

UFRRJ

**INSTITUTO DE CIÊNCIAS EXATAS
PROGRAMA DE PÓS-GRADUAÇÃO EM QUÍMICA**

DISSERTAÇÃO

**Síntese de novos naftoimidazóis derivados de β -lapachona
com potenciais atividades biológicas.**

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SEROPÉDICA – 2016

Caderno de espectros

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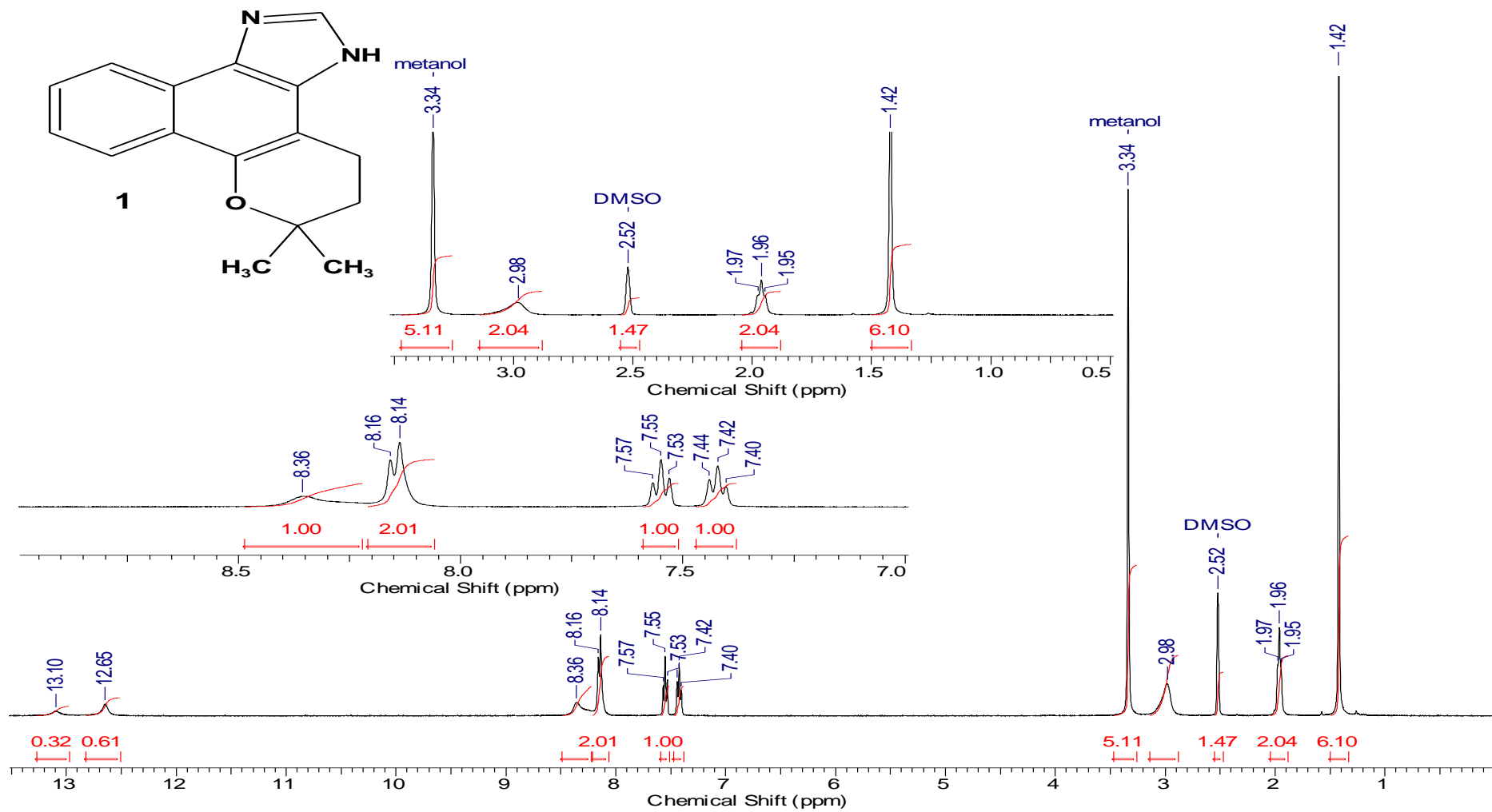
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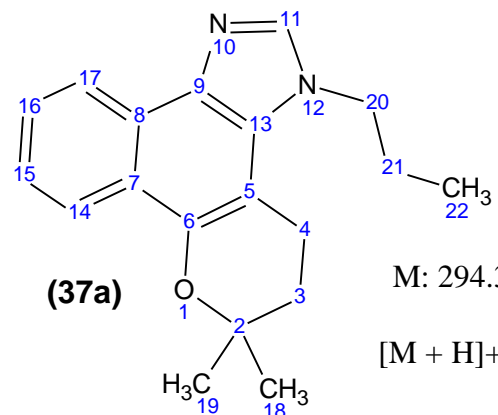
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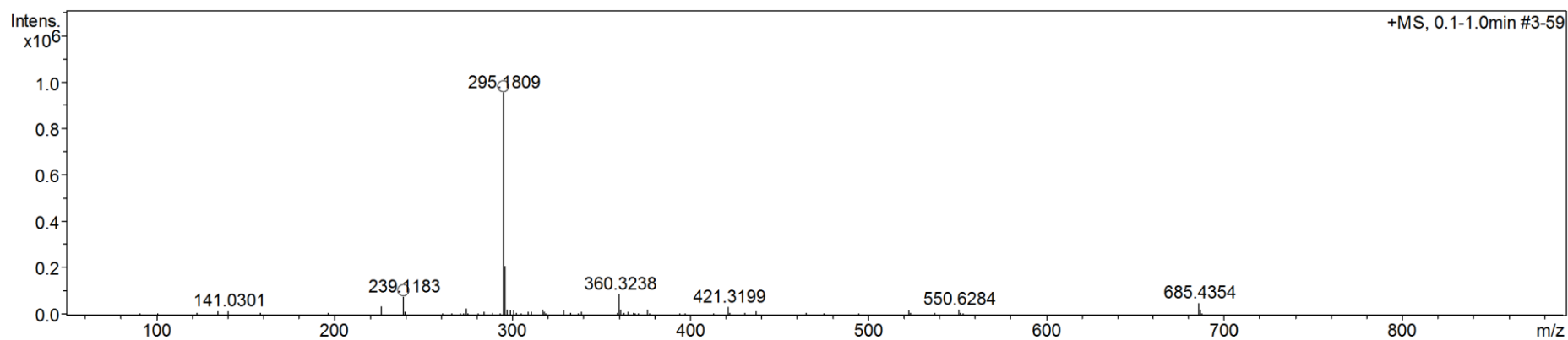


Espectro 1. RMN-¹H (400 MHz, DMSO-*d*₆) do BLI-H (1).

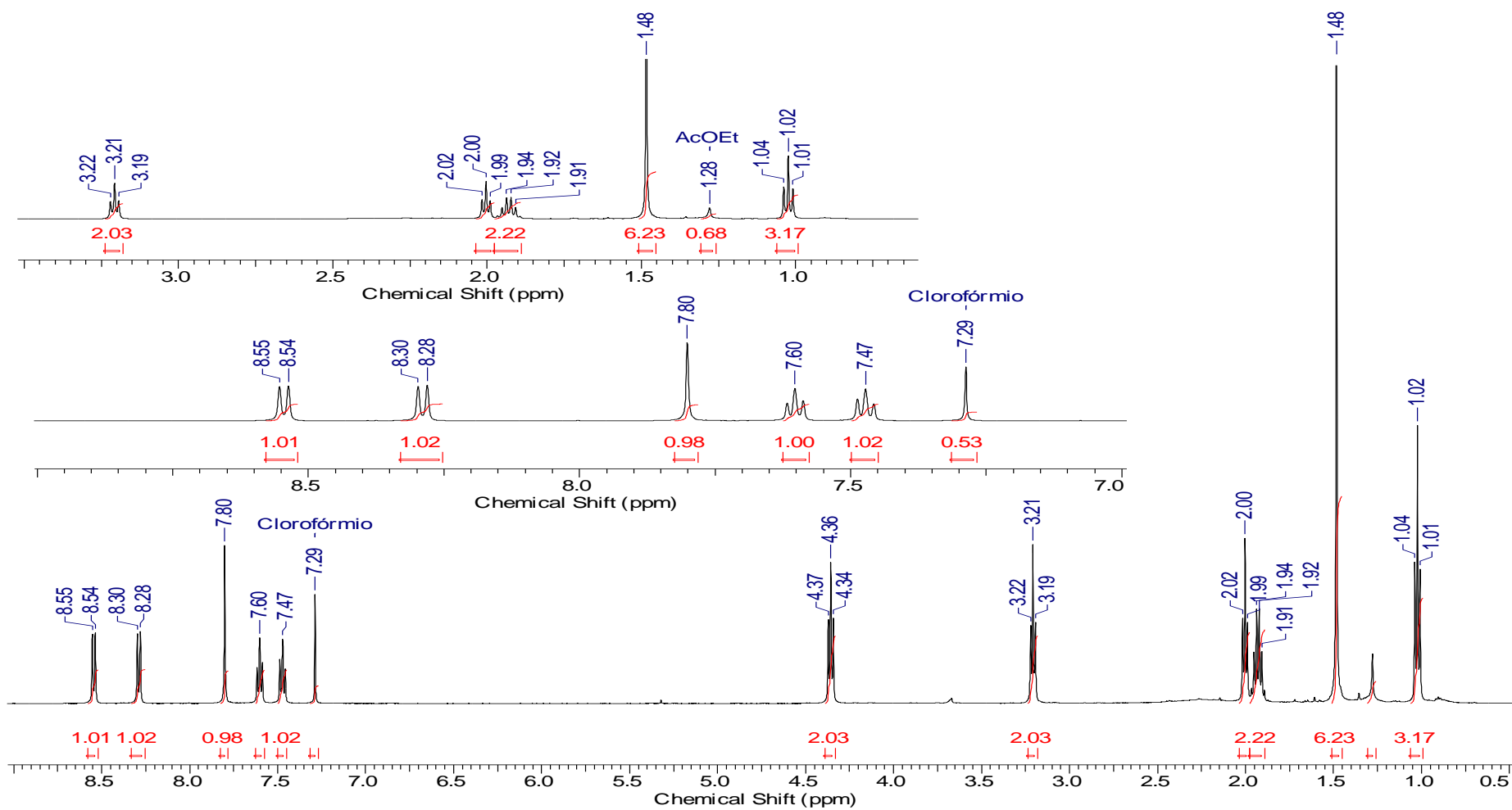


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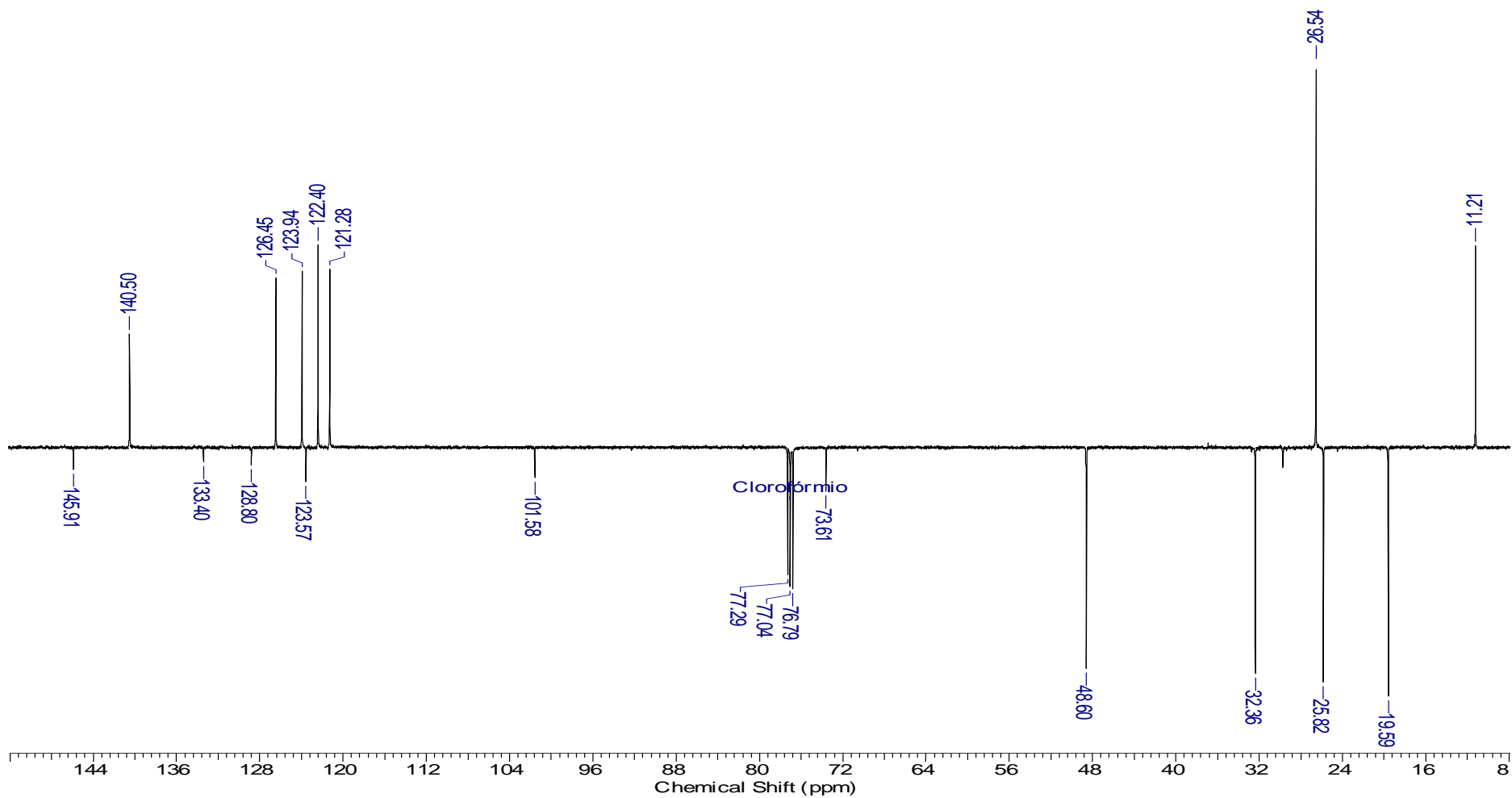
[M + H]⁺ = 295.1805Da; err [ppm] = -1,5



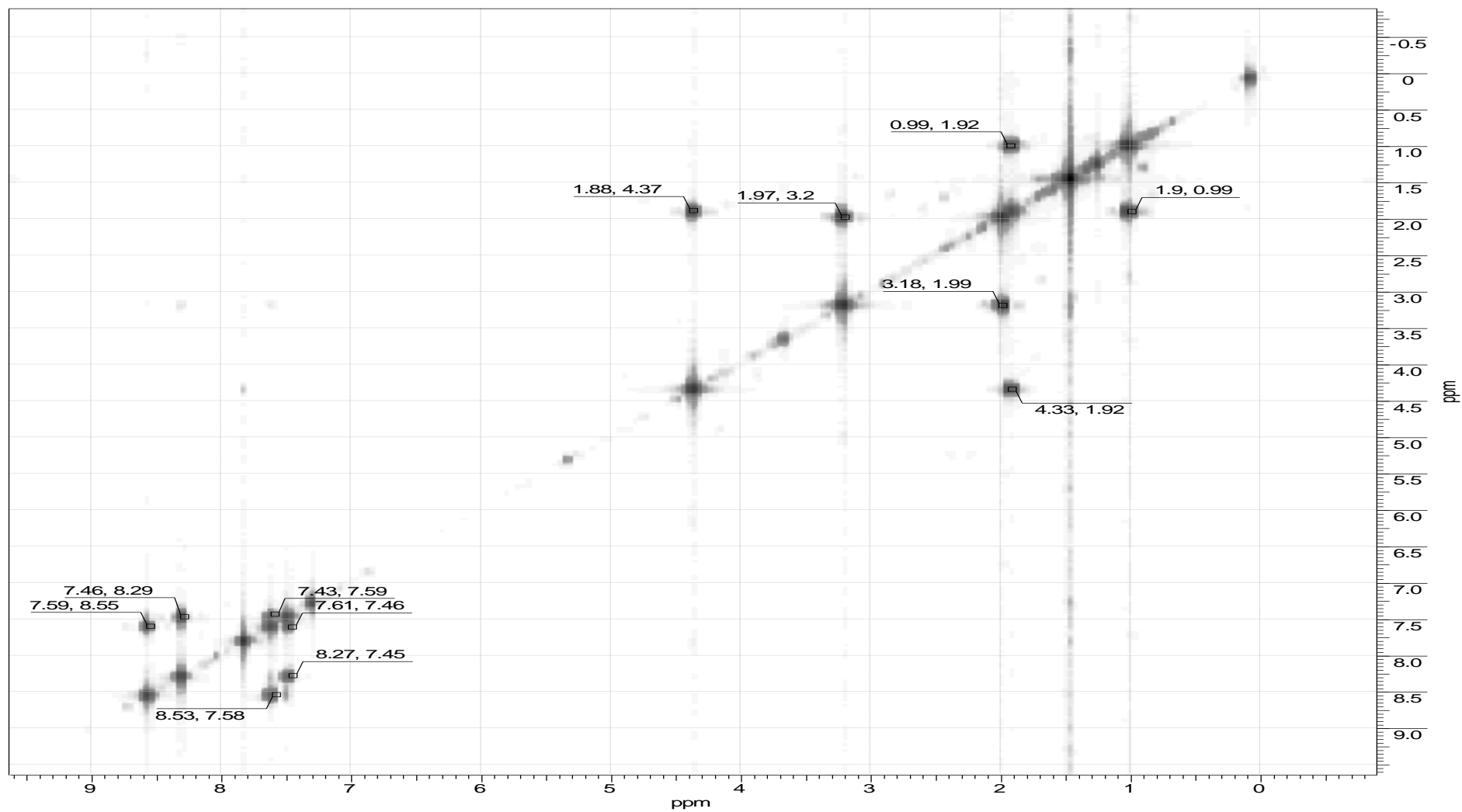
Espectro 2. EM-IES do composto 37a.



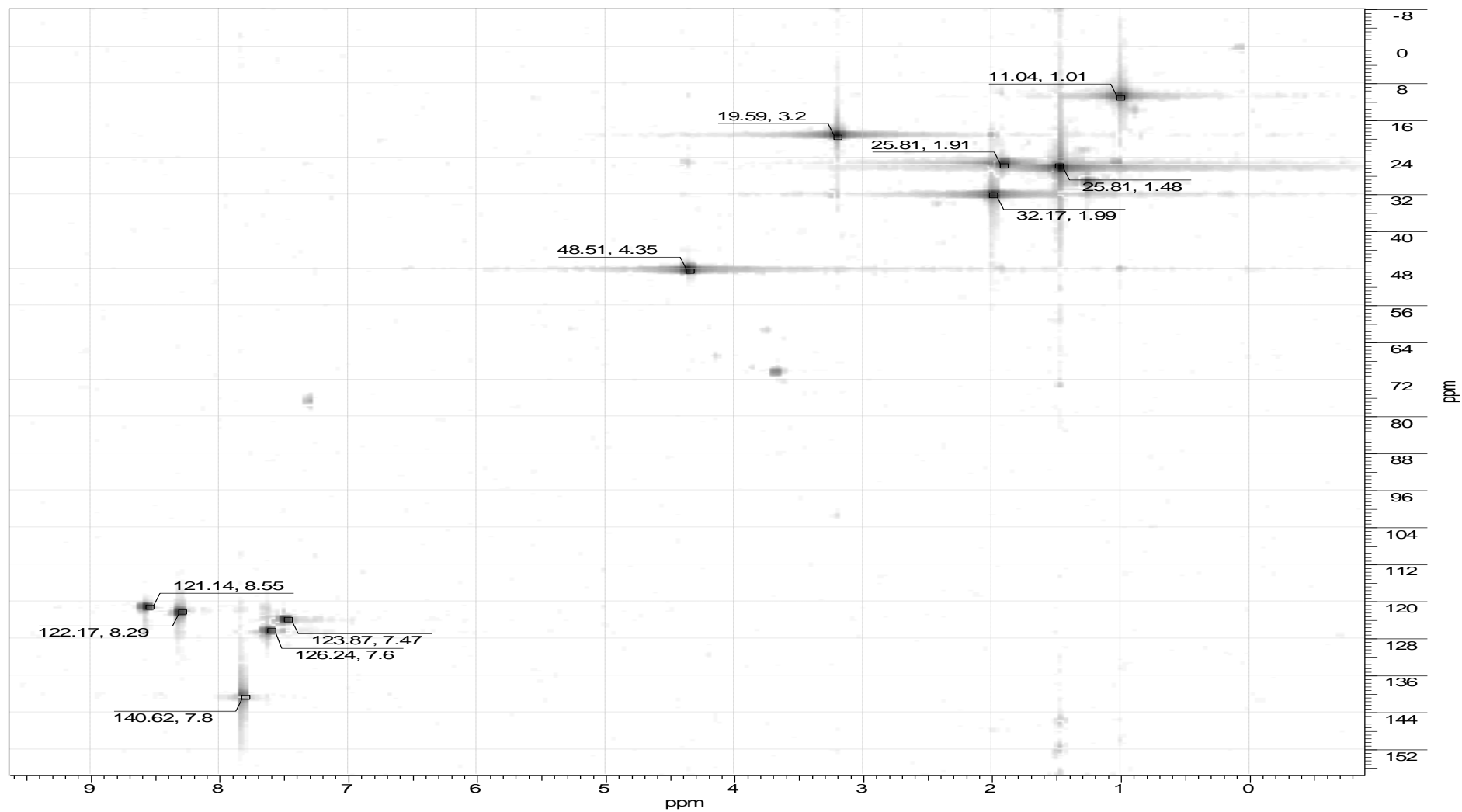
Espectro 3. RMN-¹H (500 MHz, CDCl₃)do composto 37a.



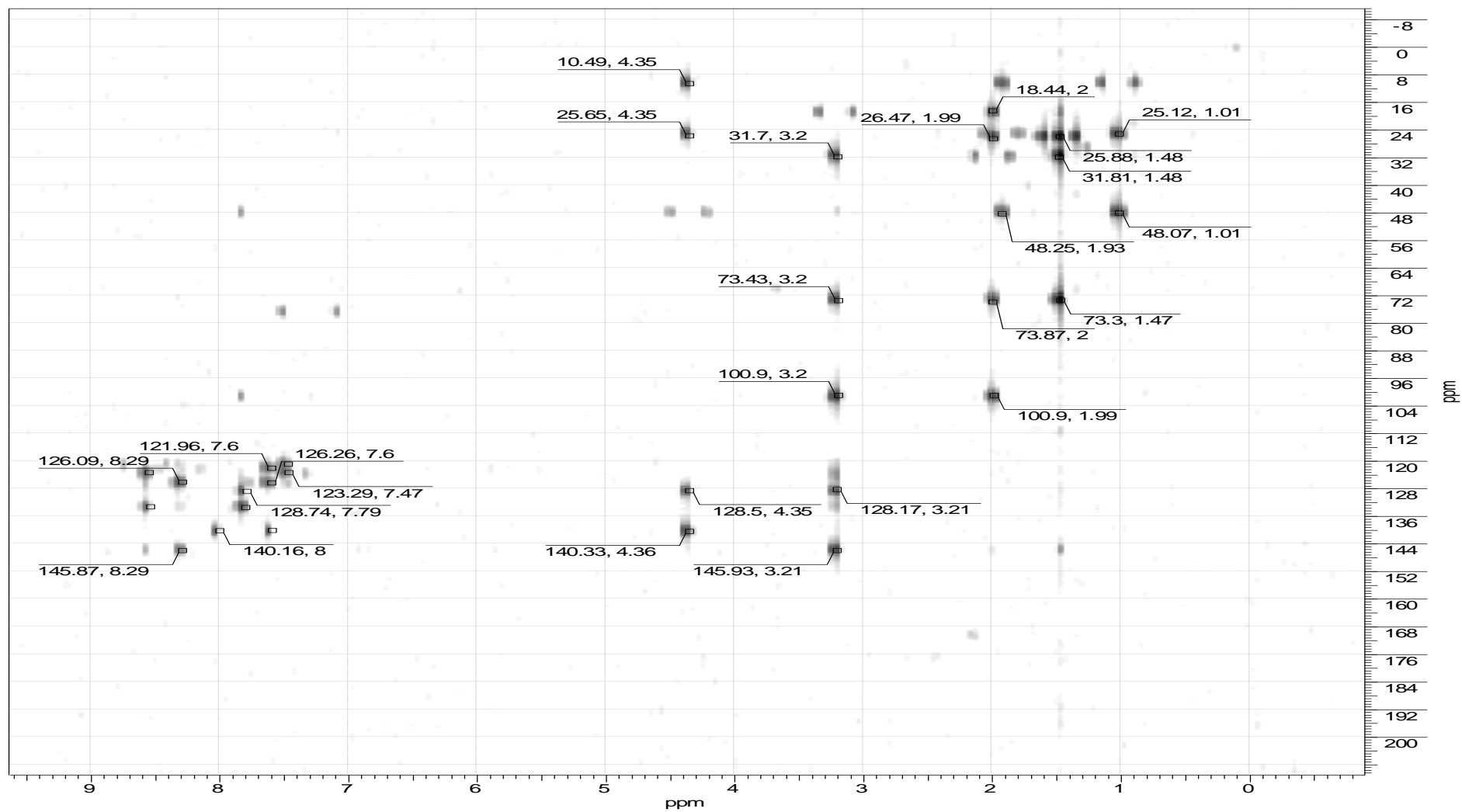
Espectro 4. DEPTQ (500 MHz, CDCl₃) do composto 37a.



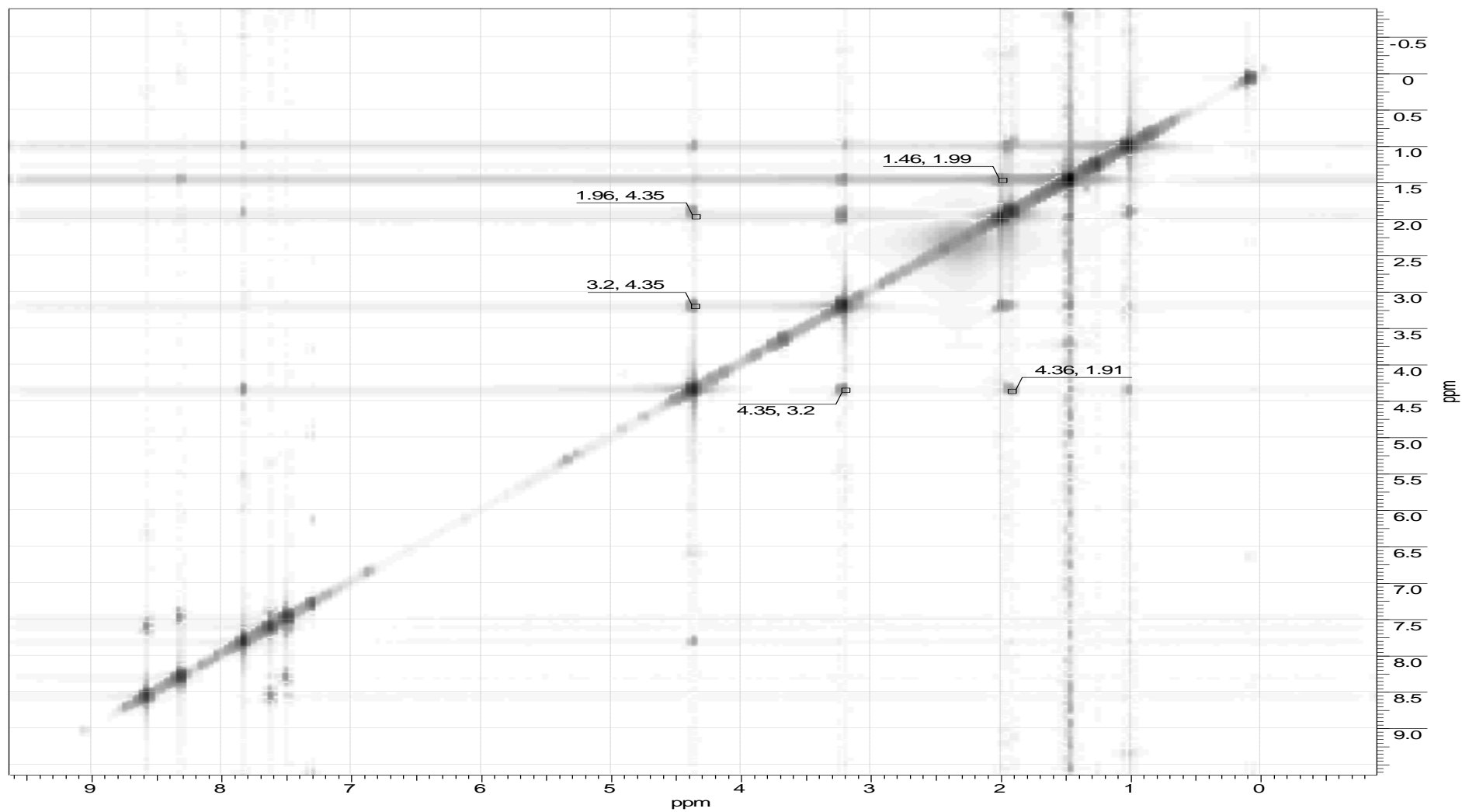
Espectro 5. ^1H -COSY (500 MHz, CDCl_3) do composto 37a.



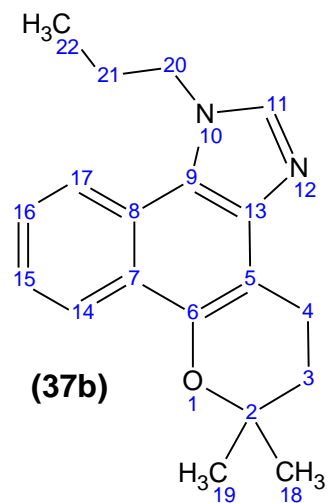
Espectro 6. HSQC (500 MHz, CDCl₃) do composto 37a.



Espectro 7.HMBC (500 MHz, CDCl_3) do composto 37a.

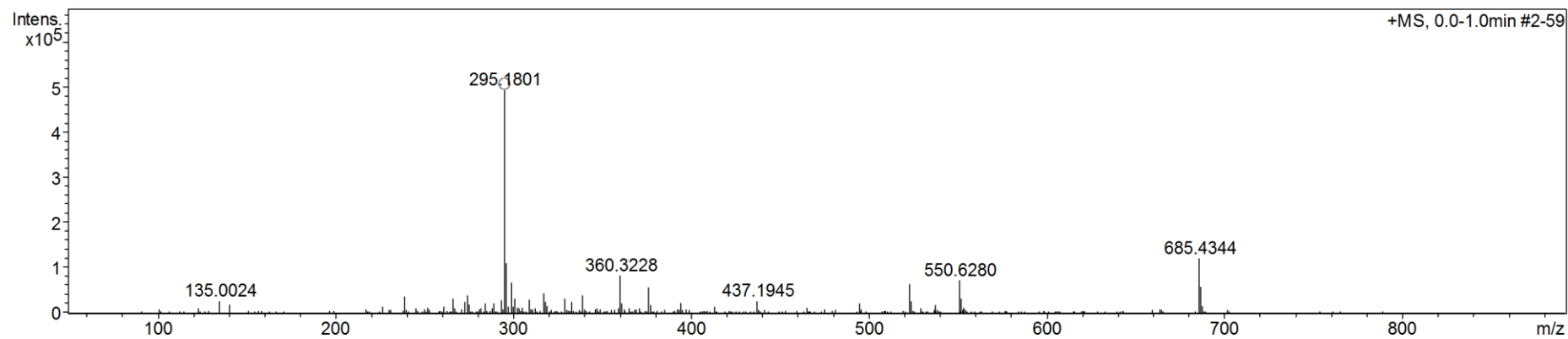


Espectro 8. NOESY (500 MHz, CDCl₃) do composto 37a.

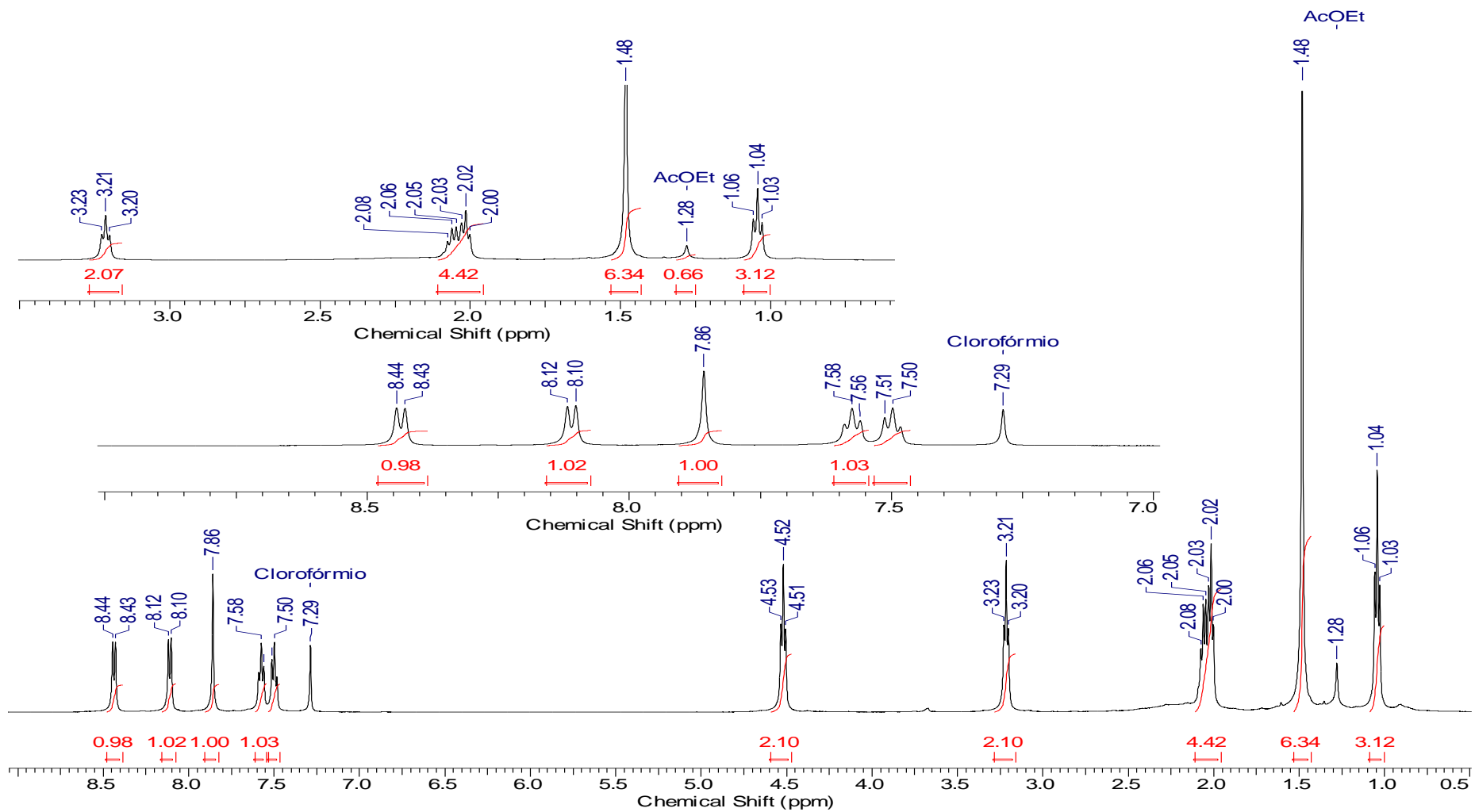


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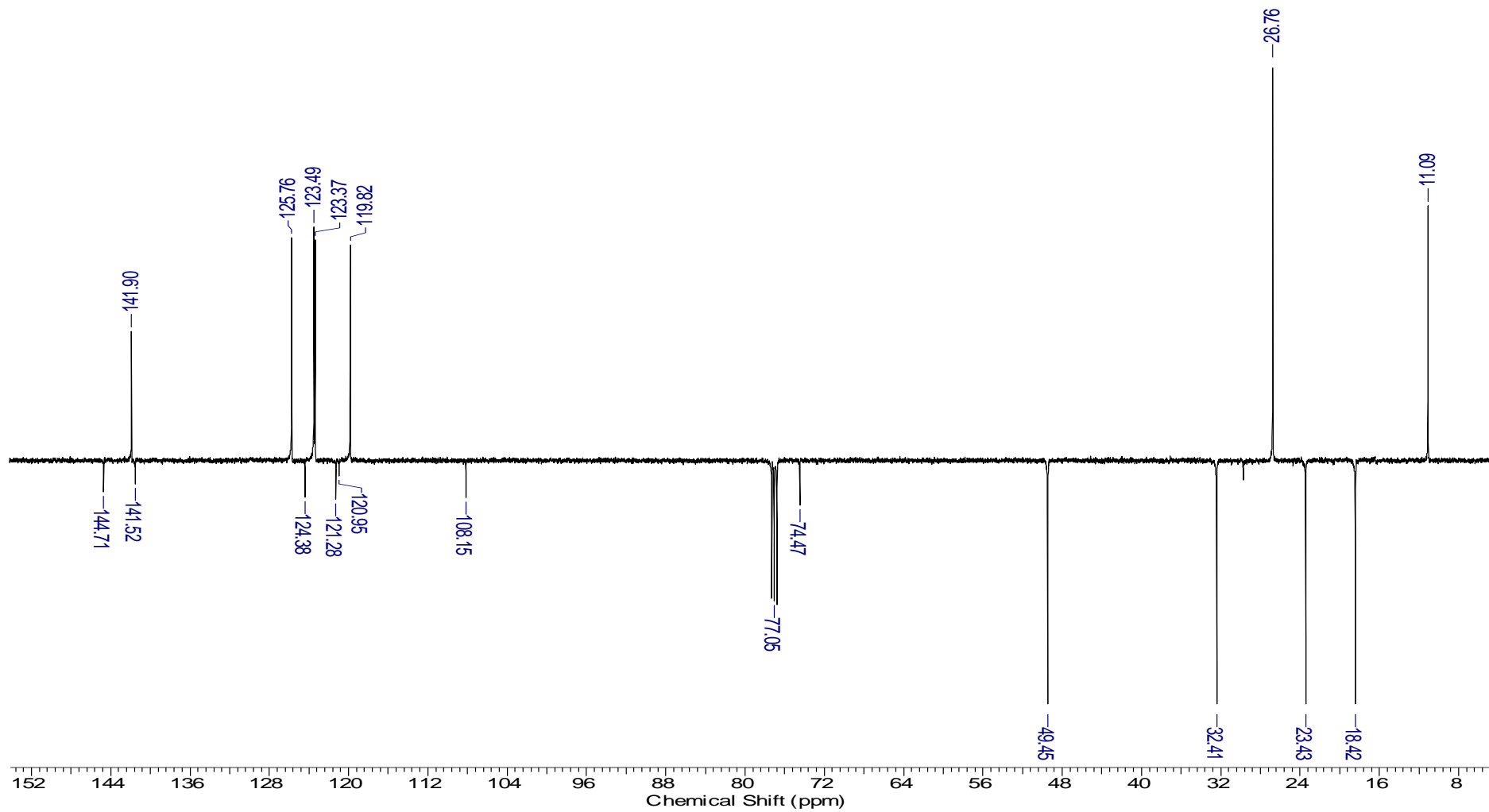
[M + H]⁺ = 295.1805Da; err [ppm] = -1,3



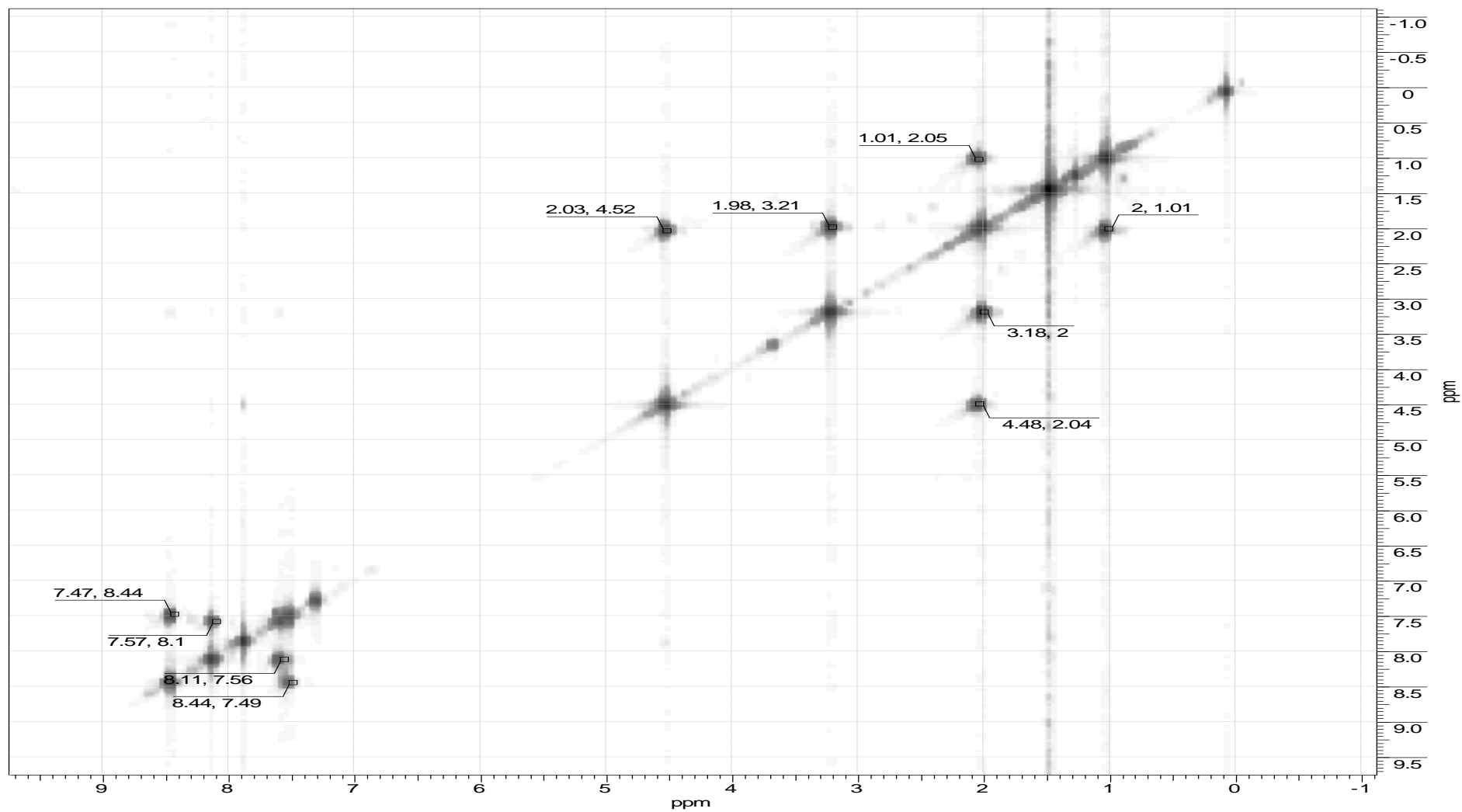
Espectro 9. EM-IES (500 MHz, CDCl₃) do composto 37b.



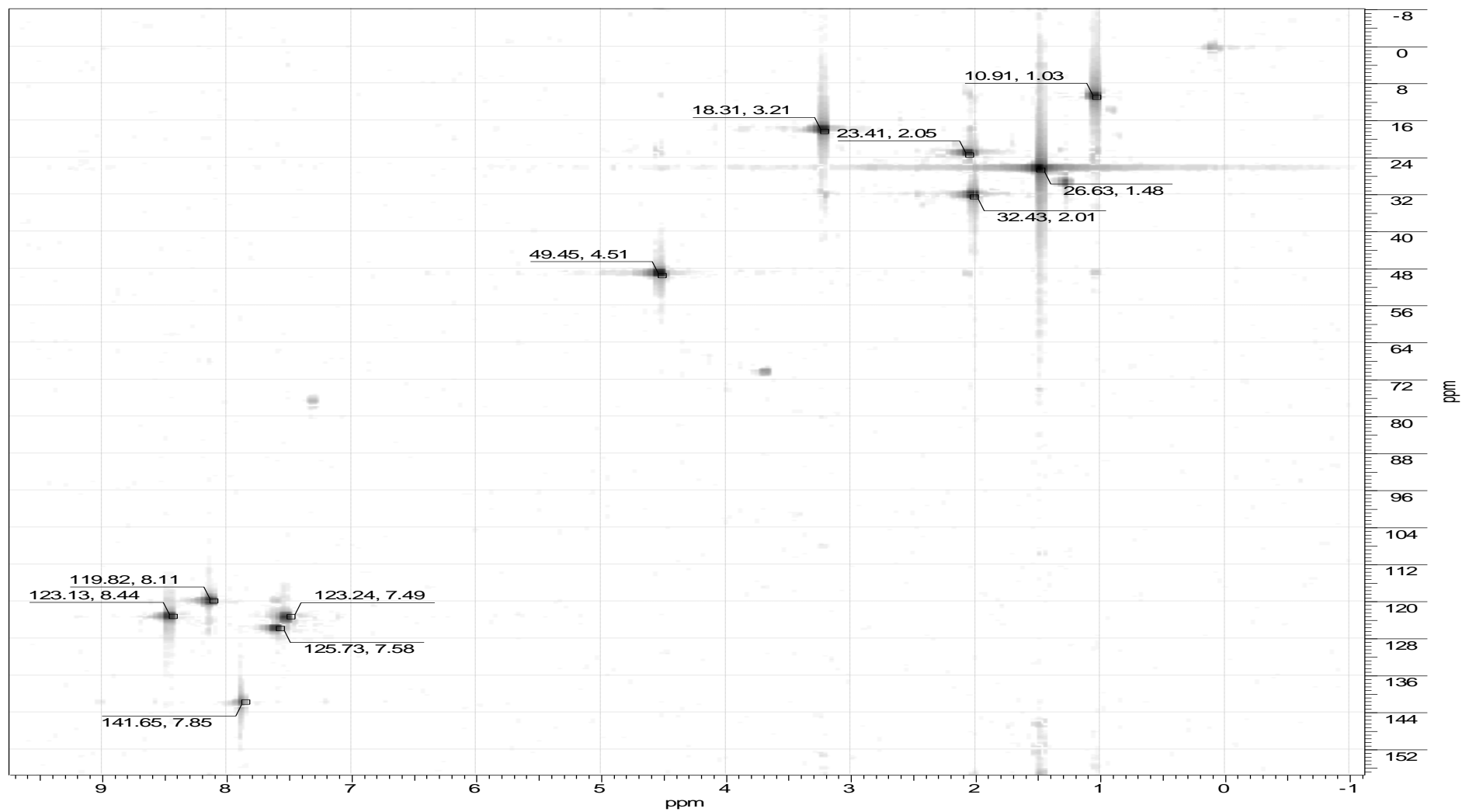
Espectro 10. RMN- ^1H (500 MHz, CDCl_3) do composto 37b.



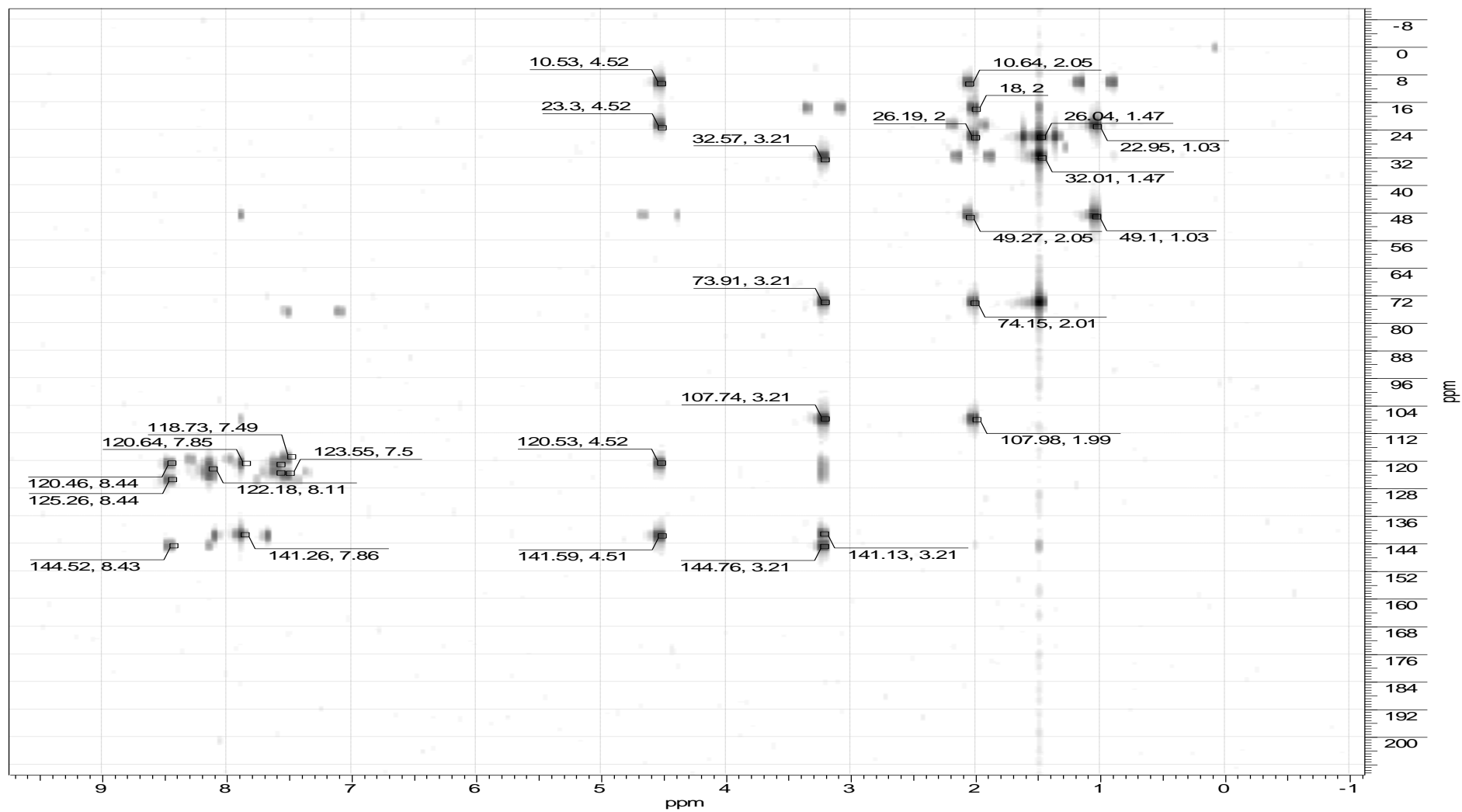
Espectro 11. RMN-¹³C (125 MHz, CDCl₃) do composto 37b.



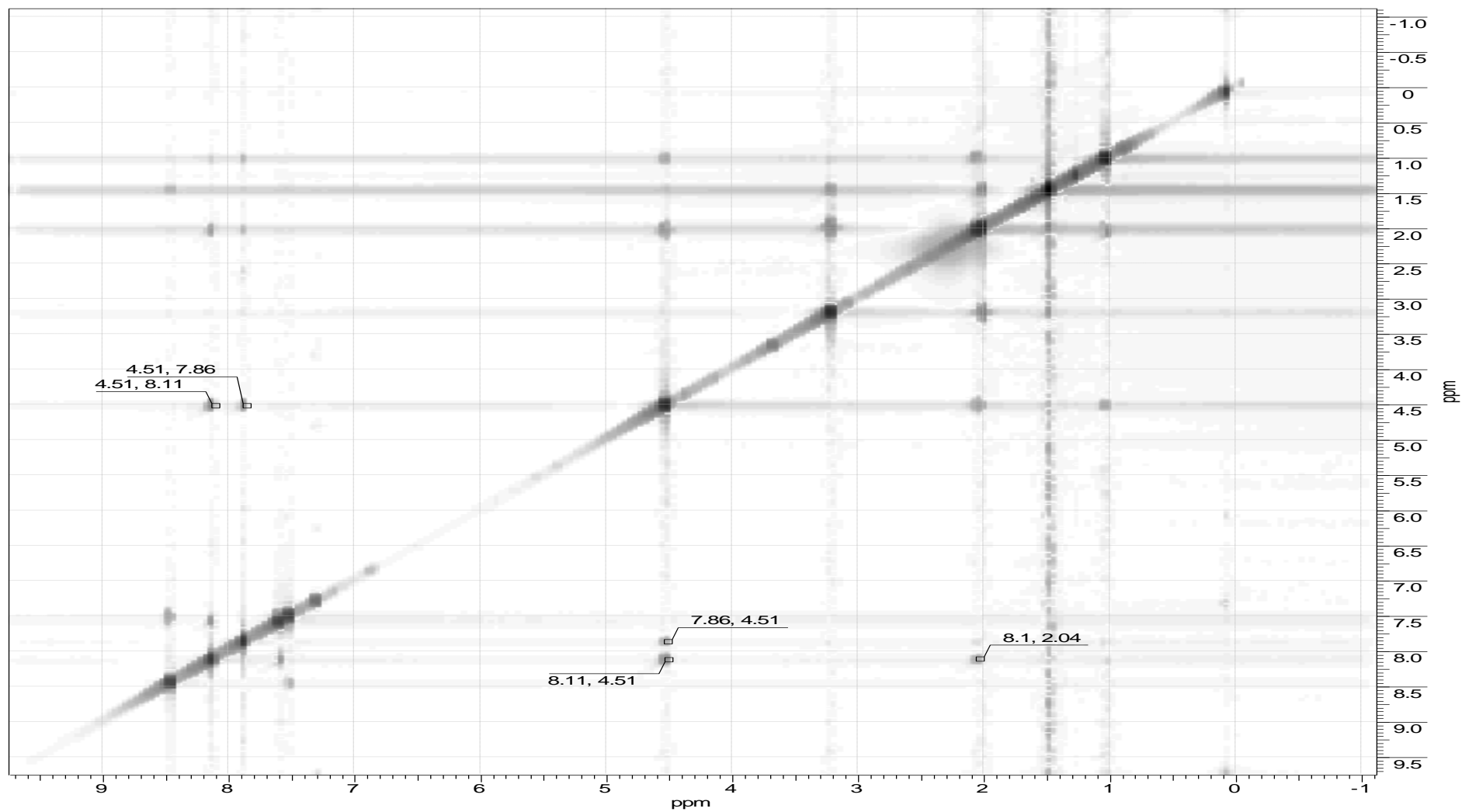
Espectro 12. ^1H -COSY(500 MHz, CDCl_3) do composto 37b.



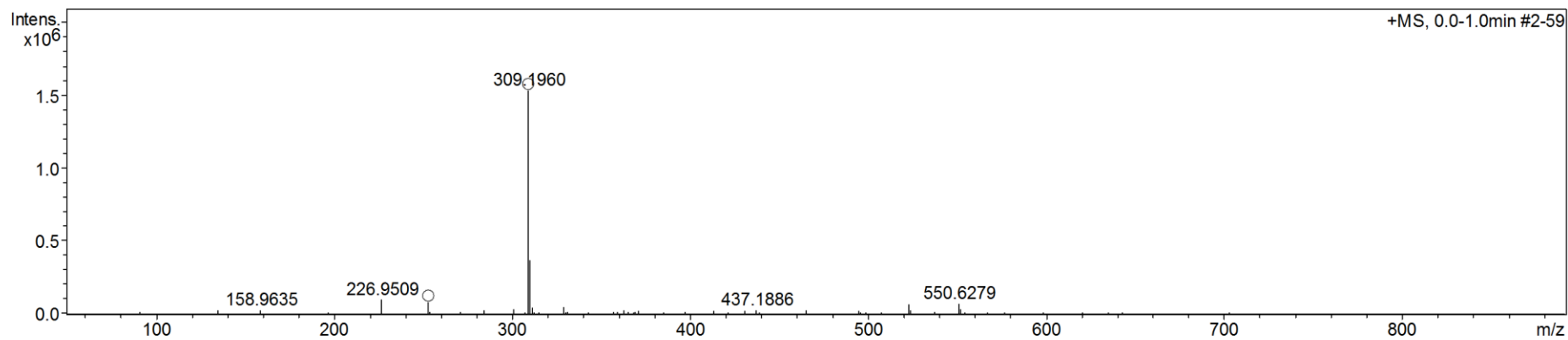
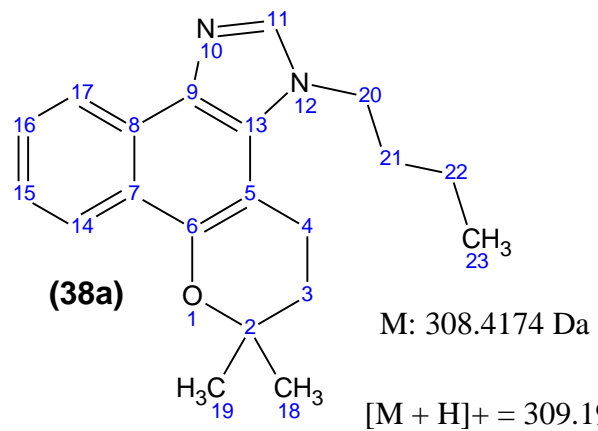
Espectro 13. HSQC (500 MHz, CDCl₃) do composto 37b.



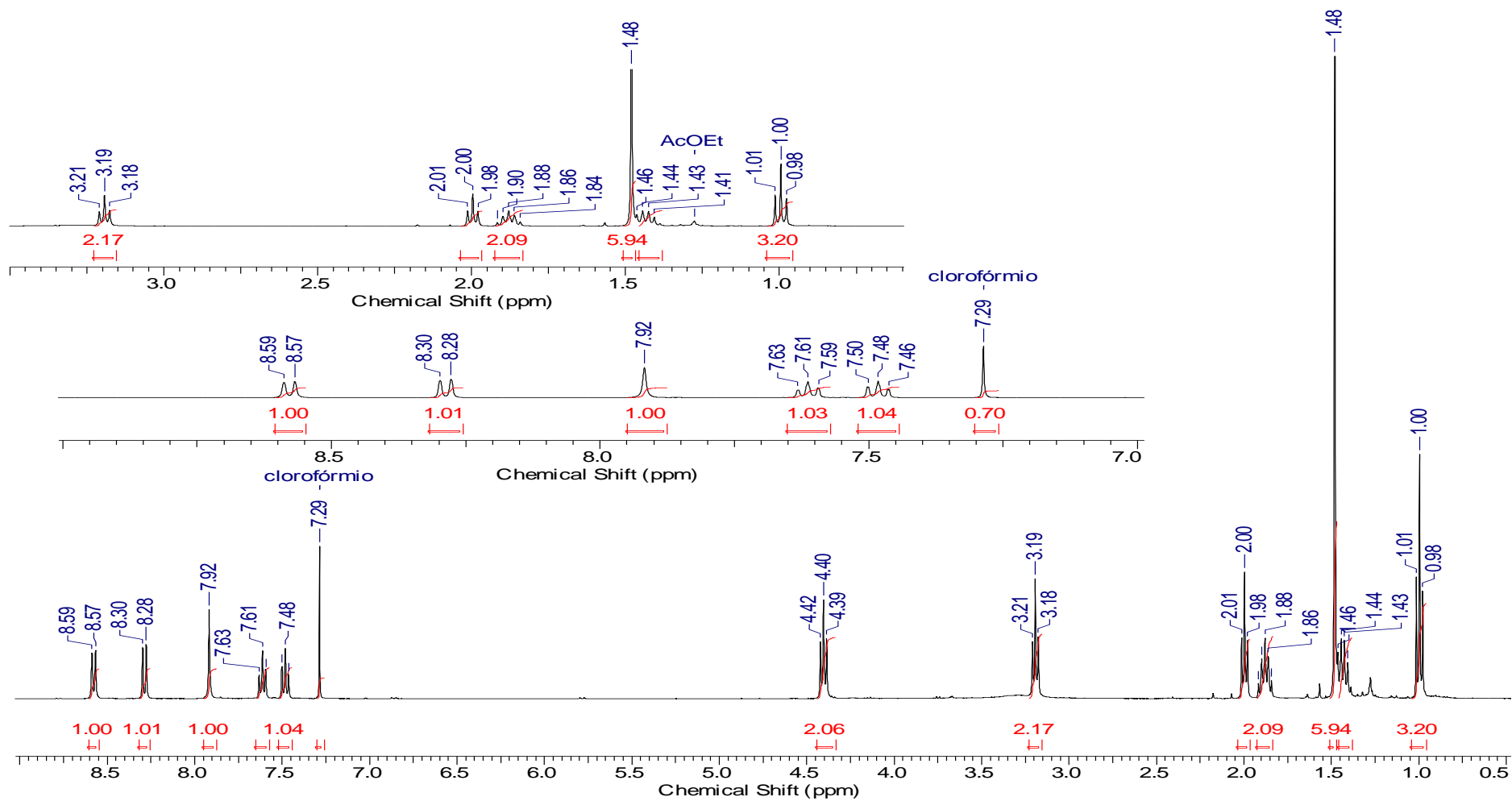
Espectro 14. HMBC (500 MHz, CDCl₃) do composto 37b.



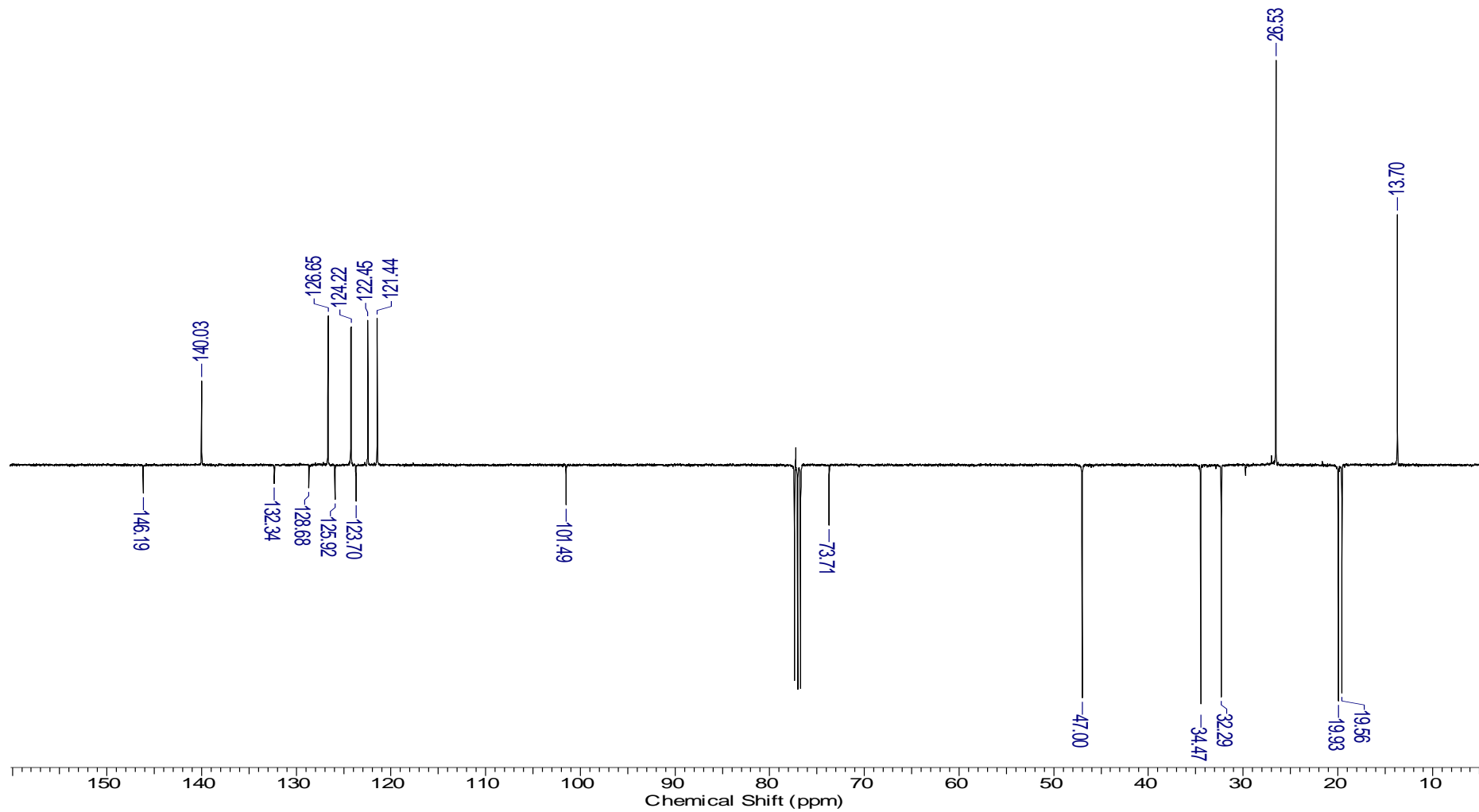
Espectro 15. NOESY (500 MHz, CDCl₃) do composto 37b.



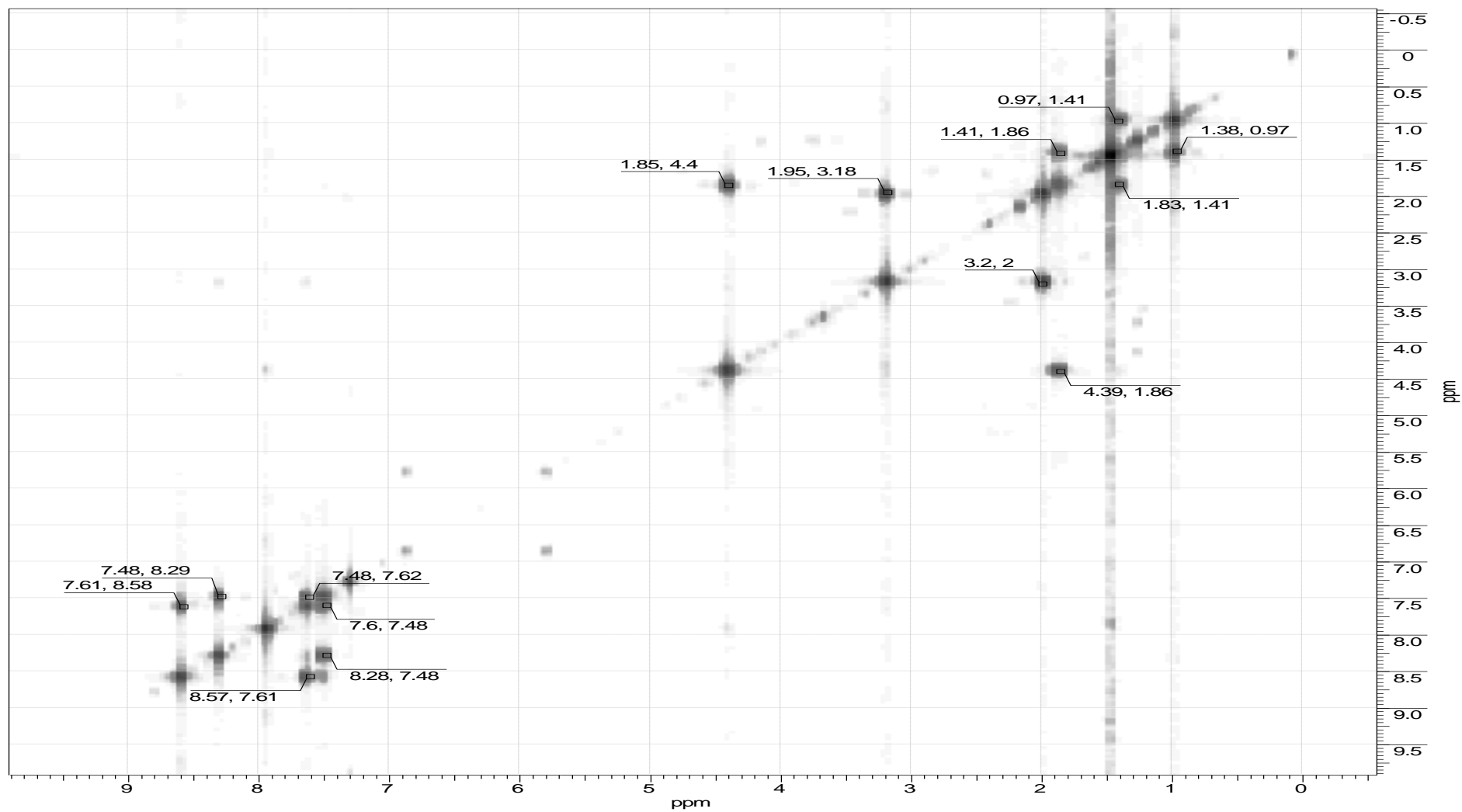
Espectro 16. EM-IES do composto 38a.



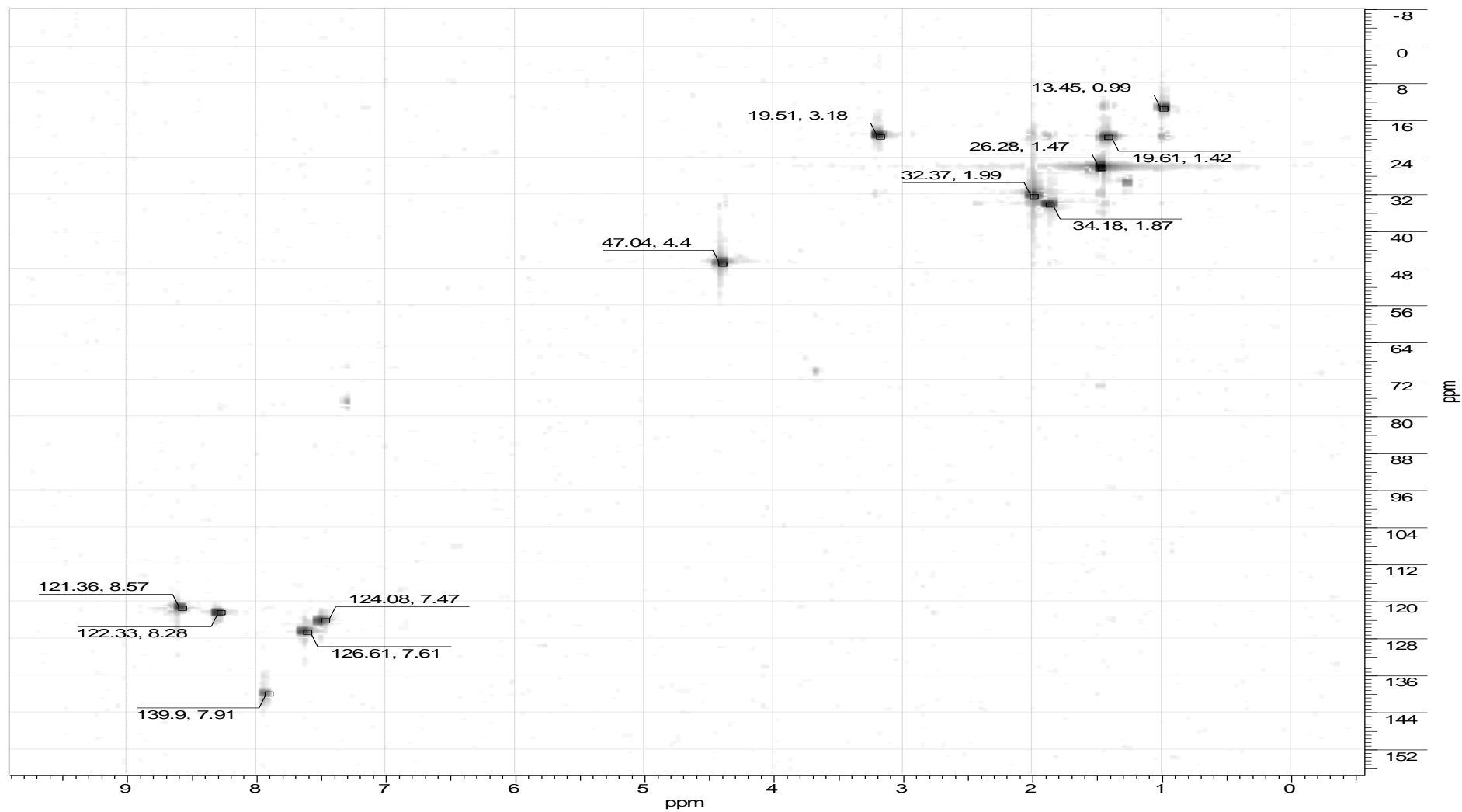
Espectro 17. RMN-¹H (400 MHz, CDCl₃) do composto 38a.



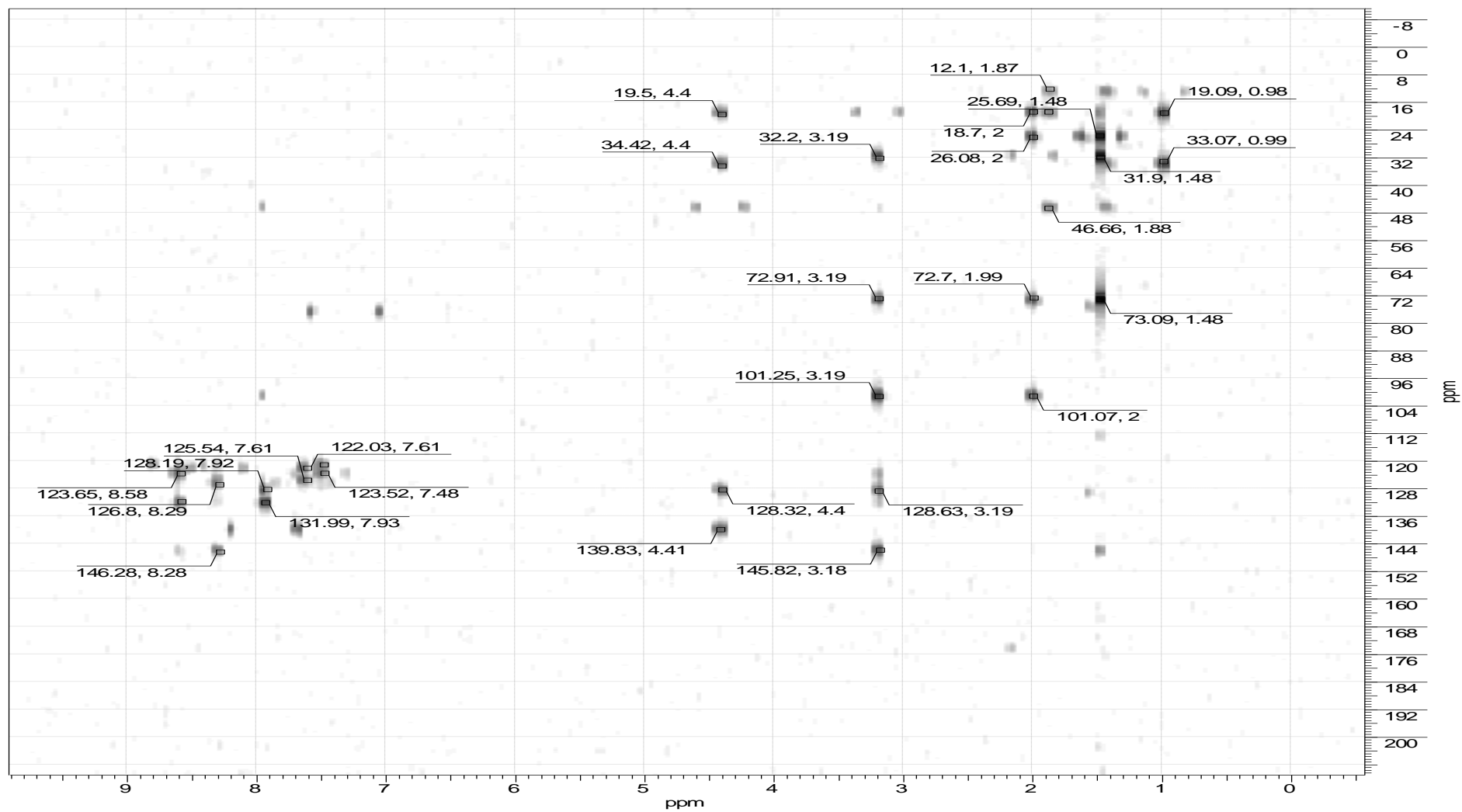
Espectro 18. RMN-¹³C (100 MHz, CDCl₃) do composto 38a.



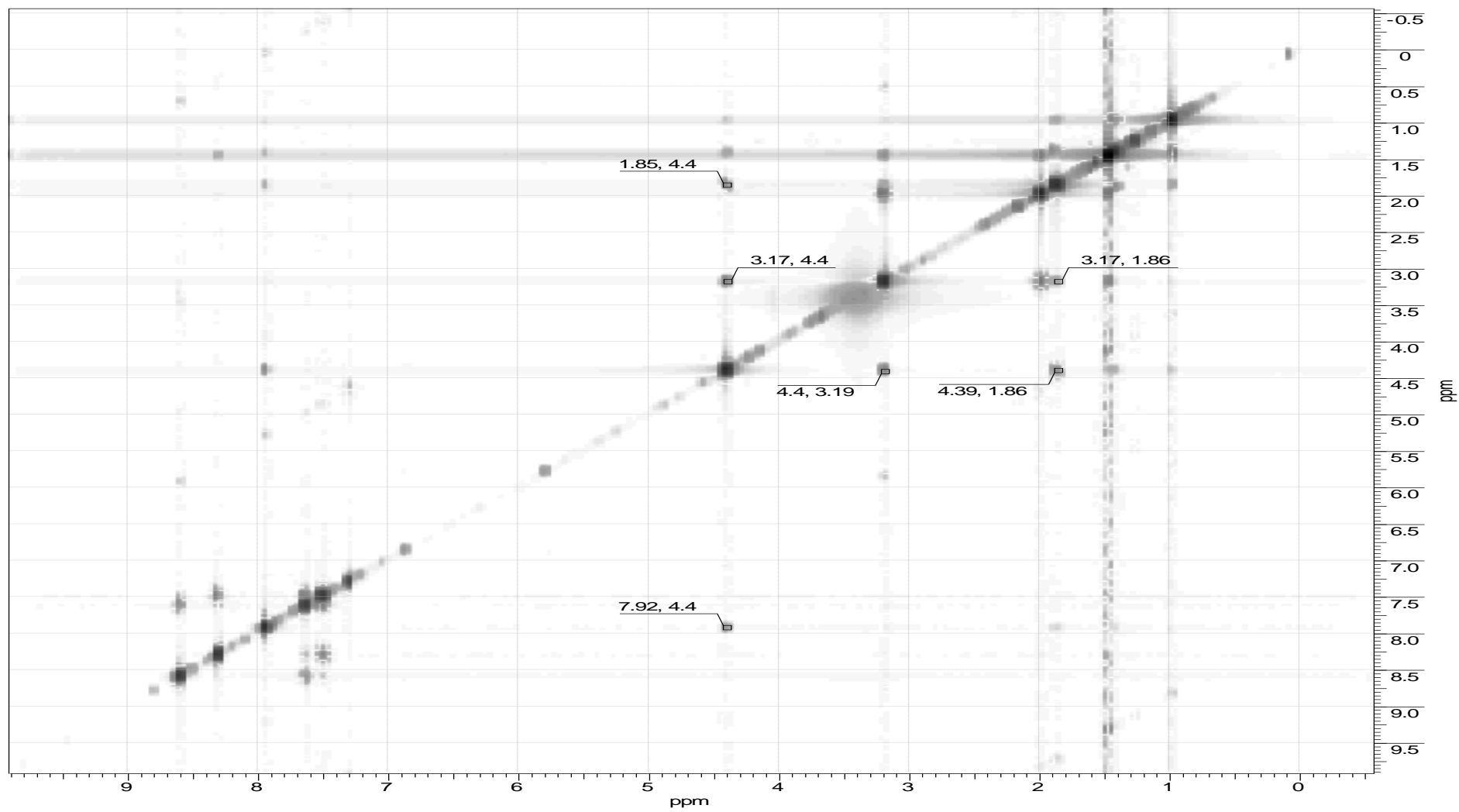
Espectro 19. ^1H -COSY (400 MHz, CDCl_3) do composto 38a.



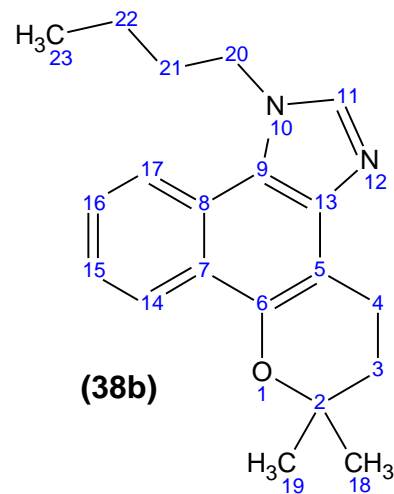
Espectro 20. HSQC (400 MHz, CDCl_3) do composto 38a.



Espectro 21. HMBC (400 MHz, CDCl_3) do composto 38a.

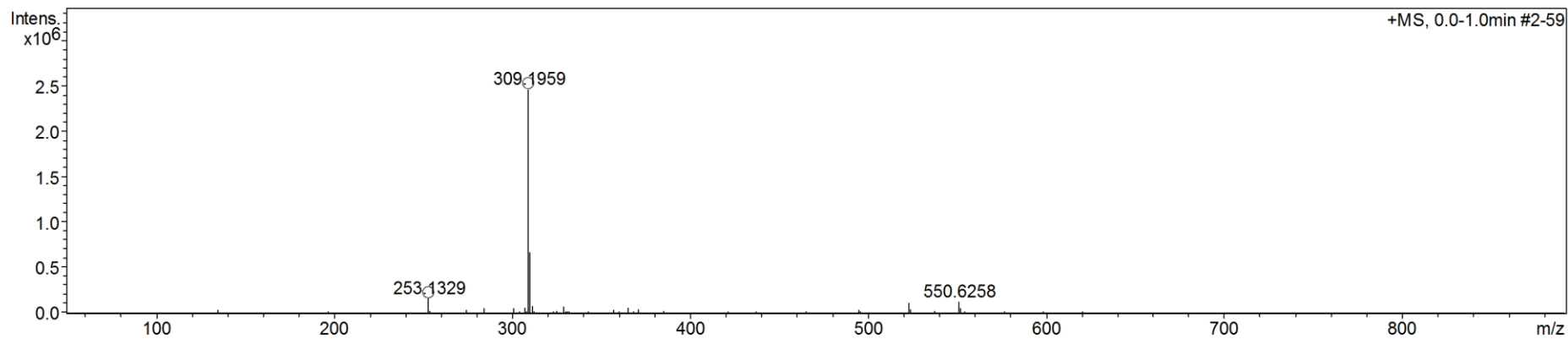


Espectro 22. NOESY (400 MHz, CDCl₃) do composto 38a.

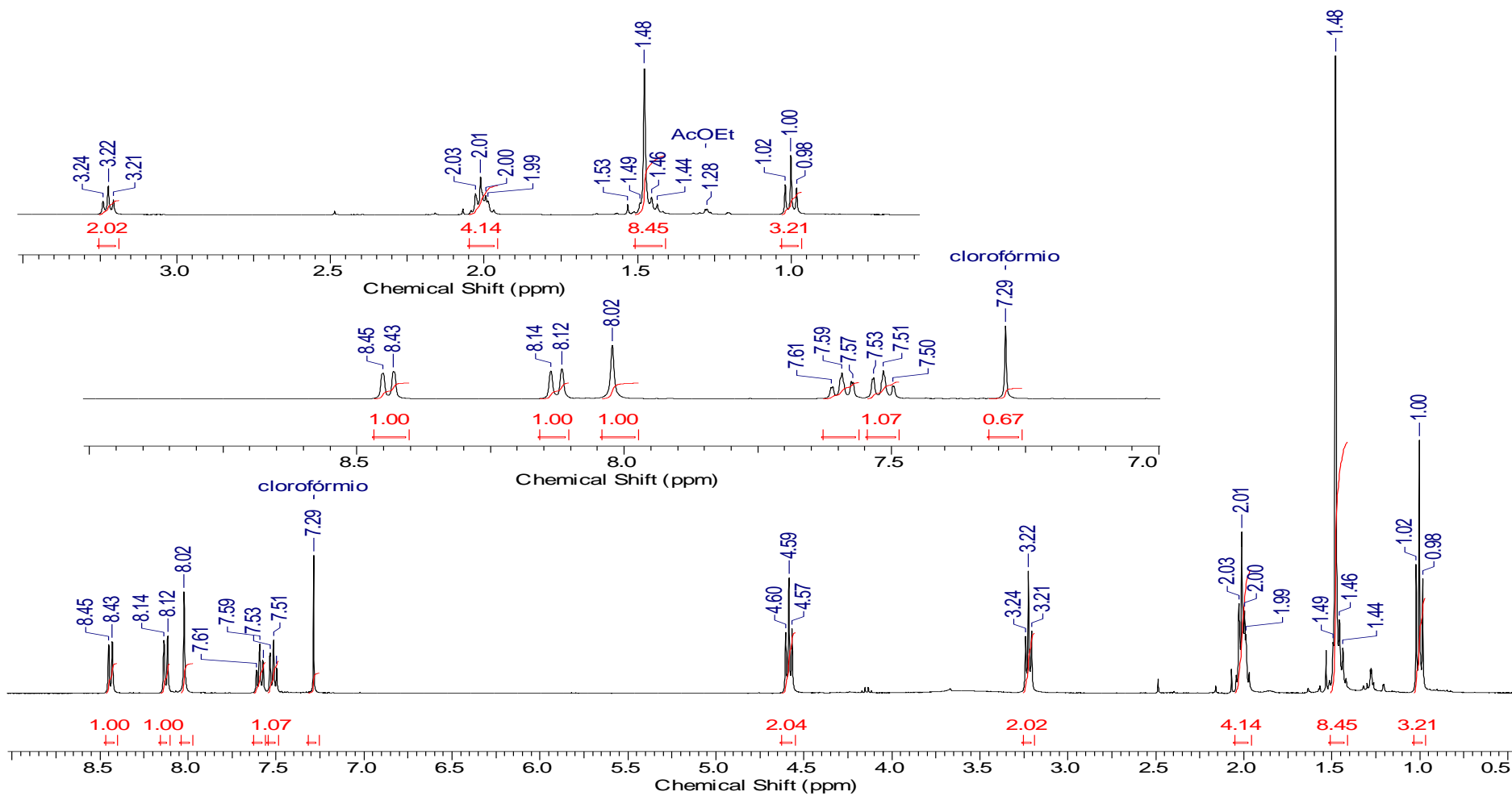


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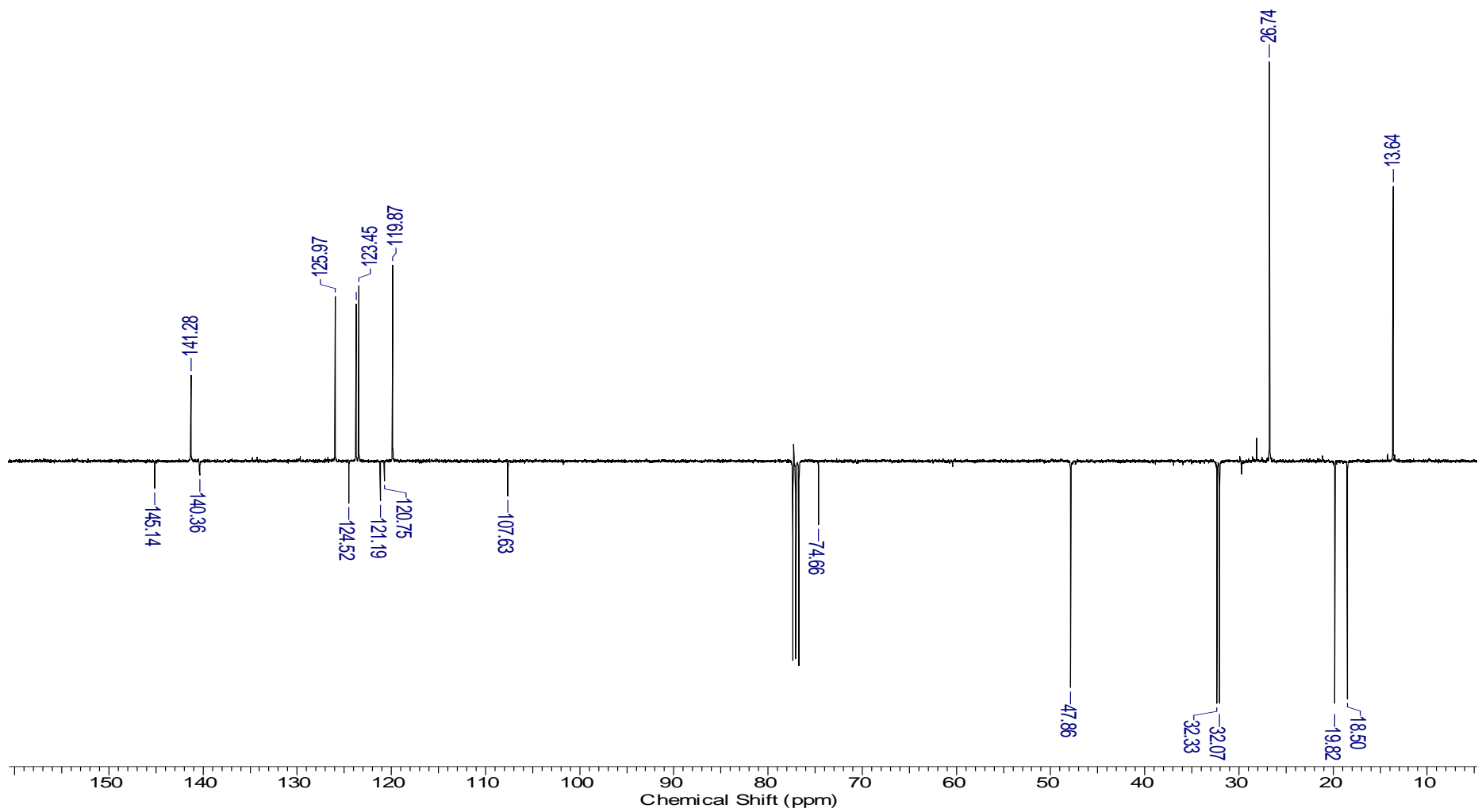
[M + H]⁺ = 309.1961Da; err [ppm] = 0,6



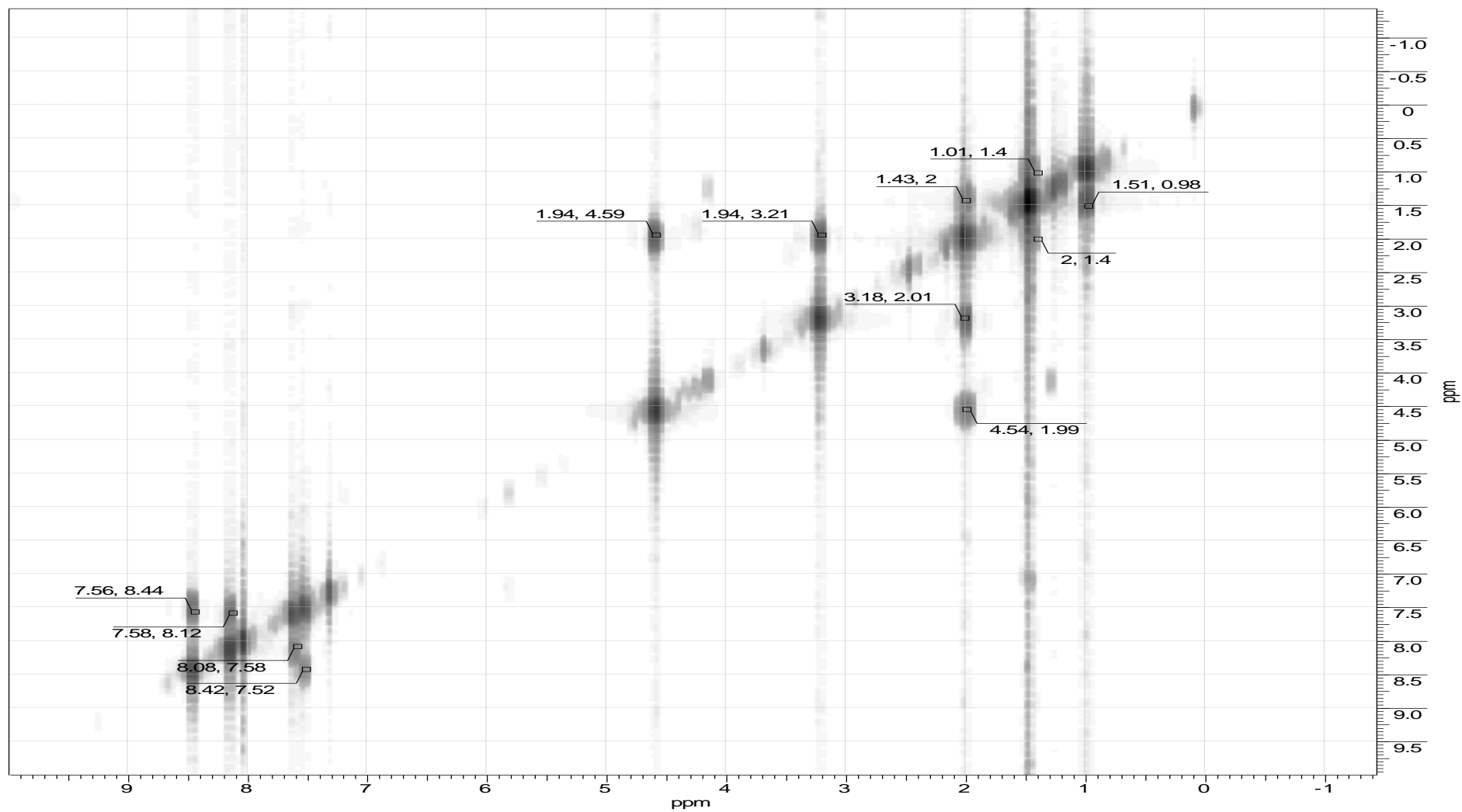
Espectro 23. EM-IES do composto 38b.



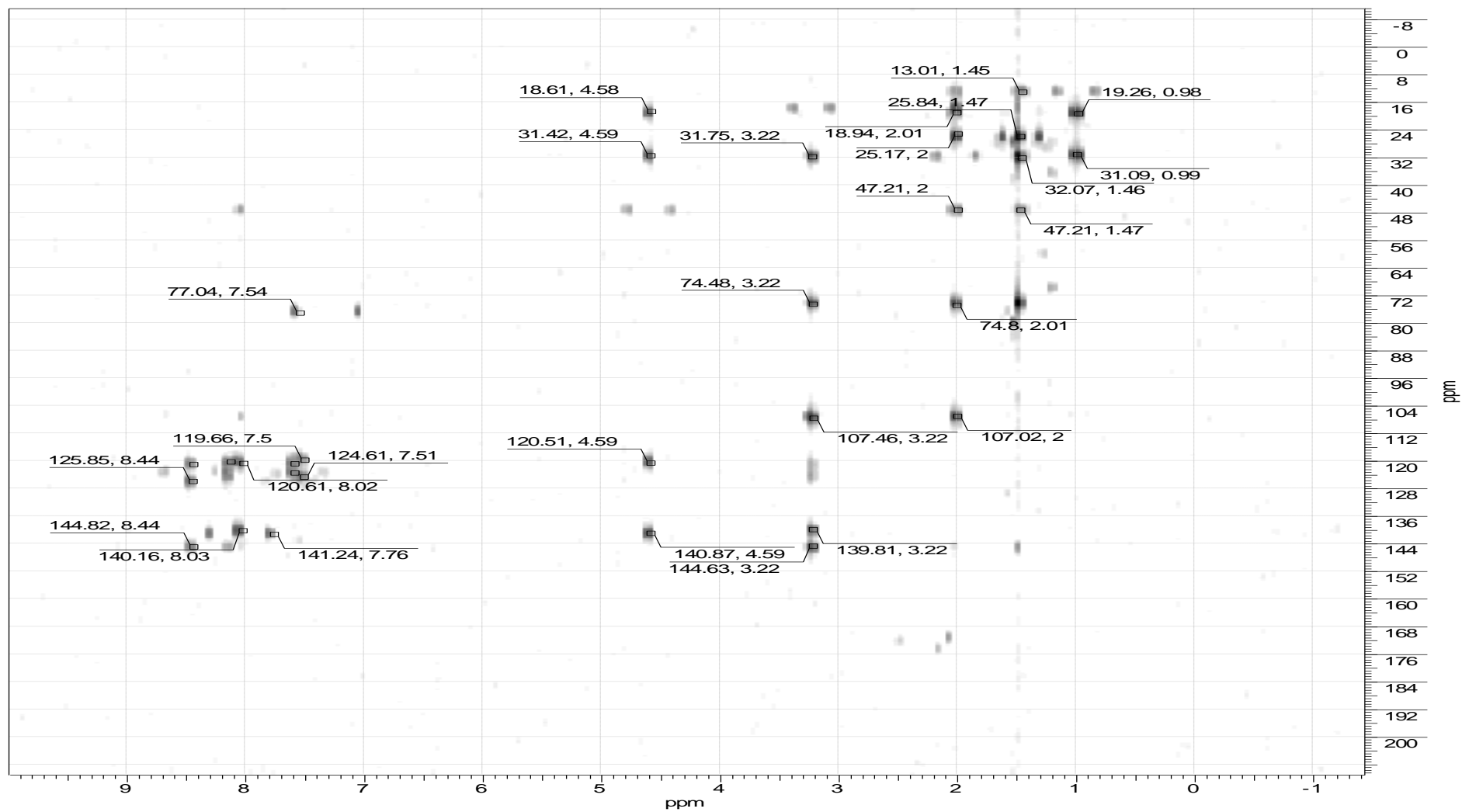
Espectro 24. RMN- ^1H (400 MHz, CDCl_3) do composto 38b.



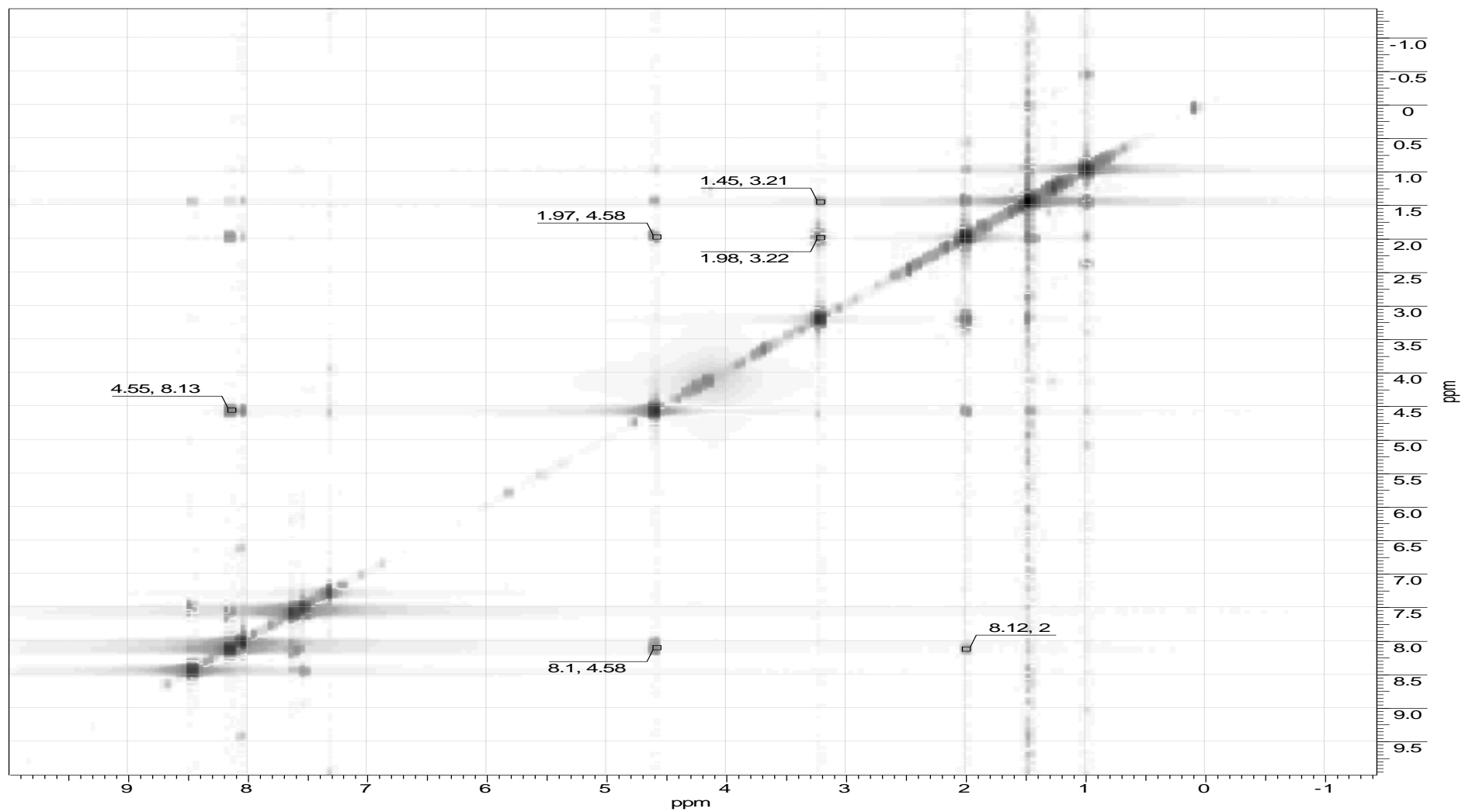
Espectro 25. RMN-¹³C (100 MHz, CDCl₃) do composto 38b.



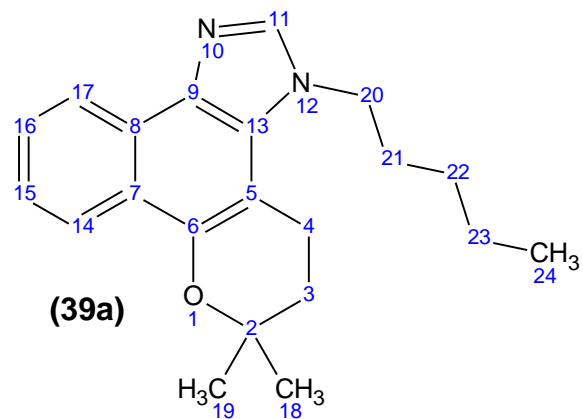
Espectro 26. ^1H -COSY (400 MHz, CDCl_3) do composto 38b.



Espectro 27. HMBC (400 MHz, CDCl_3) do composto 38b.

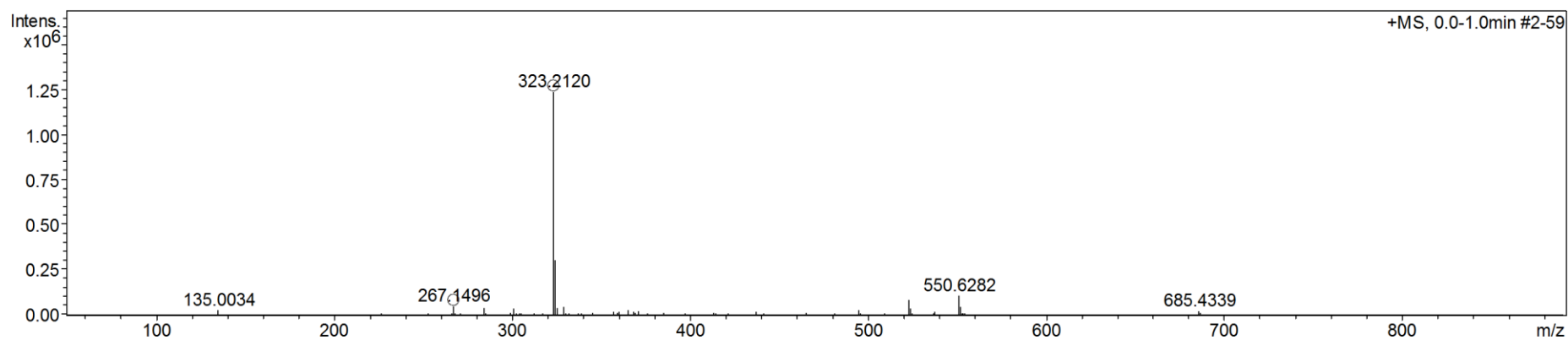


Espectro 28. NOESY (400 MHz, CDCl₃) do composto 38b.

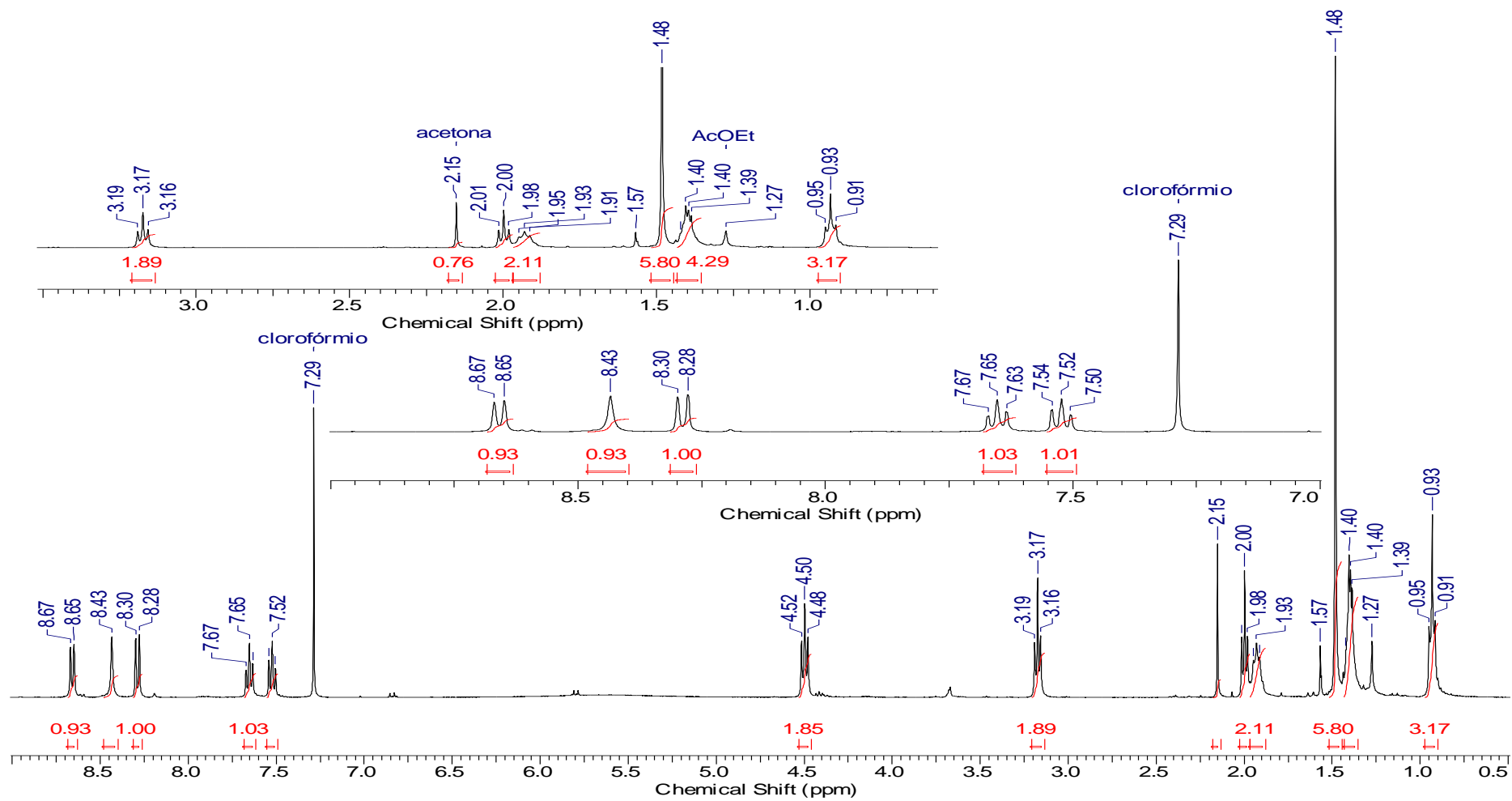


M: 322.444 Da

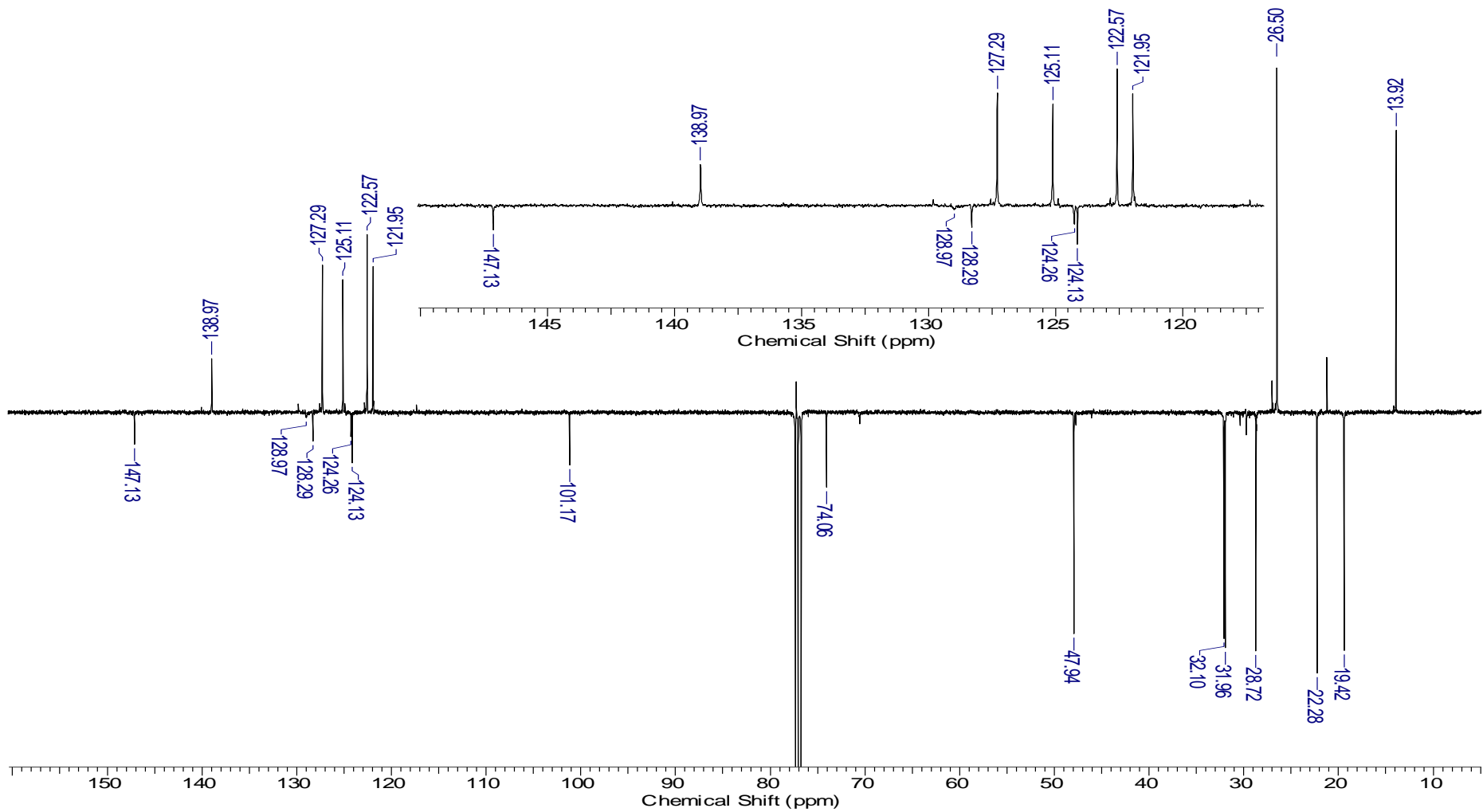
[M + H]⁺ = 323.2118Da; err [ppm] = -0,8



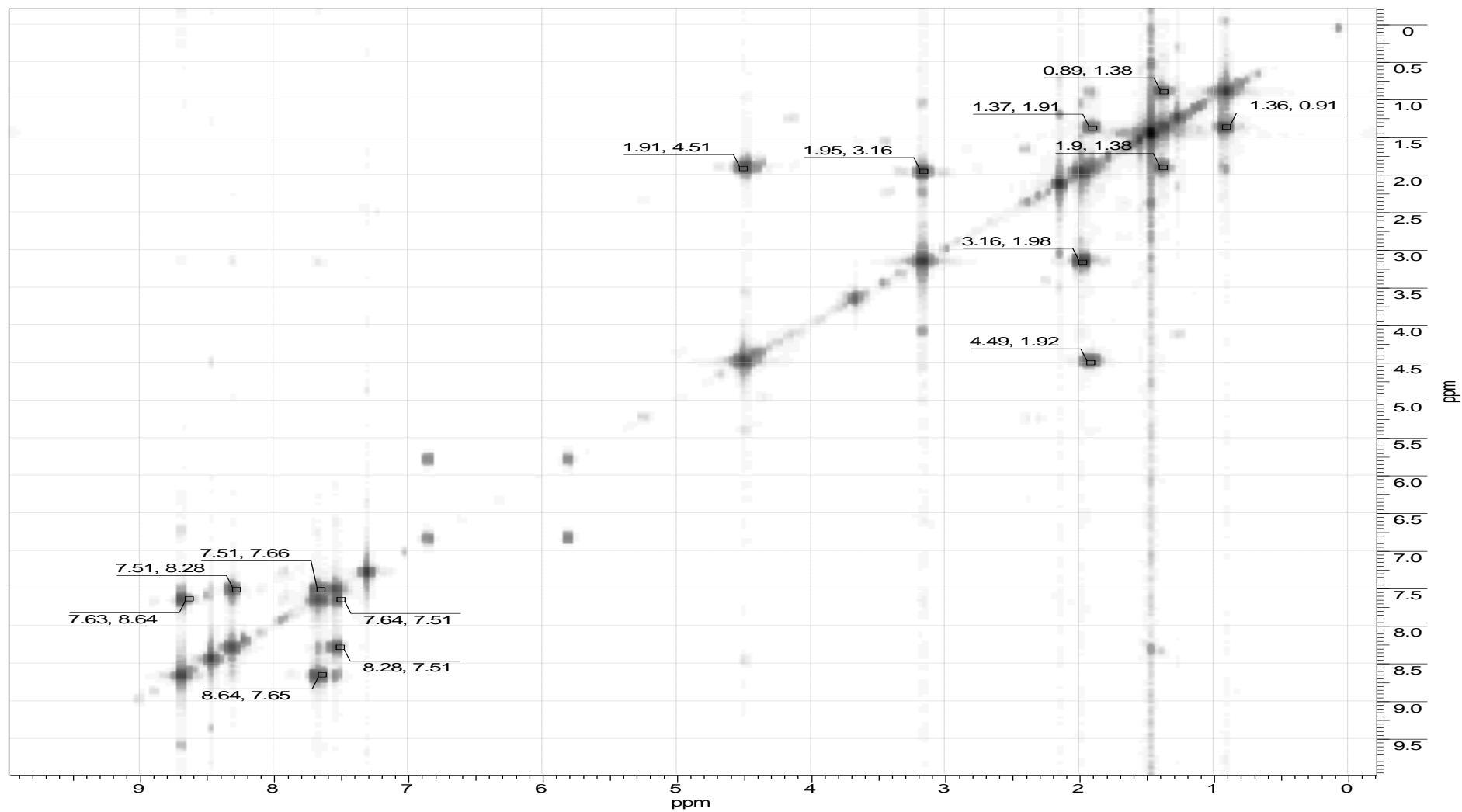
Espectro 29. EM-IES do composto 39a.



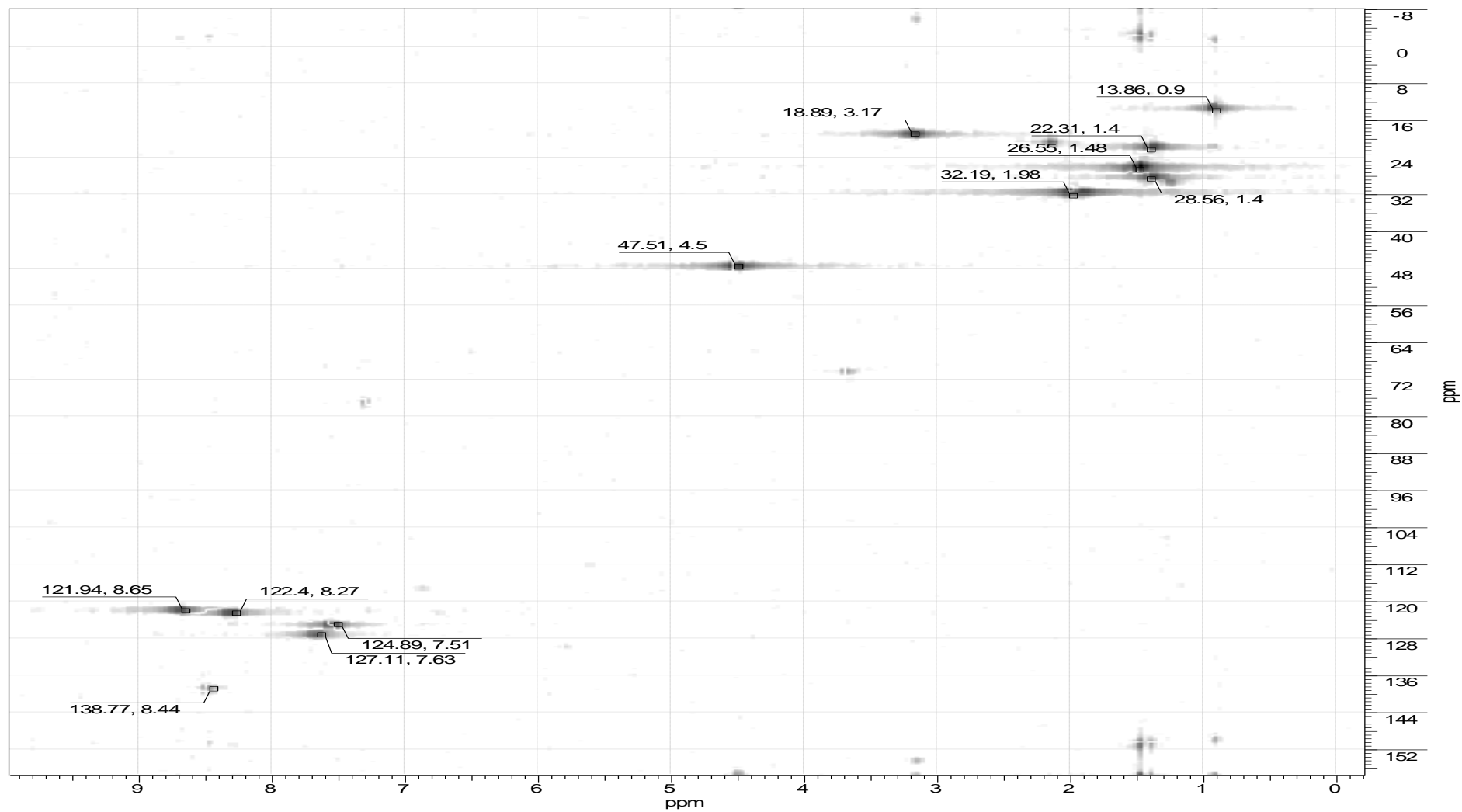
Espectro 30. RMN- ^1H (400 MHz, CDCl_3) do composto 39a.



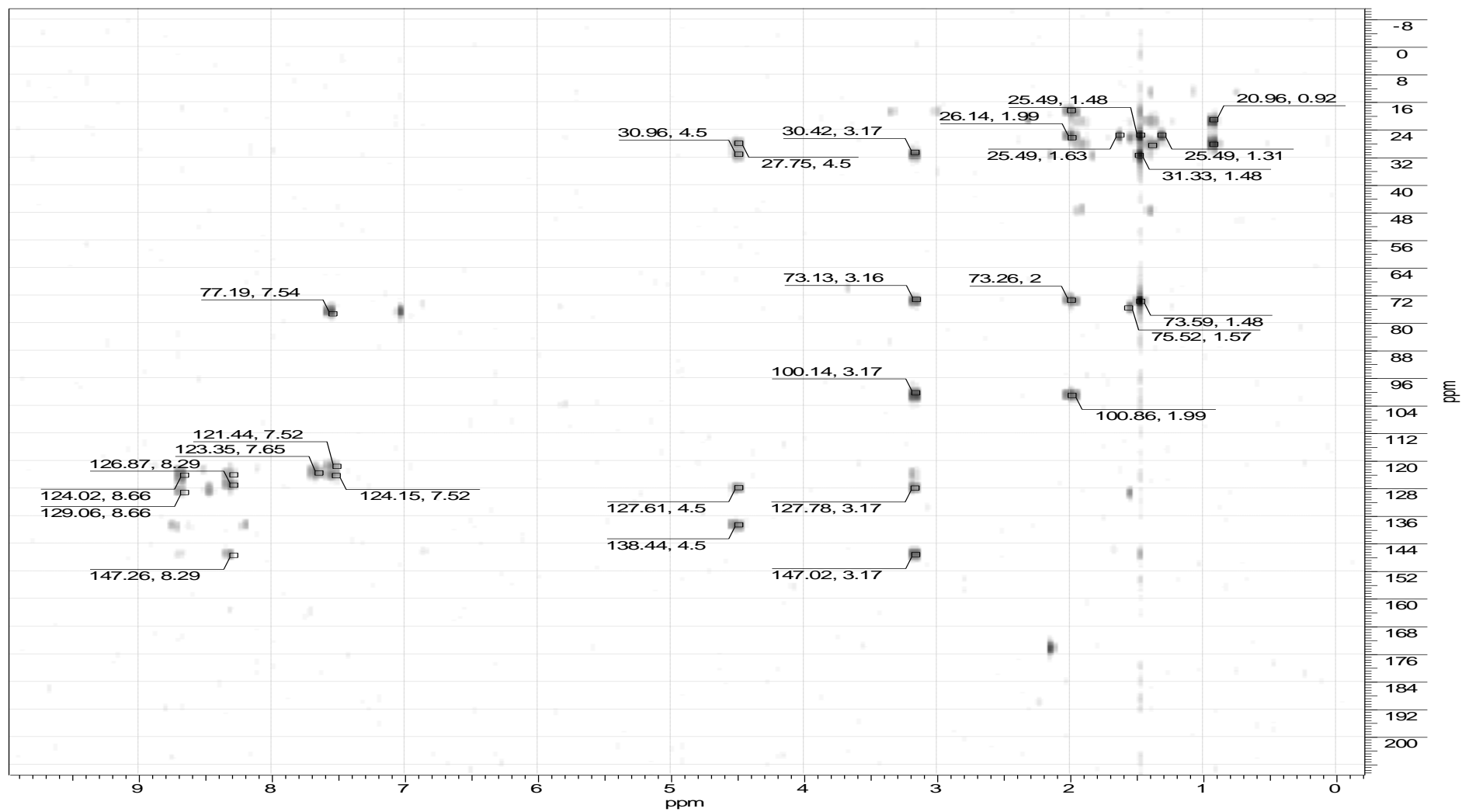
Espectro 31. RMN- ^{13}C (100 MHz, CDCl_3) do composto 39a.



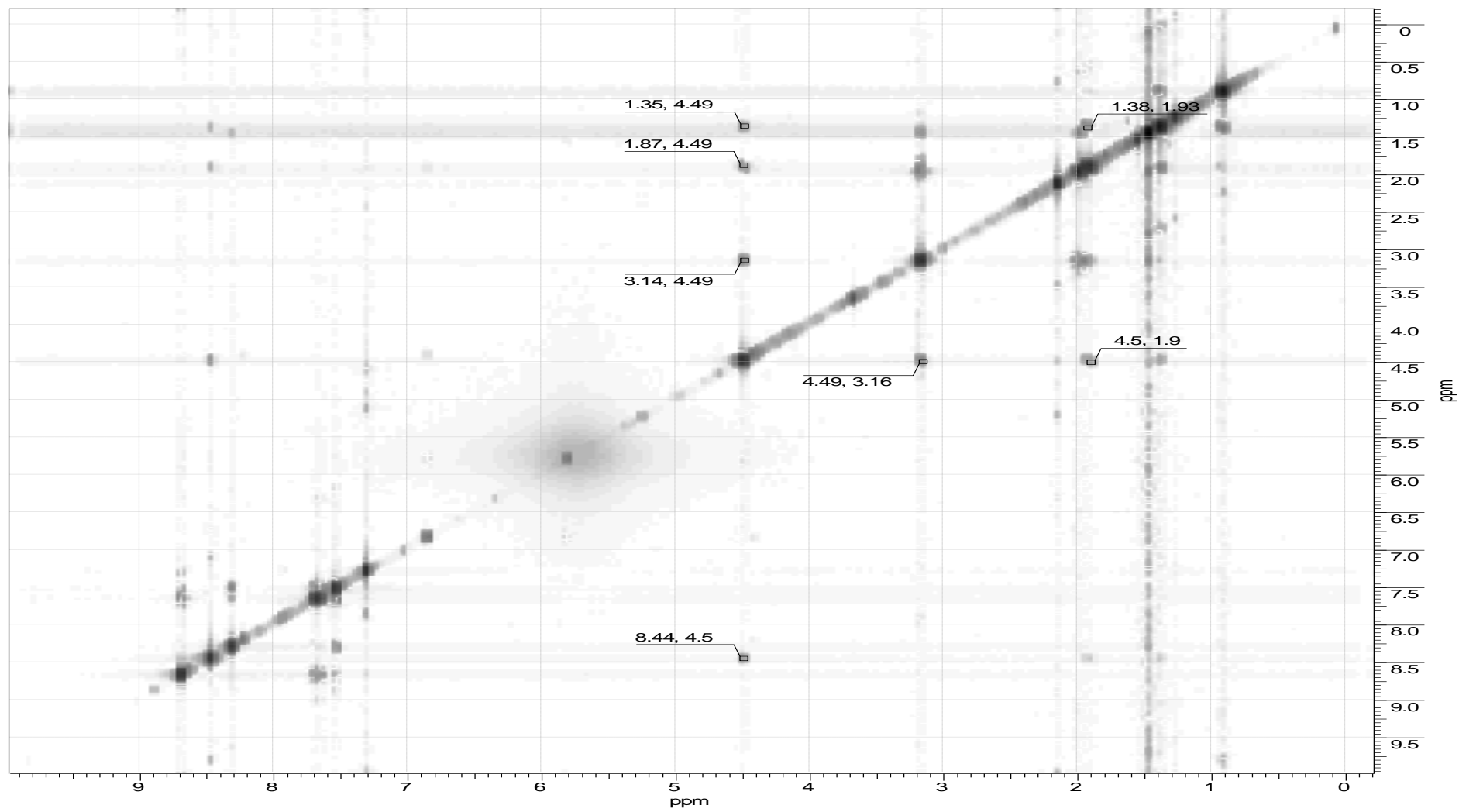
Espectro 32. ¹H-COSY (400 MHz, CDCl₃) do composto 39a.



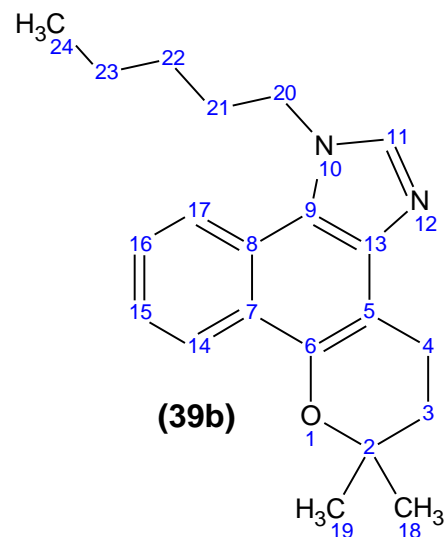
Espectro 33. HSQC (400 MHz, CDCl₃) do composto 39a.



Espectro 34. HMBC (400 MHz, CDCl₃) do composto 39a.

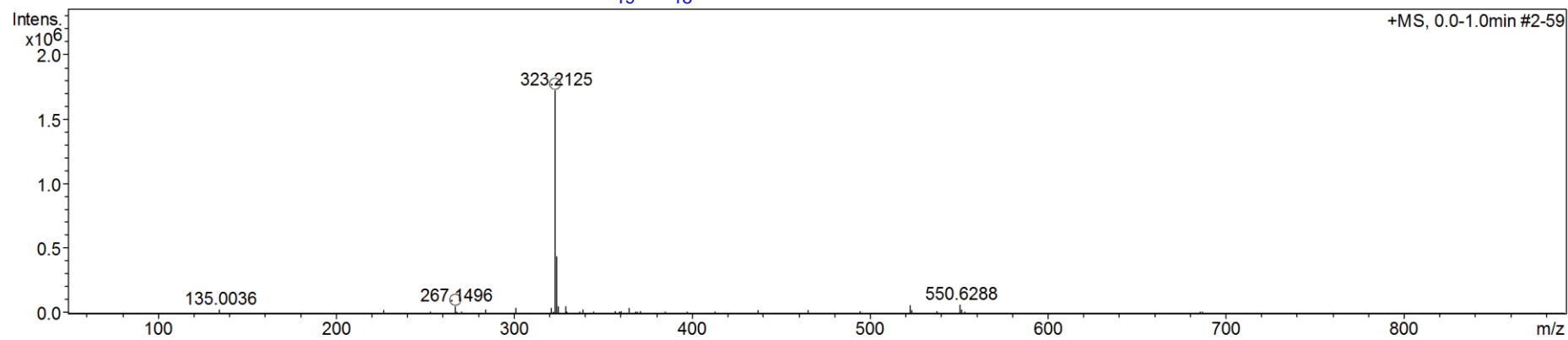


Espectro 35. NOESY (400 MHz, CDCl₃) do composto 39a.

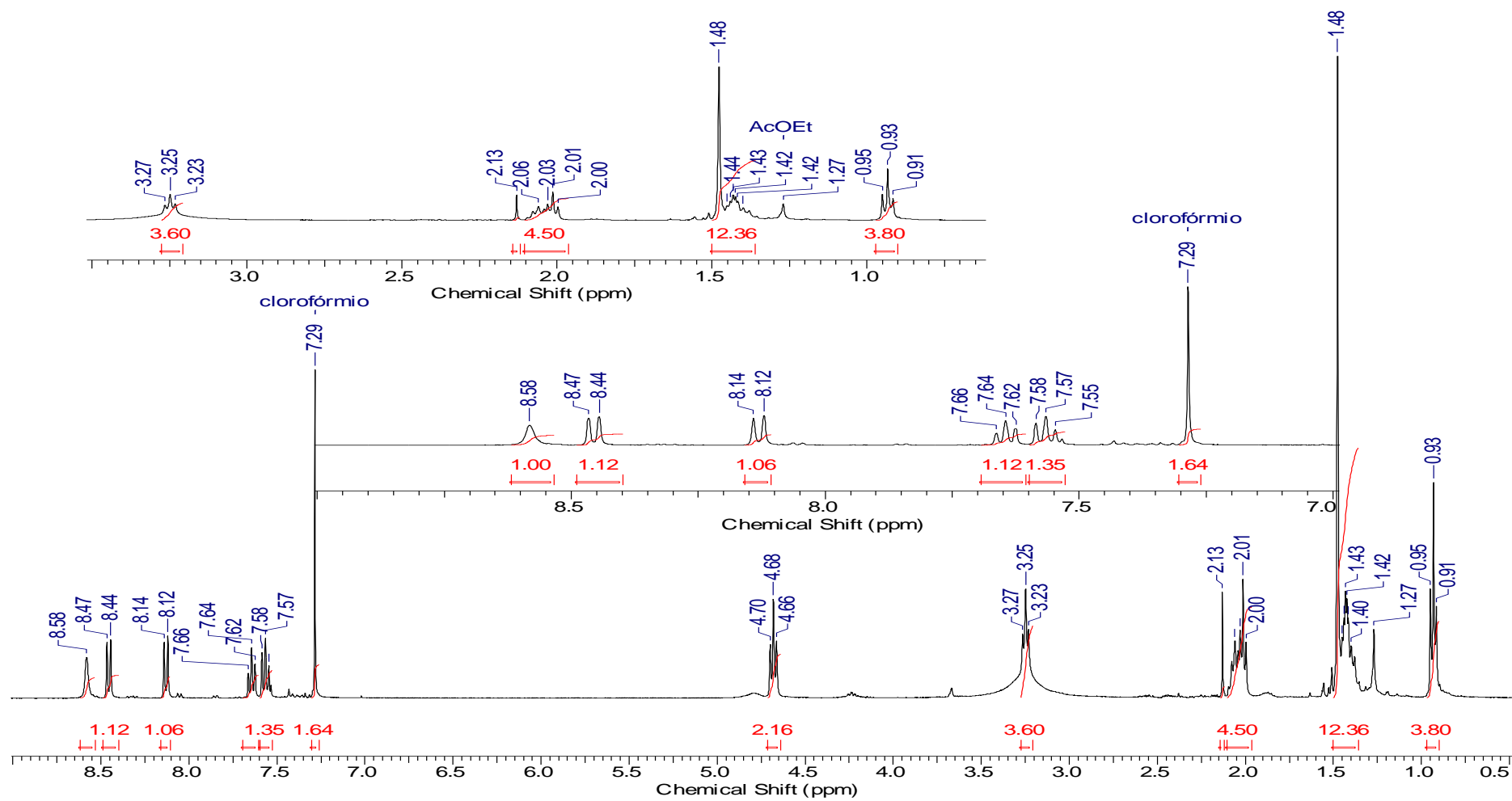


M: 322.444 Da

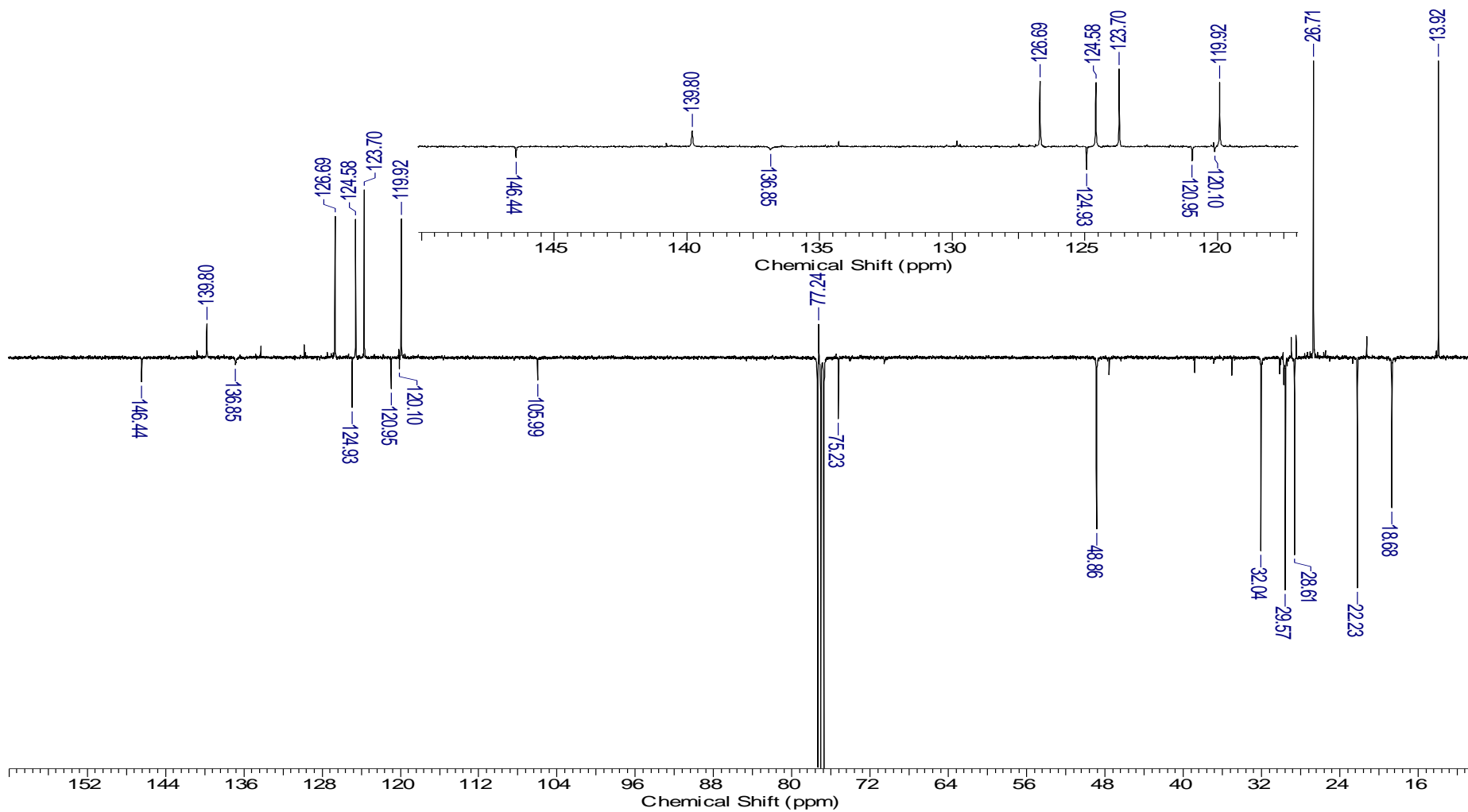
[M + H]⁺ = 323.2118 Da; err [ppm] = -2,1



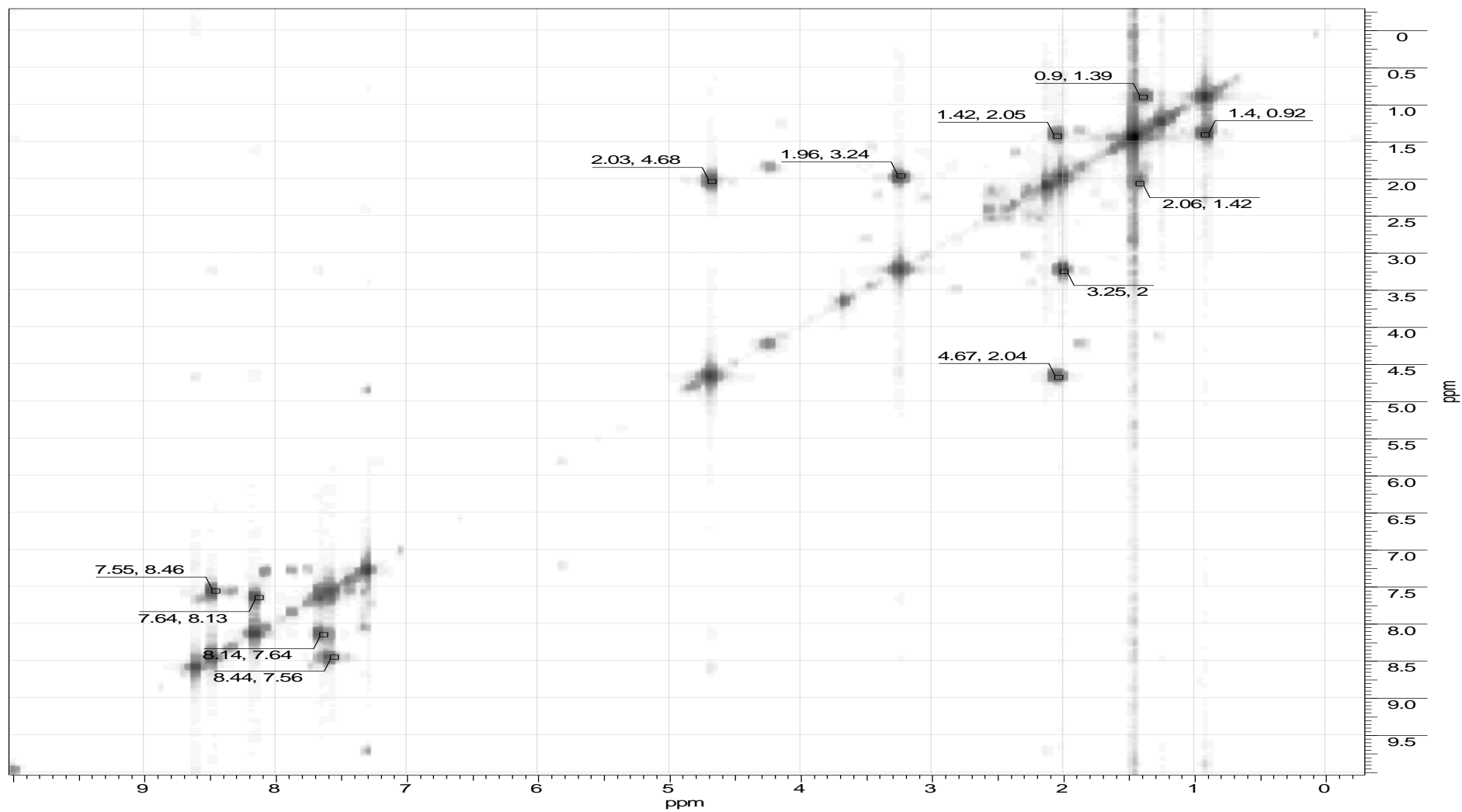
Espectro 36. EM-IES do composto 39b.



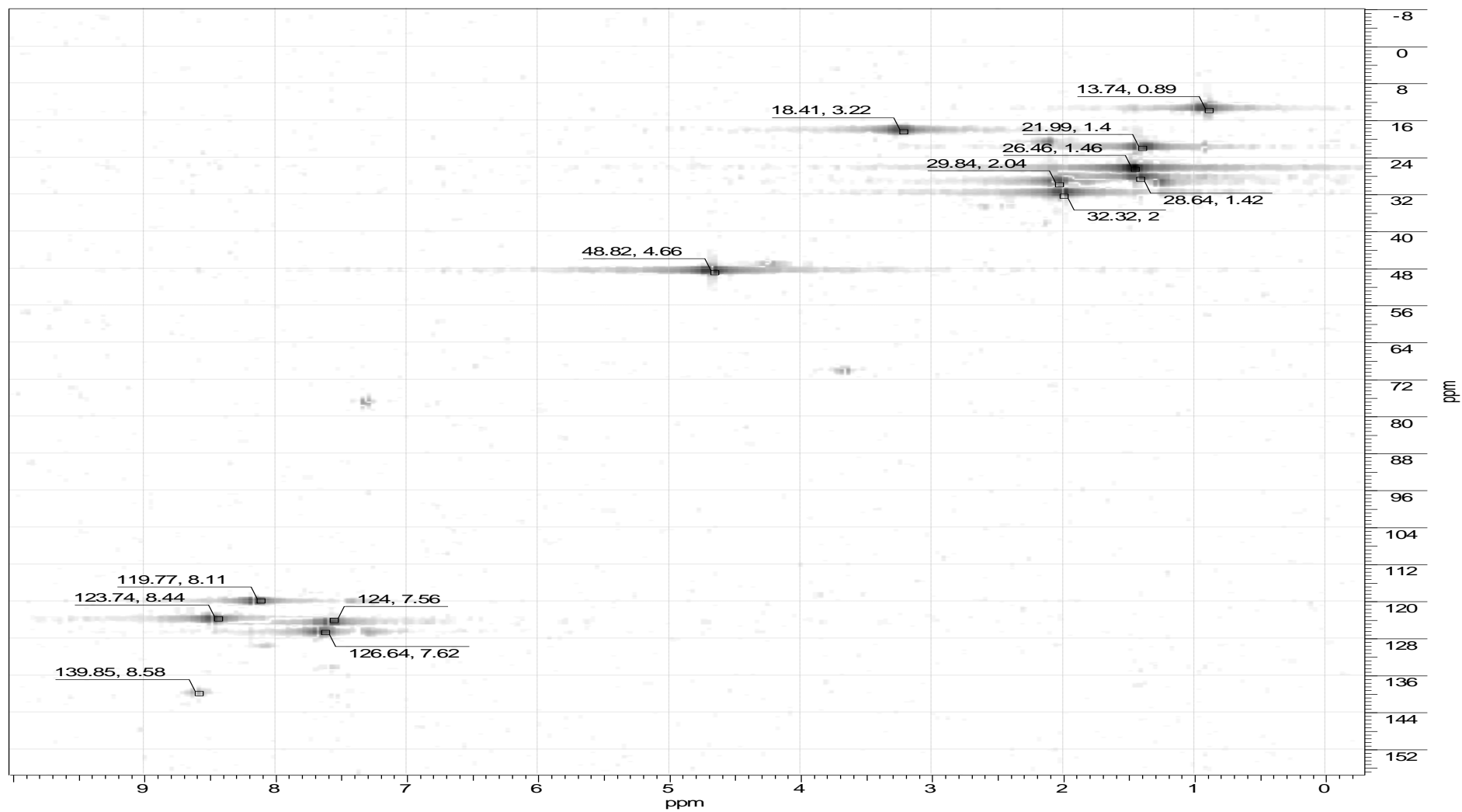
Espectro 37. RMN-¹H (400 MHz, CDCl₃) do composto 39b.



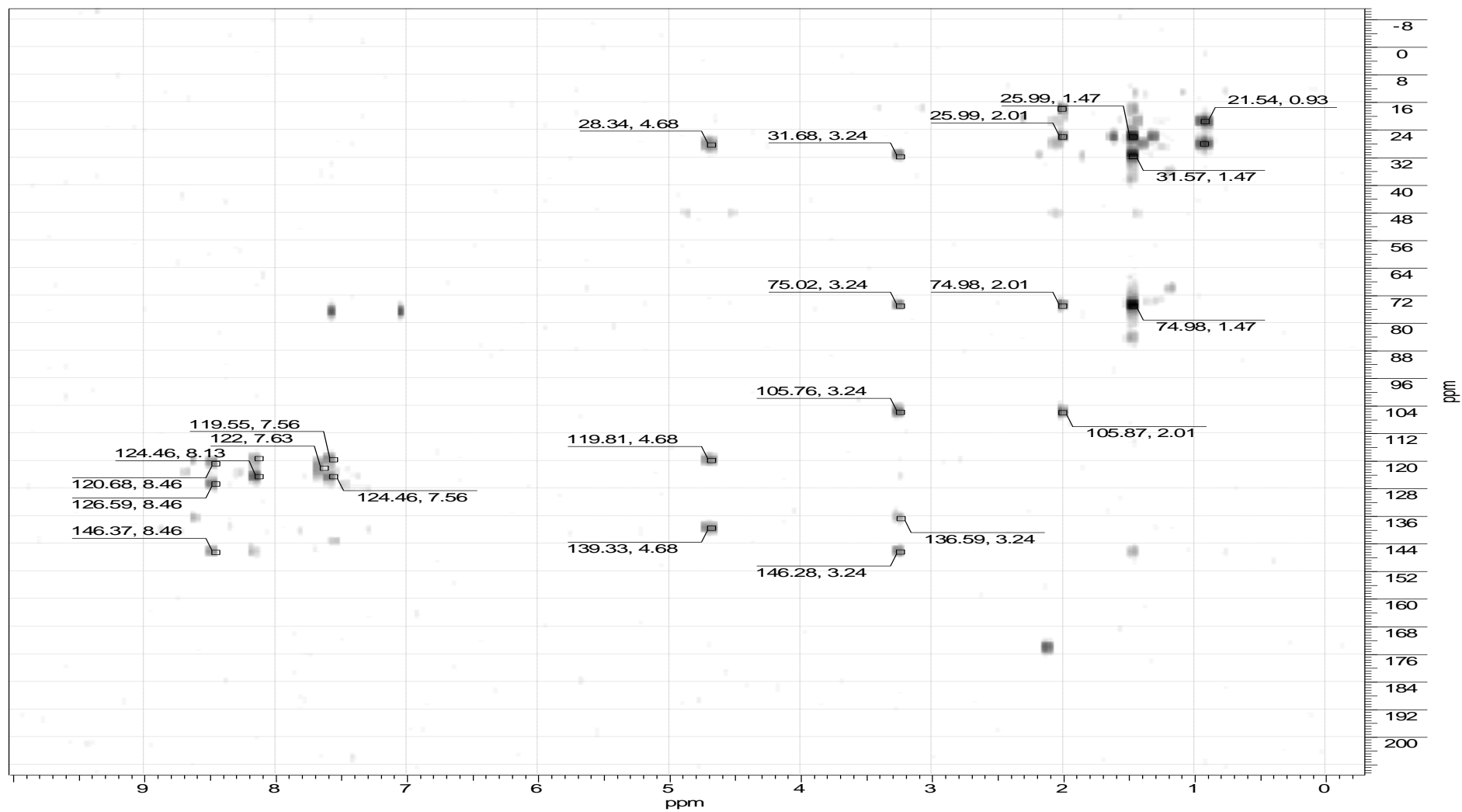
Espectro 38. RMN-¹³C (100 MHz, CDCl₃) do composto 39b.



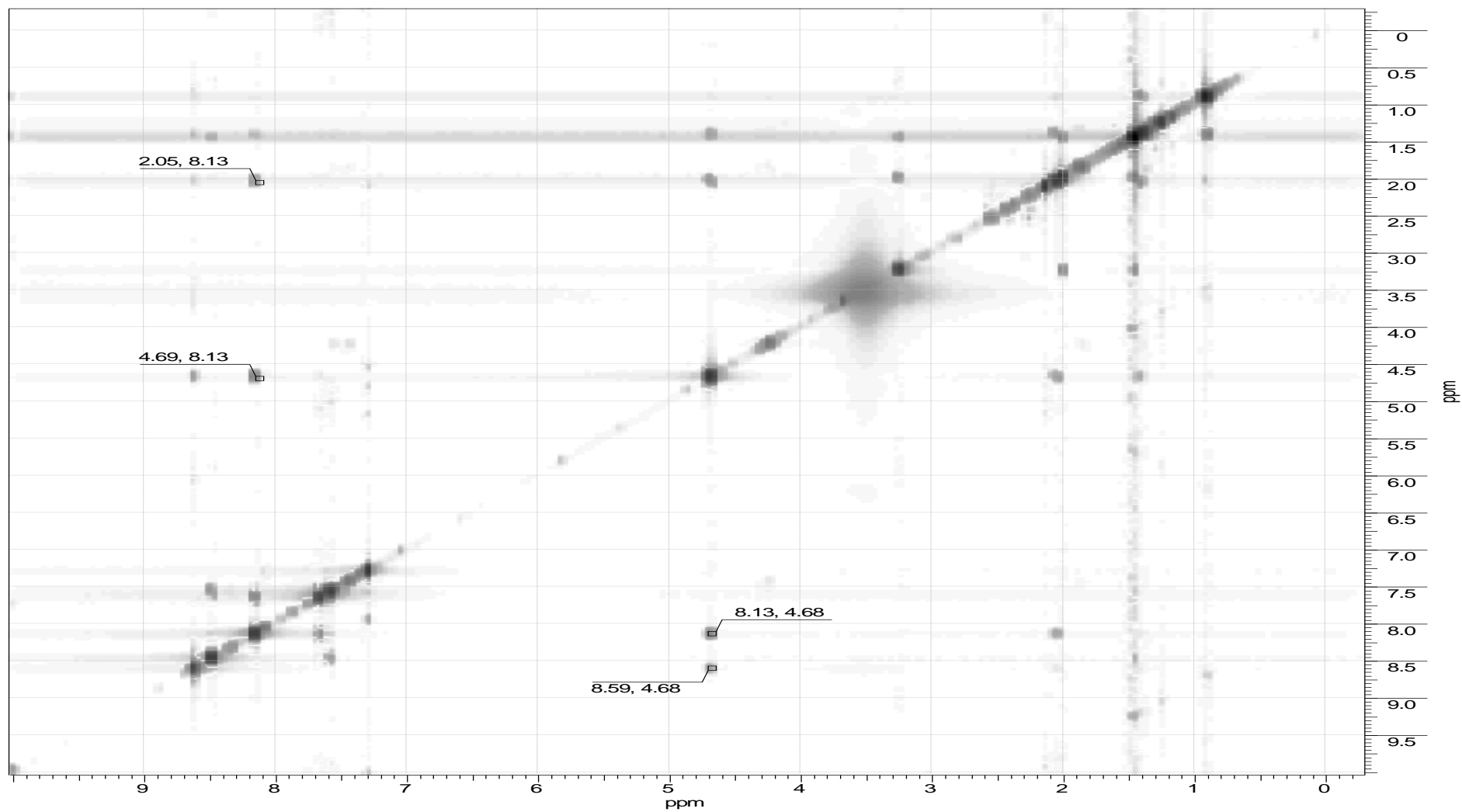
Espectro 39. ^1H -COSY (400 MHz, CDCl_3) do composto 39a.



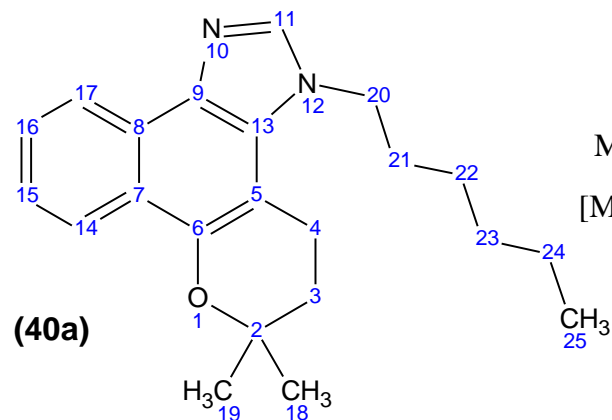
Espectro 40. HSQC (400 MHz, CDCl₃) do composto 39a.



Espectro 41. HMBC (400 MHz, CDCl_3) do composto 39a.

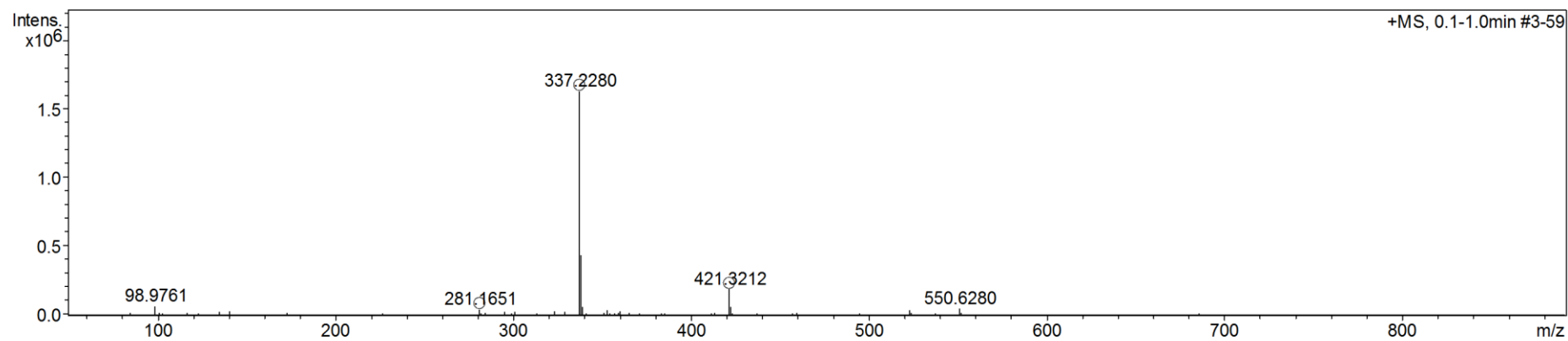


Espectro 42. NOESY (400 MHz, CDCl₃) do composto 39b.

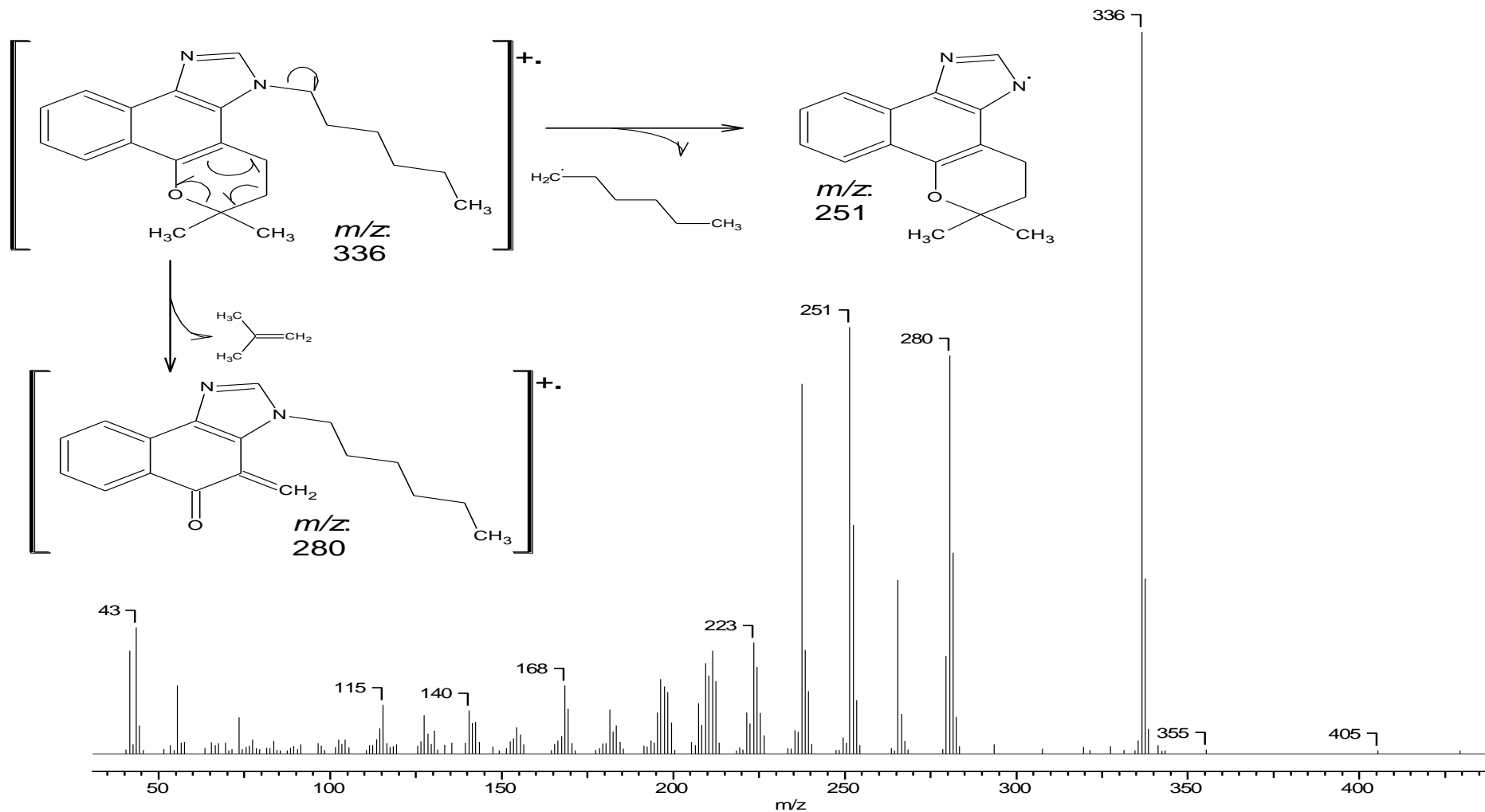


M: 336.4706 Da

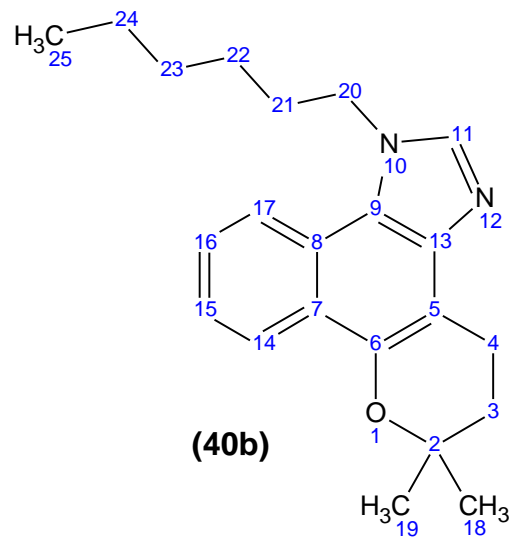
[M + H]⁺ = 337,2283 Da; err [ppm] = -2,5



Espectro 43. EM-IES do composto 40a.

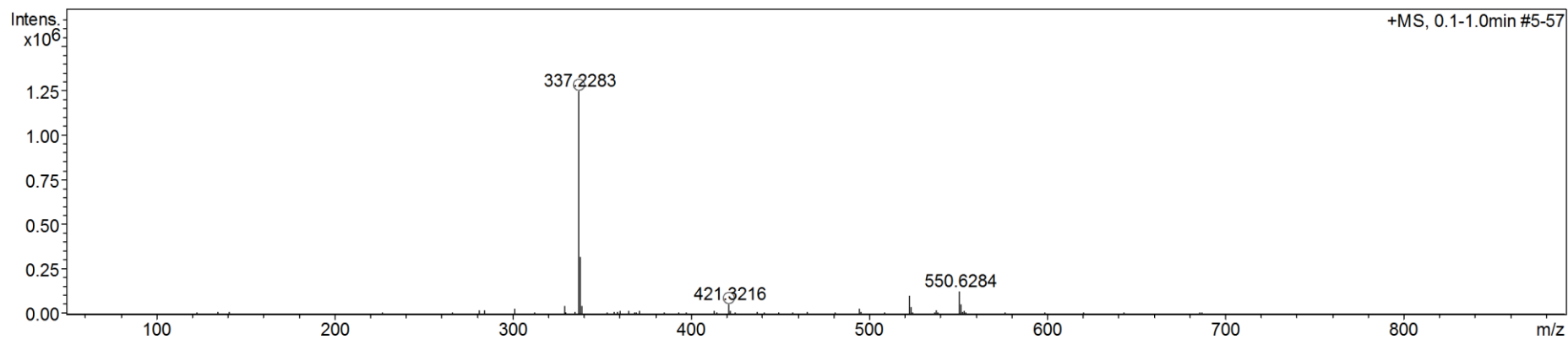


Espectro 44. EM-IE do composto 40a.

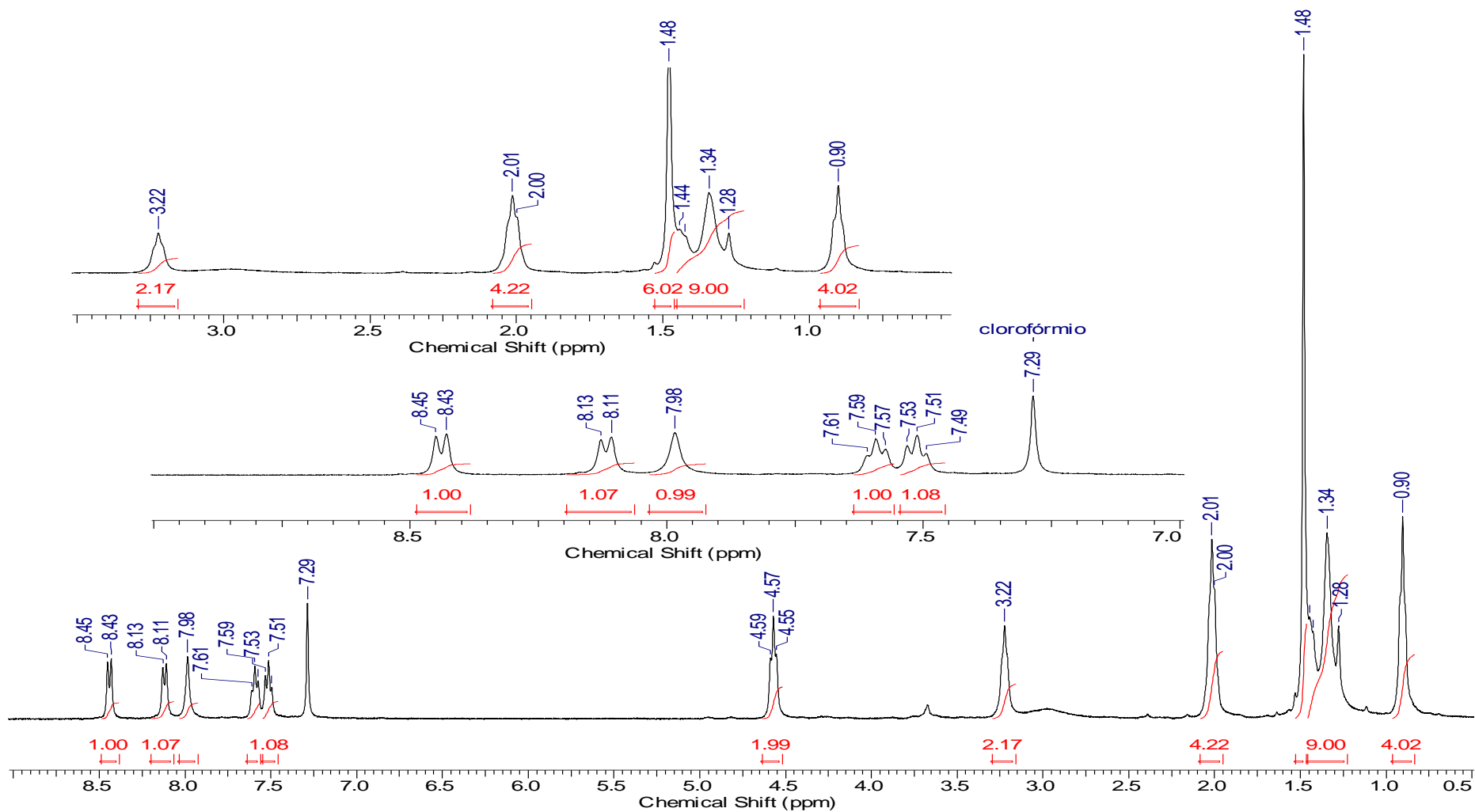


M: 336.4706 Da

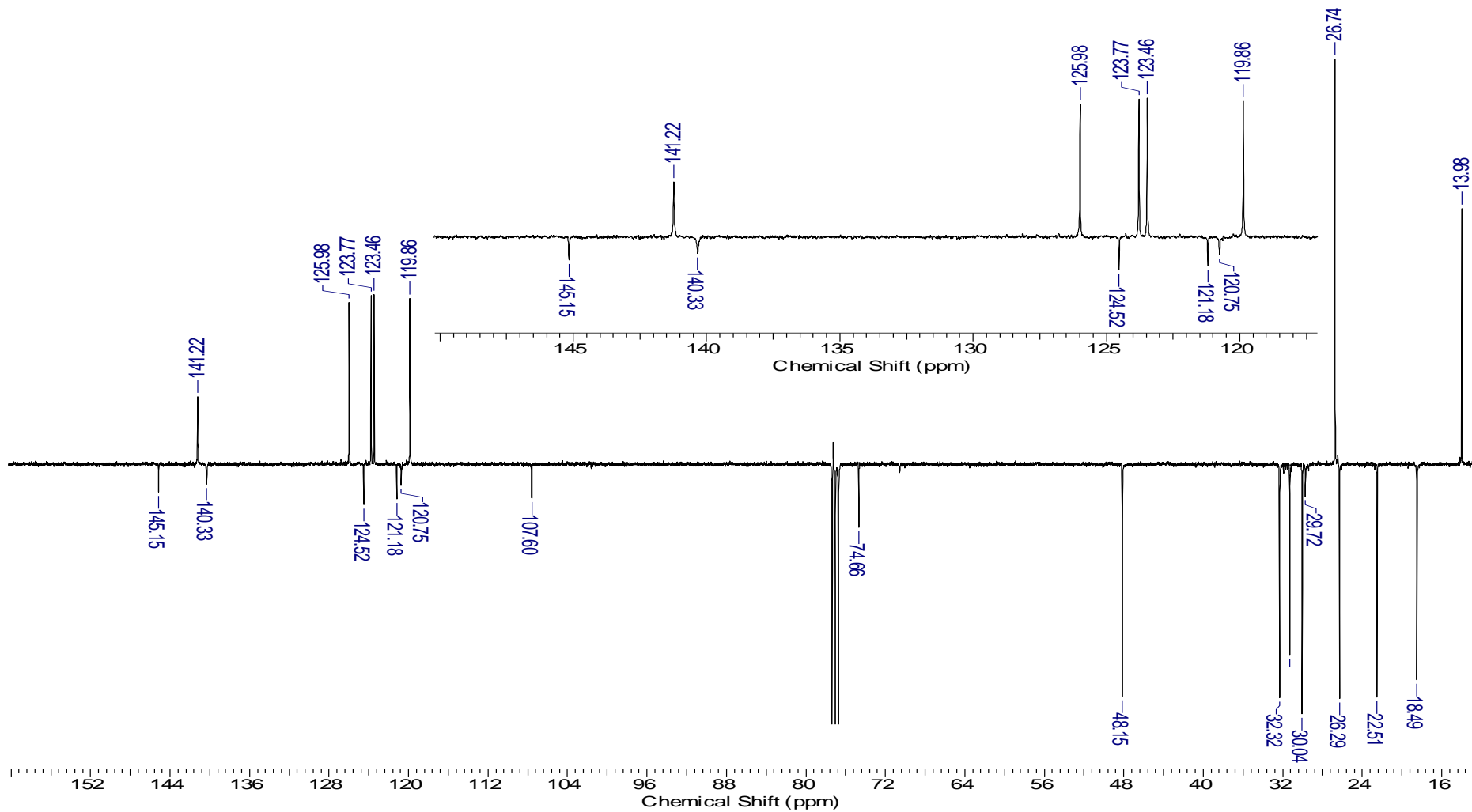
[M + H]⁺ = 337,2274 Da; err [ppm] = -2,5



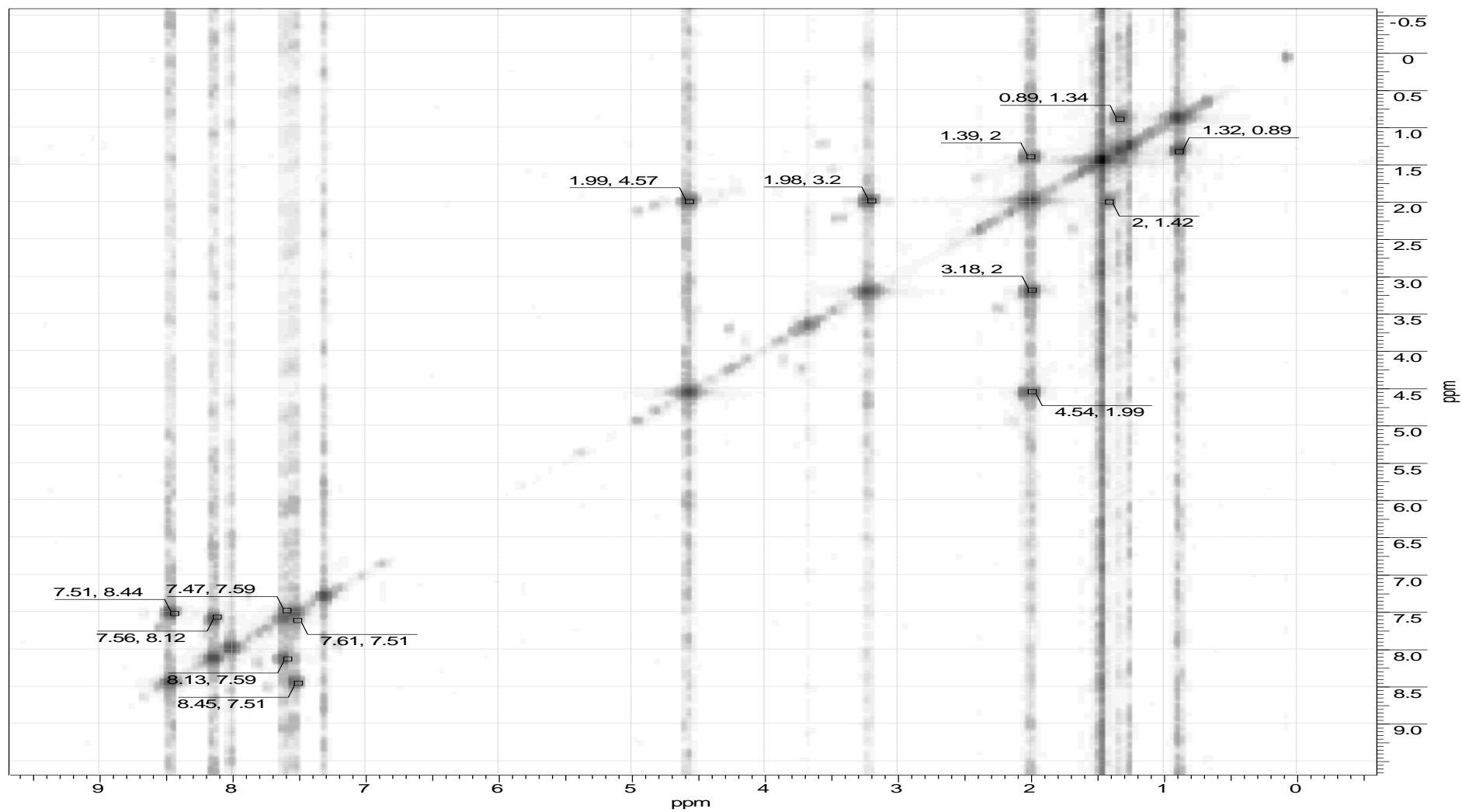
Espectro 45. EM-IES do composto 40b.



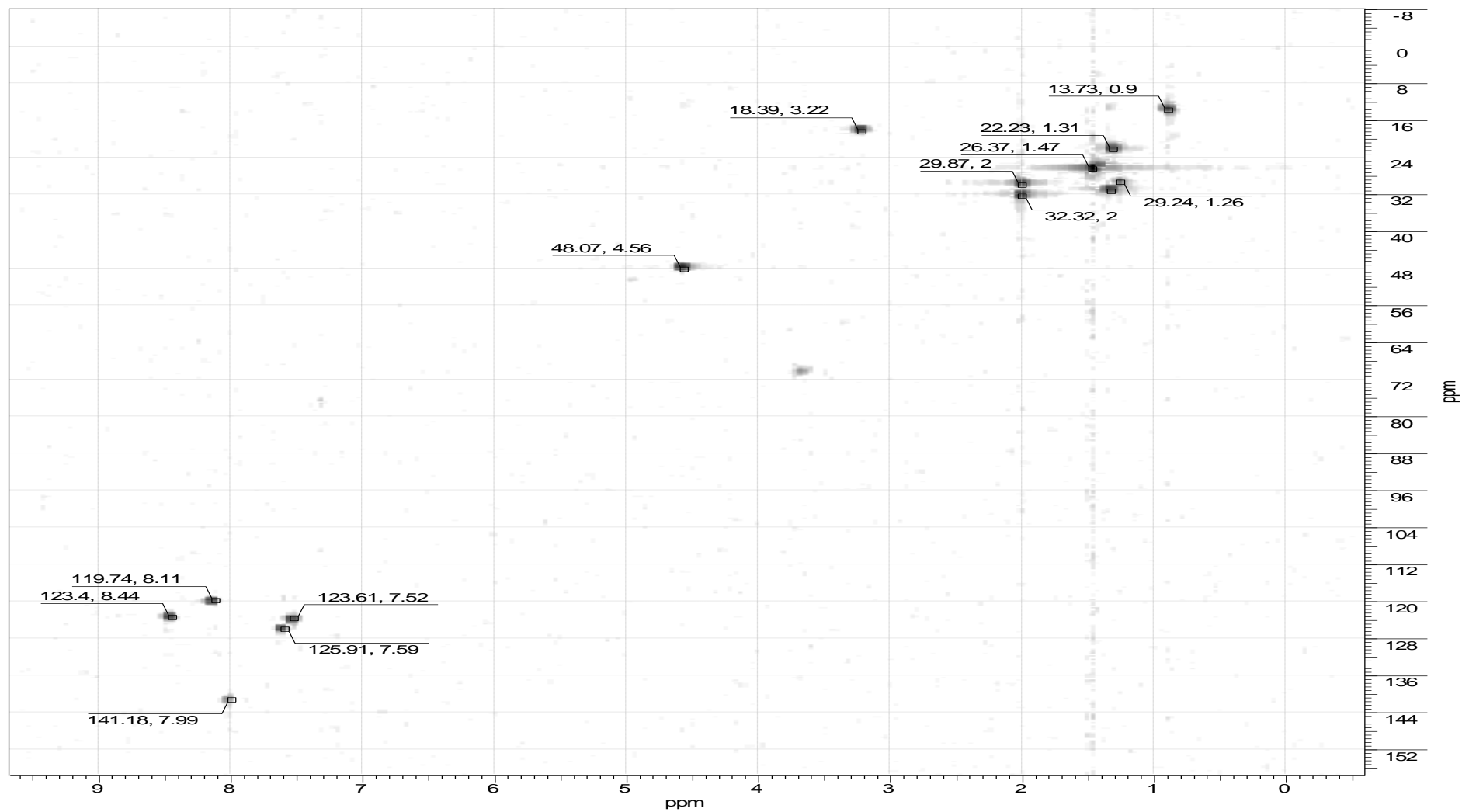
Espectro 46. RMN- ^1H (400 MHz, CDCl_3) do composto 40b.



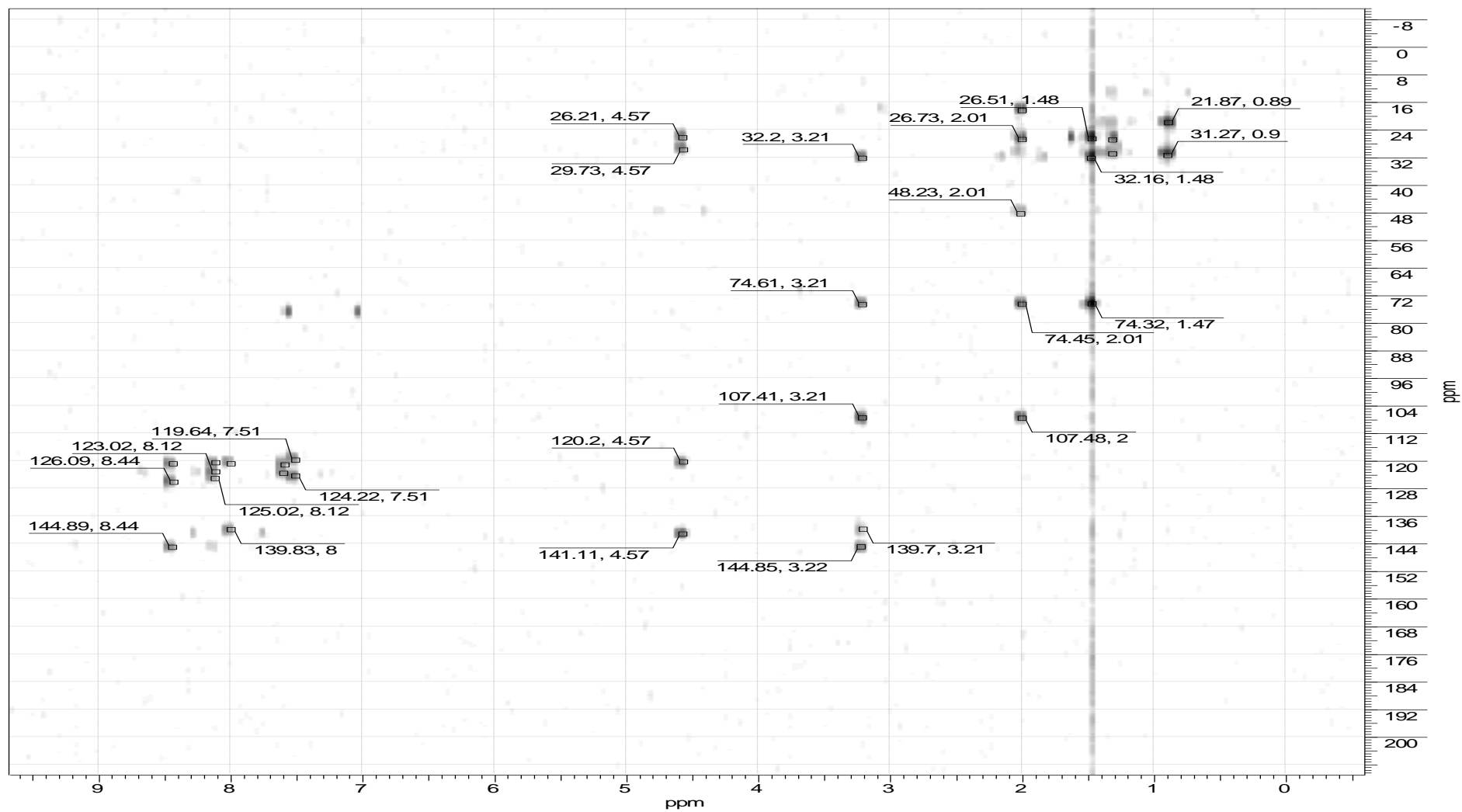
Espectro 47. RMN-¹³C (100 MHz, CDCl₃) do composto 40b.



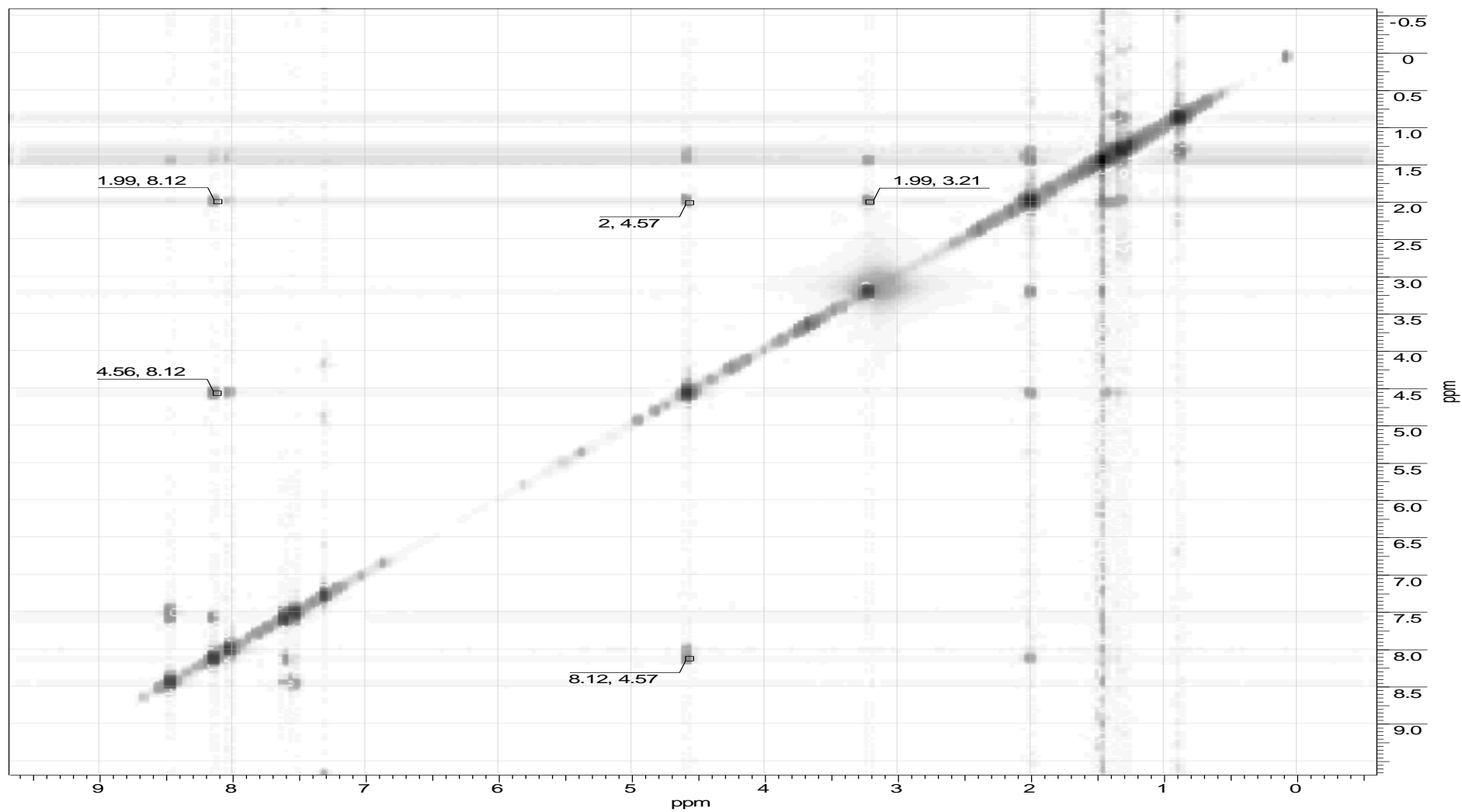
Espectro 48. ^1H -COSY (400 MHz, CDCl_3) do composto 40b.



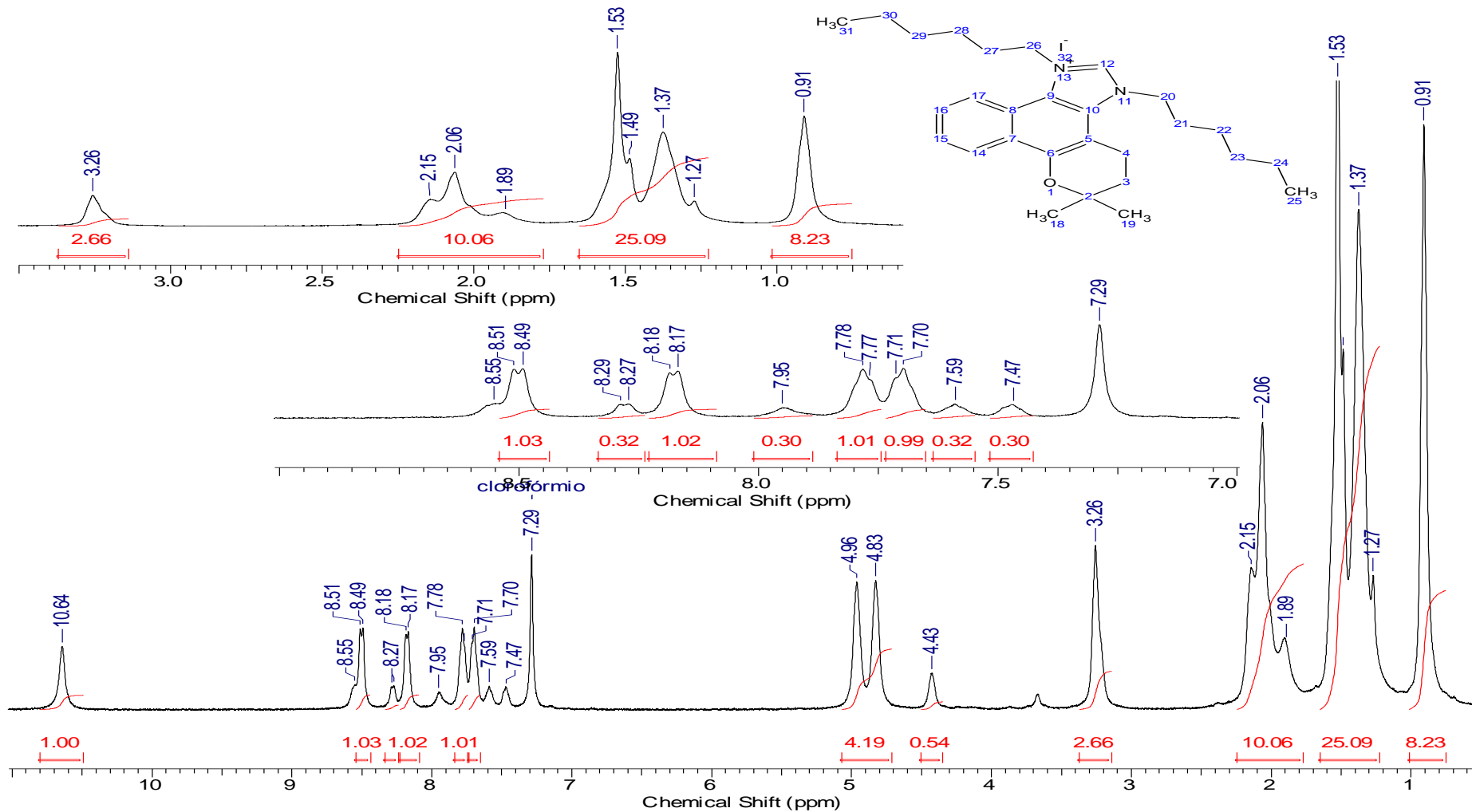
Espectro 49. HSQC (400 MHz, CDCl₃) do composto 40b.



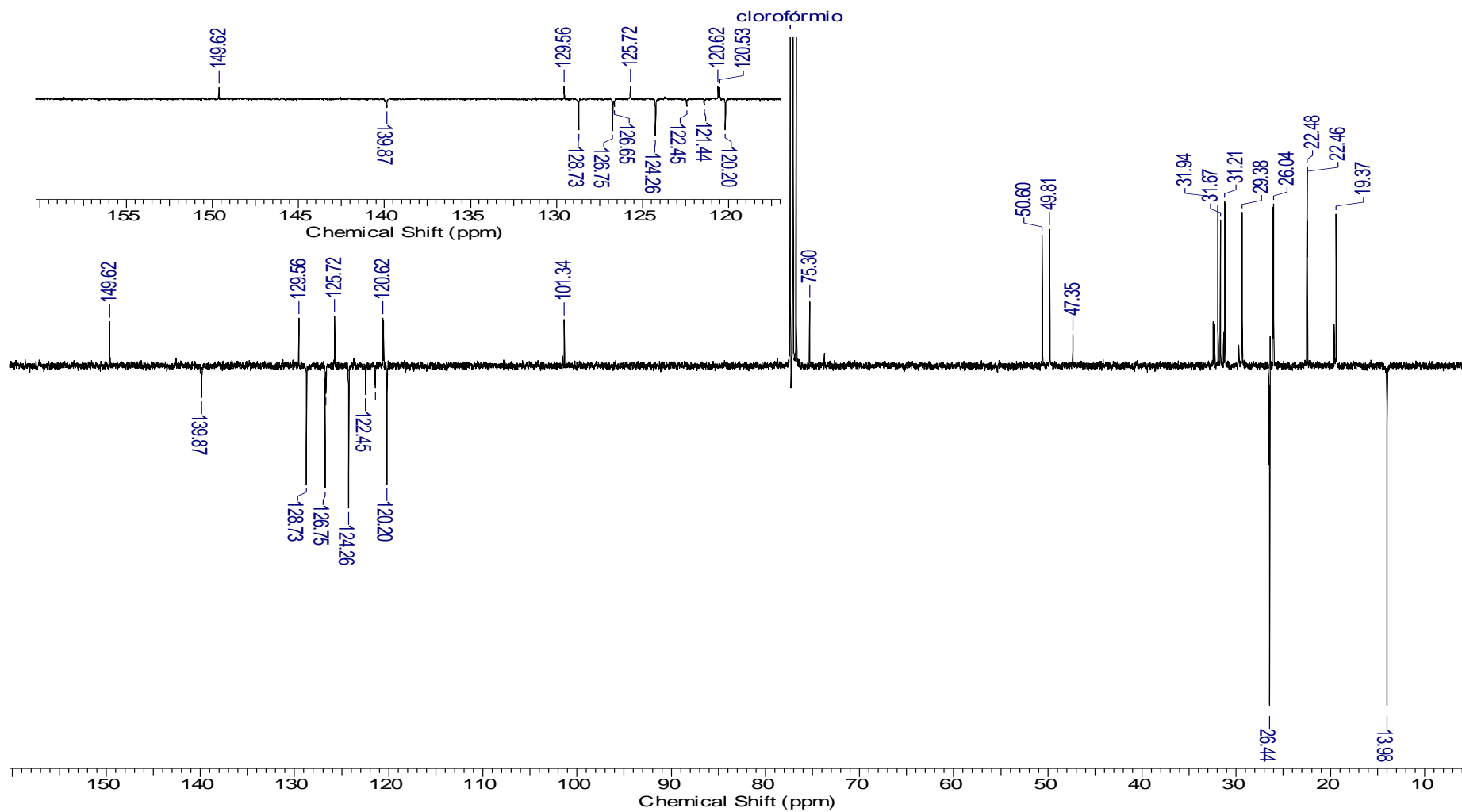
Espectro 50. HMBC (400 MHz, CDCl_3) do composto 40b.



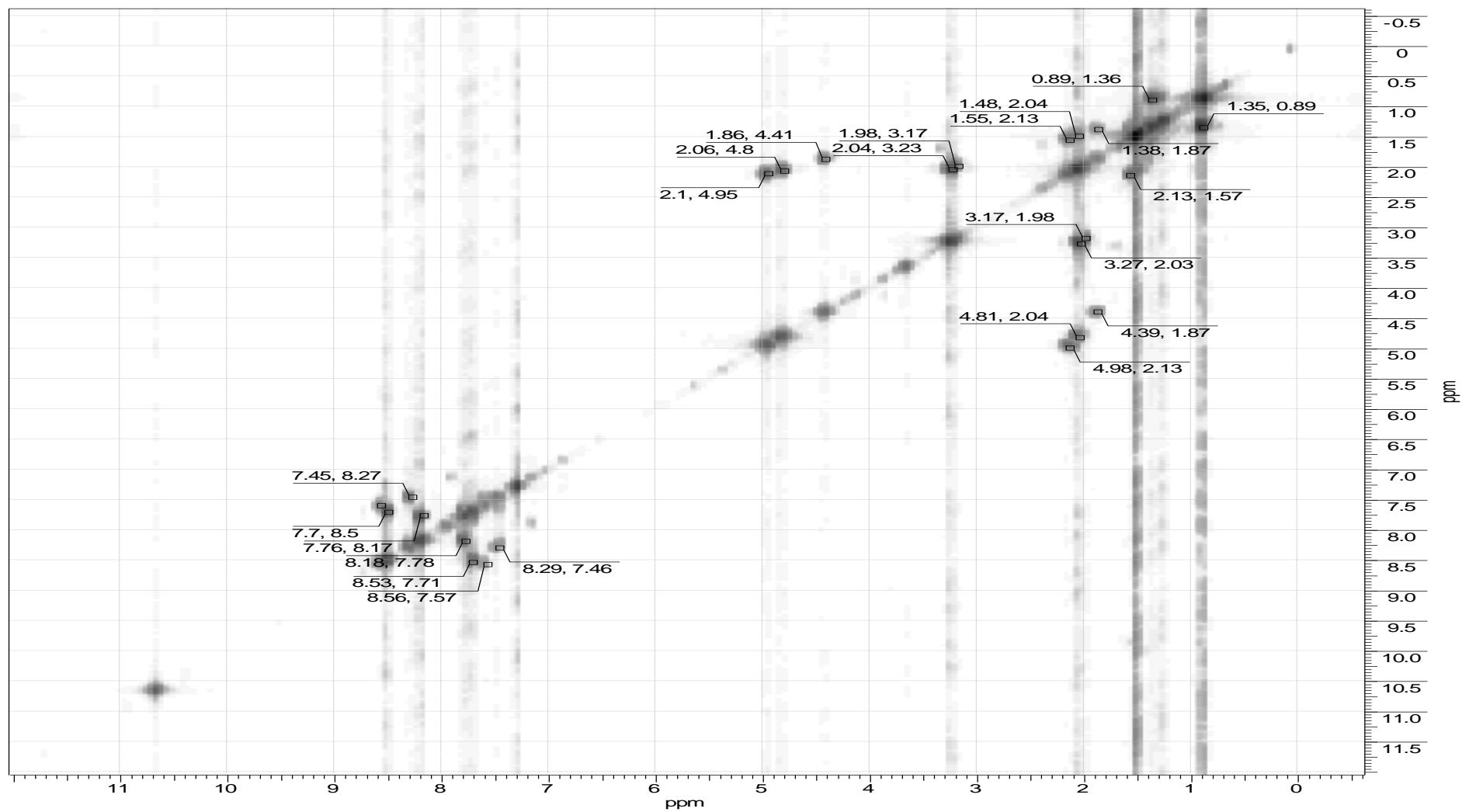
Espectro 51. NOESY (400 MHz, CDCl₃) do composto 40b.



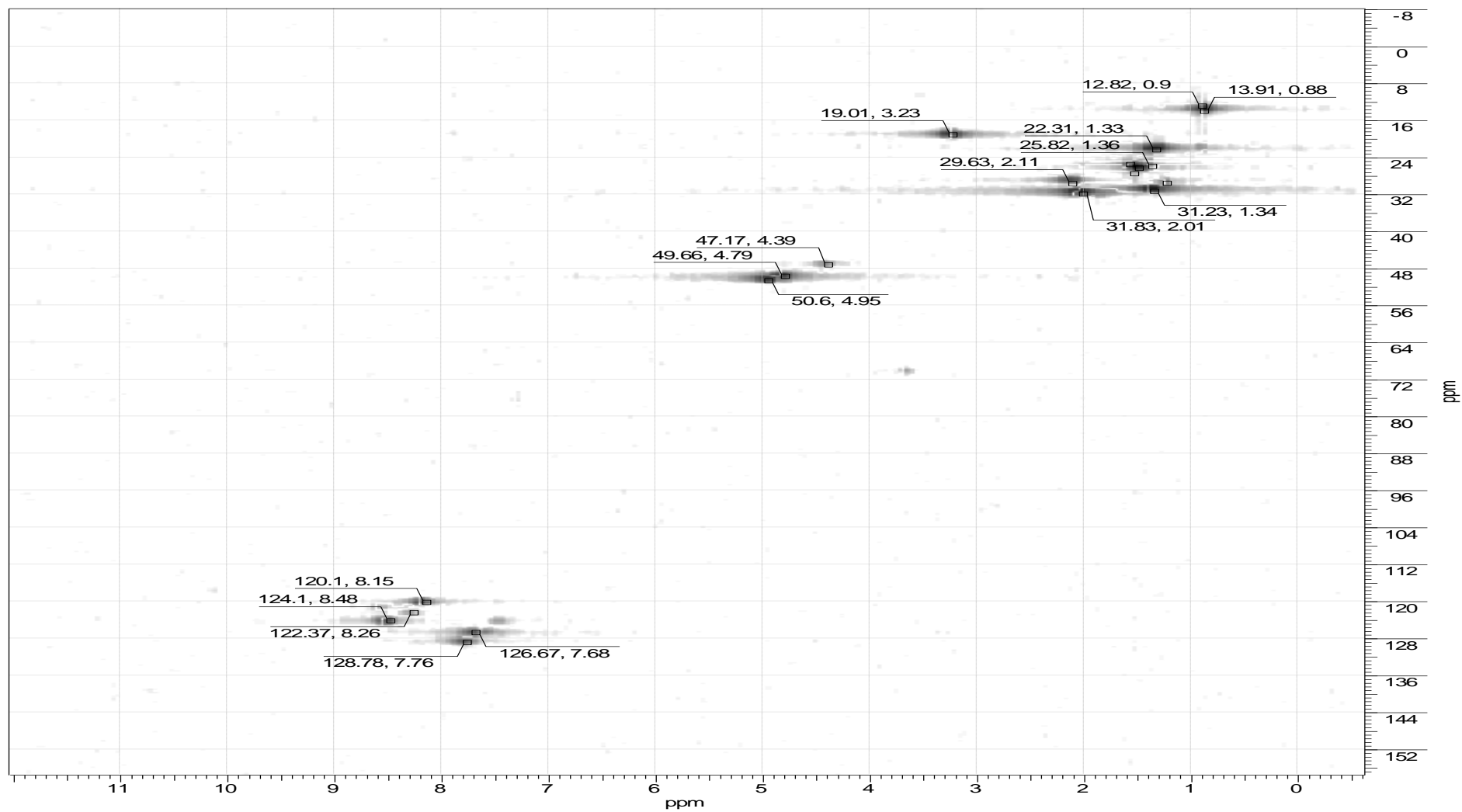
Espectro 52. RMN- ^1H (400 MHz, CDCl_3) do composto 40c.



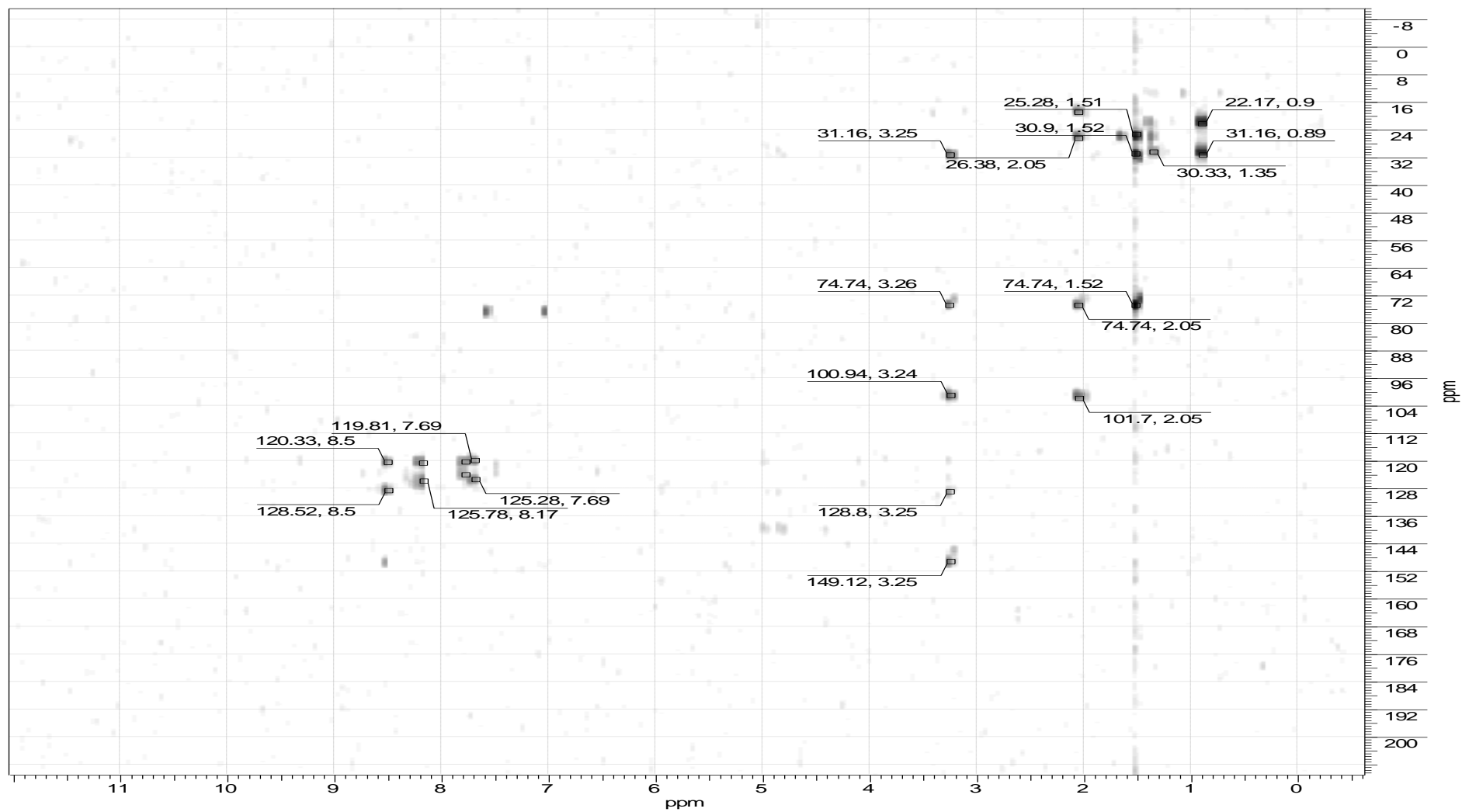
Espectro 53. RMN-¹³C (100 MHz, CDCl₃) do composto 40c.



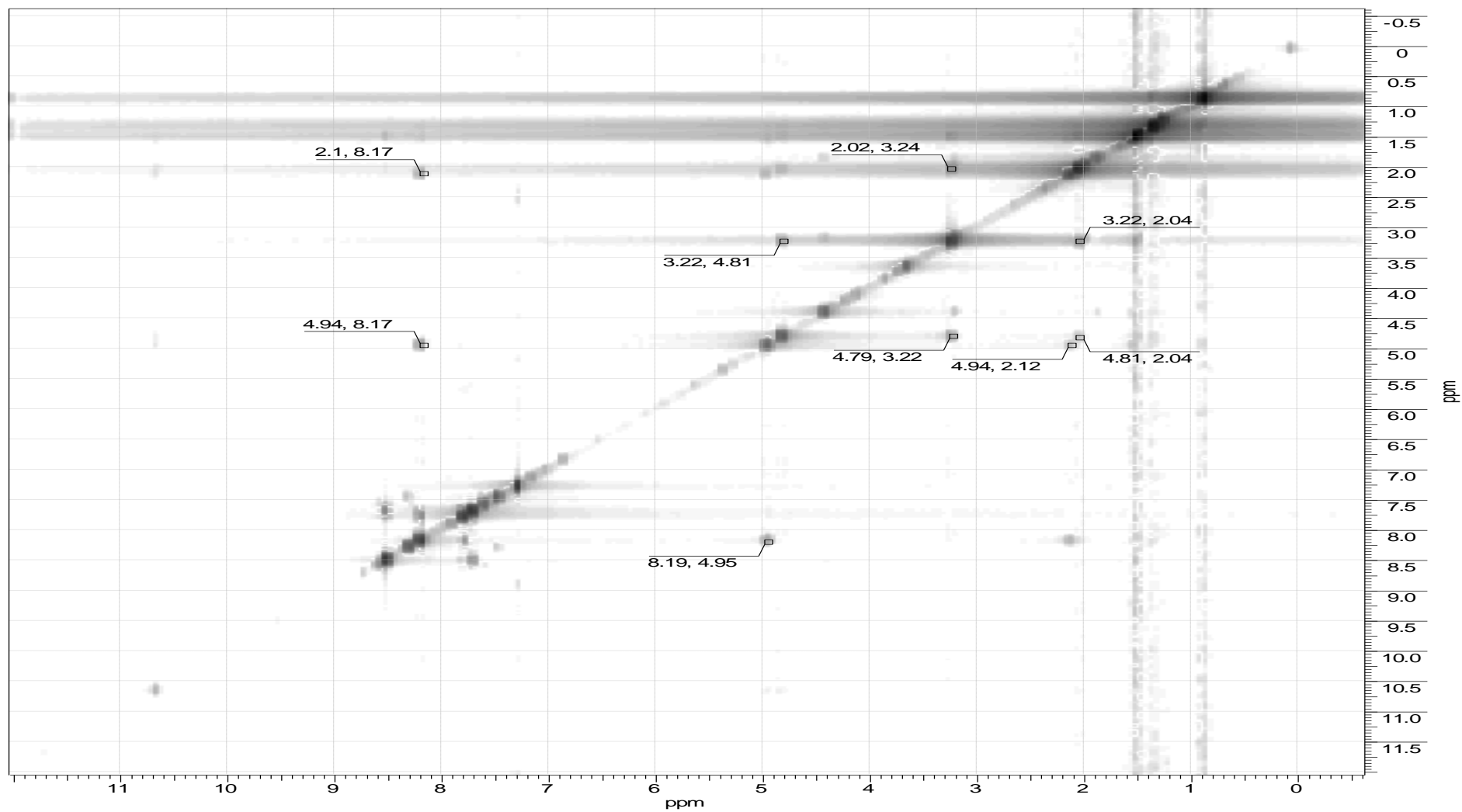
Espectro 54. ^1H -COSY (400 MHz, CDCl_3) do composto 40c.



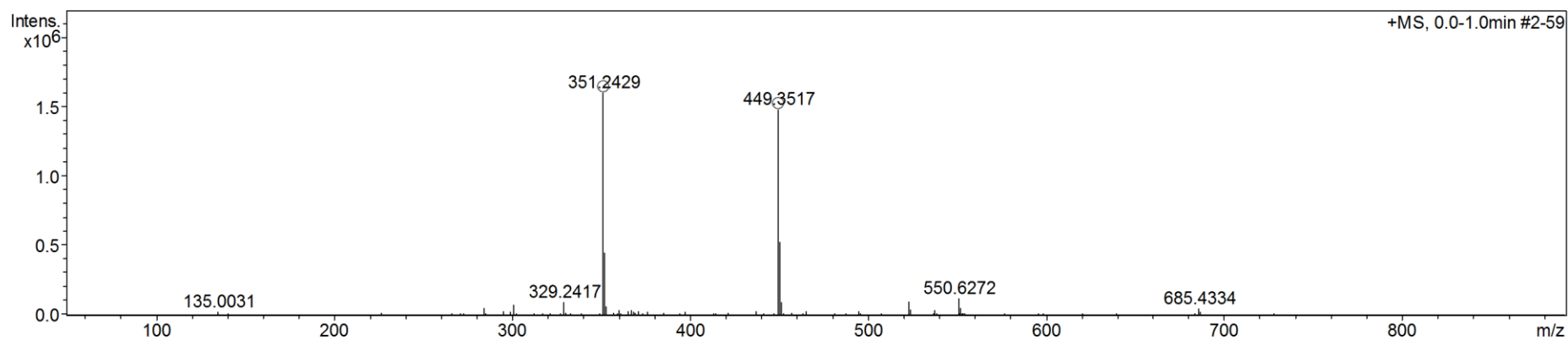
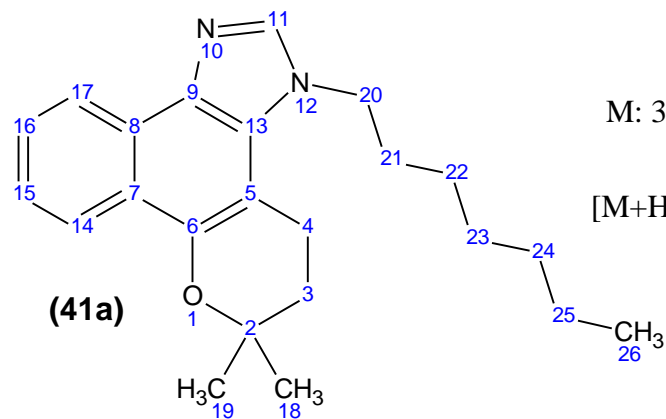
Espectro 55. HSQC (400 MHz, CDCl_3) do composto 40c.



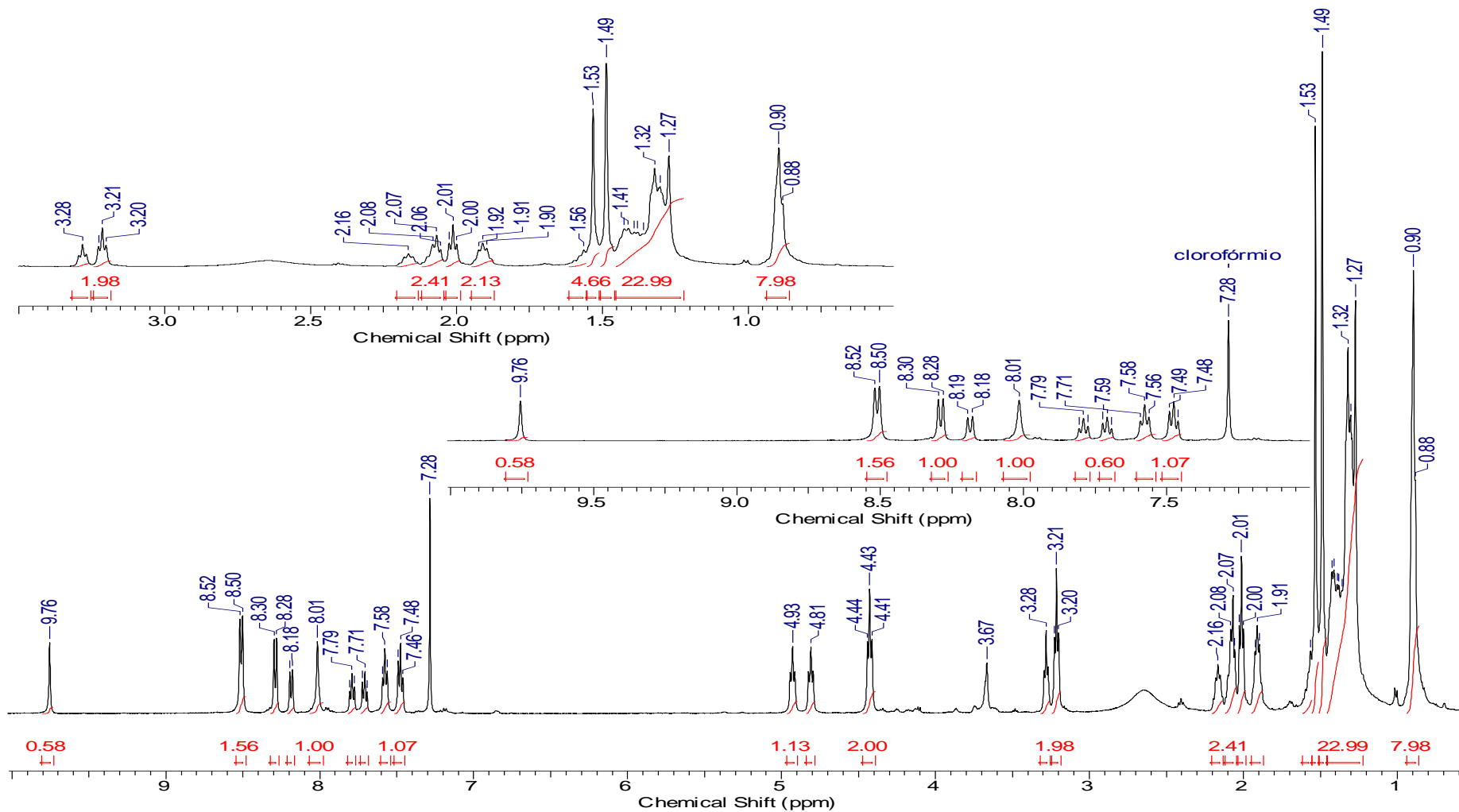
Espectro 56. HMBC (400 MHz, CDCl₃) do composto 40c.



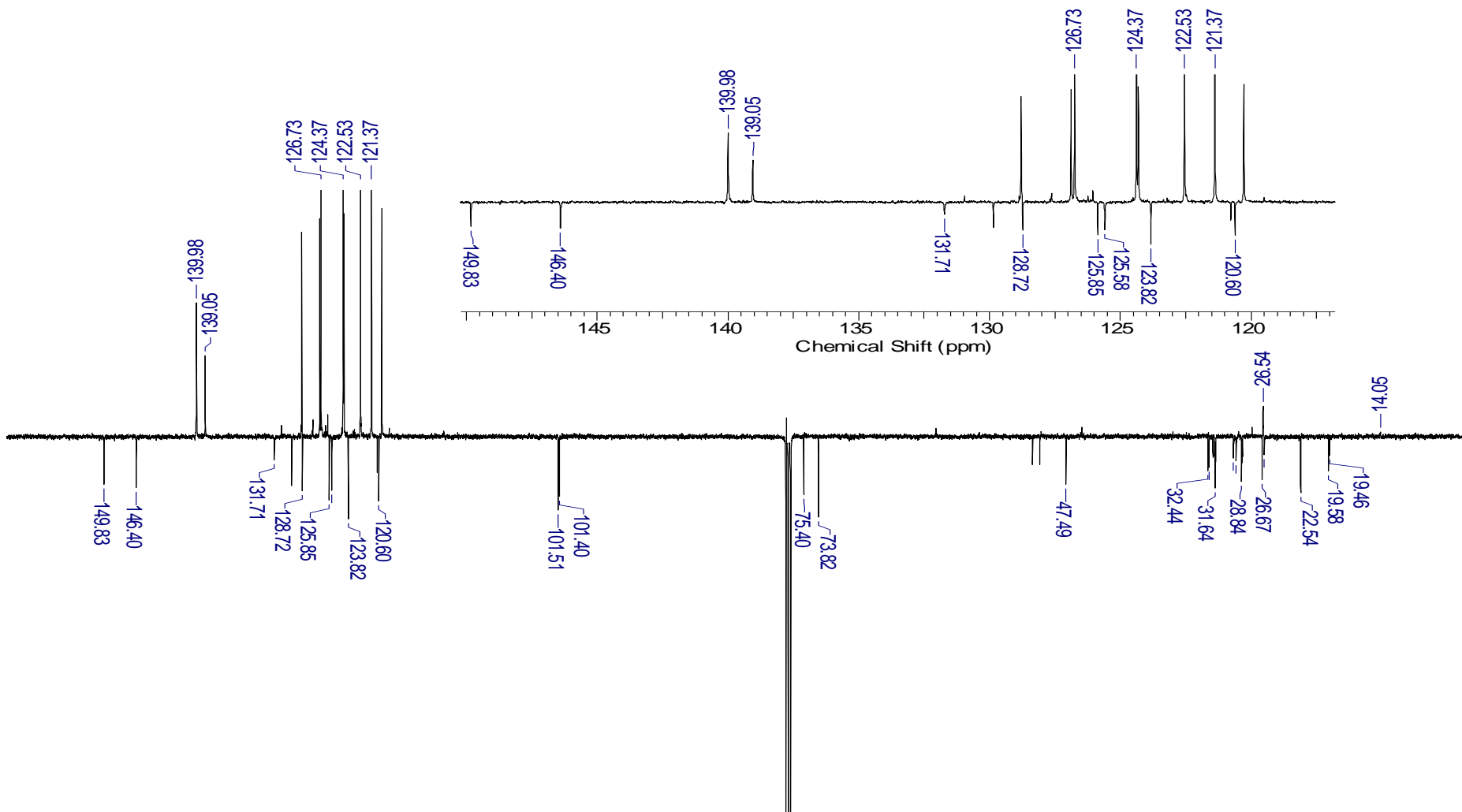
Espectro 57. NOESY (400 MHz, CDCl₃) do composto 40c.



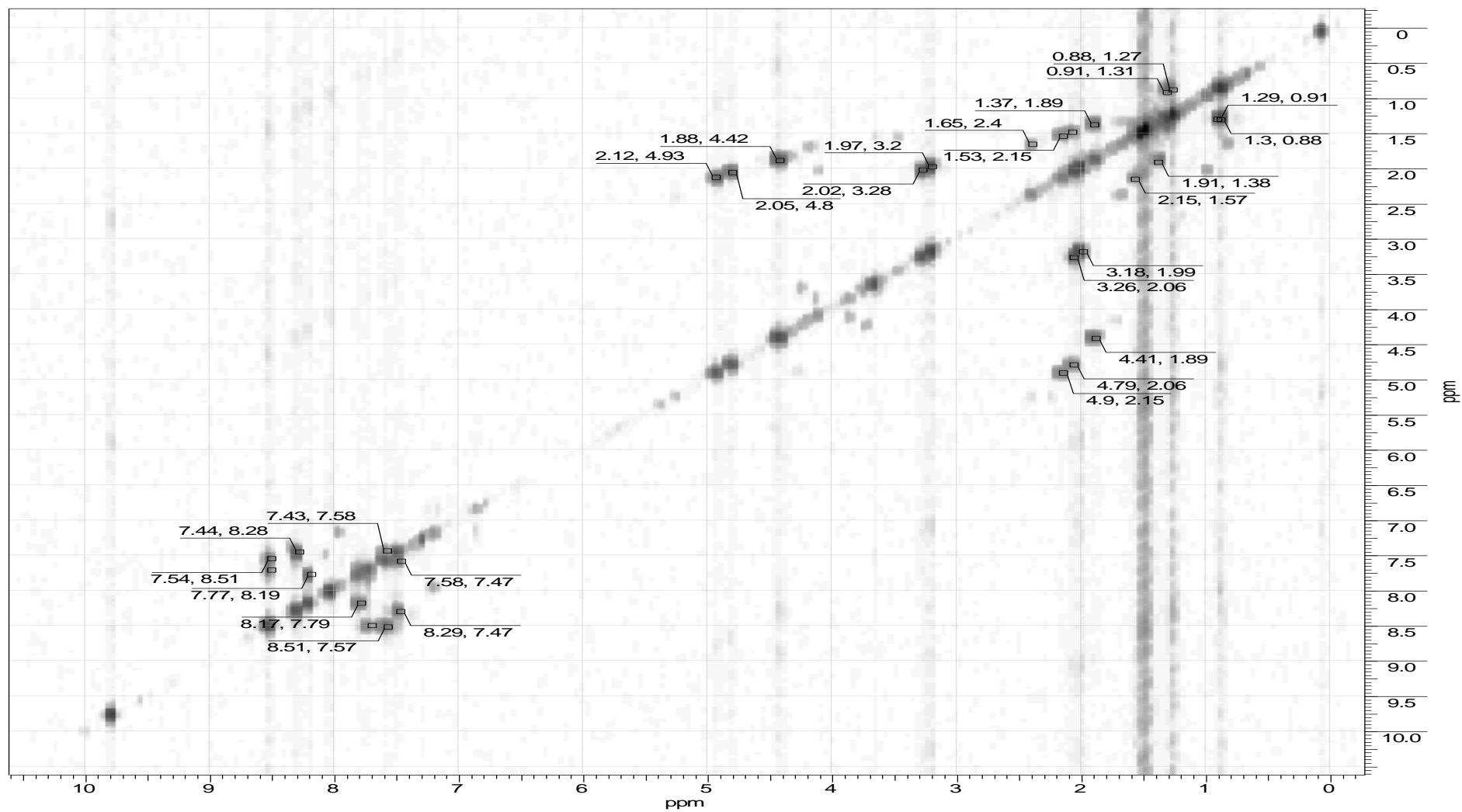
Espectro 58. EM-IES do composto 41a.



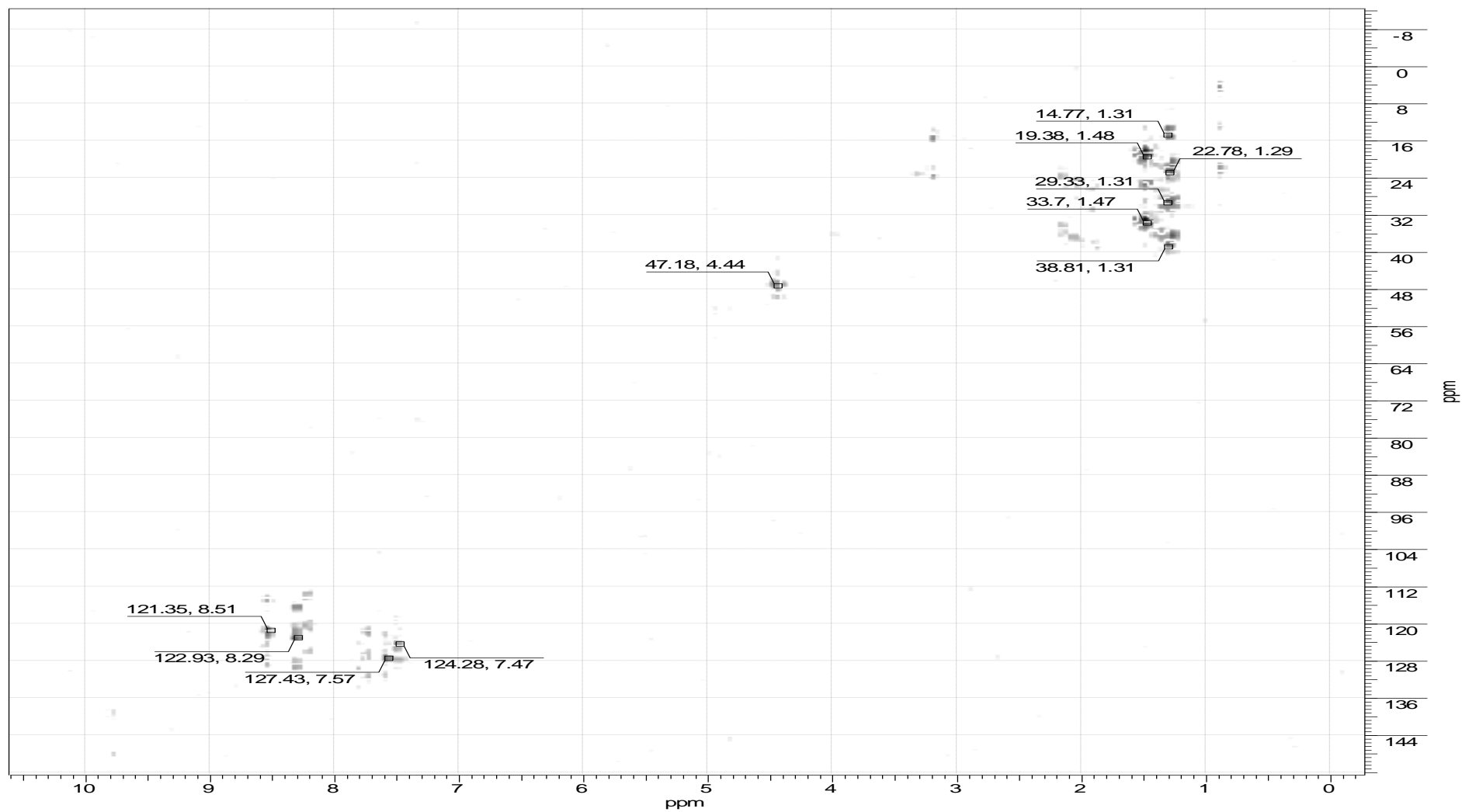
Espectro 59. RMN-¹H (500 MHz, CDCl₃) do composto 41a.



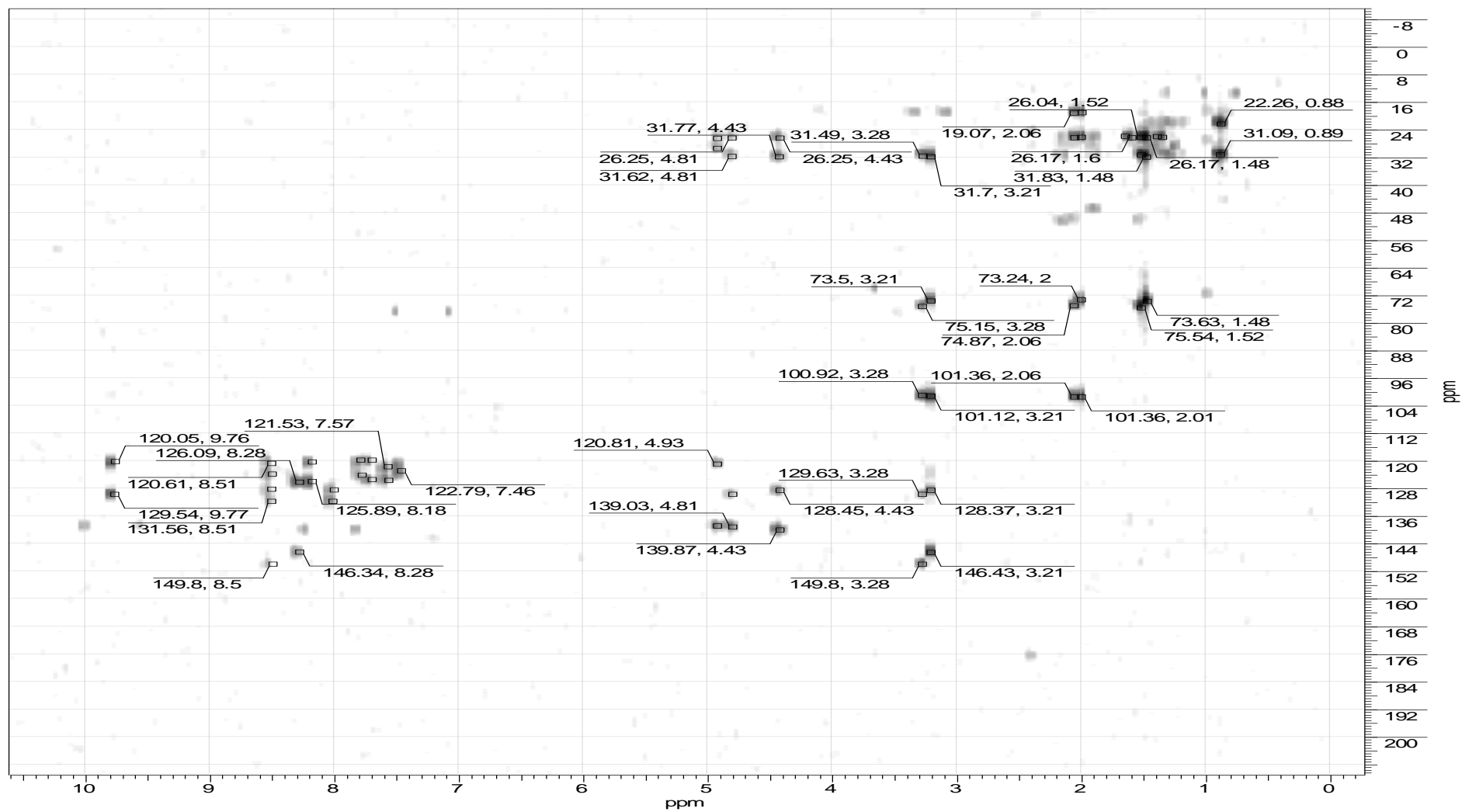
Espectro 60. RMN-¹³C (125 MHz, CDCl₃) do composto 41a.



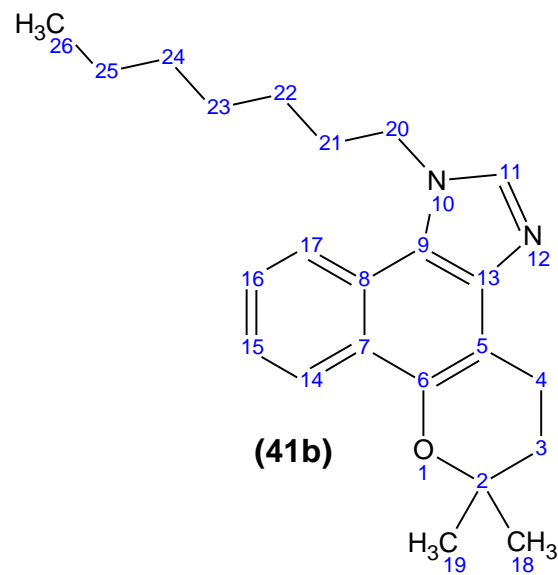
Espectro 61. ^1H -COSY (500 MHz, CDCl_3) do composto 41a.



Espectro 62. HSQC (500 MHz, CDCl₃) do composto 41a.

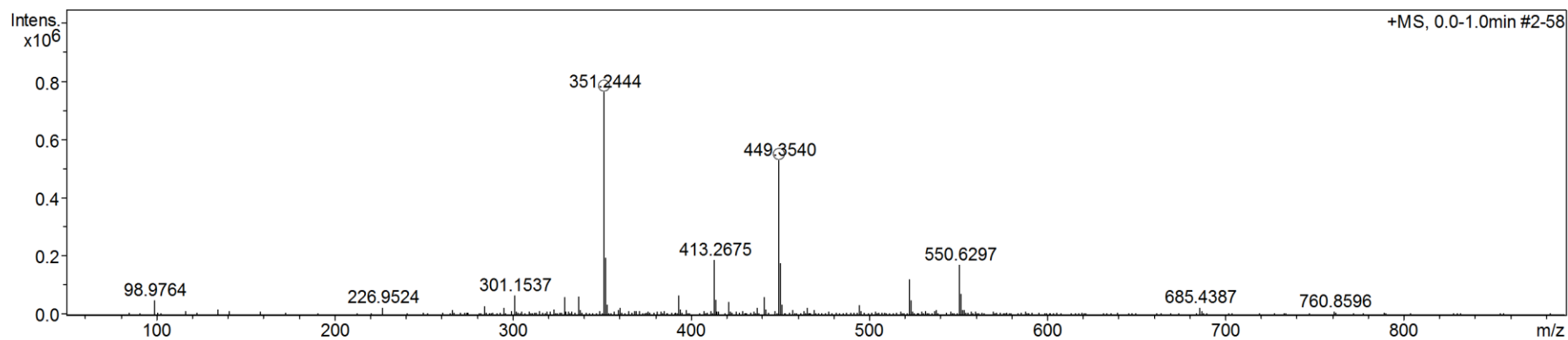


Espectro 63. HMBC (500 MHz, CDCl₃) do composto 41a.

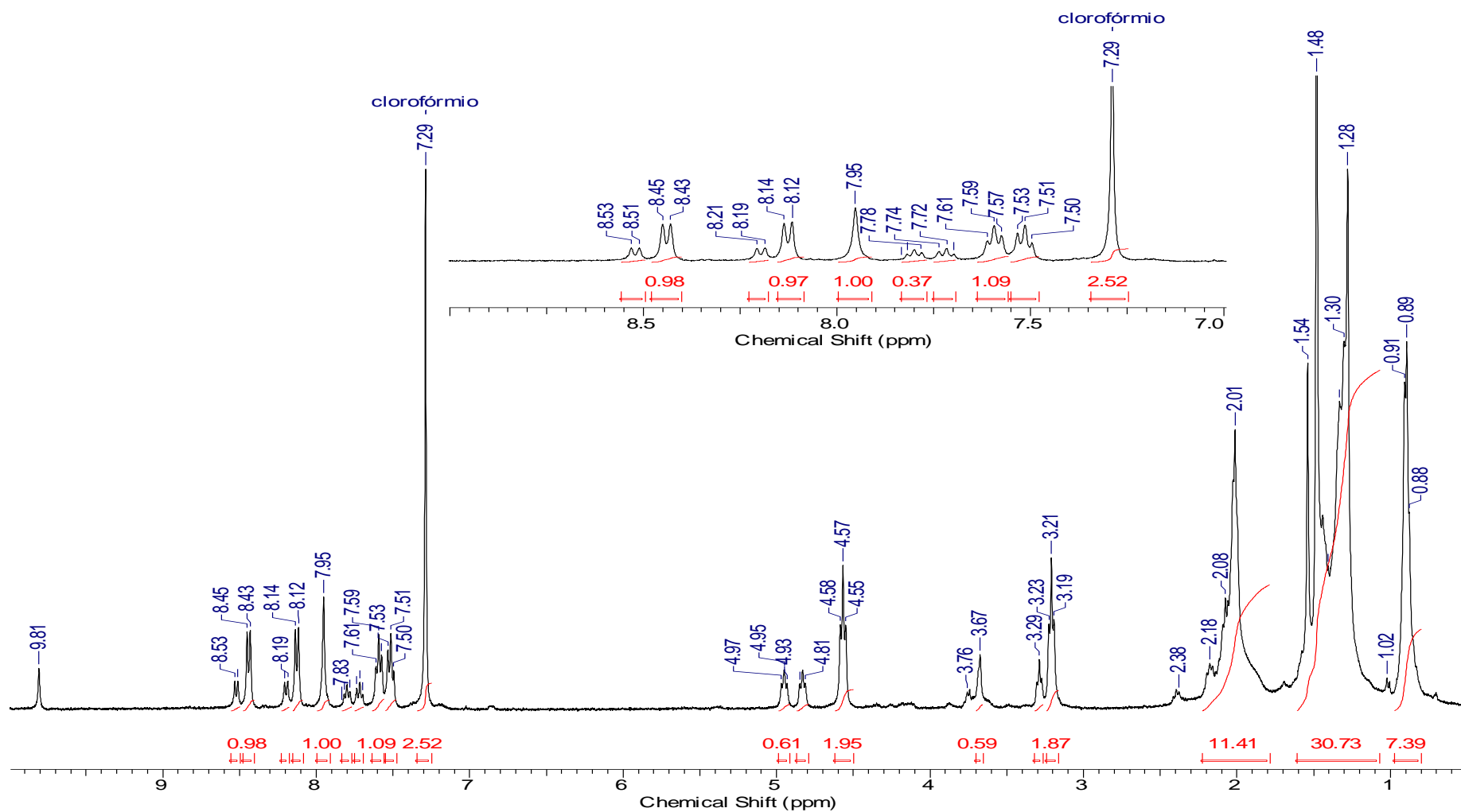


M: 350.4972 Da

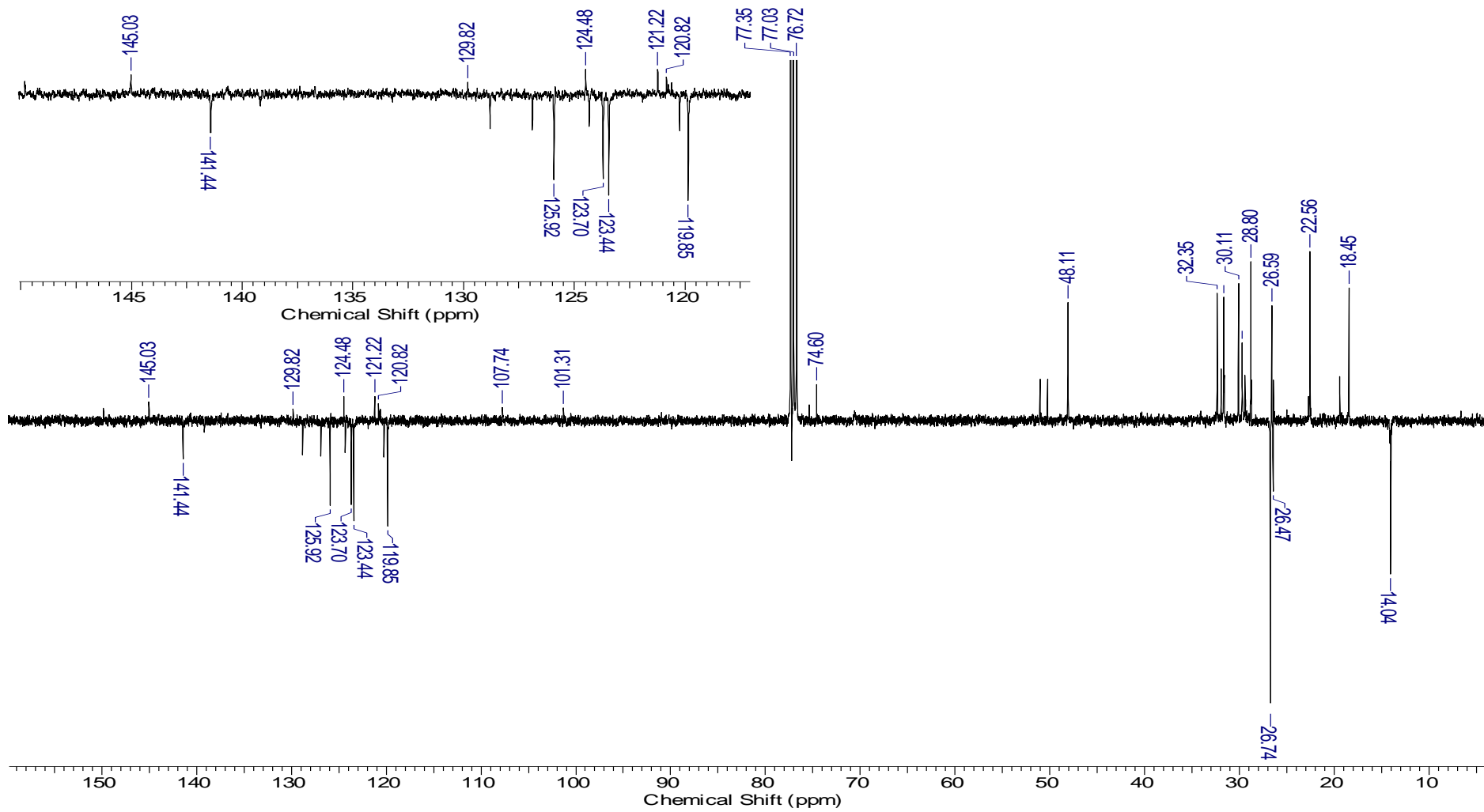
$[M+H]^+$: 351.2431 Da; err [ppm] = -3,7



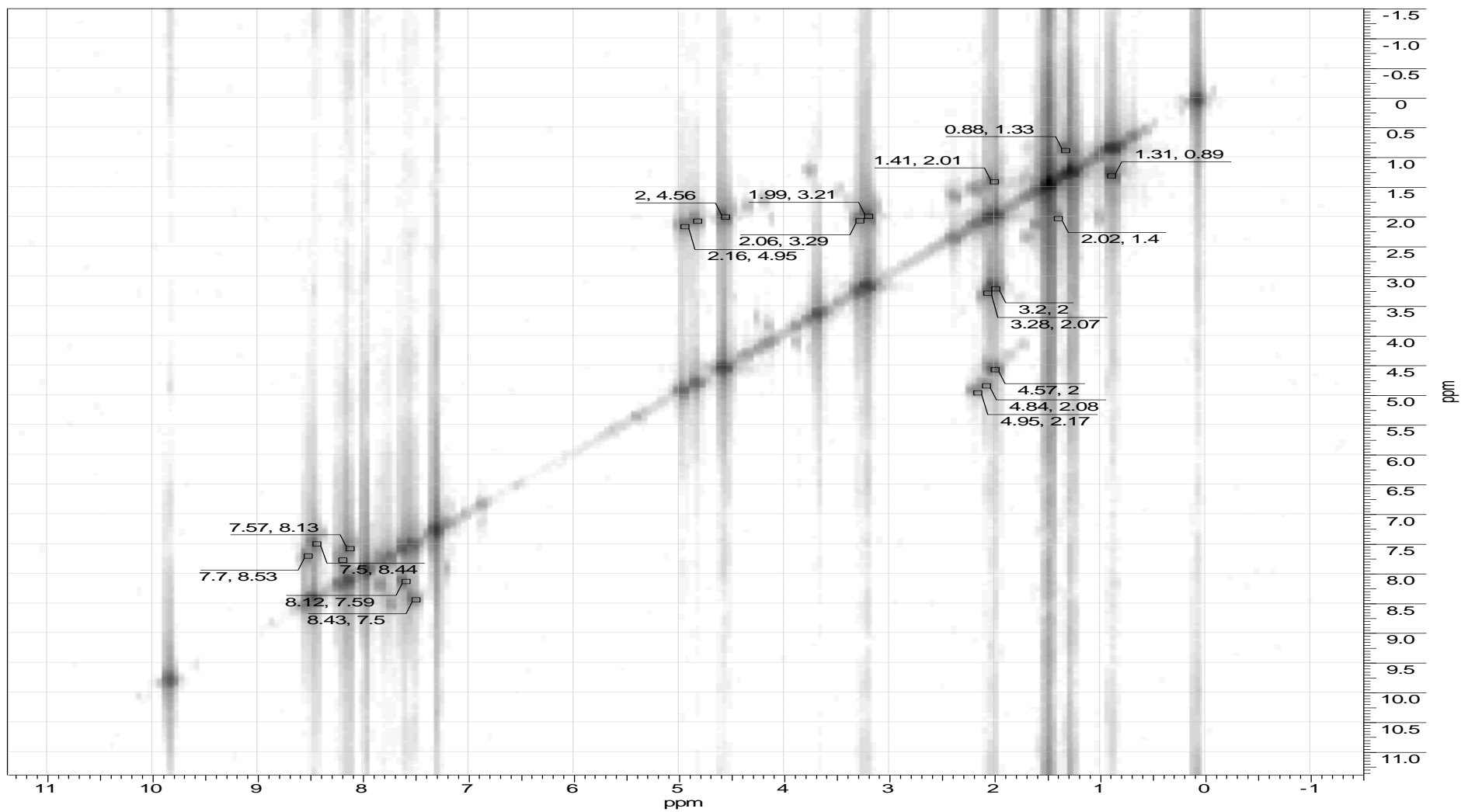
Espectro 64. EM-IES do composto 41b.



Espectro 65. RMN- ^1H (400 MHz, CDCl_3) do composto 41b.



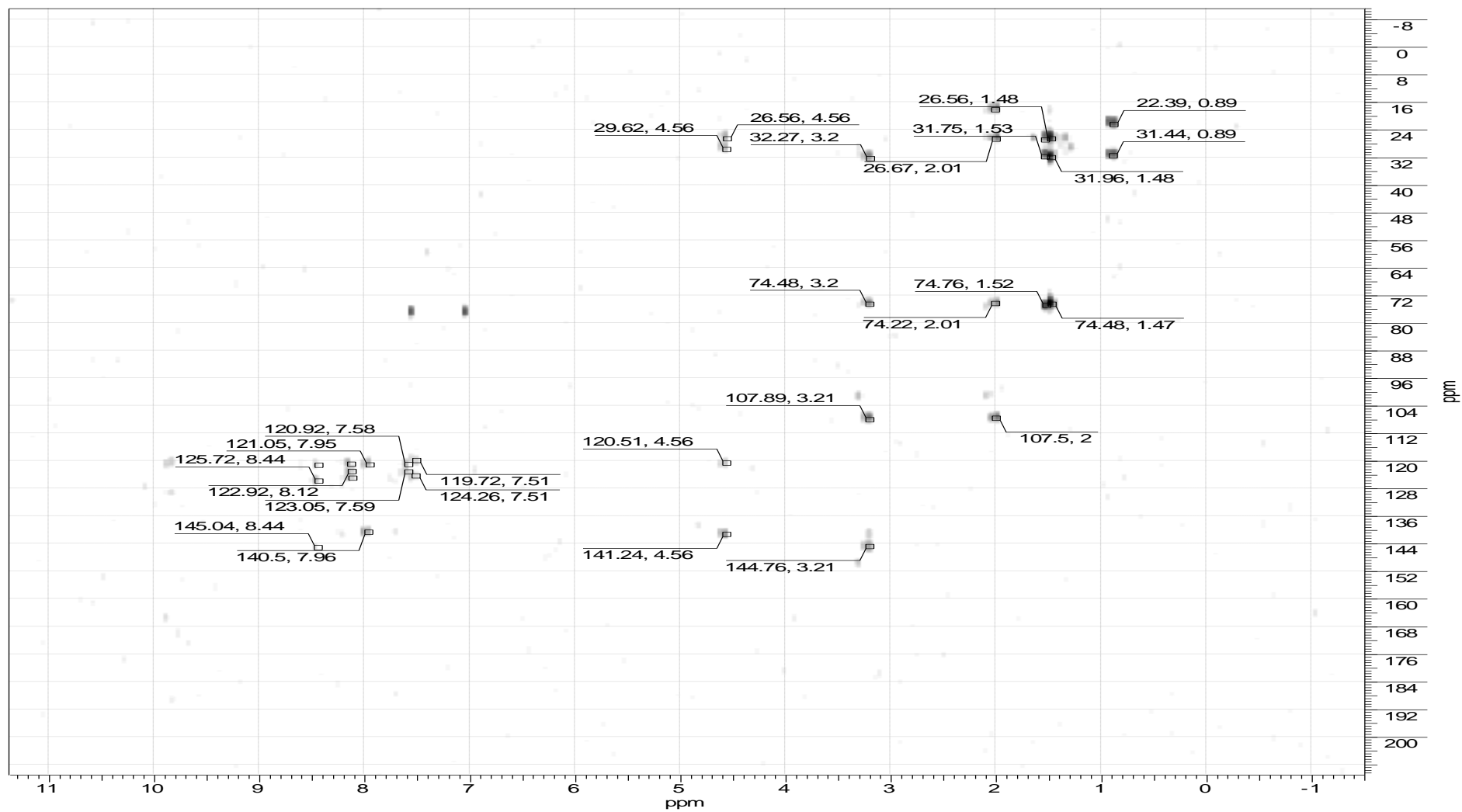
Espectro 66. RMN- ^{13}C (100 MHz, CDCl_3) do composto 41b.



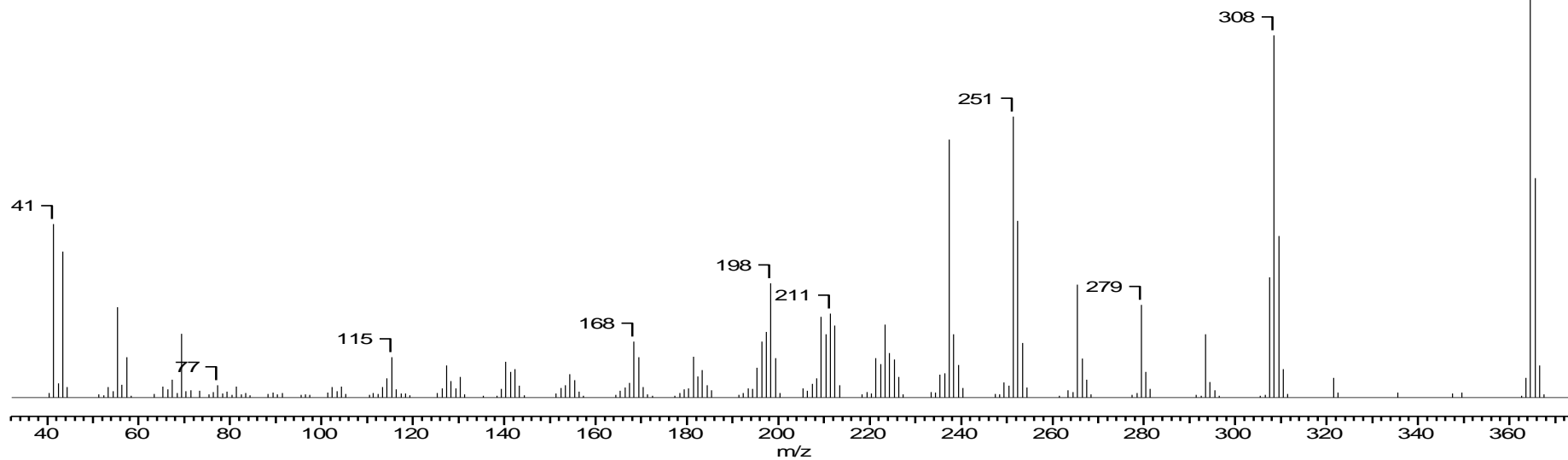
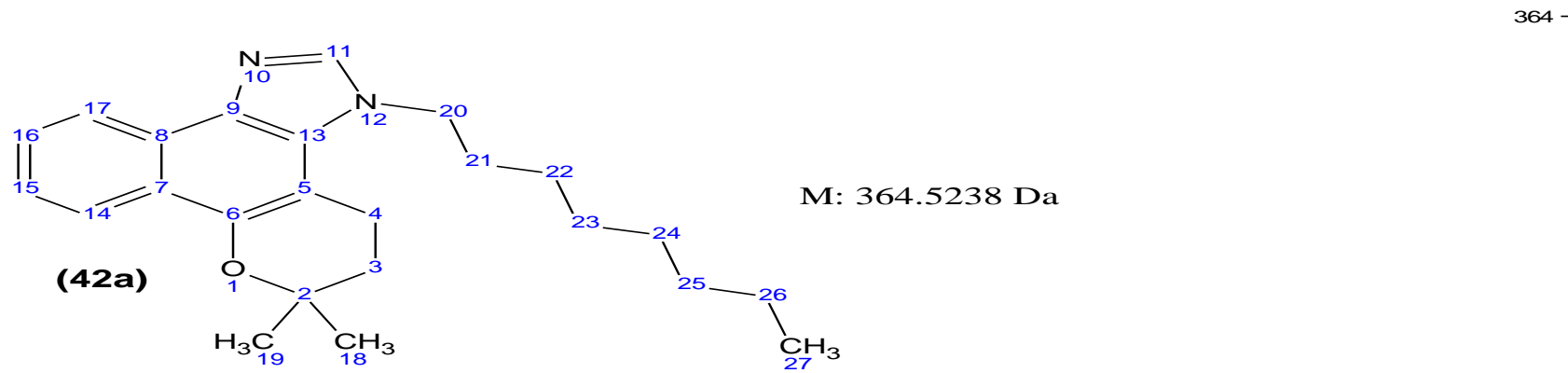
Espectro 67. ^1H -COSY (400 MHz, CDCl_3) do composto 41b.



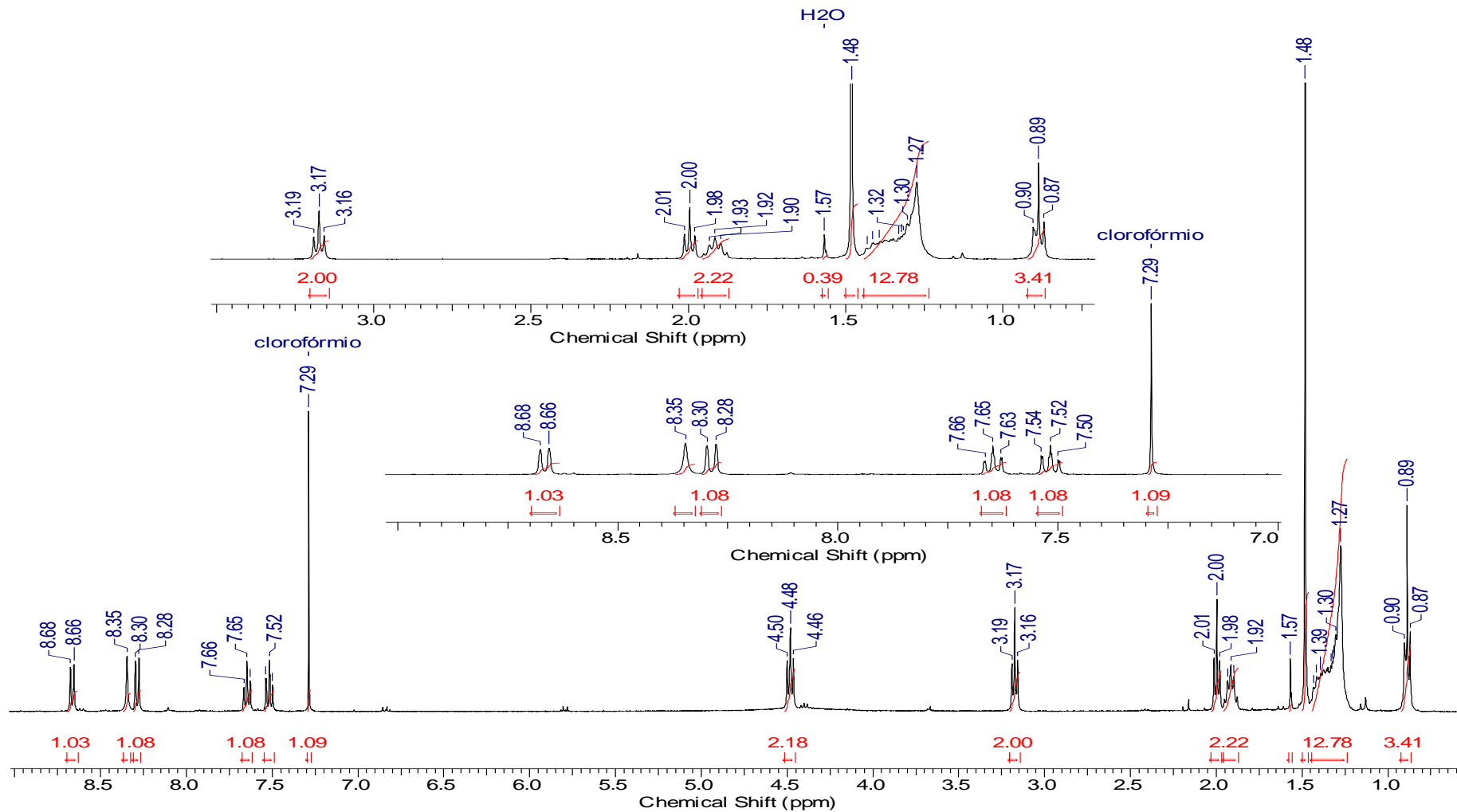
Espectro 68. HSQC (400 MHz, CDCl₃) do composto 41b.



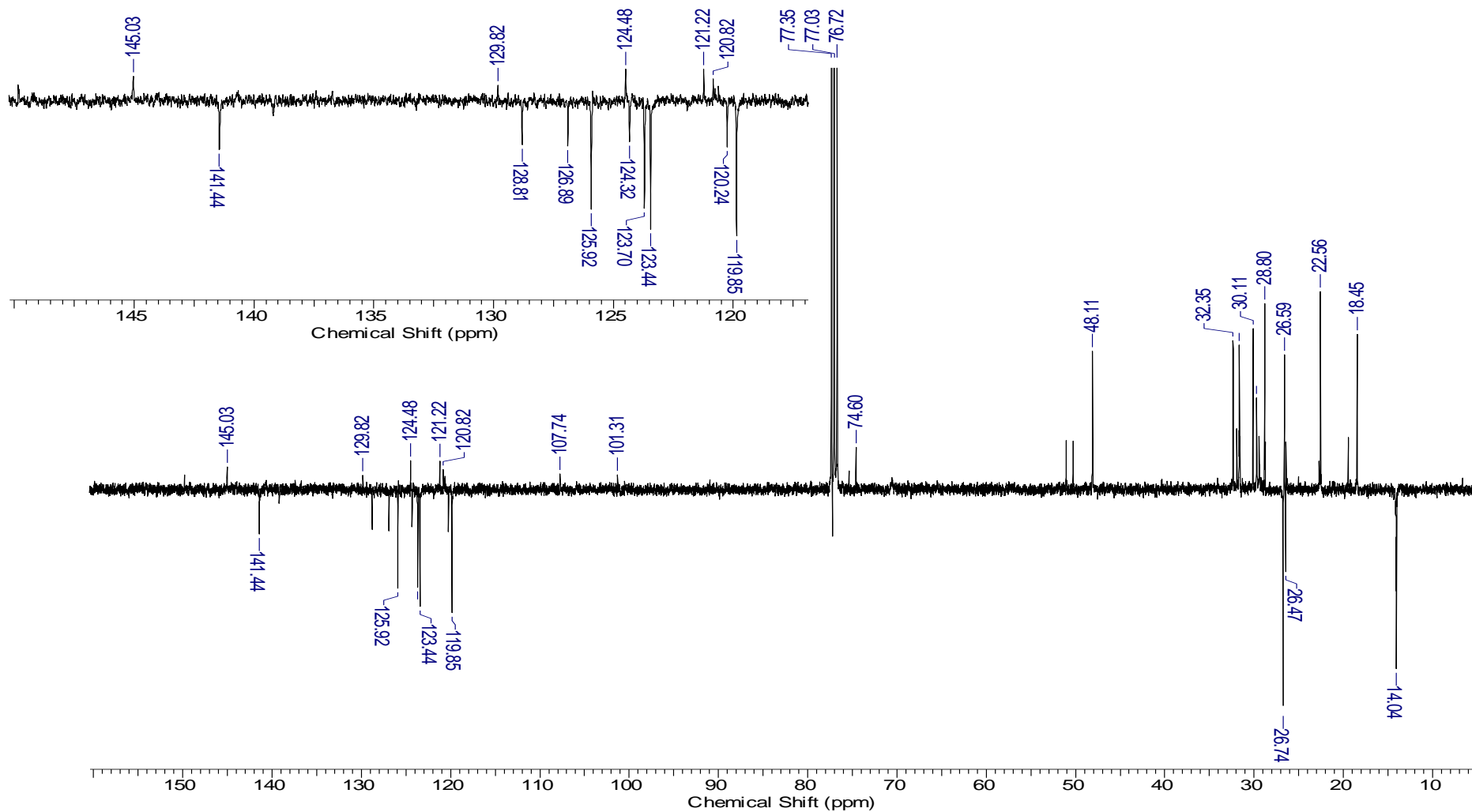
Espectro 69. HMBC (400 MHz, CDCl_3) do composto 41b.



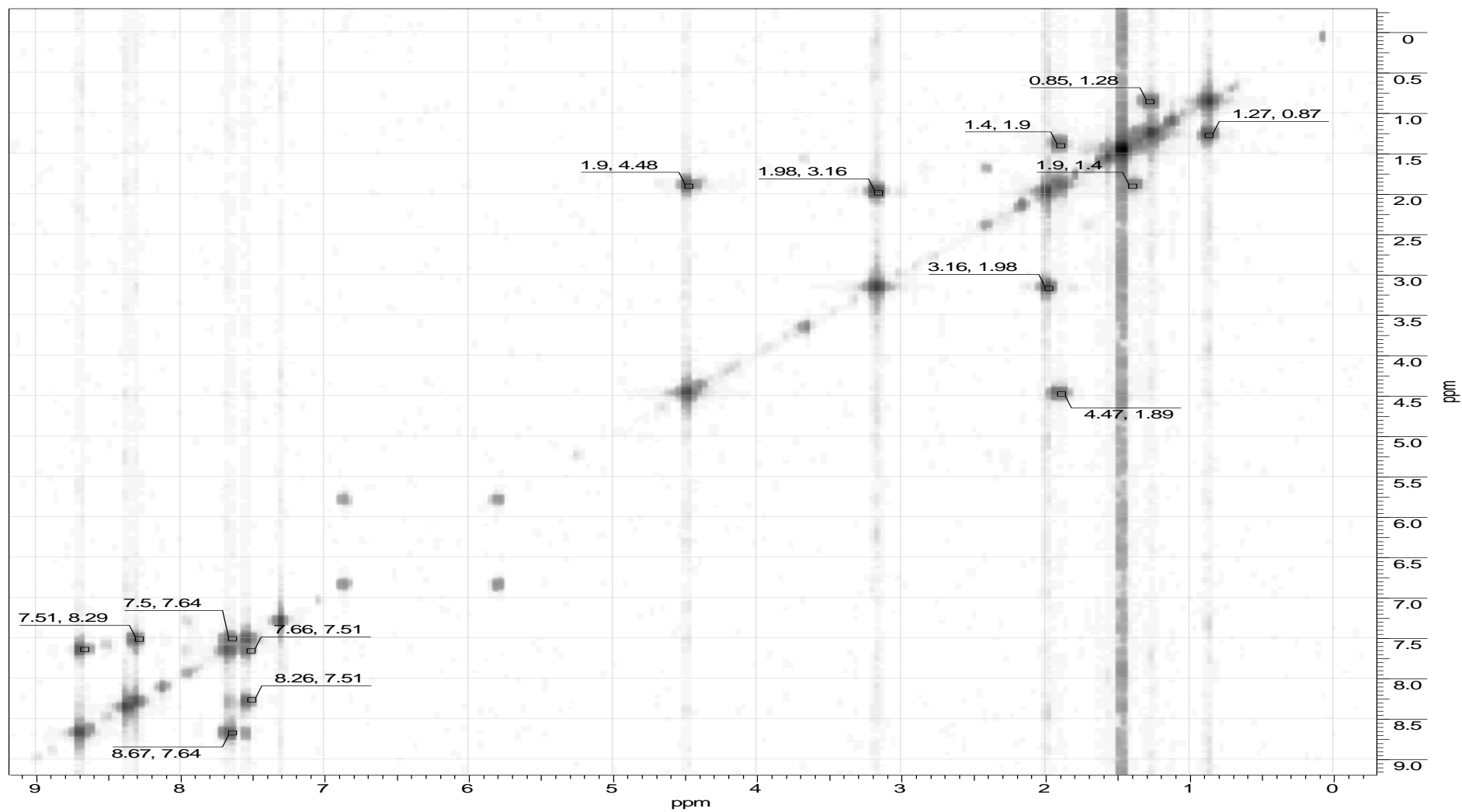
Espectro 70. EM-IE do composto 42a.



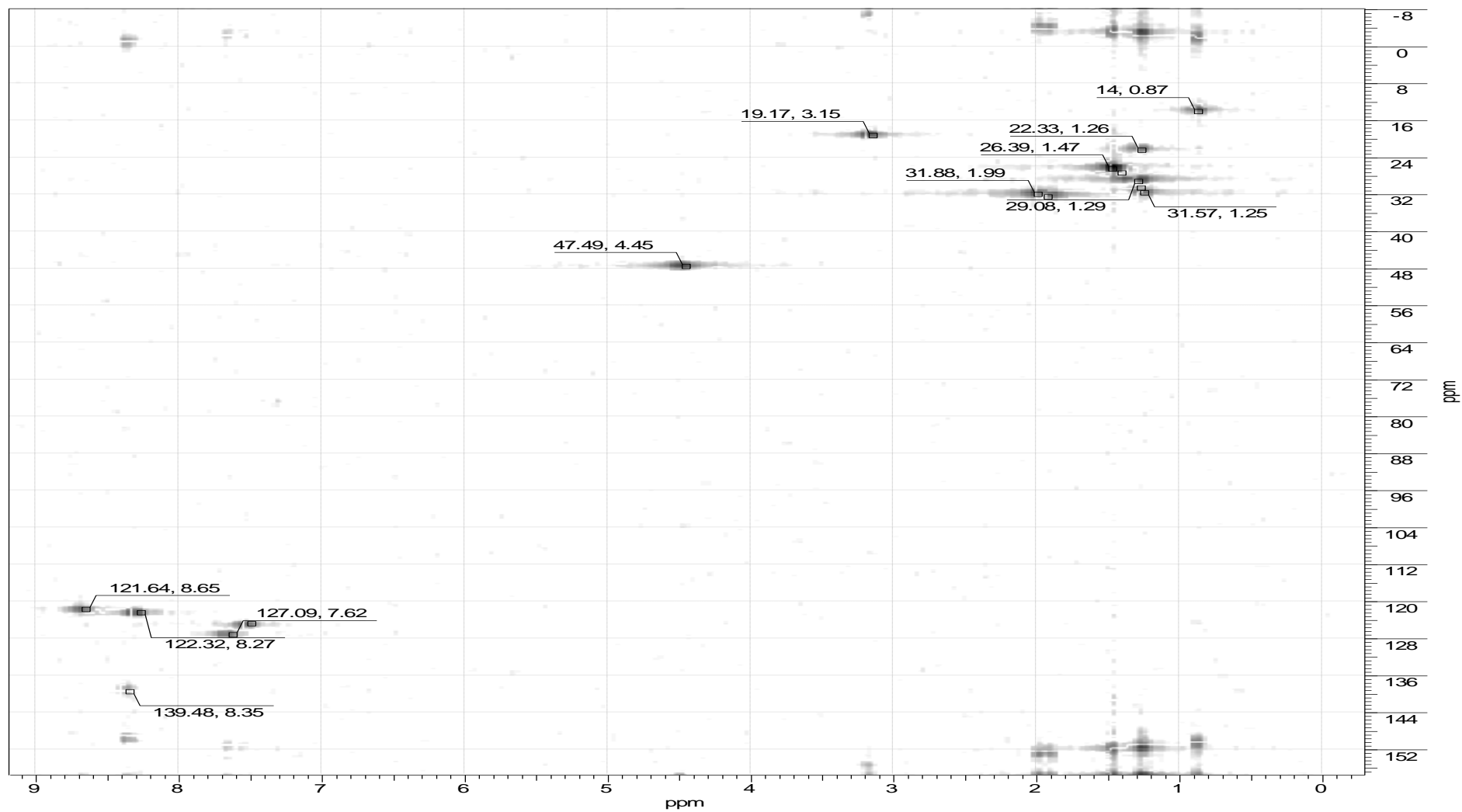
Espectro 71. RMN-¹H (400 MHz, CDCl₃) do composto 42a.



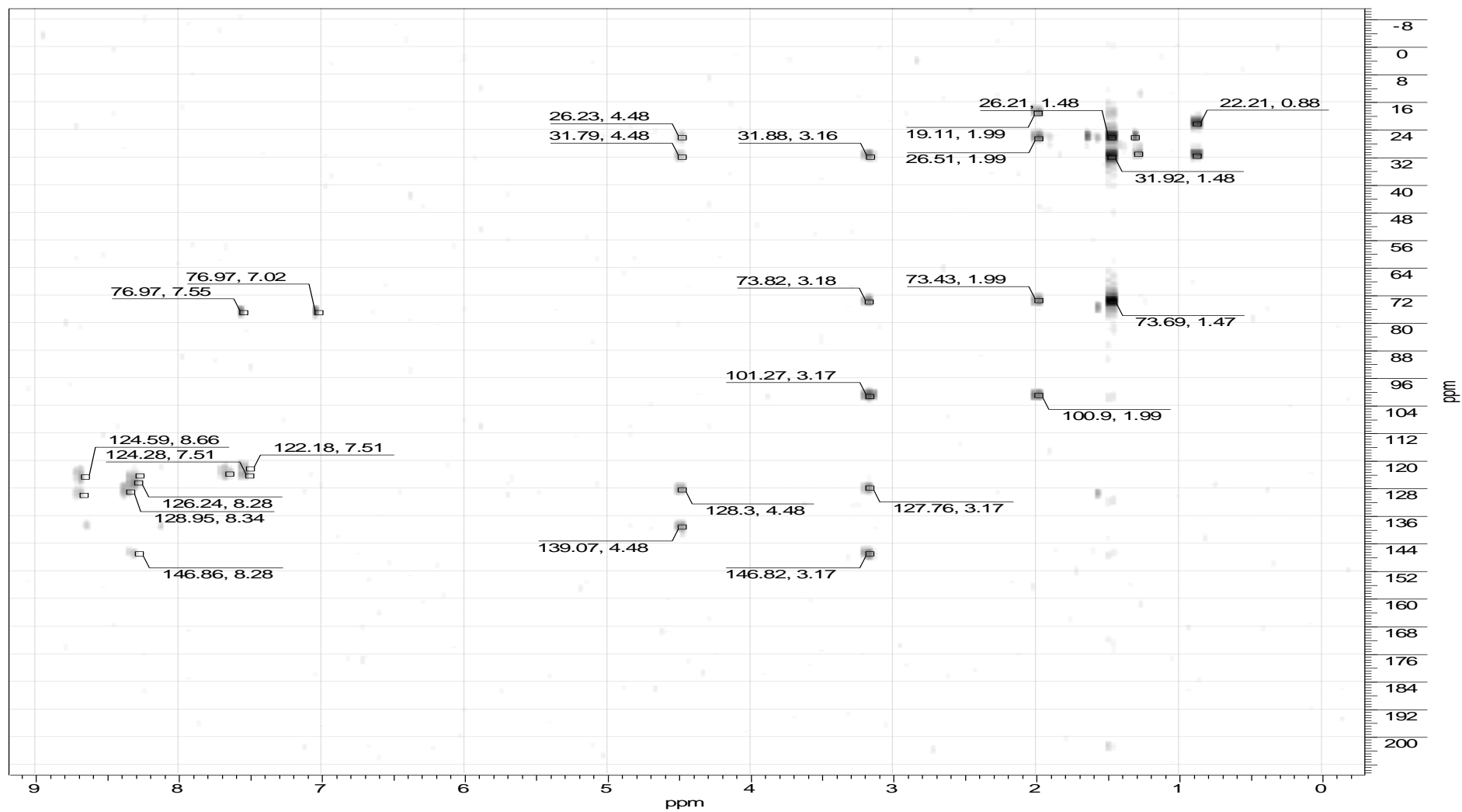
Espectro 72. RMN-¹³C (100 MHz, CDCl₃) do composto 42a.



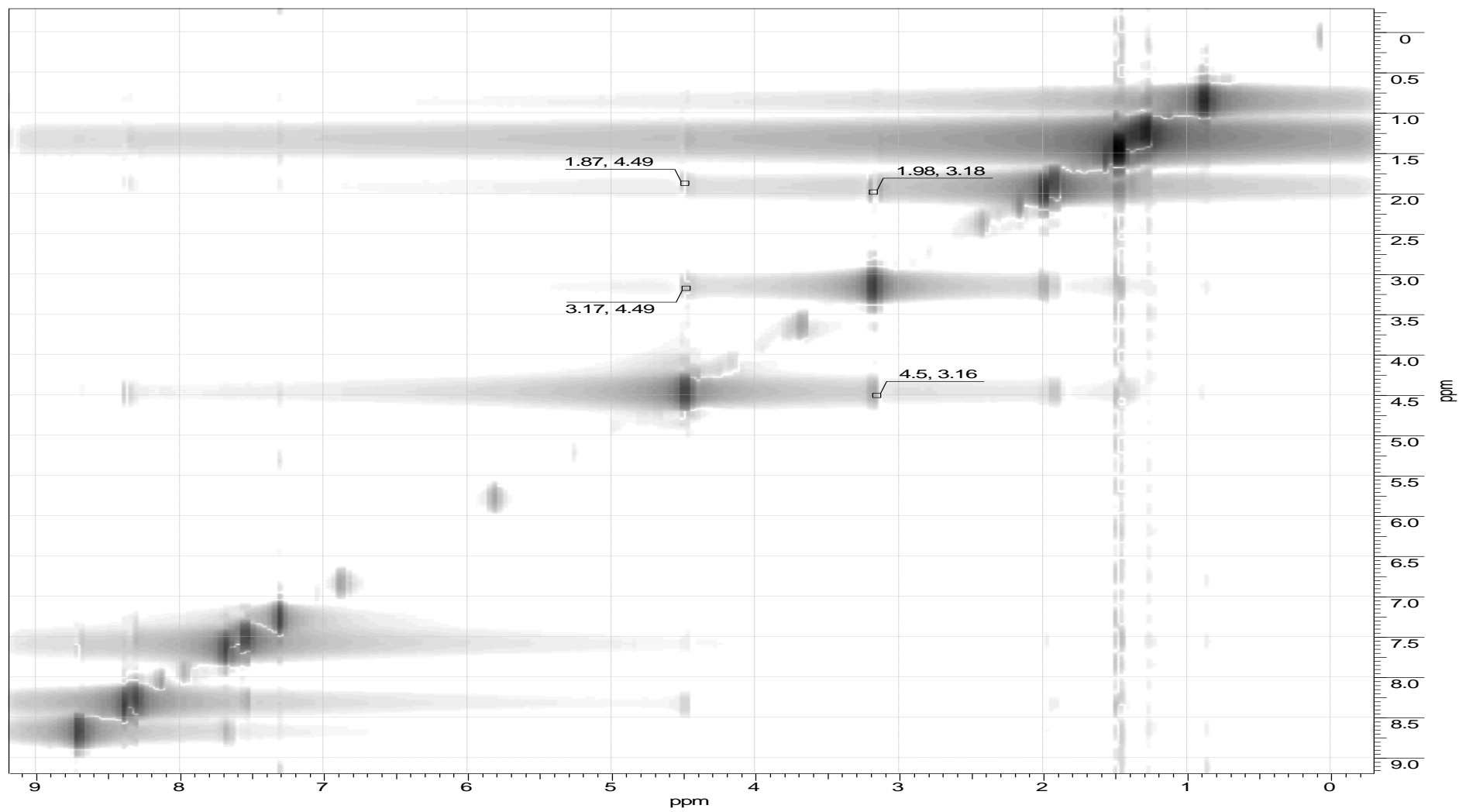
Espectro 73. ^1H -COSY (400 MHz, CDCl_3) do composto 42a.



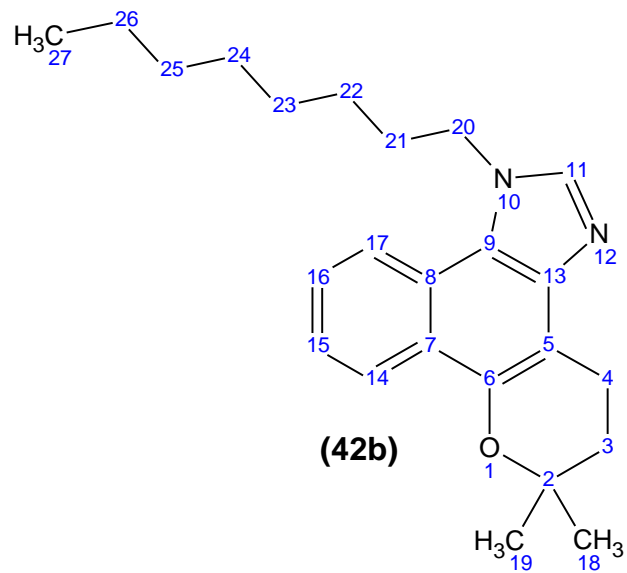
Espectro 74. HSQC (400 MHz, CDCl₃) do composto 42a.



Espectro 75. HMBC (400 MHz, CDCl_3) do composto 42a.

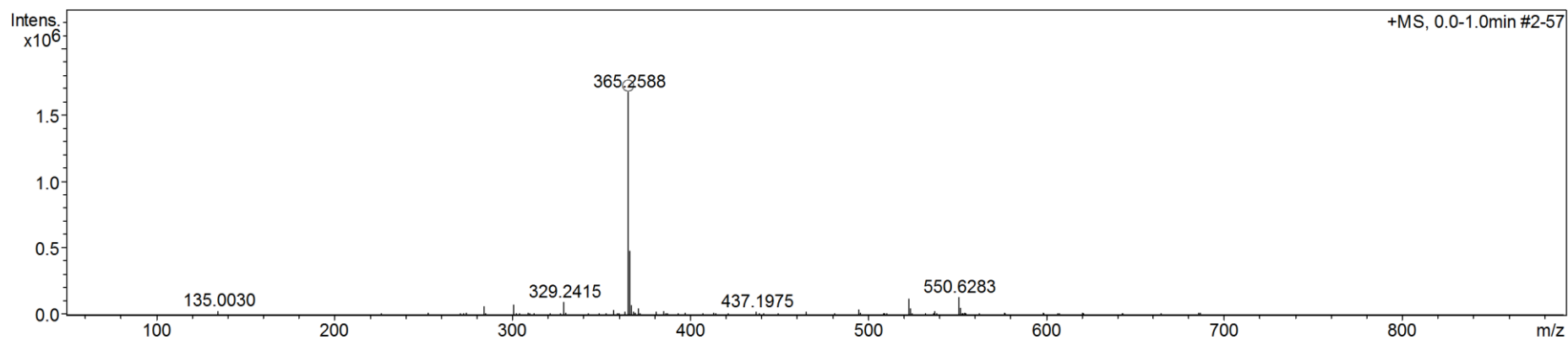


Espectro 76. NOESY (400 MHz, CDCl₃) do composto 42a.

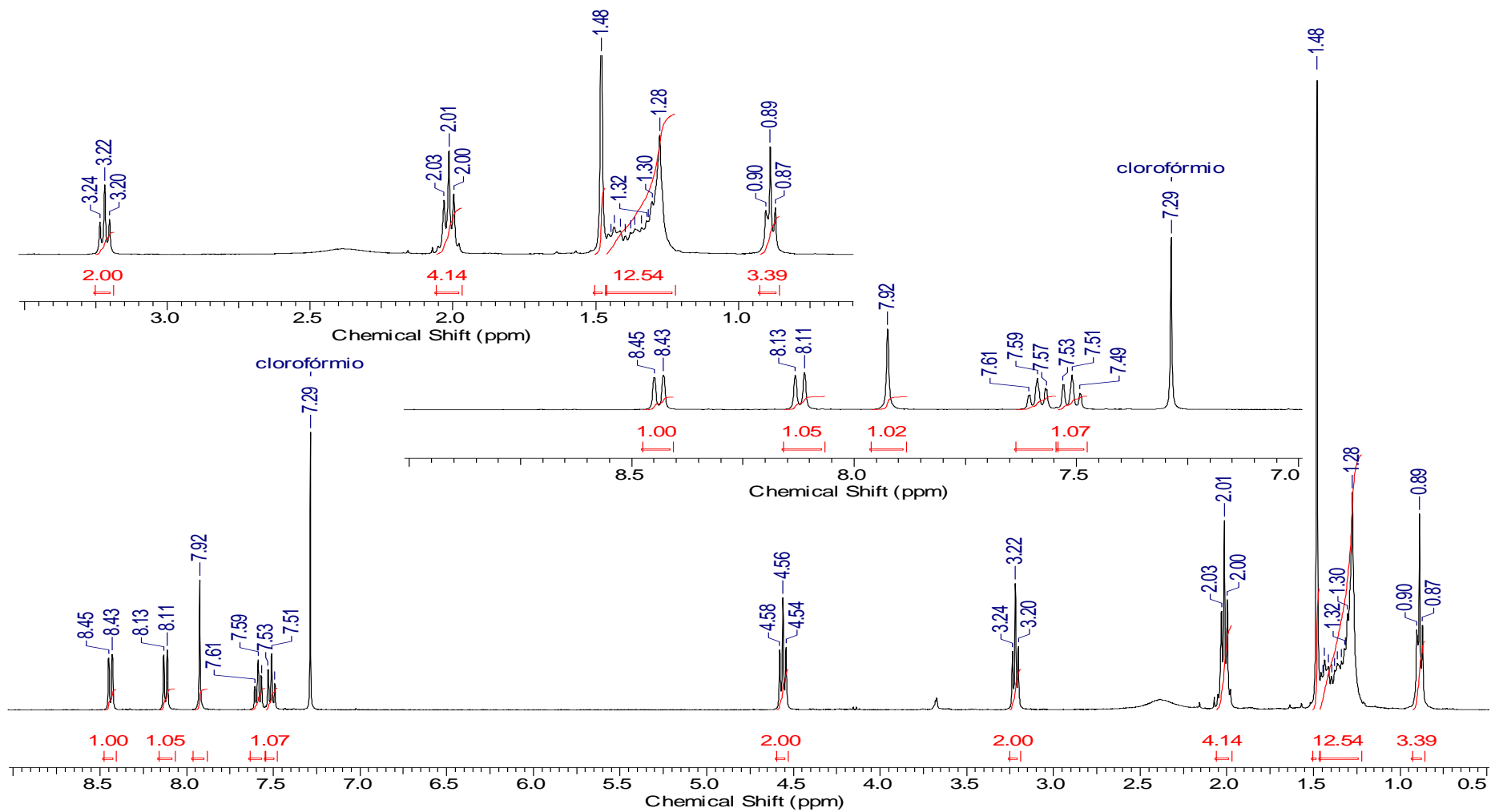


M: 364.5238 Da

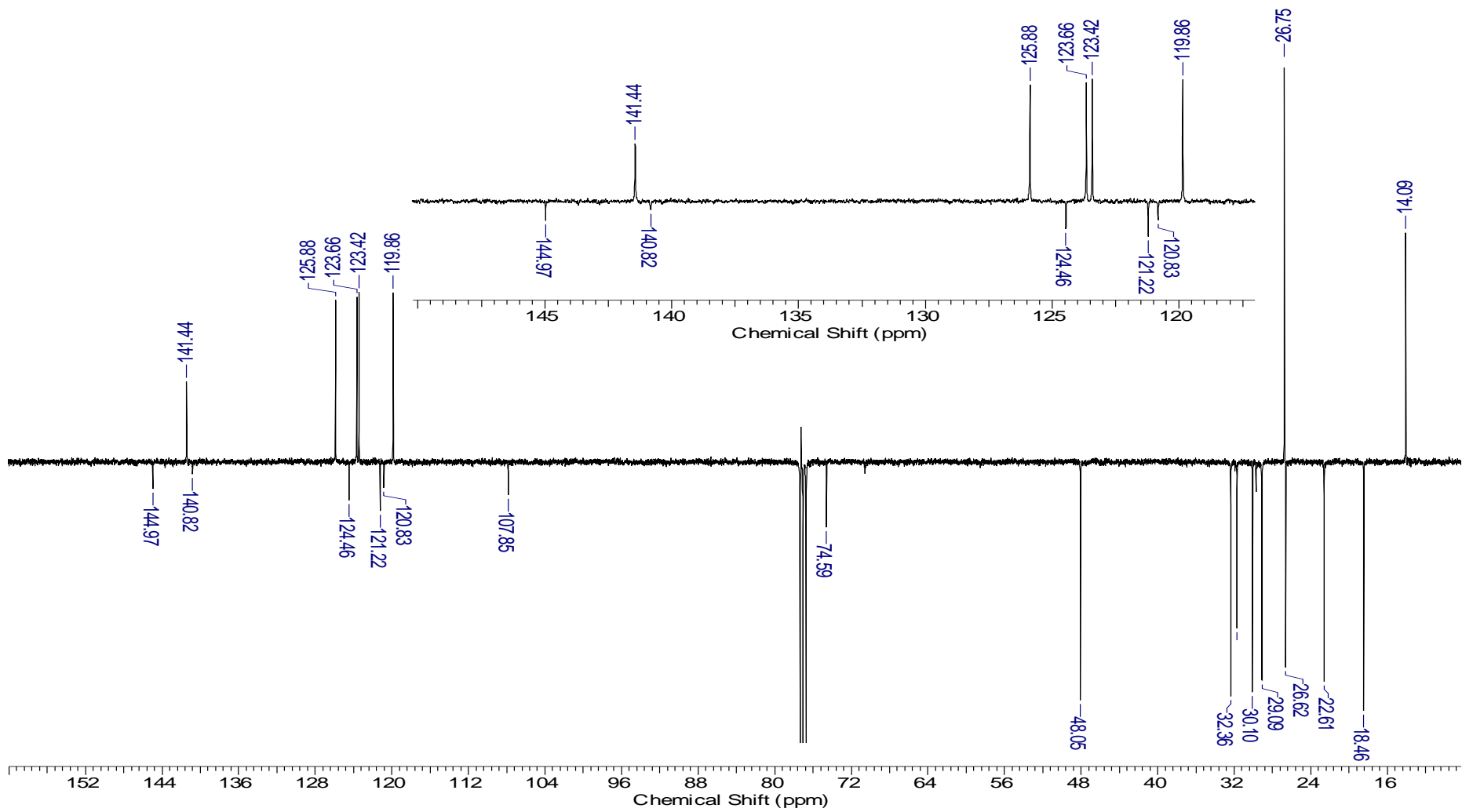
$[M+H]^+ = 365.2587$ Da; err[ppm] = -0,3



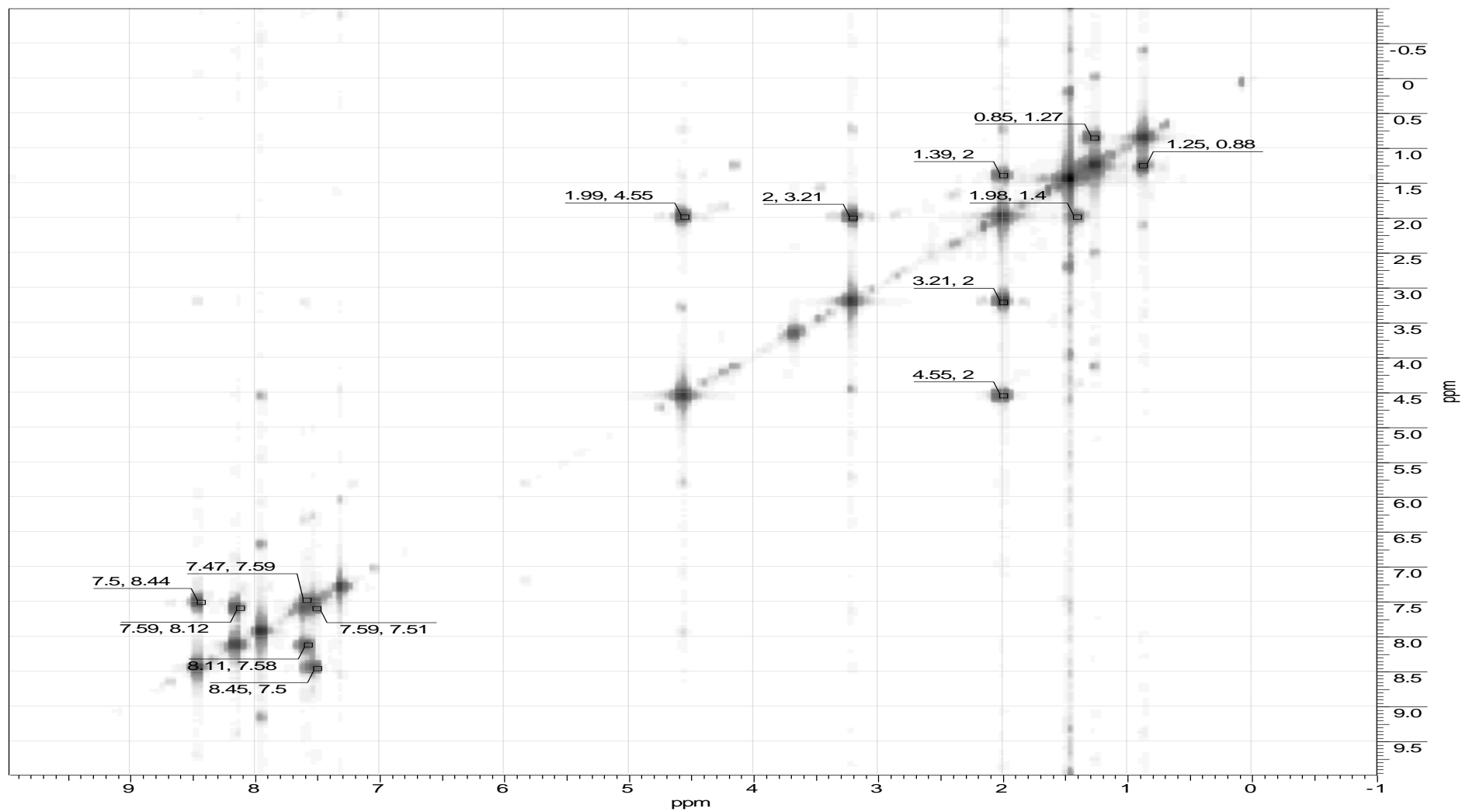
Espectro 77. EM-IES do composto 42b.



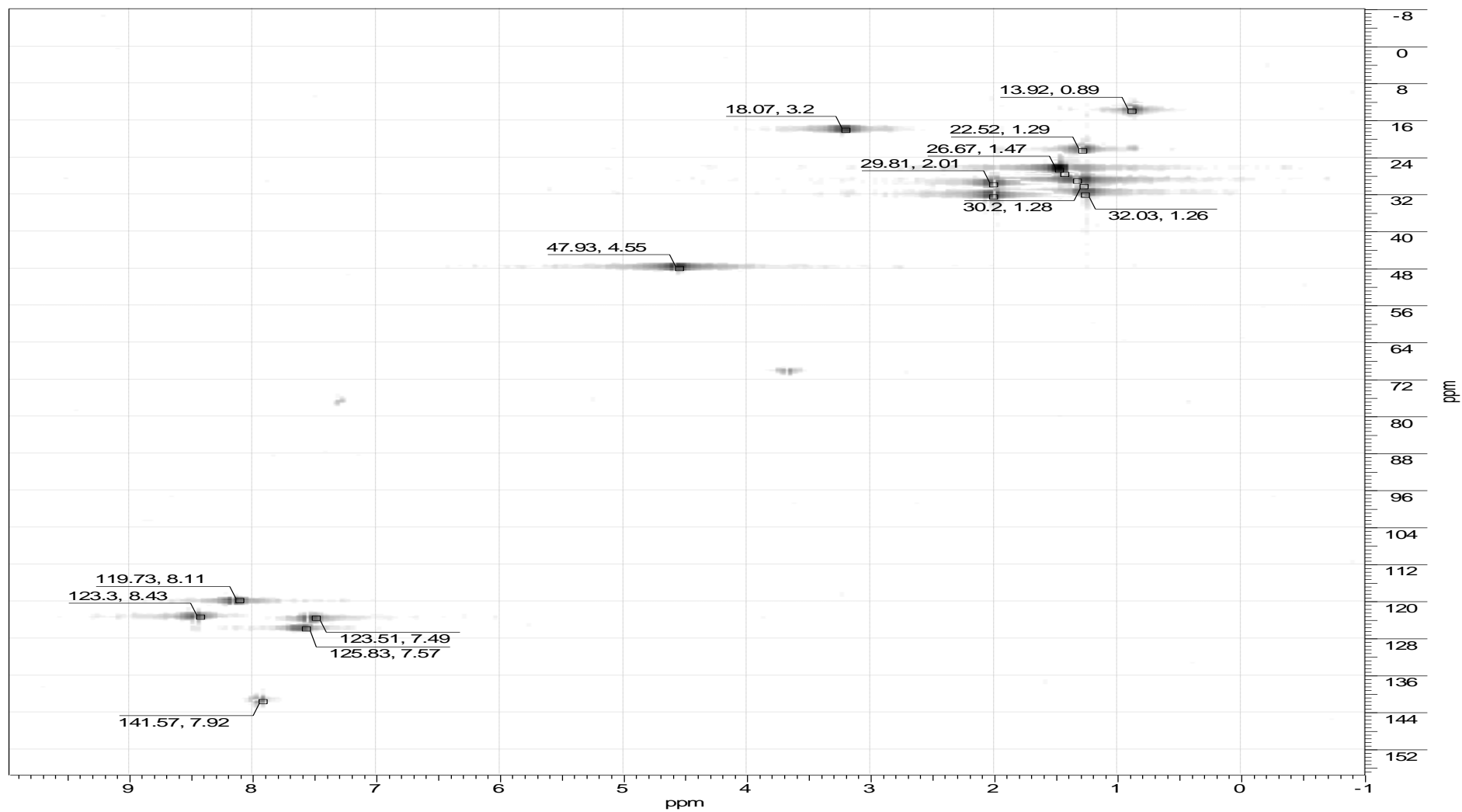
Espectro 78. RMN- ^1H (400 MHz, CDCl_3) do composto 42b.



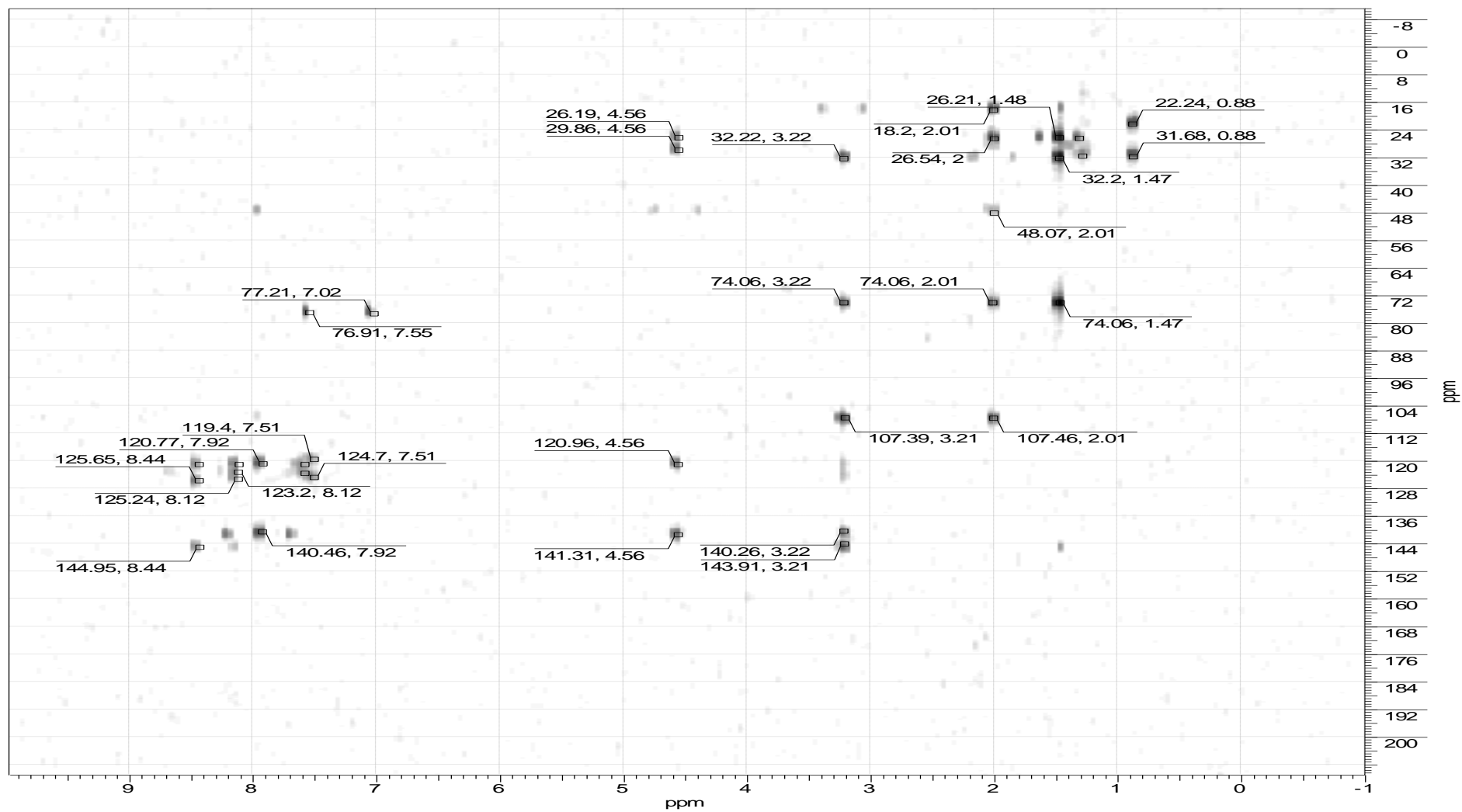
Espectro 79. RMN- ^{13}C (100 MHz, CDCl_3) do composto 42b.



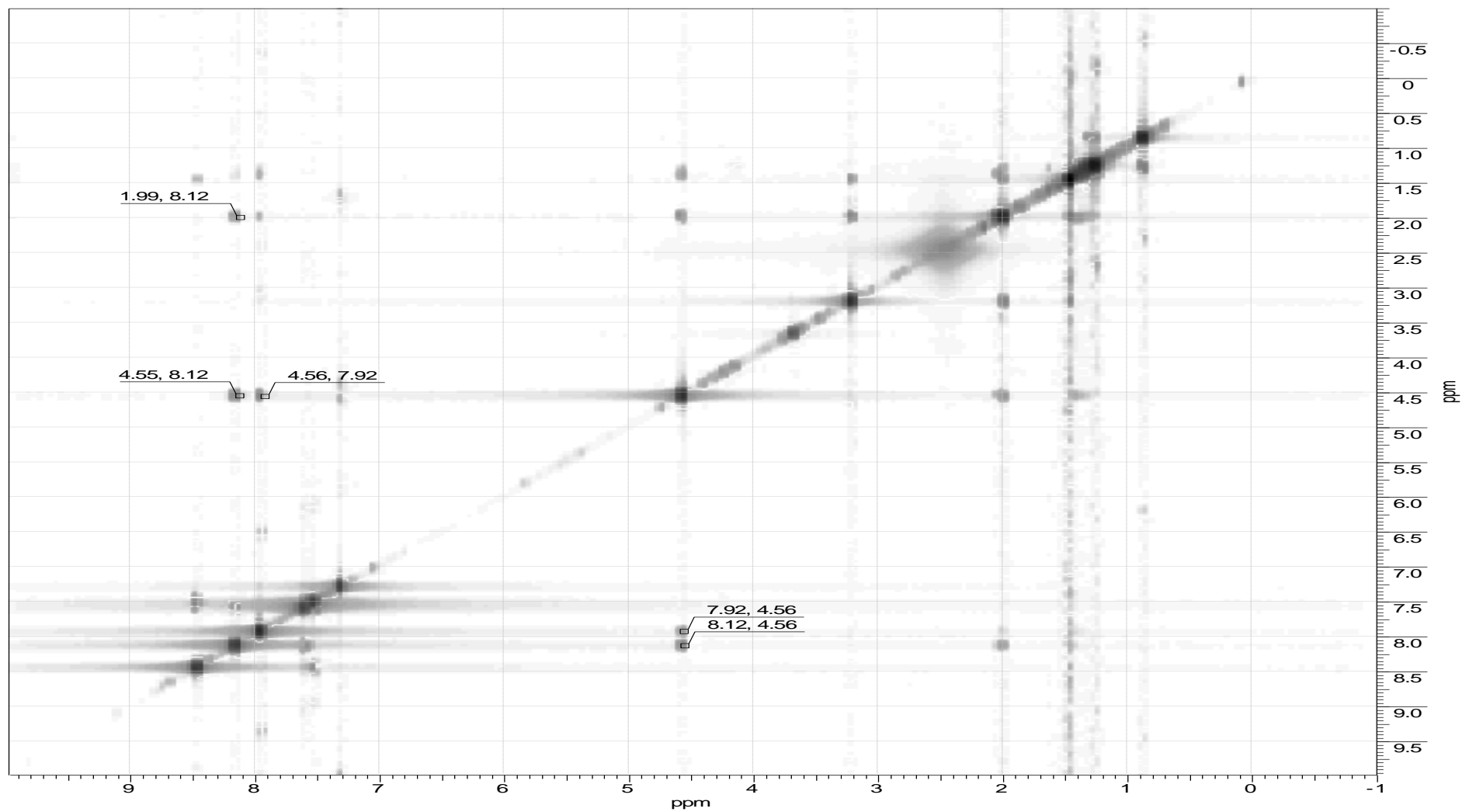
Espectro 80. ^1H -COSY (400 MHz, CDCl_3) do composto 42a.



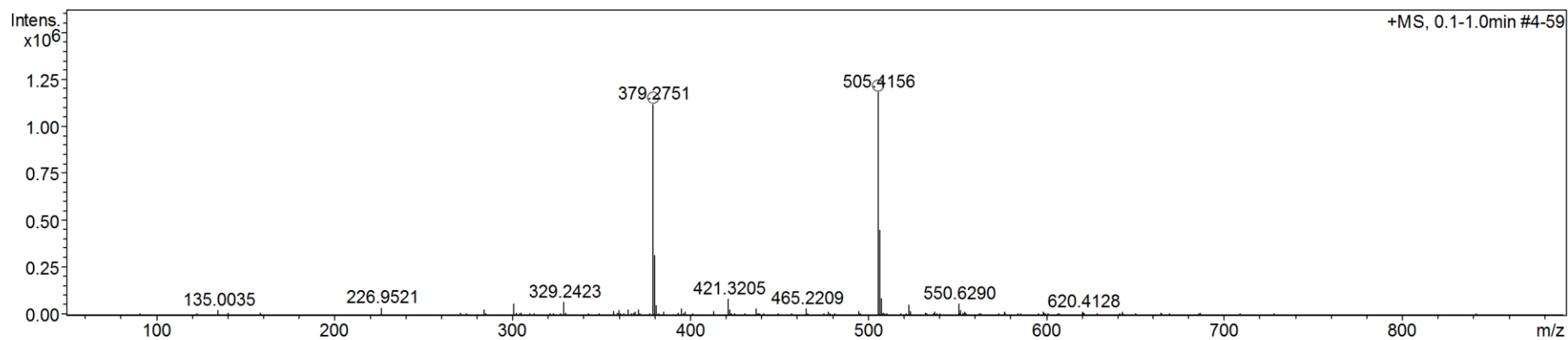
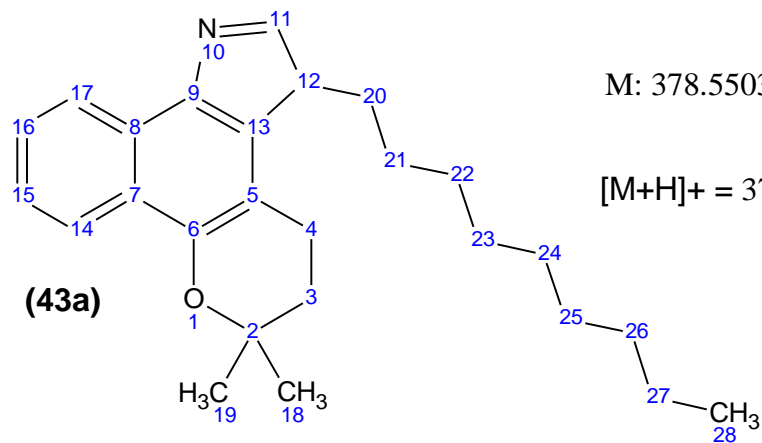
Espectro 81. HSQC (400 MHz, CDCl₃) do composto 42a.



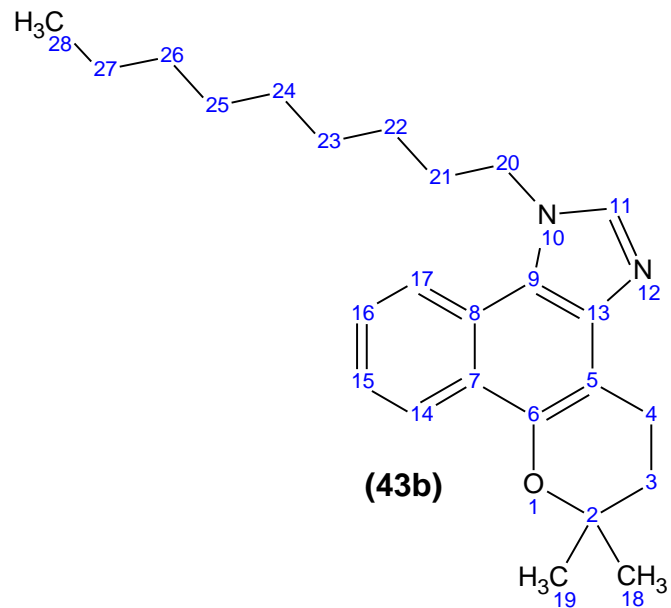
Espectro 82. HMBC (400 MHz, CDCl₃) do composto 42a.



Espectro 83. NOESY (400 MHz, CDCl₃) do composto 42a.

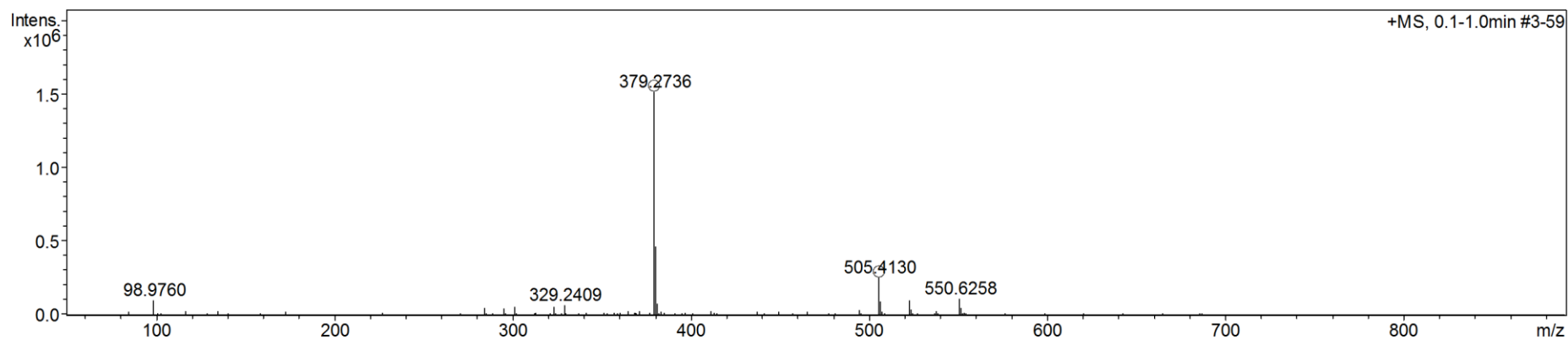


Espectro 84. EM-IES do composto 43a.

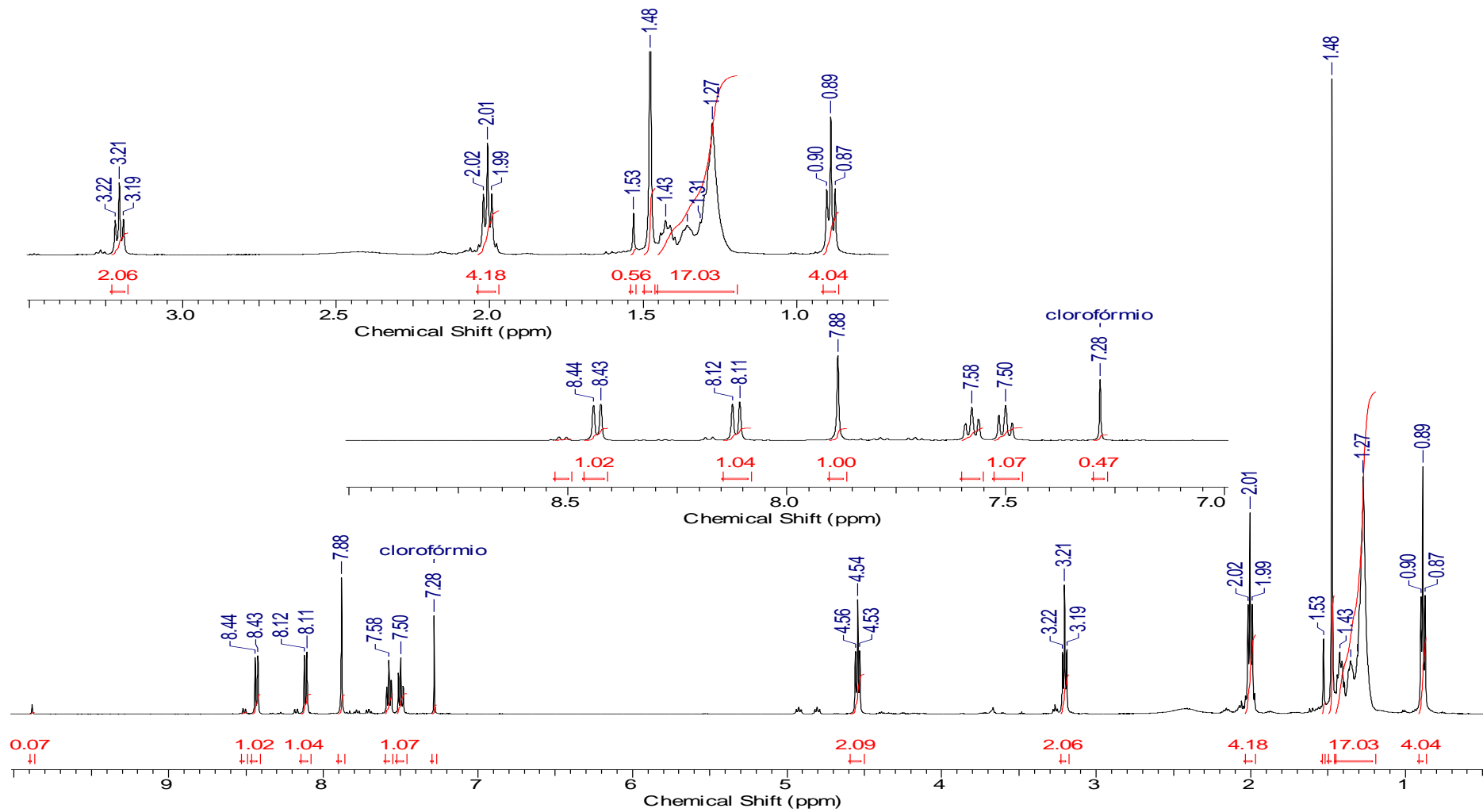


M: 378.5503 Da

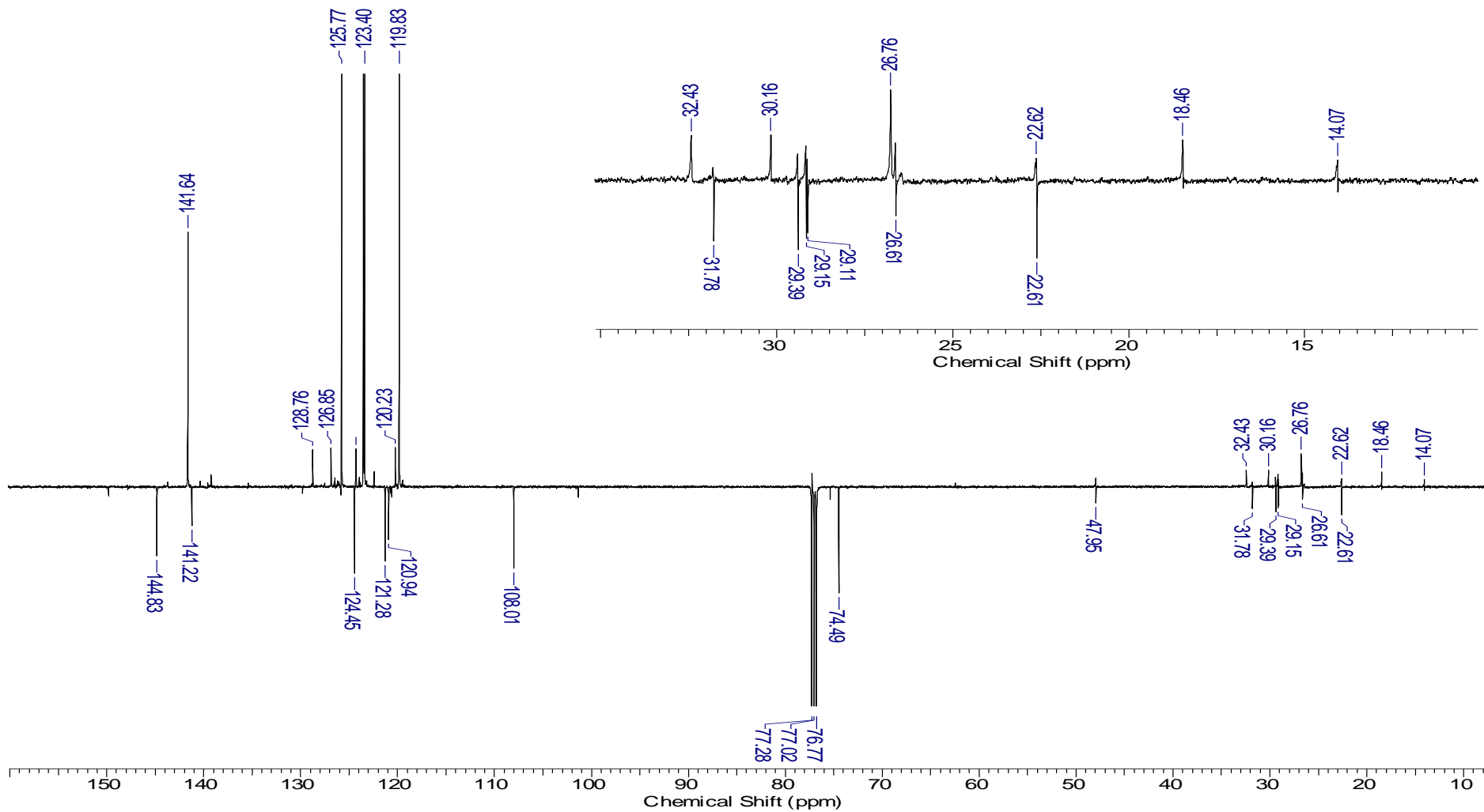
[M+H]⁺ = 379.2744 Da; err[ppm] = 2,2



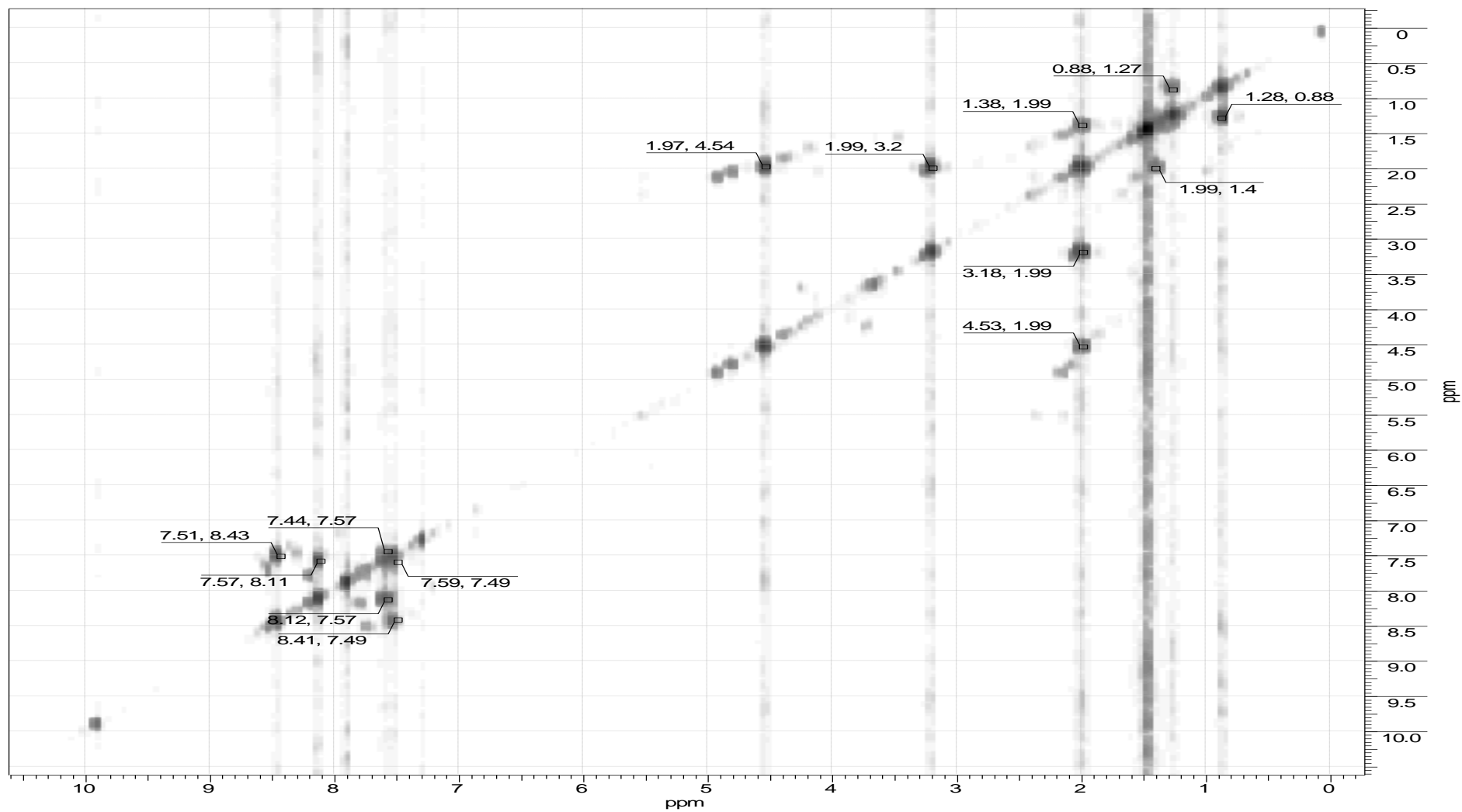
Espectro 85. EM-IES do composto 43b.



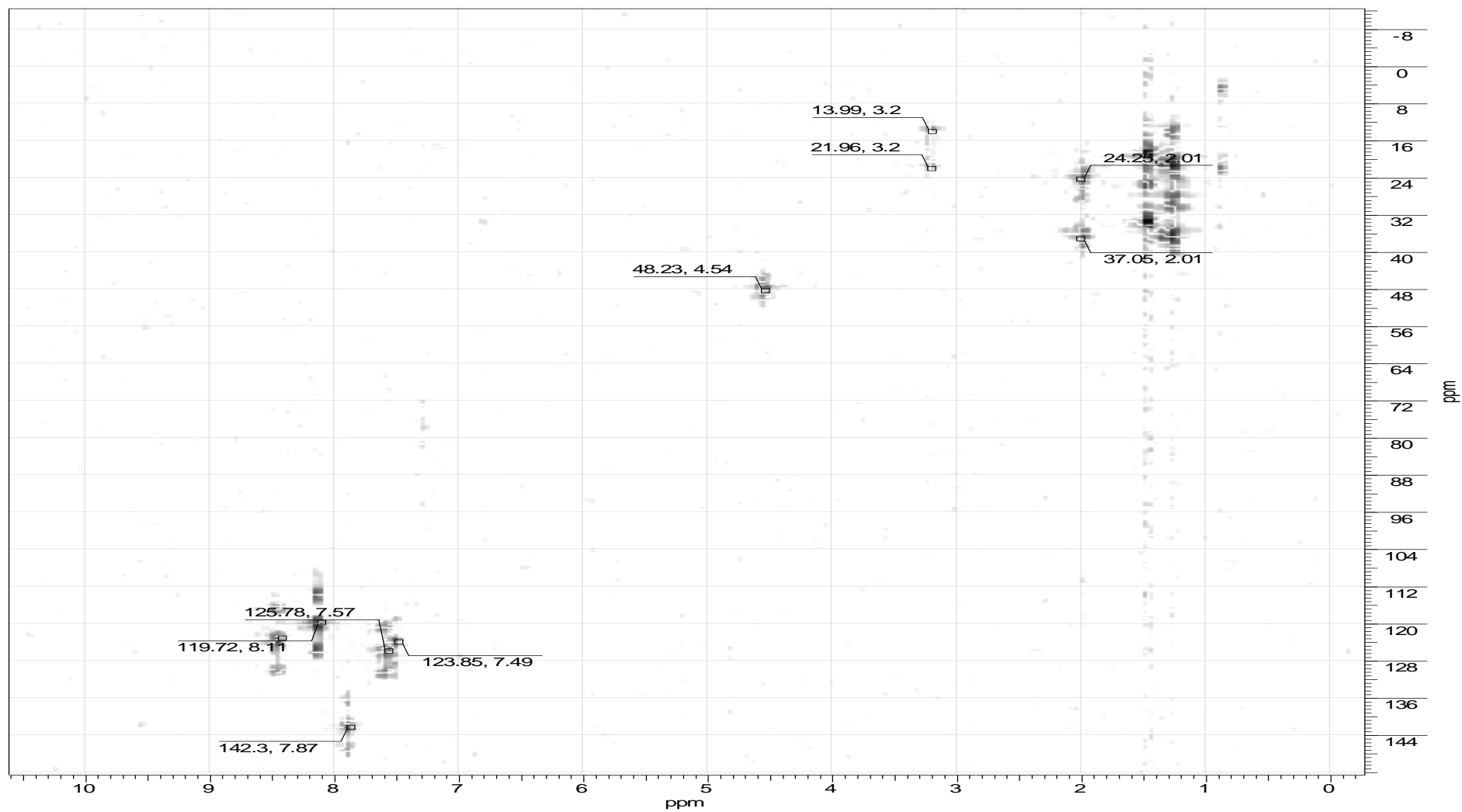
Espectro 86. RMN- ^1H (500 MHz, CDCl_3) do composto 43b.



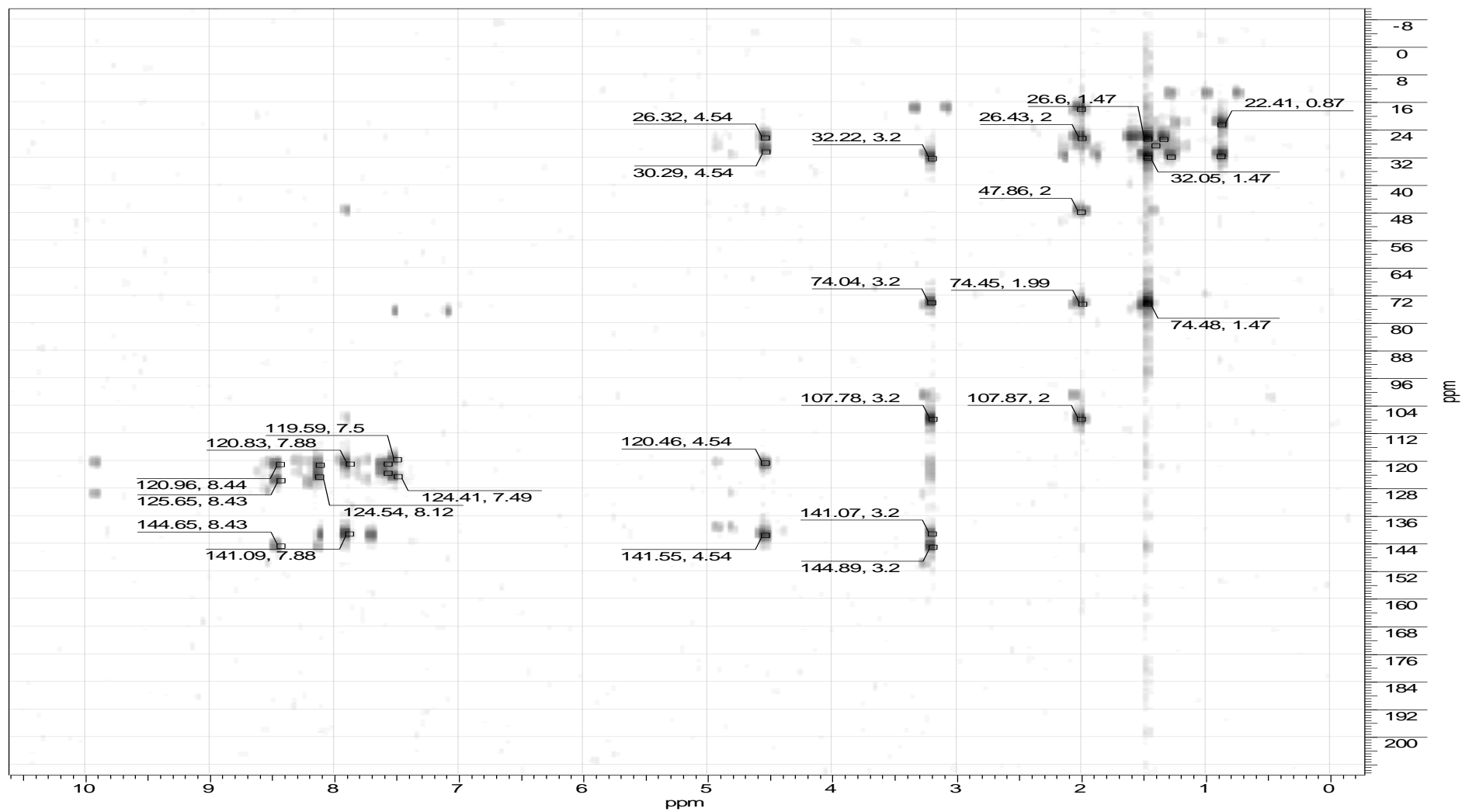
Espectro 87. RMN- ^{13}C (125 MHz, CDCl_3) do composto 43b.



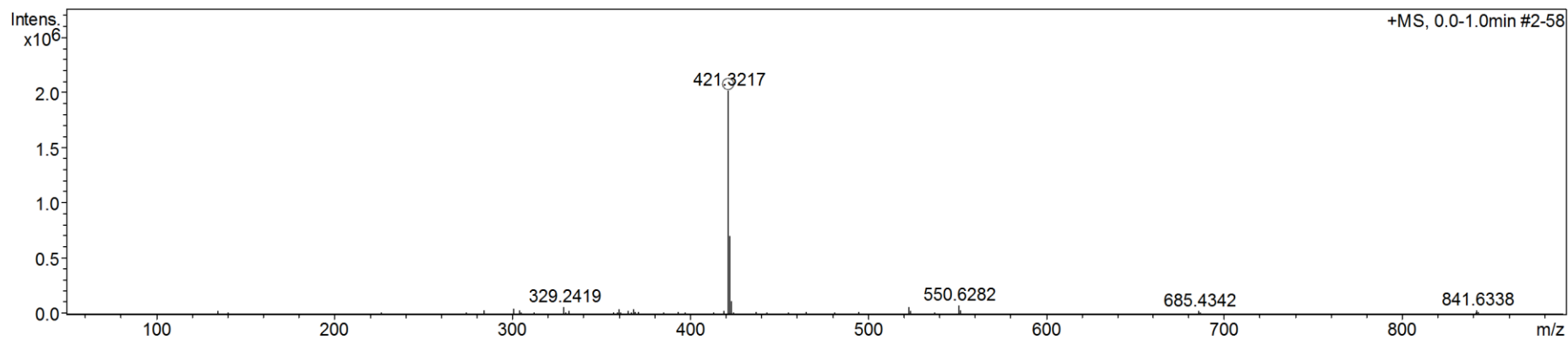
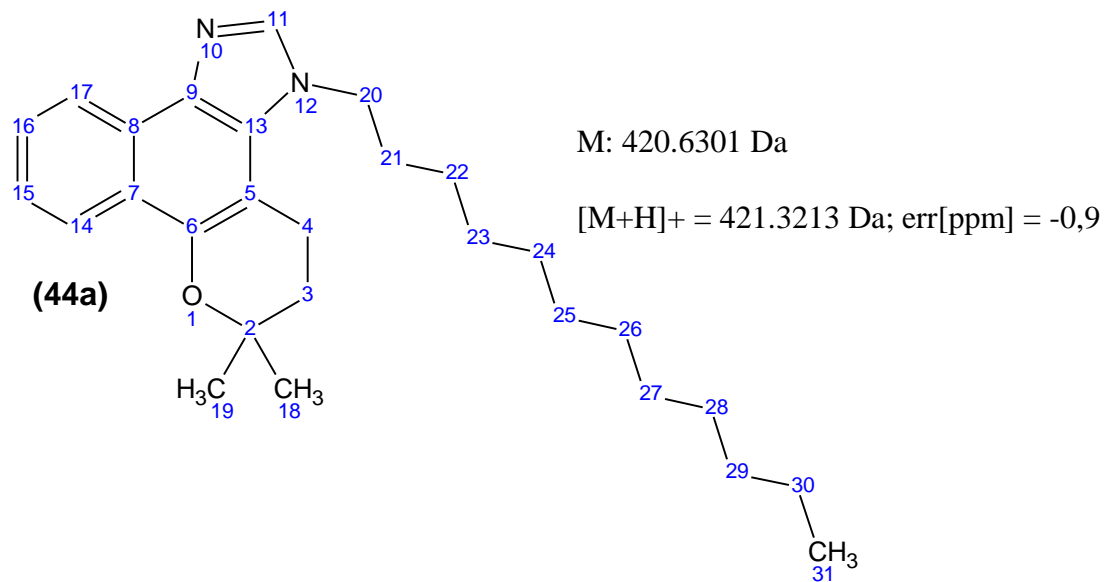
Espectro 88. ^1H -COSY (500 MHz, CDCl_3) do composto 43b.



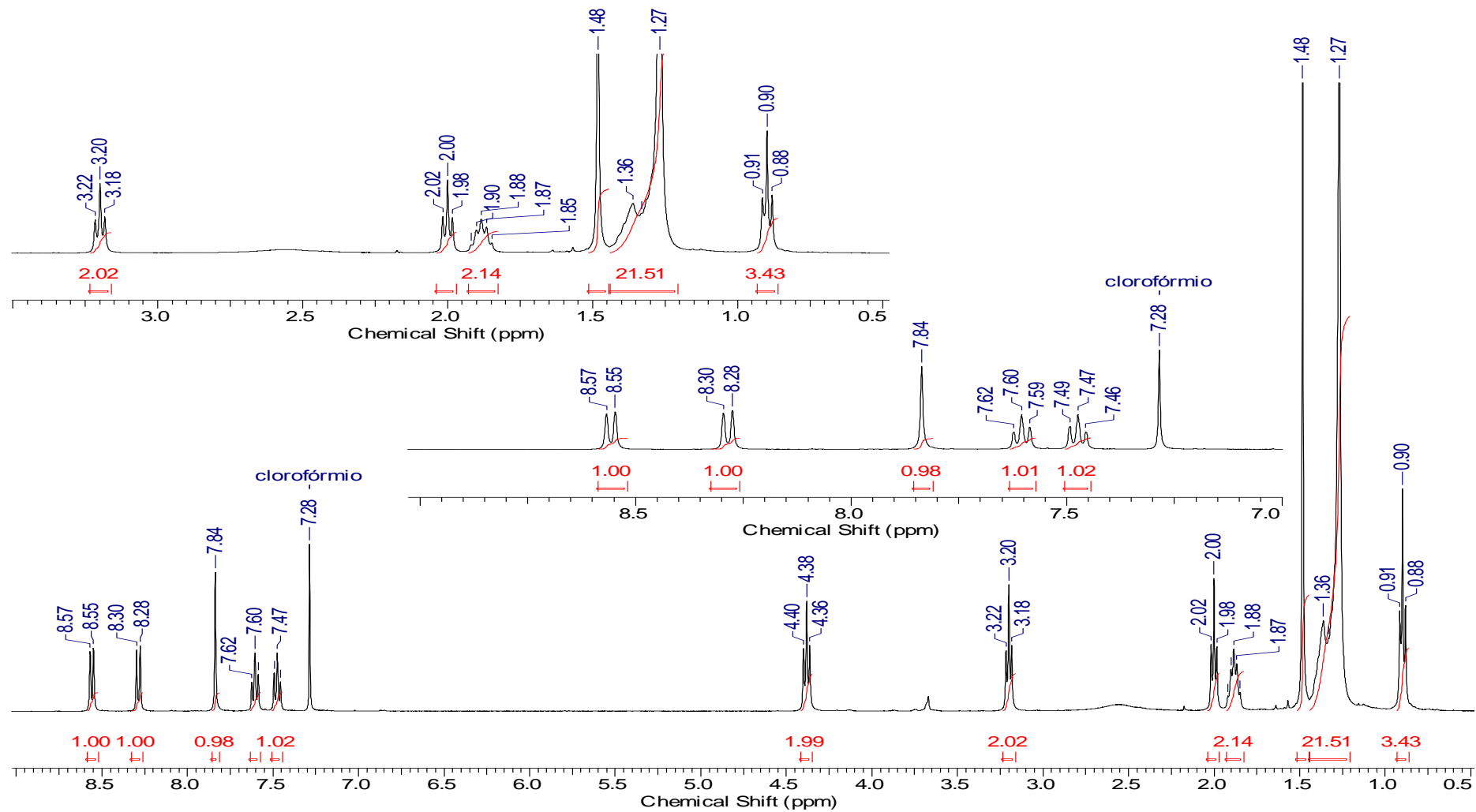
Espectro 89. HSQC (500 MHz, CDCl₃) do composto 43b.



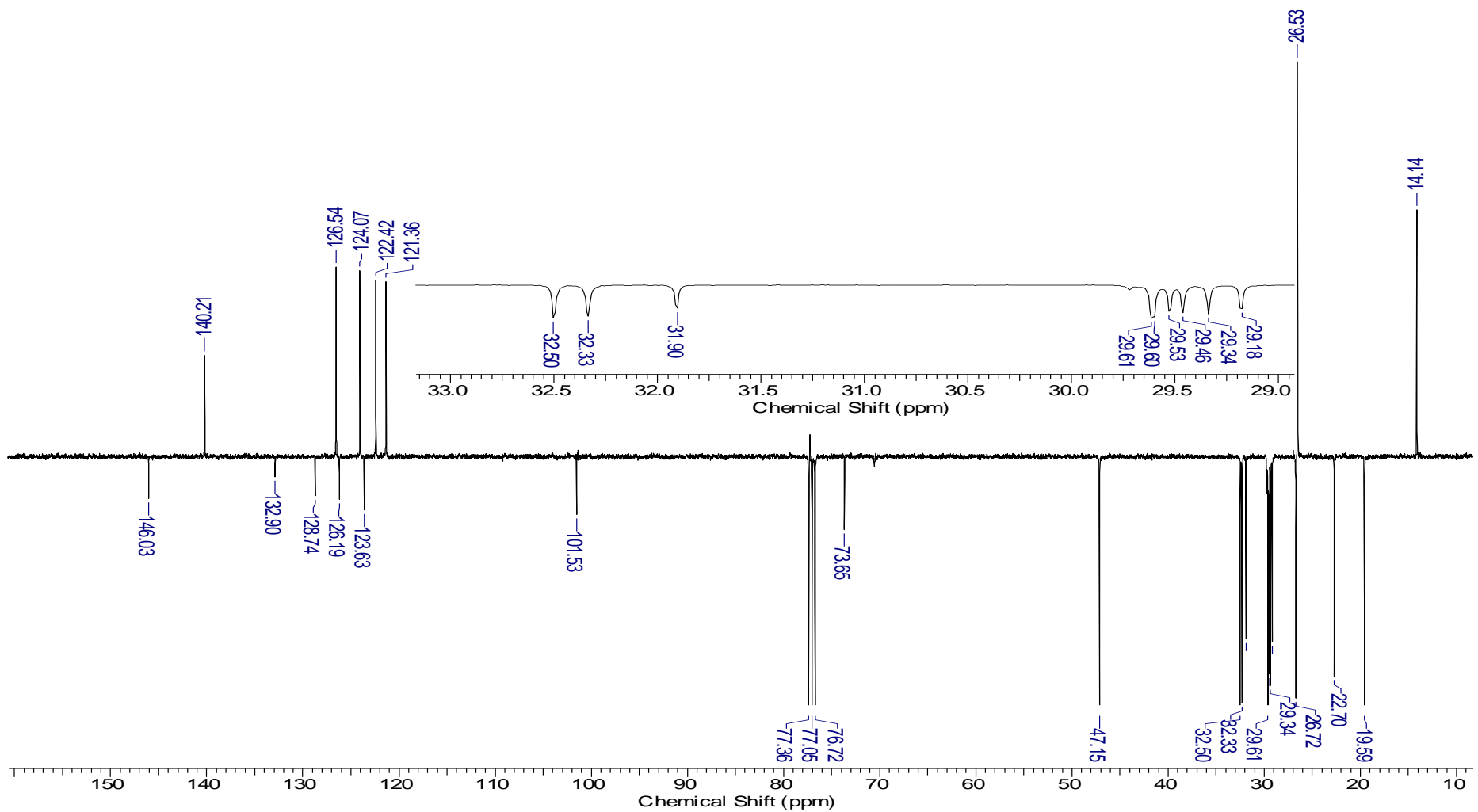
Espectro 90. HMBC (500 MHz, CDCl_3) do composto 43b.



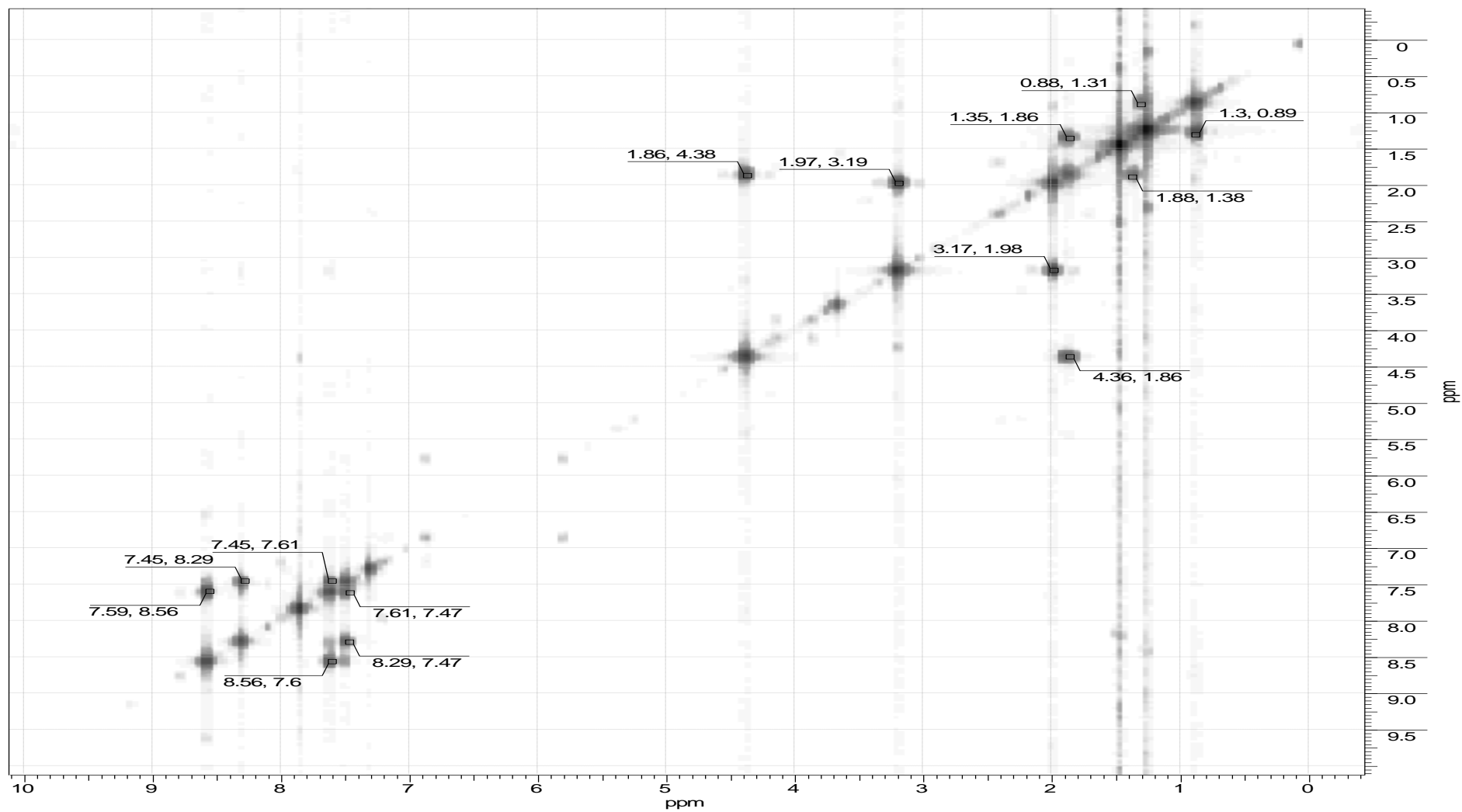
Espectro 91. EM-IES do composto 44a.



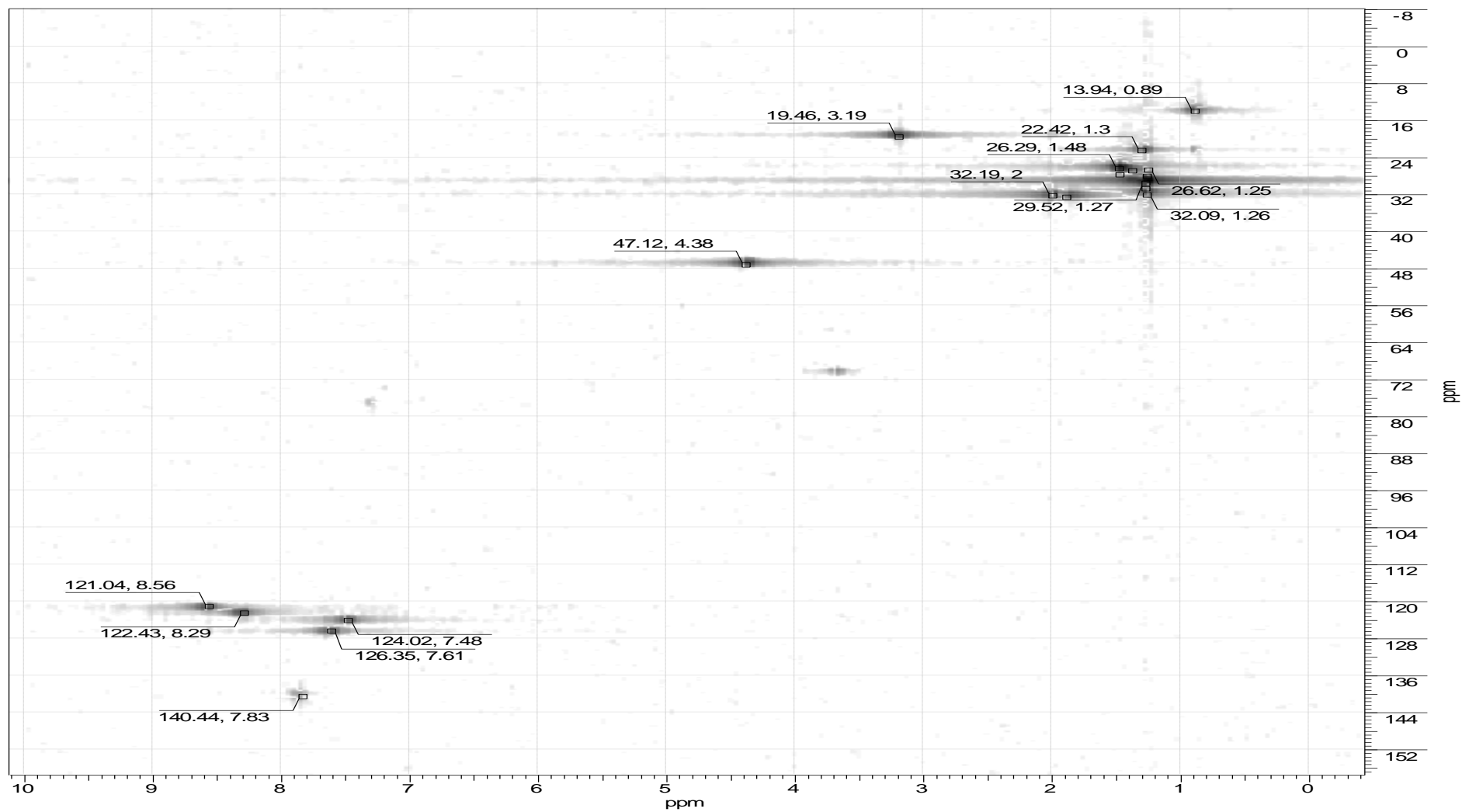
Espectro 92. RMN-¹H (400 MHz, CDCl₃) do composto 44a.



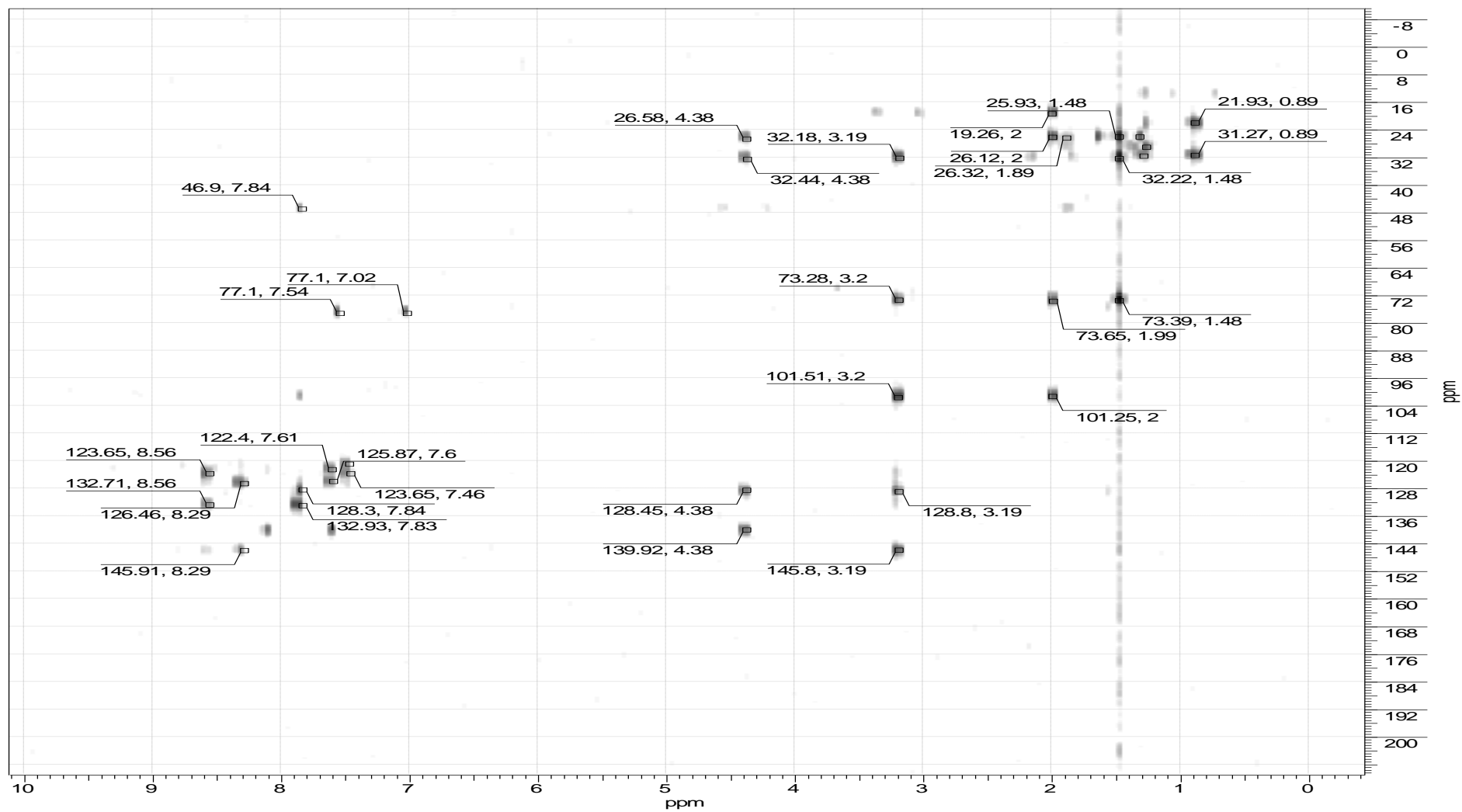
Espectro 93. RMN-¹³C (100 MHz, CDCl₃) do composto 44a.



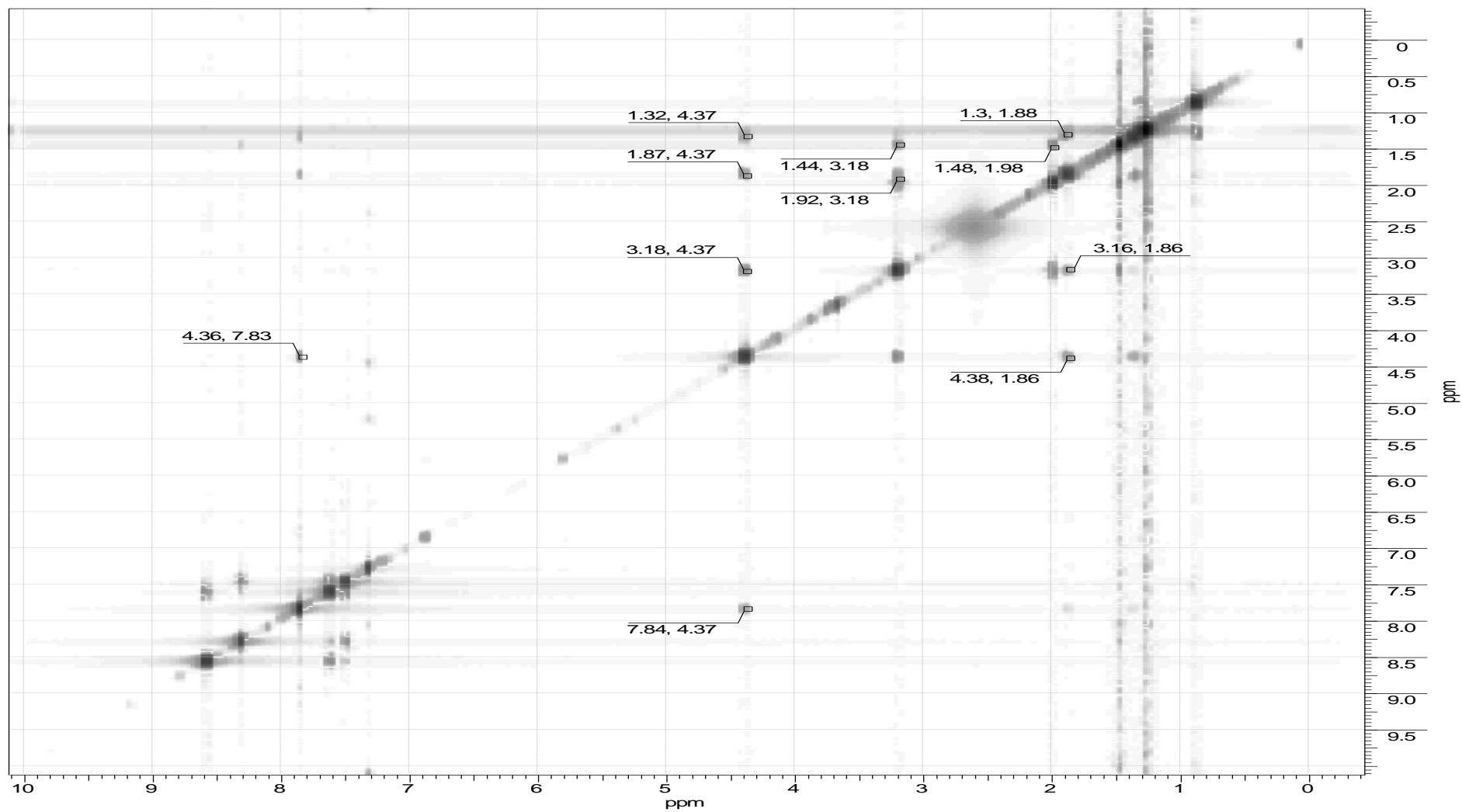
Espectro 94. ^1H -COSY (400 MHz, CDCl_3) do composto 44a.



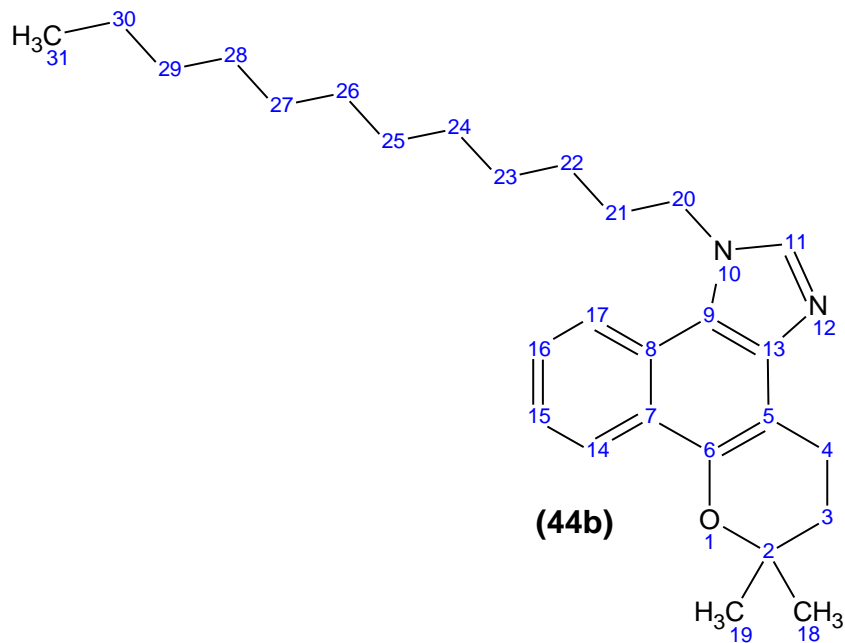
Espectro 95. HSQC (400 MHz, CDCl₃) do composto 44a.



Espectro 96. HMBC (400 MHz, CDCl_3) do composto 44a.

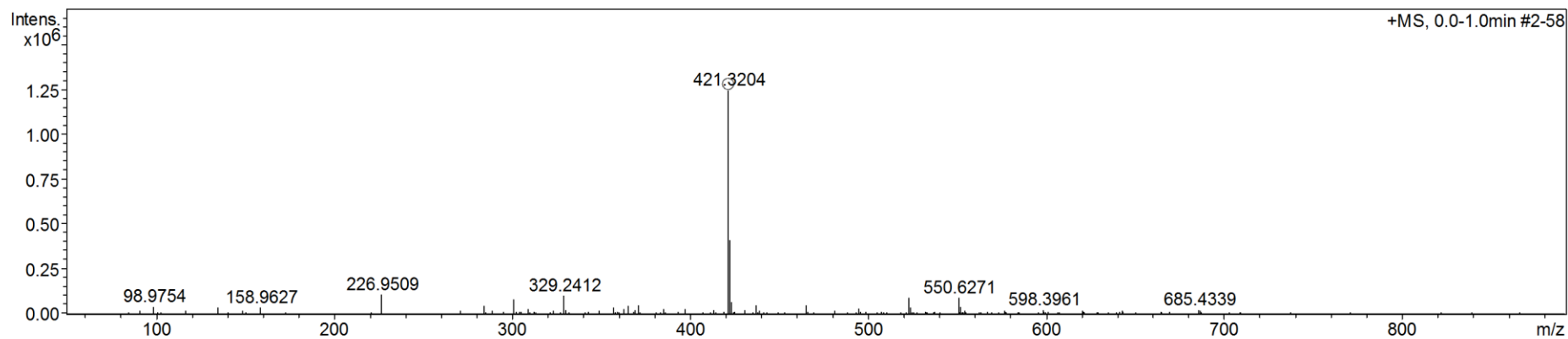


Espectro 97. NOESY (400 MHz, CDCl₃) do composto 44a.

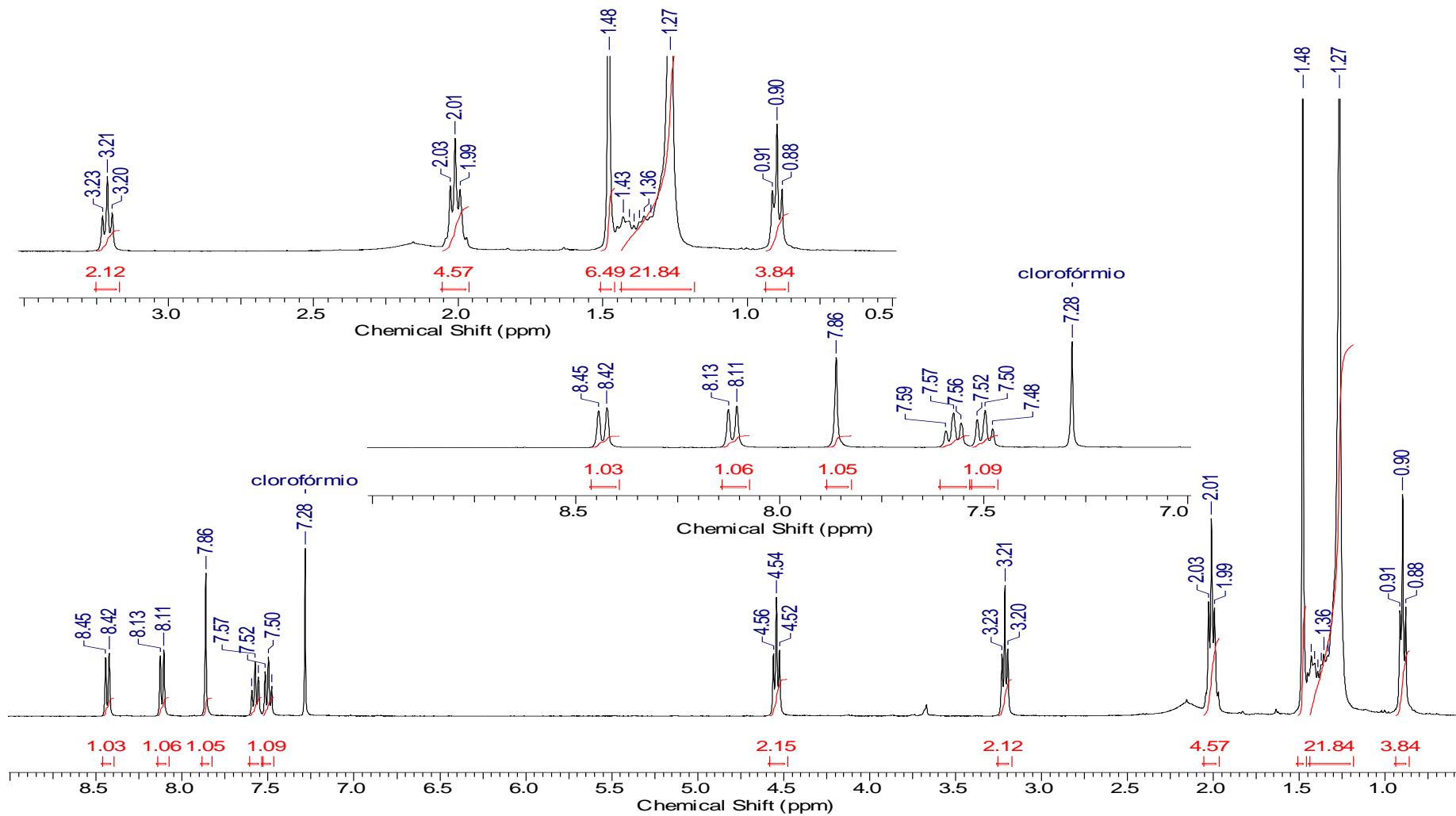


M: 420.6301 Da

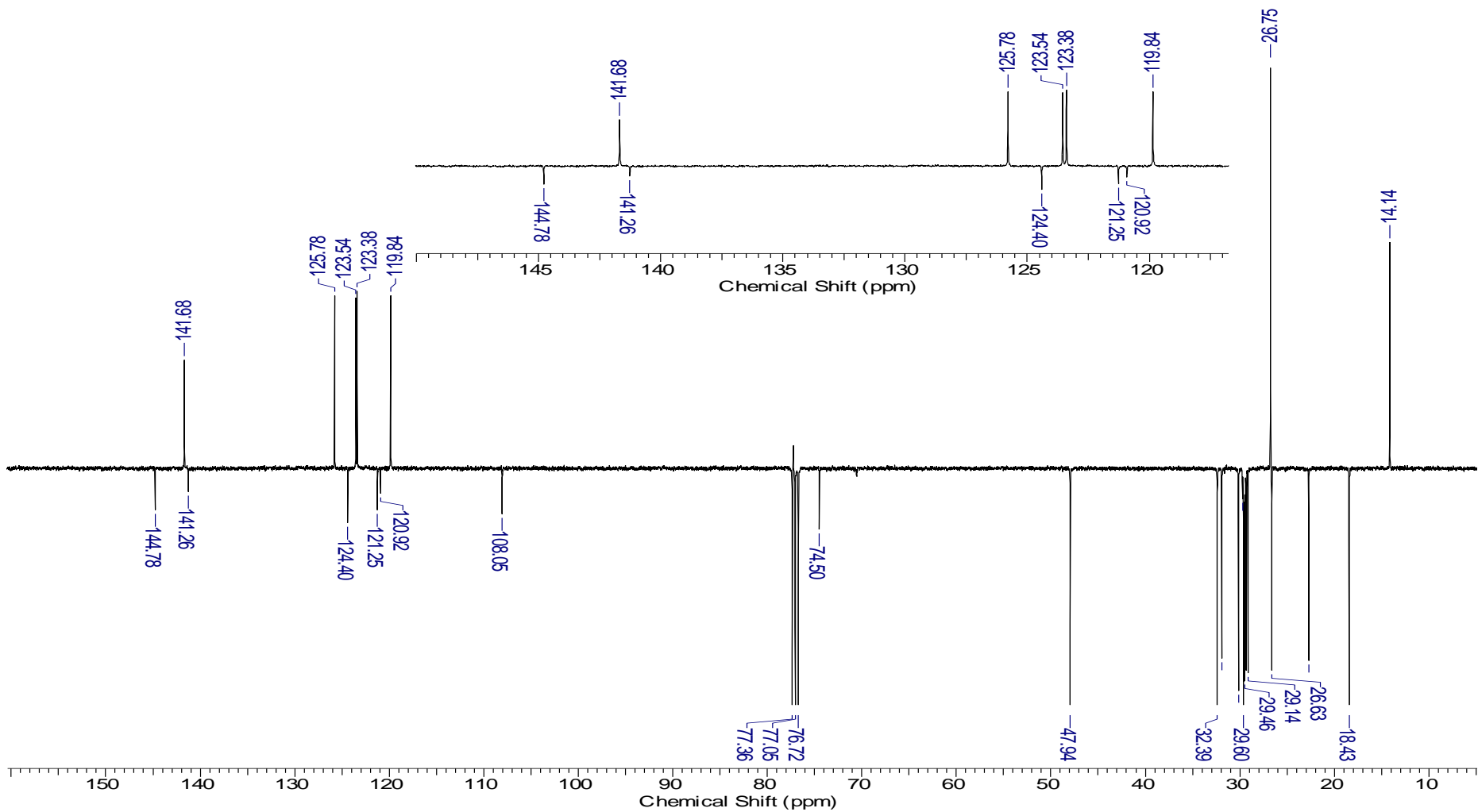
[M+H]⁺ = 421.3213 Da; err[ppm] = 2,3



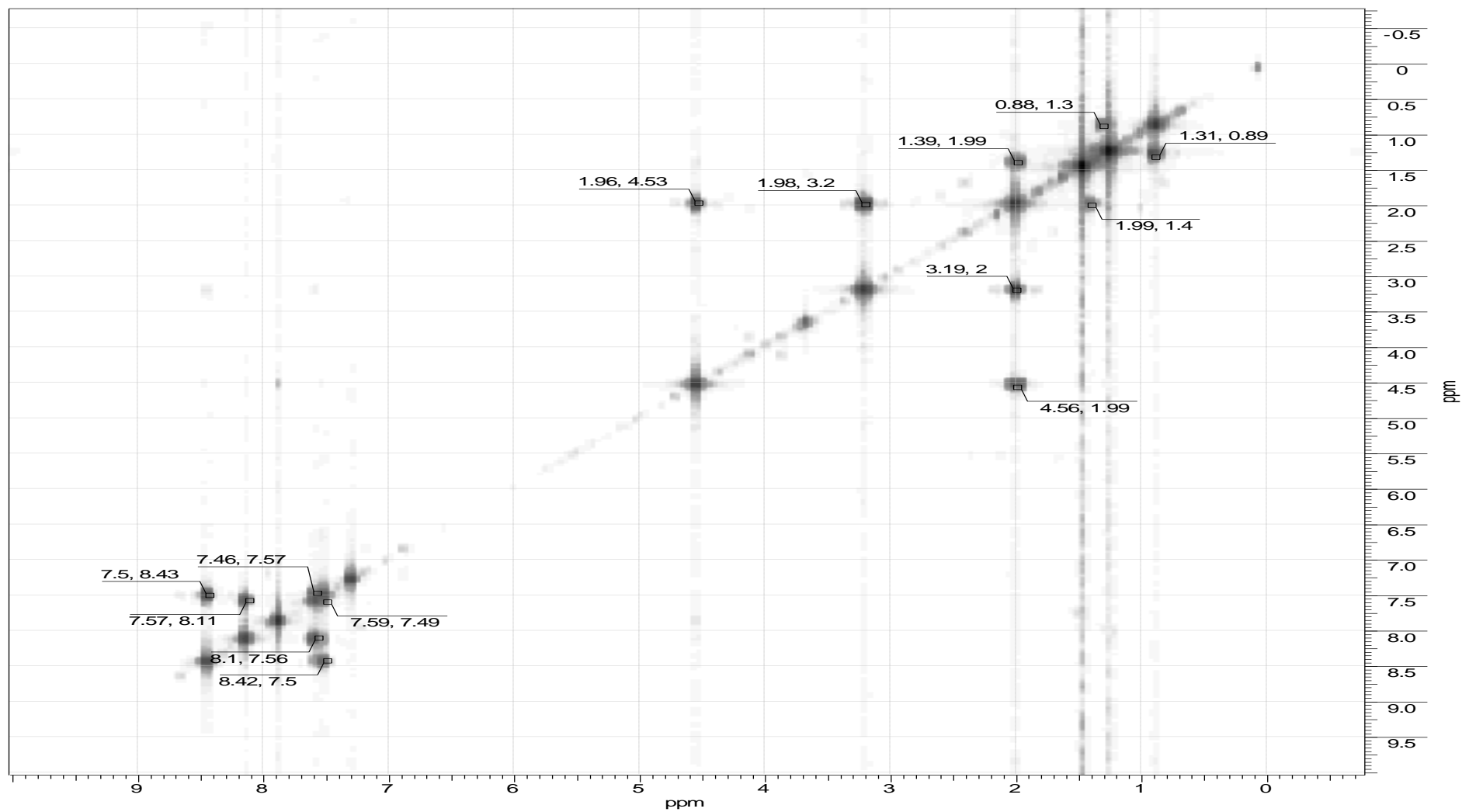
Espectro 98. EM-IES do composto 44b.



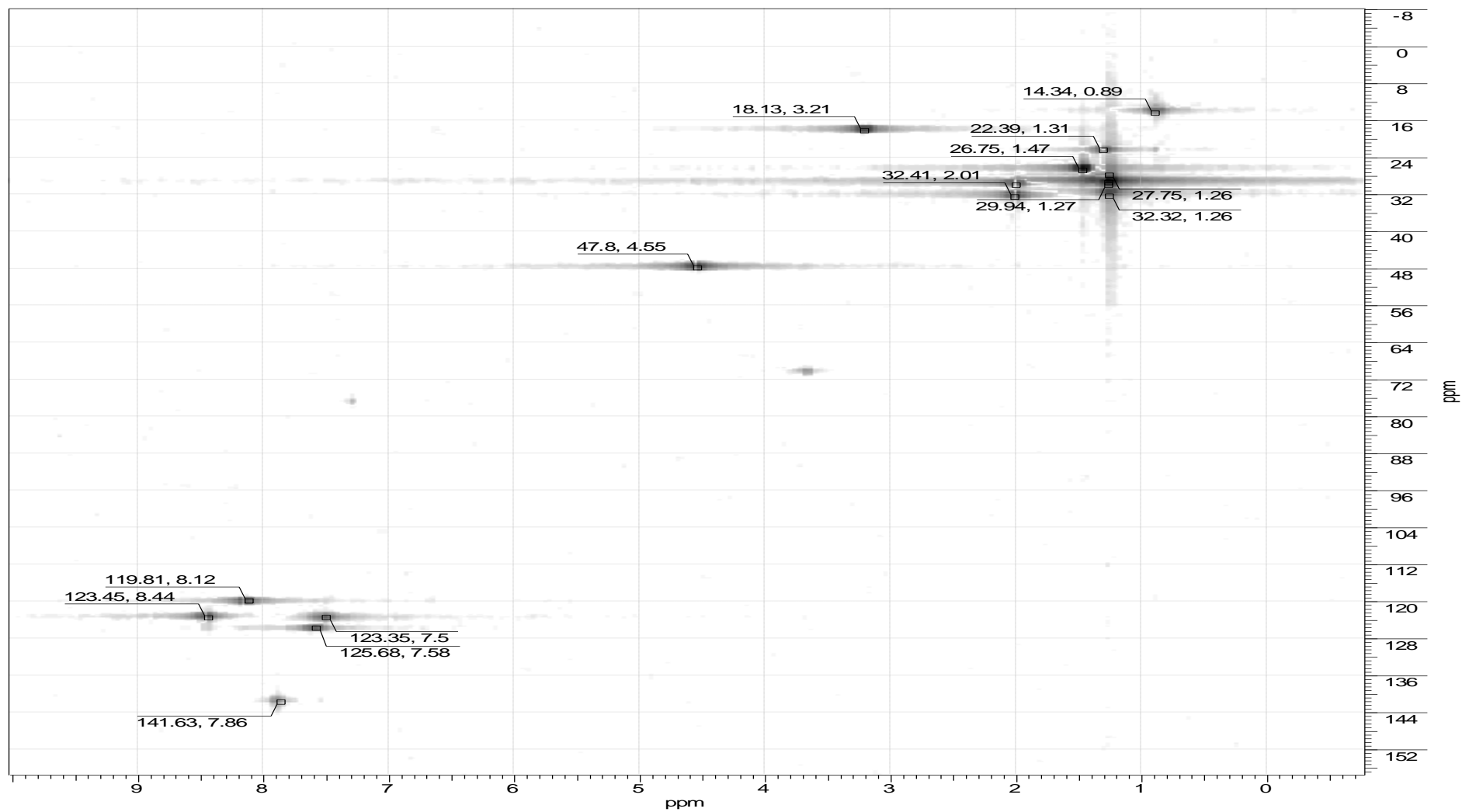
Espectro 99. RMN- ^1H (400 MHz, CDCl_3) do composto 44b.



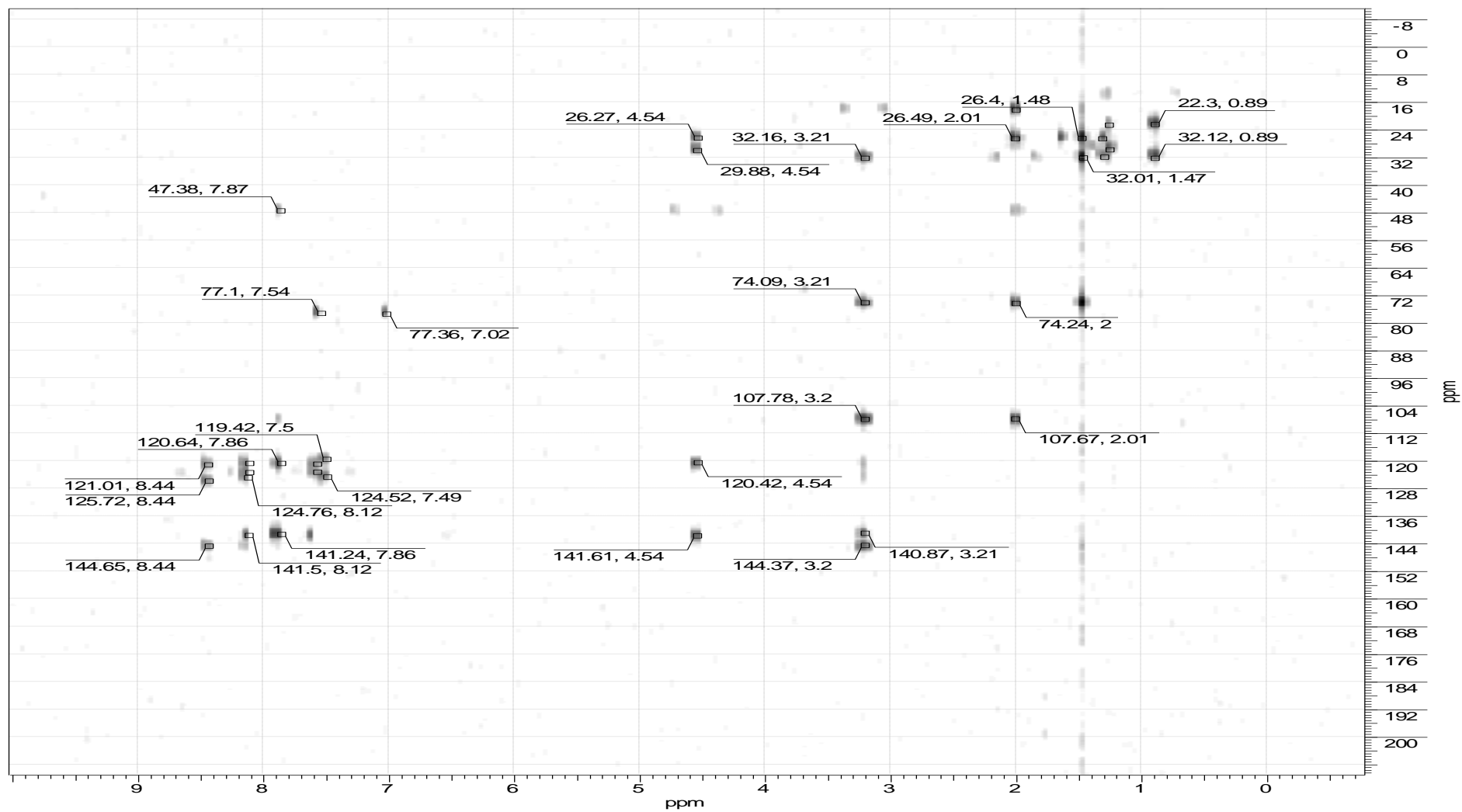
Espectro 100. RMN- ^{13}C (100 MHz, CDCl_3) do composto 44b.



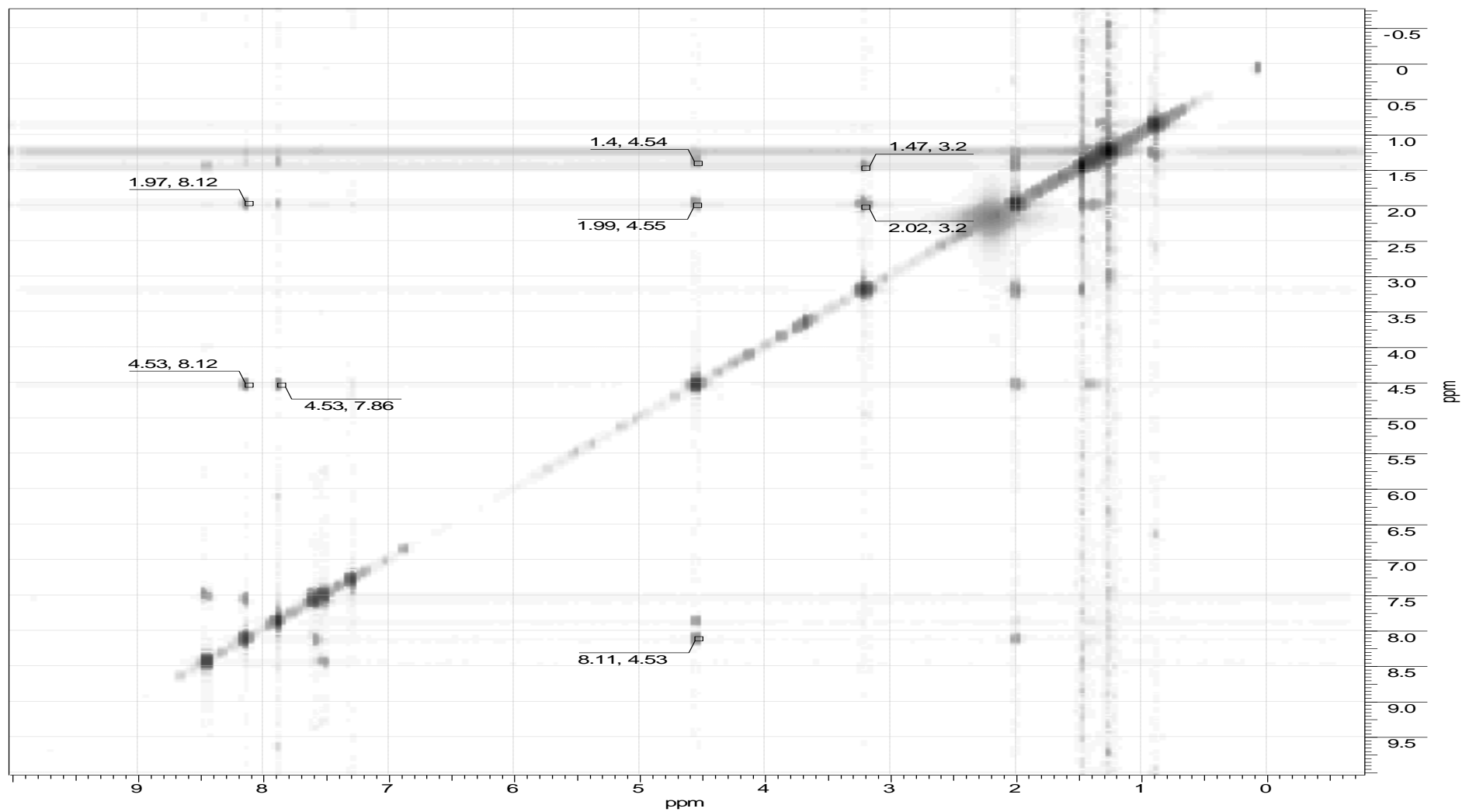
Espectro 101. ^1H -COSY (400 MHz, CDCl_3) do composto 44b.



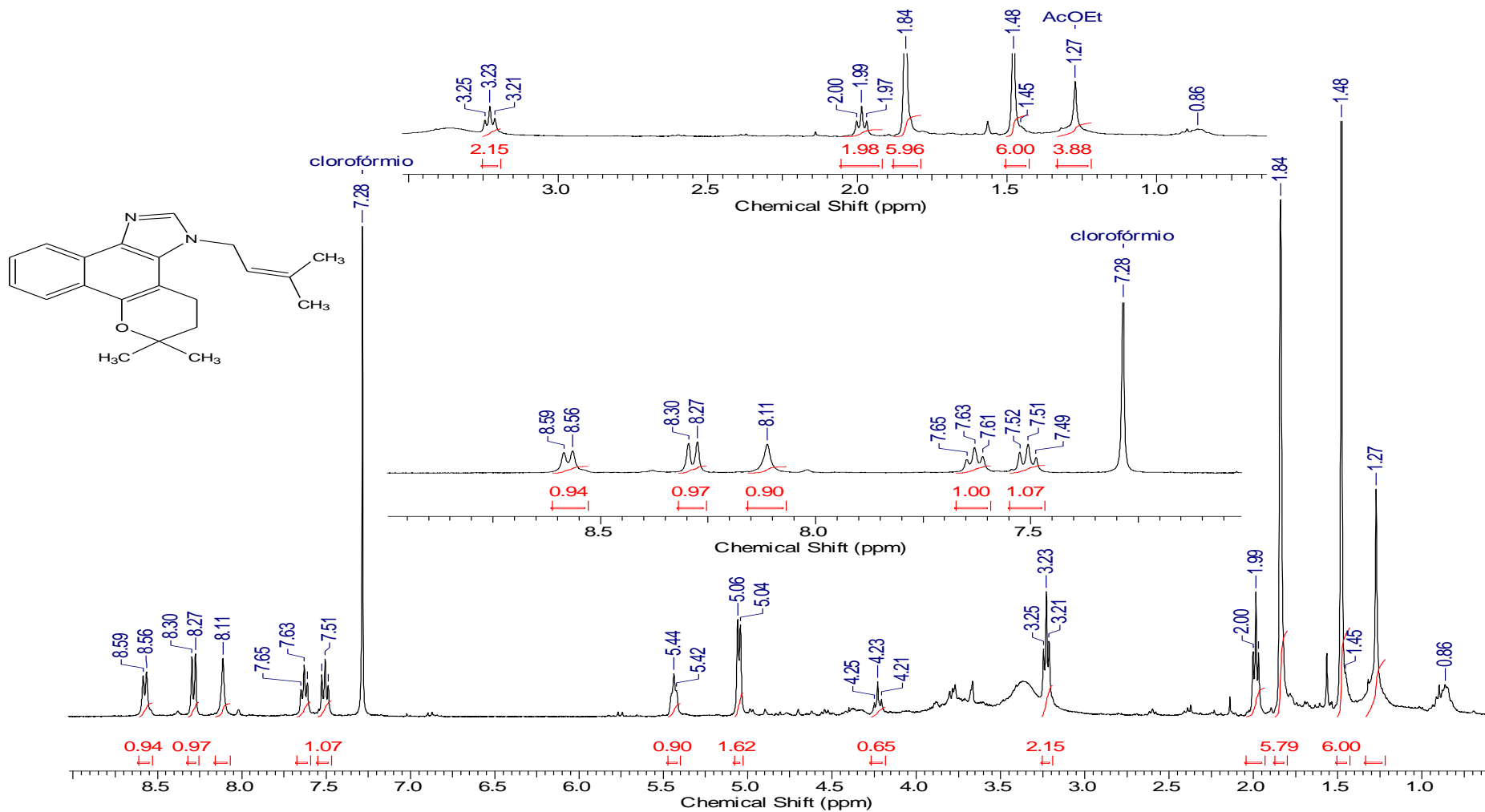
Espectro 102. HSQC (400 MHz, CDCl_3) do composto 44b.



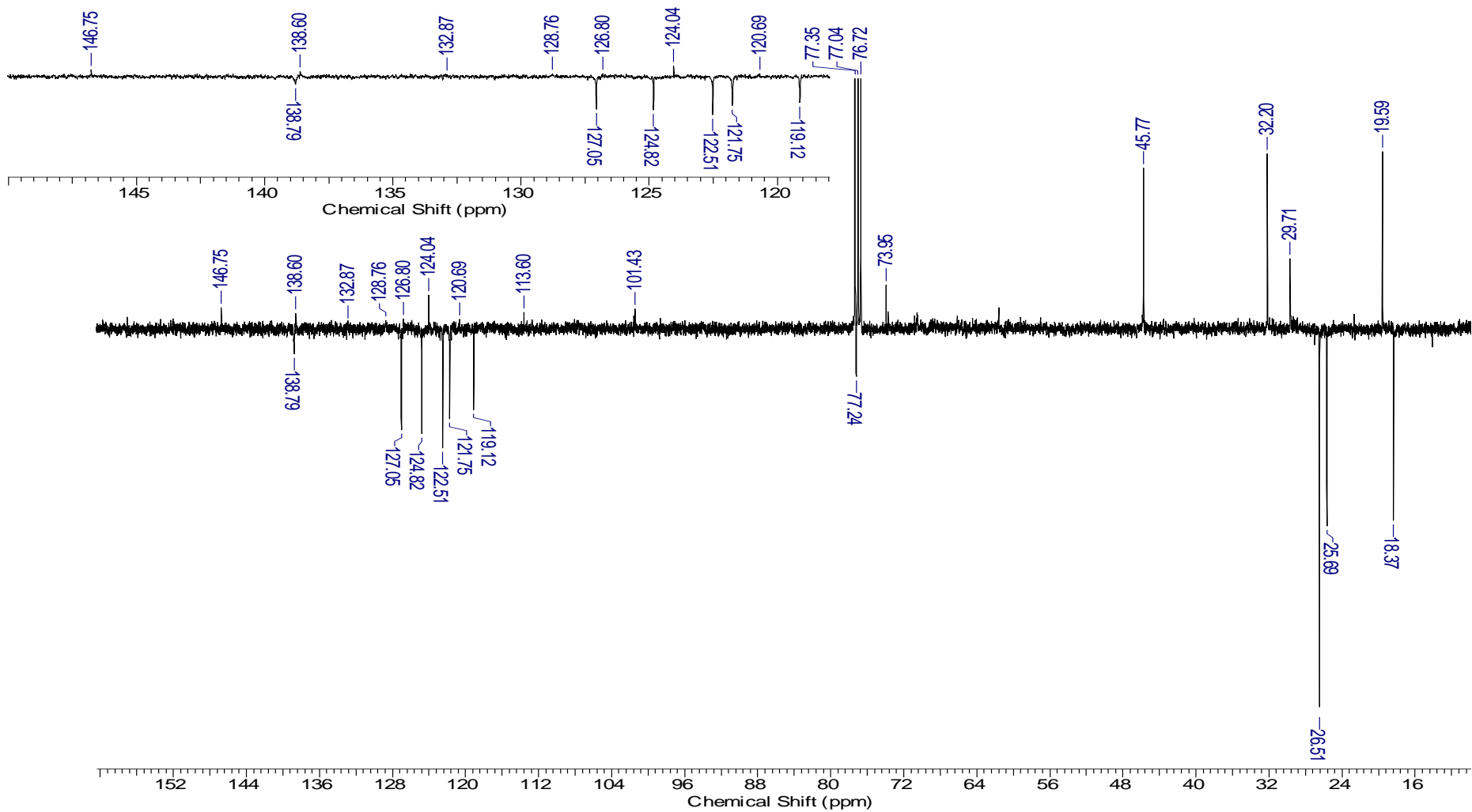
Espectro 103. HMBC (400 MHz, CDCl₃) do composto 44b.



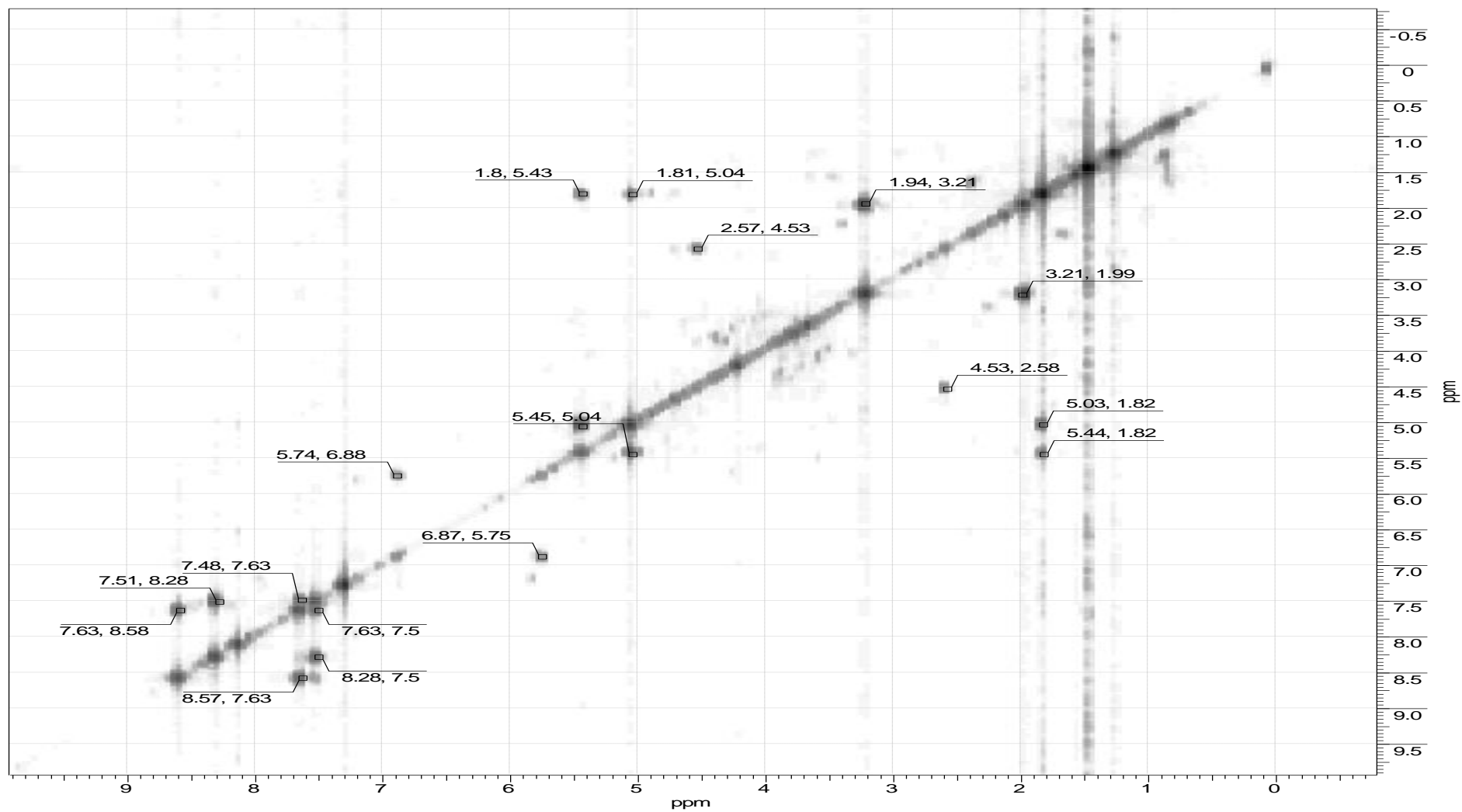
Espectro 104. NOESY (400 MHz, CDCl₃) do composto 44b.



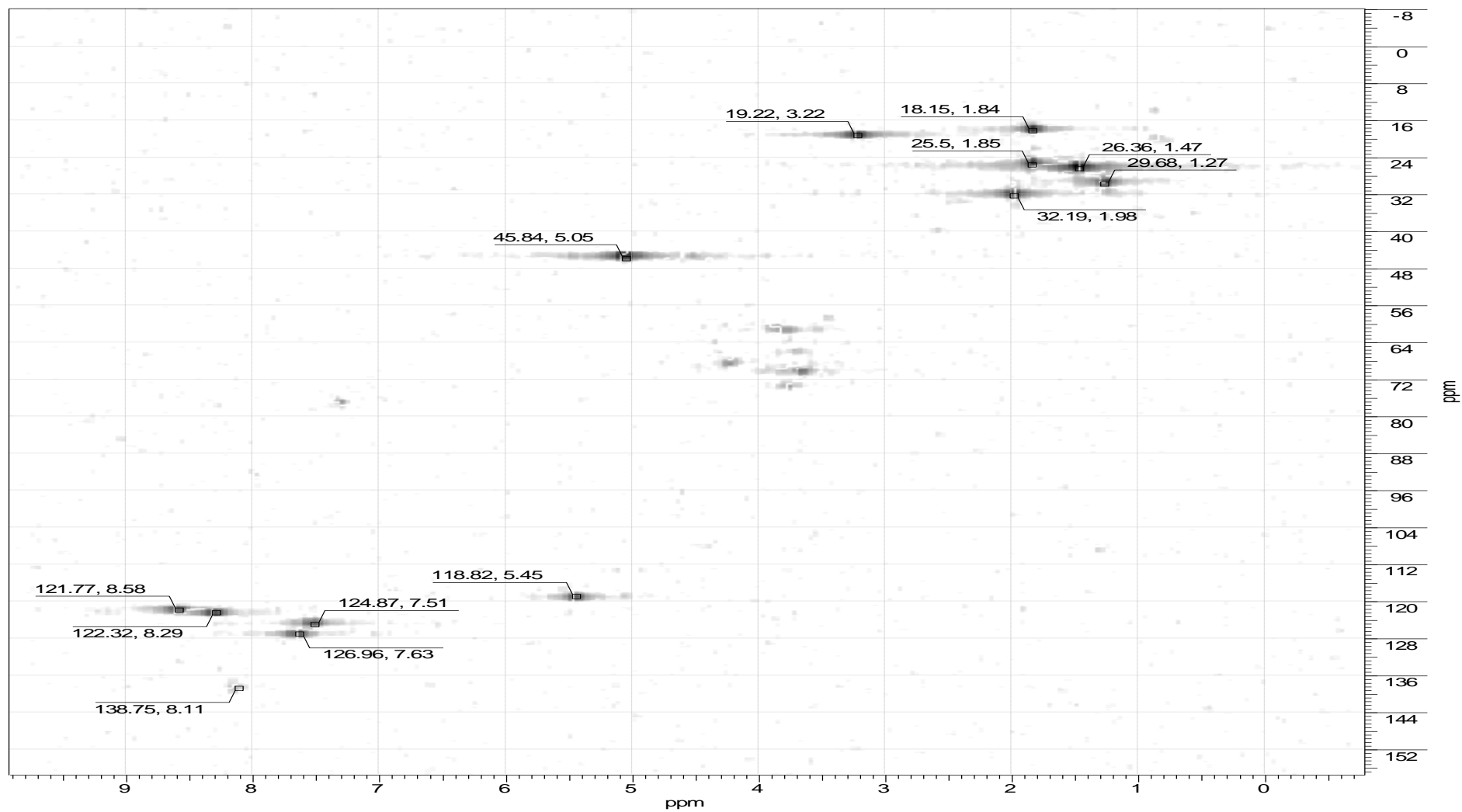
Espectro 105. RMN- ^1H (400 MHz, CDCl_3) do composto 46a.



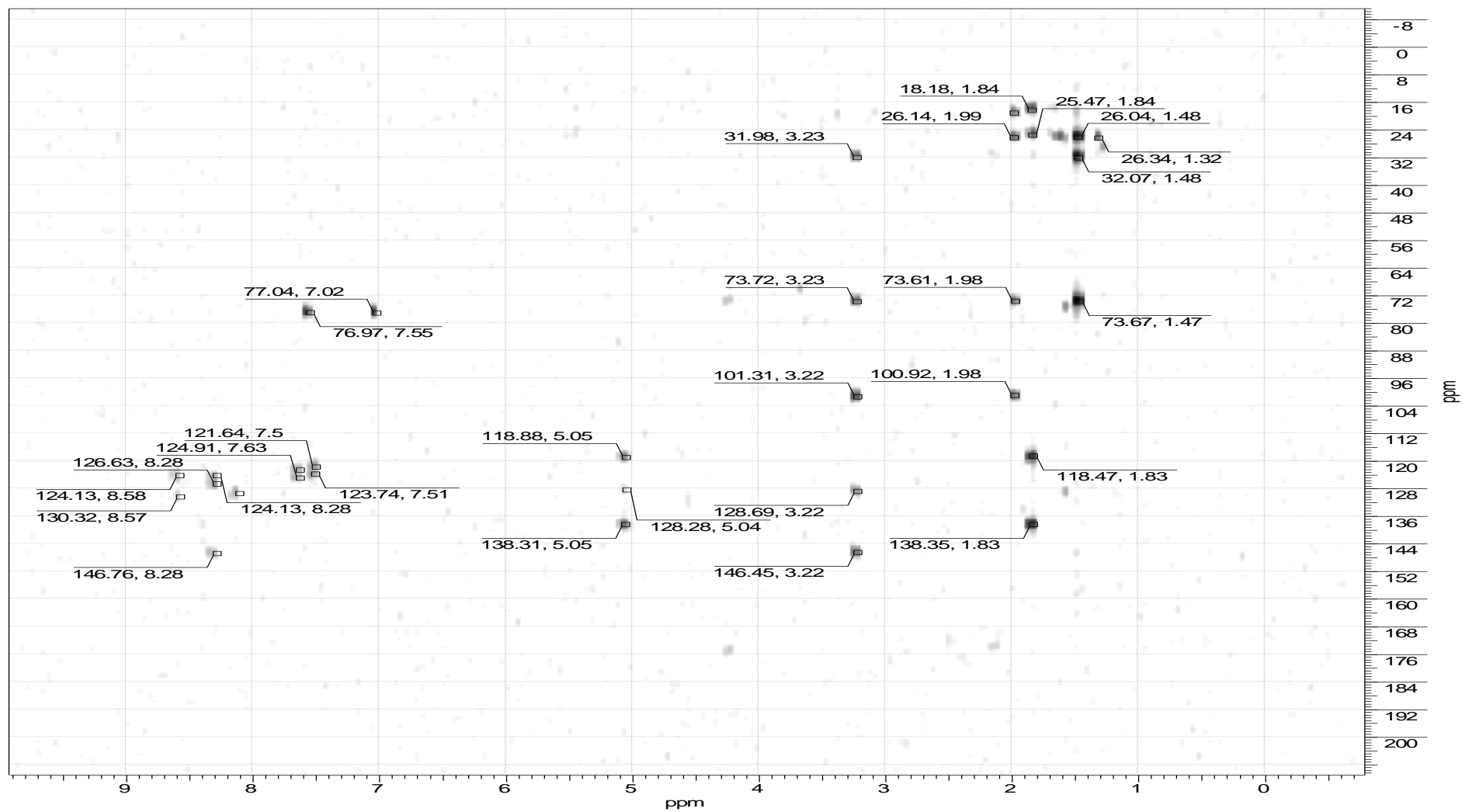
Espectro 106. RMN- ^{13}C (100 MHz, CDCl_3) do composto 46a.



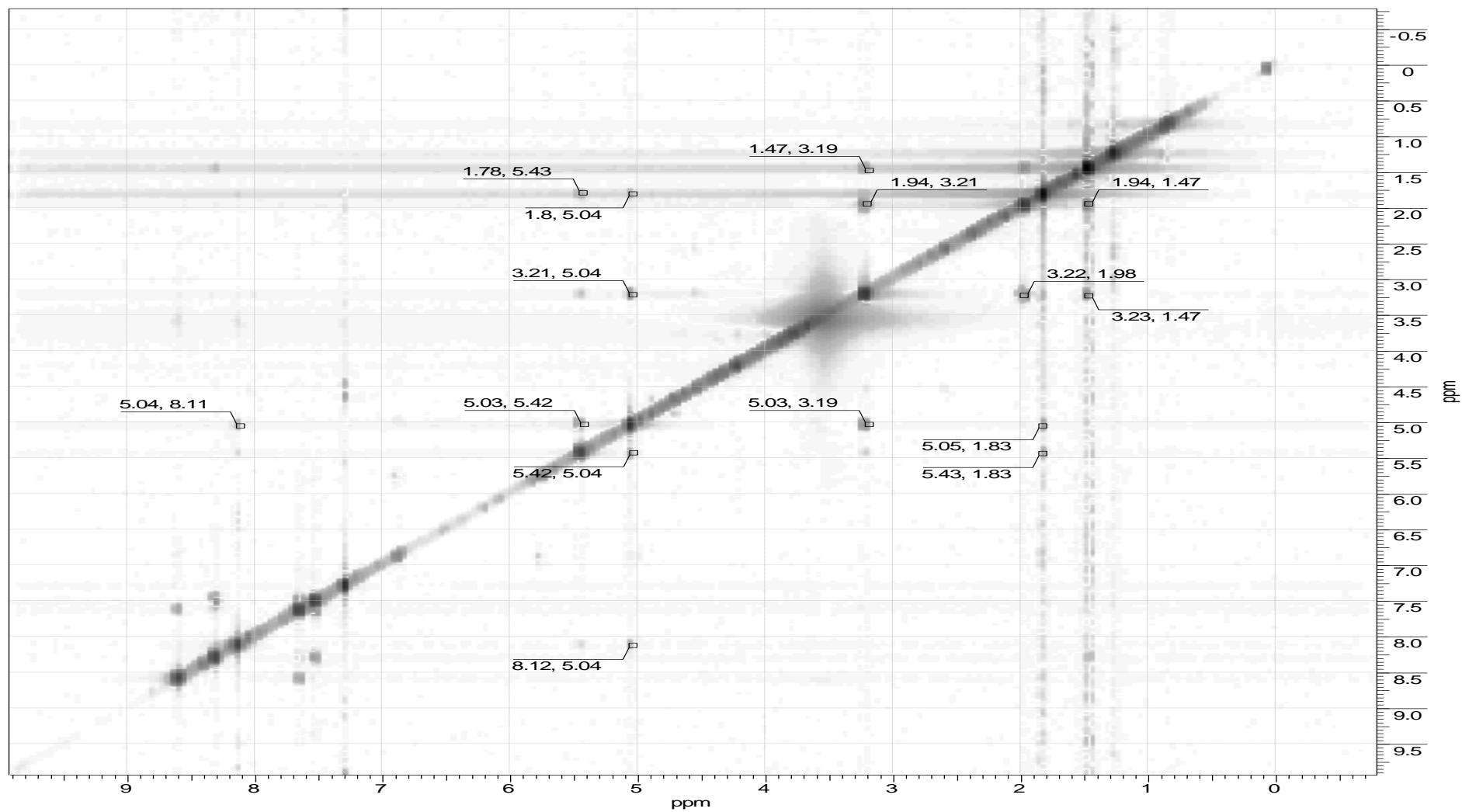
Espectro 107. ^1H -COSY (400 MHz, CDCl_3) do composto 46a.



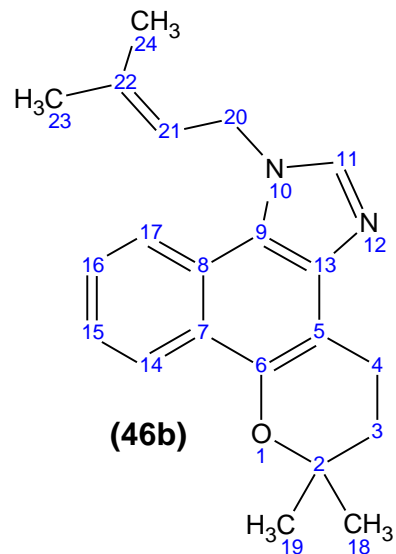
Espectro 108. HSQC (400 MHz, CDCl_3) do composto 46a.



Espectro 109. HMBC (400 MHz, CDCl₃) do composto 46a.

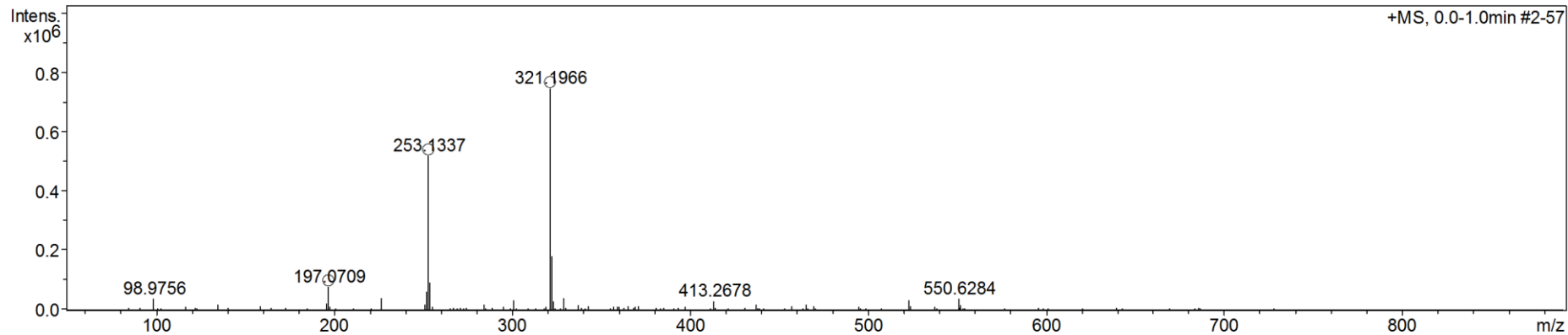


Espectro 110. NOESY (400 MHz, CDCl₃) do composto 46a.

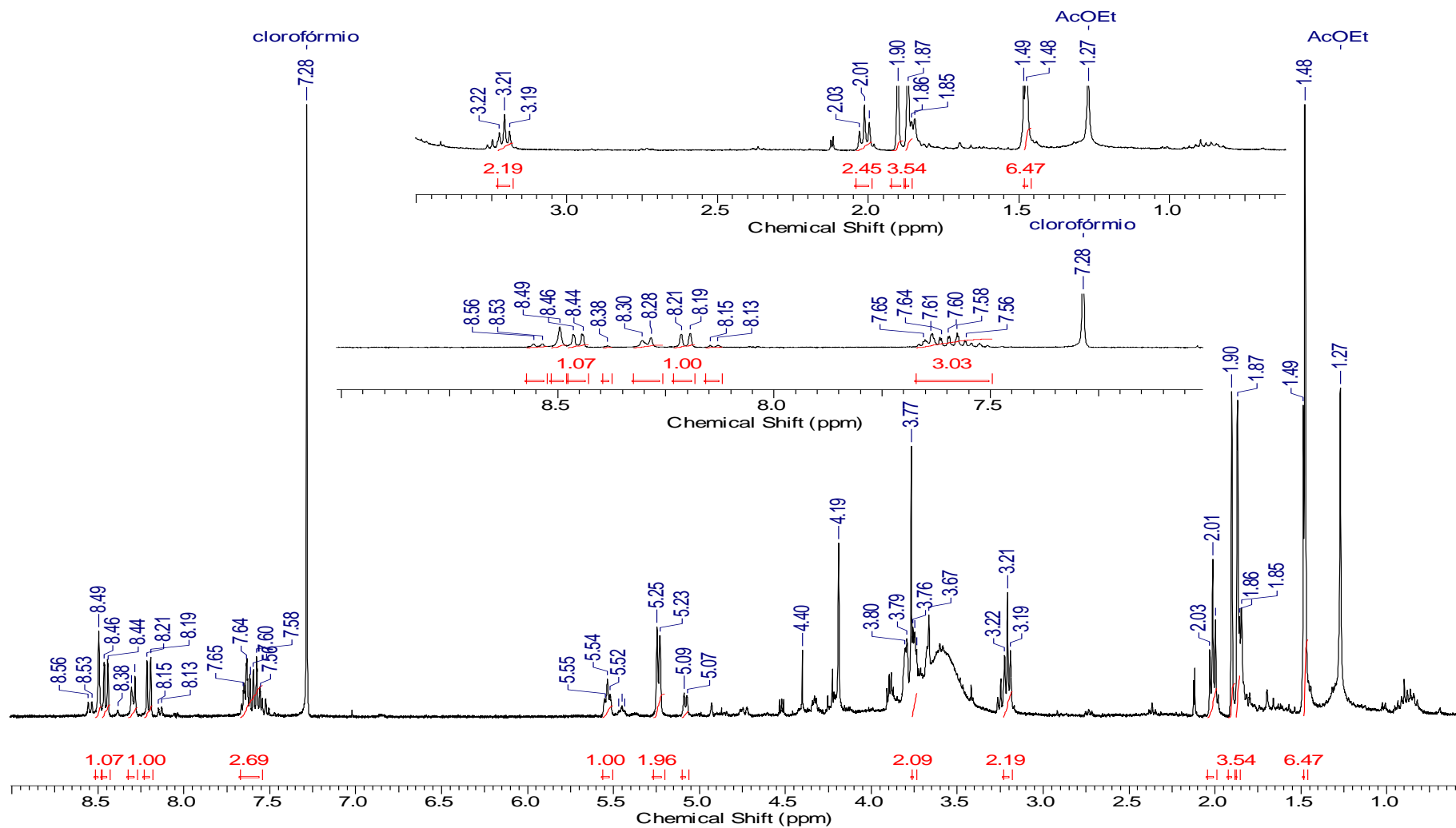


M: 320.4281 Da

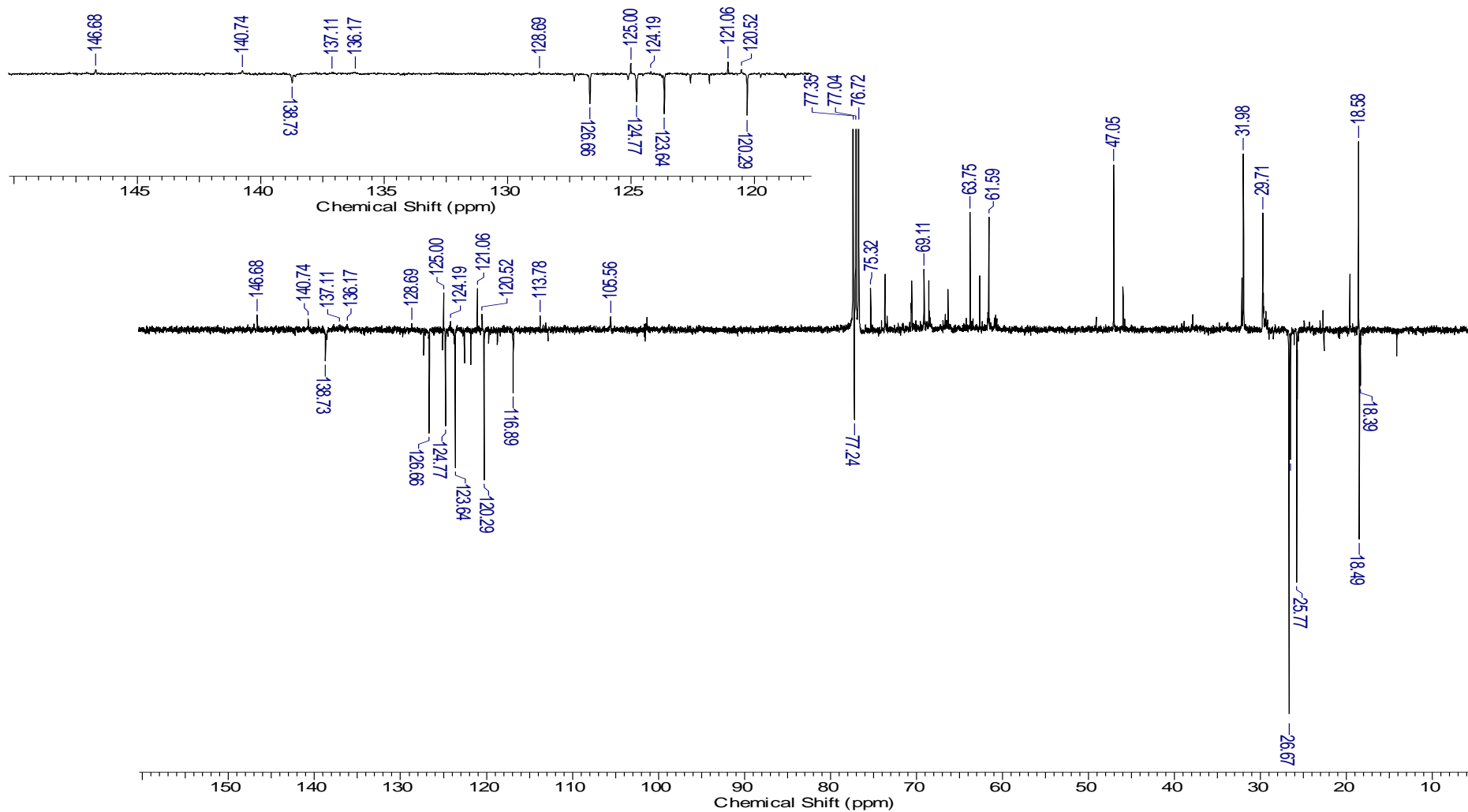
[M+H]⁺ = 321.1961 Da; err[ppm] = -1,3



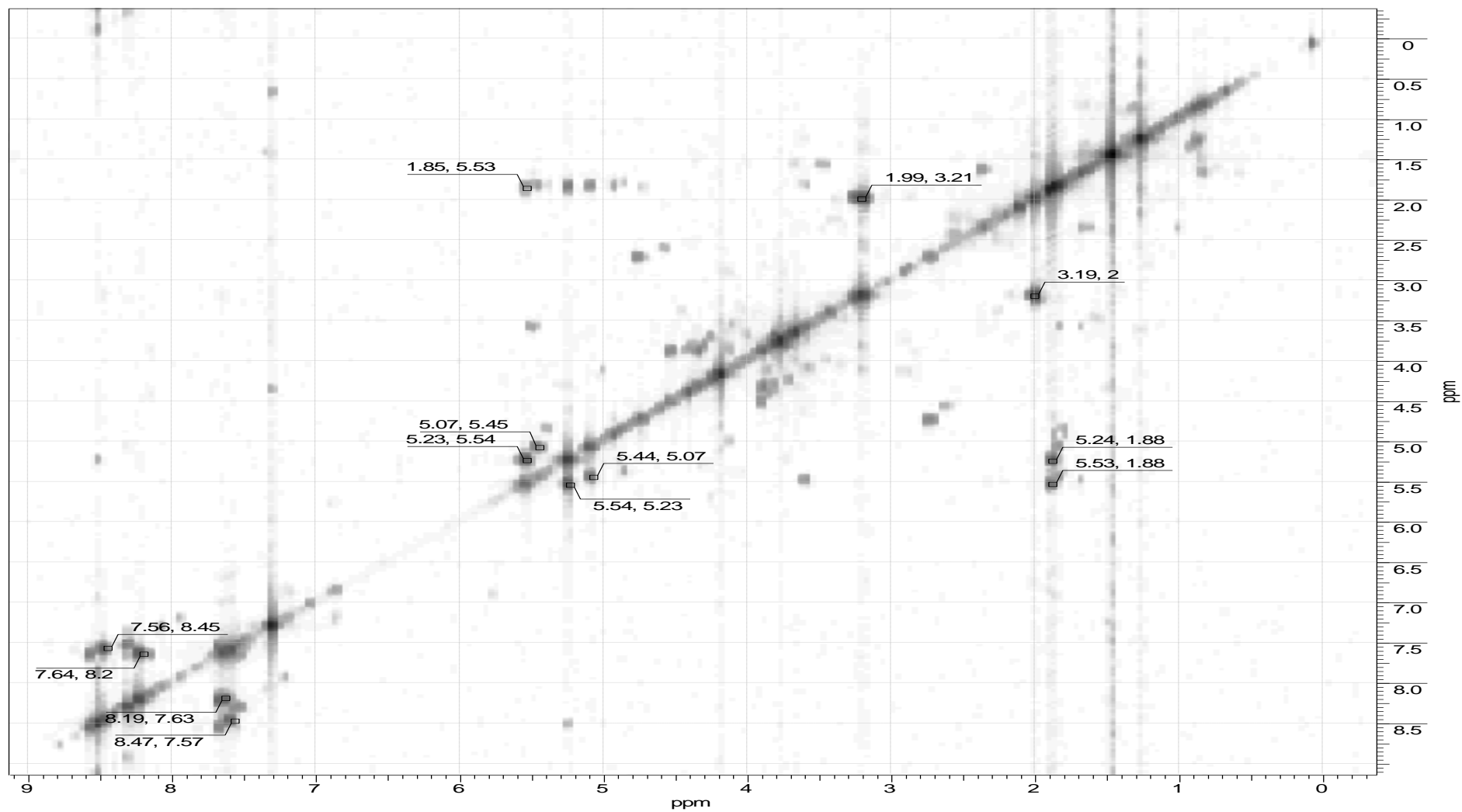
Espectro 111. EM-IES do composto 46b.



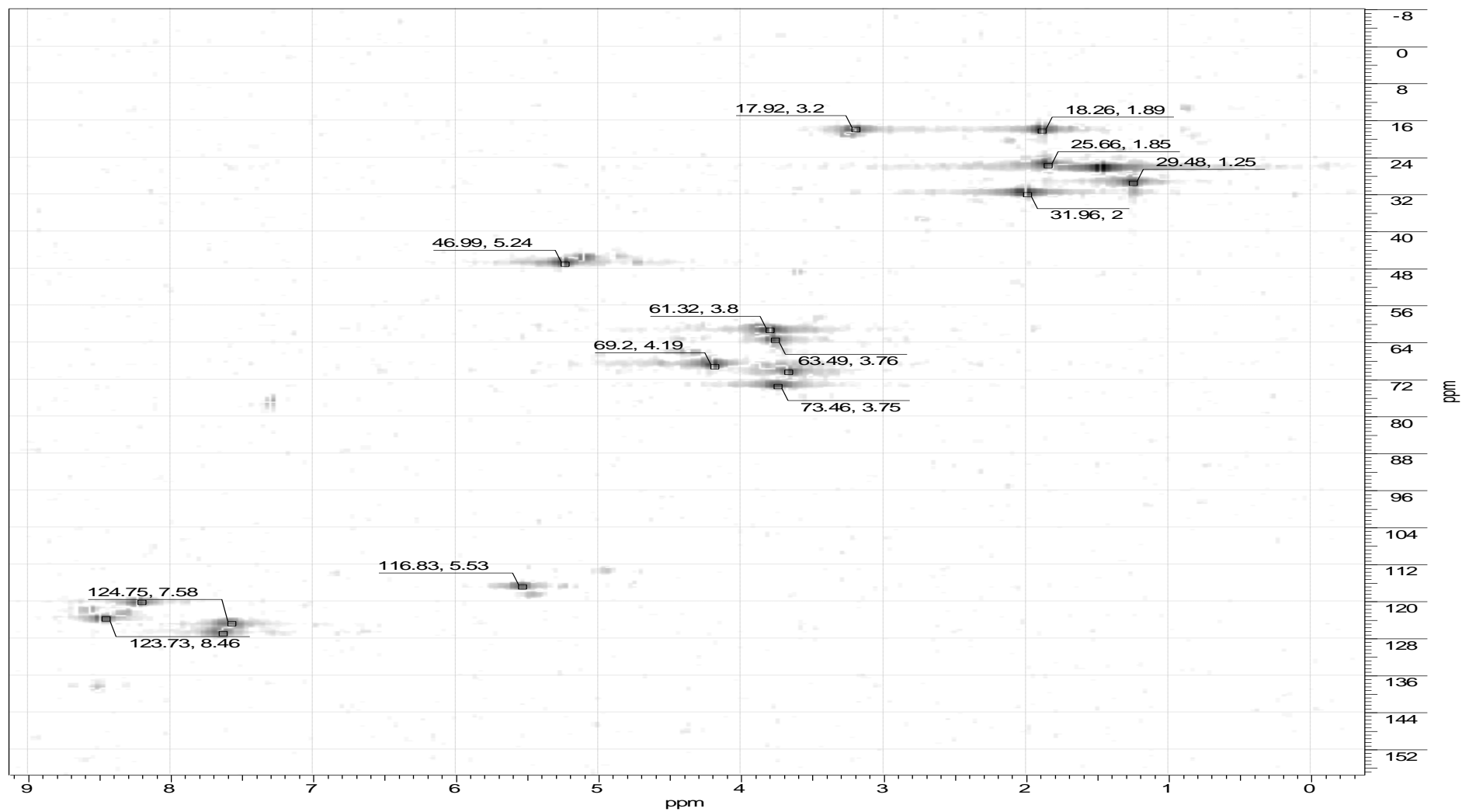
Espectro 112. RMN- ^1H (400 MHz, CDCl_3) do composto 46b.



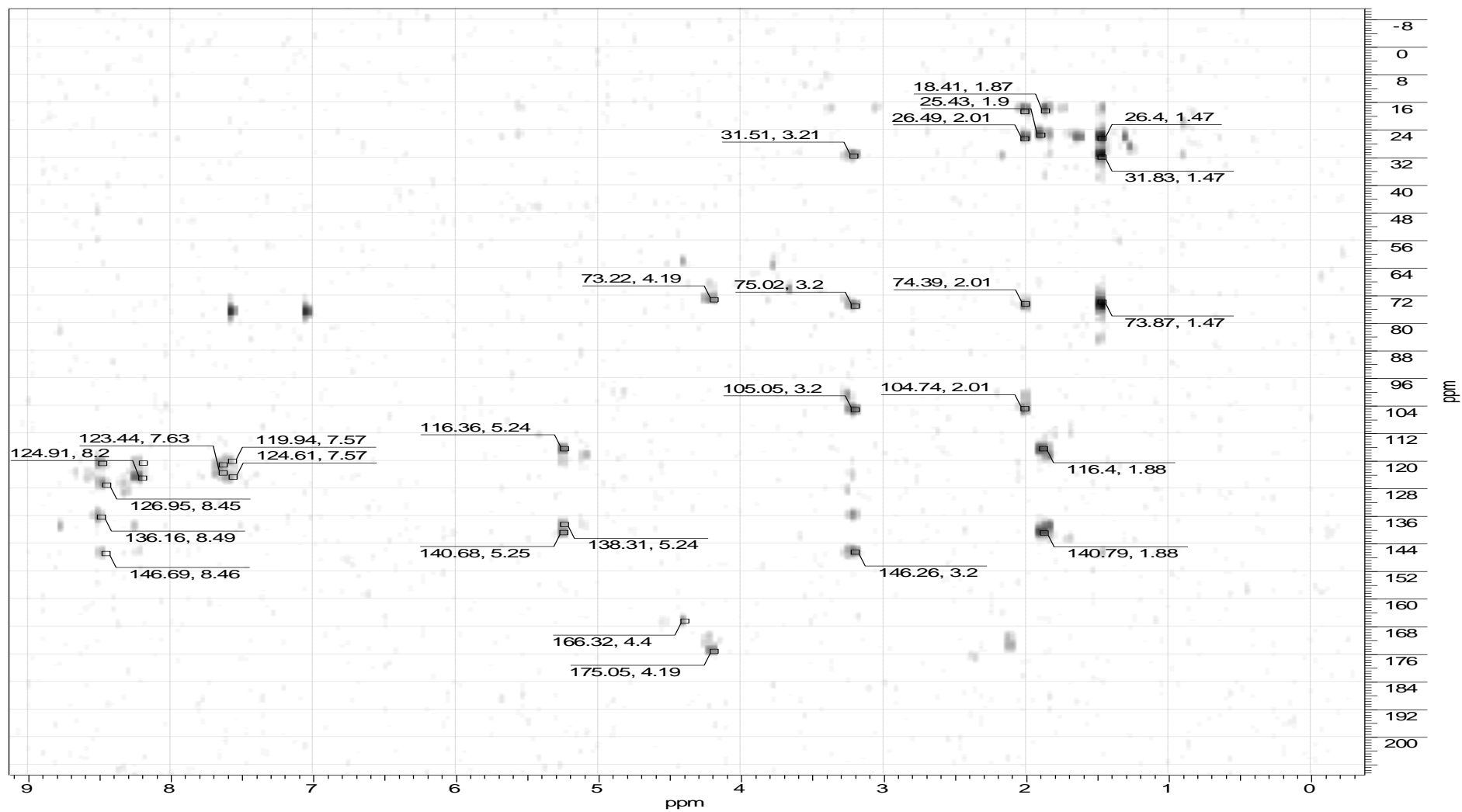
Espectro 113. RMN-¹³C (100 MHz, CDCl₃) do composto 46b.



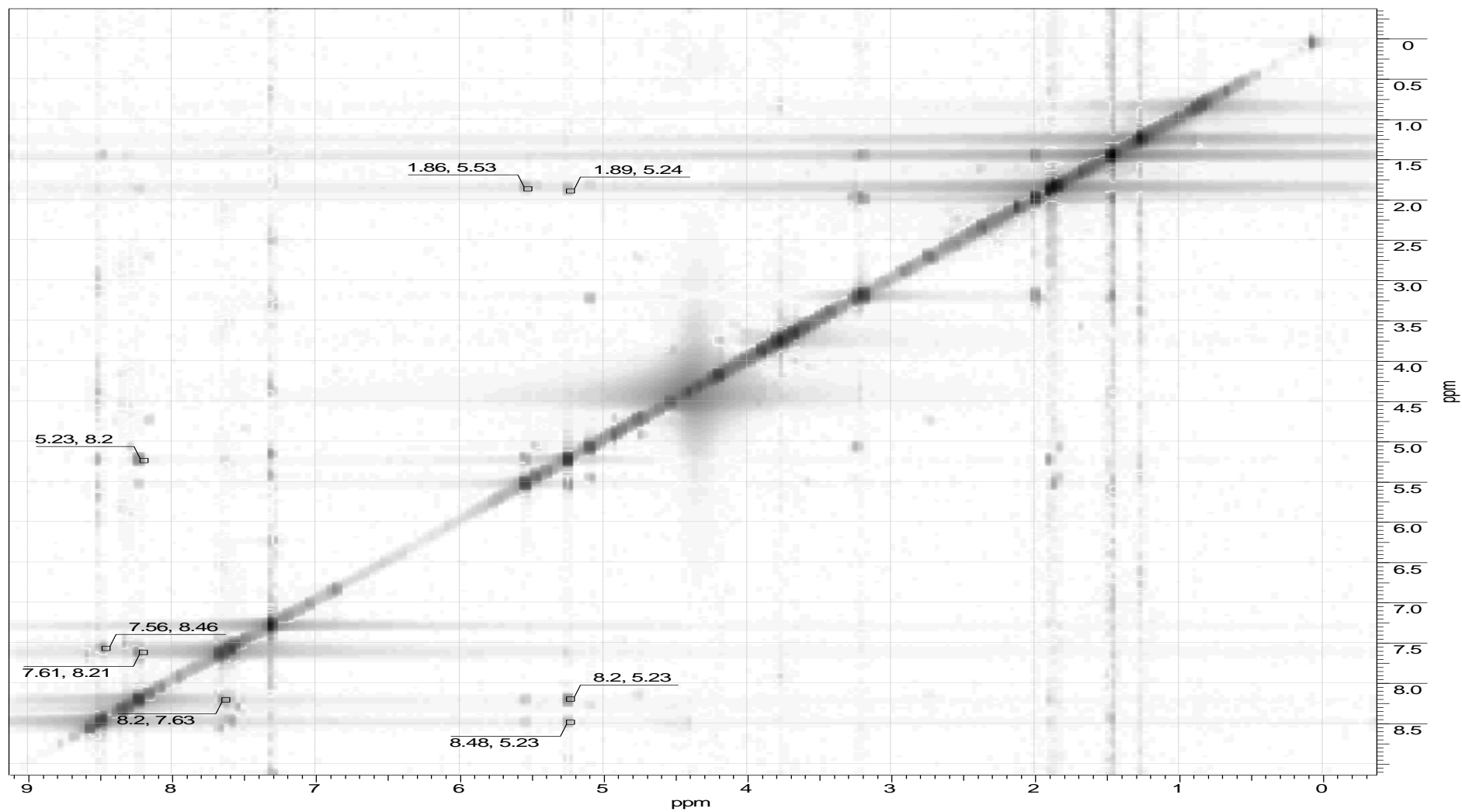
Espectro 114. ^1H -COSY (400 MHz, CDCl_3) do composto 46b.



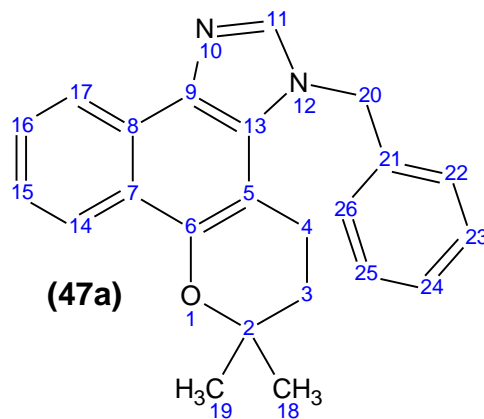
Espectro 115. HSQC (400 MHz, CDCl₃) do composto 46b.



Espectro 116. HMBC (400 MHz, CDCl₃) do composto 46b.

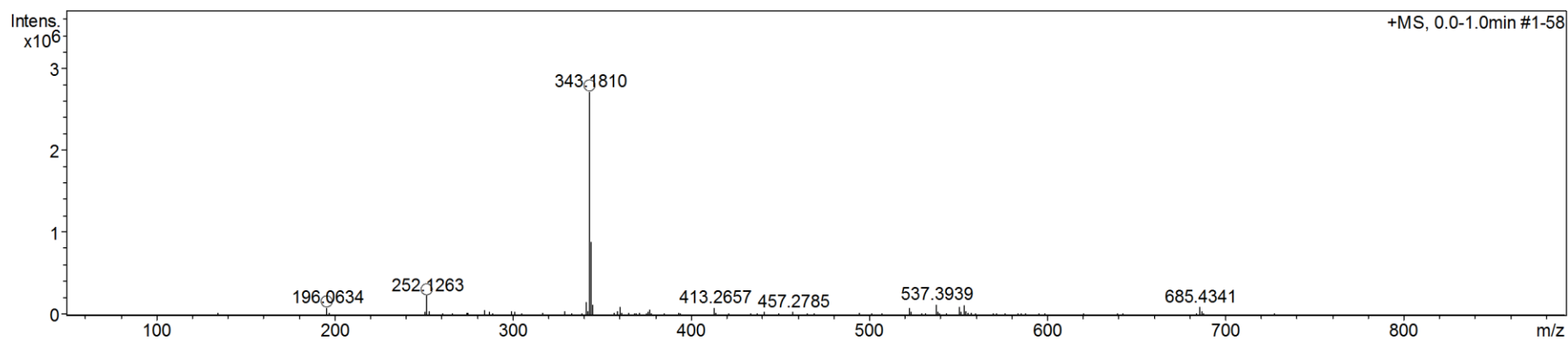


Espectro 117. NOESY (400 MHz, CDCl₃) do composto 46b.

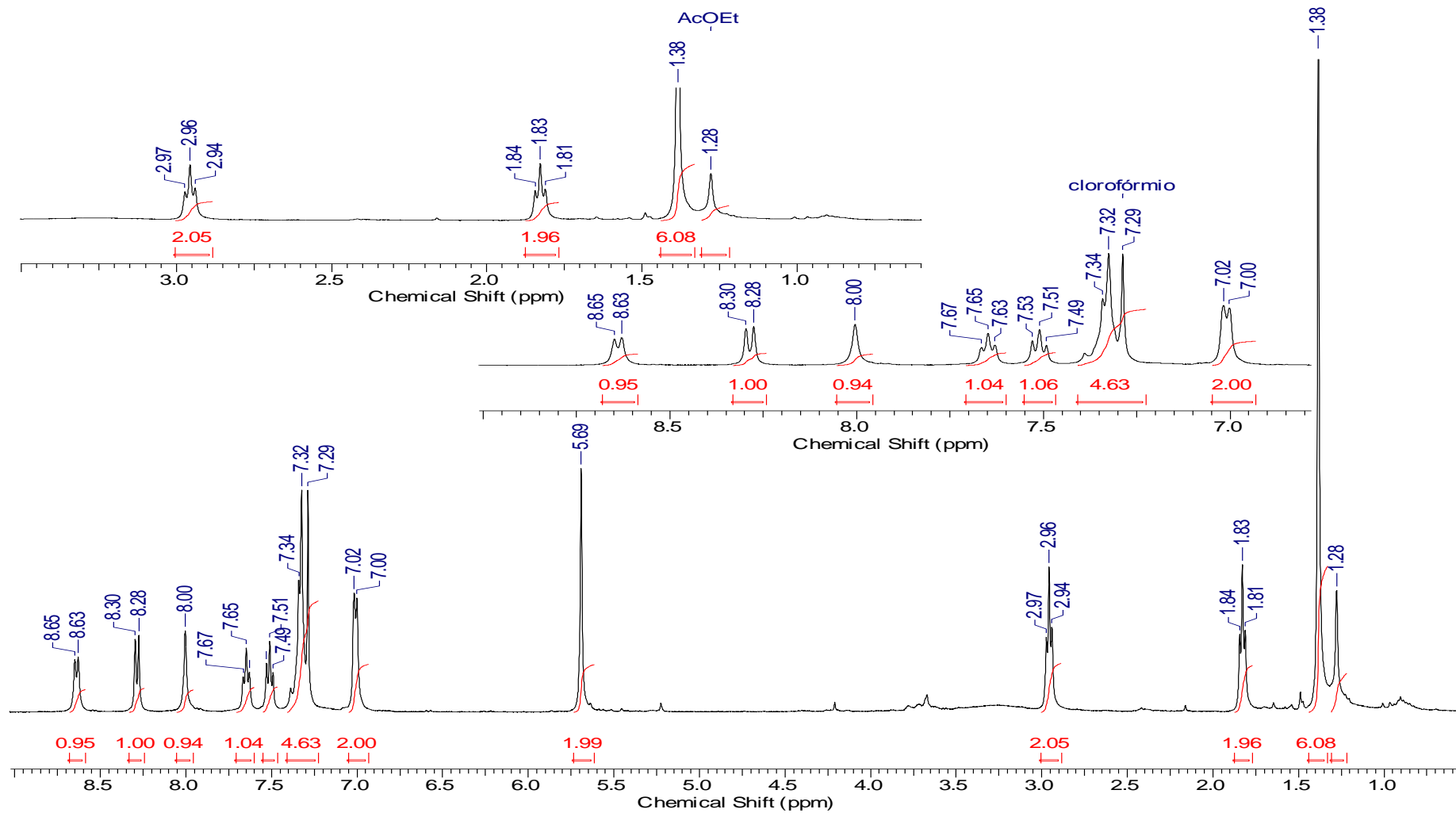


M: 342.4337 Da

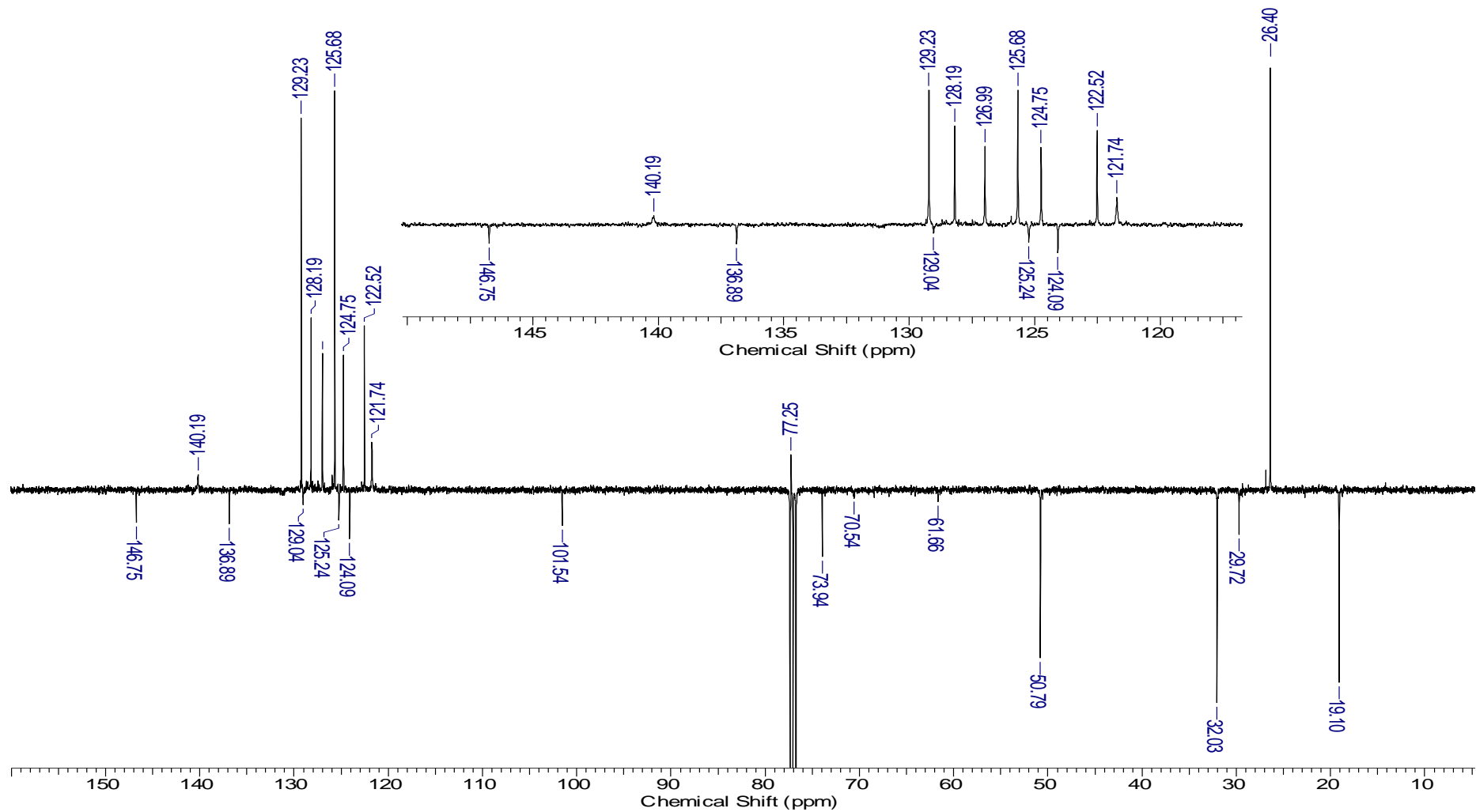
[M+H]⁺ = 343.1805 Da; err[ppm] = -1,6



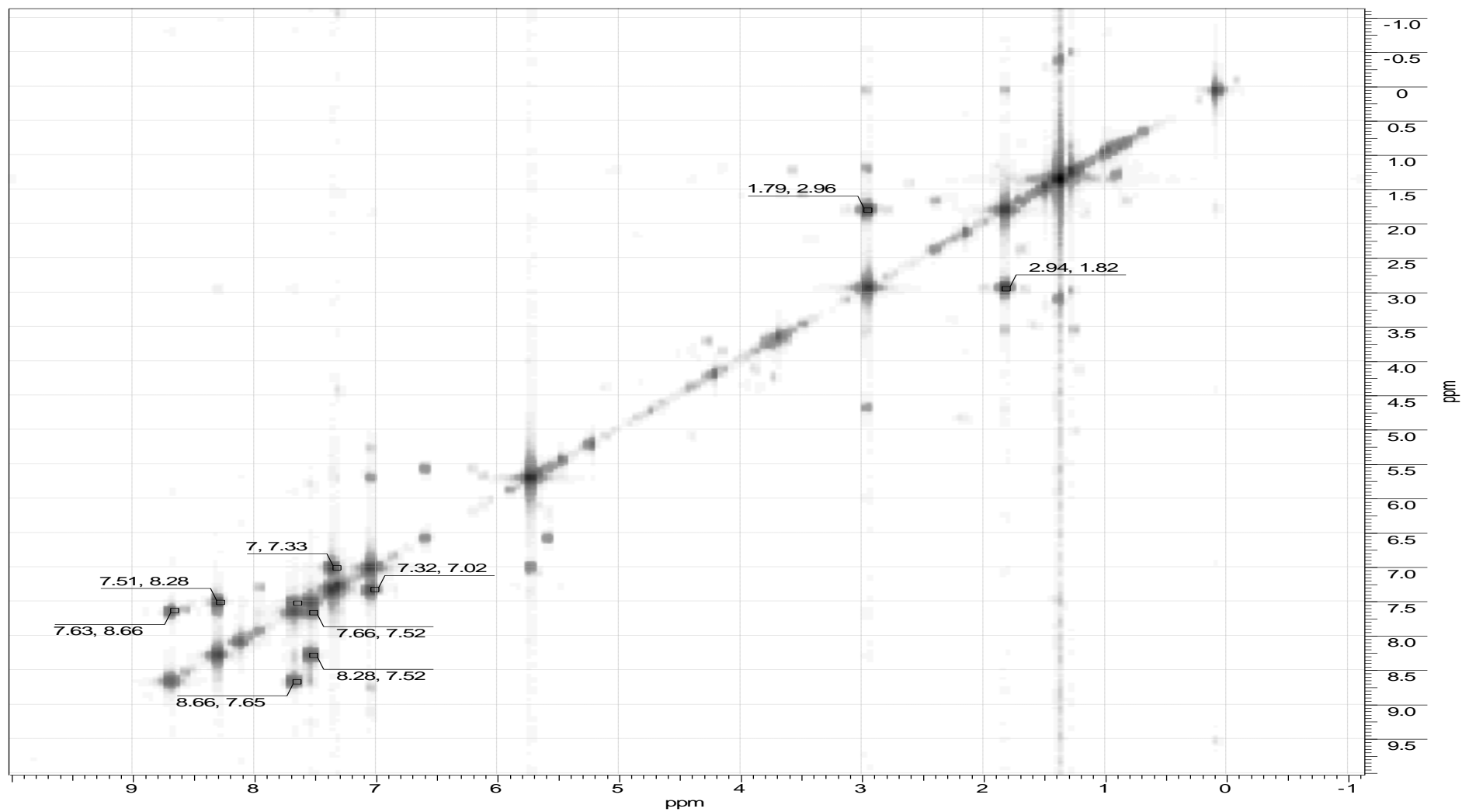
Espectro 118. EM-IES do composto 47a.



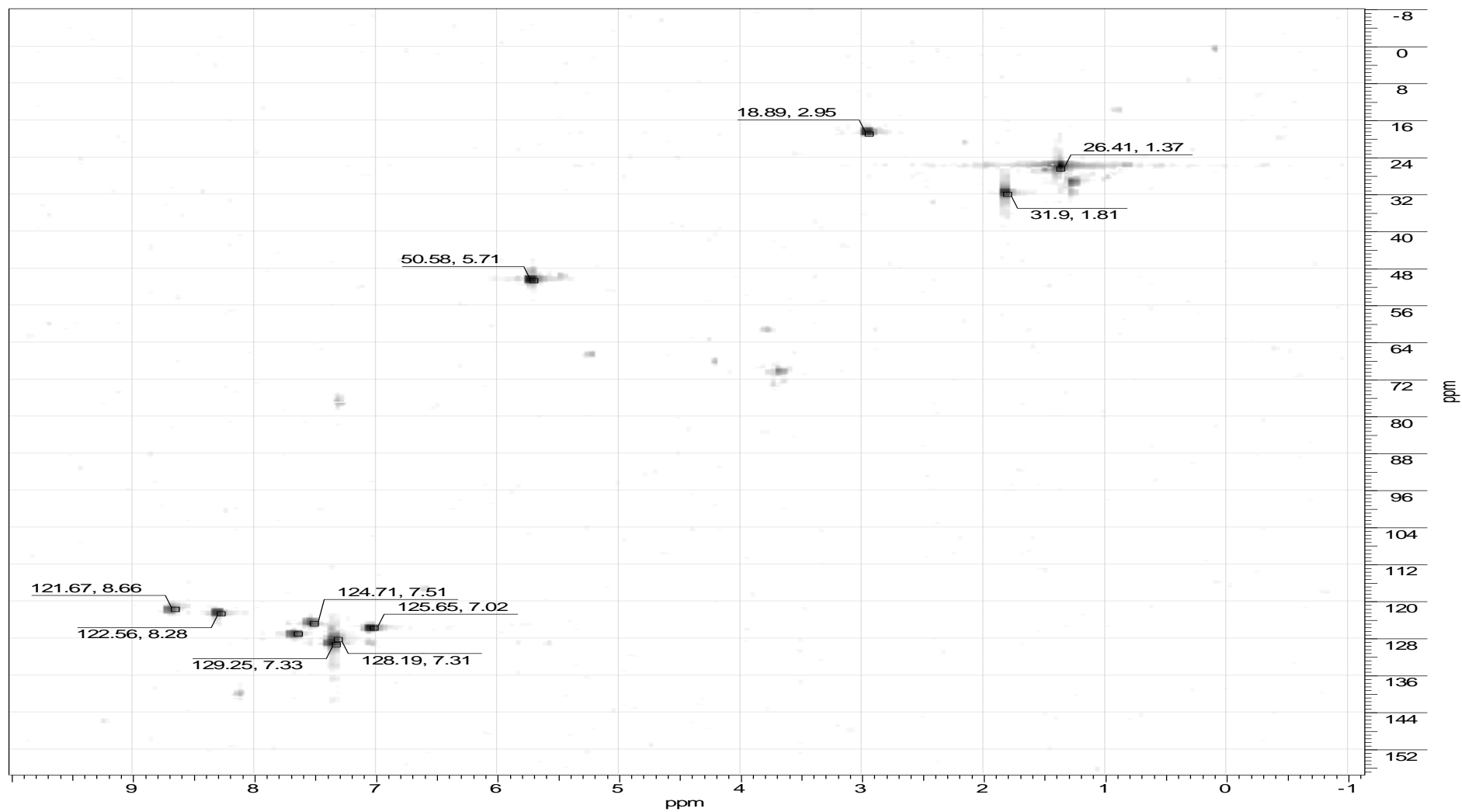
Espectro 119. RMN-¹H (400 MHz, CDCl₃) do composto 47a.



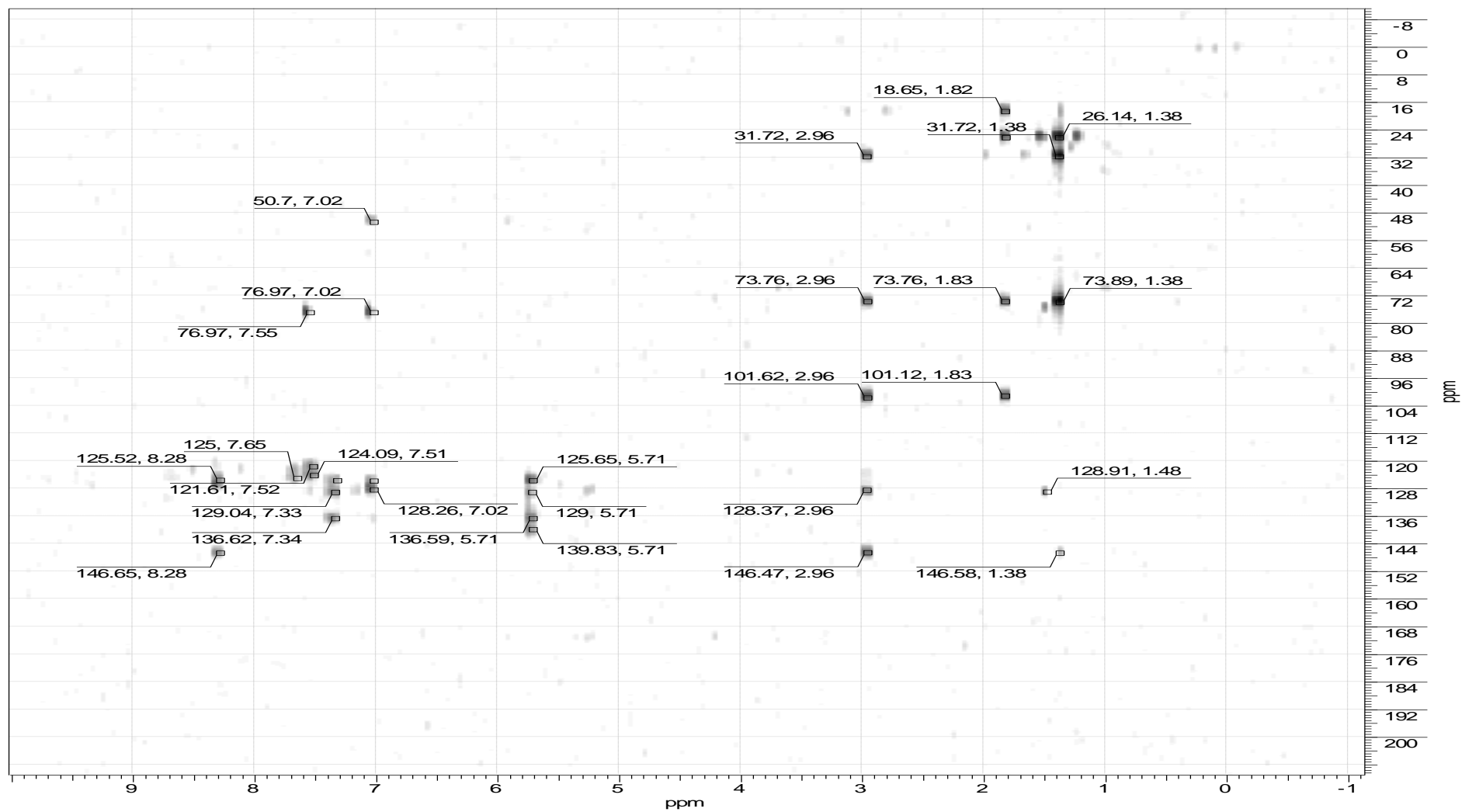
Espectro 120. RMN- ^{13}C (100 MHz, CDCl_3) do composto 47a.



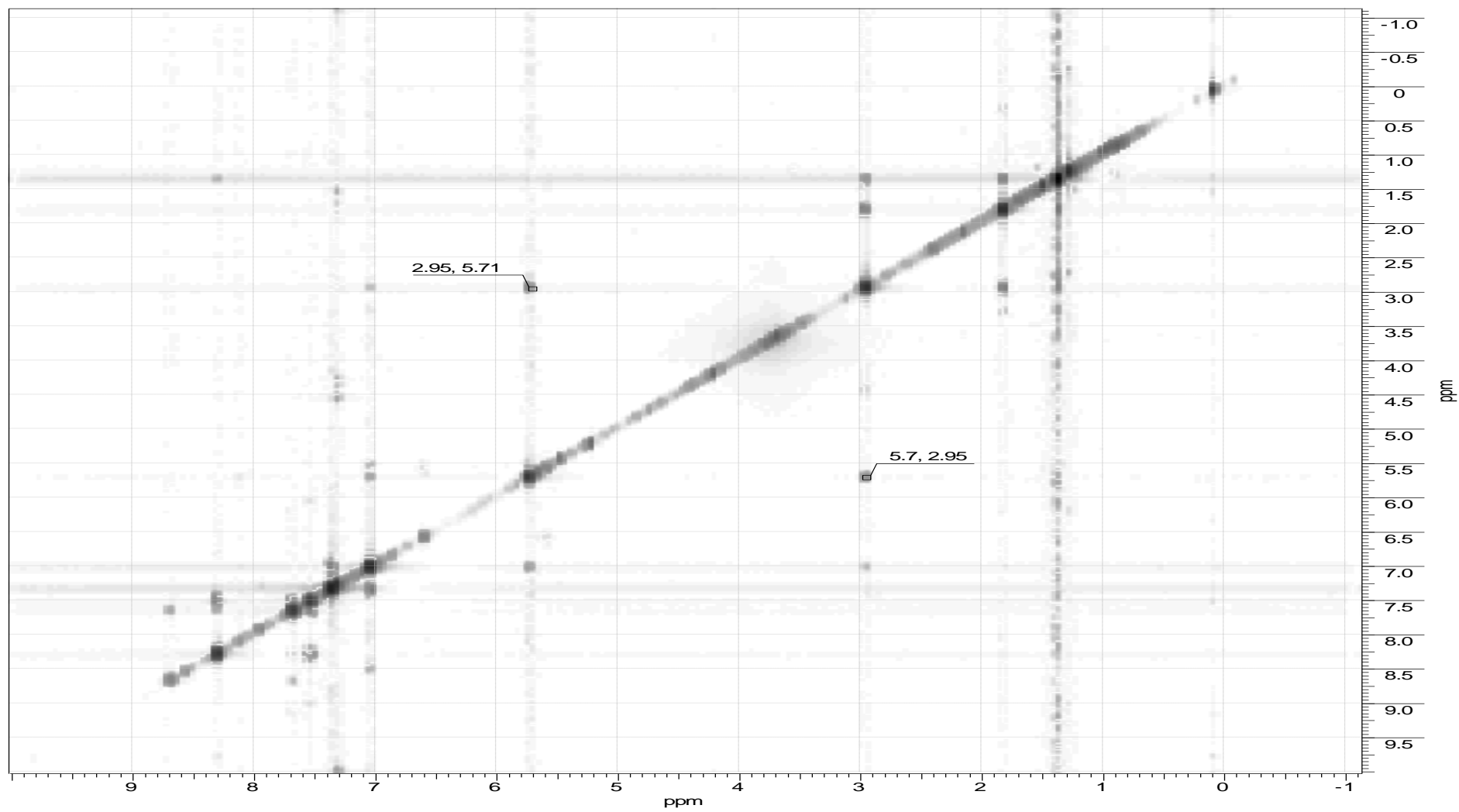
Espectro 121. ^1H -COSY (400 MHz, CDCl_3) do composto 47a.



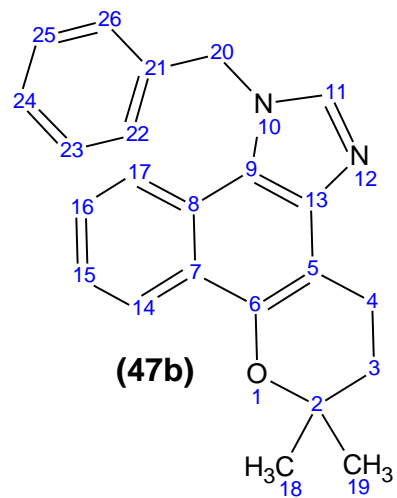
Espectro 122. HSQC (400 MHz, CDCl₃) do composto 47a.



Espectro 123. HMBC (400 MHz, CDCl₃) do composto 47a.

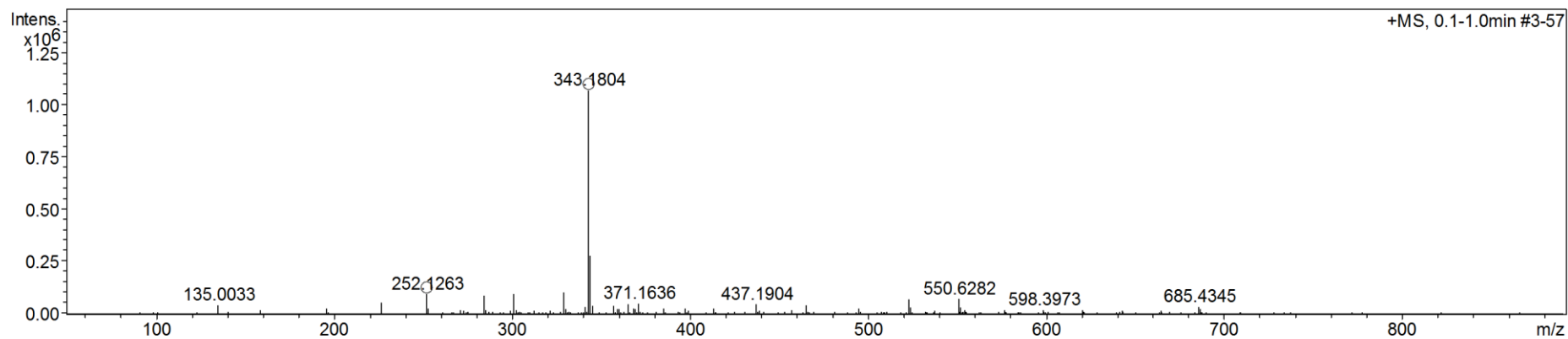


Espectro 124. NOESY (400 MHz, CDCl₃) do composto 47a.

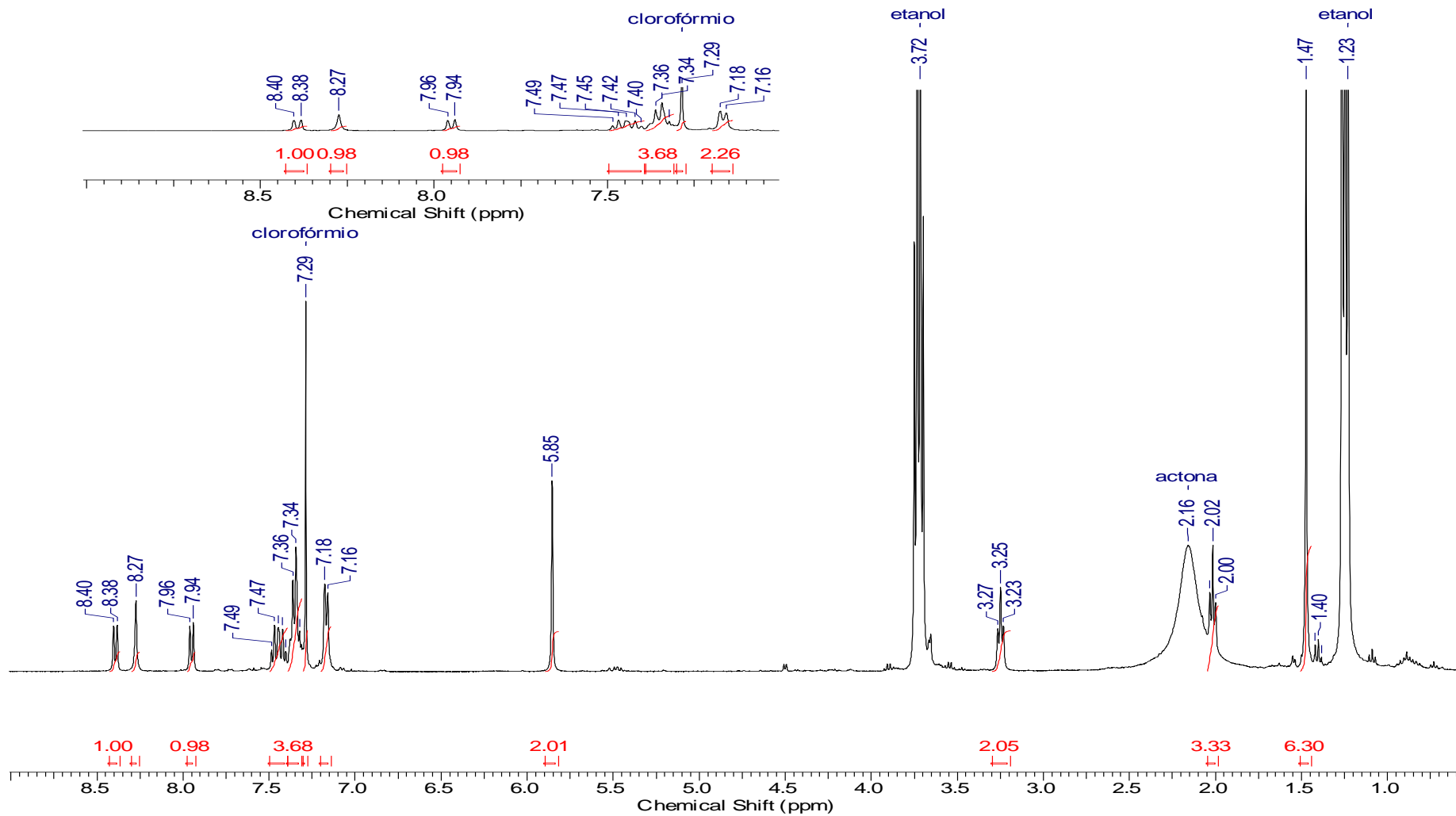


M: 342.4337 Da

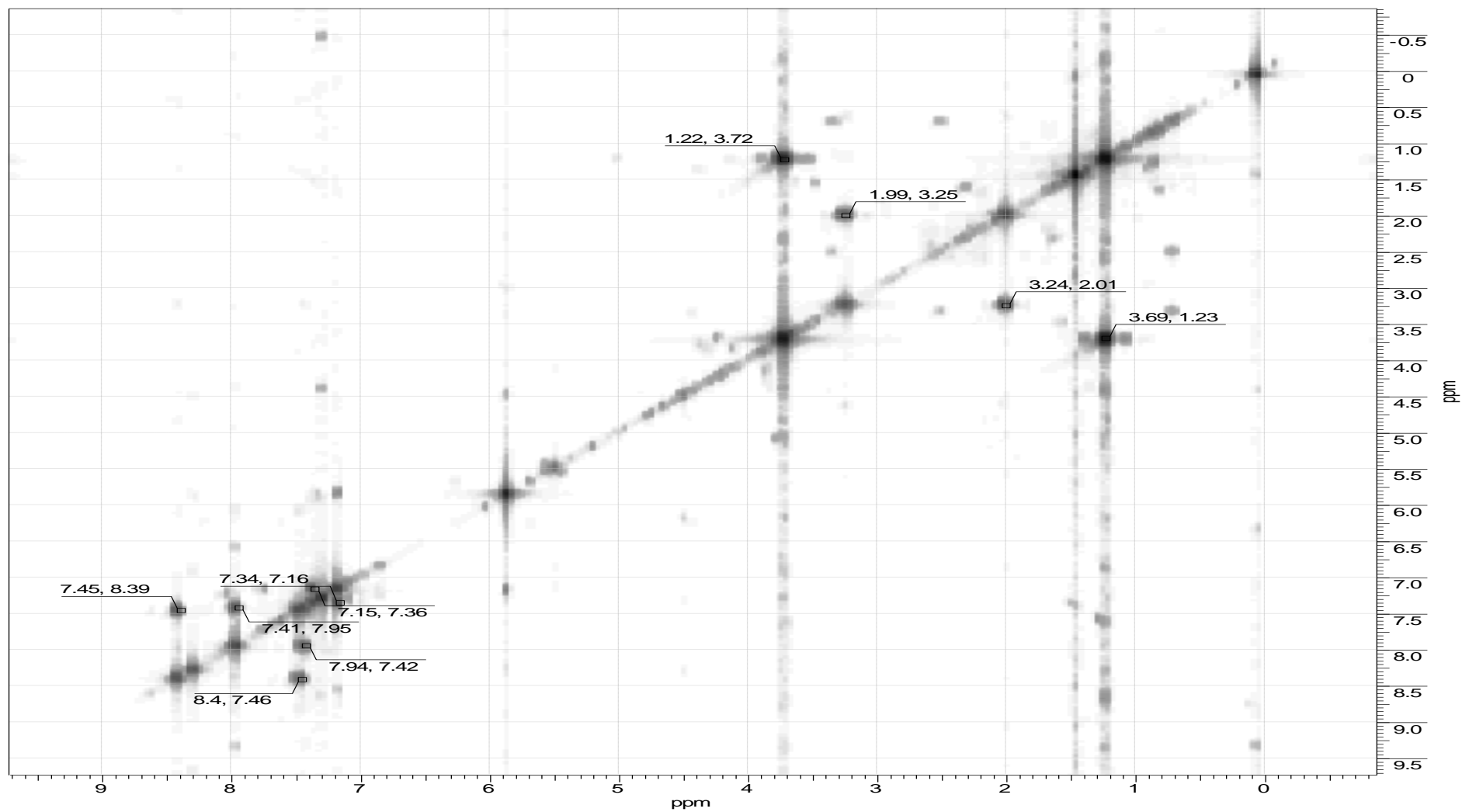
[M+H]⁺ = 343.1805 Da; err[ppm] = 0,4



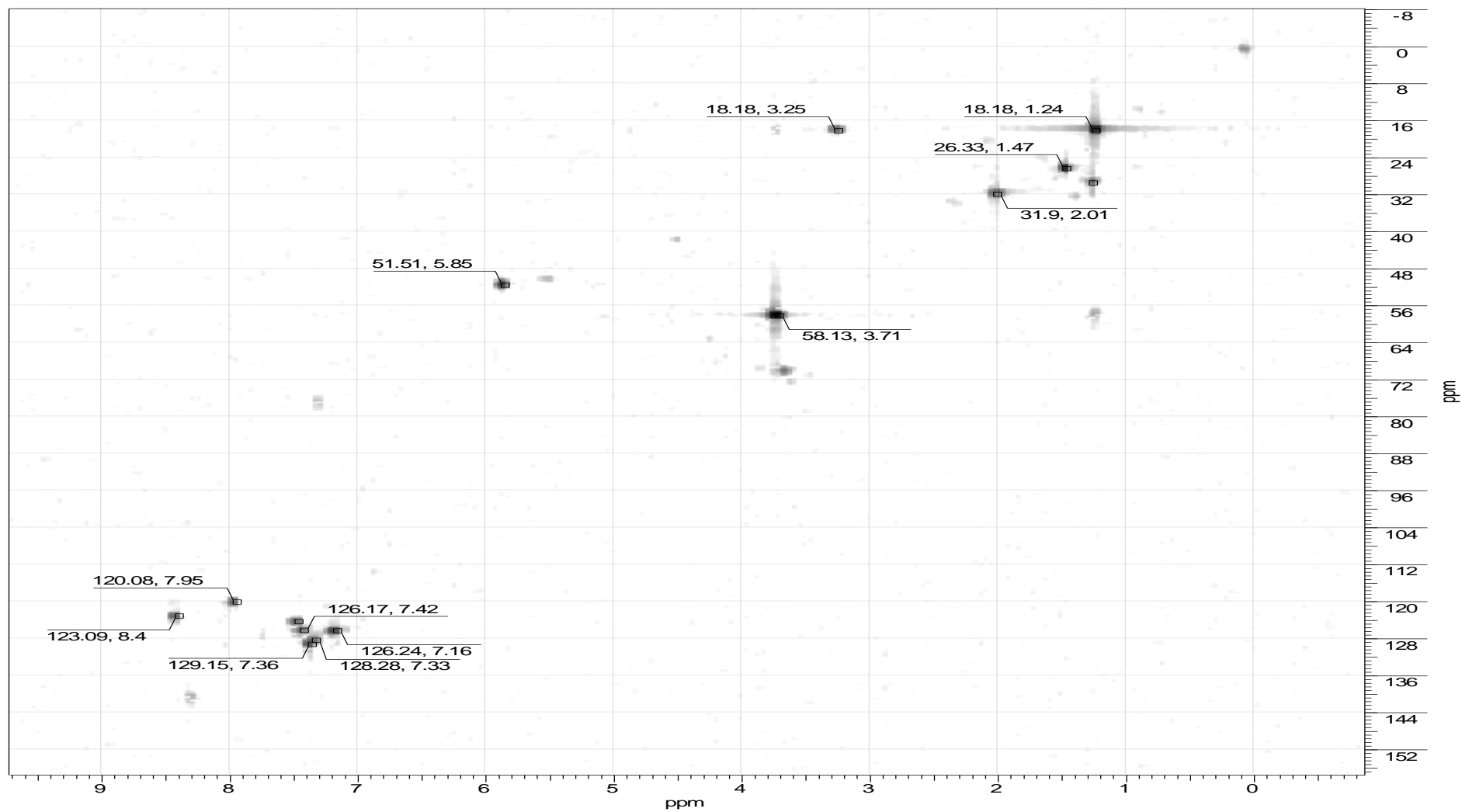
Espectro 125. EM-IES do composto 47b.



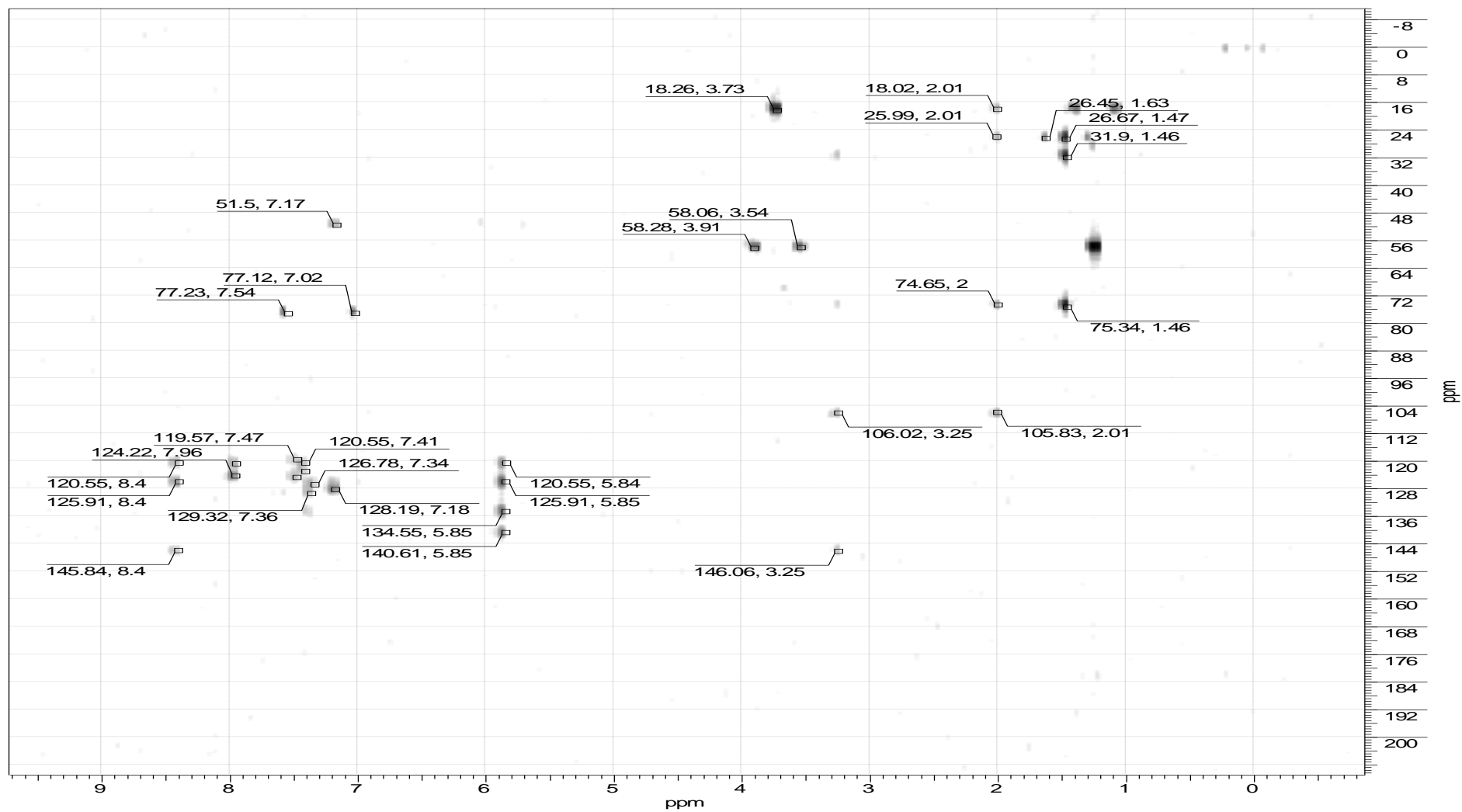
Espectro 126. RMN- ^1H (400 MHz, CDCl_3) do composto 47b.



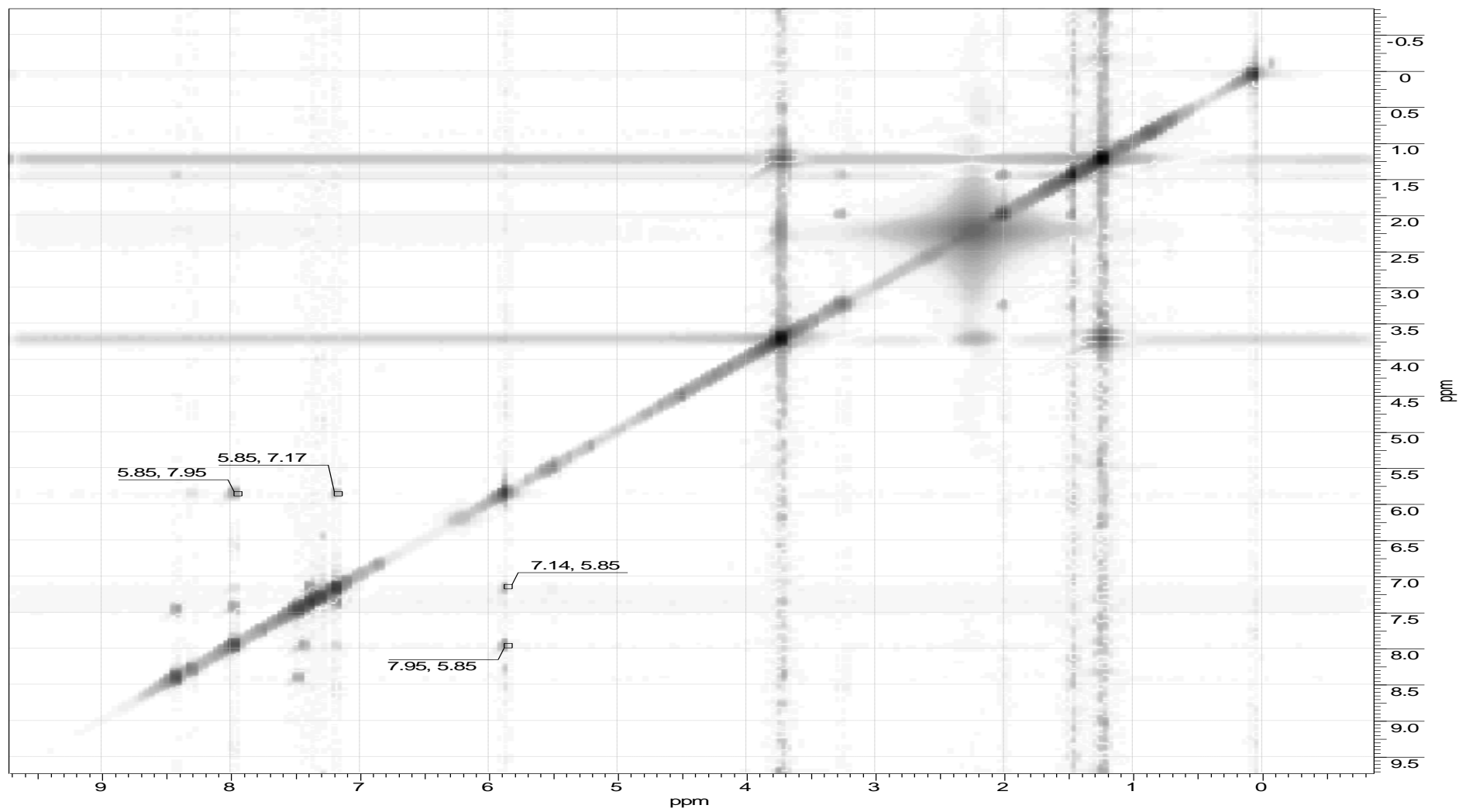
Espectro 128. ^1H -COSY (400 MHz, CDCl_3) do composto 47b.



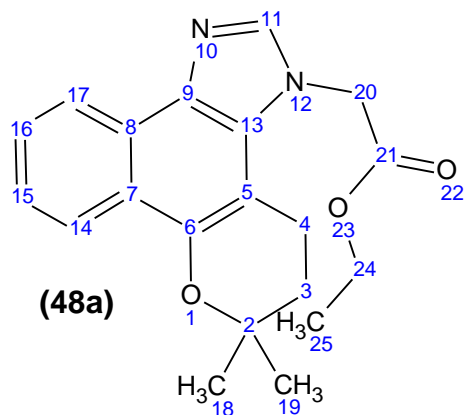
Espectro 129. HSQC (400 MHz, CDCl₃) do composto 47b.



Espectro 130. HMBC (400 MHz, CDCl₃) do composto 47b.

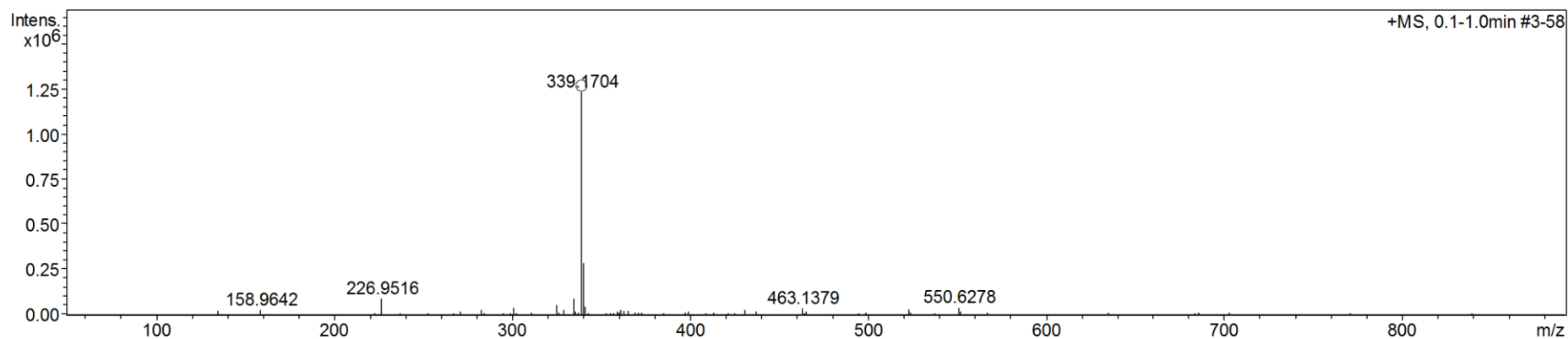


Espectro 131. NOESY (400 MHz, CDCl₃) do composto 47b.

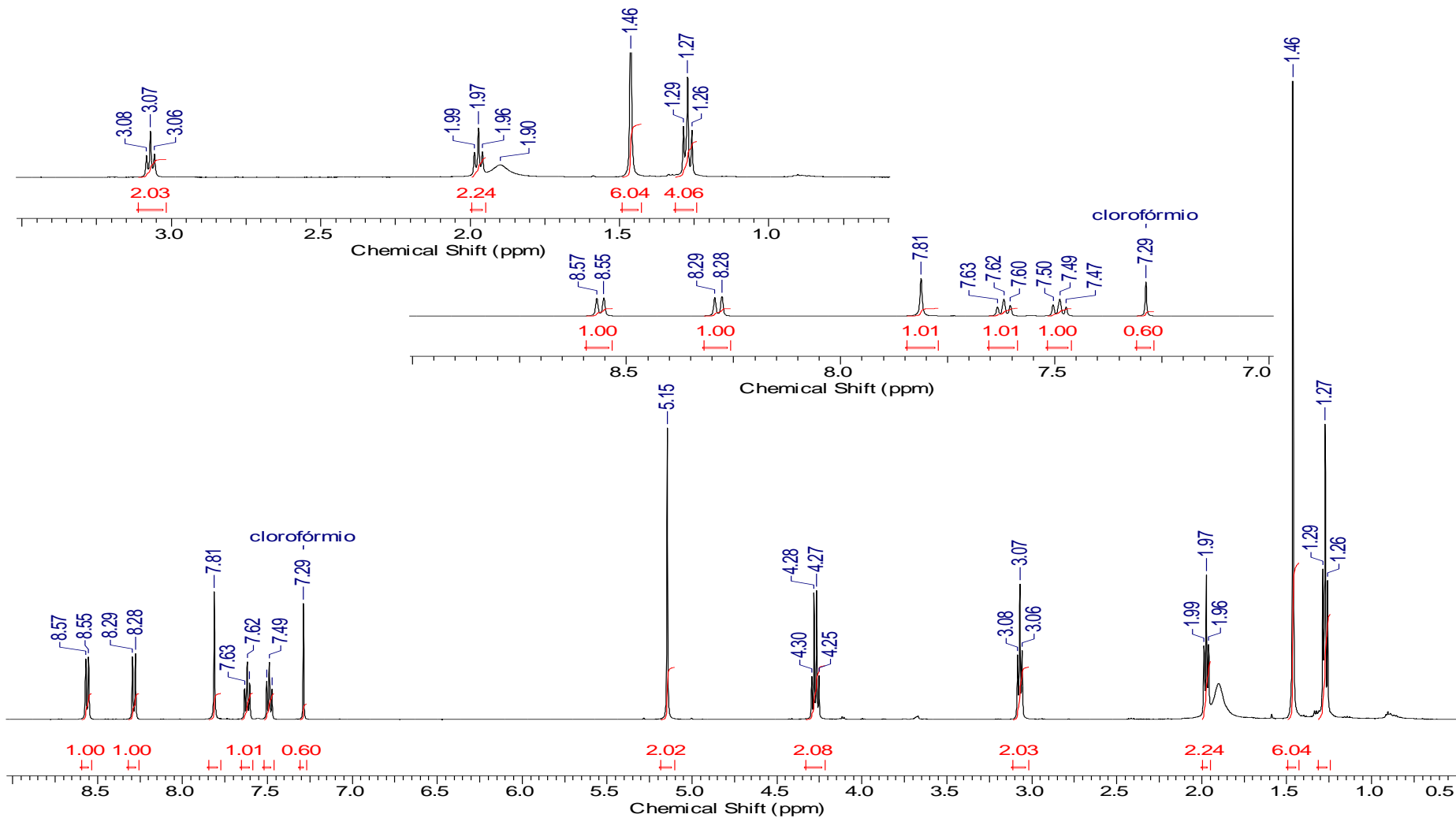


M: 338.4004 Da

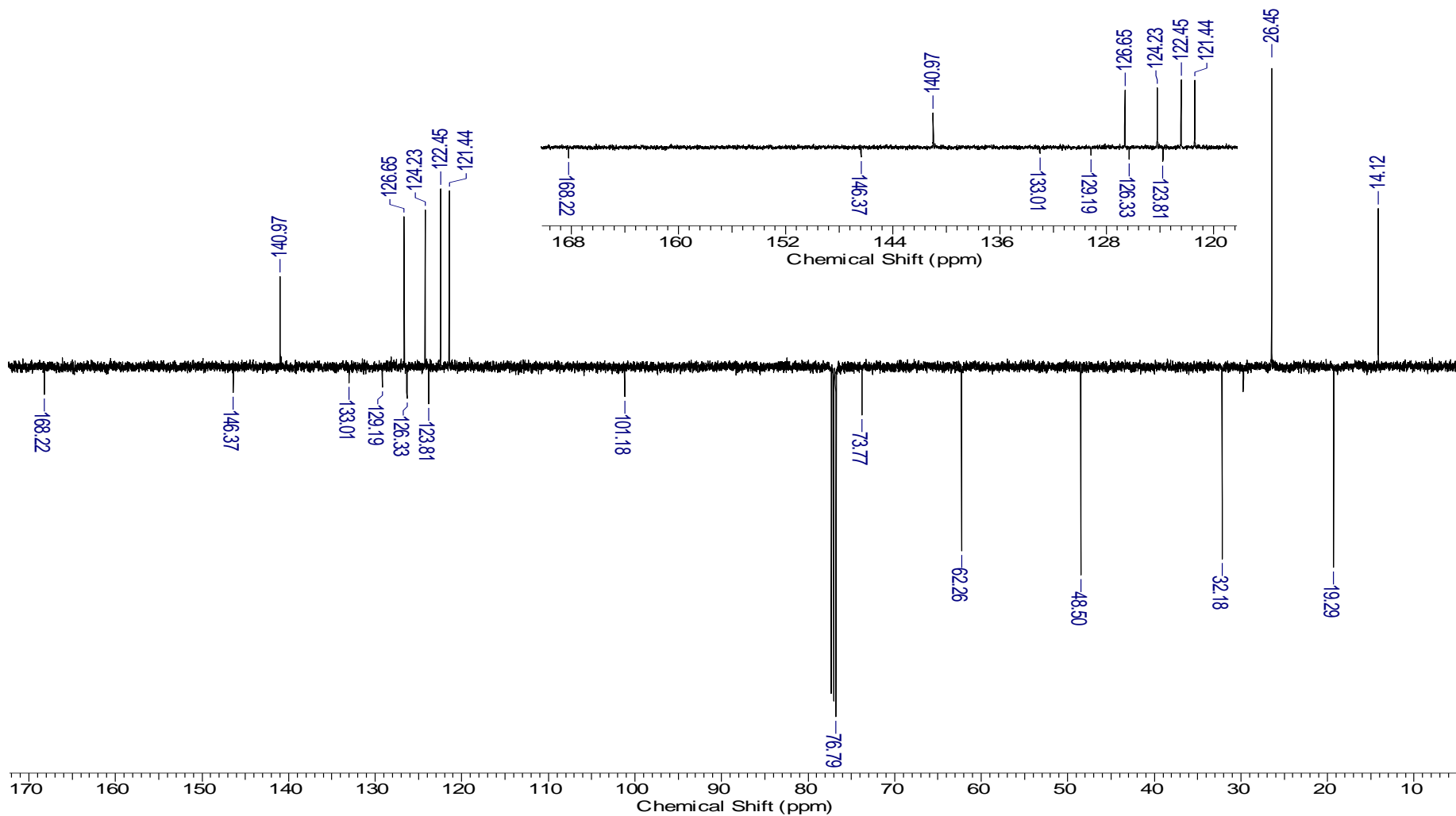
[M+H]⁺ = 339.1703 Da; err[ppm] = -0,1



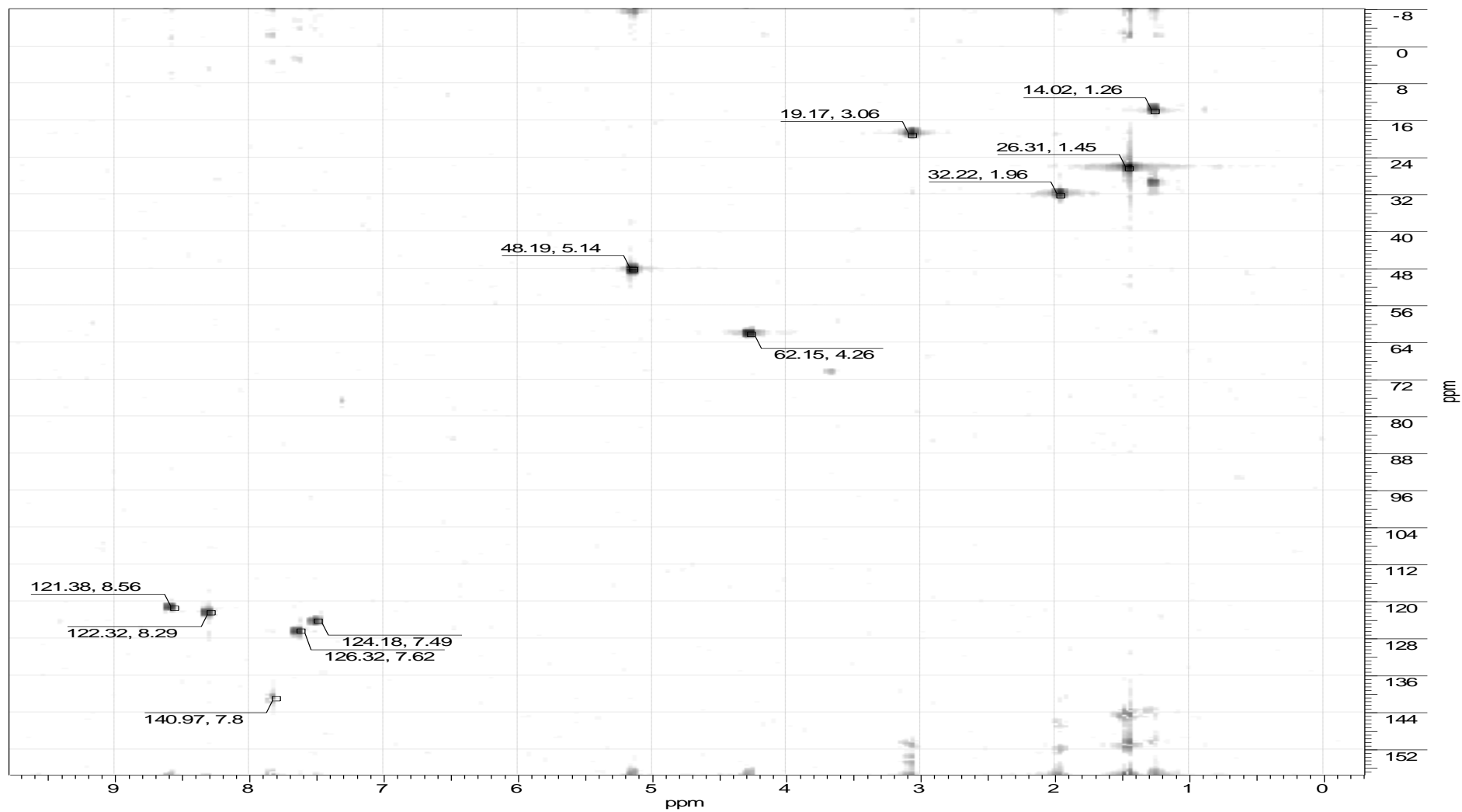
Espectro 132. EM-IES do composto 48a.



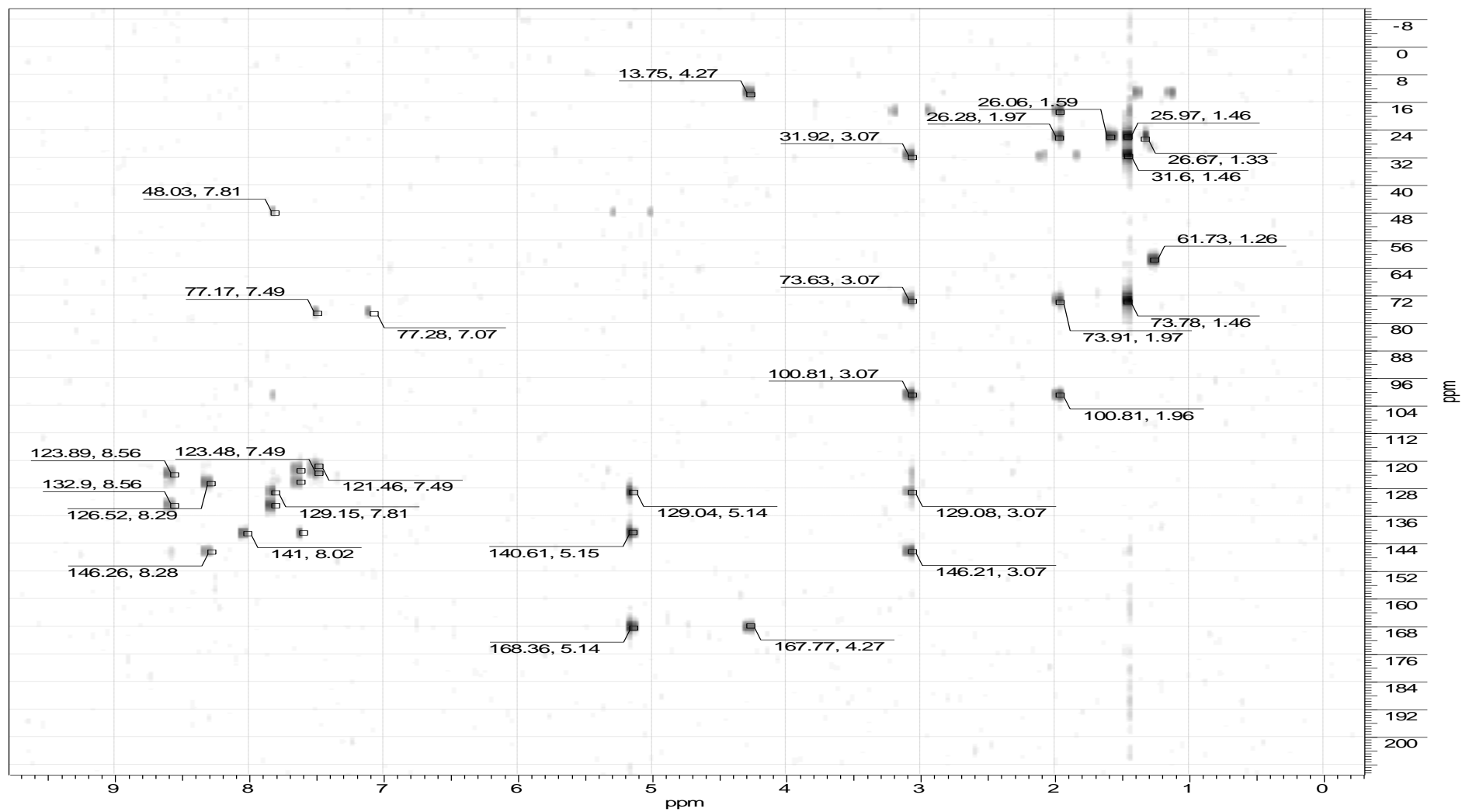
Espectro 133. RMN-¹H (500 MHz, CDCl₃) do composto 48a.



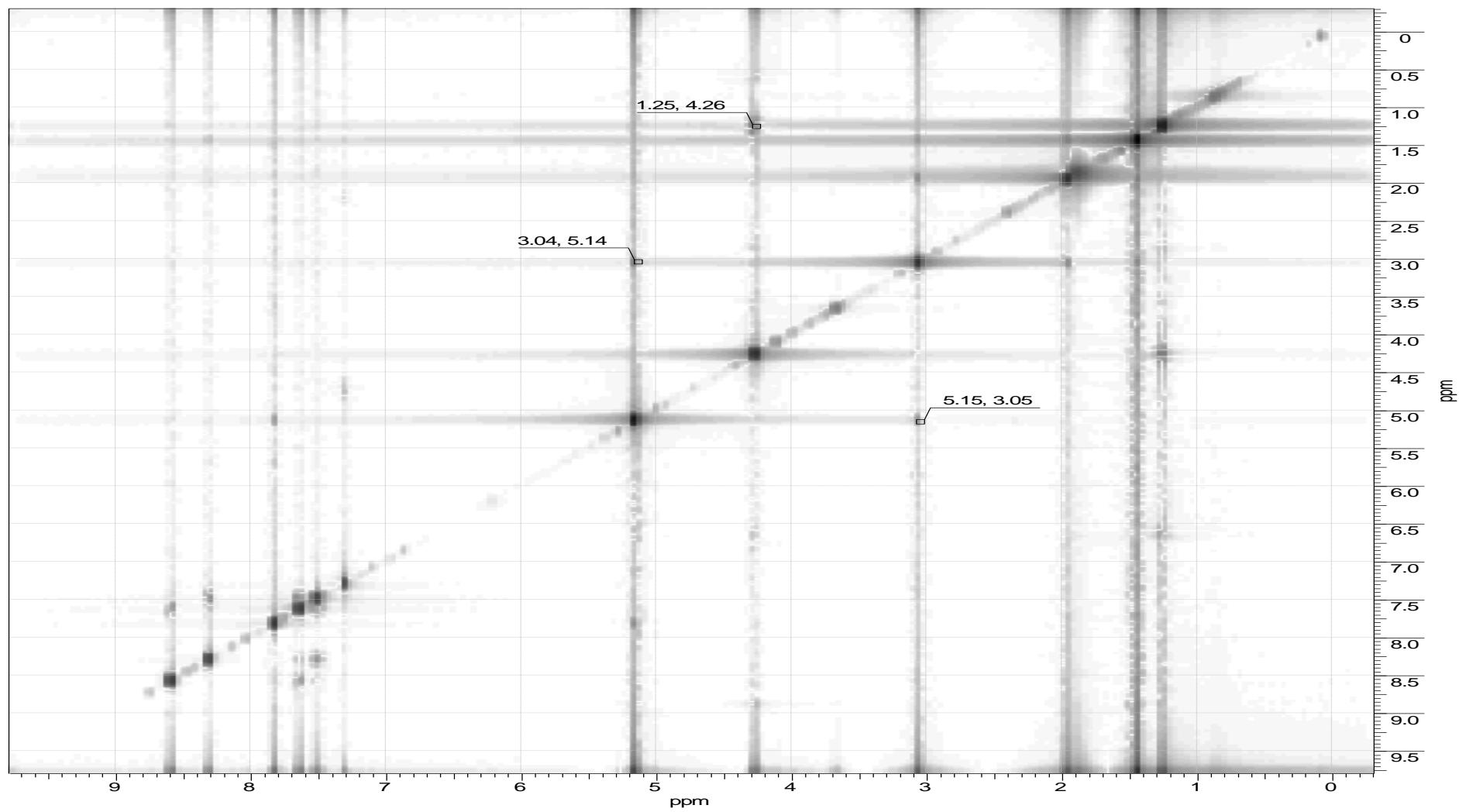
Espectro 134. RMN-¹³C (125 MHz, CDCl₃) do composto 48a.



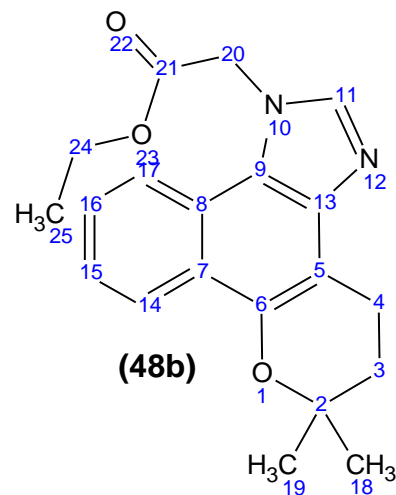
Espectro 135. HSQC (500 MHz, CDCl₃) do composto 48a.



Espectro 136. HMBC (500 MHz, CDCl₃) do composto 48a.

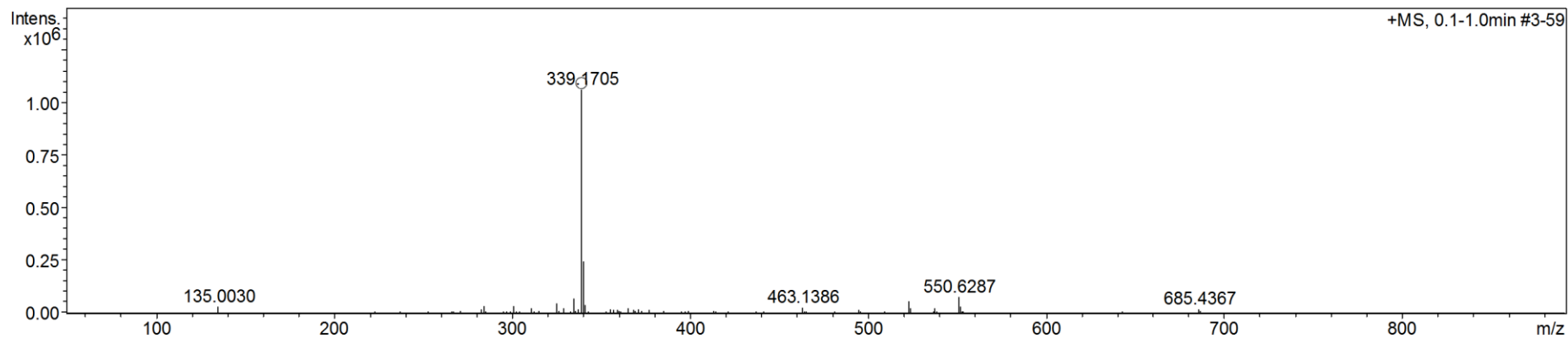


Espectro 137. NOESY (500 MHz, CDCl₃) do composto 48a.

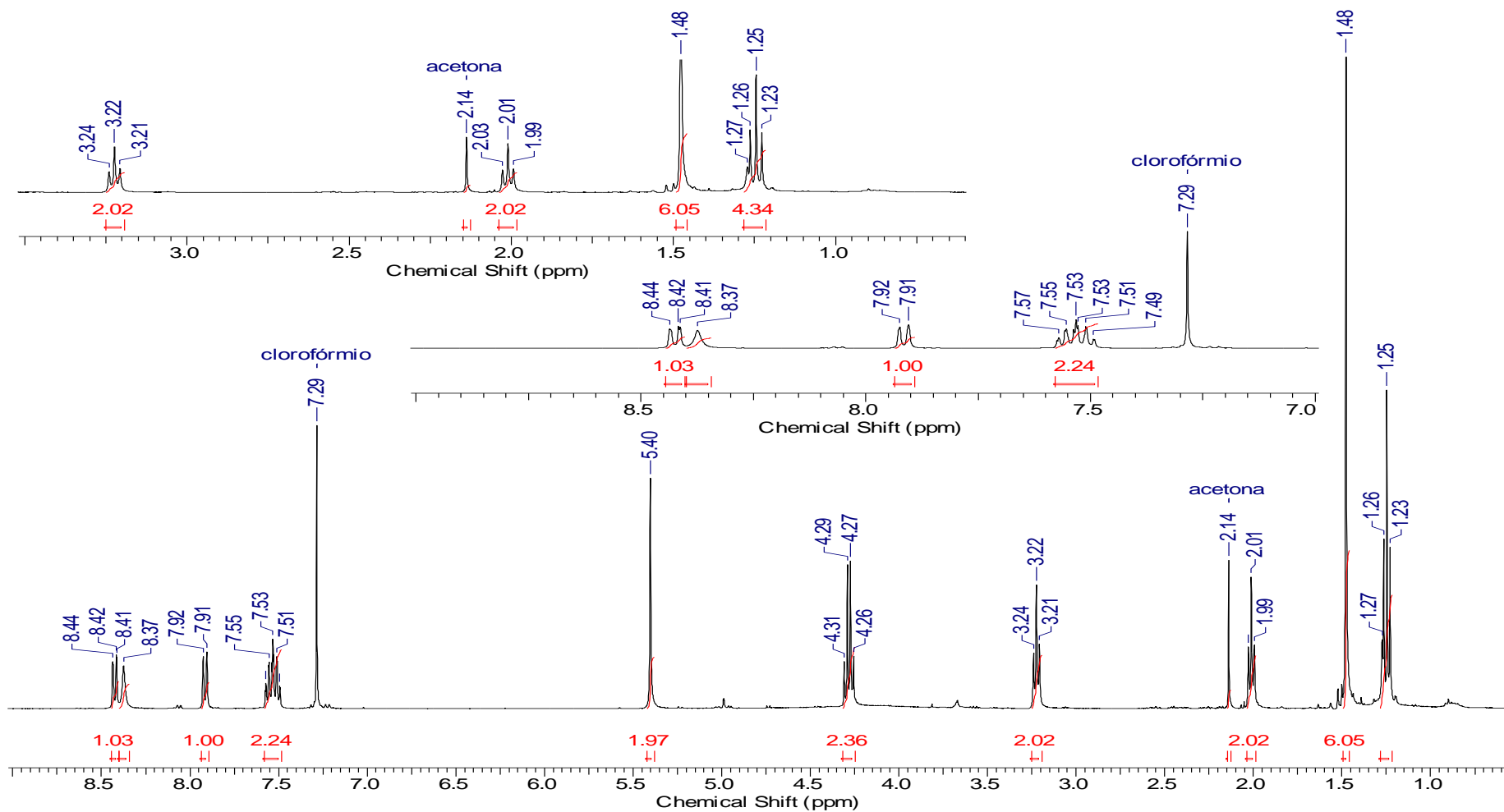


M: 338.4004 Da

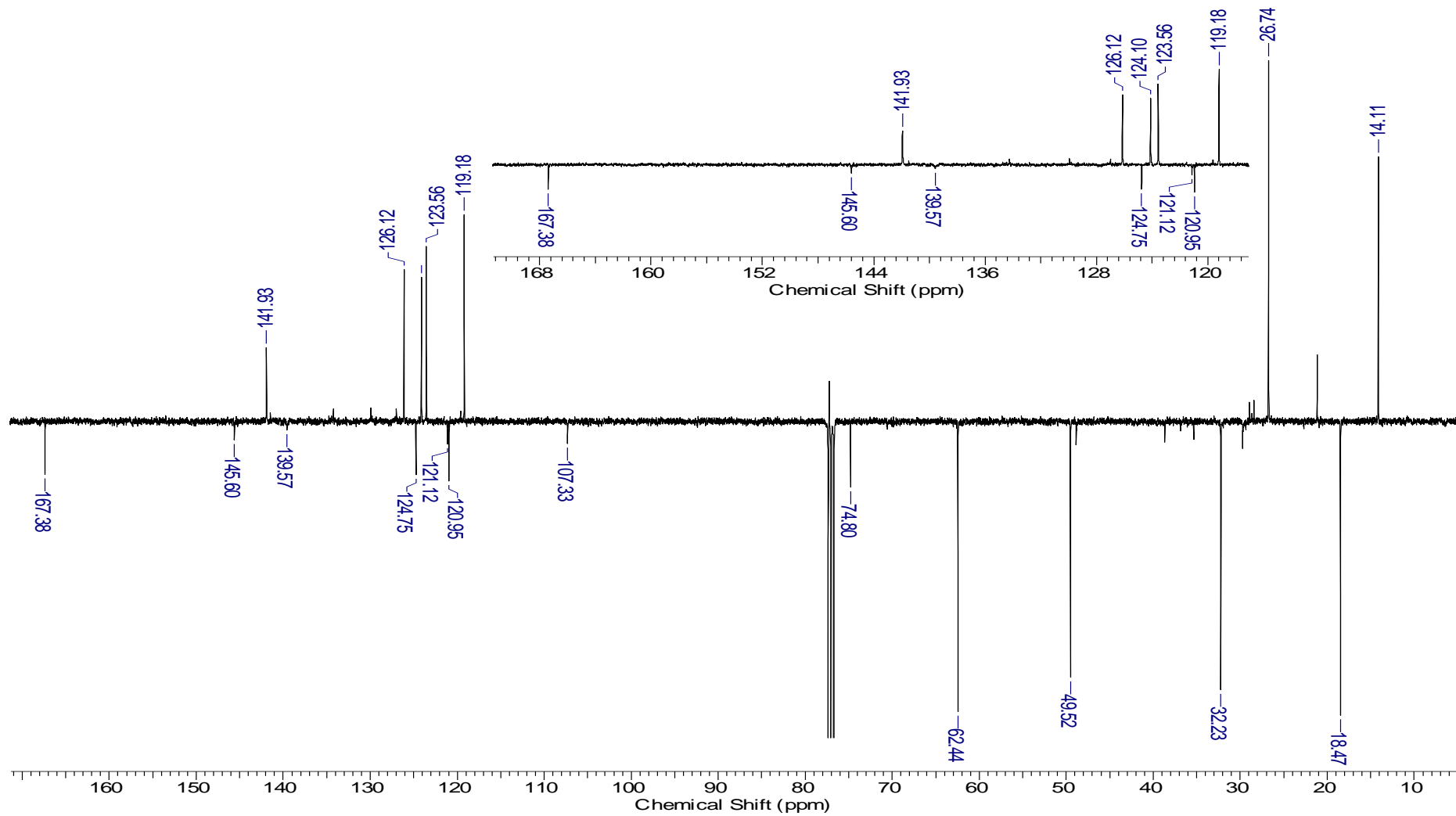
[M+H]⁺ = 339.1703 Da; err[ppm] = -0,4



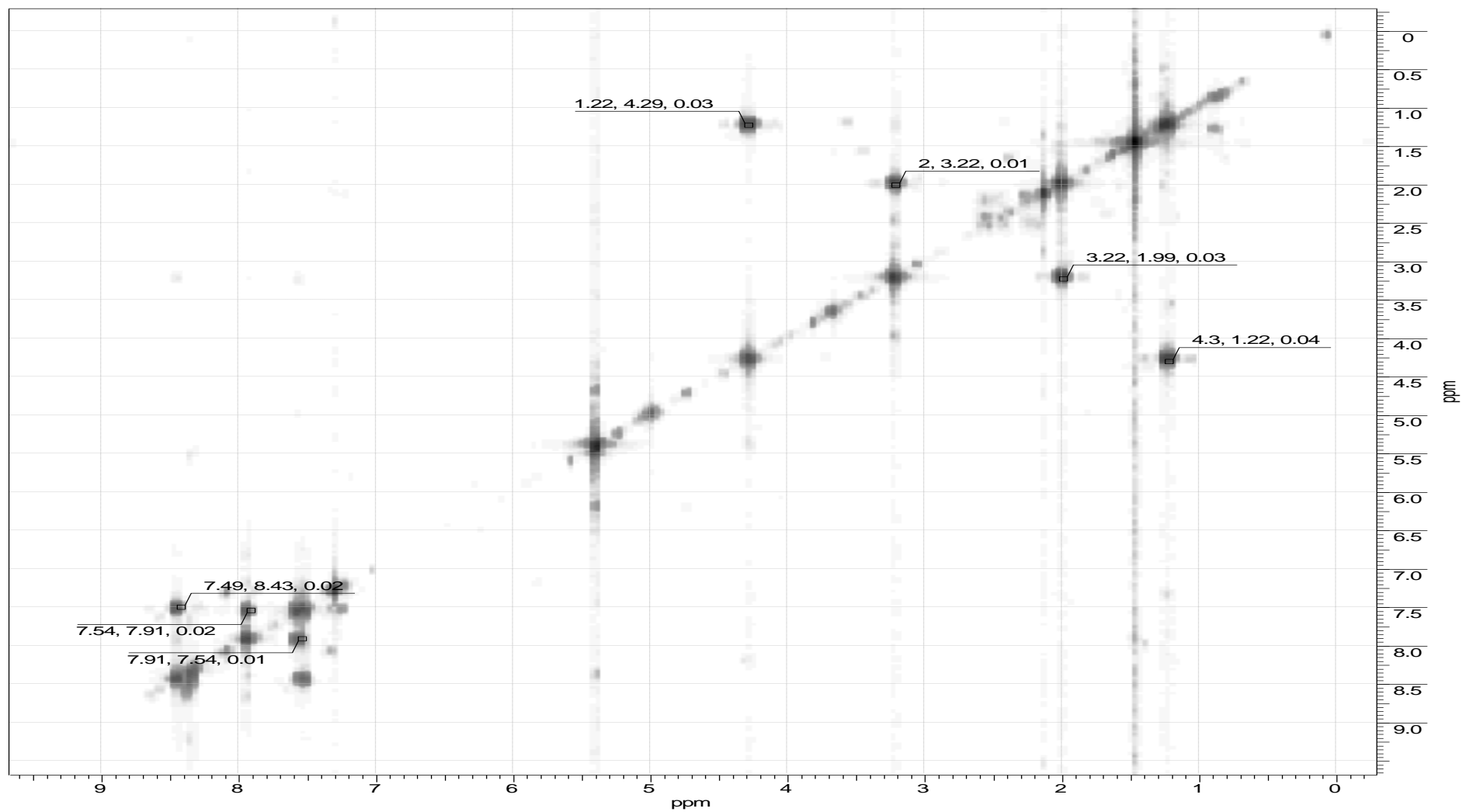
Espectro 138. EM-IES do composto 48b.



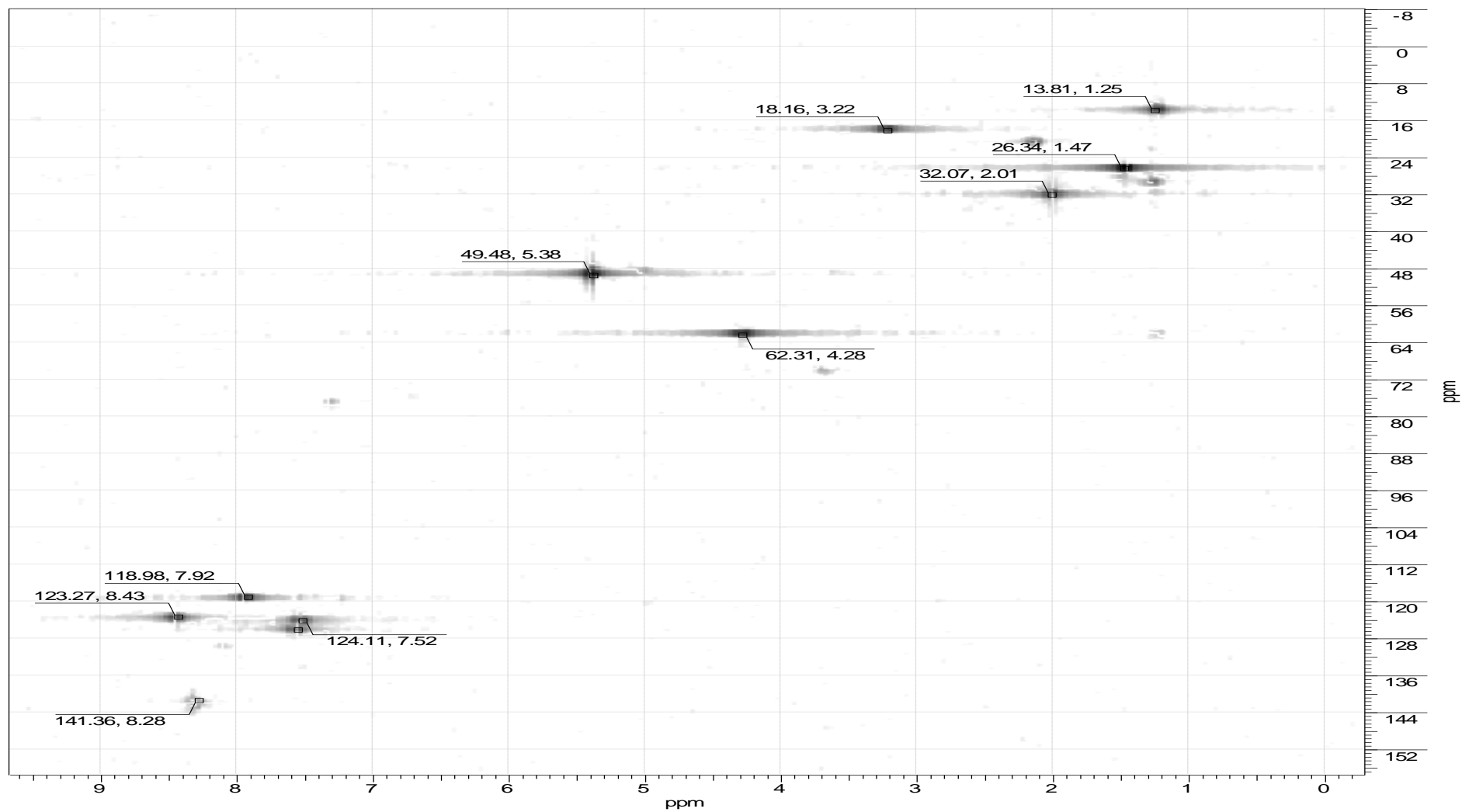
Espectro 139. RMN- ^1H (400 MHz, CDCl_3) do composto 48b.



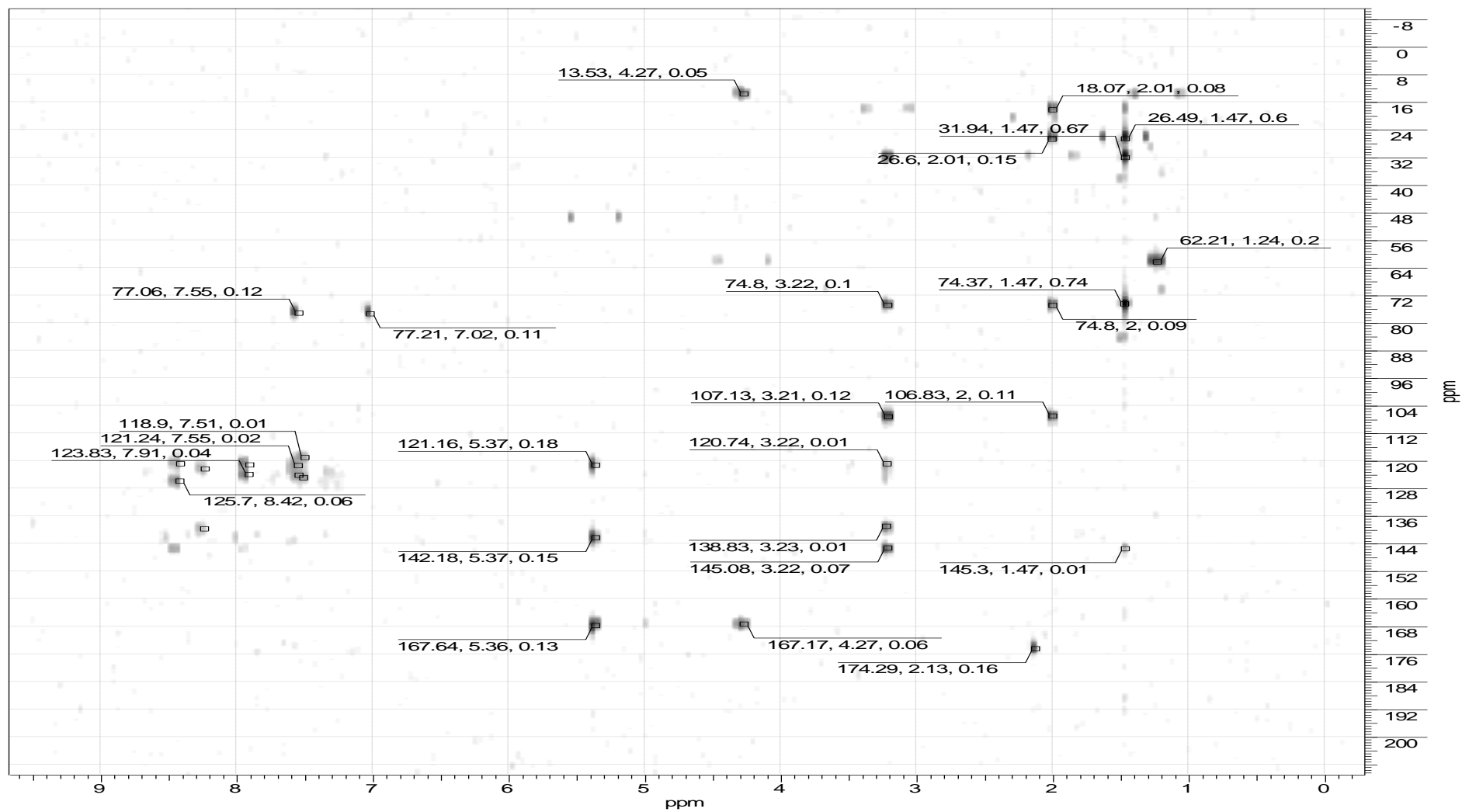
Espectro 140. RMN-¹³C (100 MHz, CDCl₃) do composto 48b.



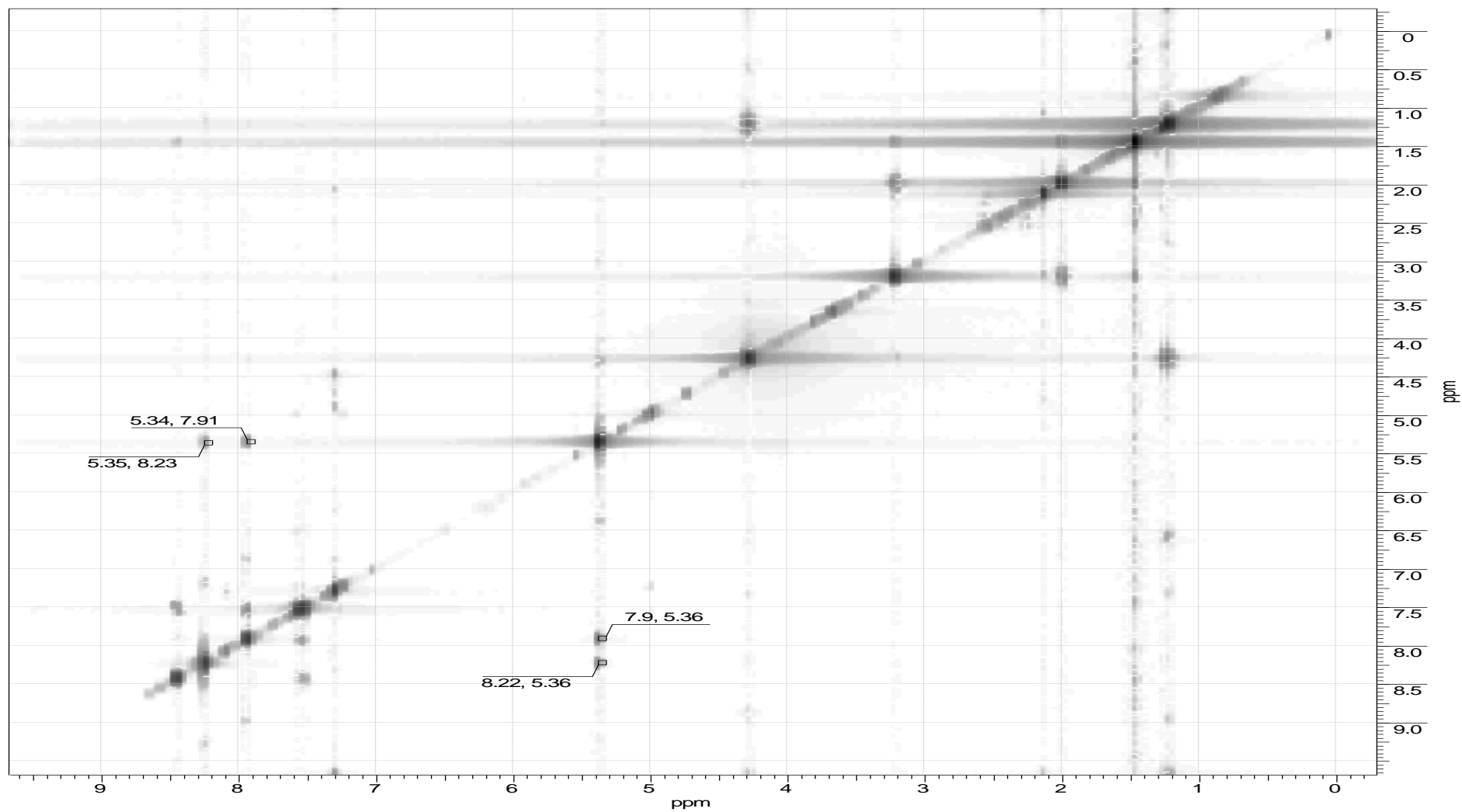
Espectro 141. ^1H -COSY (400 MHz, CDCl_3) do composto 48b.



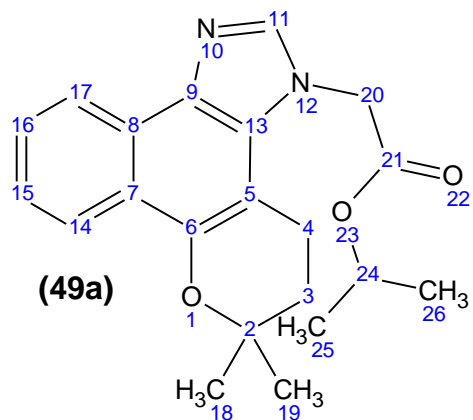
Espectro 142. HSQC (400 MHz, CDCl₃) do composto 48b.



Espectro 143. HMBC (400 MHz, CDCl₃) do composto 48b.



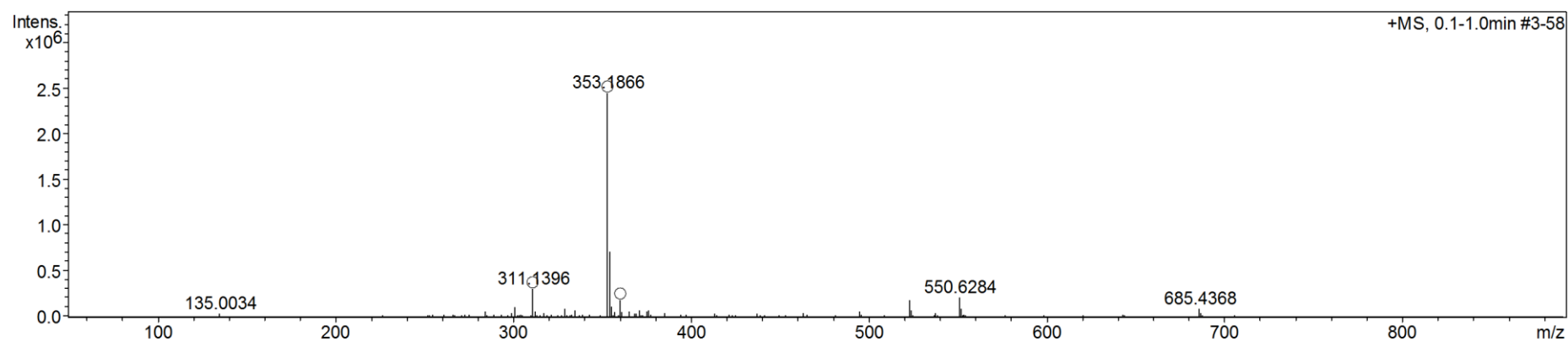
Espectro 144. NOESY (400 MHz, CDCl₃) do composto 48b.



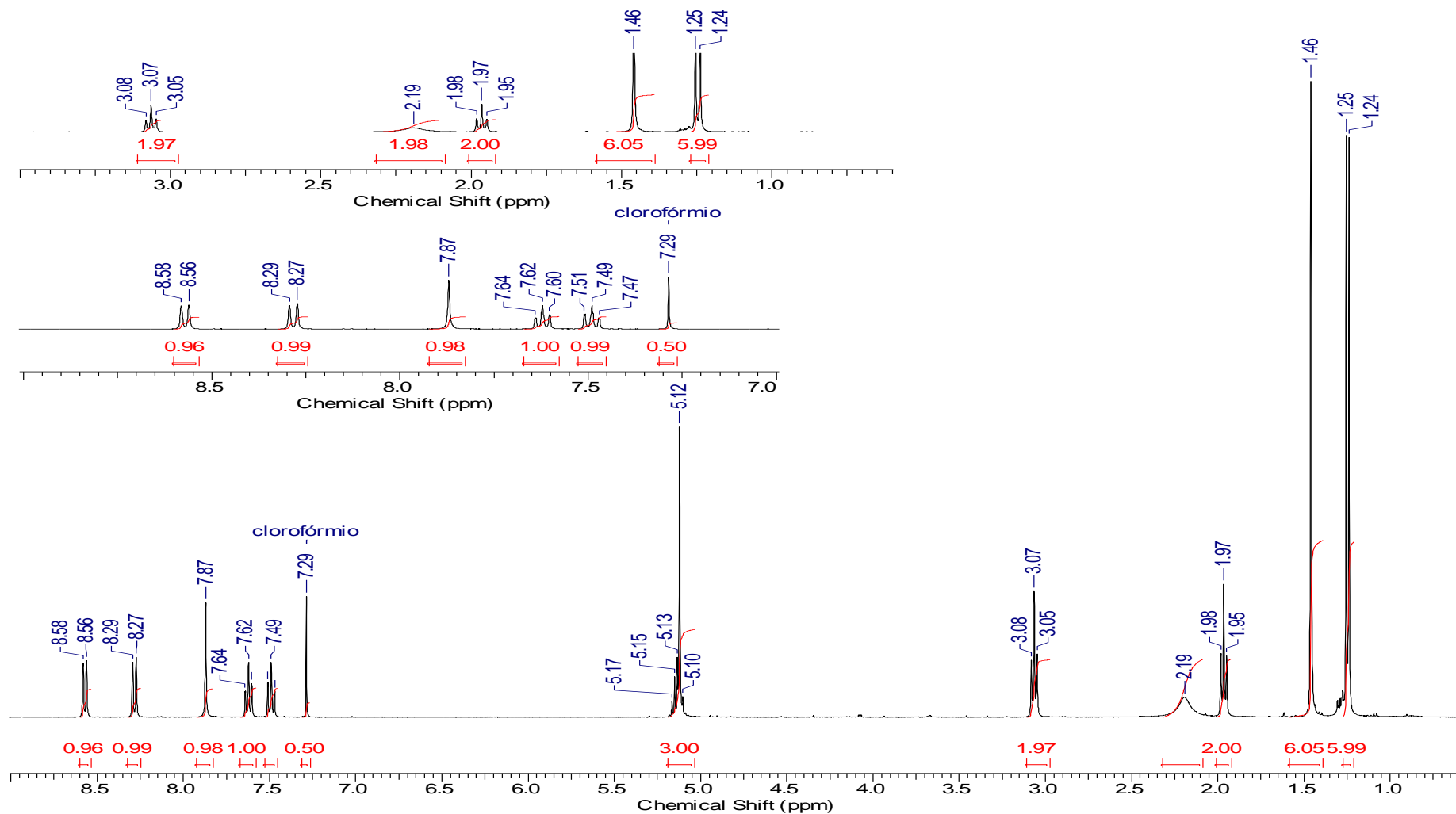
(49a)

M: 352.4269 Da

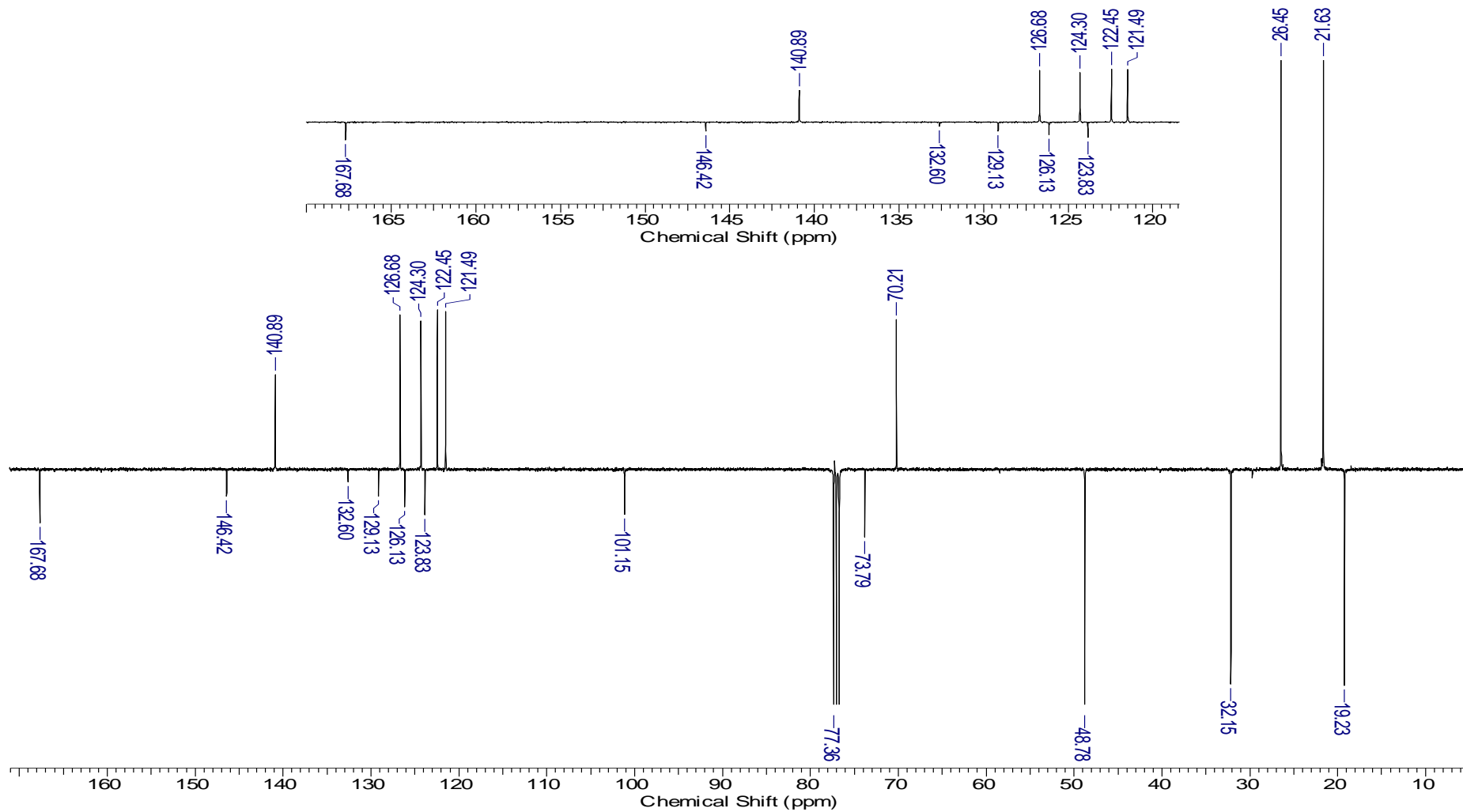
$[M+H]^+ = 353.1860$ Da; err[ppm] = -1,8



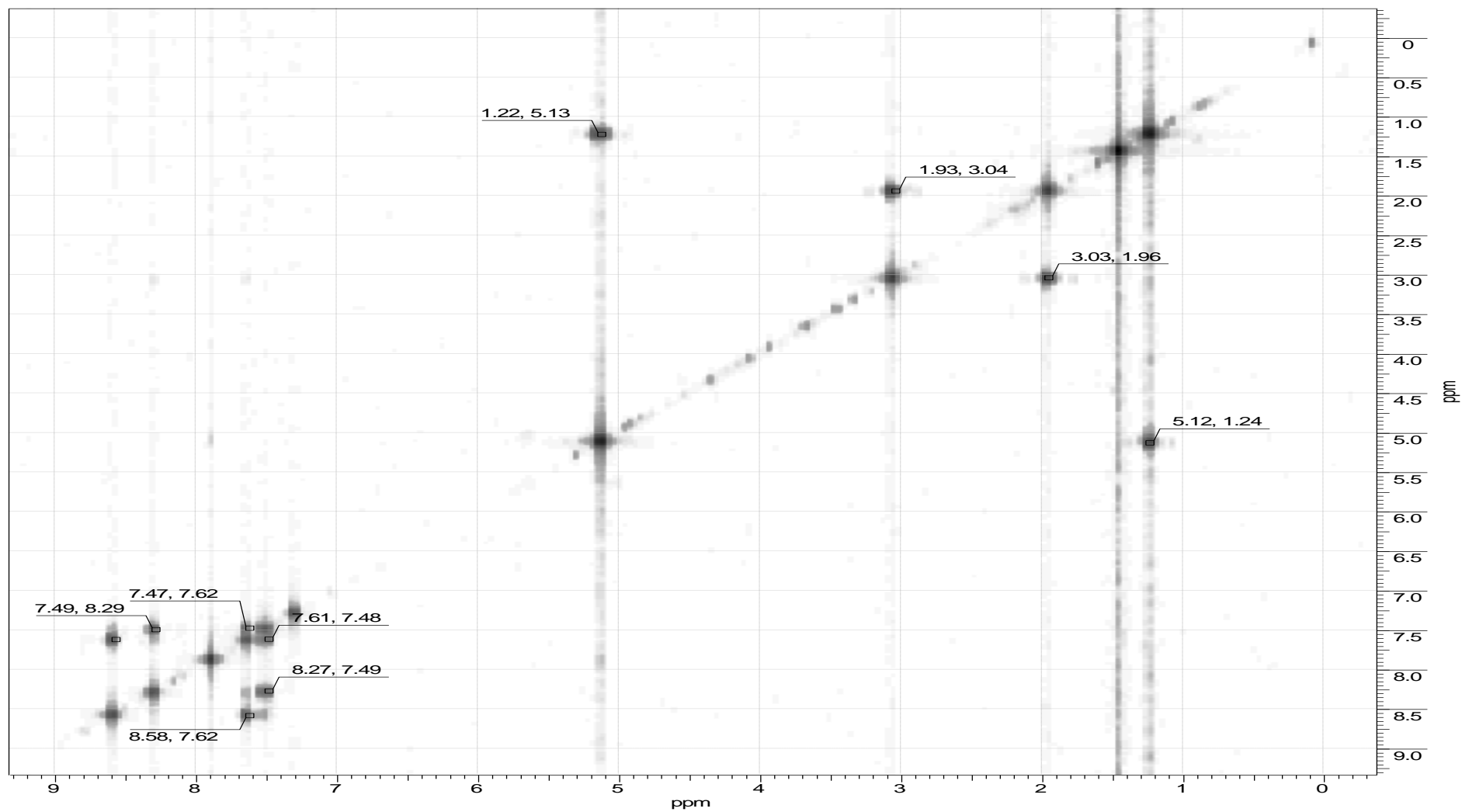
Espectro 145. EM-IES do composto 49a.



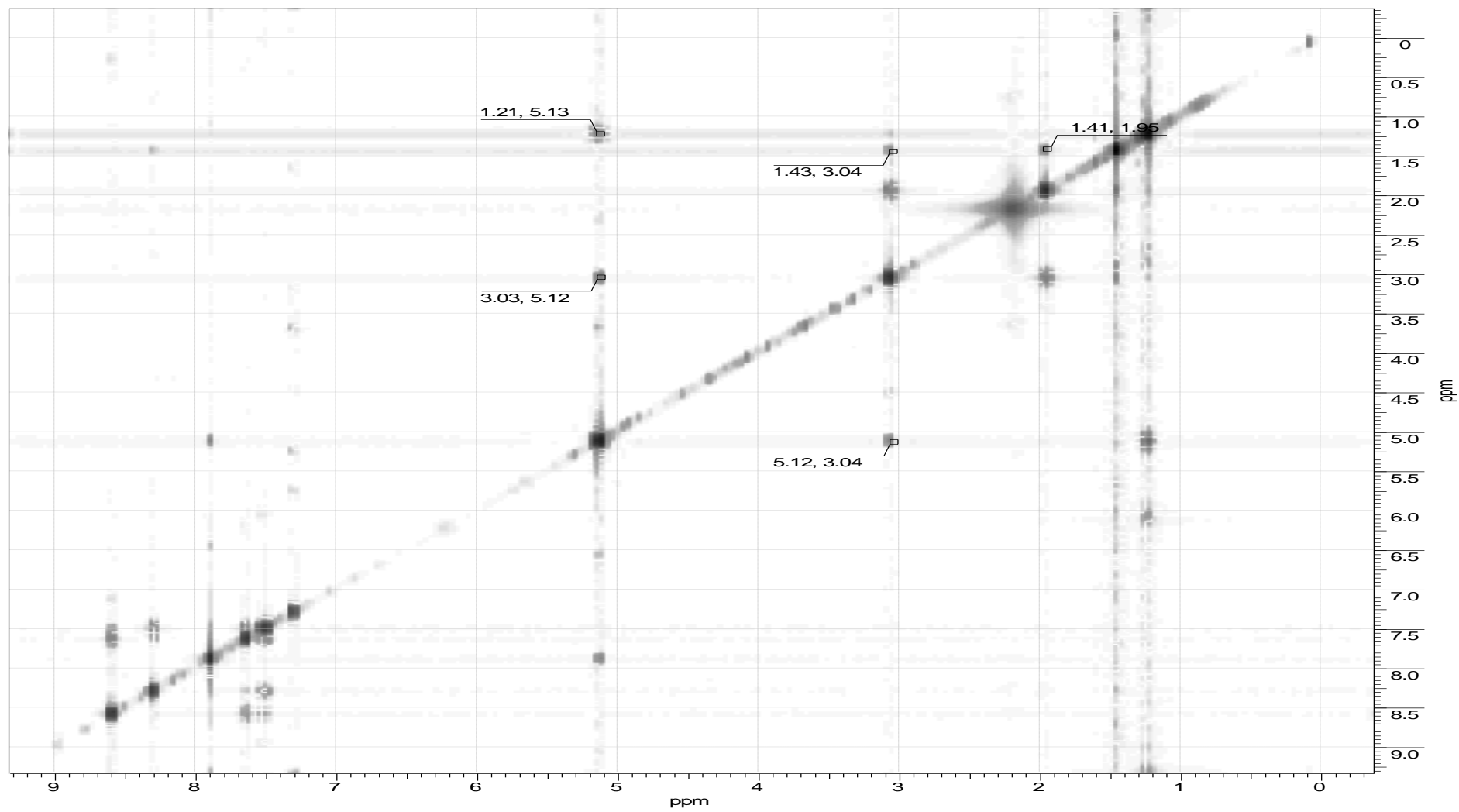
Espectro 146. RMN-¹H (400 MHz, CDCl₃) do composto 49a.



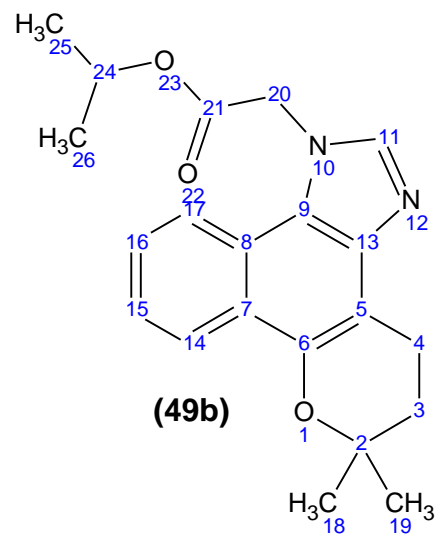
Espectro 147. RMN-¹³C (100 MHz, CDCl₃) do composto 49a.



Espectro 148. ^1H -COSY (400 MHz, CDCl_3) do composto 49a.

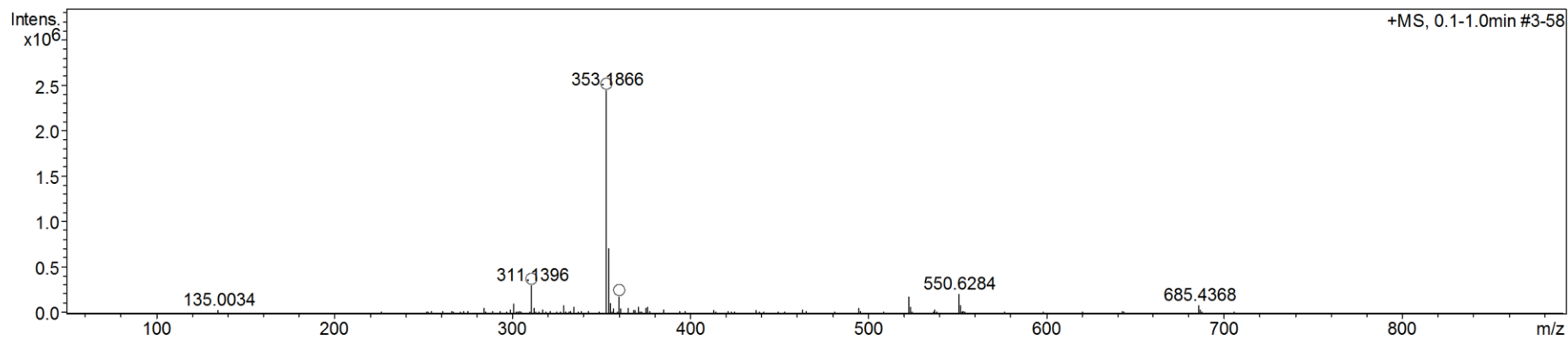


Espectro 149. NOESY (400 MHz, CDCl₃) do composto 49a.

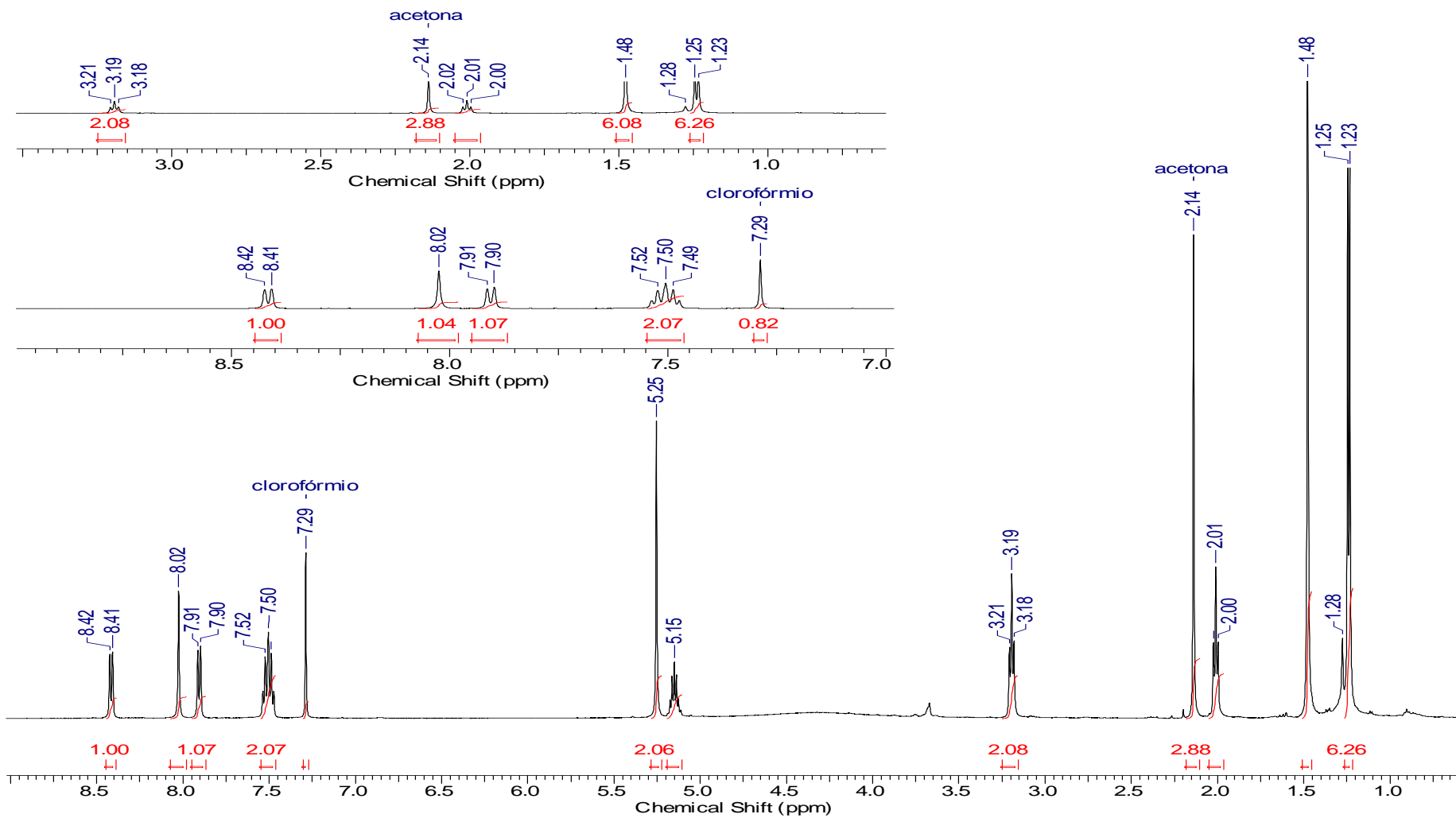


M: 352.4269 Da

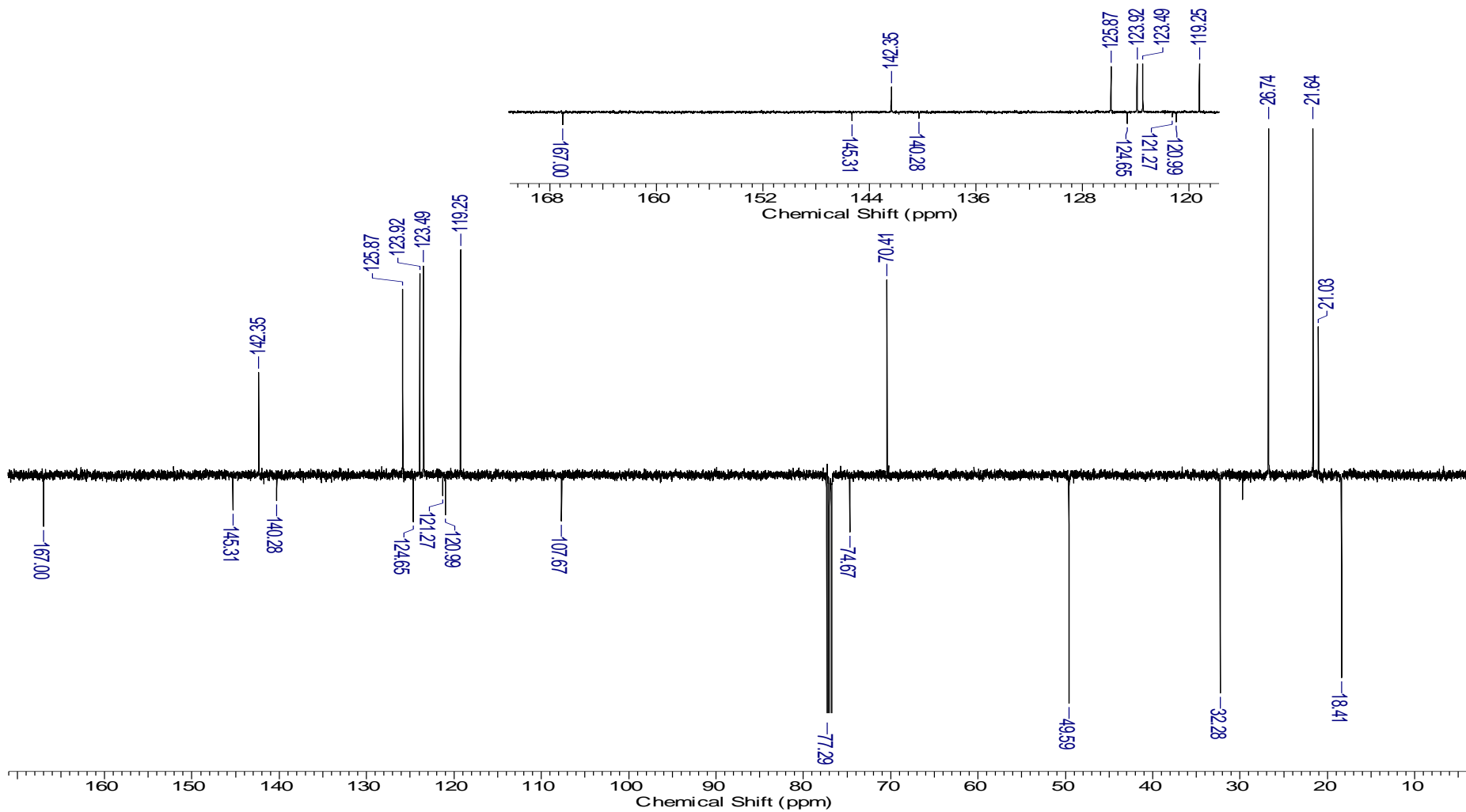
[M+H]⁺ = 353.1876 Da; err[ppm] = 1,6



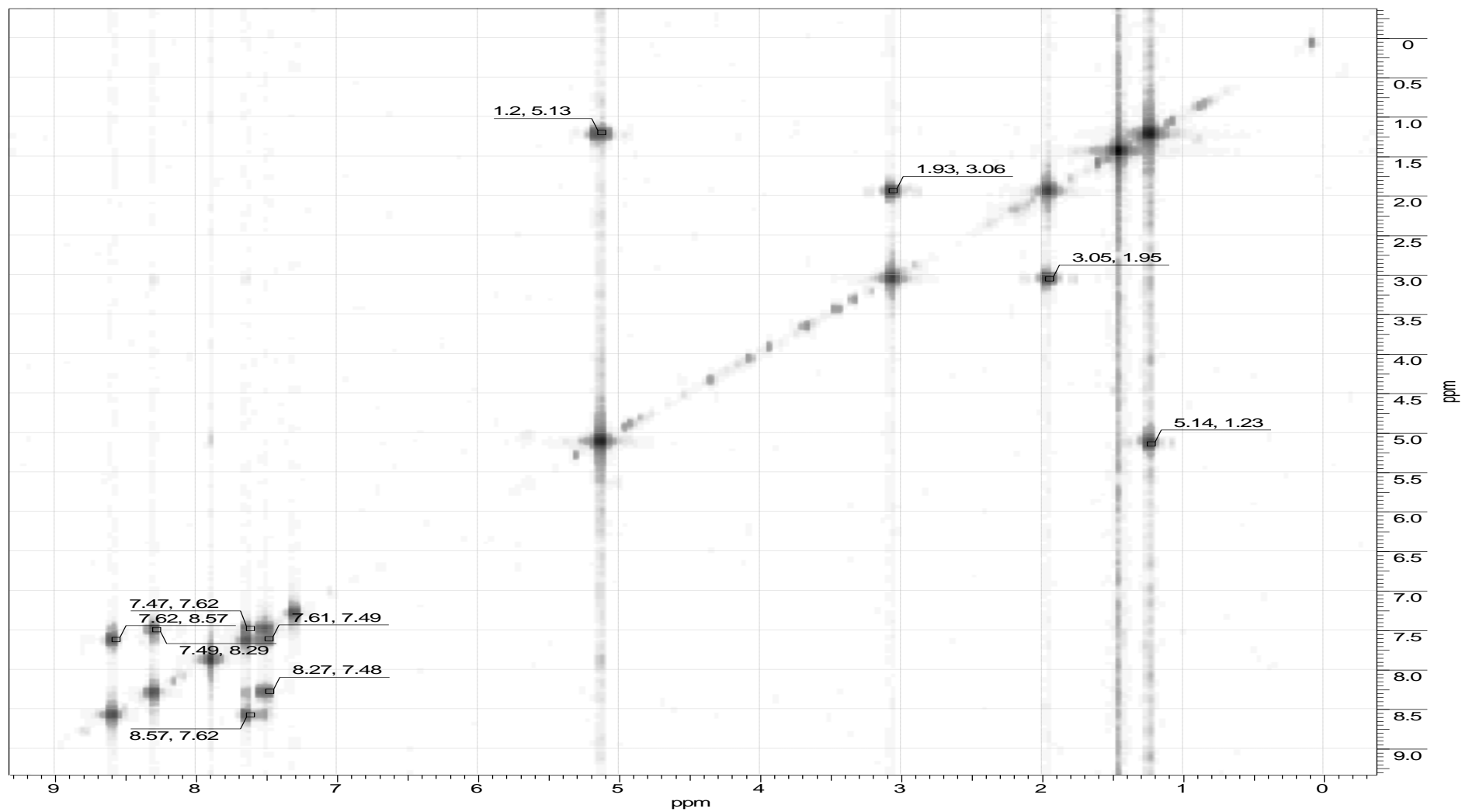
Espectro 150. EM-IES do composto 49b.



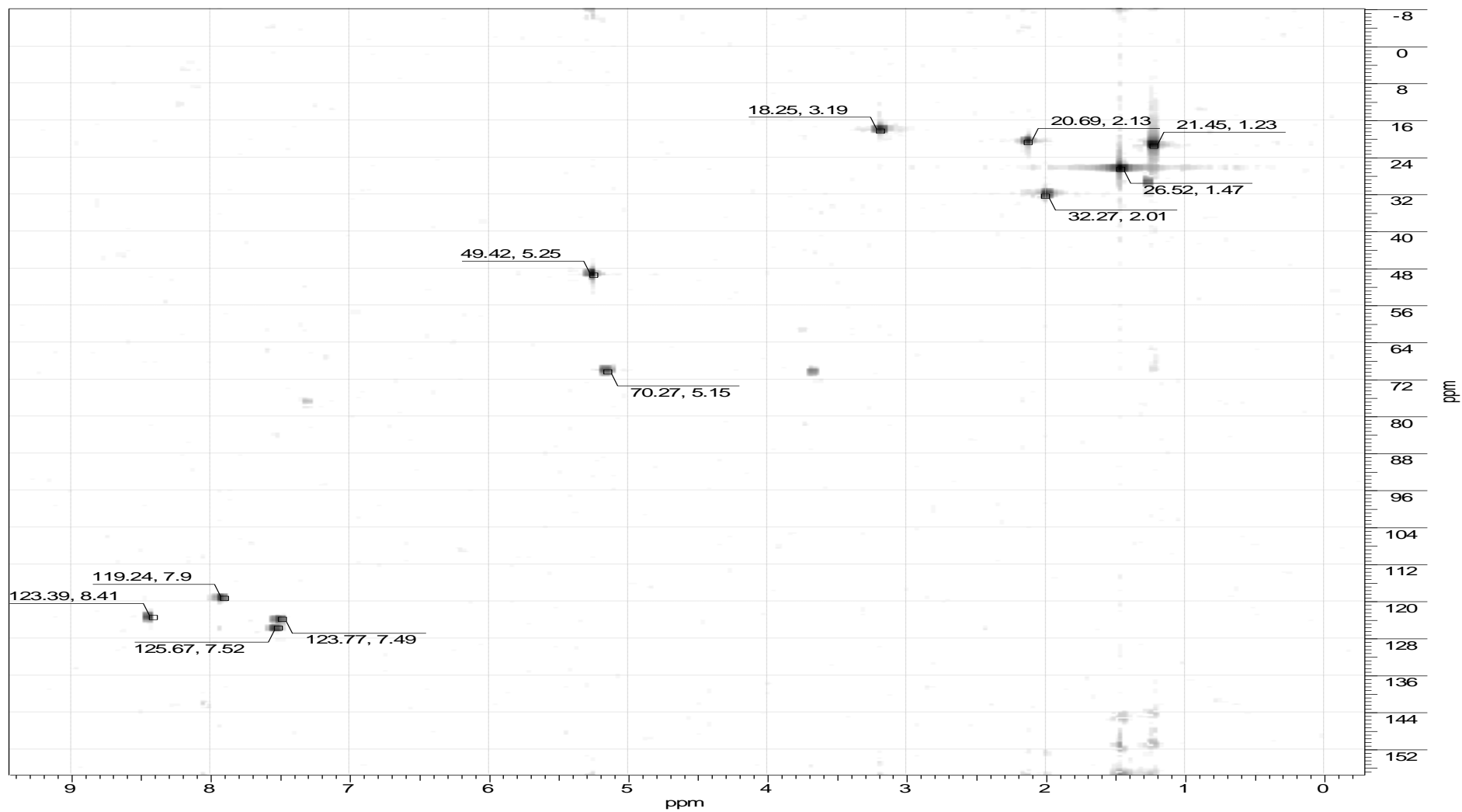
Espectro 151. RMN- ^1H (500 MHz, CDCl_3) do composto 49b.



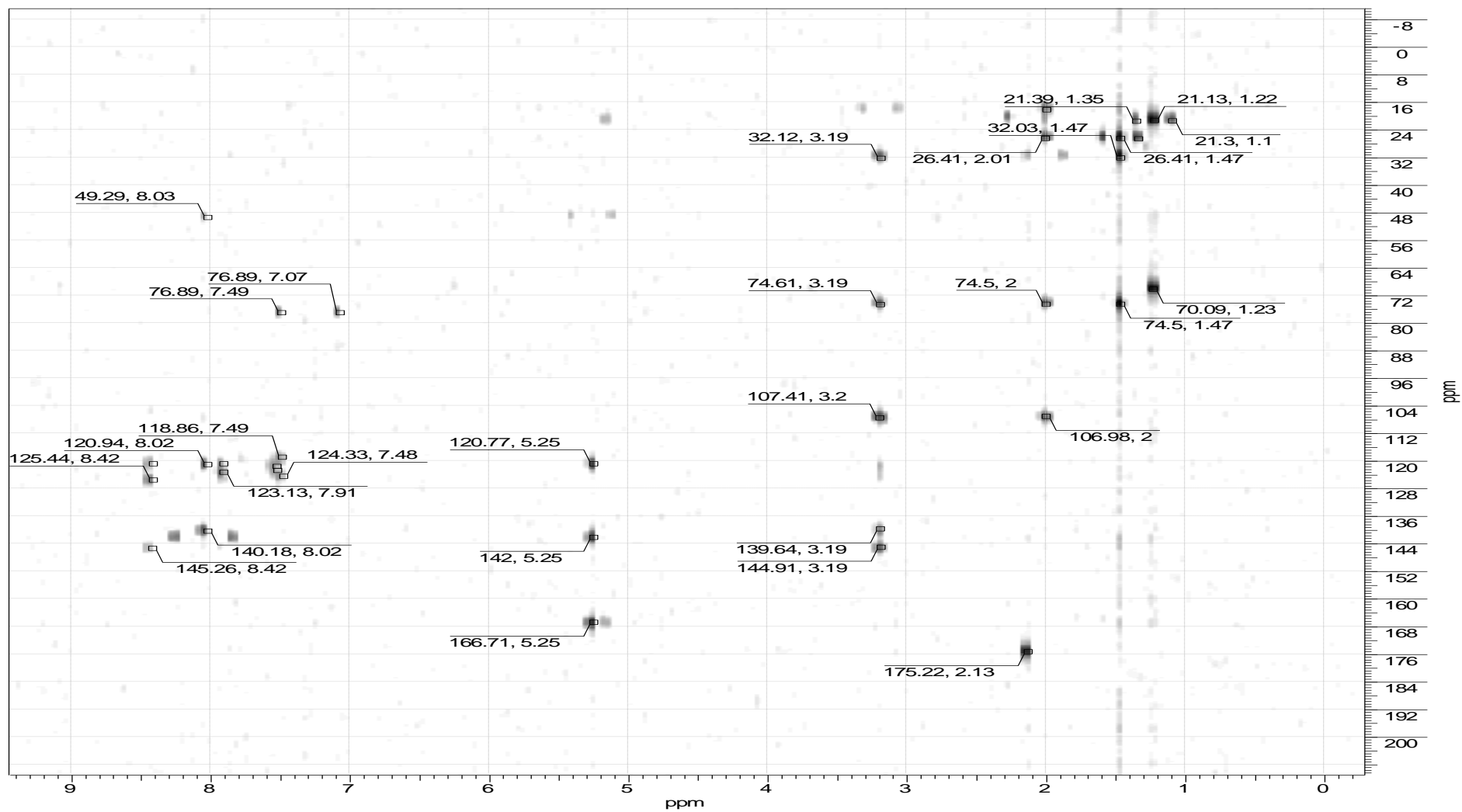
Espectro 152. RMN- ^{13}C (125 MHz, CDCl_3) do composto 49b.



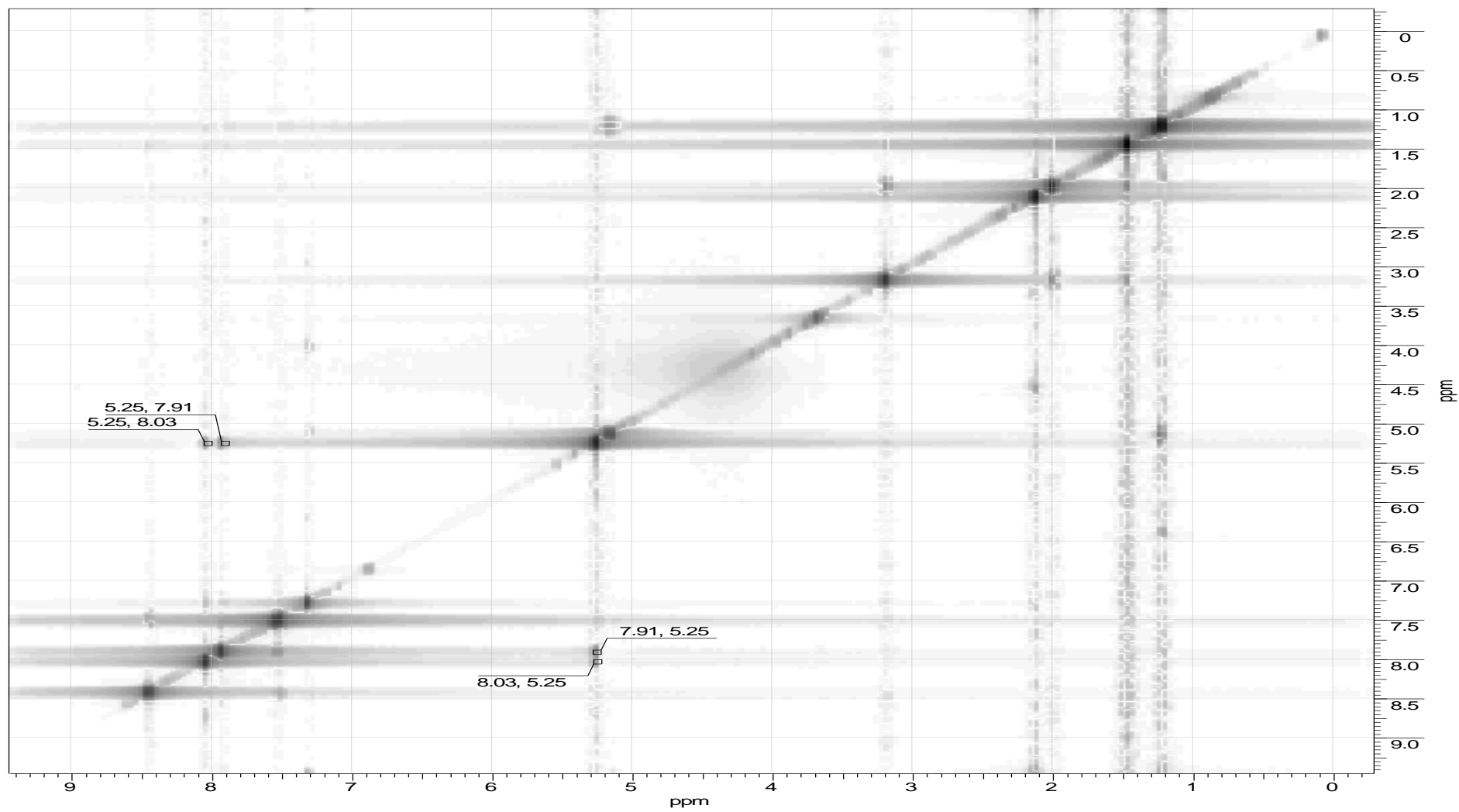
Espectro 153. ^1H -COSY (500 MHz, CDCl_3) do composto 49b.



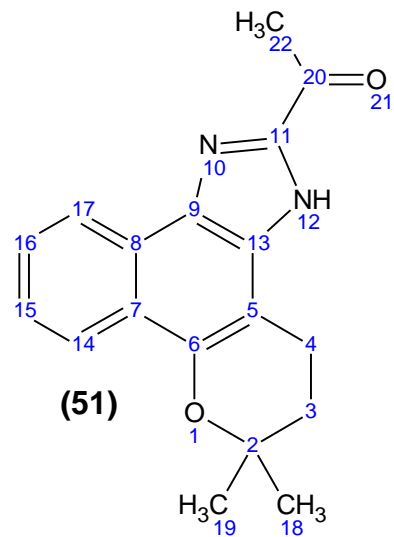
Espectro 154. HSQC (500 MHz, CDCl₃) do composto 49b.



Espectro 155. HMBC (500 MHz, CDCl_3) do composto 49b.

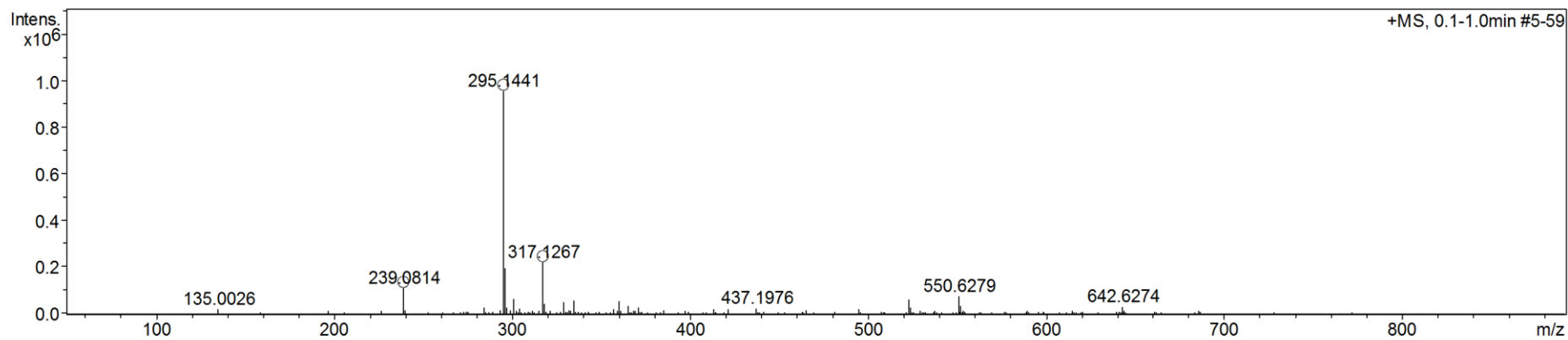


Espectro 156. NOESY (500 MHz, CDCl₃) do composto 49b.

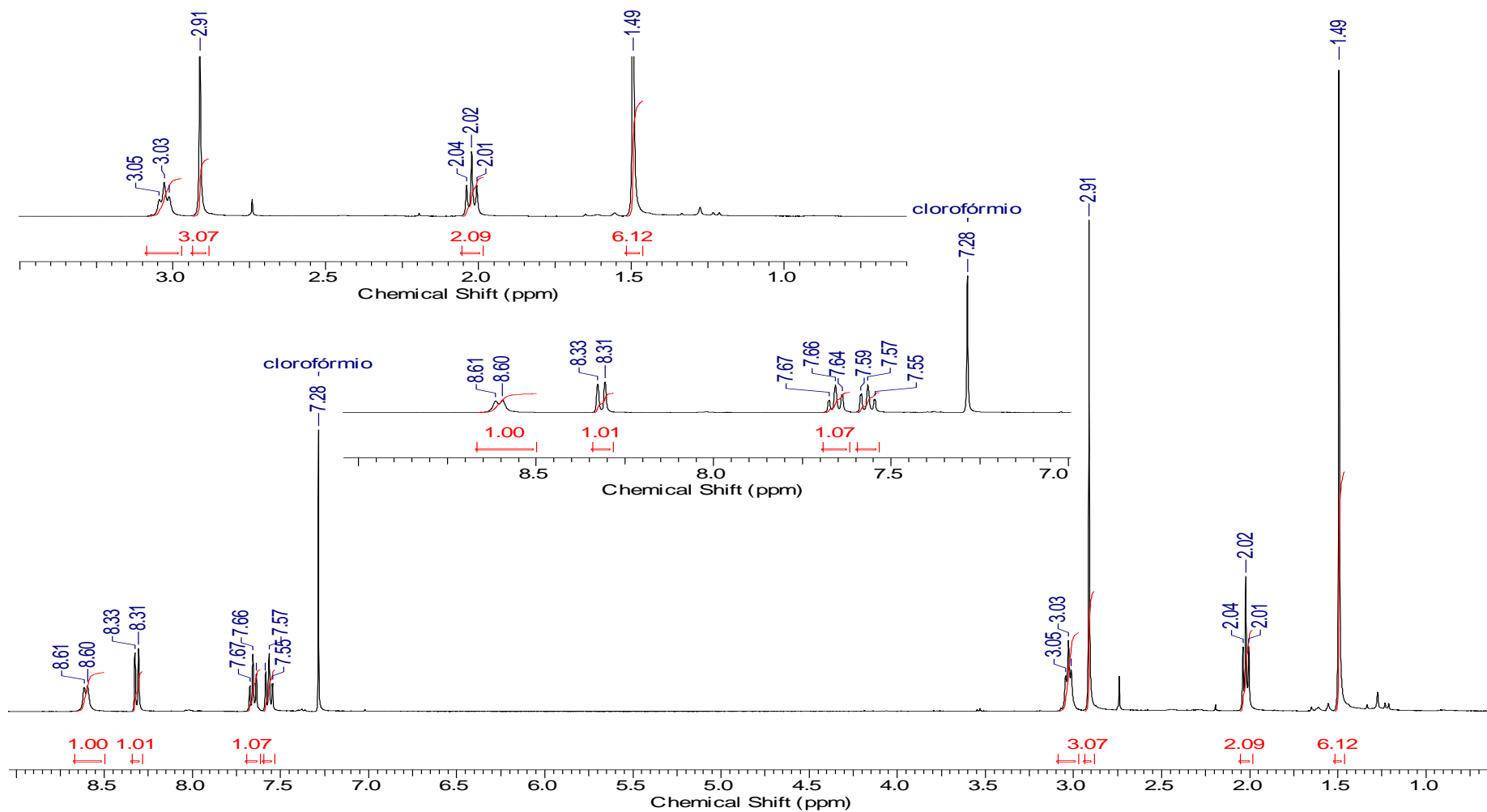


M: 294.3478 Da

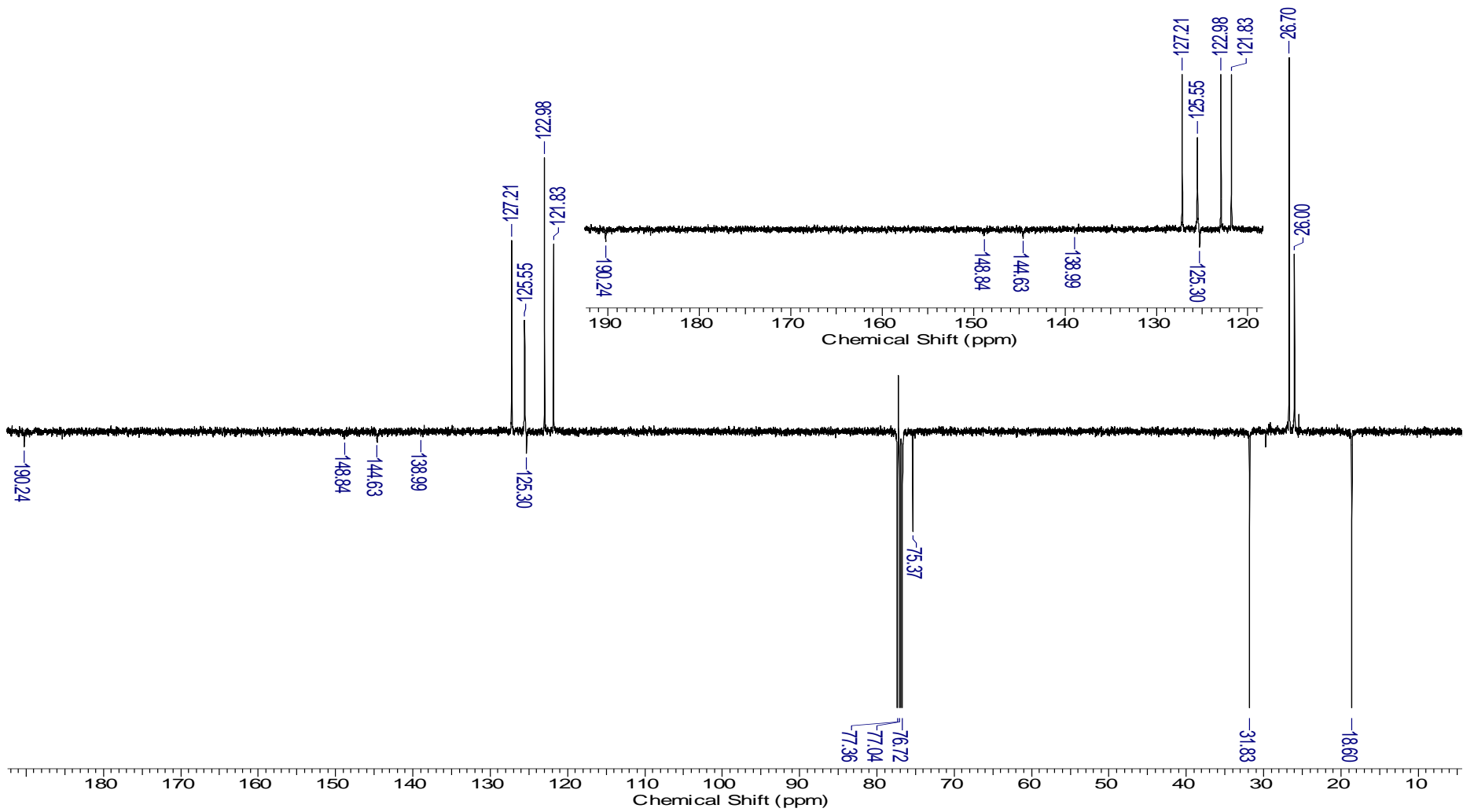
$[M+H]^+ = 295.1441$ Da; err[ppm] = 0,1



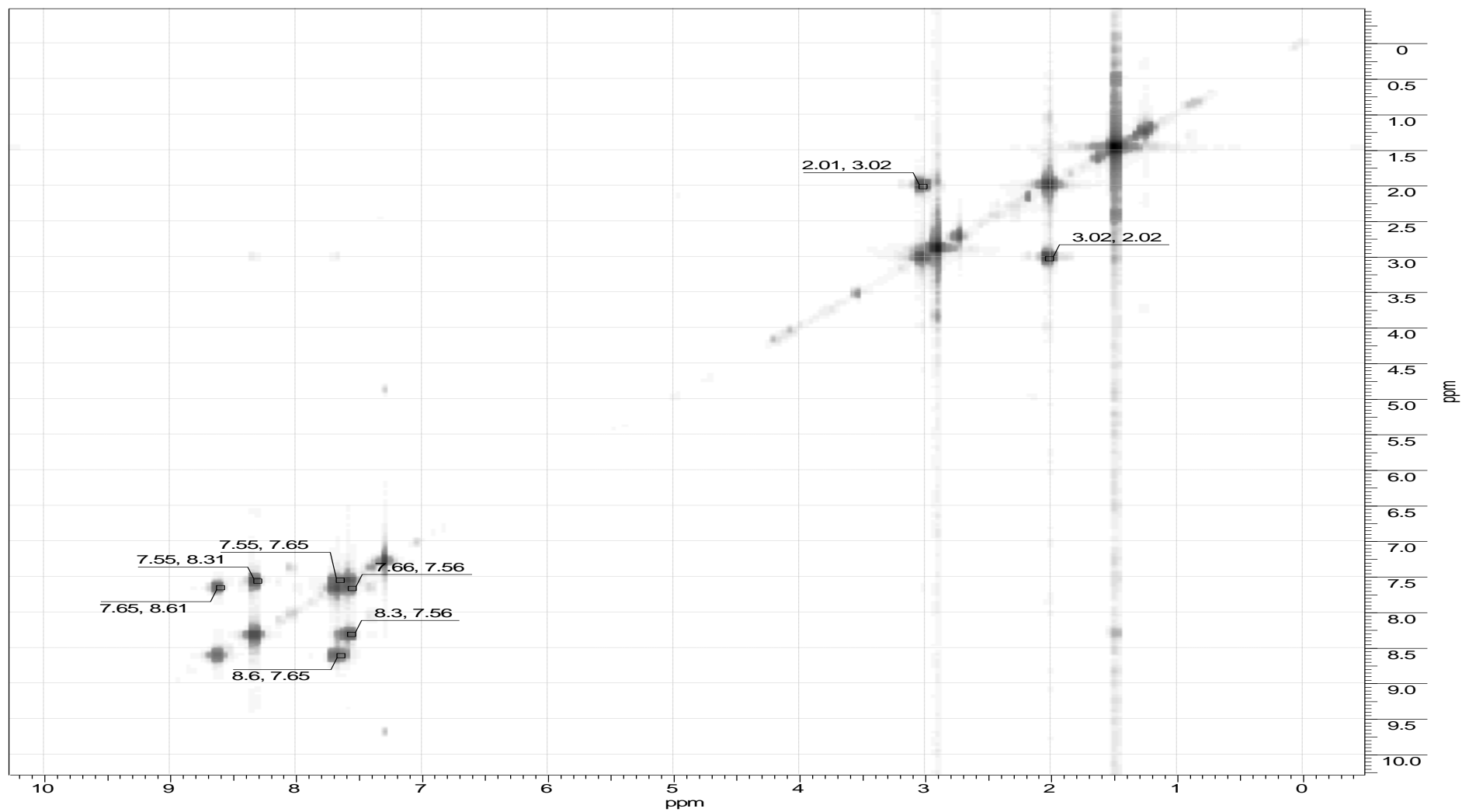
Espectro 157. EM-IES do composto 51.



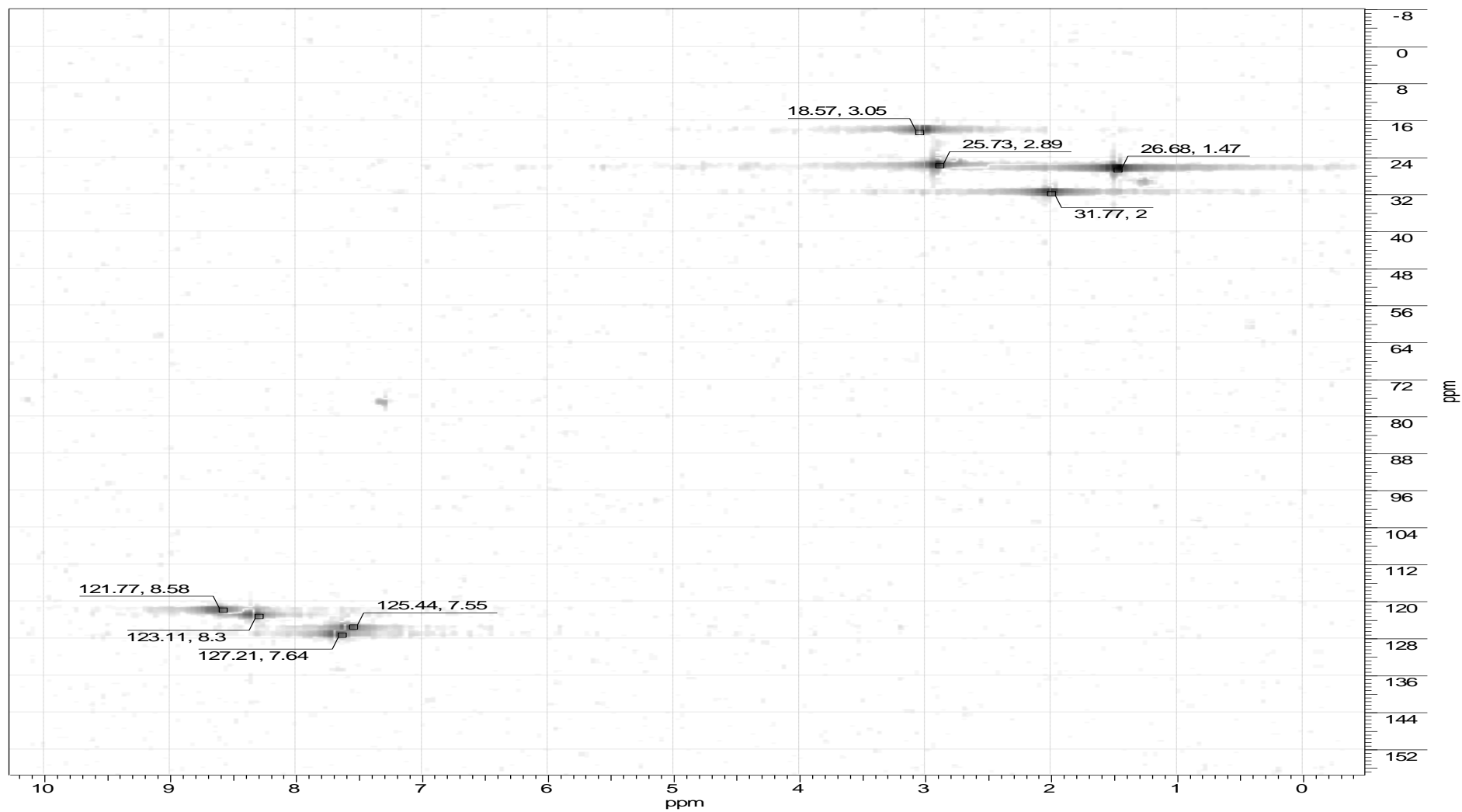
Espectro 158. RMN- ^1H (400 MHz, CDCl_3) do composto 51.



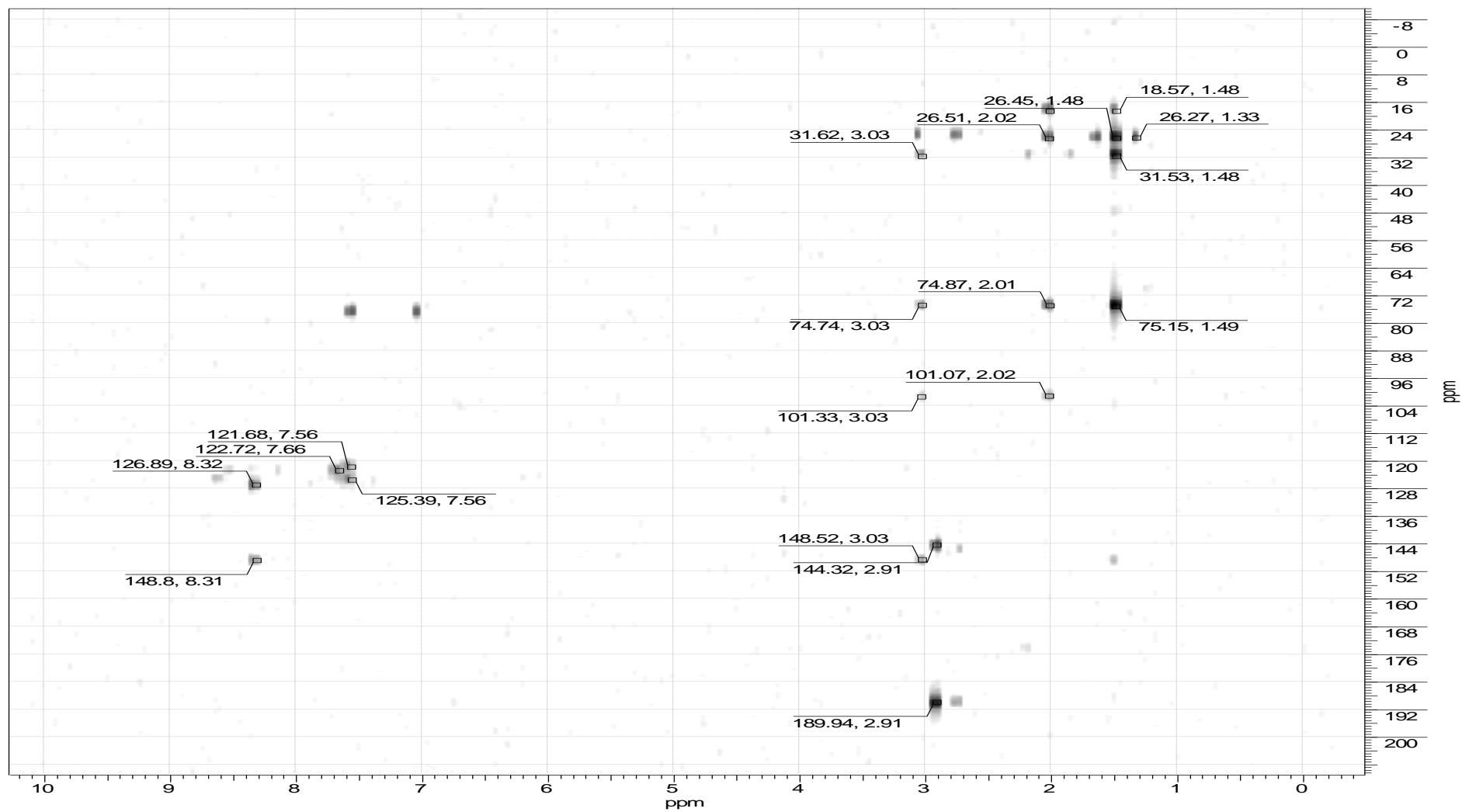
Espectro 159. RMN-¹³C (100 MHz, CDCl₃) do composto 51.



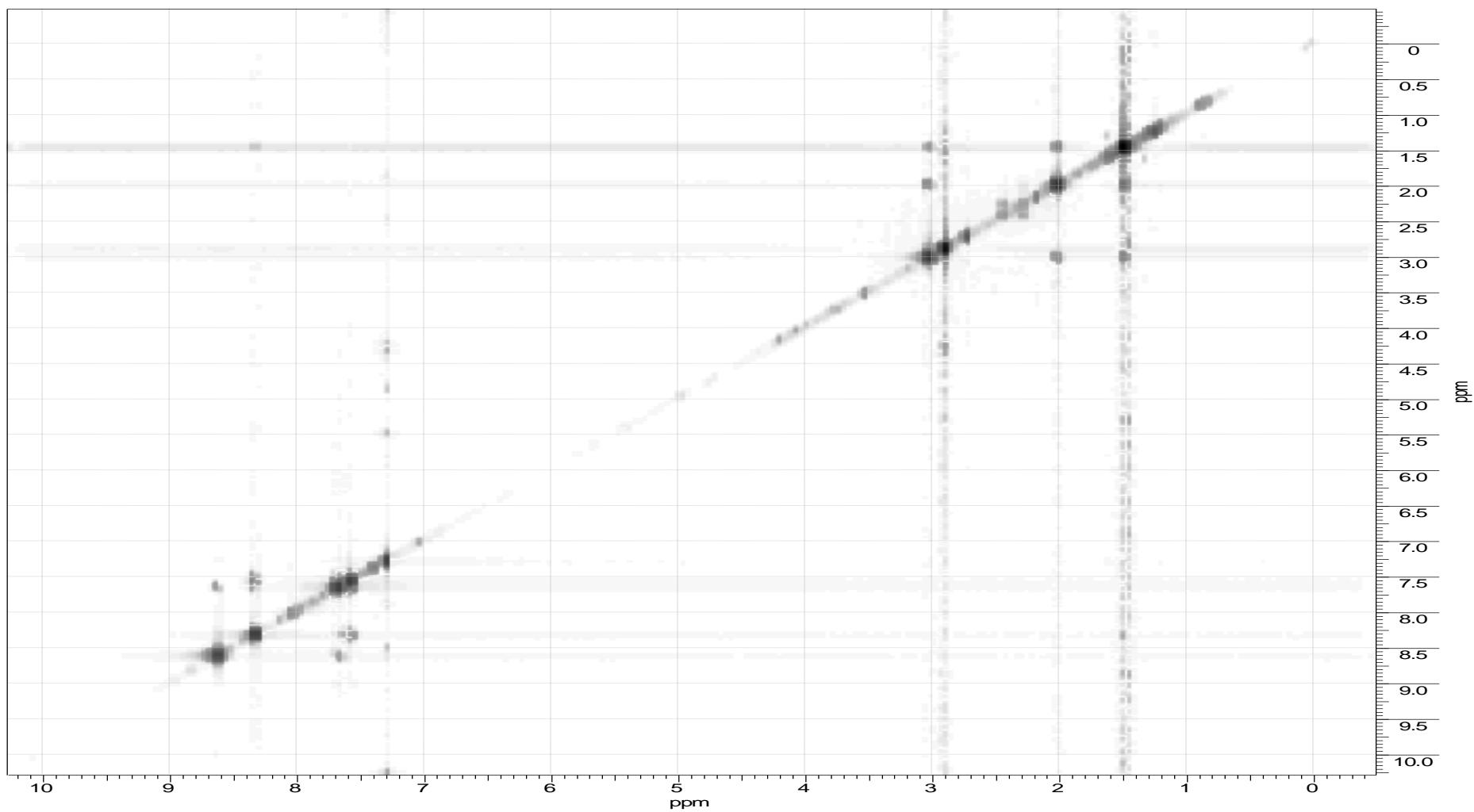
Espectro 160. ^1H -COSY (400 MHz, CDCl_3) do composto 51.



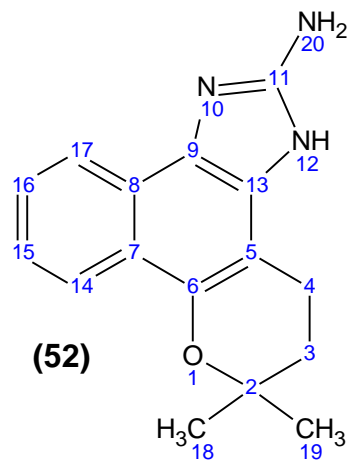
Espectro 161. HSQC (400 MHz, CDCl_3) do composto 51.



Espectro 162. HMBC (400 MHz, CDCl₃) do composto 51.

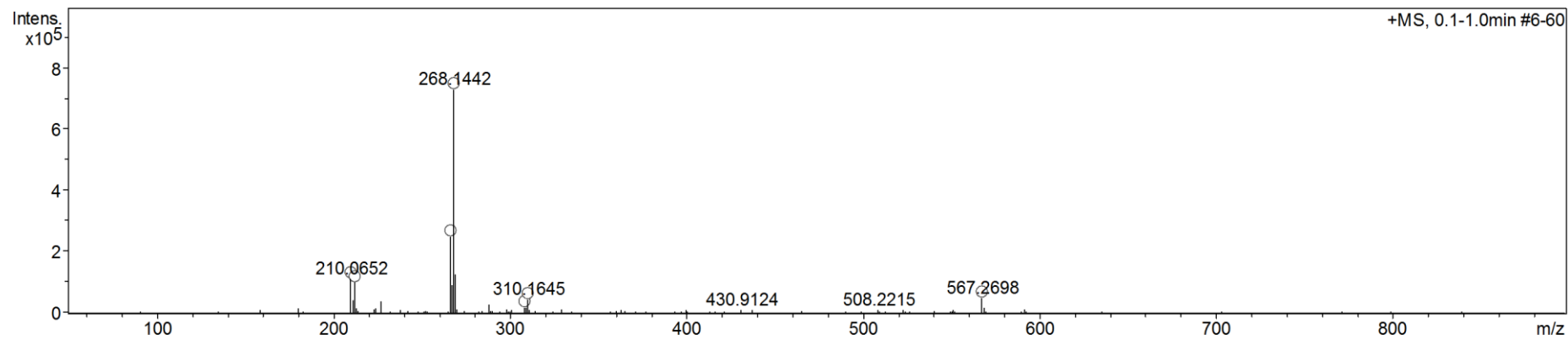


Espectro 163. NOESY (400 MHz, CDCl₃) do composto 51.

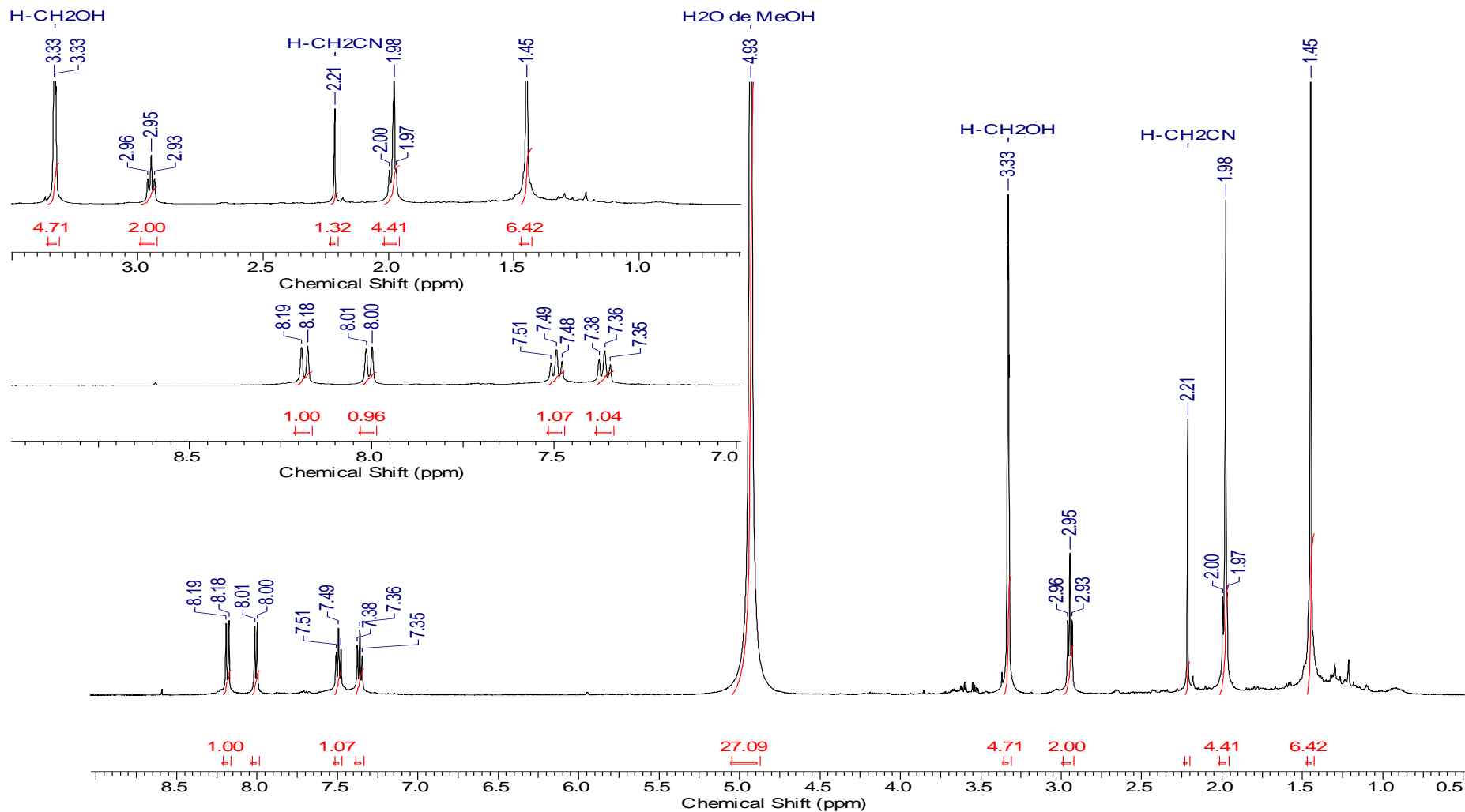


M: 267.3258 Da

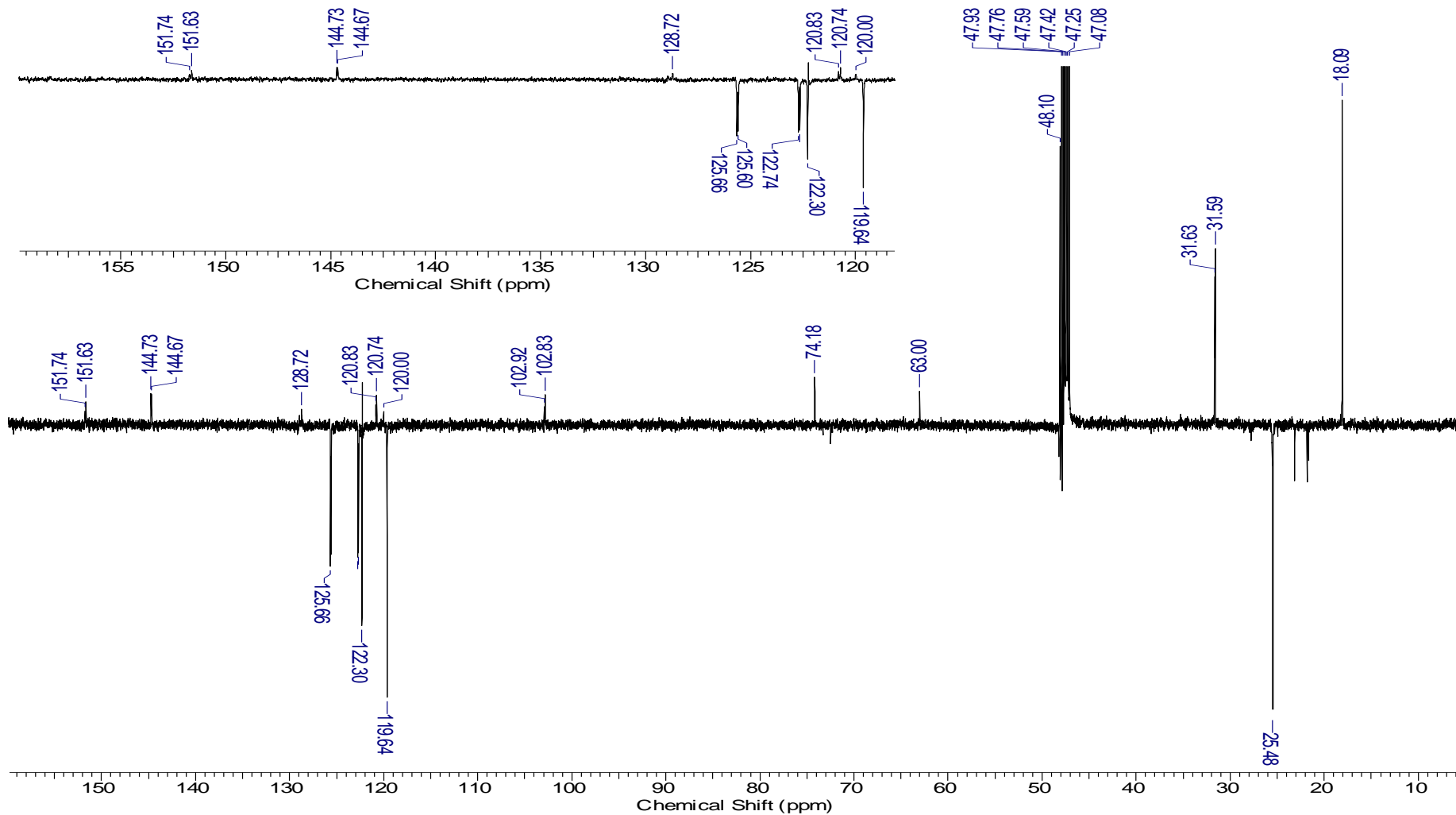
[M+H]⁺ = 268.1444 Da; err[ppm] = 1,0



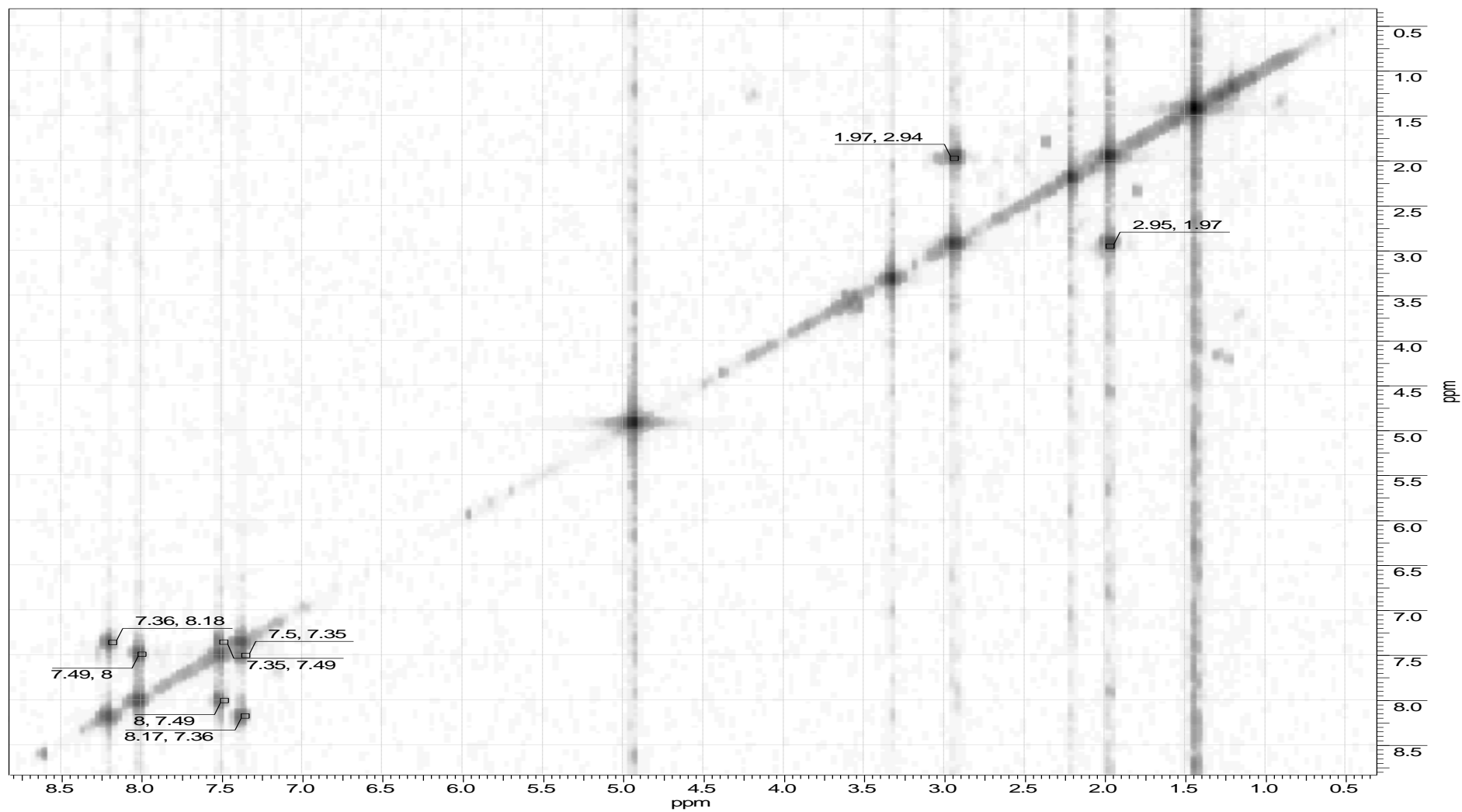
Espectro 164. EM-IES do composto 52.



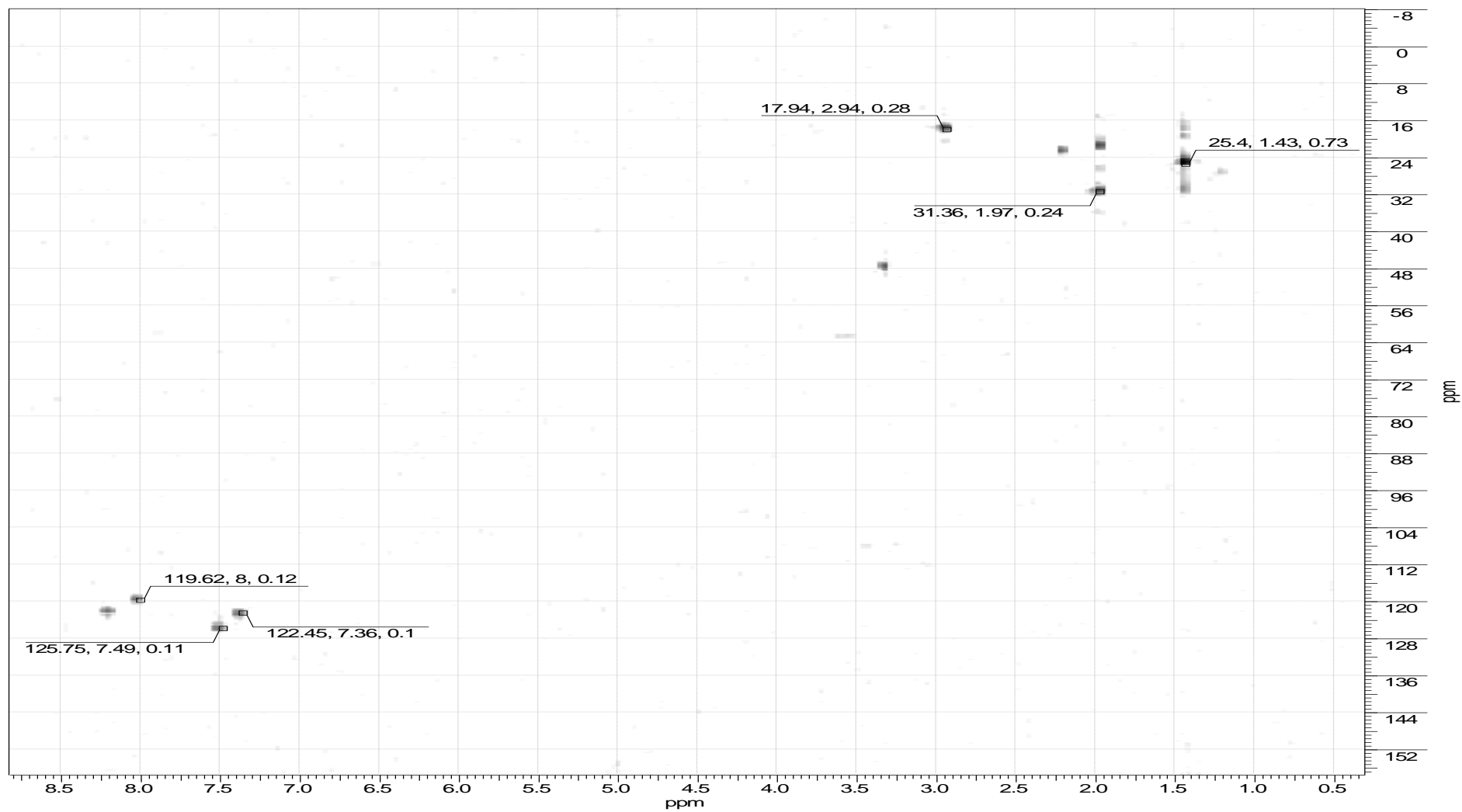
Espectro 165. RMN- ^1H (500 MHz, CDCl_3) do composto 52.



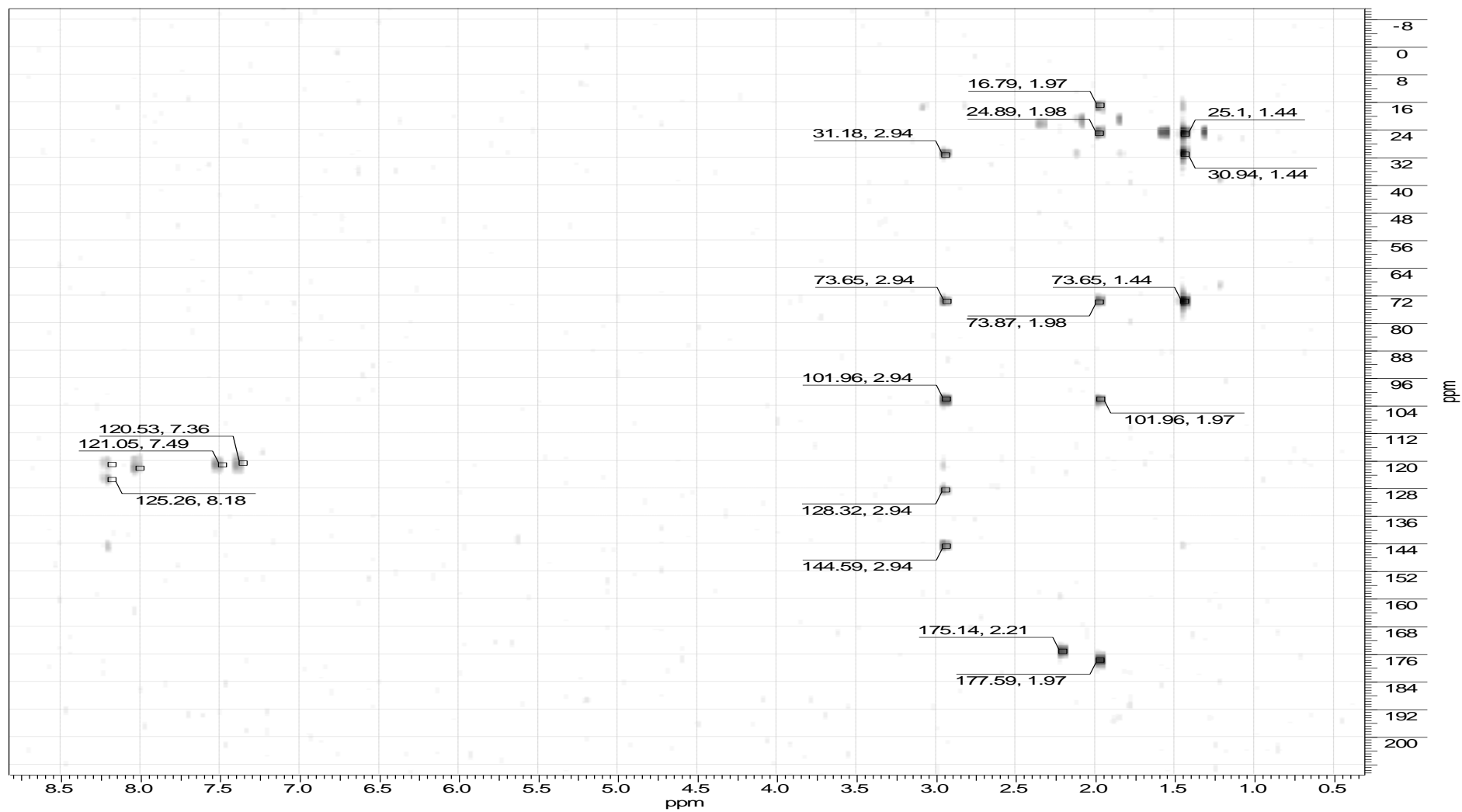
Espectro 166. RMN-¹³C (125 MHz, CDCl₃) do composto 52.



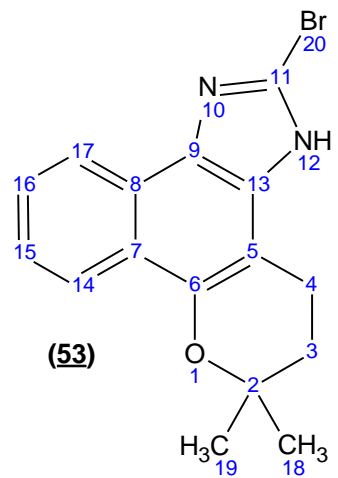
Espectro 167. ^1H -COSY (500 MHz, CDCl_3) do composto 52.



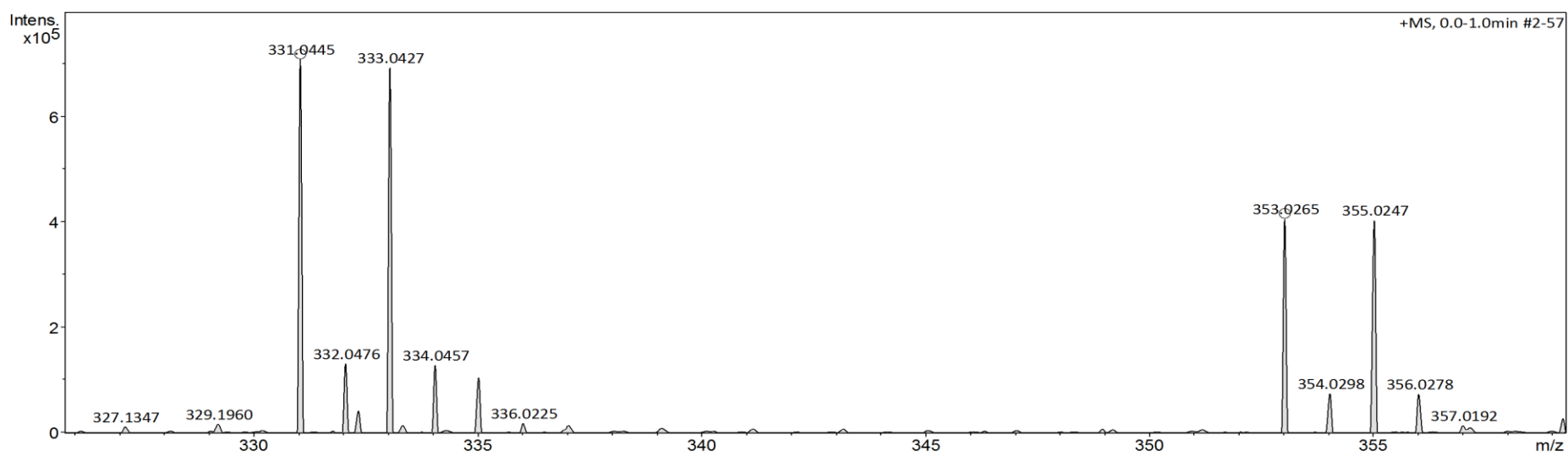
Espectro 168. HSQC (500 MHz, CDCl_3) do composto 52.



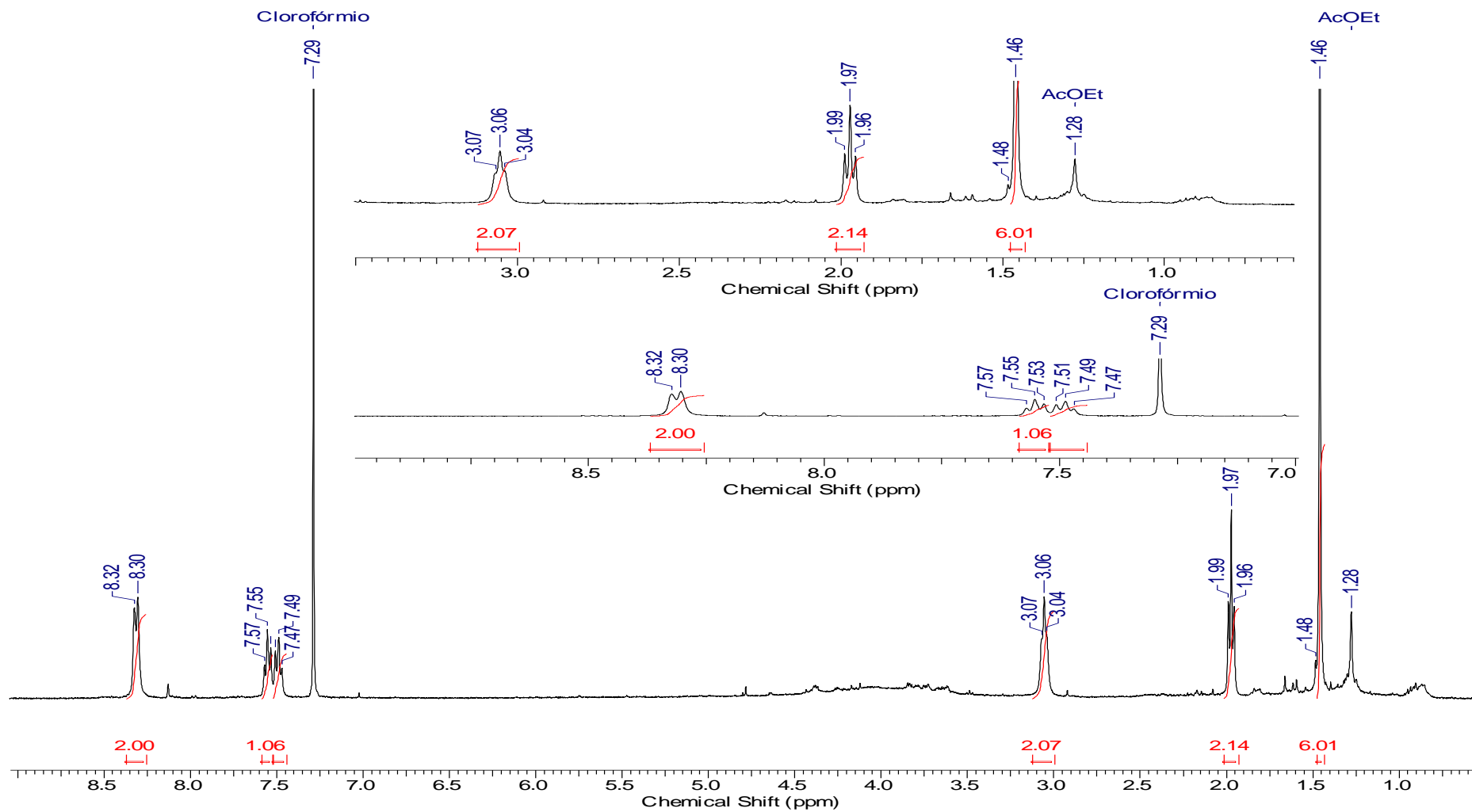
Espectro 169. HMBC (500 MHz, CDCl_3) do composto 52.



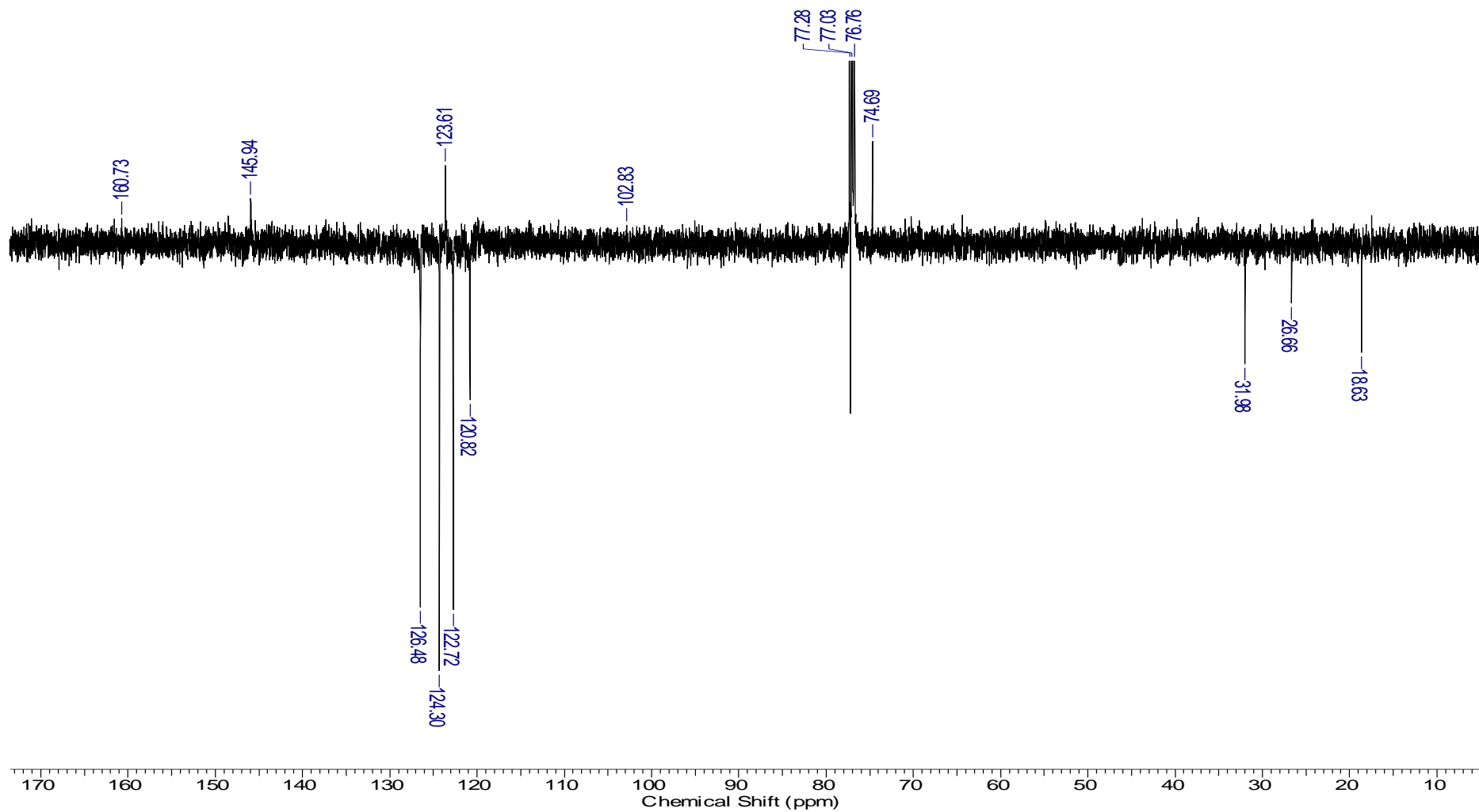
M: 330.0368 Da



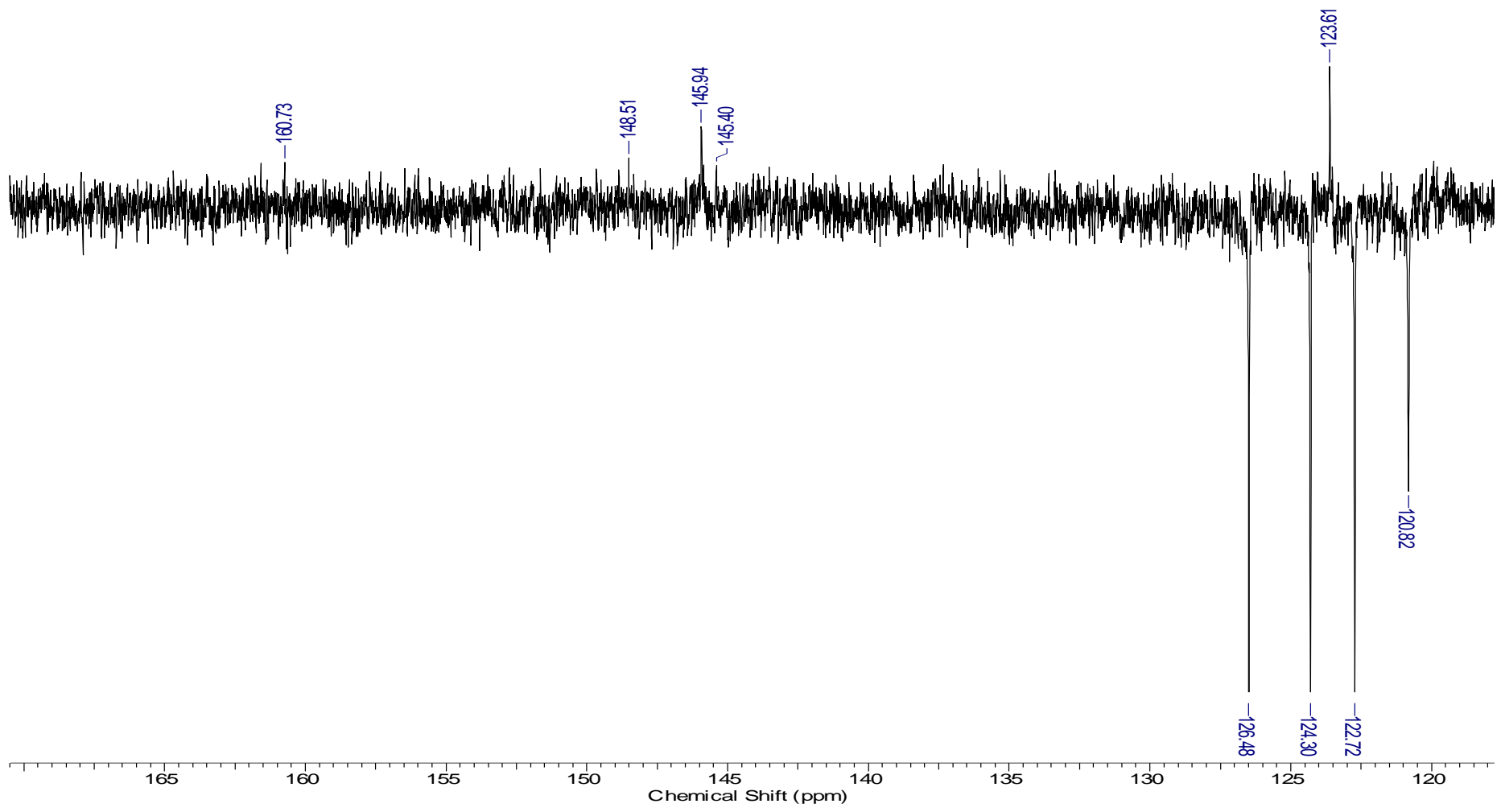
Espectro 170. EM-IES do composto 53.



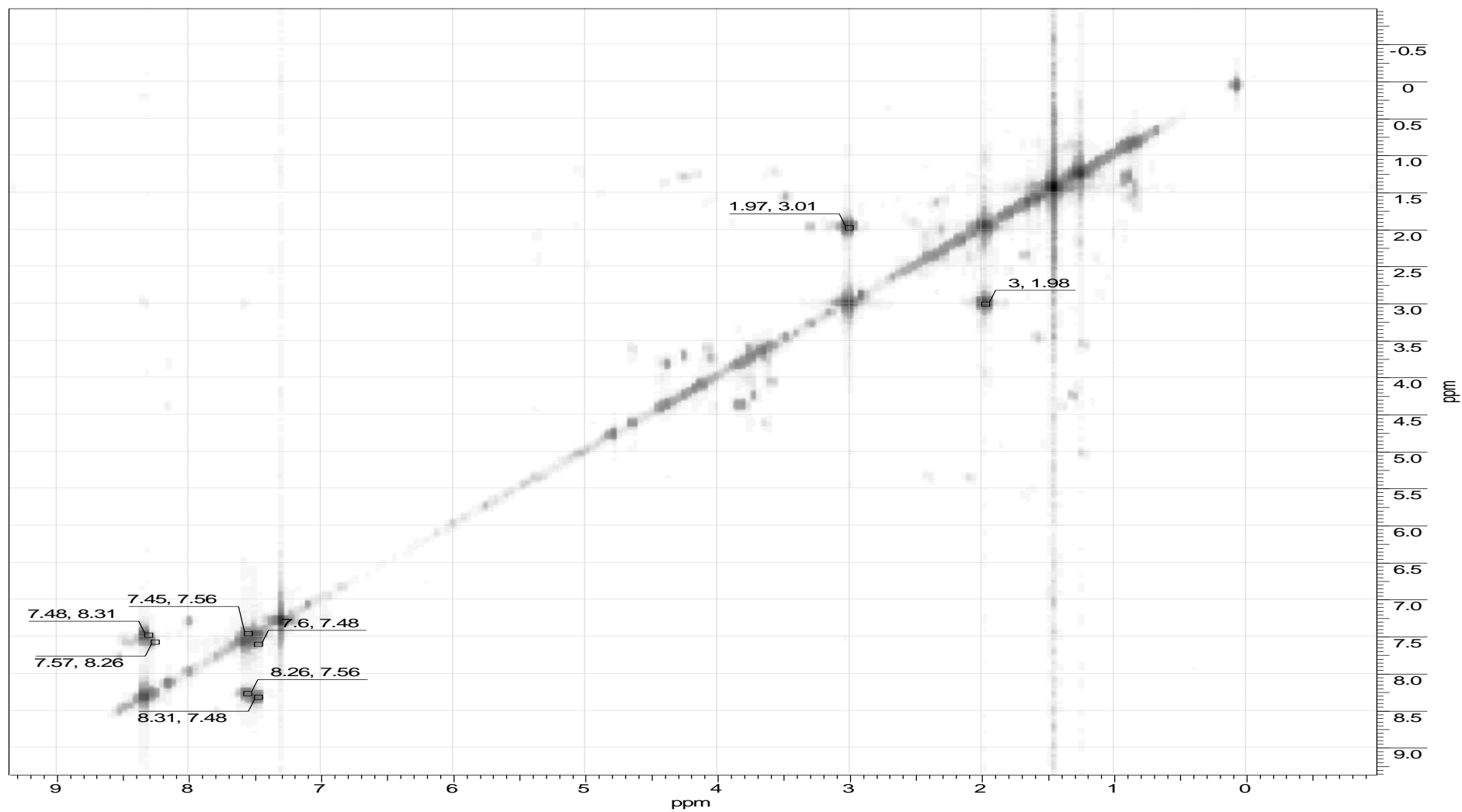
Espectro 171. RMN- ^1H (400 MHz, CDCl_3) do composto 53.



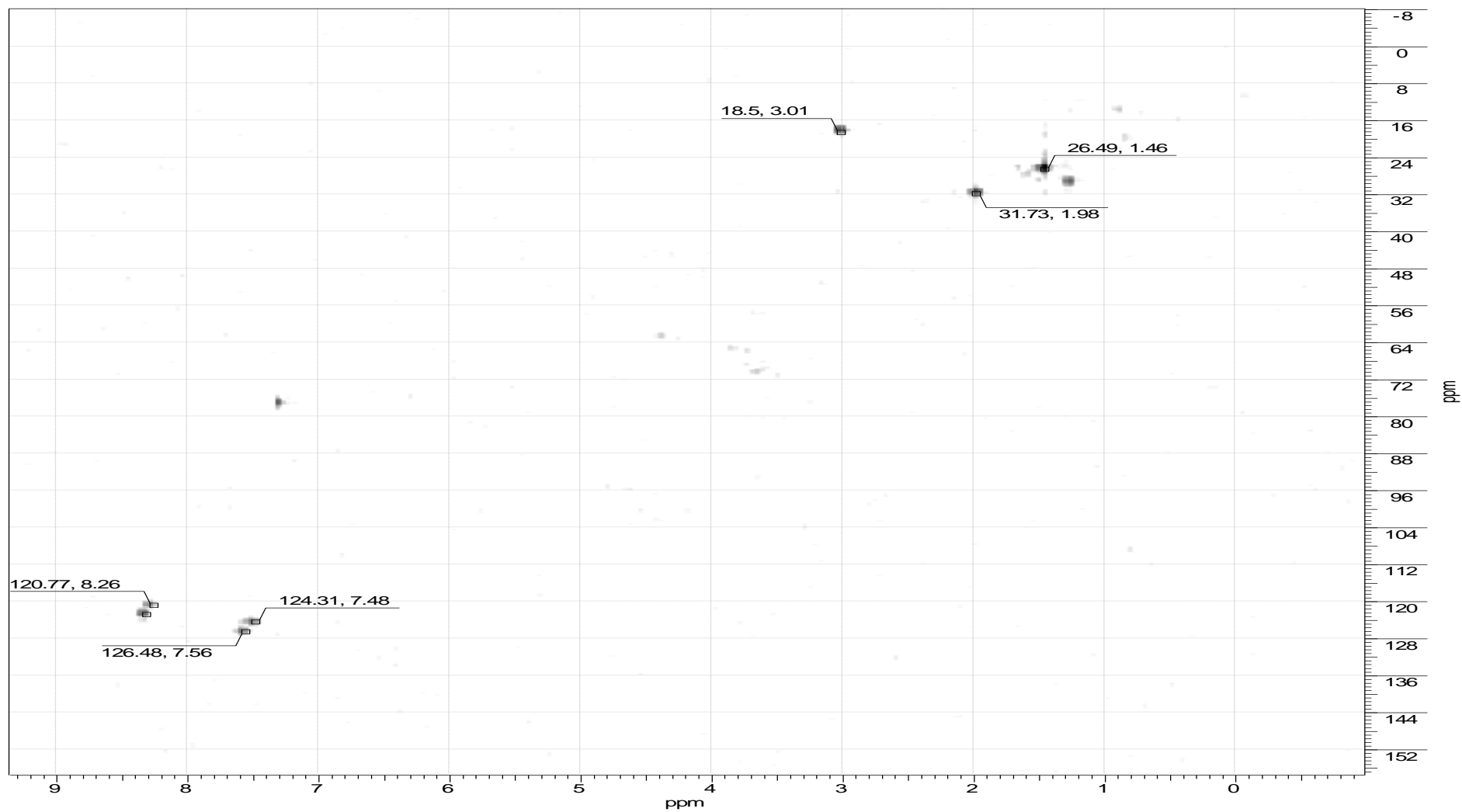
Espectro 172. RMN-¹³C (100 MHz, CDCl₃) do composto 53.



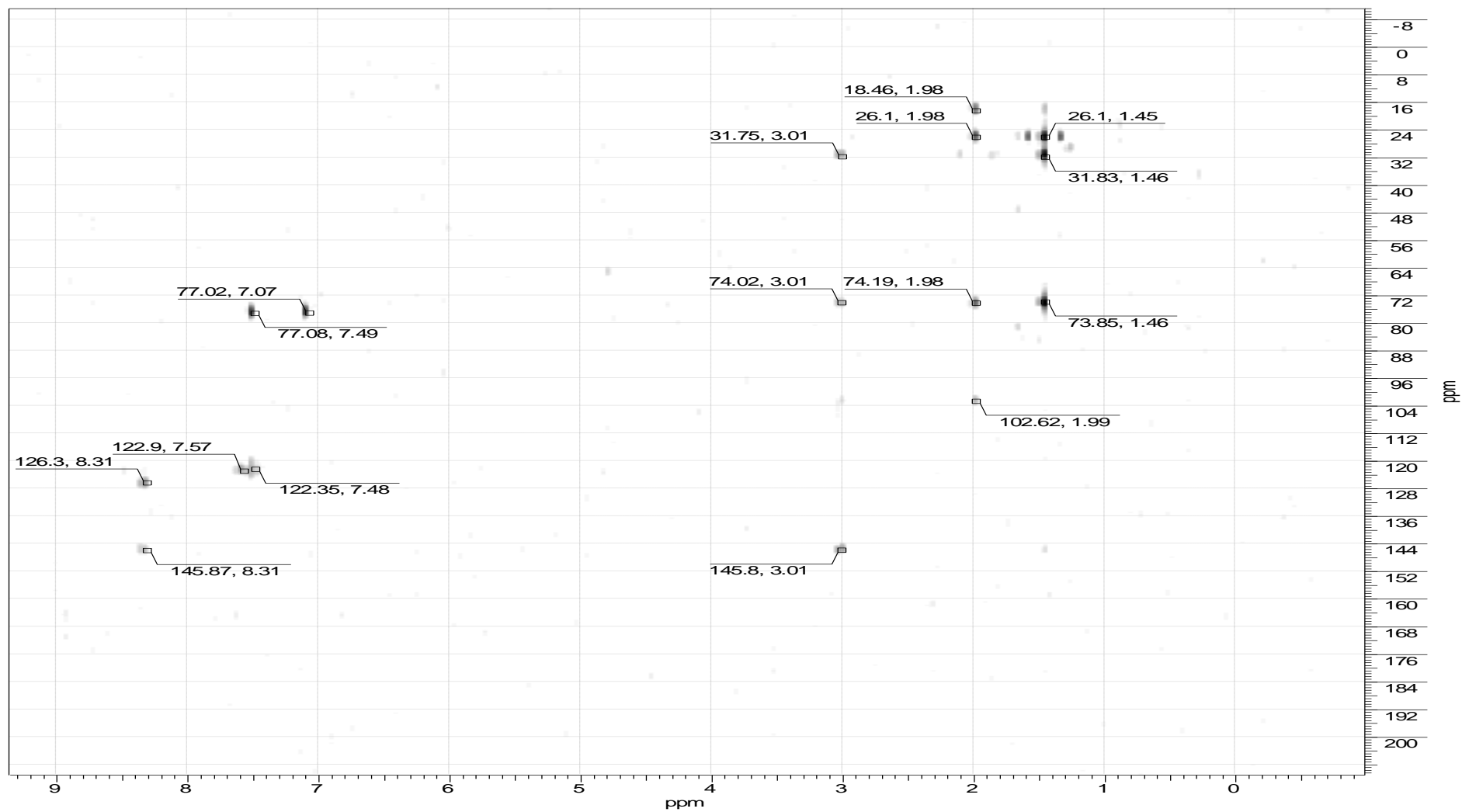
Espectro 173. RMN-¹³C (100 MHz, CDCl₃) do composto 53 – ampliação de 118 à 170 ppm.



Espectro 174. ^1H -COSY (400 MHz, CDCl_3) do composto 53.



Espectro 175. HSQC (400 MHz, CDCl_3) do composto 53.



Espectro 176. HMBC (400 MHz, CDCl₃) do composto 53.