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**METABÓLITOS ESPECIAIS ISOLADOS DE MADEIRA DE *Simira
grazielae* (RUBIACEAE) E ATIVIDADES BIOLÓGICAS**

Volume 2

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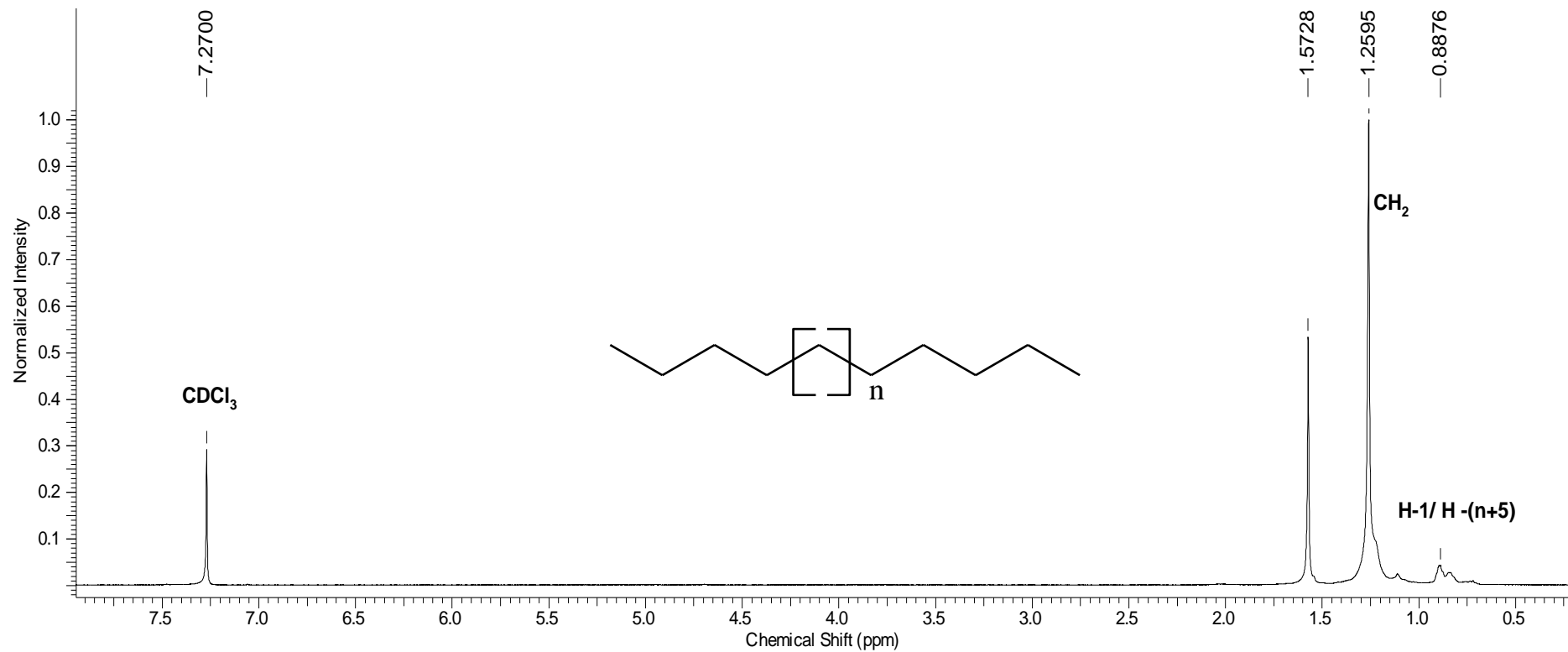
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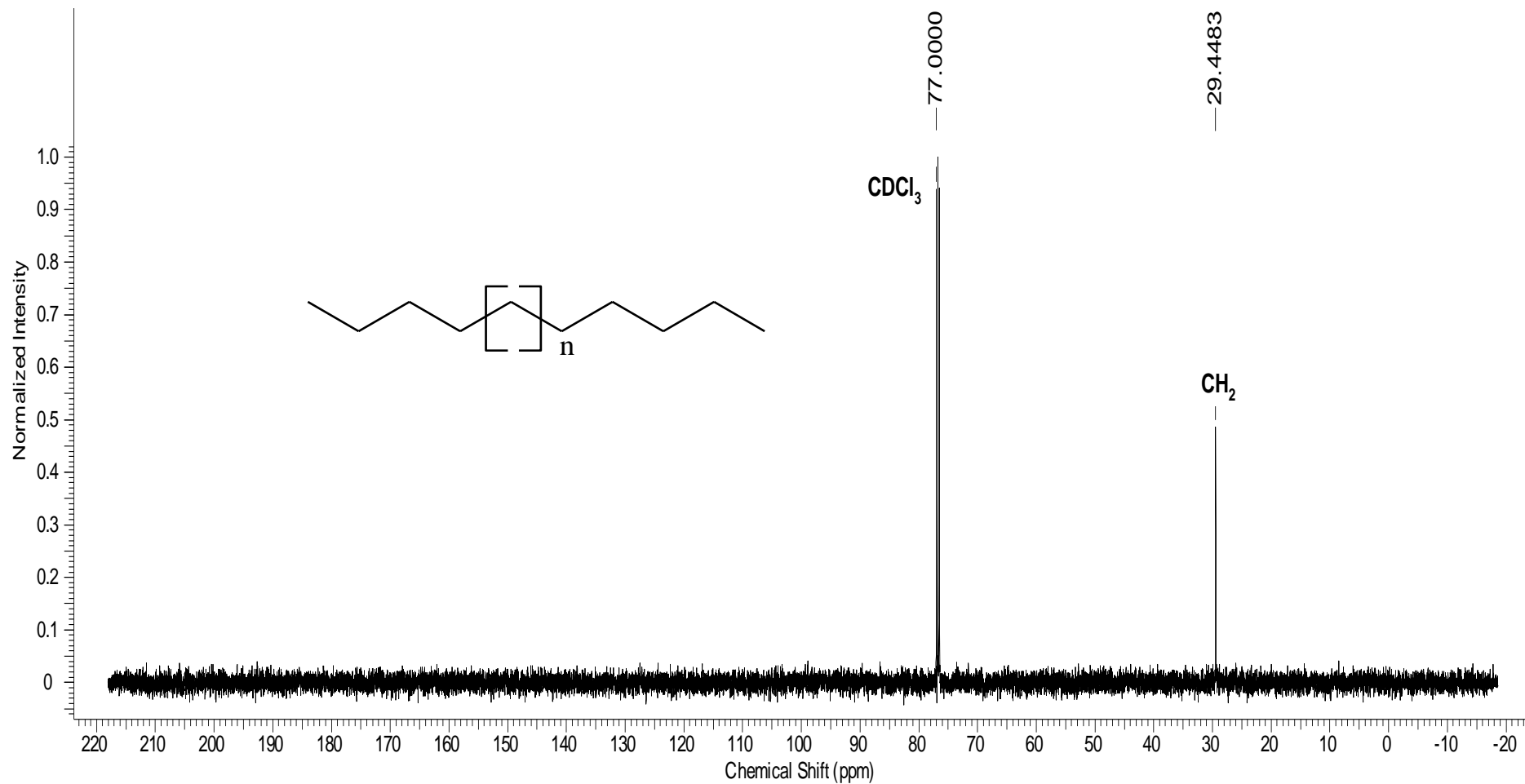
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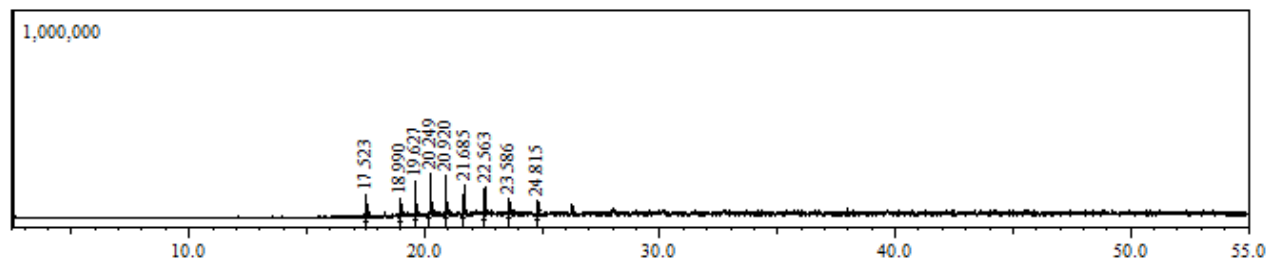
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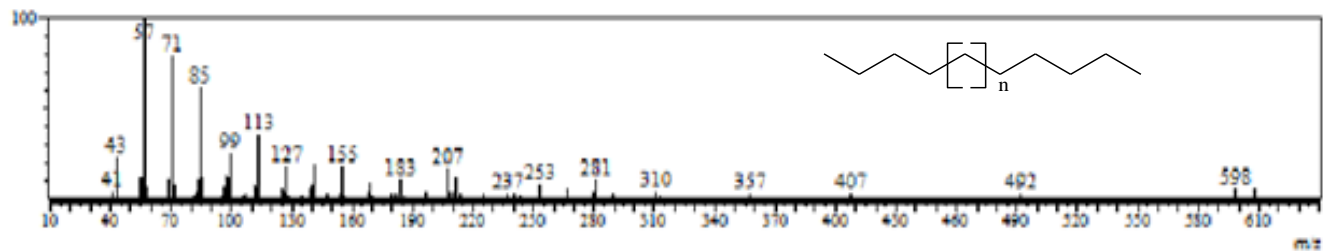
Espectro 1. RMN-¹H (500 MHz, CDCl₃) da substância **SGMD-1**.



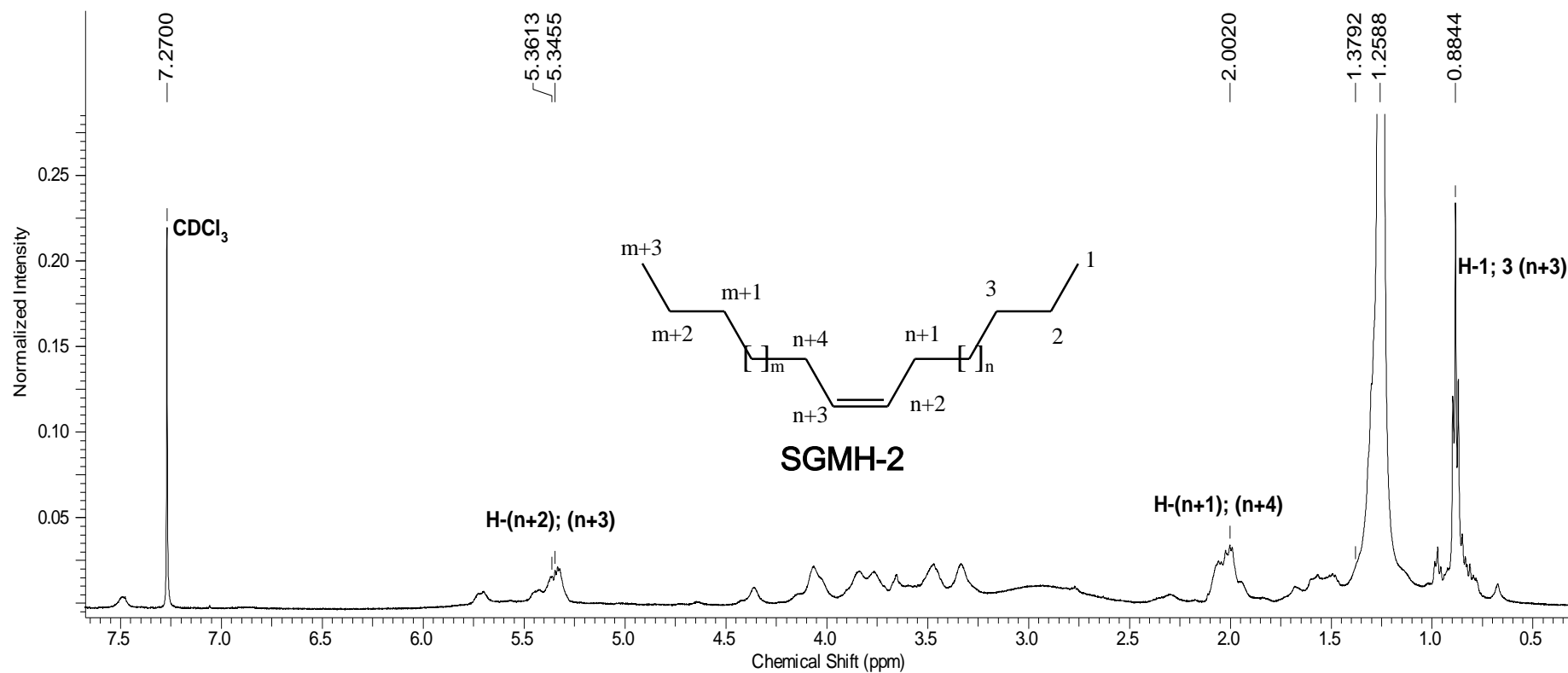
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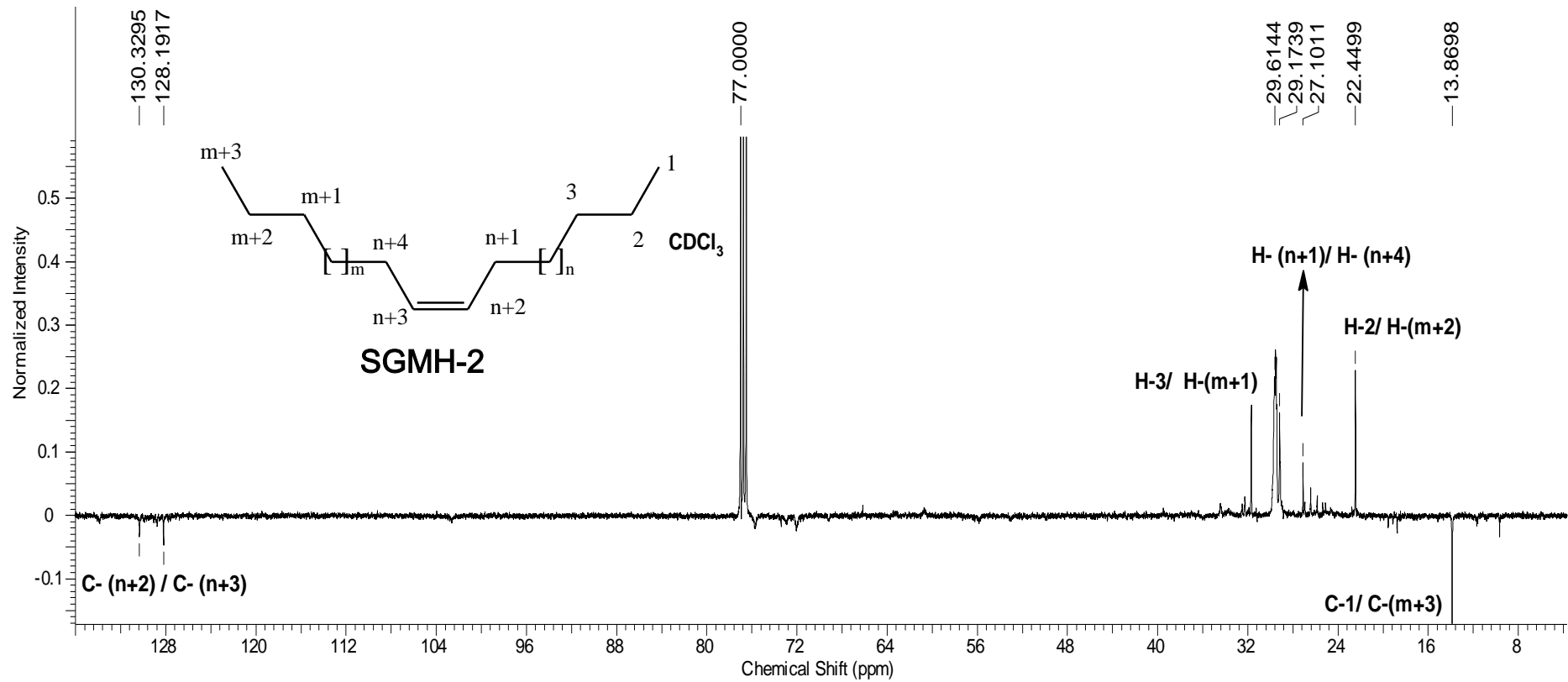
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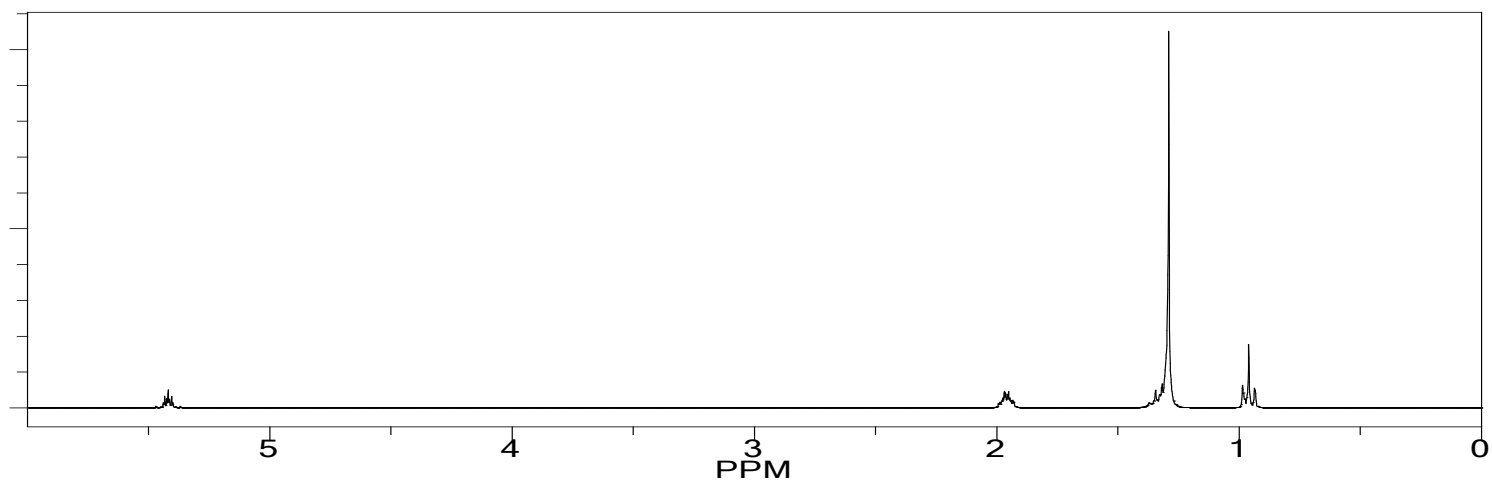
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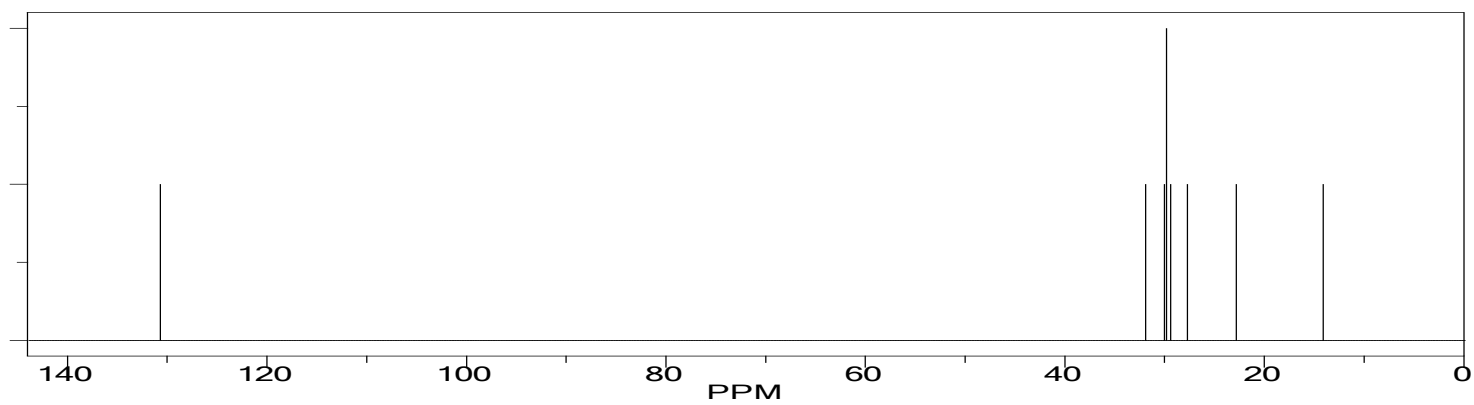
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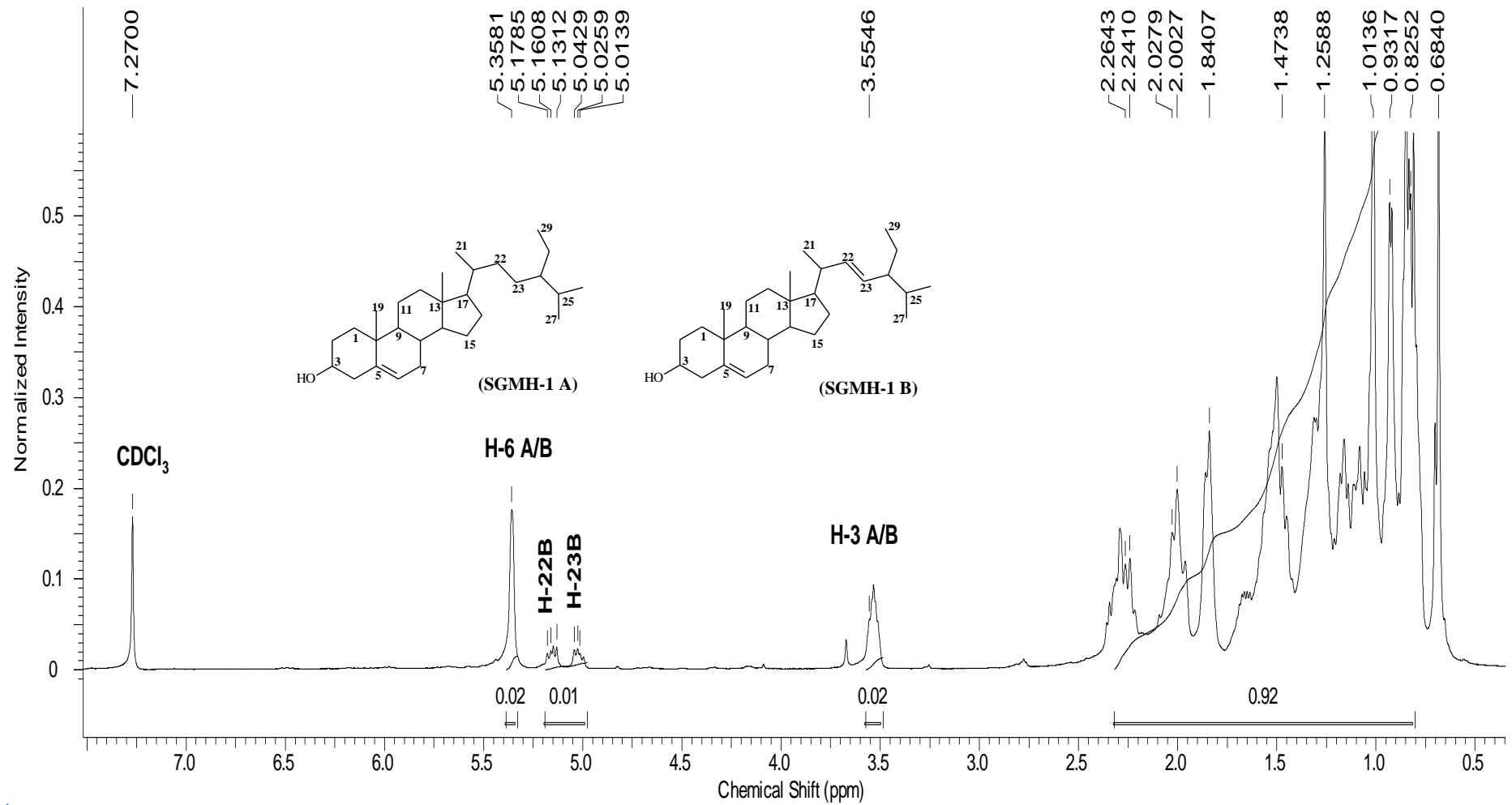
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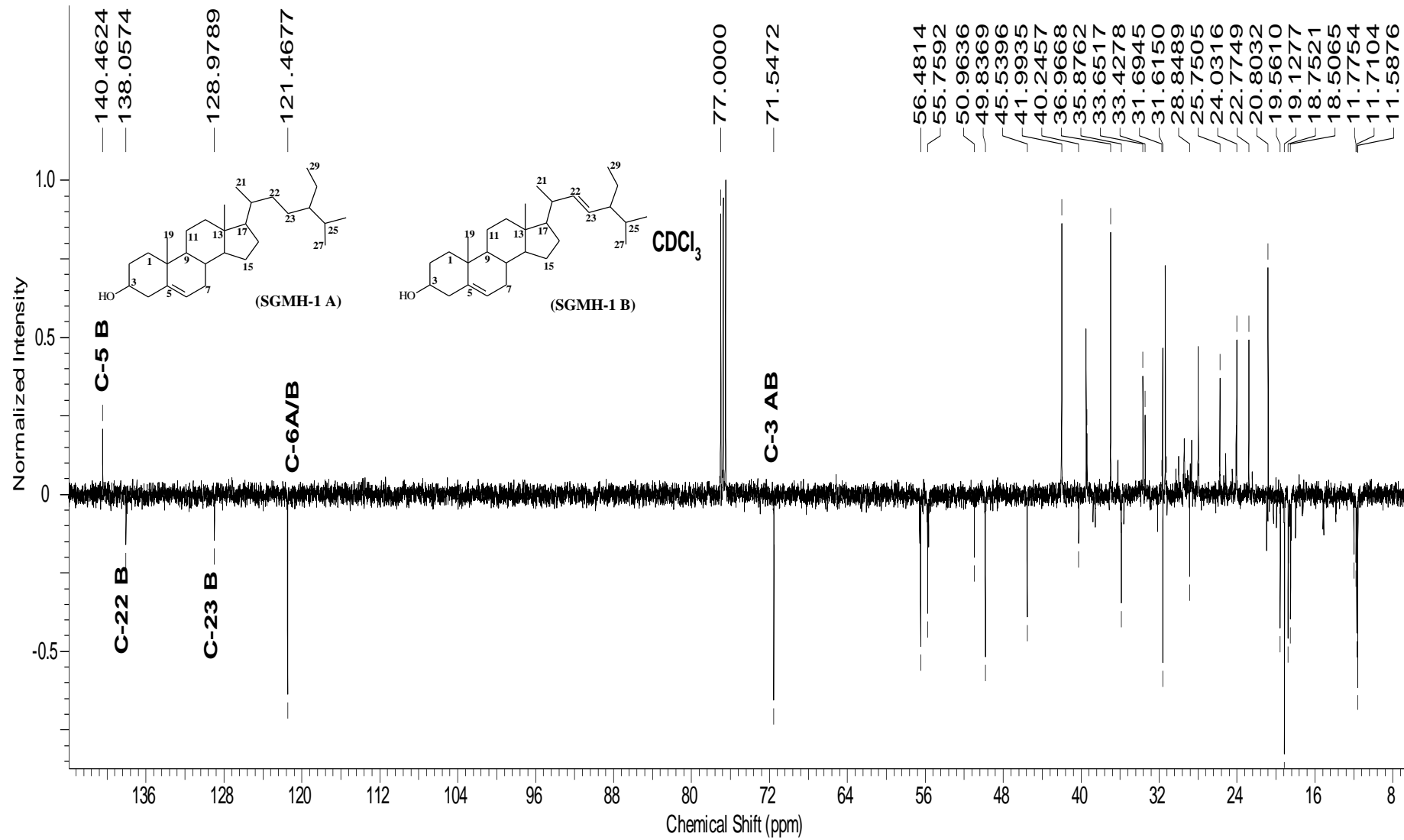
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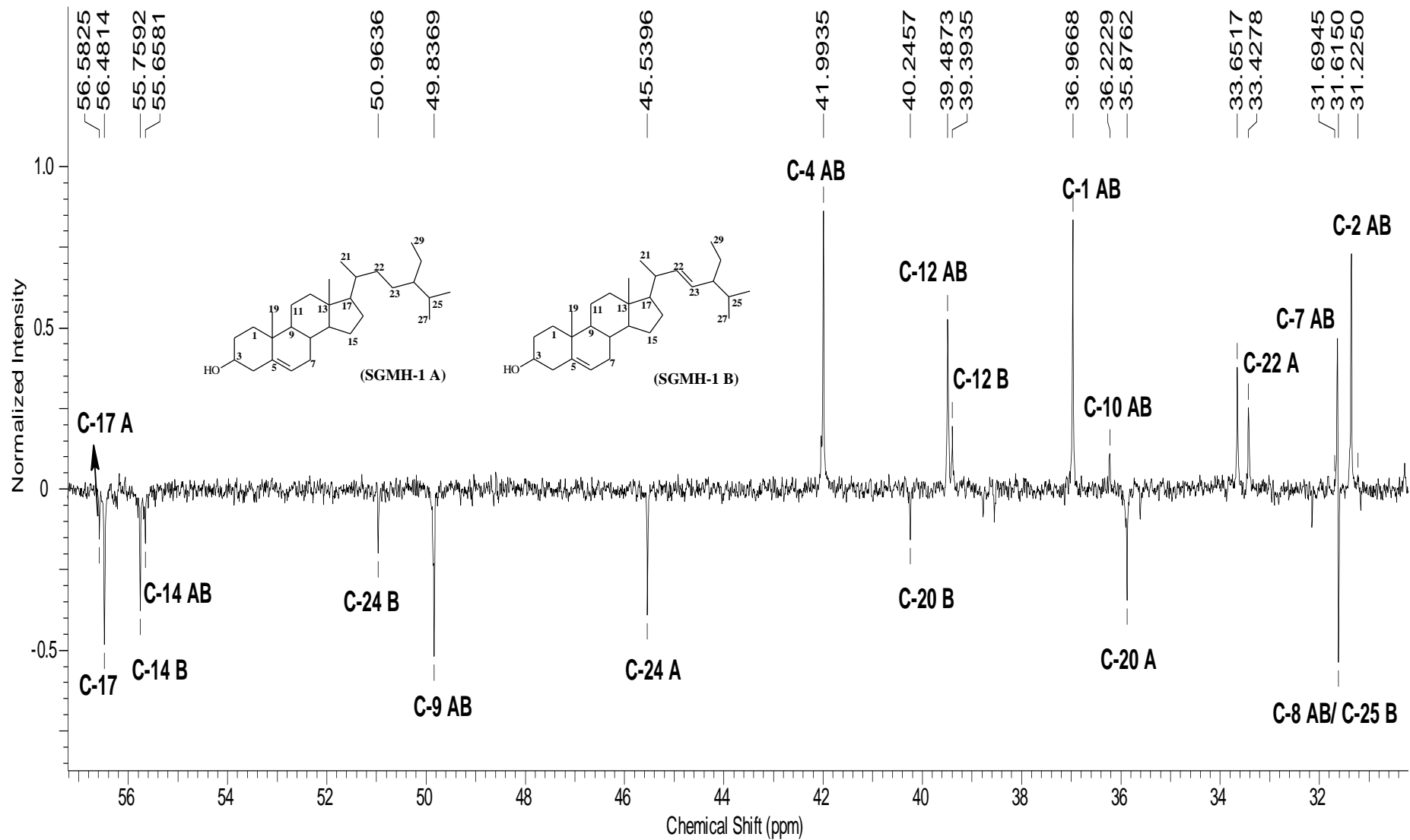
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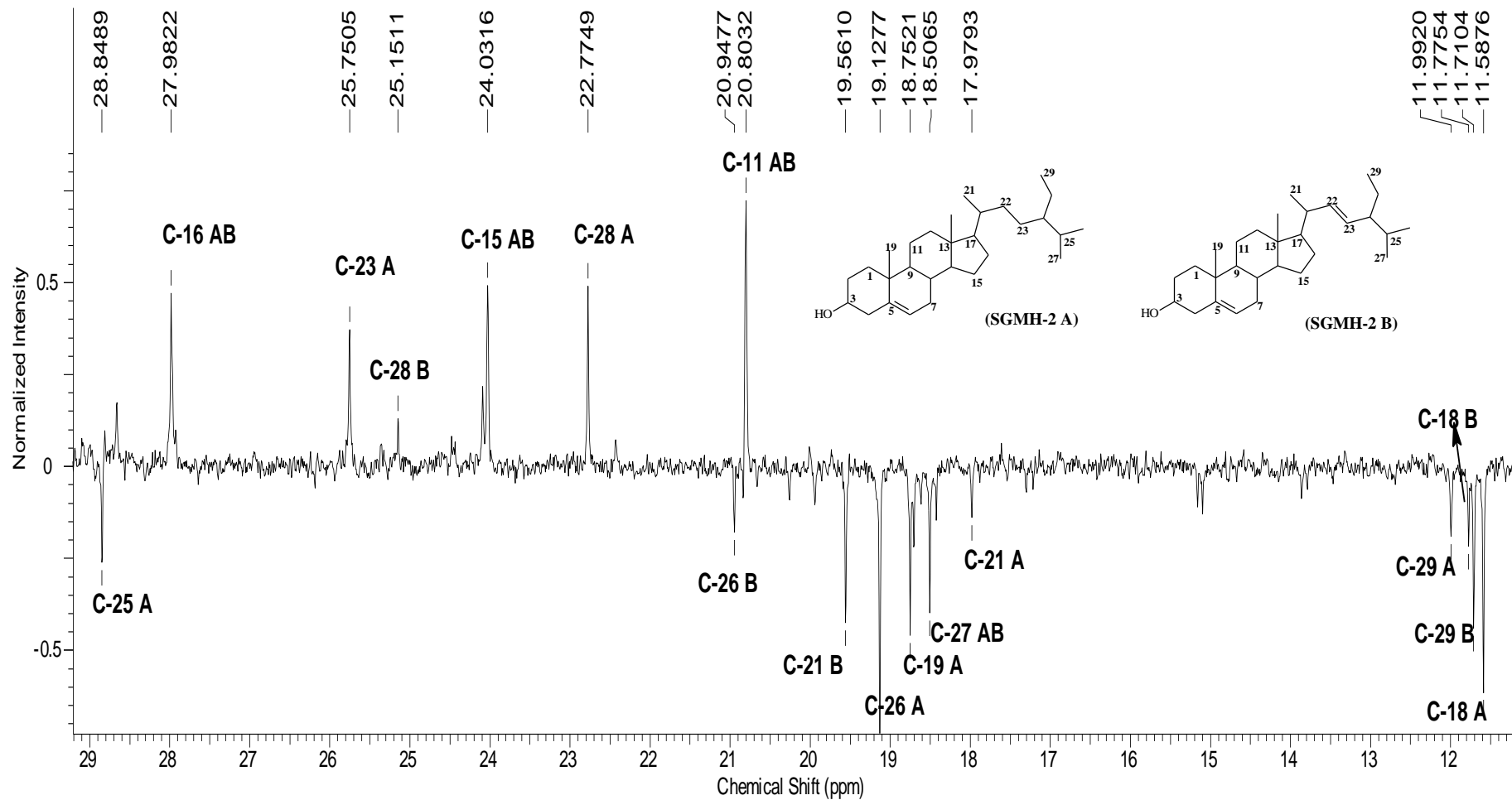
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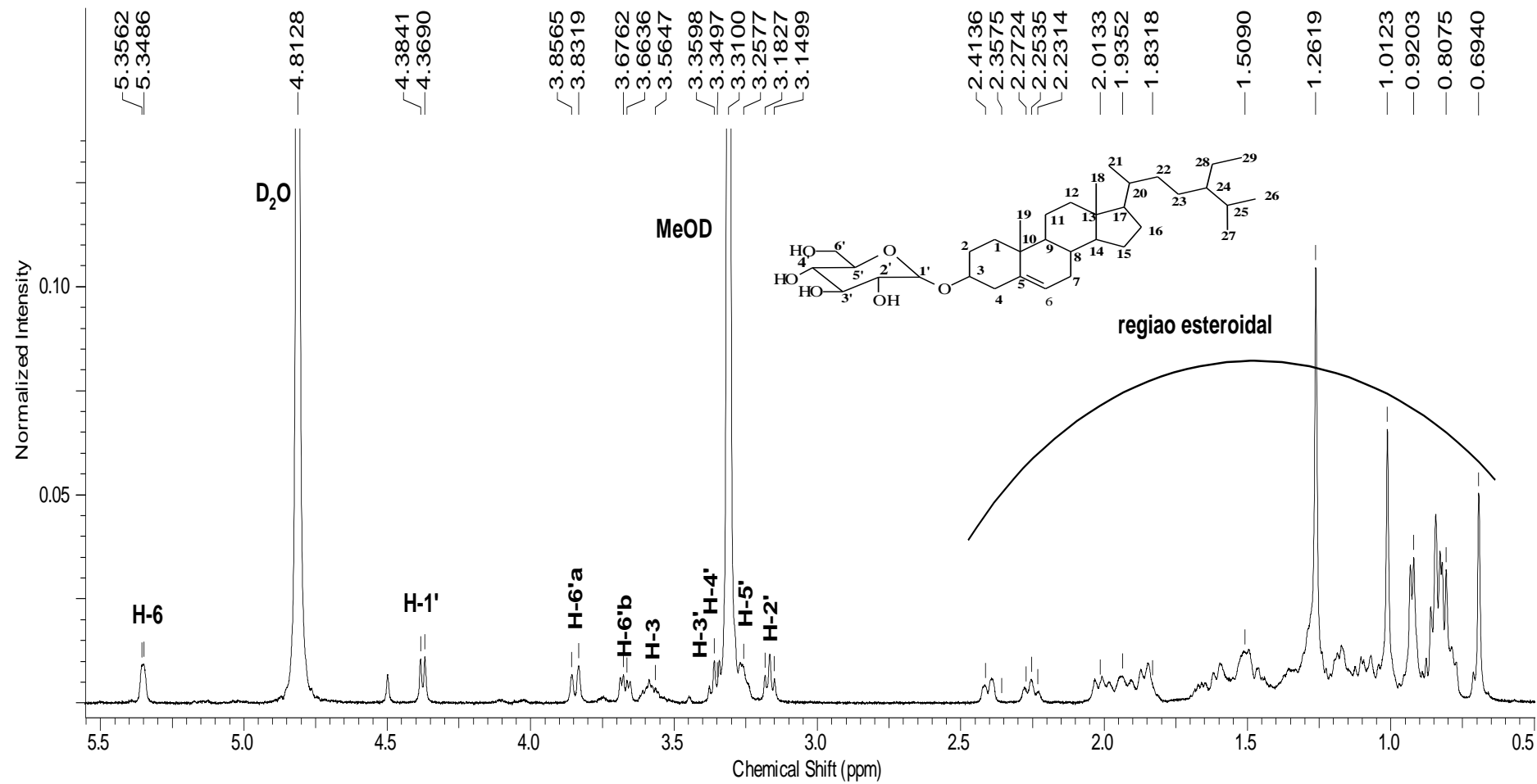
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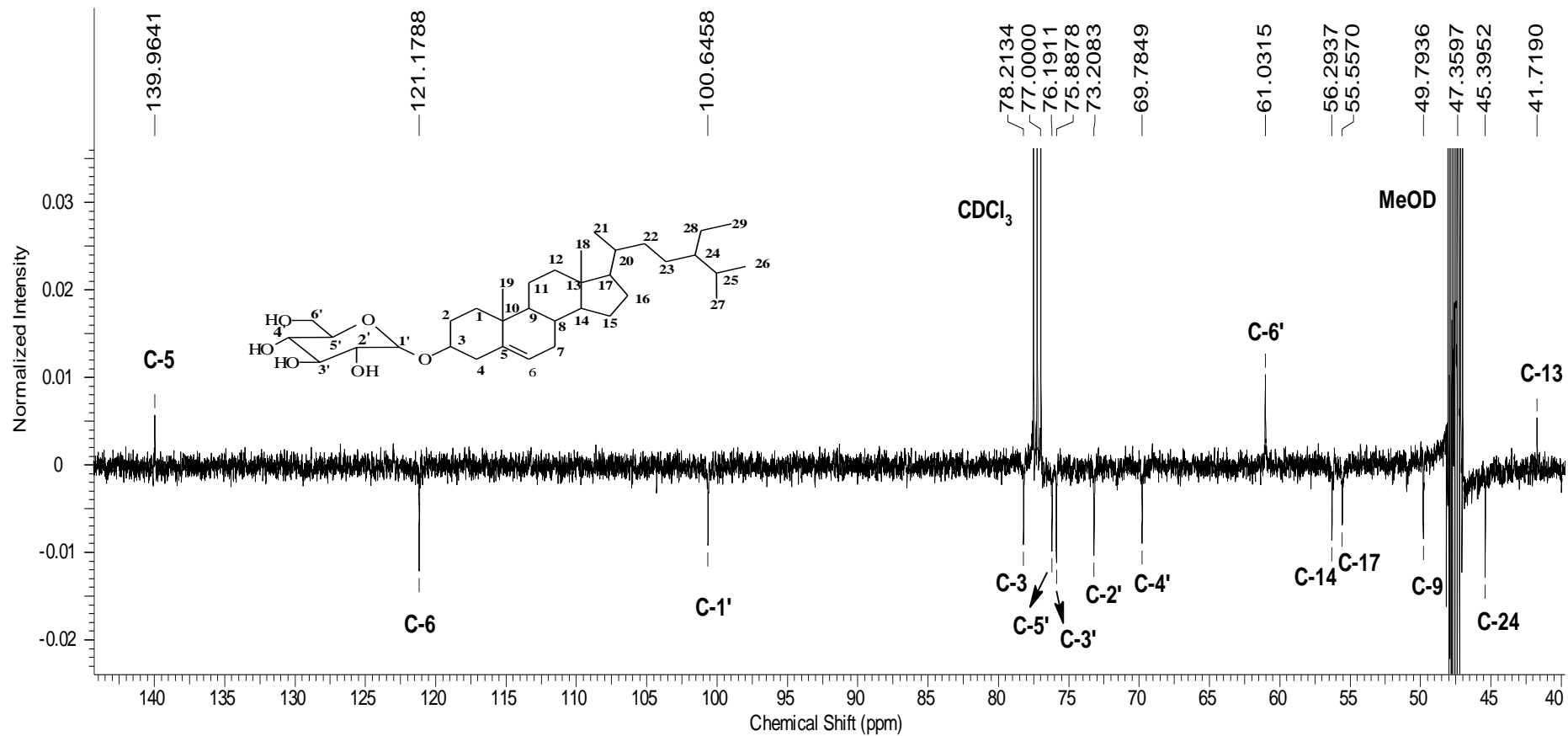
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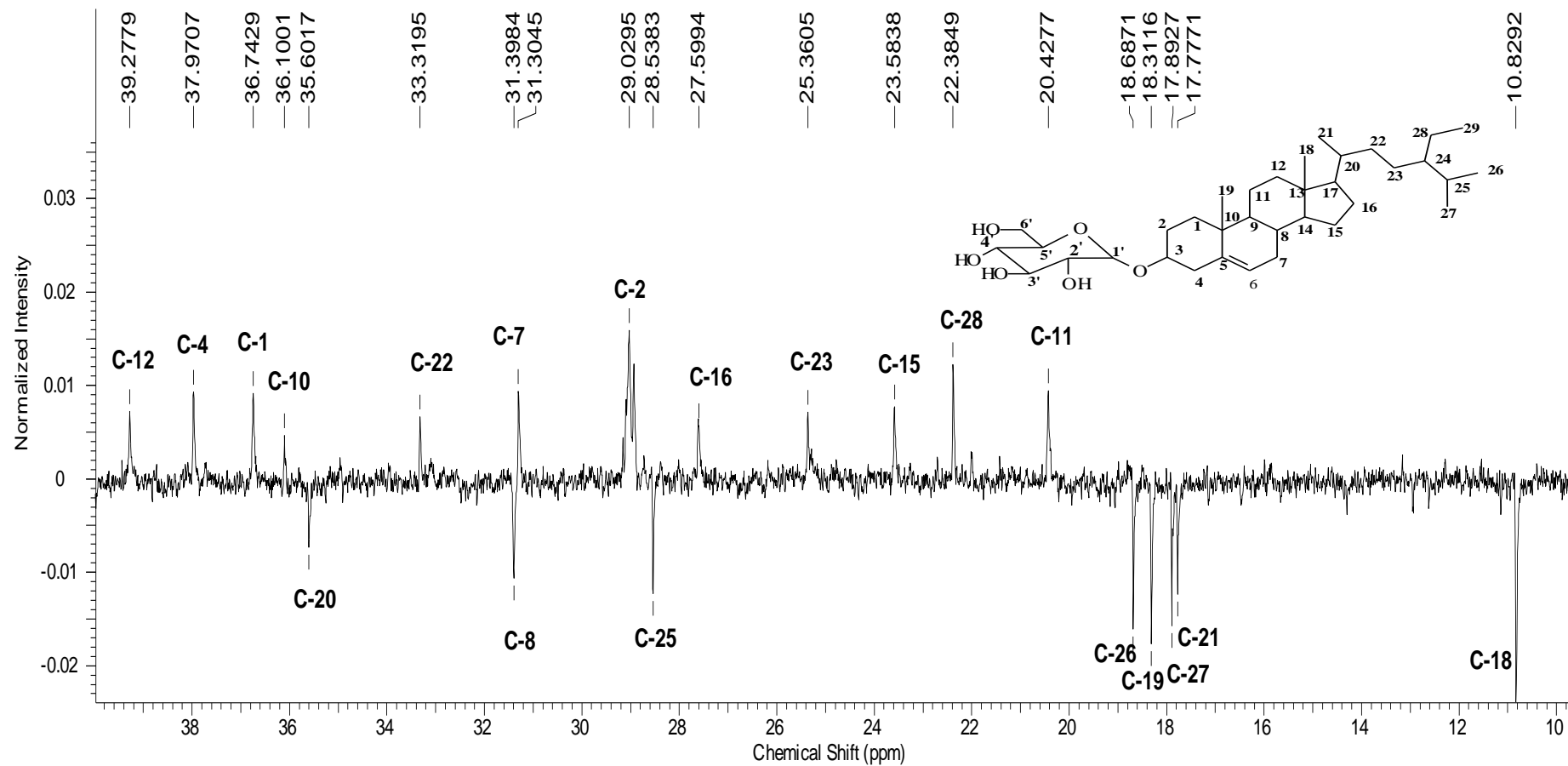
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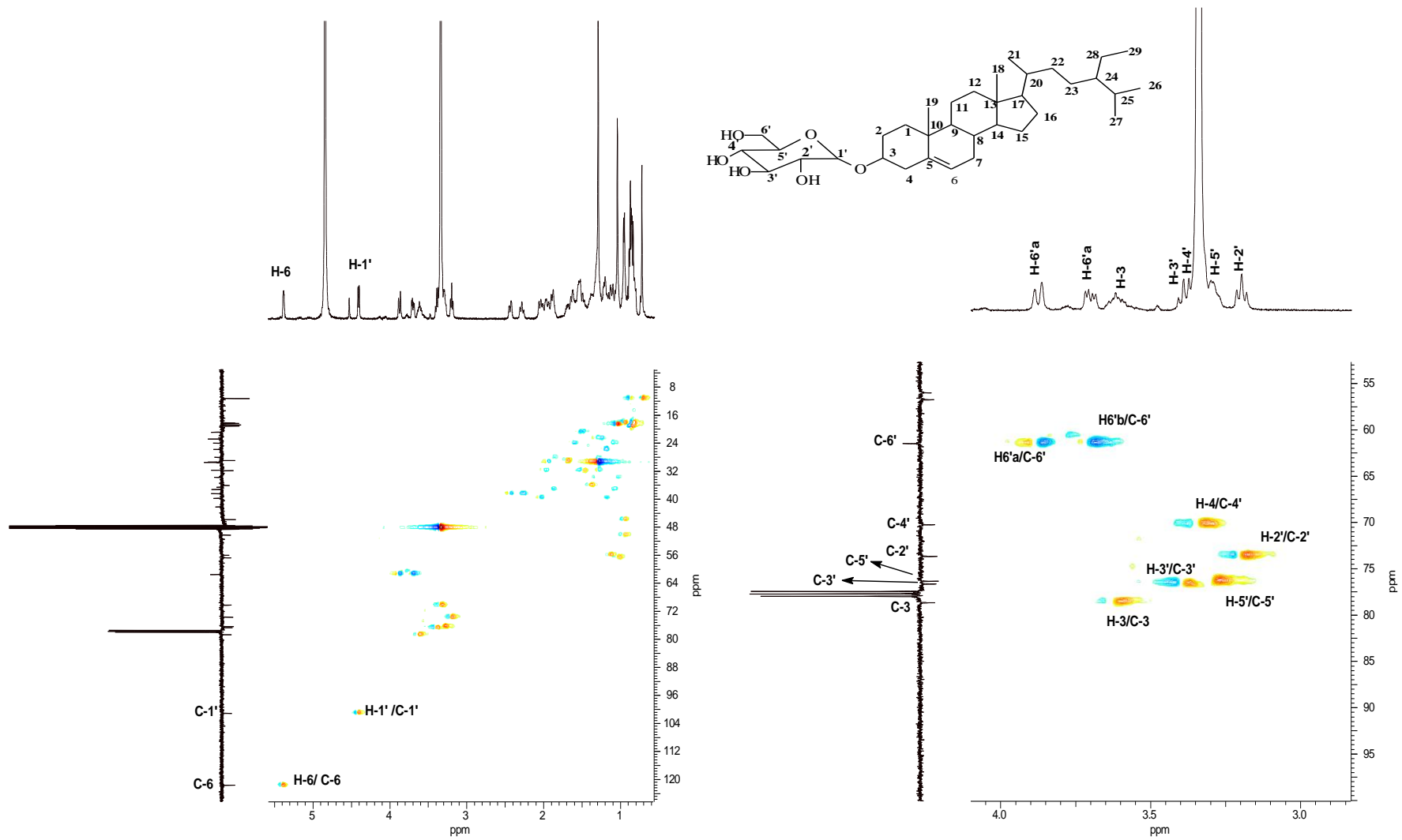
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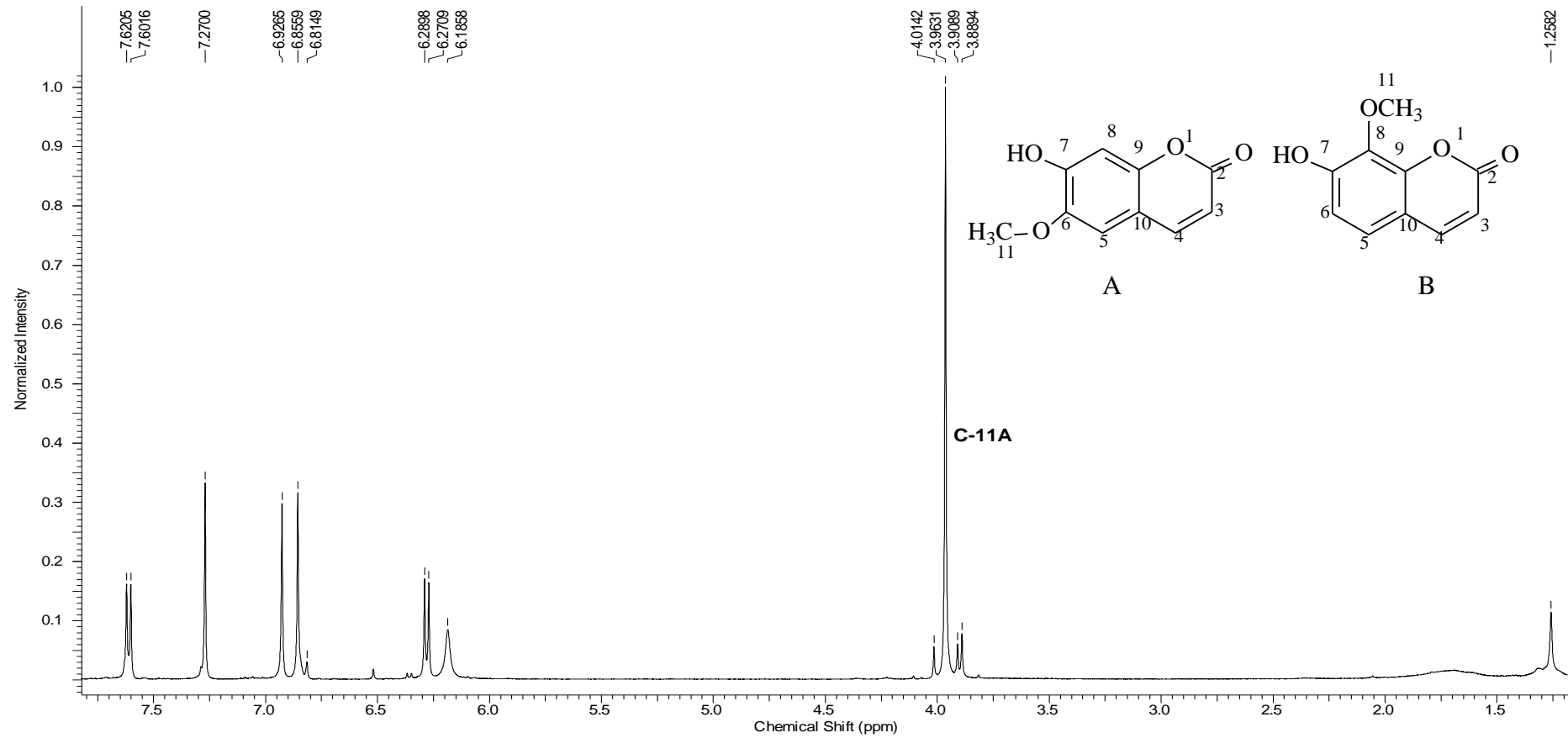
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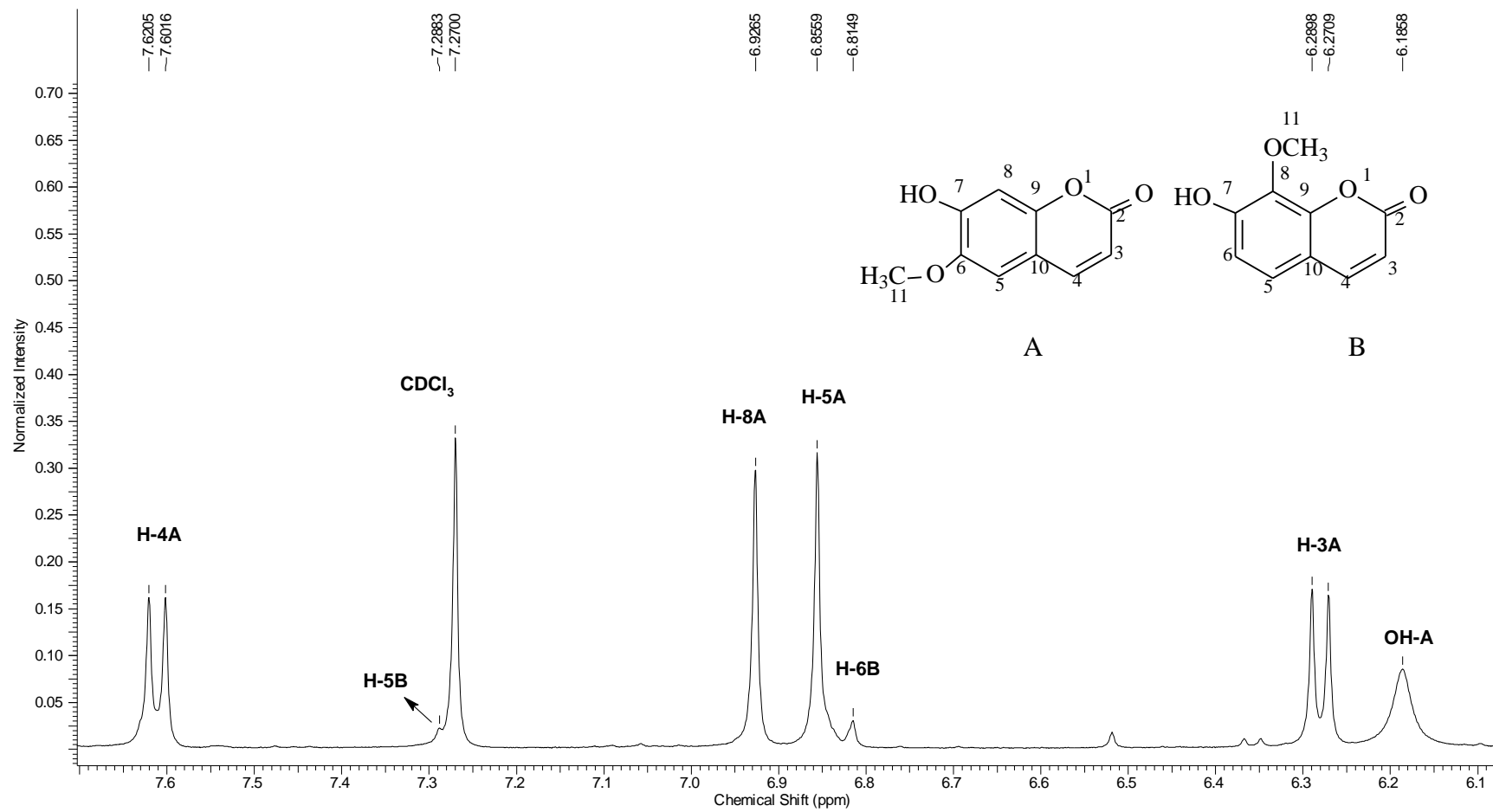
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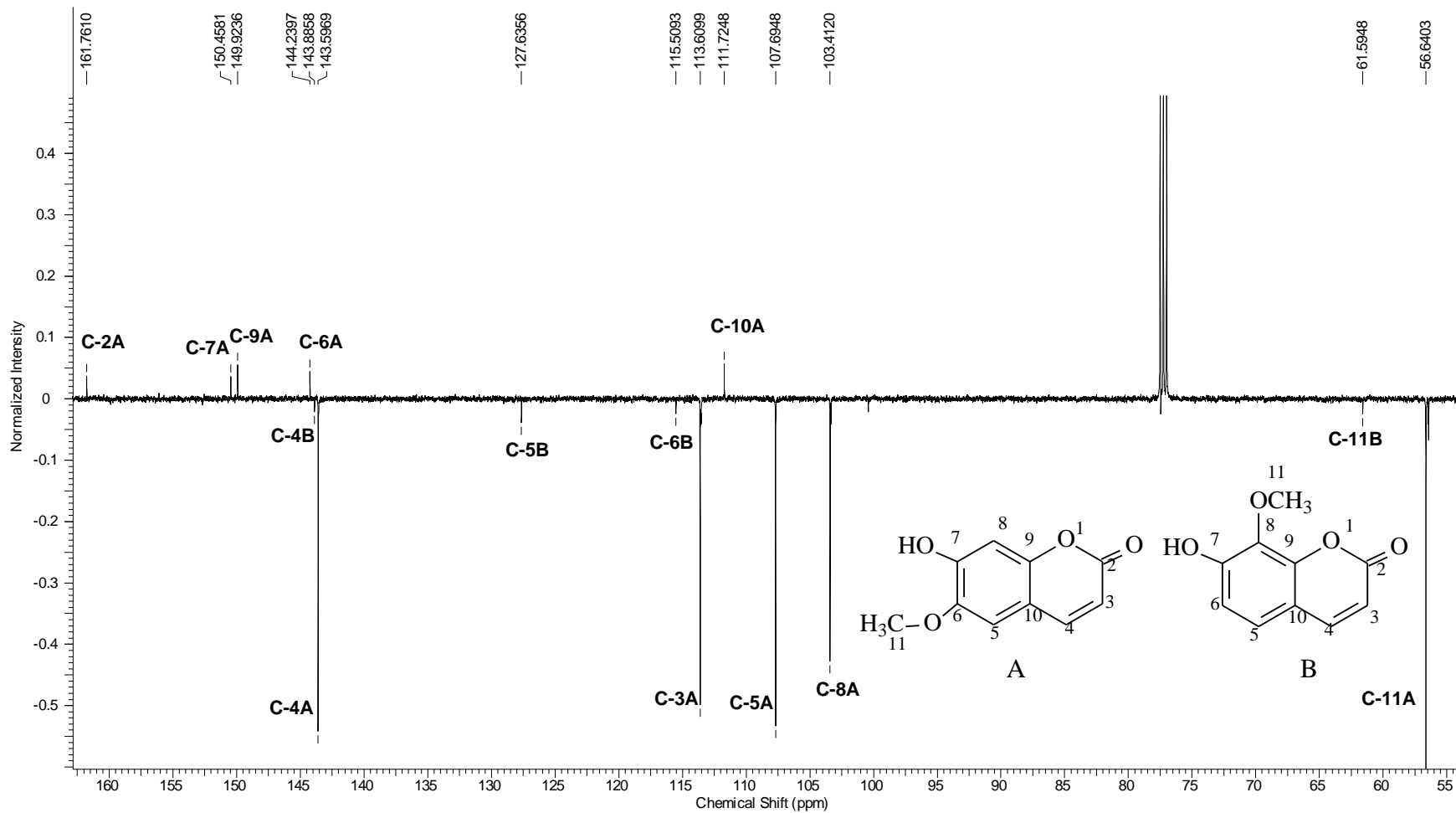
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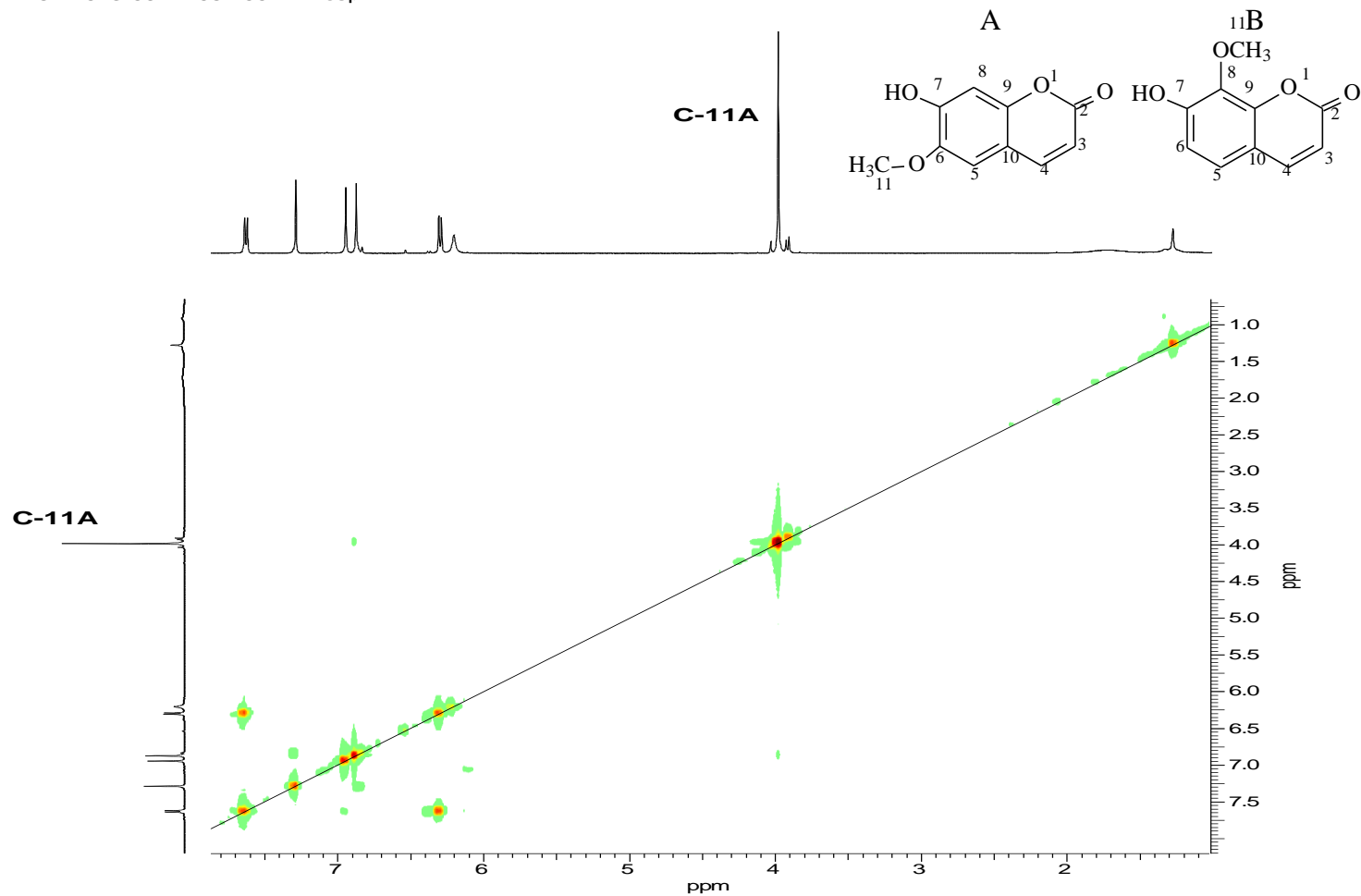
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Espectro 18. Expansão entre δ_H 7.6-6.1 do espectro de RMN-¹H (500 MHz, CDCl₃) da mistura **SGMD-2**.

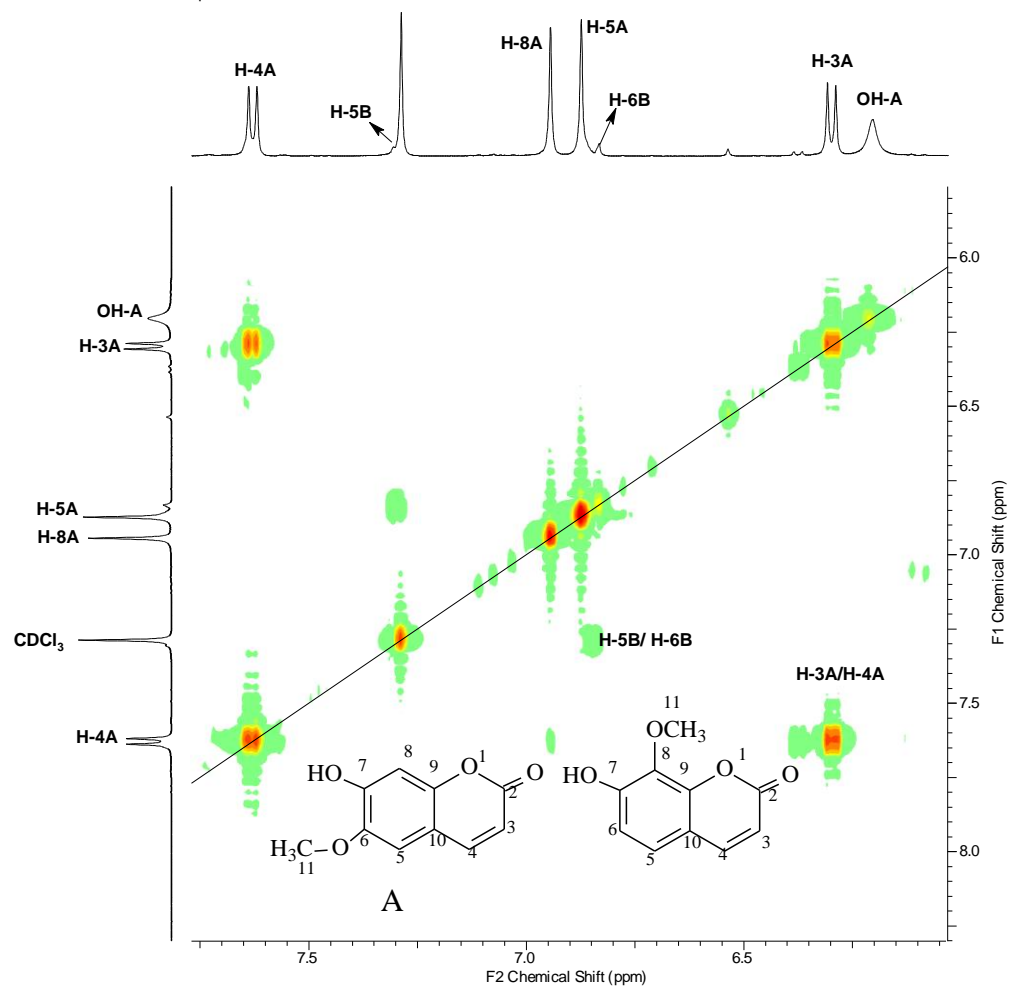


Espectro 19. RMN-¹³C-DEPTQ (125 MHz, CDCl₃) da mistura **SGMD-2**

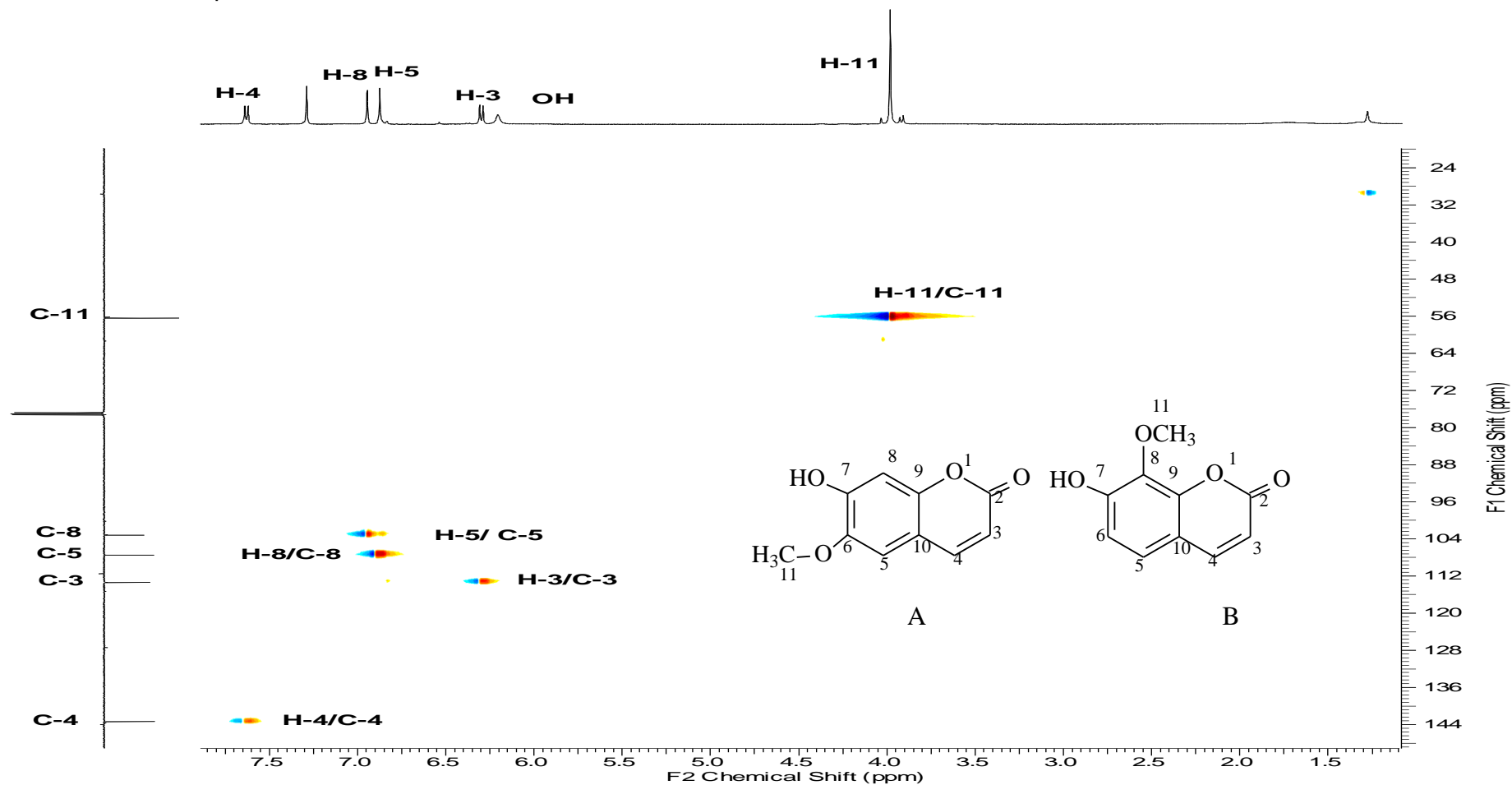


Espectro 20. ^1H - ^1H -COSY (500 MHz, CDCl_3) da mistura **SGMD-2**.

RMN.054.001.2rr.esp

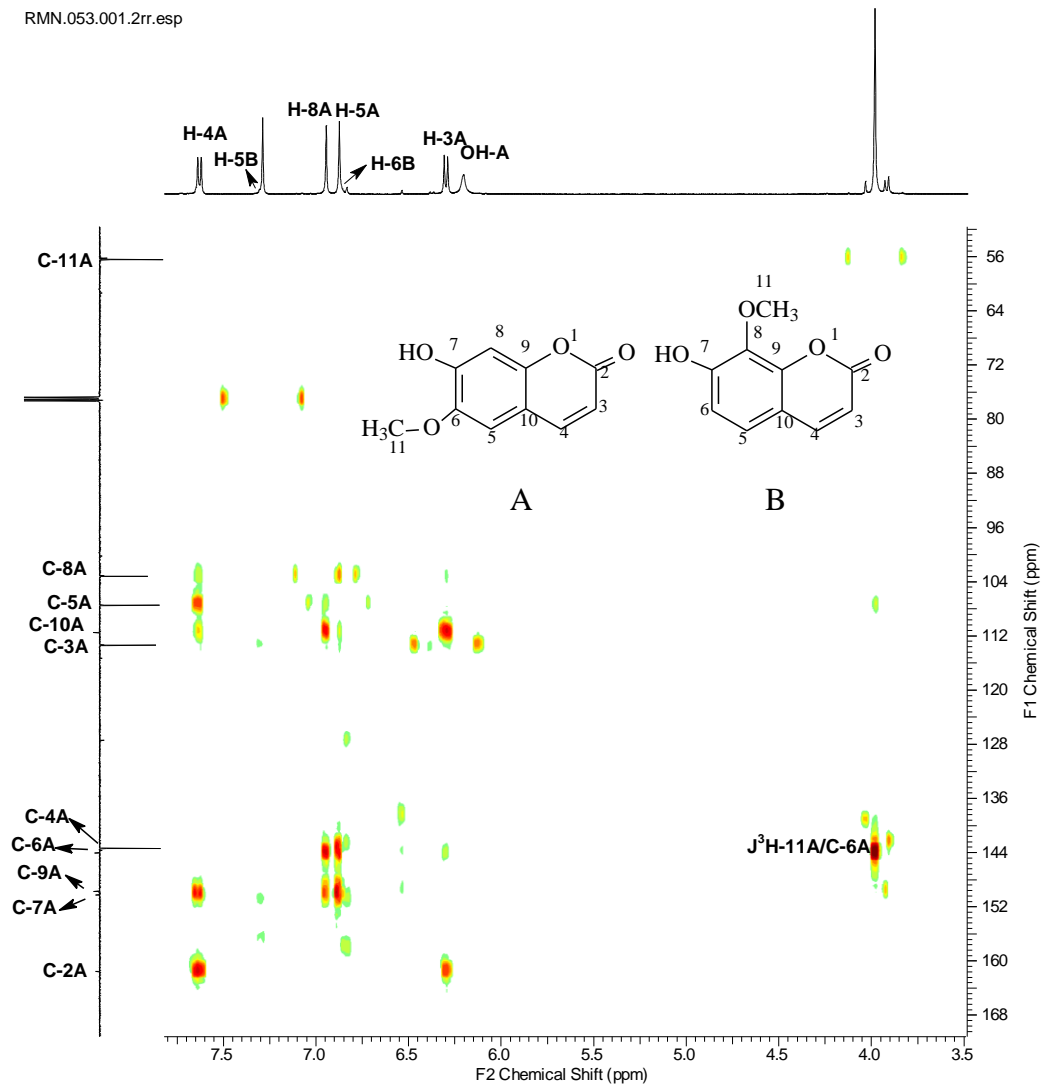


Espectro 21. Expansão entre δ_H 8.0- 6.0 do espectro de ¹H-¹H-COSY (500 MHz, CDCl₃) da mistura SGMD-2.

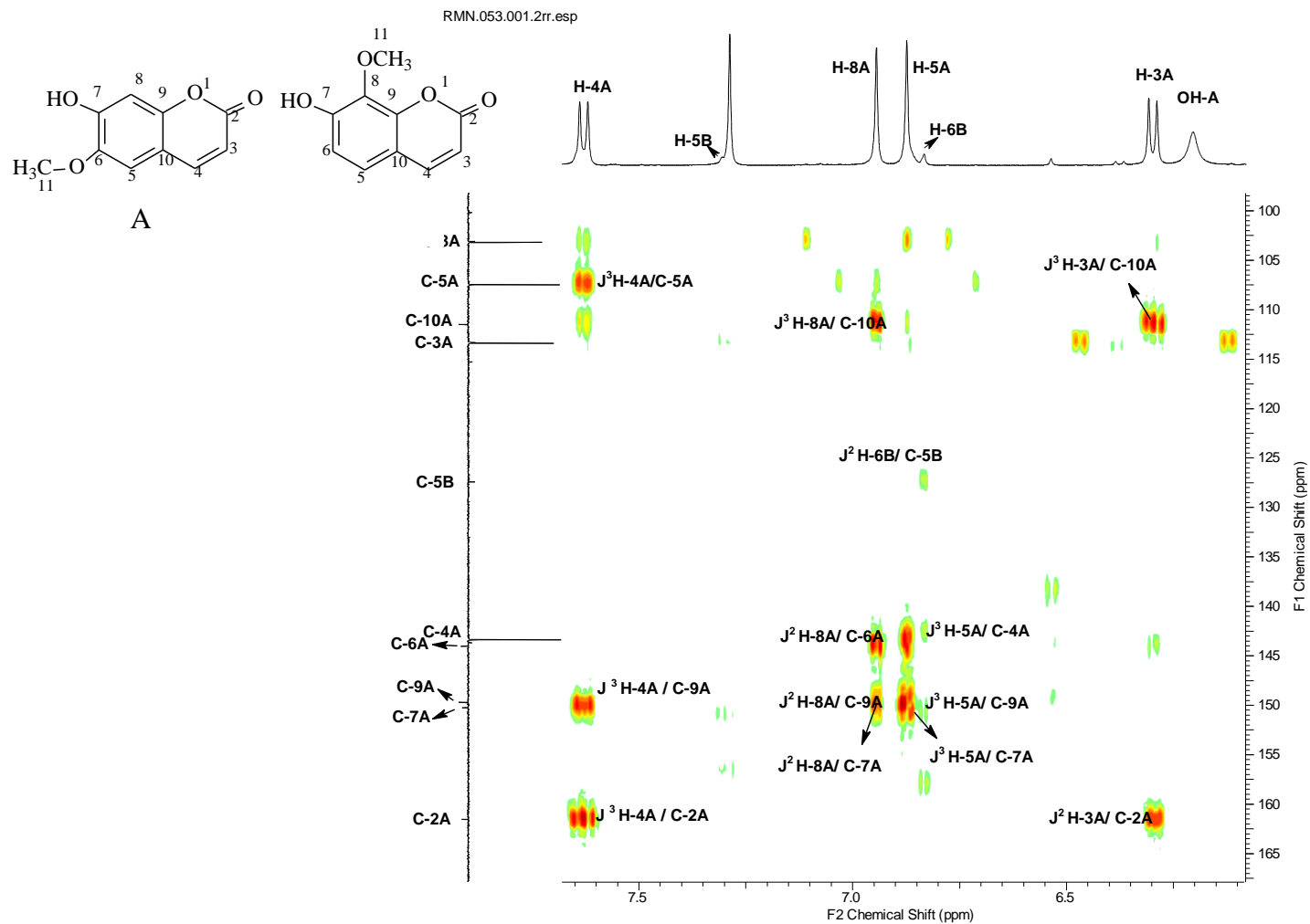


Espectro 22. 2D de ^1H - ^{13}C -COSY- $^1\text{J}_{\text{CH}}$ (HSQC, em CDCl_3) da mistura **SGMD-2**.

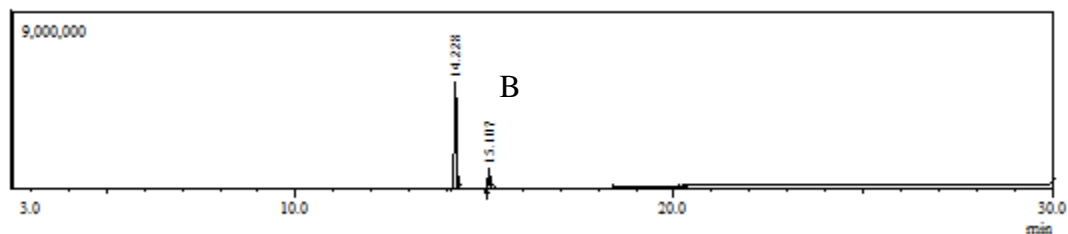
RMN.053.001.2rr.esp



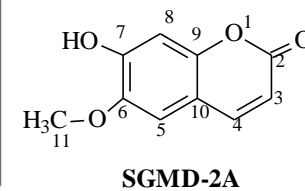
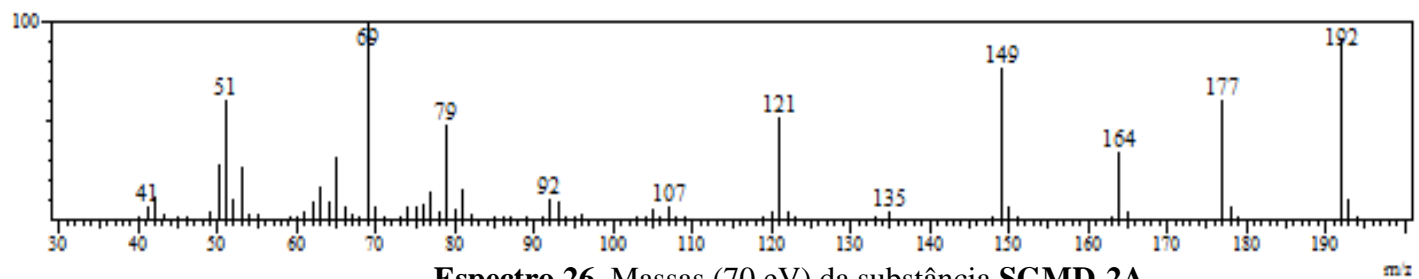
Espectro 23. 2 D de $^1\text{H-}^{13}\text{C-COSY-}^n\text{J}_{\text{CH}}$ ($n=2$ e $n=3$, HMBC, em CDCl_3) da mistura **SGMD-2**.



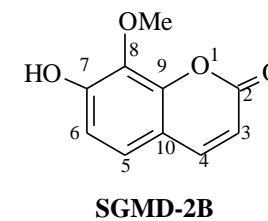
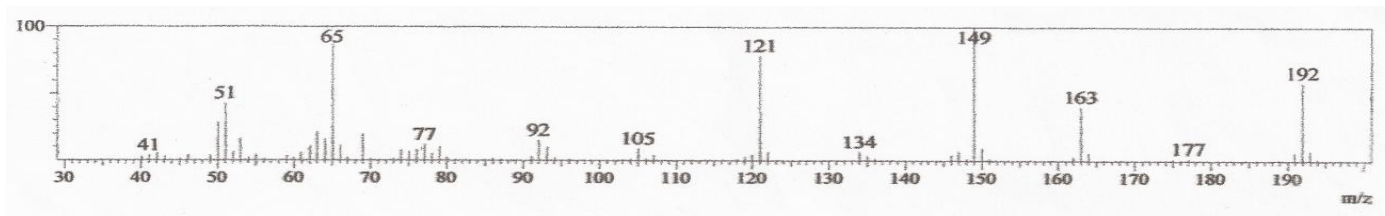
Espectro 24. Expansão entre δ_{H} 6.0-7.6 e δ_{C} 100.0-170.0 do espectro de ^1H - ^{13}C -COSY- $^n\text{J}_{\text{CH}}$ ($n=2$ e $n=3$, HMBC, em CDCl_3) da mistura **SGMD-2**.



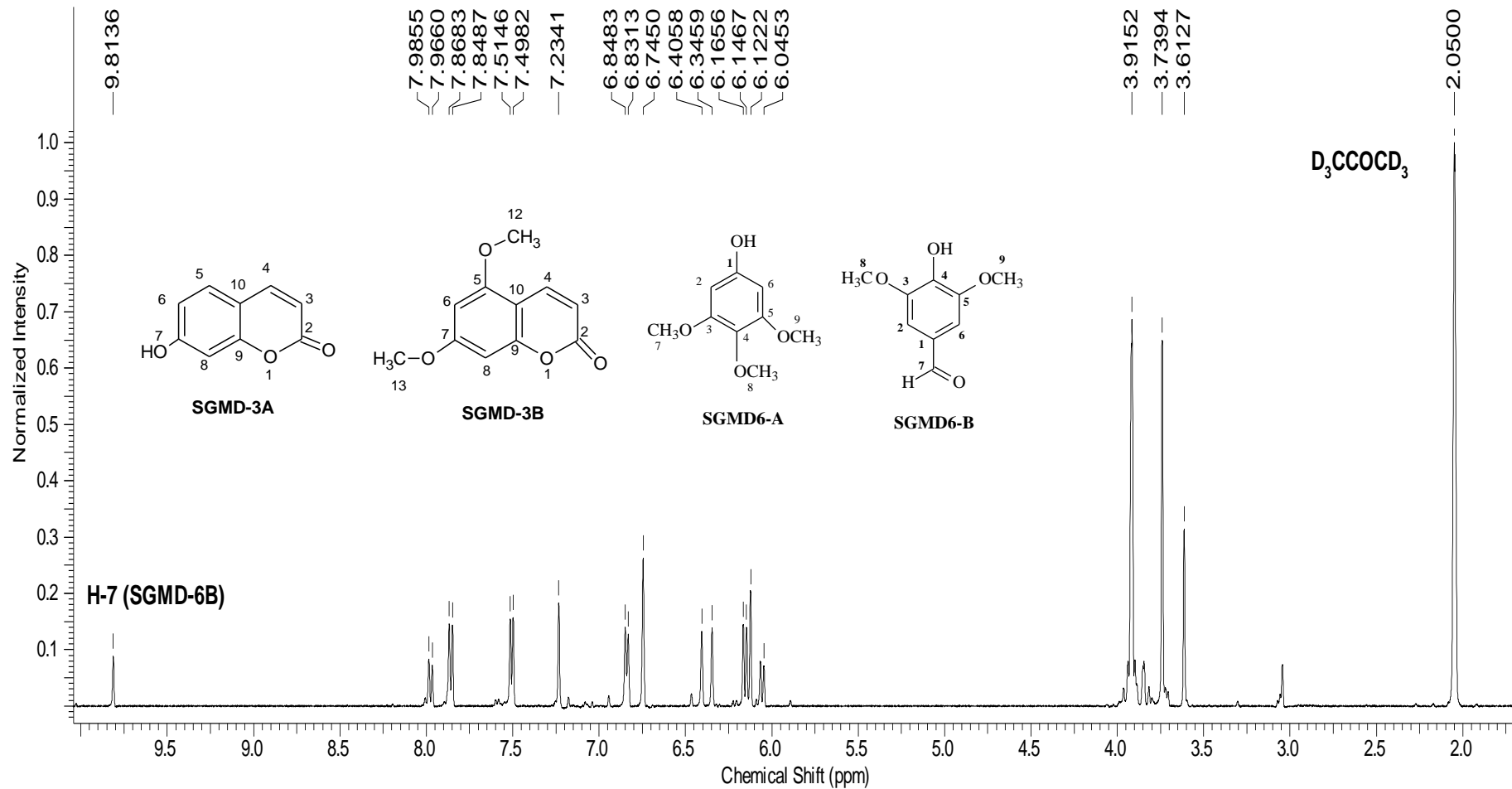
Espectro 25. Cromatograma por CG da mistura de **SGMD-2**.



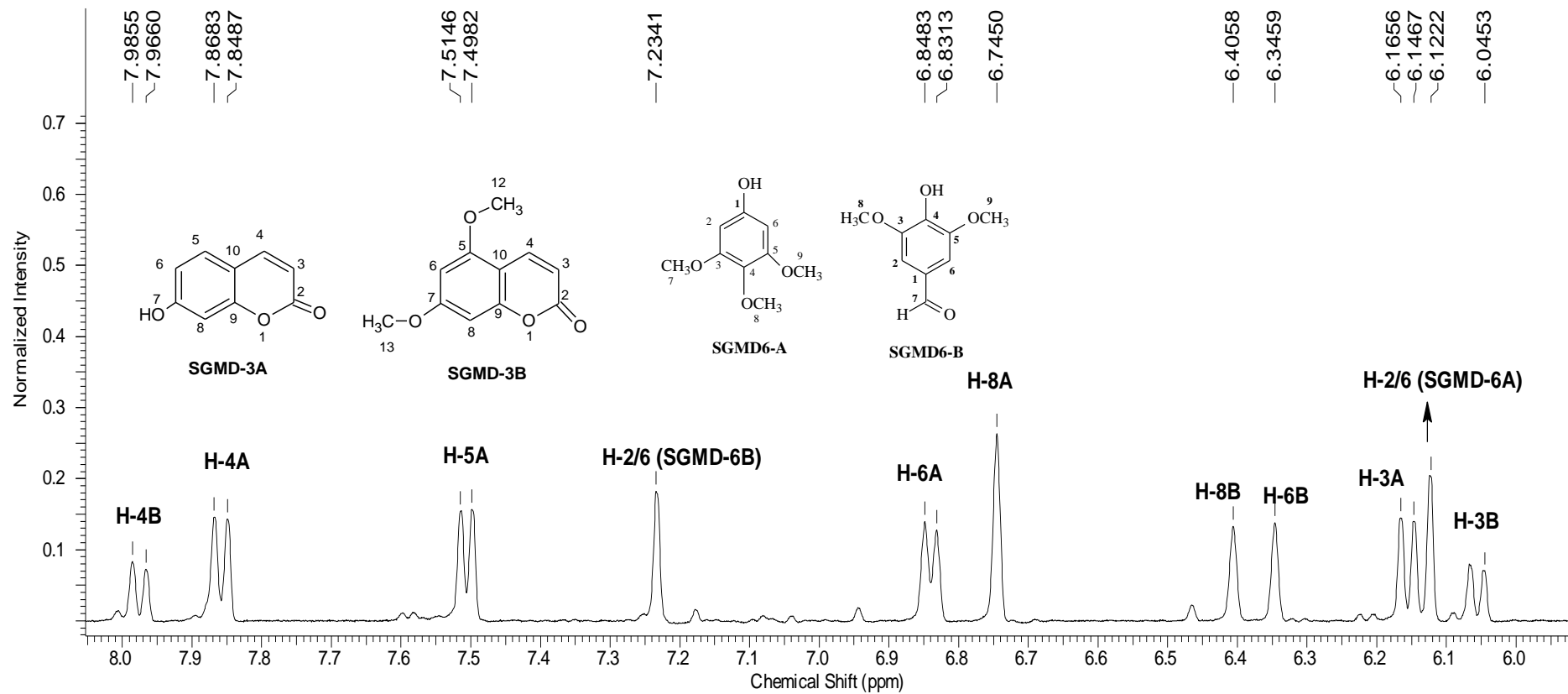
Espectro 26. Massas (70 eV) da substância **SGMD-2A**.



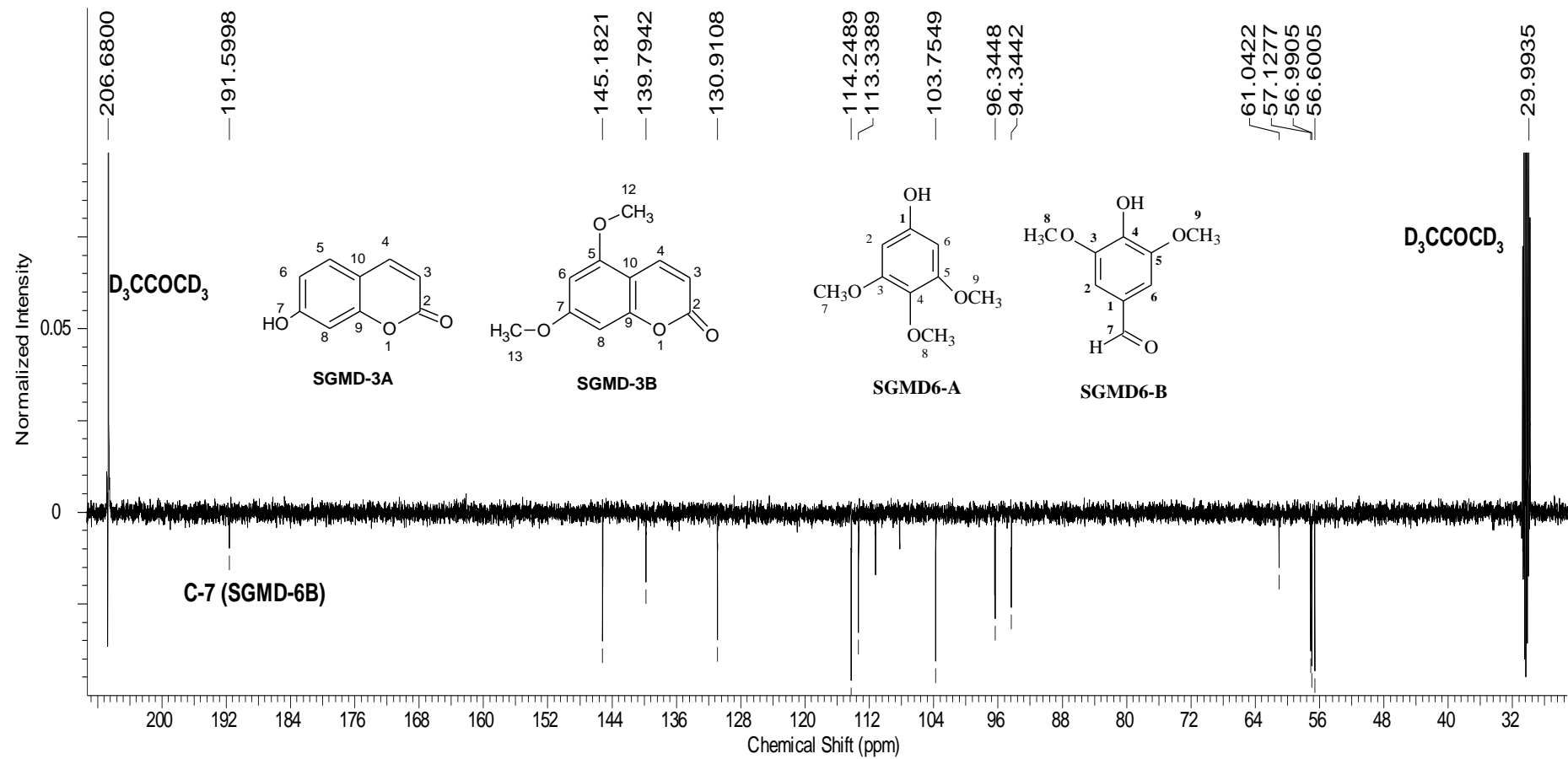
Espectro 27. Massas (70 eV) da substância **SGMD-2B**.



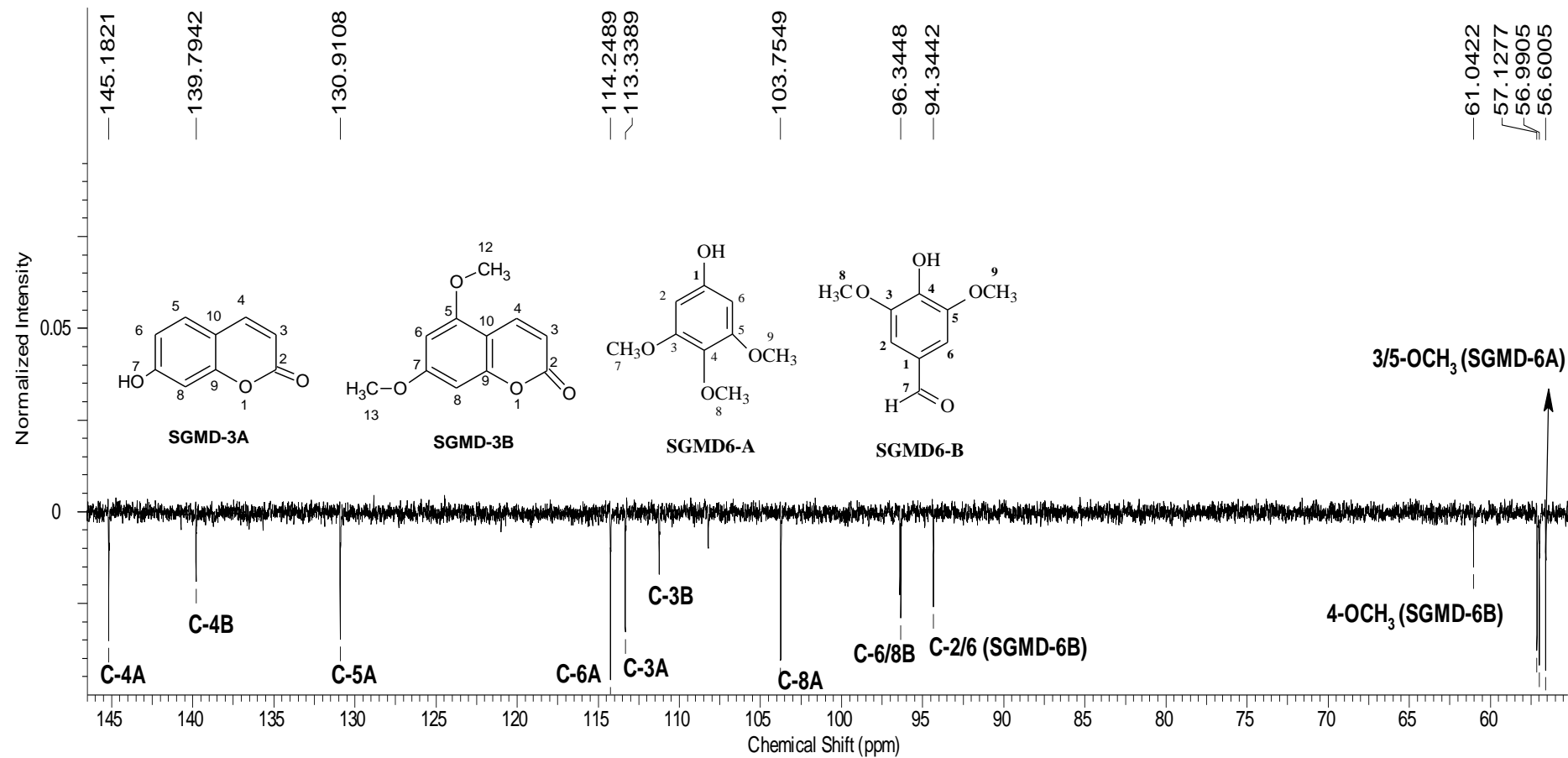
Espectro 28. RMN-¹H (500 MHz, D₃CCOCD₃) da mistura de **SGMD-3**.



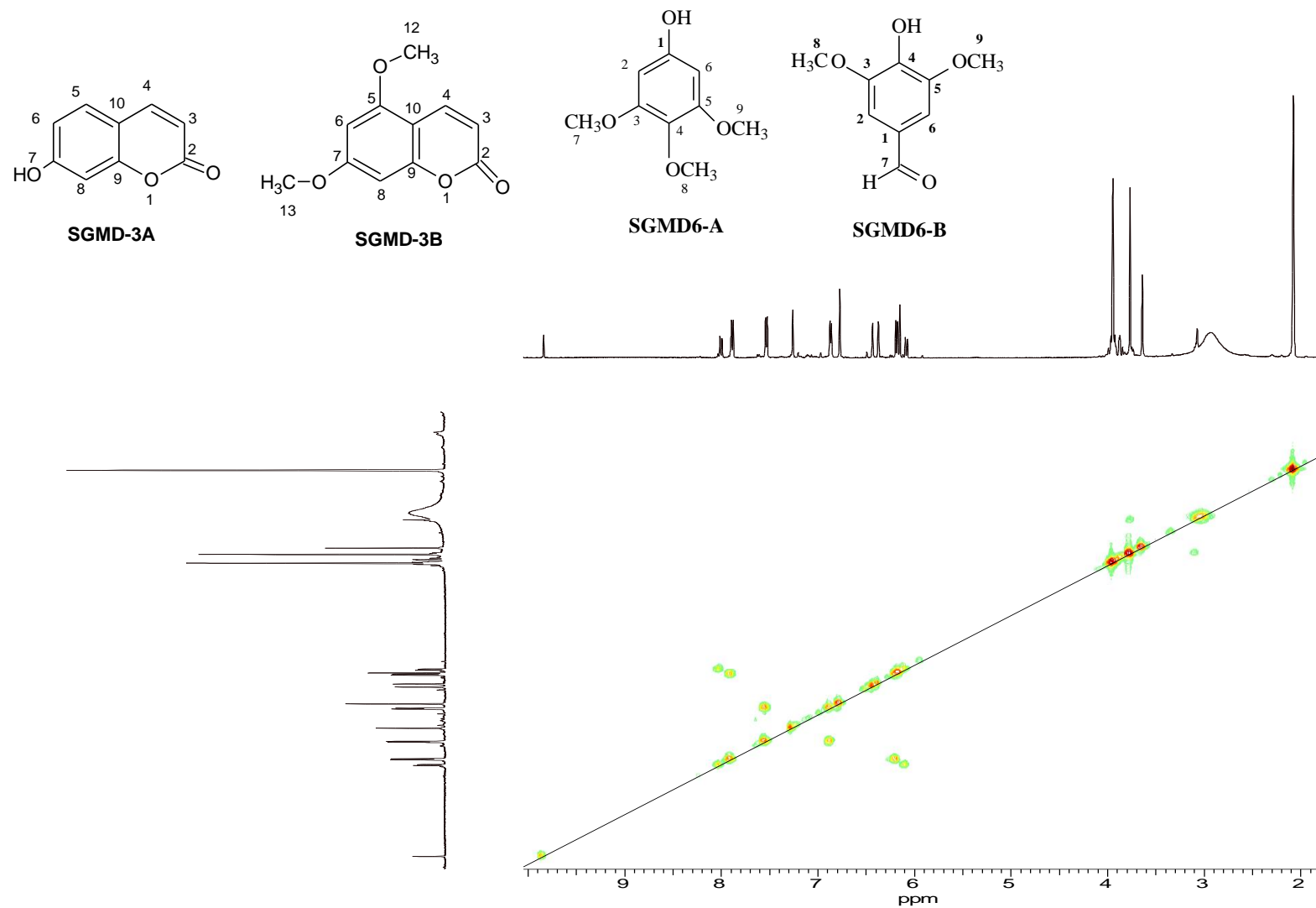
Espectro 29. Expansão entre δ_H 8.0-6.0 do espectro de RMN- 1H (500 MHz, D_3CCOCD_3) da mistura de **SGMD-3**.



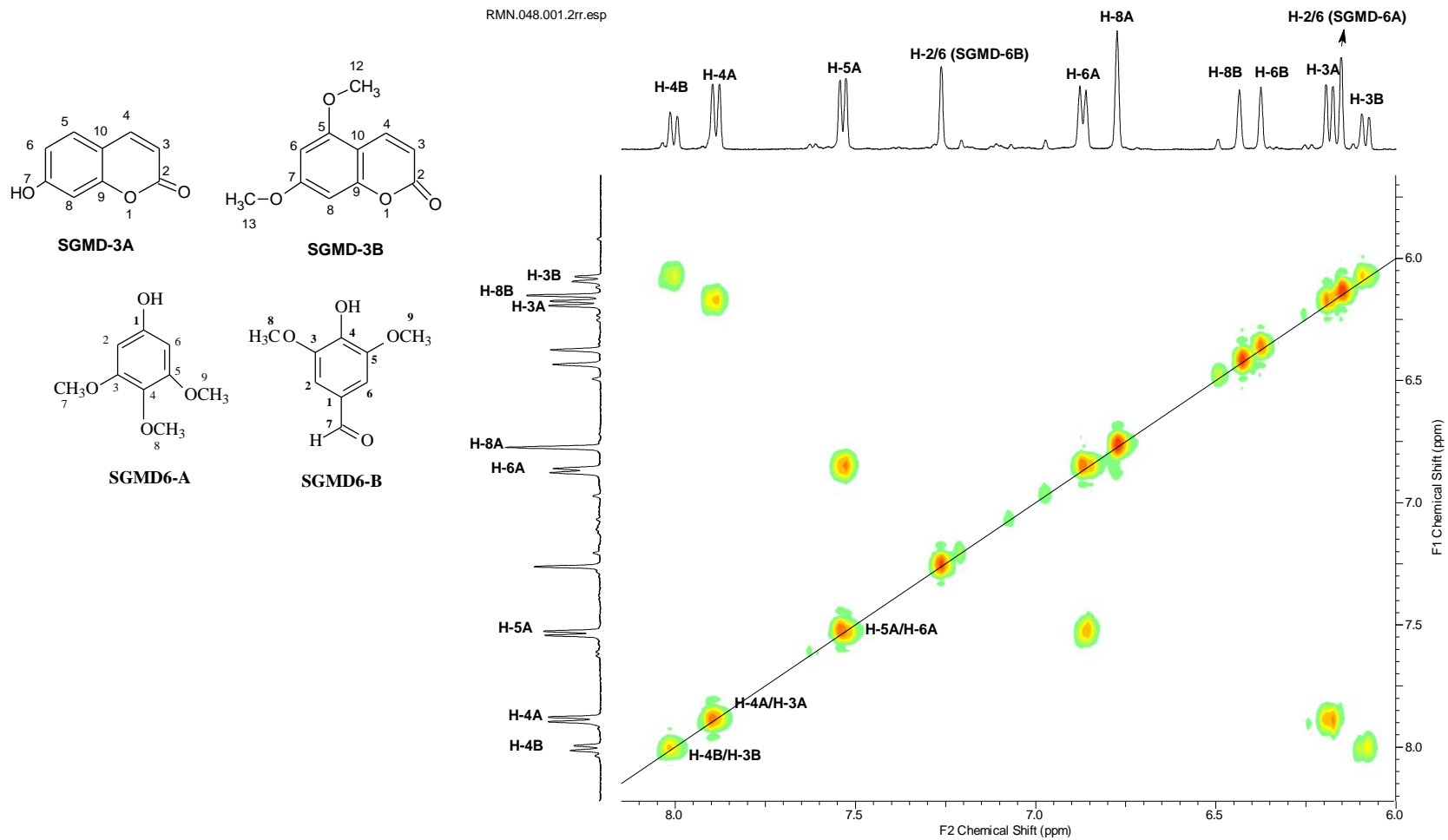
Espectro 30. Expansão entre δ_C 206.68-29.99 do espectro de RMN- ^{13}C (500 MHz, D_3CCOCD_3) da mistura de SGMD-3.



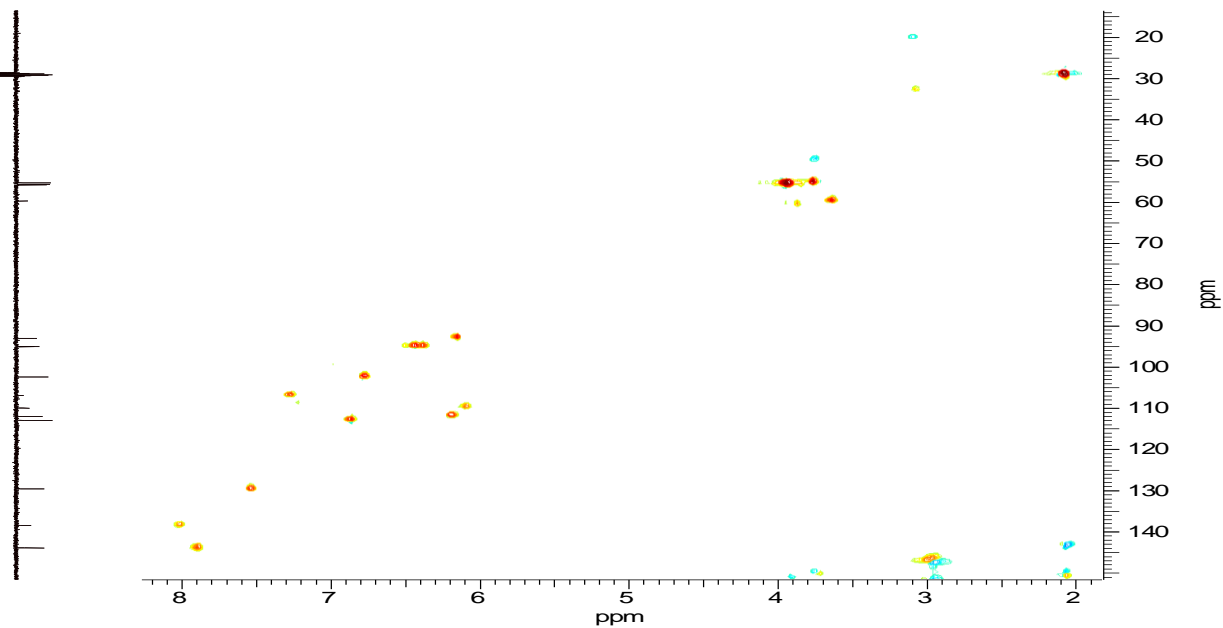
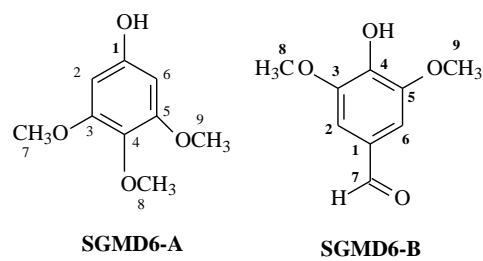
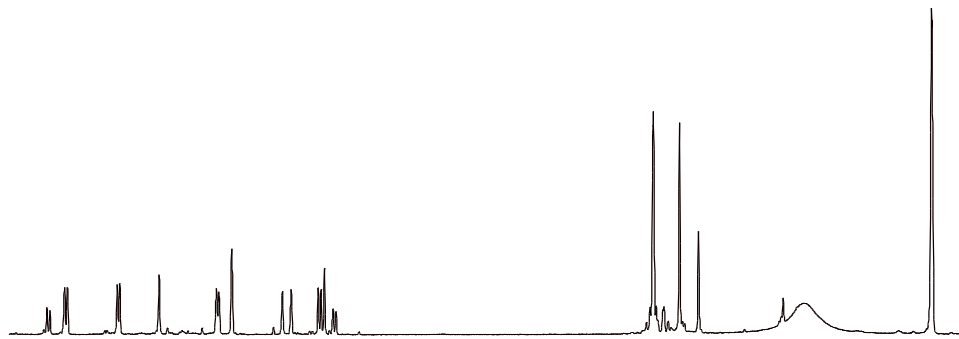
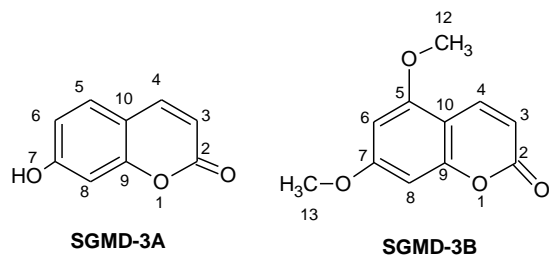
Espectro 31. Expansão entre δ_C 145.0-60.0 do espectro de RMN-¹³C (500 MHz, D₃CCOCD₃) da mistura de **SGMD-3**.



Espectro 32. RMN-¹H-¹H-COSY (500 MHz, D₃CCOCD₃) da mistura de **SGMD-3**.

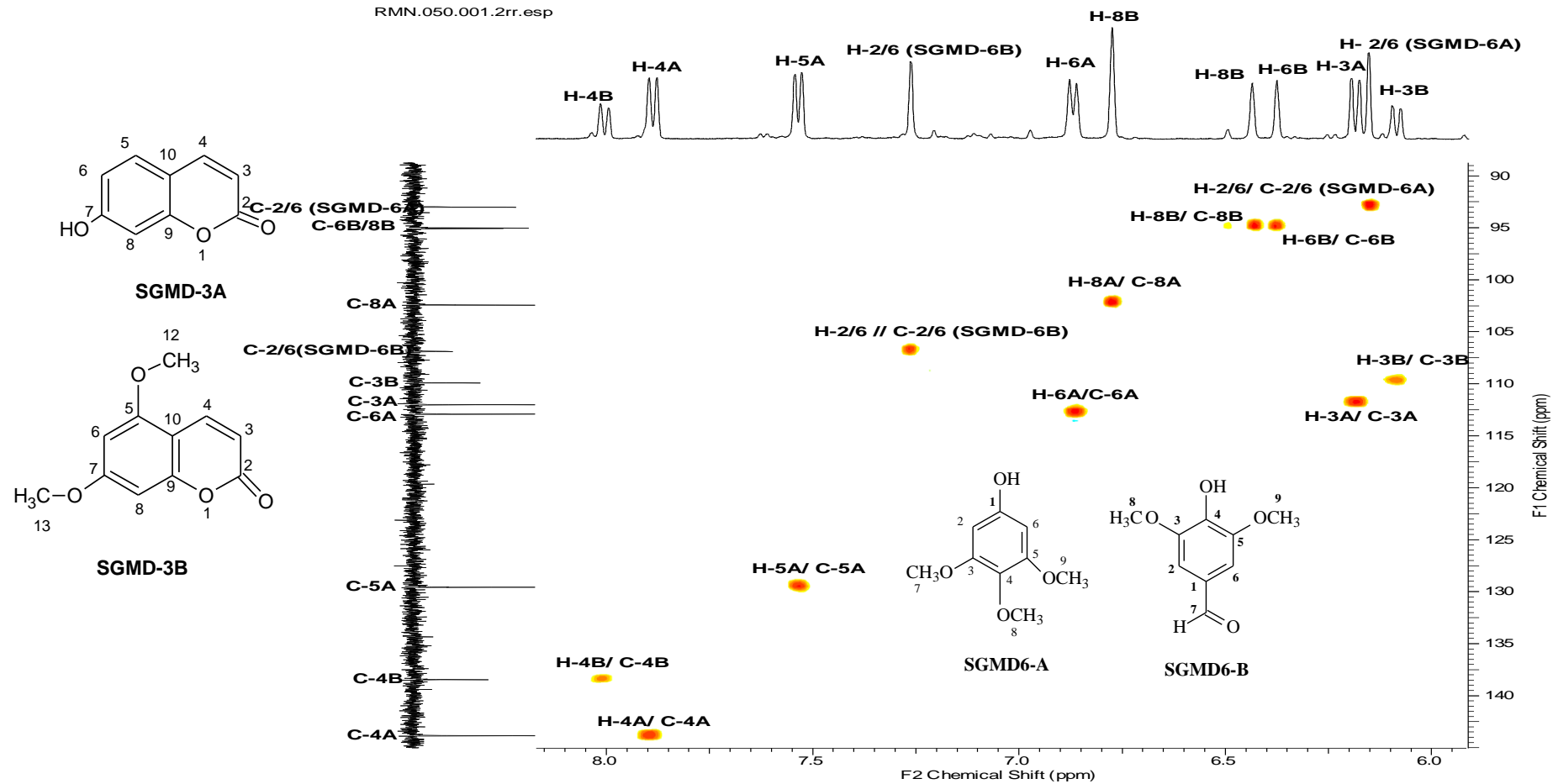


Espectro 33. Expansão entre δ_{H} 8.0-6.0 do espectro de RMN- ^1H - ^1H -COSY (500 MHz, D_3CCOCD_3) da mistura de **SGMD-3**.

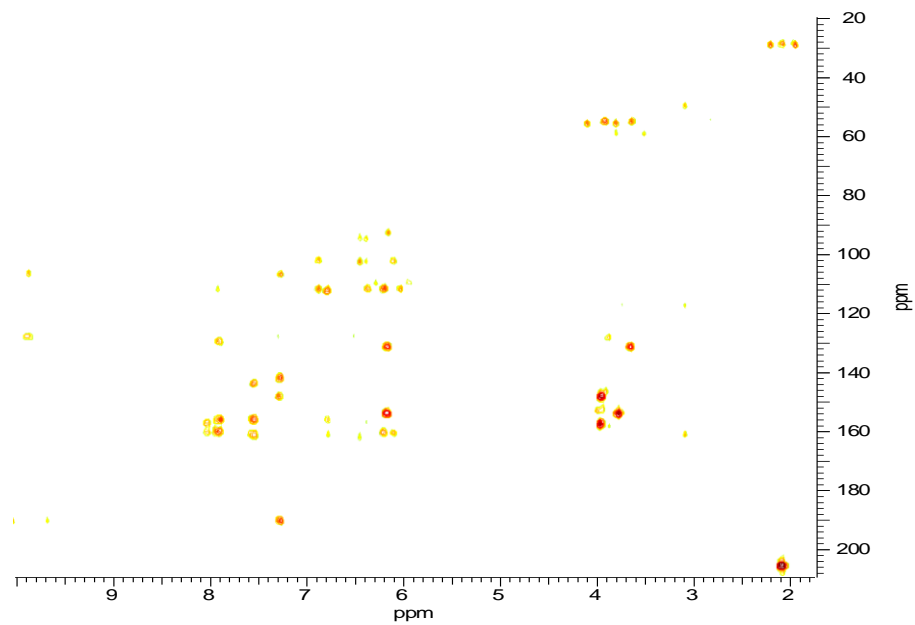
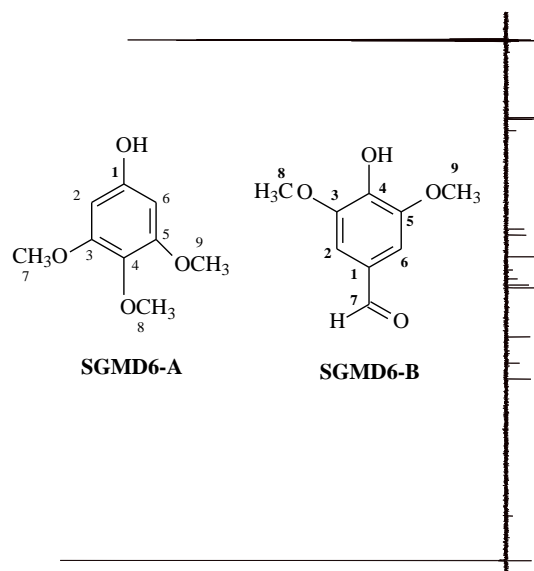
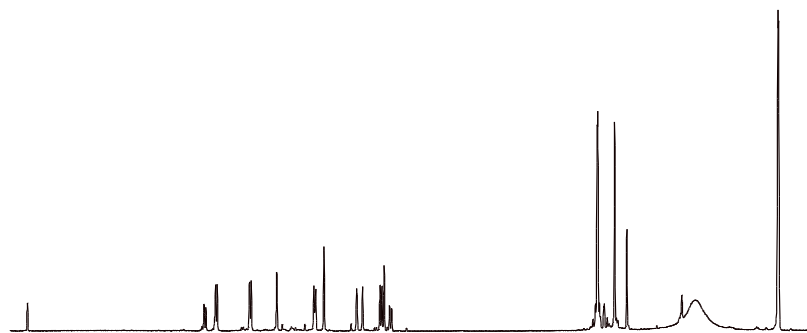
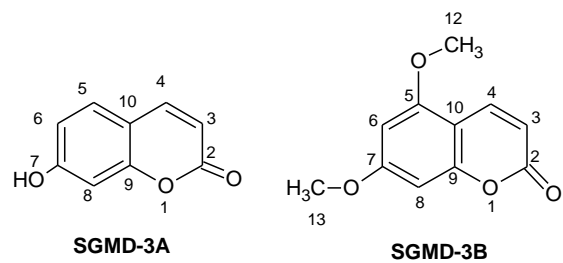


Espectro 34. 2D de ¹H-¹³C-COSY-¹J_{CH} (HSQC, em D₃CCOCD₃) da mistura **SGMD-3**.

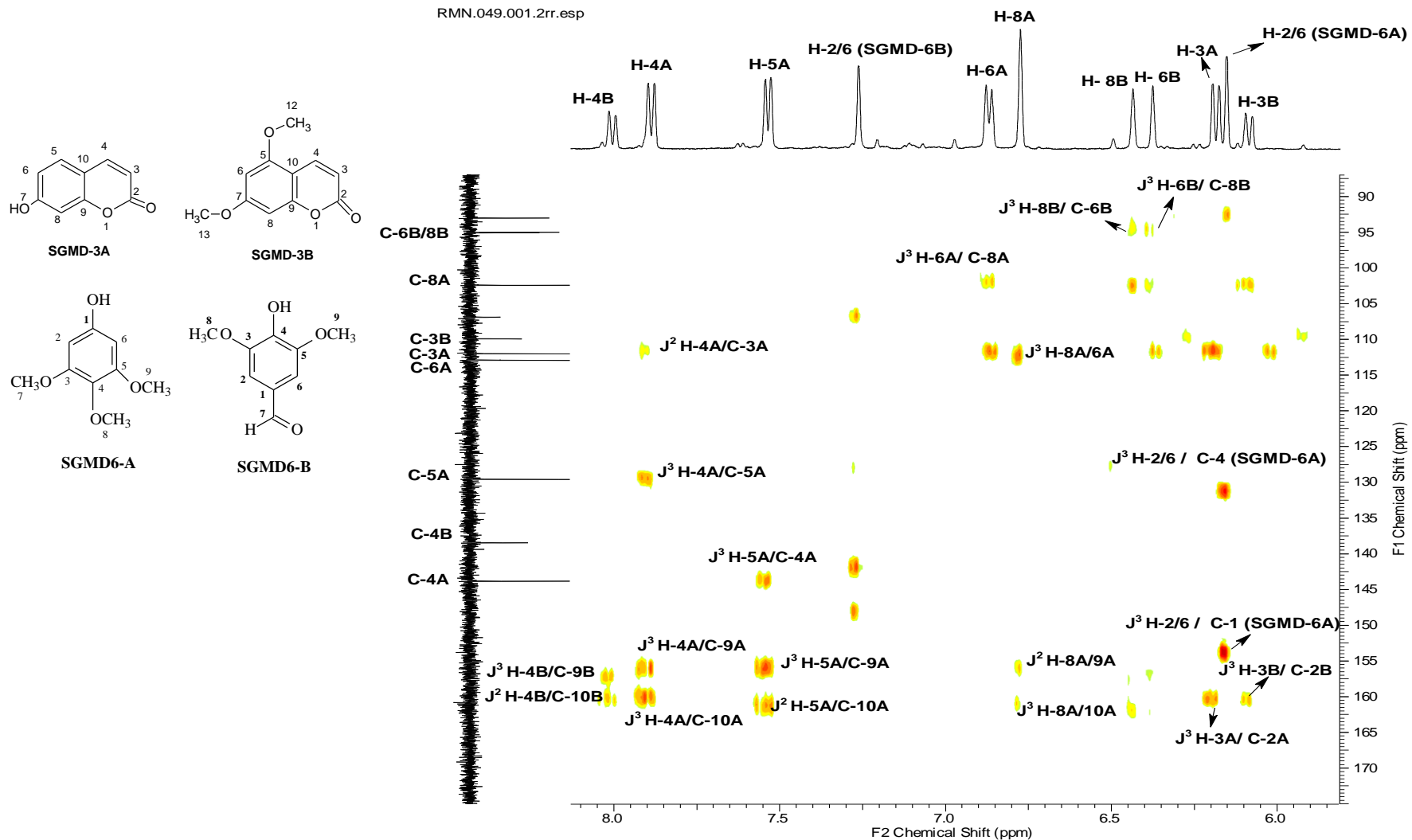
RMN.050.001.2rr.esp



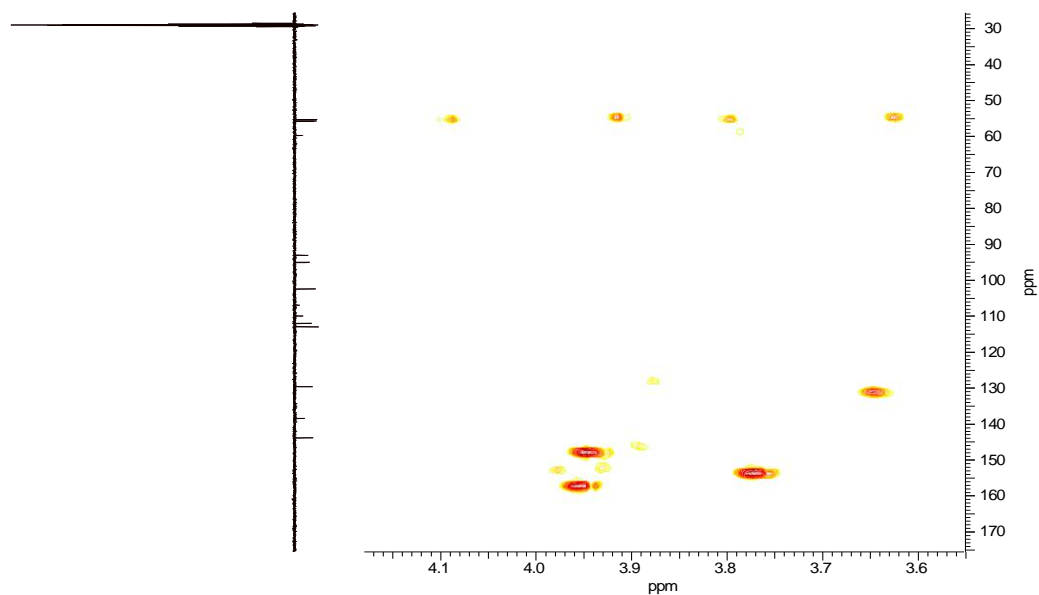
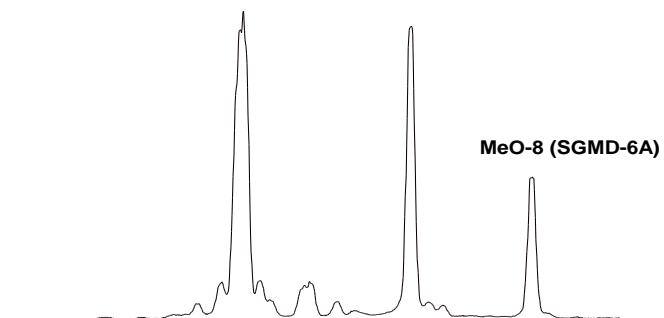
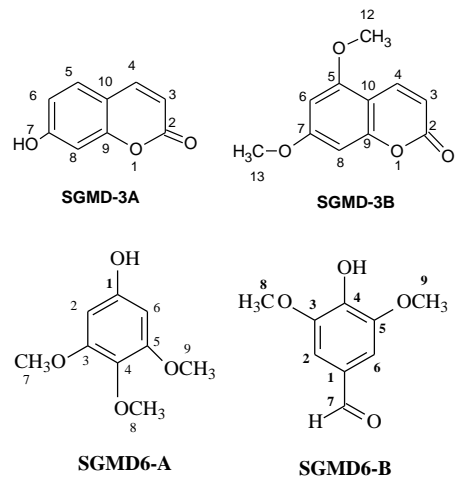
Espectro 35. Expansão entre δ_{H} 8.50 -6.10 e δ_{C} 85.0-145.5 do espectro 2D de ^1H - ^{13}C -COSY- $^n\text{J}_{\text{CH}}$ (HSQC, em D_3CCOCD_3) da mistura **SGMD-3**.



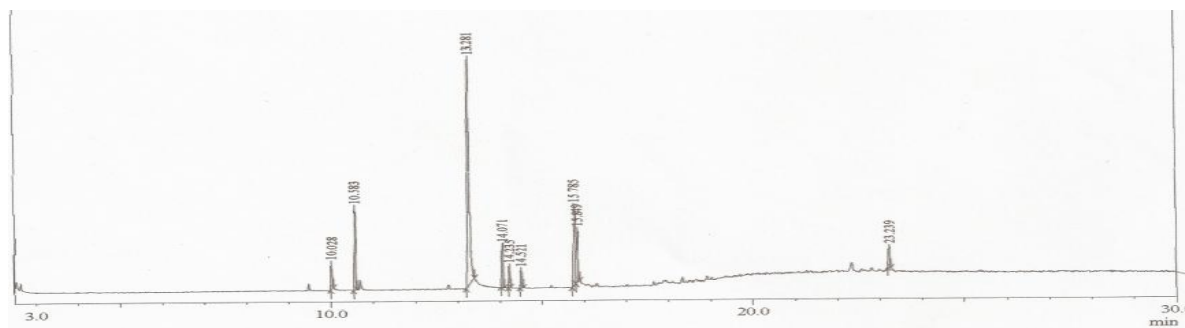
Espectro 36. 2 D de ^1H - ^{13}C -COSY- $^n\text{J}_{\text{CH}}$ ($n=2$ e $n=3$, HMBC, em D_3CCOCD_3) da mistura de **SGMD-3**.



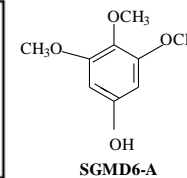
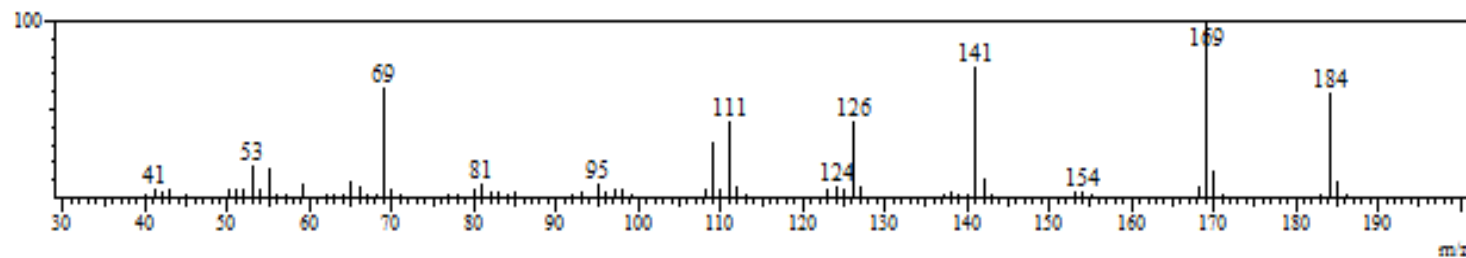
Espetro 37. Expansão entre δ_{H} 8.0-6.0 e δ_{C} 170.0-70.0 do espectro de 2D de ^1H - ^{13}C COSY- ^1JCH ($n=2$ e $n=3$, HMBC, em D_3CCOCD_3) da mistura de **SGMD-3**.



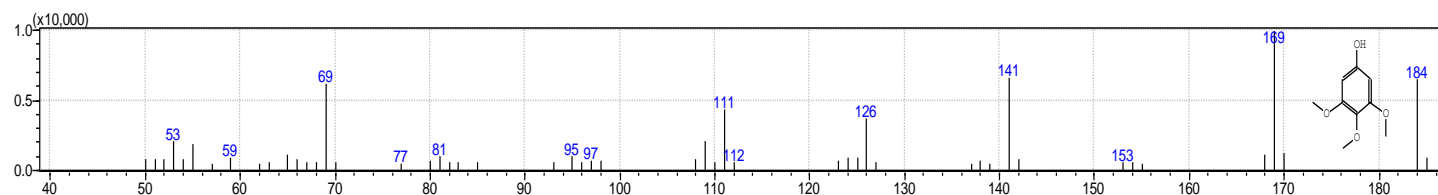
Espectro 38. Expansão entre δ_{H} 4.0-2.6.0 e δ_{C} 170.0-30.0 do espectro de 2D de ^1H - ^{13}C -COSY- $^n\text{J}_{\text{CH}}$ ($n=2$ e $n=3$, HMBC, em D_3CCOCD_3) da mistura de **SGMD-3**.



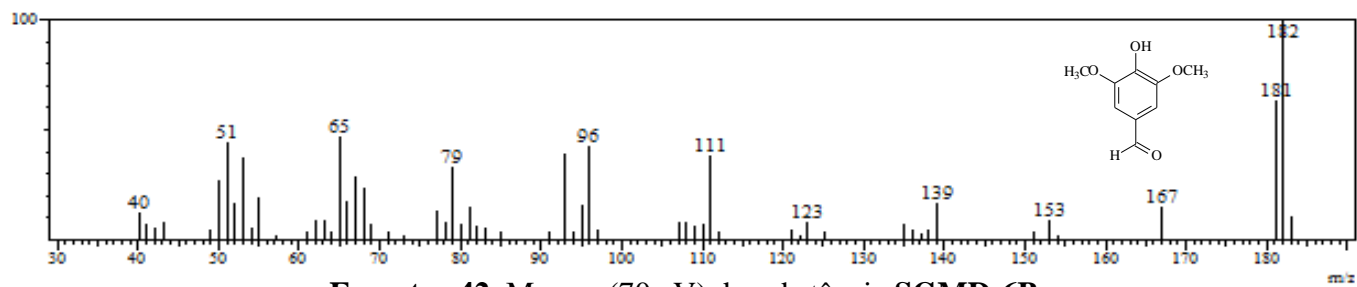
Espectro 39. Cromatograma por CG da mistura **SGMD-3**.



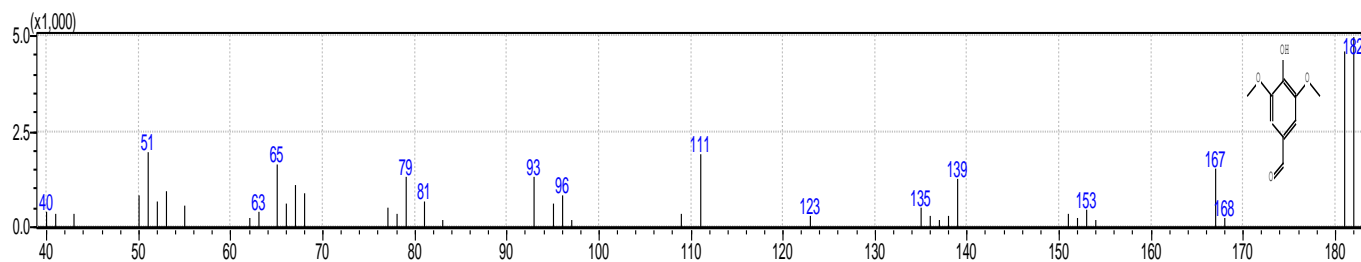
Espectro 40. Massas (70 eV) da substância **SGMD-6A**.



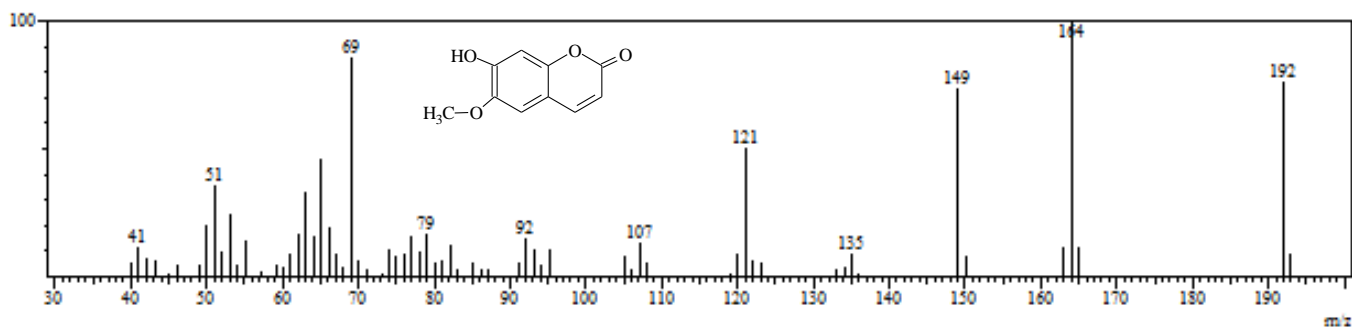
Espectro 41. Massas postulado pela análise biblioteca GCMS Postrun Analysis, para substância **SGMD-6A**.



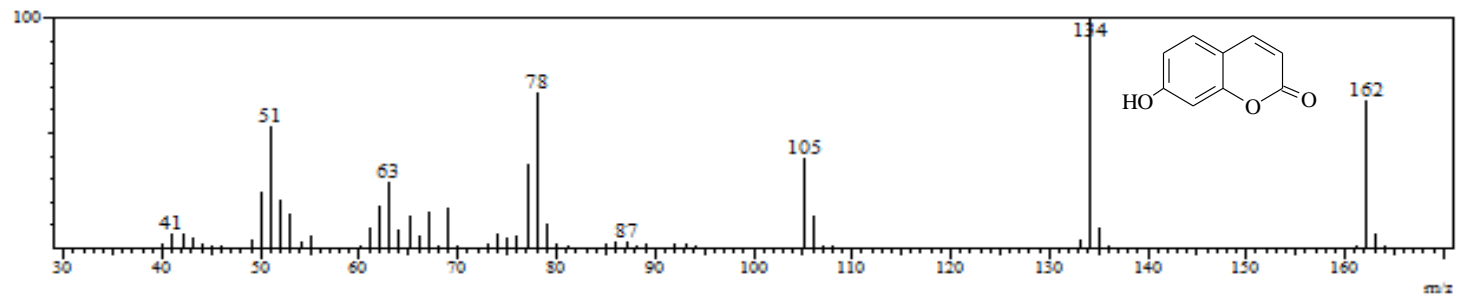
Espectro 42. Massas (70 eV) da substância **SGMD-6B**.



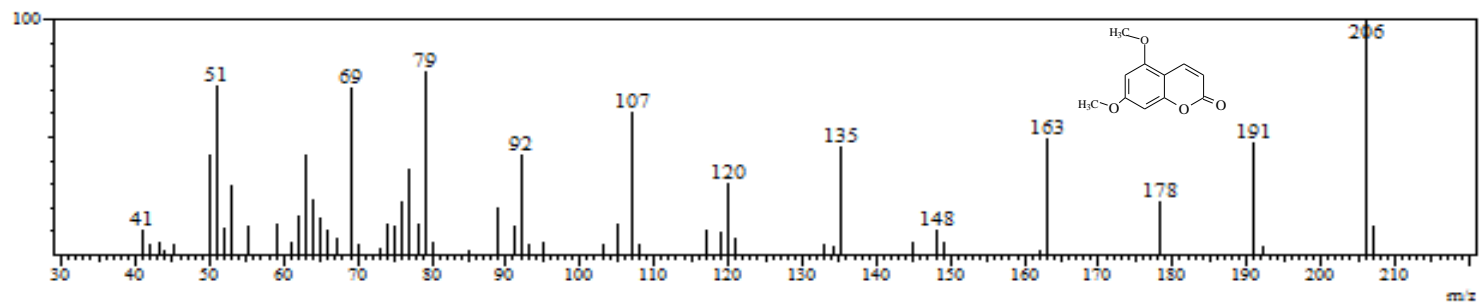
Espectro 43. Massas postulado pela análise biblioteca GCMS Postrun Analysis, para substância **SGMD-6B**.



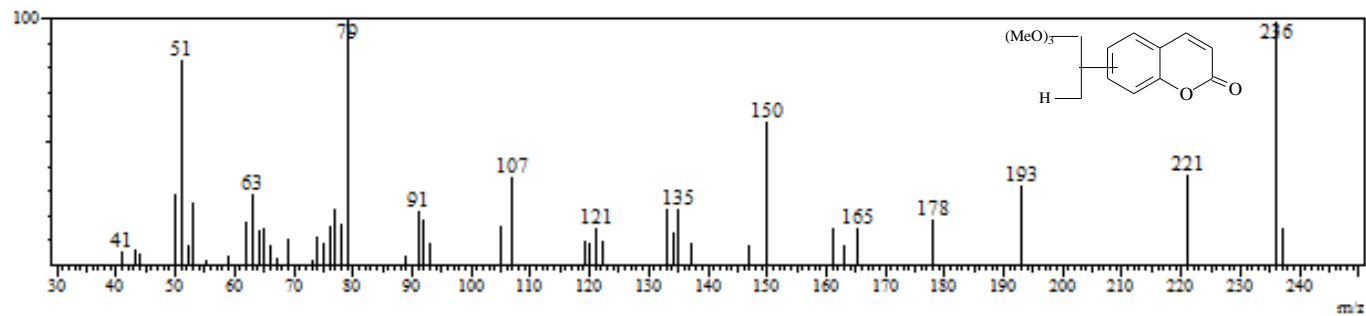
Espectro 44. Massas (70 eV) da substância **SGMD-2A**.



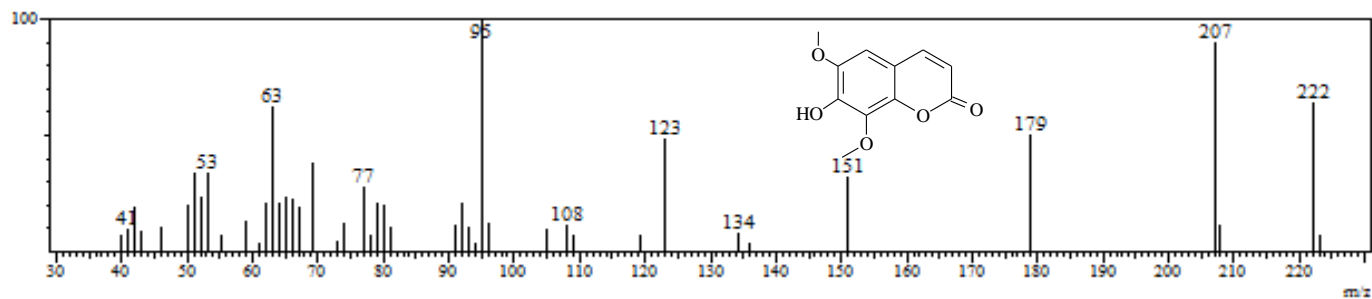
Espectro 45. Massas (70 eV) da substância **SGMD-3A**.



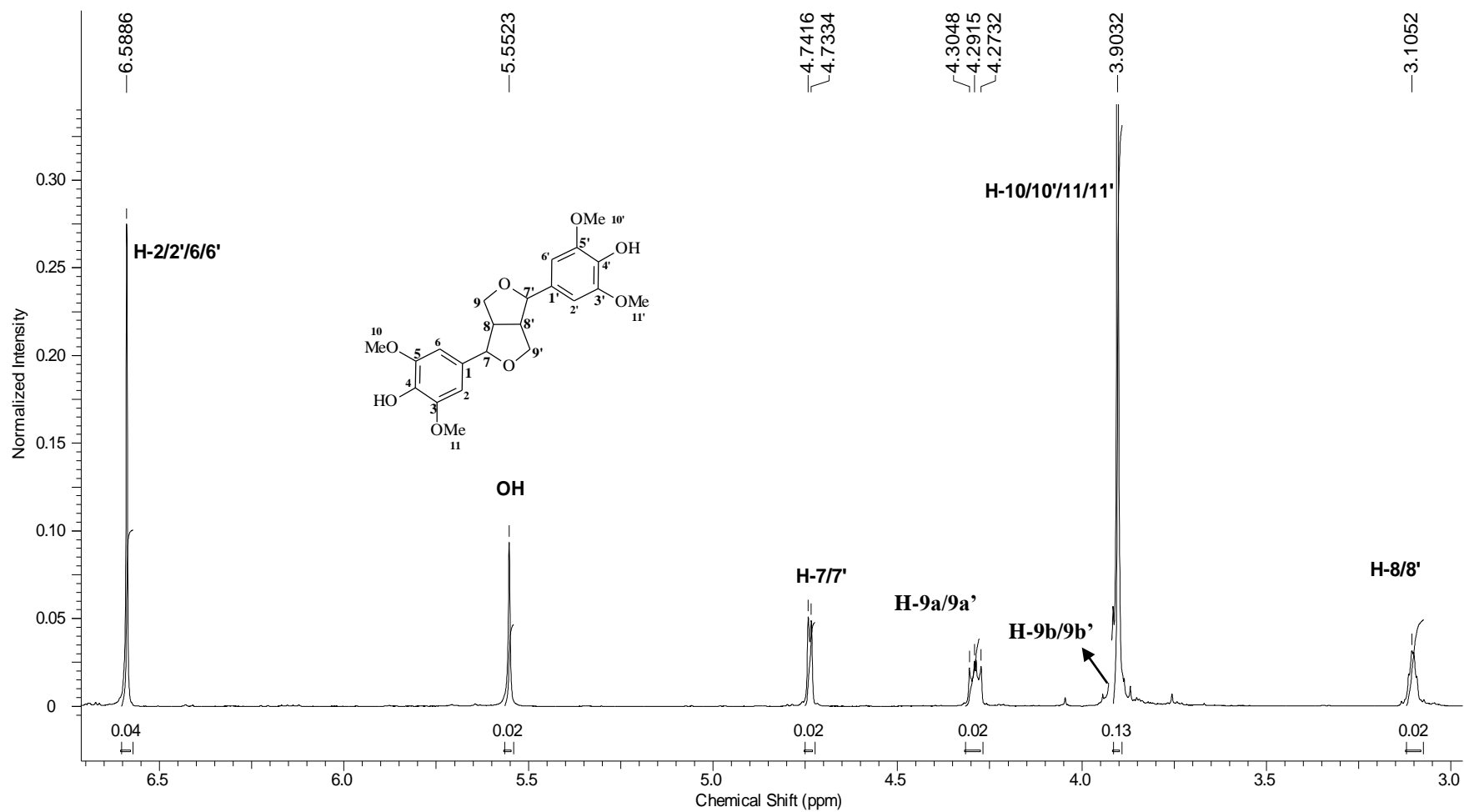
Espectro 46. Massas (70 eV) da substância **SGMD-3B**.



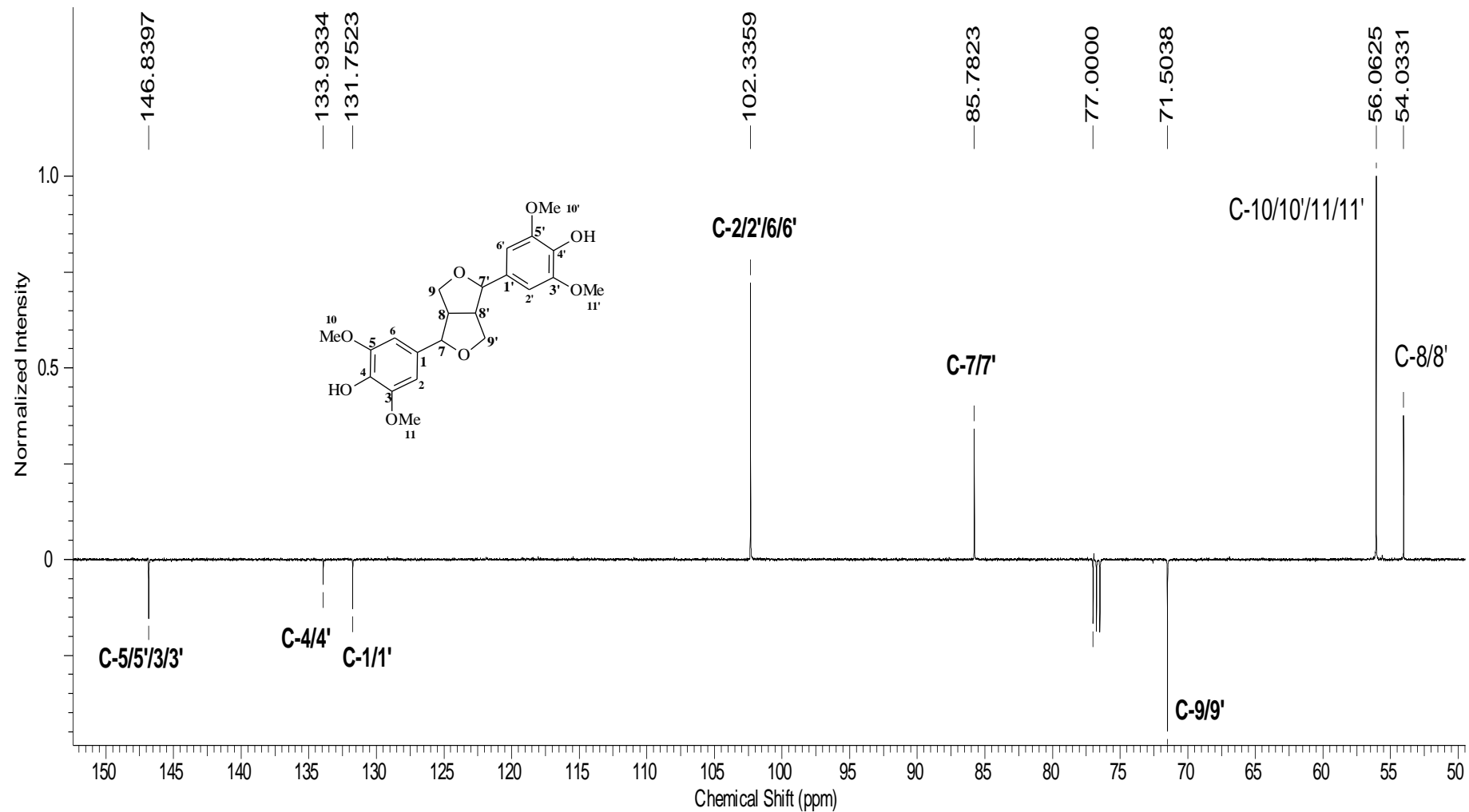
Espectro 47. Massas (70 eV) da substância **SGMD-3C**.



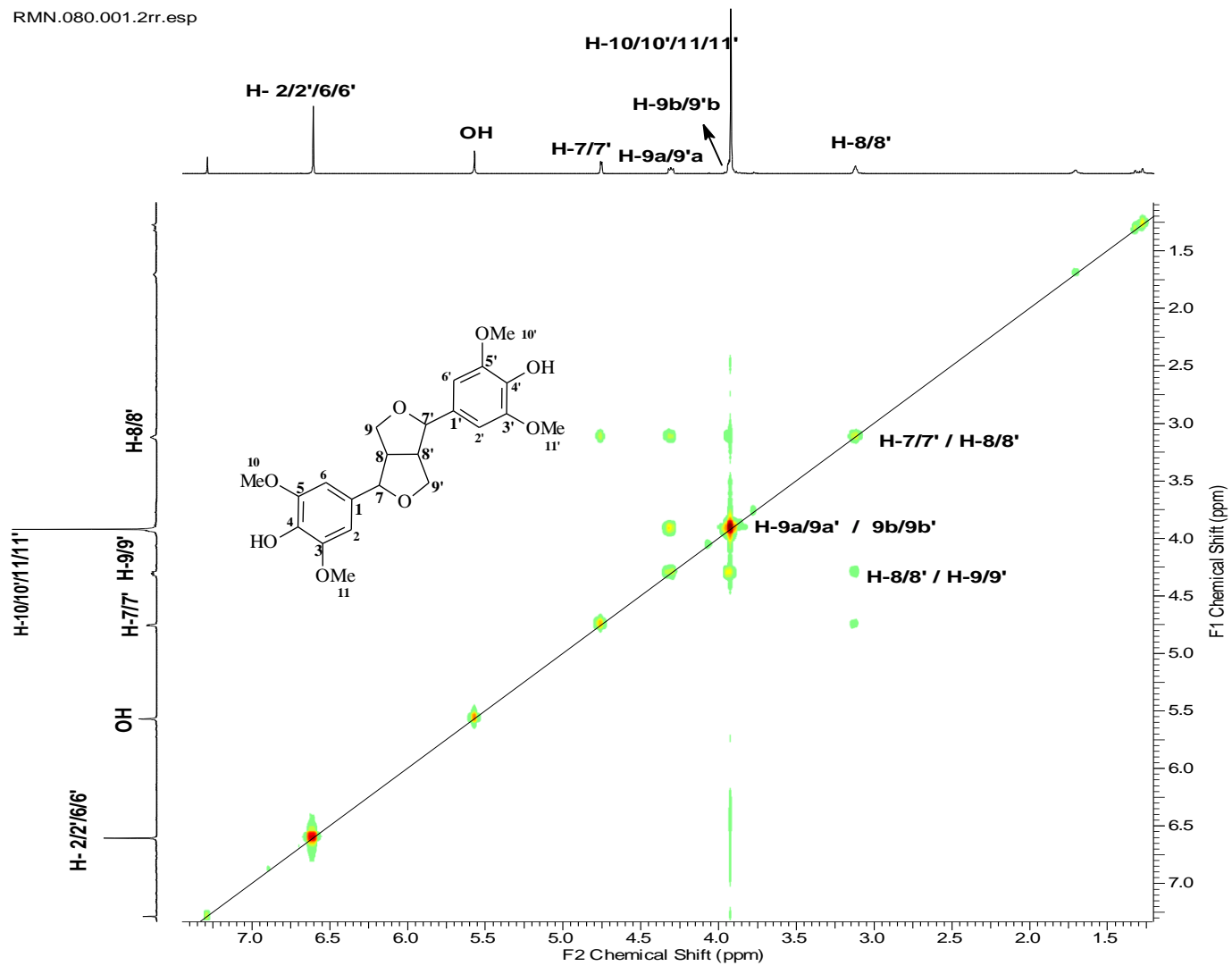
Espectro 48. Massas (70 eV) da substância **SGMD-3D**.



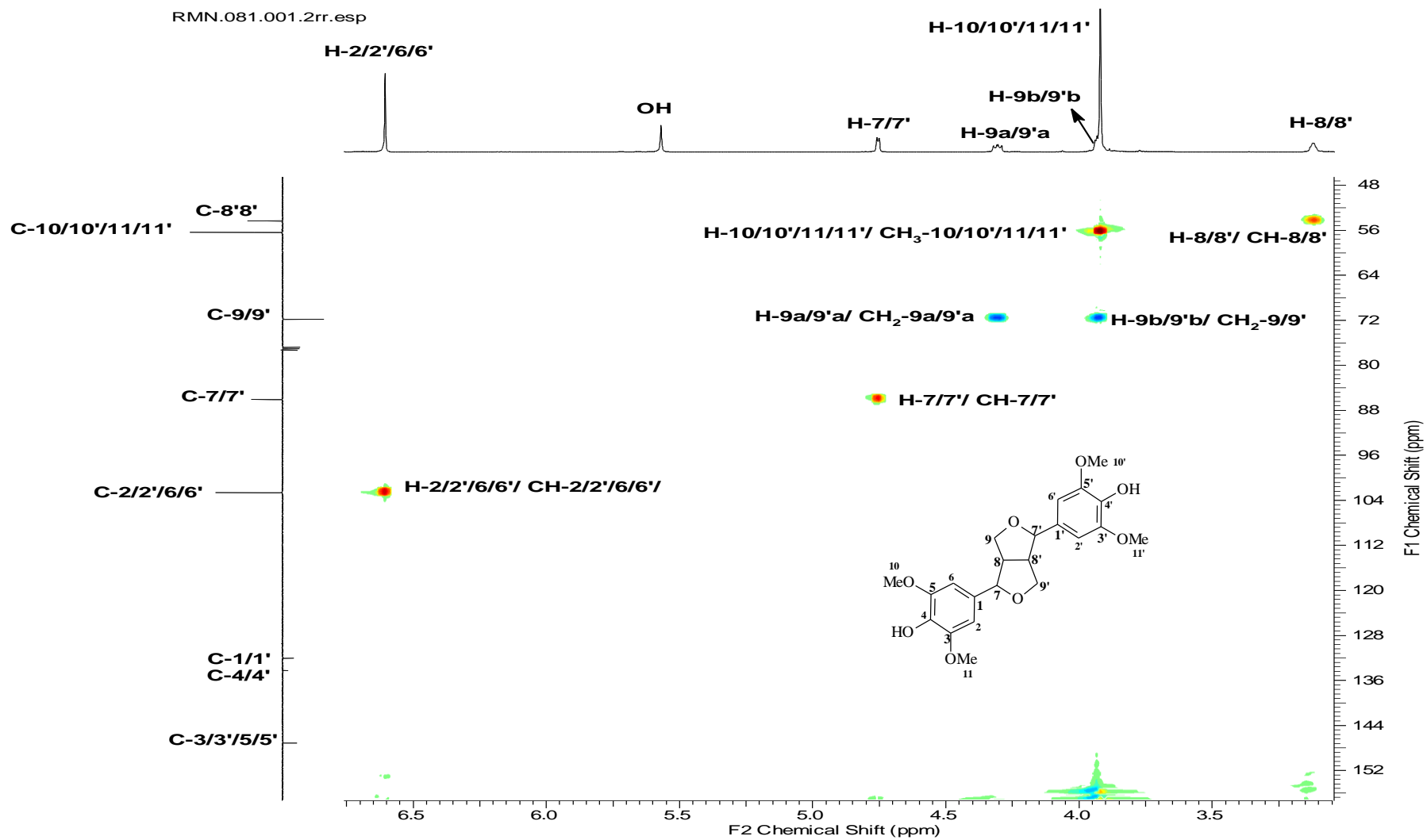
Espectro 49. RMN-¹H (500 MHz, CDCl₃) da substância SGMD-4.



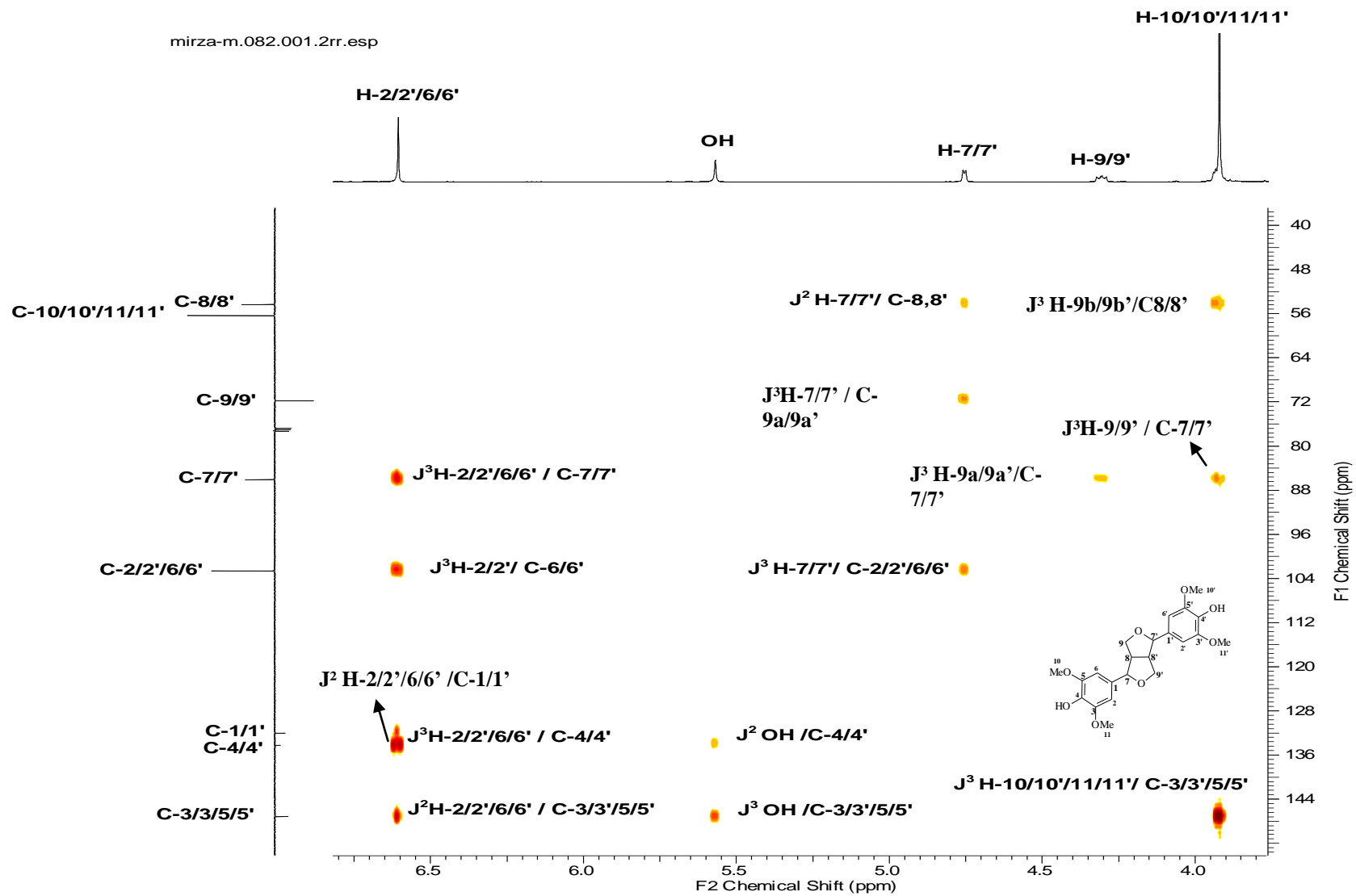
Espectro 50. RMN-¹³C-DEPTQ (125 MHz, CDCl₃) da substância **SGMD-4**.



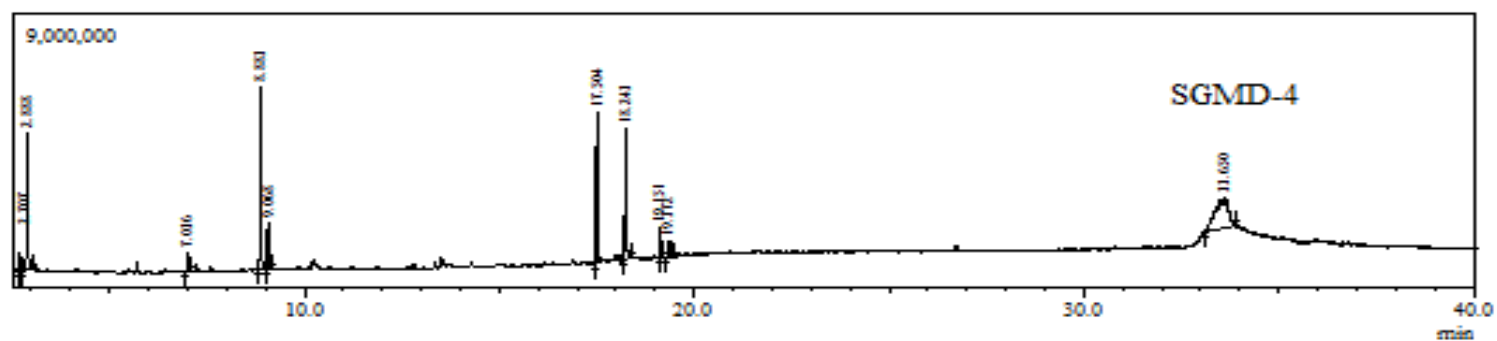
Espectro 51. 2D ^1H - ^1H -COSY (500 MHz, CDCl_3) da substância **SGMD-4**.



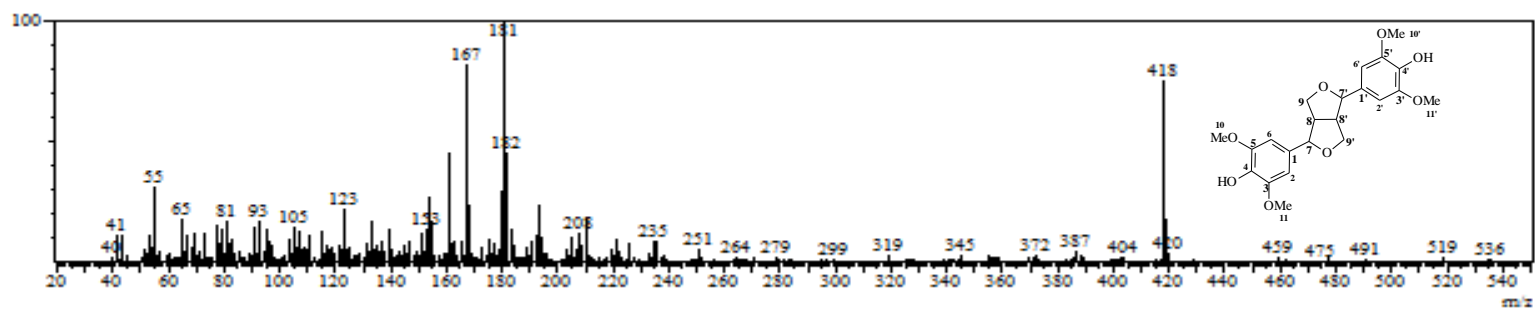
Espectro 52. 2D de ^1H - ^{13}C -COSY- ^1JCH (HSQC, em CDCl_3) da substância **SGMD-4**.



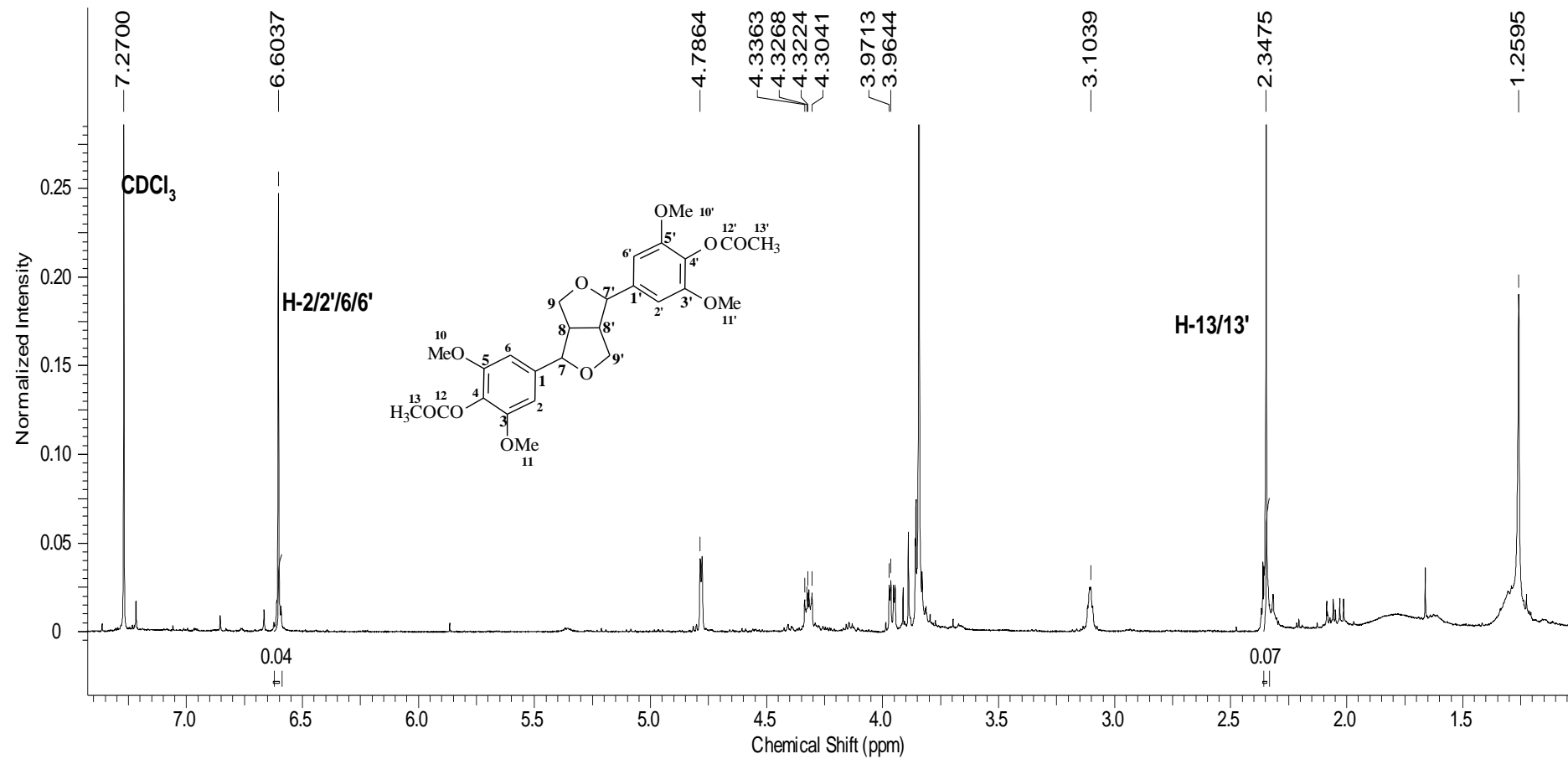
Espectro 53. 2 D de ^1H - ^{13}C -COSY- $^n\text{J}_{\text{CH}}$ (n=2 e n=3, HMBC, em CDCl_3) da substância **SGMD-4**.



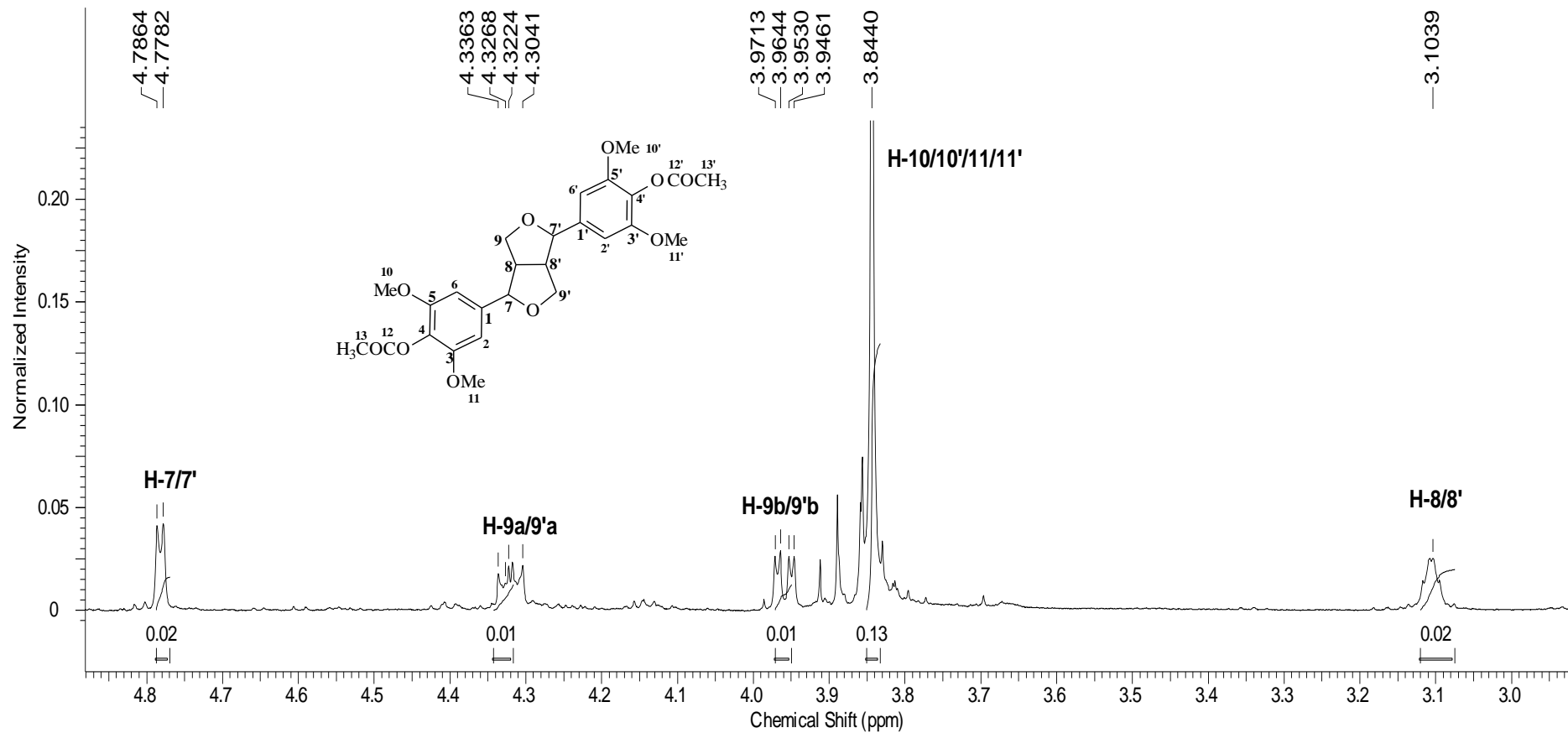
Espectro 54. Cromatograma por CG das Substâncias SGMD-4.



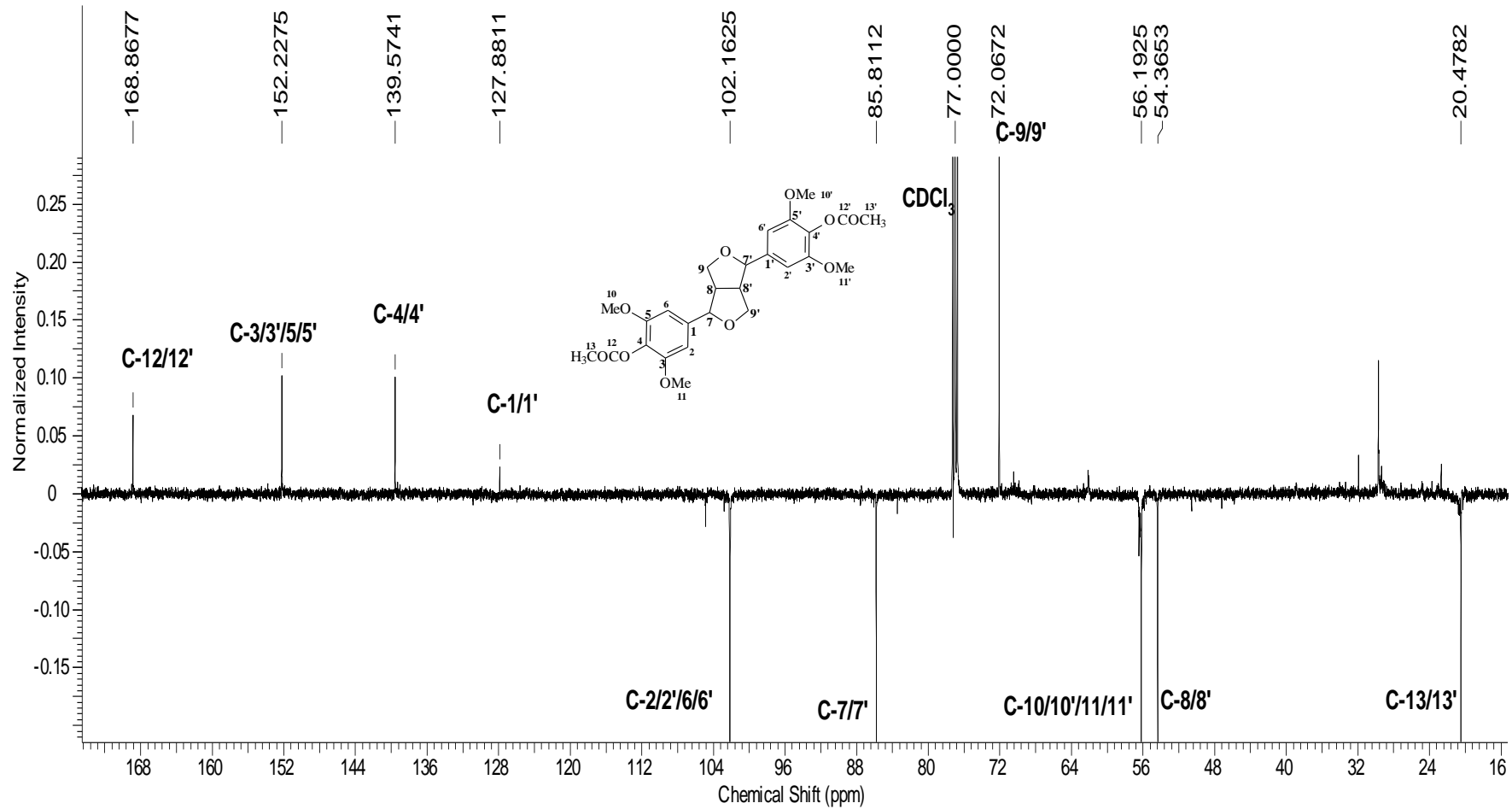
Espectro 55. Massas (70 eV) da substância SGMD-4.



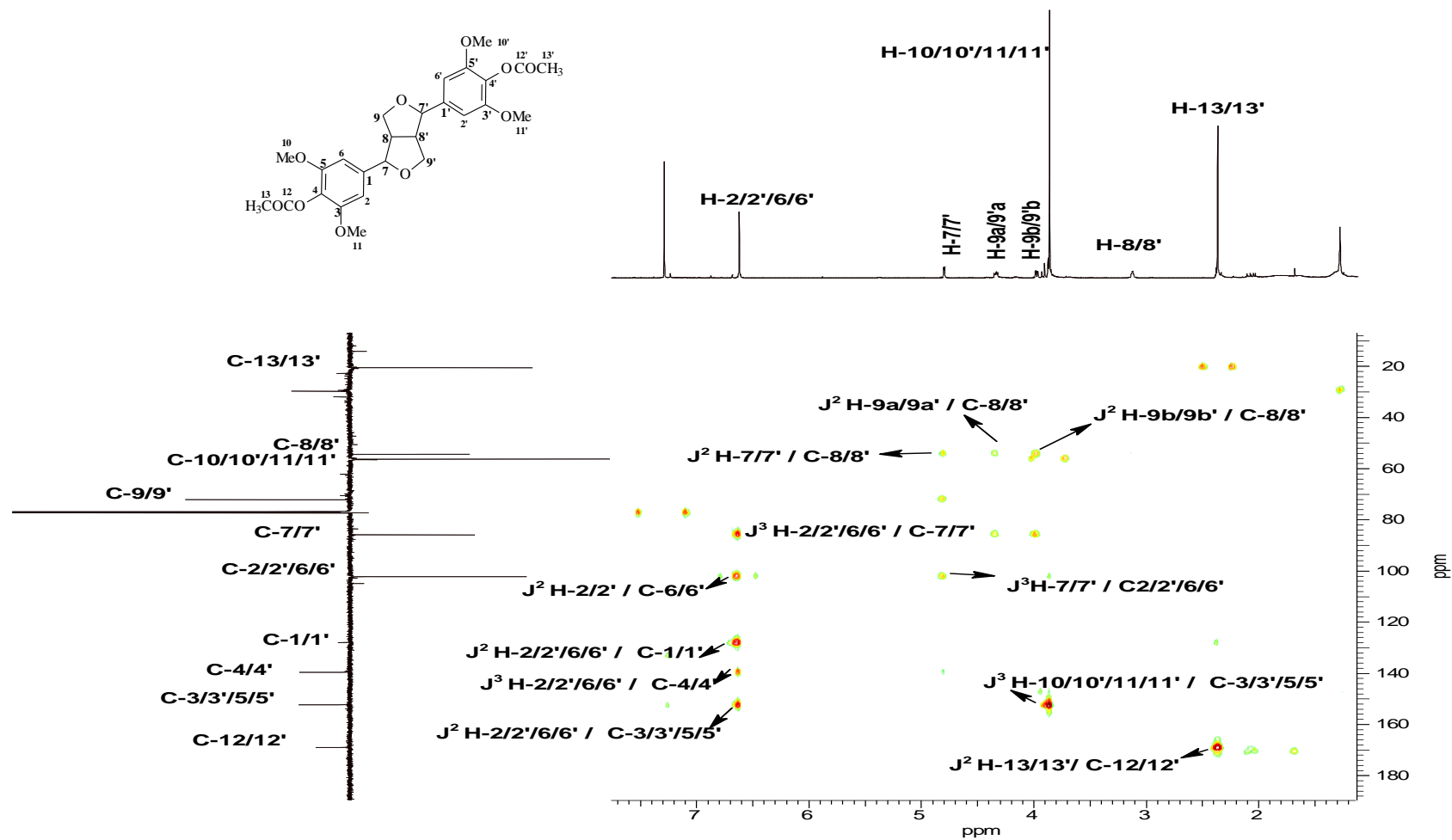
Espetro 56. RMN-¹H (500 MHz, CDCl₃) do derivado SGMD-4a.



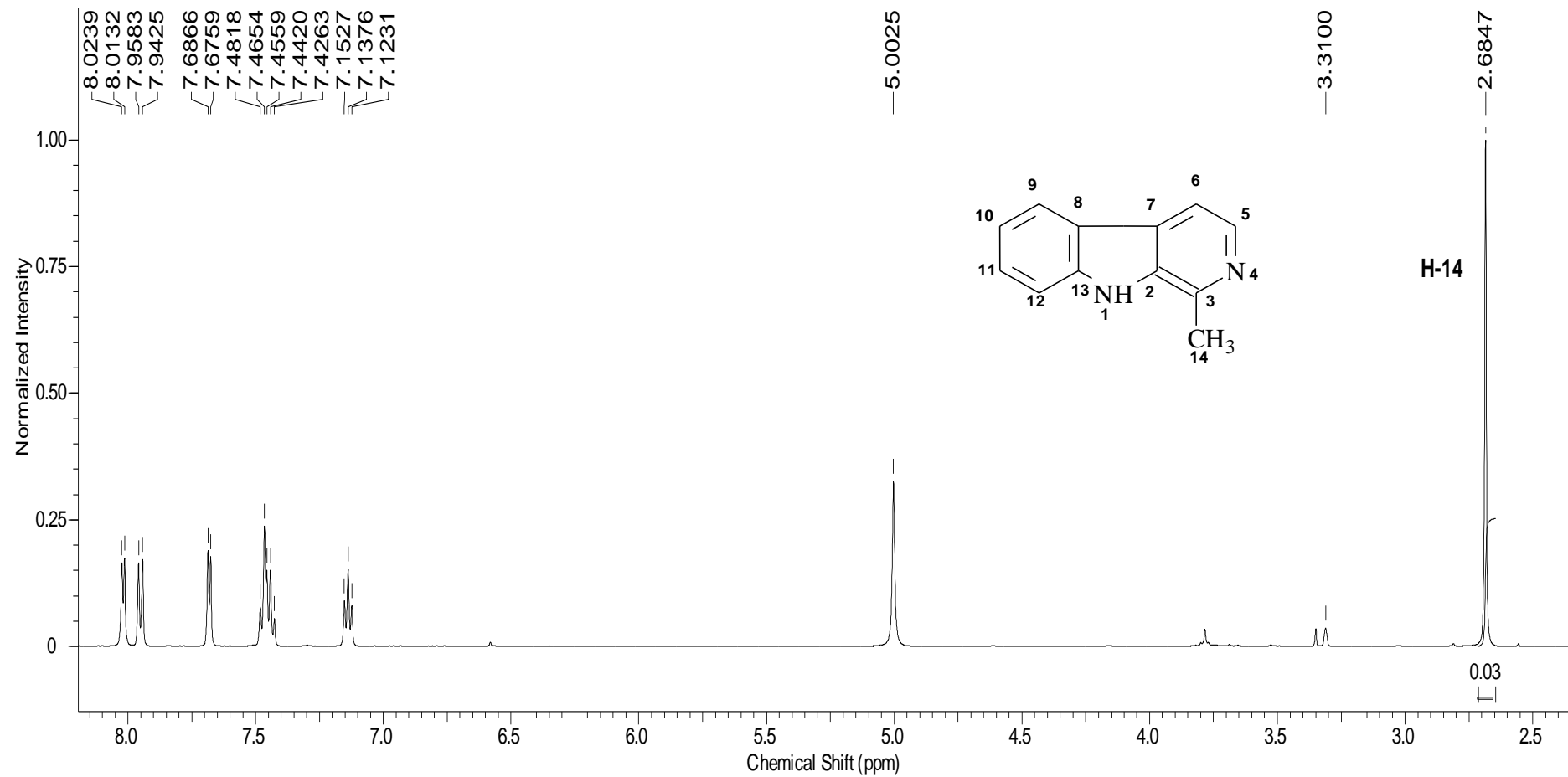
Espectro 57. Expansão entre δ_H 5.0- 3.1 do espectro de RMN-¹H (500 MHz, CDCl₃) do derivado **SGMD-4a**.



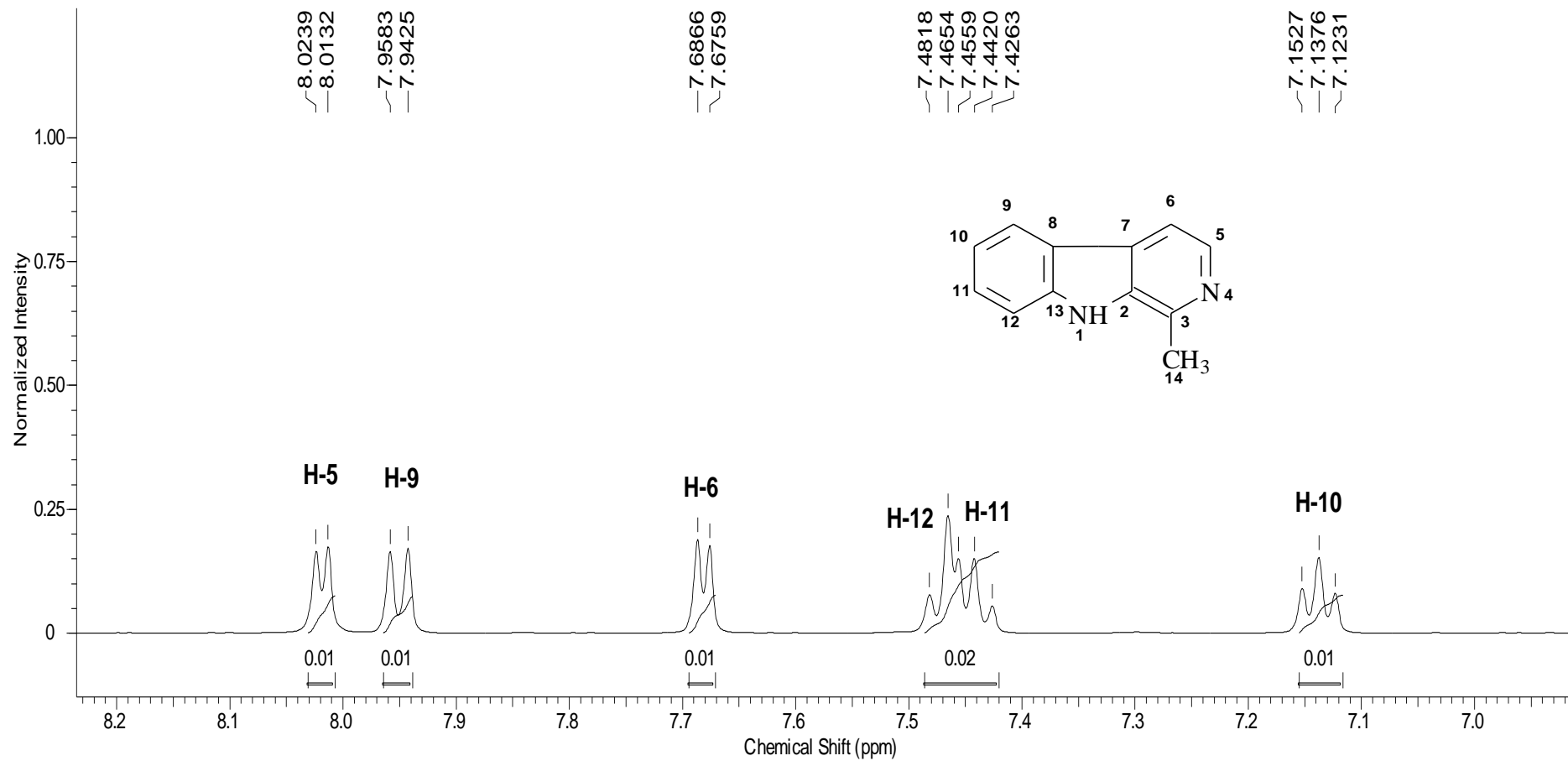
Espectro 58. RMN-¹³C-DEPTQ (125 MHz, CDCl₃) do derivado **SGMD-4a**.



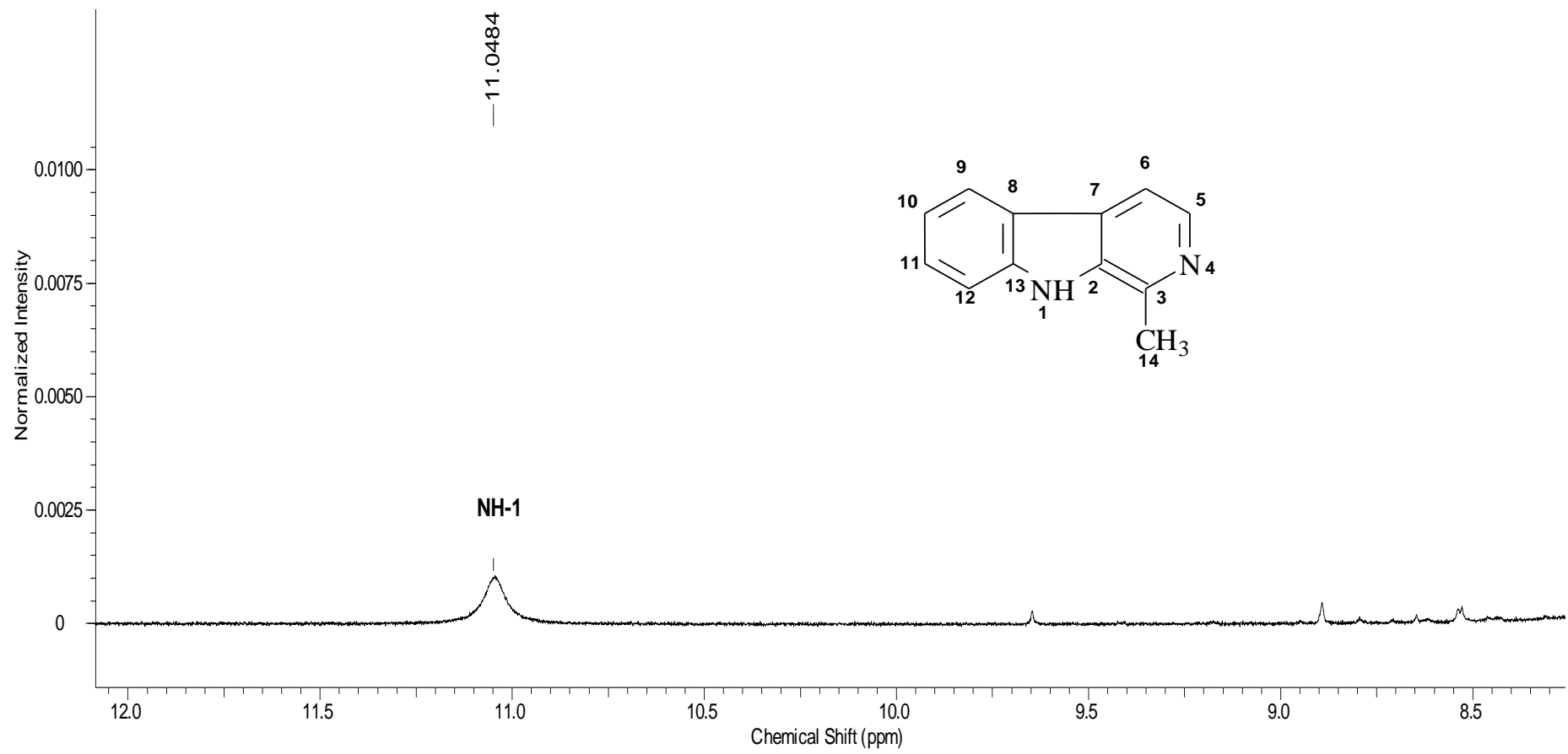
Espetro 59.2 D de ¹H-¹³C-COSY-ⁿJCH (n=2 e n=3, HMBC, em CDCl₃) do derivado **SGMD-4a**.



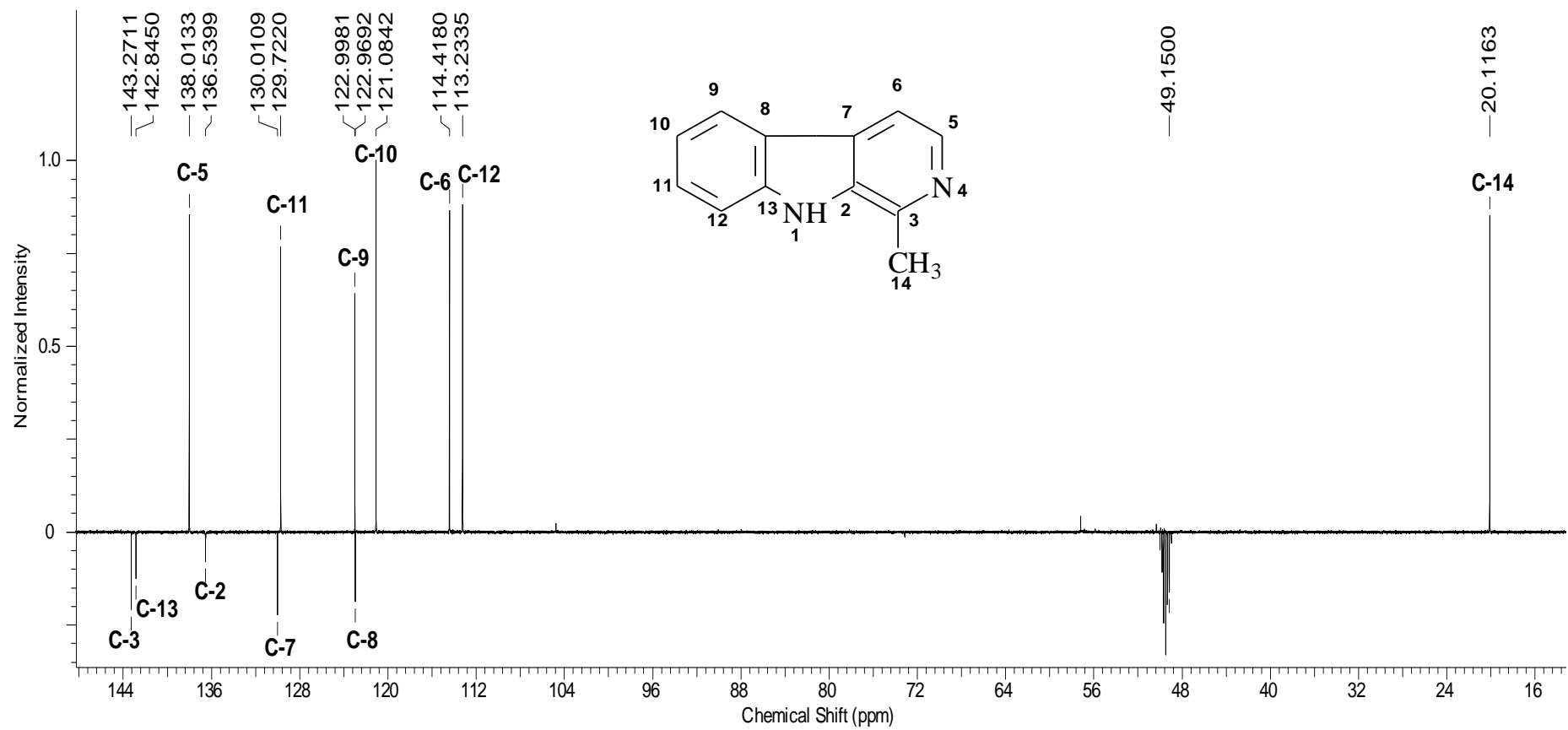
Espectro 60. RMN-¹H (500 MHz, MeOD) da substância **SGMD-5**.



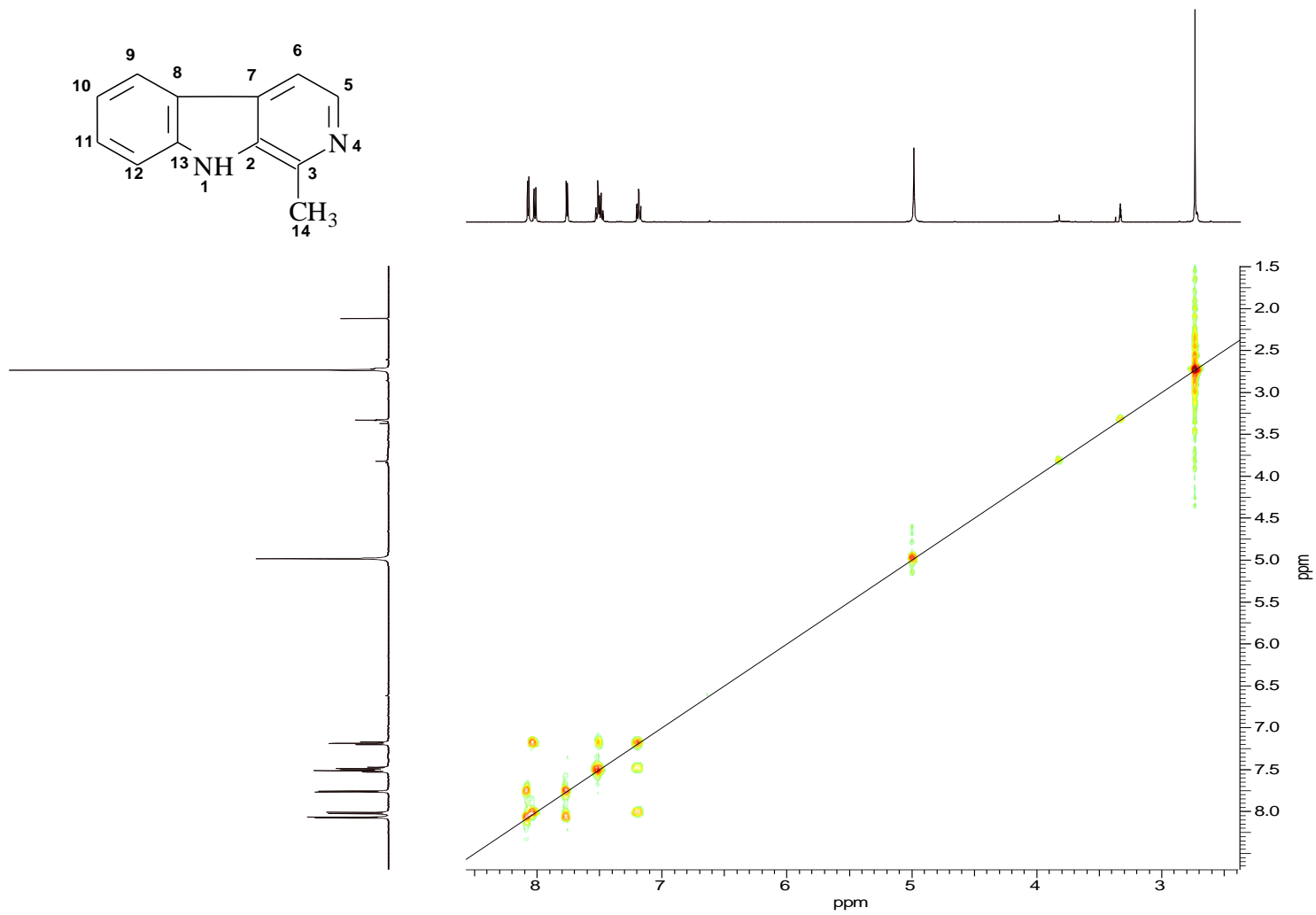
Espectro 61. Expansão entre δ_H 8.1- 7.0 do espectro de RMN-¹H (500 MHz, MeOD) da substância **SGMD-5**.



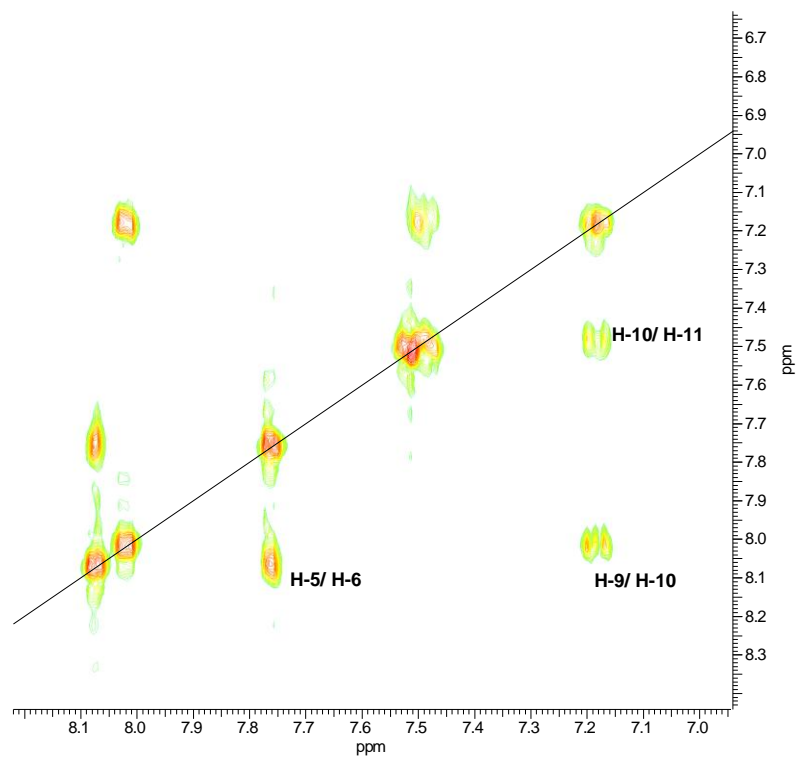
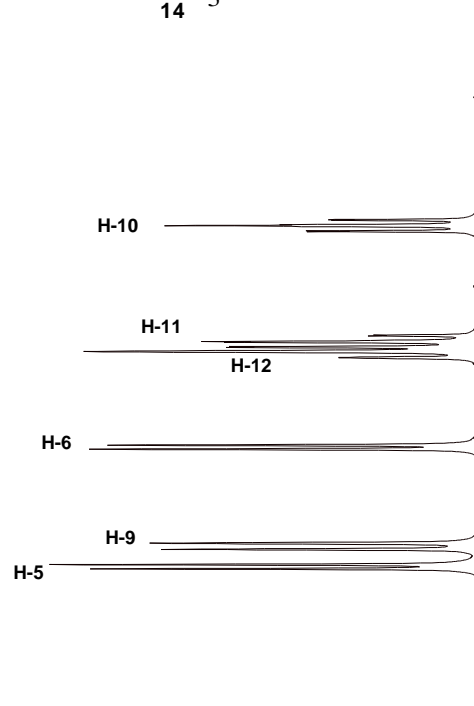
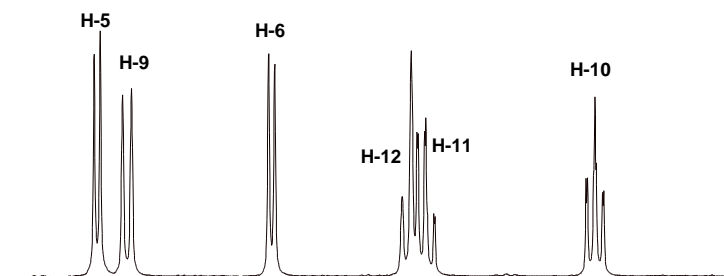
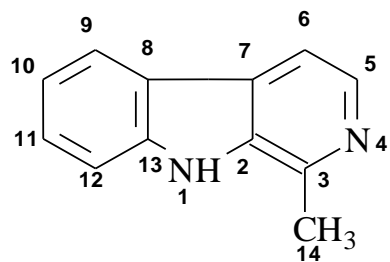
Espectro 62. Expansão entre δ_H 11.5- 9.5 do espectro de RMN-¹H (500 MHz, MeOD) da substância **SGMD-5**.



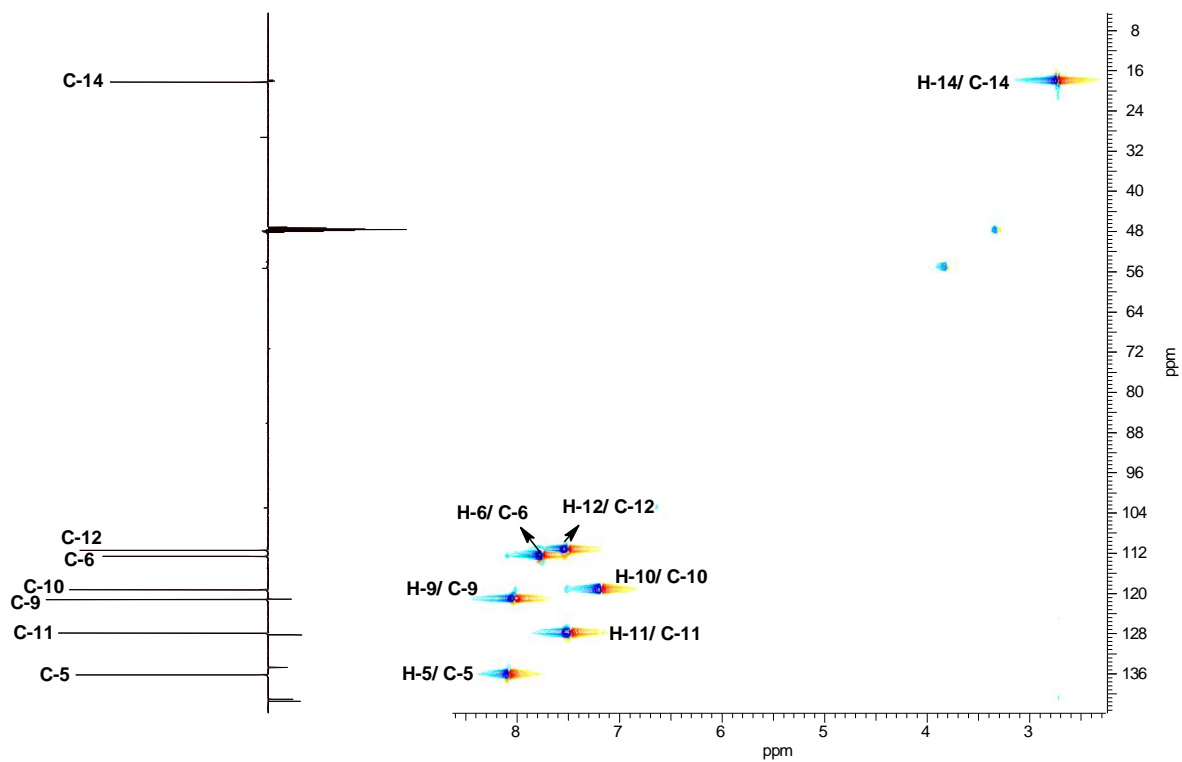
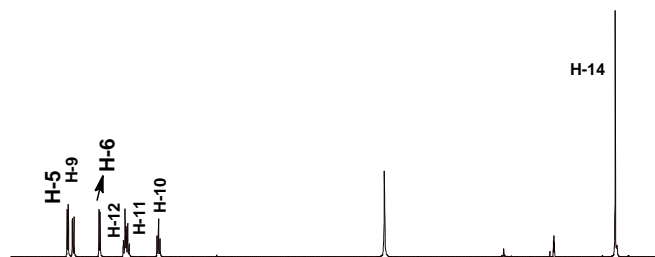
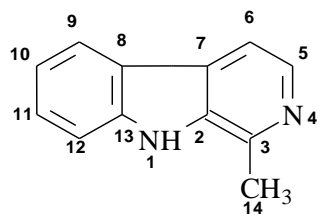
Espectro 63. RMN-¹³C-DEPTQ (125 MHz, MeOD) da substância **SGMD-5**.



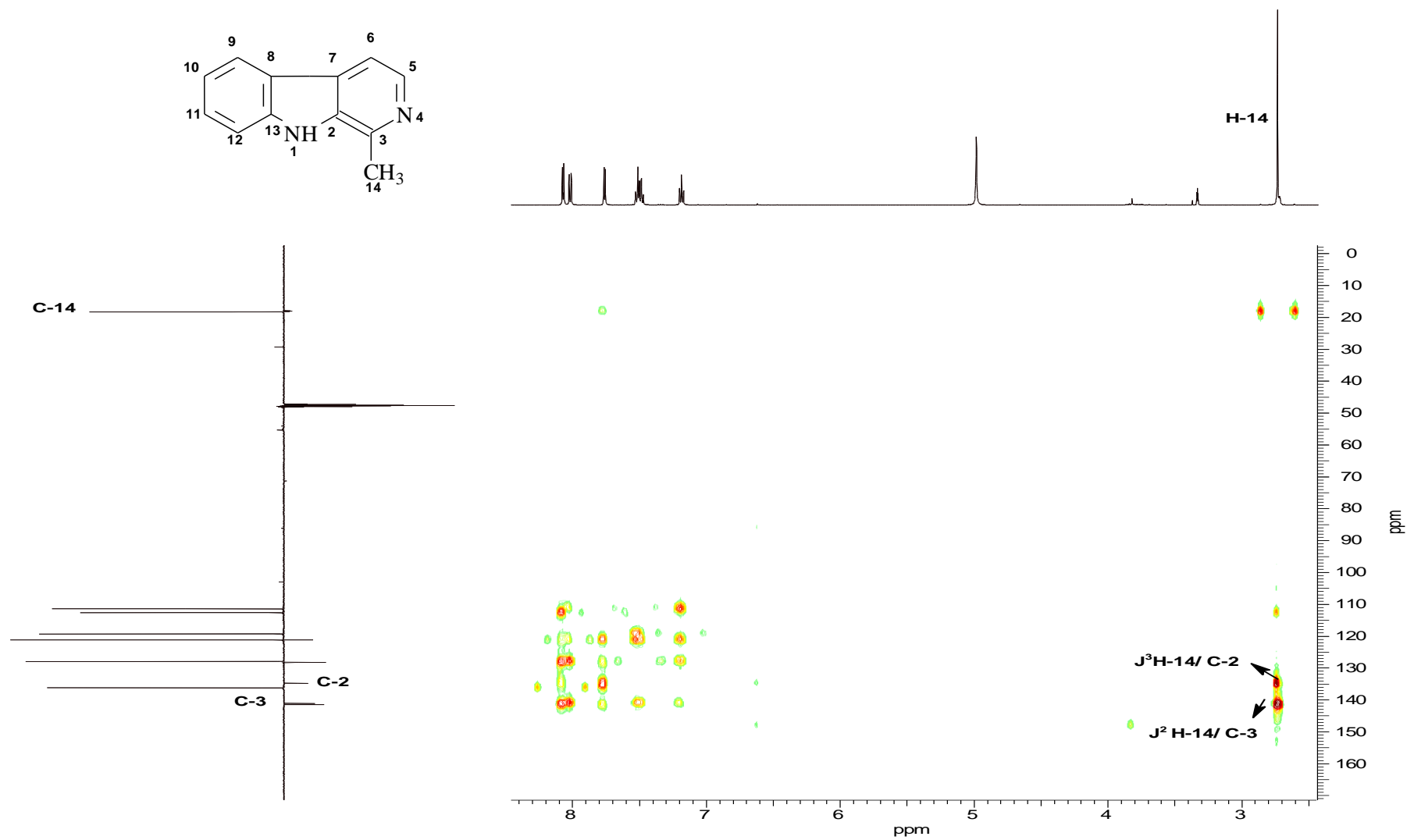
Espectro 64. RMN ^1H - ^1H -COSY (500 MHz, MeOD) da substância **SGMD-5**.



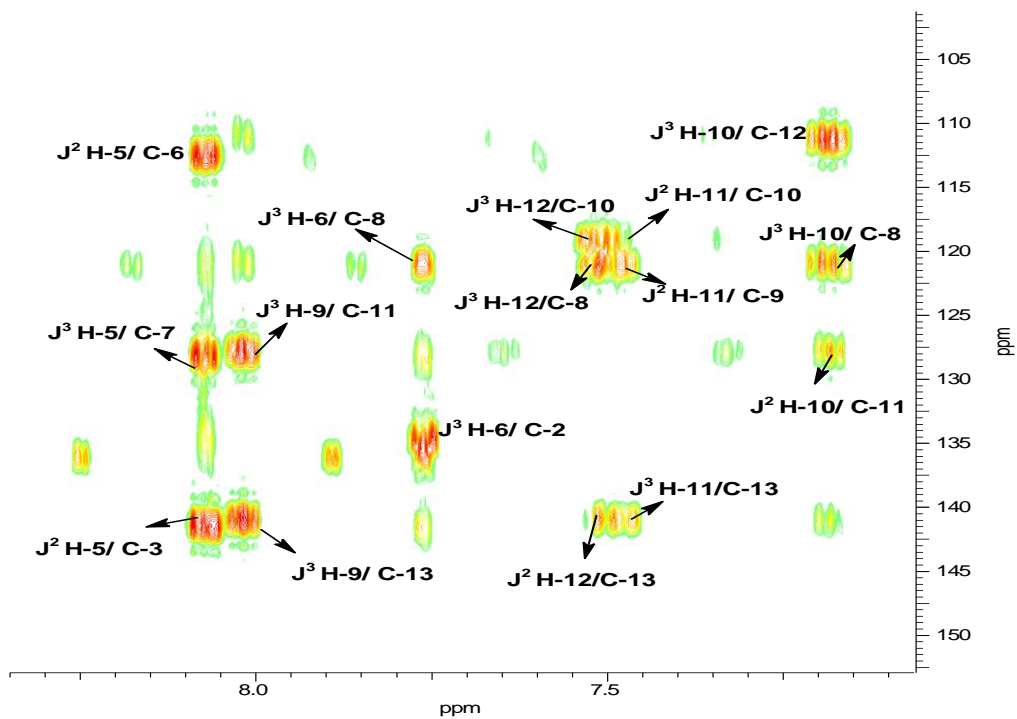
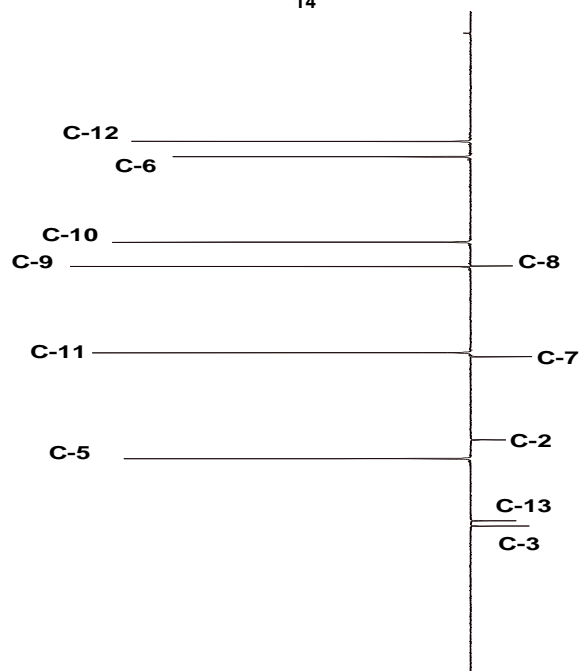
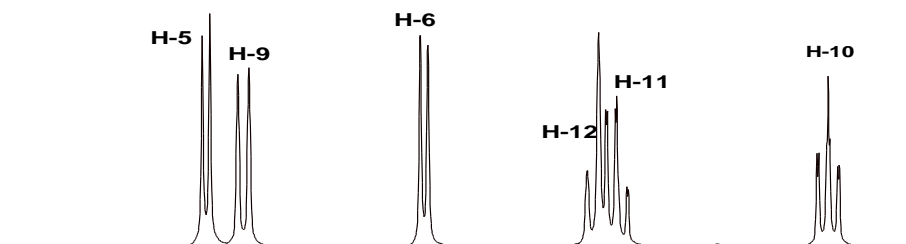
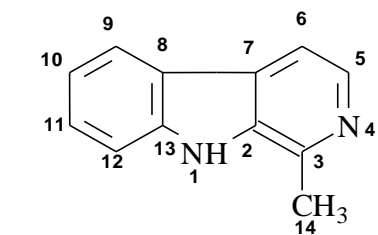
Espectro 65. Expansão entre δ_{H} 8.5-7.0 do espectro de RMN- ^1H - ^1H -COSY (500 MHz, MeOD) da substância **SGMD-5**.



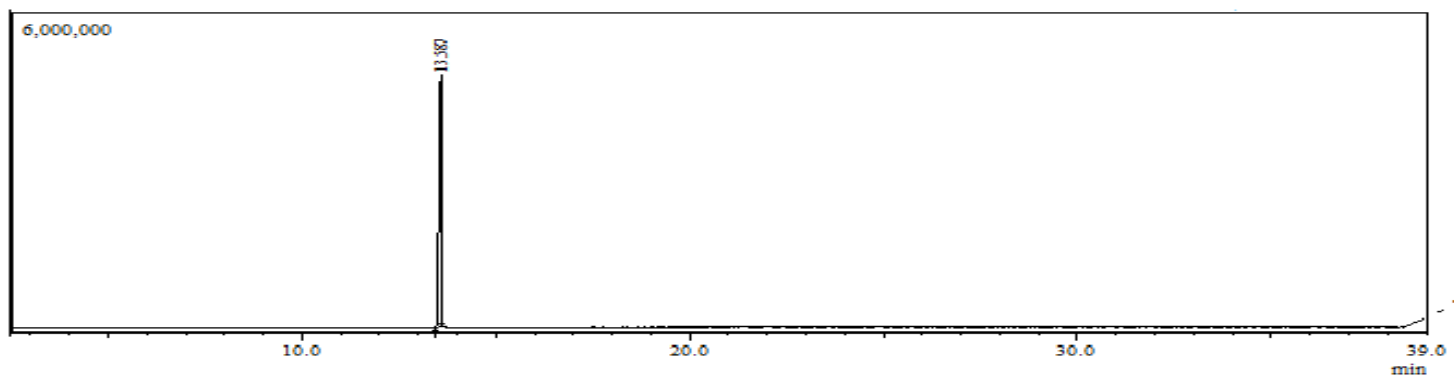
Espectro 66. ^1H - ^{13}C -COSY- $^1\text{J}_{\text{CH}}$ (HSQC, em MeOD) da substância **SGMD-5**.



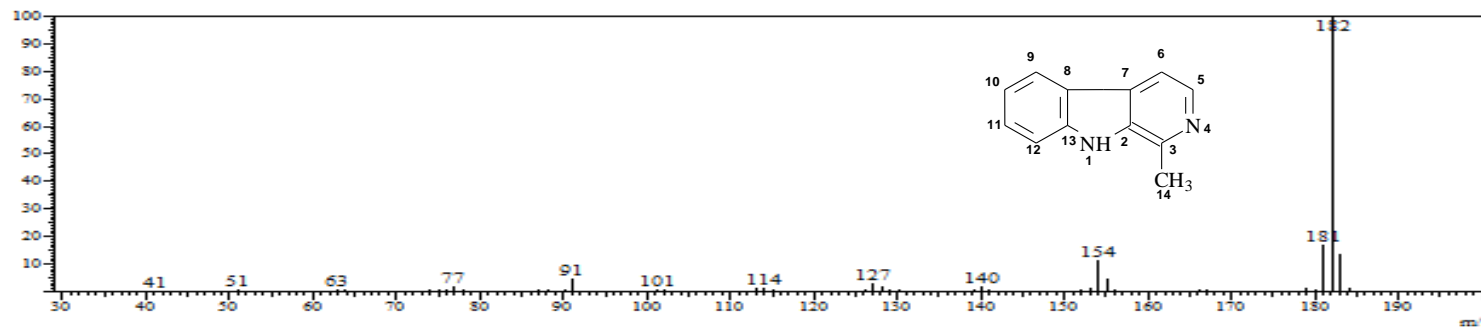
Espectro 67. 2D de ^1H - ^{13}C -COSY- ^nJCH ($n=2$ e $n=3$, HMBC, em MeOD_3) da substância **SGMD-5**.



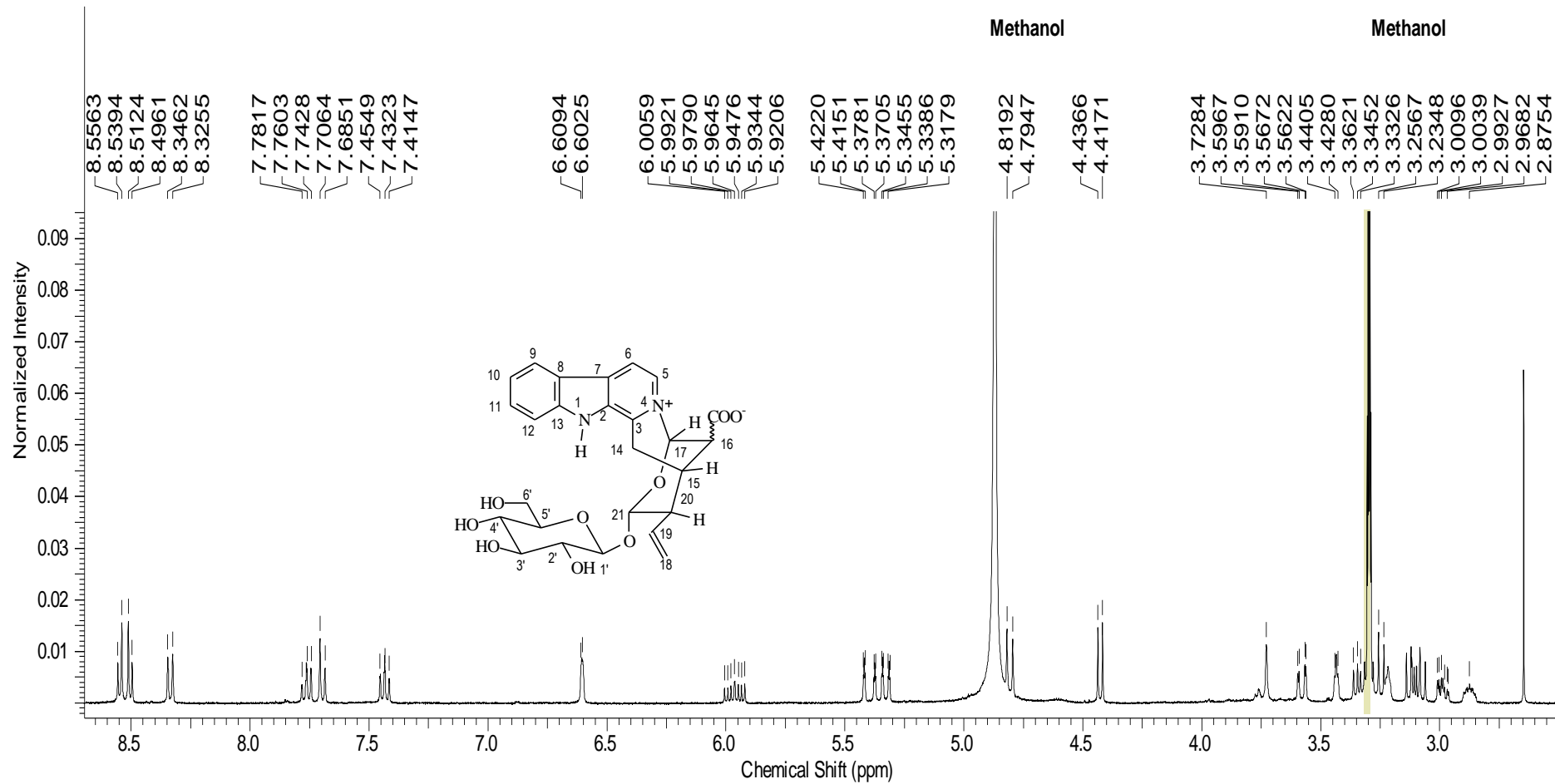
Espectro 68. Expansão entre δ_H 8.5-7.0 e δ_C 150.0-105.0 do espectro de 2D de 1H - ^{13}C -COSY- n JCH ($n=2$ e $n=3$, HMBC, em MeOD) da substância SGMD-5.



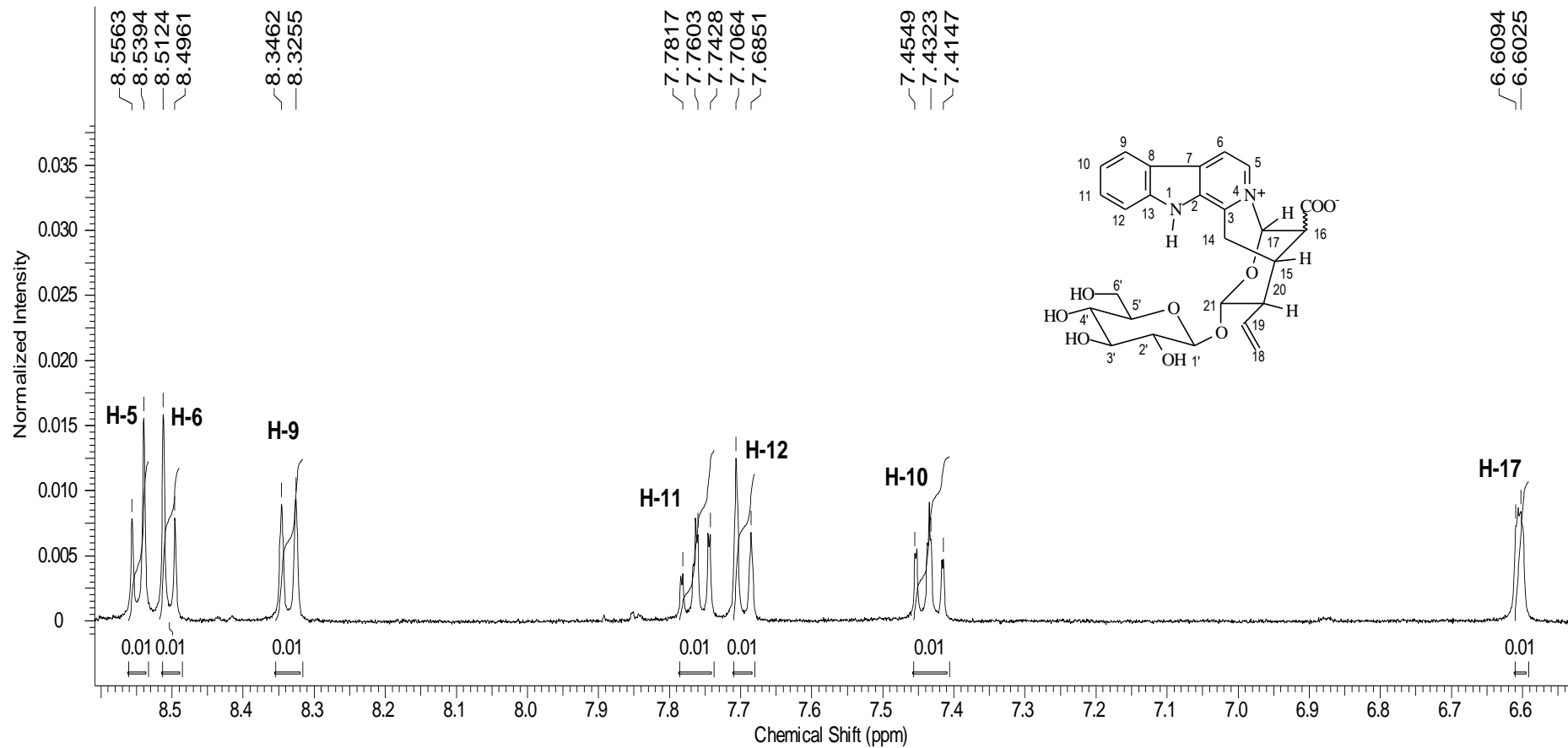
Espectro 69. Cromatograma por CG da substância **SGMD-5**.



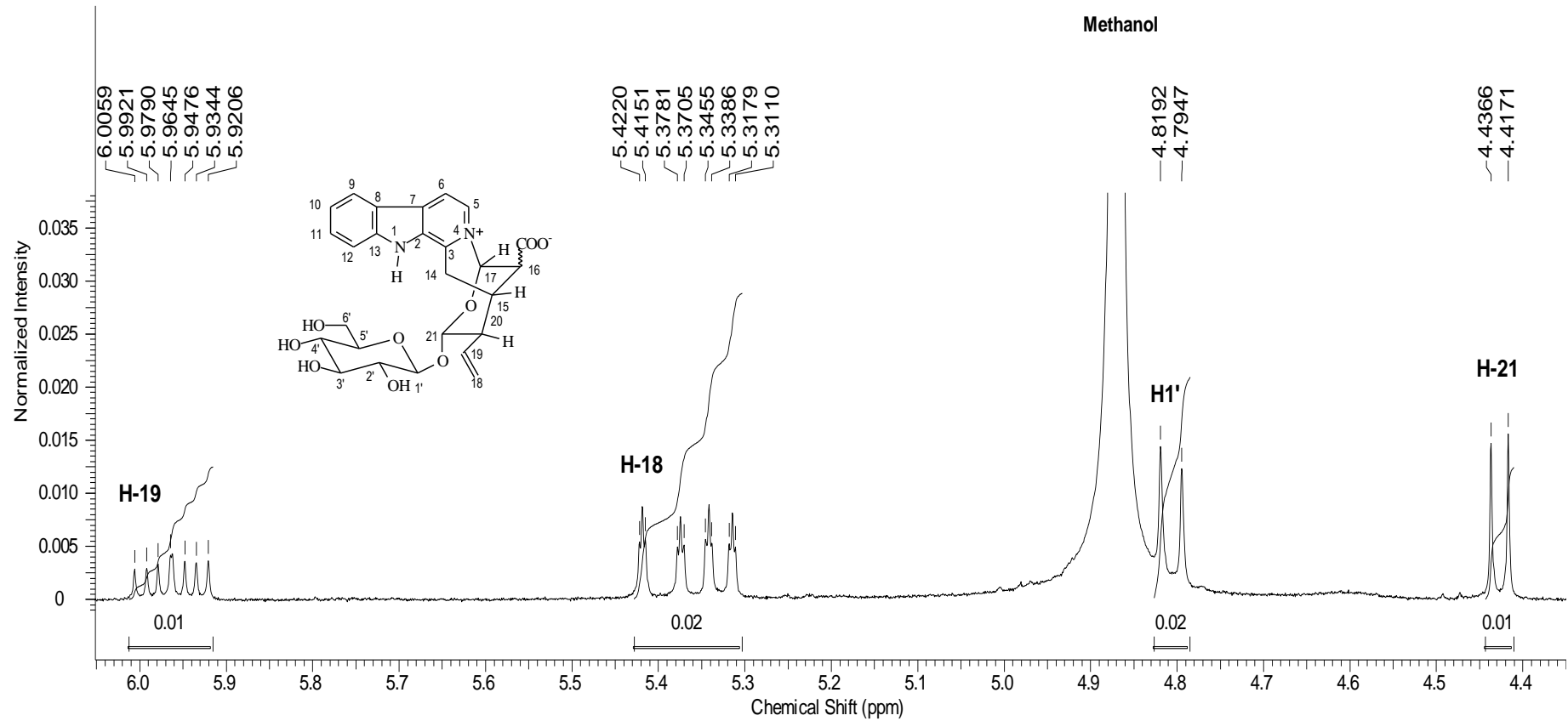
Espectro 70. Massas (70 eV) da substância **SGMD-5**.



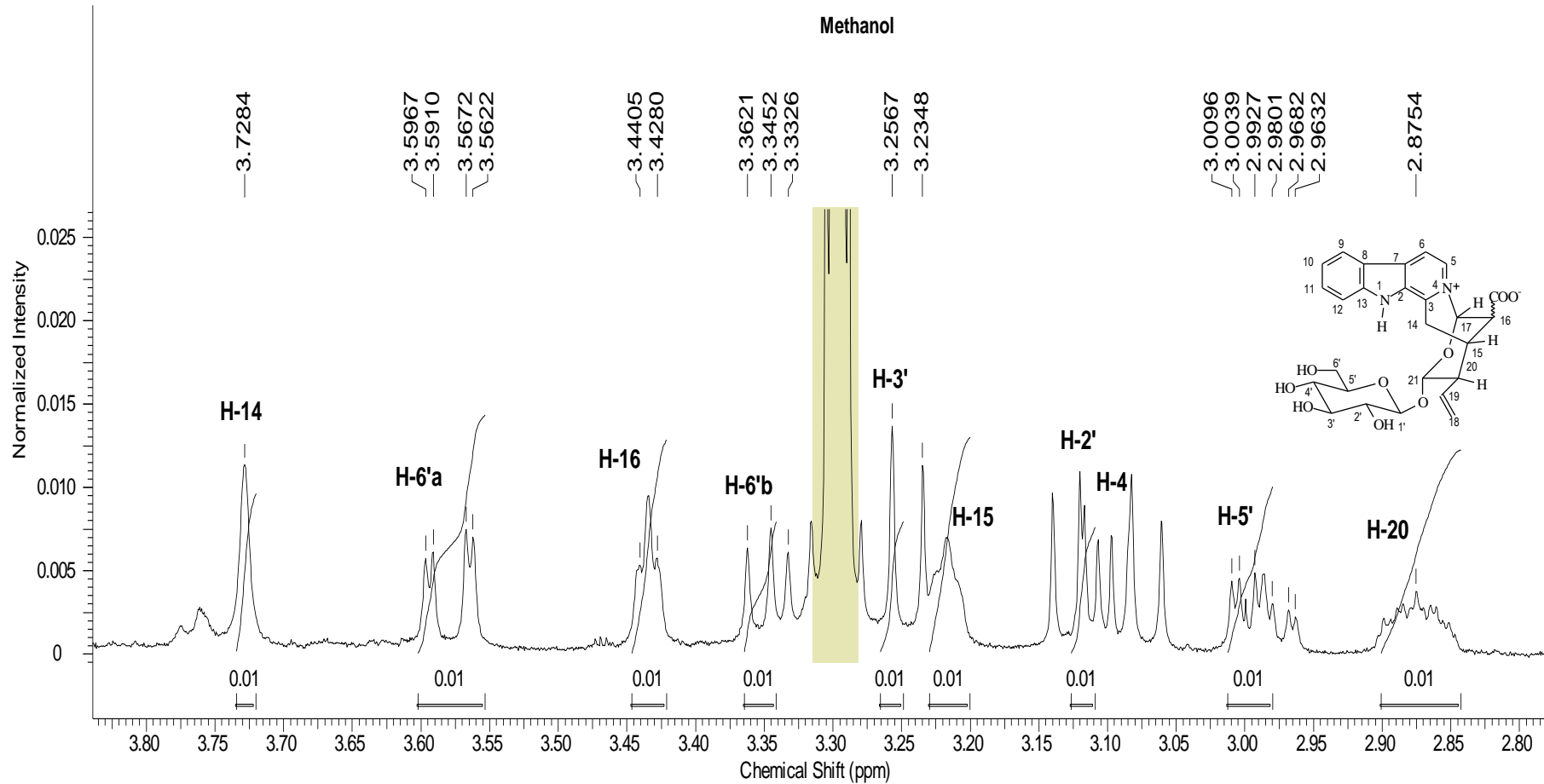
Espectro 71. RMN-¹H (400 MHz, MeOD) da substância **SGMH-4**.



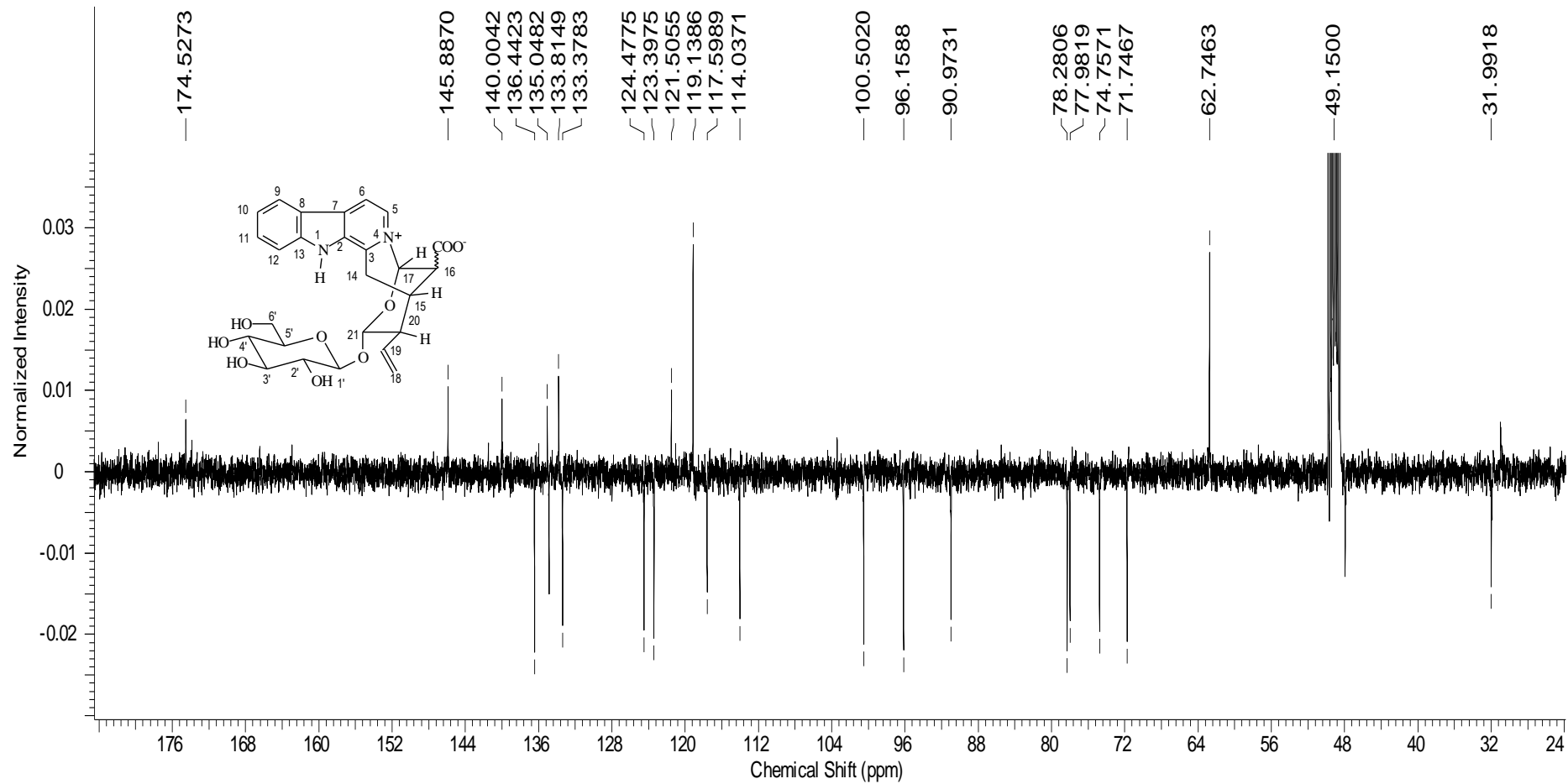
Espectro 72. Expansão entre δ_H 8.50- 6.60 do espectro de RMN- 1H (400 MHz, MeOD) da substância **SGMH-4**.



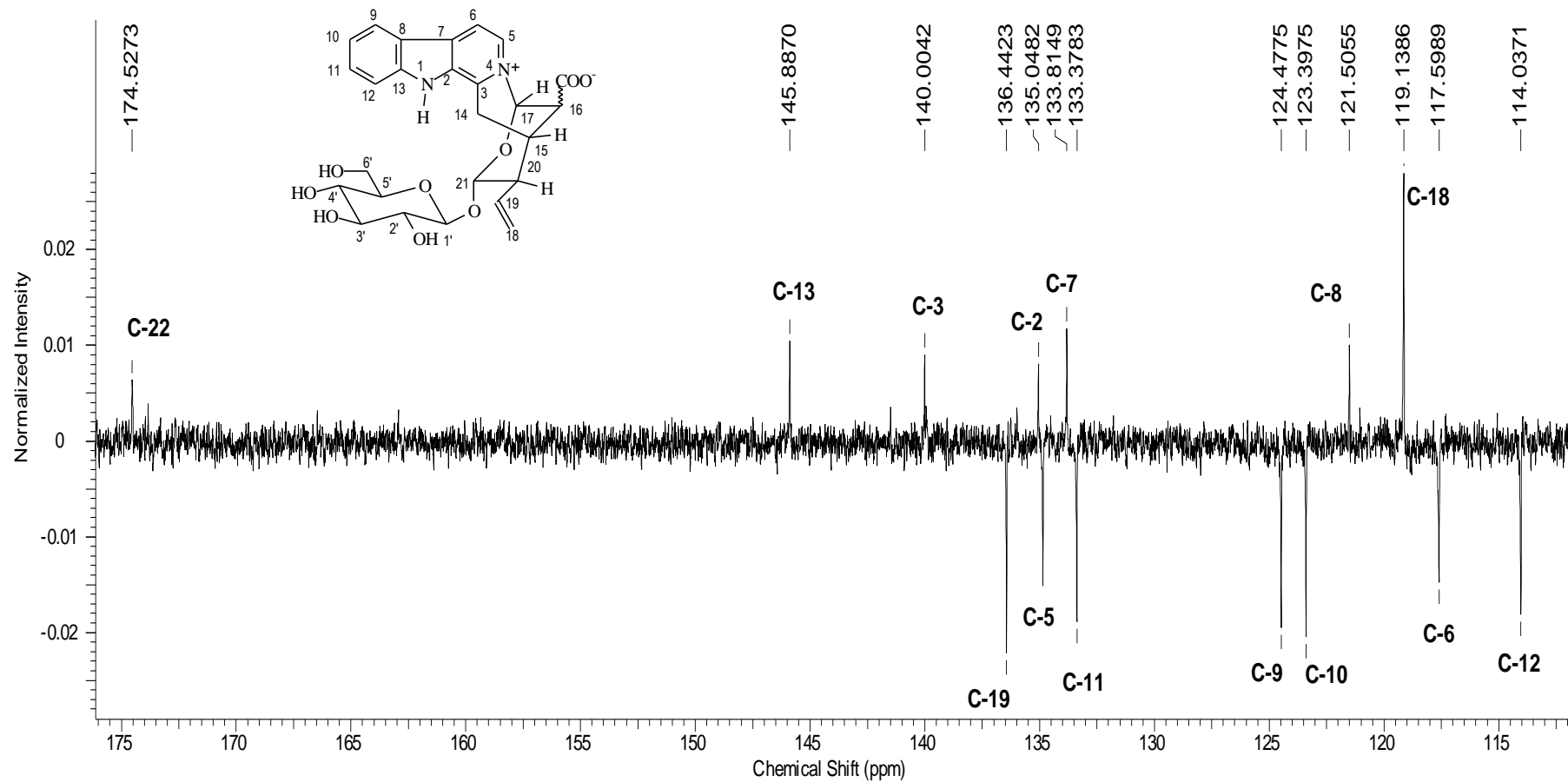
Espectro 73. Expansão entre δ_H 6.0- 4.0 do espectro de RMN-¹H (400 MHz, MeOD) da substância **SGMH-4**.



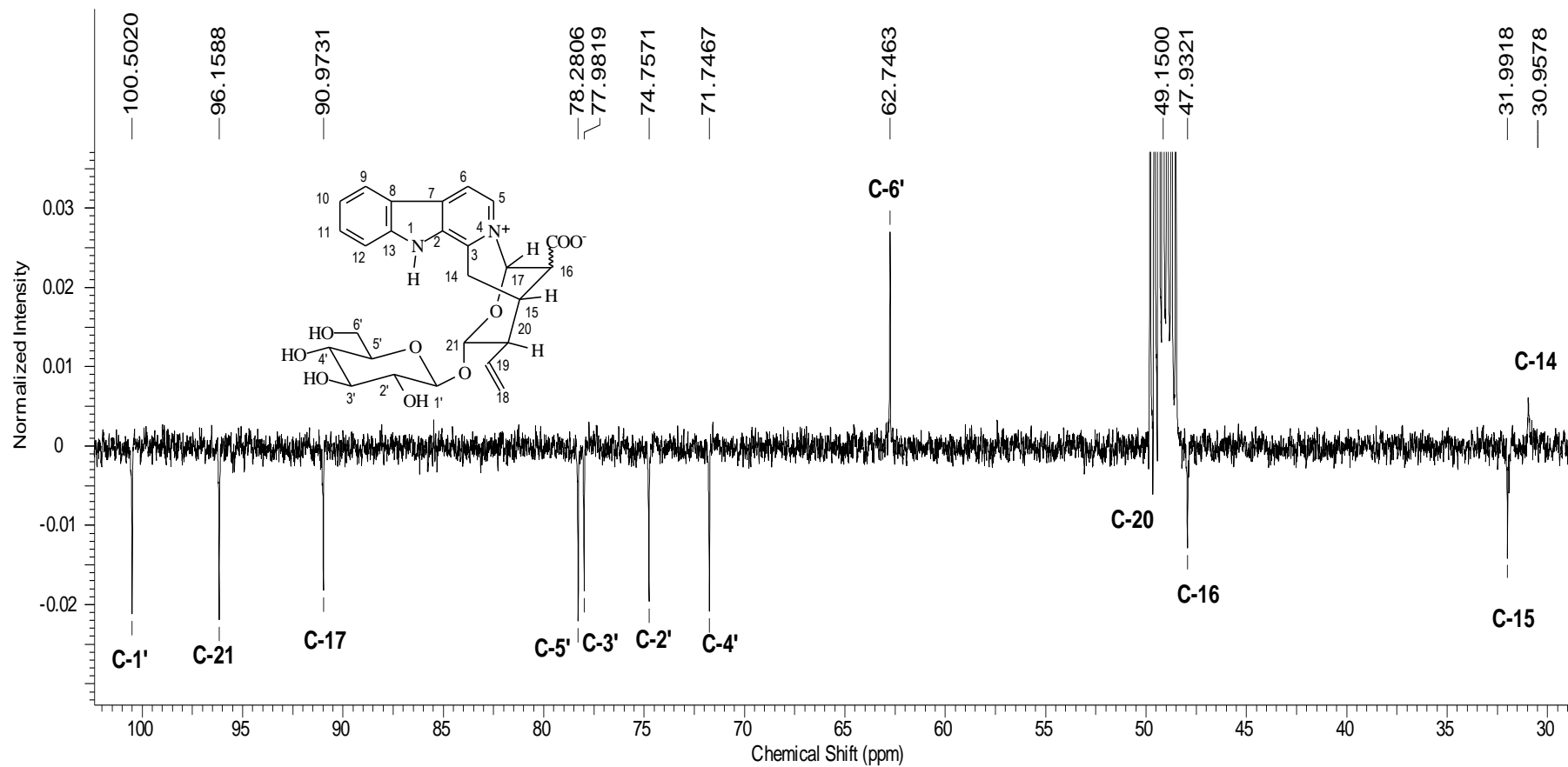
Espectro 74. Expansão entre δ_H 3.80- 2.80 do espectro de RMN- 1H (400 MHz, MeOD) da substância **SGMH-4**.



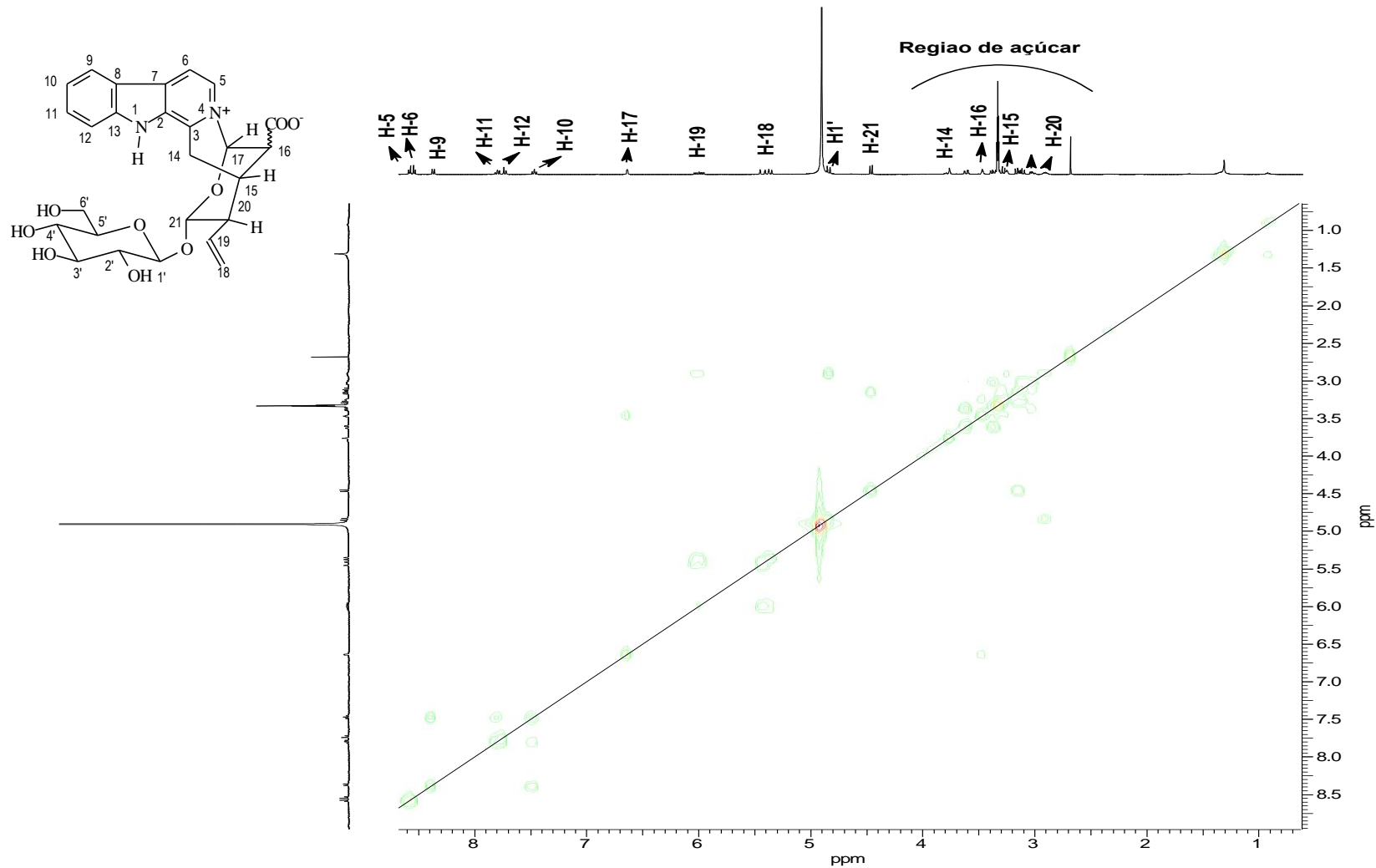
Espetro 75. RMN-¹³C-DEPTQ (100 MHz, MeOD) da substância SGMH-4.



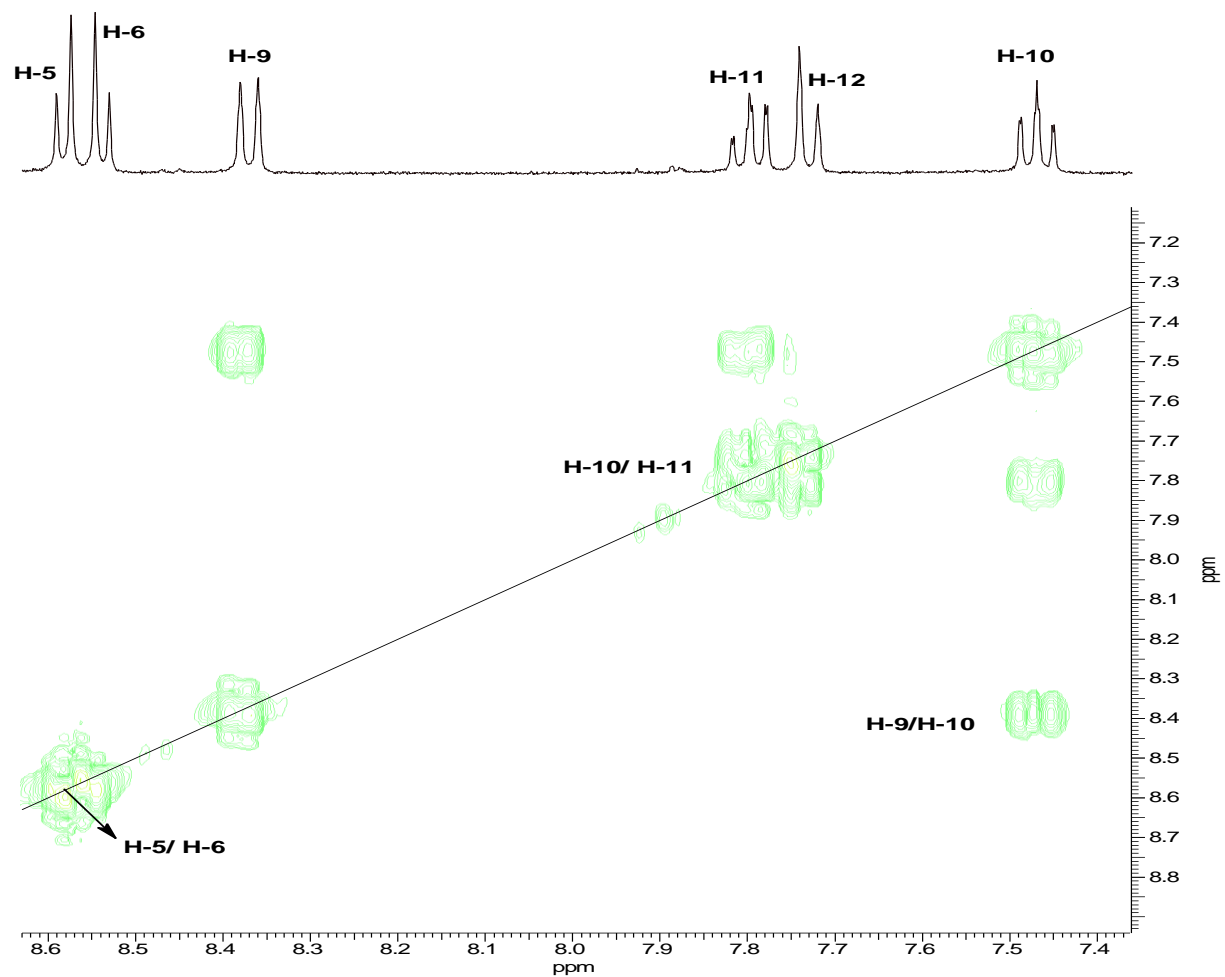
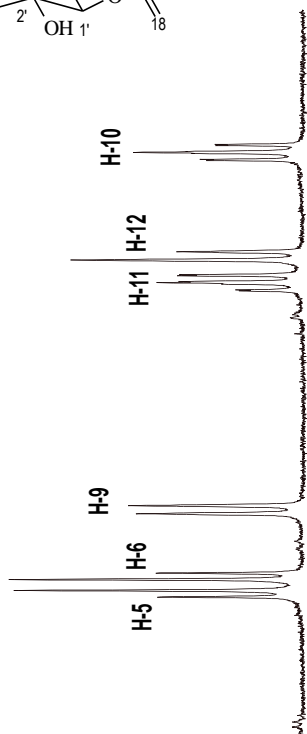
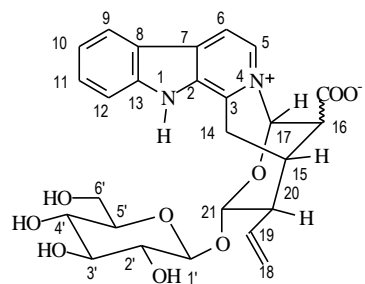
Espectro 76. Expansão entre δ_C 175.0- 115.5 do espectro de RMN- ^{13}C -DEPTQ (100 MHz, MeOD) da substância **SGMH-4**.



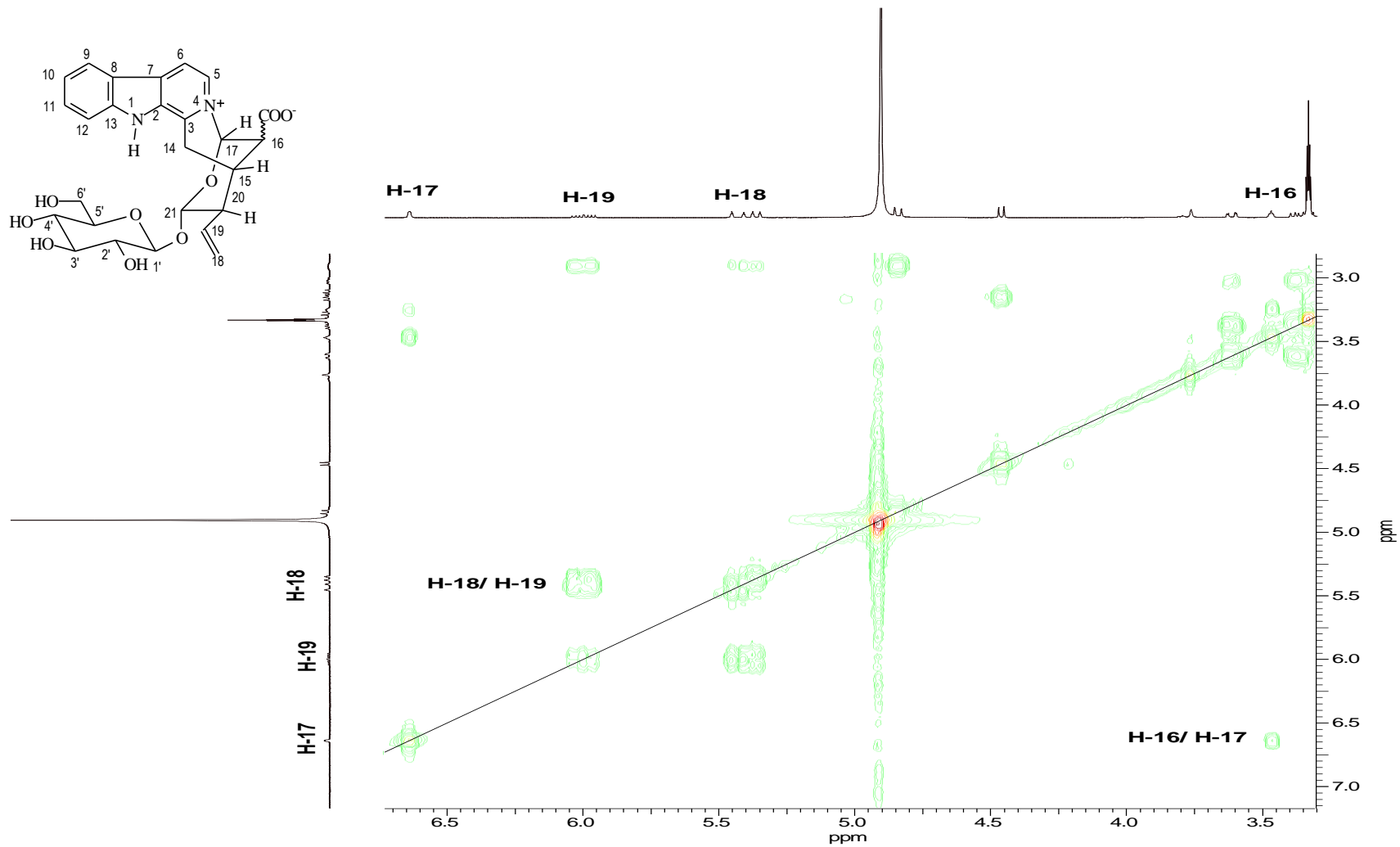
Espectro 77. Expansão entre δ_C 100.5- 30.0 do espectro de RMN- ^{13}C -DEPTQ (100 MHz, MeOD) da substância **SGMH-4**.



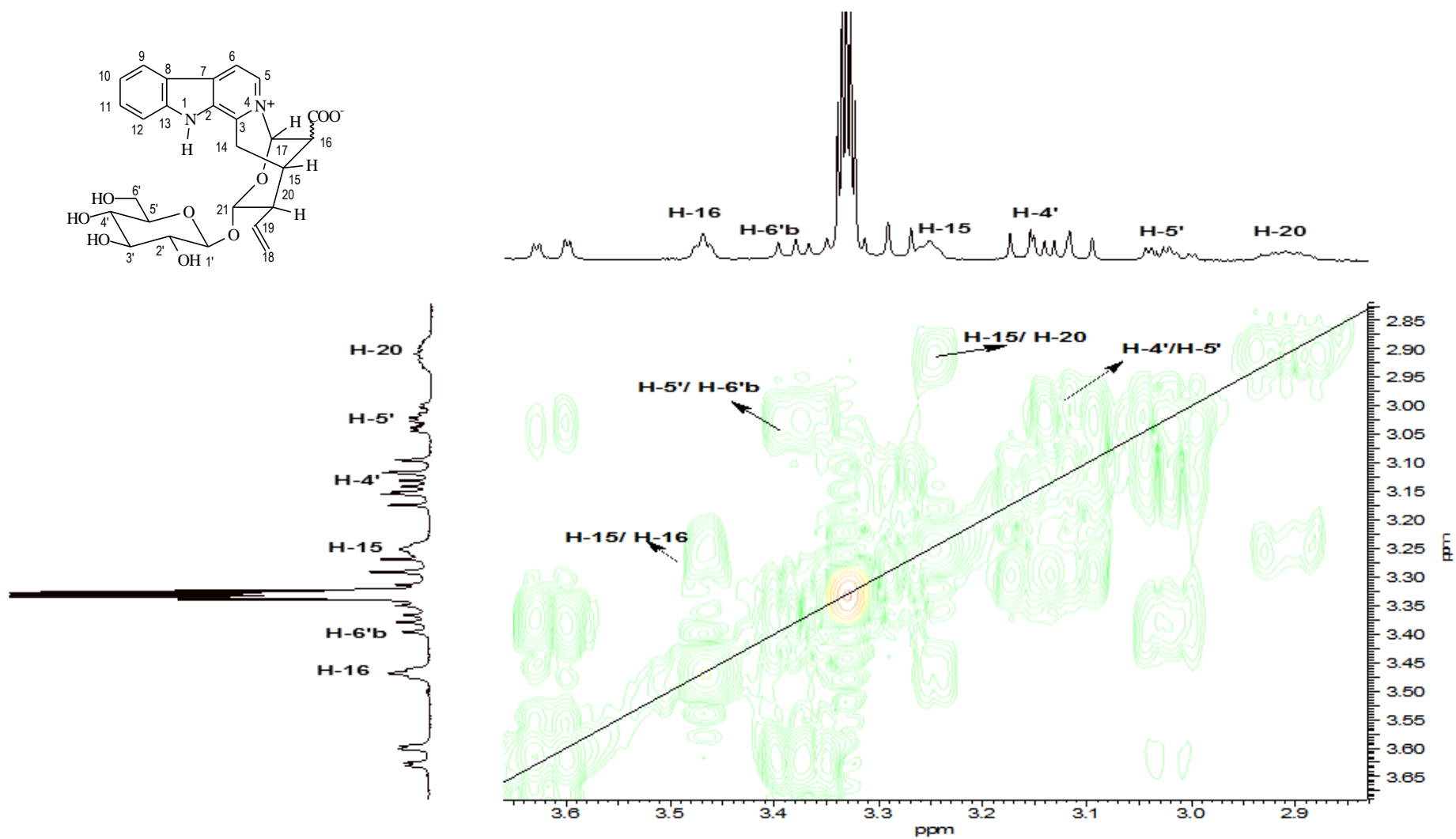
Espectro 78. RMN ^1H - ^1H -COSY (400 MHz, MeOD) da substância **SGMH-4**.



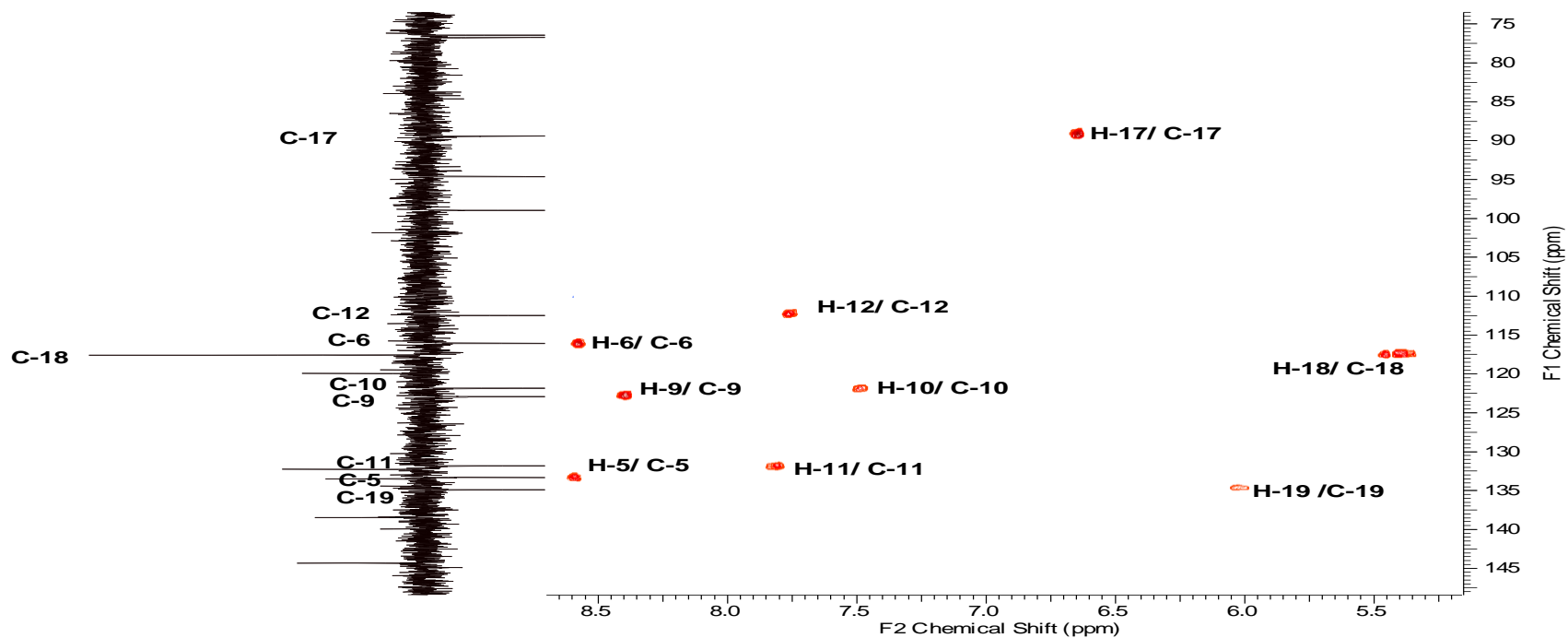
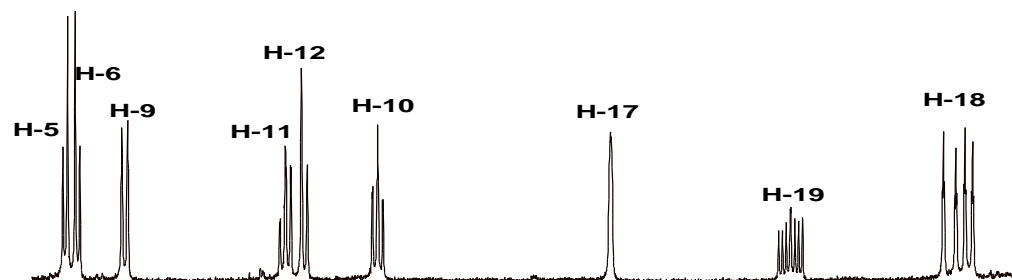
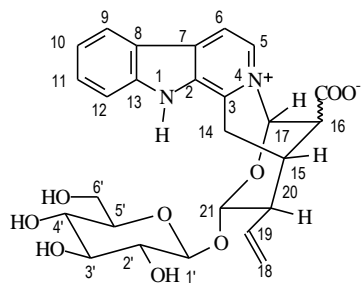
Espectro 79. Expansão entre δ_H 8.0- 6.0 do espectro de 1H - 1H -COSY (400 MHz, MeOD) da substância **SGMH-4**.



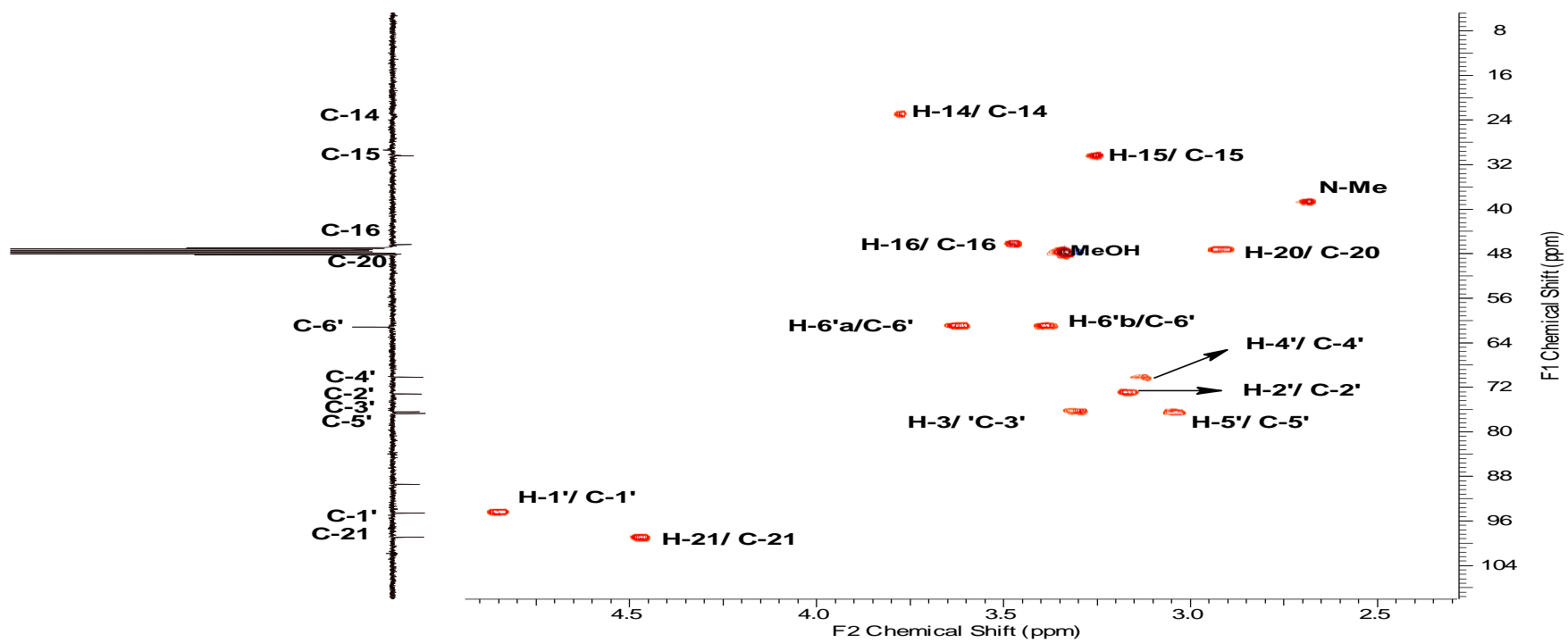
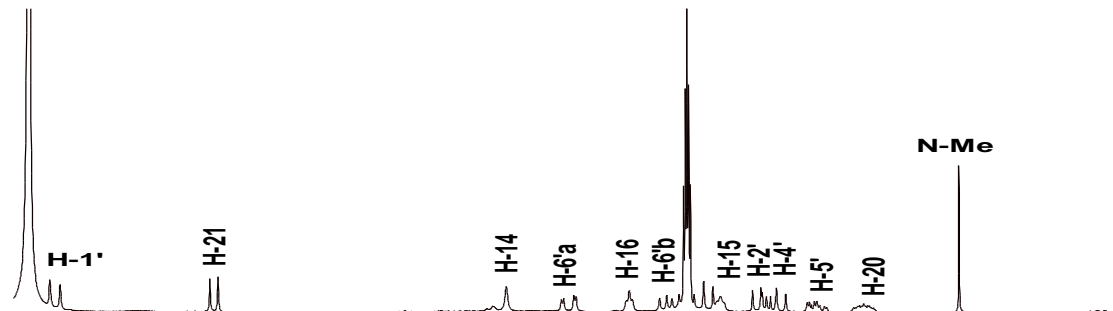
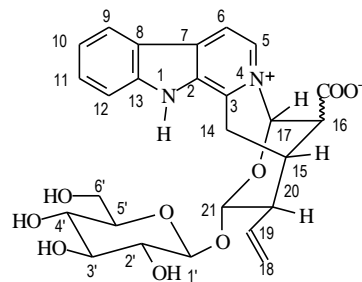
Espectro 80. Expansão entre δ_{H} 6.50-3.5 do espectro de ^1H - ^1H -COSY (400 MHz, MeOD) da substância **SGMH-4**.



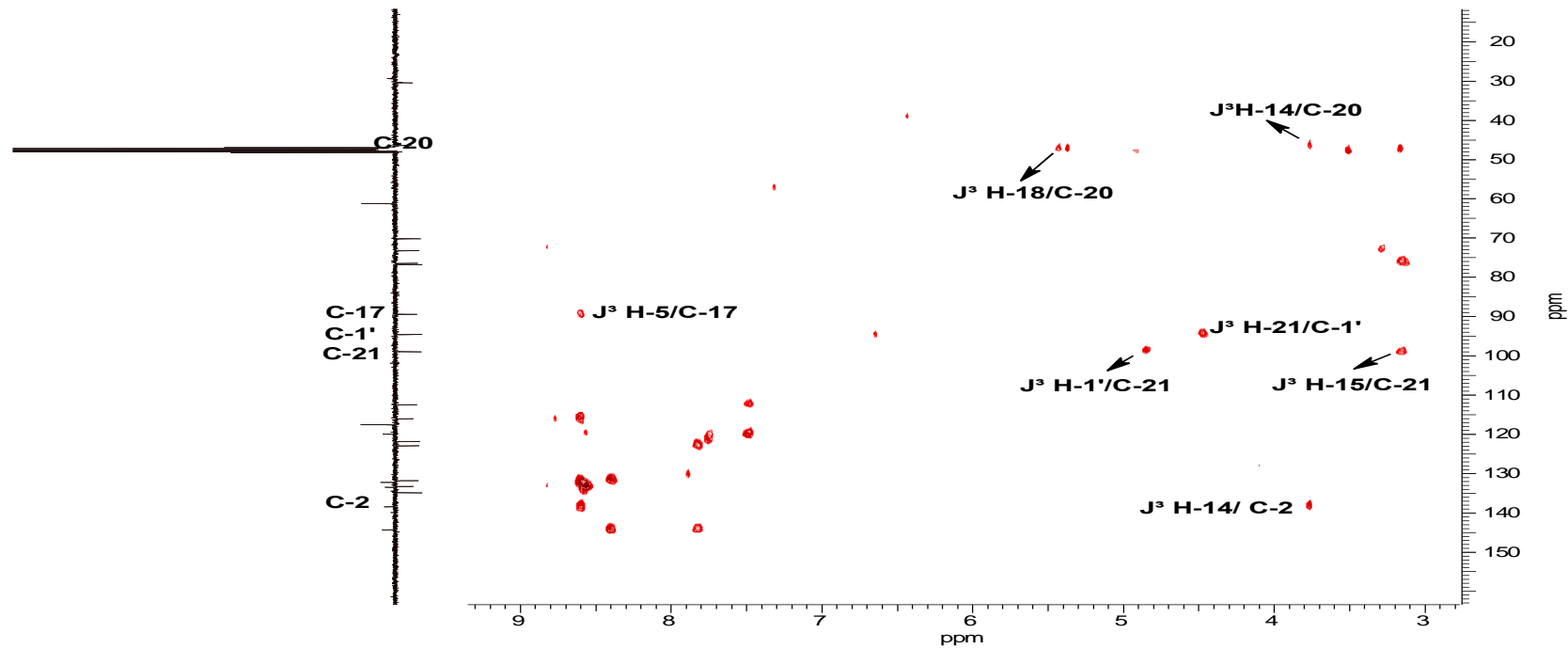
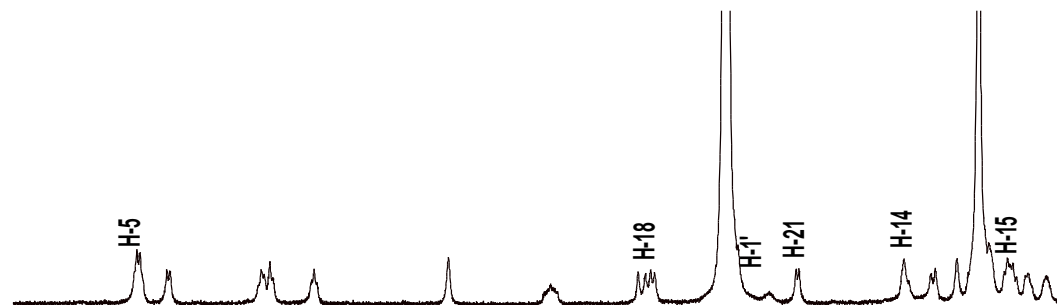
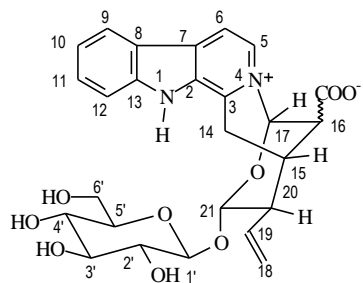
Espectro 81. Expansão entre δ_{H} 3.6.-2.9 do espectro de ^1H - ^1H -COSY (400 MHz, em MeOD) da substância **SGMH-4**.



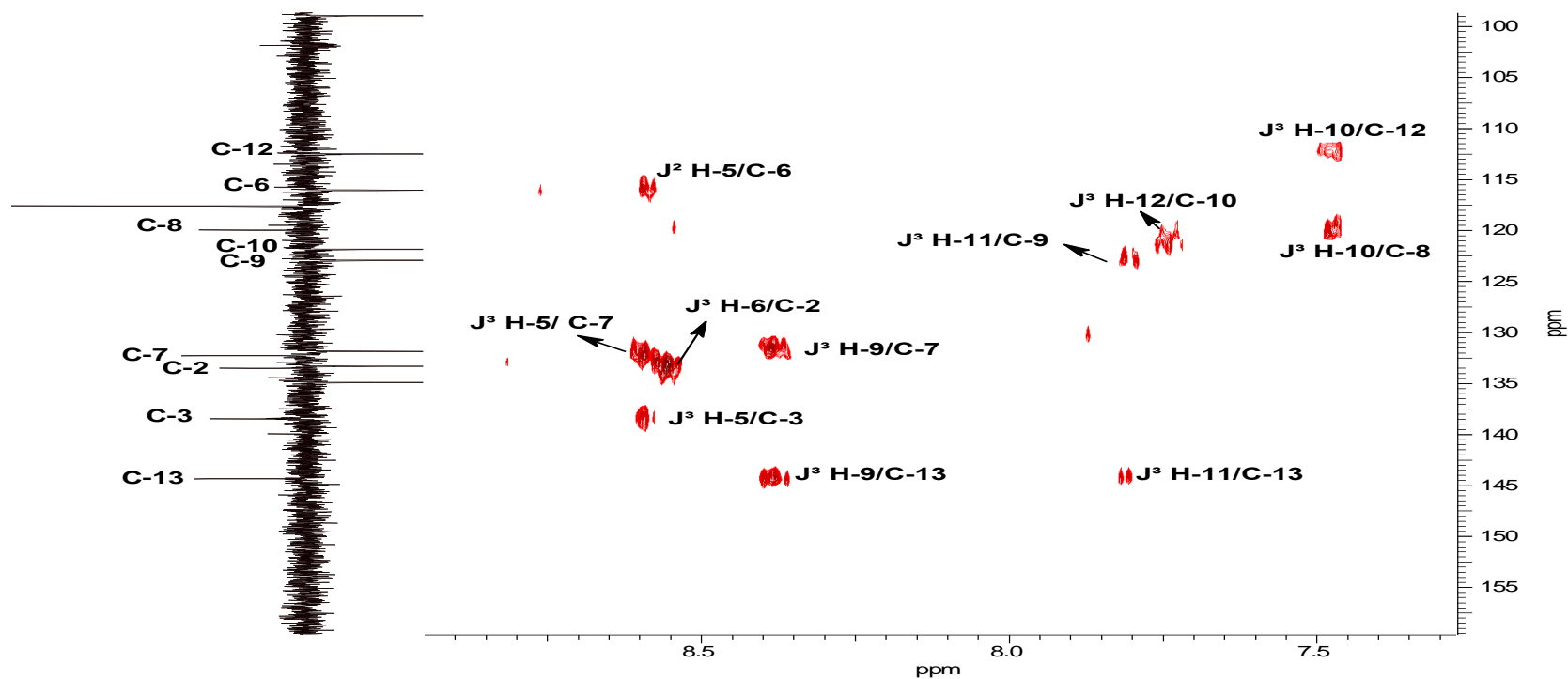
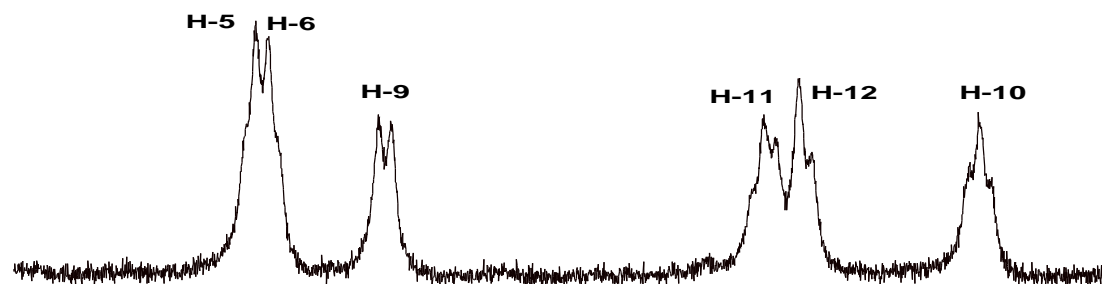
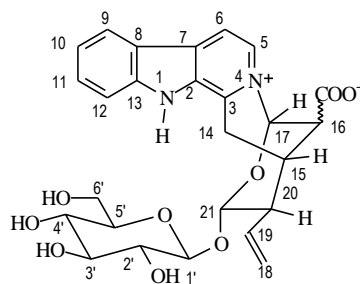
Espectro 82. Expansão entre δ_H 8.5-5.0 e δ_C 145.5-75.0 de 1H - ^{13}C -COSY- $^1J_{CH}$ (HSQC, em MeOD) da substância **SGMH-4**.



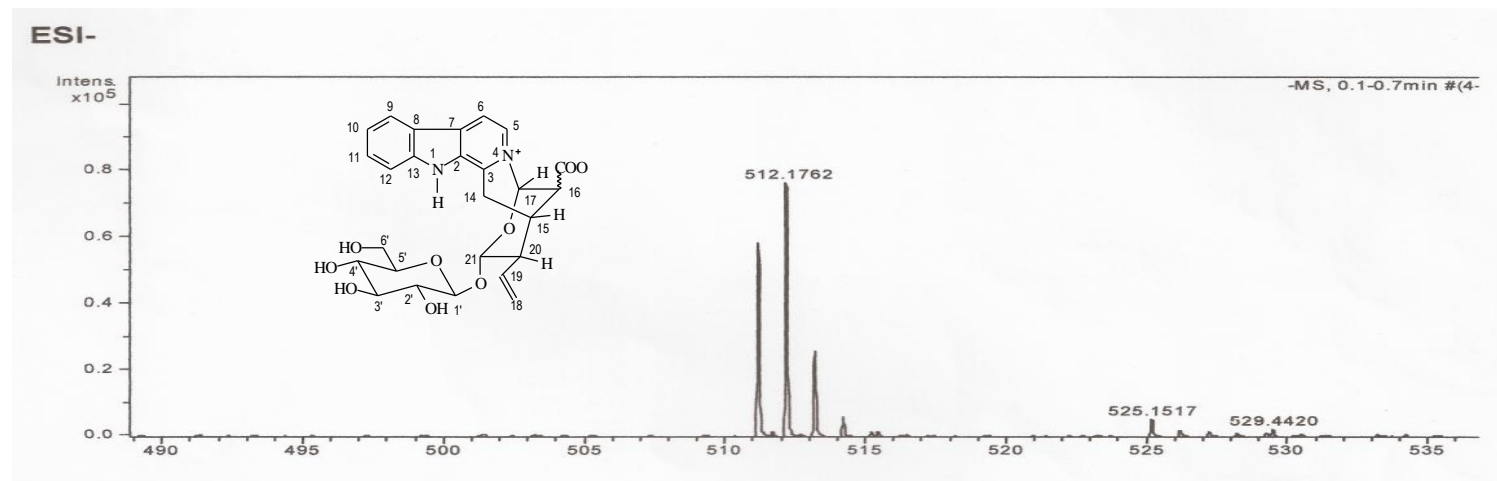
Espectro 83. Expansão entre δ_H 5.0-2.0 e δ_C 104.5-8.0 de 1H - ^{13}C -COSY- $^1J_{CH}$ (HSQC, em MeOD) da substância **SGMH-4**.



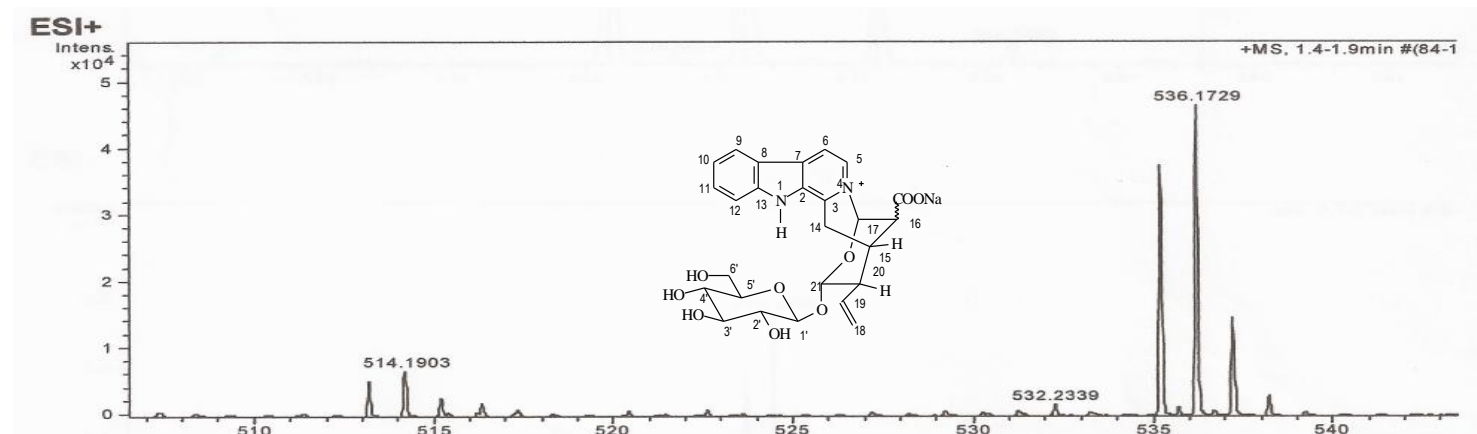
Espectro 84. 2 D de ^1H - ^{13}C -COSY- $^n\text{J}_{\text{CH}}$ ($n=2$ e $n=3$, HMBC, em MeOD) da substância **SGMH-4**.



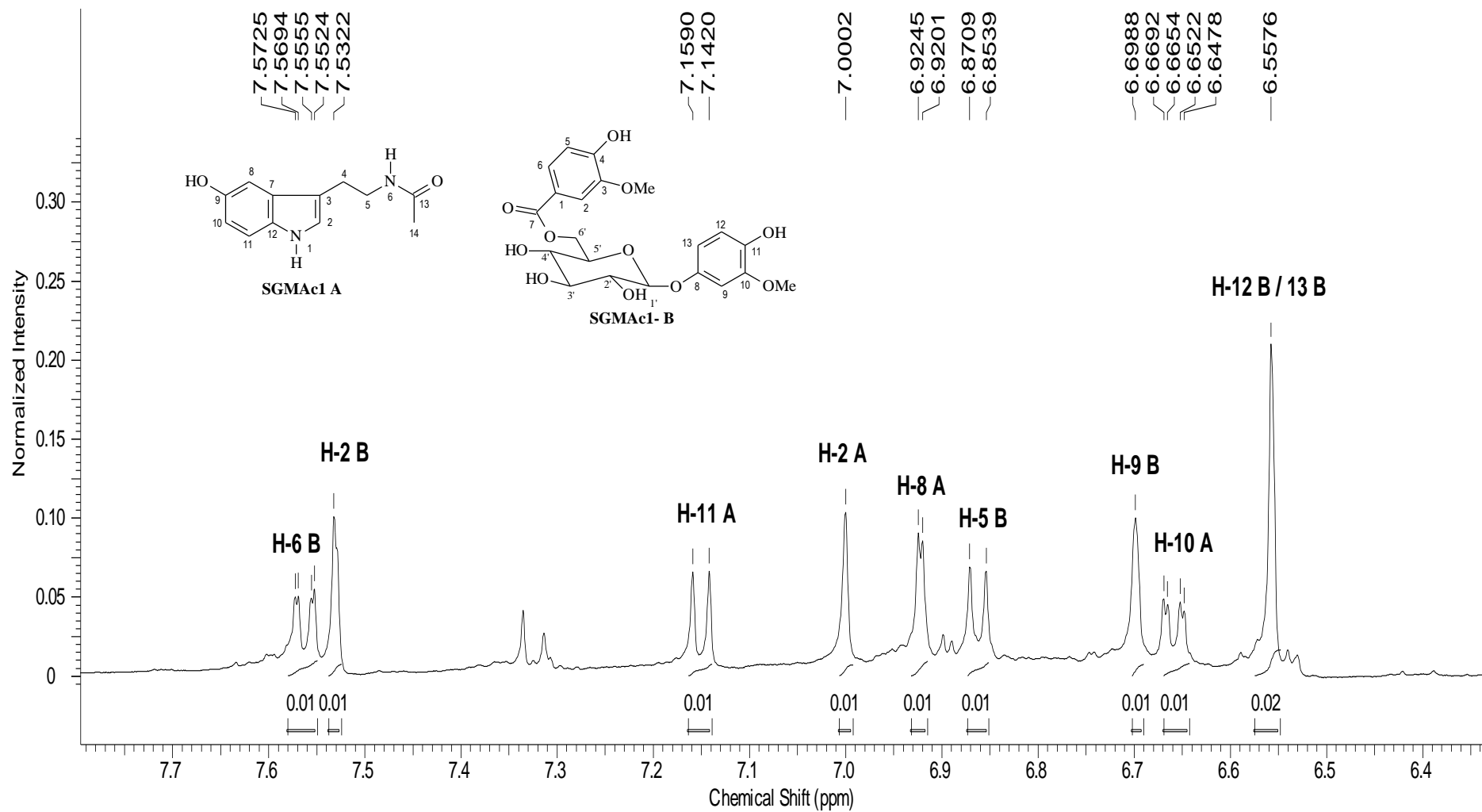
Espectro 85. Expansão entre δ_H 9.0-7.0 e δ_C 155.0-100.0 de 1H - ^{13}C -COSY- nJCH ($n=2$ e $n=3$, HMBC, em MeOD) da substância **SGMH-4**.



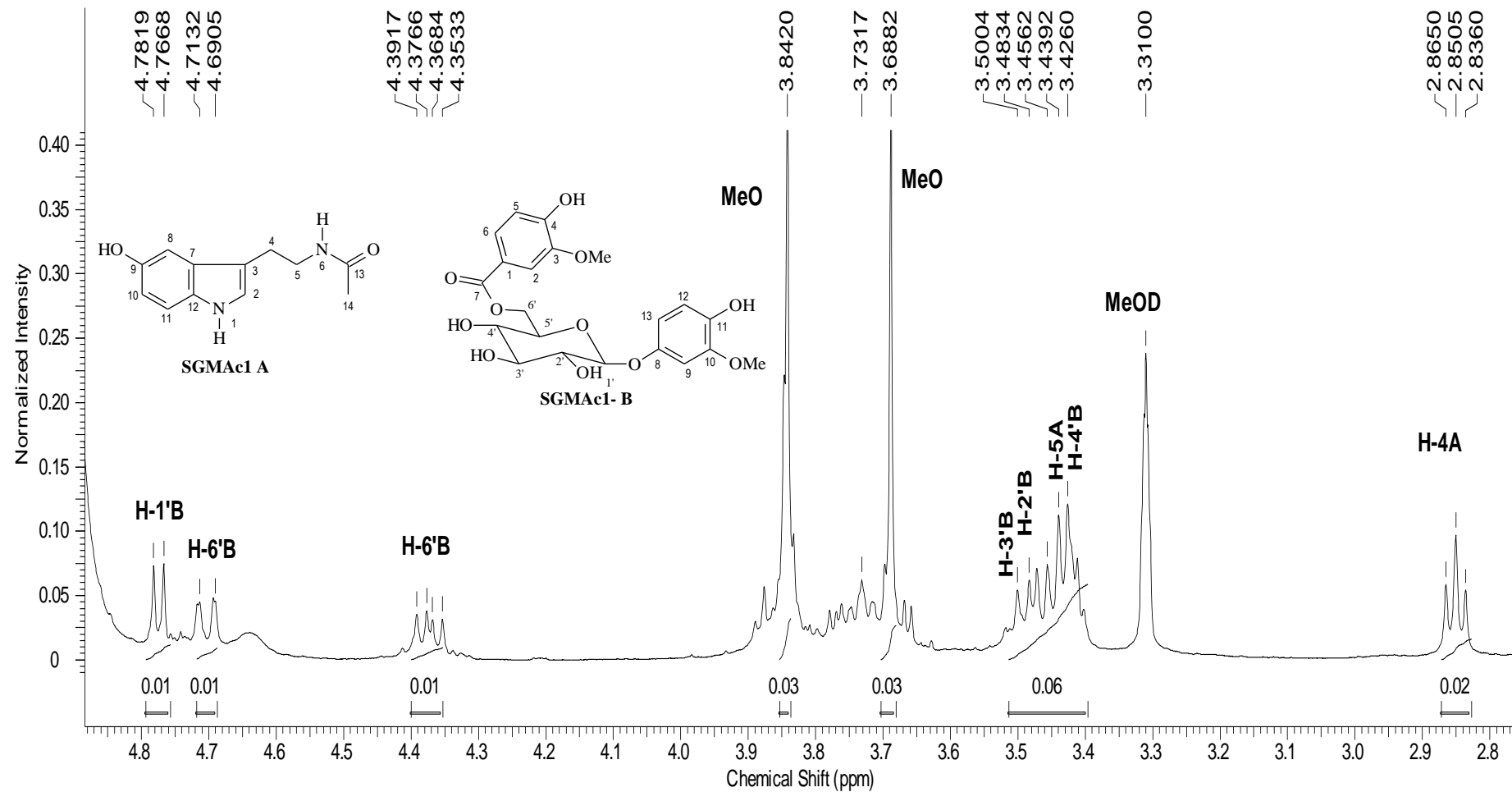
Espetro 86. ESI-MS $[M+H]^+$ da substância SGMH-4.



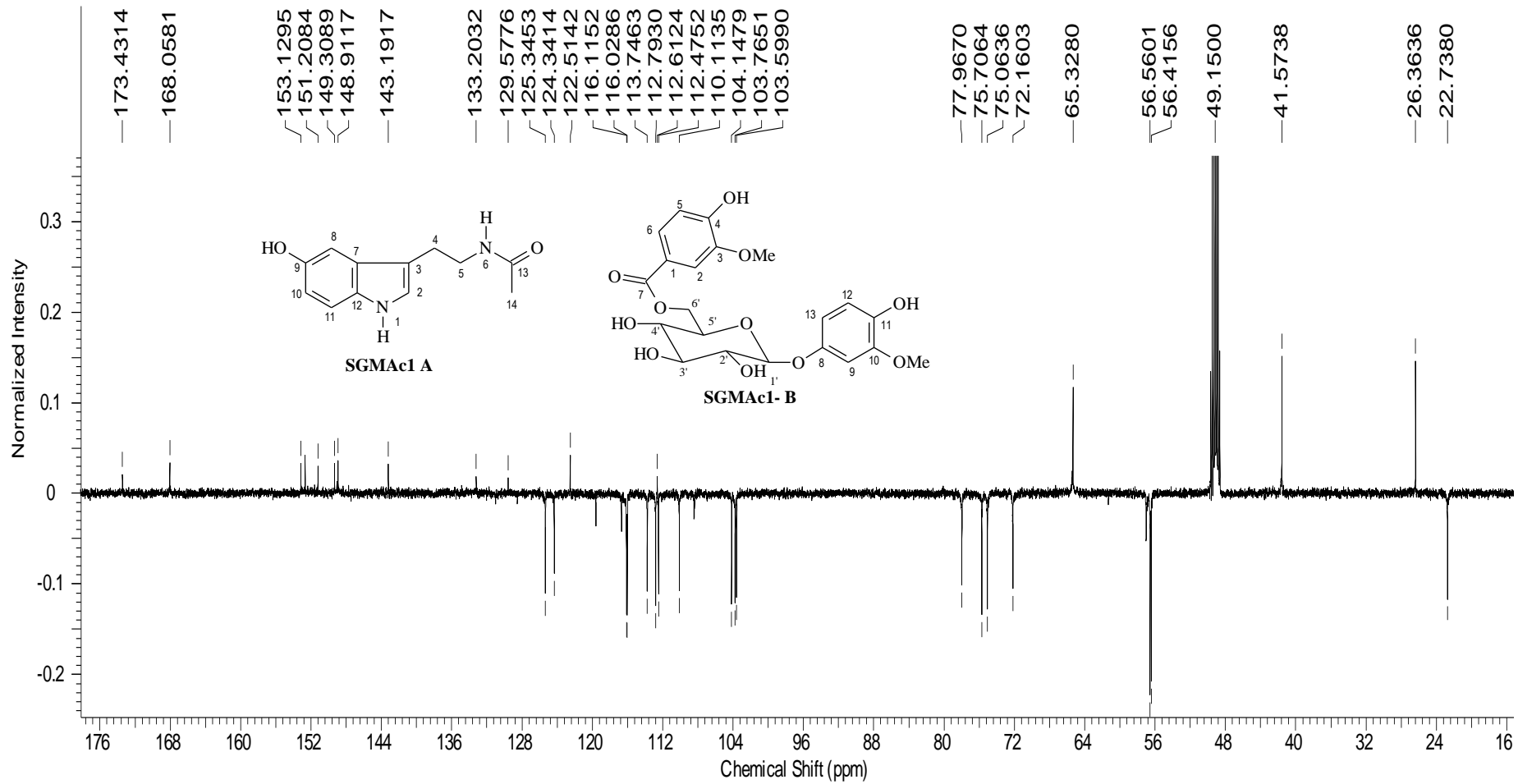
Espetro 87. ESI-MS $[M+Na]^+$ da substância SGMH-4.



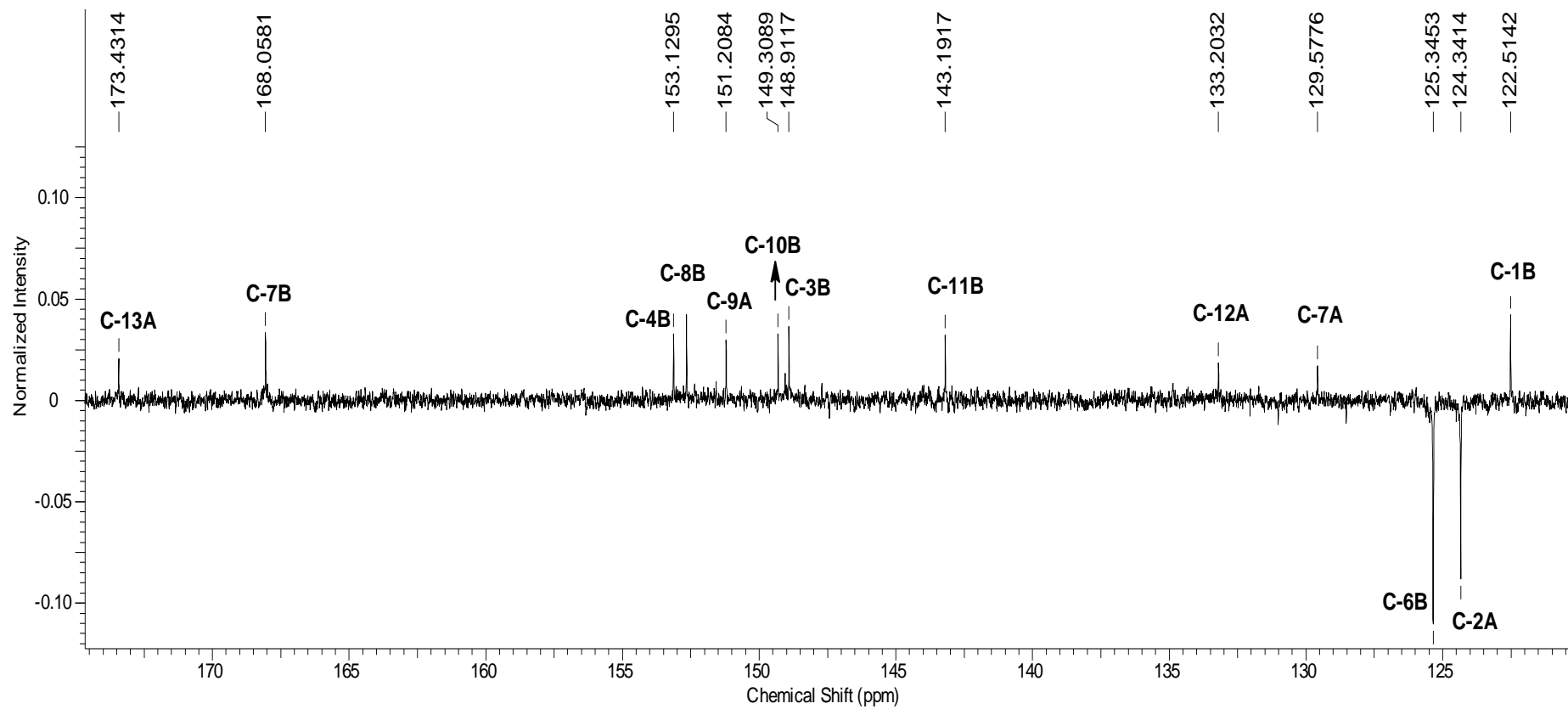
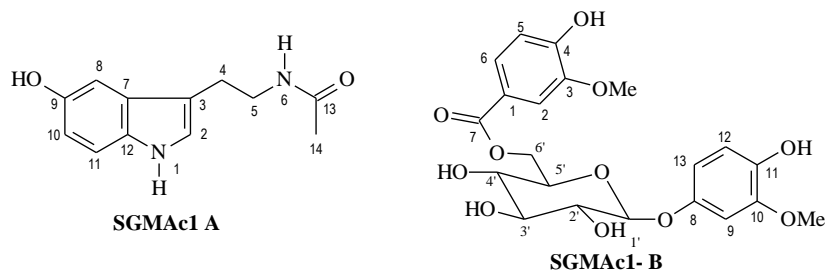
Espectro 89. Expansão entre δ_H 7.7- 6.4 do espectro de RMN- 1H (500 MHz, MeOD) da mistura de **SGMAc-1**.



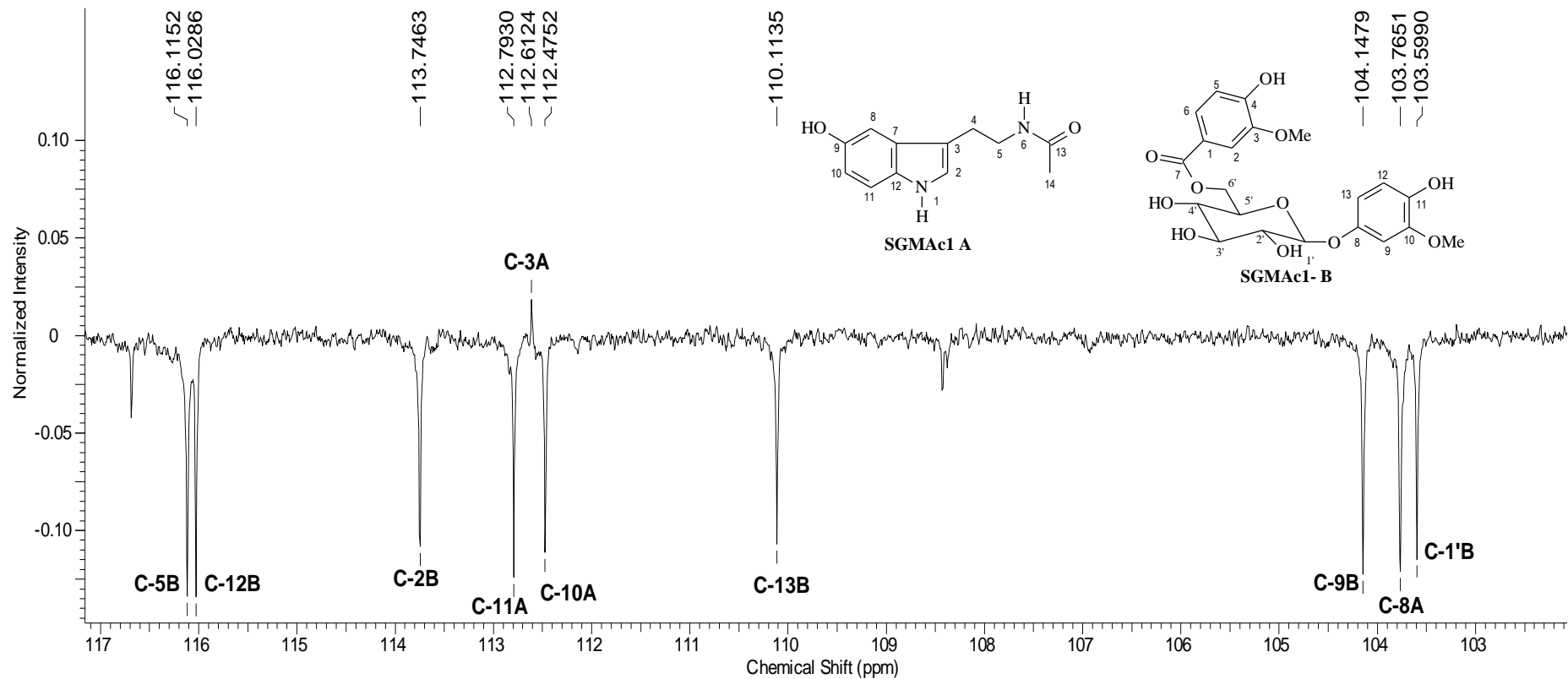
Espectro 90. Expansão entre δ_H 4.8- 2.8 do espectro de RMN- 1H (500 MHz, MeOD) da mistura de **SGMAc-1**.



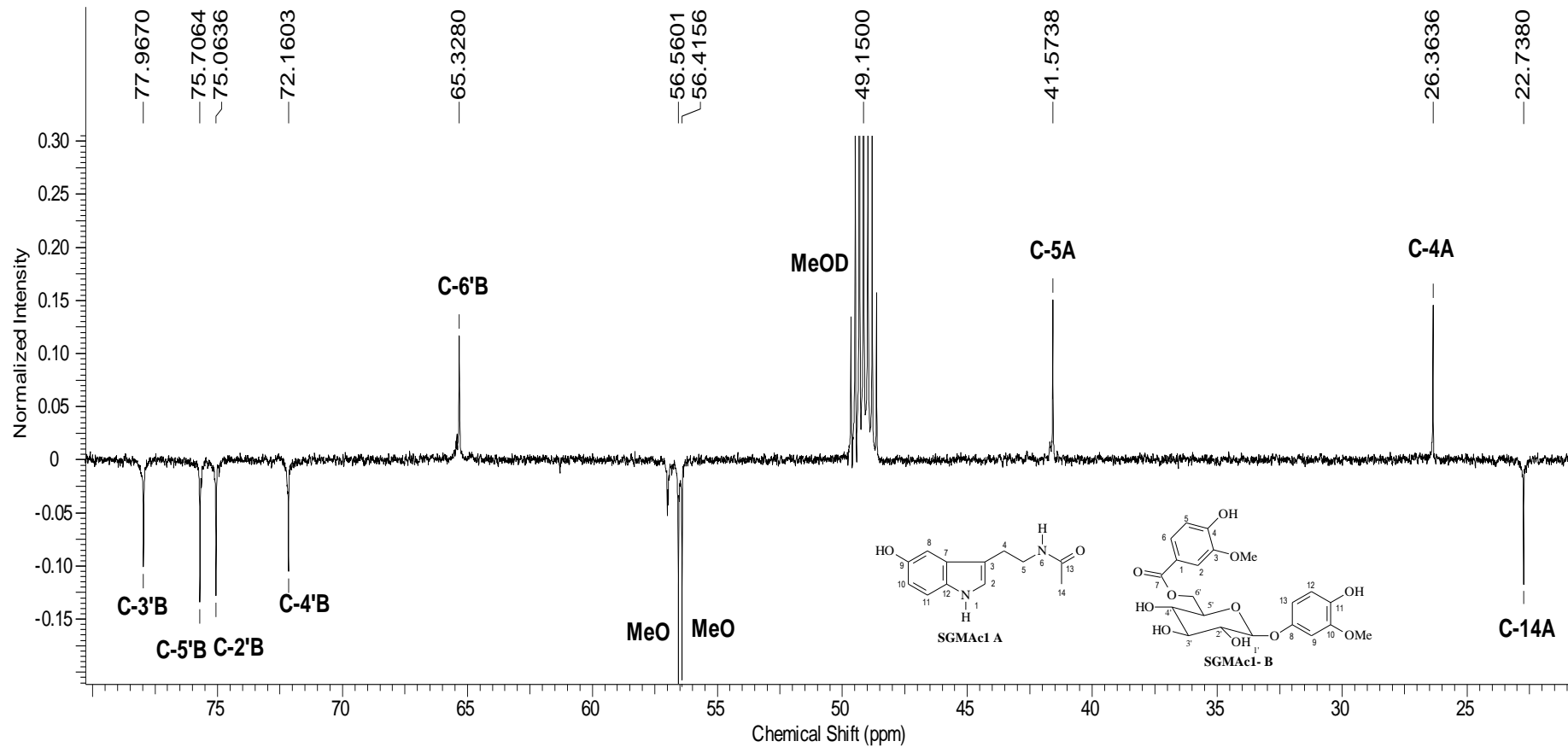
Espectro 91. RMN-¹³C-DEPTQ (125 MHz, MeOD) da mistura de **SGMac-1**.



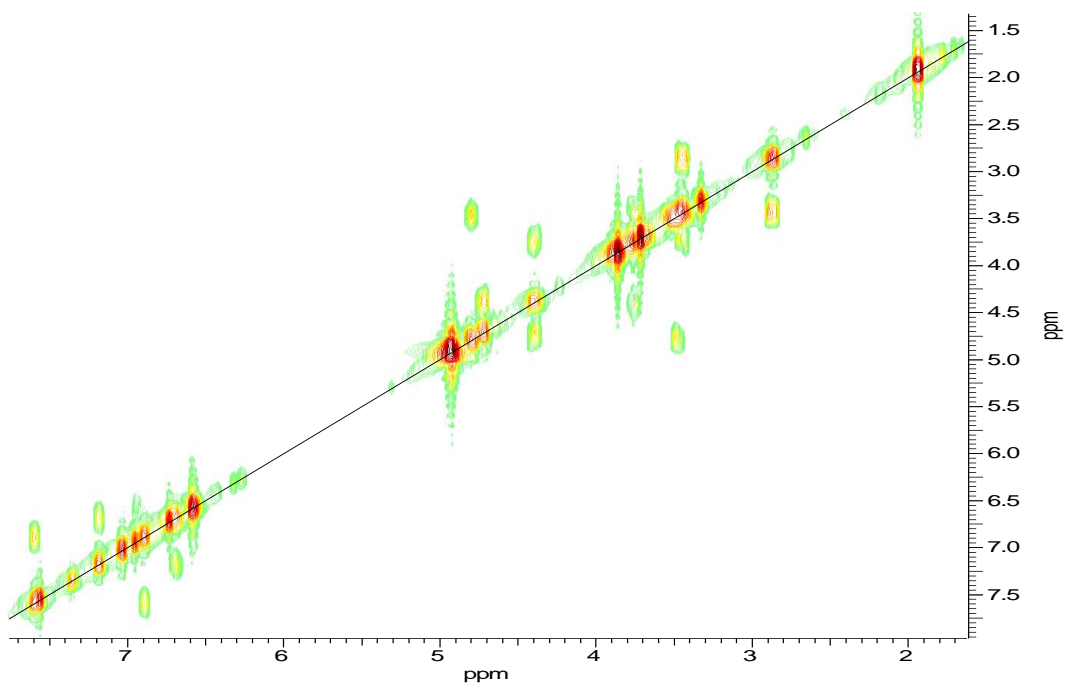
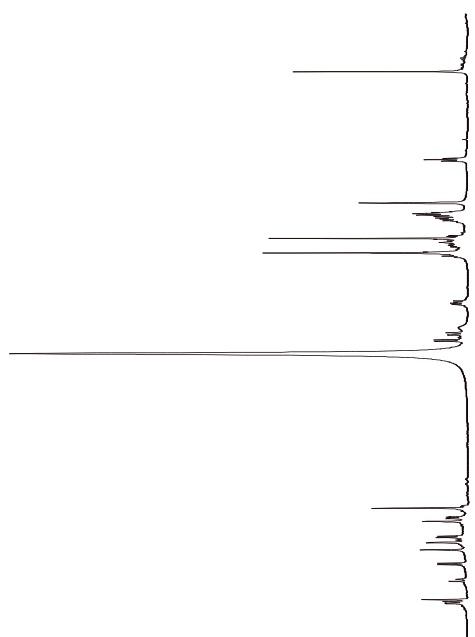
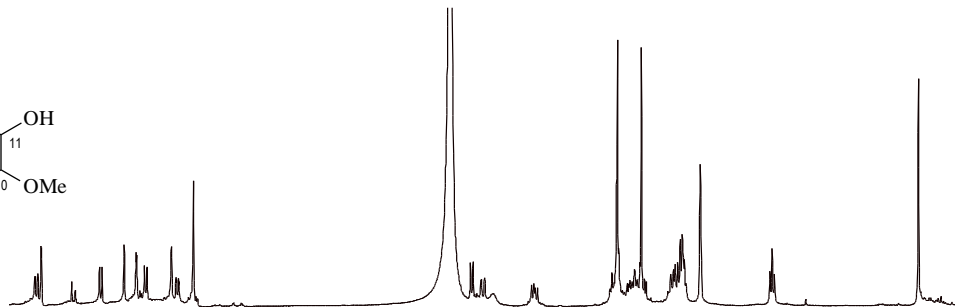
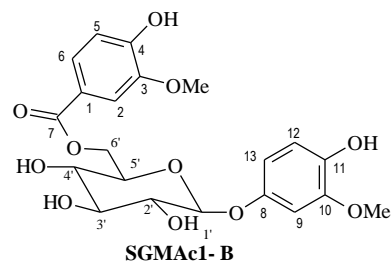
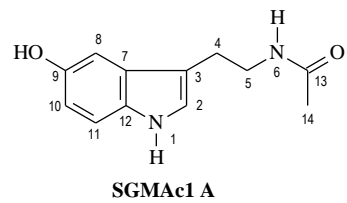
Espectro 92. Expansão entre δ_C 175.0- 120.0 do espectro de RMN- ^{13}C -DEPTQ (125 MHz, MeOD) da mistura de **SGMAc-1**.



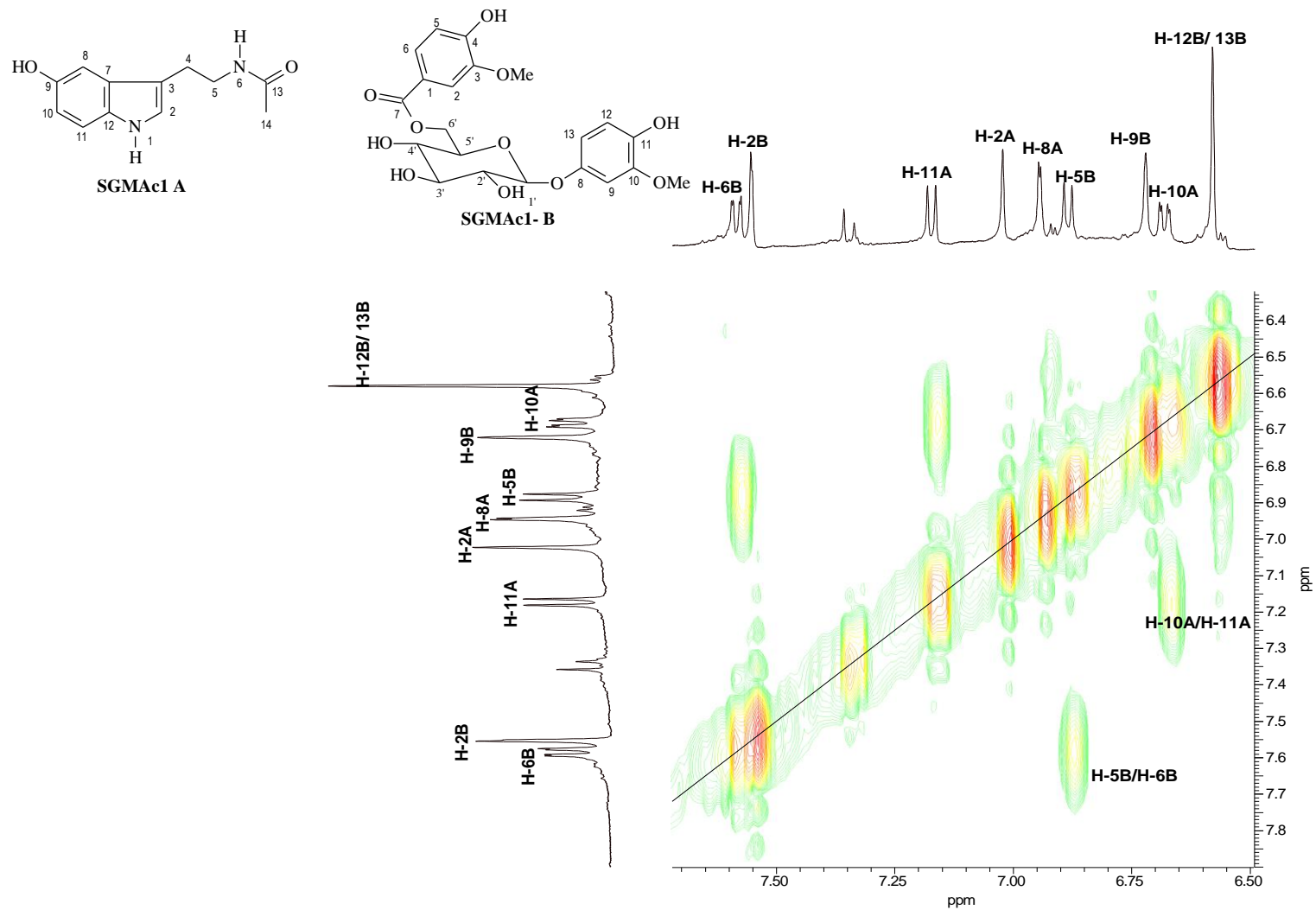
Espectro 93. Expansão entre δ_c 117.0- 102.0 do espectro de RMN- ^{13}C -DEPTQ (125 MHz, MeOD) da mistura de **SGMAc-1**.



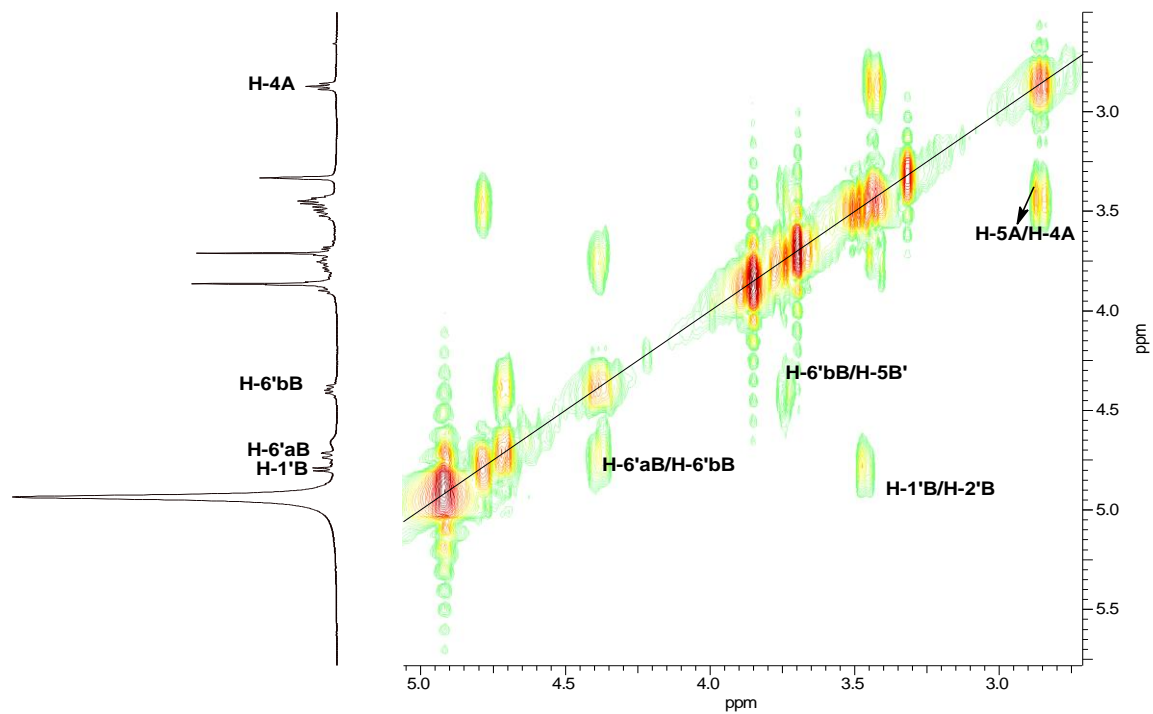
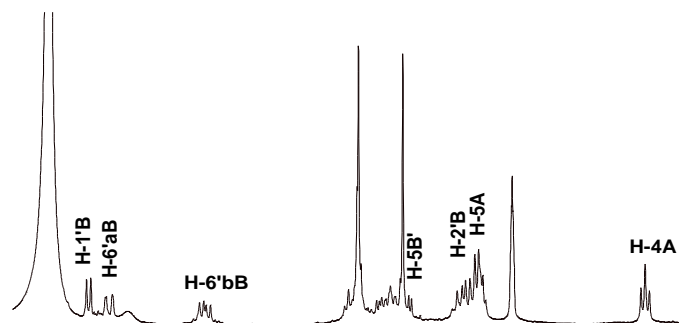
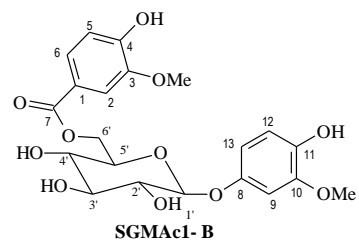
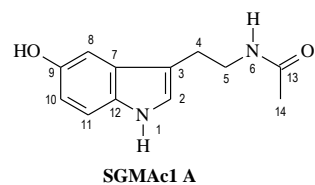
Espectro 94. Expansão entre δ_c 78.0- 20.0 do espectro de RMN- ^{13}C -DEPTQ (125 MHz, MeOD) da mistura de **SGMAc-1**.



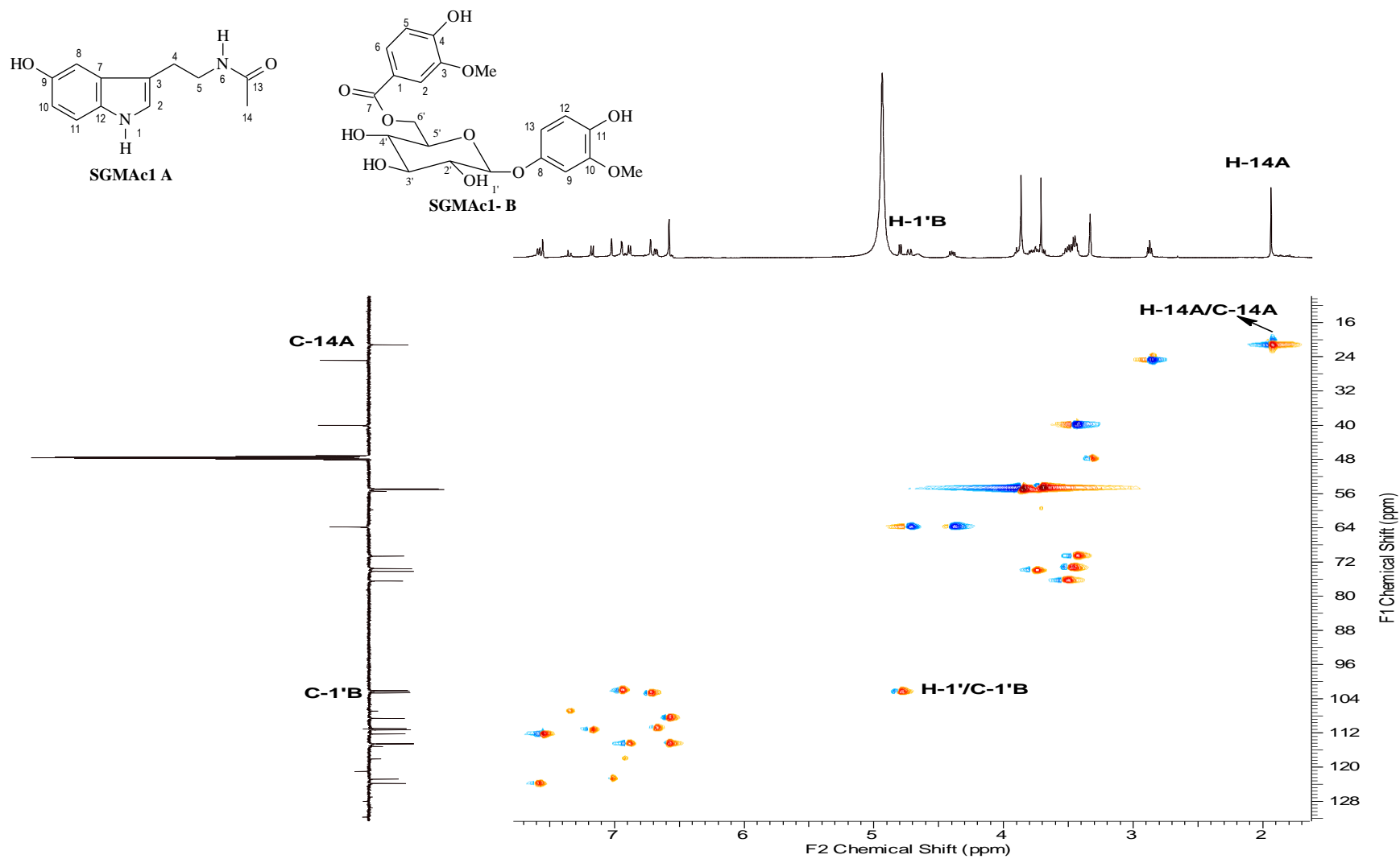
Espectro 95. 2D¹H-¹H-COSY (500 MHz, MeOD) da mistura de **SGMac-1**.



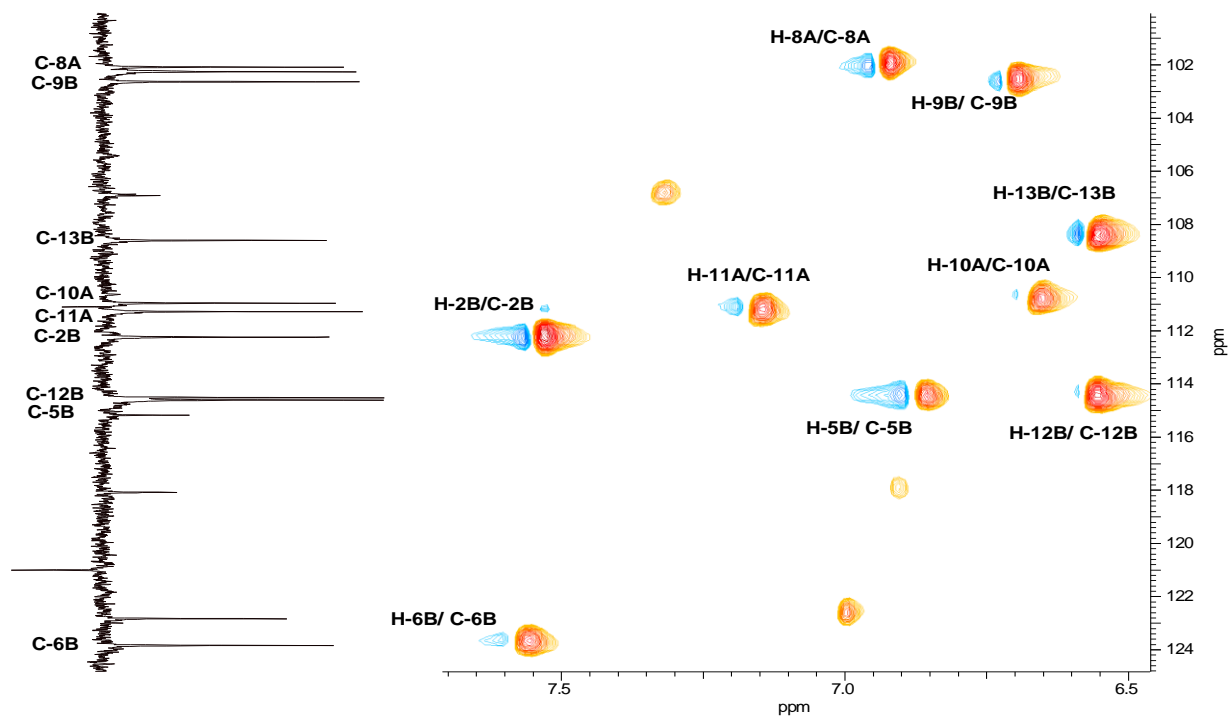
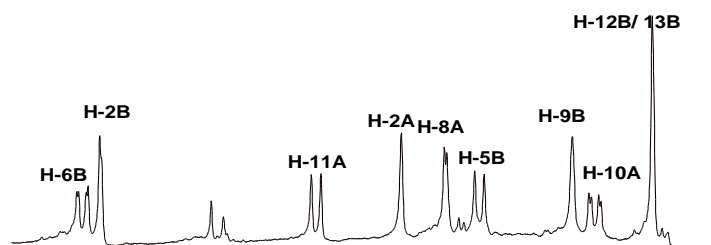
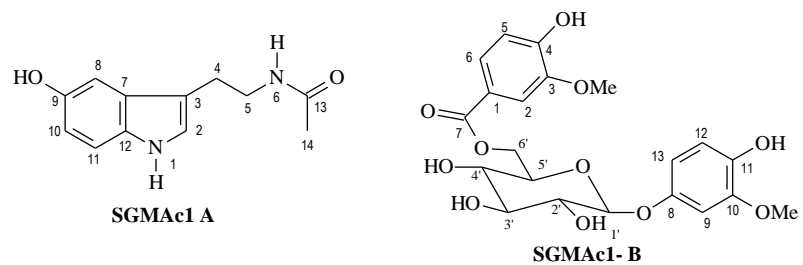
Espetro 96. Expansão entre δ_H 8.0.-6.5 do espectro de ^1H - ^1H -COSY (500 MHz, em MeOD) da mistura de SGMac-1.



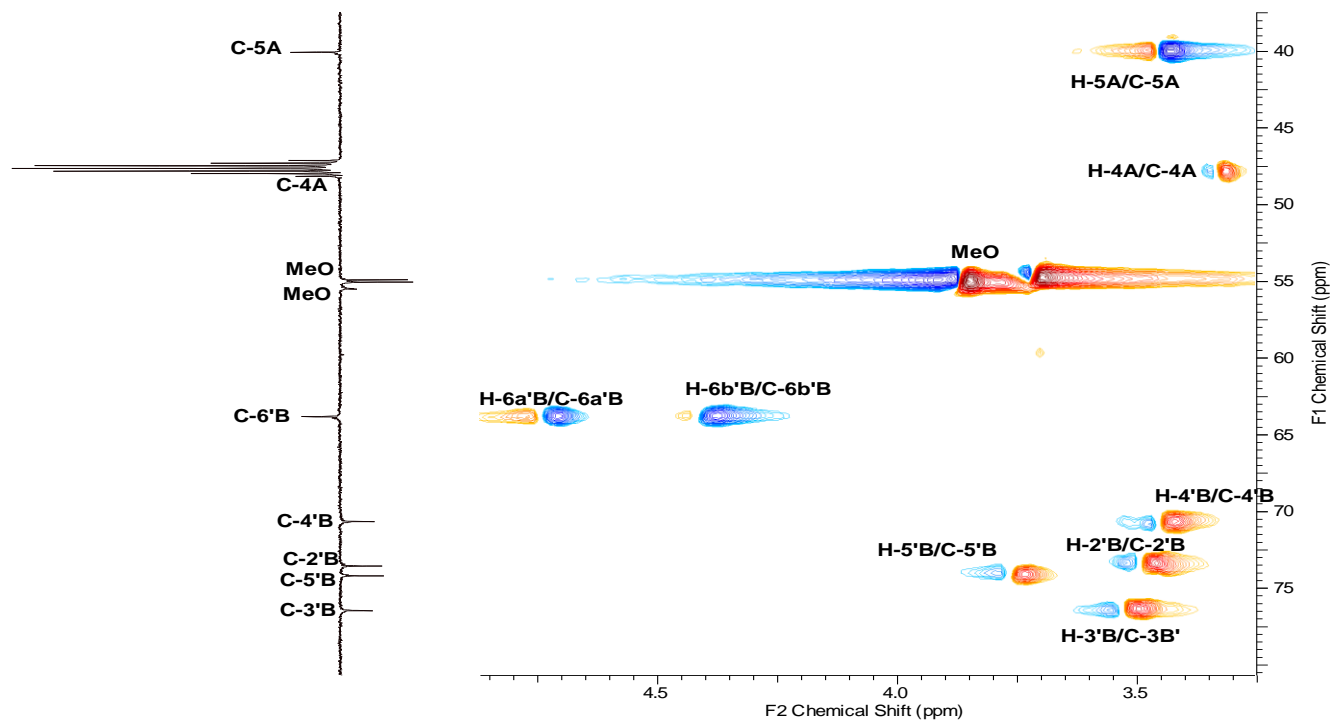
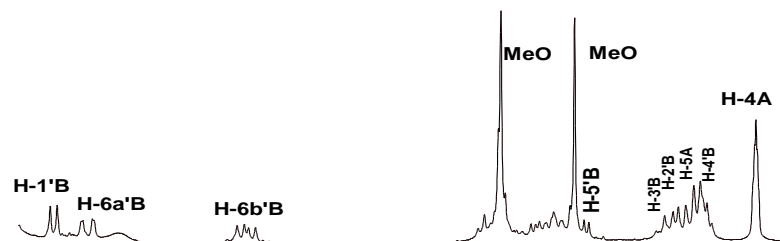
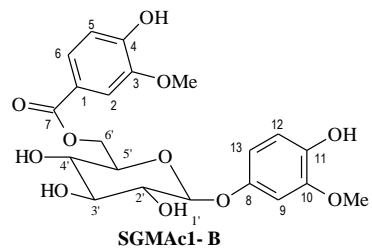
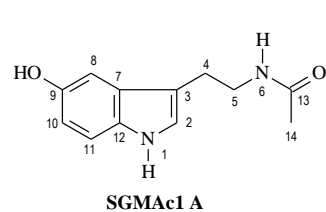
Espetro 97. Expansão entre δ_H 5.0-2.0 do espectro de 1H - 1H -COSY (500 MHz, em MeOD) da mistura de **SGMac-1**.



Espectro 98. 2 D de ¹H-¹³C-COSY-¹J_{CH} (HSQC, em MeOD) da mistura de SGMac-1.

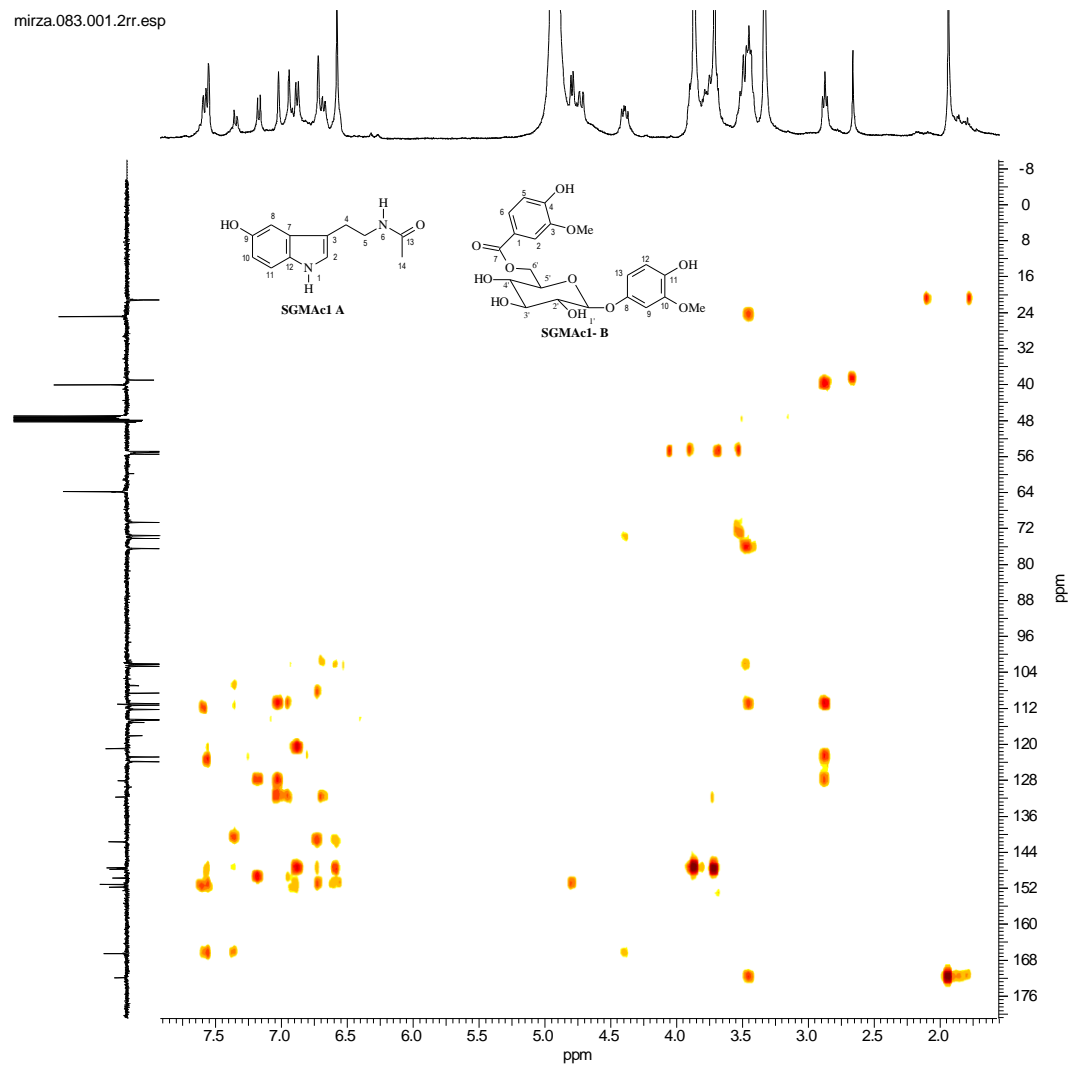


Espectro 99. Expansão entre δ_H 8.0-6.5 e δ_C 124.0-102.0 de 1H - ^{13}C -COSY- $^1J_{CH}$ (HSQC, em MeOD) da mistura de **SGMac-1**.

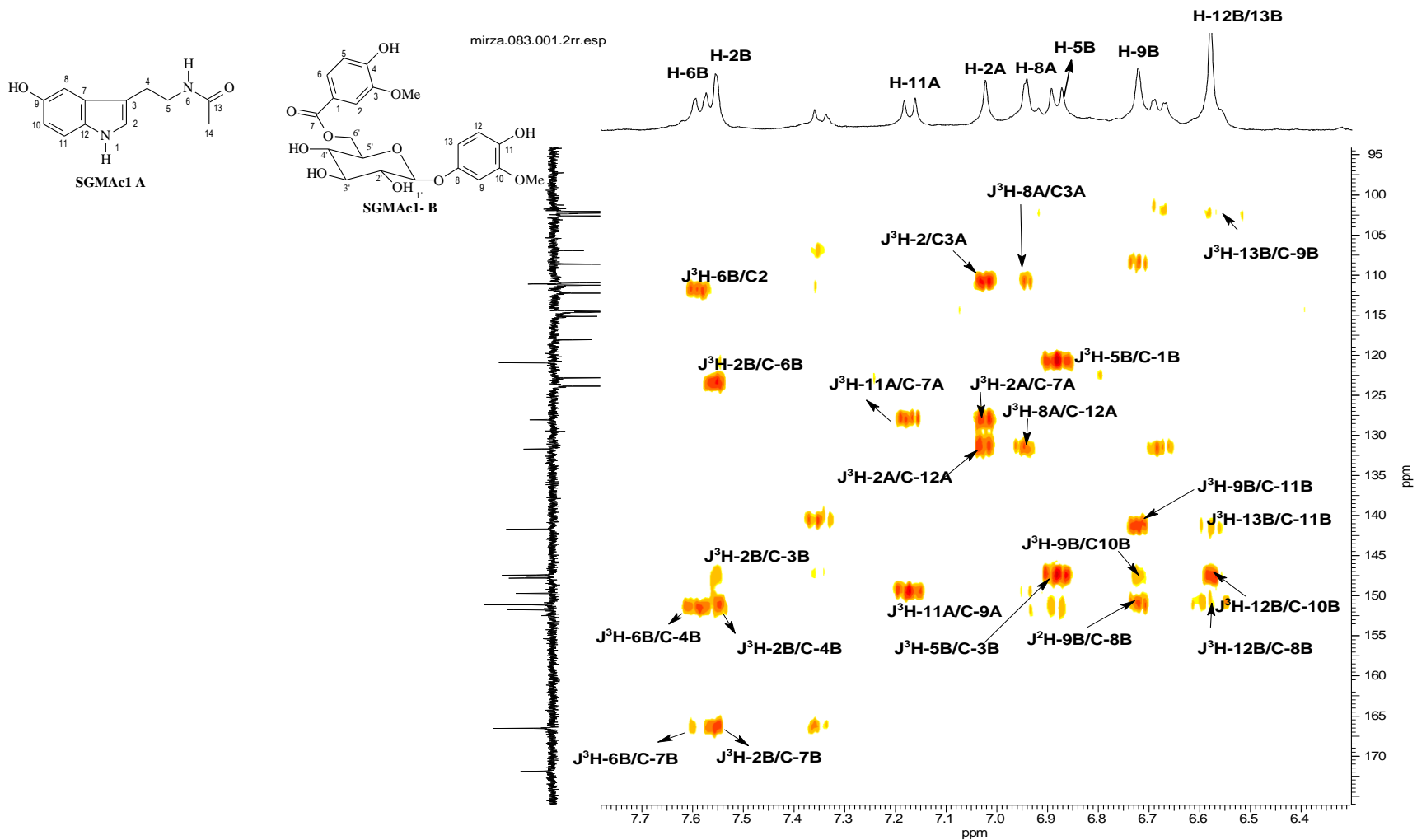


Espectro 100. Expansão entre δ_H 5.0-2.0 e δ_C 80.0.-40.0 de 1H - ^{13}C -COSY- $^1J_{CH}$ (HSQC, em MeOD) da mistura de SGMac-1.

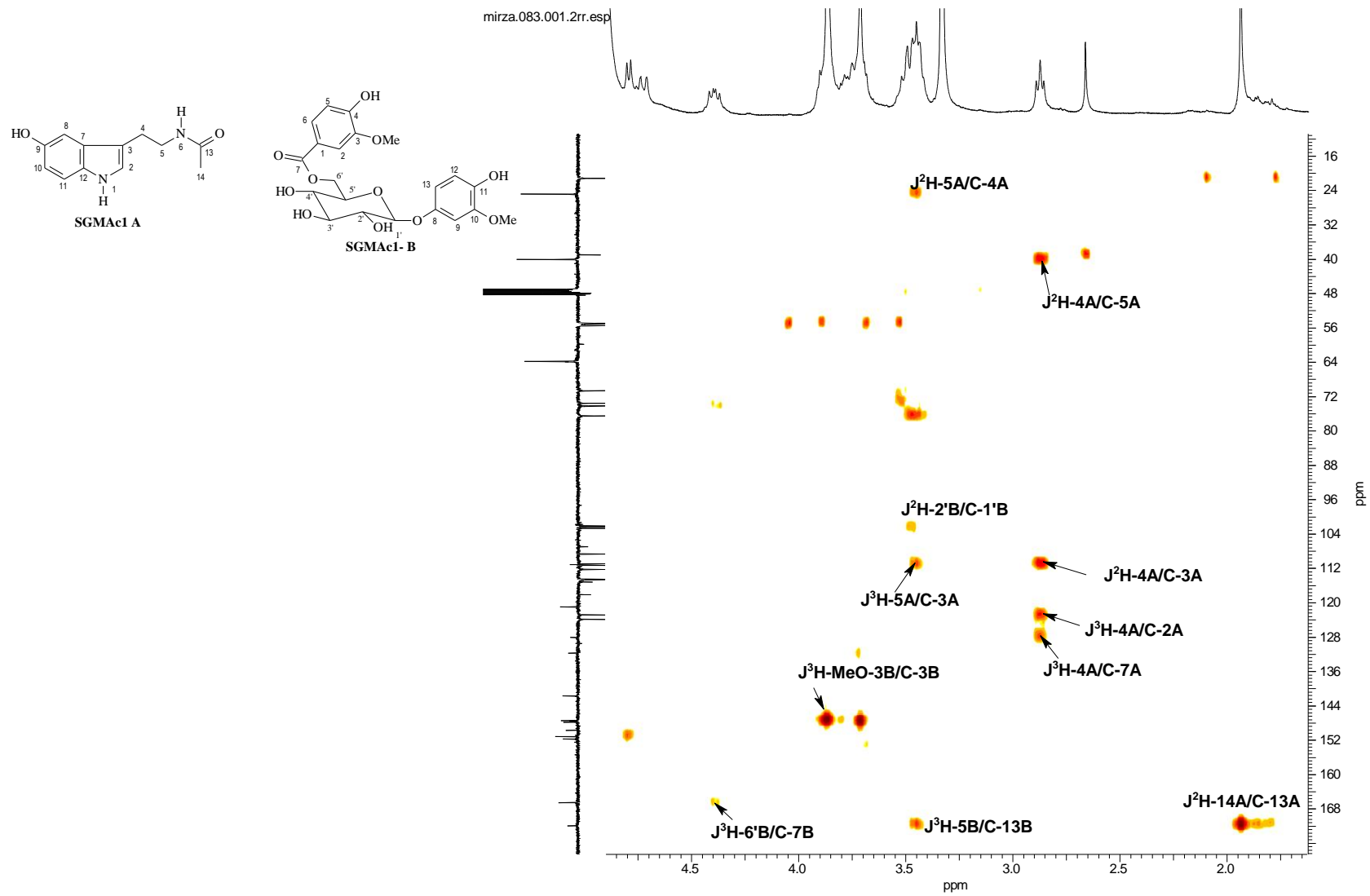
mirza.083.001.2rr.esp



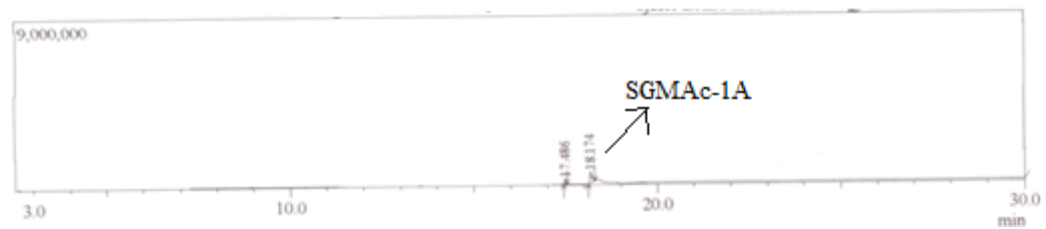
Espectro 101. 2 D de ^1H - ^{13}C -COSY- $^n\text{J}_{\text{CH}}$ (n=2 e n=3, HMBC, em MeOD) da mistura de **SGMAc-1**.



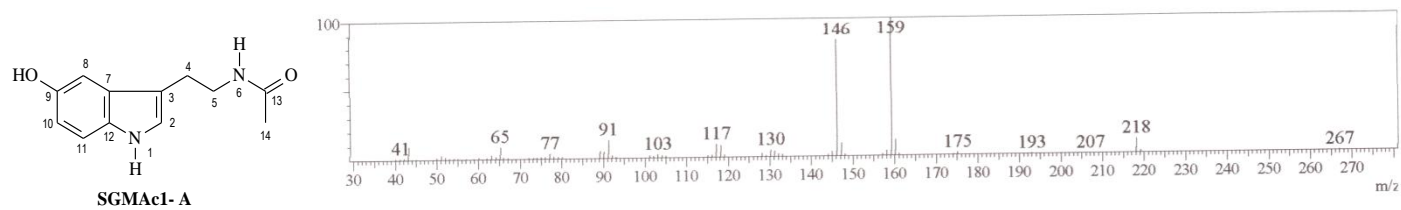
Espectro 102. Expansão entre δ_H 7.8-6.3 e δ_C 180.0-95.0 2 D de 1H - ^{13}C -COSY- $^nJ_{CH}$ ($n=2$ e $n=3$, HMBC, em MEOD) da mistura de SGMac-1.



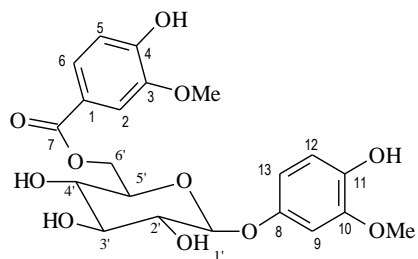
Espectro 103. Expansão entre δ_{H} 4.5-2.0 e δ_{C} 168-16. 2 D de ^1H - ^{13}C -COSY- $^n\text{J}_{\text{CH}}$ ($n=2$ e $n=3$, HMBC, em MeOD) da mistura de **SGMAc-1**.



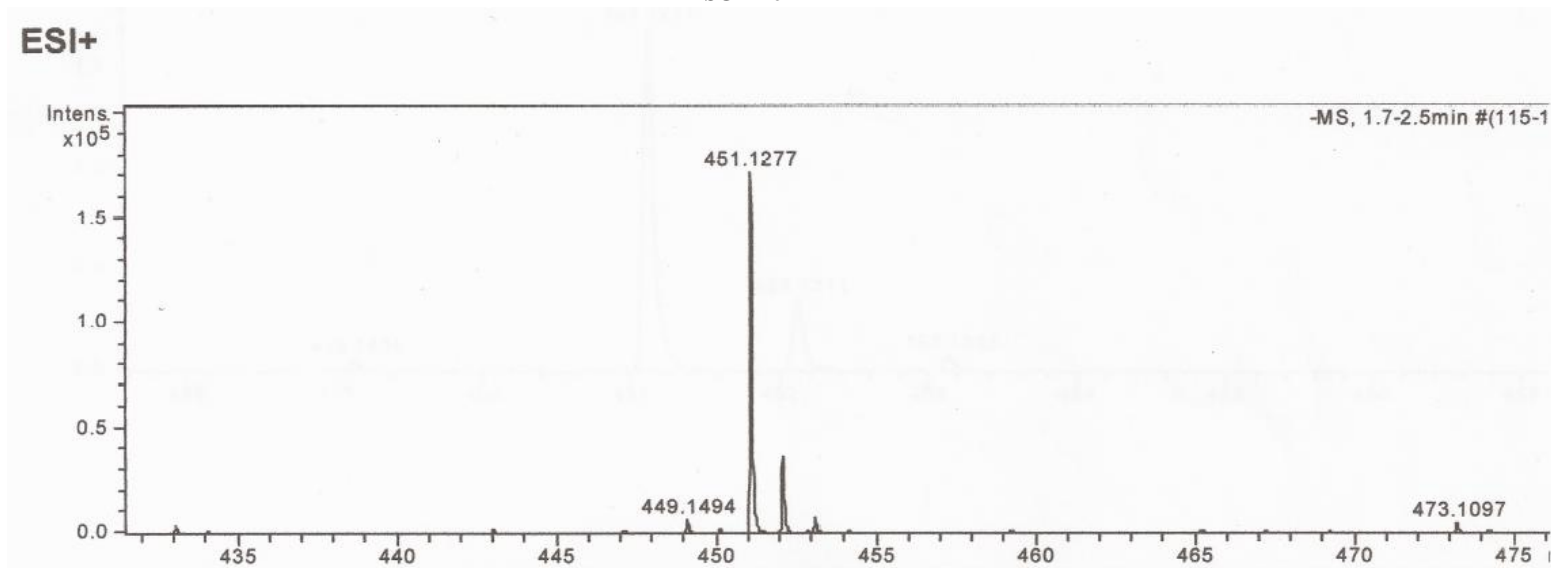
Espectro 104. Cromatograma por CG da substância SGMac-1A.



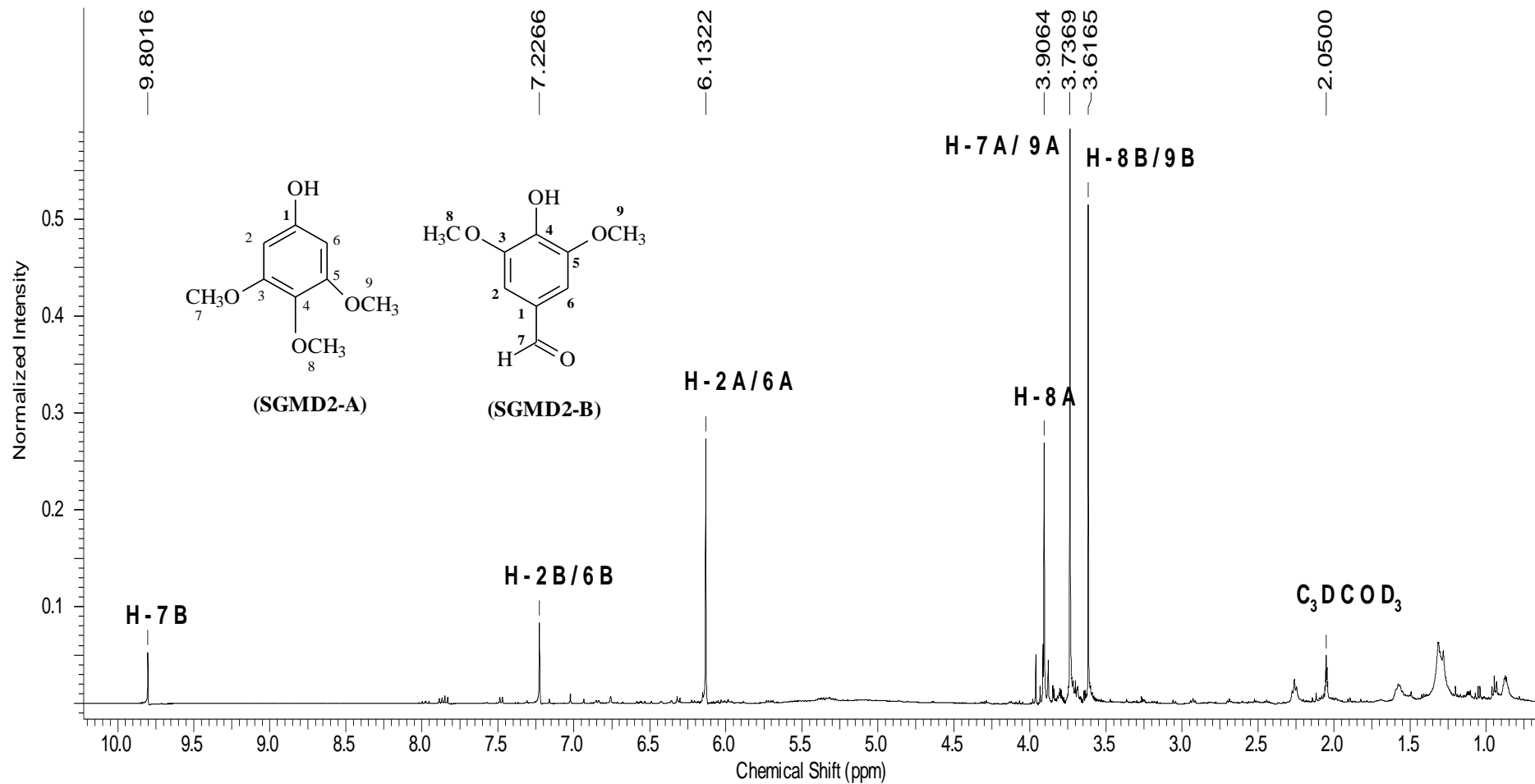
Espectro 105. Massas (70 eV) da substância SGMac-1A.



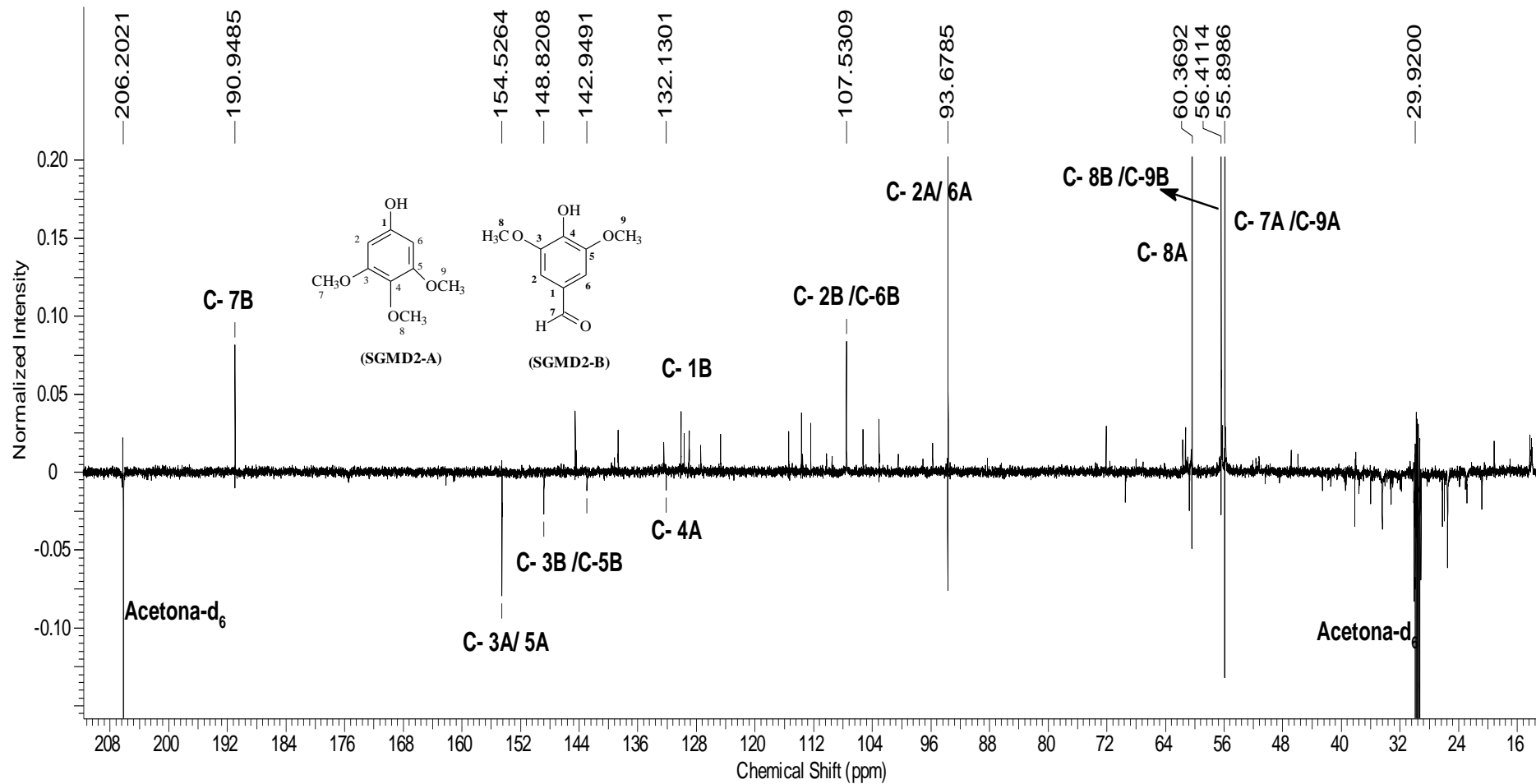
SGMAc-1 B



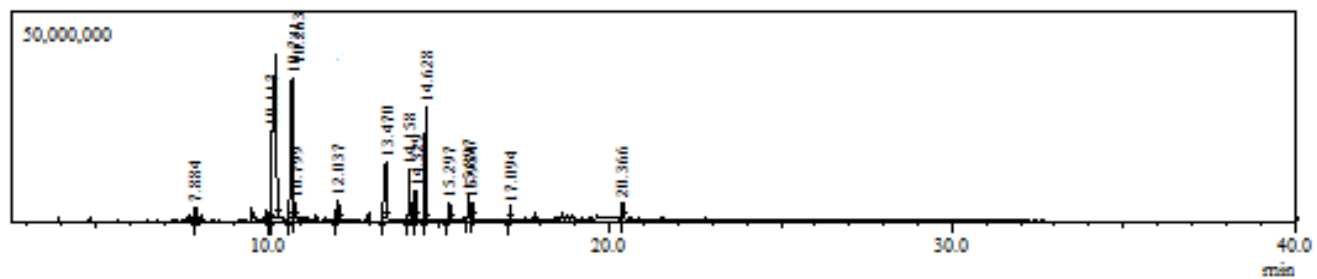
Espetro 106. ESI-MS $[M+H]^+$ da substância SGMAc-1B.



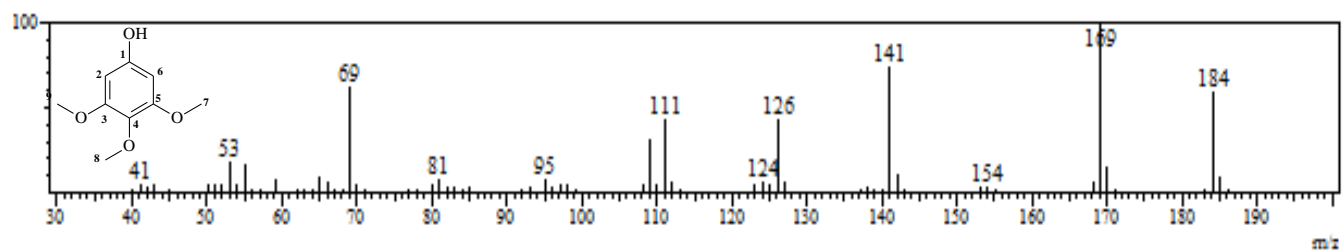
Espectro 107. RMN-¹H (500 MHz, C₃DCOCD₃) da mistura da **SGMD-6**.



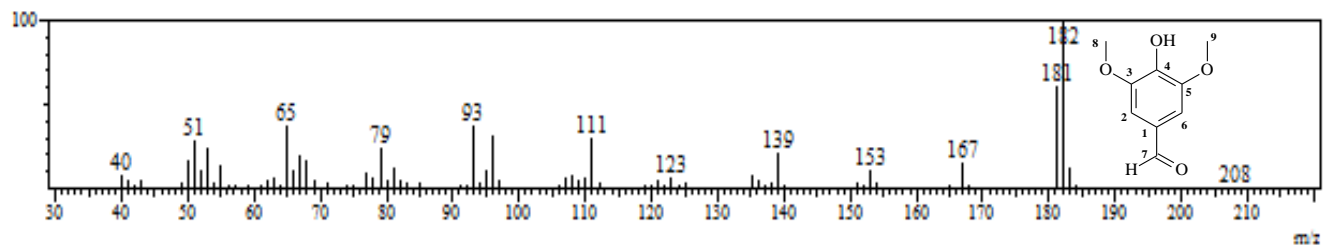
Espectro 108. RMN-¹³C-DEPTQ (125 MHz, em C₃DCOCD₃) da mistura de **SGMD-6**.



Espectro 109. Cromatograma por CG da mistura de **SGMD-6**.



Espectro 110. Massas por I.E. (70 eV) de **SGMD-6A**.



Espectro 111. Massas por I.E. (70 eV) da substância **SGMD6-B**.