

ANEXO

Autoensamblaje de nuevos ciclofanos catiónicos

Self-assembly of new cationic cyclophanes

Ángel Fernández Blanco

INDICE

DAL1	1
DI1	8
1CM1-4Br: 1,5-DIHIDROXINAFTALENO	11
2CM1-4Br: 2,7-DIHIDROXINAFTALENO	14
3CM1-4Br: CARBAZOL	17
4CM1-4Br: ANTRACENO	20
5CM1-4Br: FENANTRENO	23
6CM1-4Br: PIRENO	26
1CM2-4Br: 1,5-DIHIDROXINAFTALENO	29
2CM2-4Br: 2,7-DIHIDROXINAFTALENO	32
3CM2-4Br: CARBAZOL	35
4CM2-4Br: ANTRACENO	38
5CM2-4Br: FENANTRENO	41
6CM2-4Br: PIRENO	44
1CM1-4PF ₆	47
1CM1-4NO ₃	48
1CM1-4Cl	49
1CM1-4Cl (sólido gris obtenido en la columna flash)	49
1CM1-4PF ₆ (Purificado por columna flash)	50
1,5-DIHIDROXINAFTALENO	50
2,7-DIHIDROXINAFTALENO	51

DAL1

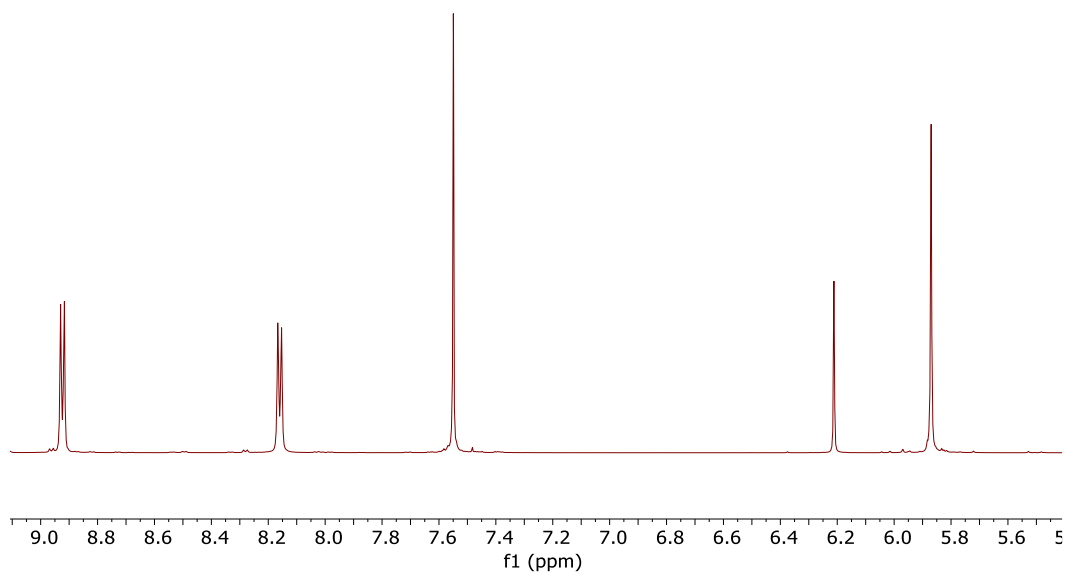


Figura 1. Espectro parcial de RMN- ^1H (D_2O , 500 MHz, 25°C) de DAL1

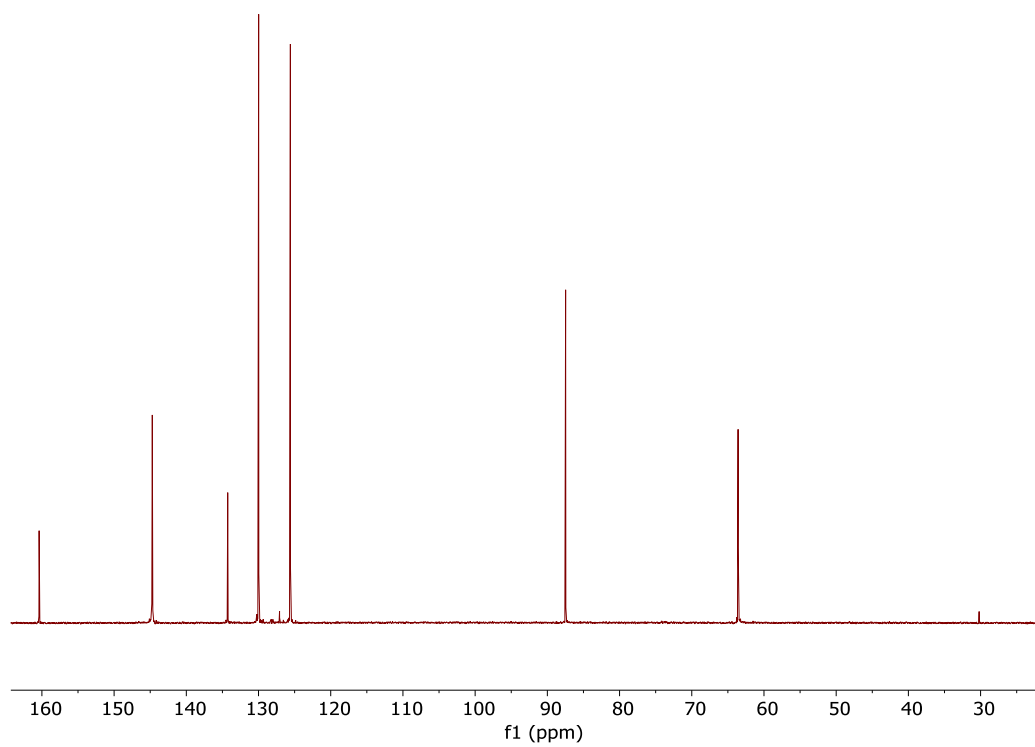


Figura 2. Espectro parcial de RMN- ^{13}C (D_2O , 125 MHz, 25°C) de DAL1

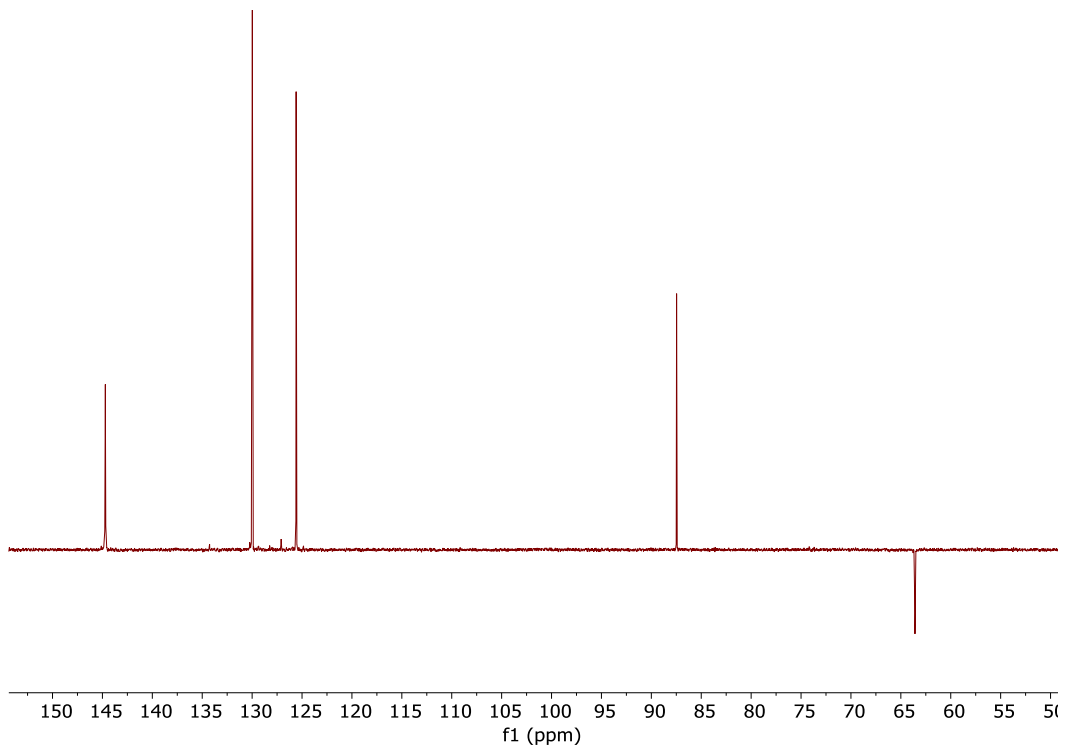


Figura 3. Espectro DEPT (D_2O , 125 MHz, 25°C) de DAL1

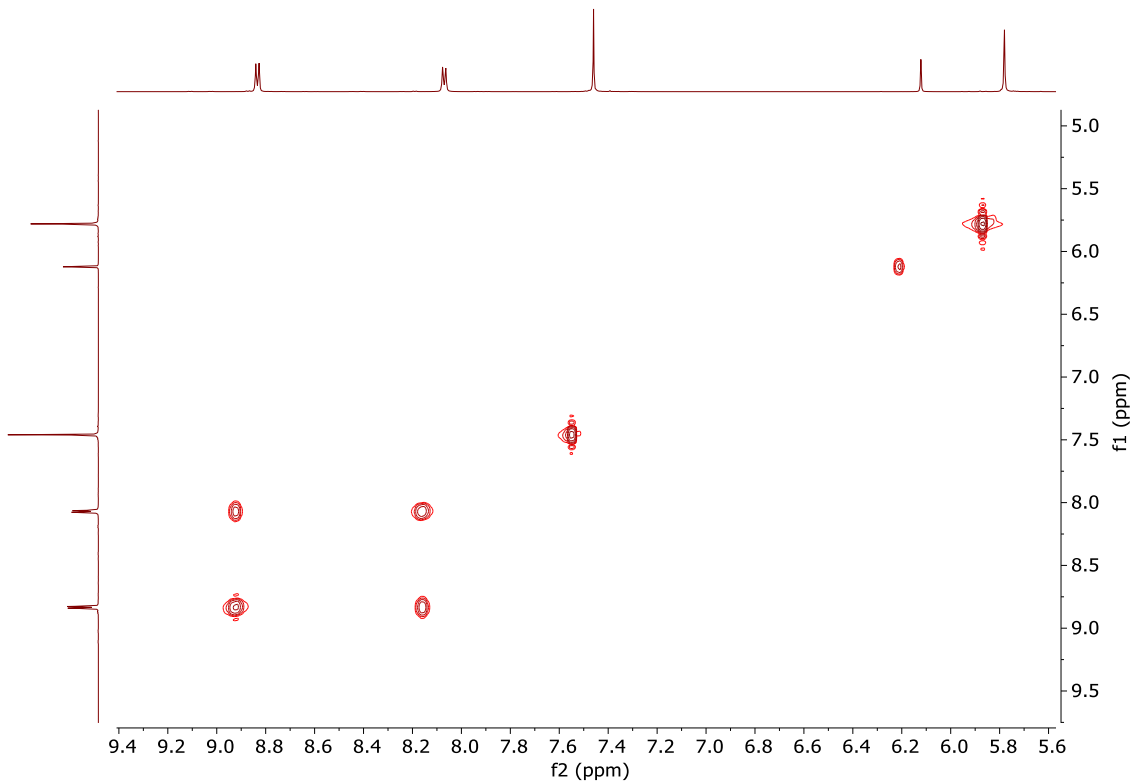


Figura 4. Espectro parcial COSY (D_2O , 500 MHz, 25°C) del DAL1

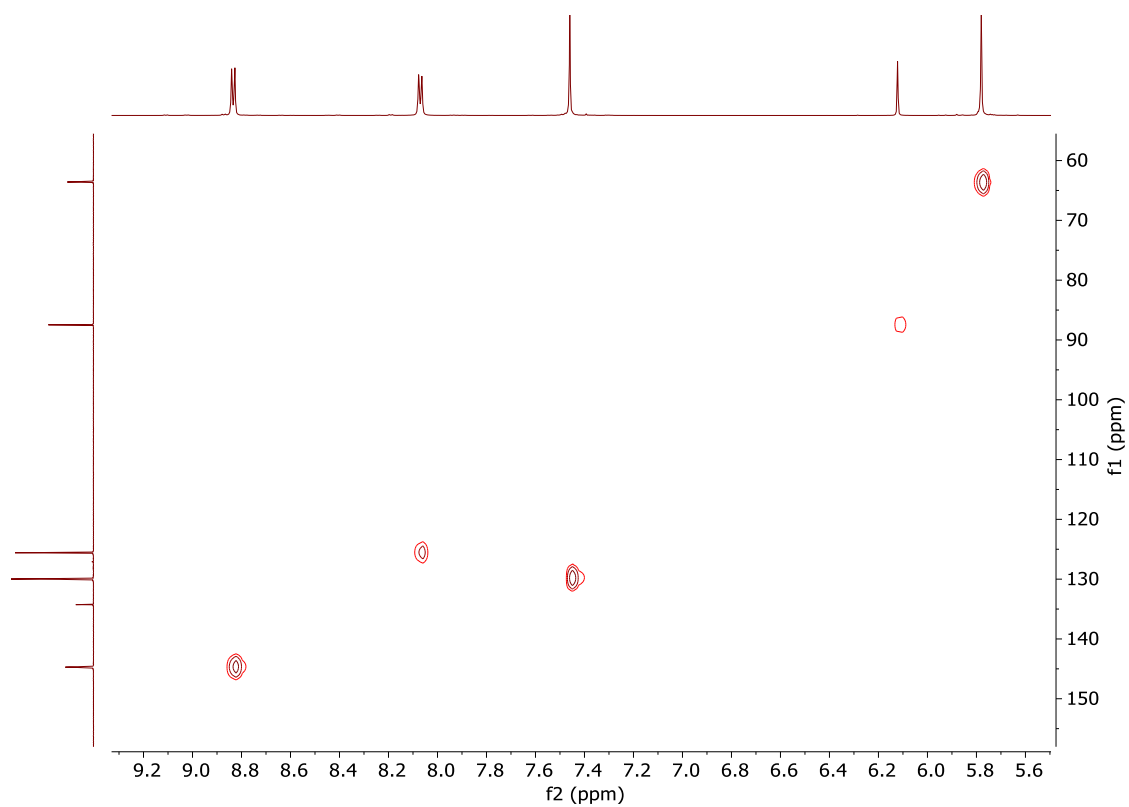


Figura 5. Espectro HSQC (D_2O , 500 MHz, 25°C) del DAL1

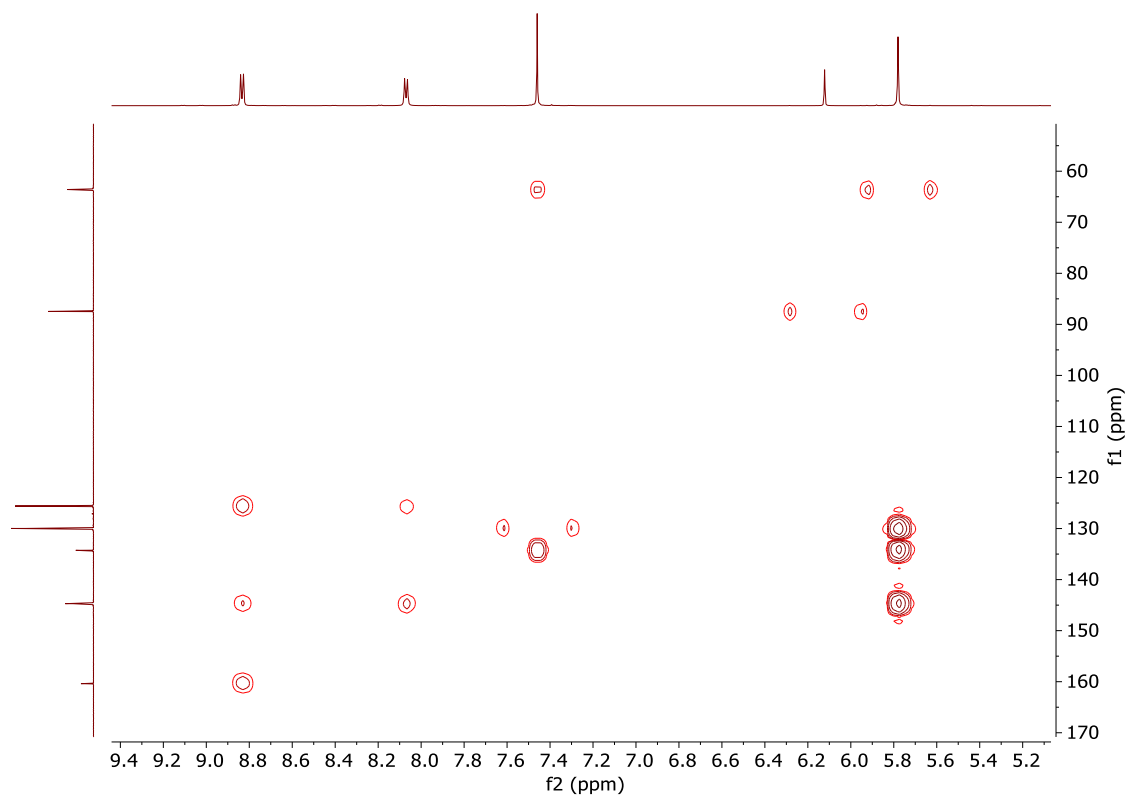
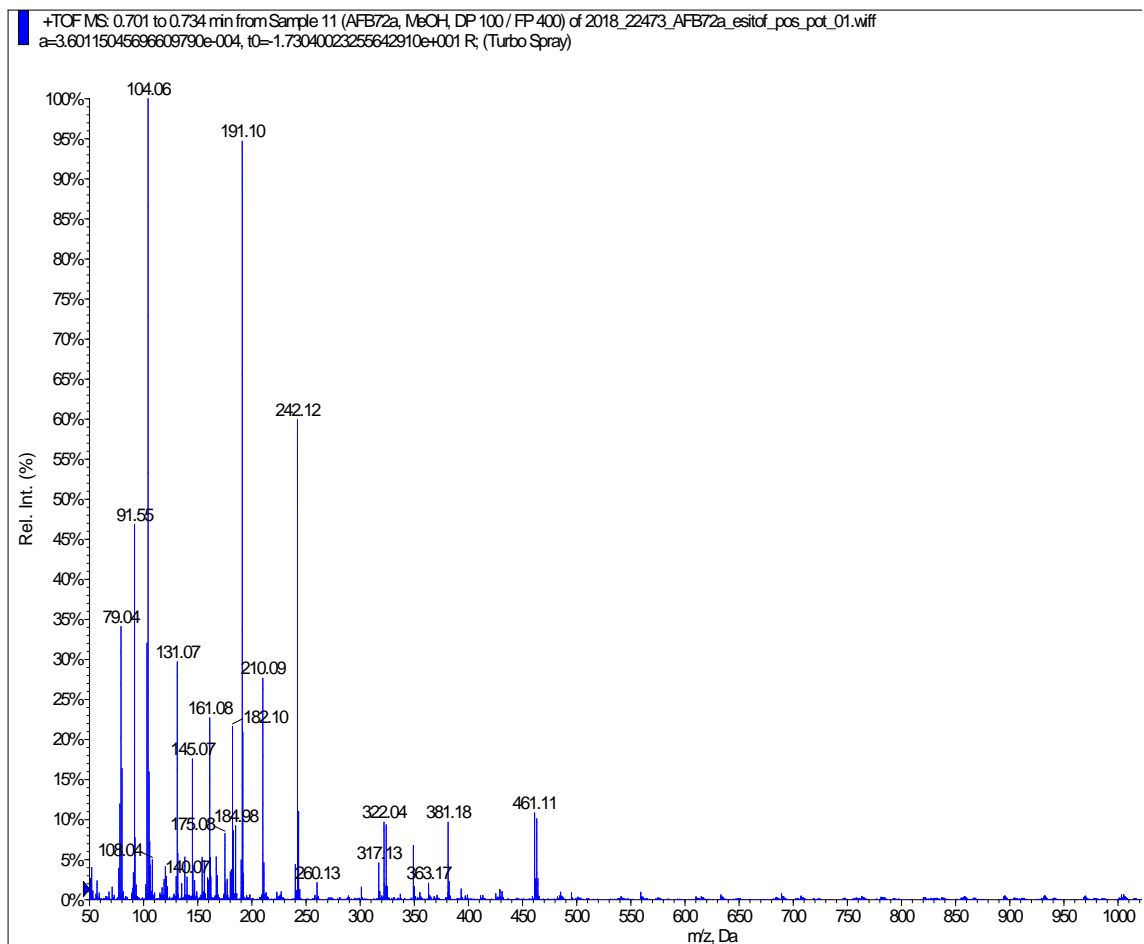


Figura 6. Espectro parcial de HMBC (D_2O , 500 MHz, 25°C) del DAL1



DAL2

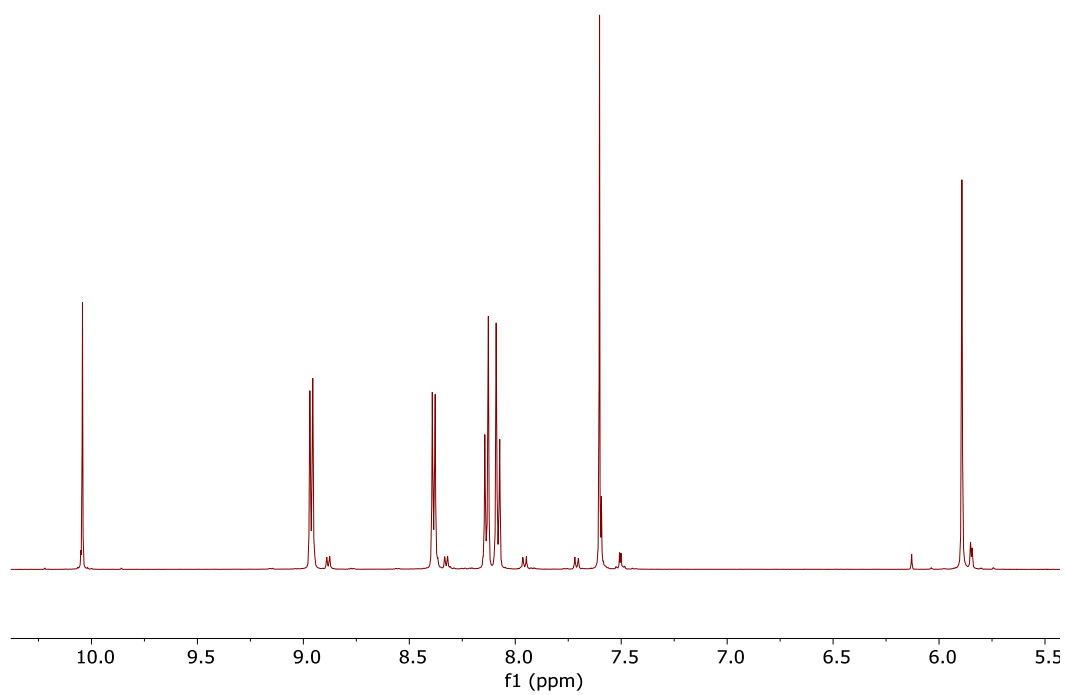


Figura 7. Espectro parcial de RMN-¹H (D₂O, 500 MHz, 25°C) de DAL2

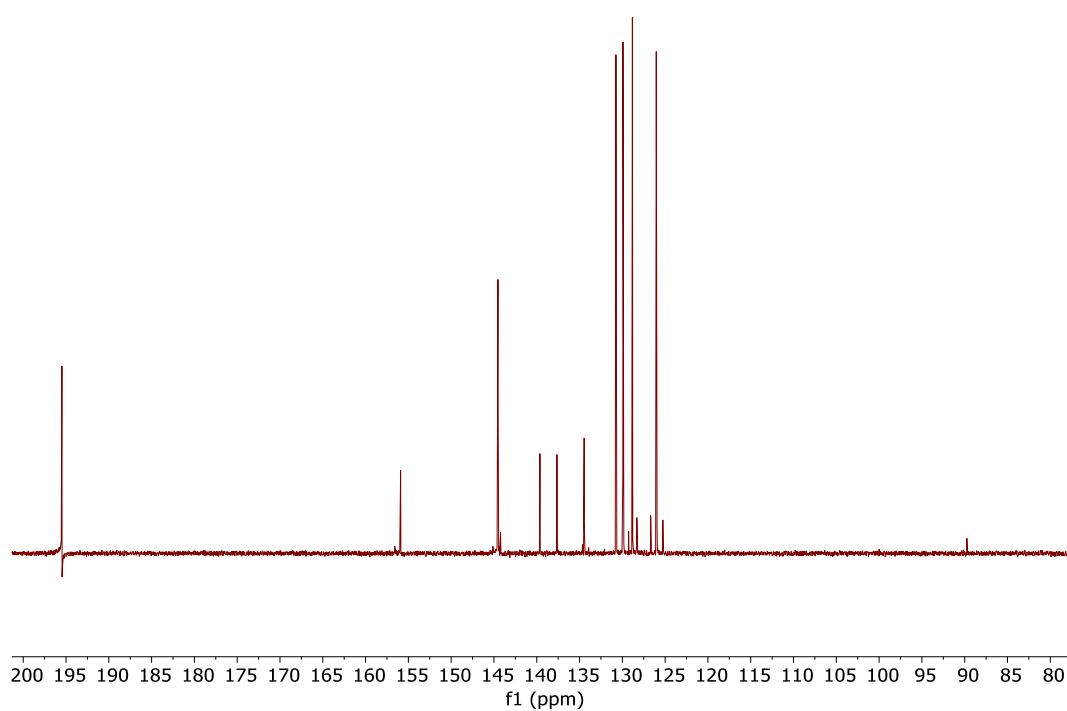


Figura 8. Espectro parcial de RMN- ^{13}C (D_2O , 125 MHz, 25°C) de DAL2

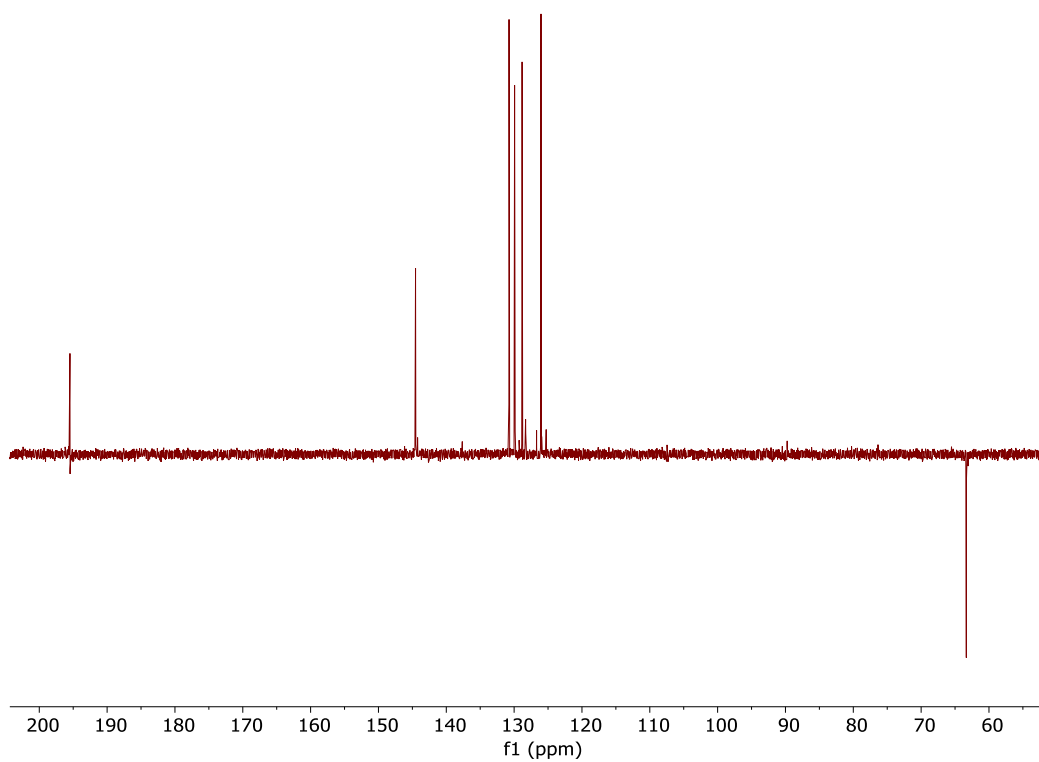


Figura 9. Espectro DEPT (D_2O , 125 MHz, 25°C) de DAL2

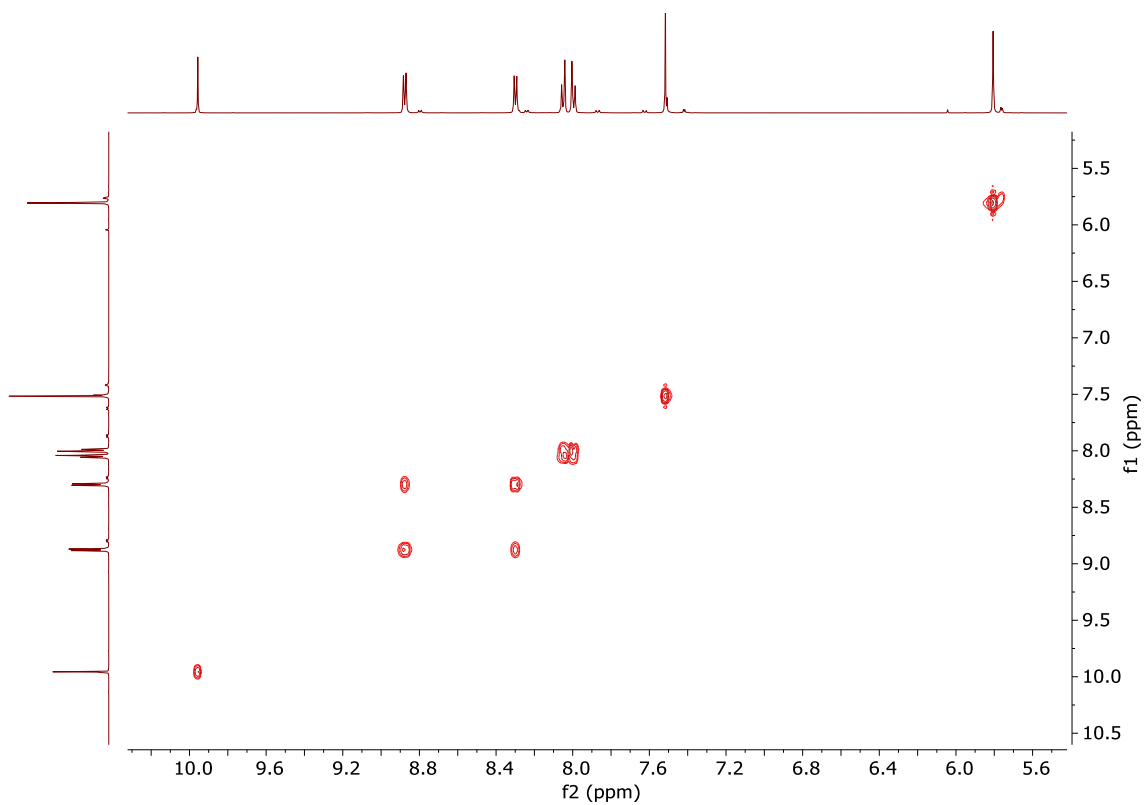


Figura 10. Espectro parcial COSY (D₂O, 500 MHz, 25°C) del DAL2

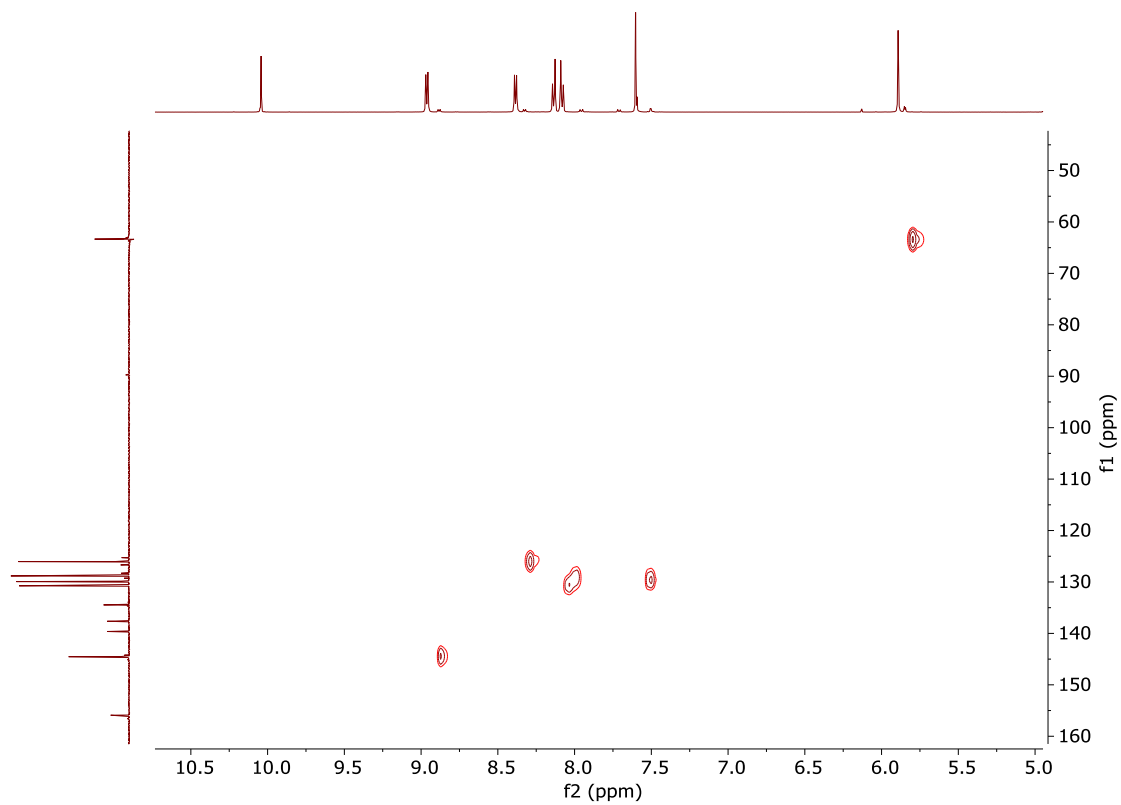


Figura 11. Espectro HSQC (D₂O, 500 MHz, 25°C) del DAL2

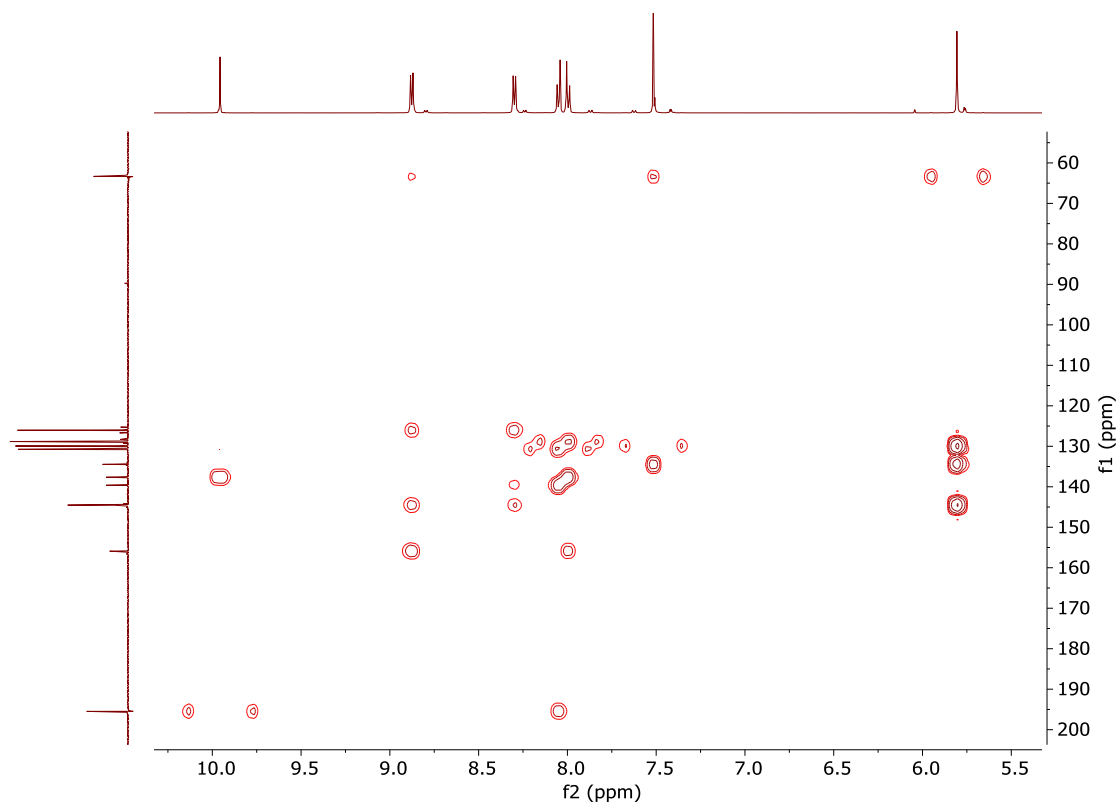
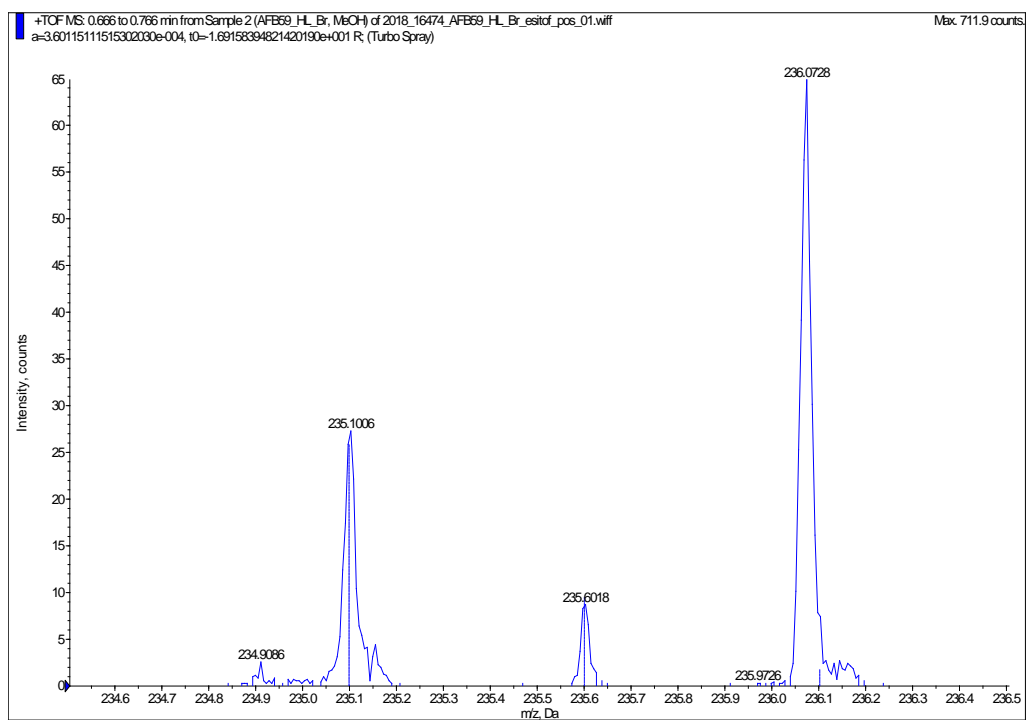


Figura 12. Espectro parcial de HMBC (D_2O , 500 MHz, 25°C) del DAL2



m/z experimental	235.1006	Notas:		
Fórmula	m/z teórico	Erro, mDa	Erro en ppm	Equivalencia de dobles enlaces
C32 H26 N2 O2	235.0991	2.8688	6.1012	21

DI1

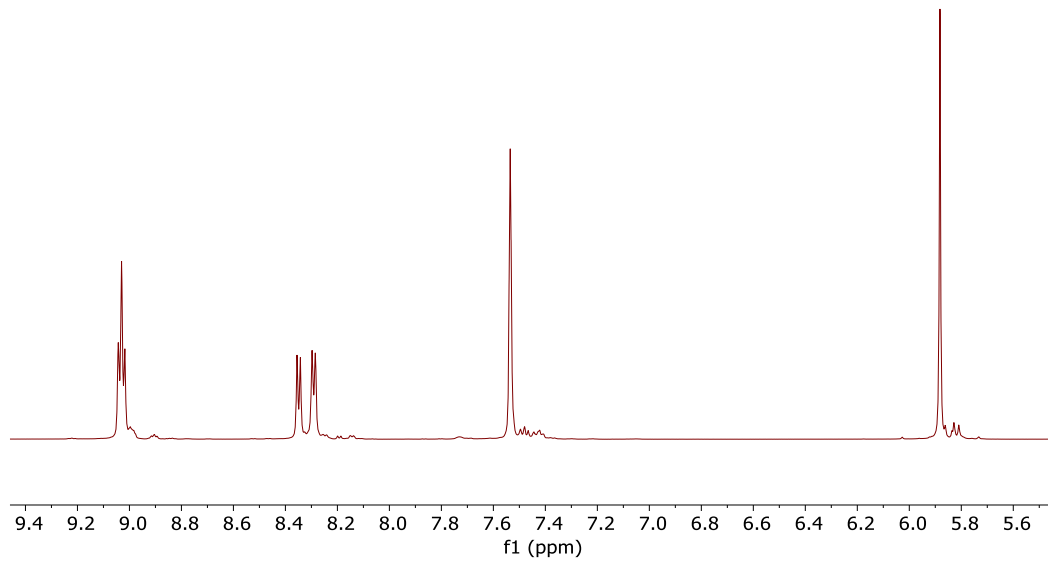


Figura 13. Espectro parcial de RMN- ^1H (D_2O , 500 MHz, 25°C) de DI1

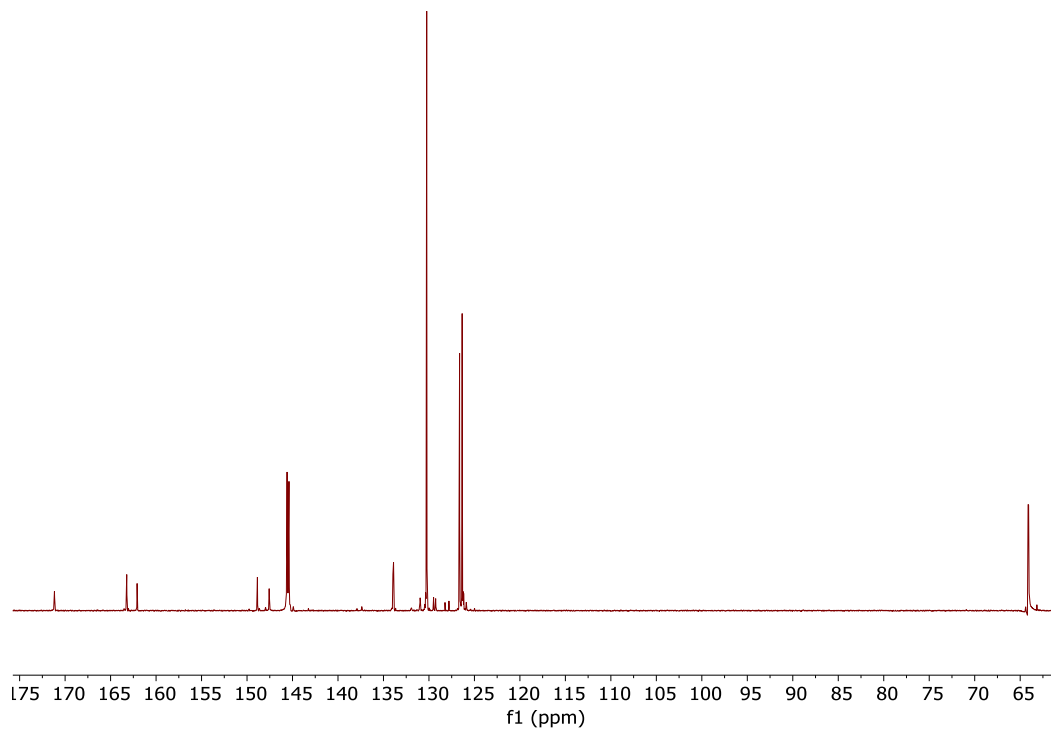


Figura 14. Espectro parcial de RMN- ^{13}C (D_2O , 125 MHz, 25°C) de DI1

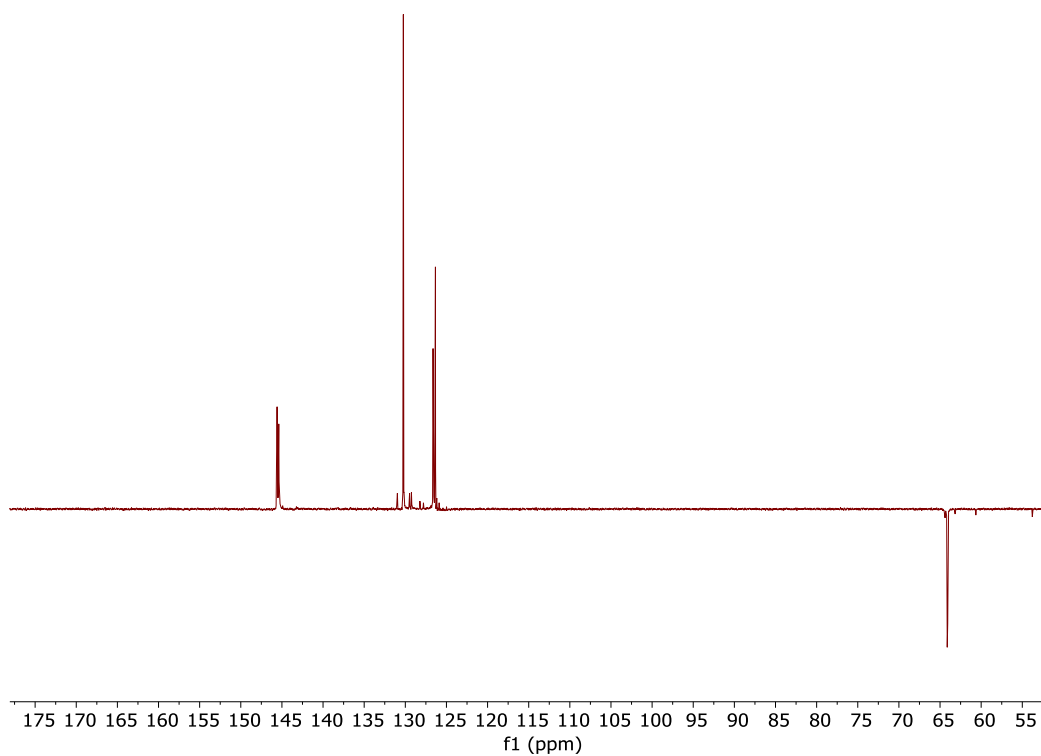


Figura 15. Espectro DEPT (D_2O , 125 MHz, 25°C) de DI1

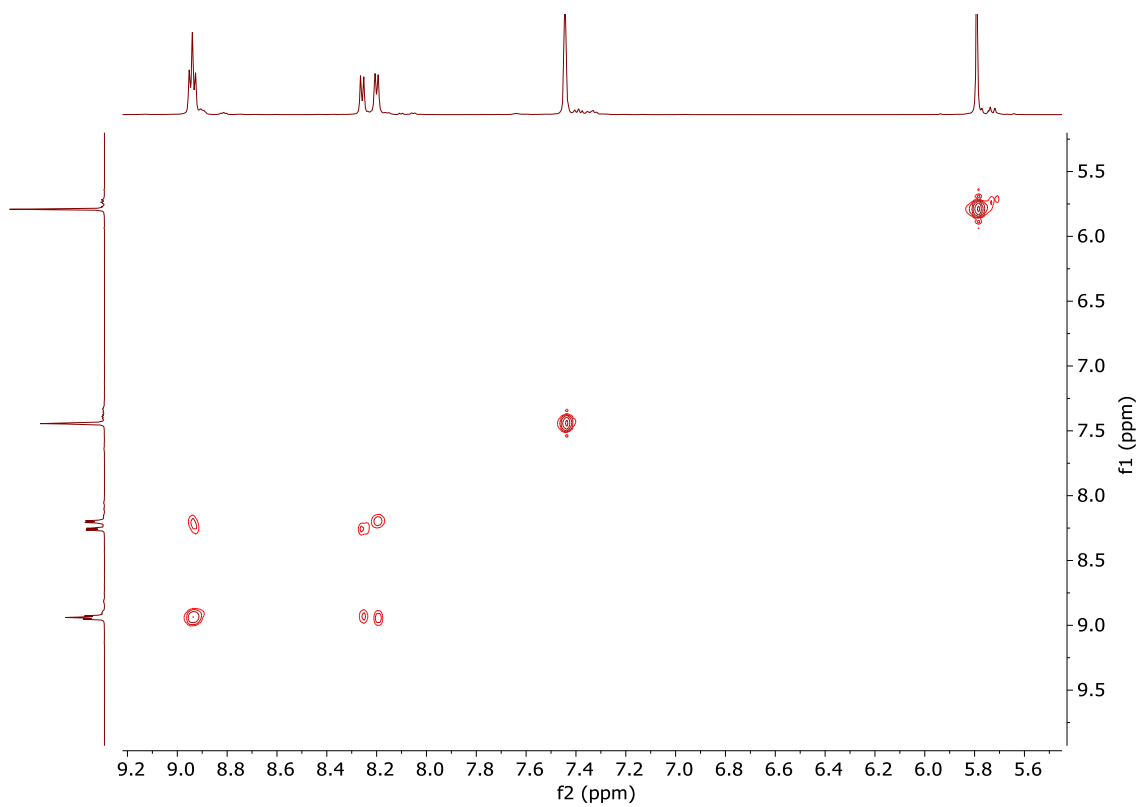


Figura 16. Espectro parcial COSY (D_2O , 500 MHz, 25°C) del DI1

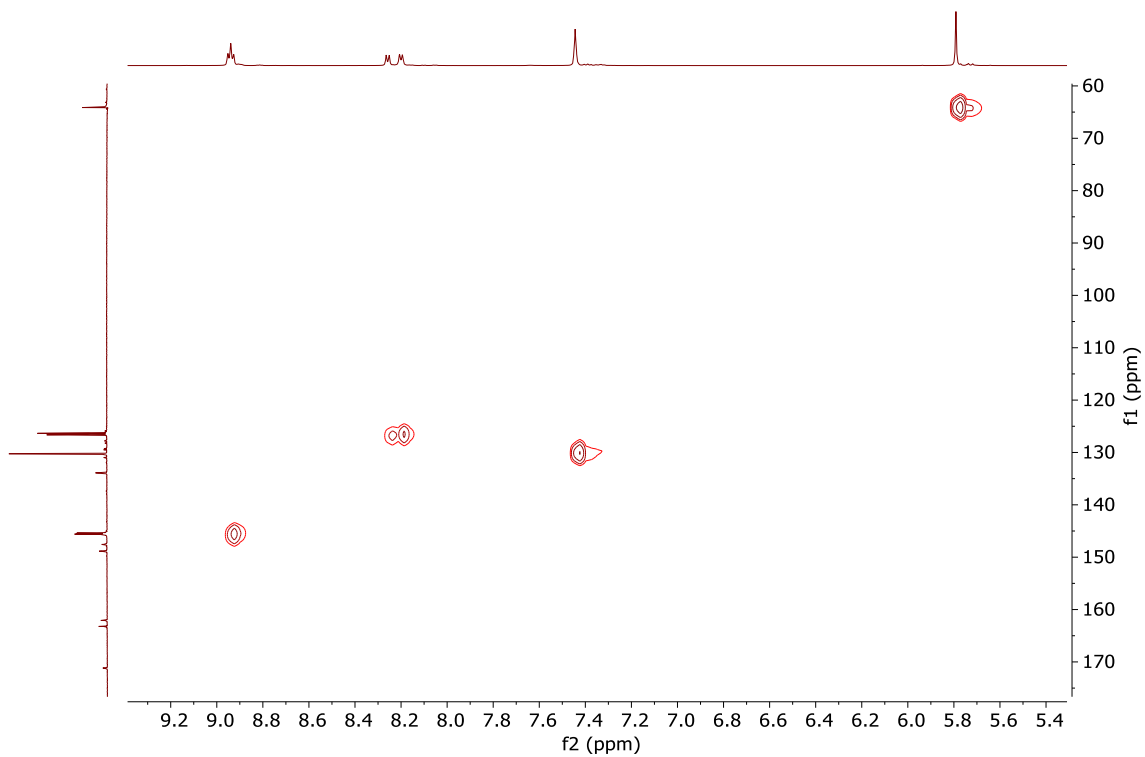


Figura 17. Espectro HSQC (D_2O , 500 MHz, 25°C) del DI1

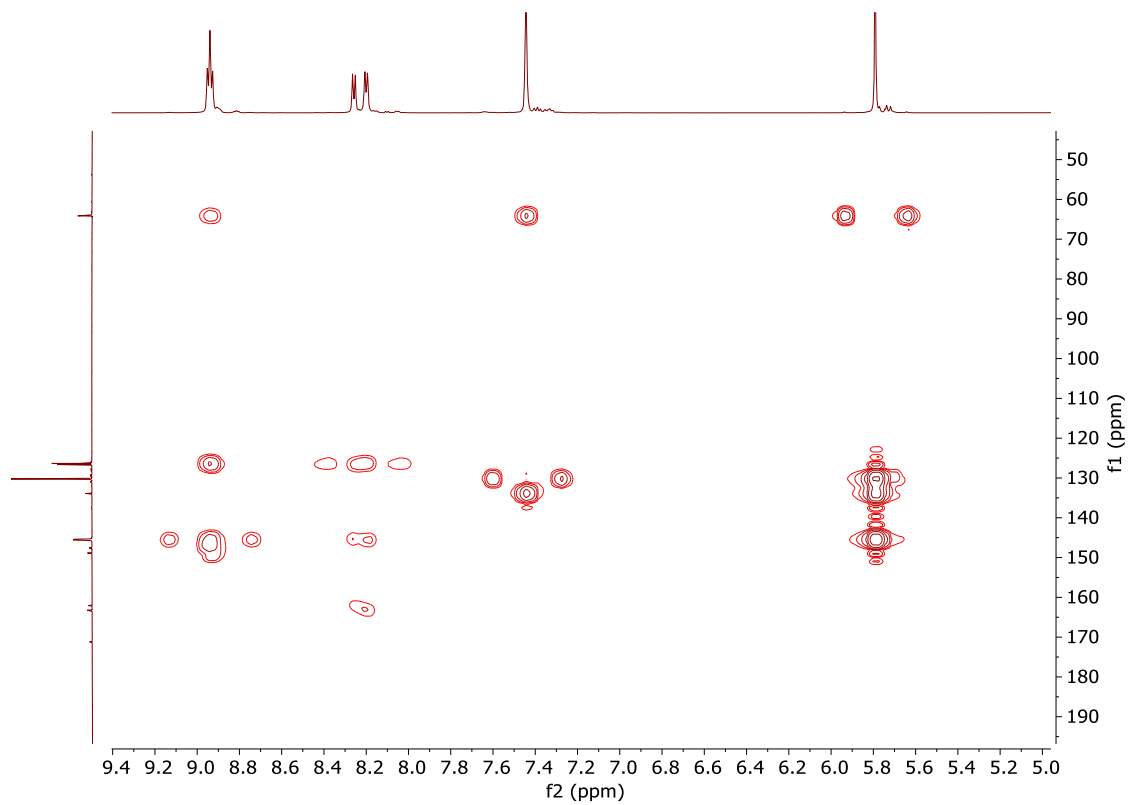
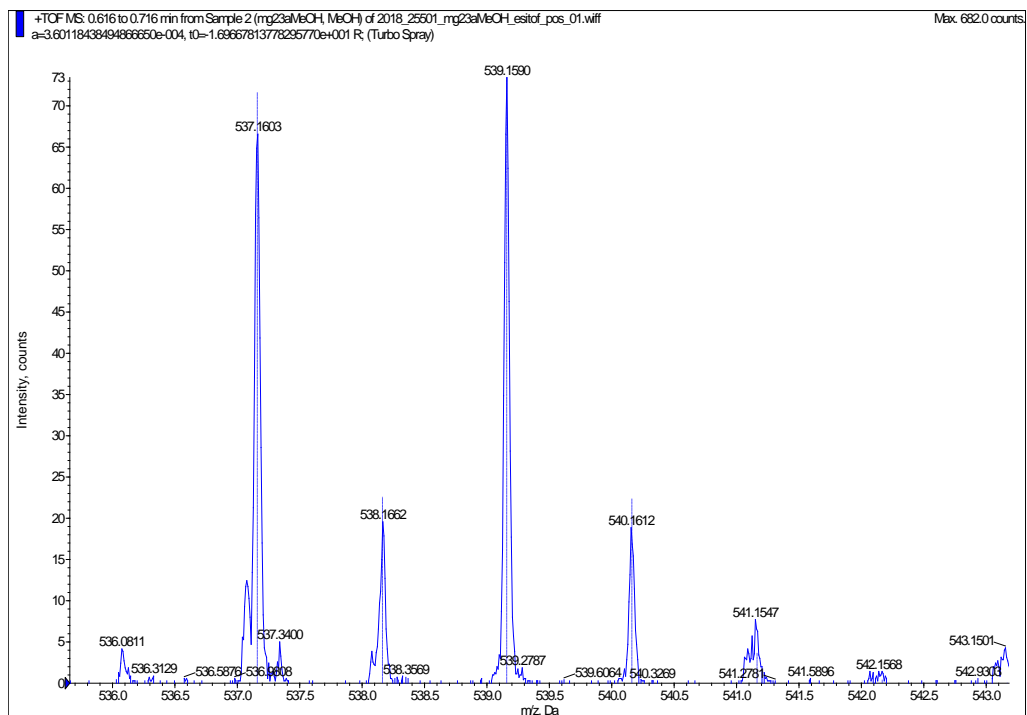


Figura 18. Espectro parcial de HMBC (D_2O , 500 MHz, 25°C) del DI1



m/z experimental	537.1603	Notas:		
Fórmula	m/z teórico	Erro, mDa	Erro en ppm	Equivalencia de dobles enlaces
C ₂₆ H ₃₀ N ₆ O ₂ Br	537.1608	-0.512	-0.9532	14.5

1CM1·4Br: 1,5-DIHIDROXINAFTALENO

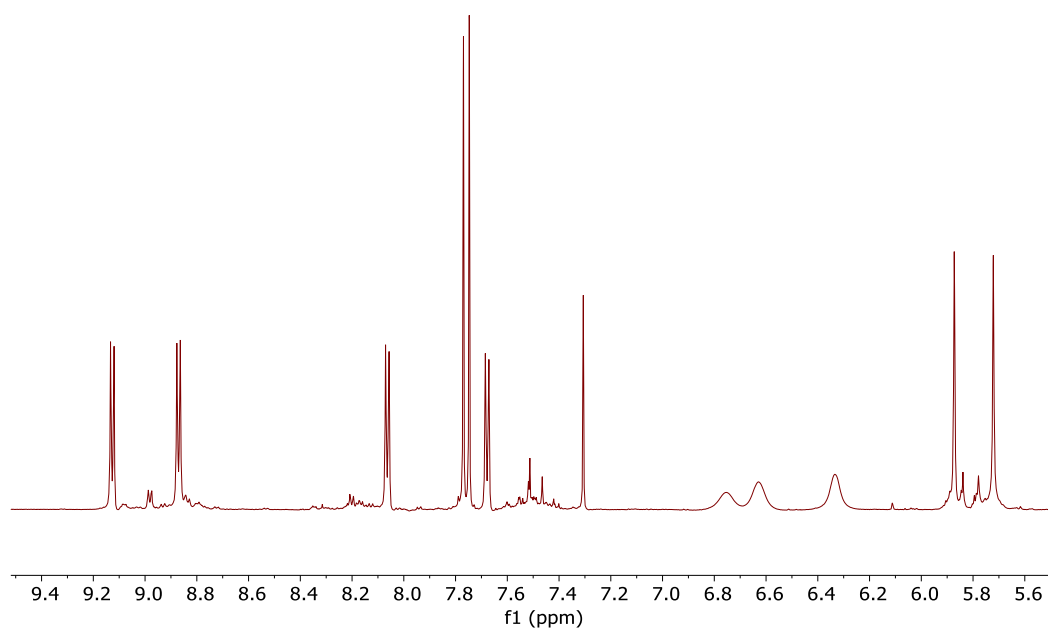


Figura 19. Espectro parcial de RMN-¹H (D₂O, 500 MHz, 25°C) de 1CM1·4Br

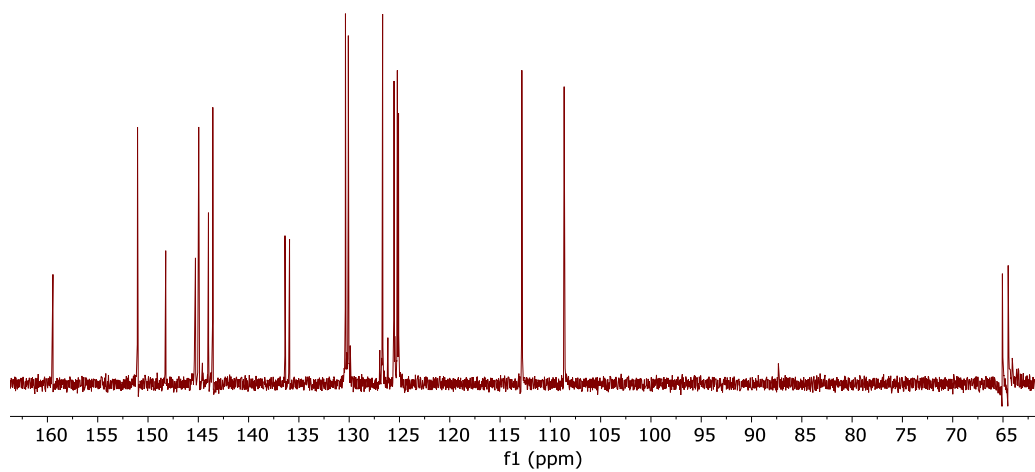


Figura 20. Espectro parcial de RMN^{13}C (D_2O , 125 MHz, 25°C) de 1CM1-4Br

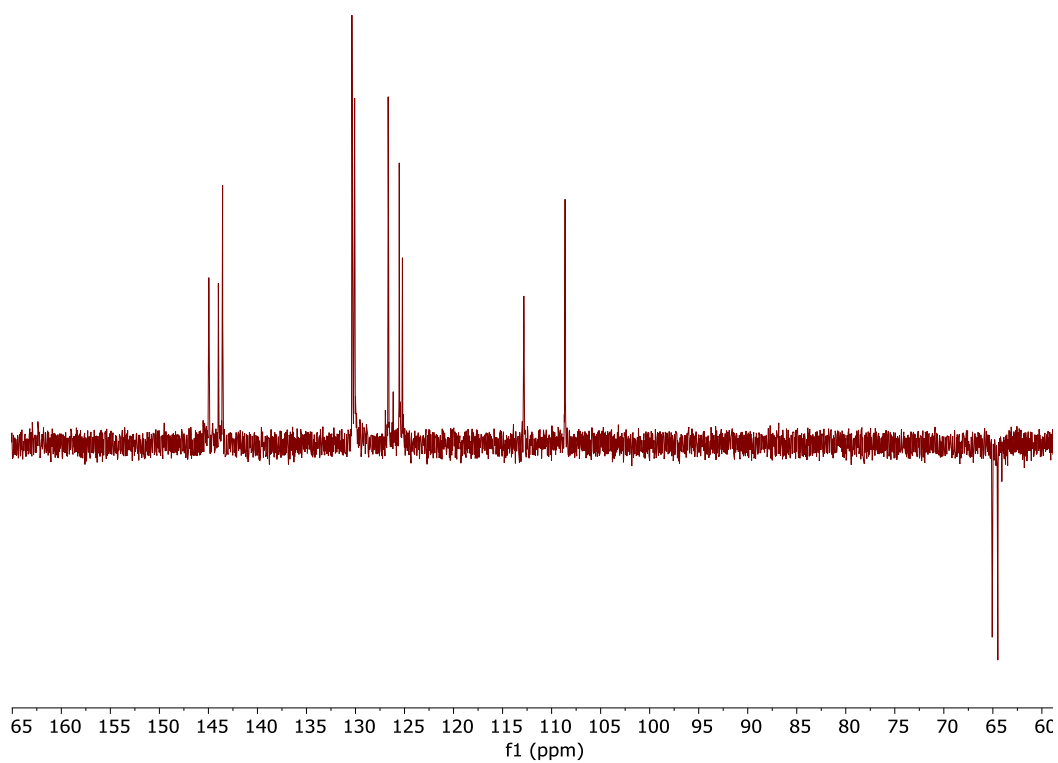


Figura 21. Espectro DEPT (D_2O , 125 MHz, 25°C) 1CM1-4Br

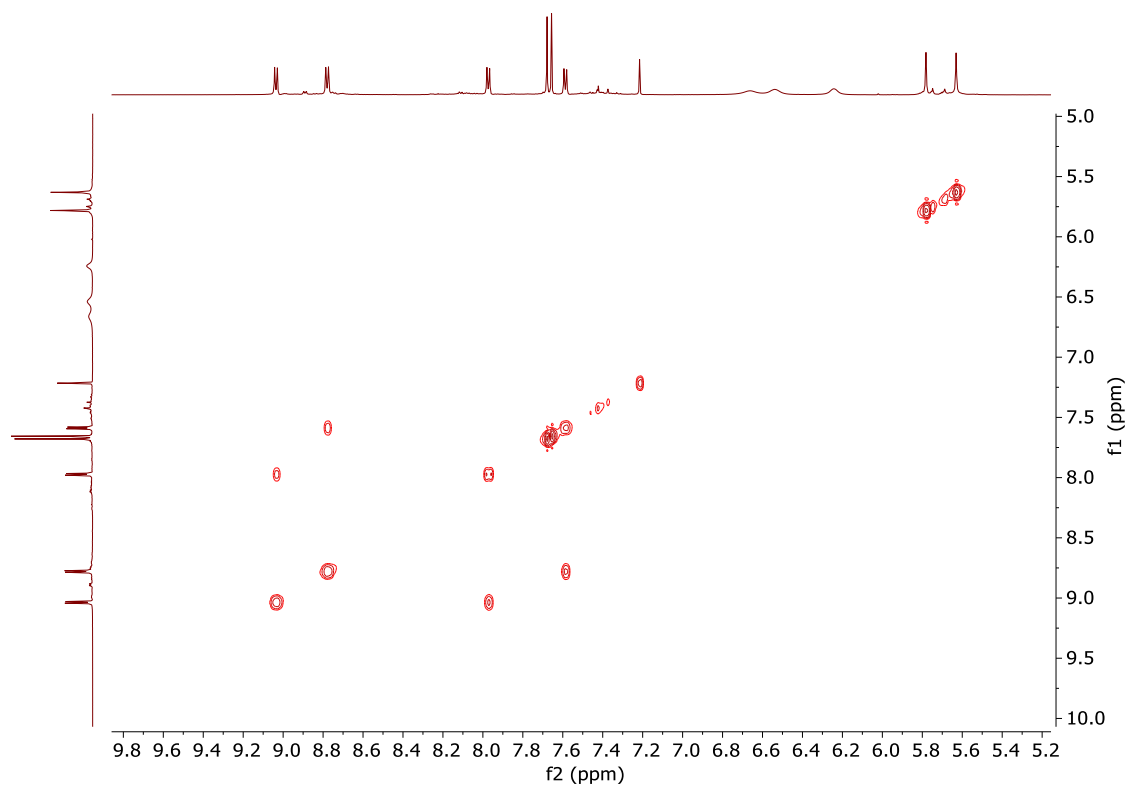


Figura 22. Espectro parcial COSY (D₂O, 500 MHz, 25°C) del 1CM1-4Br

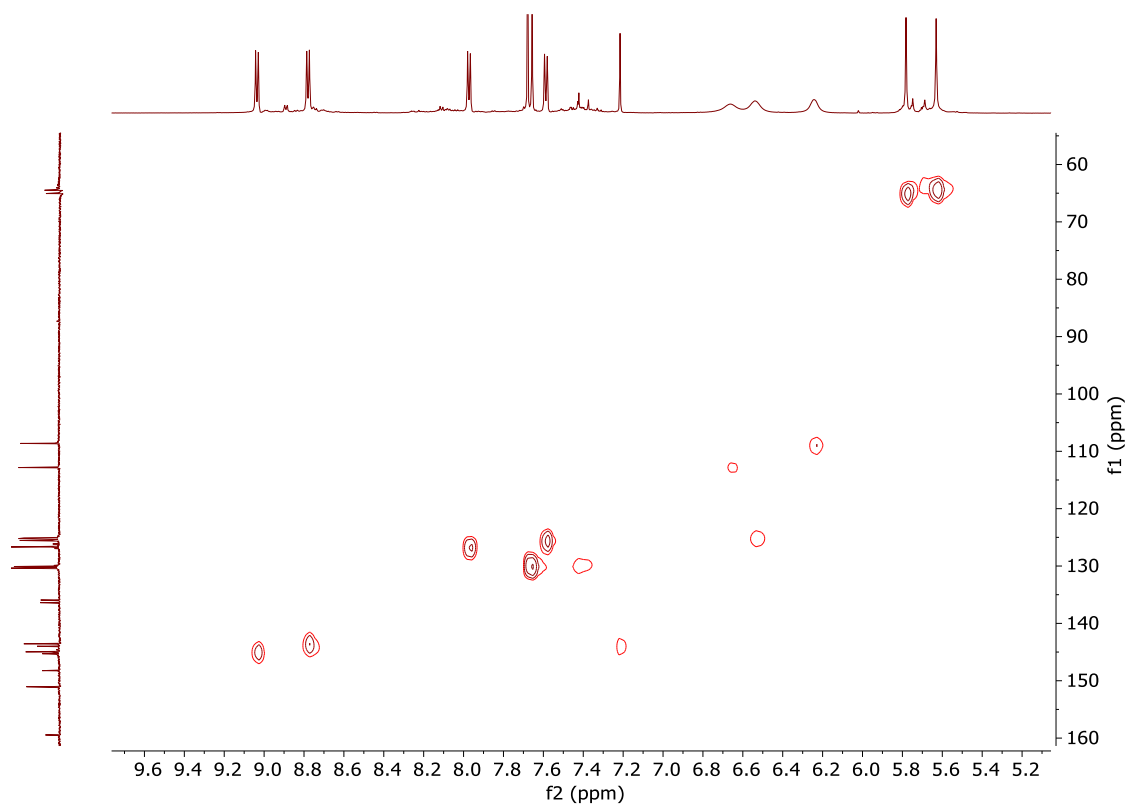


Figura 23. Espectro HSQC (D₂O, 500 MHz, 25°C) del 1CM1-4Br

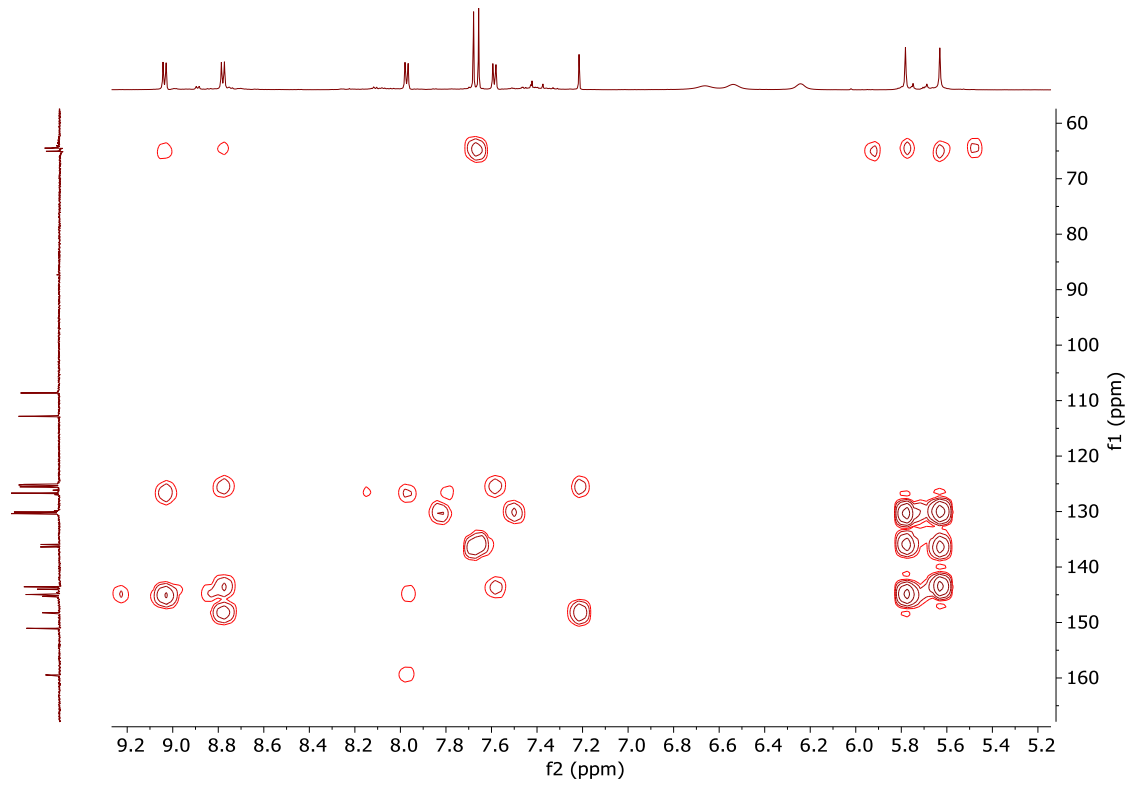


Figura 24. Espectro parcial de HMBC (D₂O, 500 MHz, 25°C) del 1CM1-4Br

2CM1-4Br: 2,7-DIHIDROXINAFTALENO

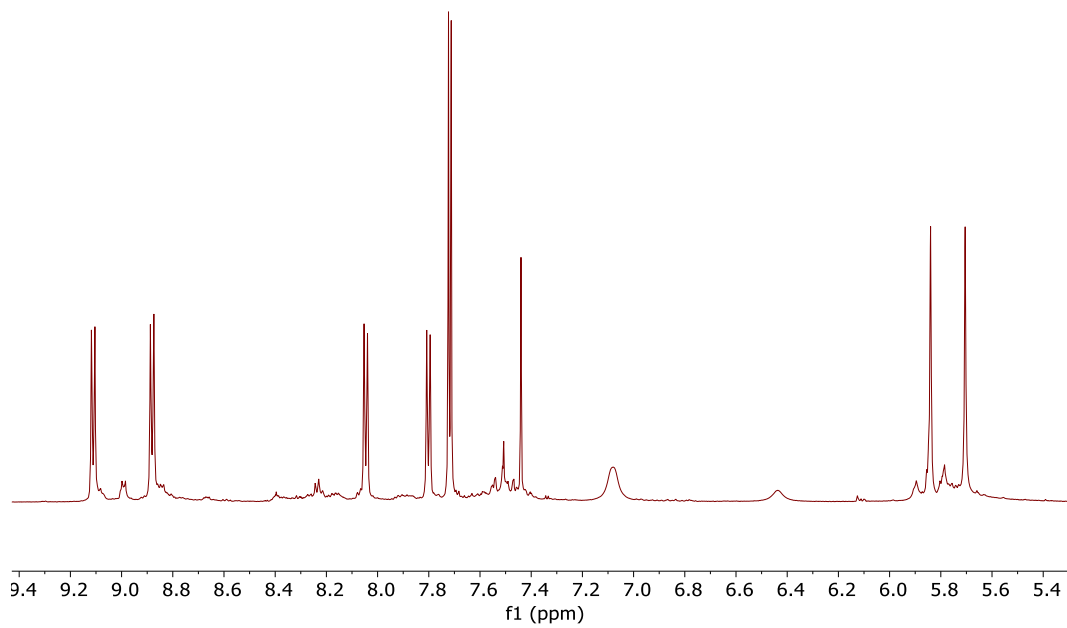


Figura 25. Espectro parcial de RMN-¹H (D₂O, 500 MHz, 25°C) de 2CM1-4Br

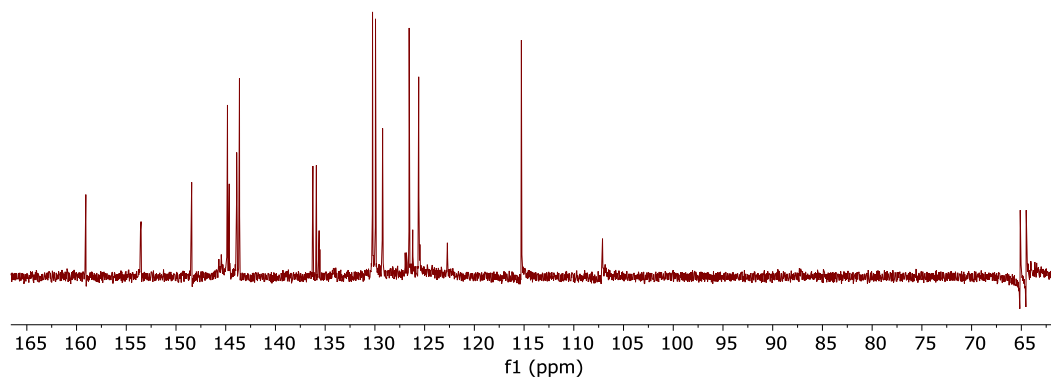


Figura 26. Espectro parcial de RMN- ^{13}C (D_2O , 125 MHz, 25°C) de 2CM1-4Br

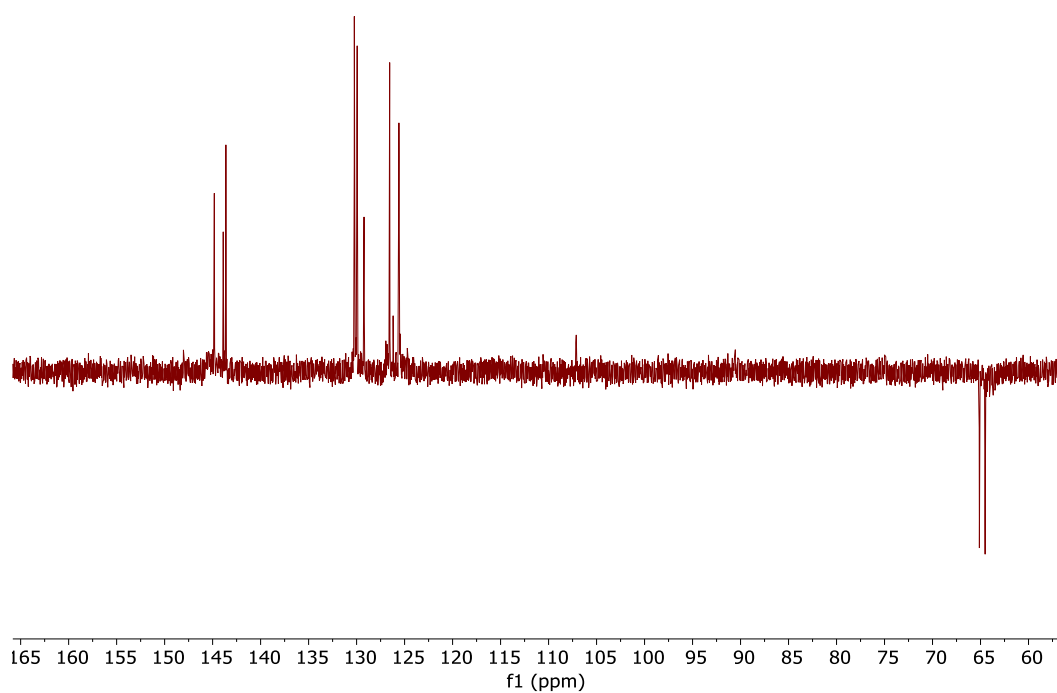


Figura 27. Espectro DEPT (D_2O , 125 MHz, 25°C) 2CM1-4Br

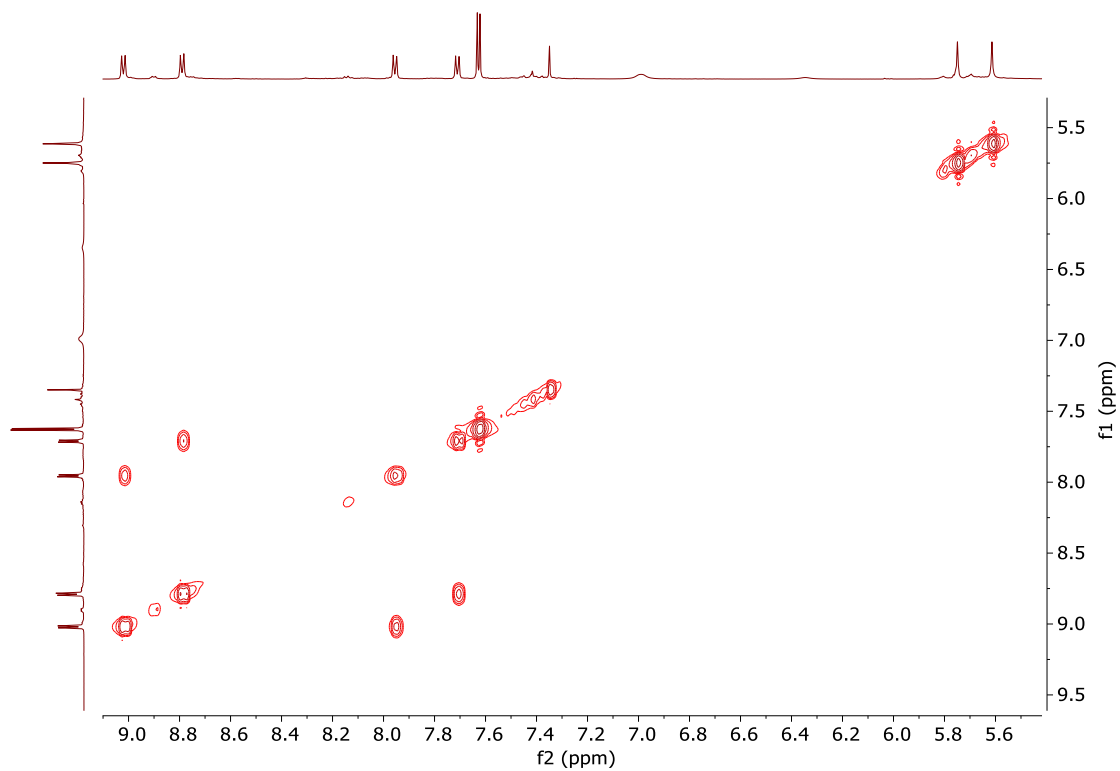


Figura 28. Espectro parcial COSY (D_2O , 500 MHz, 25°C) del 2CM1-4Br

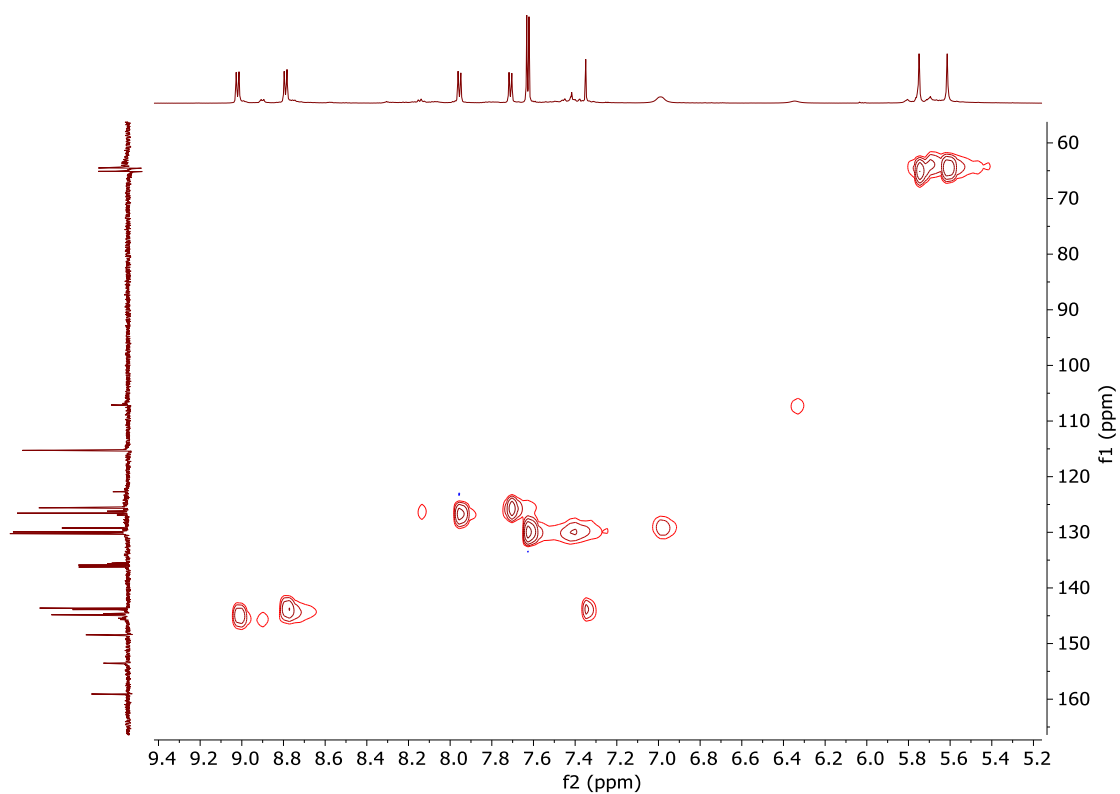


Figura 29. Espectro HSQC (D_2O , 500 MHz, 25°C) del 2CM1-4Br

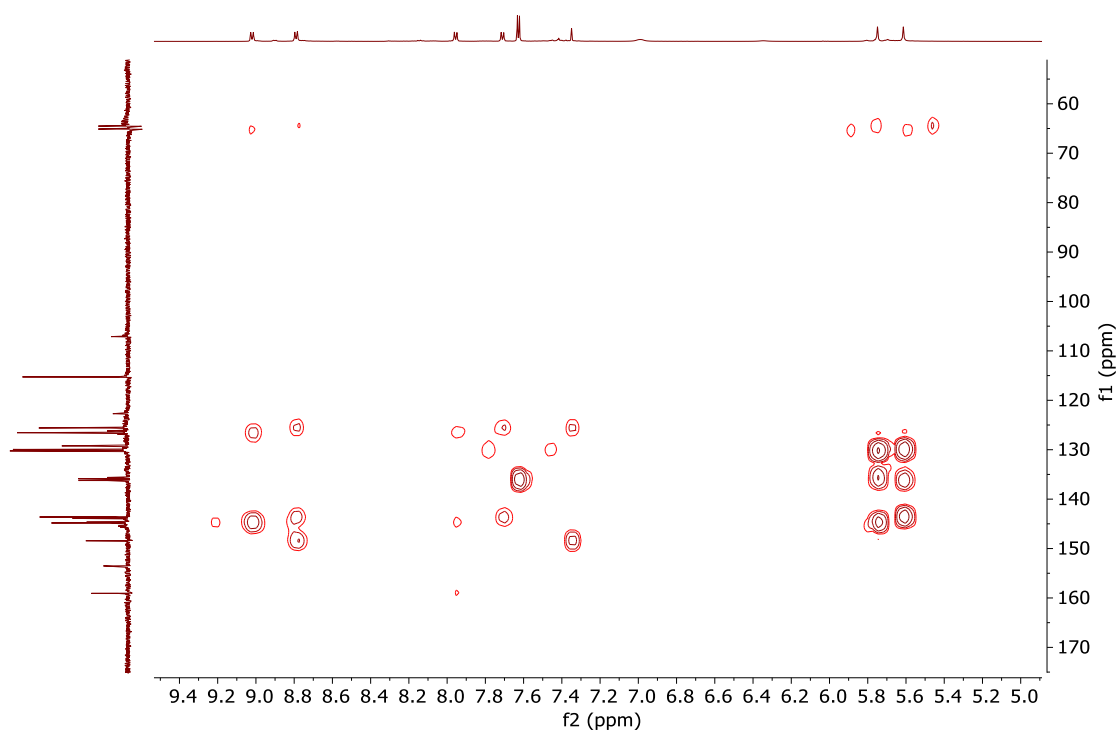


Figura 30. Espectro parcial de HMBC (D_2O , 500 MHz, 25°C) del 2CM1-4Br

3CM1-4Br: CARBAZOL

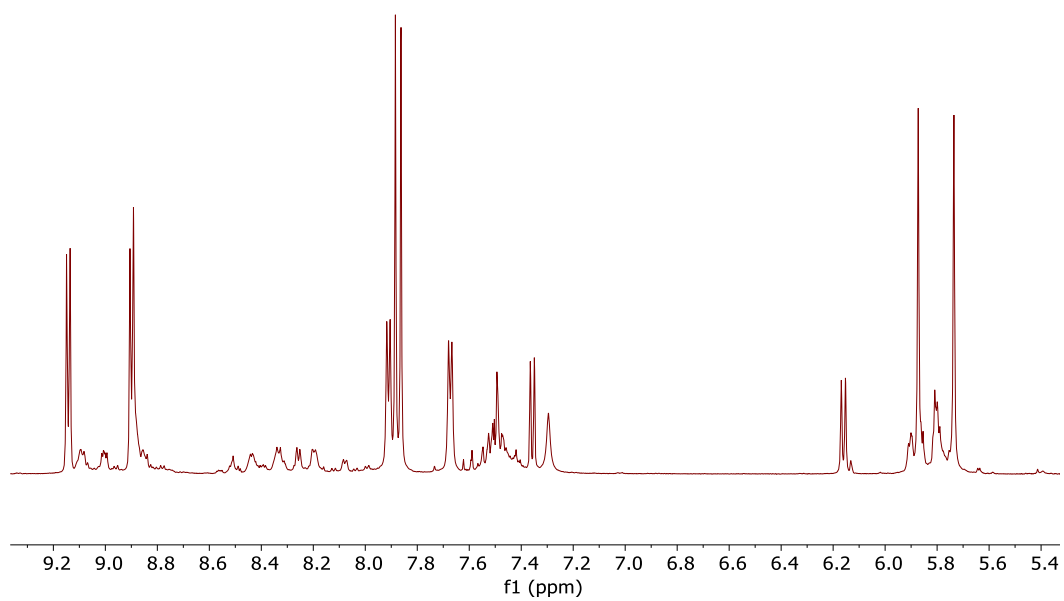


Figura 31 .Espectro parcial de RMN- 1H (D_2O , 500 MHz, 25°C) de 3CM1-4Br

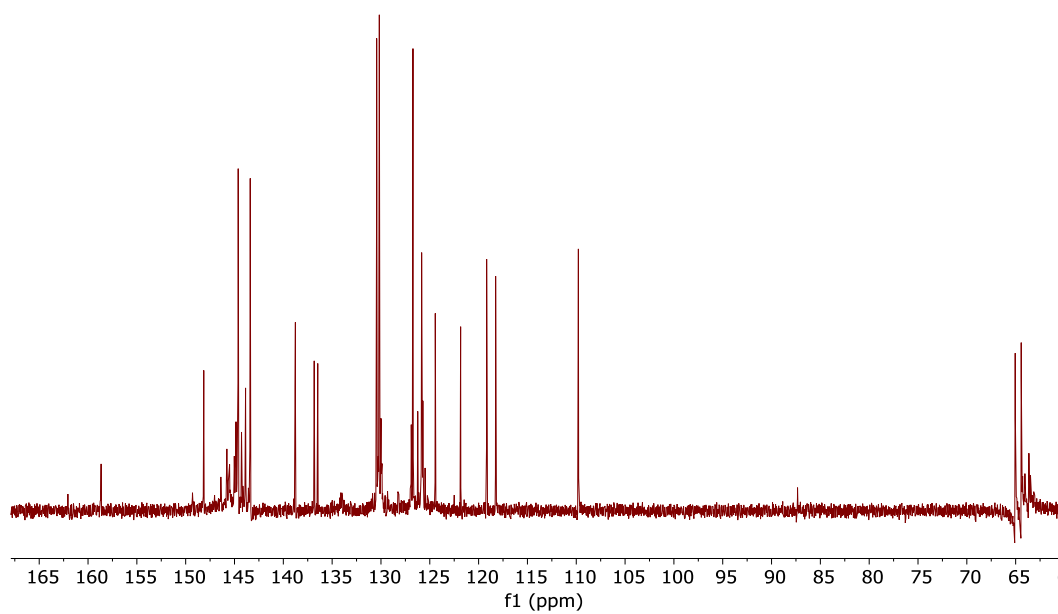


Figura 32. Espectro parcial de RMN- ^{13}C (D_2O , 125 MHz, 25°C) de 3CM1-4Br

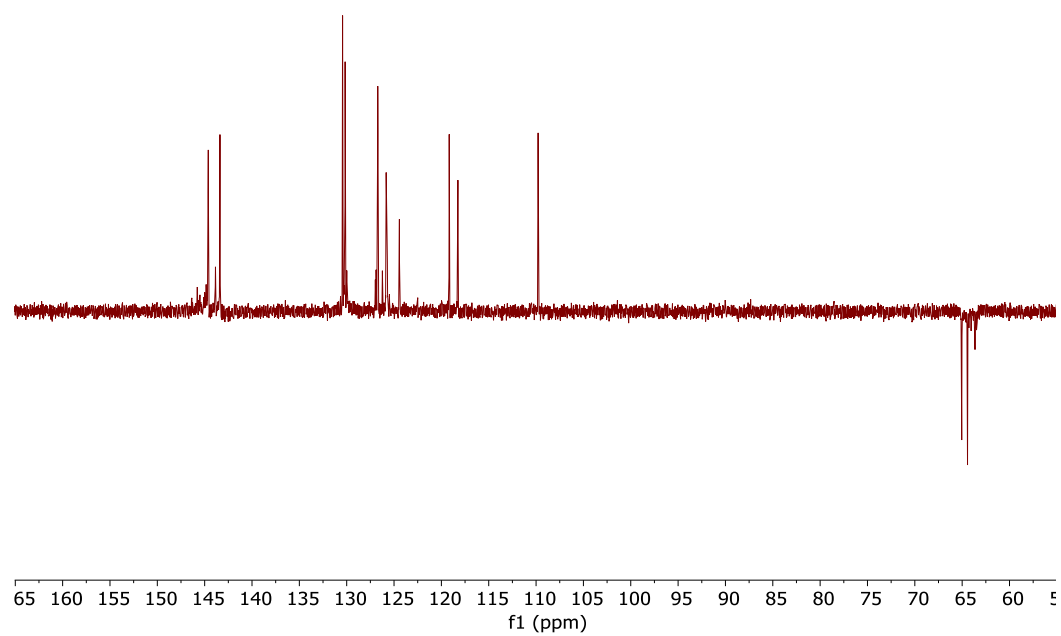


Figura 33. Espectro DEPT (D_2O , 125 MHz, 25°C) 3CM1-4Br

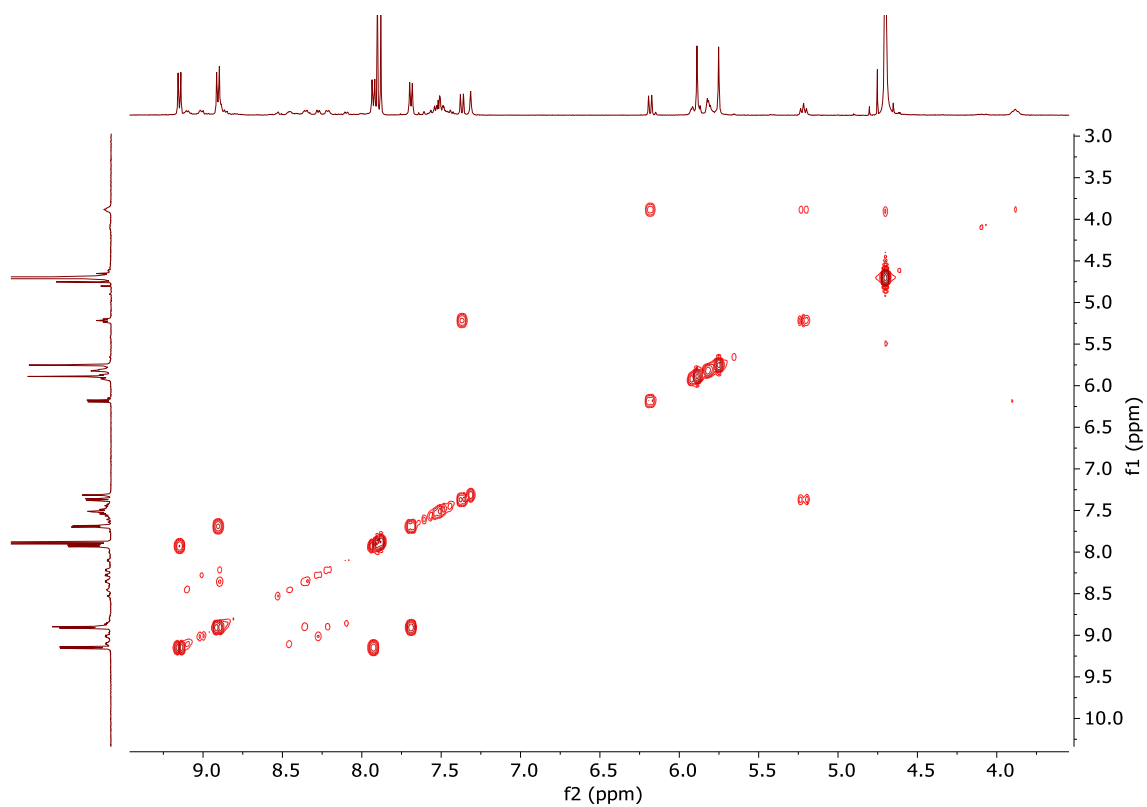


Figura 34. Espectro parcial COSY (D_2O , 400 MHz, 25°C) del 3CM1-4Br

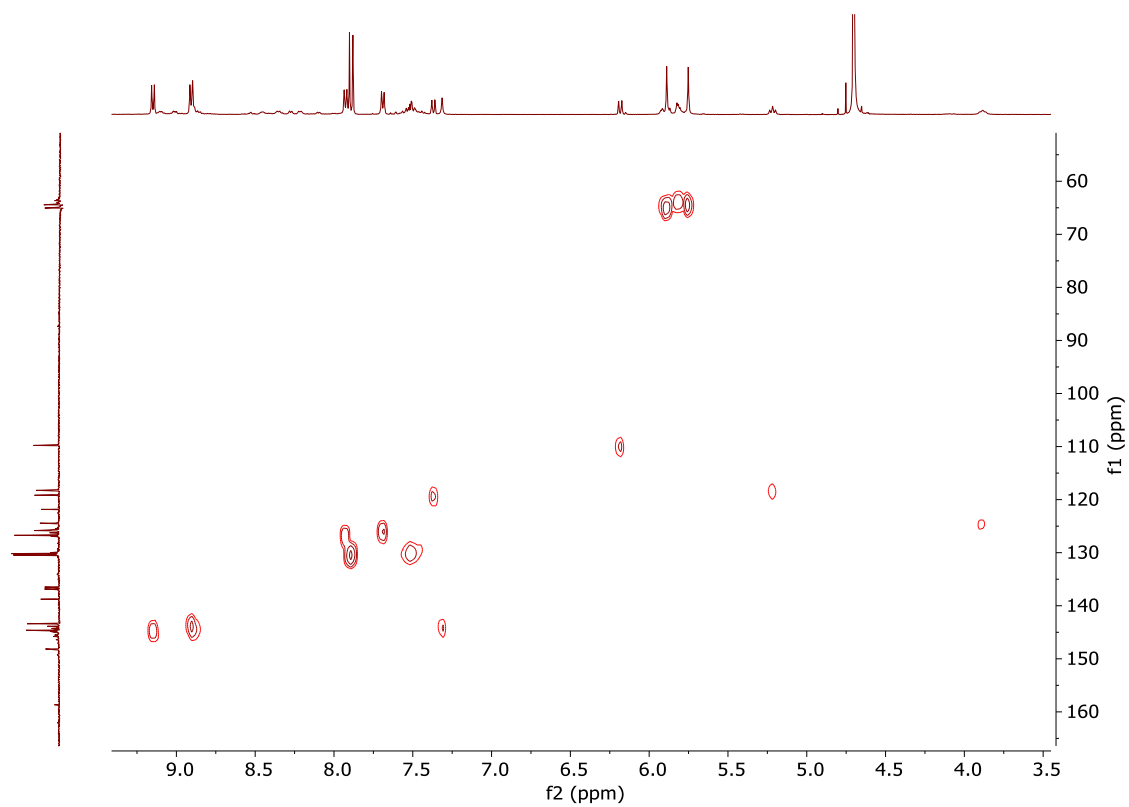


Figura 35. Espectro HSQC (D_2O , 400 MHz, 25°C) del 3CM1-4Br

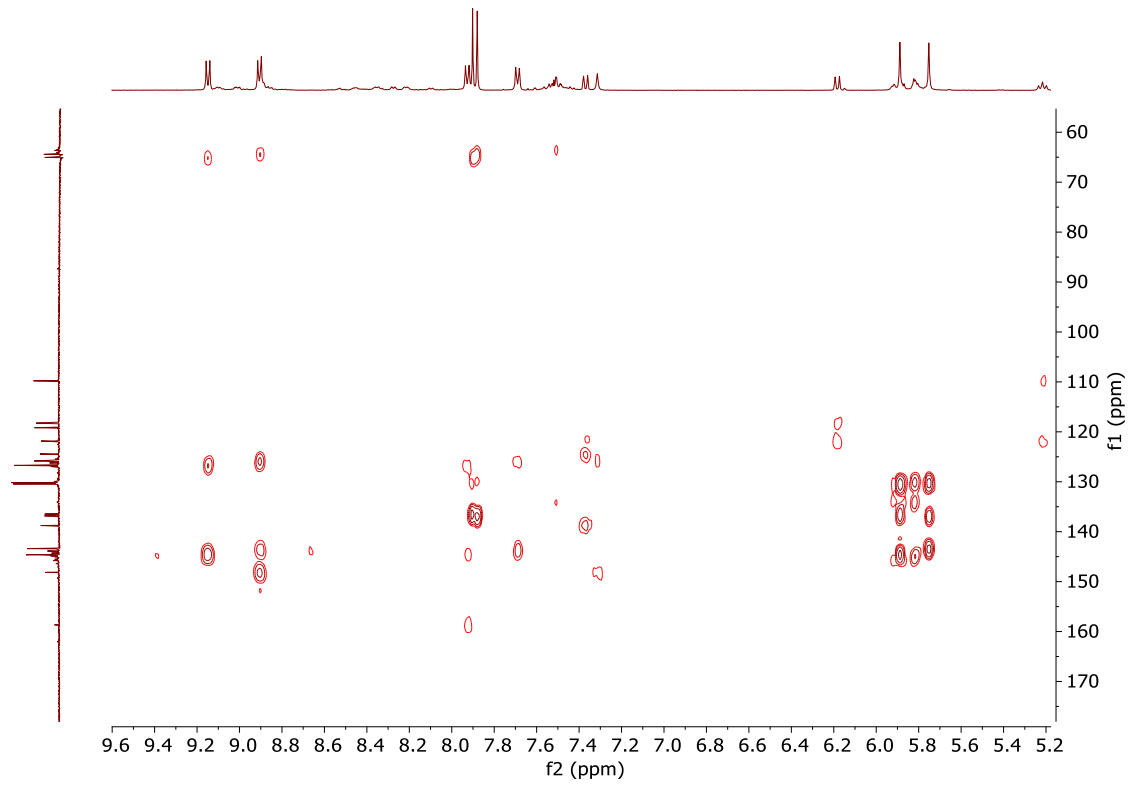


Figura 36. Espectro parcial de HMBC (D_2O , 400 MHz, 25°C) del 3CM1-4Br

4CM1-4Br: ANTRACENO

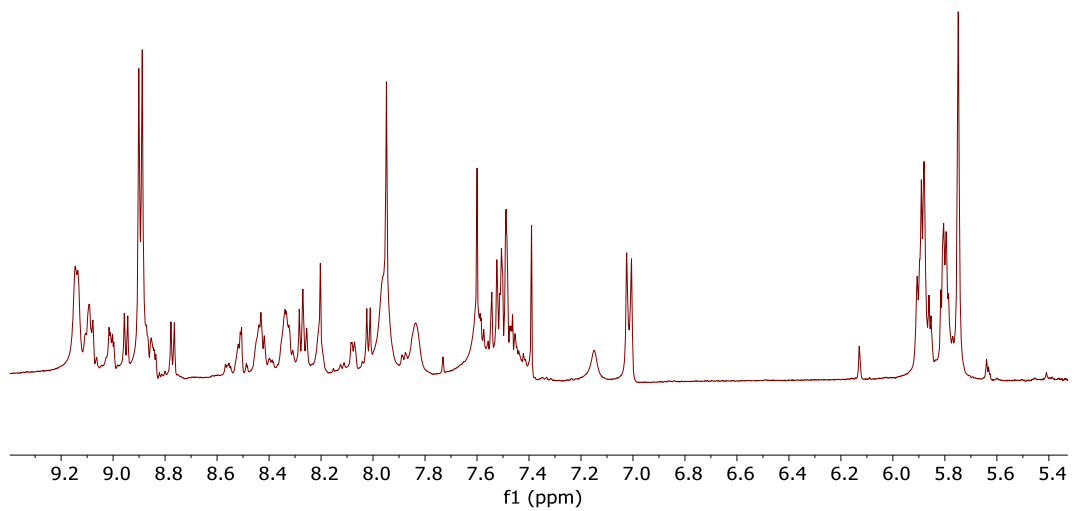


Figura 37. Espectro parcial de RMN-¹H (D_2O , 500 MHz, 25°C) de 4CM1-4Br

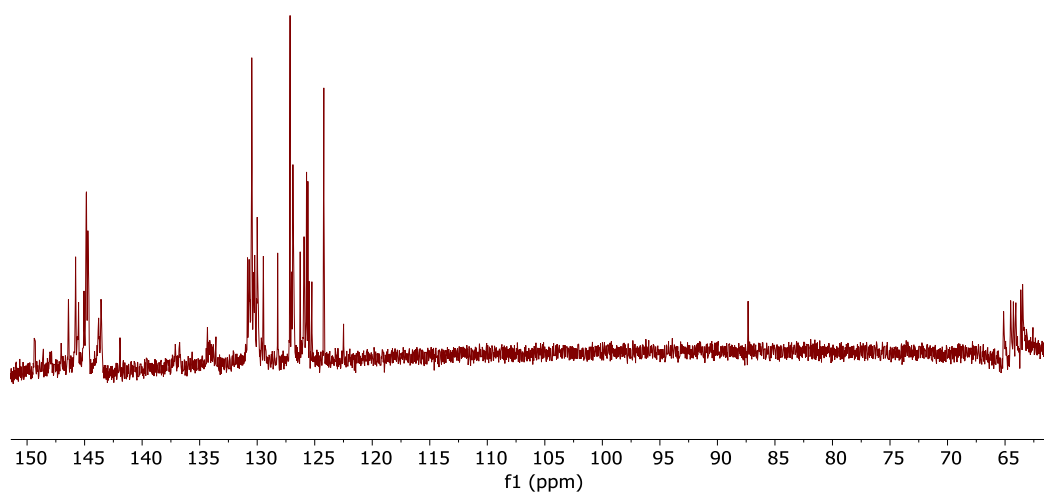


Figura 38. Espectro parcial de RMN- ^{13}C (D_2O , 125 MHz, 25°C) de 4CM1-4Br

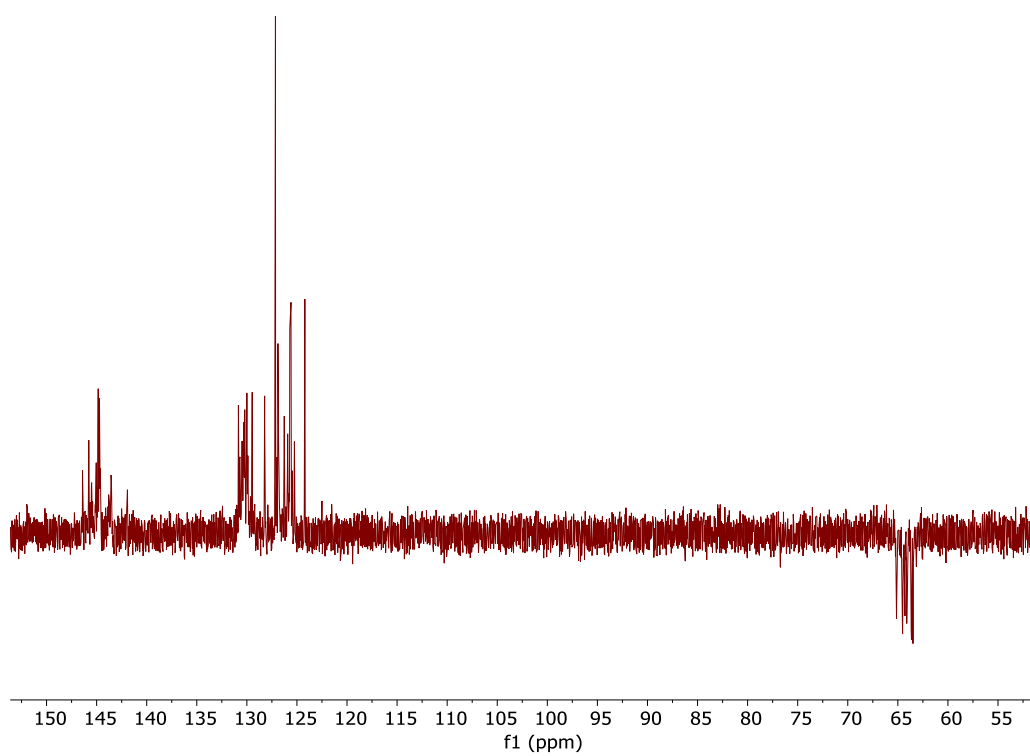


Figura 39. Espectro DEPT (D_2O , 125 MHz, 25°C) 4CM1-4Br

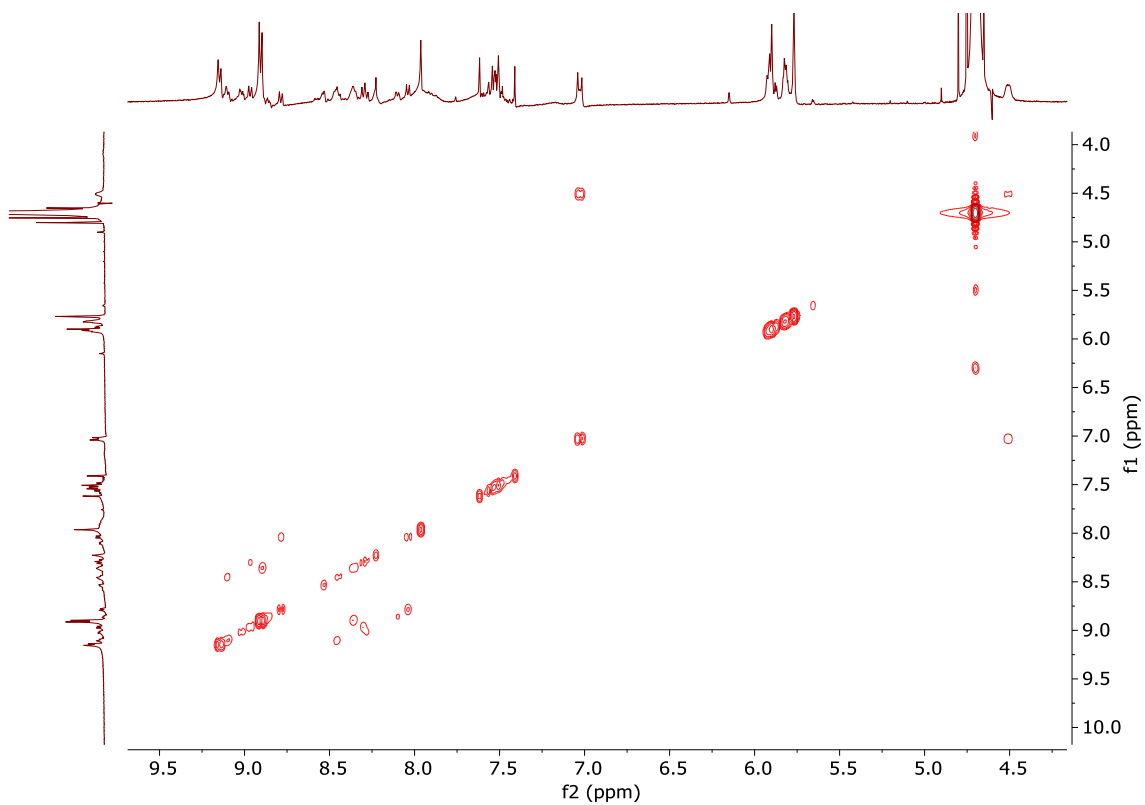


Figura 40. Espectro parcial COSY (D_2O , 400 MHz, 25°C) del 4CM1-4Br

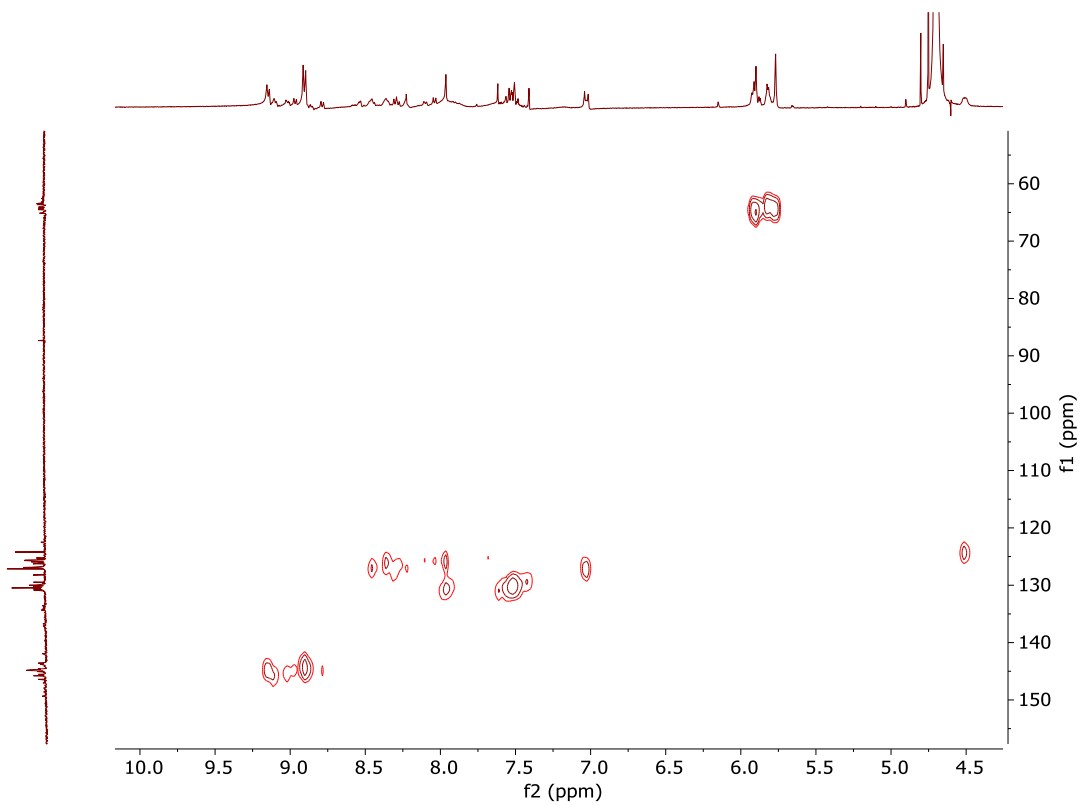


Figura 41. Espectro HSQC (D_2O , 400 MHz, 25°C) del 4CM1-4Br

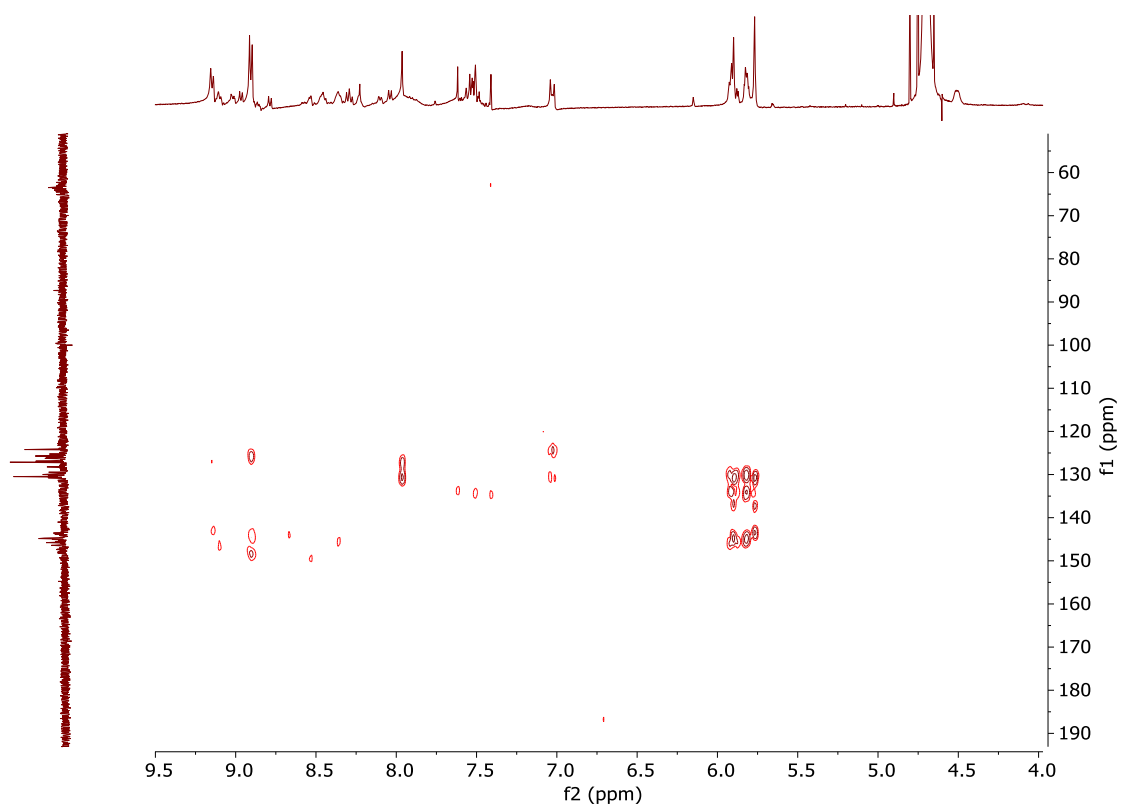


Figura 42. Espectro parcial de HMBC (D₂O, 400 MHz, 25°C) del 4CM1·4Br

5CM1·4Br: FENANTRENO

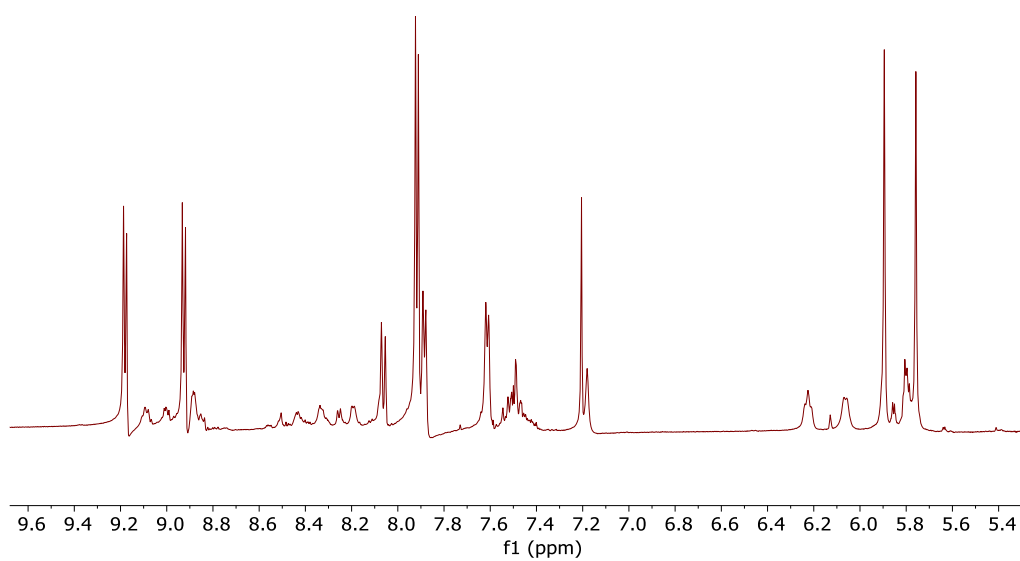


Figura 43. Espectro parcial de RMN-¹H (D₂O, 500 MHz, 25°C) de 5CM1·4Br

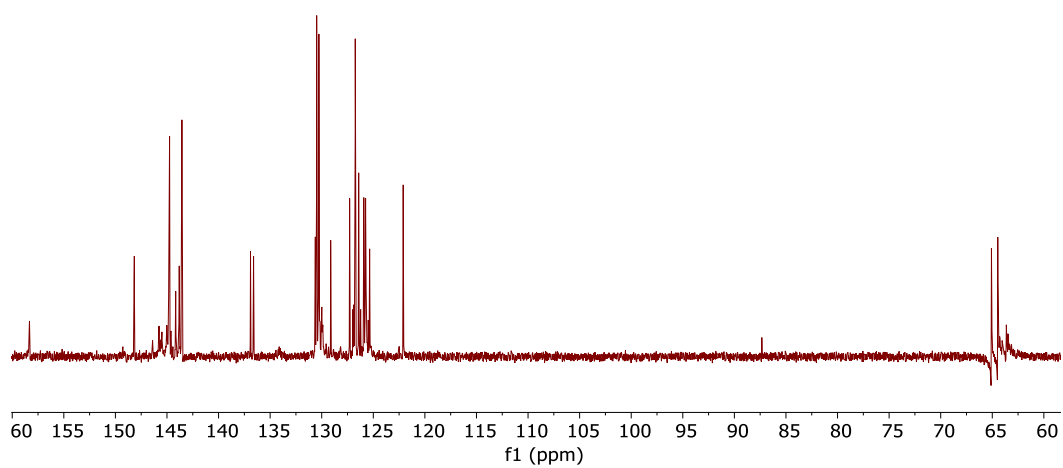


Figura 44. Espectro parcial de RMN- ^{13}C (D_2O , 125 MHz, 25°C) de 5CM1-4Br

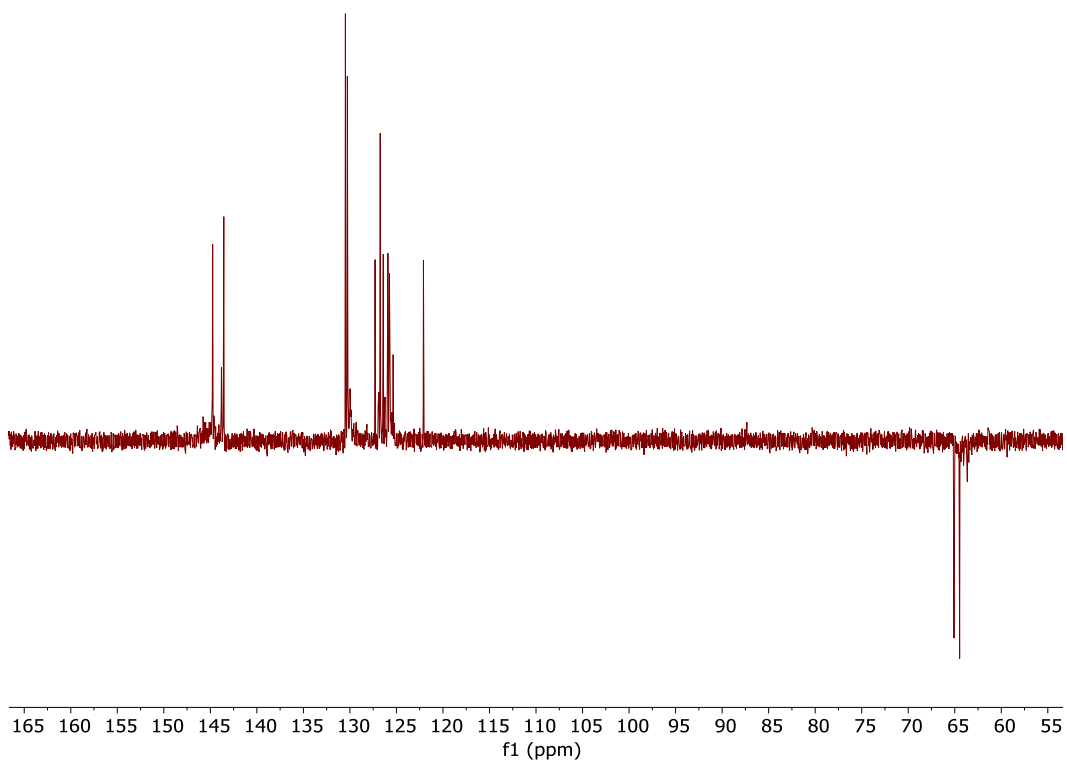


Figura 45. Espectro DEPT (D_2O , 125 MHz, 25°C) 5CM1-4Br

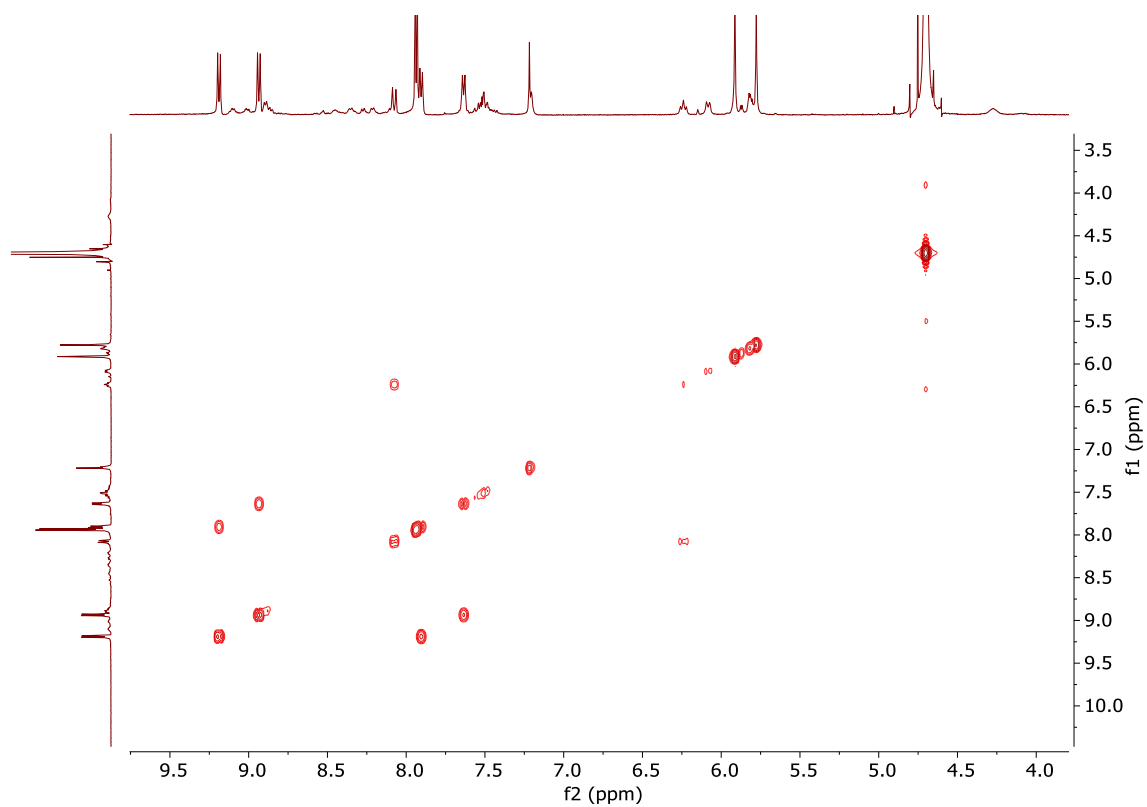


Figura 46. Espectro parcial COSY (D_2O , 400 MHz, 25°C) del 5CM1-4Br

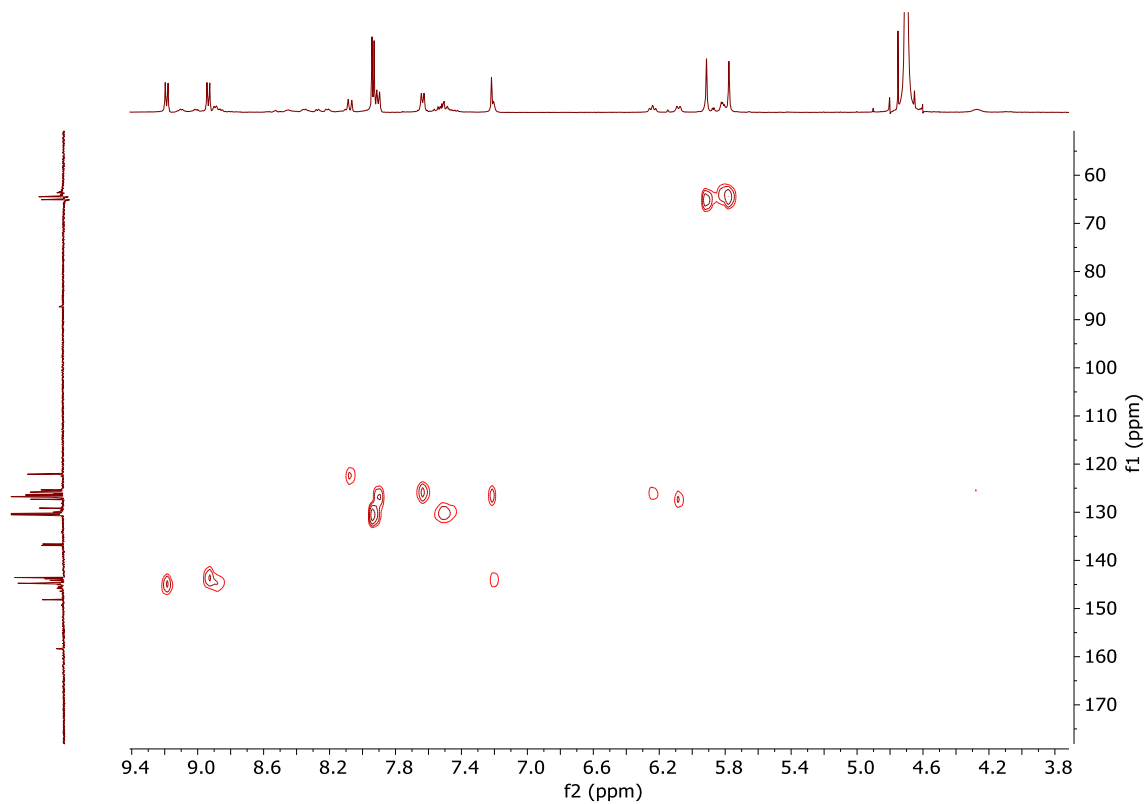


Figura 47. Espectro HSQC (D_2O , 400 MHz, 25°C) del 5CM1-4Br

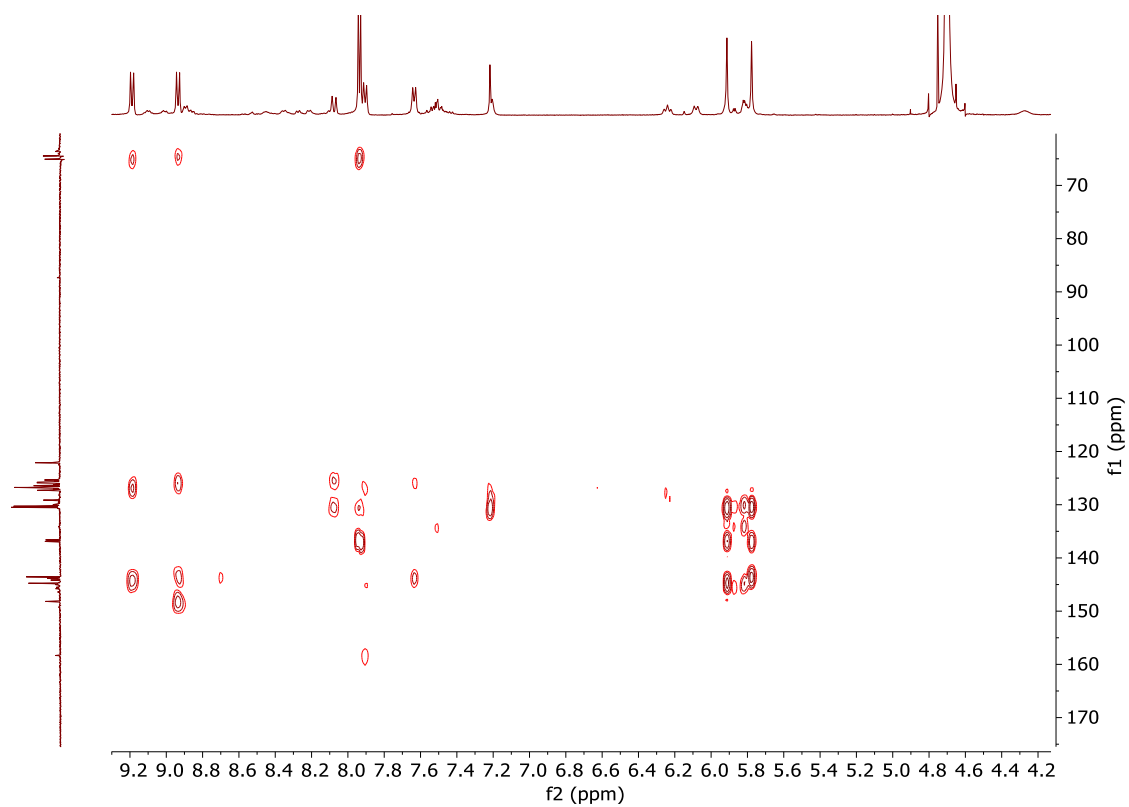


Figura 48. Espectro parcial de HMBC (D₂O, 400 MHz, 25°C) del 4CM1-4Br

6CM1-4Br: PIRENO

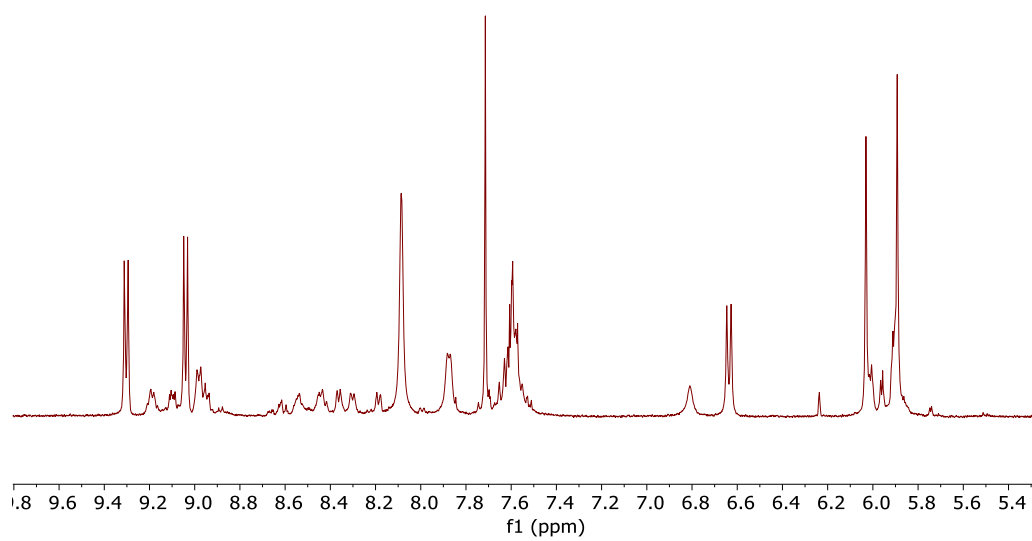


Figura 49. Espectro parcial de RMN-¹H (D₂O, 500 MHz, 25°C) de 6CM1-4Br

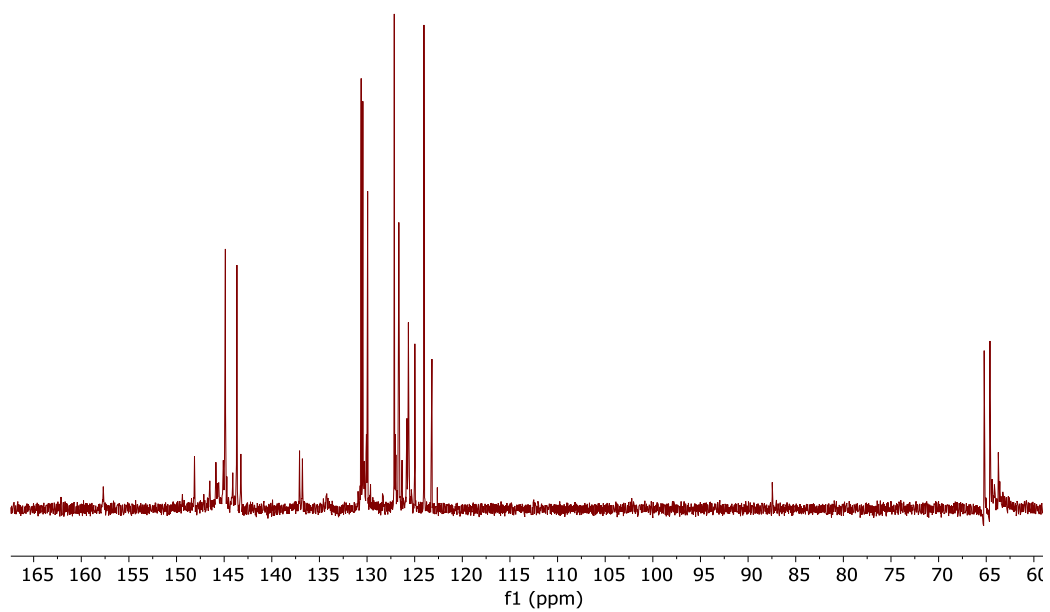


Figura 50. Espectro parcial de RMN- ^{13}C (D_2O , 125 MHz, 25°C) de 6CM1-4Br

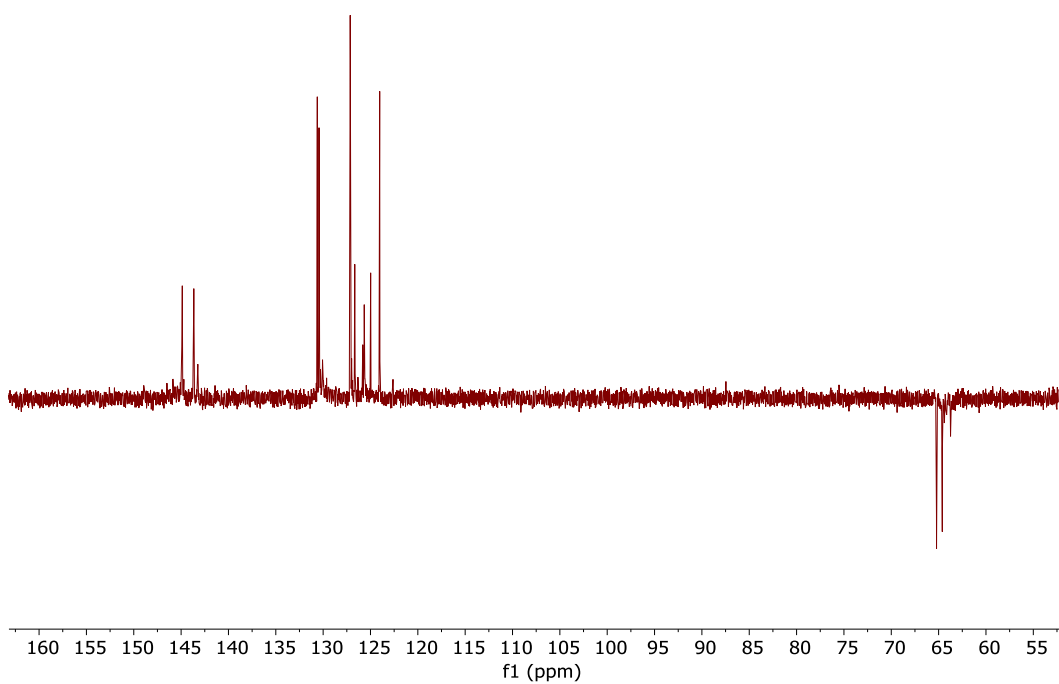


Figura 51. Espectro DEPT (D_2O , 125 MHz, 25°C) 6CM1-4Br

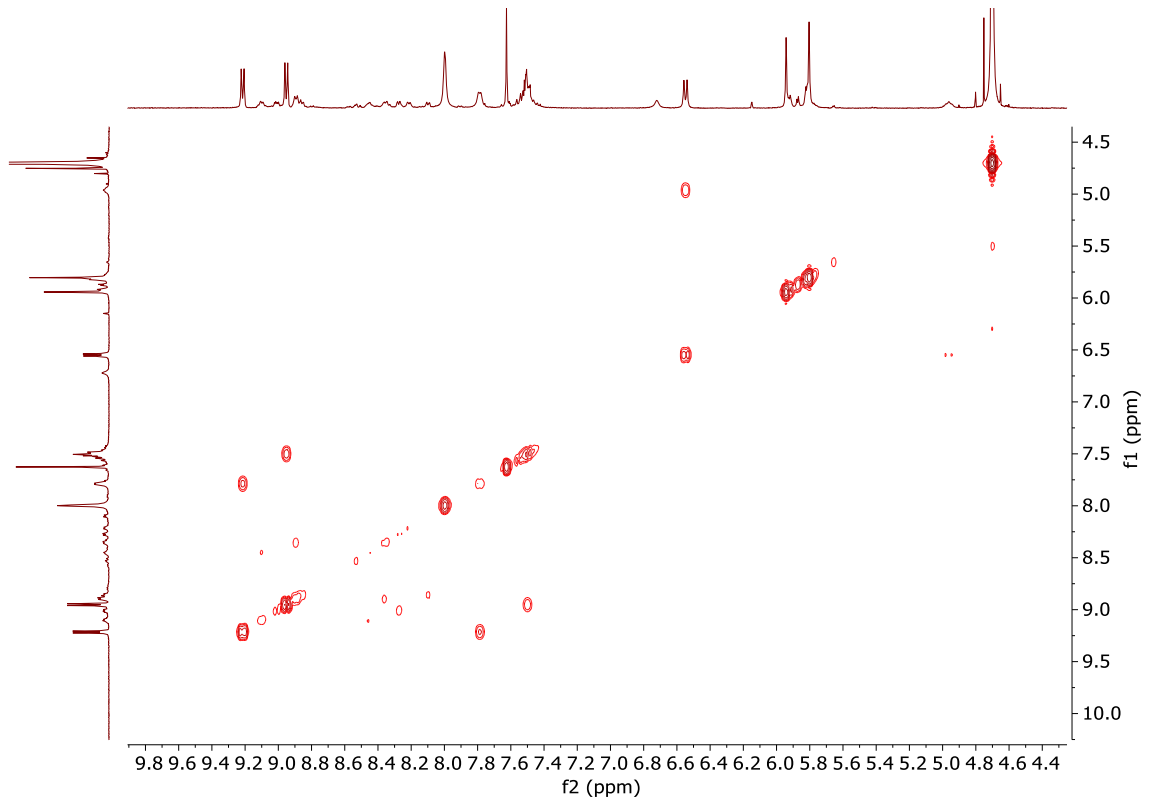


Figura 52. Espectro parcial COSY (D₂O, 400 MHz, 25°C) del 6CM1-4Br

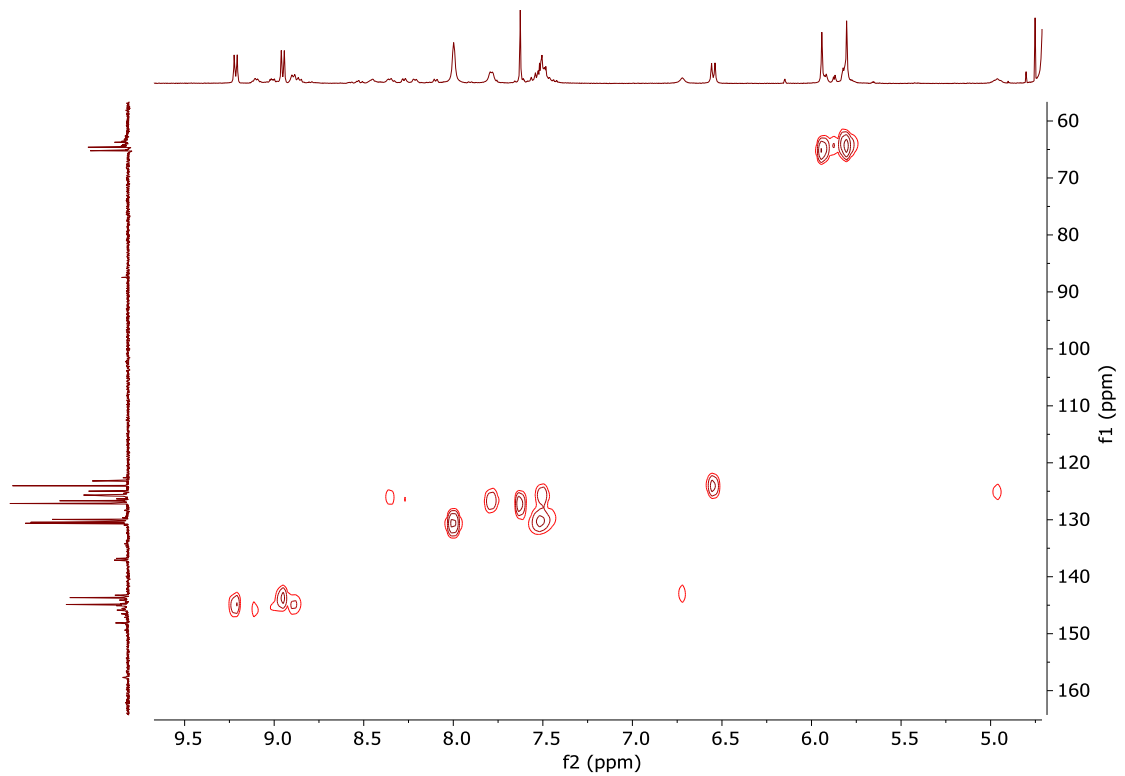


Figura 53. Espectro HSQC (D₂O, 400 MHz, 25°C) del 6CM1-4Br

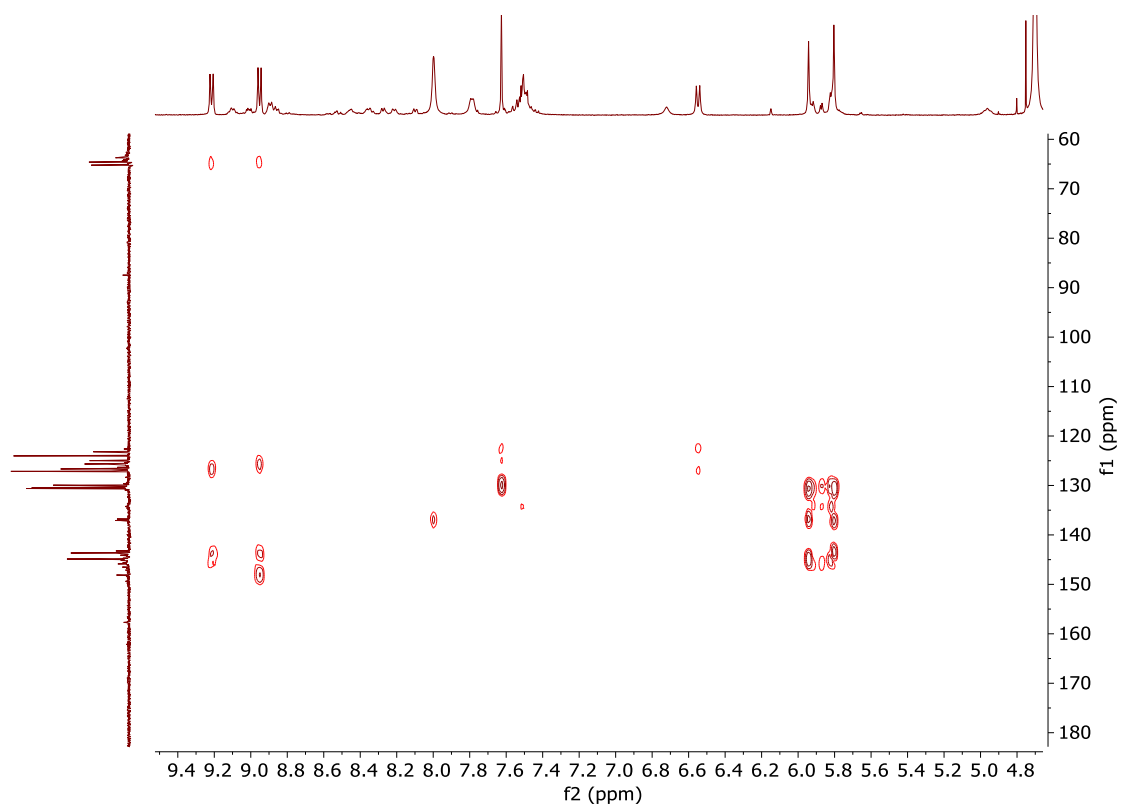


Figura 54. Espectro parcial de HMBC (D_2O , 400 MHz, 25°C) del 6CM1-4Br

1CM2-4Br: 1,5-DIHIDROXINAFTALENO

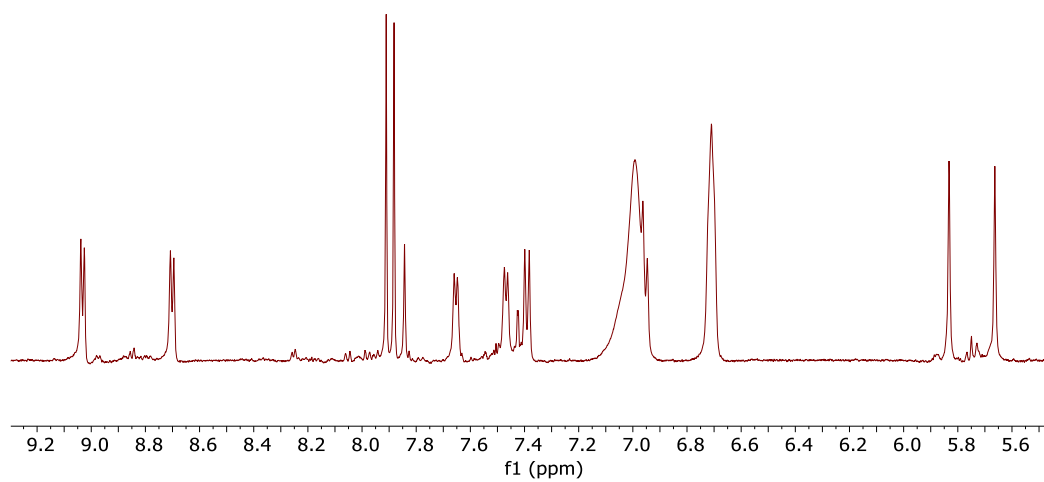


Figura 55. Espectro parcial de RMN-¹H (D_2O , 500 MHz, 25°C) de 1CM2-4Br

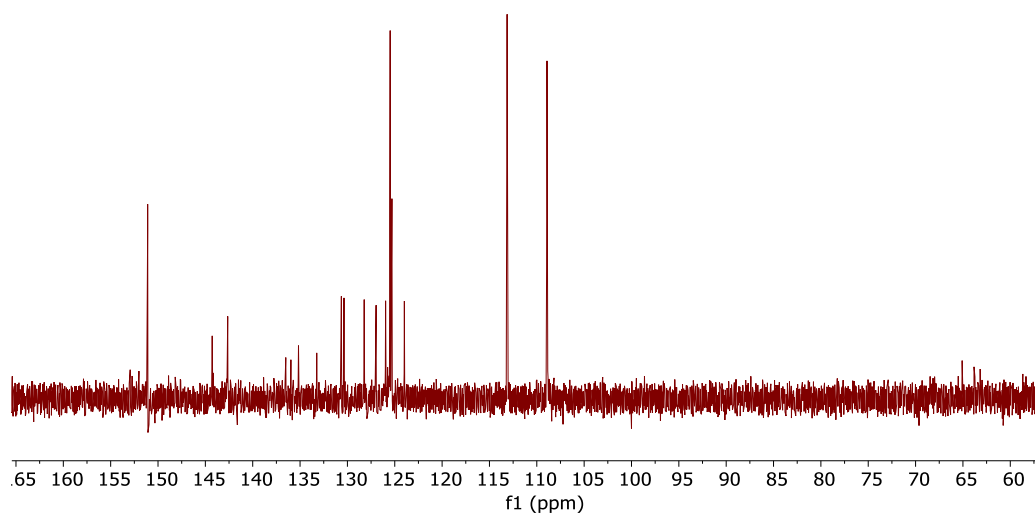


Figura 56. Espectro parcial de RMN- ^{13}C (D_2O , 125 MHz, 25°C) de 1CM2-4Br

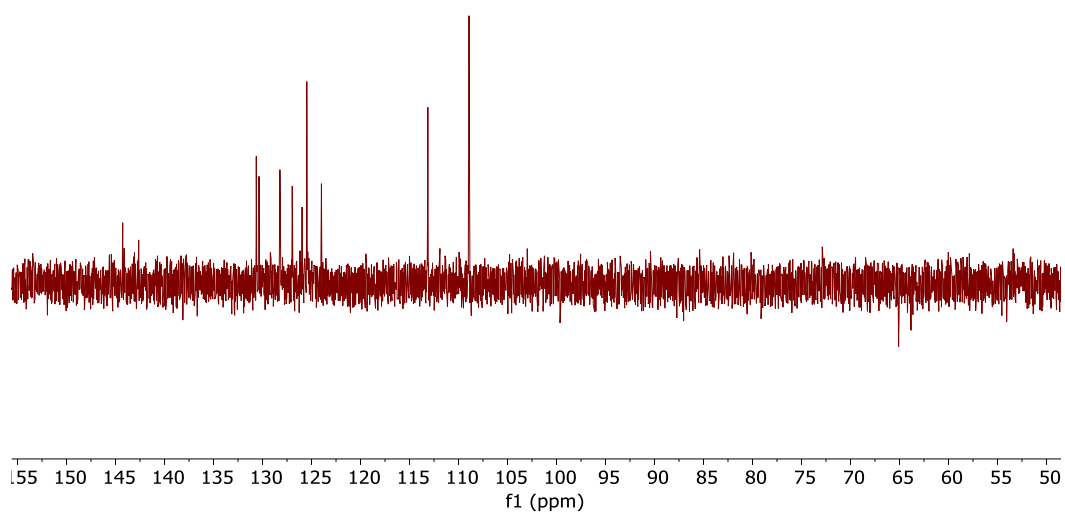


Figura 57. Espectro DEPT (D_2O , 125 MHz, 25°C) 1CM2-4Br

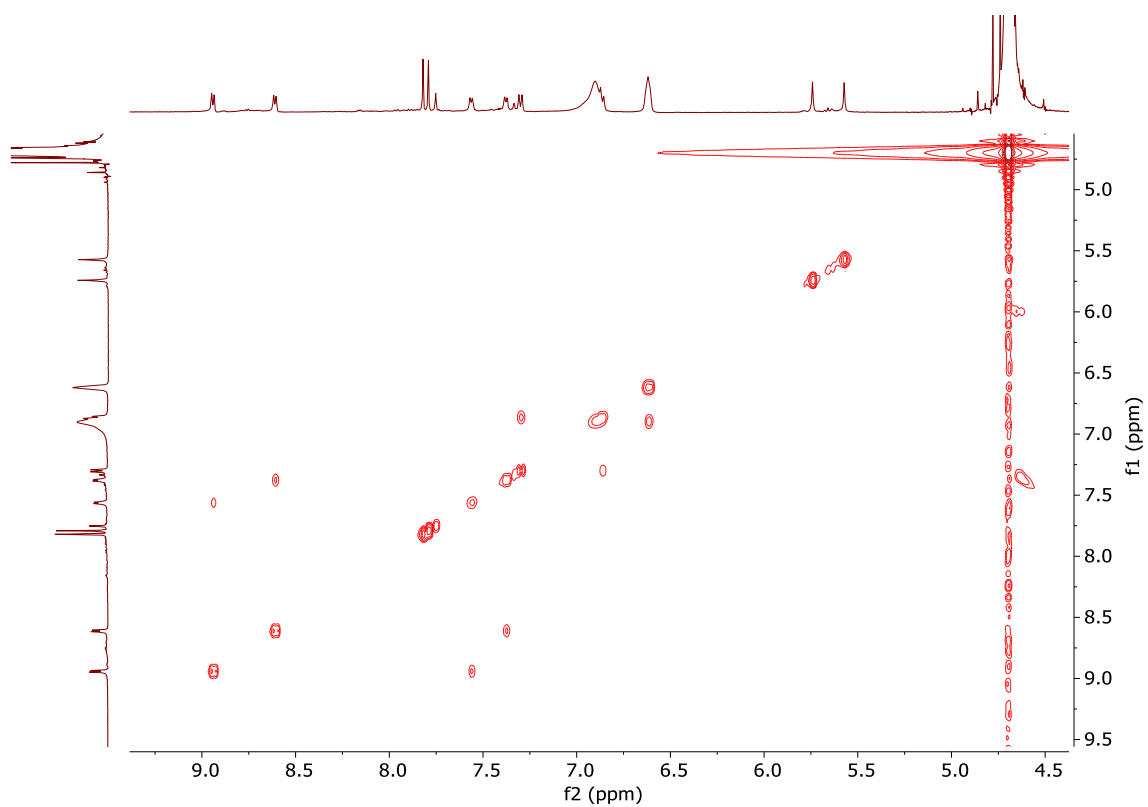


Figura 58. Espectro parcial COSY (D_2O , 400 MHz, 25°C) del 1CM2-4Br

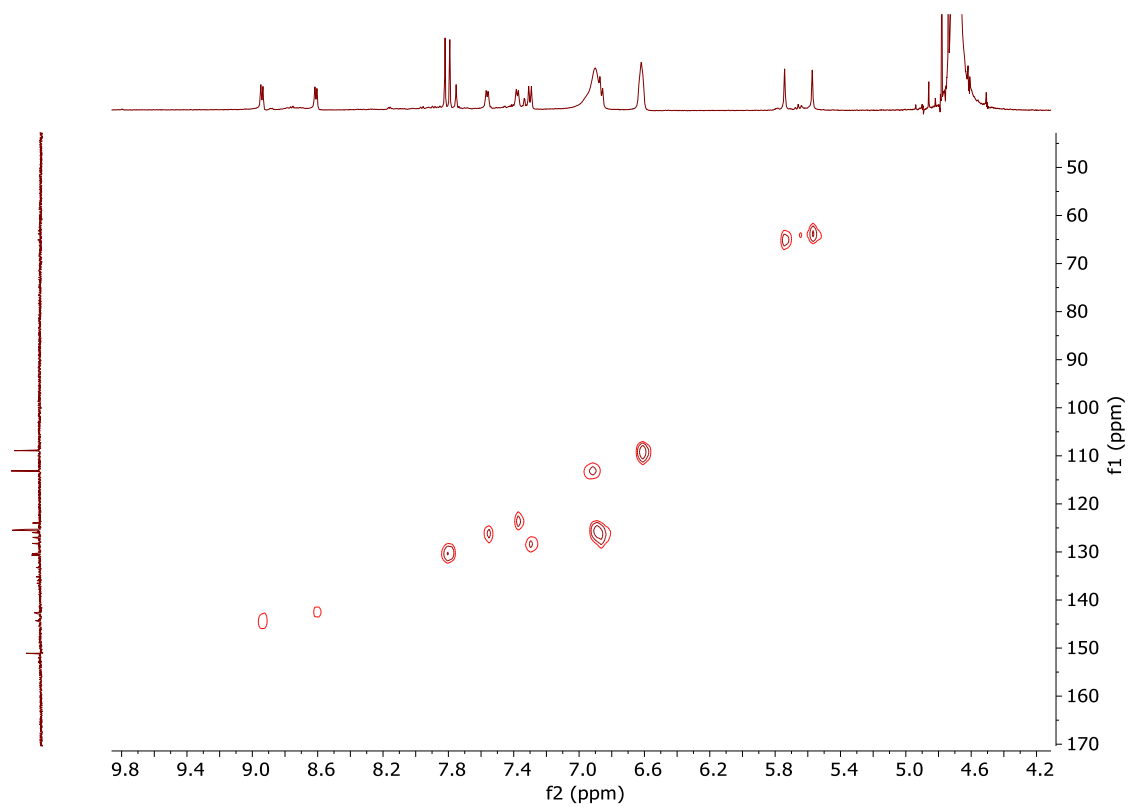


Figura 59. Espectro HSQC (D_2O , 400 MHz, 25°C) del 1CM2-4Br

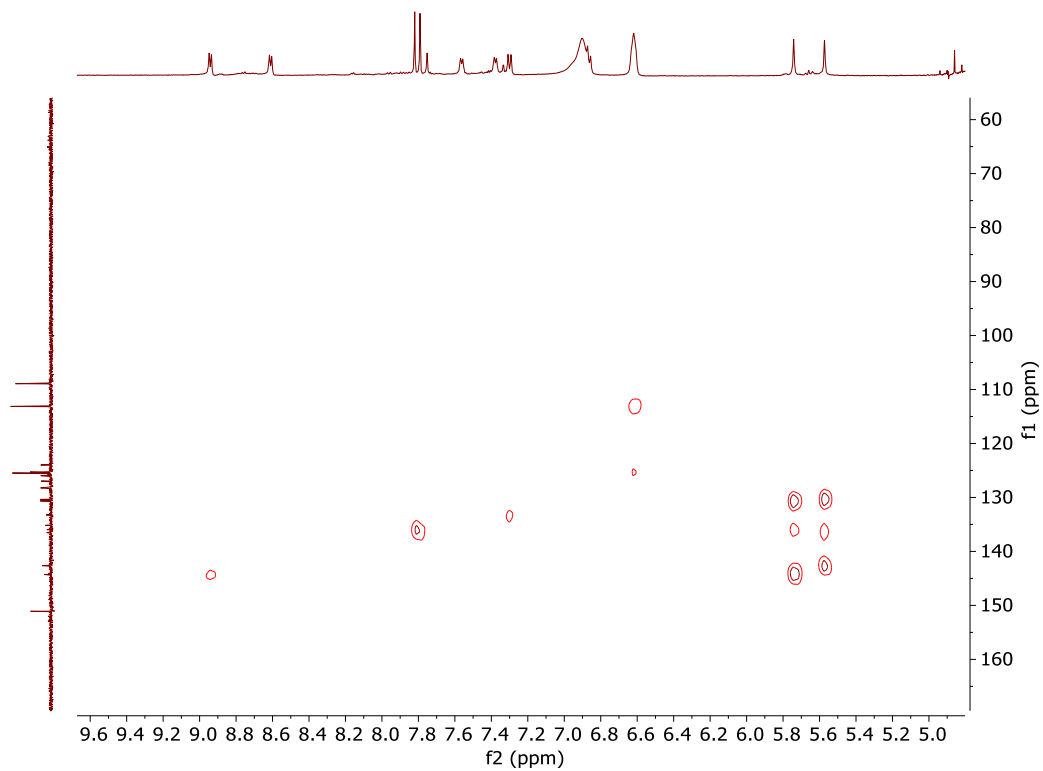


Figura 60. Espectro parcial de HMBC (D_2O , 400 MHz, 25°C) del 1CM2·4Br

2CM2·4Br: 2,7-DIHIDROXINAFTALENO

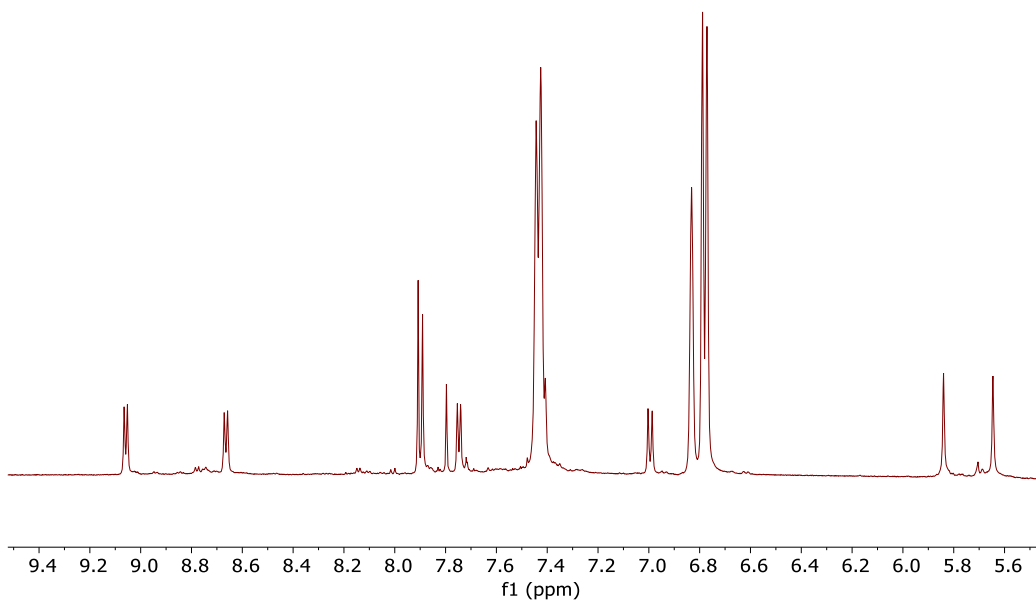


Figura 61. Espectro parcial de RMN- 1H (D_2O , 500 MHz, 25°C) de 2CM2·4Br

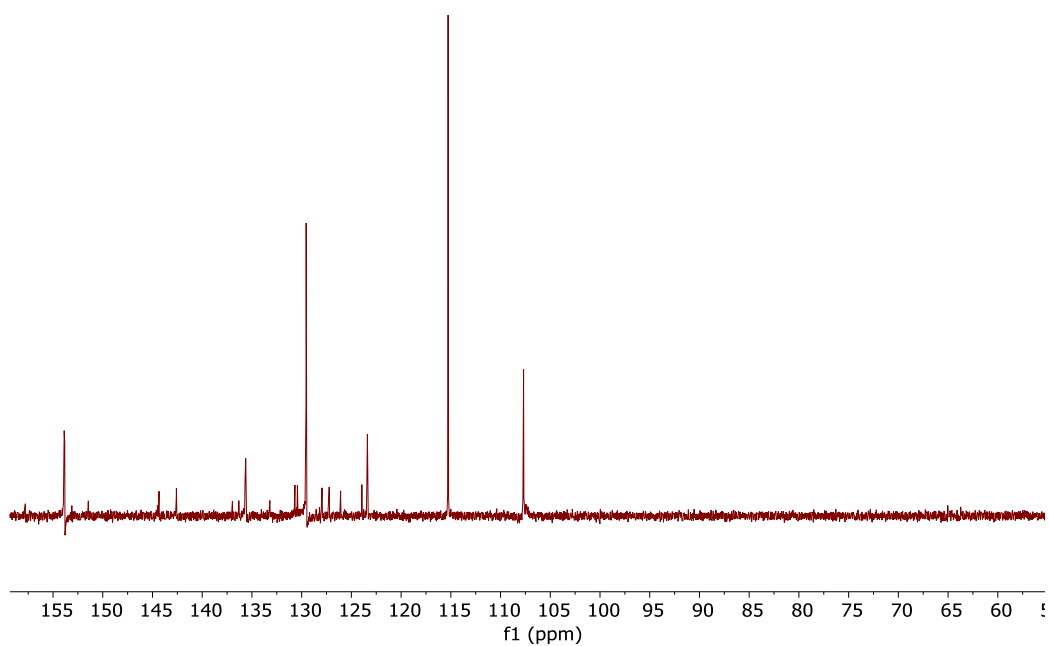


Figura 62. Espectro parcial de RMN- ^{13}C (D_2O , 125 MHz, 25°C) de 2CM2-4Br

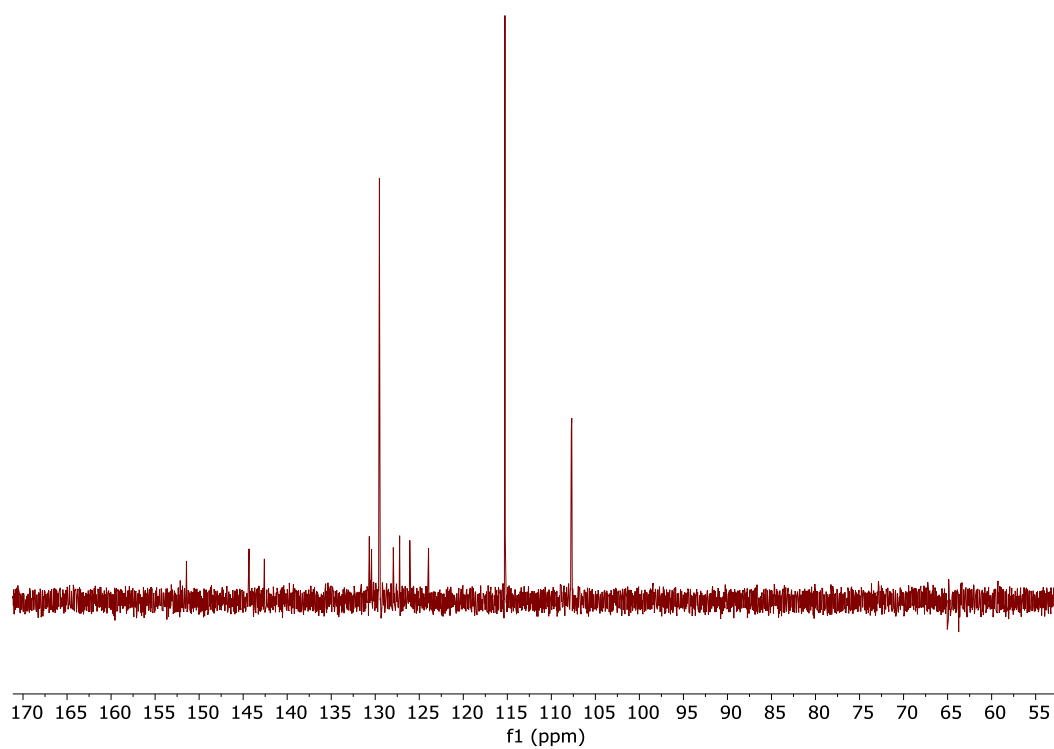


Figura 63. Espectro DEPT (D_2O , 125 MHz, 25°C) 2CM2-4Br

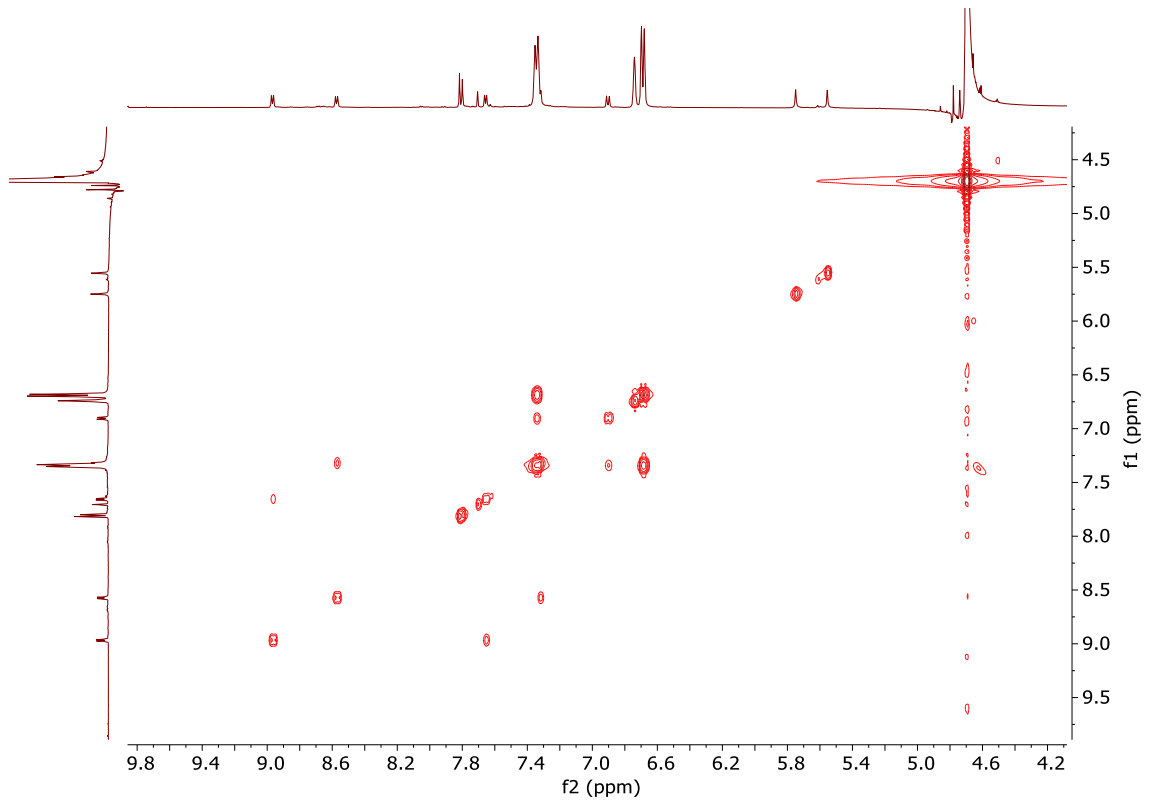


Figura 64. Espectro parcial COSY (D₂O, 400 MHz, 25°C) del 2CM2-4Br

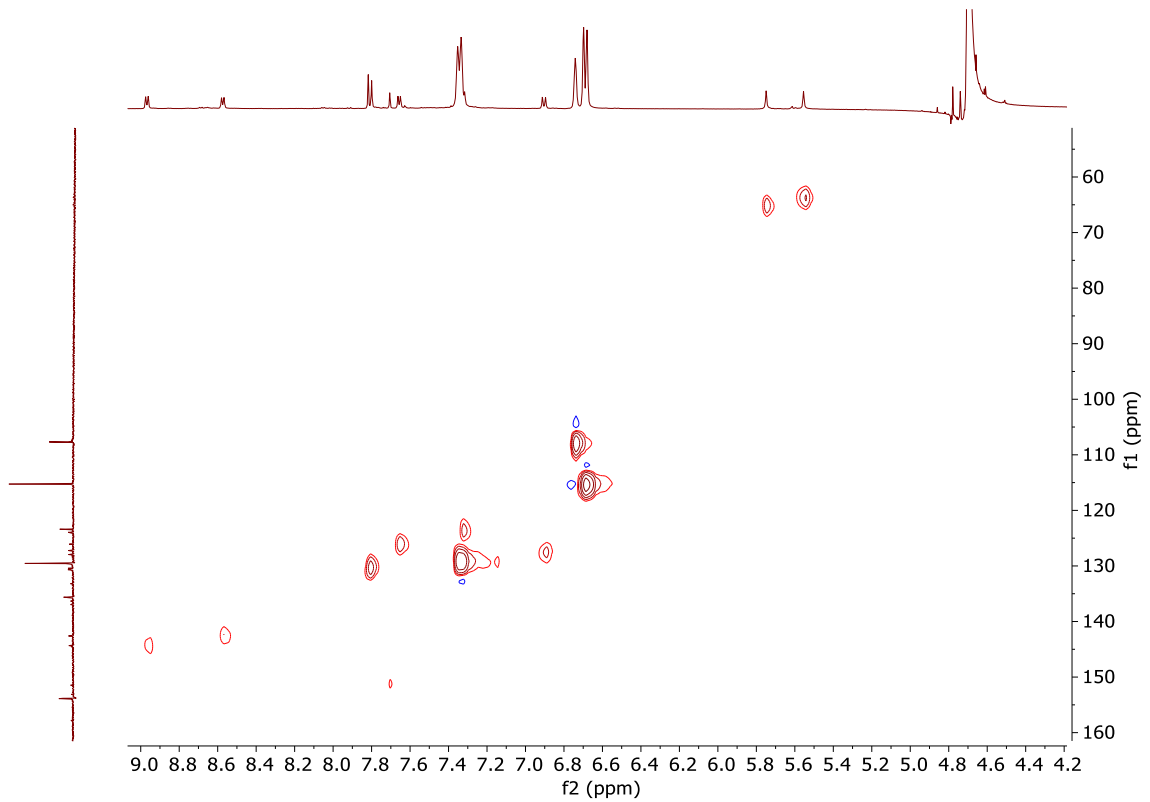


Figura 65. Espectro HSQC (D₂O, 400 MHz, 25°C) del 2CM2-4Br

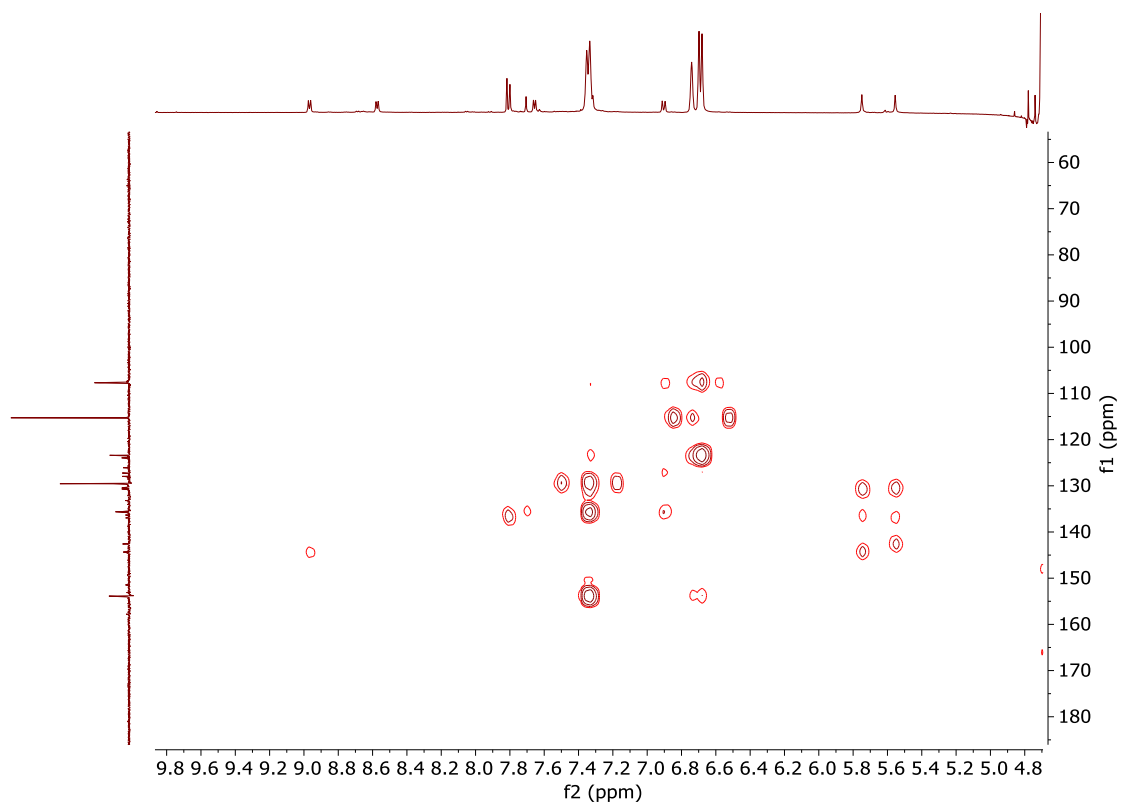


Figura 66. Espectro parcial de HMBC (D₂O, 400 MHz, 25°C) del 2CM2·4Br

3CM2·4Br: CARBAZOL

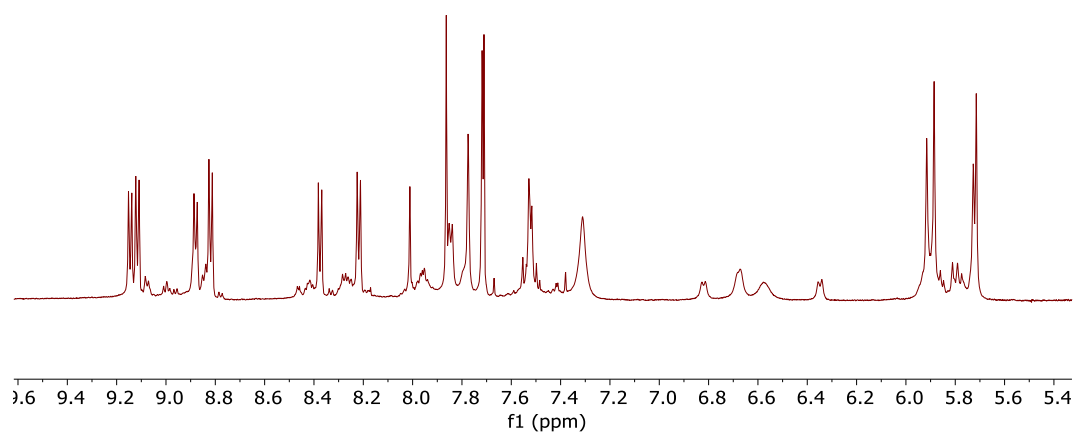


Figura 67. Espectro parcial de RMN-¹H (D₂O, 500 MHz, 25°C) de 3CM2·4Br

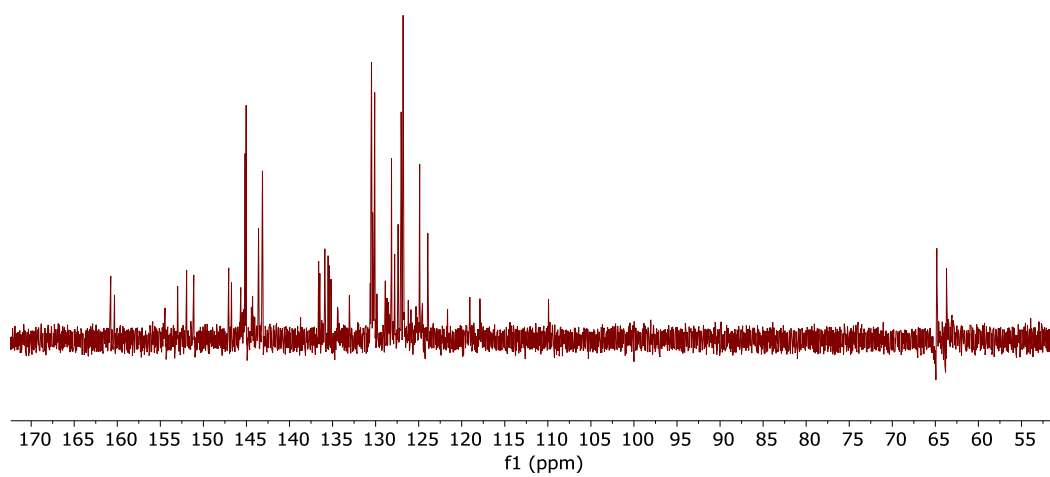


Figura 68. Espectro parcial de RMN- ^{13}C (D_2O , 125 MHz, 25°C) de 3CM2-4Br

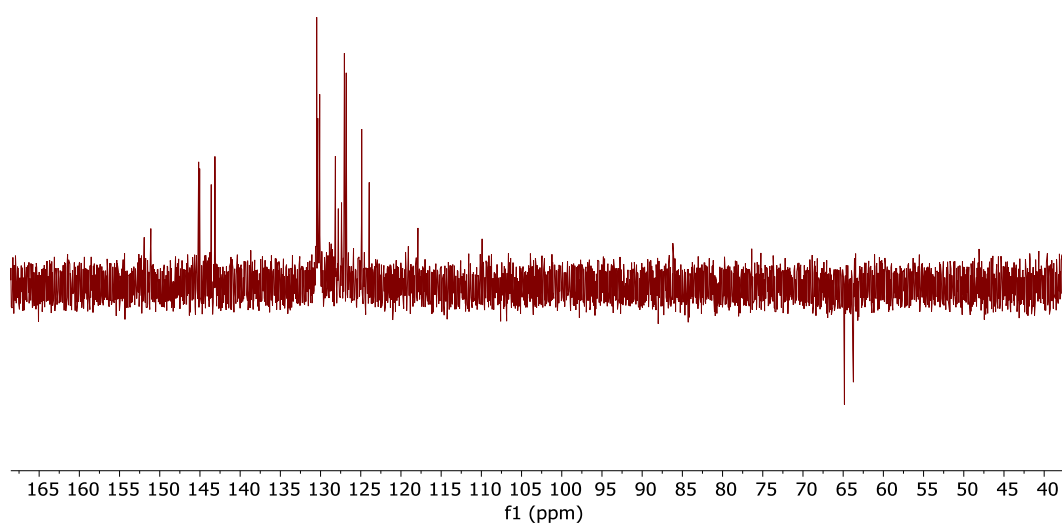


Figura 69. Espectro DEPT (D_2O , 125 MHz, 25°C) 3CM2-4Br

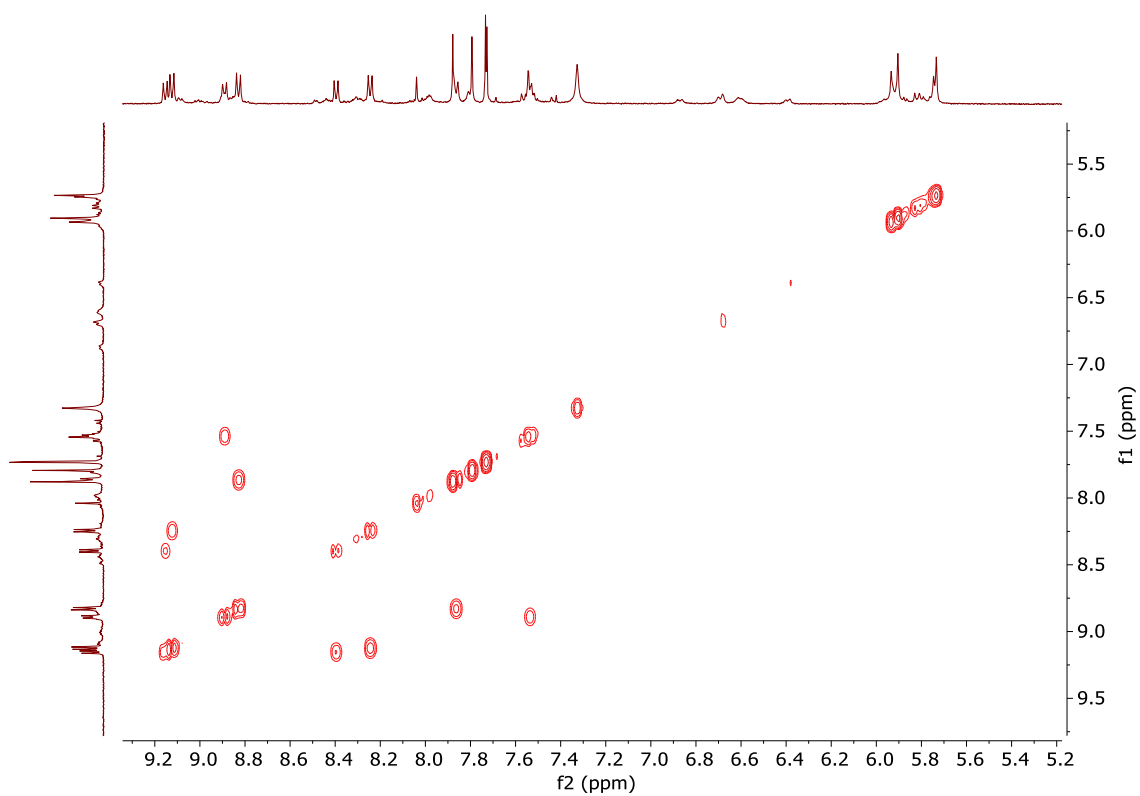


Figura 70. Espectro parcial COSY (D_2O , 400 MHz, 25°C) del 3CM2-4Br

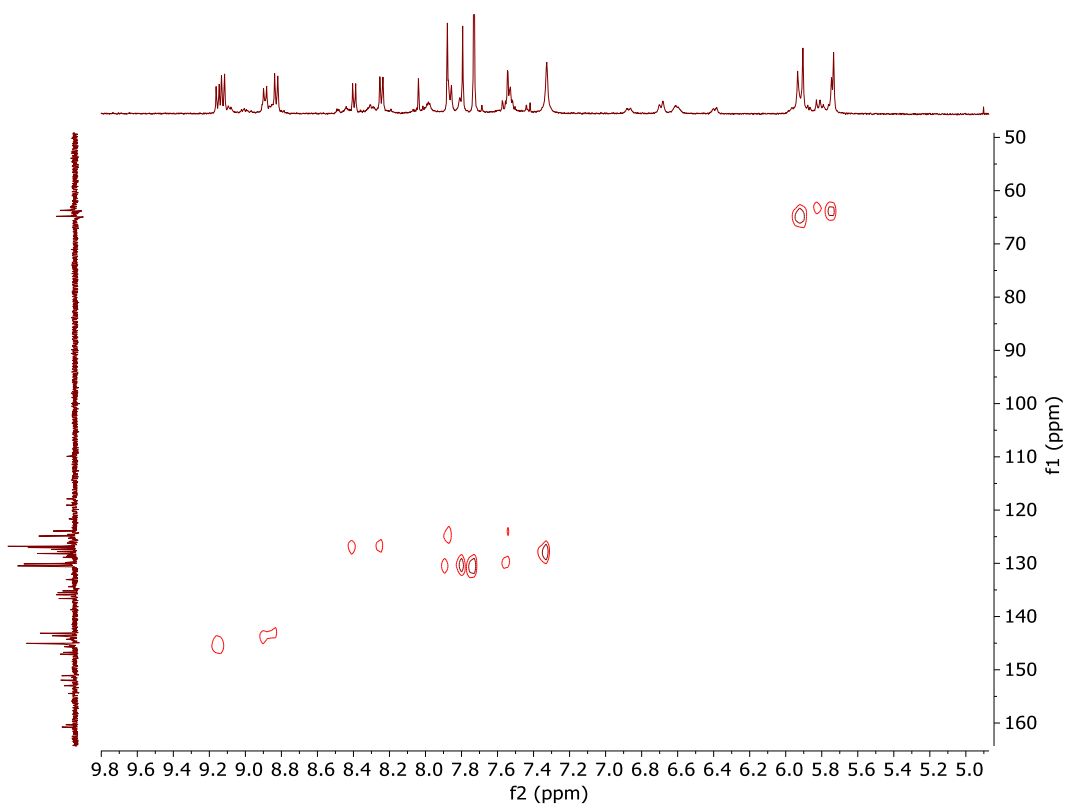


Figura 71. Espectro HSQC (D_2O , 400 MHz, 25°C) del 3CM2-4Br

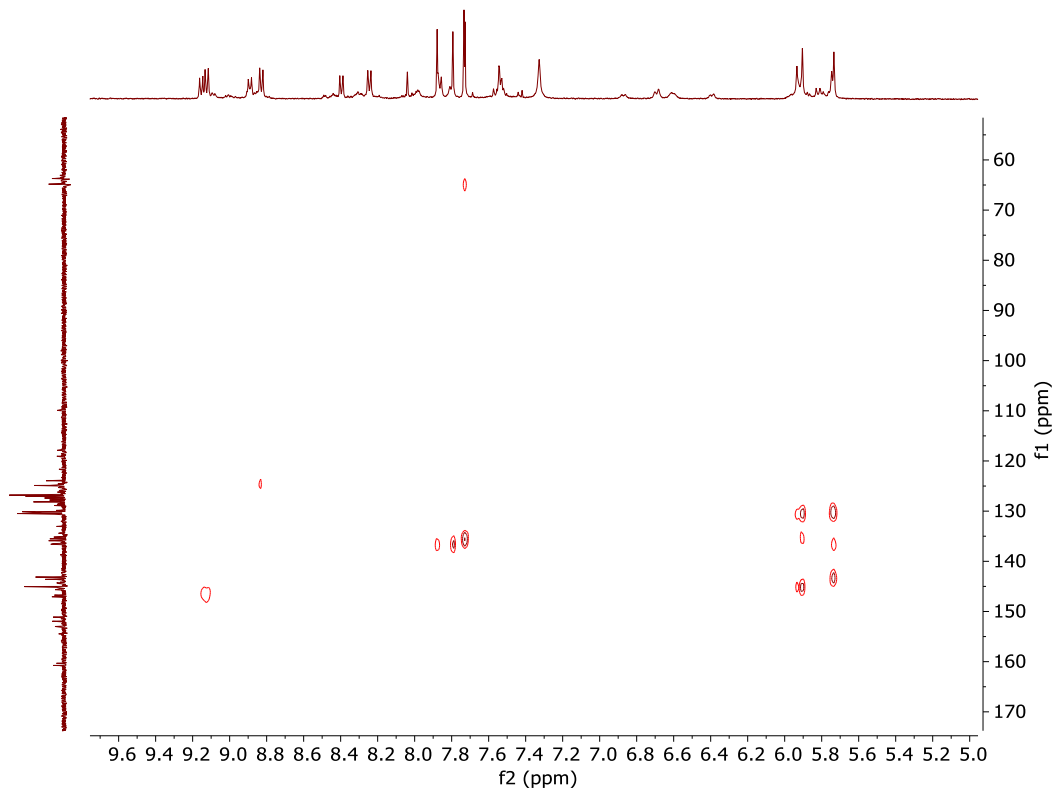


Figura 72. Espectro parcial de HMBC (D_2O , 400 MHz, 25°C) del 3CM2-4Br

4CM2-4Br: ANTRACENO

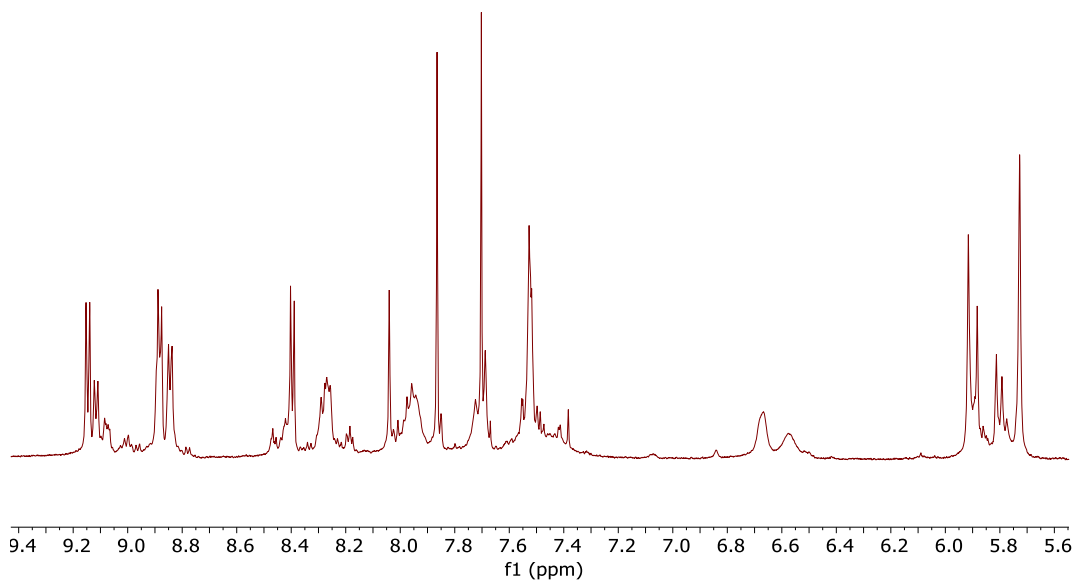


Figura 73. Espectro parcial de RMN-¹H (D_2O , 500 MHz, 25°C) de 4CM2-4Br

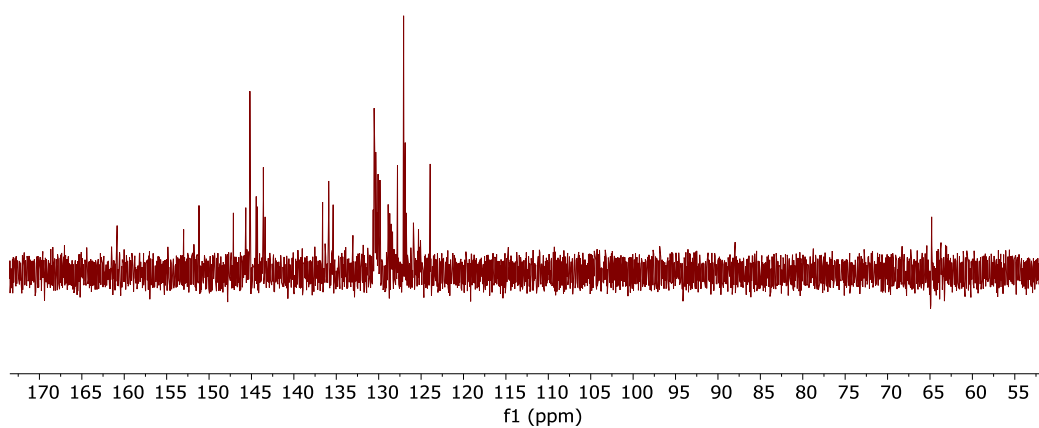


Figura 74. Espectro parcial de RMN- ^{13}C (D_2O , 125 MHz, 25°C) de 4CM2-4Br

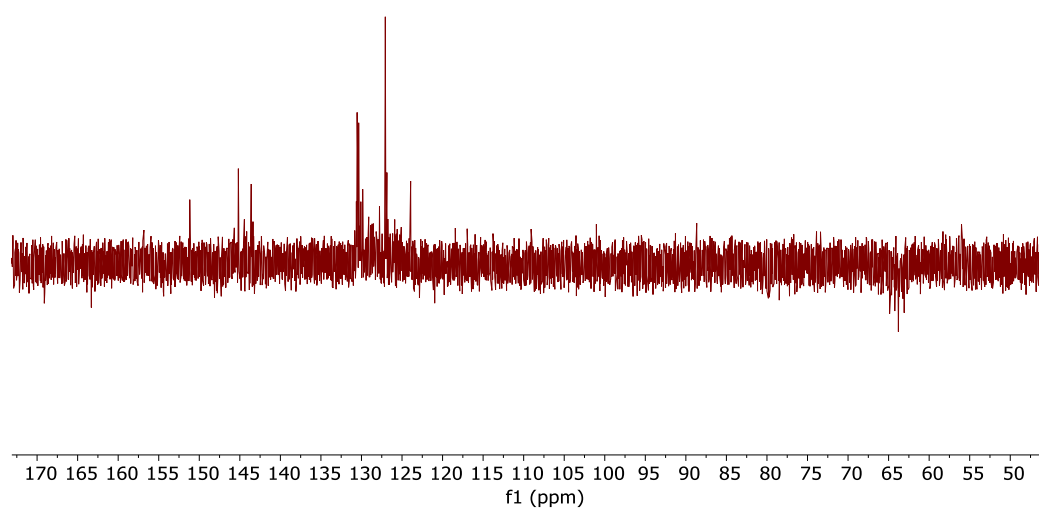


Figura 75. Espectro DEPT (D_2O , 125 MHz, 25°C) 4CM2-4Br

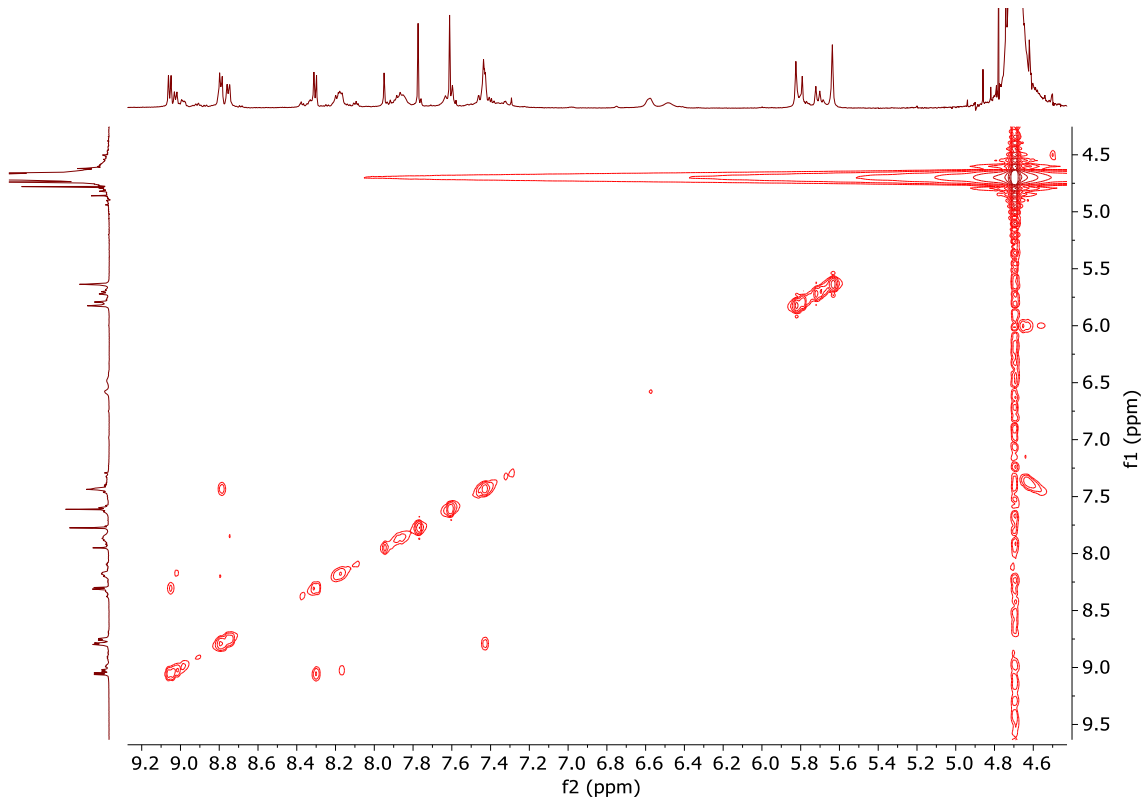


Figura 76. Espectro parcial COSY (D_2O , 500 MHz, 25°C) del 4CM2-4Br

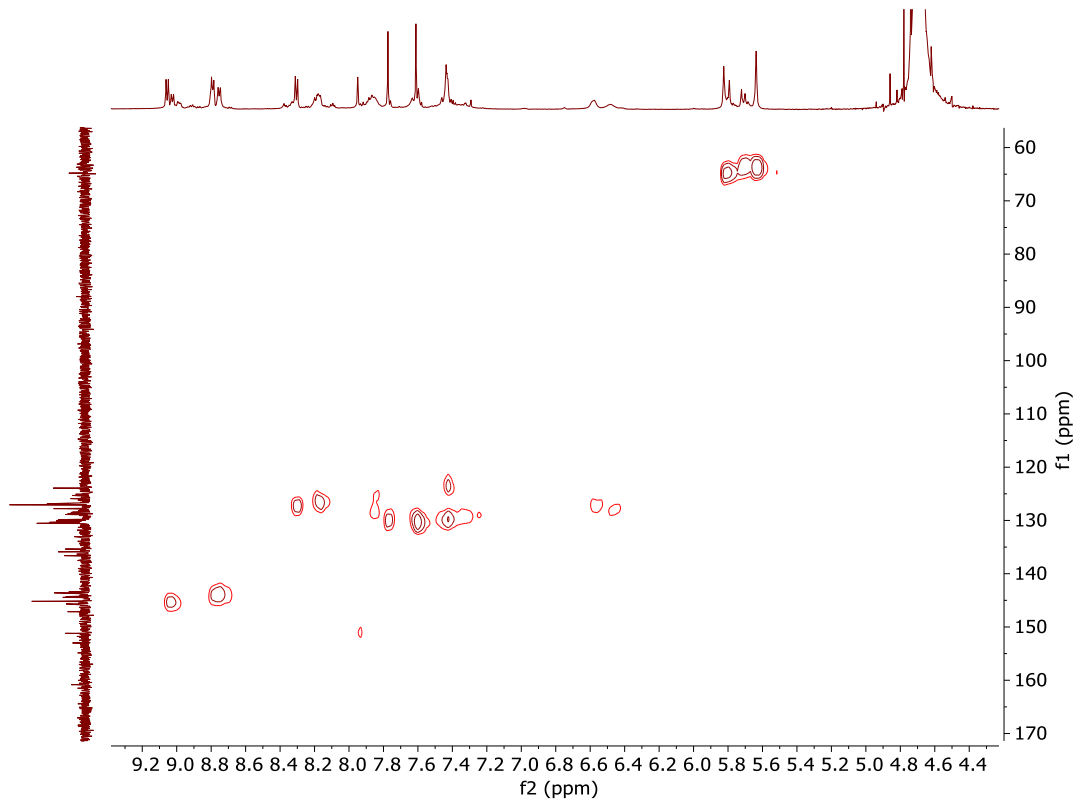


Figura 77. Espectro HSQC (D_2O , 500 MHz, 25°C) del 4CM2-4Br

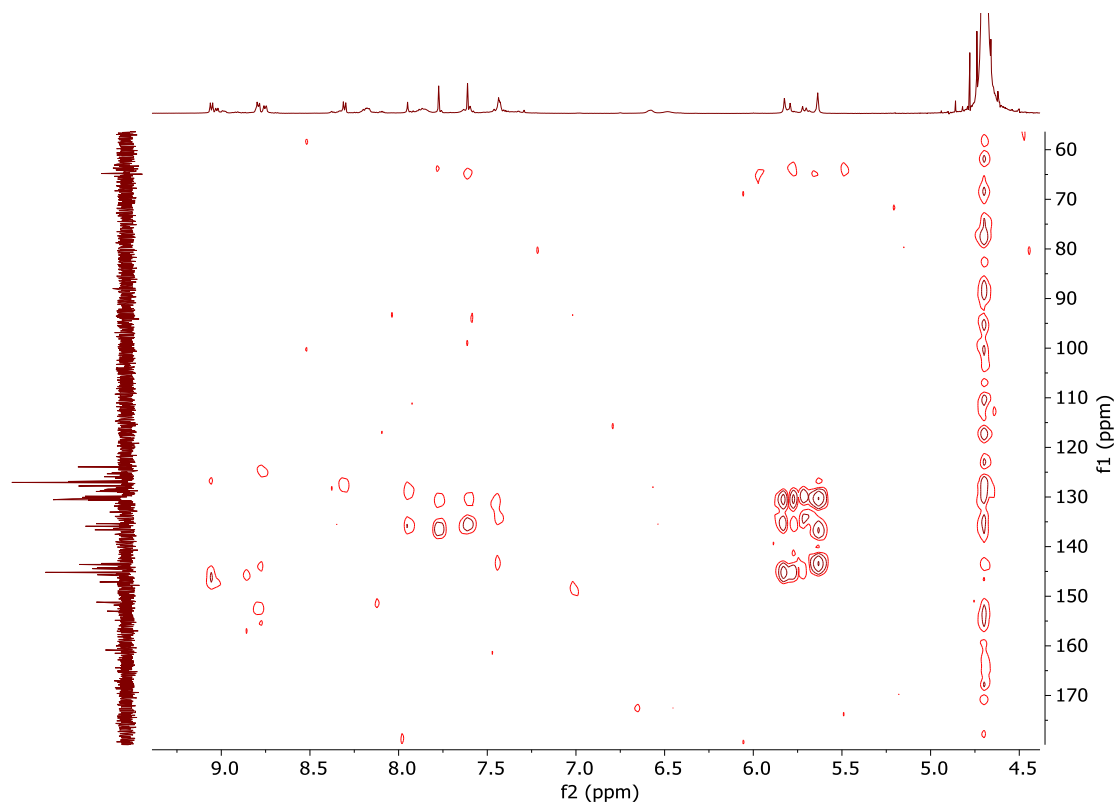


Figura 78. Espectro parcial de HMBC (D_2O , 500 MHz, 25°C) del 4CM2·4Br

5CM2·4Br: FENANTRENO

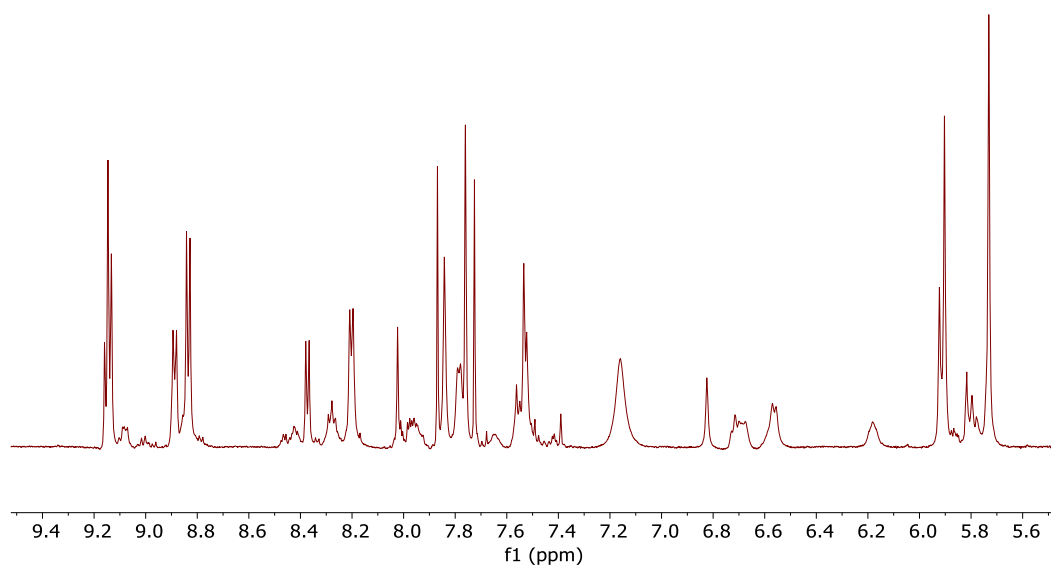


Figura 79. Espectro parcial de RMN- 1H (D_2O , 500 MHz, 25°C) de 5CM2·4Br

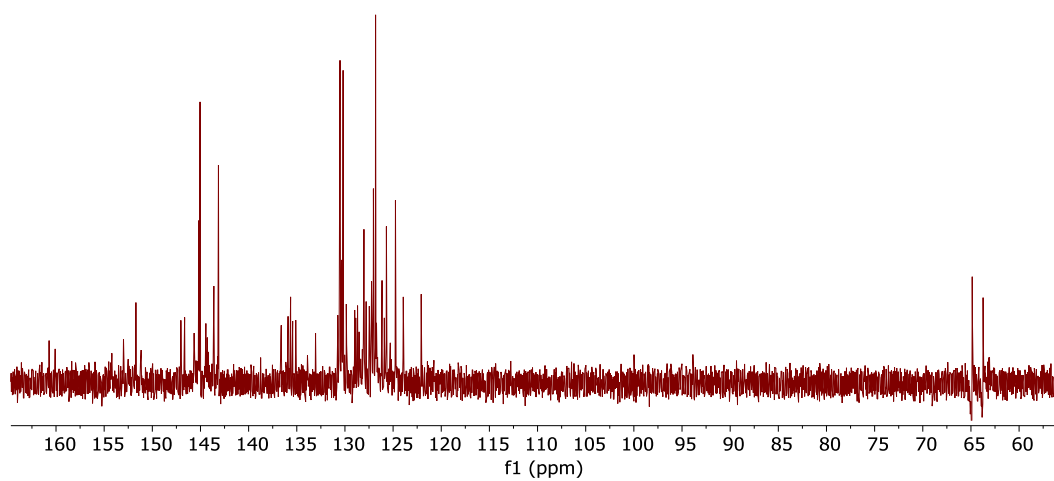


Figura 80. Espectro parcial de RMN- ^{13}C (D_2O , 125 MHz, 25°C) de 5CM2-4Br

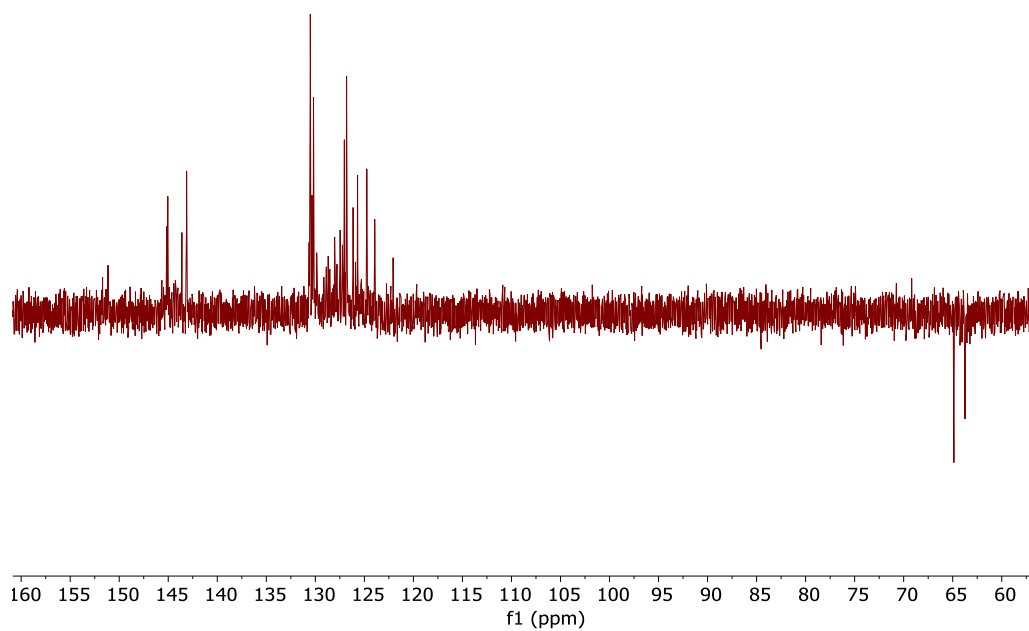


Figura 81. Espectro DEPT (D_2O , 125 MHz, 25°C) 5CM2-4Br

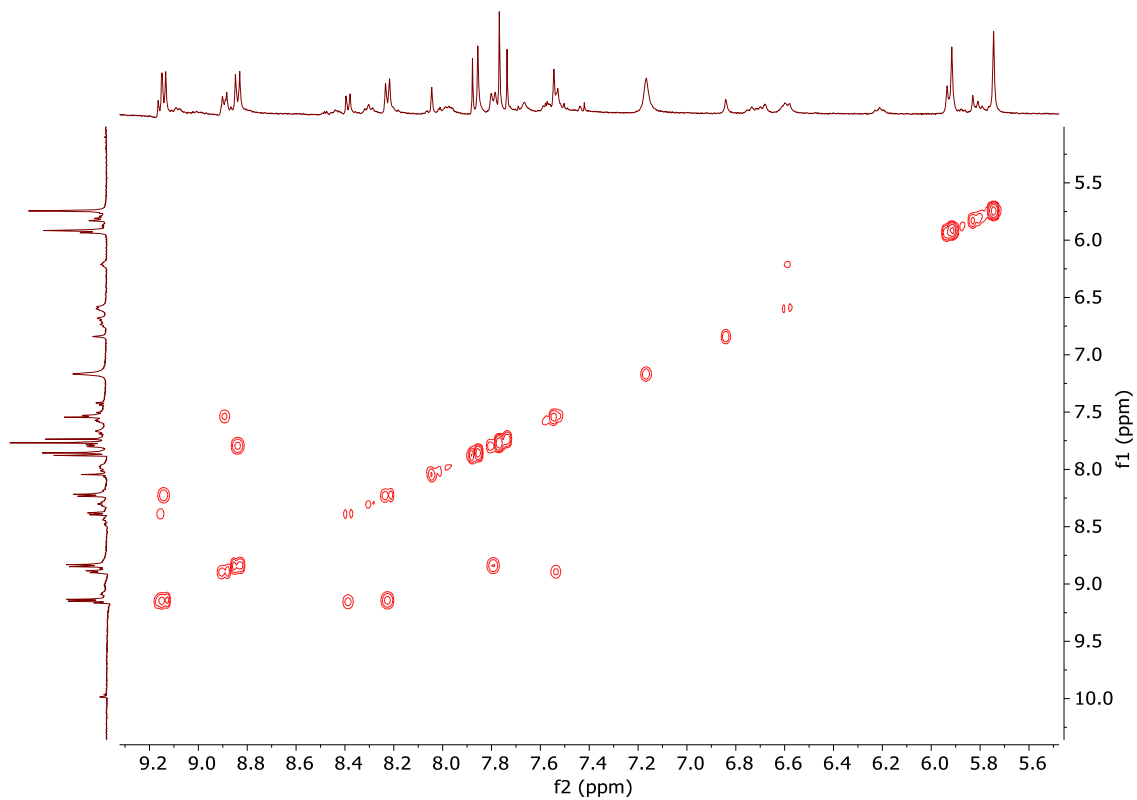


Figura 82. Espectro parcial COSY (D_2O , 400 MHz, 25°C) del 5CM2-4Br

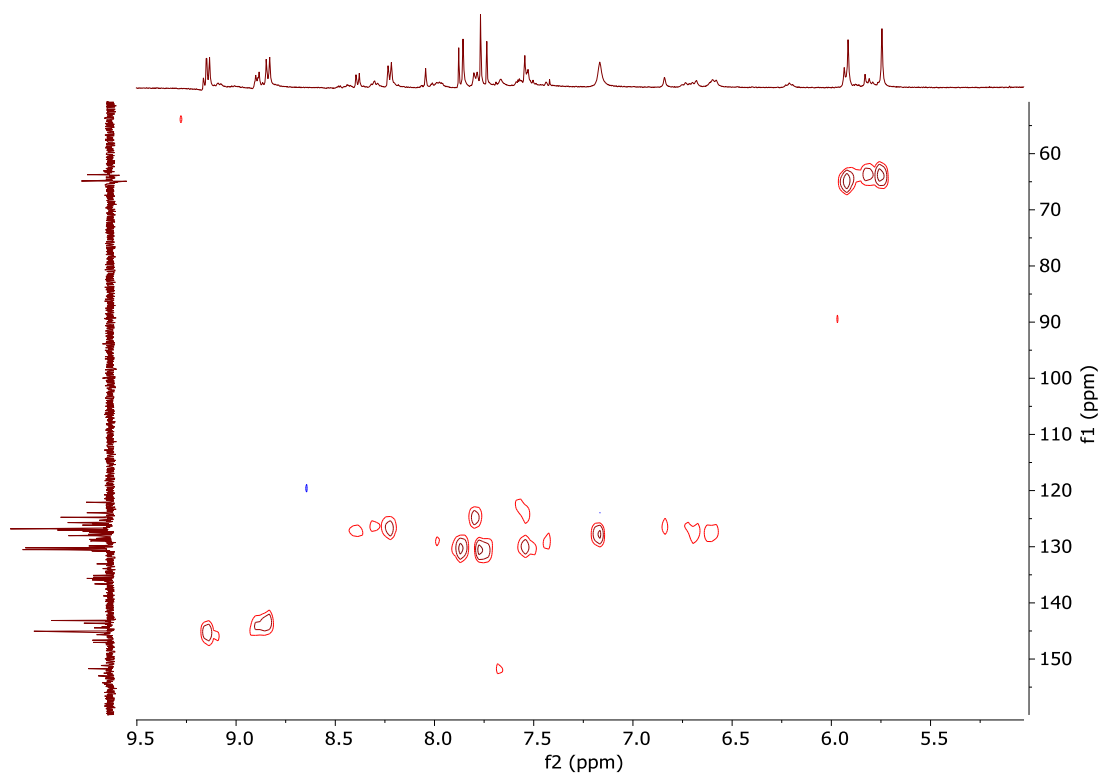


Figura 83. Espectro HSQC (D_2O , 400 MHz, 25°C) del 5CM2-4Br

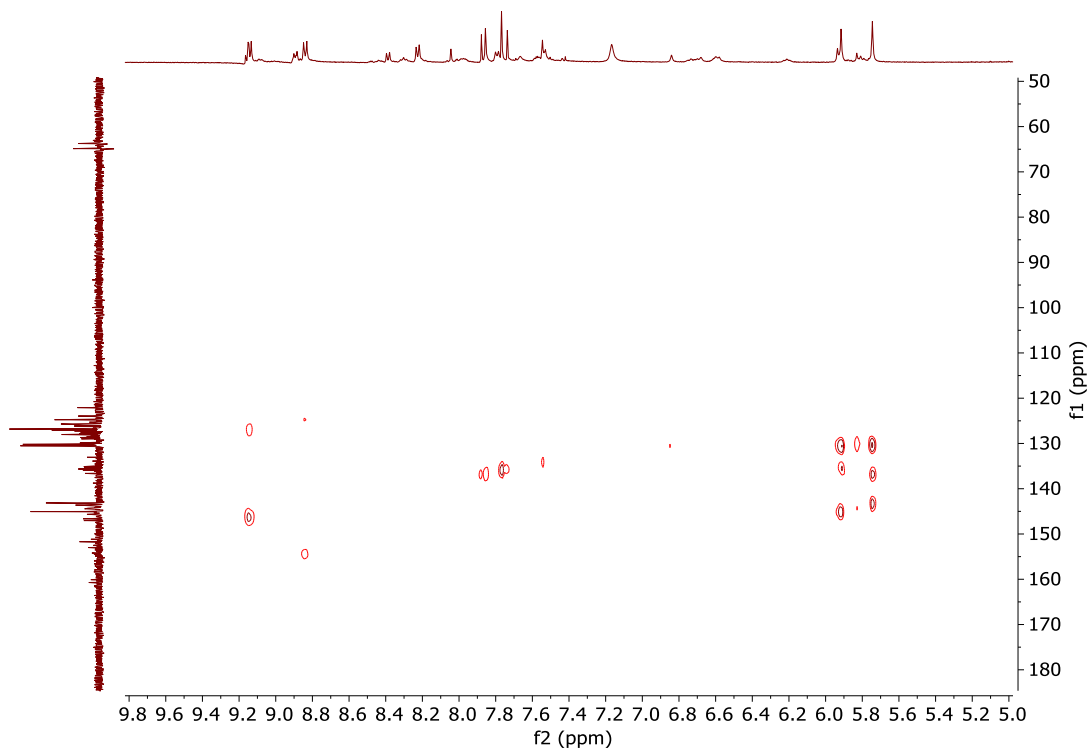


Figura 84. Espectro parcial de HMBC (D_2O , 400 MHz, 25°C) del 5CM2·4Br

6CM2·4Br: PIRENO

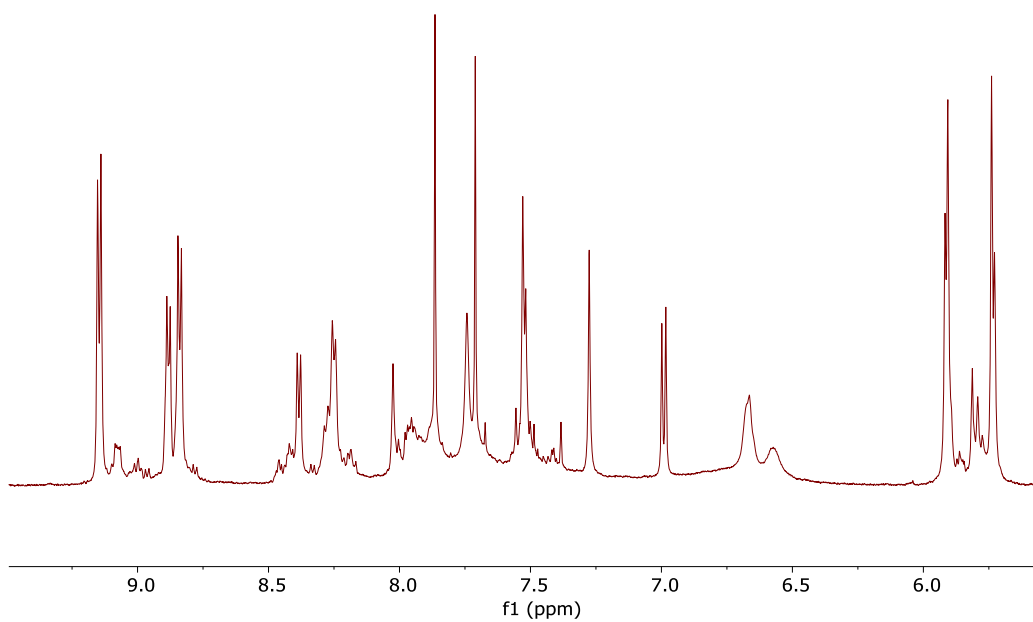


Figura 85. Espectro parcial de RMN- 1H (D_2O , 500 MHz, 25°C) de 6CM2·4Br

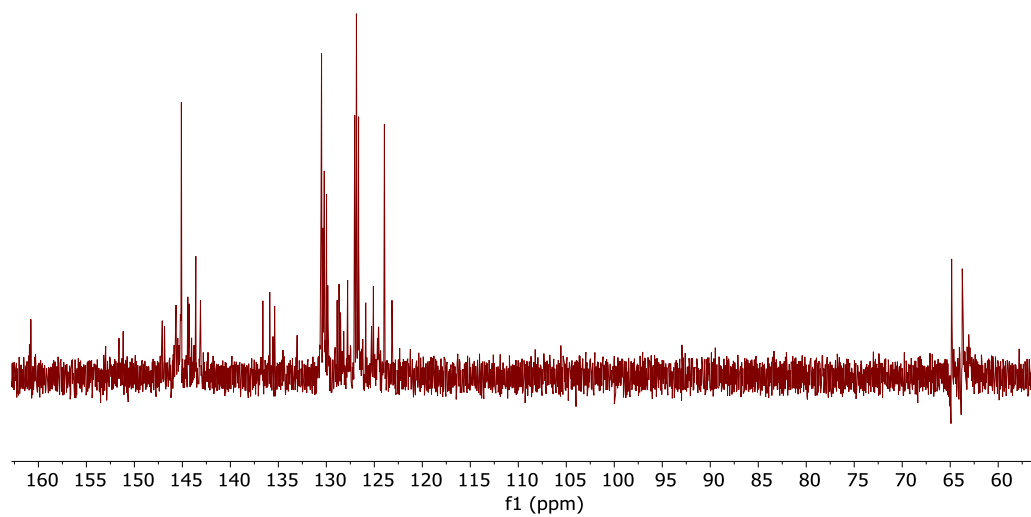


Figura 86. Espectro parcial de RMN- ^{13}C (D_2O , 125 MHz, 25°C) de 6CM2-4Br

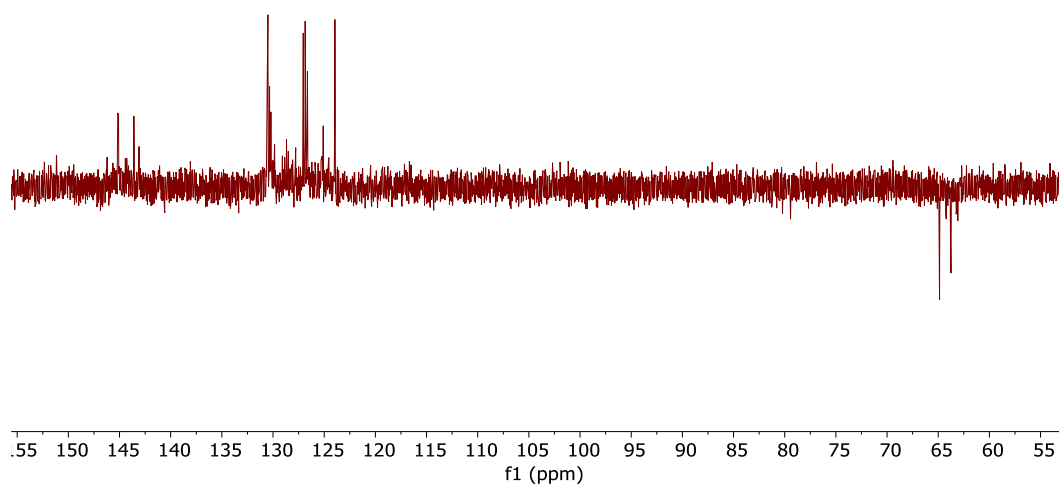


Figura 87. Espectro DEPT (D_2O , 125 MHz, 25°C) 6CM2-4Br

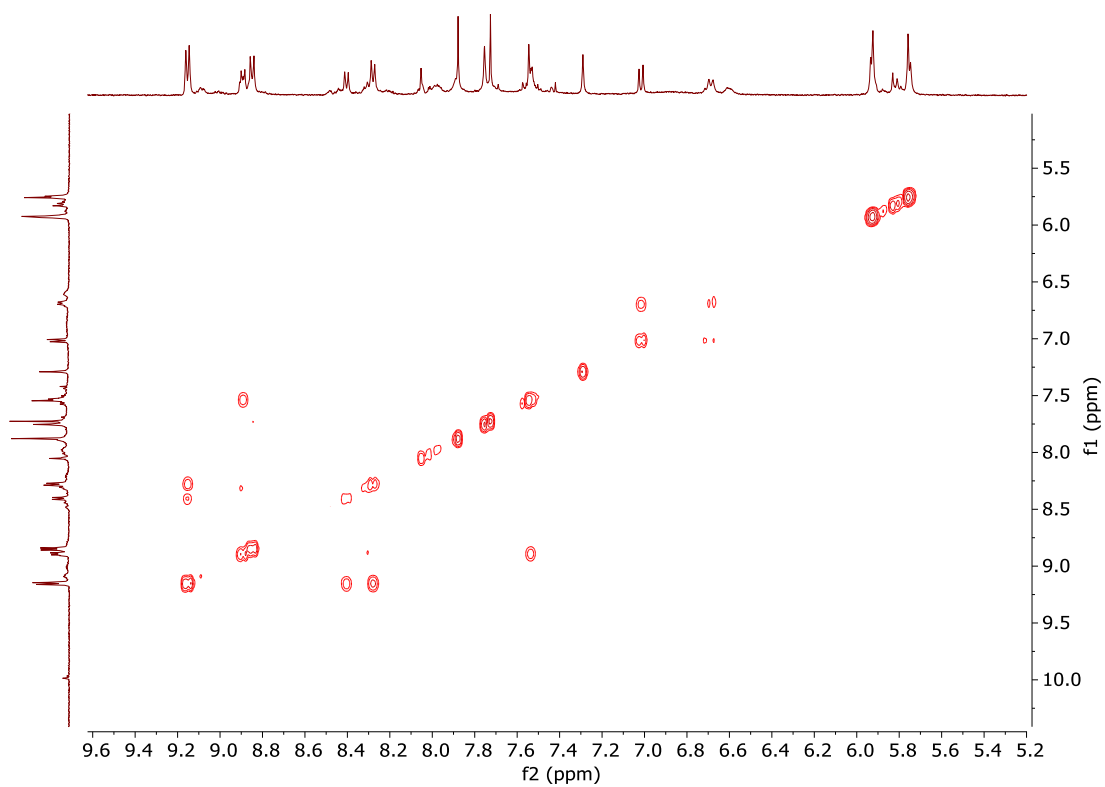


Figura 88. Espectro parcial COSY (D_2O , 400 MHz, 25°C) del 6CM2-4Br

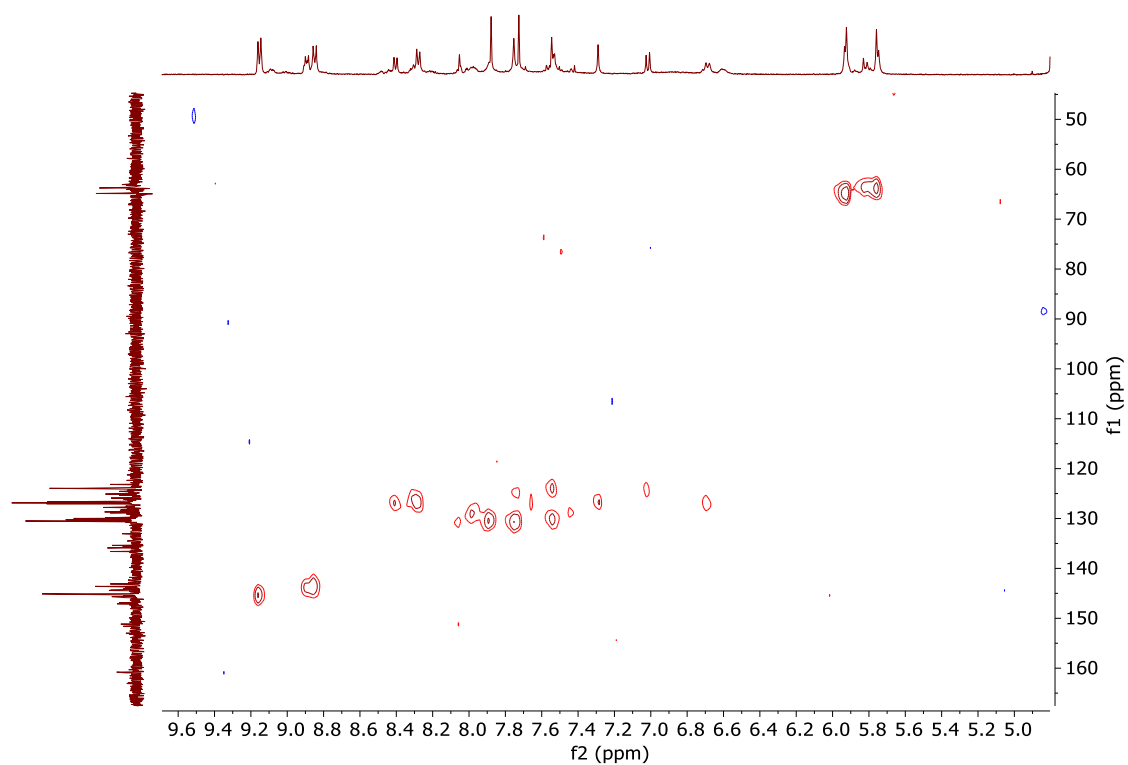


Figura 89. Espectro HSQC (D_2O , 400 MHz, 25°C) del 6CM2-4Br

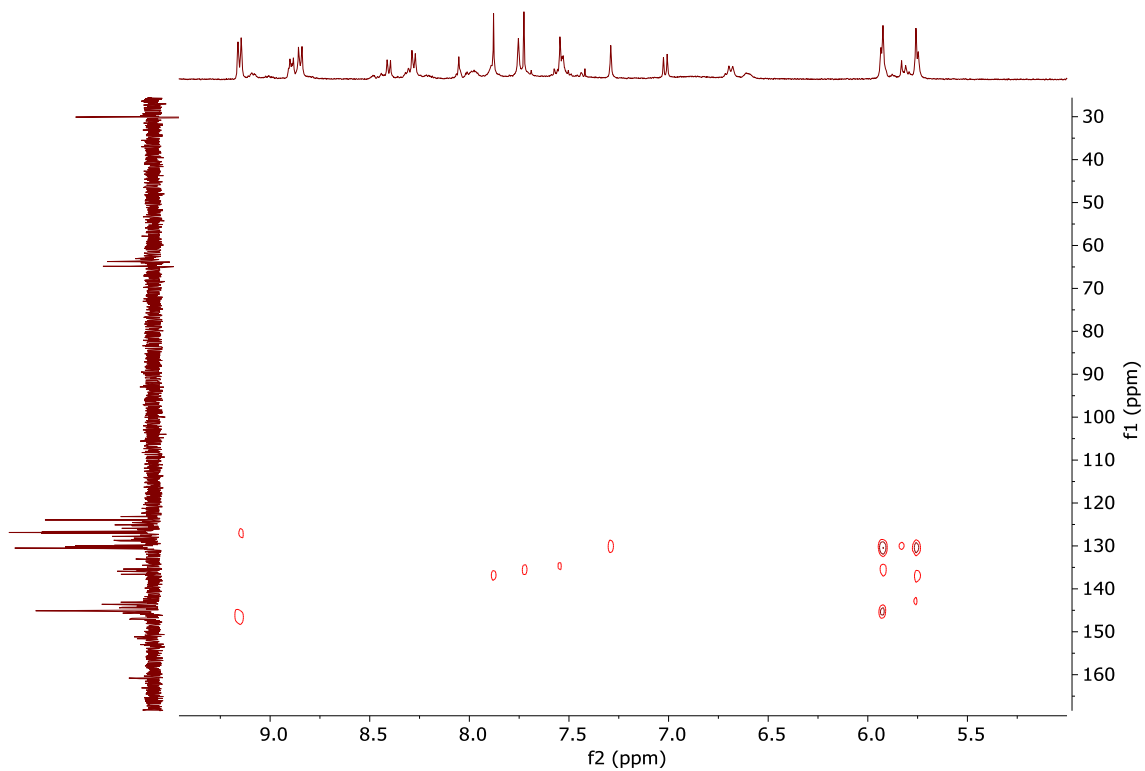


Figura 90. Espectro parcial de HMBC (D_2O , 400 MHz, 25°C) del 6CM2-4Br

1CM1.4PF₆

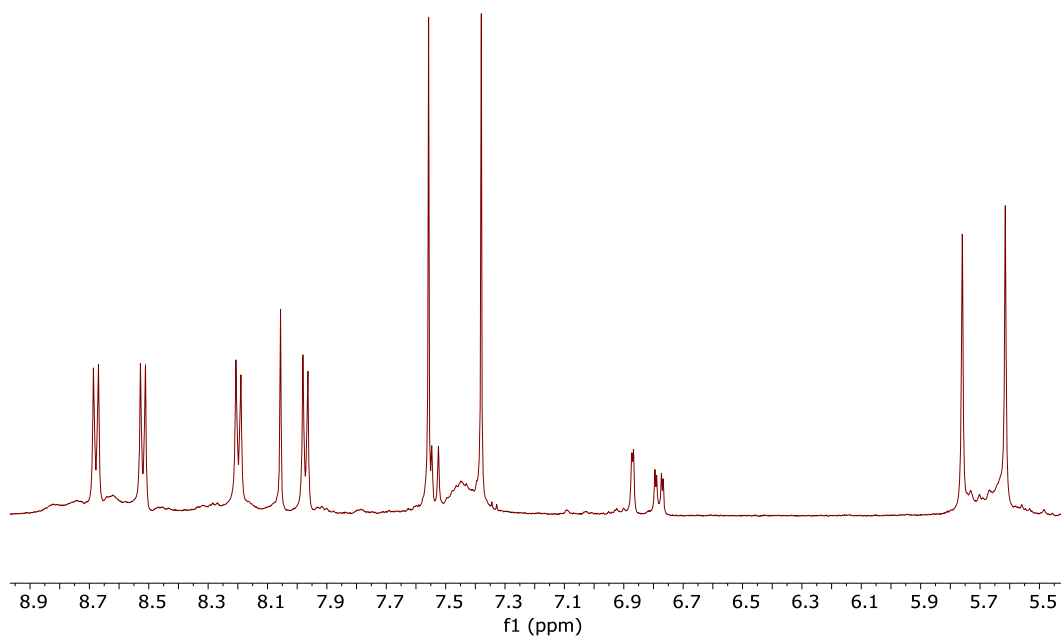
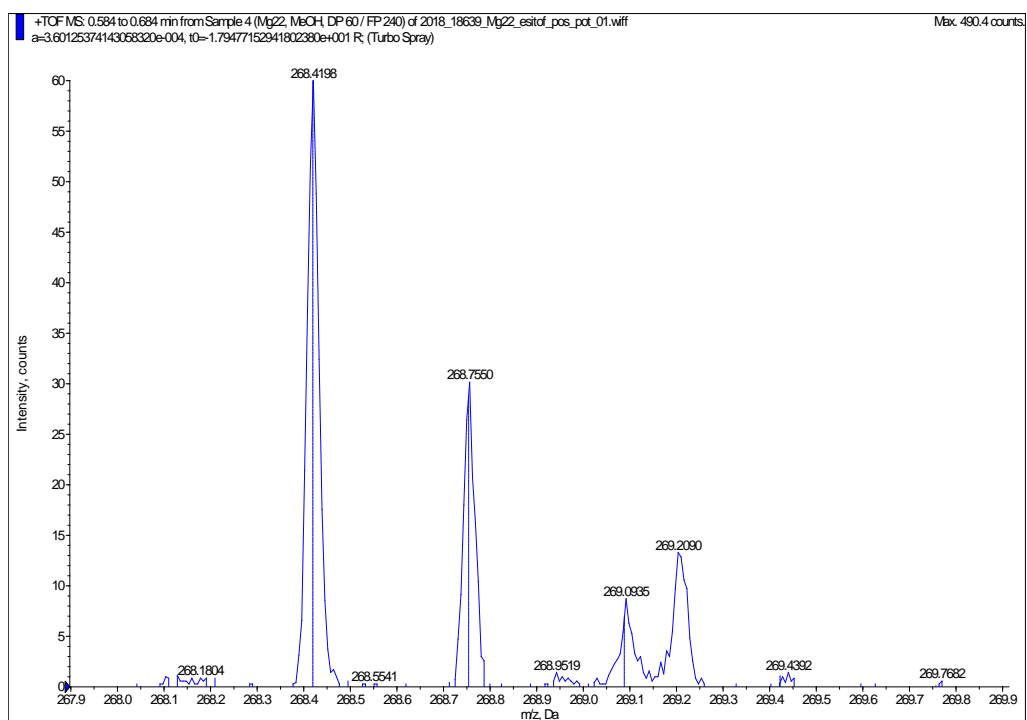


Figura 91. Espectro parcial de RMN-¹H (CD_3CN , 400 MHz, 25°C) de 1CM1.4PF₆



m/z experimental	268.4198	Notas:		
Fórmula	m/z teórico	Erro, mDa	Erro en ppm	Equivalencia de dobles enlaces
C40 H36 N8 O2 F6 P	268.4195	0.74	0.919	24.5

1CM1·4NO₃

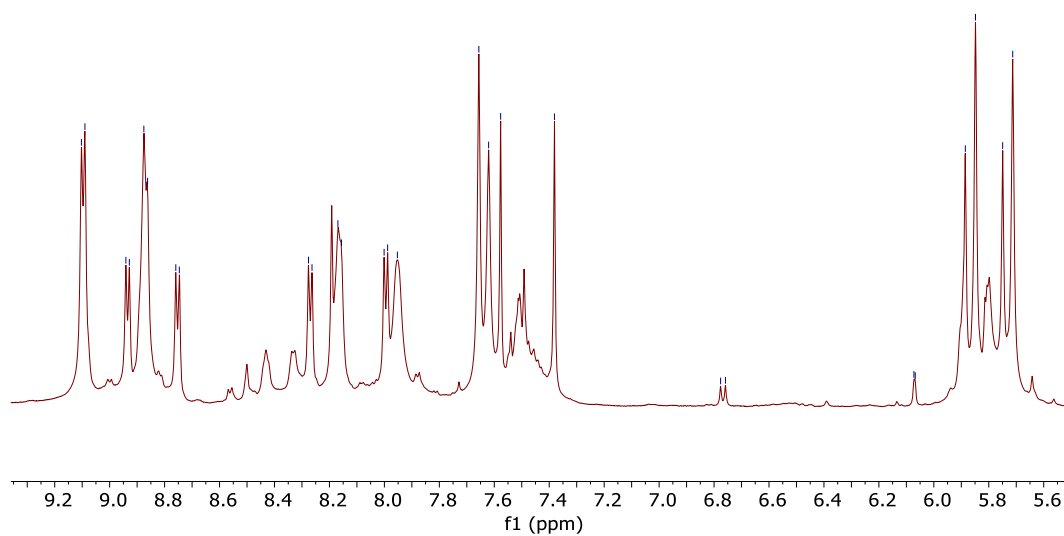


Figura 92. Espectro parcial de RMN-¹H (D₂O, 500 MHz, 25°C) de 1CM1·4NO₃

1CM1·4Cl

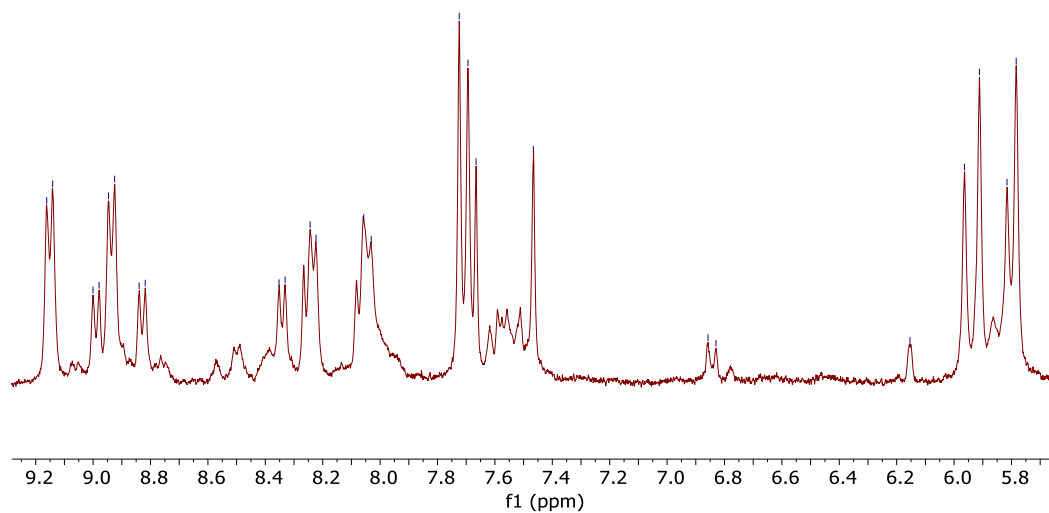


Figura 93. Espectro parcial de RMN-¹H (D₂O, 300 MHz, 25°C) de 1CM1·4Cl

1CM1·4Cl (sólido gris obtenido en la columna flash)

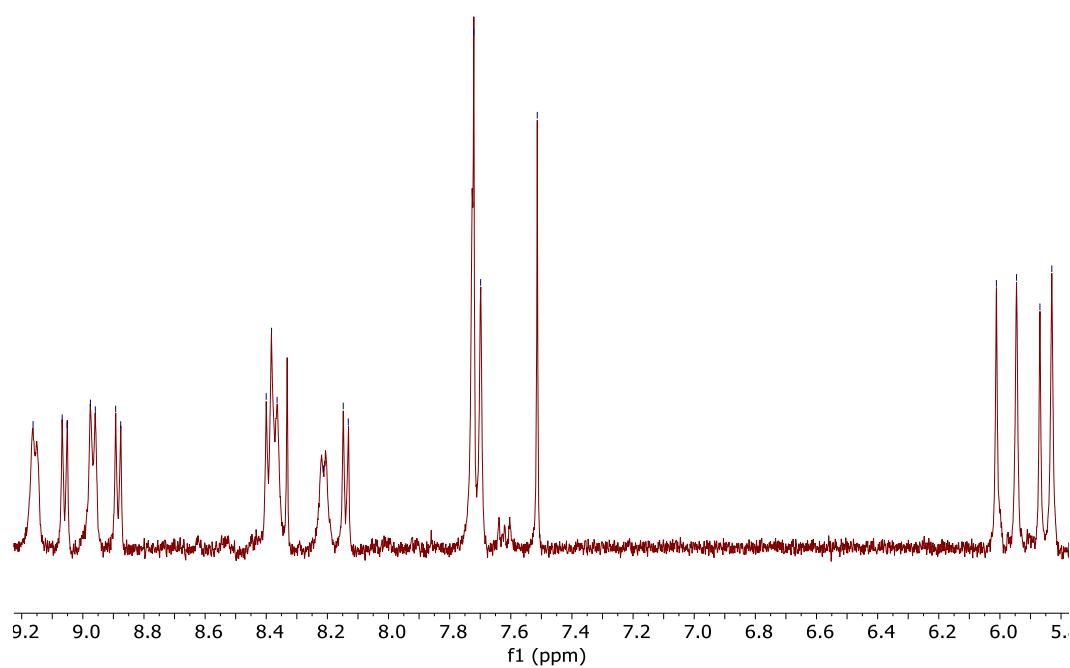
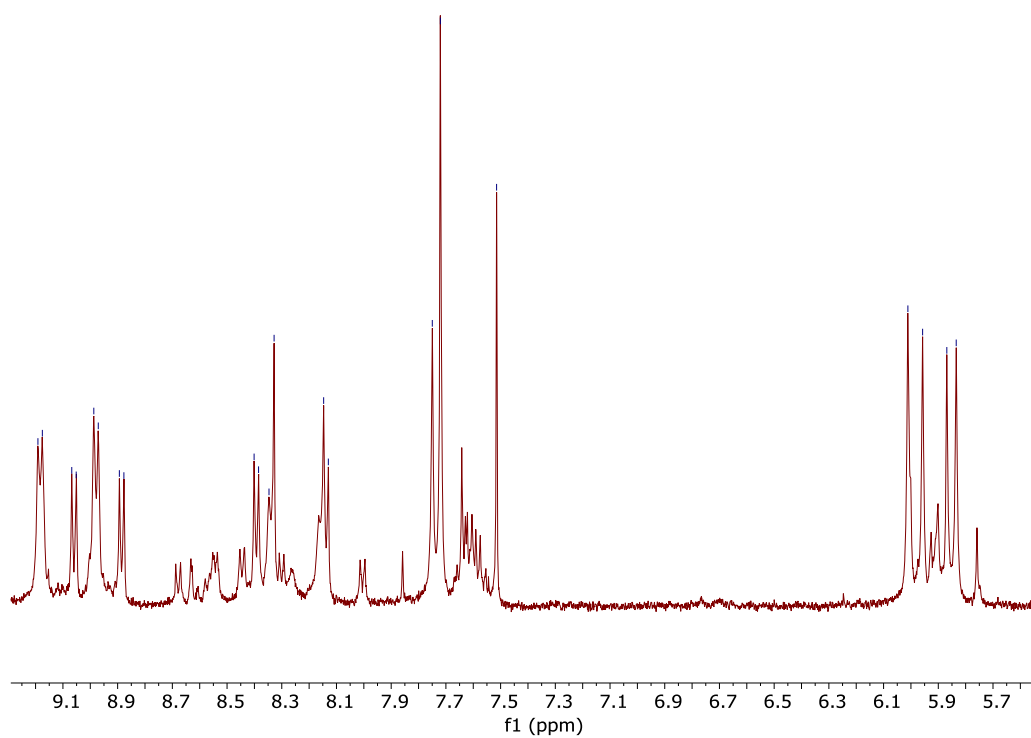
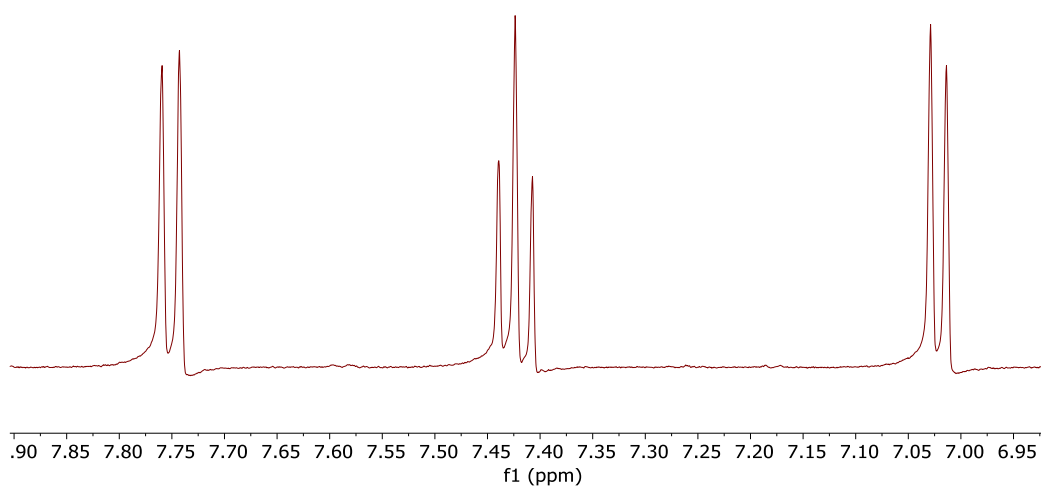


Figura 94. Espectro parcial de RMN-¹H (D₂O, 400 MHz, 25°C) de 1CM1·4Cl

1CM1·4PF₆ (Purificado por columna flash)Figura 95. Espectro parcial de RMN-¹H (D₂O, 400 MHz, 25°C) de 1CM1·4PF₆

1,5-DIHIDROXINAFTALENO

Figura 96. Espectro parcial de RMN-¹H (D₂O, 500 MHz, 25°C) de 1,5-Dihidroxi-naftaleno

2,7-DIHIDROXINAFTALENO

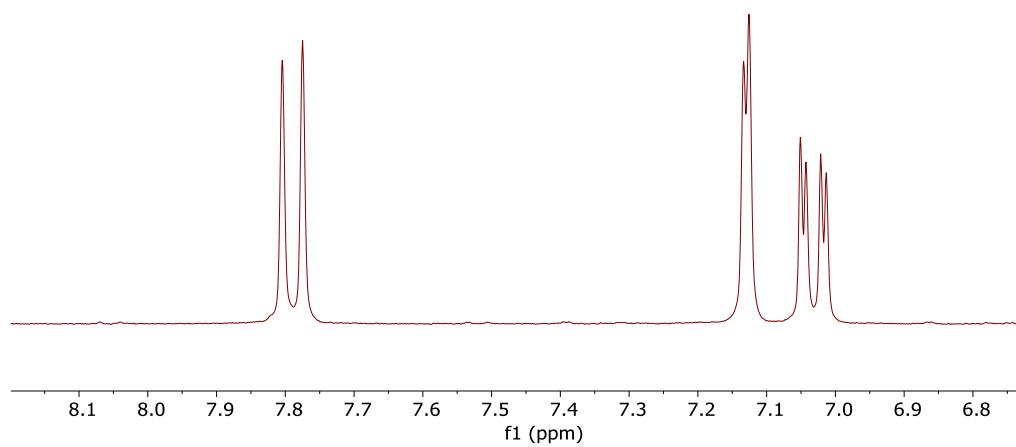


Figura 97. Espectro parcial de RMN-¹H (D₂O, 500 MHz, 25°C) de 2,7-Dihidroxi-naftaleno