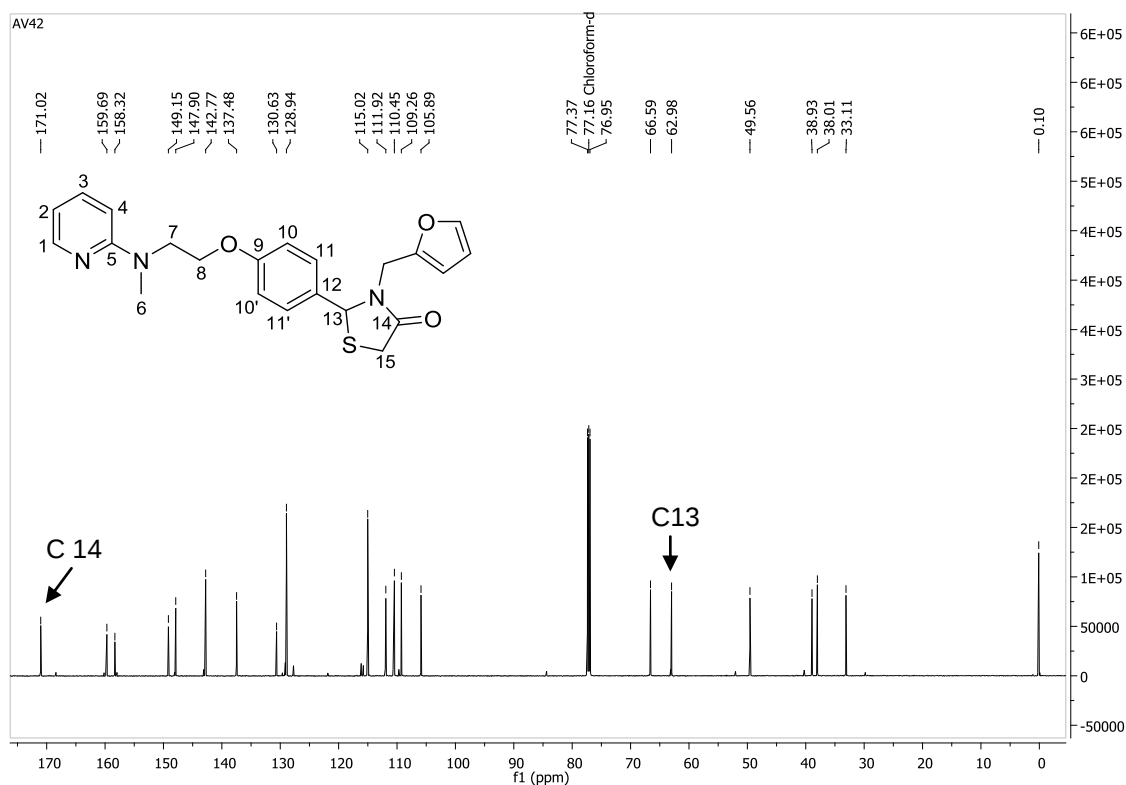


Figura 119: Espectro de ¹³C da tiazolidin-4-ona **8g** (CDCl₃ - 150 MHz).

AV56

AV56

Chemical structure of compound 14 (labeled 14 in the original image) is shown above the spectrum. The structure is a pyridine ring (atoms 1-6) connected via a methylene group (7) to an ethoxy chain (8-9), which is connected to a benzene ring (10-11). The benzene ring is also connected to a thiazolidine ring (12-15). The thiazolidine ring has a carbonyl group (14) and a sulfur atom (15). The pyridine ring is numbered 1-6, the ethoxy chain 7-9, the benzene ring 10-11, and the thiazolidine ring 12-15.

13C NMR Spectrum (CDCl₃)

Chemical shift (ppm):

- 171.58
- 159.60
- 158.24
- 155.59
- 149.54
- 147.77
- 137.53
- 136.86
- 130.64
- 128.98
- 122.62
- 122.48
- 114.96
- 111.91
- 105.96
- 77.37
- 77.16
- 76.95 (CDCl₃)
- 66.54
- 63.40
- 49.55
- 47.79
- 38.01
- 33.04

Peak assignments:

- C 14 (labeled with an arrow pointing to the peak at 171.58 ppm)
- C 13 (labeled with an arrow pointing to the peak at 66.54 ppm)

175

Anexo III: Espectroscopia de RMN

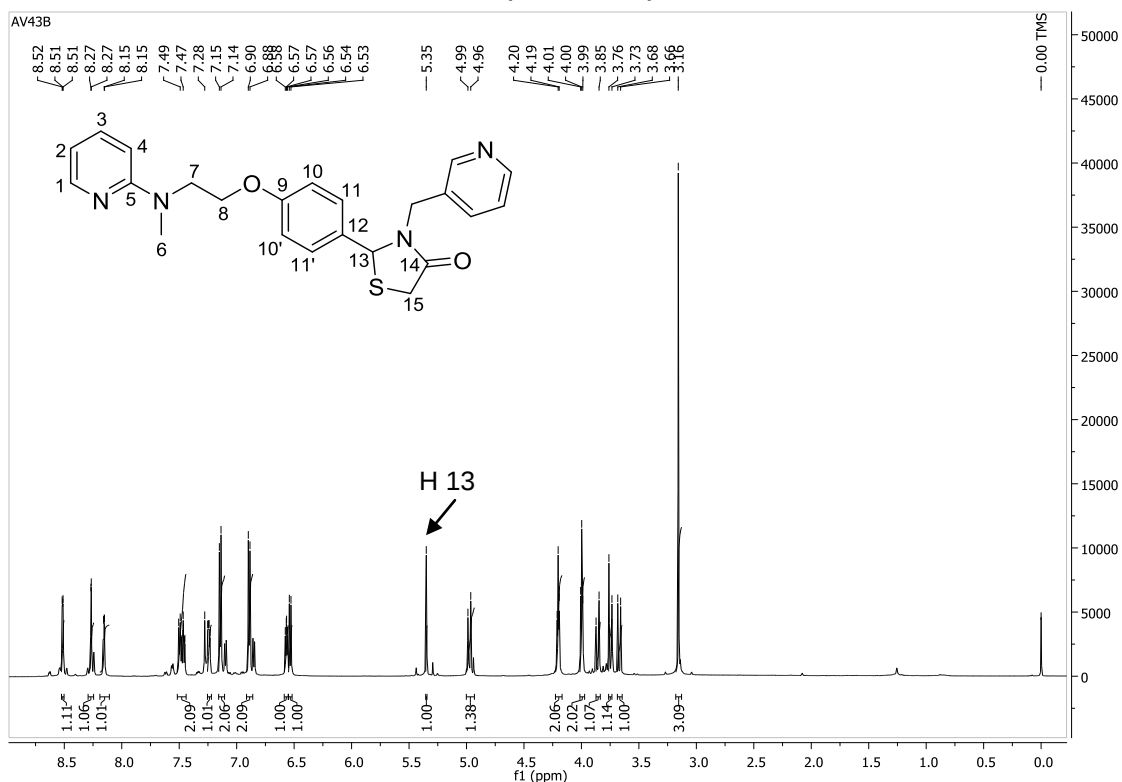


Figura 122: Espectro de RMN ^1H da tiazaolidin-4-ona **8i** (CDCl_3 - 600 MHz).

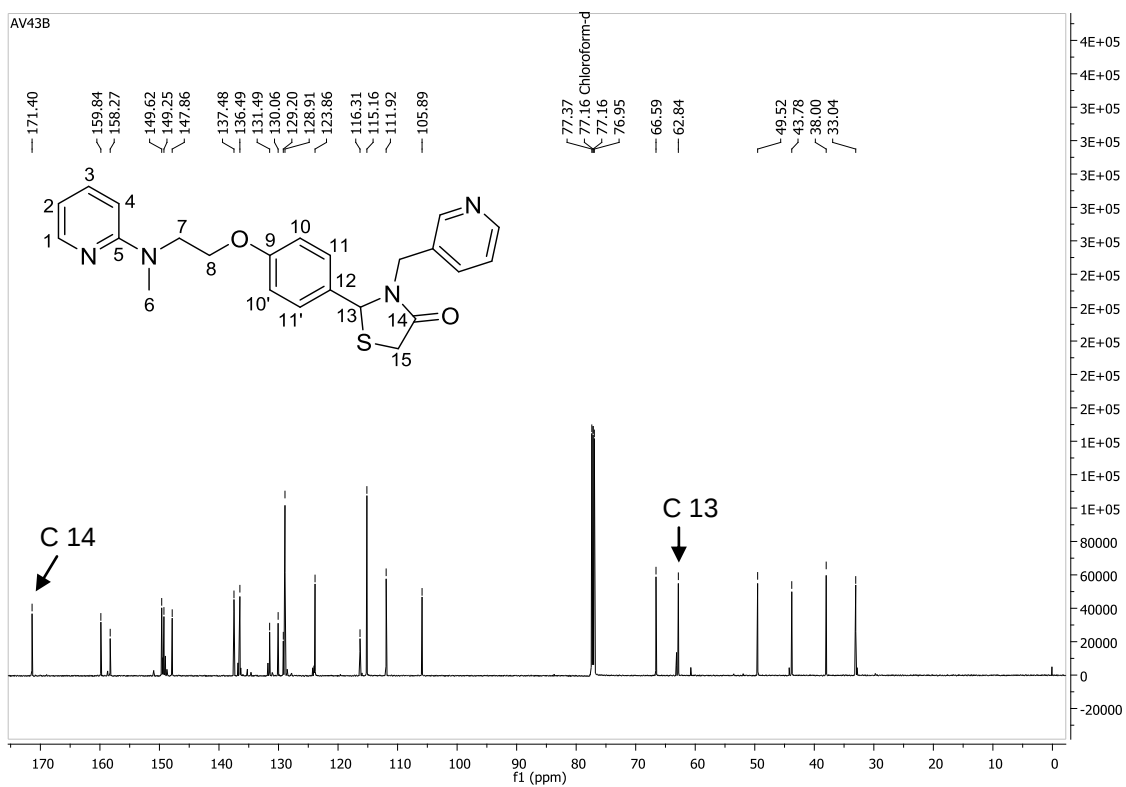


Figura 123: Espectro de ^{13}C da tiazaolidin-4-ona **8i** (CDCl_3 - 150 MHz).

Anexo III: Espectroscopia de RMN

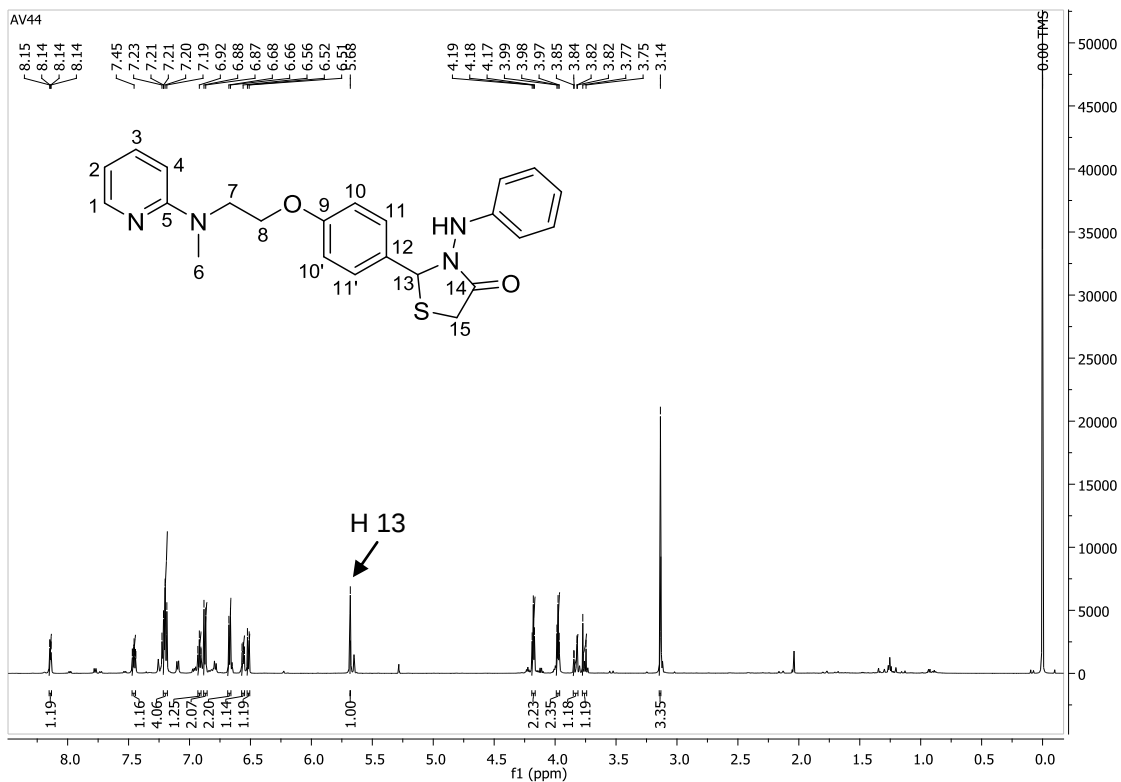


Figura 124: Espectro de RMN ^1H da tiazolidin-4-ona **8j** (CDCl_3 - 600 MHz).

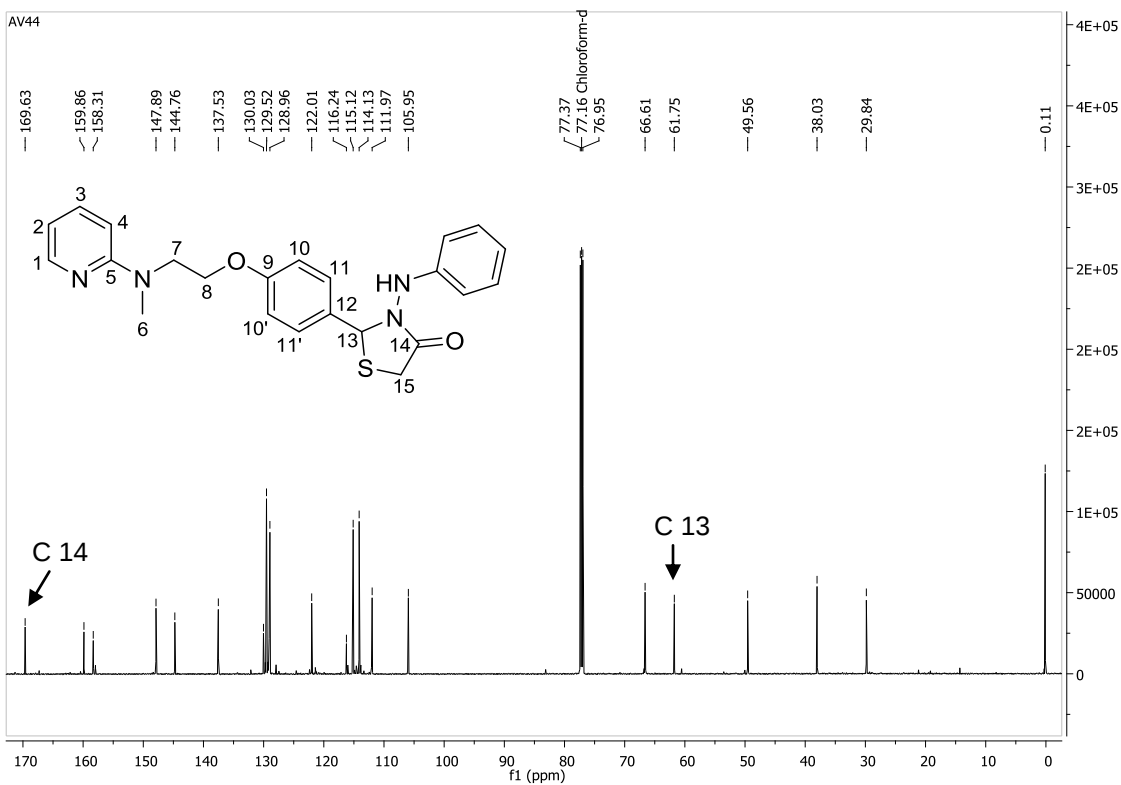


Figura 125: Espectro de ^{13}C da tiazolidin-4-ona **8j** (CDCl_3 - 150 MHz).

Anexo III: Espectroscopia de RMN

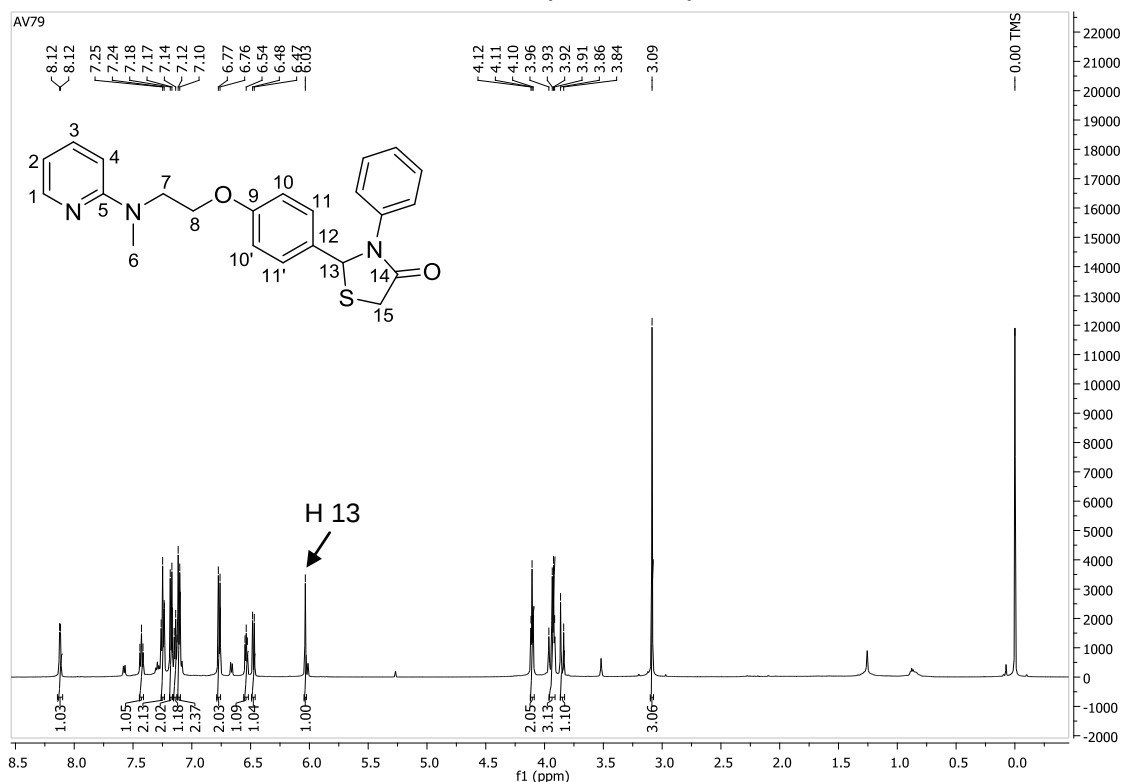


Figura 126: Espectro de RMN ^1H da tiazolidin-4-ona **8k** (CDCl₃ - 600 MHz).

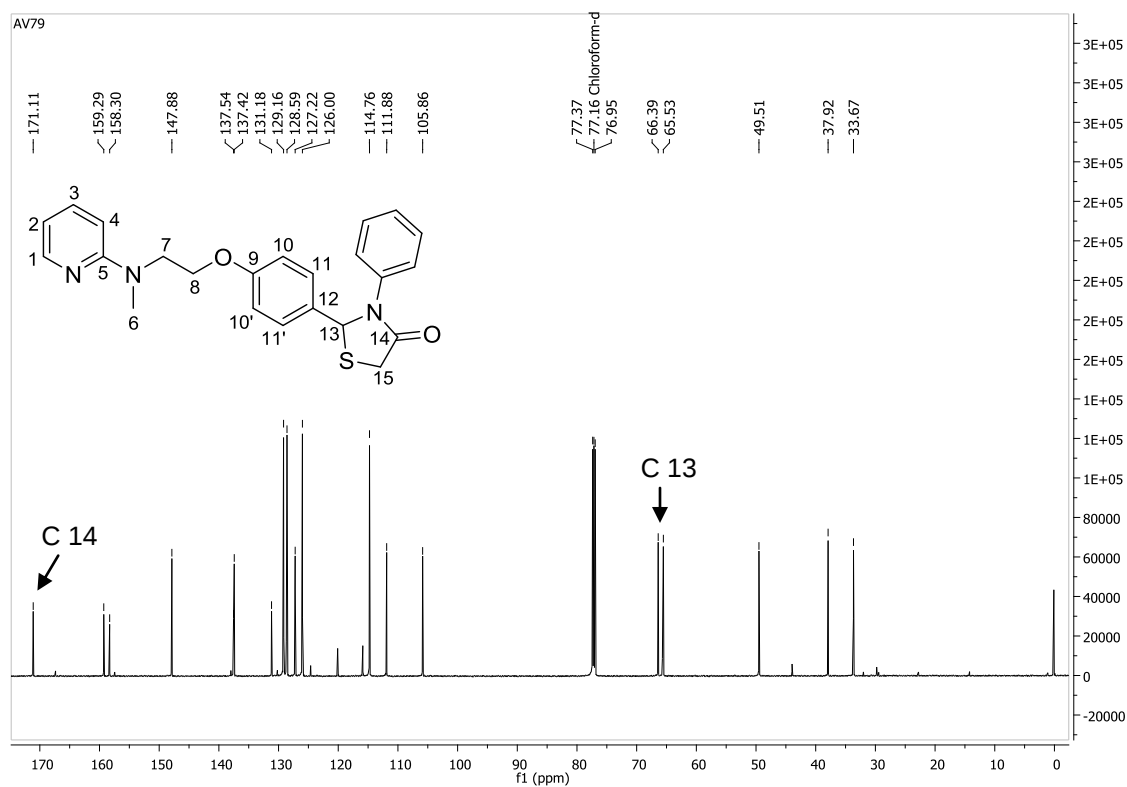


Figura 127: Espectro de ^{13}C da tiazolidin-4-ona **8k** (CDCl₃ - 150 MHz).

Anexo III: Espectroscopia de RMN

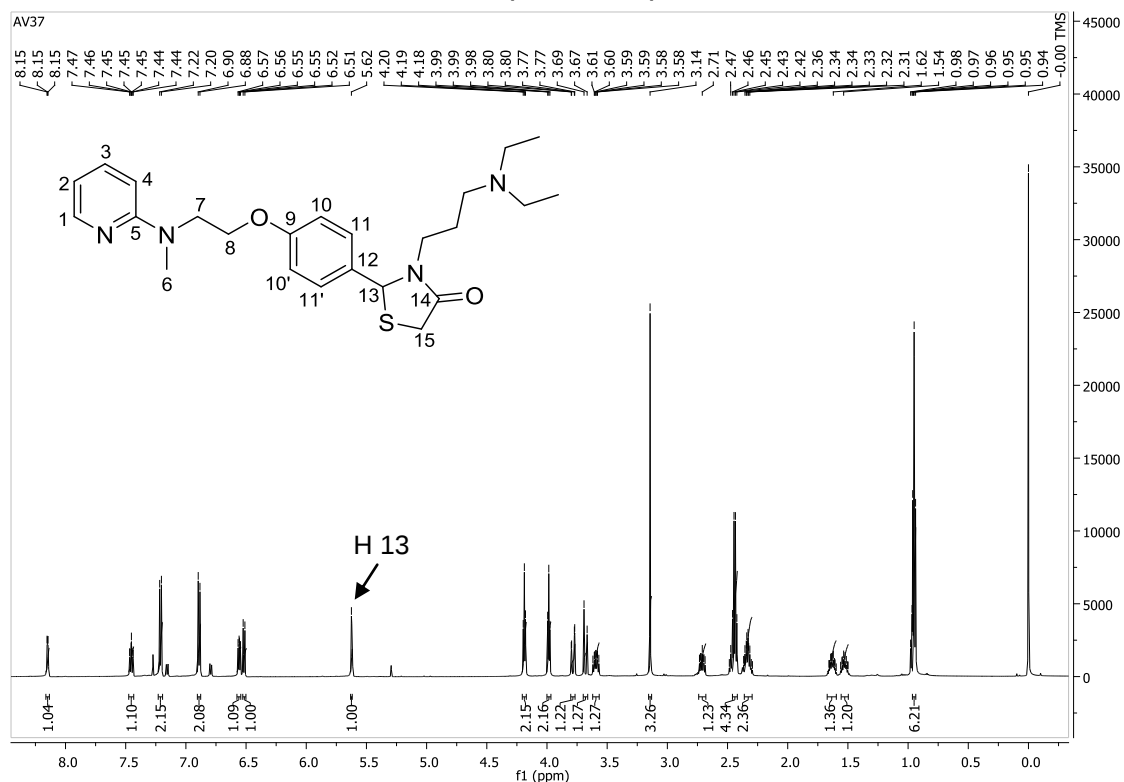


Figura 128: Espectro de RMN ¹H da tiazolidin-4-ona **8I** (CDCl₃ - 600 MHz).

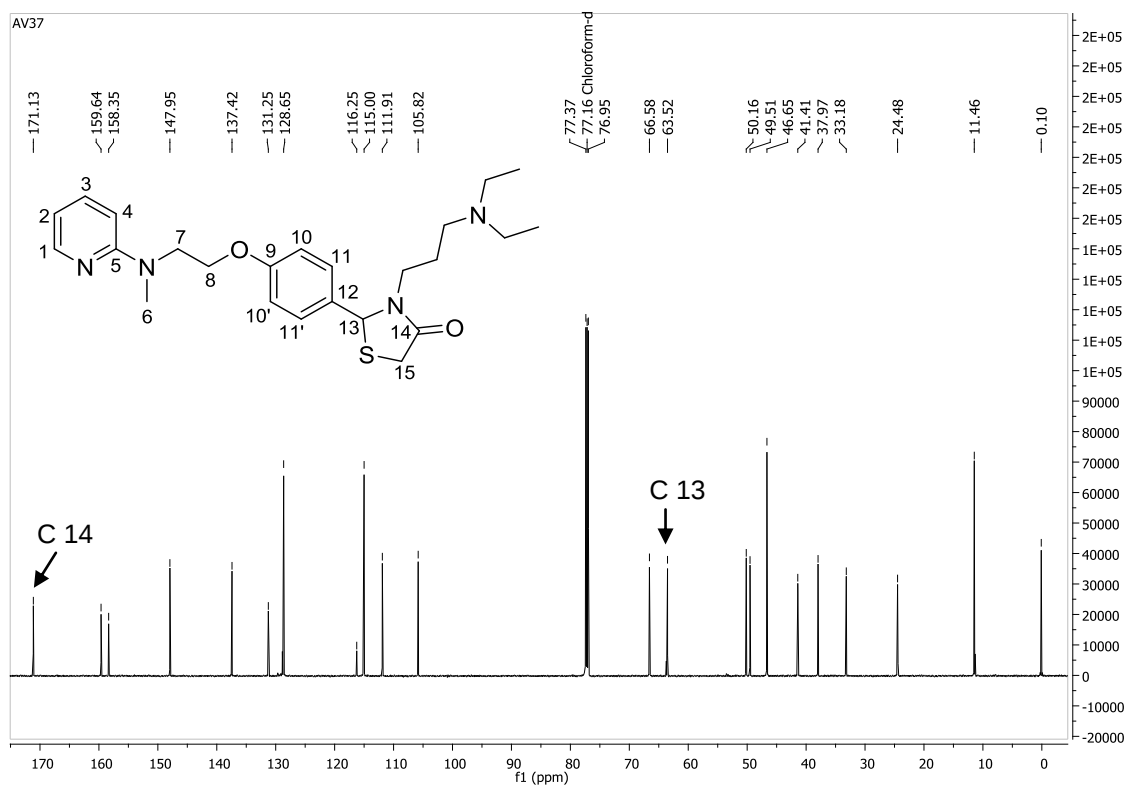


Figura 129: Espectro de ¹³C da tiazolidin-4-ona **8I** (CDCl₃ - 150 MHz).

Anexo III: Espectroscopia de RMN

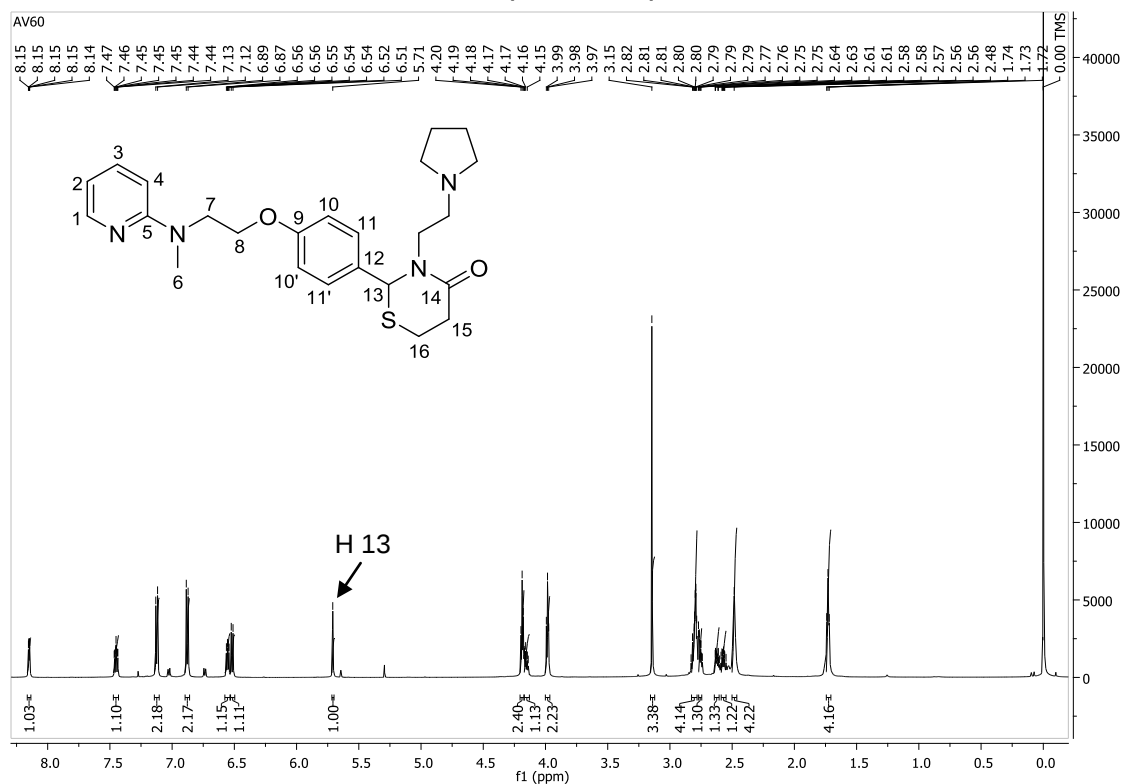


Figura 130: Espectro de ¹H da tiazinan-4-ona **9a** (CDCl₃ - 600 MHz).

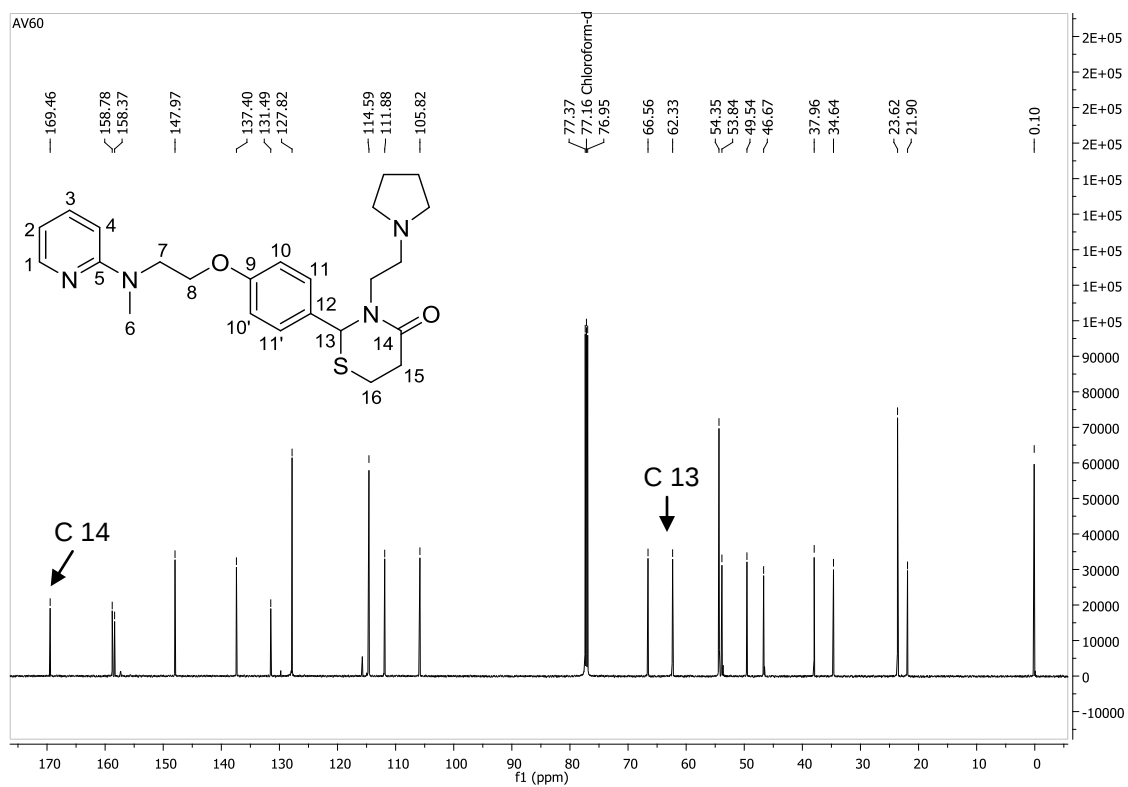


Figura 131: Espectro de ¹³C da tiazinan-4-ona **9a** (CDCl₃ - 150 MHz).

Anexo III: Espectroscopia de RMN

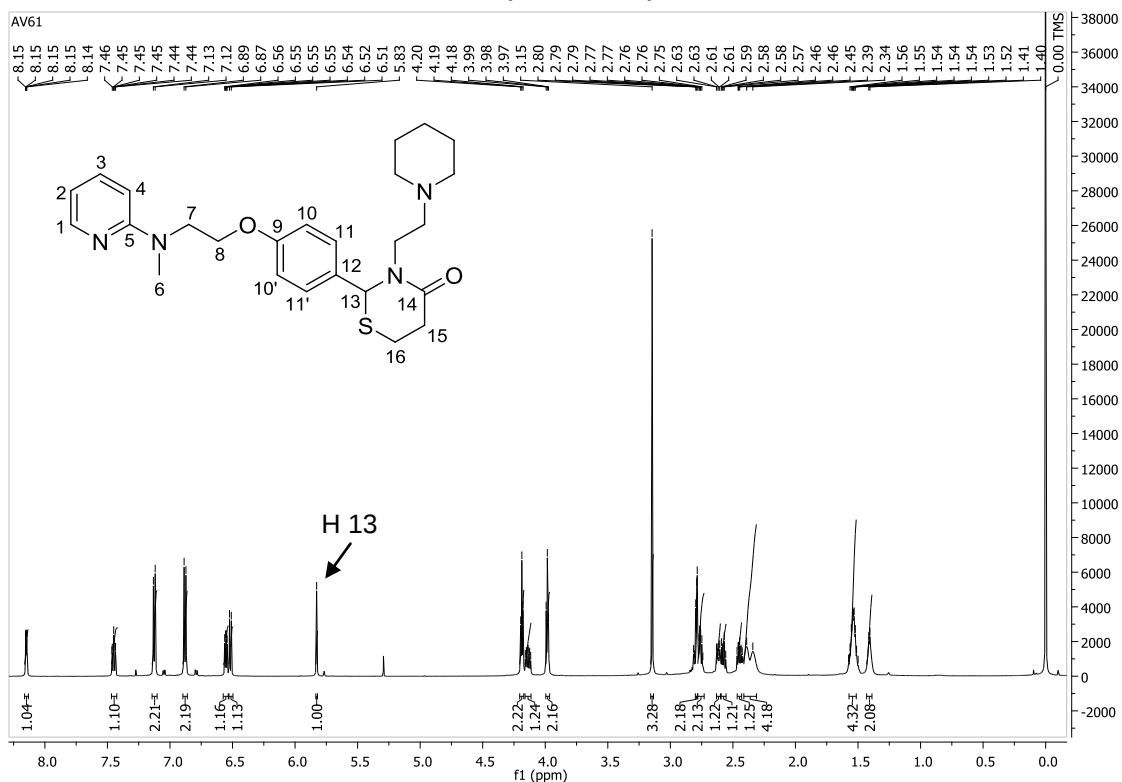


Figura 132: Espectro de ¹H da tiazinan-4-ona **9b** (CDCl₃ - 600 MHz).

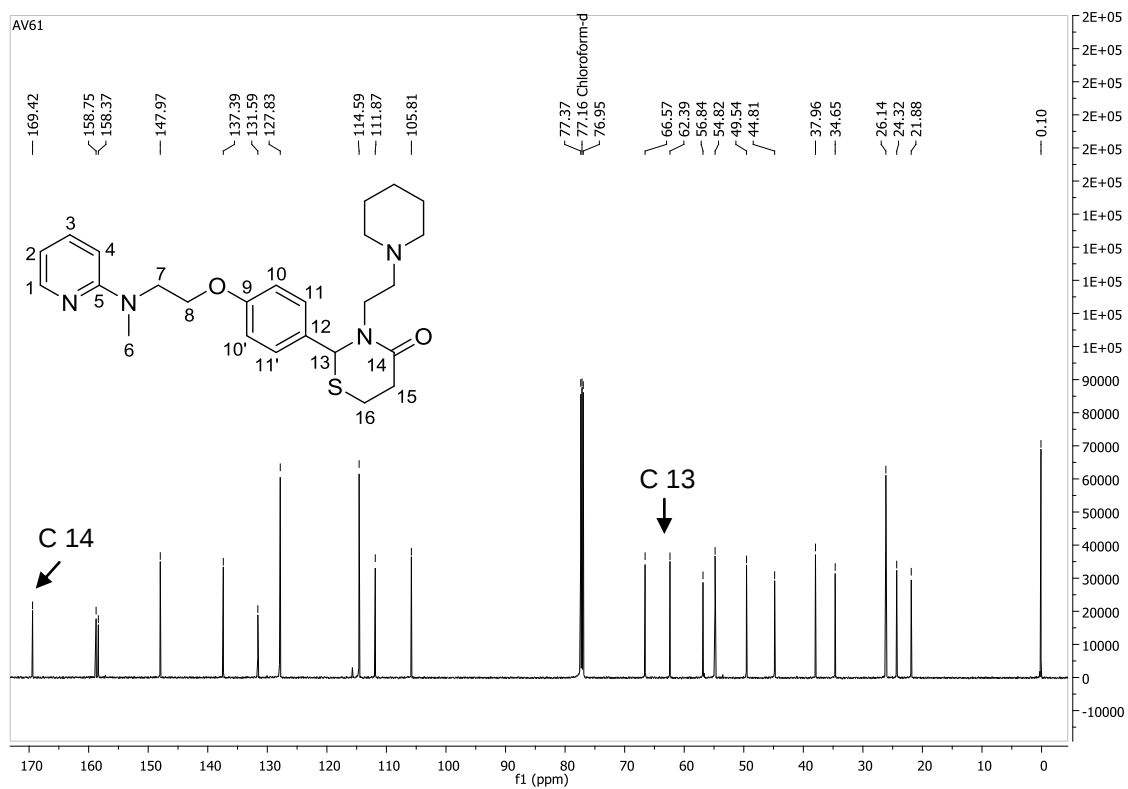


Figura 133: Espectro de ¹³C da tiazinan-4-ona **9b** (CDCl₃ - 150 MHz).

Anexo III: Espectroscopia de RMN

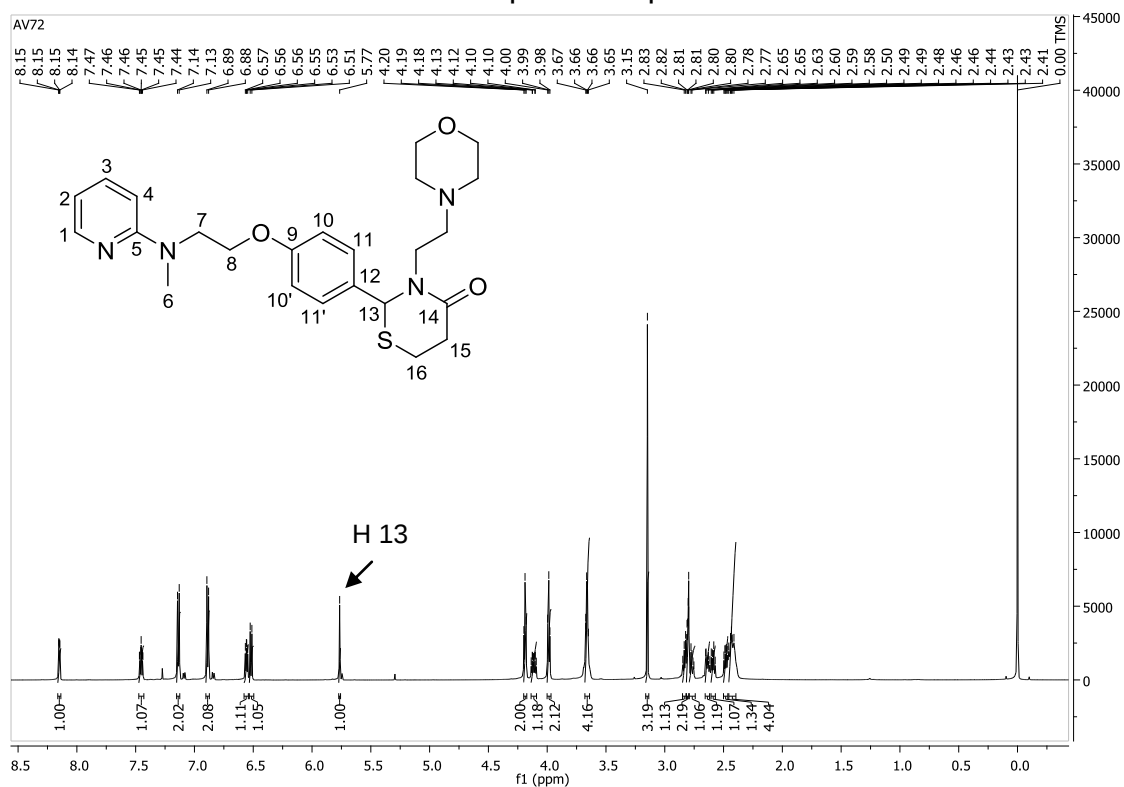


Figura 134: Espectro de ^1H da tiazinan-4-ona **9c** (CDCl_3 - 600 MHz).

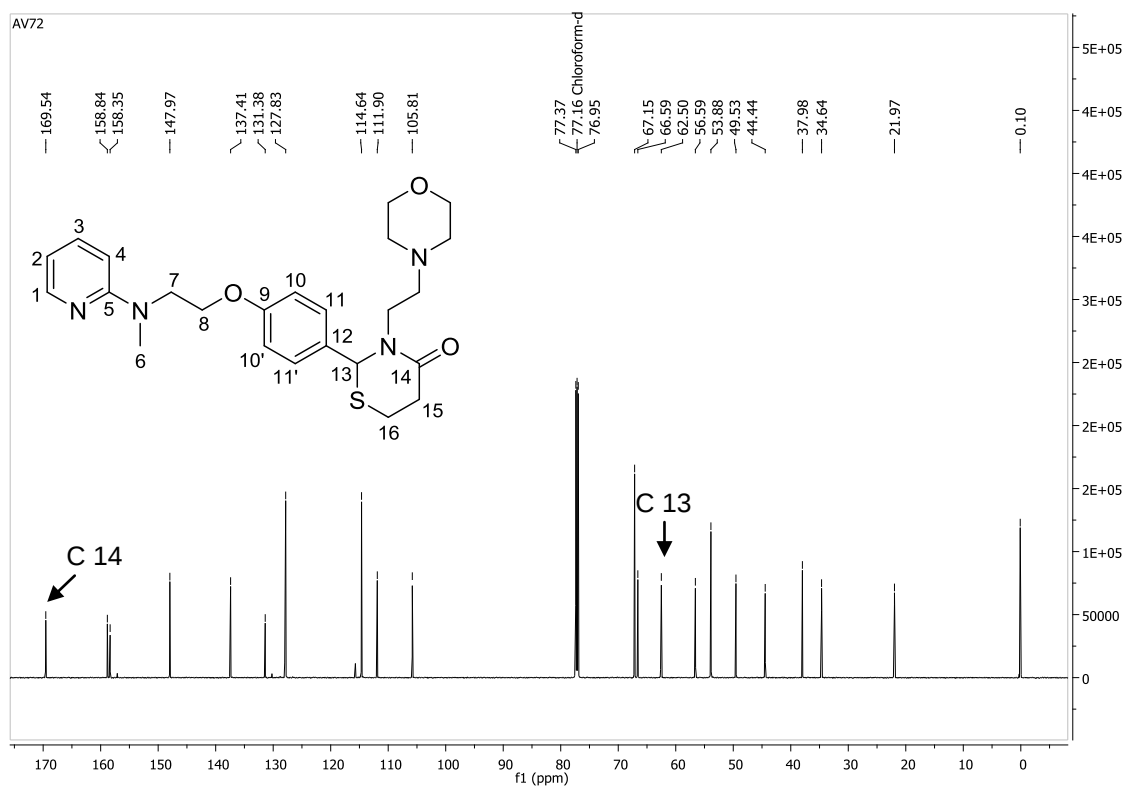


Figura 135: Espectro de ^{13}C da tiazinan-4-ona **9c** (CDCl_3 - 150 MHz).

Anexo III: Espectroscopia de RMN

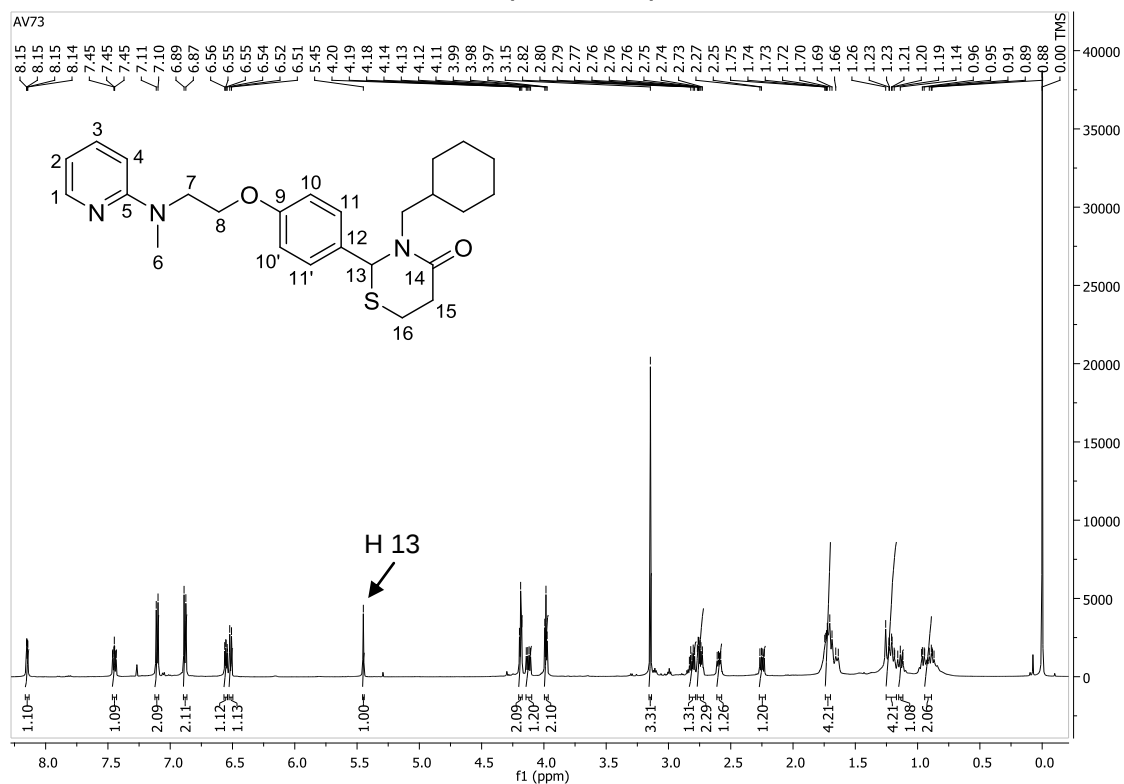


Figura 136: Espectro de ¹H da tiazinan-4-ona **9d** (CDCl₃ - 600 MHz).

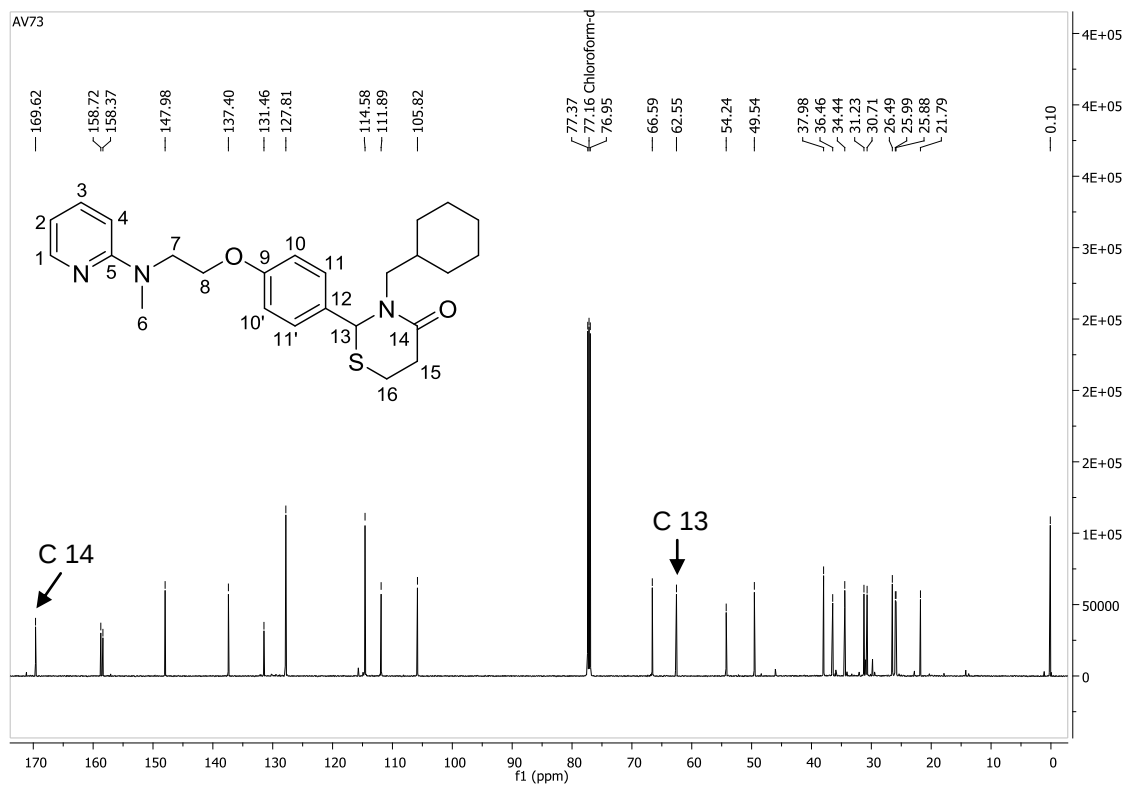


Figura 137: Espectro de ¹³C da tiazinan-4-ona **9d** (CDCl₃ - 150 MHz).

Anexo III: Espectroscopia de RMN

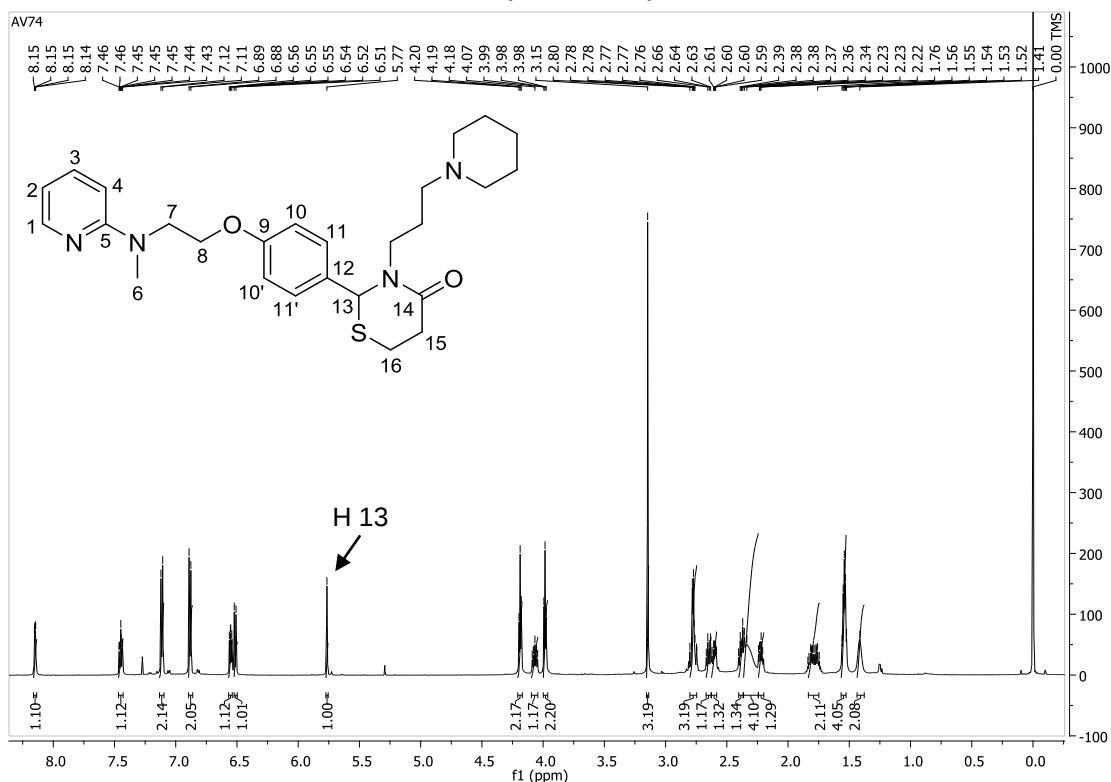


Figura 138: Espectro de ¹H da tiazinan-4-ona **9e** (CDCl₃ - 600 MHz).

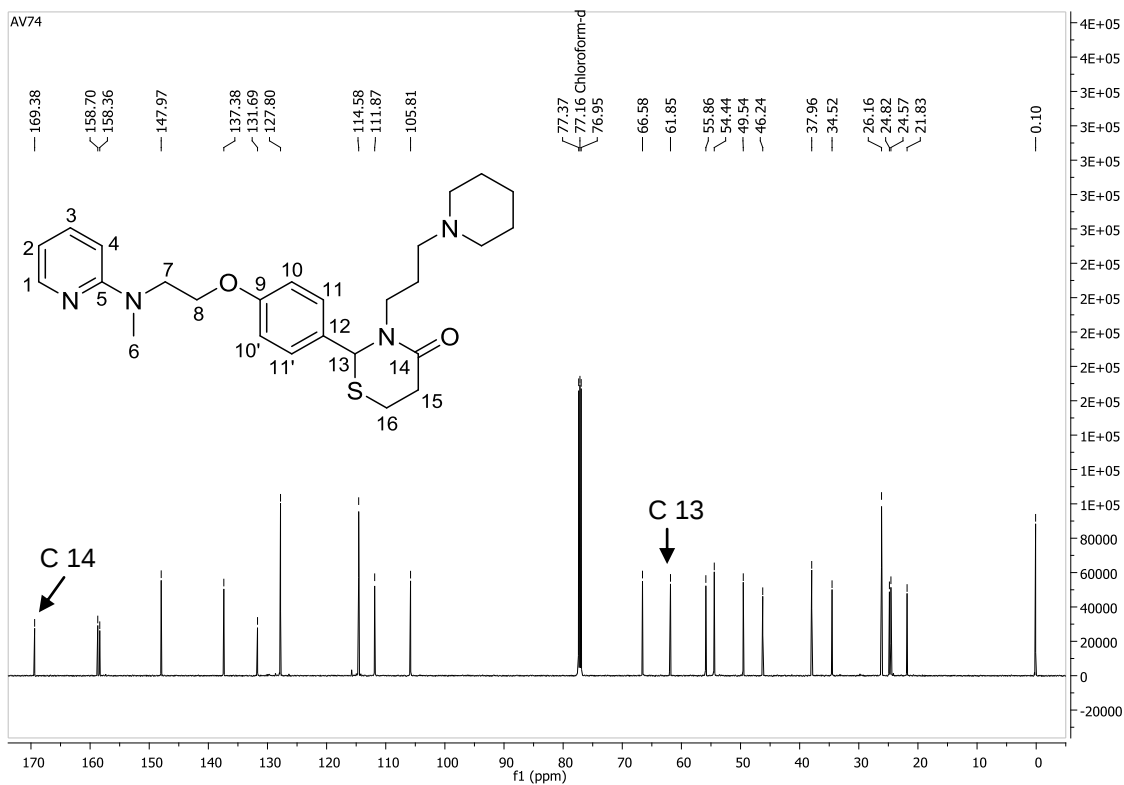


Figura 139: Espectro de ¹³C da tiazinan-4-ona **9e** (CDCl₃ - 150 MHz).

Anexo III: Espectroscopia de RMN

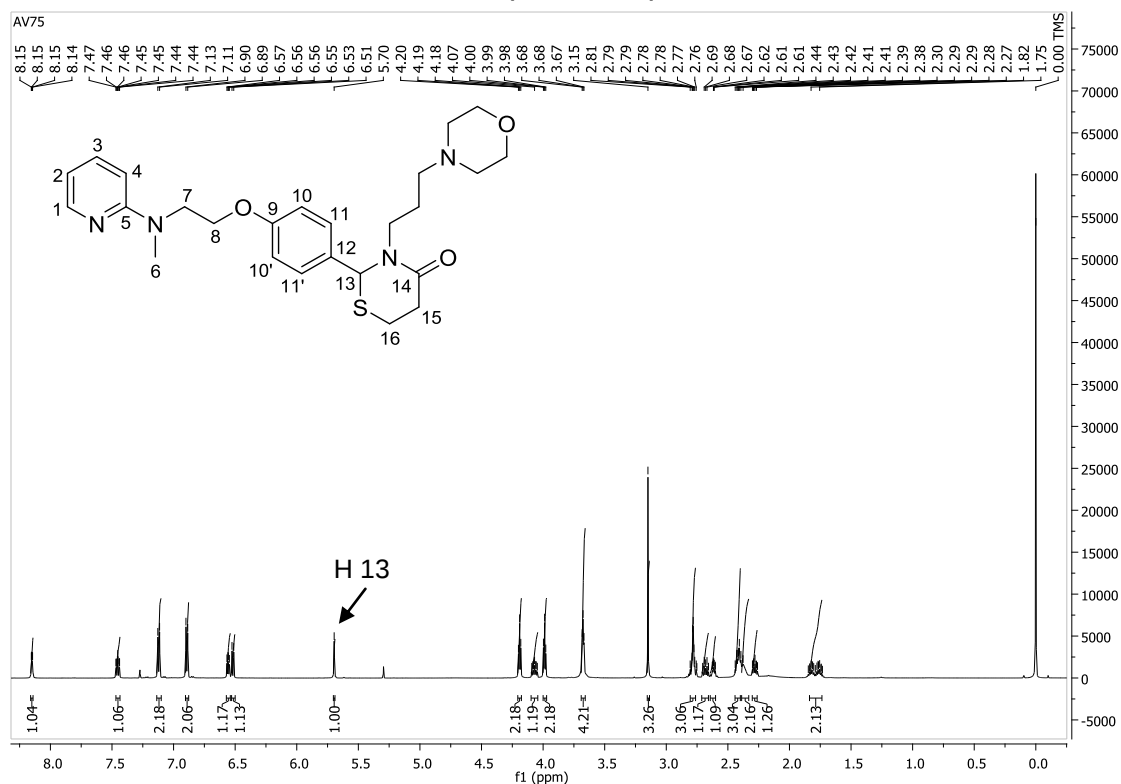


Figura 140: Espectro de ¹H da tiazinan-4-ona **9f** (CDCl₃ - 600 MHz).

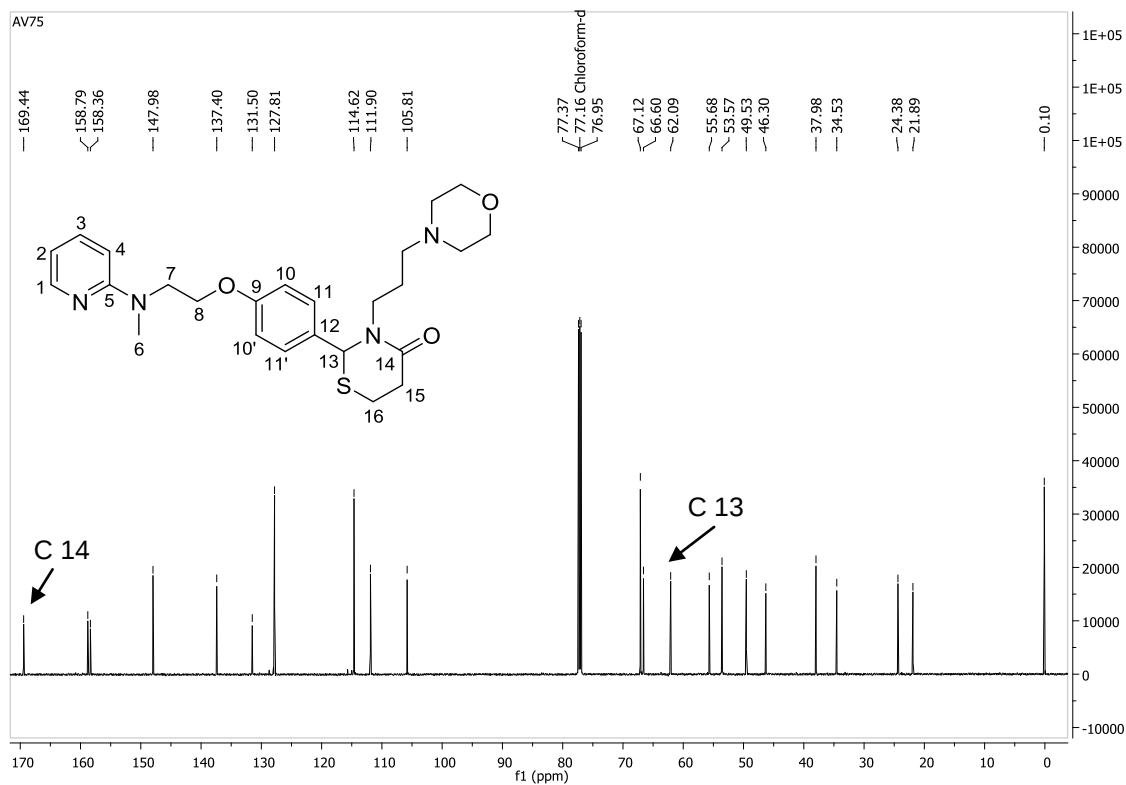


Figura 141: Espectro de ¹³C da tiazinan-4-ona **9f** (CDCl₃ - 150 MHz).

Anexo III: Espectroscopia de RMN

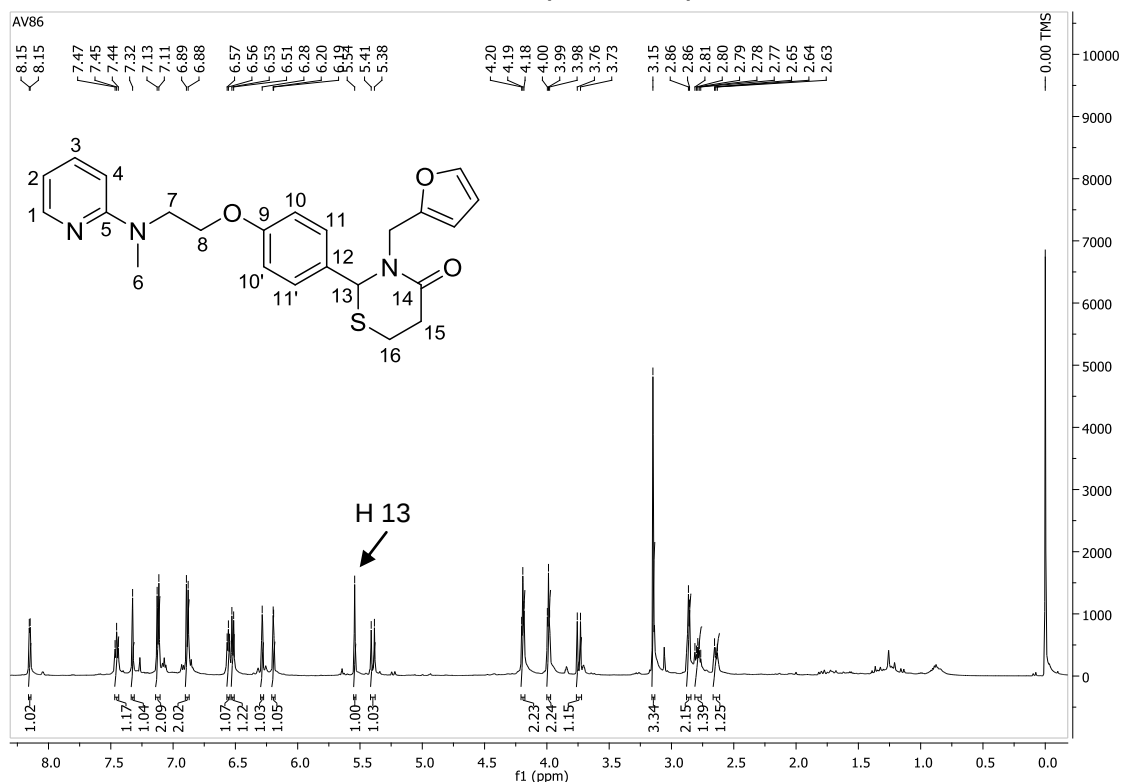


Figura 142: Espectro de ^1H da tiazinan-4-ona **9g** (CDCl_3 - 600 MHz).

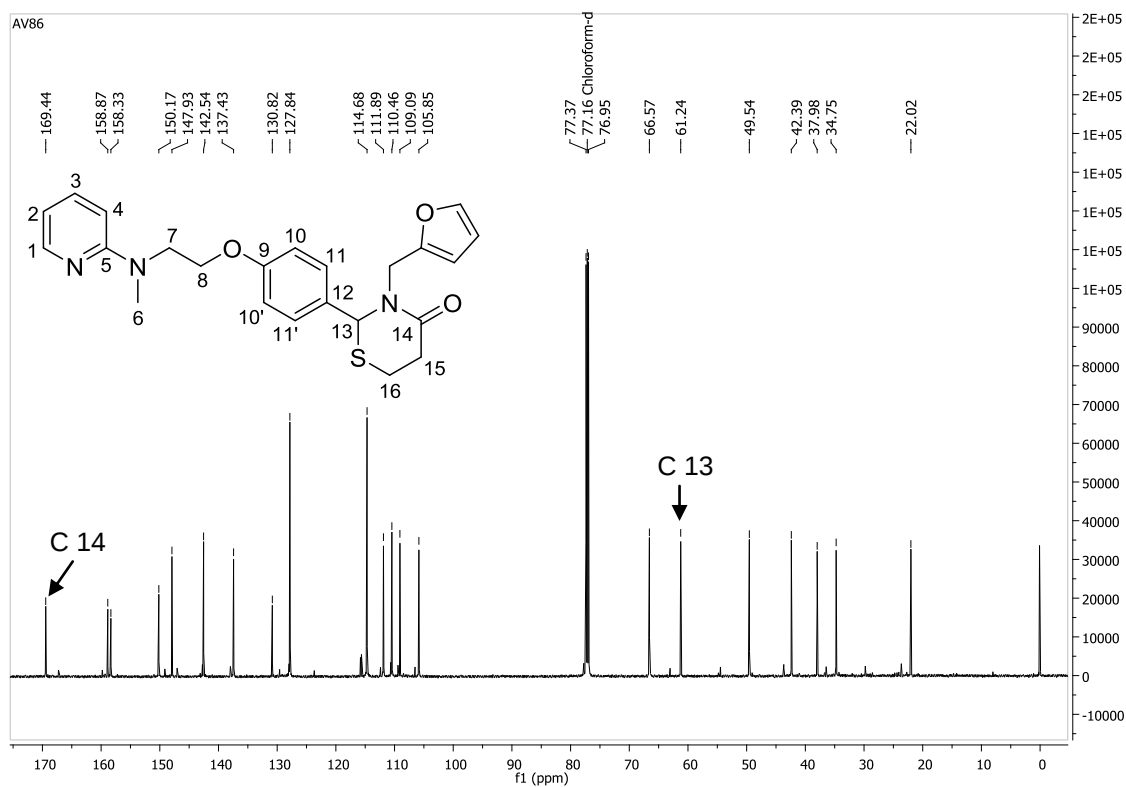


Figura 143: Espectro de ^{13}C da tiazinan-4-ona **9g** (CDCl_3 - 150 MHz).

Anexo III: Espectroscopia de RMN

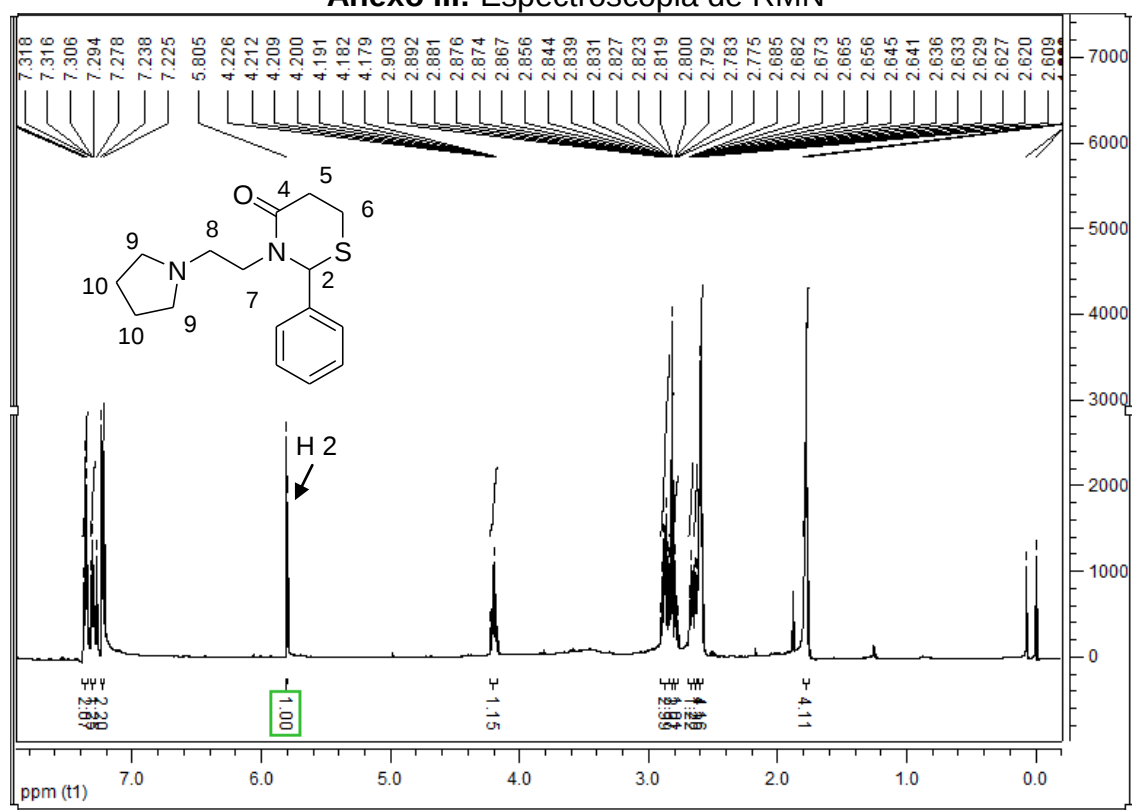


Figura 144: Espectro de ^1H da tiazinan-4-ona **11a** (CDCl_3 - 600 MHz).

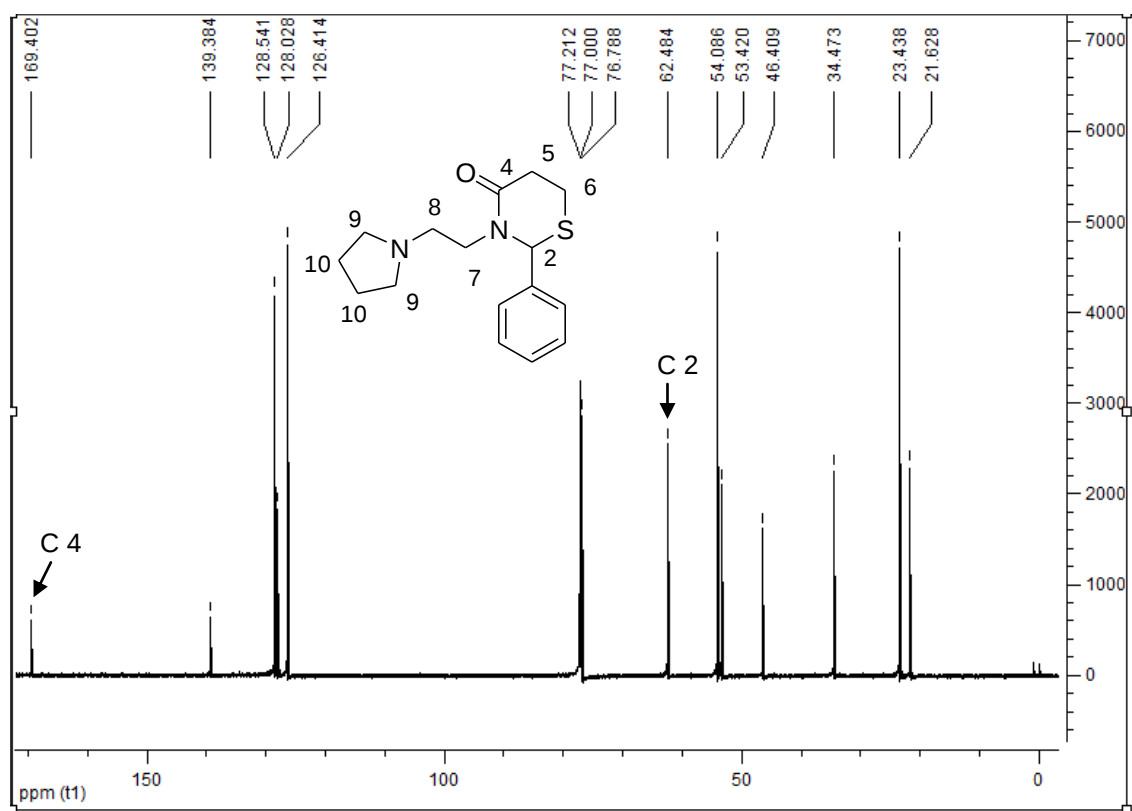


Figura 145: Espectro de ^{13}C da tiazinan-4-ona **11a** (CDCl_3 - 150 MHz).

Anexo III: Espectroscopia de RMN

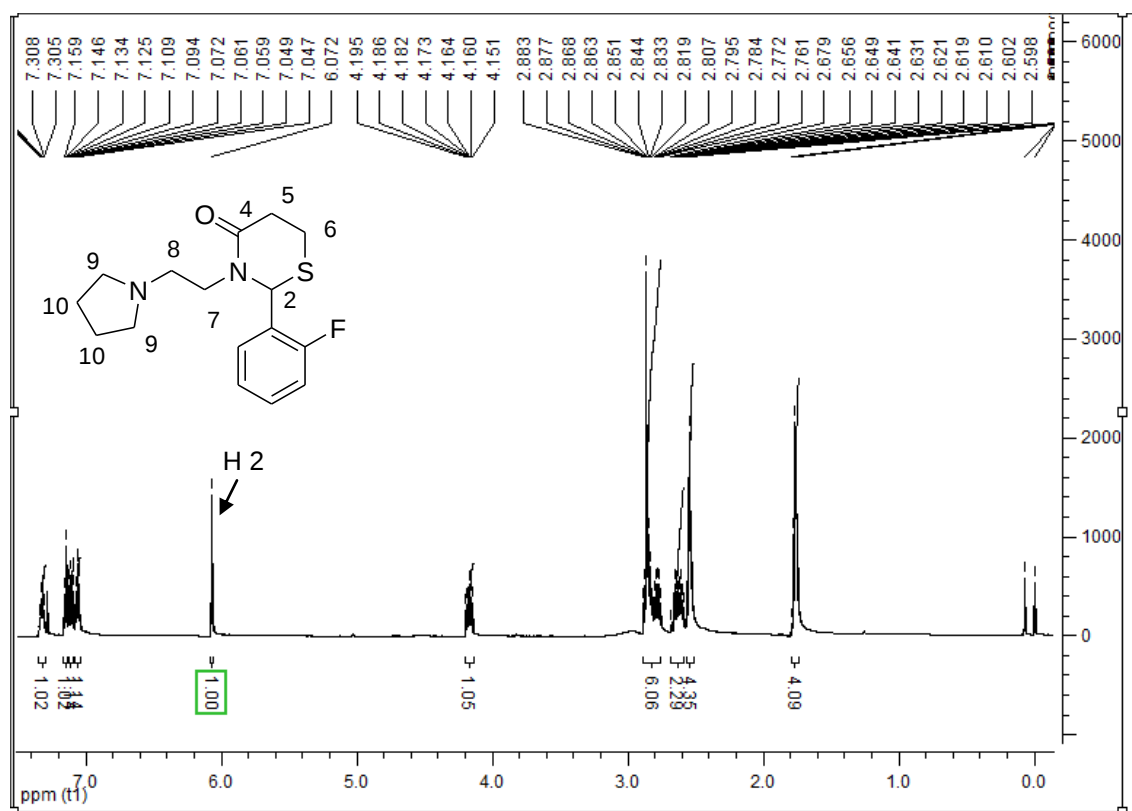


Figura 146: Espectro de ^1H da tiazinan-4-ona **11b** (CDCl_3 - 600 MHz).

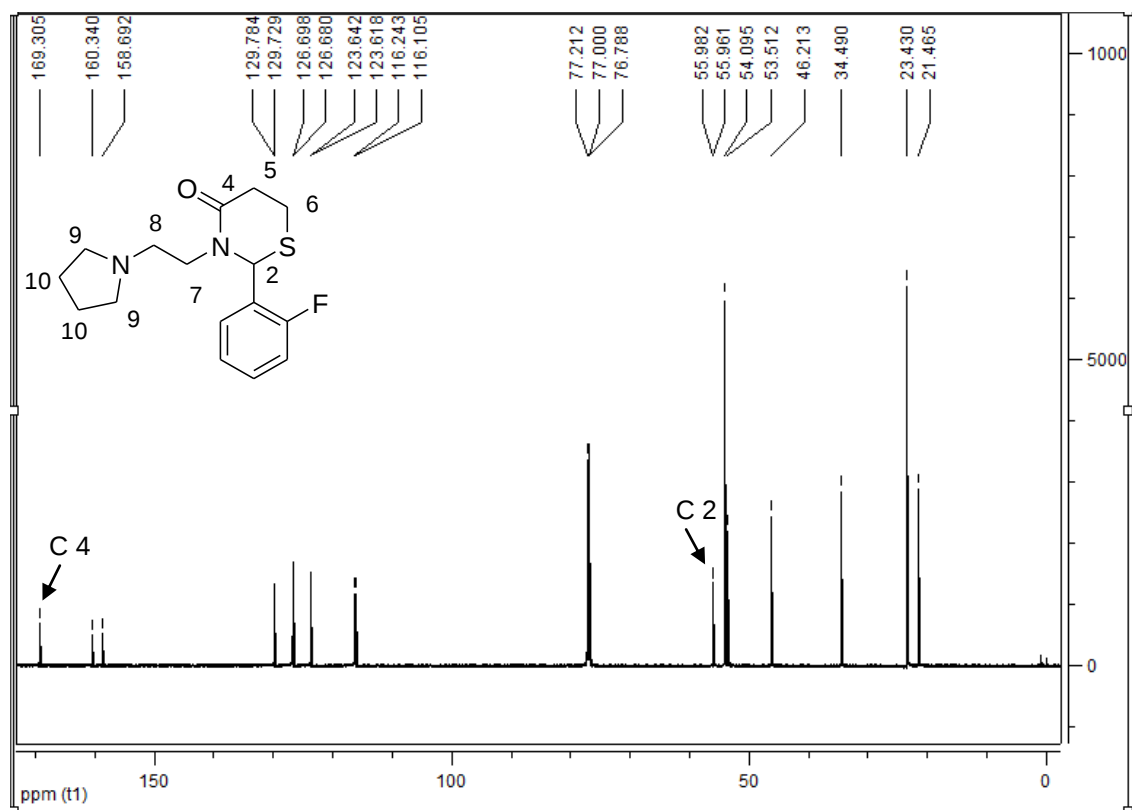


Figura 147: Espectro de ^{13}C da tiazinan-4-ona **11b** (CDCl_3 - 150 MHz).

Chemical structure of compound 10 is shown with atom numbering 1-10. The peak at 5.830 ppm is labeled 'H 2' and has an integration of 1.00. Other peaks have integrations of 1.10, 2.97, 1.05, 2.39, 4.04, and 4.19.

Chemical structure of compound 10 is shown, featuring a 4-fluorophenyl group attached to a 1,3,4-thioxazolidine ring system. The structure is labeled with atom numbers 1 through 10.

The ^{13}C NMR spectrum (ppm) shows the following peaks (labeled C 4 and C 2):

Peak Label	Chemical Shift (ppm)
C 4	169.232
	163.629
	161.989
	142.409
	142.366
	130.118
	130.064
	122.054
	122.035
	115.084
	114.944
	113.666
	113.515
	77.212
	77.000
	76.788
	61.986
	54.153
	53.534
	46.464
	34.364
	23.460
	21.671

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Anexo III: Espectroscopia de RMN

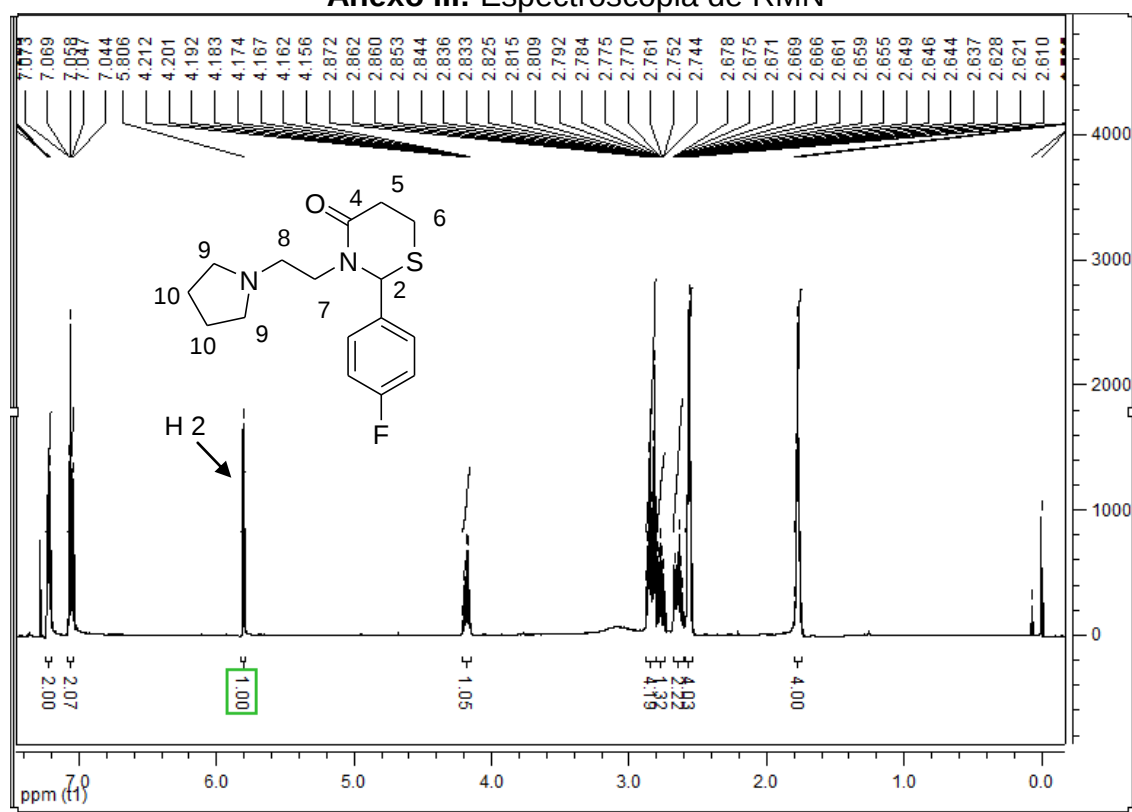


Figura 150: Espectro de ¹H da tiazinan-4-ona **11d** (CDCl₃ - 600 MHz).

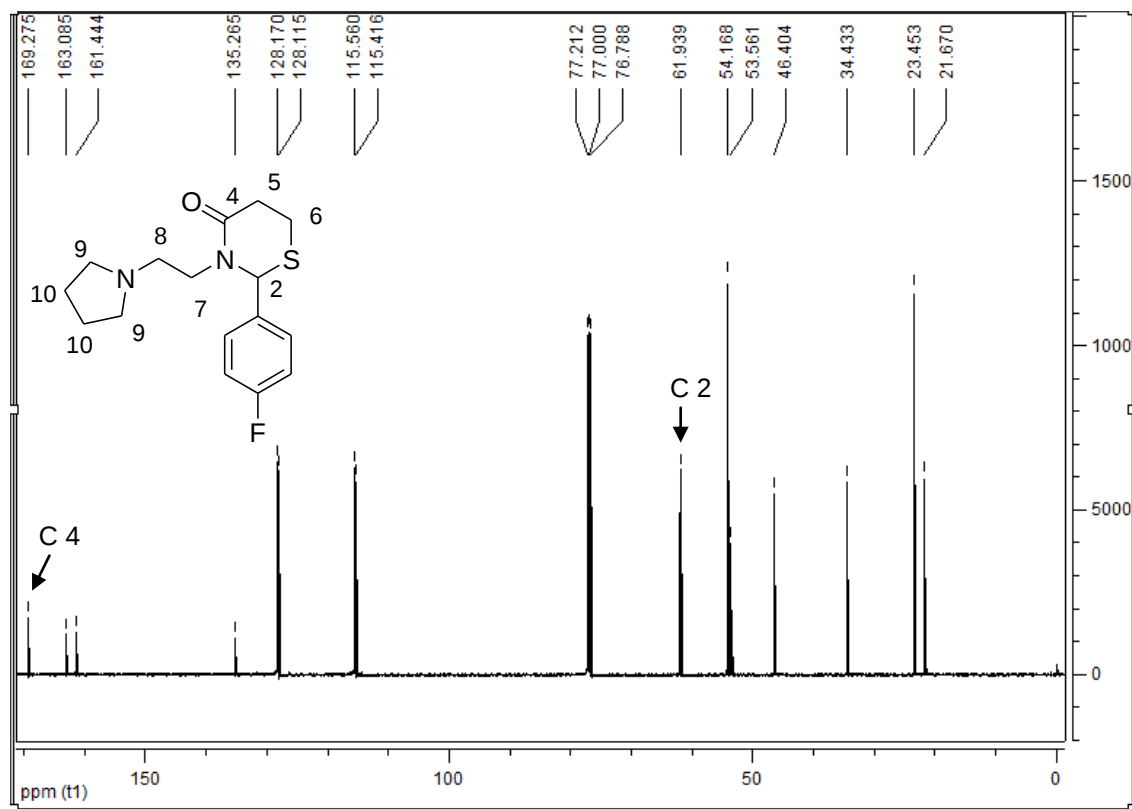


Figura 151: Espectro de ¹³C da tiazinan-4-ona **11d** (CDCl₃ - 150 MHz)..

Anexo III: Espectroscopia de RMN

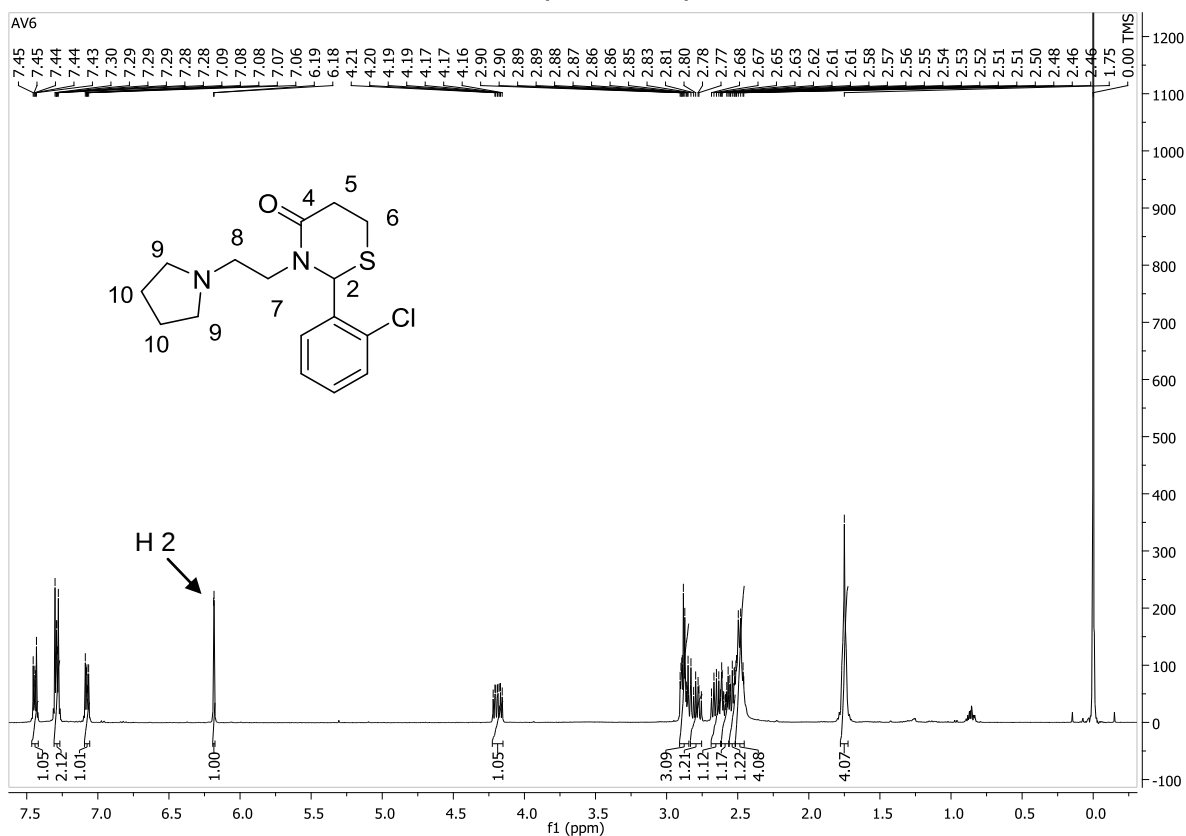


Figura 152: Espectro de ¹H da tiazinan-4-ona **11e** (CDCl₃ - 600 MHz).

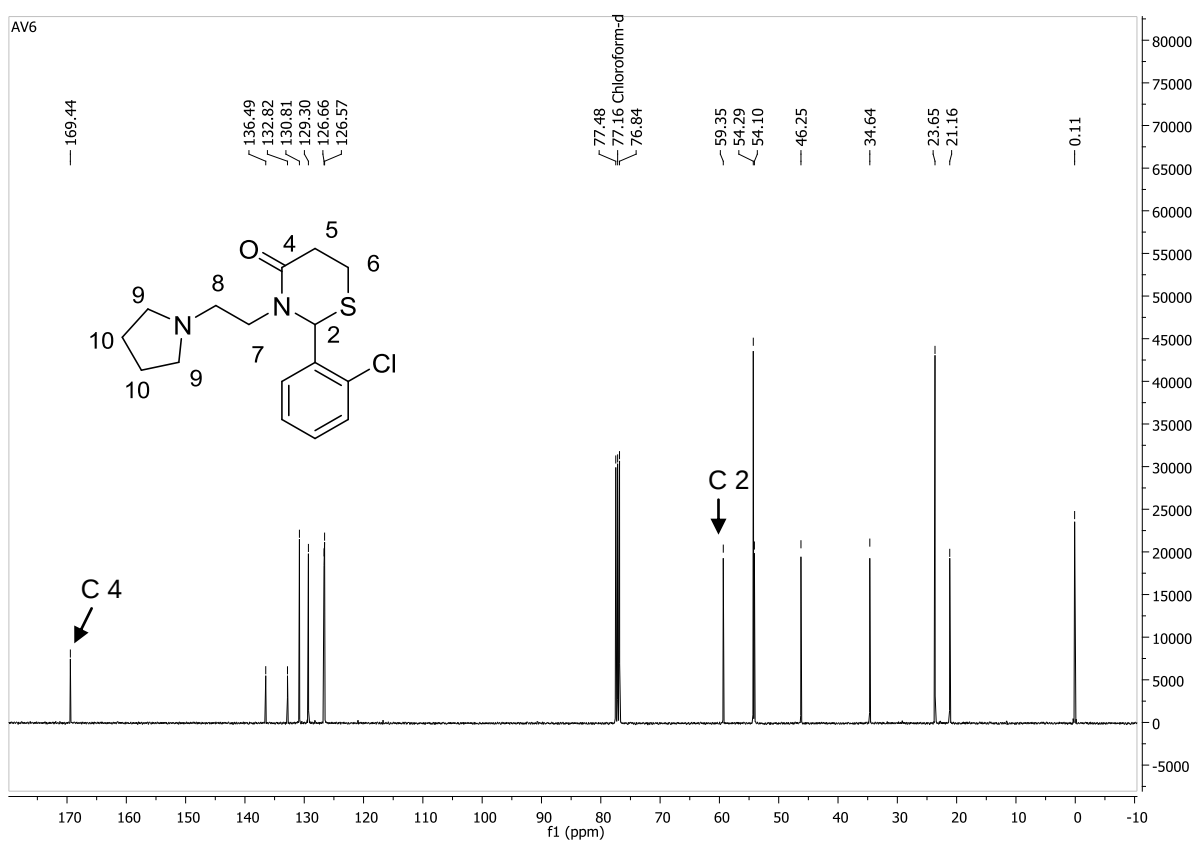


Figura 153: Espectro de ¹³C da tiazinan-4-ona **11e** (CDCl₃ - 150 MHz).

Chemical structure of compound 10 is shown, with protons labeled 1 through 10. The structure is a 2-(4-chlorophenyl)-1,3-dithiane-4-carboxamide derivative with a 2-morpholinoethyl group.

The ^1H NMR spectrum (CDCl₃) shows the following chemical shifts (ppm) and integrations:

- 7.281, 7.278, 7.246, 7.137, 7.125 (aromatic protons, integration 2.109)
- 5.804 (labeled H 2, integration 1.00, highlighted with a green box)
- 4.223, 4.216, 4.211, 4.205, 4.195, 4.186, 4.177, 4.167 (morpholine protons, integration 2.09)
- 2.886, 2.874, 2.867, 2.858, 2.851, 2.850, 2.844, 2.837, 2.827, 2.820, 2.818, 2.814, 2.811, 2.805, 2.790, 2.782, 2.773, 2.765, 2.669, 2.667, 2.665, 2.661, 2.659, 2.655, 2.653, 2.649, 2.640, 2.632, 2.623, 2.616 (aliphatic protons, integration 2.05)
- 1.425 (methyl protons, integration 4.25)

Chemical structure of compound 10 is shown. The spectrum displays peaks corresponding to the structure, with the following chemical shifts (ppm) labeled at the top:

169.164, 141.871, 134.642, 129.762, 128.197, 126.551, 124.576, 77.212, 77.000, 76.788, 61.923, 54.180, 53.631, 48.509, 34.374, 23.481, 21.675.

Key peaks are labeled: C 4 (at ~169 ppm) and C 2 (at ~61 ppm).

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Anexo III: Espectroscopia de RMN

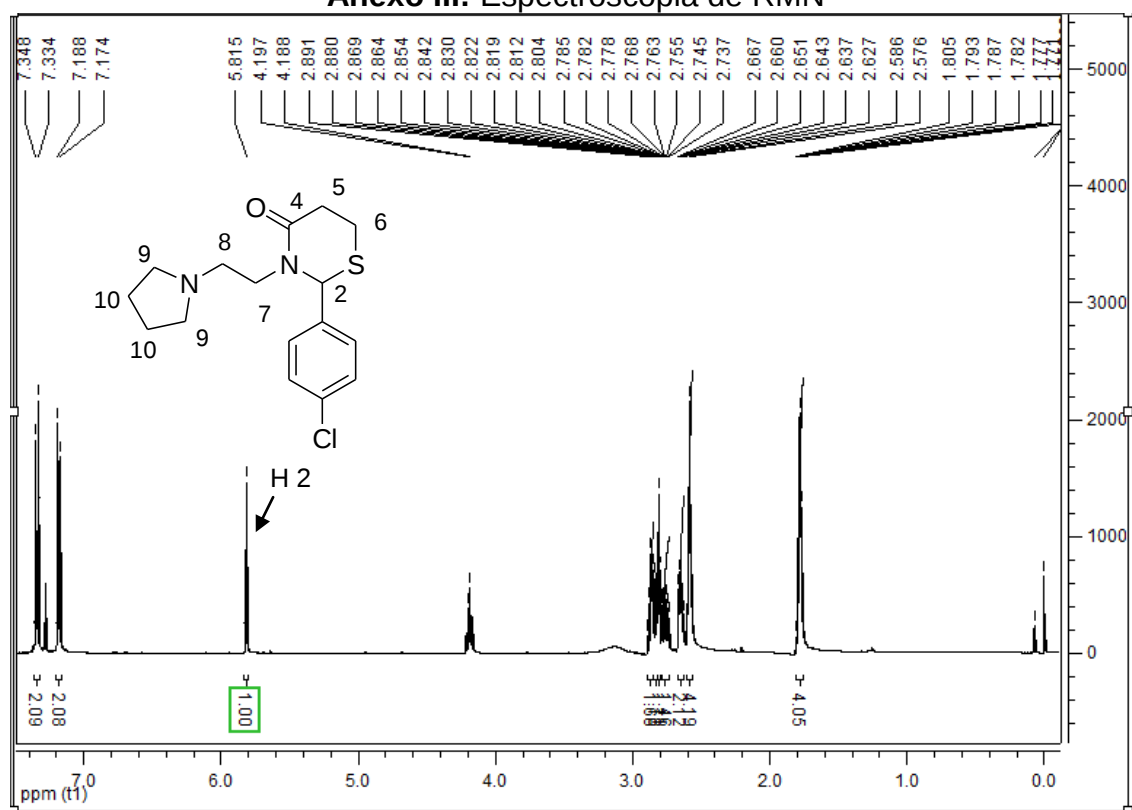


Figura 156: Espectro de ¹H da tiazinan-4-ona **11g** (CDCl₃ - 600 MHz).

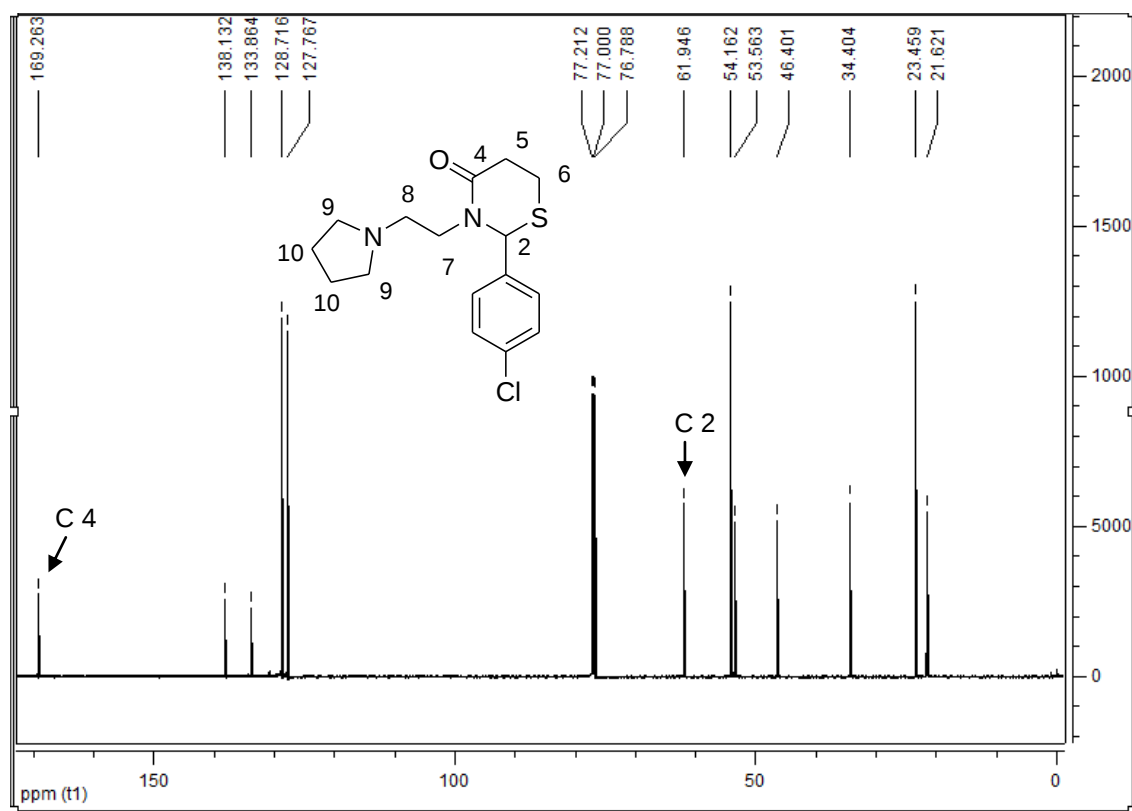


Figura 157: Espectro de ¹³C da tiazinan-4-ona **11g** (CDCl₃ - 150 MHz).

Anexo III: Espectroscopia de RMN

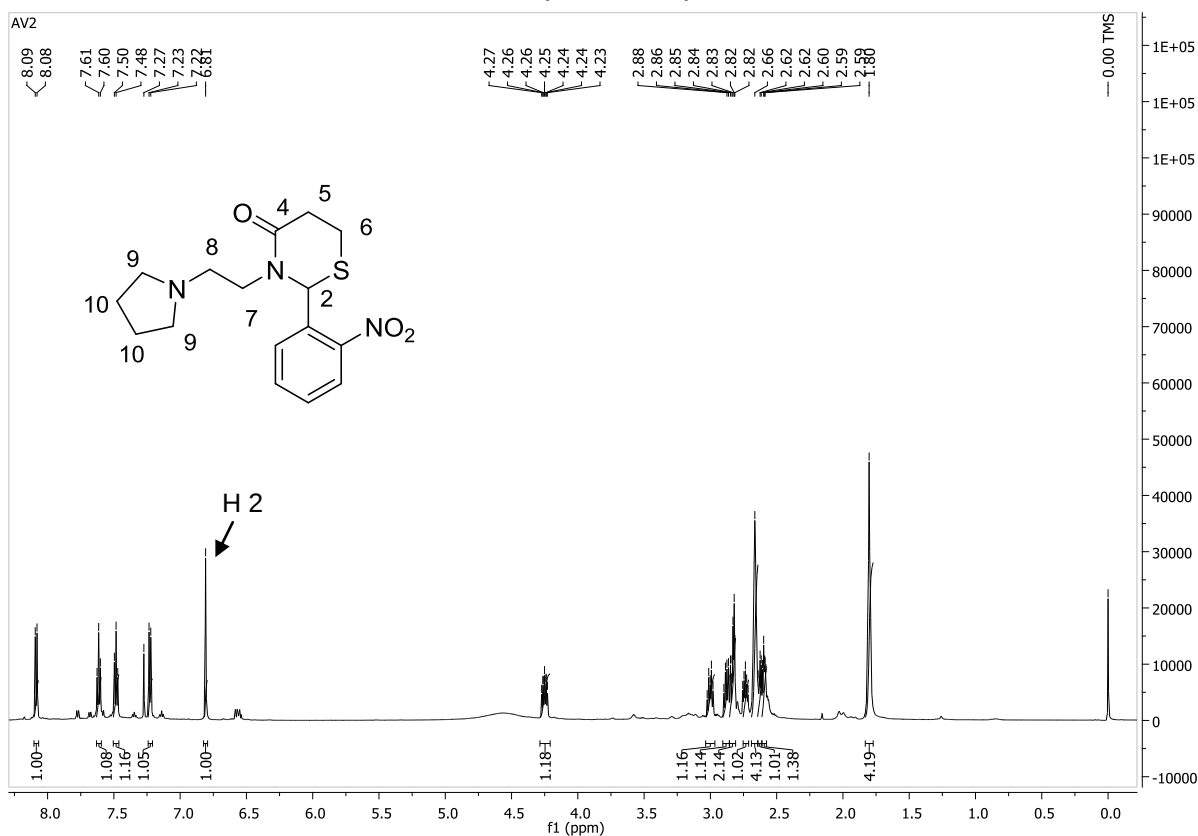


Figura 158: Espectro de ¹H da tiazinan-4-ona **11h** (CDCl₃ - 600 MHz).

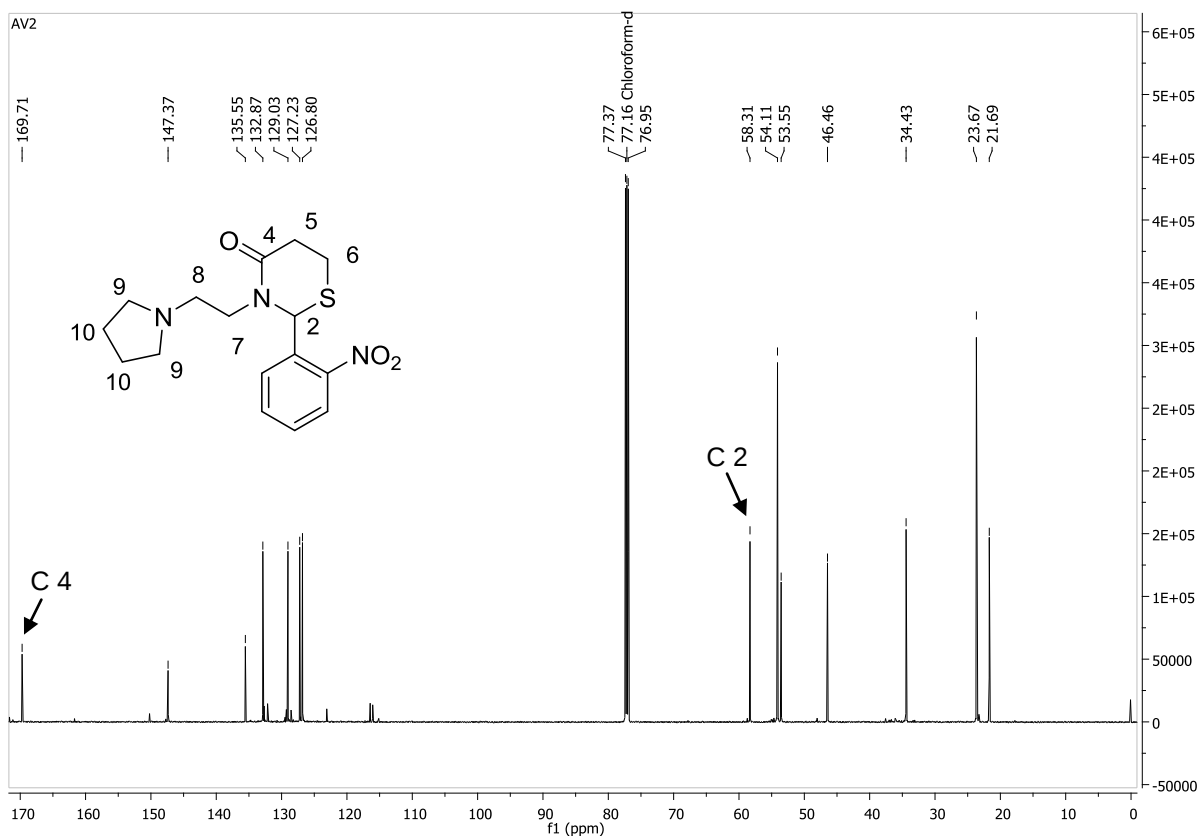


Figura 159: Espectro de ¹³C da tiazinan-4-ona **11h** (CDCl₃ - 150 MHz).

Anexo III: Espectroscopia de RMN

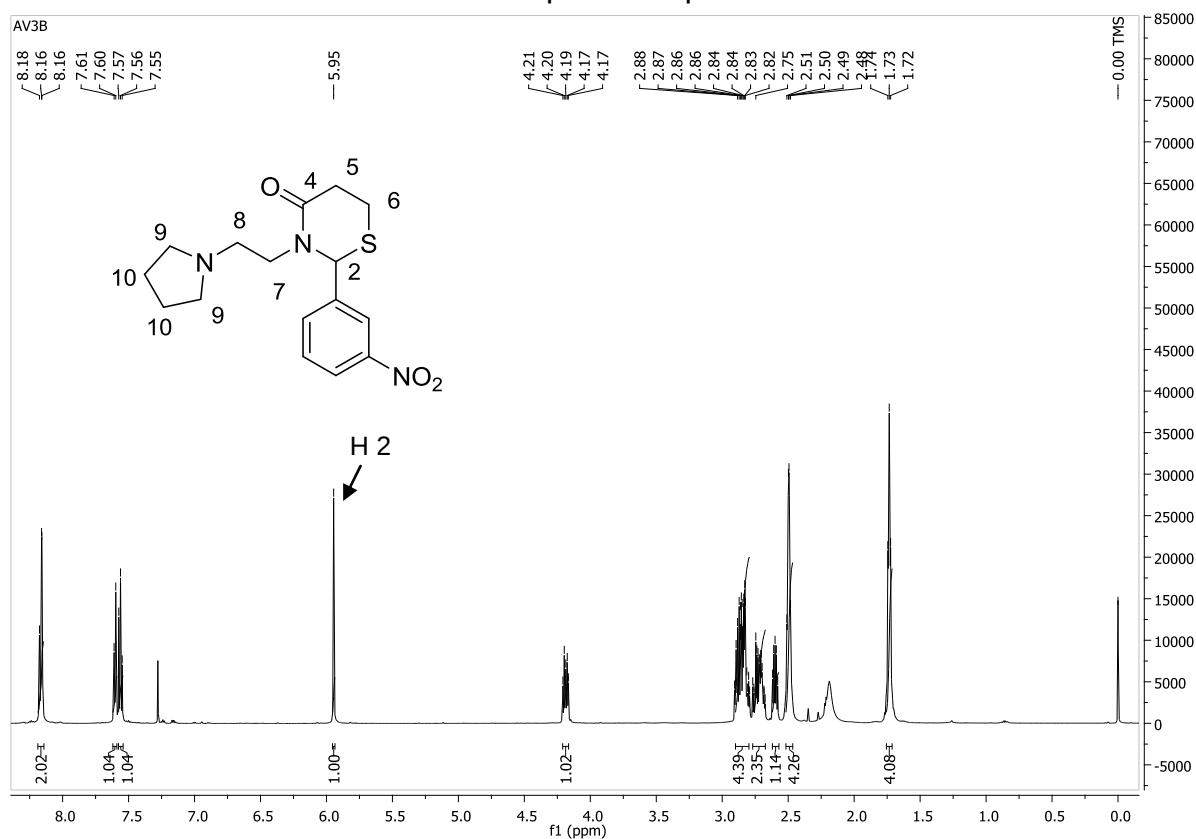


Figura 160: Espectro de ^1H da tiazinan-4-ona **11i** (CDCl_3 - 600 MHz).

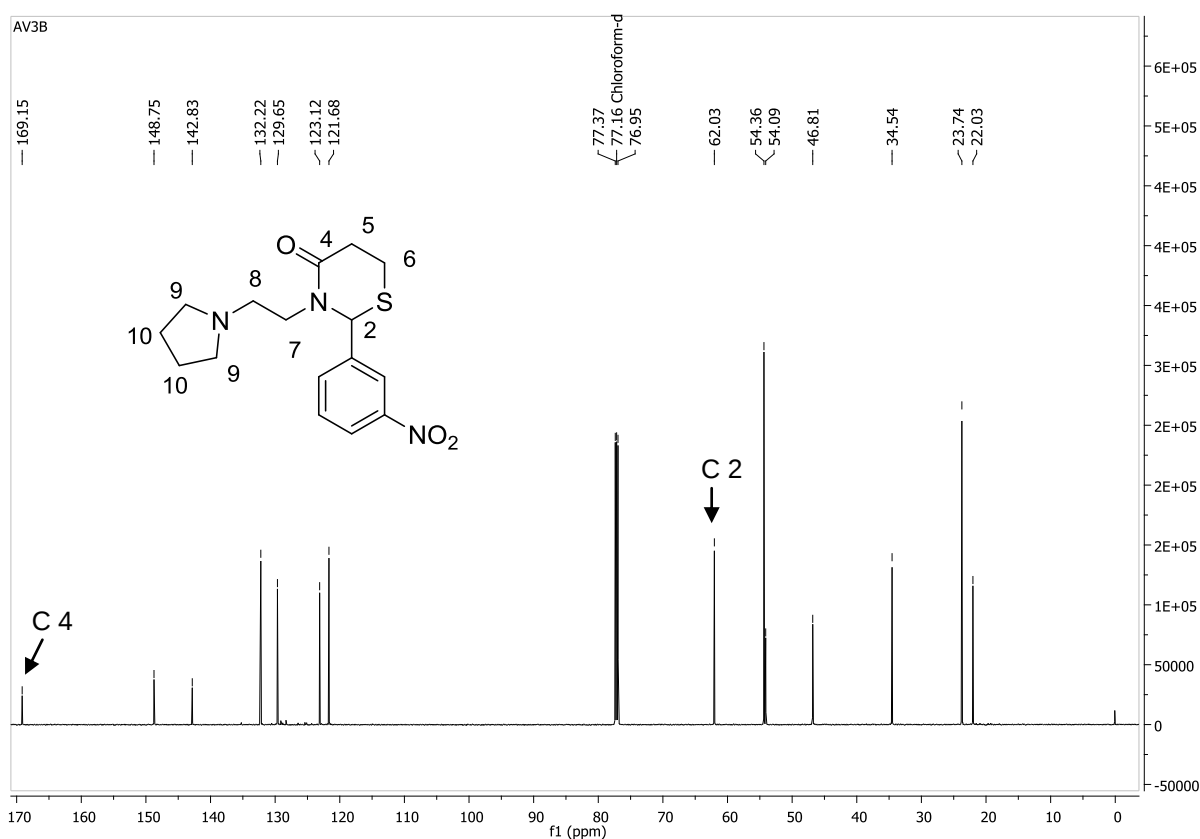


Figura 161: Espectro de ^{13}C da tiazinan-4-ona **11i** (CDCl_3 - 150 MHz).

Anexo III: Espectroscopia de RMN

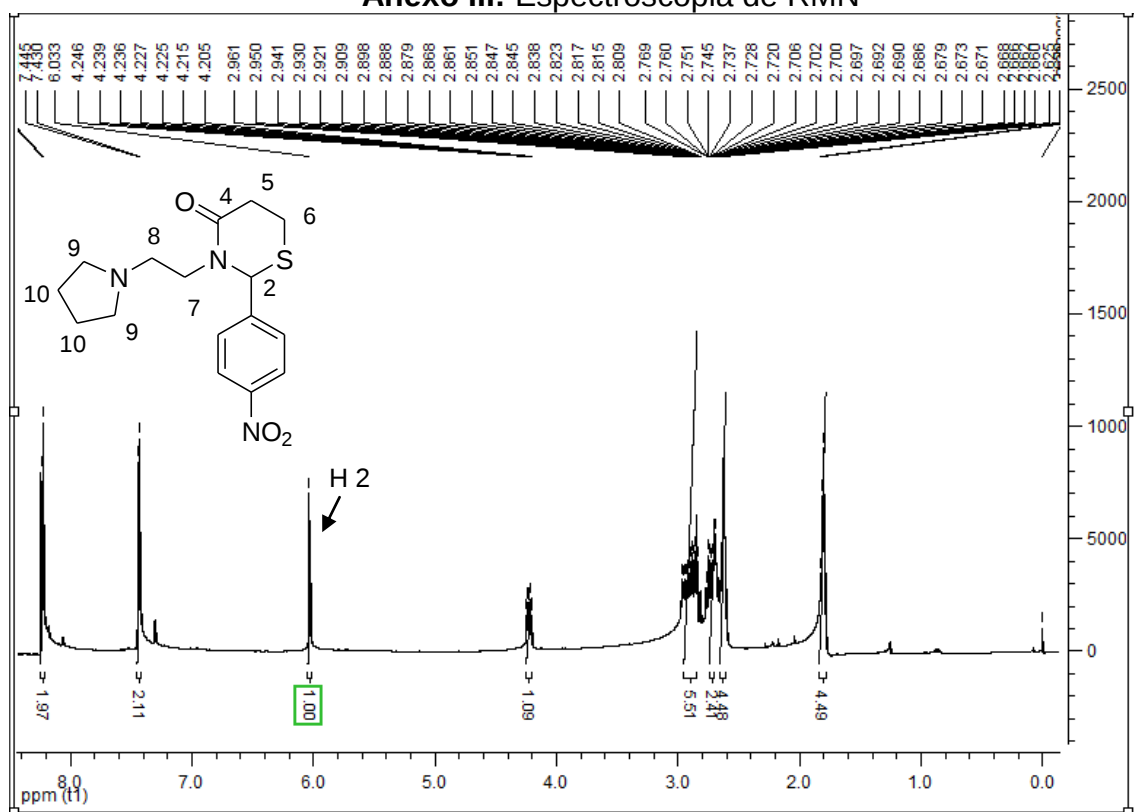


Figura 162: Espectro de ¹H da tiazinan-4-ona **11j** (CDCl₃ - 600 MHz).

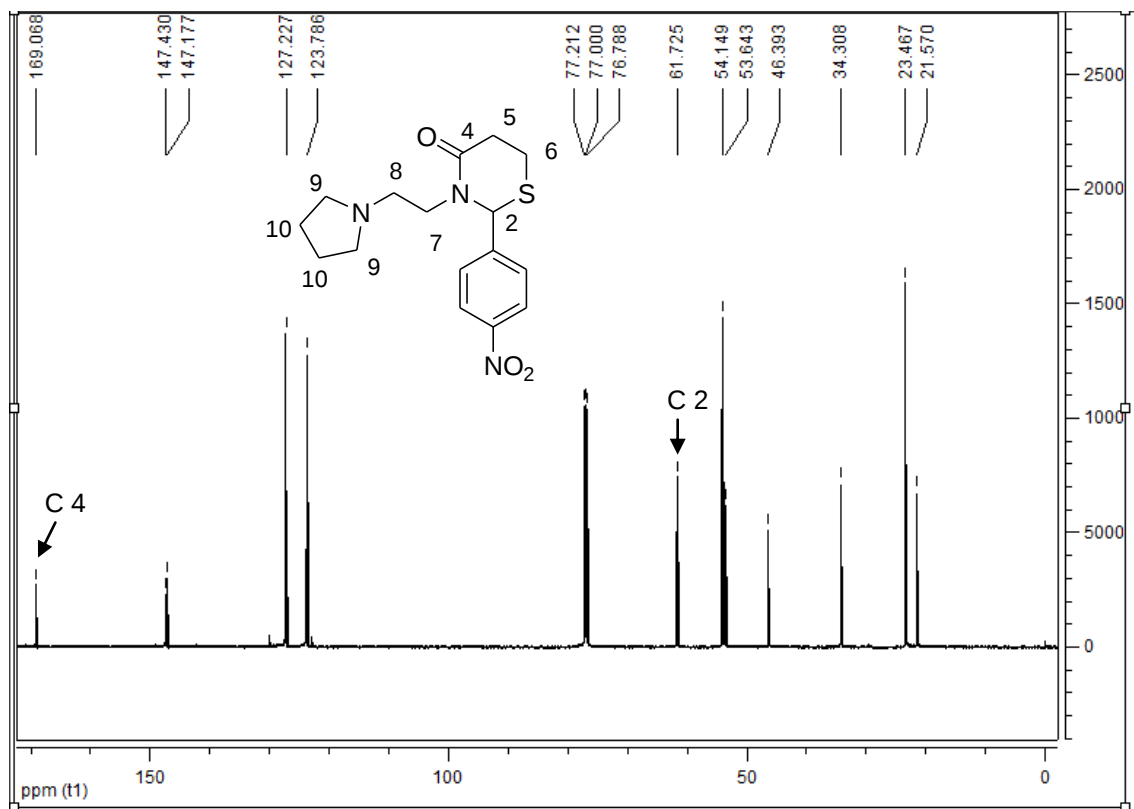


Figura 163: Espectro de ¹³C da tiazinan-4-ona **11j** (CDCl₃ - 150 MHz).

Anexo III: Espectroscopia de RMN

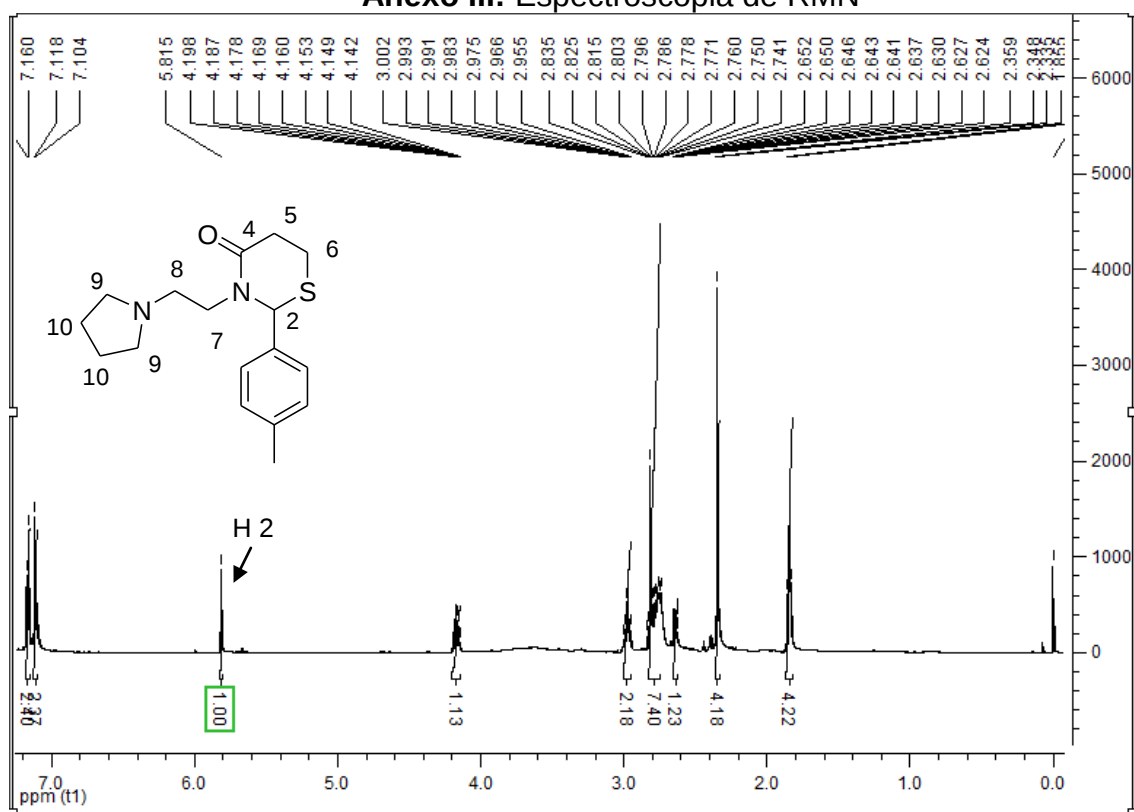


Figura 164: Espectro de ¹H da tiazinan-4-ona **11k** (CDCl₃ - 600 MHz).

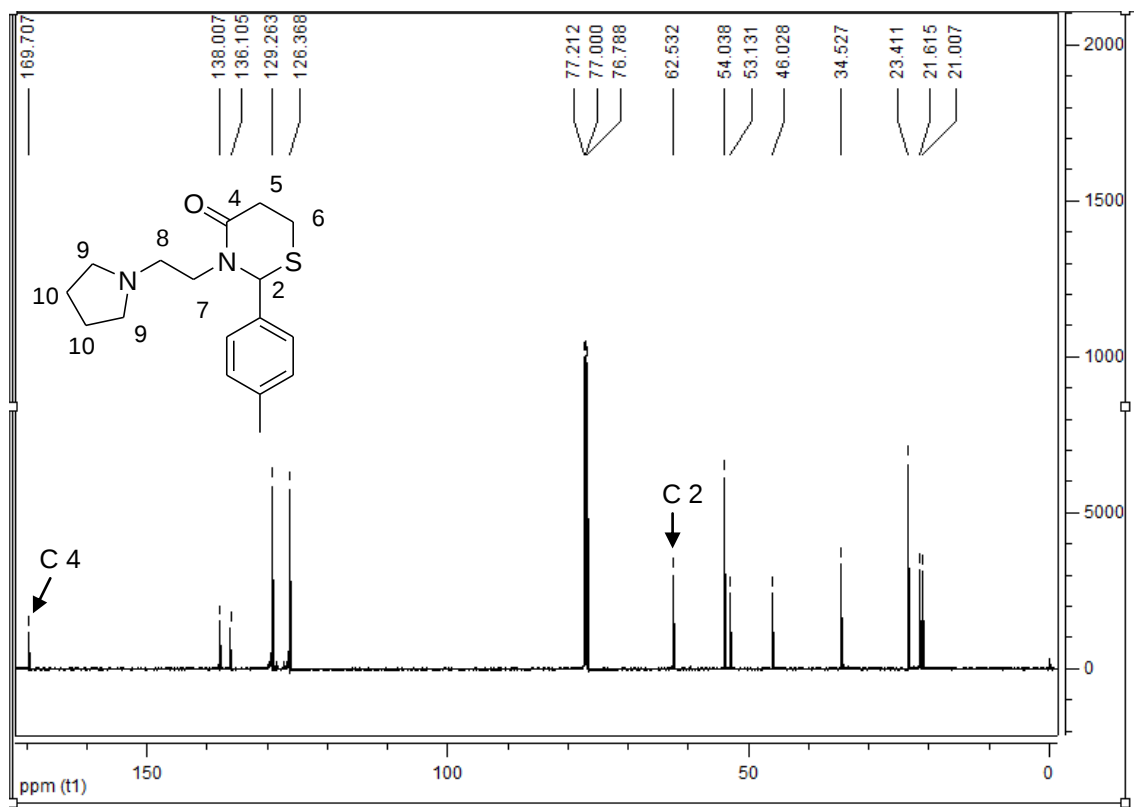


Figura 165: Espectro de ¹³C da tiazinan-4-ona **11k** (CDCl₃ - 150 MHz).

Anexo III: Espectroscopia de RMN

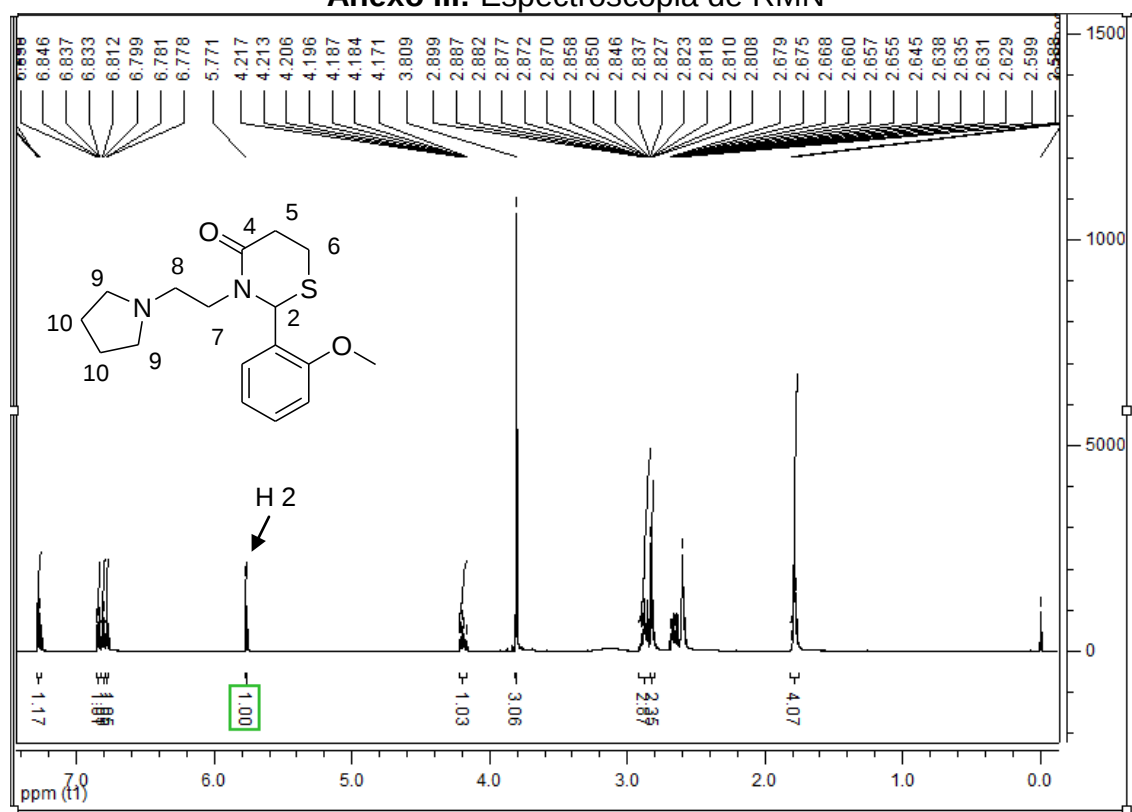


Figura 166: Espectro de ¹H da tiazinan-4-ona **11I** (CDCl₃ - 600 MHz).

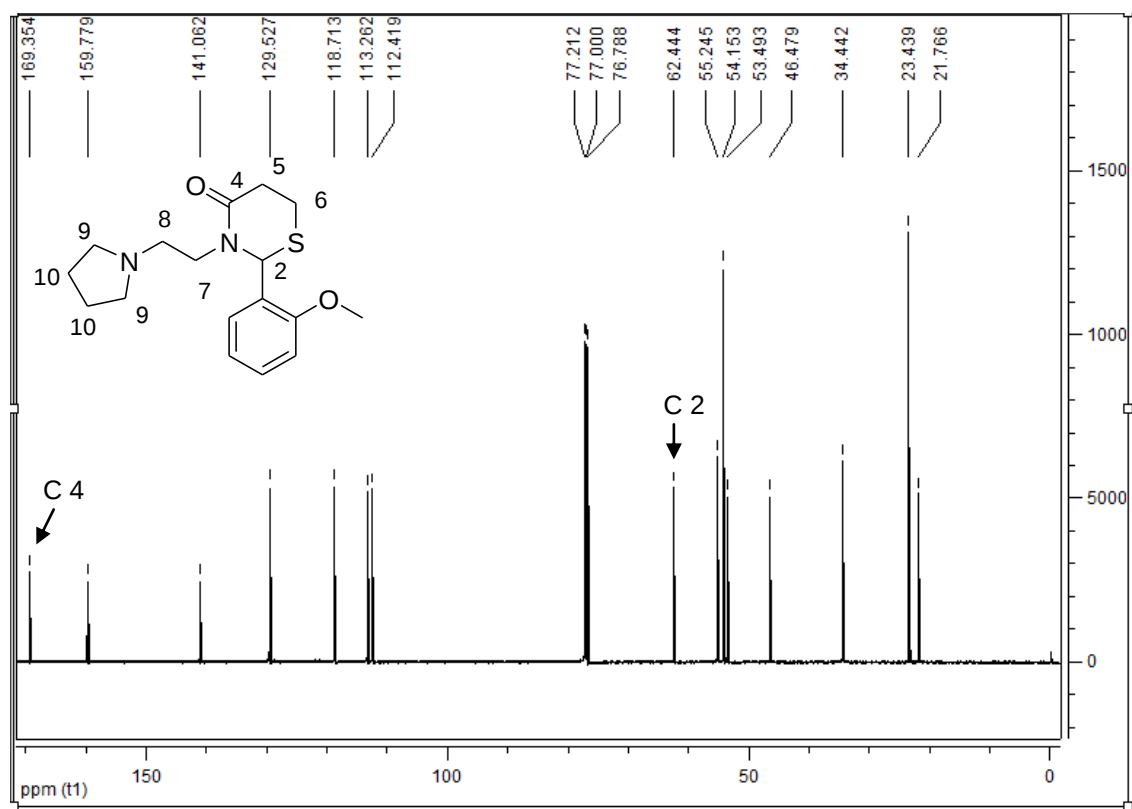


Figura 167: Espectro de ¹³C da tiazinan-4-ona **11I** (CDCl₃ - 150 MHz).

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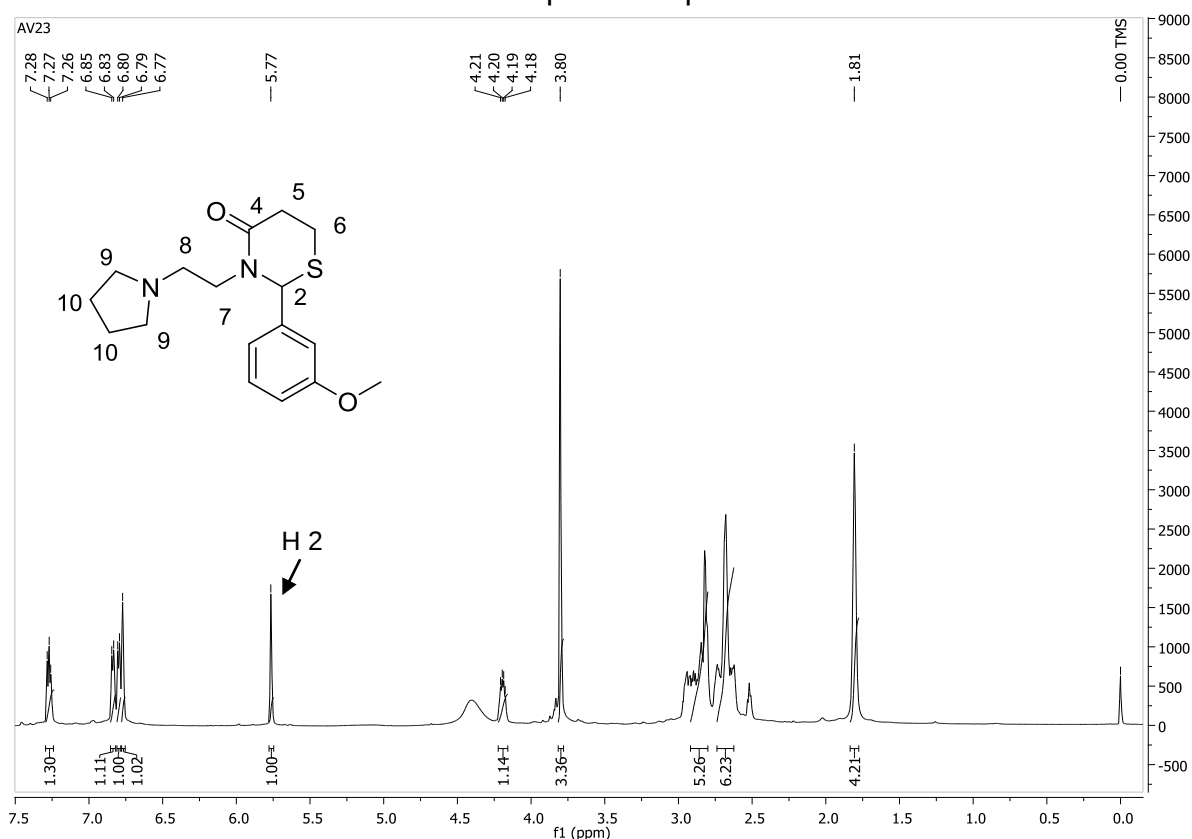


Figura 168: Espectro de ¹H da tiazinan-4-ona **11m** (CDCl₃ - 600 MHz).

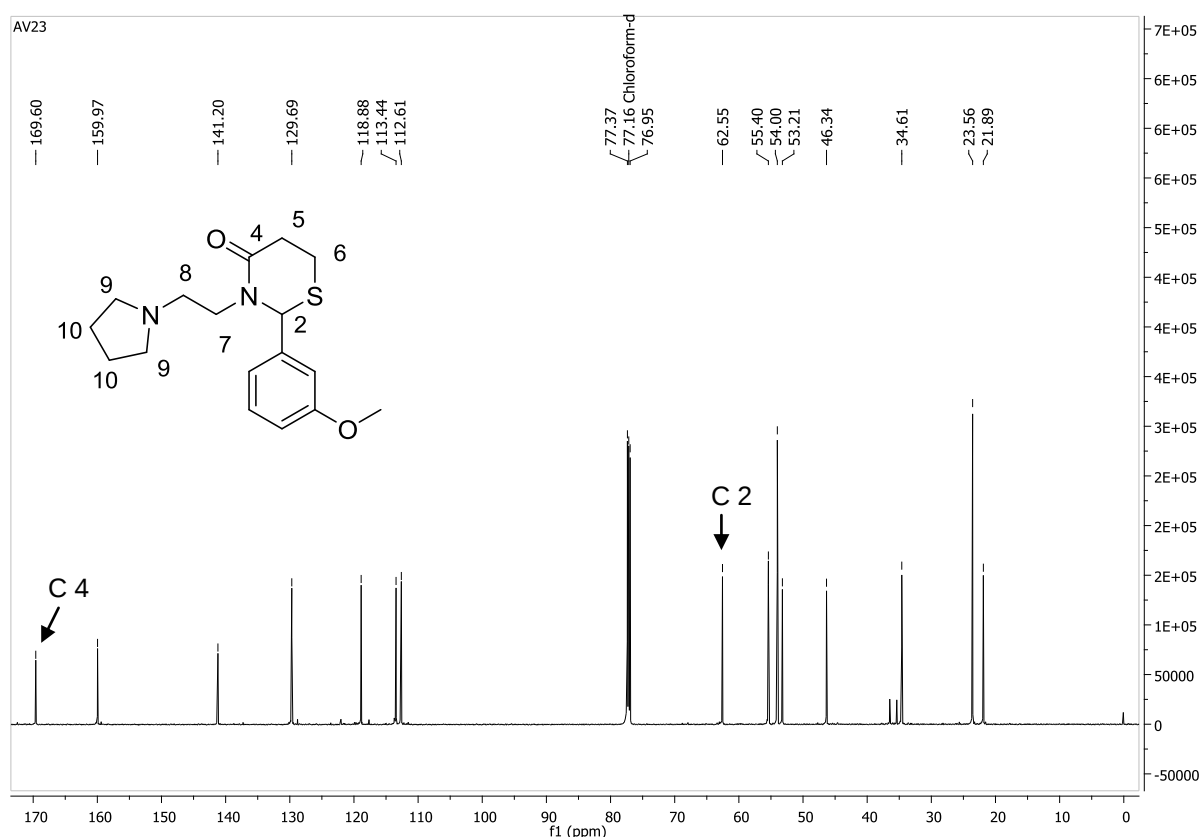
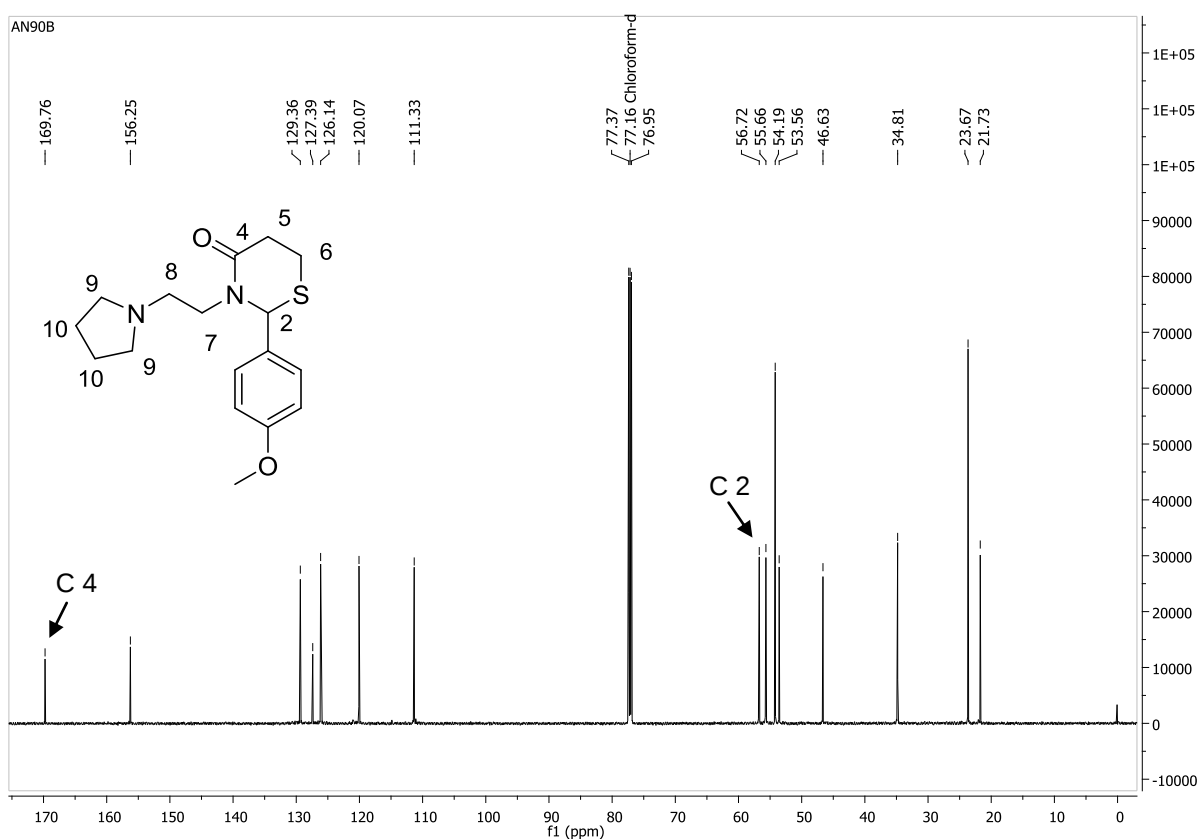
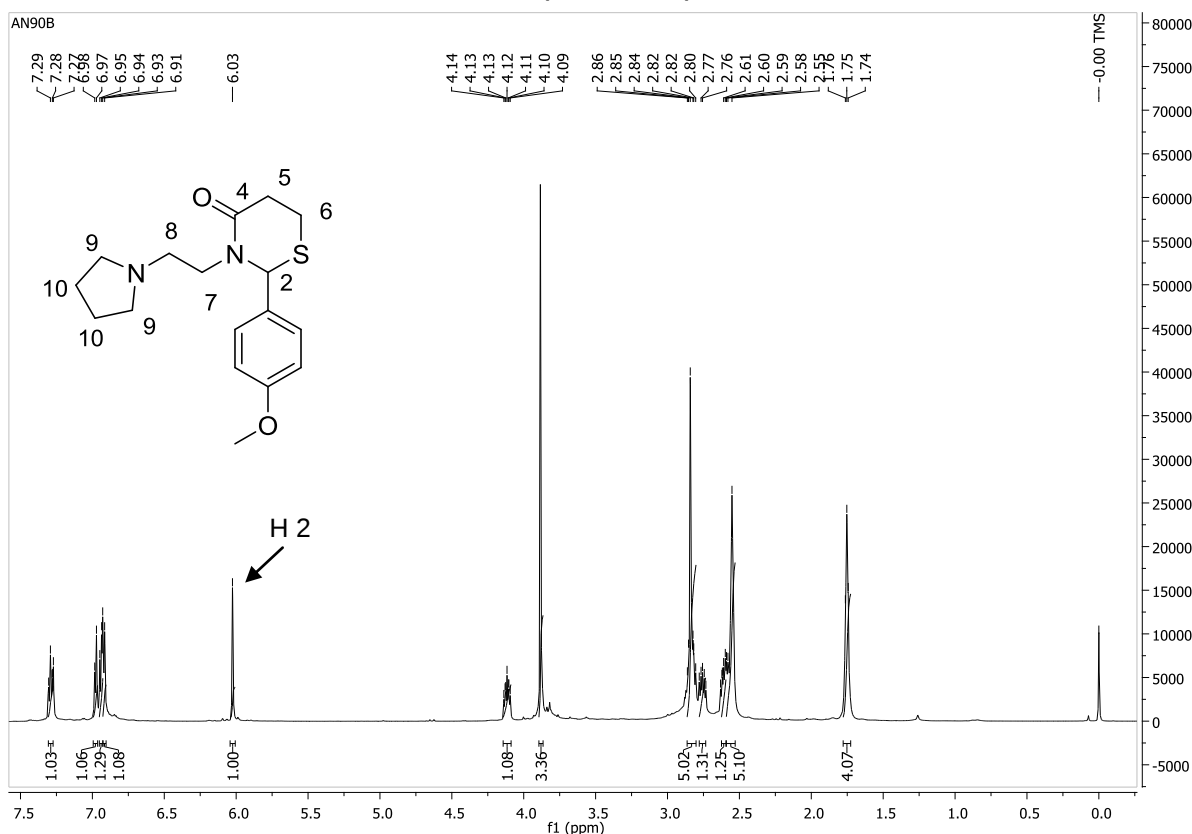


Figura 169: Espectro de ¹³C da tiazinan-4-ona **11m** (CDCl₃ - 150 MHz).

Anexo III: Espectroscopia de RMN



Anexo III: Espectroscopia de RMN

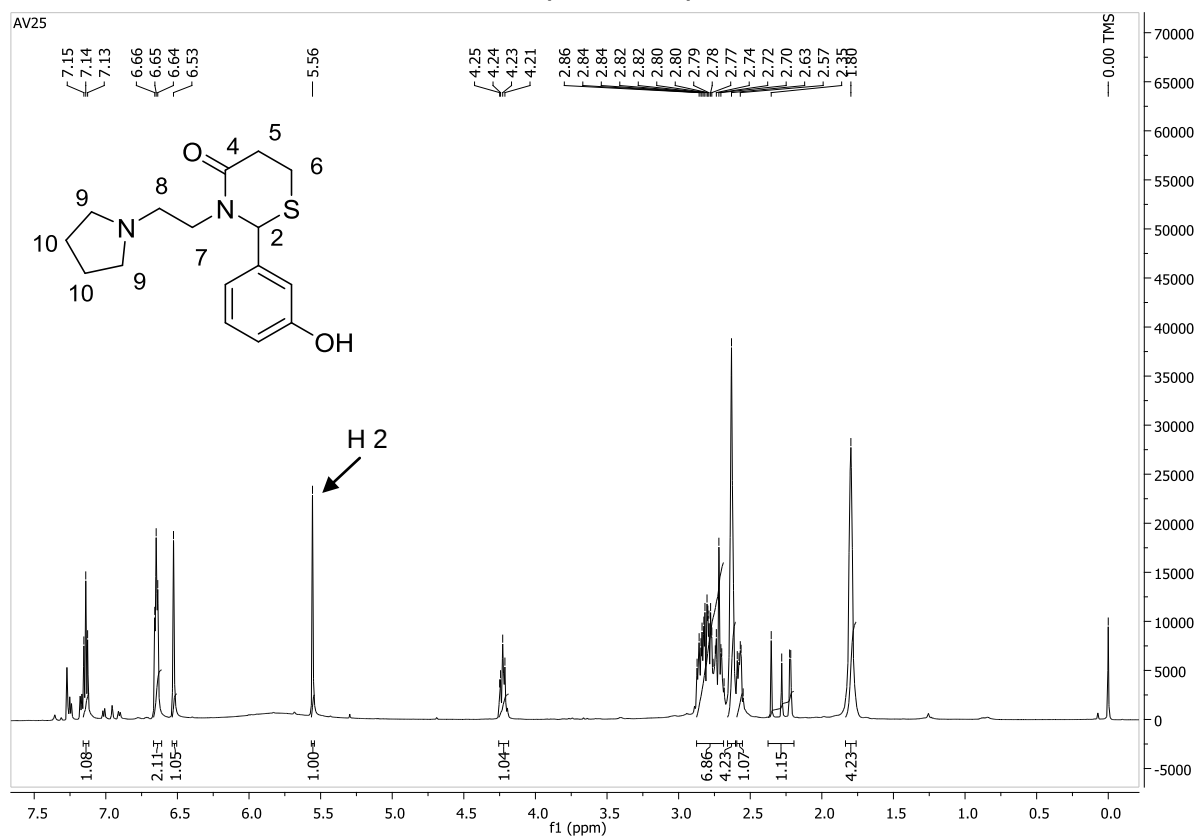


Figura 172: Espectro de ^1H da tiazinan-4-ona **11o** (CDCl₃ - 600 MHz).

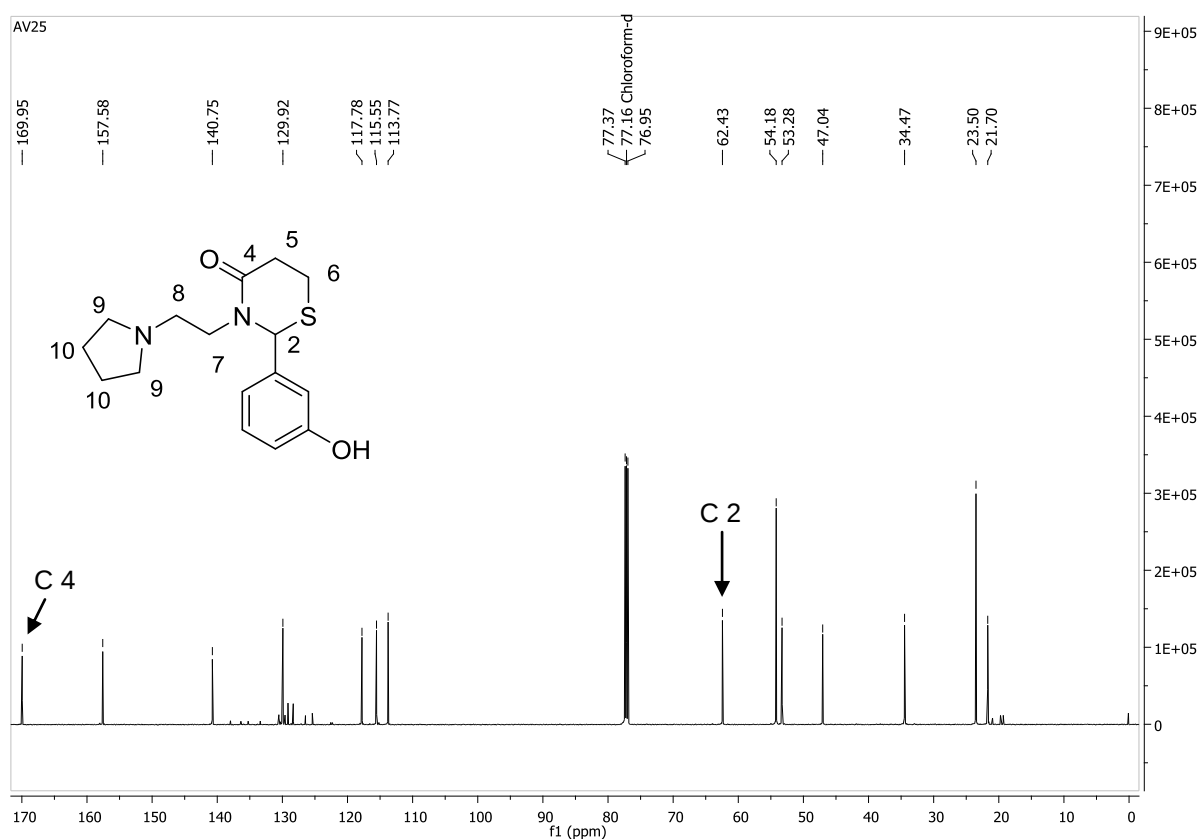


Figura 173: Espectro de ^{13}C da tiazinan-4-ona **11o** (CDCl₃ - 150 MHz).

Anexo III: Espectroscopia de RMN

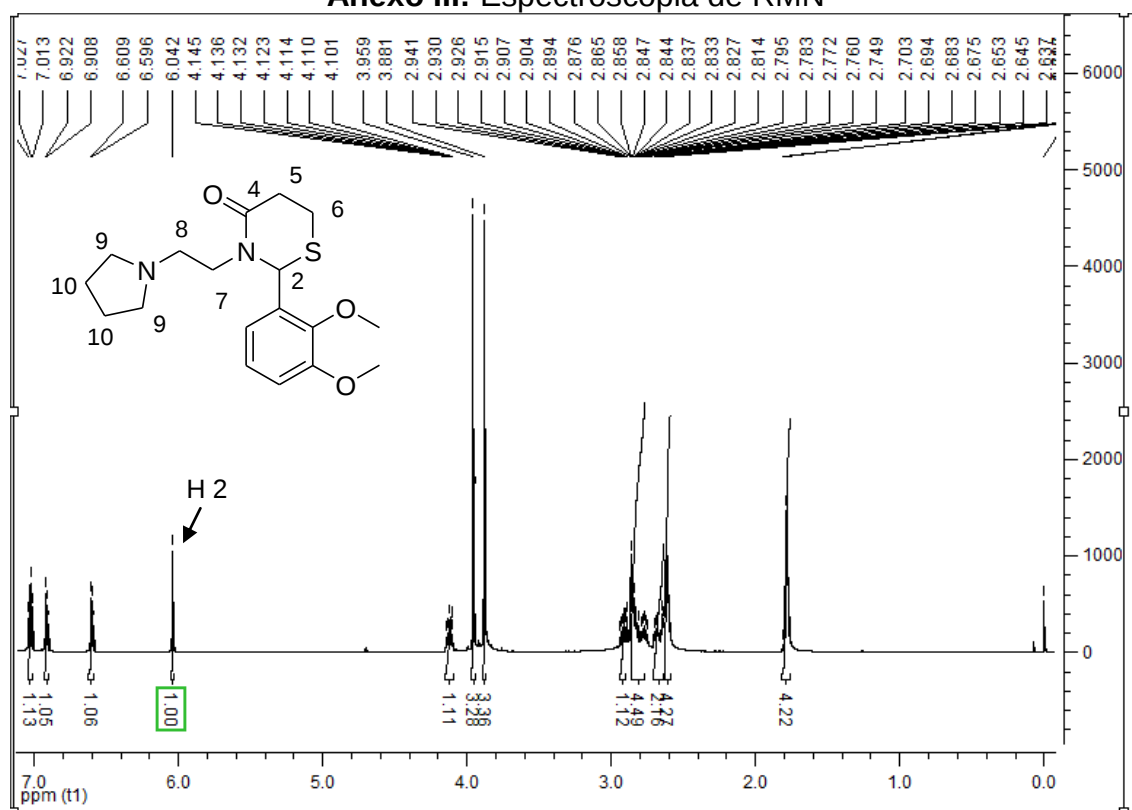


Figura 174: Espectro de ¹H da tiazinan-4-ona **11p** (CDCl₃ - 600 MHz).

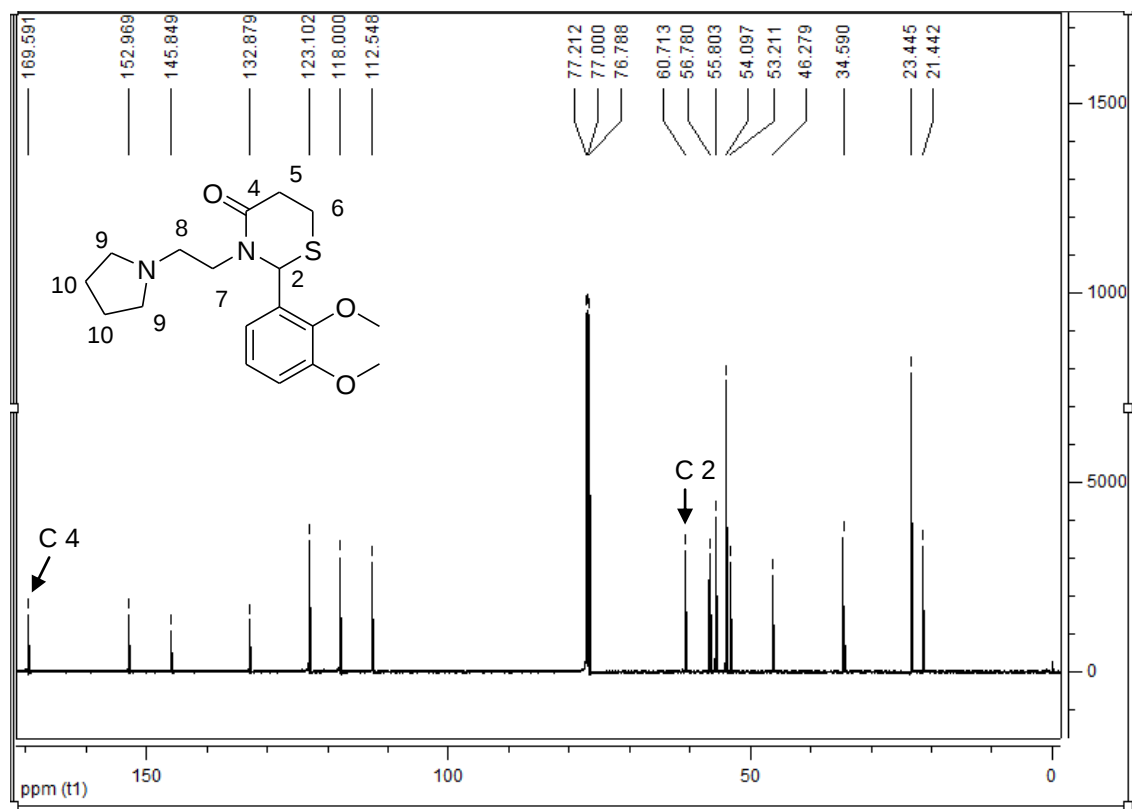


Figura 175: Espectro de ¹³C da tiazinan-4-ona **11p** (CDCl₃ - 150 MHz).

Anexo III: Espectroscopia de RMN

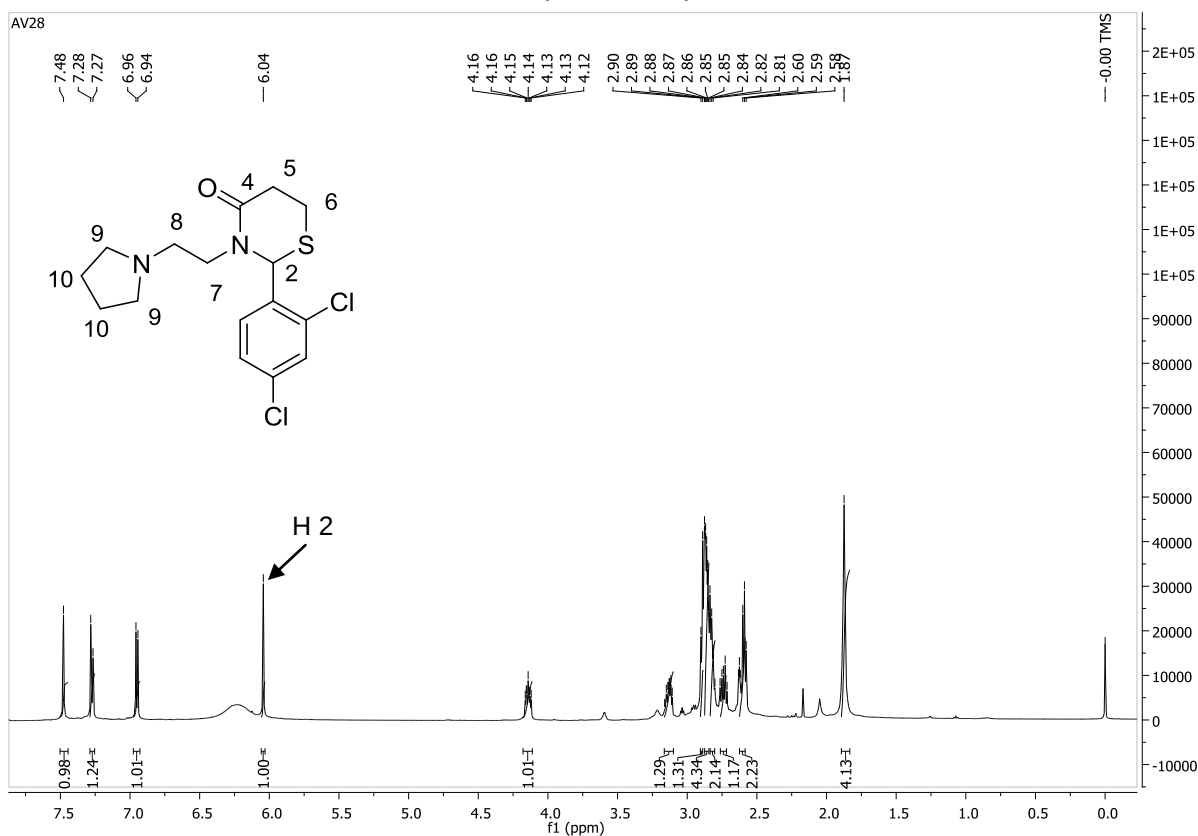


Figura 176: Espectro de ^1H da tiazinan-4-ona **11q** (CDCl_3 - 600 MHz).

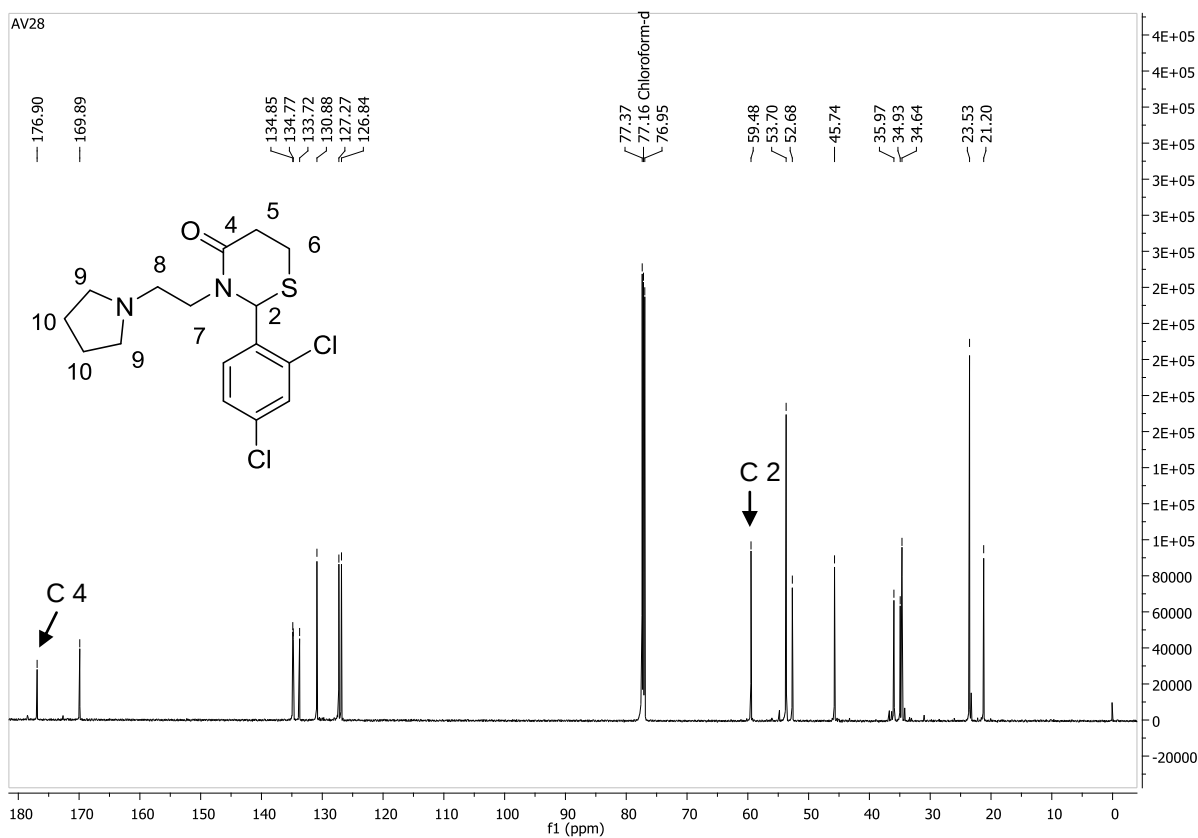


Figura 177: Espectro de ^{13}C da tiazinan-4-ona **11q** (CDCl_3 - 150 MHz).

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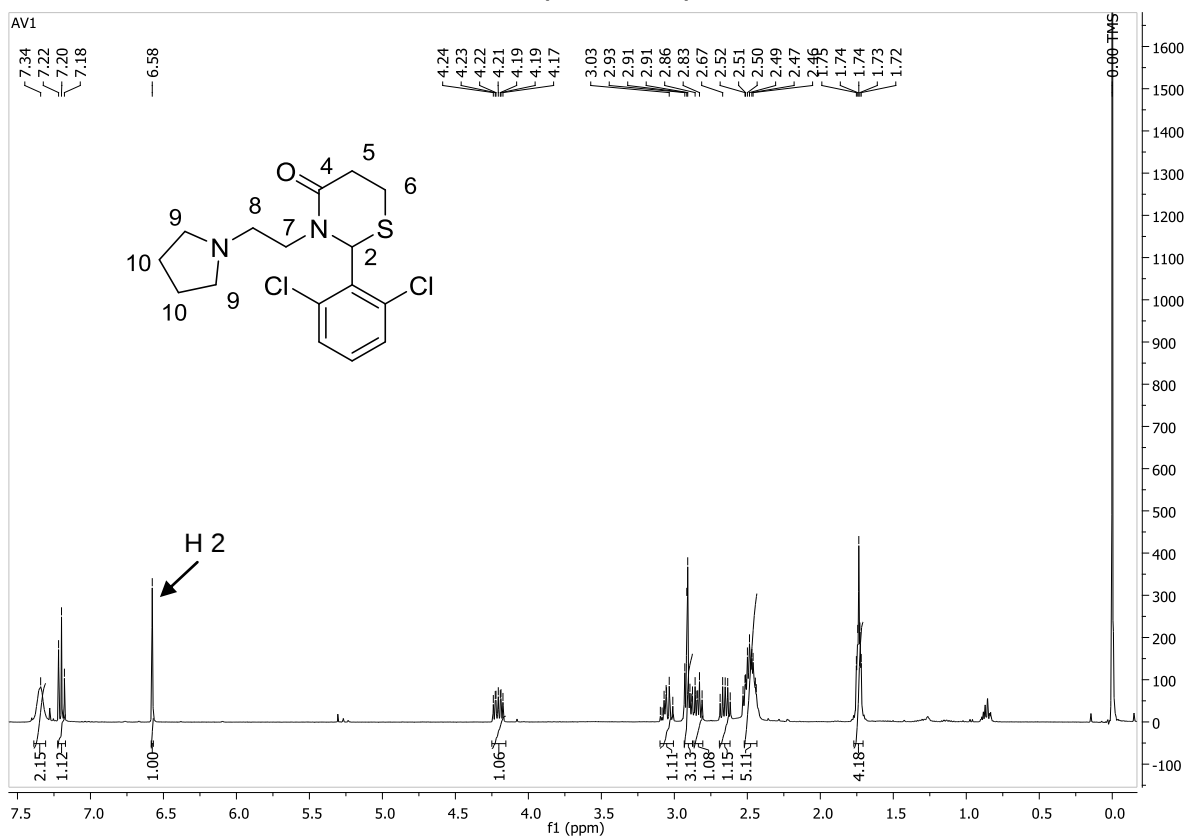


Figura 178: Espectro de ¹H da tiazinan-4-ona **11r** (CDCl₃ - 600 MHz).

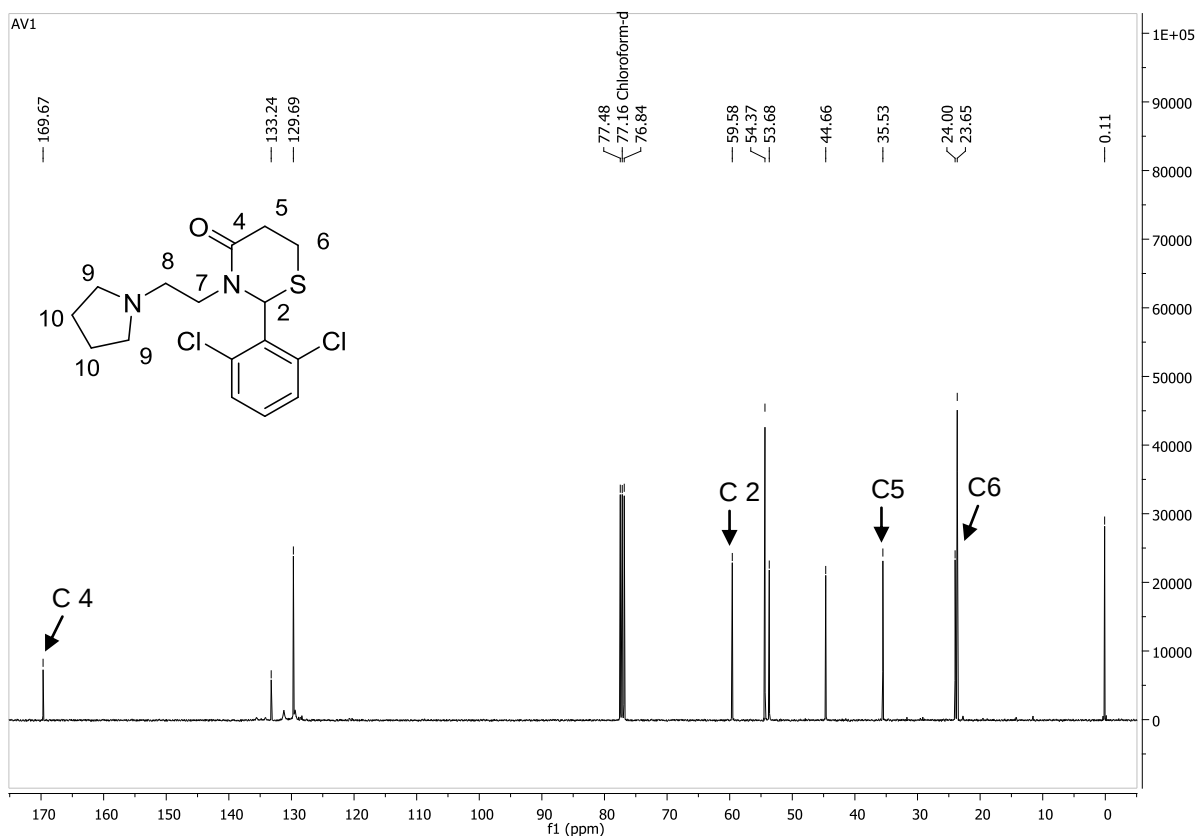


Figura 179: Espectro de ¹³C da tiazinan-4-ona **11r** (CDCl₃ - 150 MHz).

Anexo III: Espectroscopia de RMN

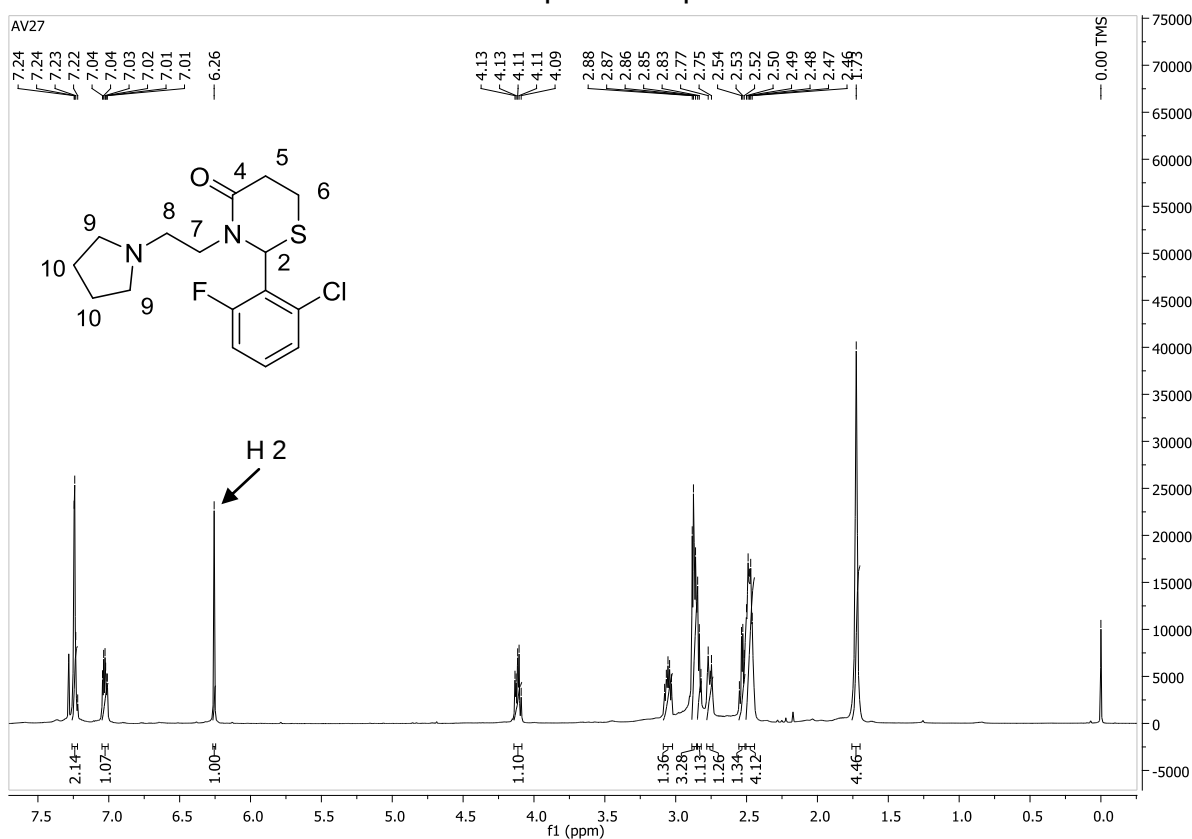


Figura 180: Espectro de ^1H da tiazinan-4-ona **11s** (CDCl_3 - 600 MHz).

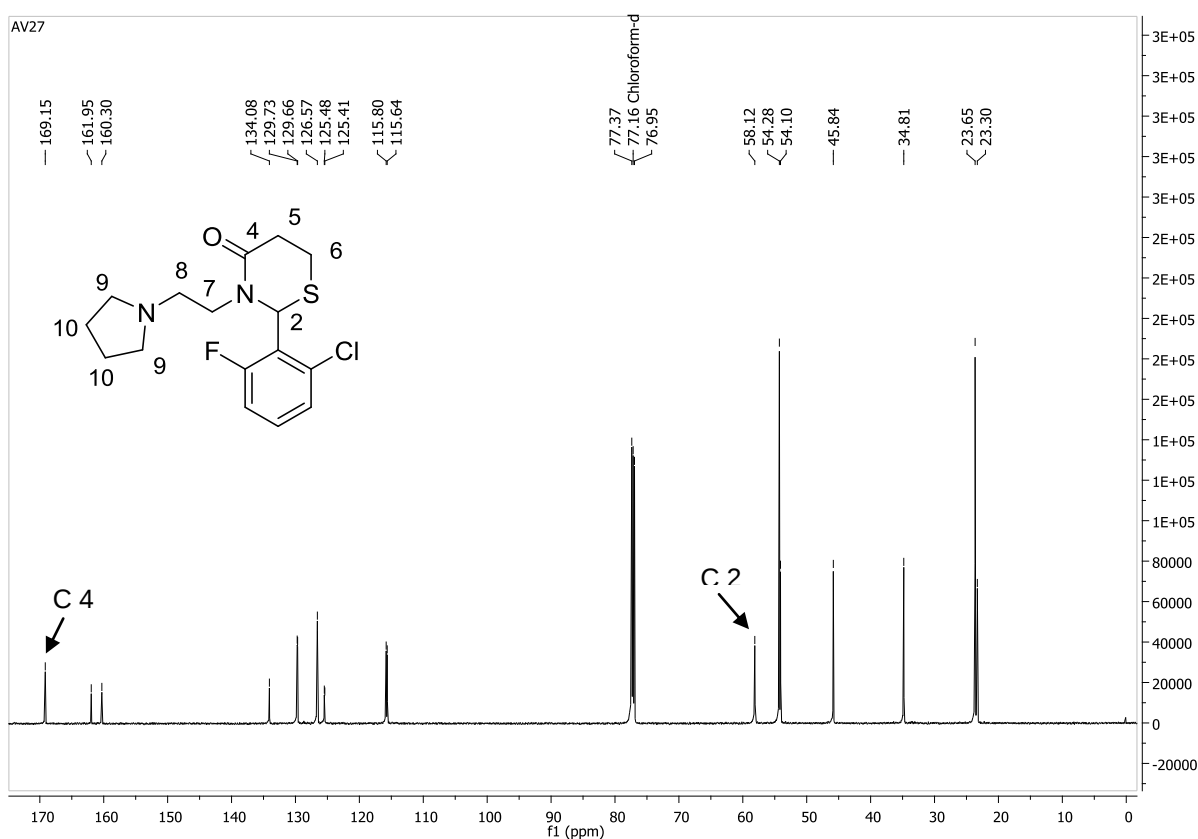


Figura 181: Espectro de ^{13}C da tiazinan-4-ona **11s** (CDCl_3 - 150 MHz).

Anexo III: Espectroscopia de RMN

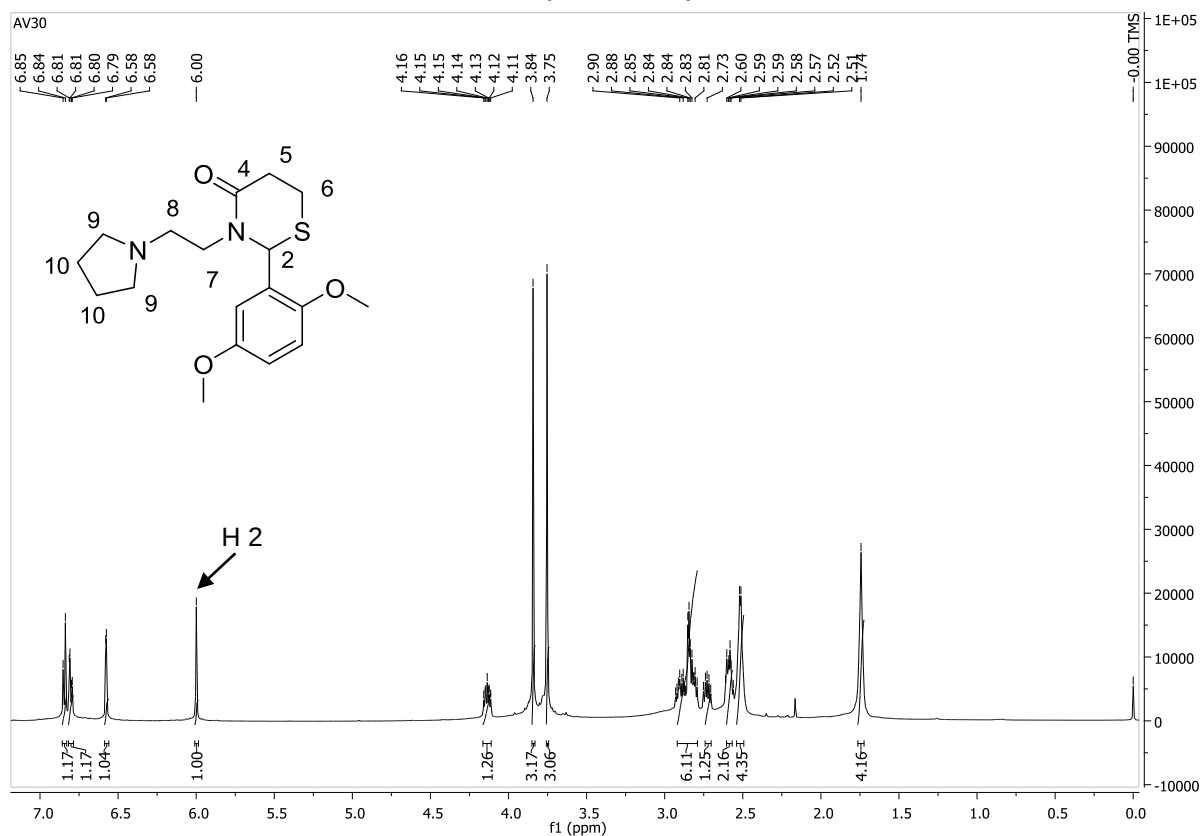


Figura 182: Espectro de ¹H da tiazinan-4-ona **11t** (CDCl₃ - 600 MHz).

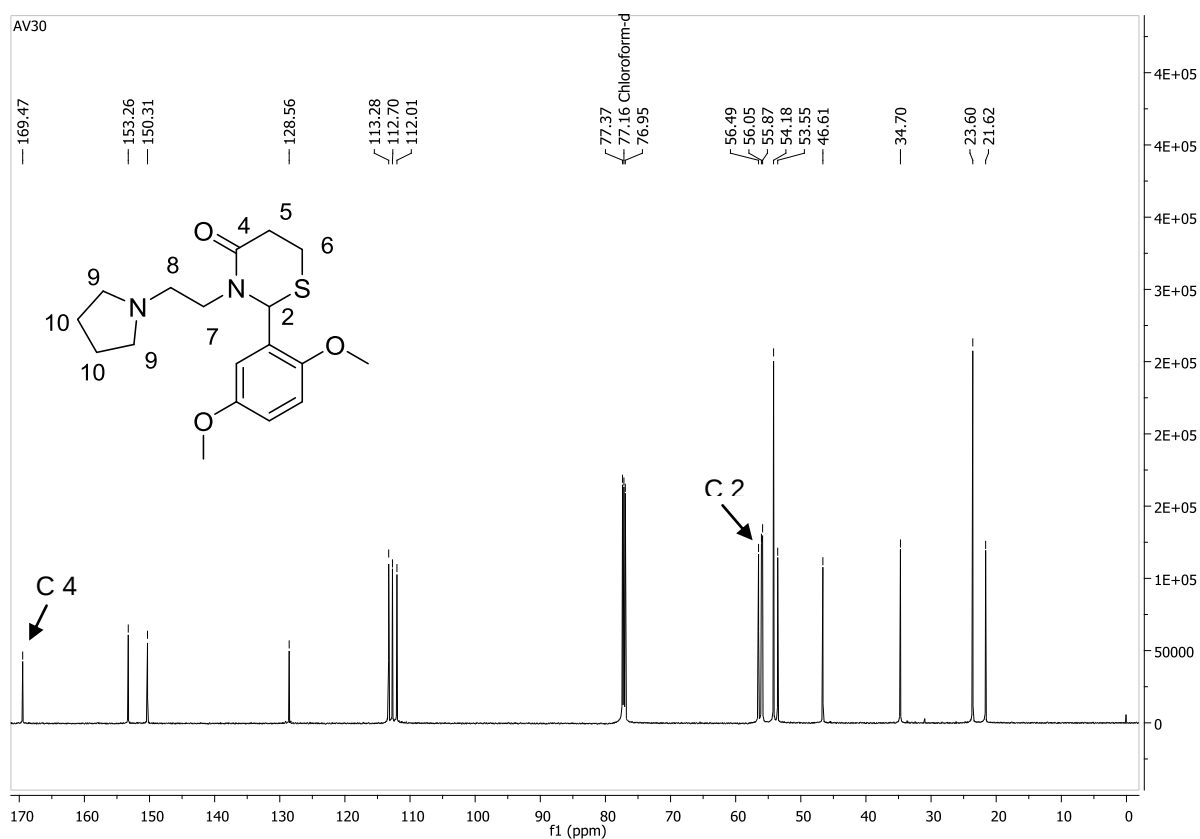


Figura 183: Espectro de ¹³C da tiazinan-4-ona **11t** (CDCl₃ - 150 MHz).

Anexo III: Espectroscopia de RMN

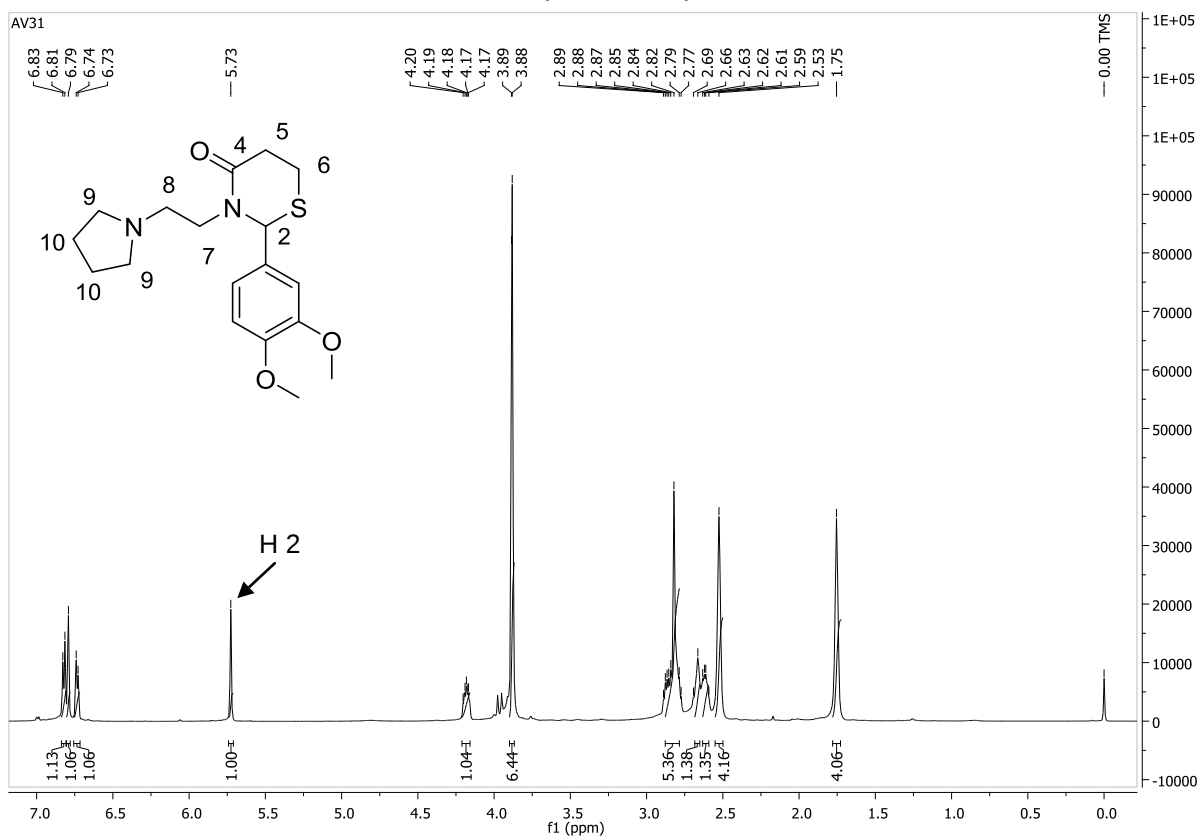


Figura 184: Espectro de ¹H da tiazinan-4-ona **11u** (CDCl₃ - 600 MHz).

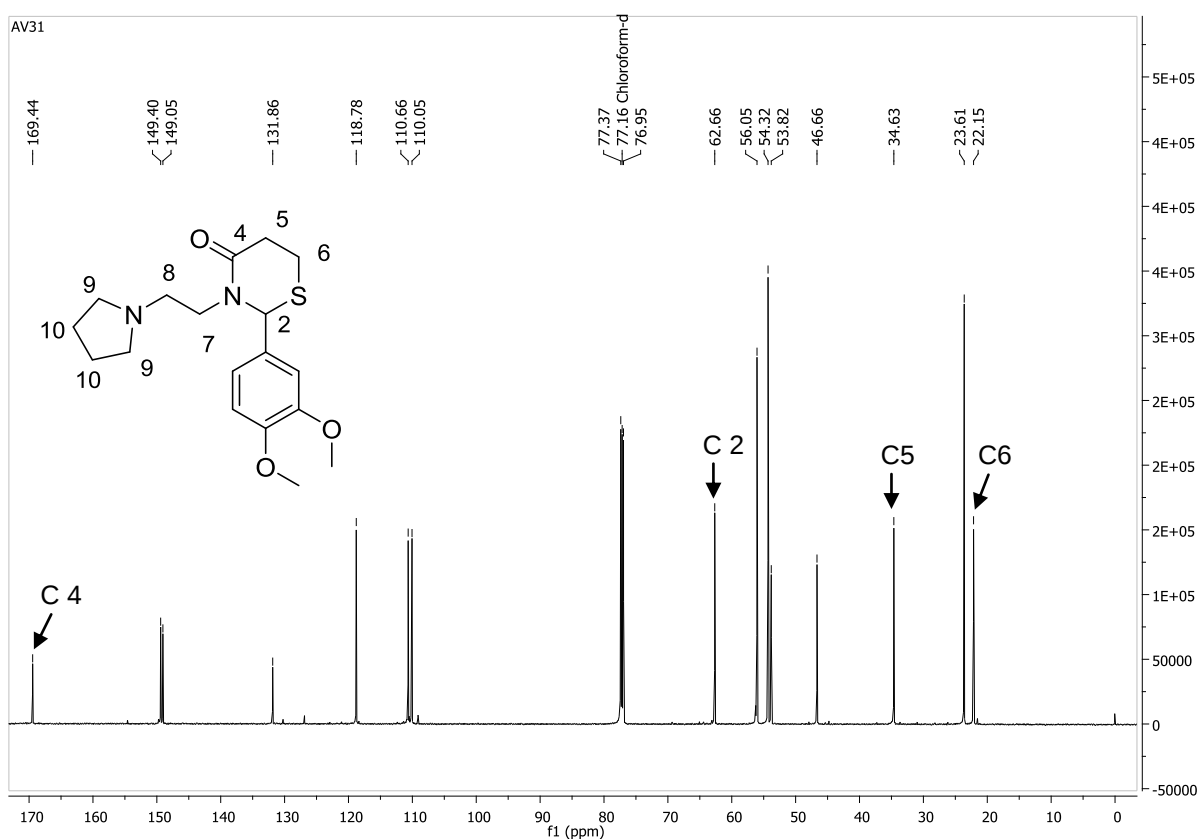


Figura 185: Espectro de ¹³C da tiazinan-4-ona **11u** (CDCl₃ - 150 MHz).