

Supplementary Material

Lactones from the Sponge-Derived Fungus *Talaromyces rugulosus*

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§ L. Küppers and W. Ebrahim contributed equally to this study

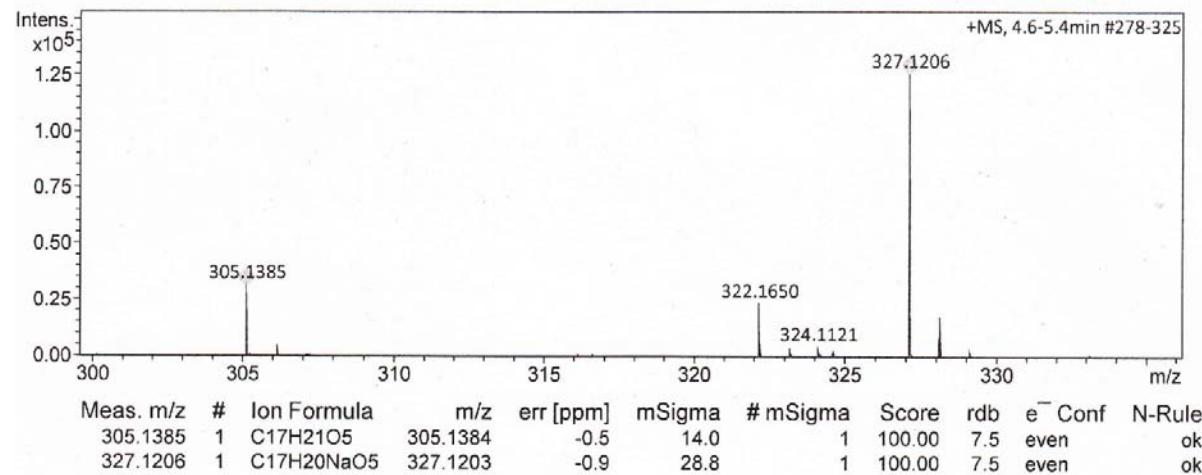
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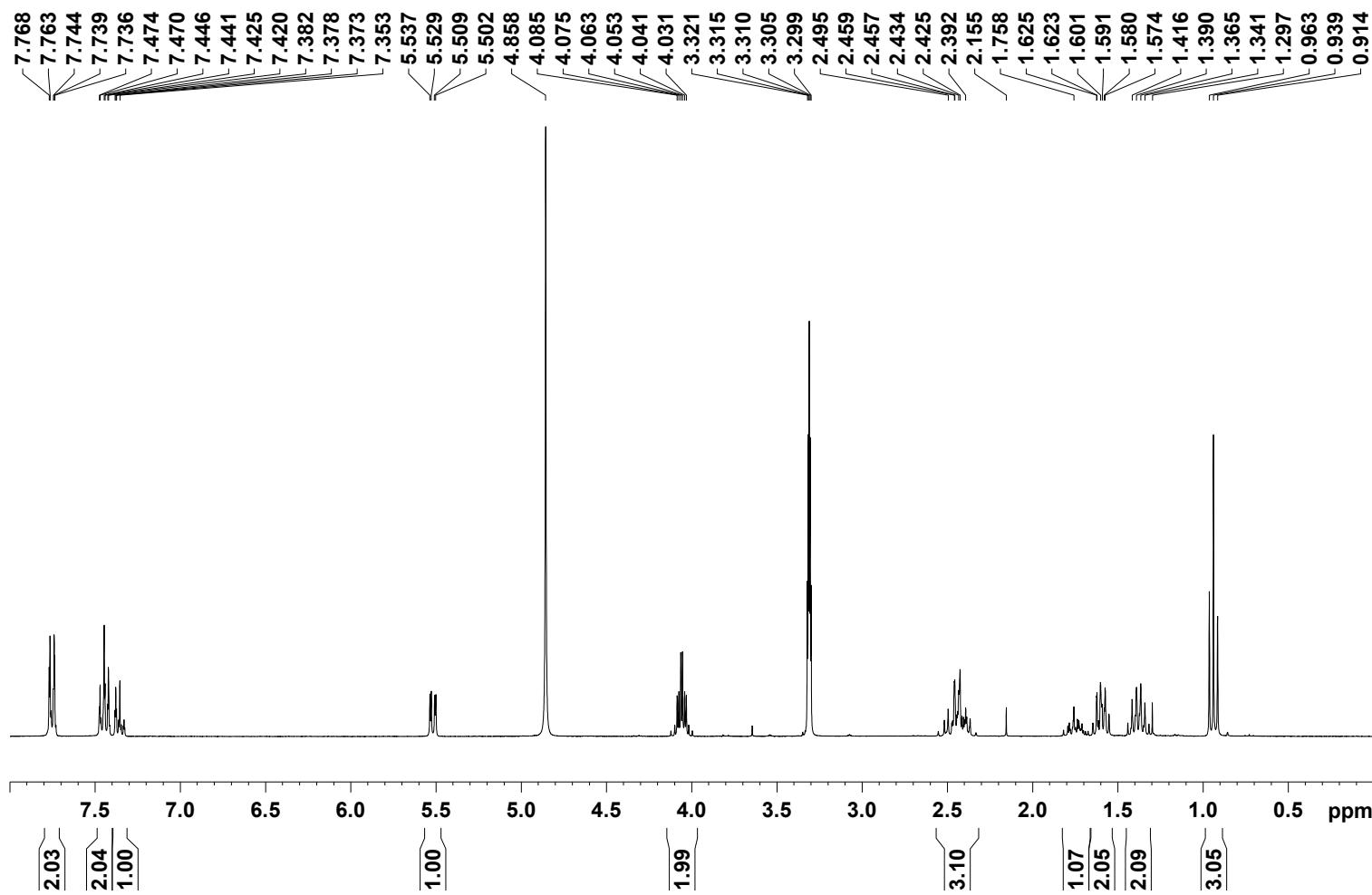
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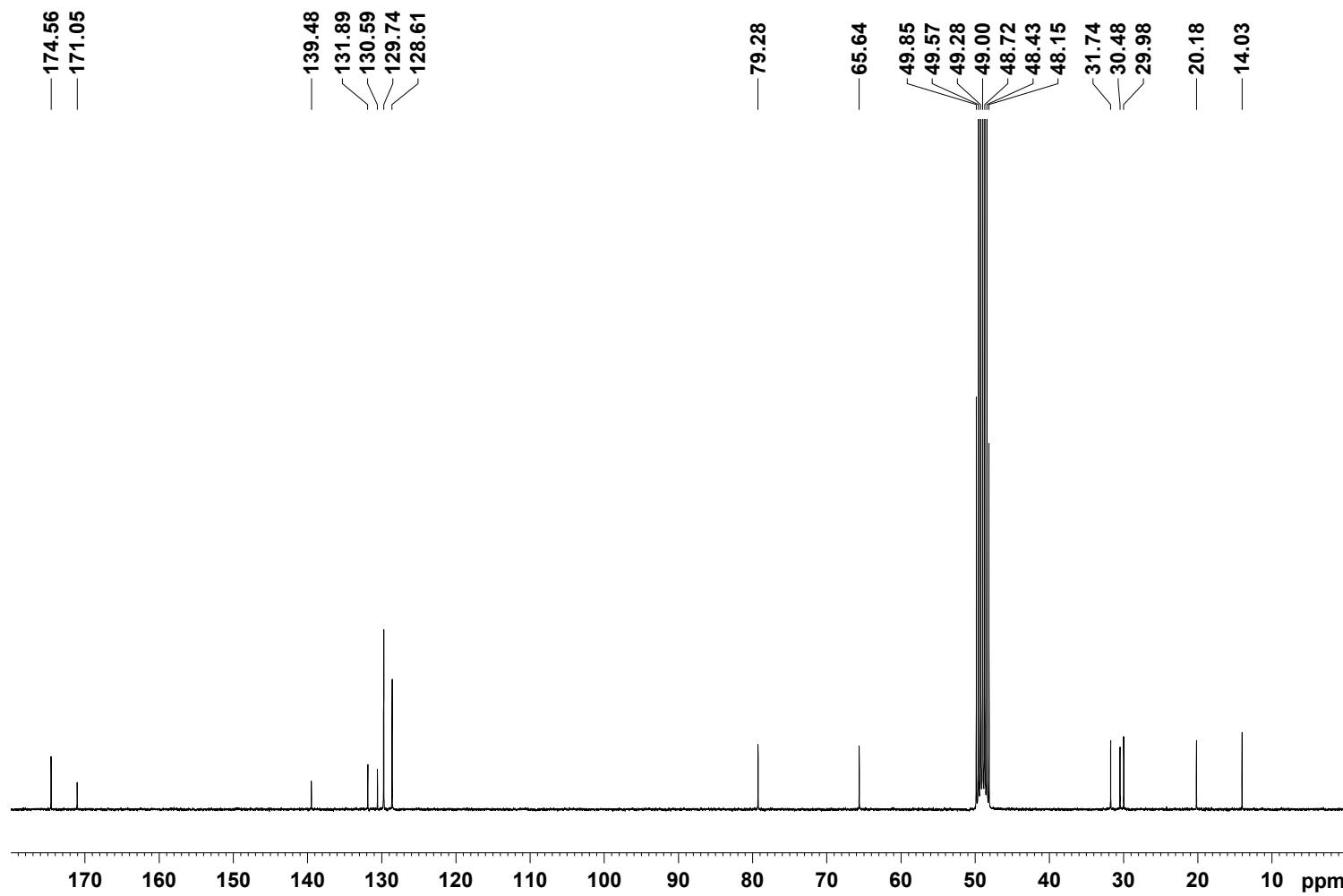
S1. HRESIMS spectrum of compound **1**.

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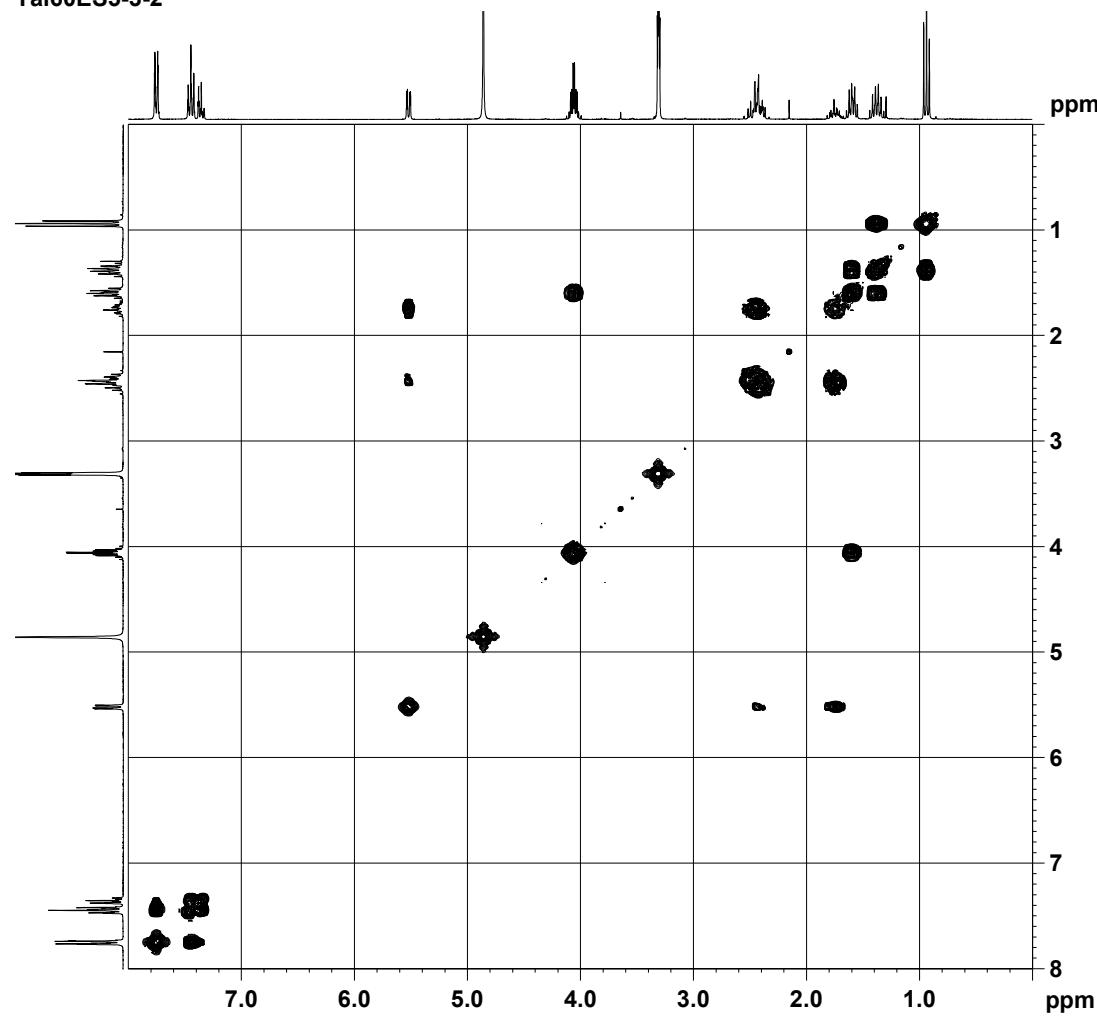
S2. ^1H NMR (300 MHz, CD_3OD) spectrum of compound 1.

Tal60ES5-3-2

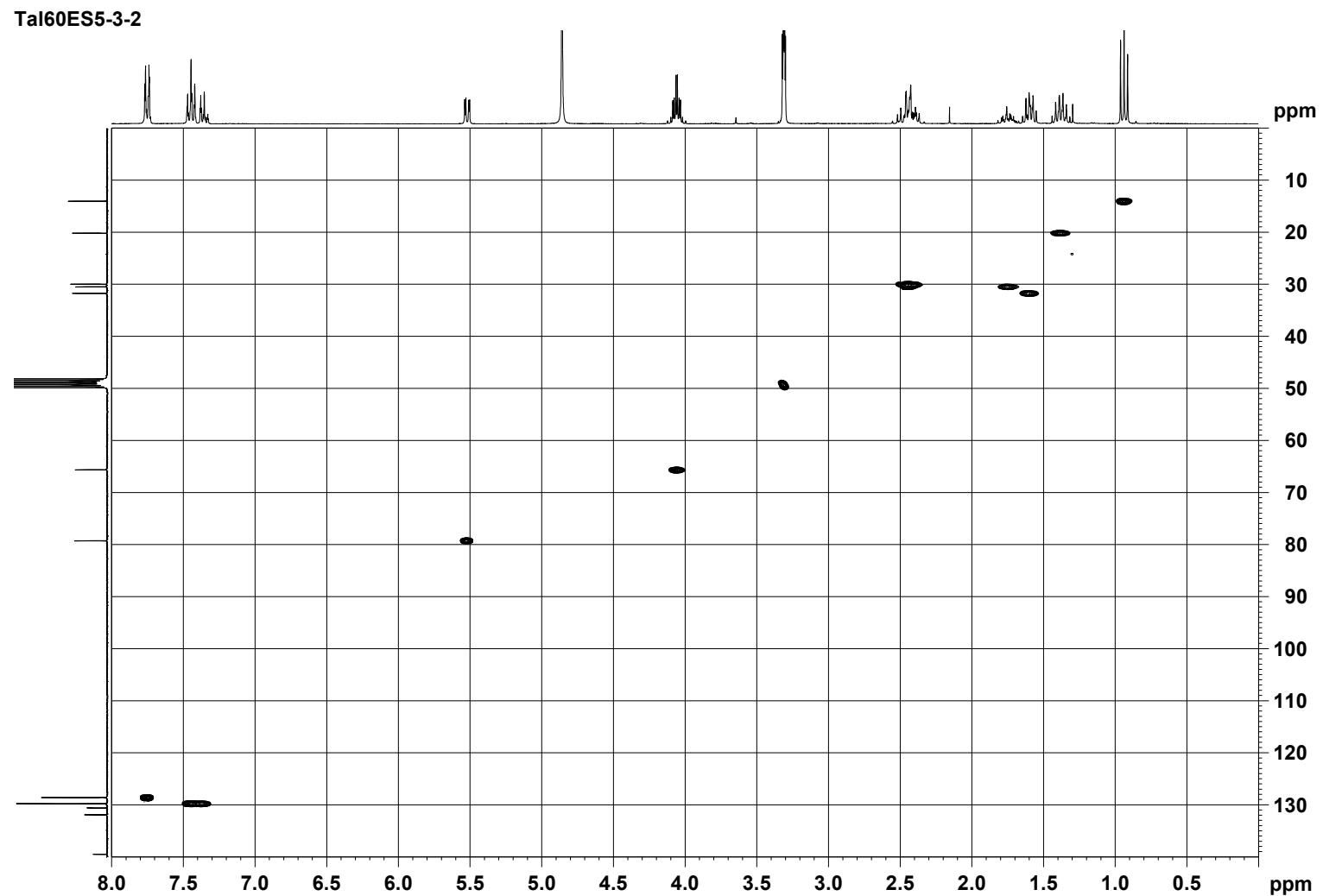


S3. ^{13}C NMR (75 MHz, CD_3OD) spectrum of compound 1.

Tal60ES5-3-2

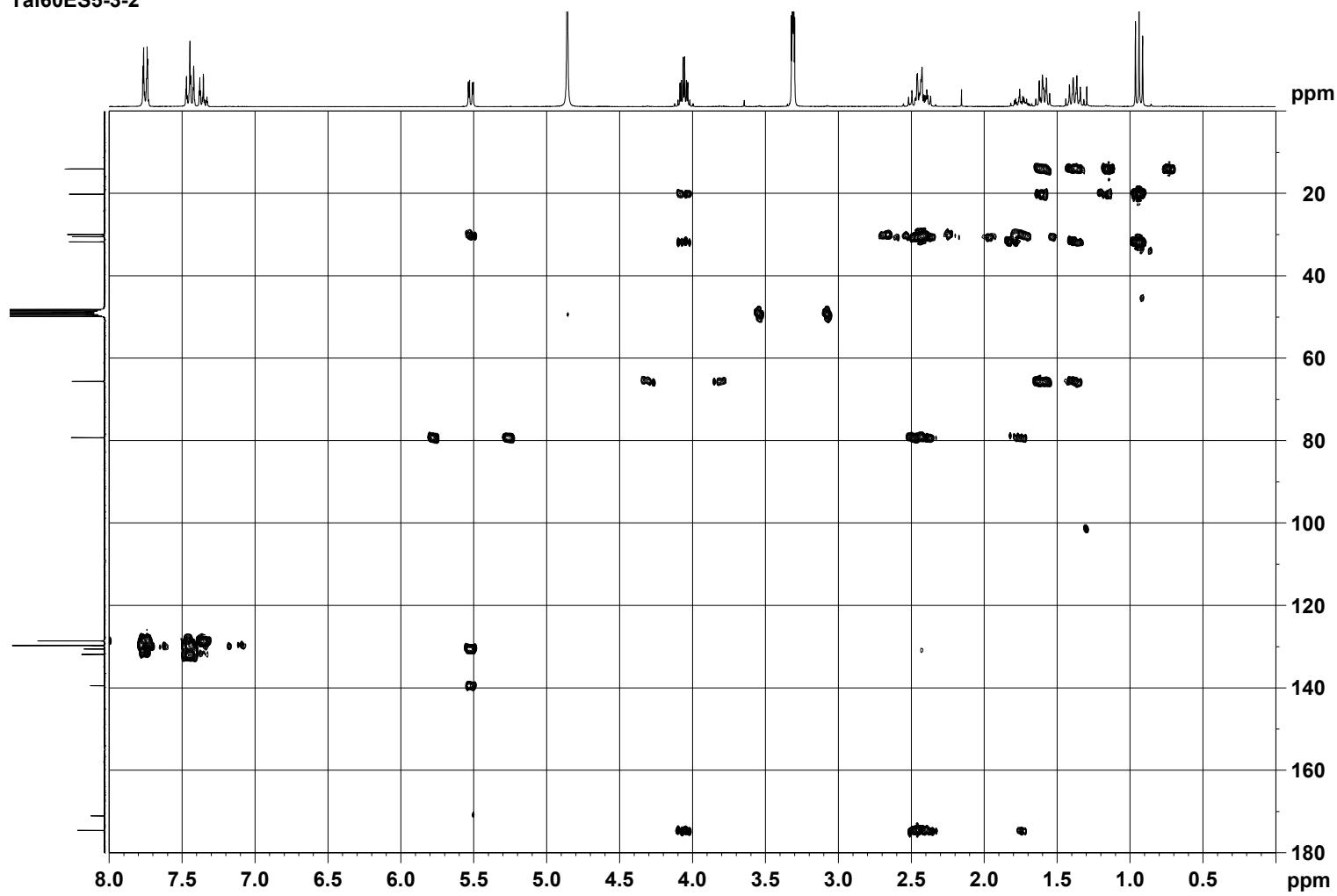


S4. ^1H - ^1H COSY (300 MHz, CD_3OD) spectrum of compound 1.

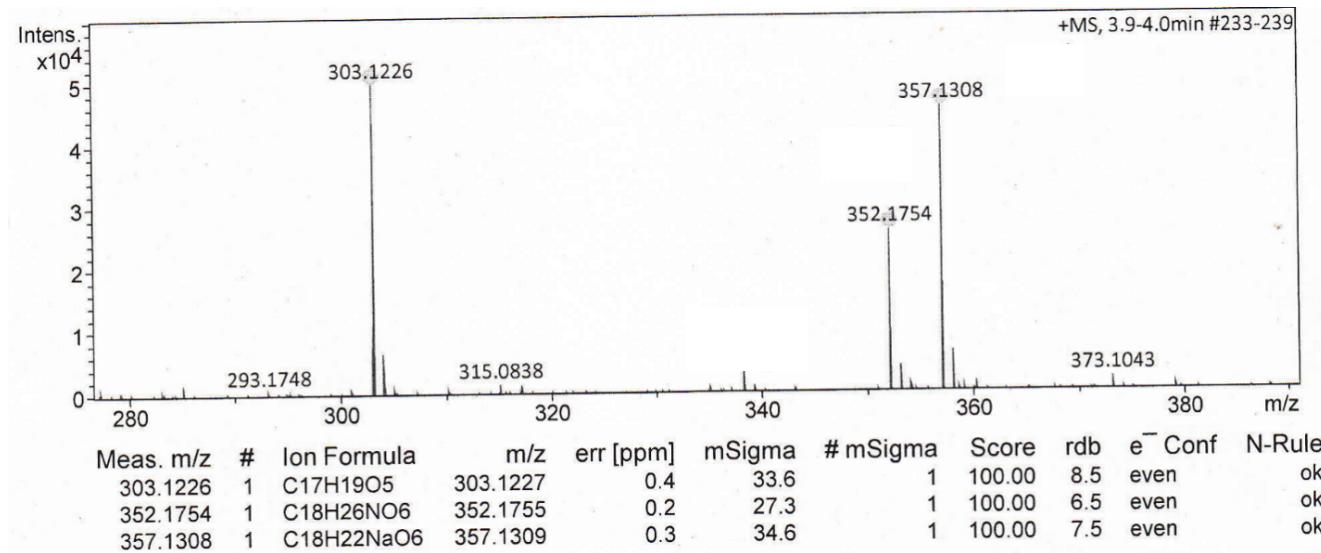


S5. HSQC (300 and 75 MHz, CD₃OD) spectrum of compound **1**.

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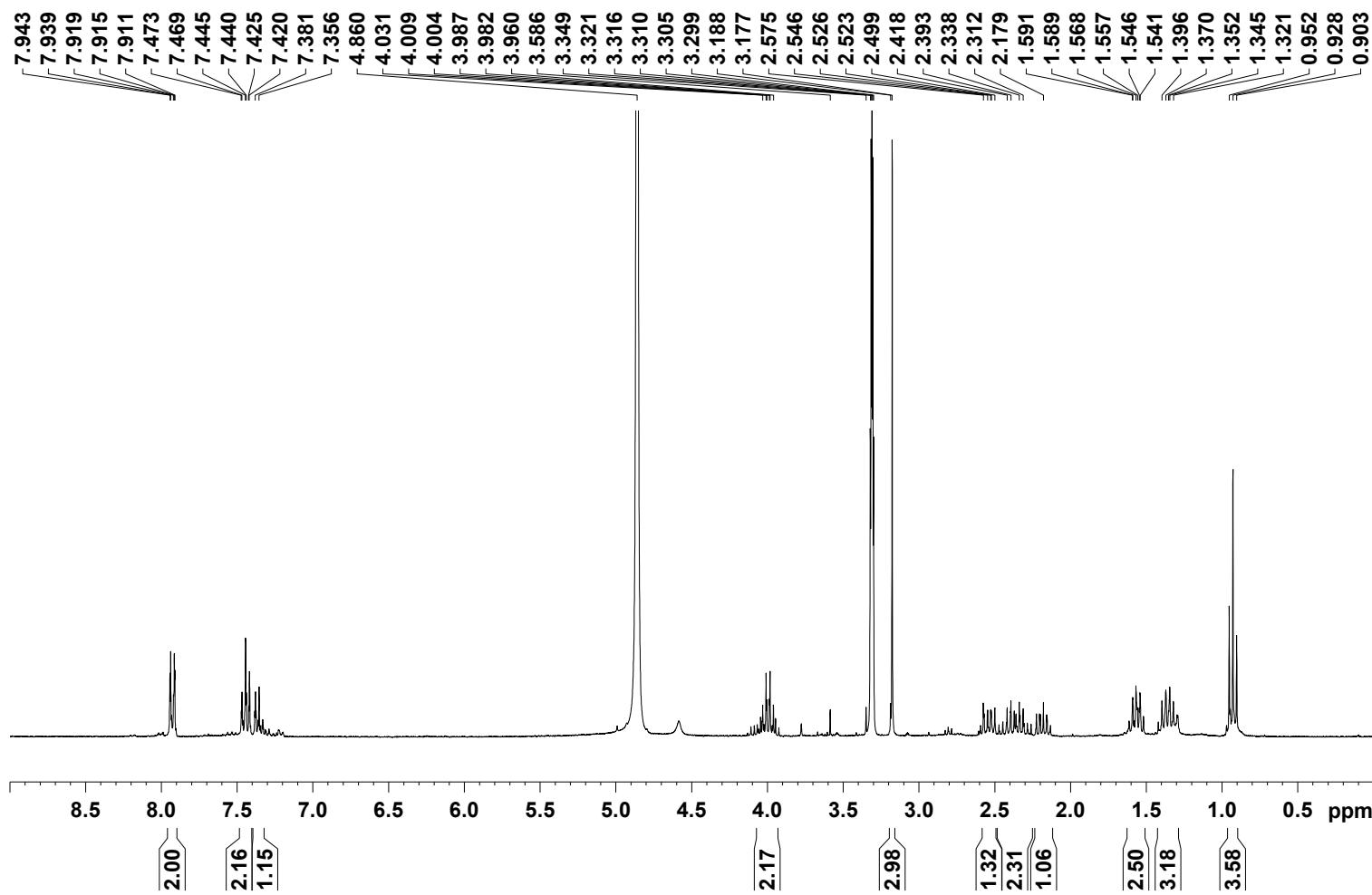


S6. HMBC (300 and 75 MHz, CD_3OD) spectrum of compound 1.



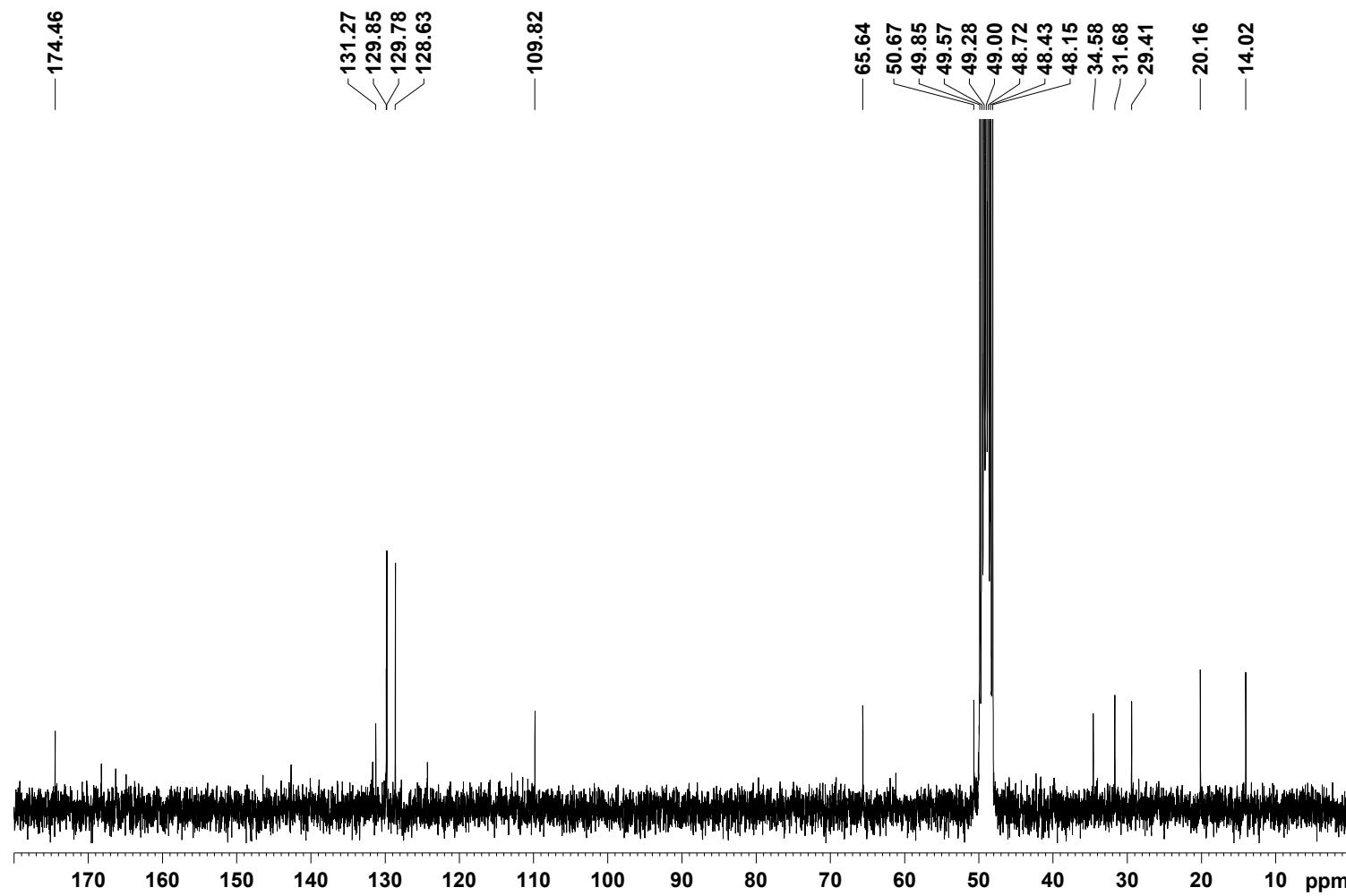
S7. HRESIMS spectrum of compound 2.

Tal80ES 3-3-6-15/15'



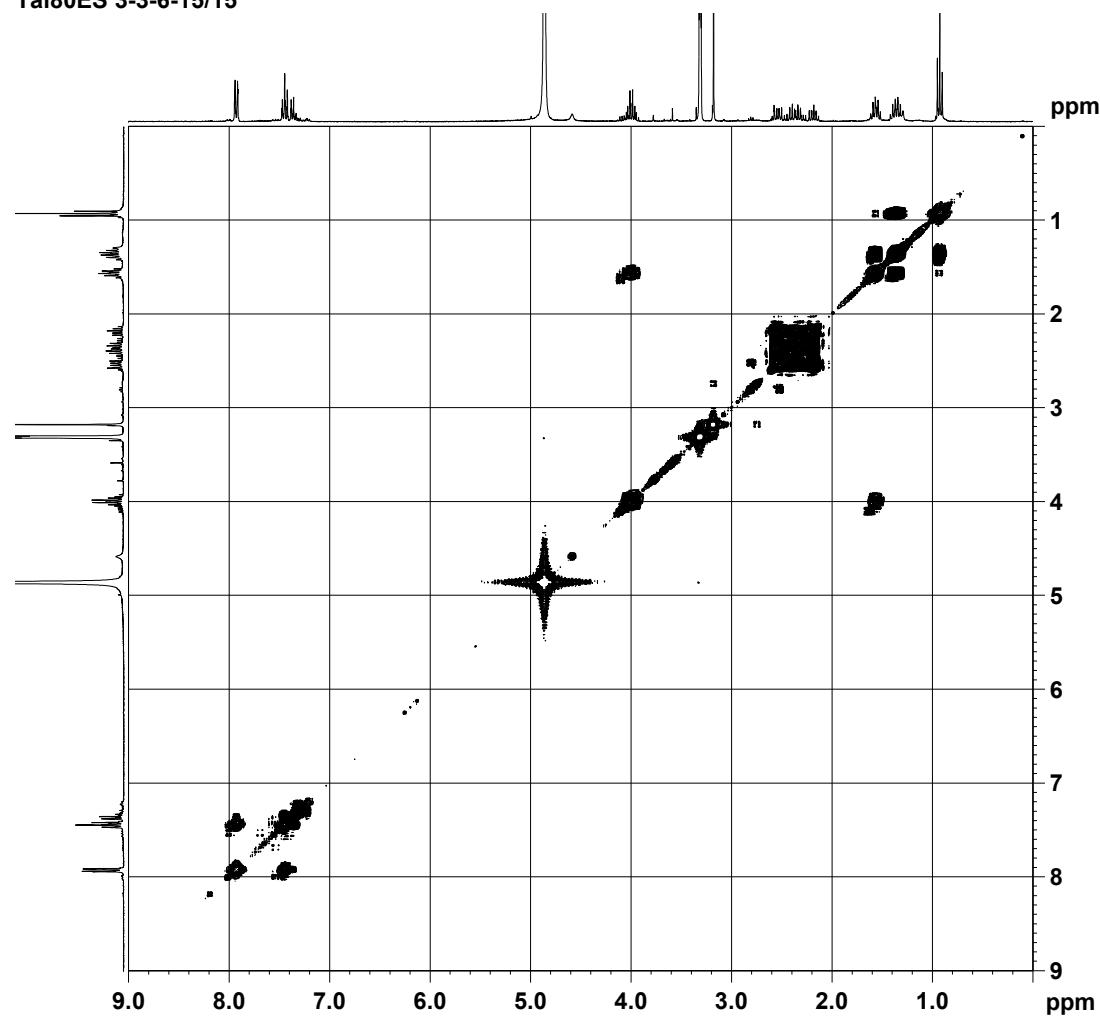
S8. ^1H NMR (300 MHz, CD_3OD) spectrum of compound 2.

Tal80ES 3-3-6-15/15'



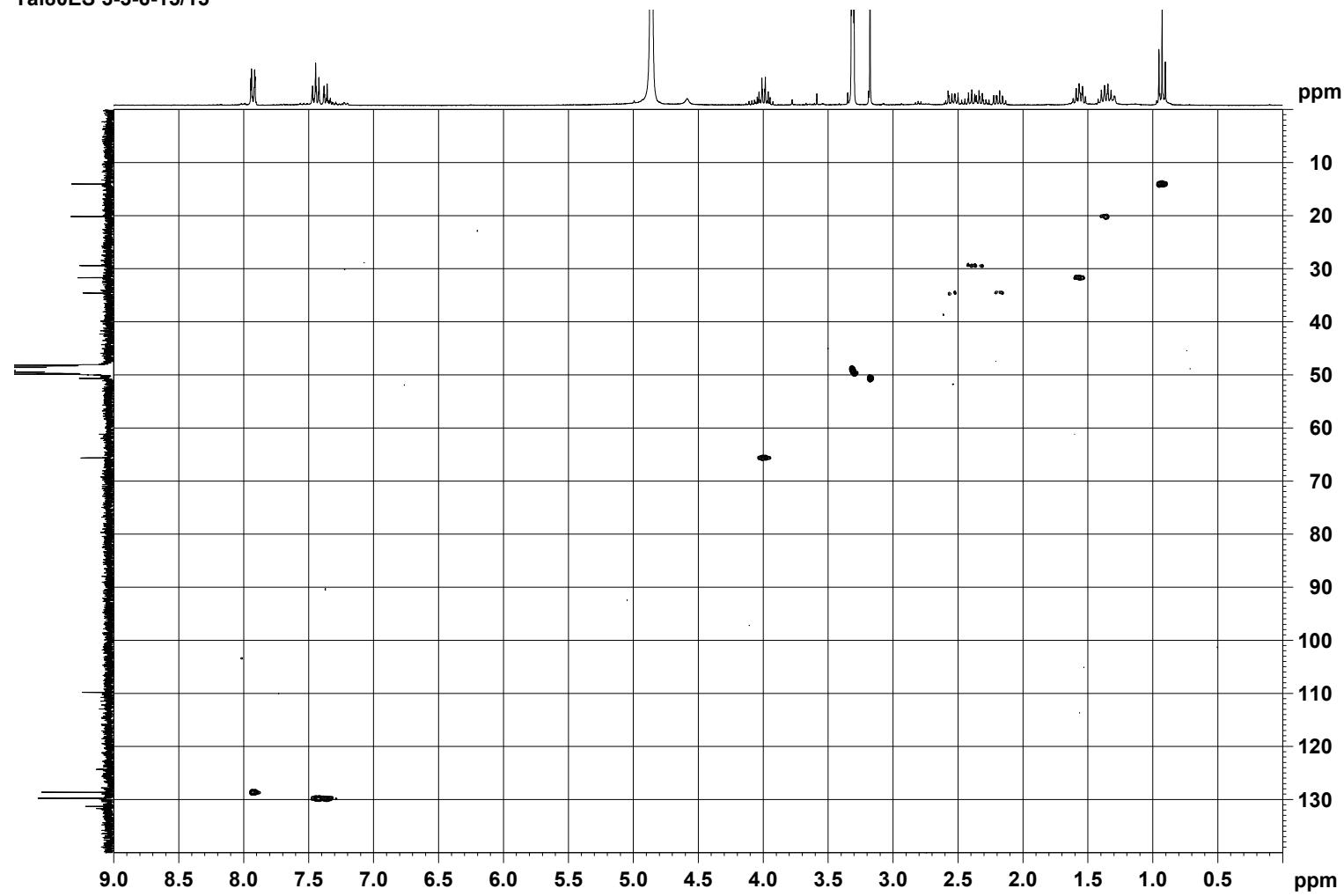
S9. ^{13}C NMR (75 MHz, CD_3OD) spectrum of compound 2.

Tal80ES 3-3-6-15/15'



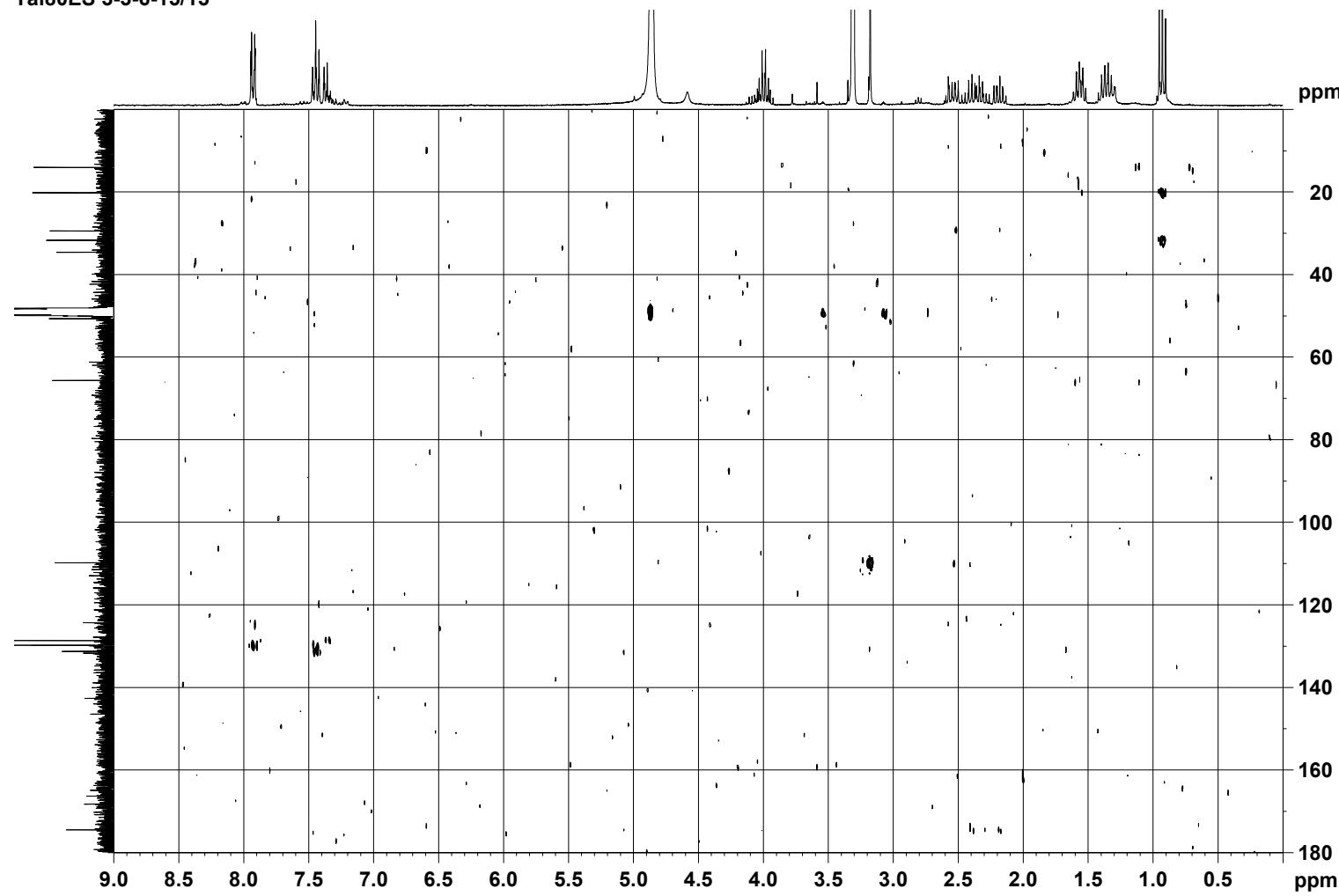
S10. ^1H - ^1H COSY (300 MHz, CD_3OD) spectrum of compound 2.

Tal80ES 3-3-6-15/15'

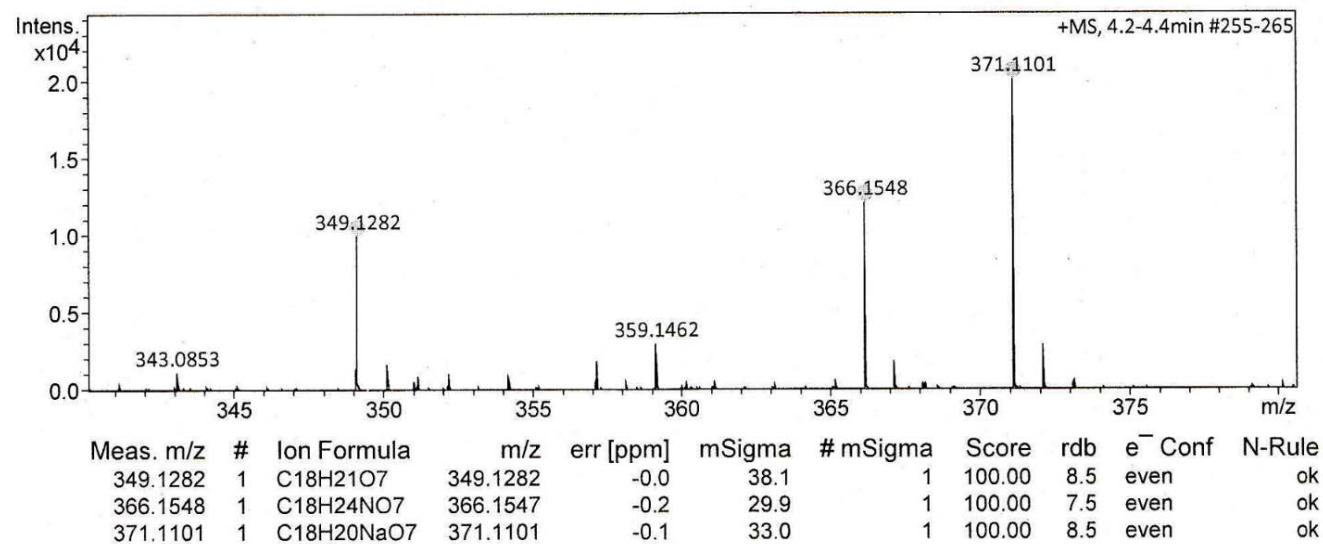


S11. HSQC (300 and 75 MHz, CD₃OD) spectrum of compound 2.

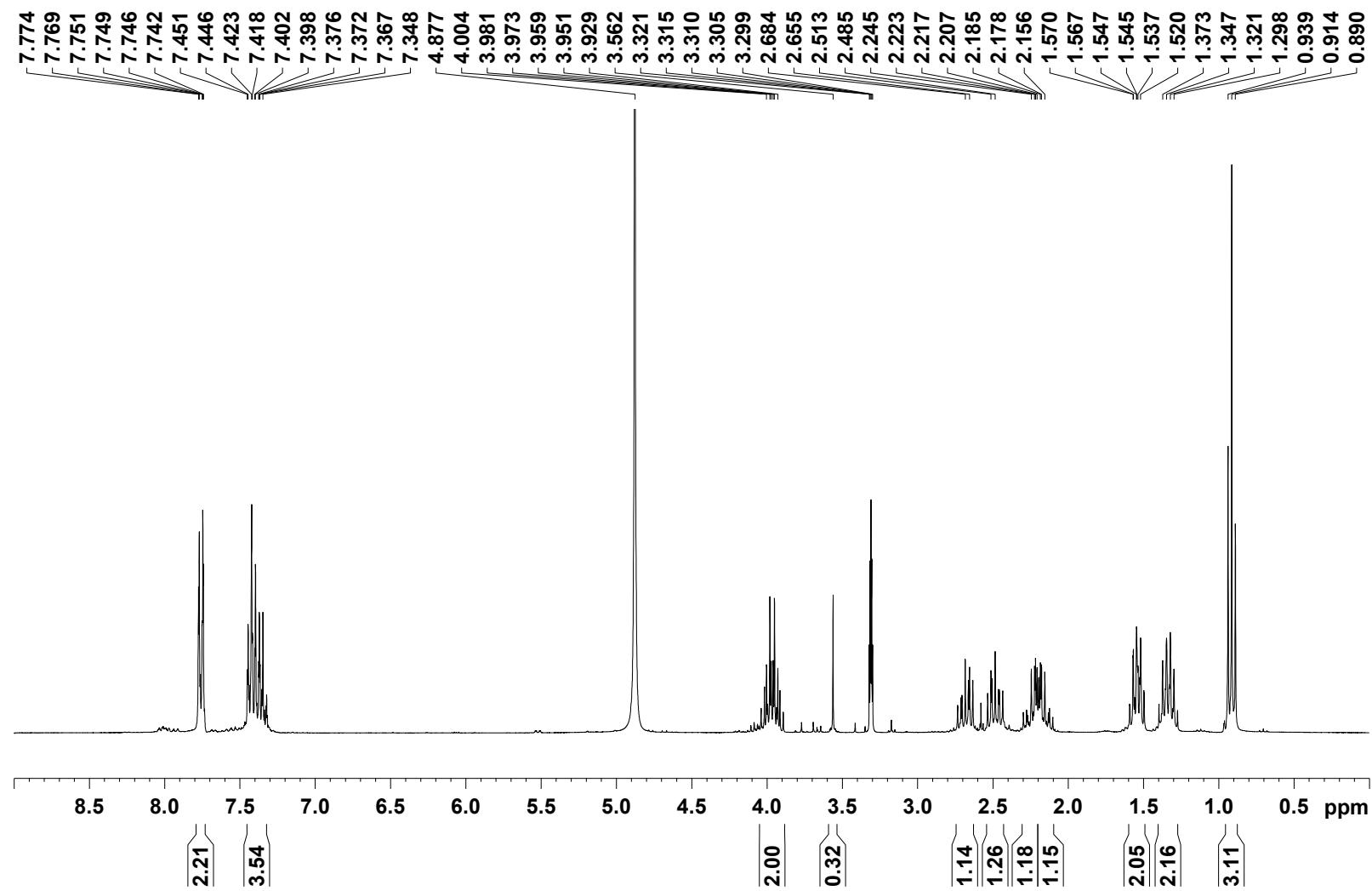
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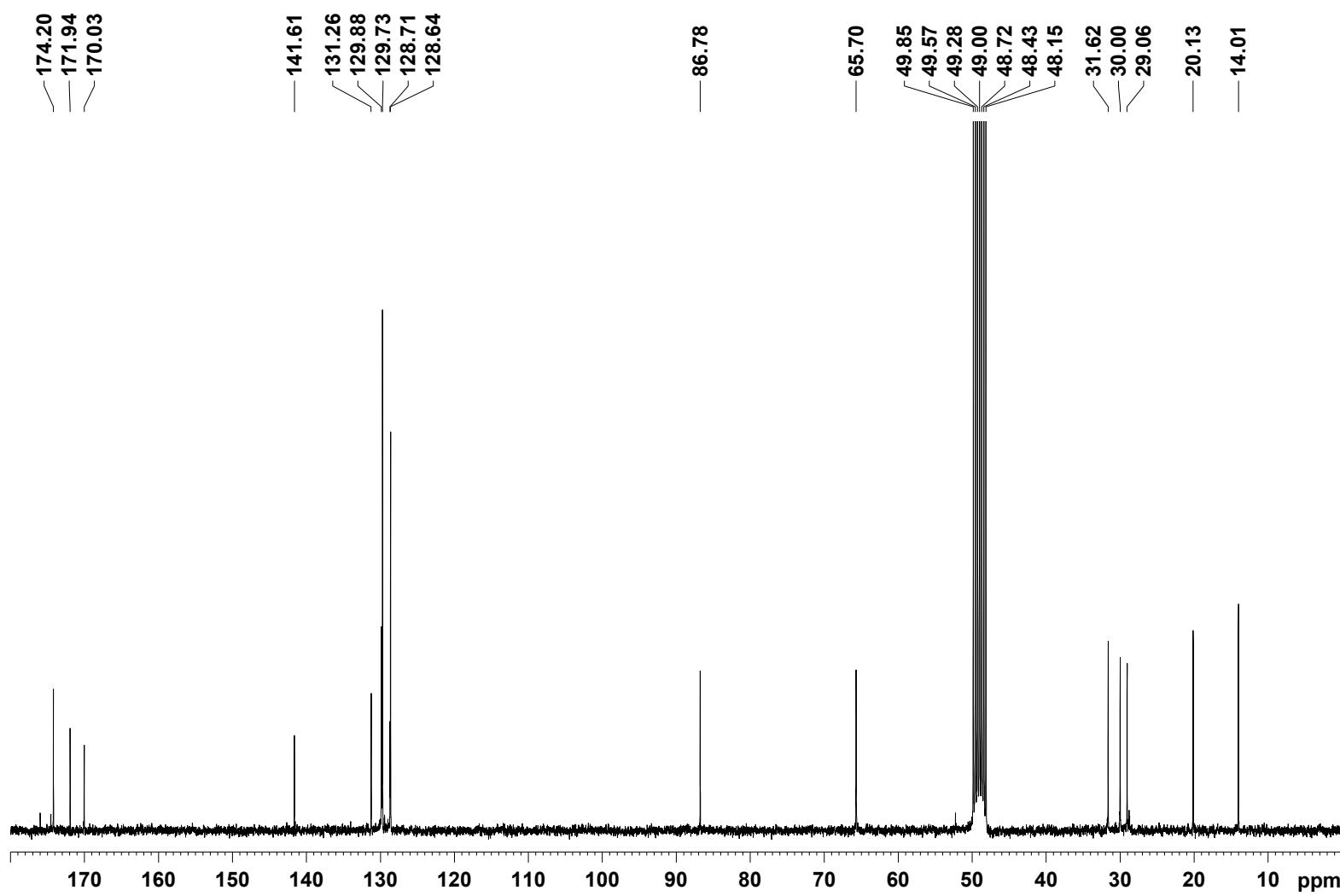
S12. HMBC (300 and 75 MHz, CD₃OD) spectrum of compound 2.



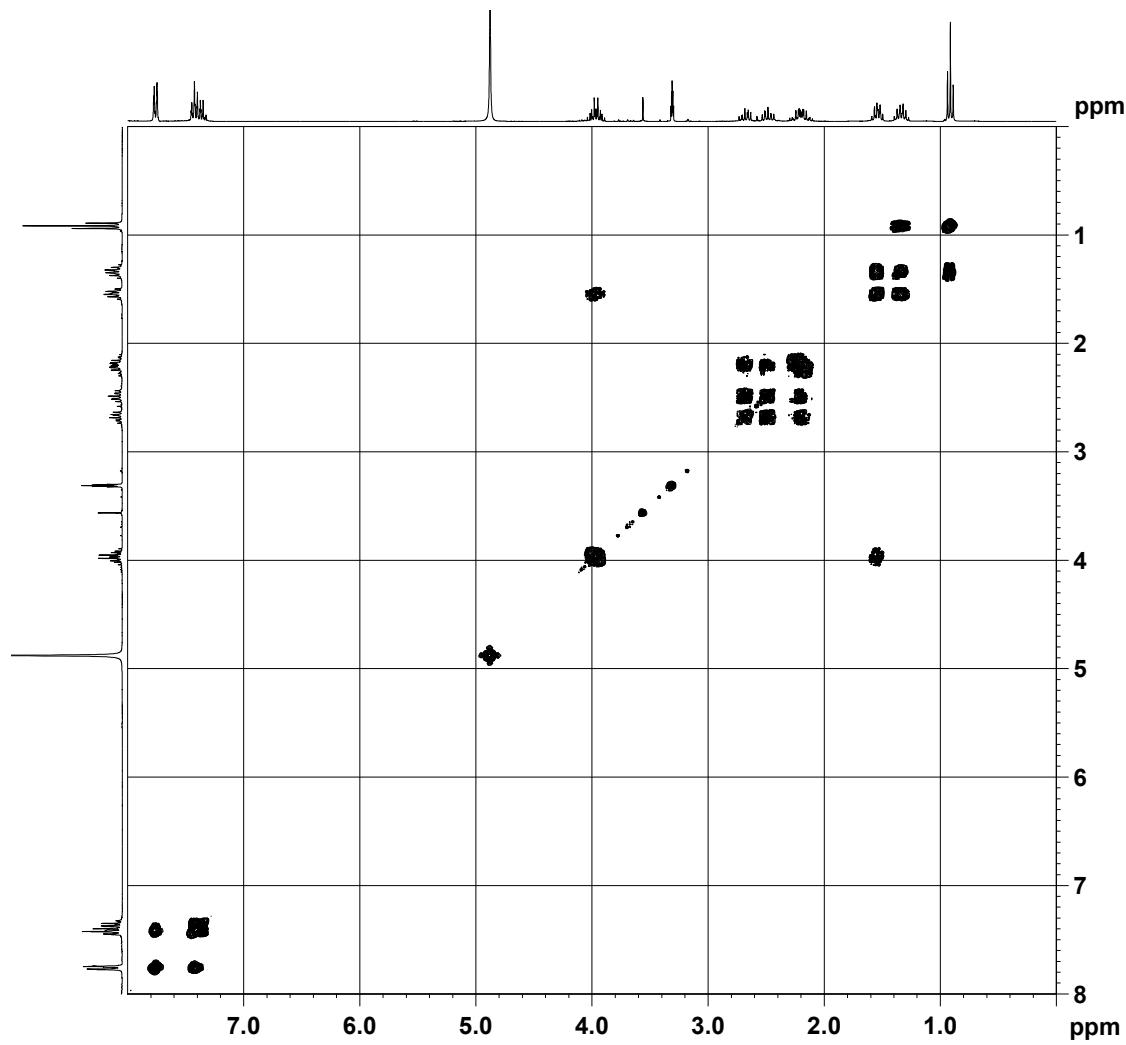
S13. HRESIMS spectrum of compound 3.



S14. ^1H NMR (300 MHz, CD_3OD) spectrum of compound 3.

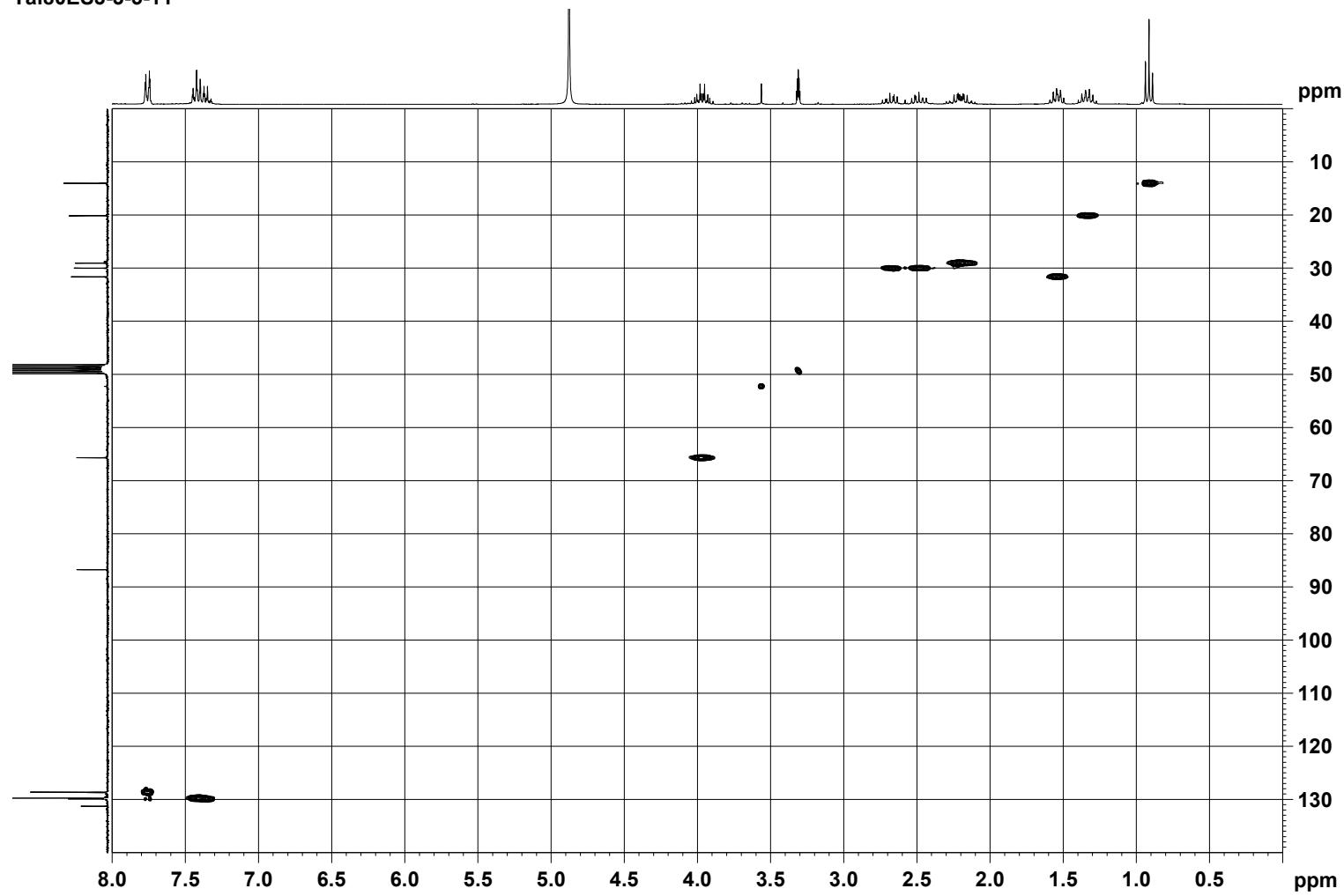


S15. ^{13}C NMR (75 MHz, CD_3OD) spectrum of compound 3.

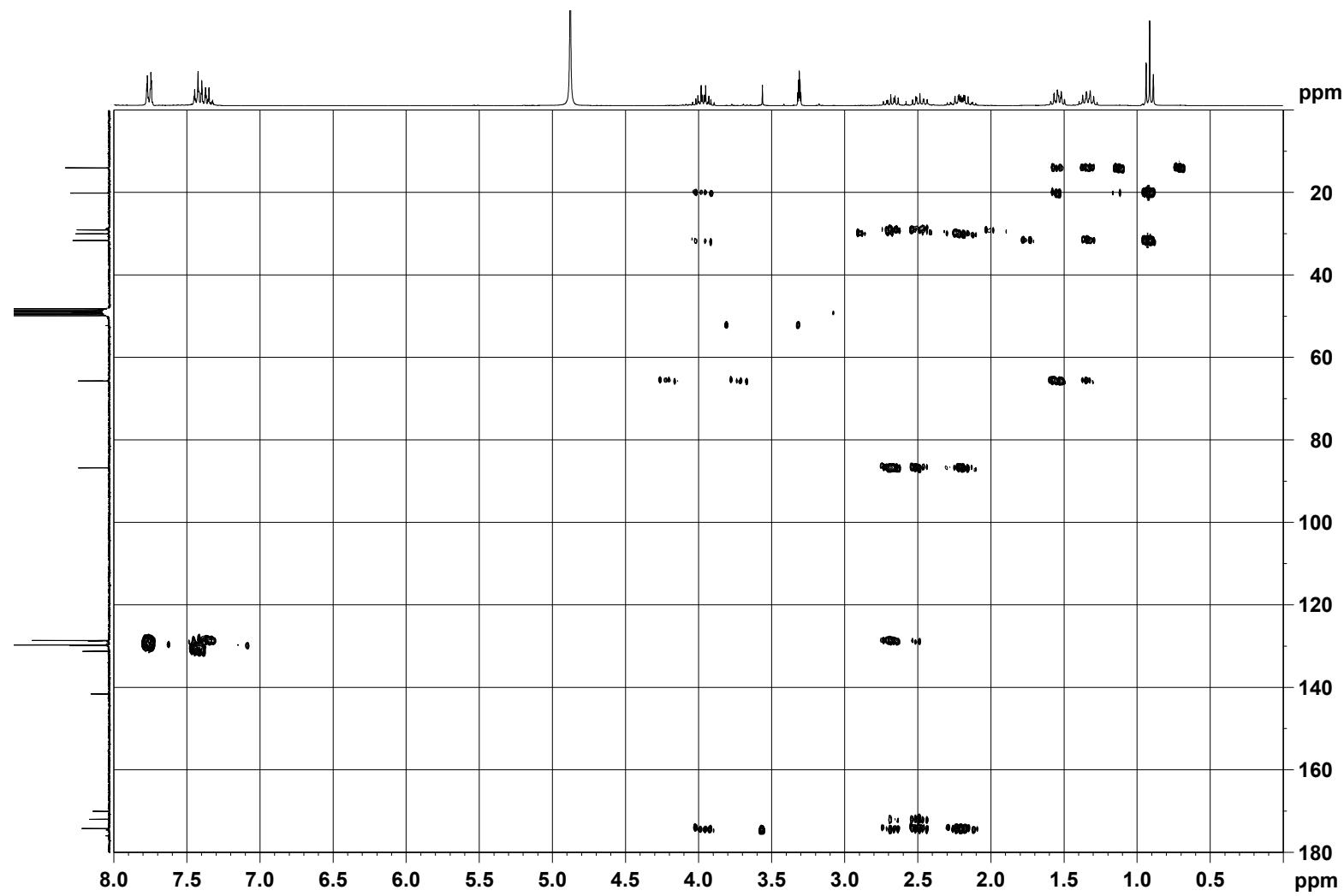


S16. ^1H - ^1H COSY (300 MHz, CD_3OD) spectrum of compound 3.

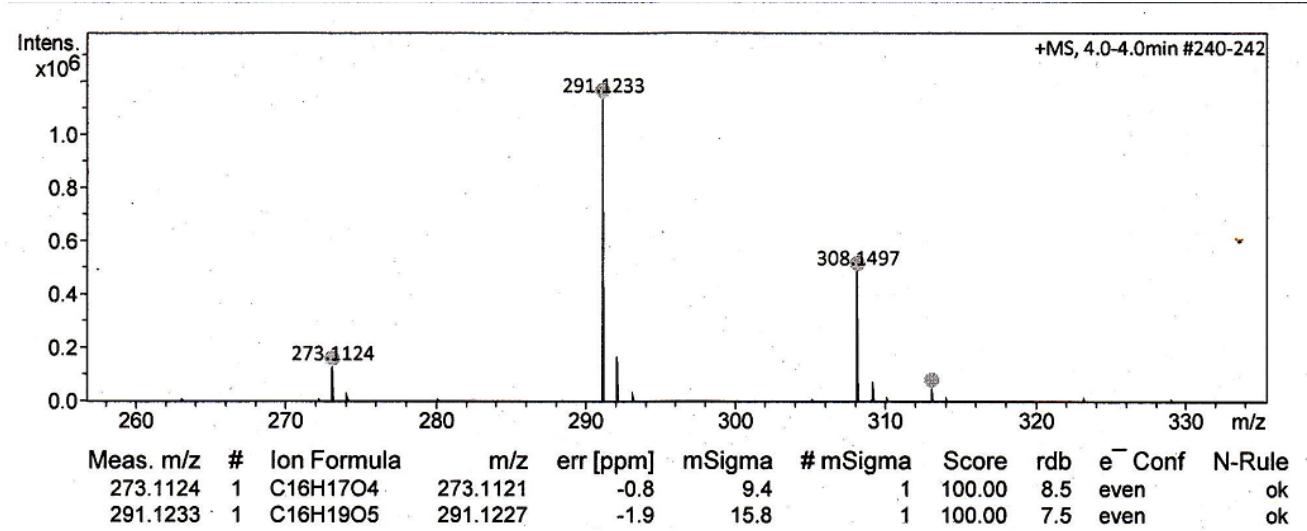
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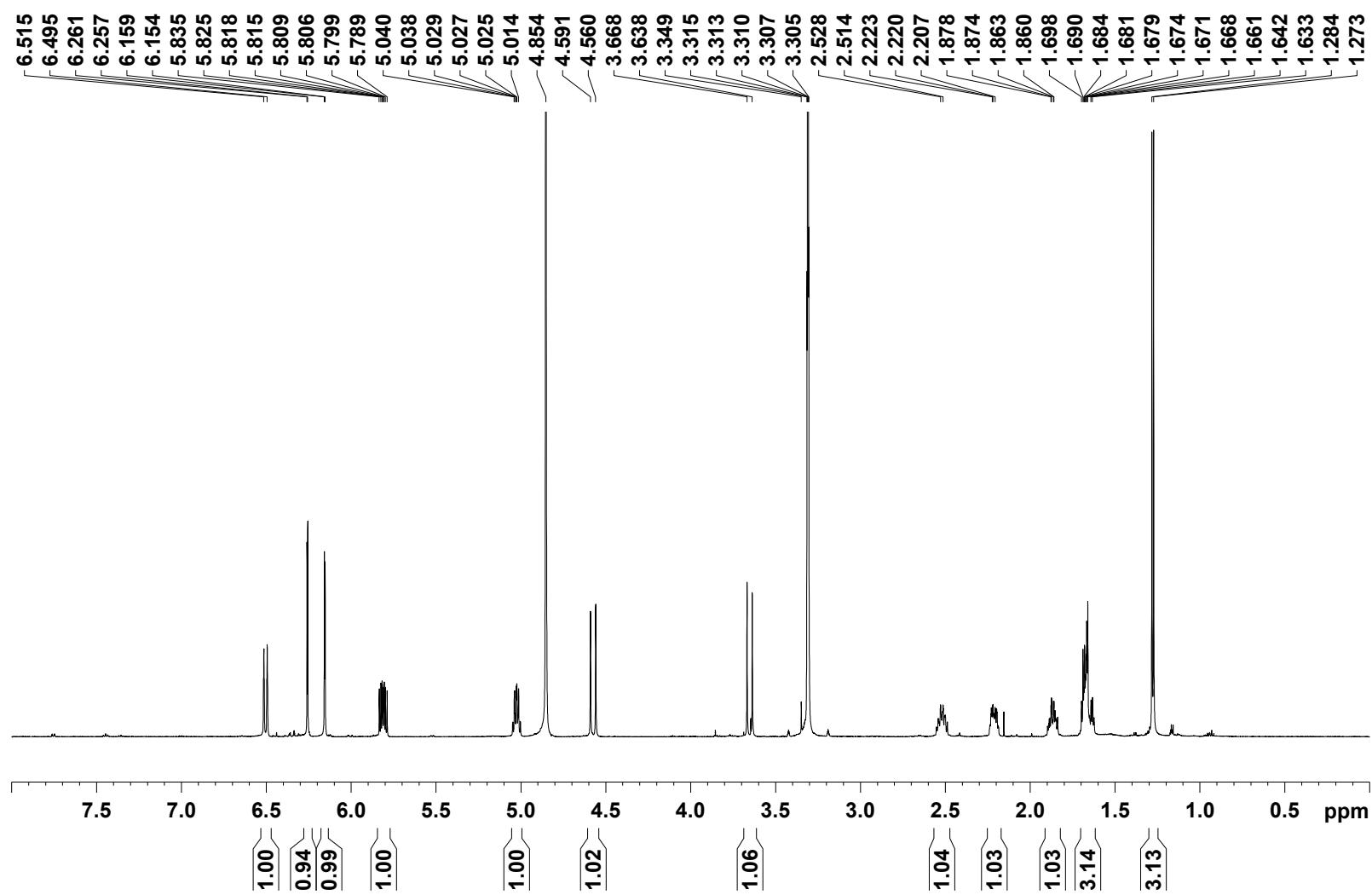
S17. HSQC (300 and 75 MHz, CD_3OD) spectrum of compound 3.



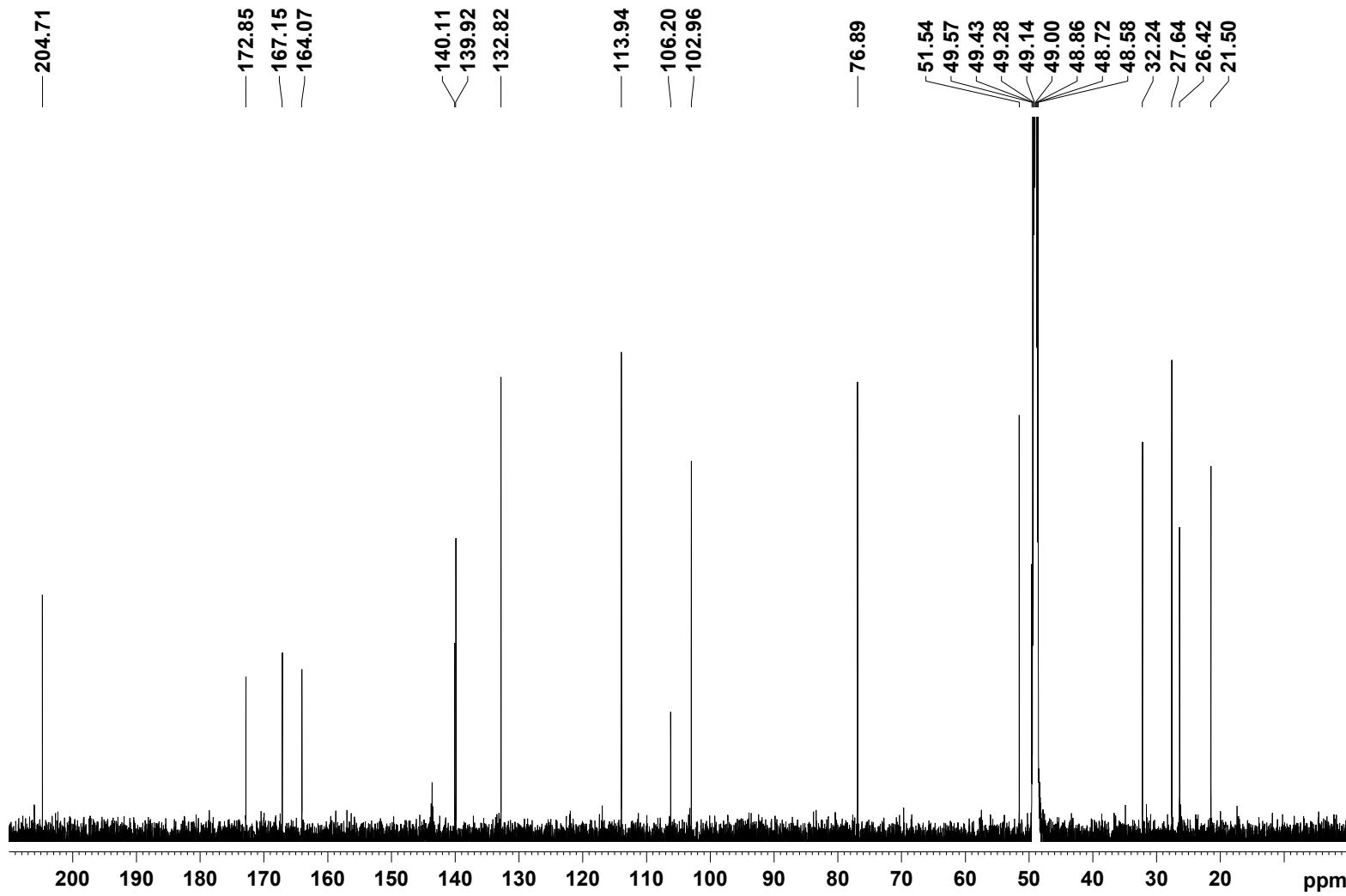
S18. HMBC (300 and 75 MHz, CD_3OD) spectrum of compound 3.



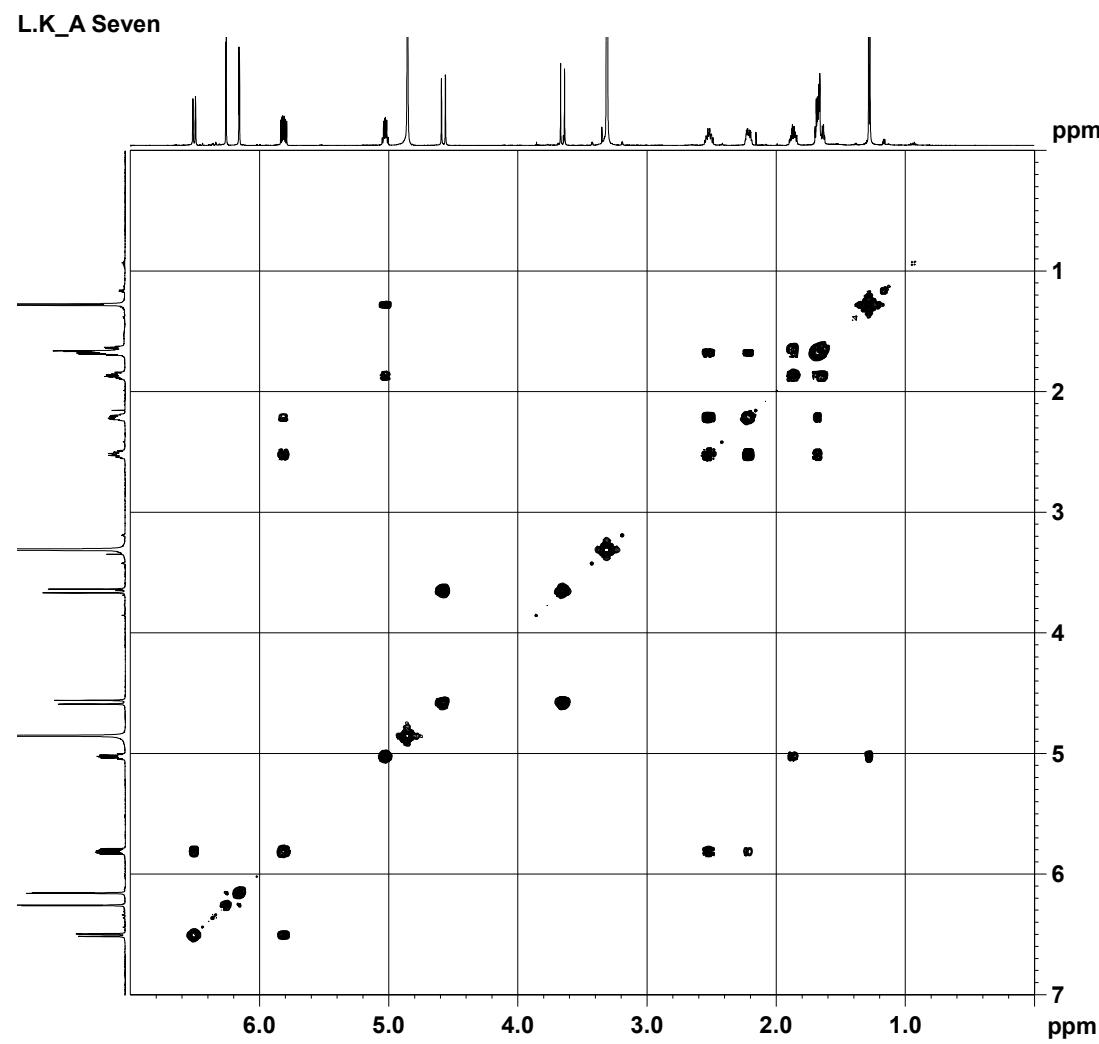
S19. HRESIMS spectrum of compound 6.



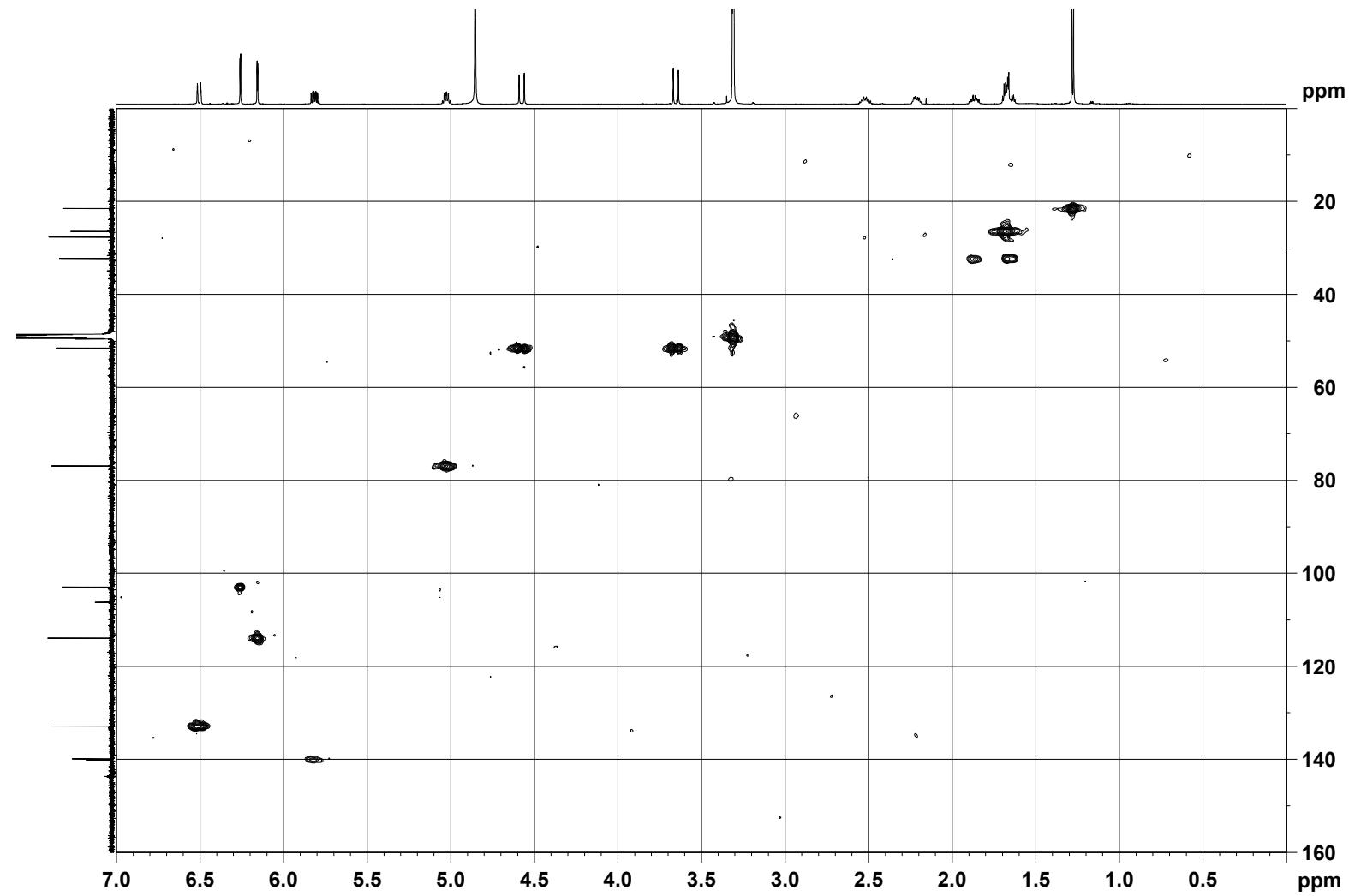
S20. ^1H NMR (600 MHz, CD_3OD) spectrum of compound 6.



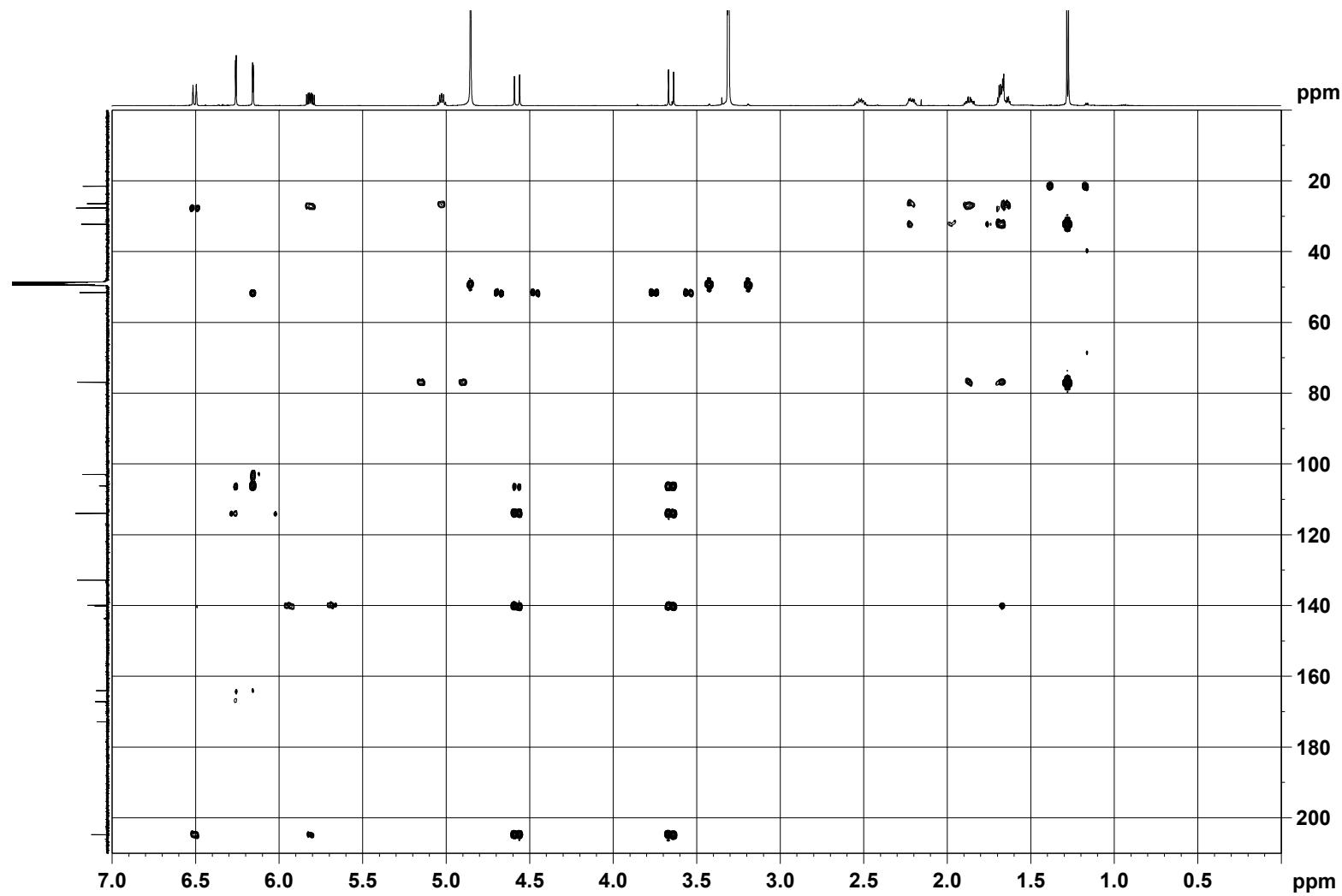
S21. ^{13}C NMR (150 MHz, CD_3OD) spectrum of compound 6.



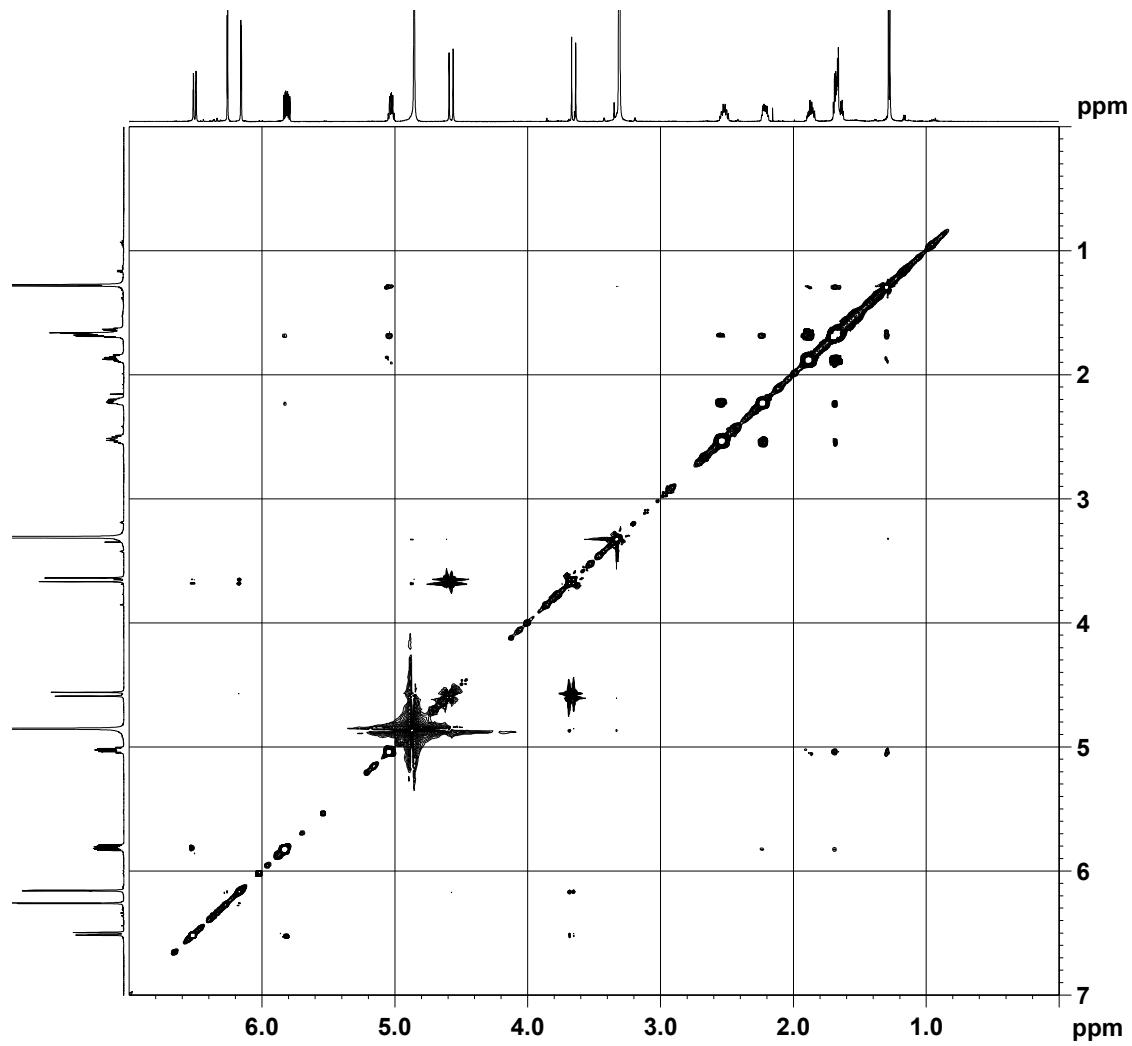
S22. ^1H - ^1H COSY (600 MHz, CD_3OD) spectrum of compound **6**.



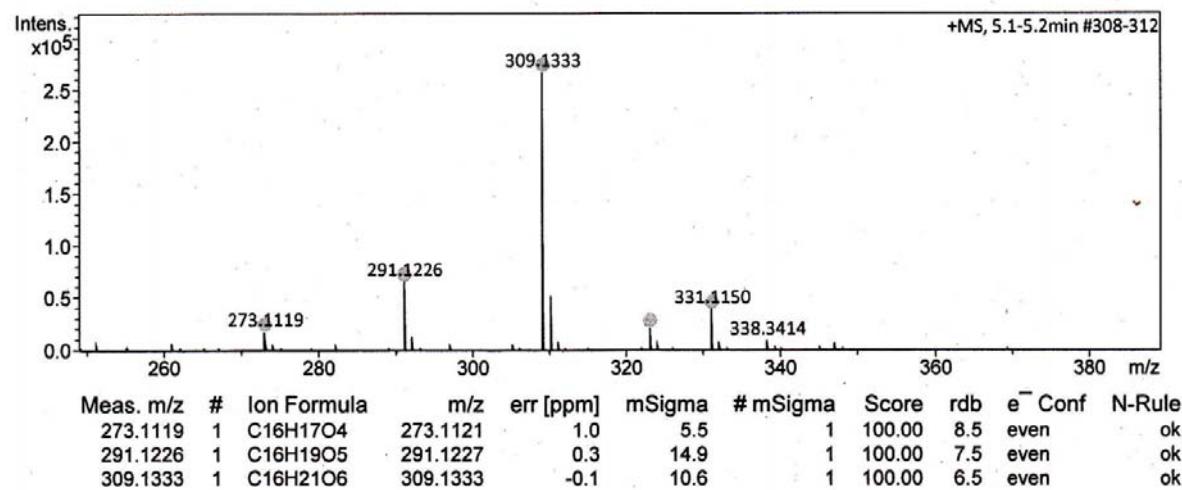
S23. HSQC (600 and 150 MHz, CD_3OD) spectrum of compound 6.



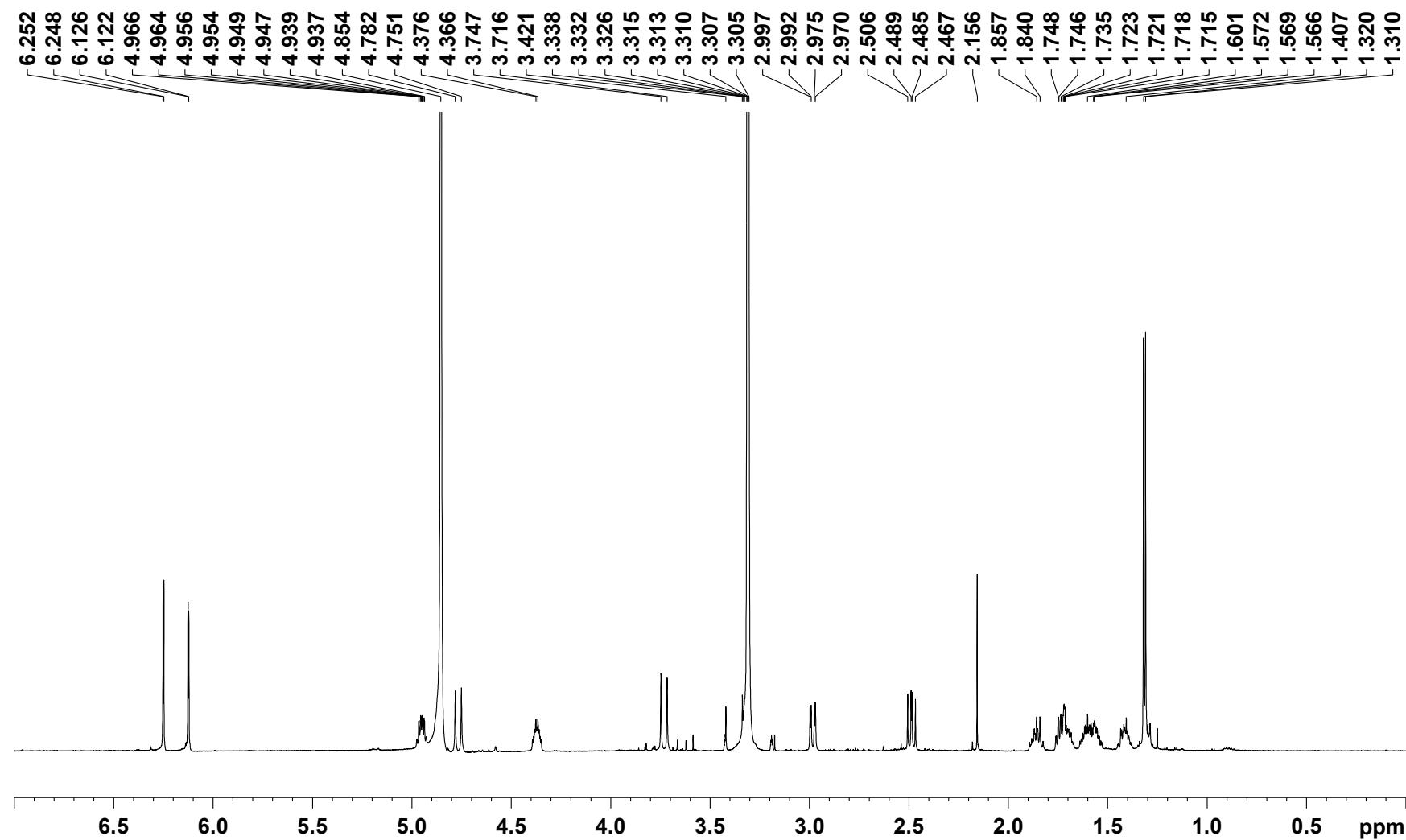
S24. HMBC (600 and 150 MHz, CD_3OD) spectrum of compound 6.



S25. ROESY (600 MHz, CD₃OD) spectrum of compound 6.

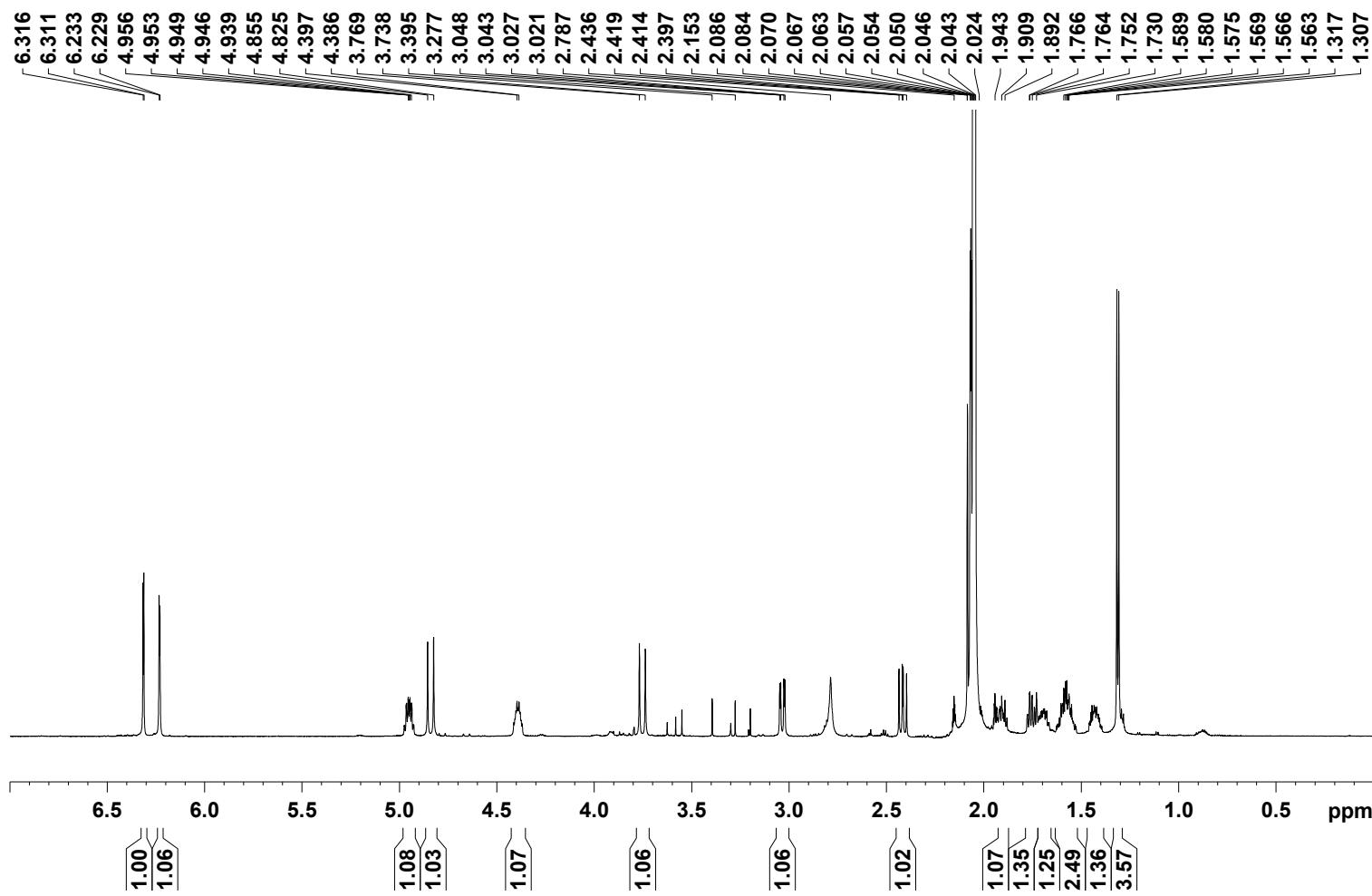


S26. HRESIMS spectrum of compound 7.



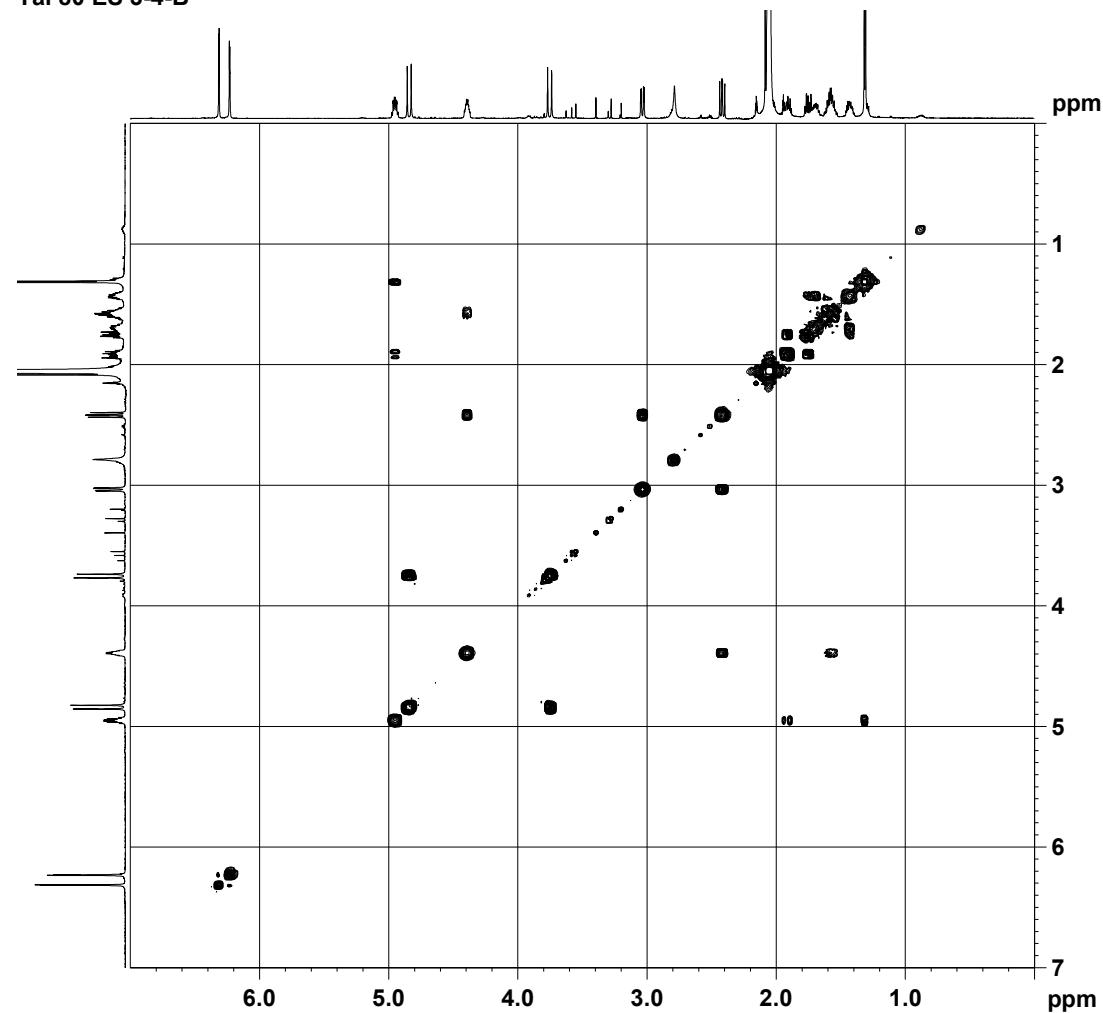
S27. ^1H NMR (600 MHz, CD_3OD) spectrum of compound 7.

Tal 80 ES 3-4-B



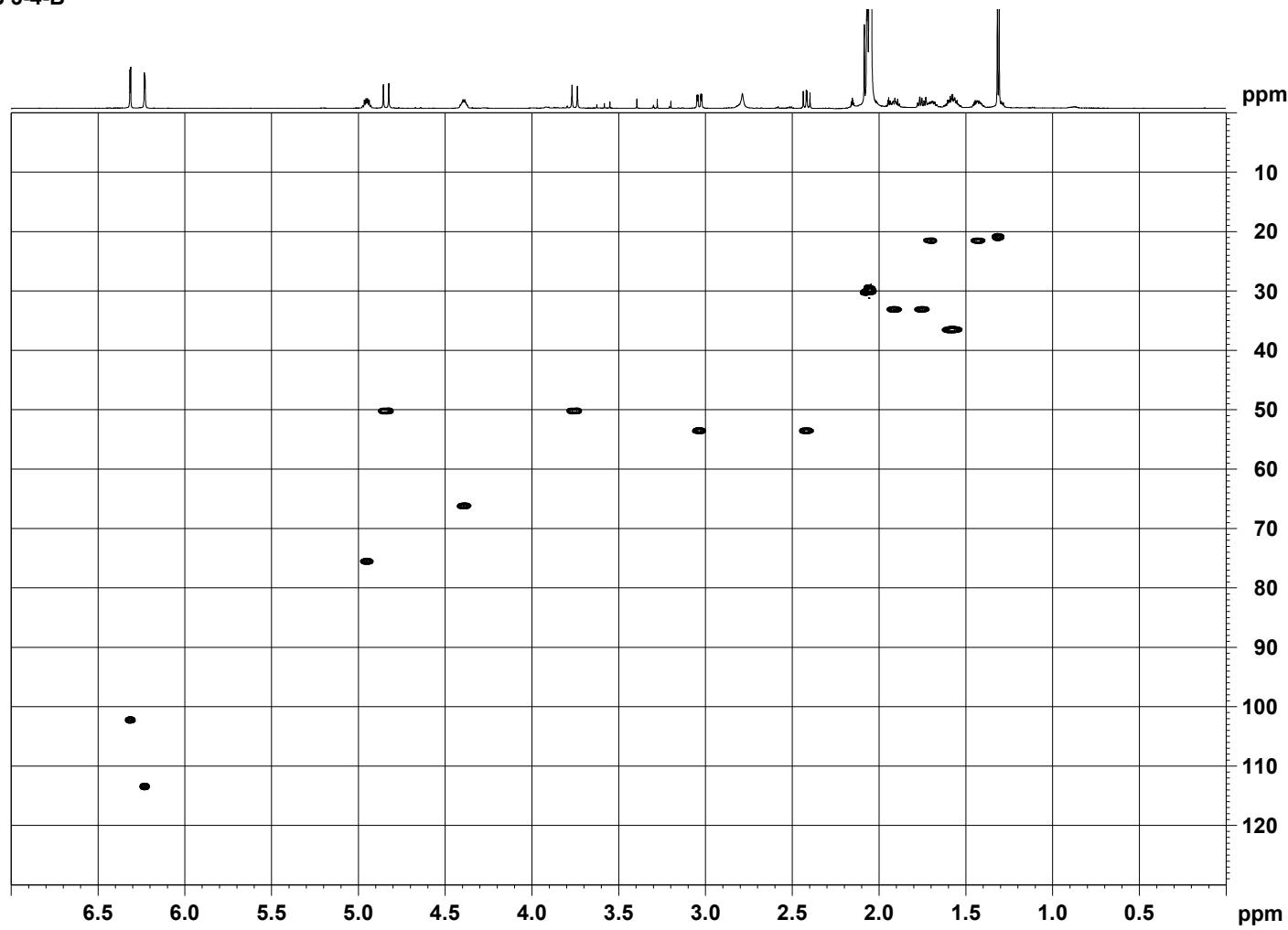
S28. ^1H NMR (600 MHz, CD_3COCD_3) spectrum of compound 7.

Tal 80 ES 3-4-B



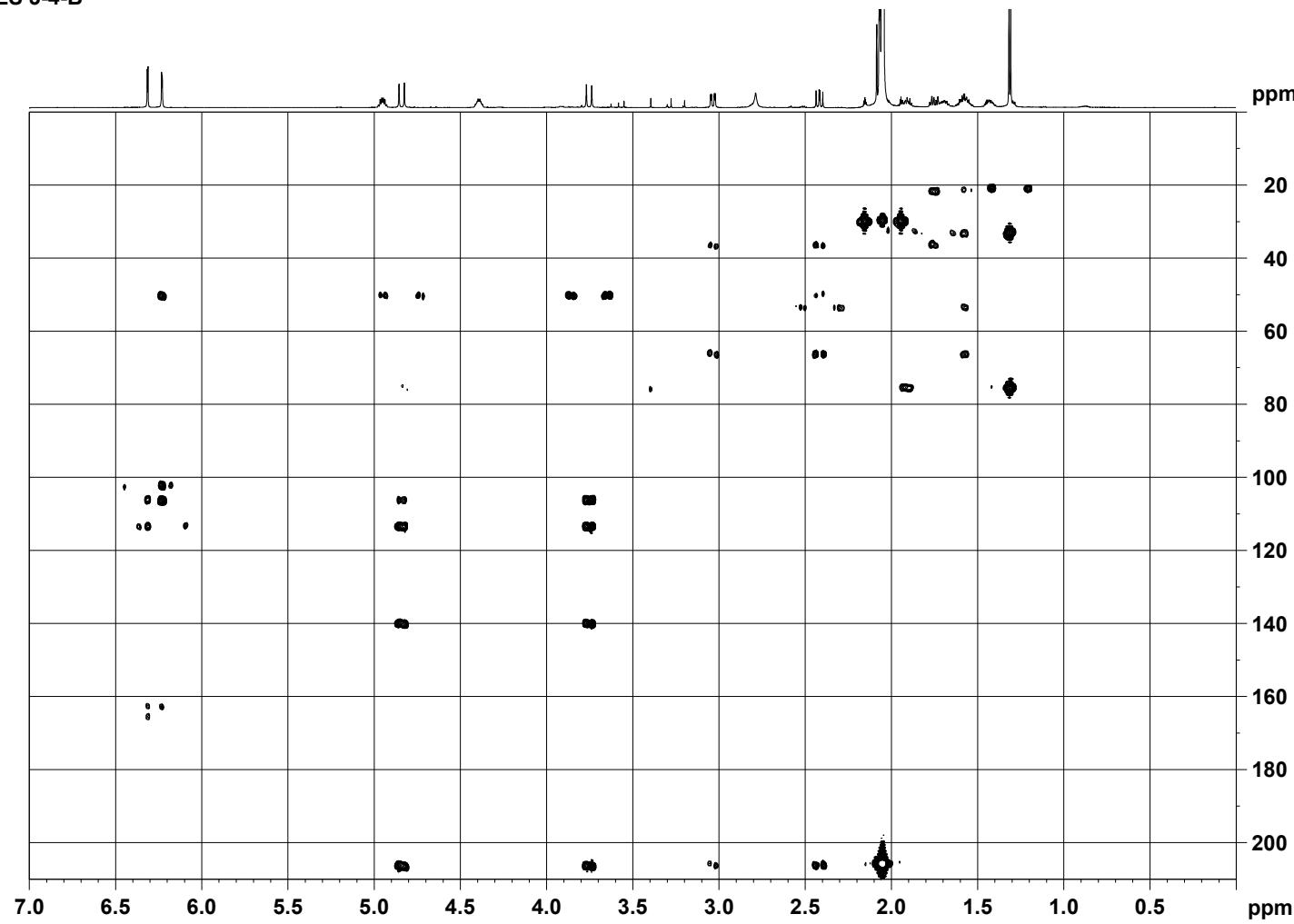
S29. ^1H - ^1H COSY (600 MHz, CD_3COCD_3) spectrum of compound 7.

Tal 80 ES 3-4-B



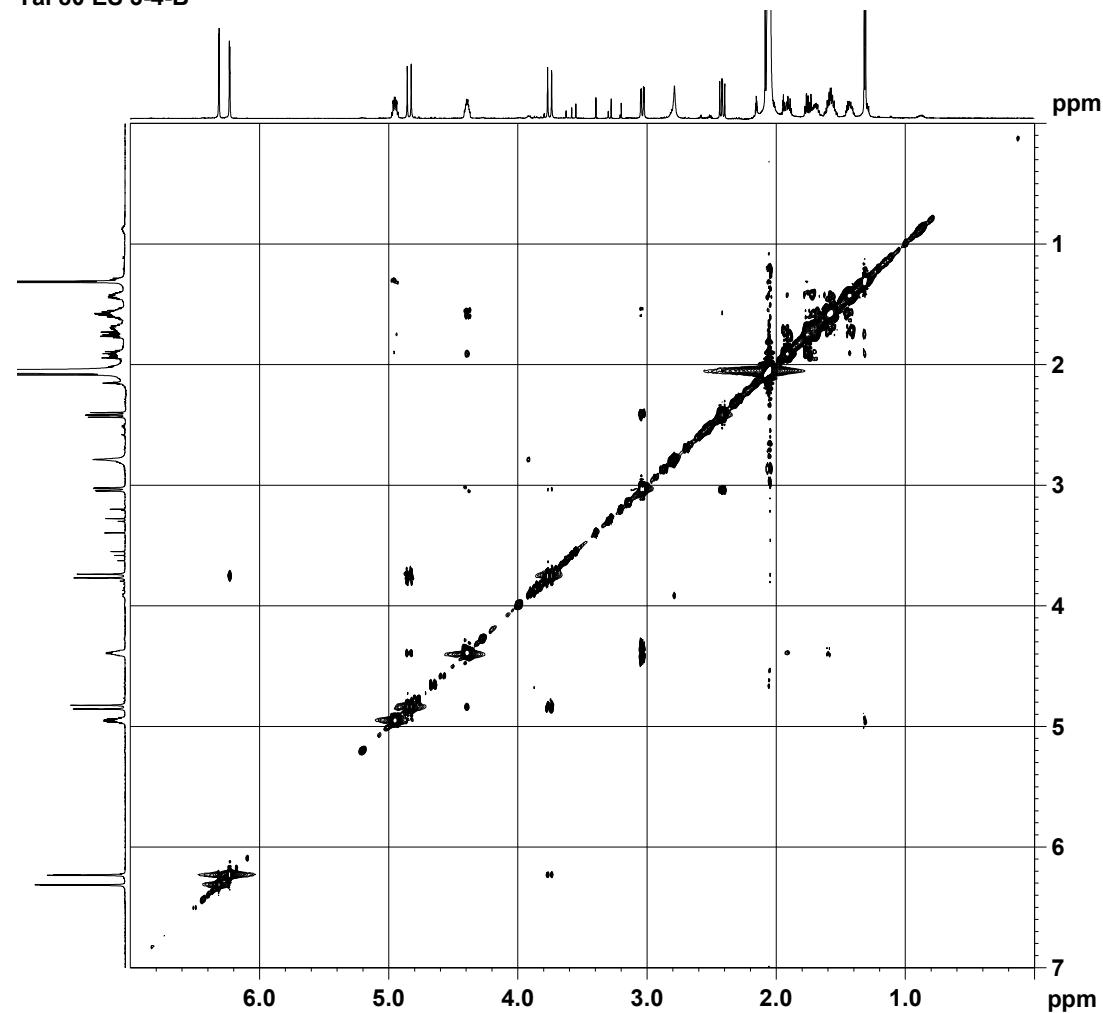
S30. HSQC (600 and 150 MHz, CD_3COCD_3) spectrum of compound 7.

Tal 80 ES 3-4-B

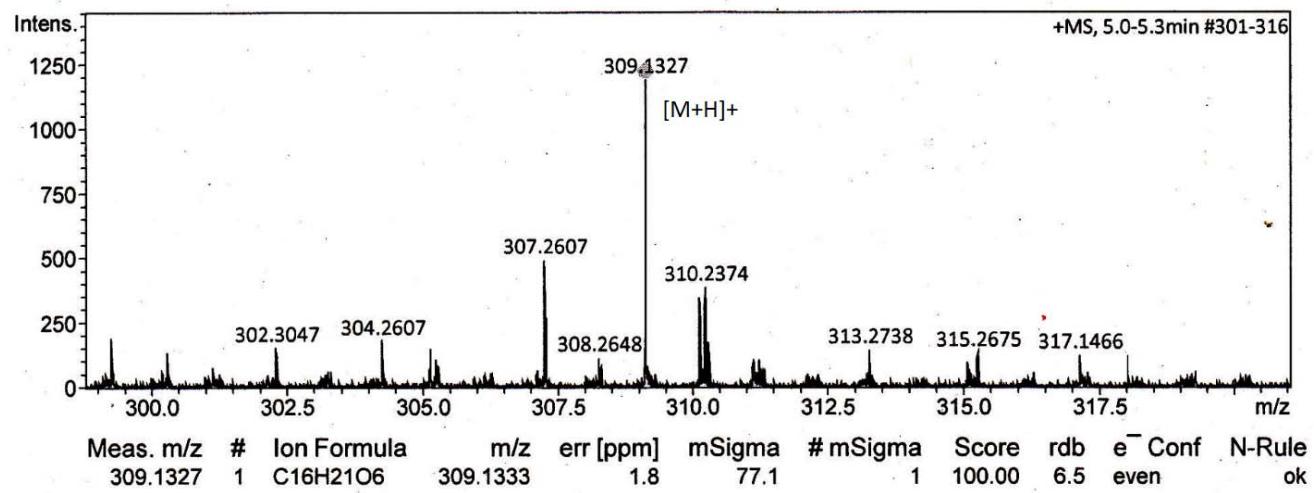


S31. HMBC (600 and 150 MHz, CD_3COCD_3) spectrum of compound 7.

Tal 80 ES 3-4-B

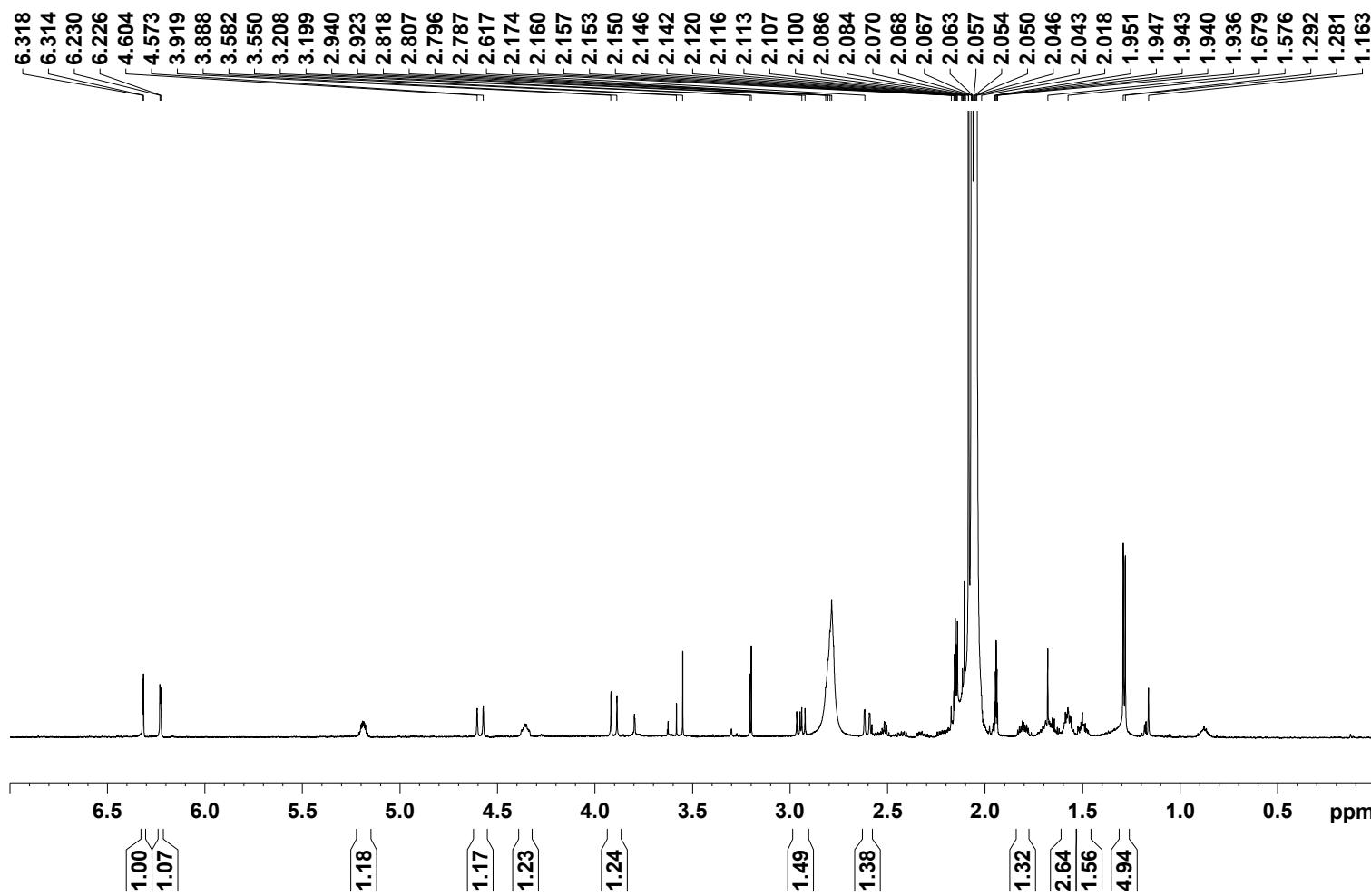


S32. ROESY (600 MHz, CD₃COCD₃) spectrum of compound 7.

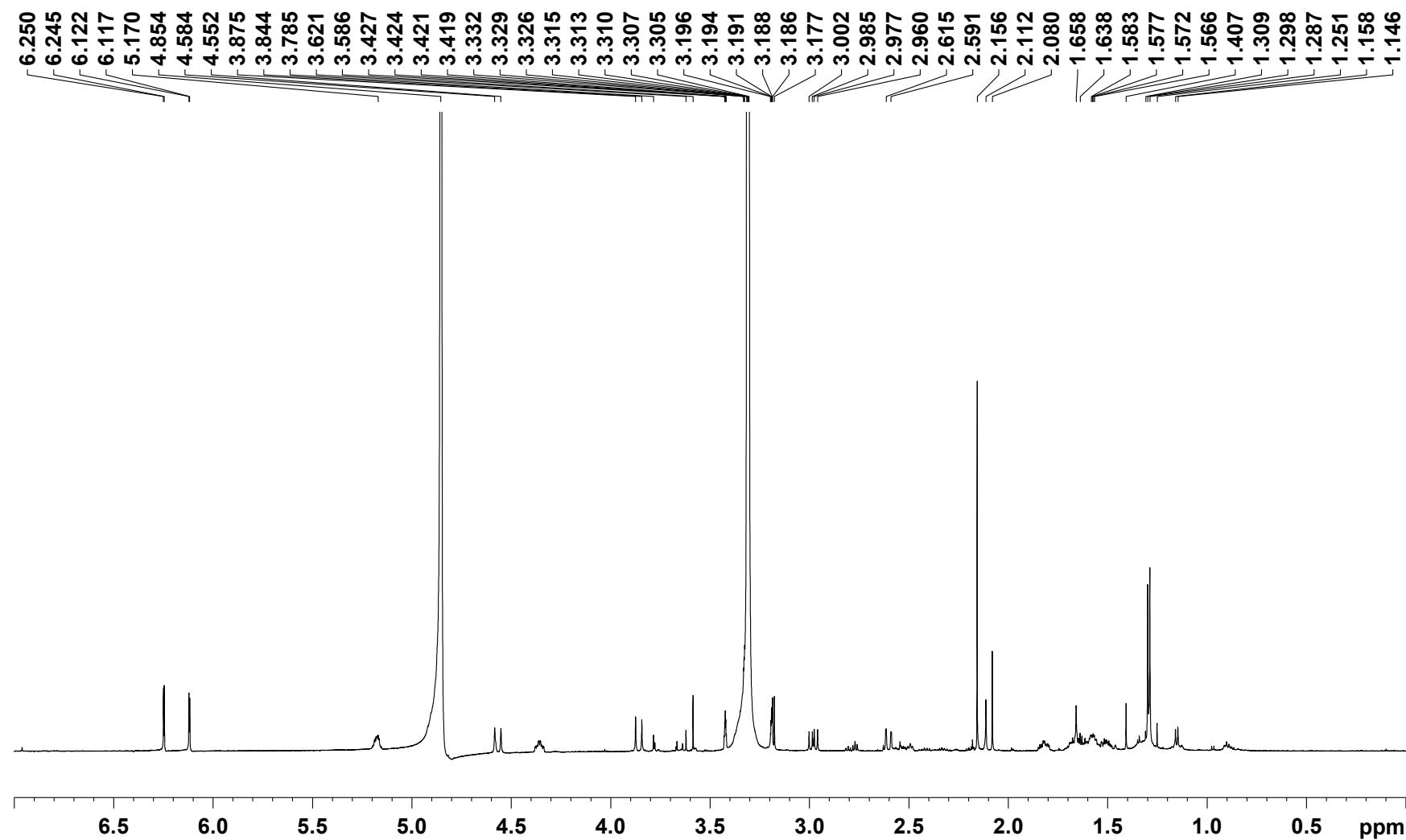


S33. HRESIMS spectrum of compound 8.

Tal 80 ES 4-5-6

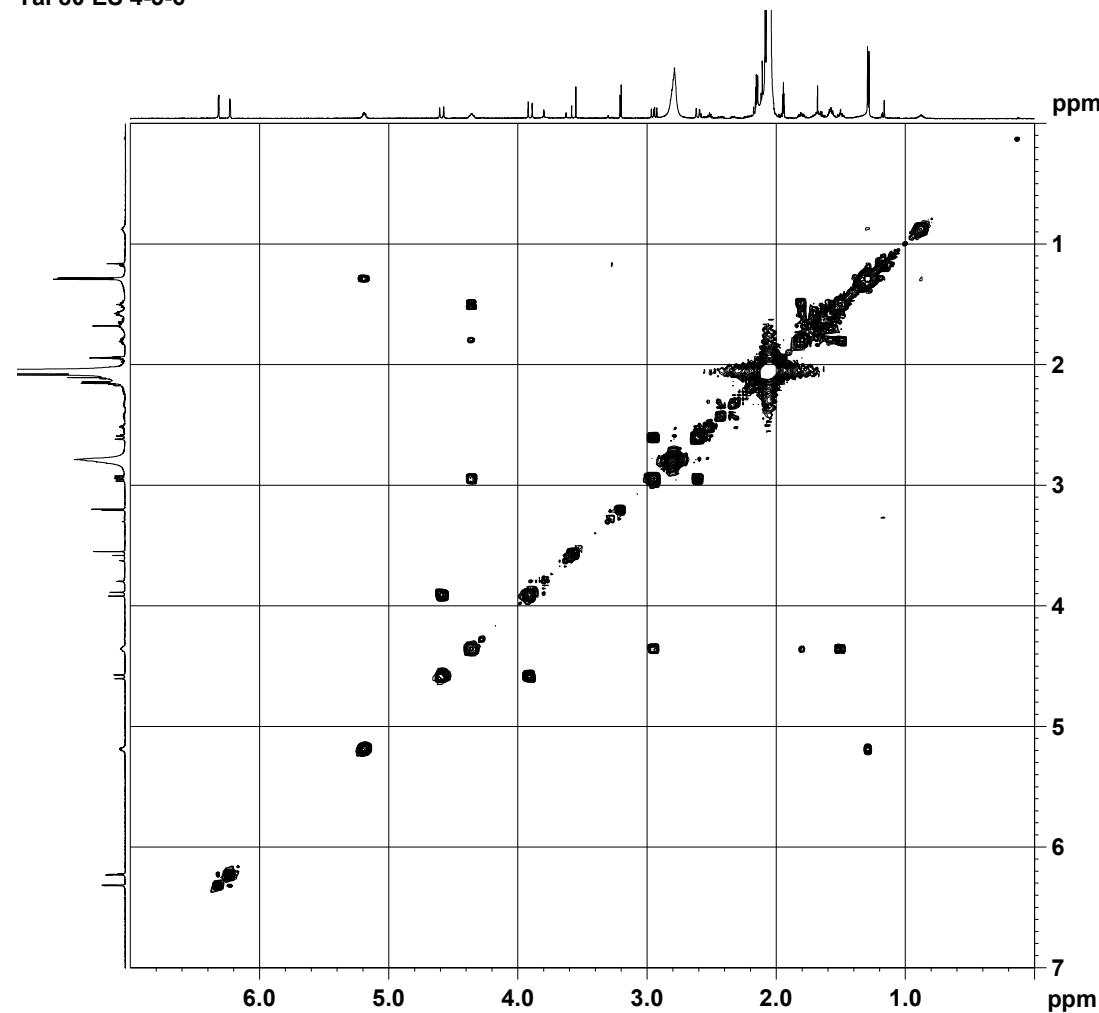


S34. ^1H NMR (600 MHz, CD_3COCD_3) spectrum of compound 8.



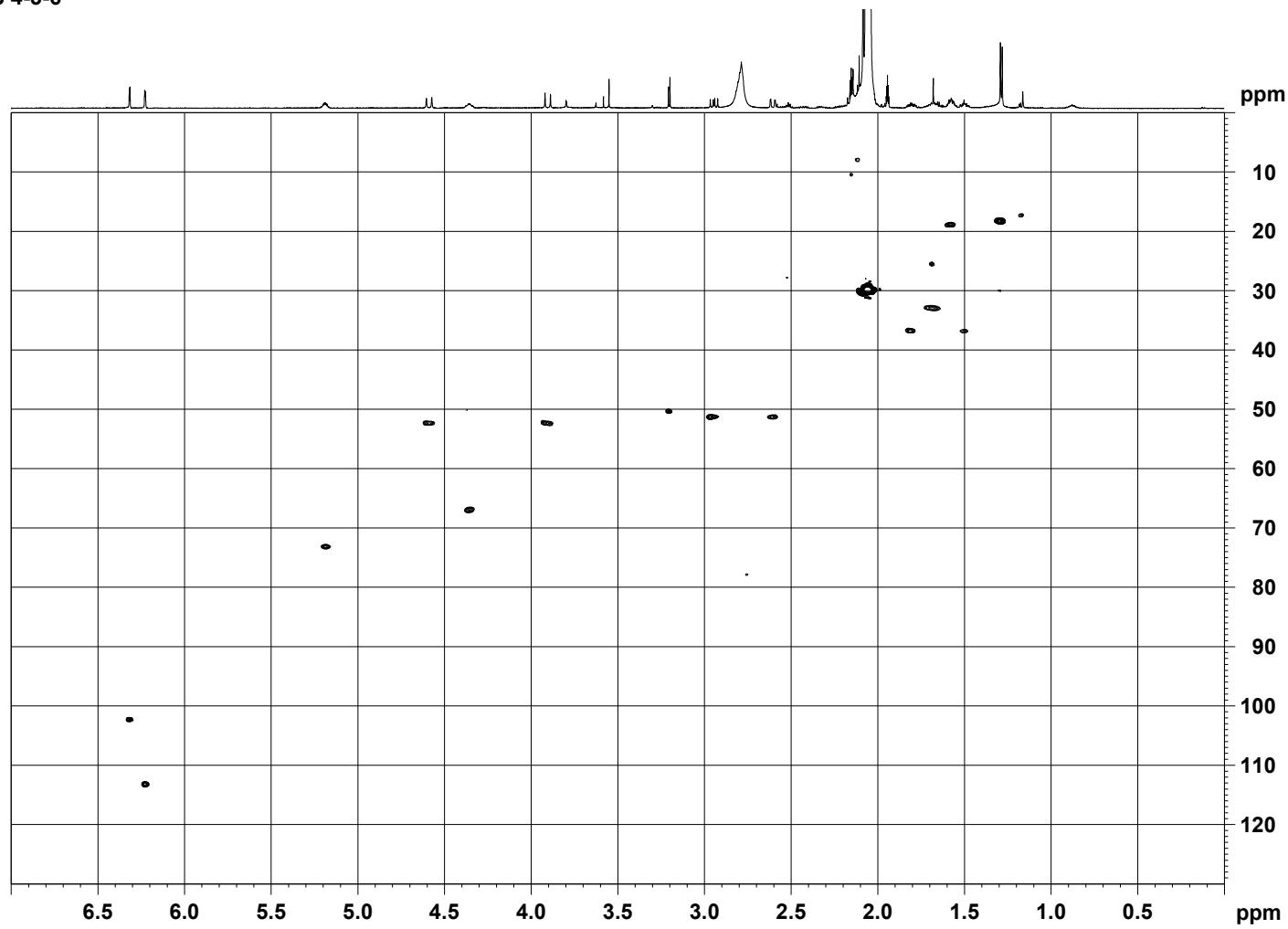
S35. ^1H NMR (600 MHz, CD_3OD) spectrum of compound 8.

Tal 80 ES 4-5-6



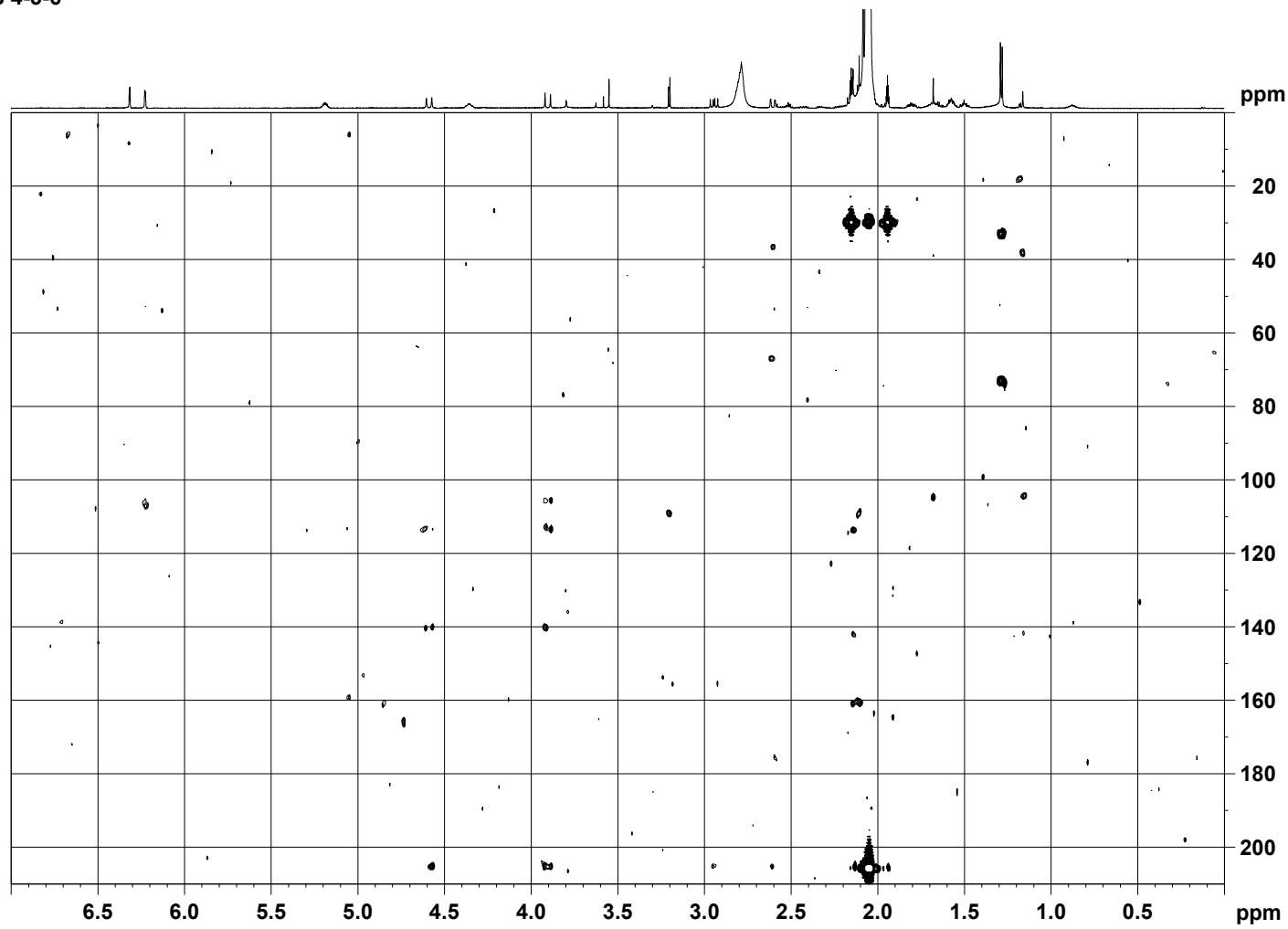
S36. ^1H - ^1H COSY (600 MHz, CD_3COCD_3) spectrum of compound 8.

Tal 80 ES 4-5-6



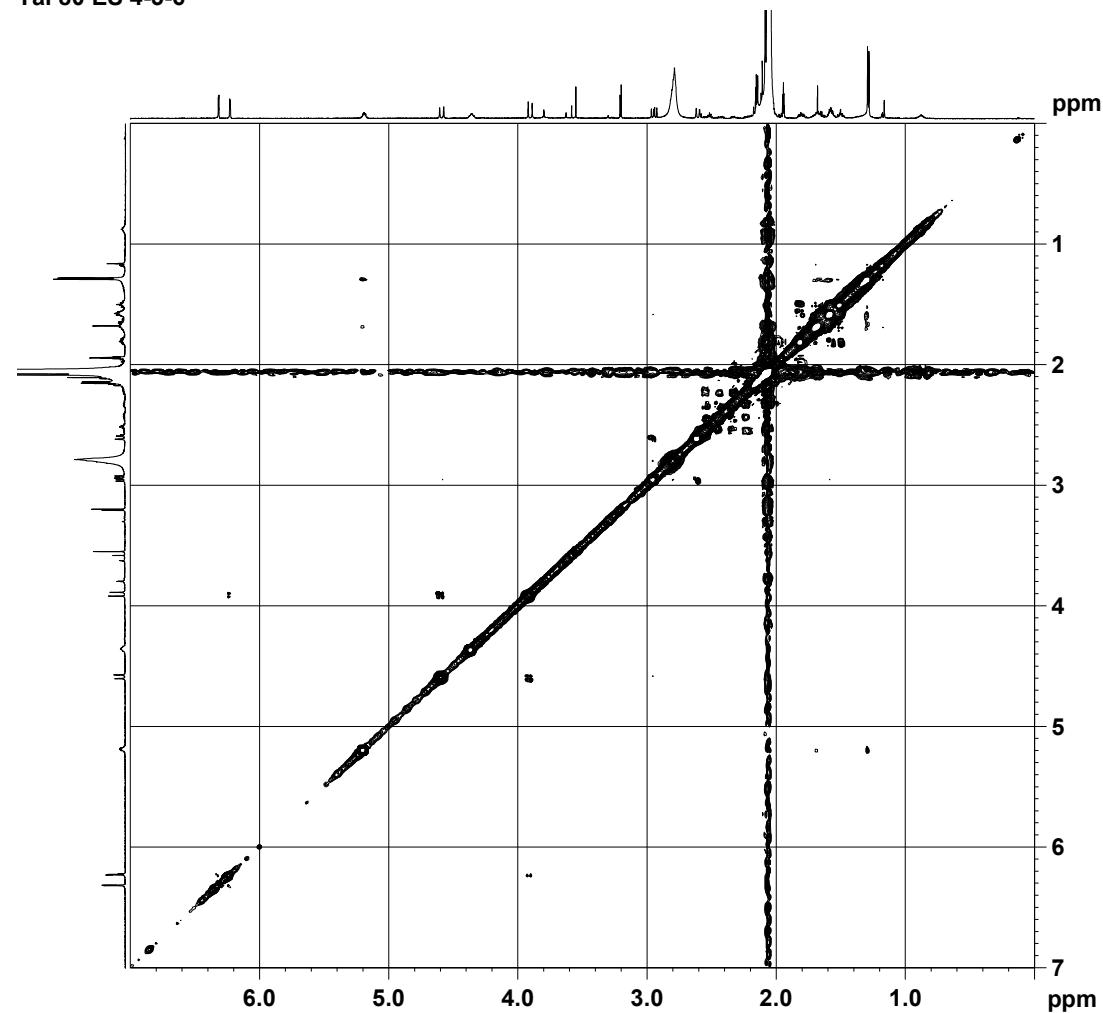
S37. HSQC (600 and 150 MHz, CD_3COCD_3) spectrum of compound 8.

Tal 80 ES 4-5-6

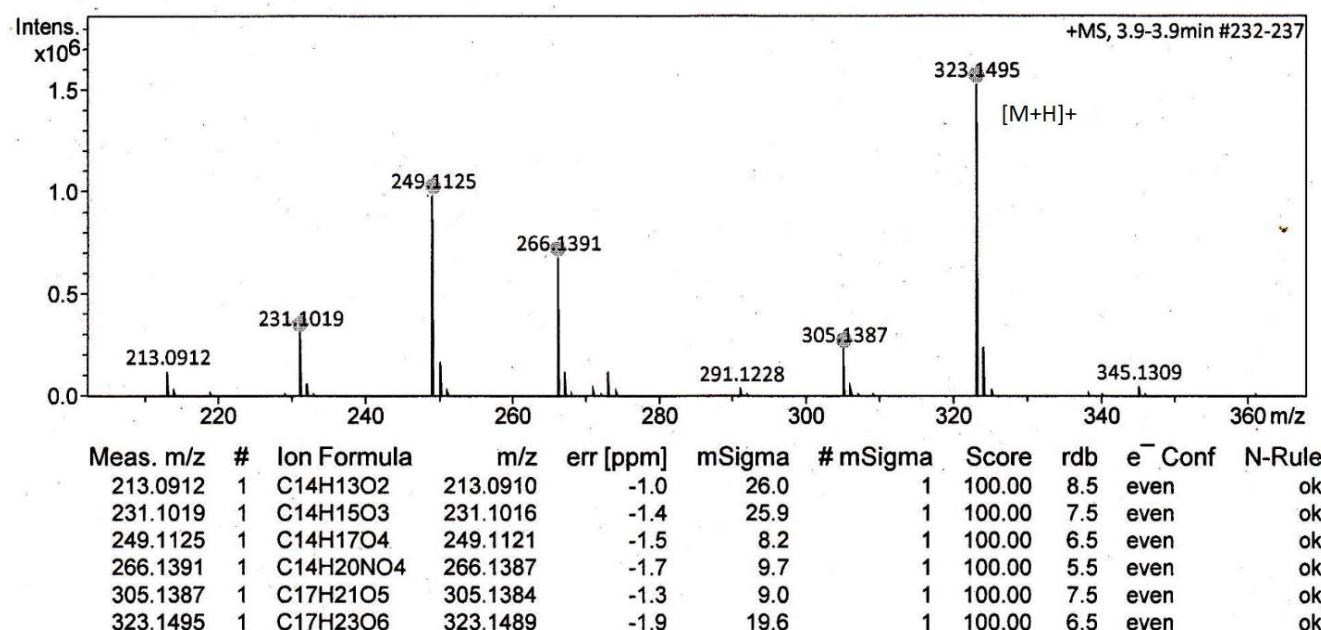


S38. HMBC (600 and 150 MHz, CD_3COCD_3) spectrum of compound 8.

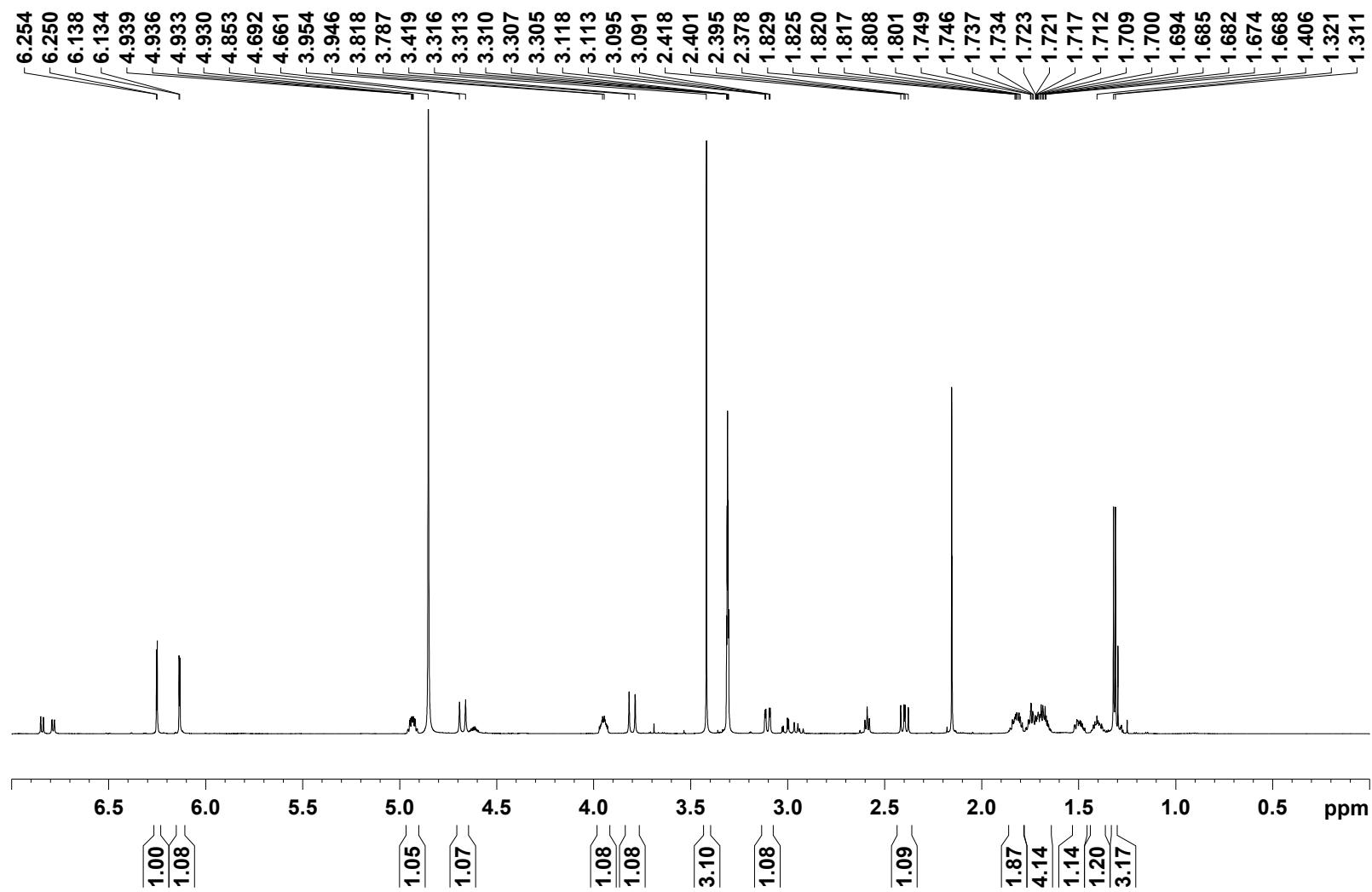
Tal 80 ES 4-5-6



S39. ROESY (600 MHz, CD_3COCD_3) spectrum of compound 8.

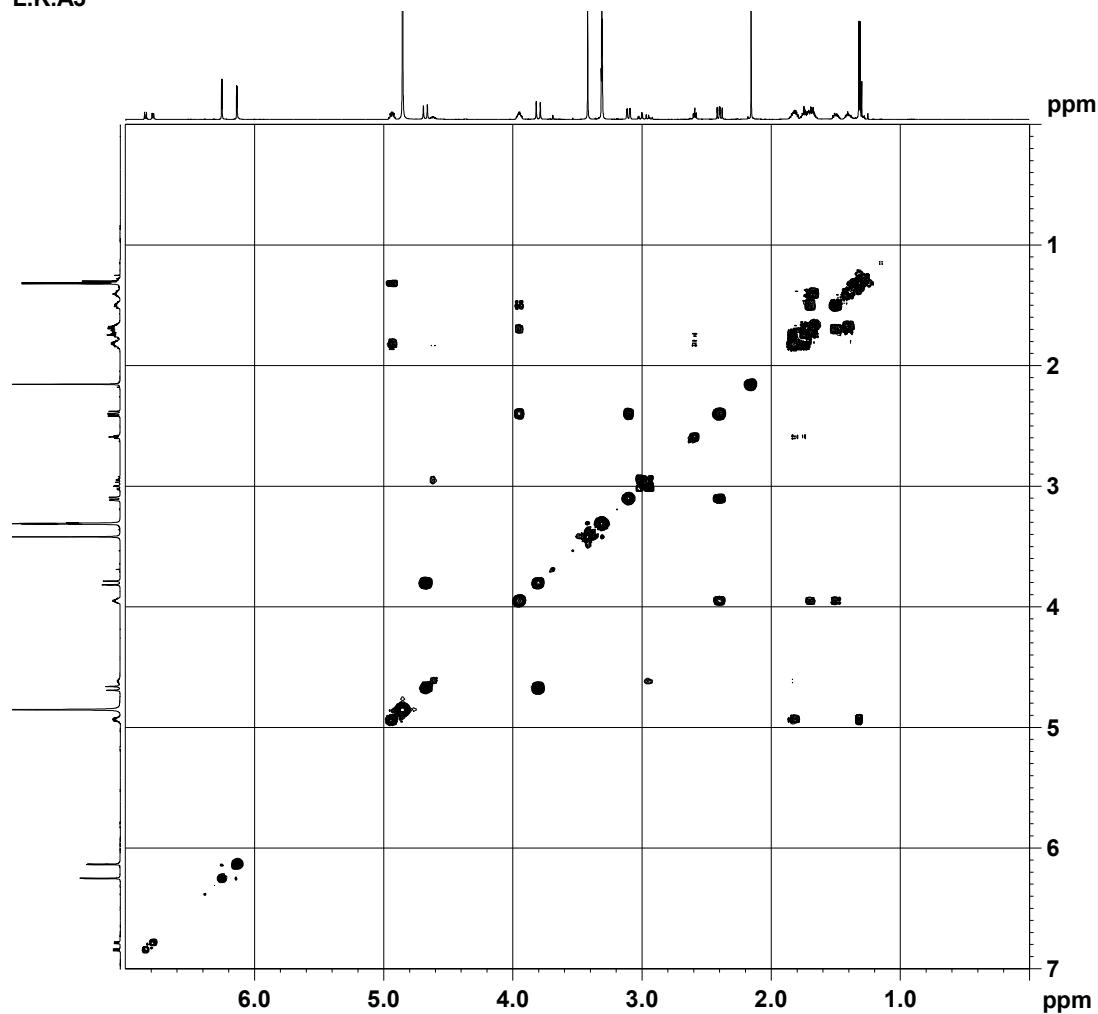


S40. HRESIMS spectrum of compound 9.

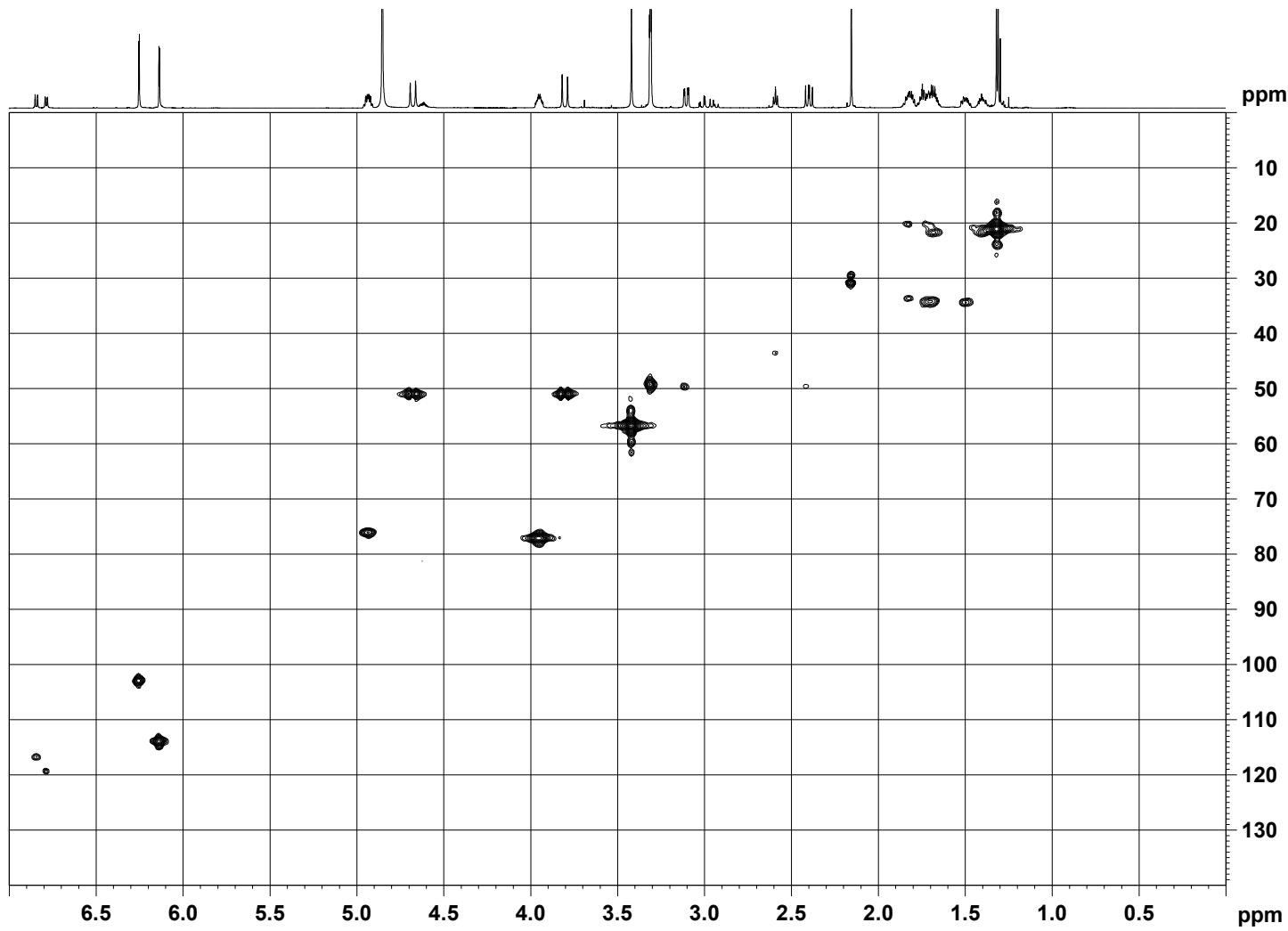


S41. ^1H NMR (600 MHz, CD_3OD) spectrum of compound 9.

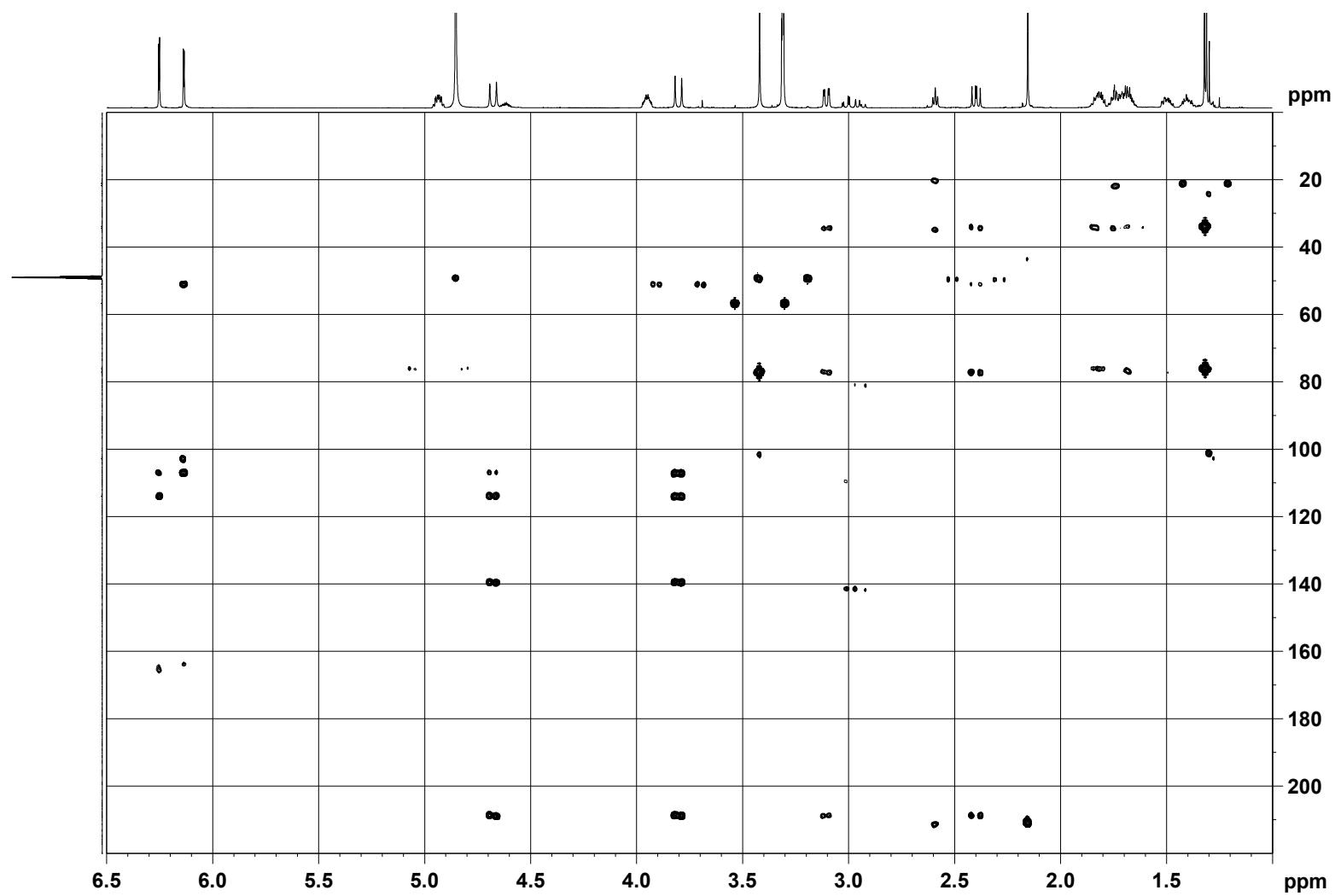
L.K.A3



S42. ^1H - ^1H COSY (600 MHz, CD_3OD) spectrum of compound 9.

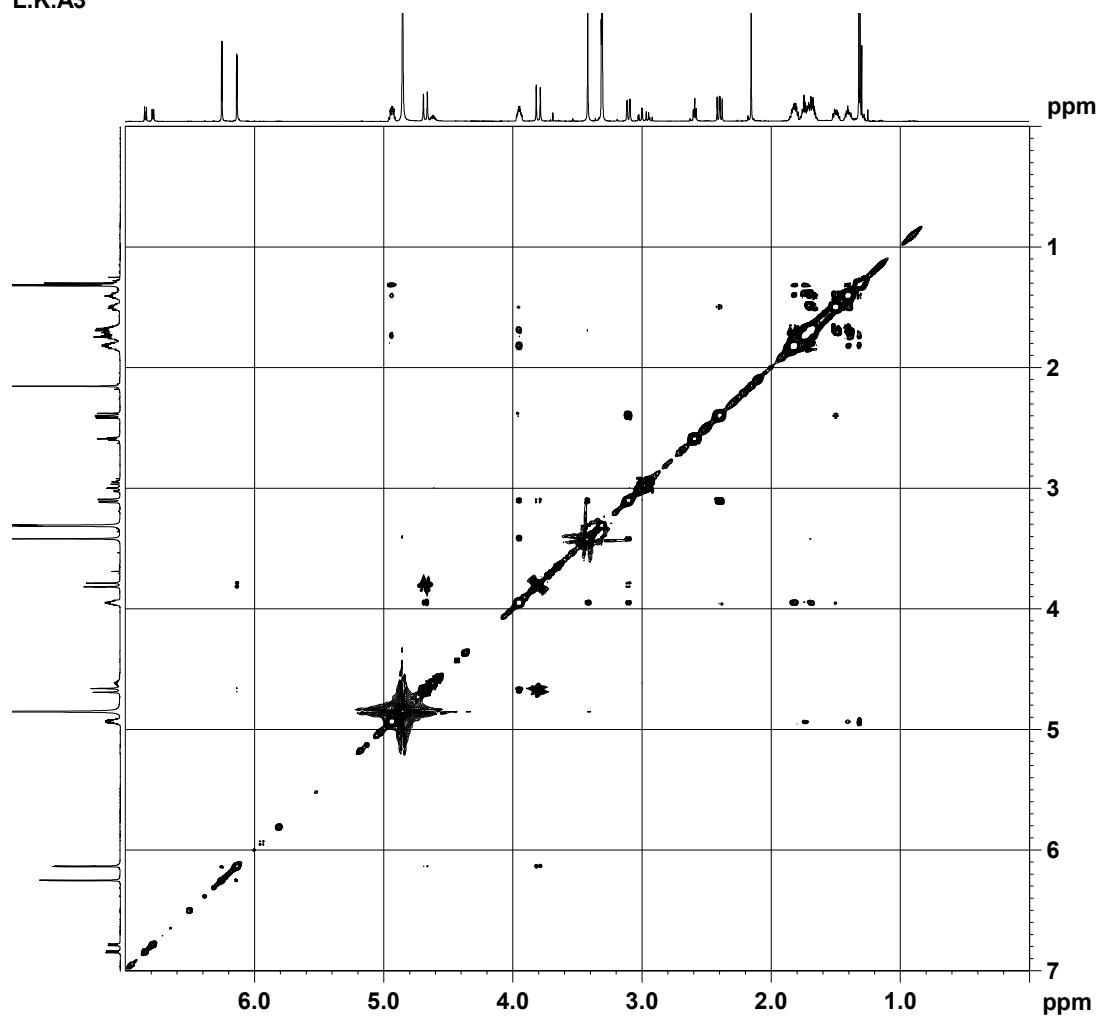


S43. HSQC (600 and 150 MHz, CD₃OD) spectrum of compound 9.

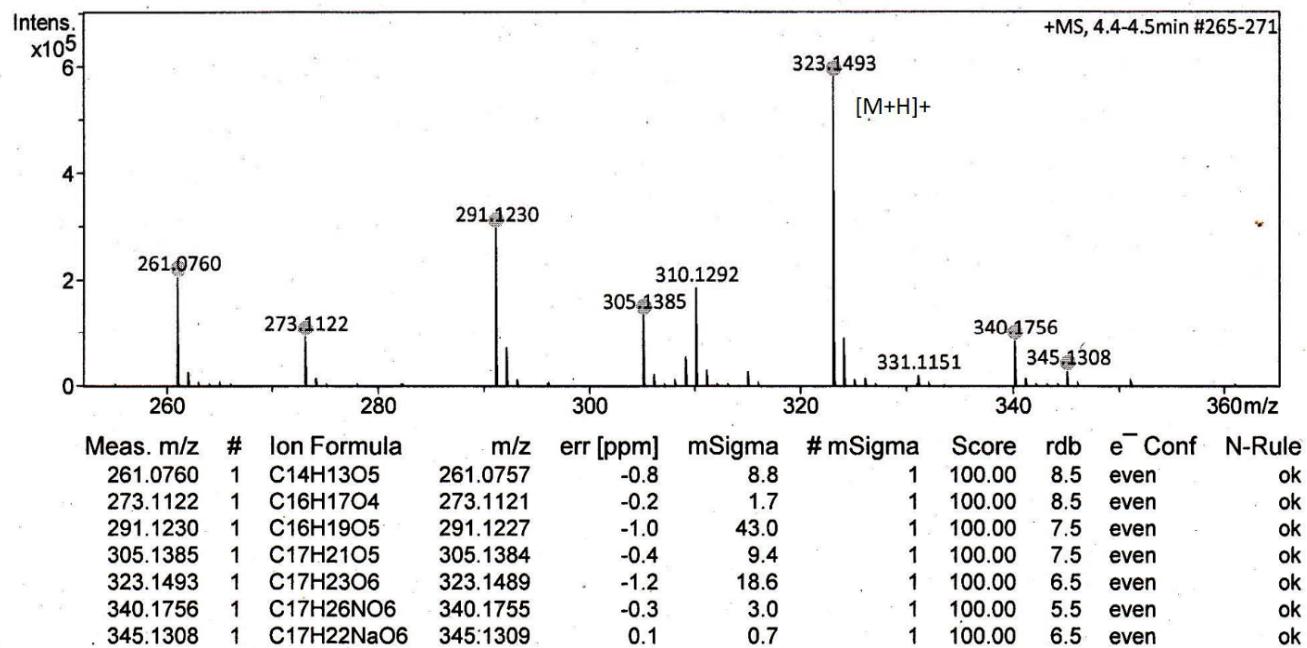


S44. HMBC (600 and 150 MHz, CD_3OD) spectrum of compound 9.

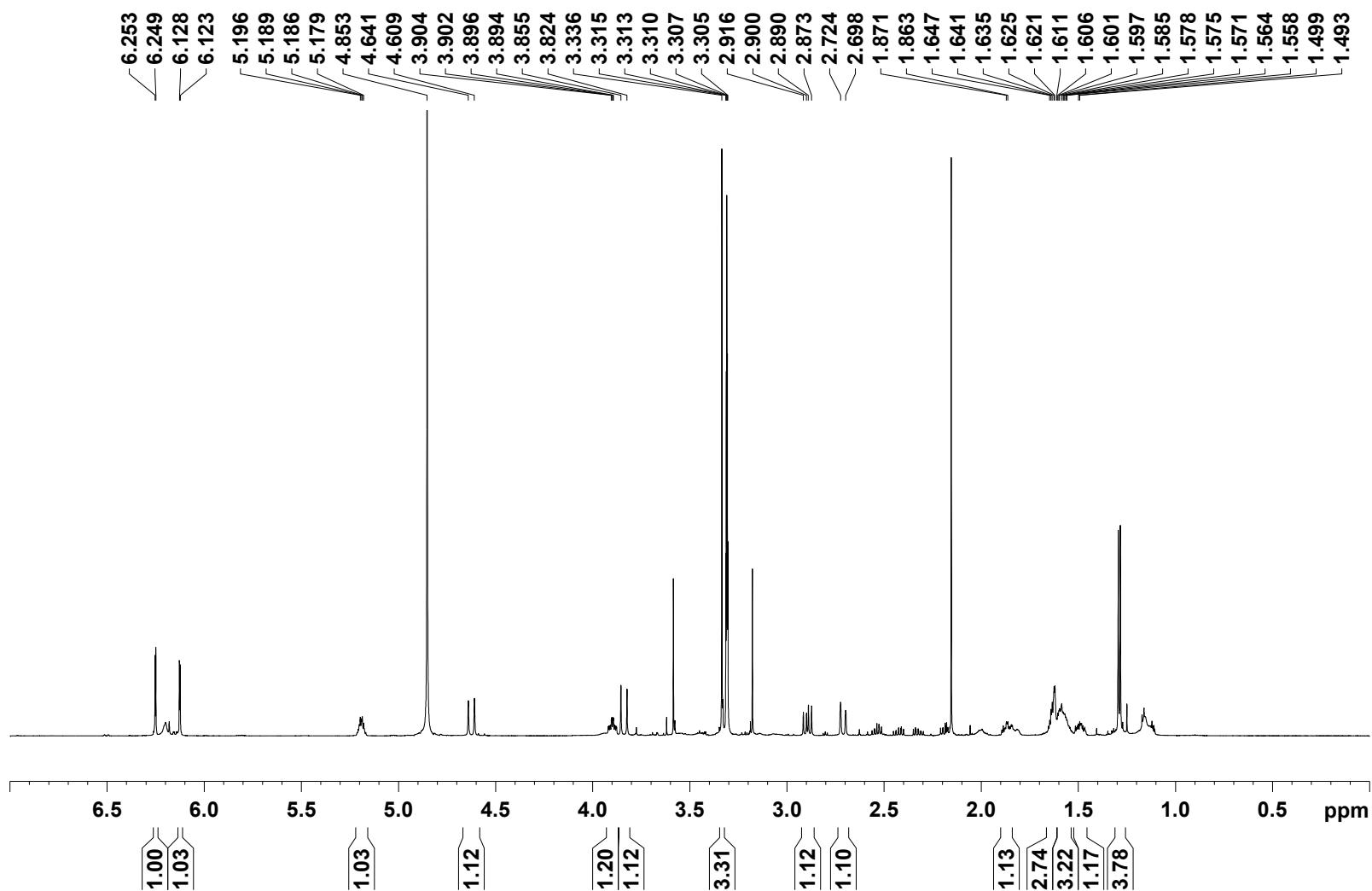
L.K.A3



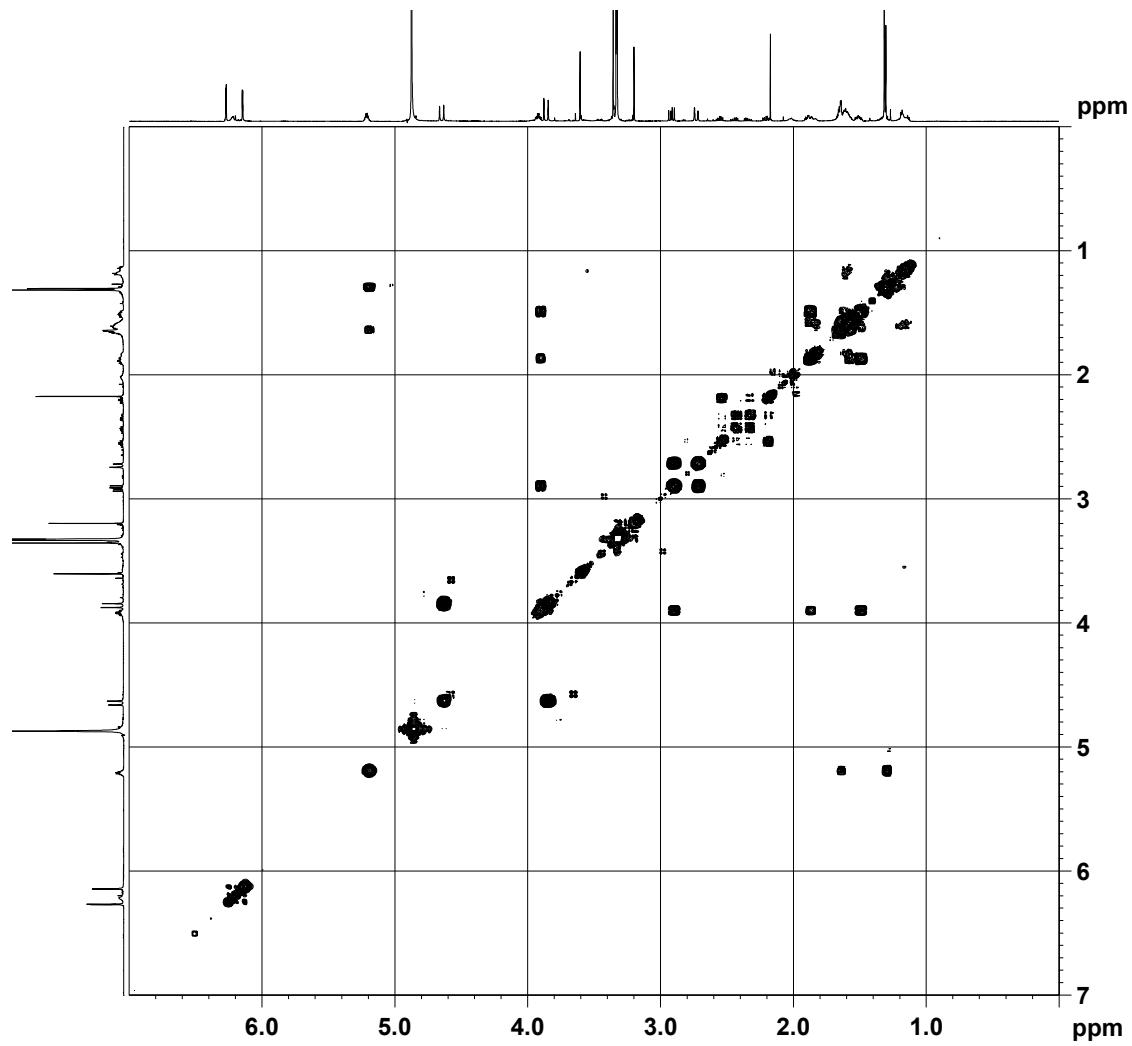
S45. ROESY (600 MHz, CD₃OD) spectrum of compound 9.



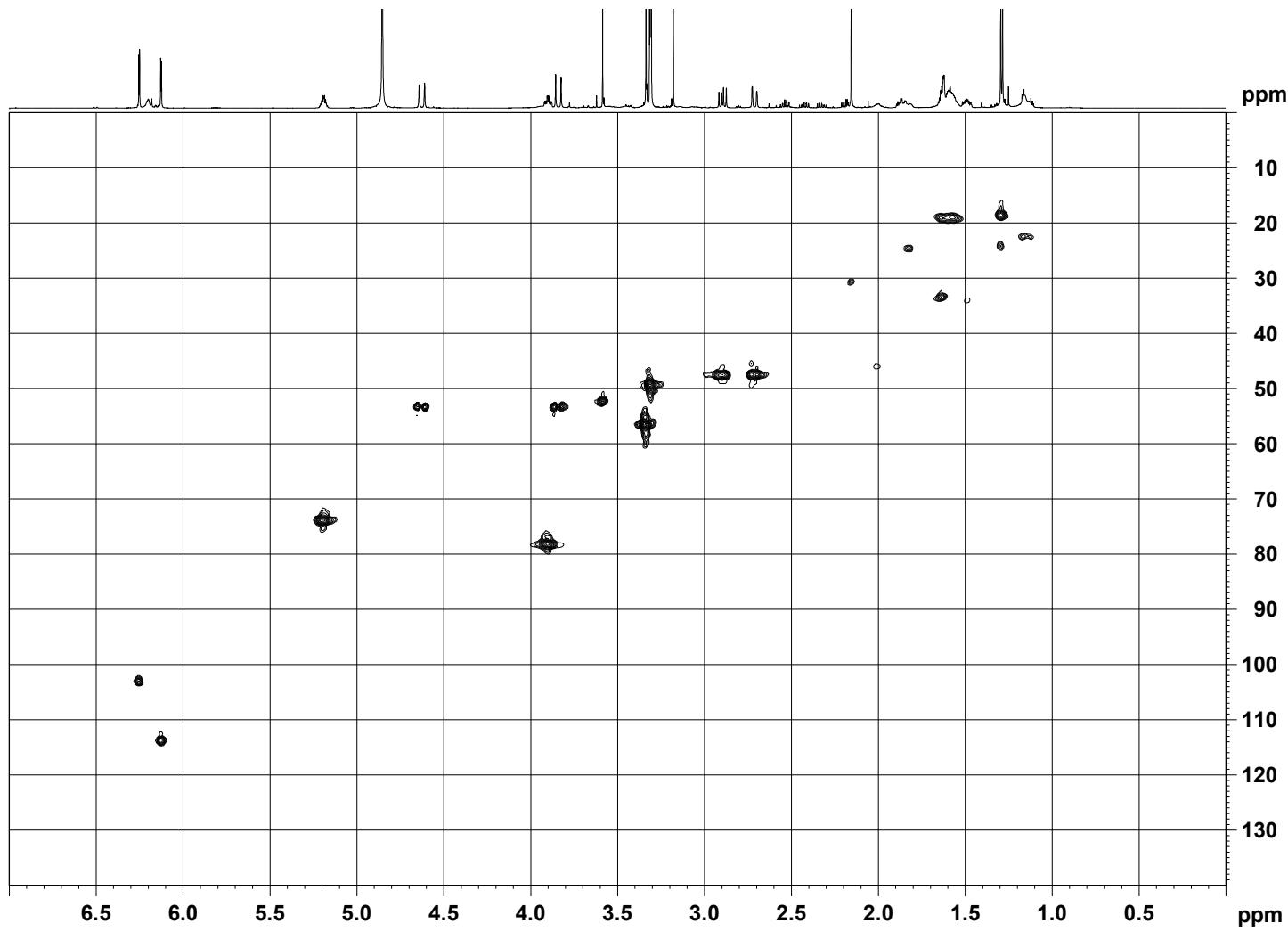
S46. HRESIMS spectrum of compound 10.



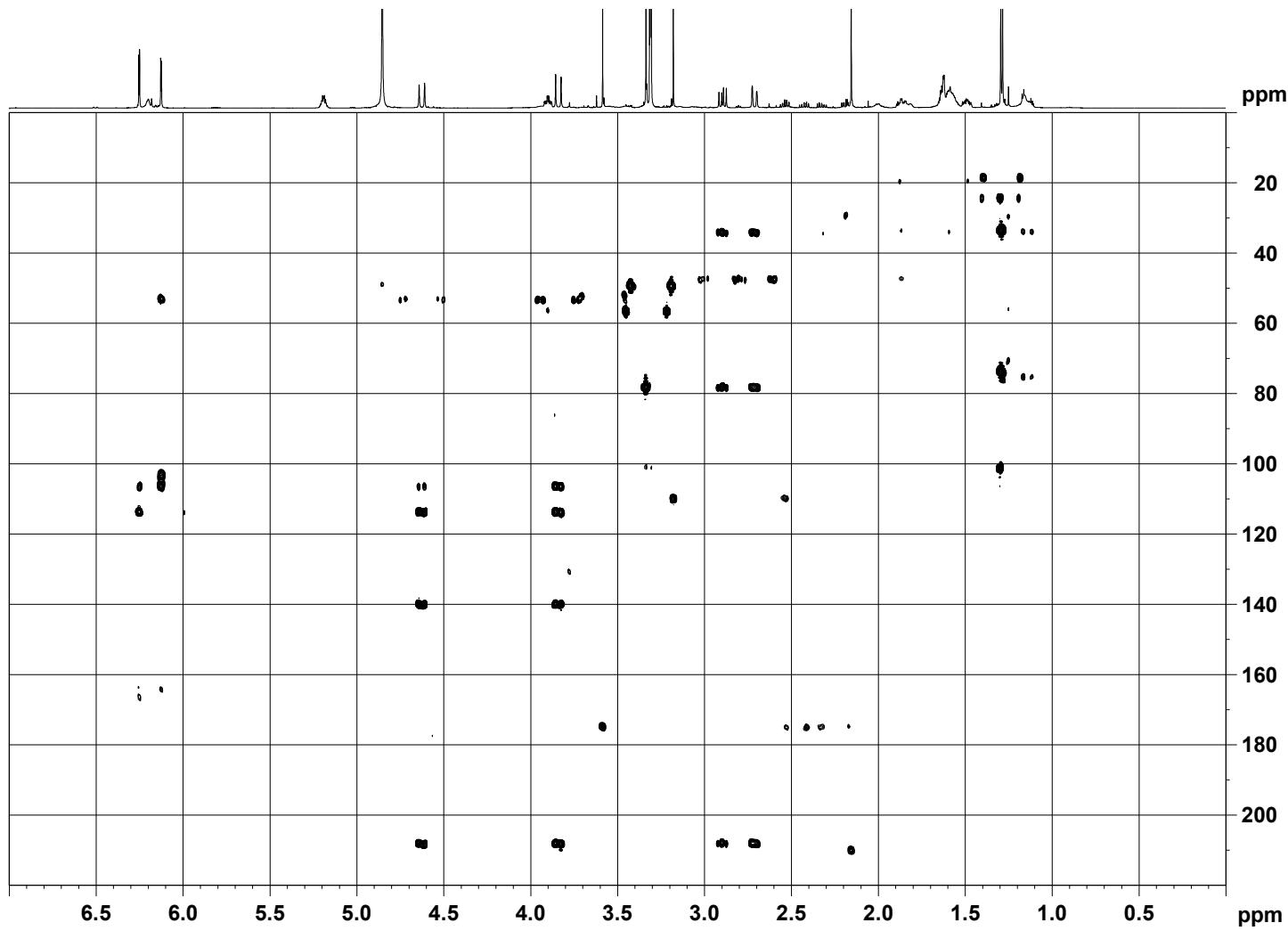
S47. ^1H NMR (600 MHz, CD_3OD) spectrum of compound **10**.



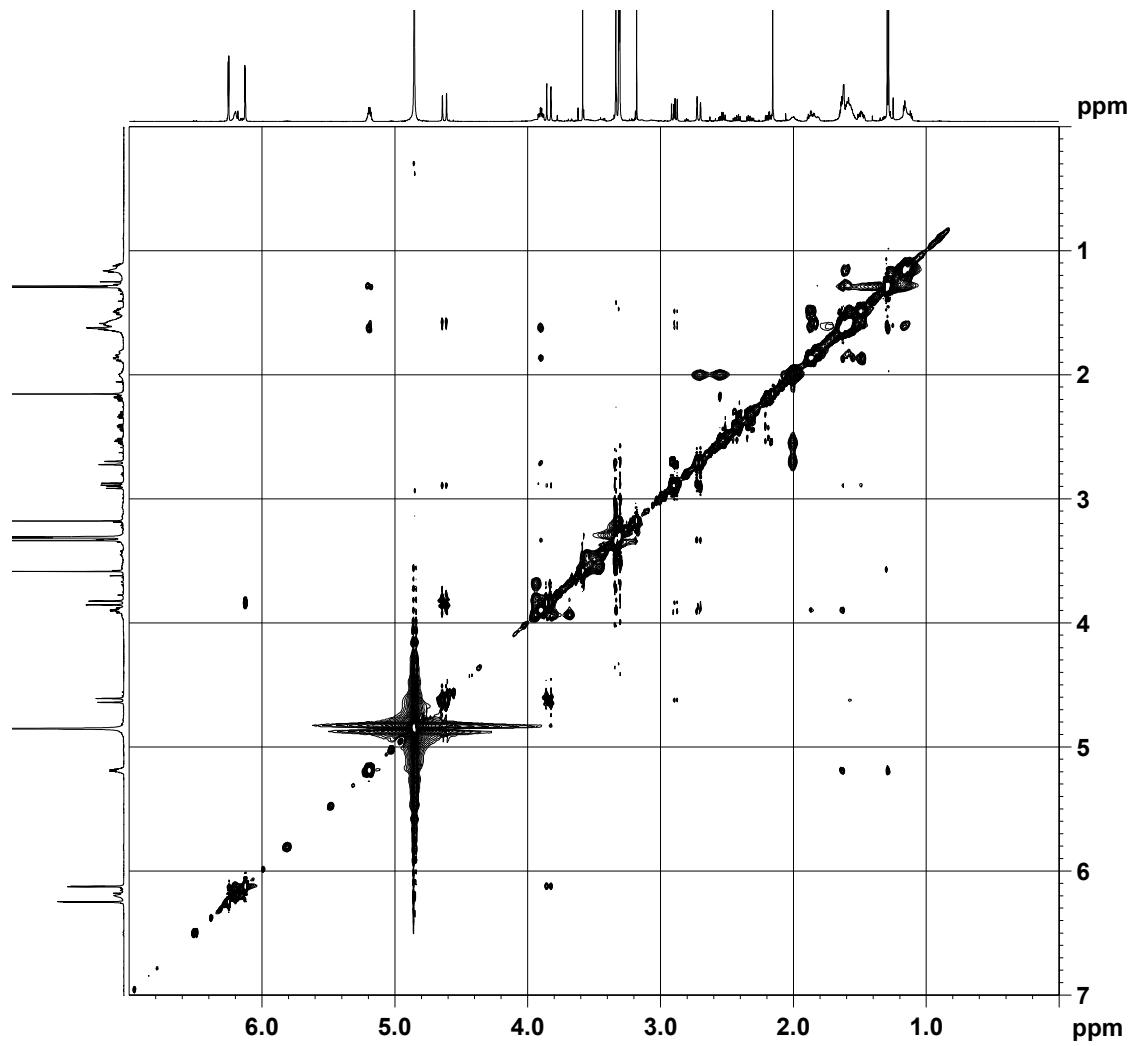
S48. ^1H - ^1H COSY (600 MHz, CD_3OD) spectrum of compound **10**.



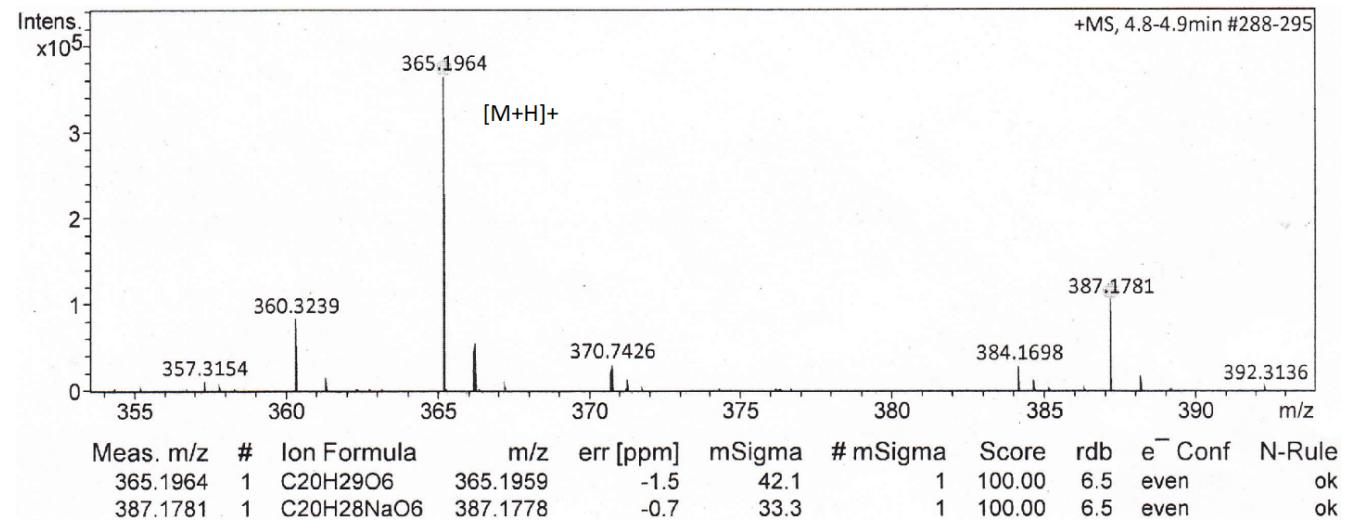
S49. HSQC (600 and 150 MHz, CD_3OD) spectrum of compound **10**.



S50. HMBC (600 and 150 MHz, CD_3OD) spectrum of compound **10**.

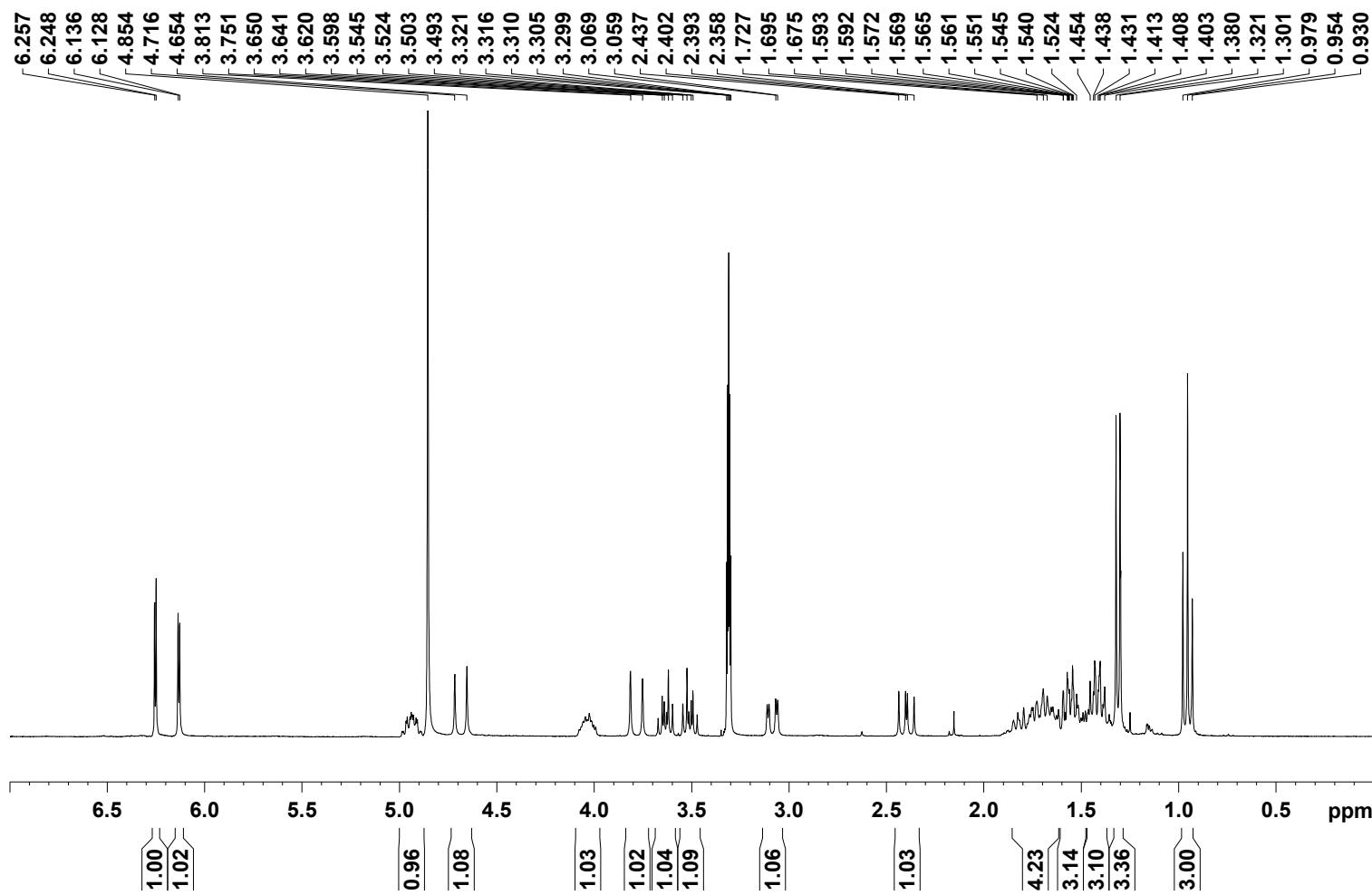


S51. ROESY (600 MHz, CD_3OD) spectrum of compound **10**.



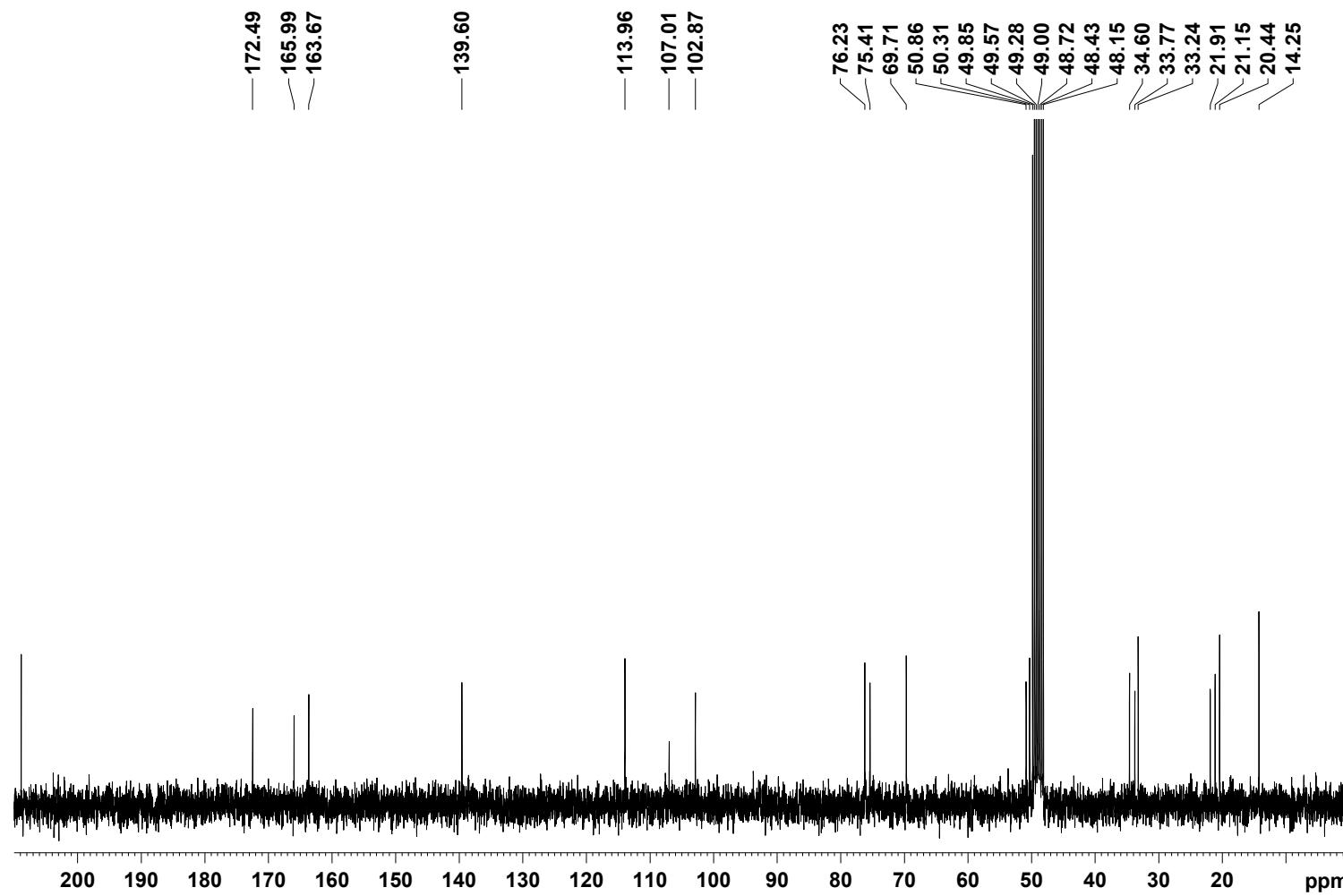
S52. HRESIMS spectrum of compound 11.

Tal60ES5-3-3



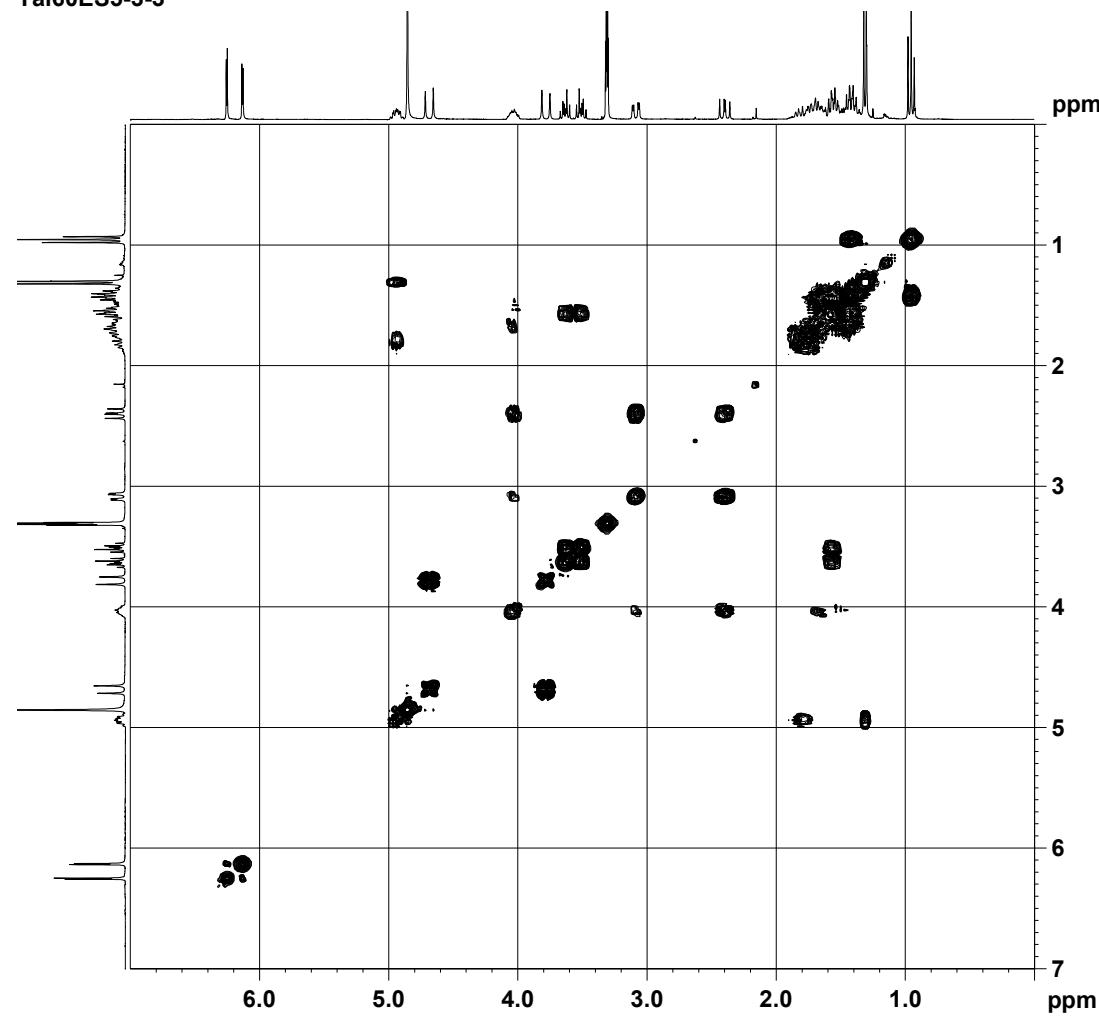
S53. ¹H NMR (300 MHz, CD₃OD) spectrum of compound 11.

Tal60ES5-3-3



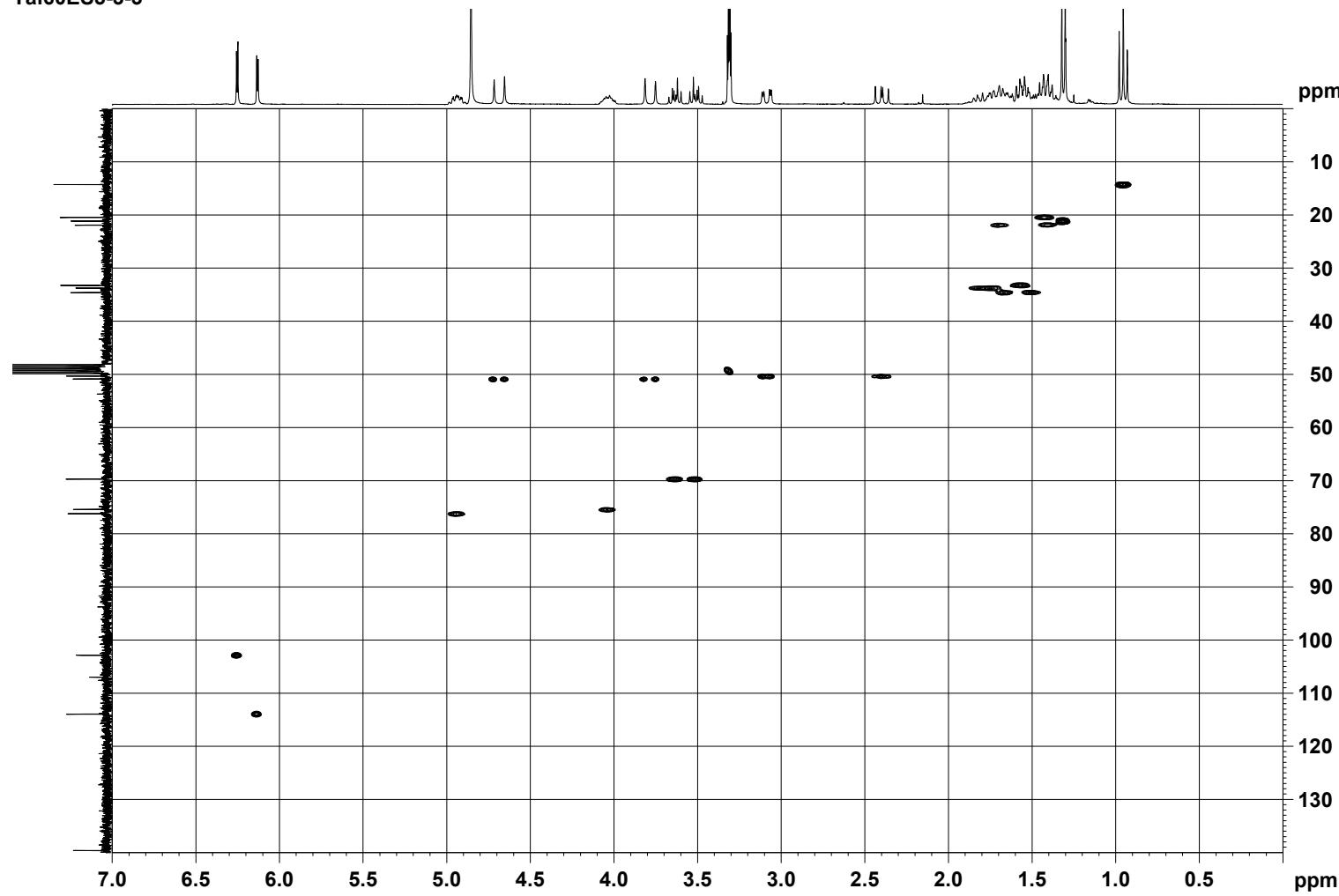
S54. ¹³C NMR (75 MHz, CD₃OD) spectrum of compound 11.

Tal60ES5-3-3



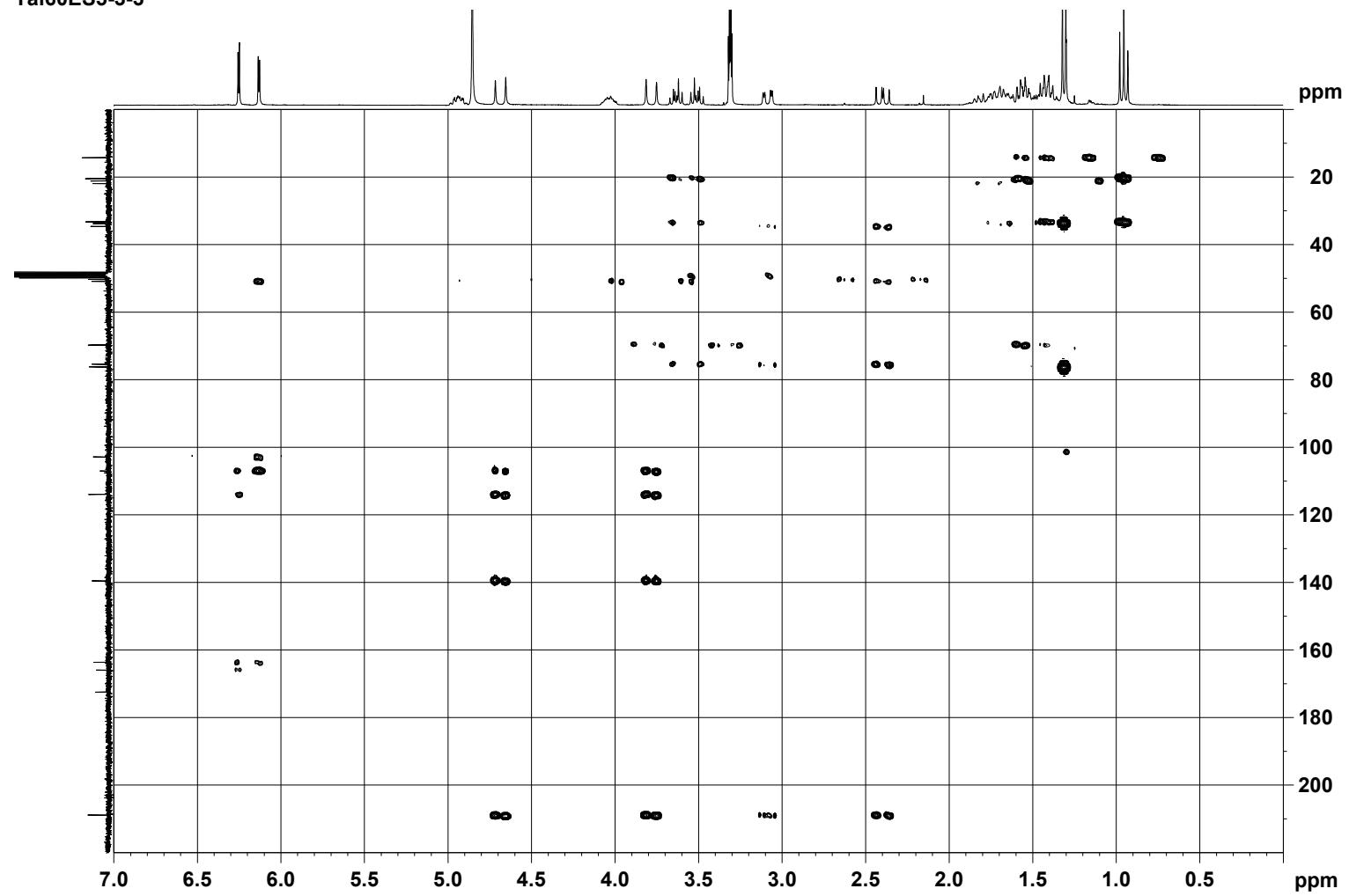
S55. ^1H - ^1H COSY (300 MHz, CD_3OD) spectrum of compound 11.

Tal60ES5-3-3



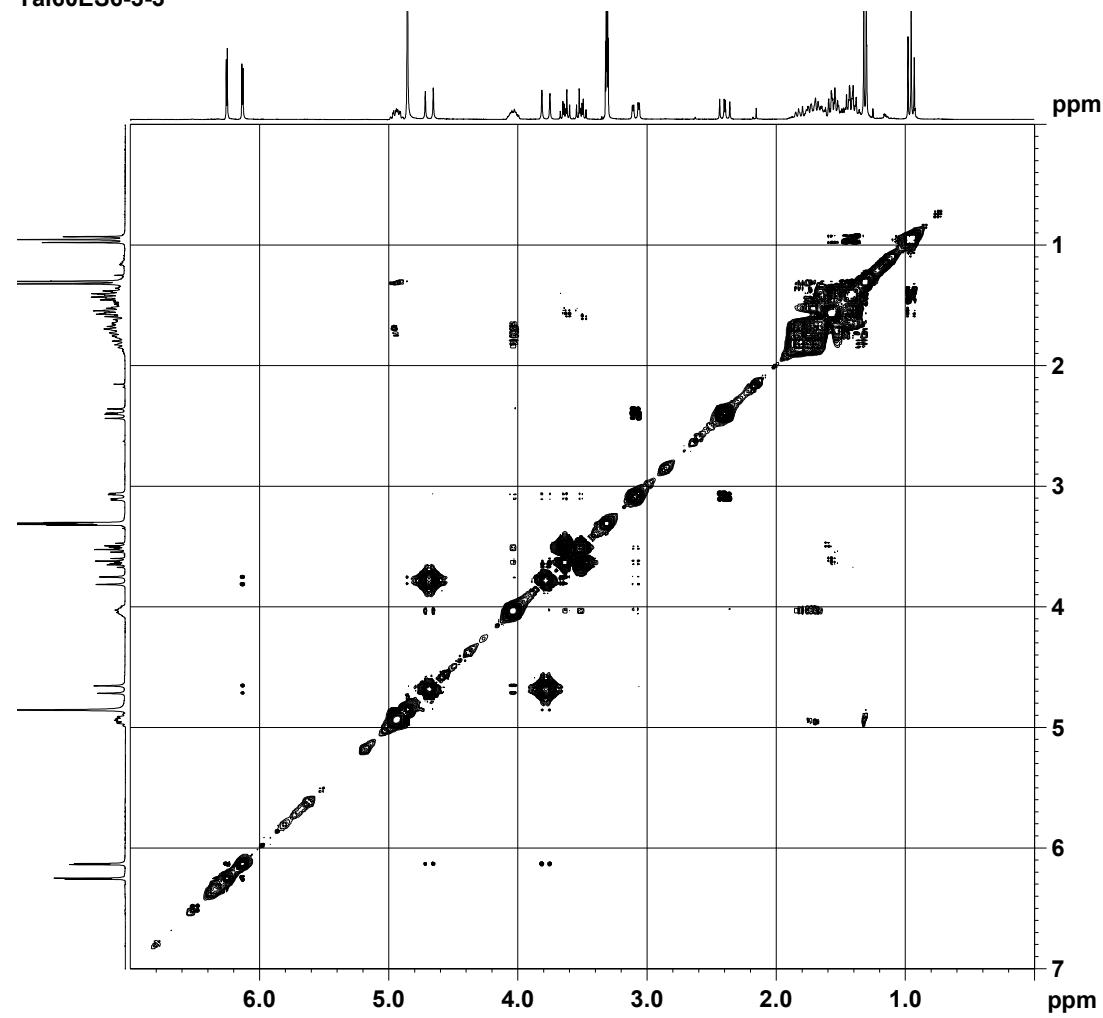
S56. HSQC (300 and 75 MHz, CD₃OD) spectrum of compound 11.

Tal60ES5-3-3

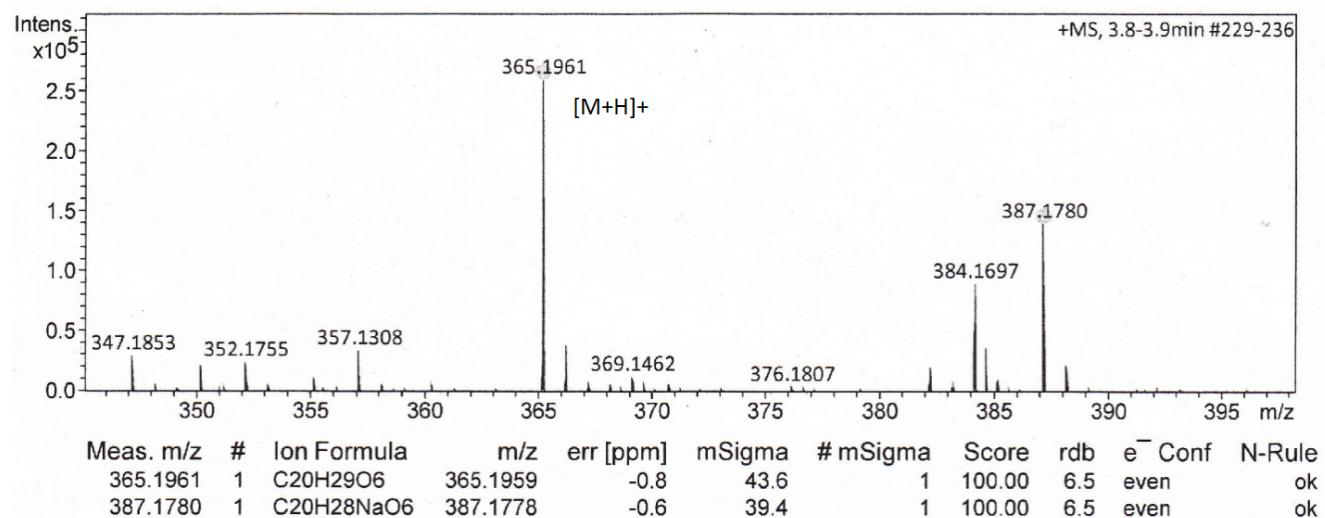


S57. HMBC (300 and 75 MHz, CD_3OD) spectrum of compound 11.

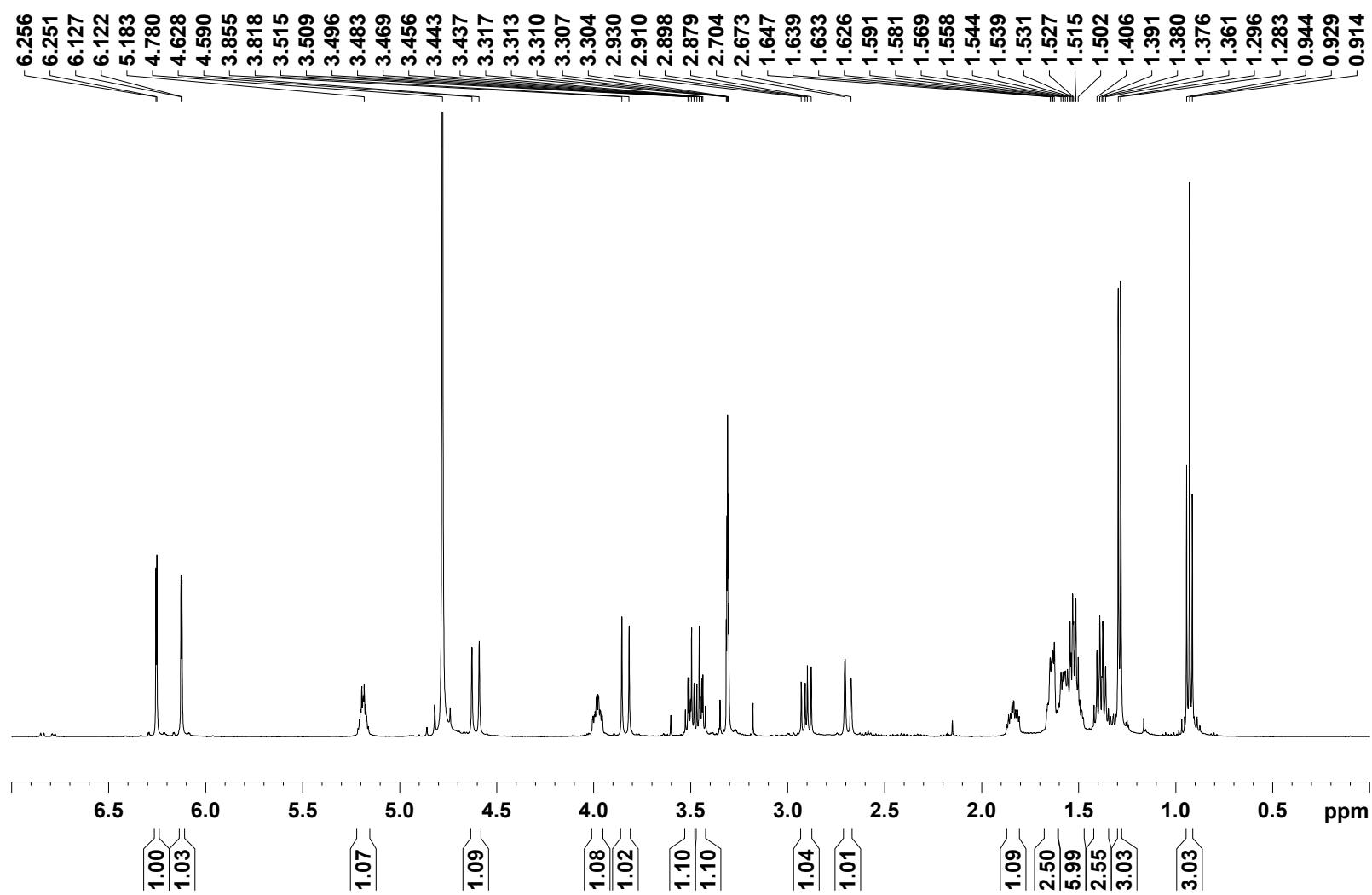
Tal60ES6-3-3



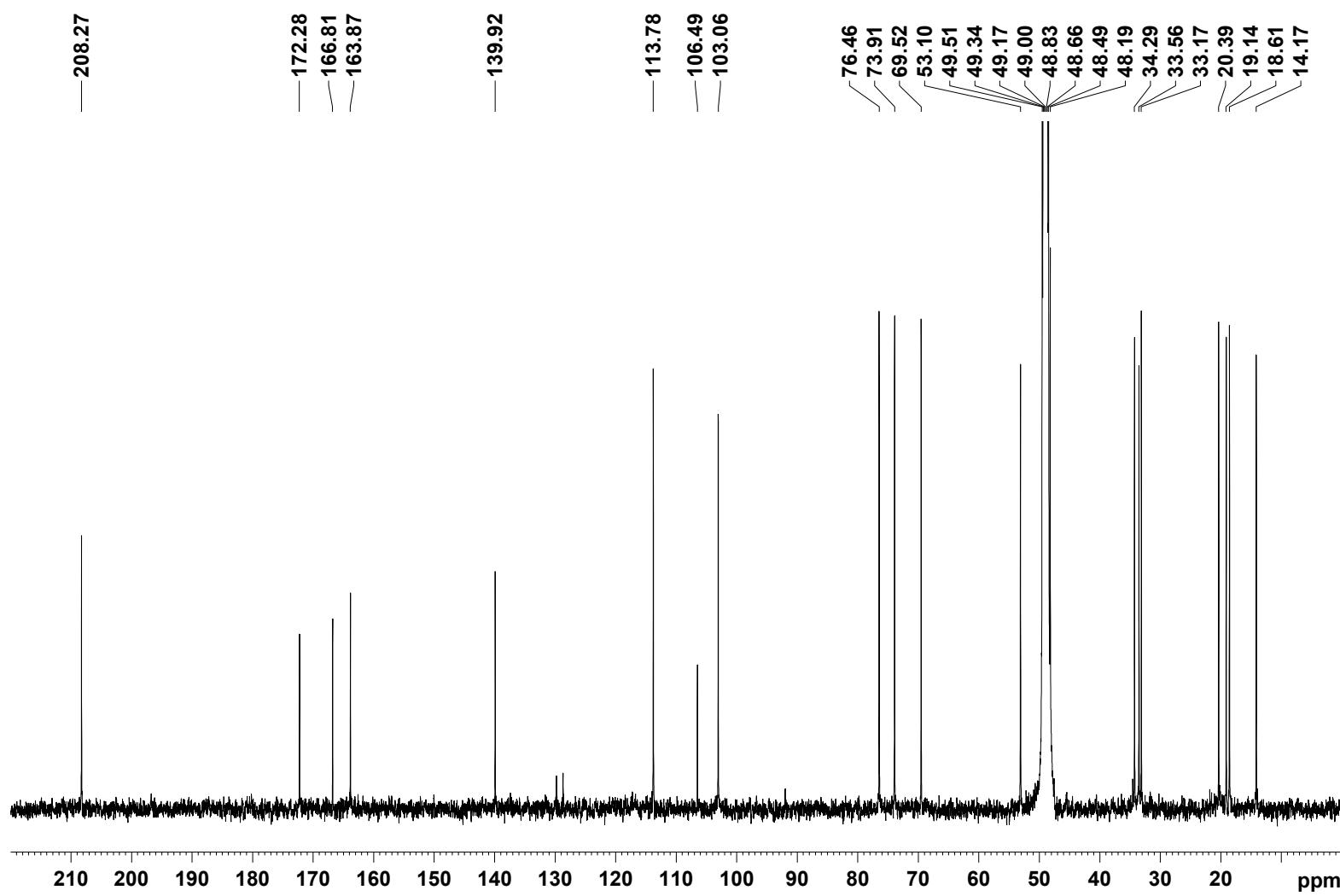
S58. ROESY (300 MHz, CD_3OD) spectrum of compound **11**.



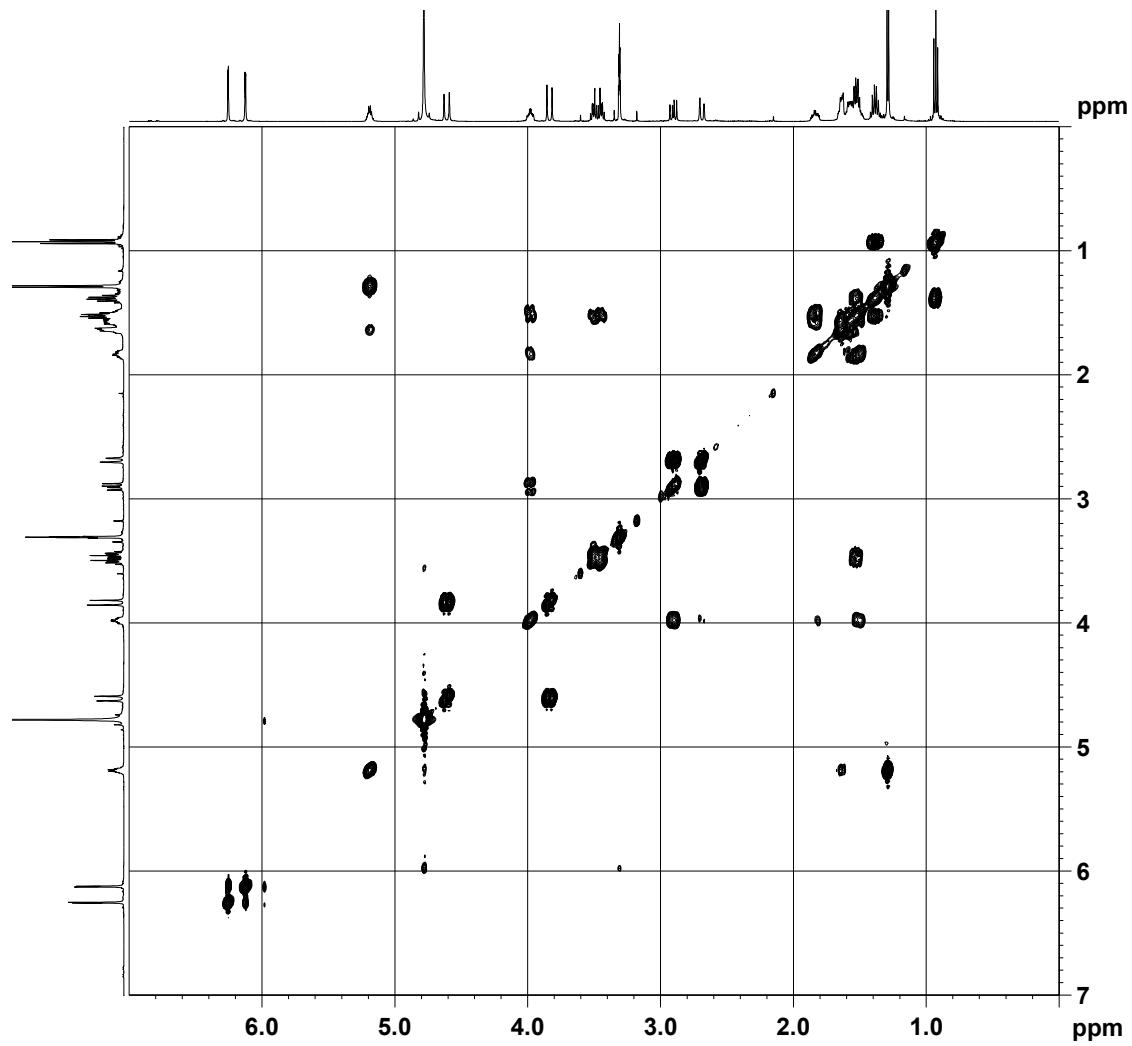
S59. HRESIMS spectrum of compound 12.



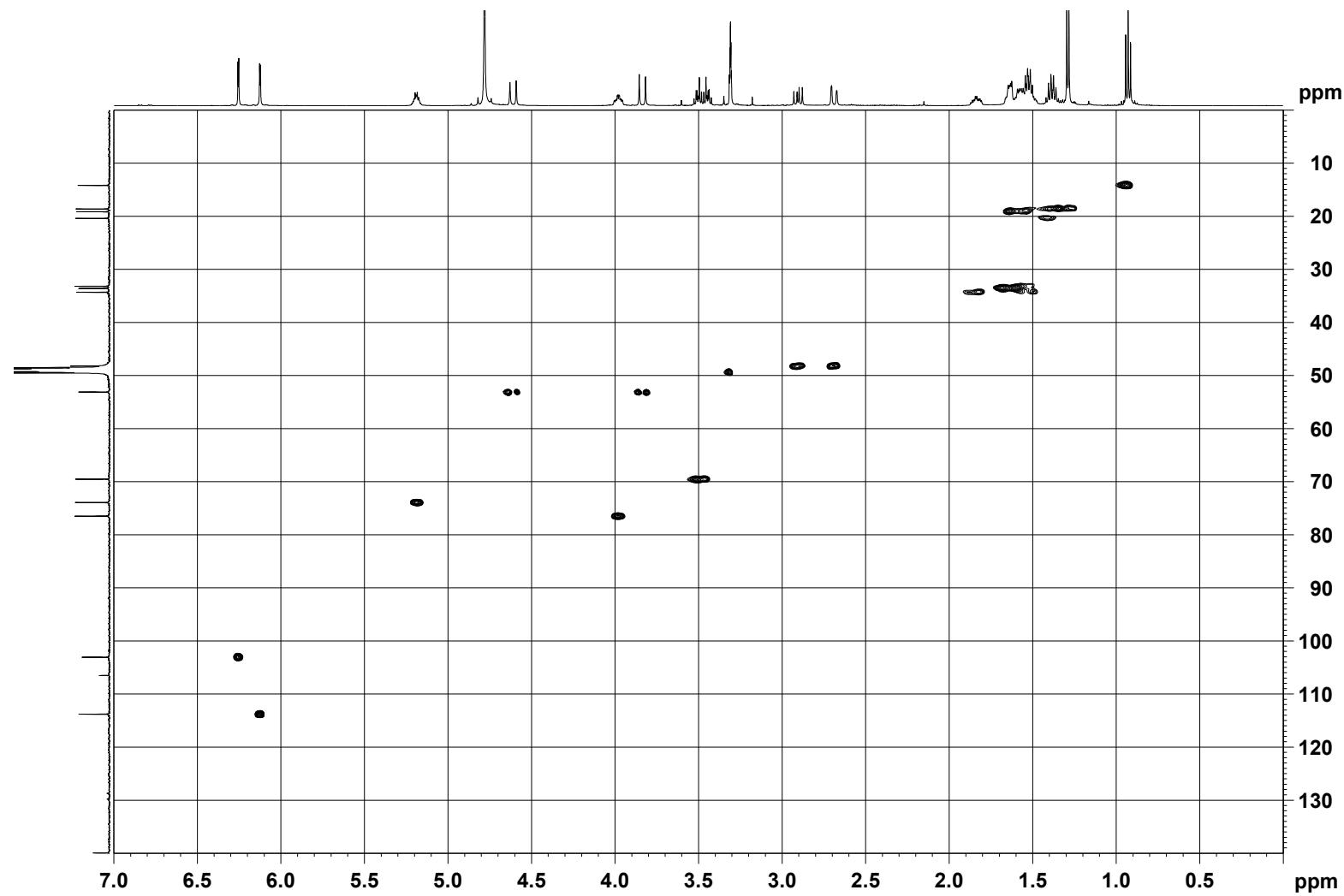
S60. ^1H NMR (500 MHz, CD_3OD) spectrum of compound 12.



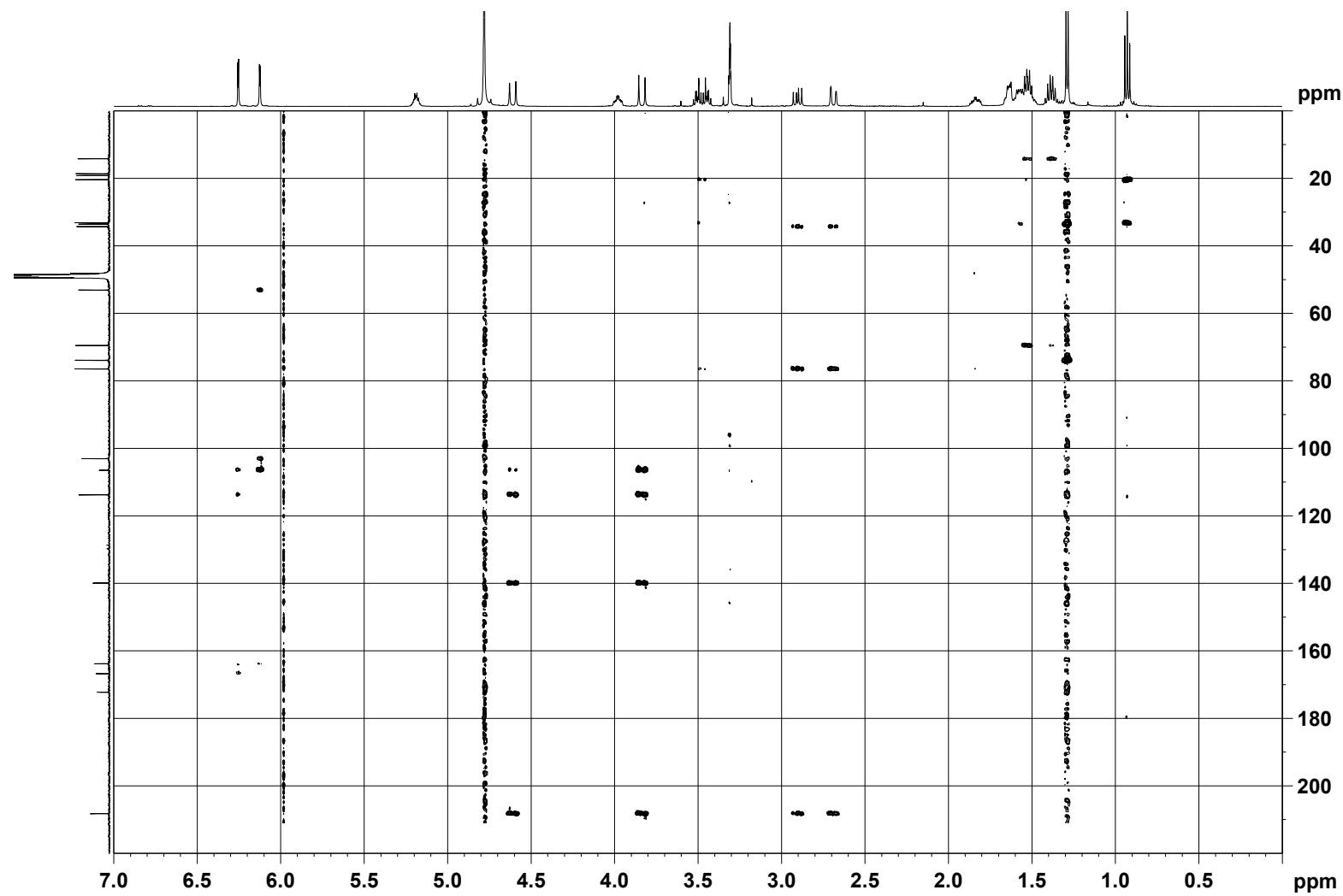
S61. ^{13}C NMR (125 MHz, CD_3OD) spectrum of compound 12.



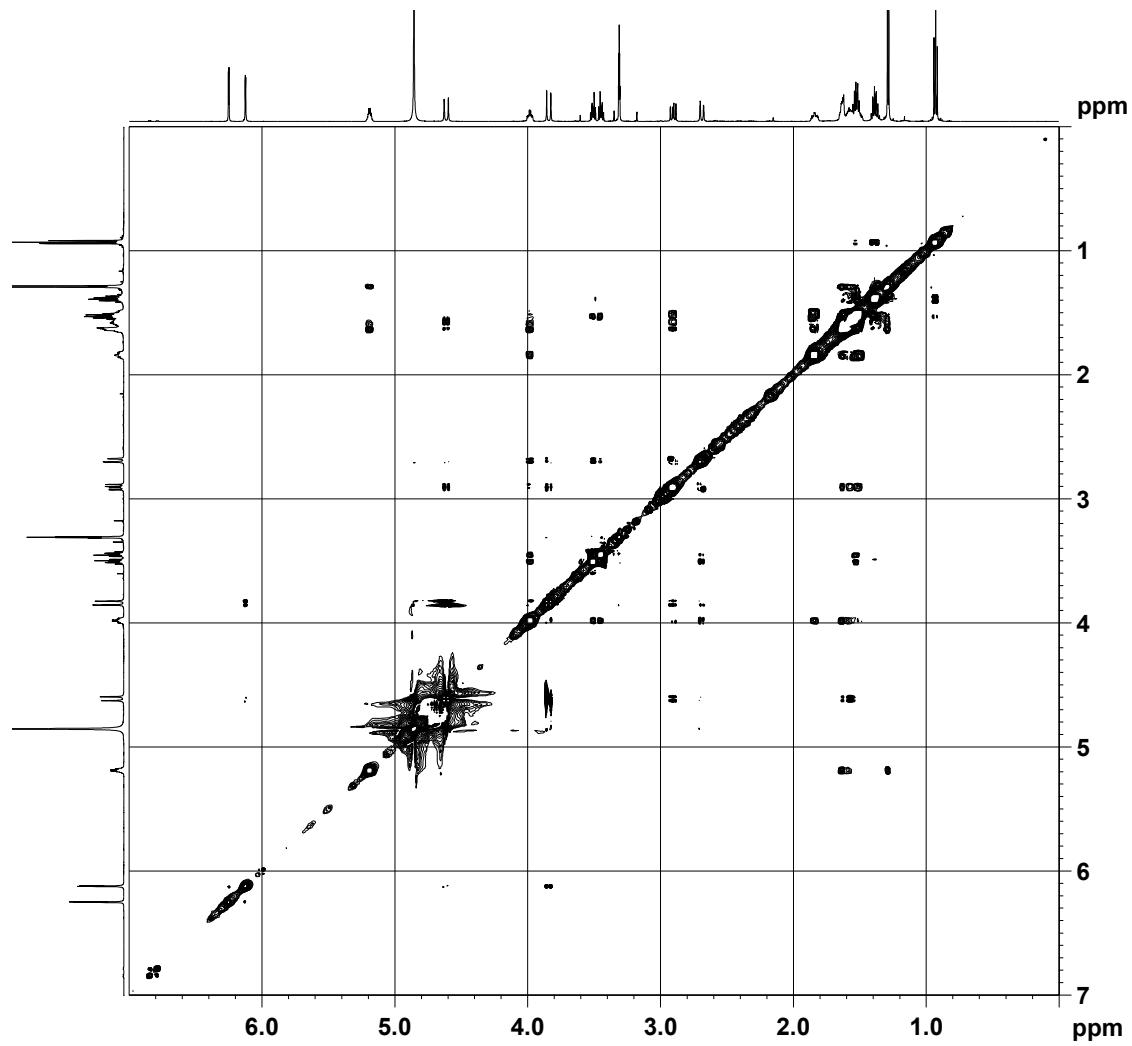
S62. ^1H - ^1H COSY (500 MHz, CD_3OD) spectrum of compound **12**.



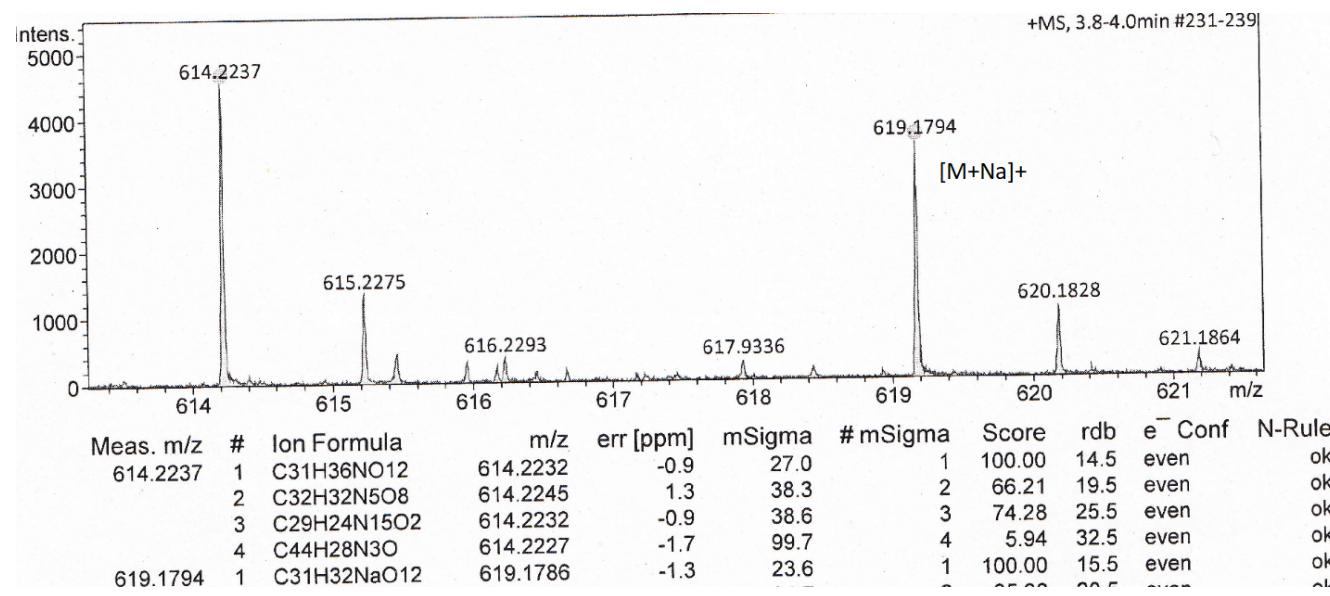
S63. HSQC (500 and 125 MHz, CD₃OD) spectrum of compound **12**.



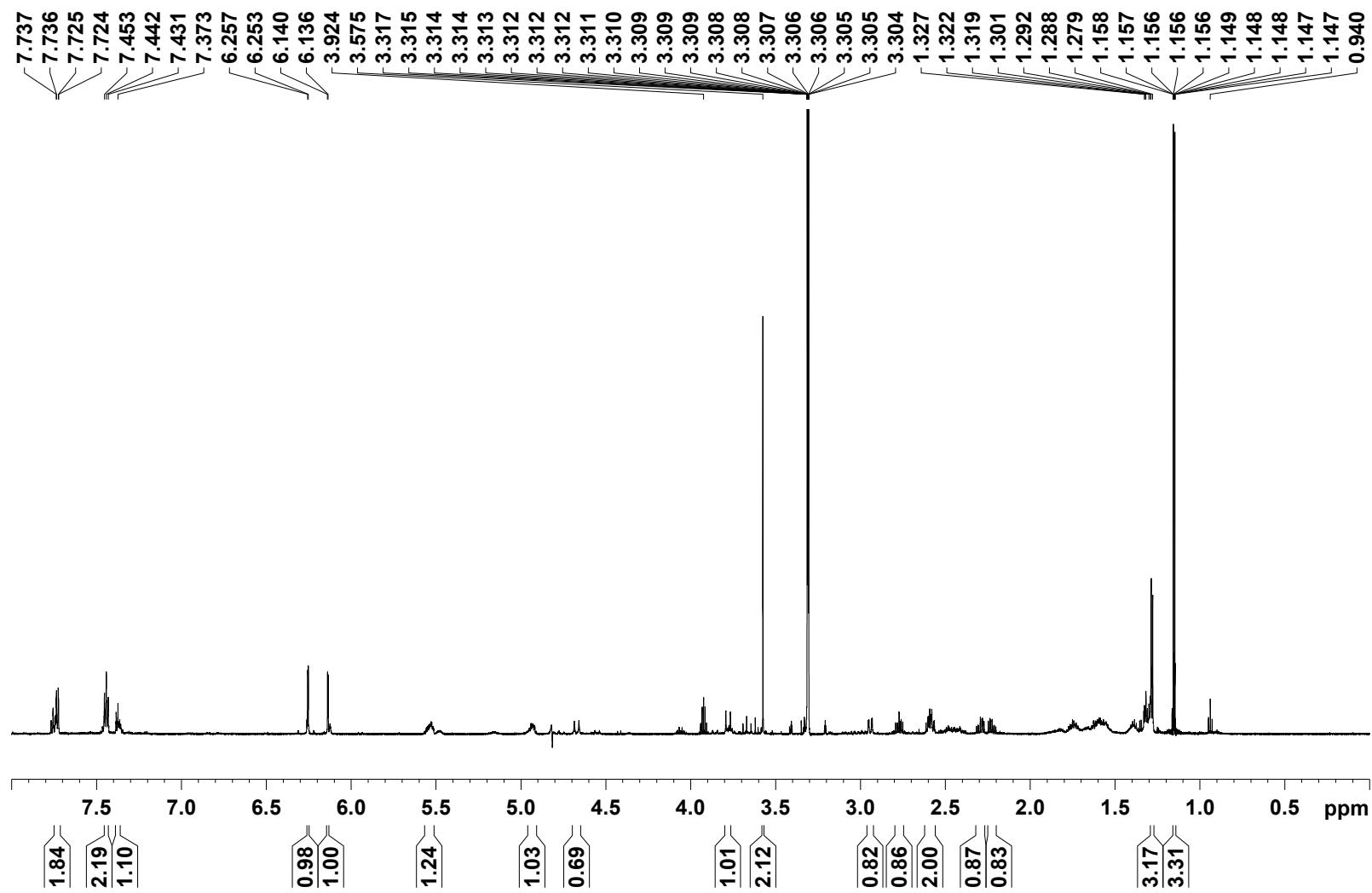
S64. HMBC (500 and 125 MHz, CD₃OD) spectrum of compound 12.



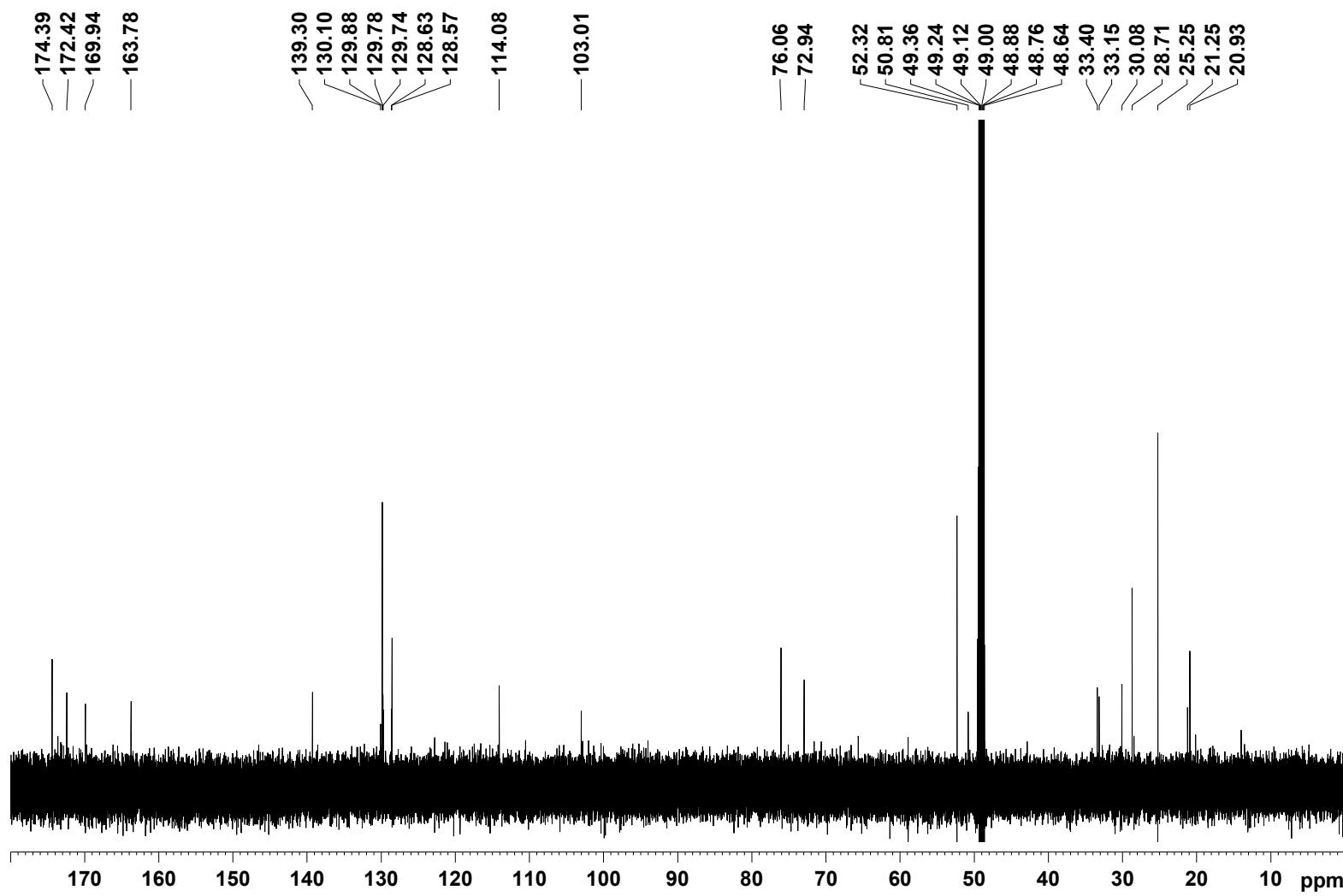
S65. ROESY (500 MHz, CD₃OD) spectrum of compound **12**



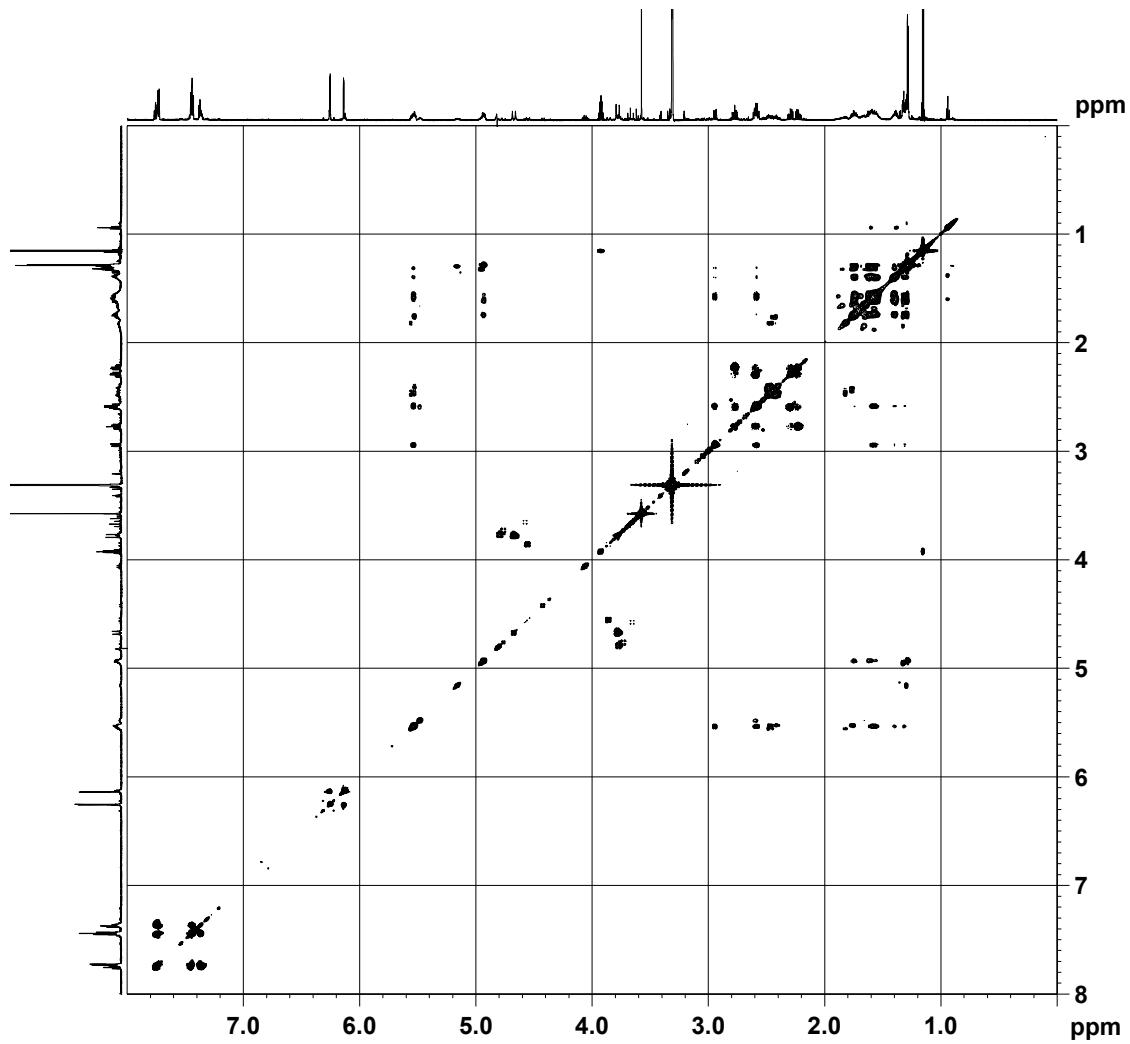
S66. HRESIMS spectrum of compound **13**.



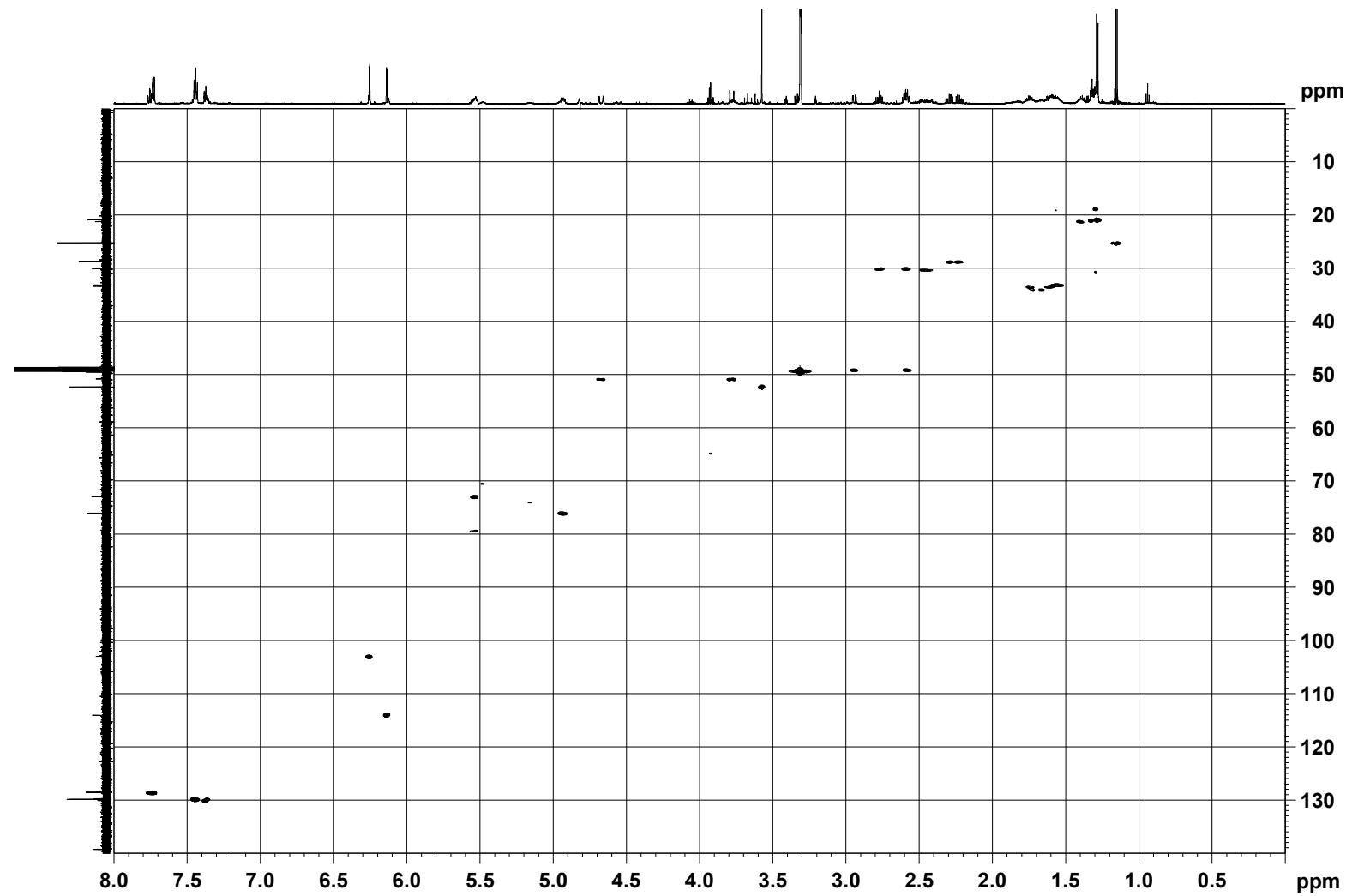
S67. ^1H NMR (700 MHz, CD_3OD) spectrum of compound 13.



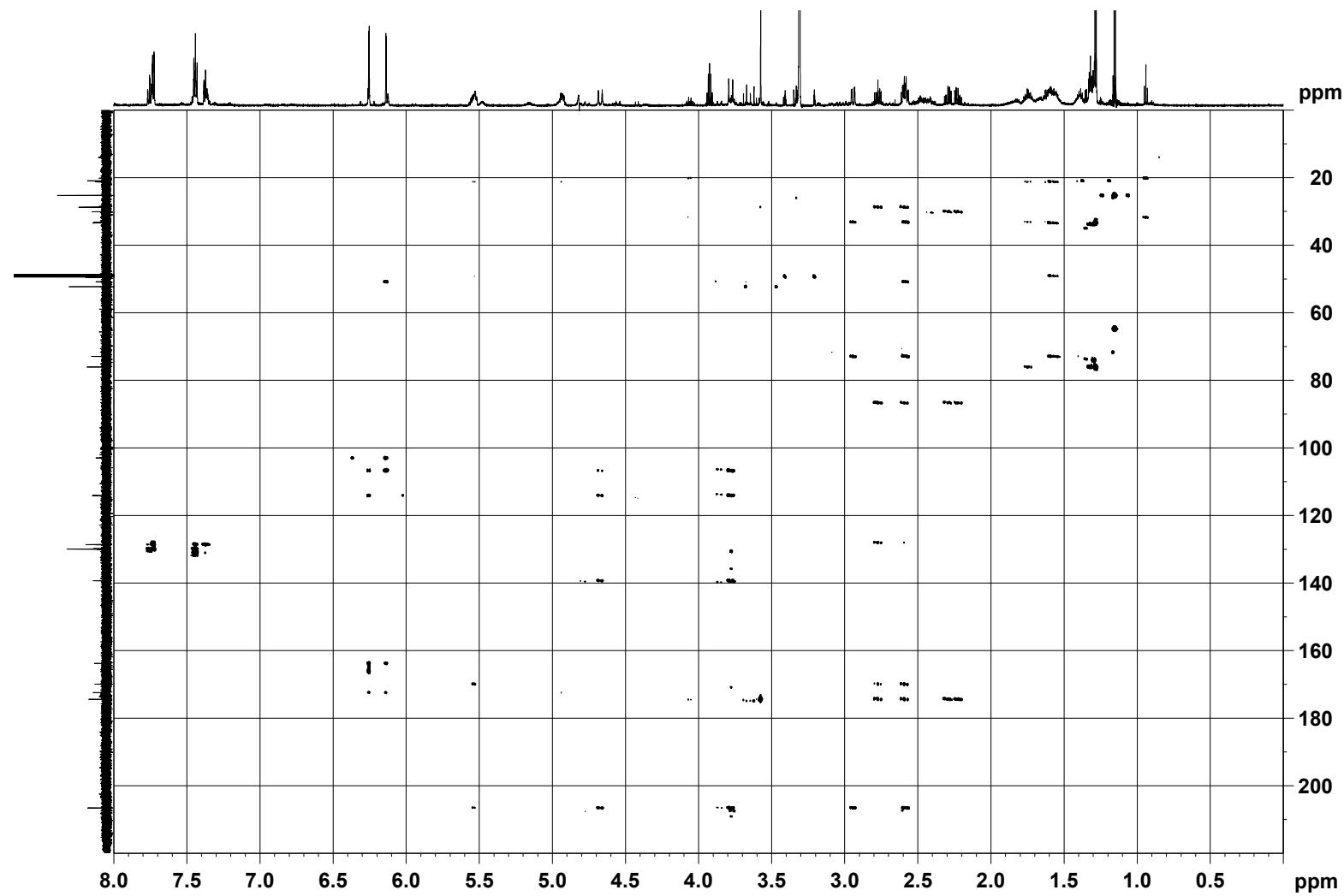
S68. ^{13}C NMR (175 MHz, CD_3OD) spectrum of compound **13**.



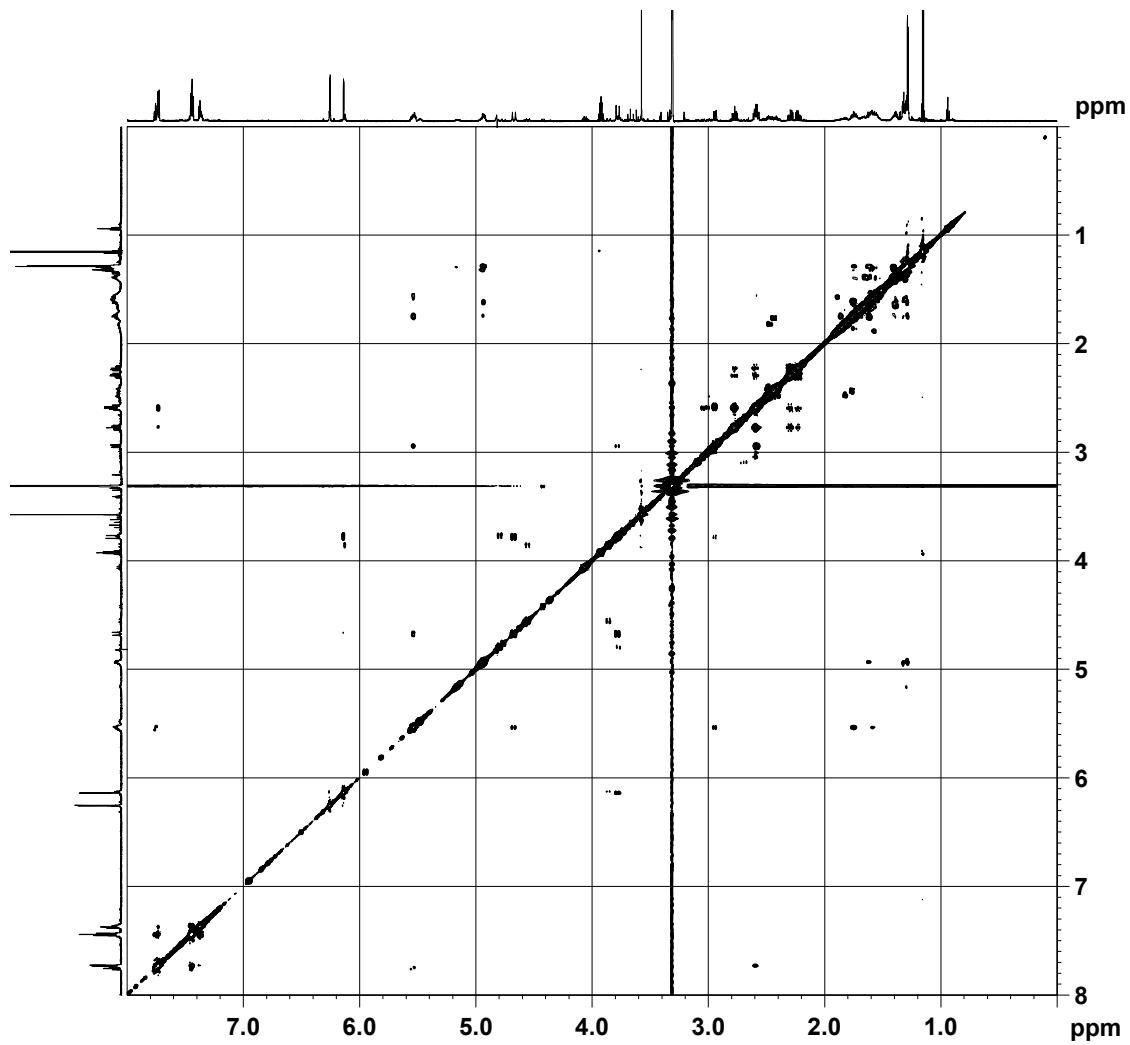
S69. ^1H - ^1H TOCSY NMR (700 MHz, CD_3OD) spectrum of compound 13.



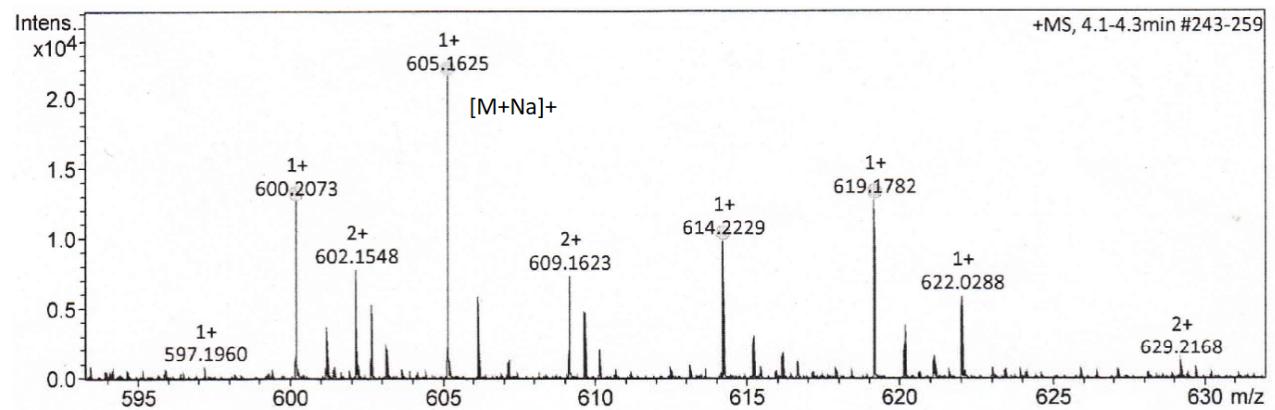
S70. HSQC (700 and 175 MHz, CD_3OD) spectrum of compound 13.



S71. HMBC (700 and 175 MHz, CD₃OD) spectrum of compound 13.

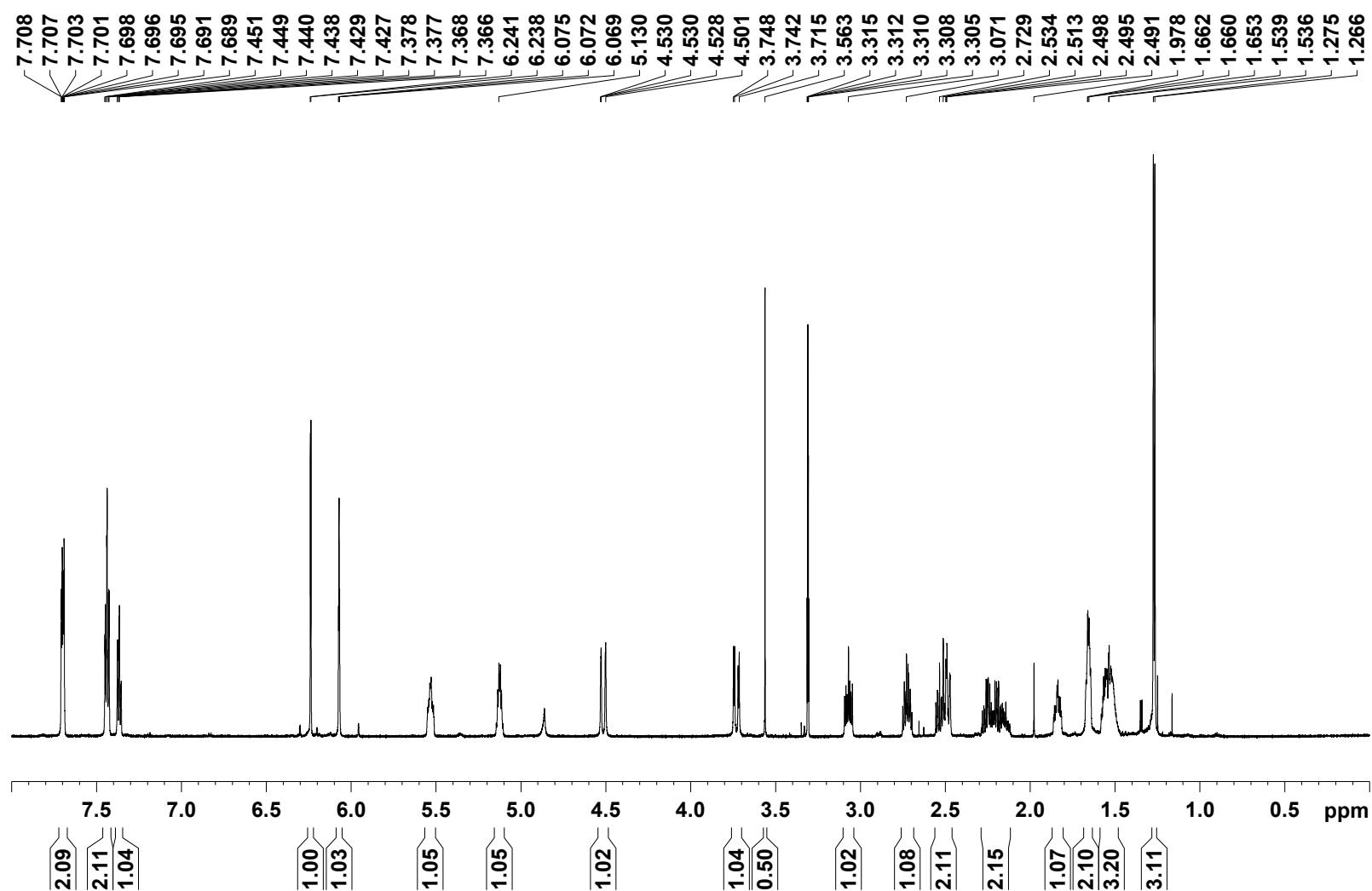


S72. ROESY (700 MHz, CD_3OD) spectrum of compound **13**.

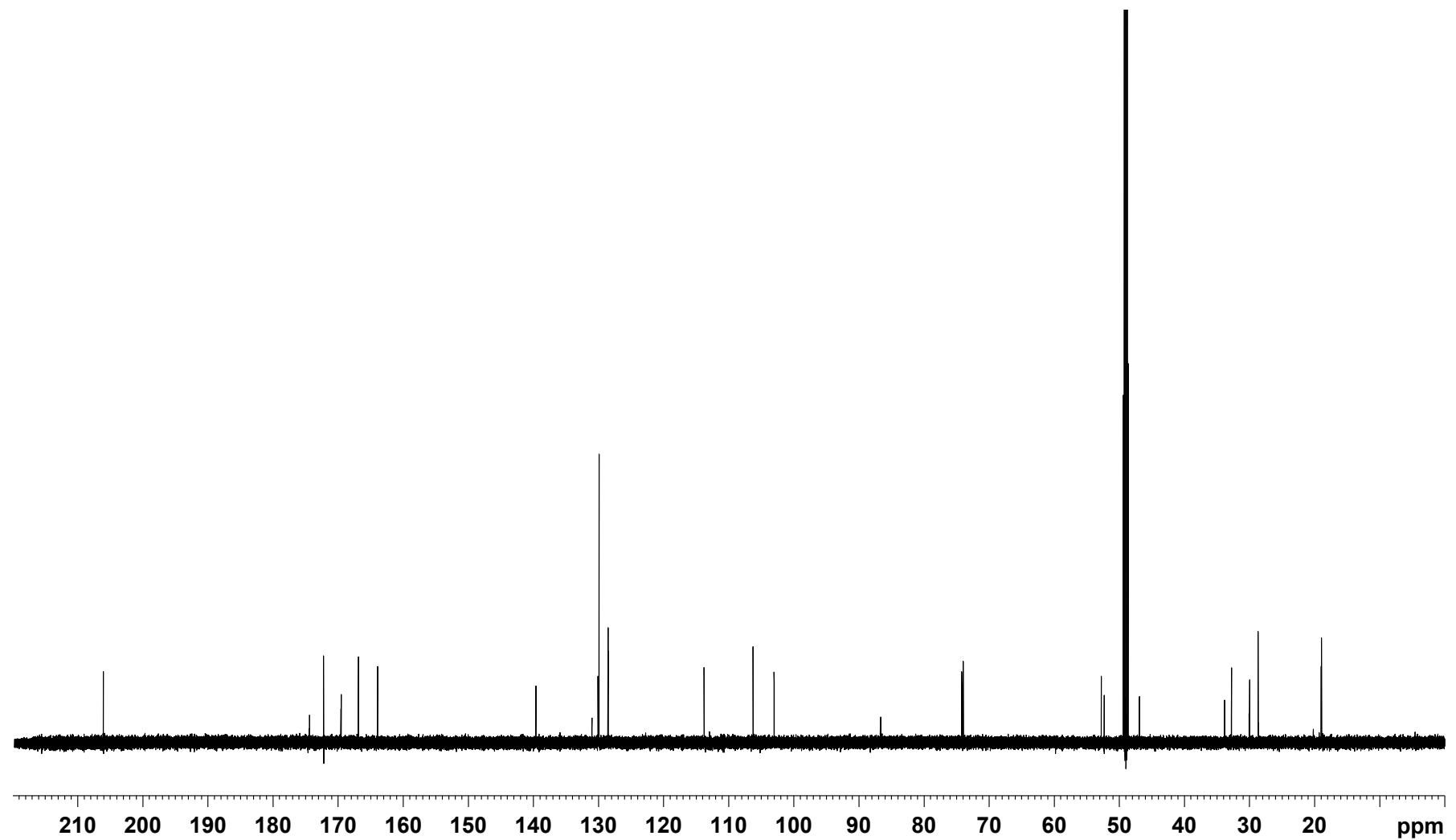


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
600.2073	1	C ₃₀ H ₃₄ NO ₁₂	600.2076	0.4	22.1	1	100.00	14.5	even	ok
	2	C ₂₇ H ₂₆ N ₁₁ O ₆	600.2062	-1.8	23.1	2	62.59	20.5	even	ok
	3	C ₂₈ H ₂₂ N ₁₅ O ₂	600.2075	0.4	34.7	3	74.53	25.5	even	ok
	4	C ₄₃ H ₂₆ N ₃ O	600.2070	-0.5	95.3	4	8.46	32.5	even	ok
605.1625	1	C ₂₇ H ₂₉ N ₂ O ₁₄	605.1613	-1.9	19.8	1	77.84	14.5	even	ok
	2	C ₂₅ H ₁₇ N ₁₆ O ₄	605.1613	-1.9	30.5	2	60.55	25.5	even	ok
	3	C ₂₈ H ₂₅ N ₆ O ₁₀	605.1627	0.3	30.6	3	100.00	19.5	even	ok
	4	C ₂₇ H ₂₂ N ₁₀ NaO ₆	605.1616	-1.5	31.1	4	70.12	21.5	even	ok
	5	C ₃₀ H ₃₀ NaO ₁₂	605.1629	0.8	31.7	5	85.94	15.5	even	ok

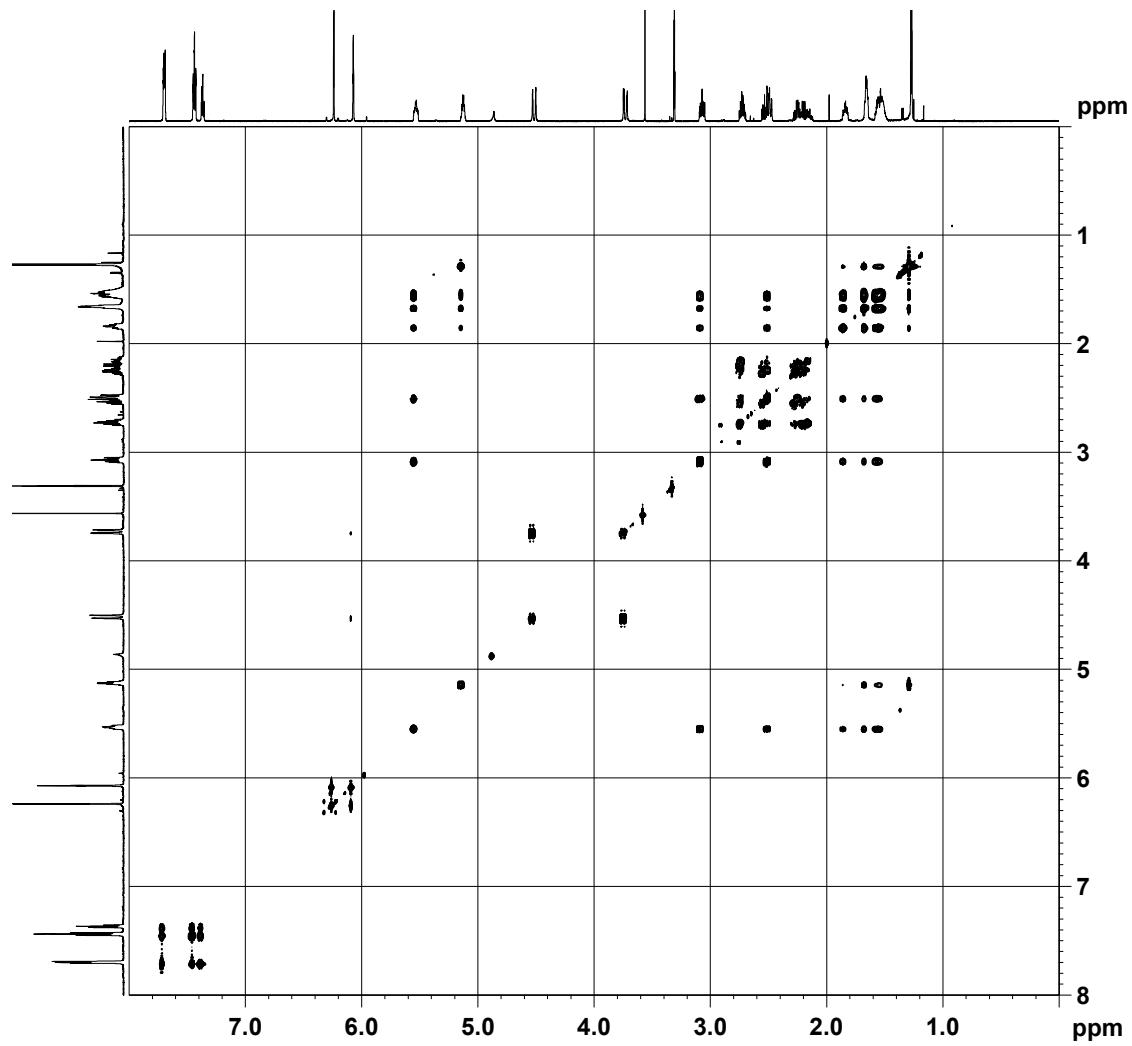
S73. HRESIMS spectrum of compound 14.



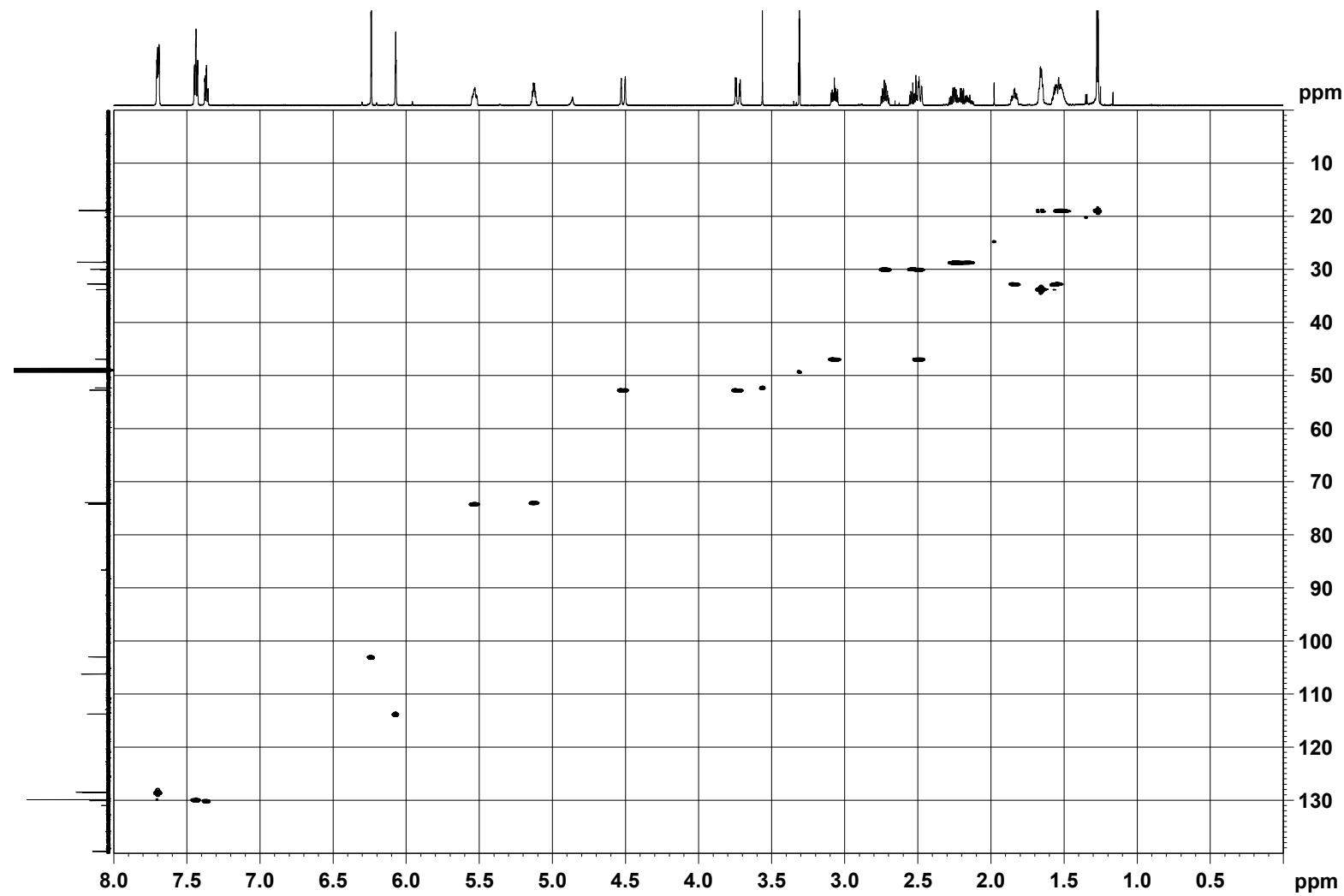
S74. ^1H NMR (700 MHz, CD_3OD) spectrum of compound 14.



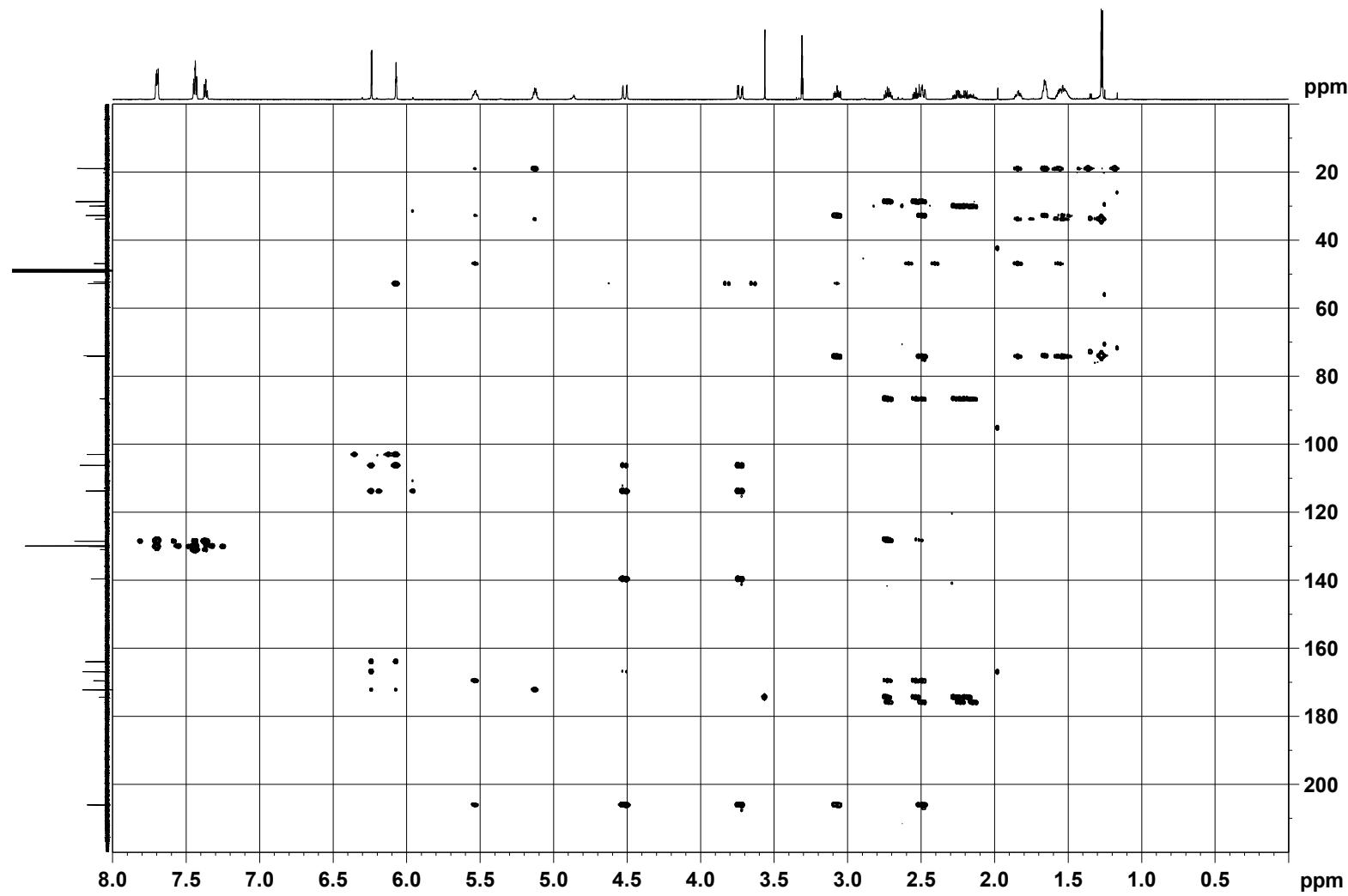
S75. ^{13}C NMR (175 MHz, CD_3OD) spectrum of compound 14.



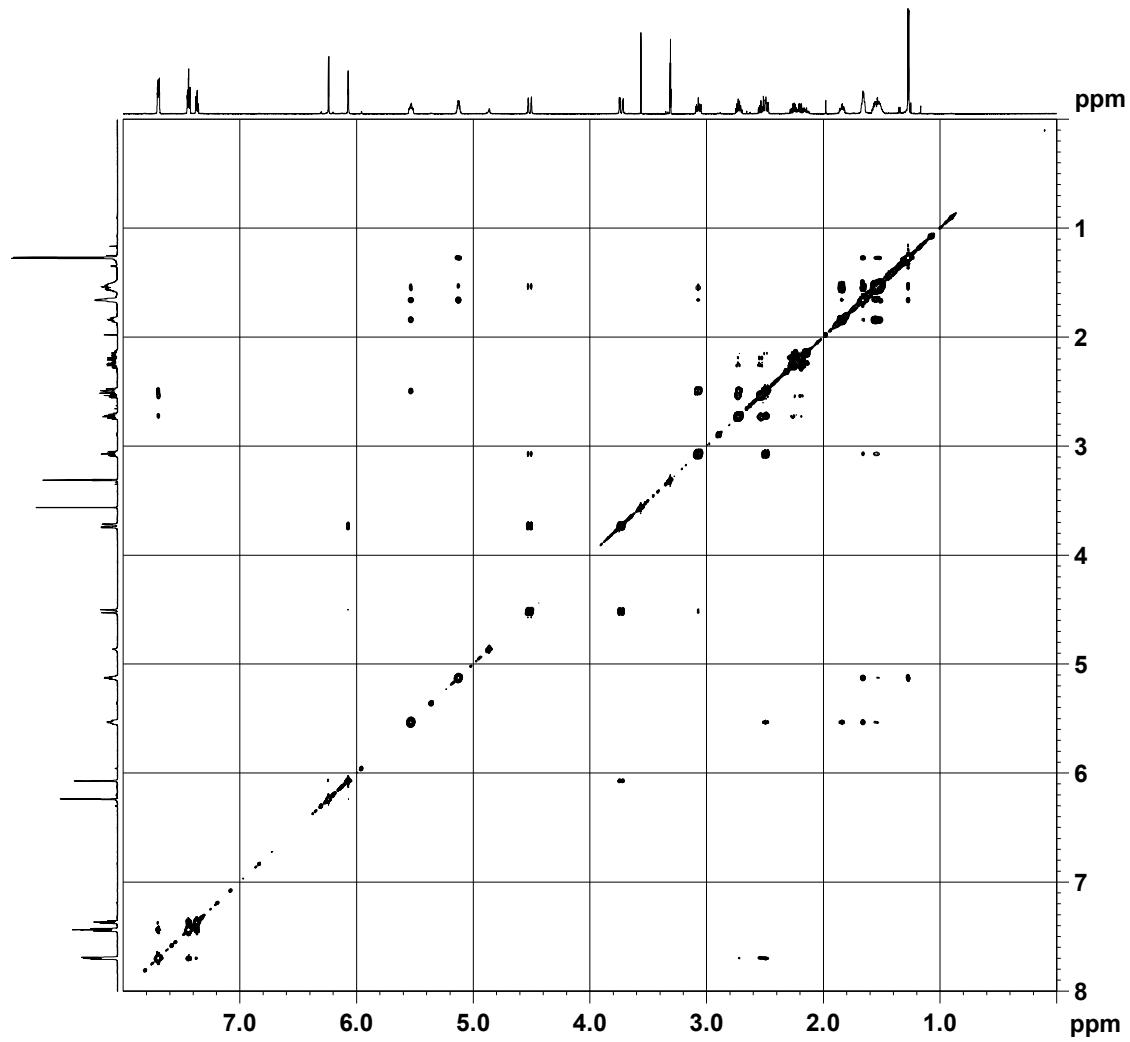
S76. ^1H - ^1H TOCSY (700 MHz, CD_3OD) spectrum of compound **14**.



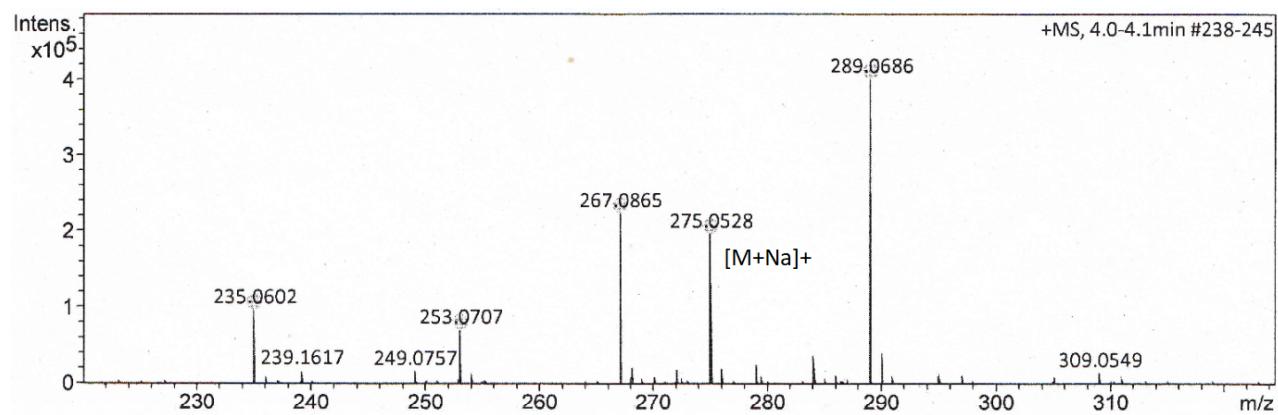
S77. HSQC (700 and 175 MHz, CD_3OD) spectrum of compound 14.



S78. HMBC (700 and 175 MHz, CD₃OD) spectrum of compound 14.



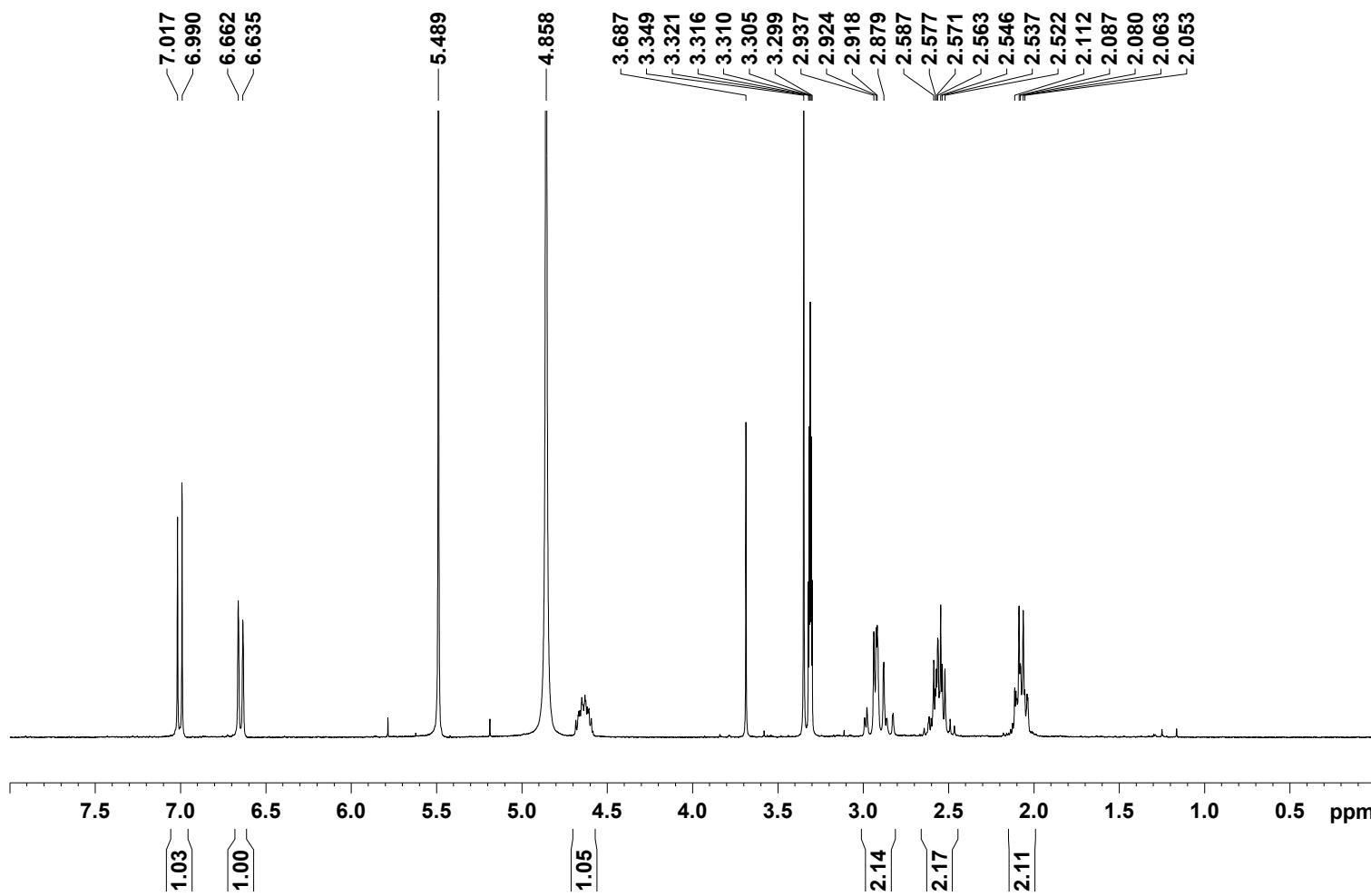
S79. ROESY (700 MHz, CD₃OD) spectrum of compound **14**.



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e ⁻ Conf	N-Rule
235.0602	1	C ₁₂ H ₁₁ O ₅	235.0601	-0.2	20.8	1	100.00	7.5	even	ok
	2	C ₁₁ H ₈ N ₄ NaO	235.0590	-4.8	21.8	2	57.43	9.5	even	ok
	3	C ₁₃ H ₇ N ₄ O	235.0614	5.4	34.1	3	39.02	12.5	even	ok
253.0707	1	C ₁₂ H ₁₃ O ₆	253.0707	-0.2	10.9	1	100.00	6.5	even	ok
	2	C ₉ H ₅ N ₁₀	253.0693	-5.5	12.6	2	47.98	12.5	even	ok
	3	C ₁₃ H ₉ N ₄ O ₂	253.0720	5.1	24.4	3	39.68	11.5	even	ok
267.0865	1	C ₁₃ H ₁₅ O ₆	267.0863	-0.8	28.2	1	100.00	6.5	even	ok
	2	C ₁₀ H ₇ N ₁₀	267.0850	-5.9	28.4	2	47.28	12.5	even	ok
	3	C ₁₂ H ₁₂ N ₄ NaO ₂	267.0852	-4.8	28.9	3	56.01	8.5	even	ok
	4	C ₁₄ H ₁₁ N ₄ O ₂	267.0877	4.2	41.4	4	44.75	11.5	even	ok
275.0528	1	C ₉ H ₁₁ N ₂ O ₈	275.0510	-6.5	7.7	1	51.17	5.5	even	ok
	2	C ₁₀ H ₇ N ₆ O ₄	275.0523	-1.7	19.6	2	89.93	10.5	even	ok
	3	C ₁₂ H ₁₂ NaO ₆	275.0526	-0.7	20.5	3	100.00	6.5	even	ok

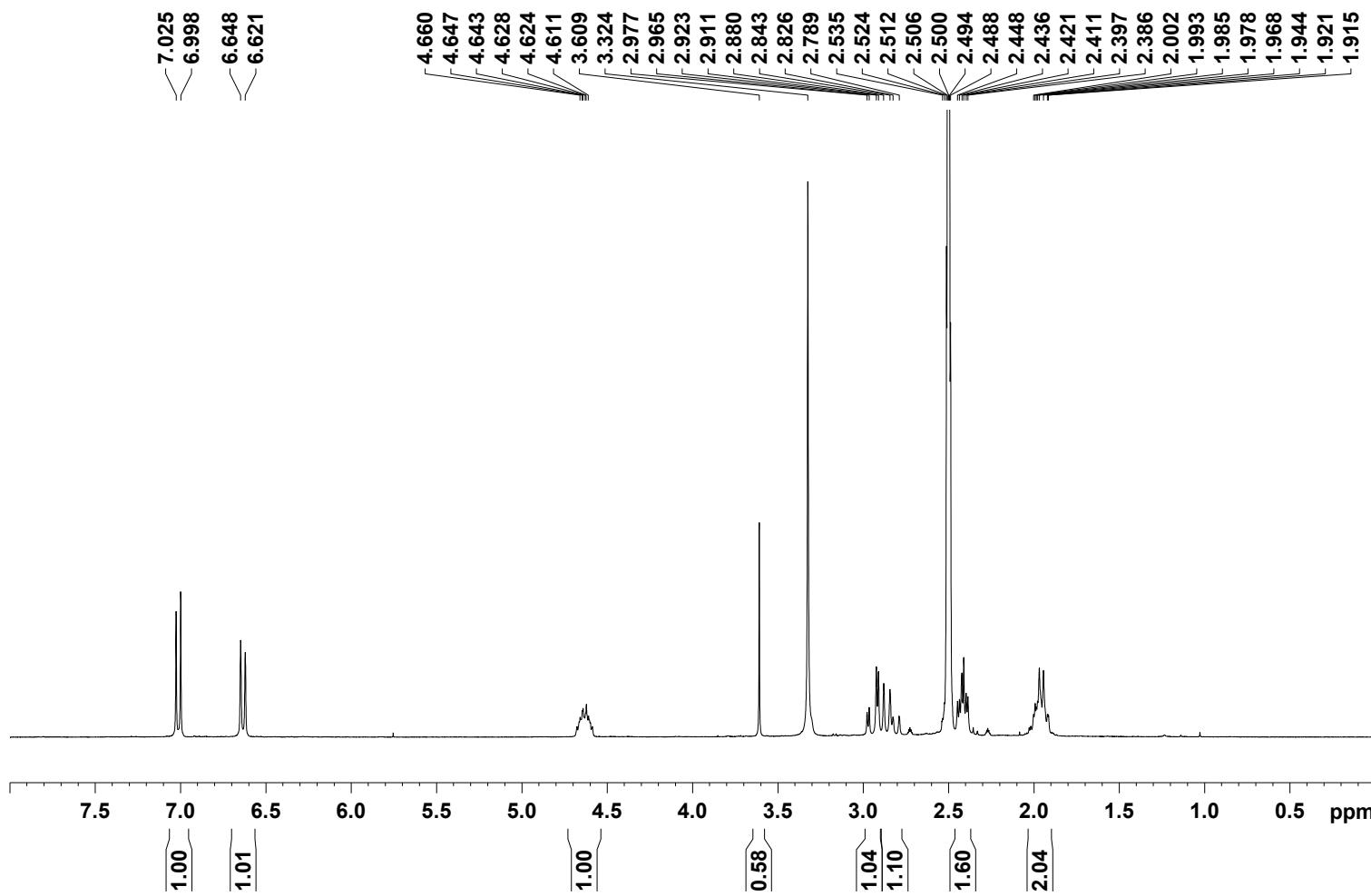
S80. HRESIMS spectrum of compound 15.

Tal80CS6-3



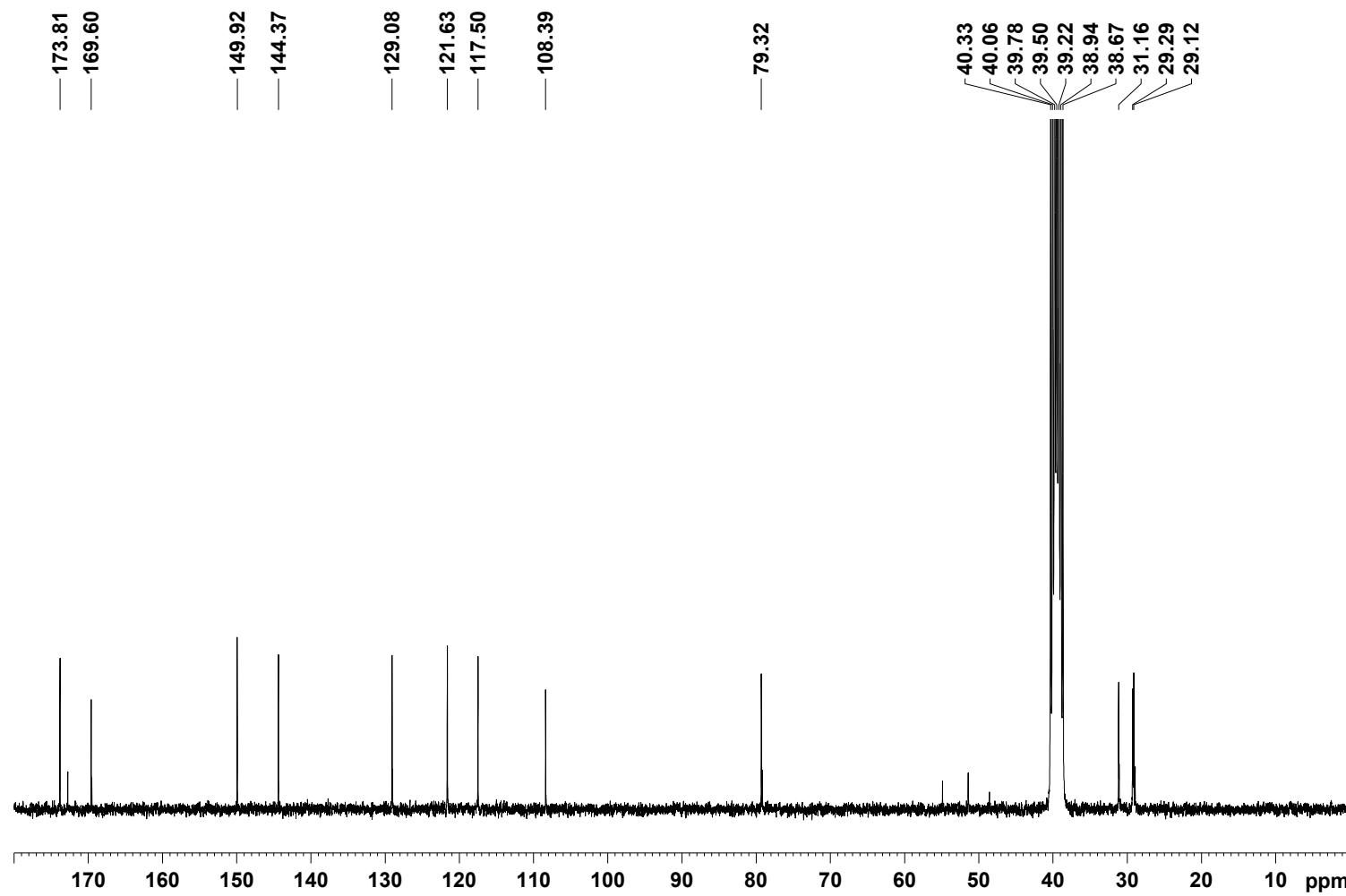
S81. ^1H NMR (300 MHz, CD_3OD) spectrum of compound **15**.

Tal80ES6-3

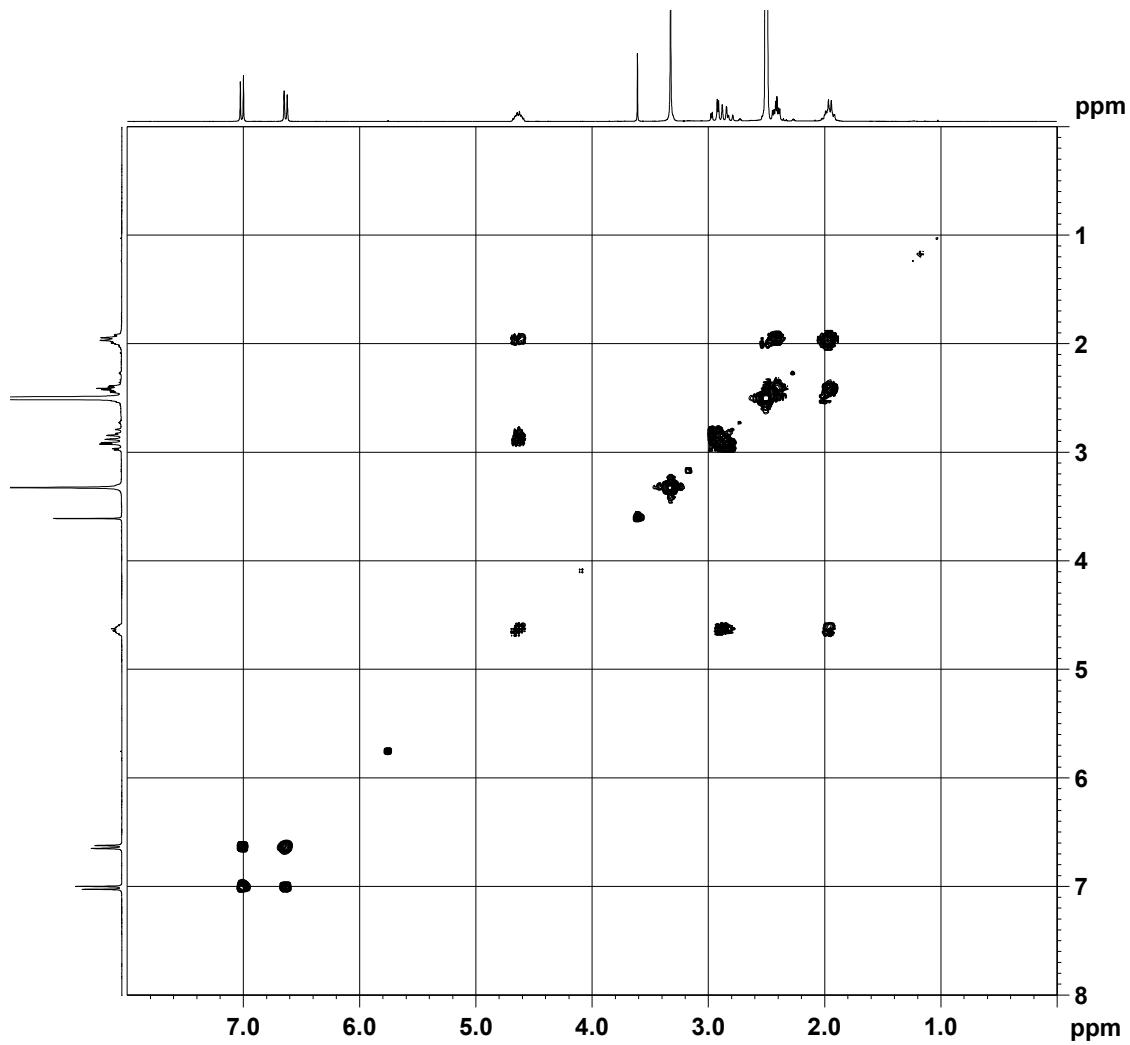


S82. ^1H NMR (300 MHz, $\text{DMSO}-d_6$) spectrum of compound 15.

Tal80Es6-3

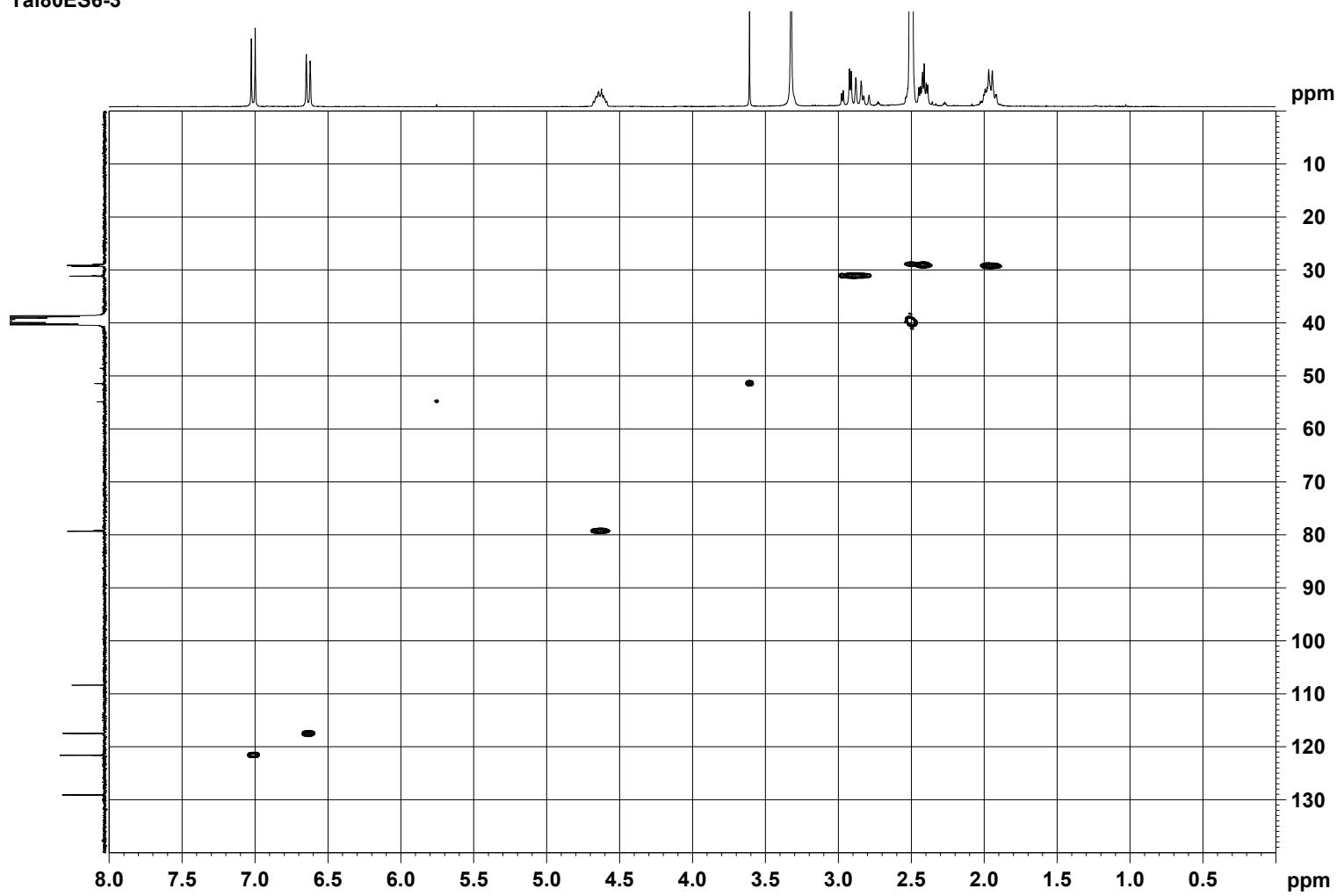


S83. ^{13}C NMR (75 MHz, $\text{DMSO}-d_6$) spectrum of compound **15**.



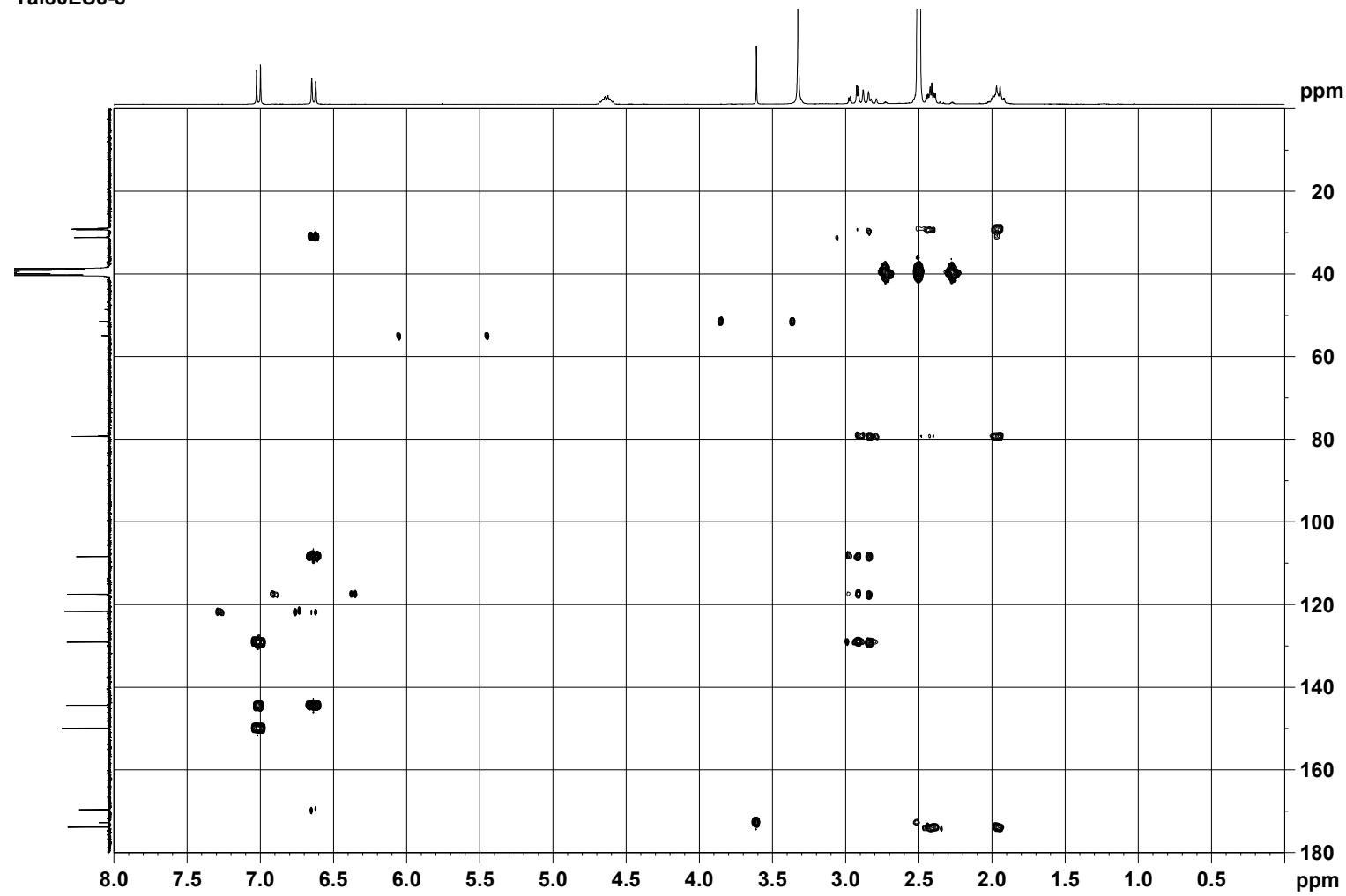
S84. ^1H - ^1H COSY (300 MHz, $\text{DMSO}-d_6$) spectrum of compound **15**.

Tal80ES6-3

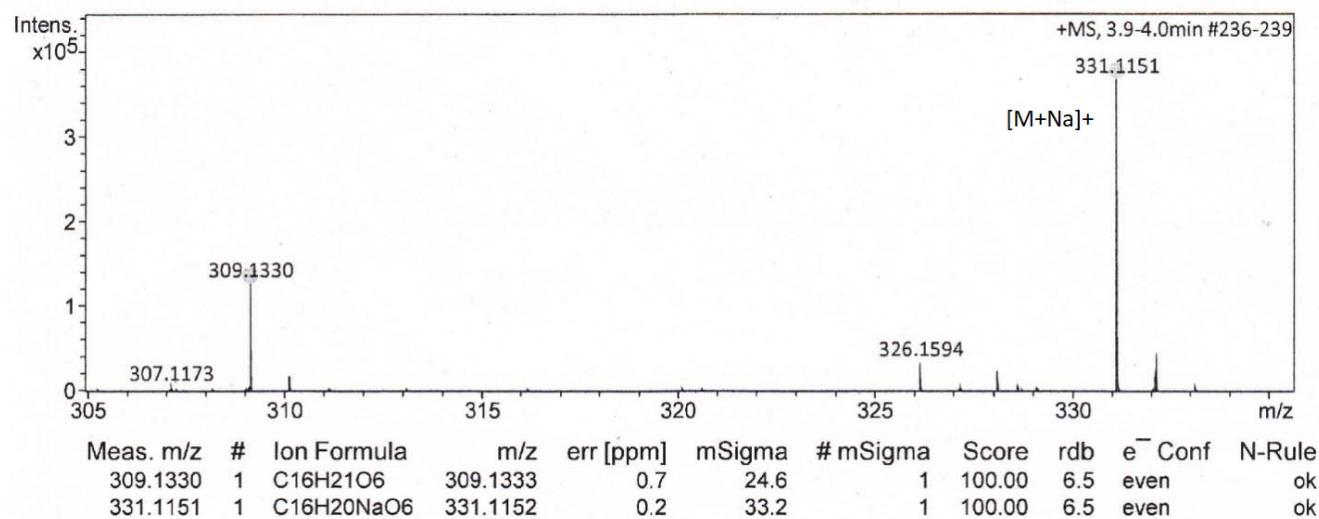


S85. HSQC (300 and 75 MHz, DMSO-*d*₆) spectrum of compound **15**.

Tal80ES6-3

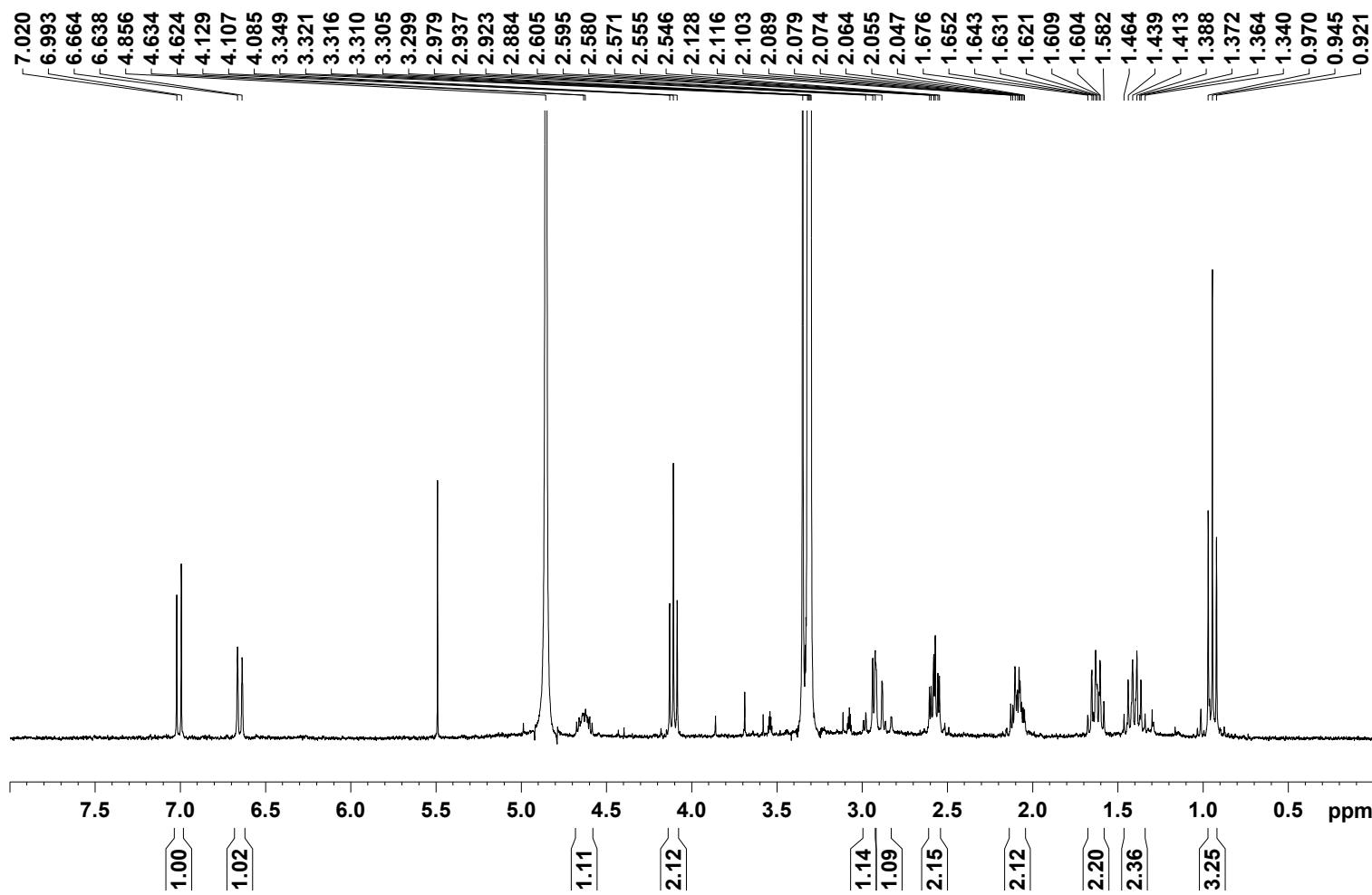


S86. HMBC (300 and 75 MHz, $\text{DMSO}-d_6$) spectrum of compound **15**.



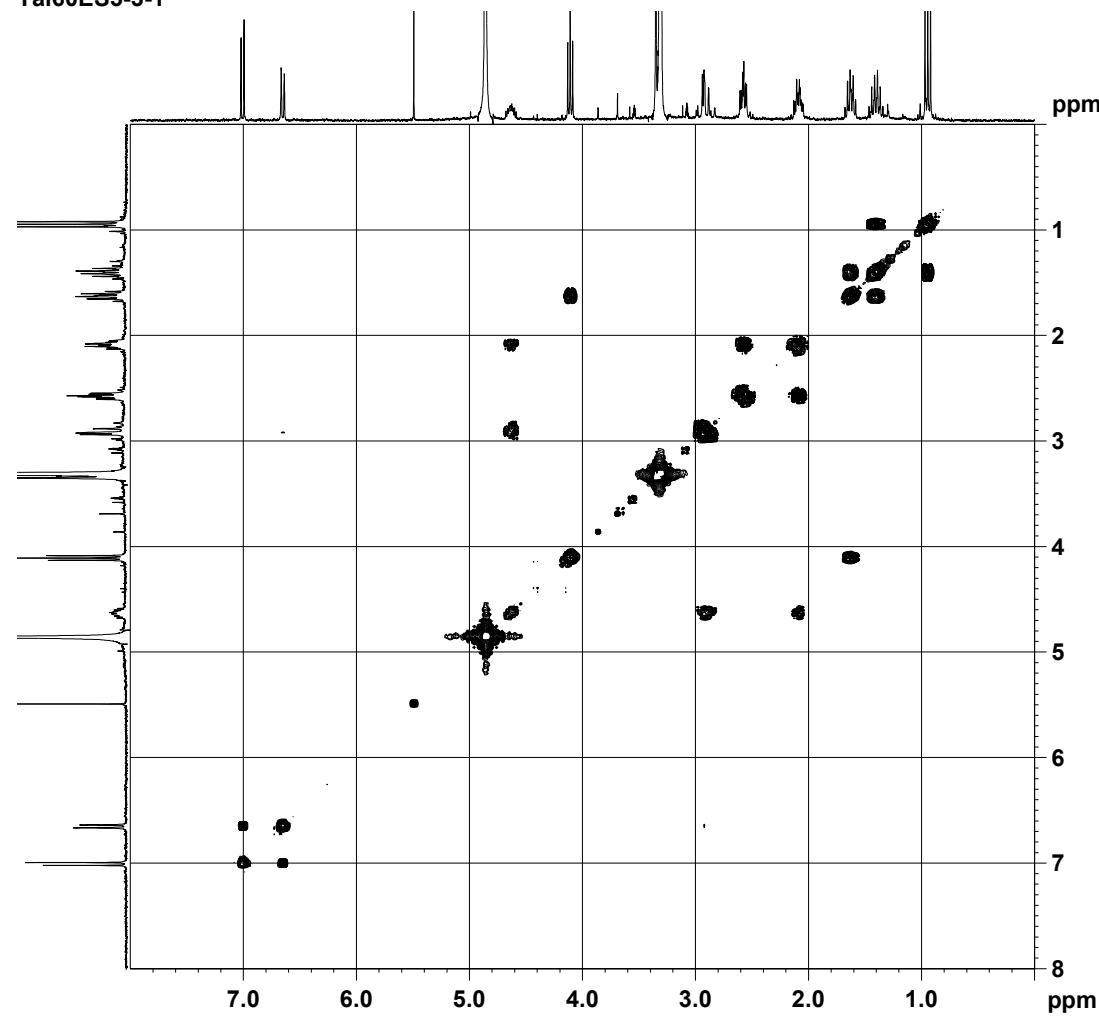
S87. HRESIMS spectrum of compound **16**.

Tal60ES5-3-1



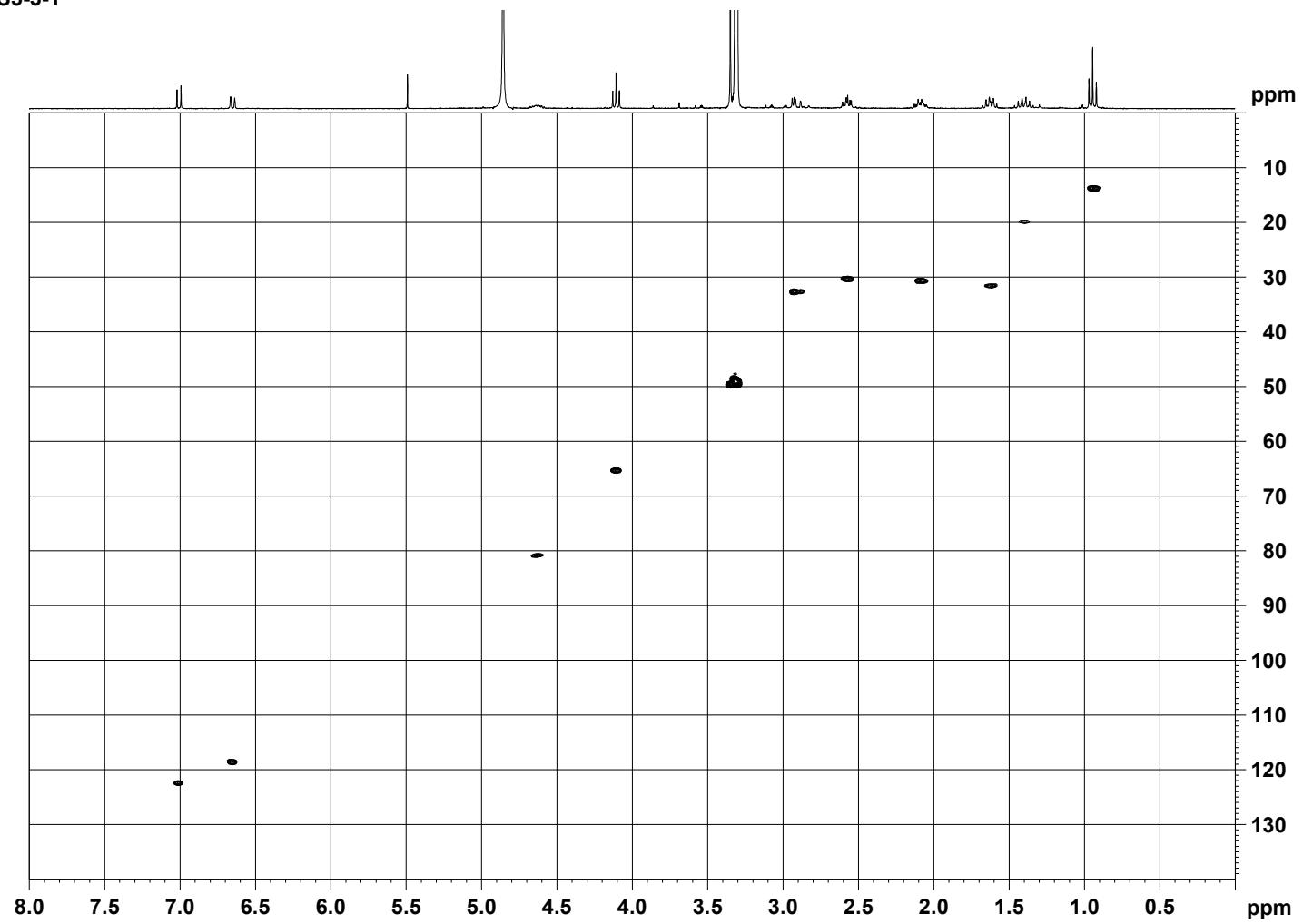
S88. ^1H NMR (300 MHz, CD_3OD) spectrum of compound 16.

Tal60ES5-3-1



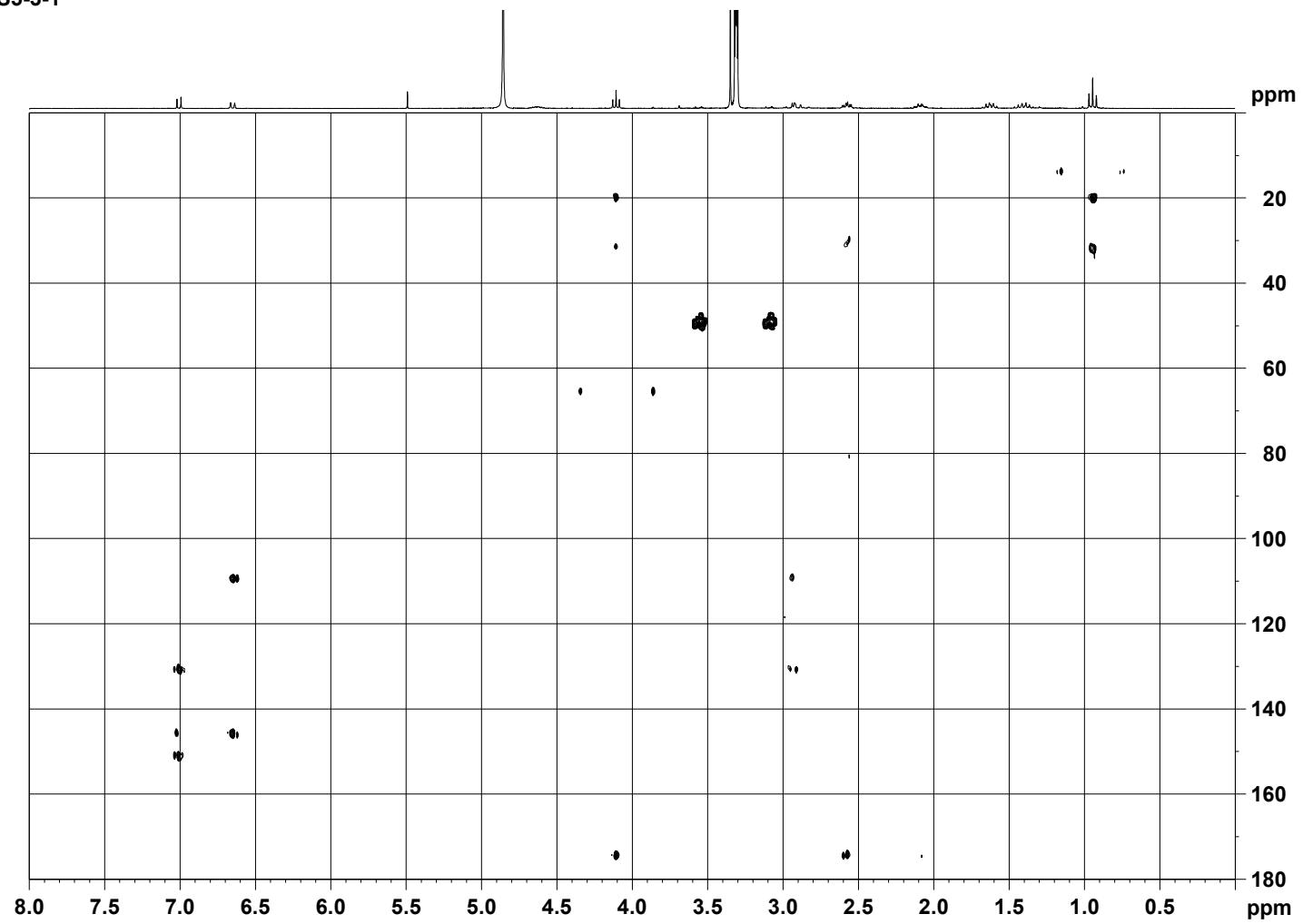
S89. ^1H - ^1H COSY (300 MHz, CD_3OD) spectrum of compound **16**.

Tal60ES5-3-1

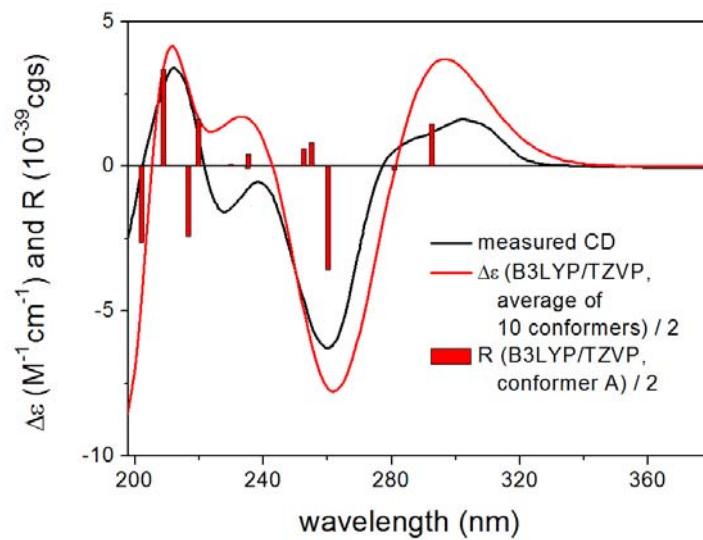


S90. HSQC (300 and 75 MHz, CD₃OD) spectrum of compound **16**.

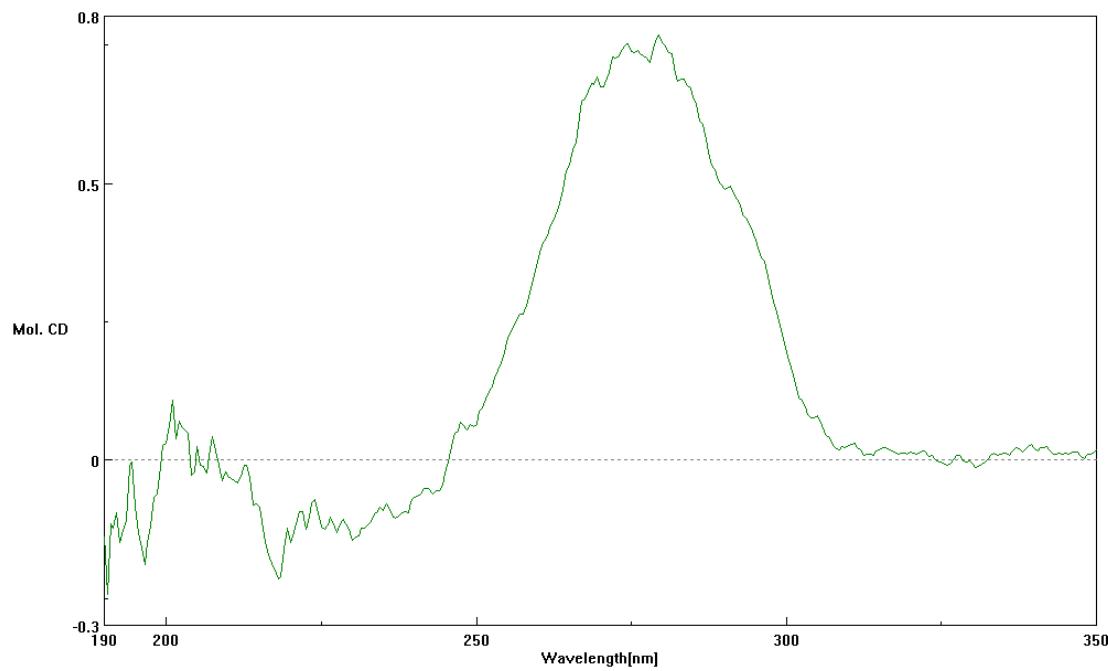
Tal60ES5-3-1



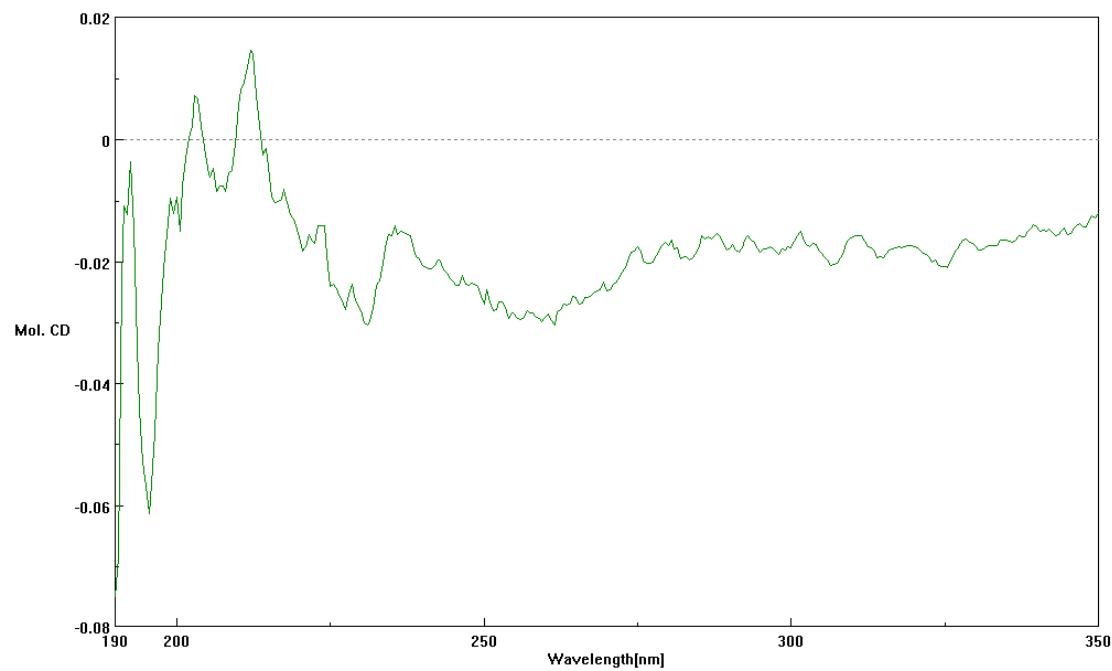
S91. HMBC (300 and 75 MHz, CD_3OD) spectrum of compound **16**.



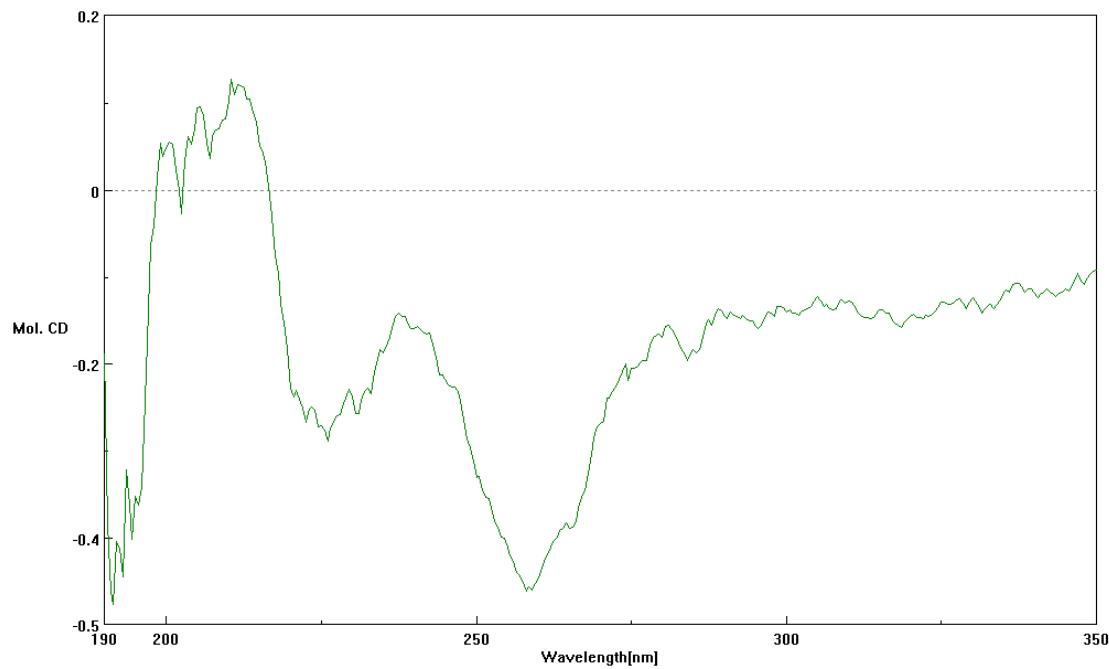
S92. Experimental ECD spectrum of **9** in MeCN compared with the Boltzmann-weighted B3LYP/TZVP PCM/MeCN ECD spectrum of (*3S,7S*)-**9** computed for the B97D/TZVP PCM/MeCN conformers. Bars represent the rotational strength values of the lowest-energy conformer.



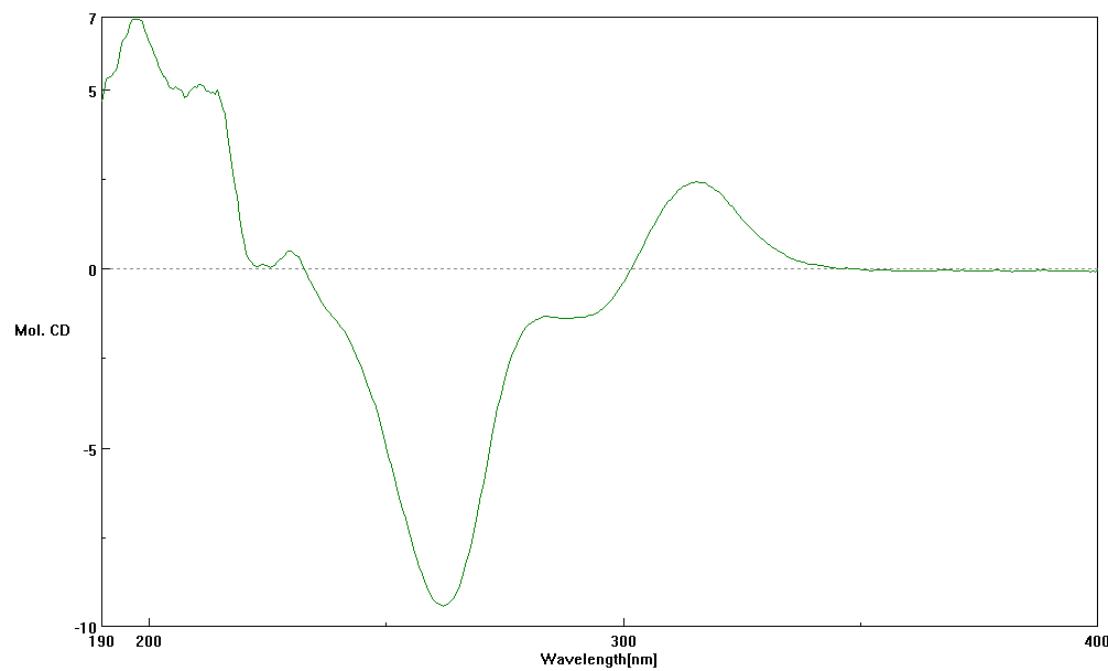
S93. Experimental ECD spectrum of **1** in MeCN



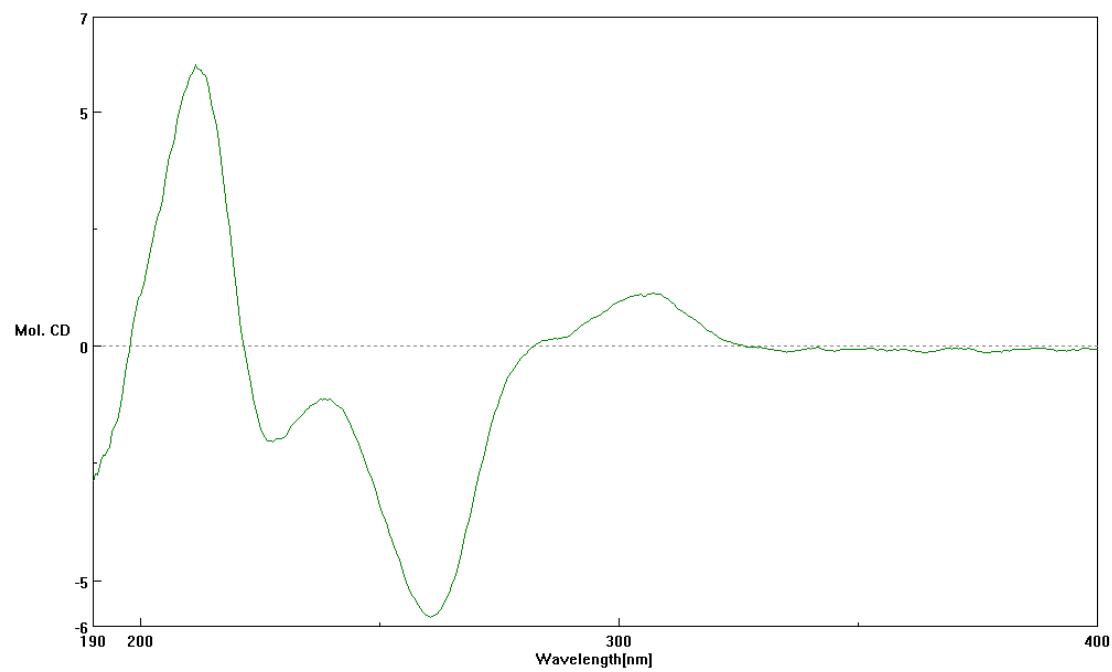
S94. Experimental ECD spectrum of **2** in MeCN



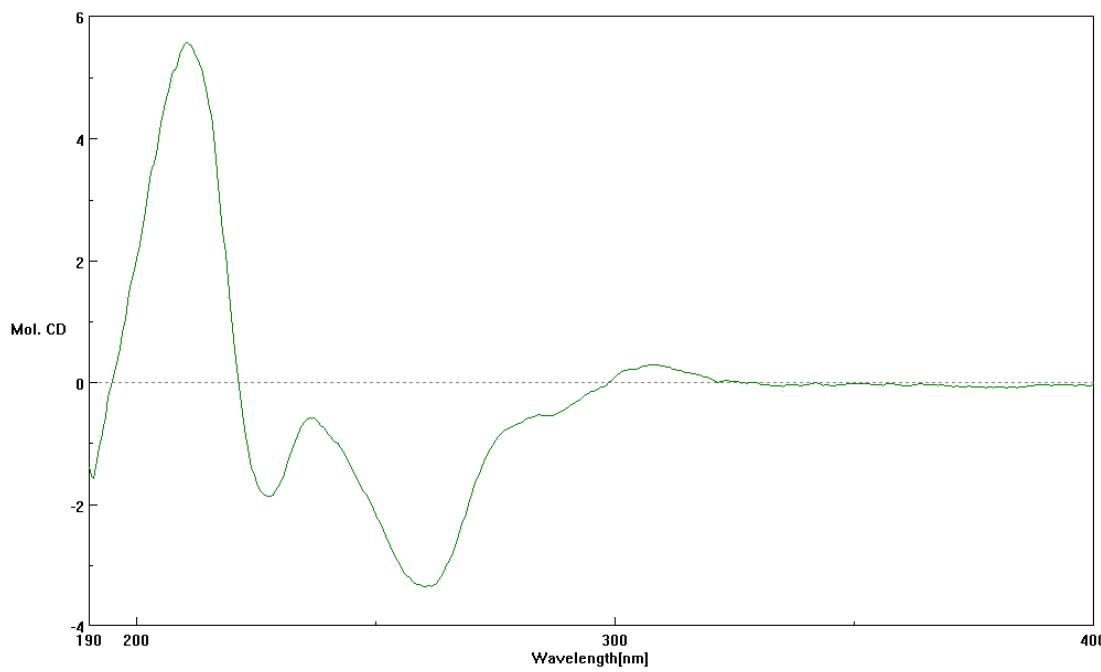
S95. Experimental ECD spectrum of **5** in MeCN



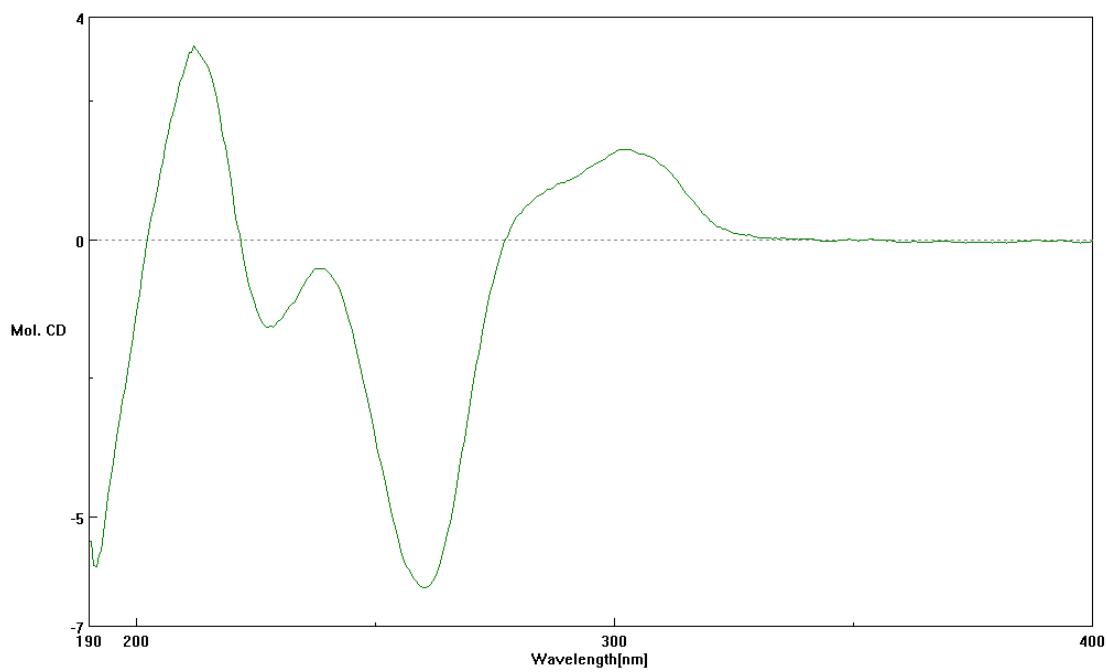
S96. Experimental ECD spectrum of **6** in MeCN



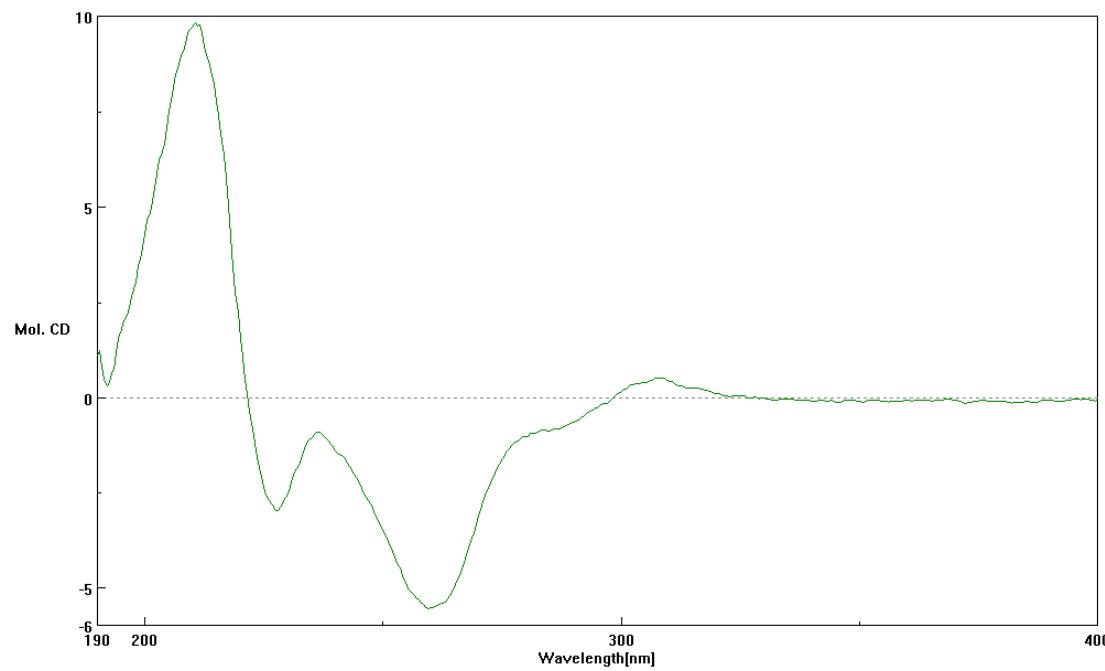
S97. Experimental ECD spectrum of **7** in MeCN



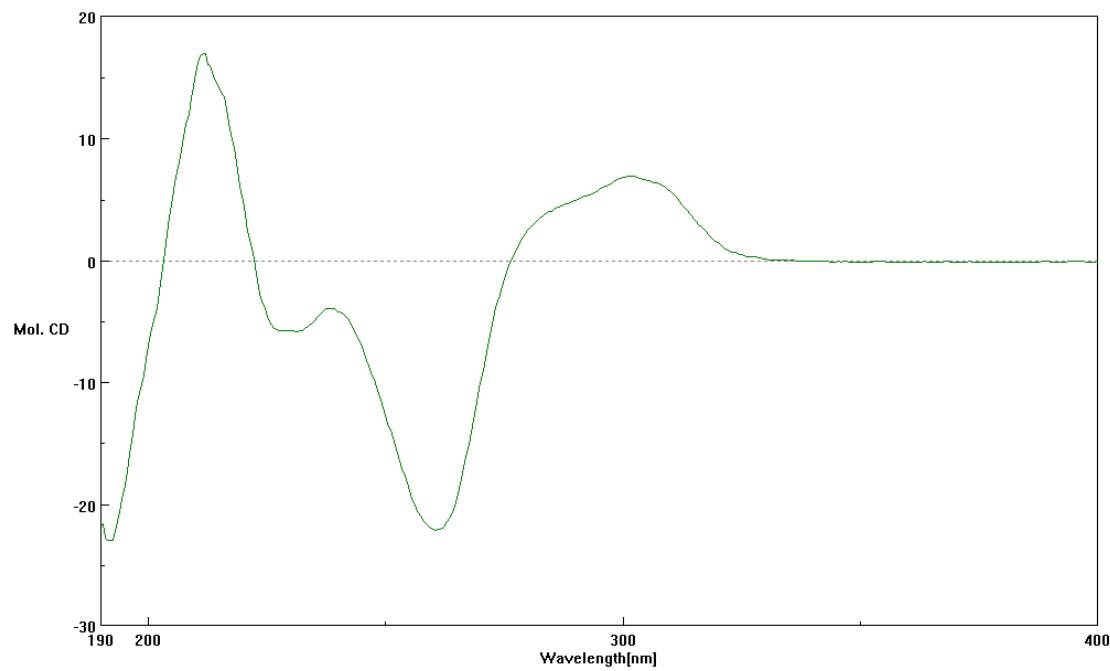
S98. Experimental ECD spectrum of **8** in MeCN



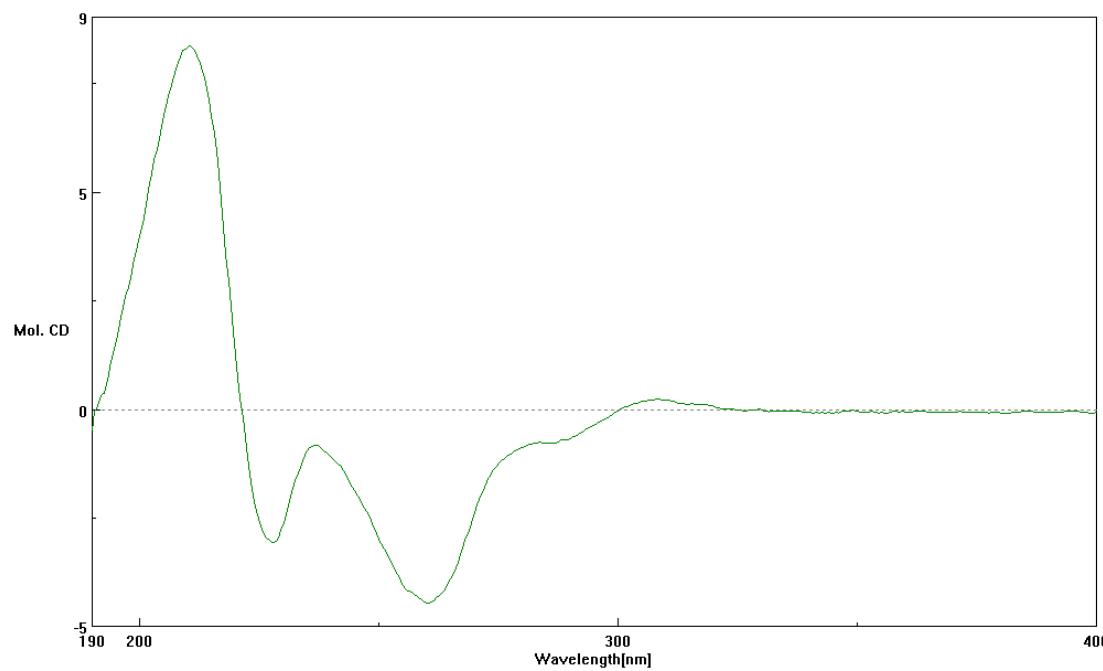
S99. Experimental ECD spectrum of **9** in MeCN



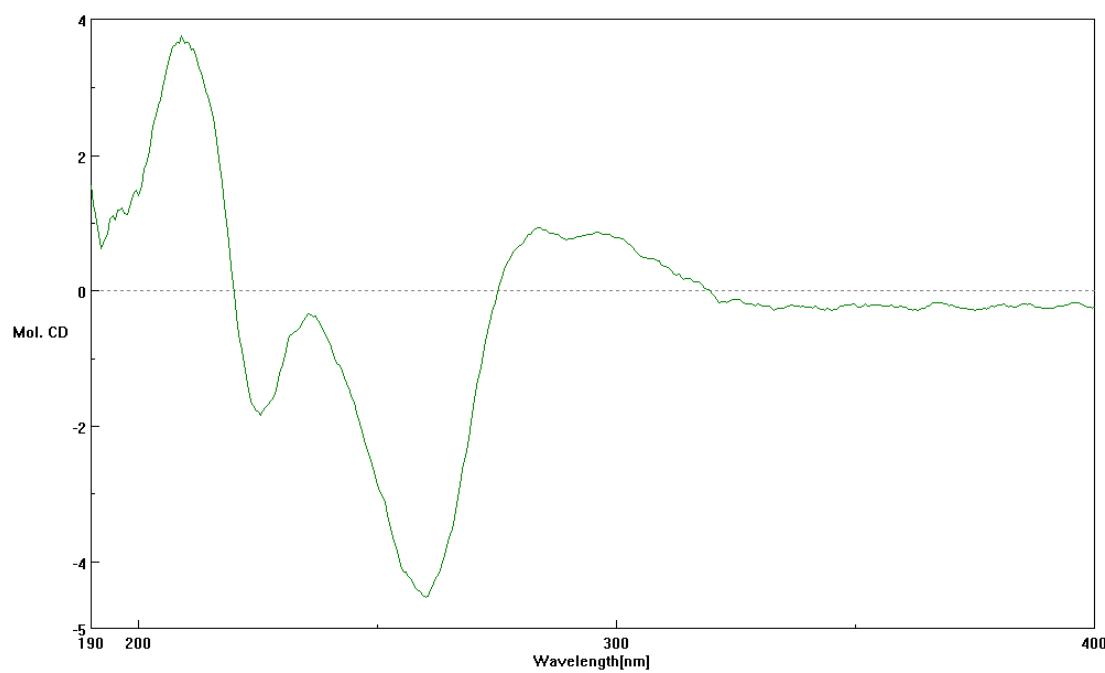
S100. Experimental ECD spectrum of **10** in MeCN



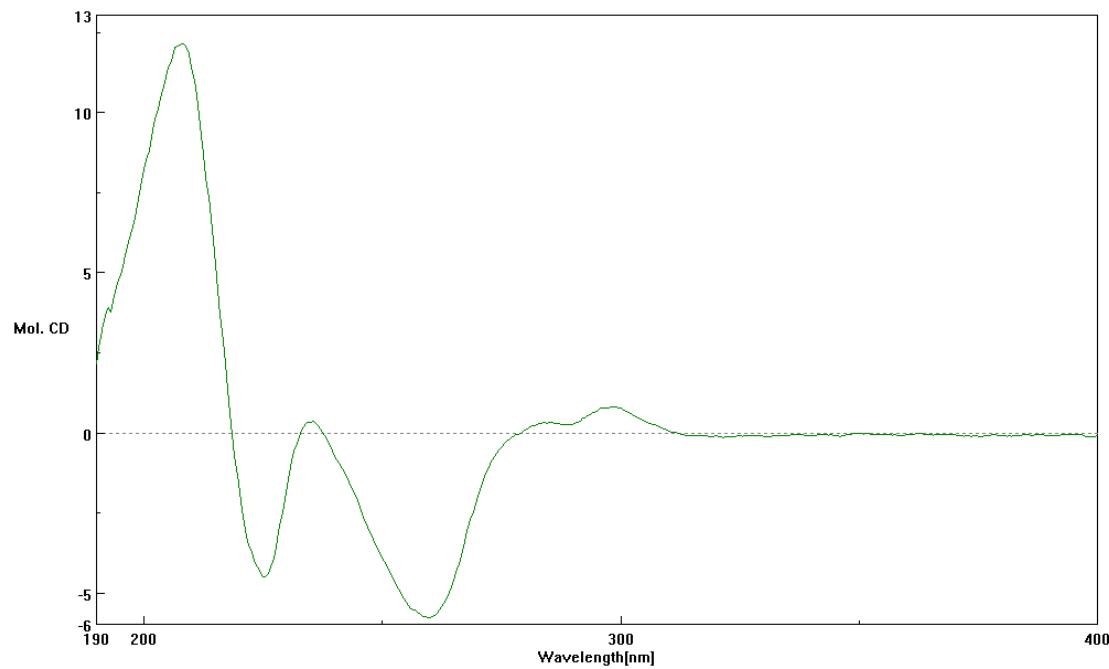
S101. Experimental ECD spectrum of **11** in MeCN



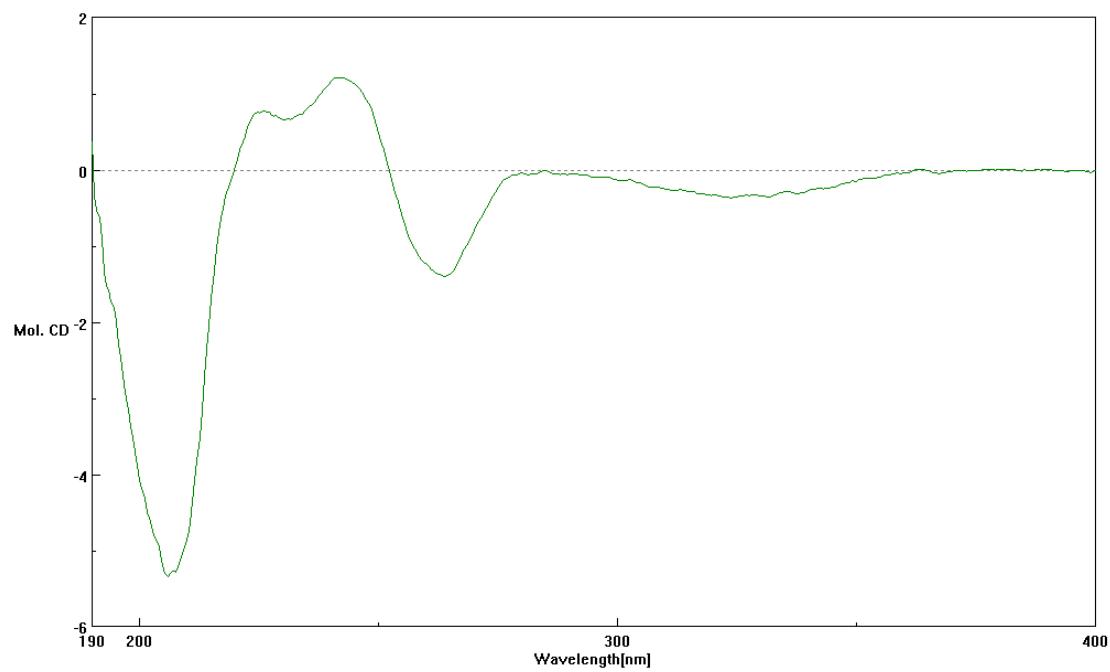
S102. Experimental ECD spectrum of **12** in MeCN



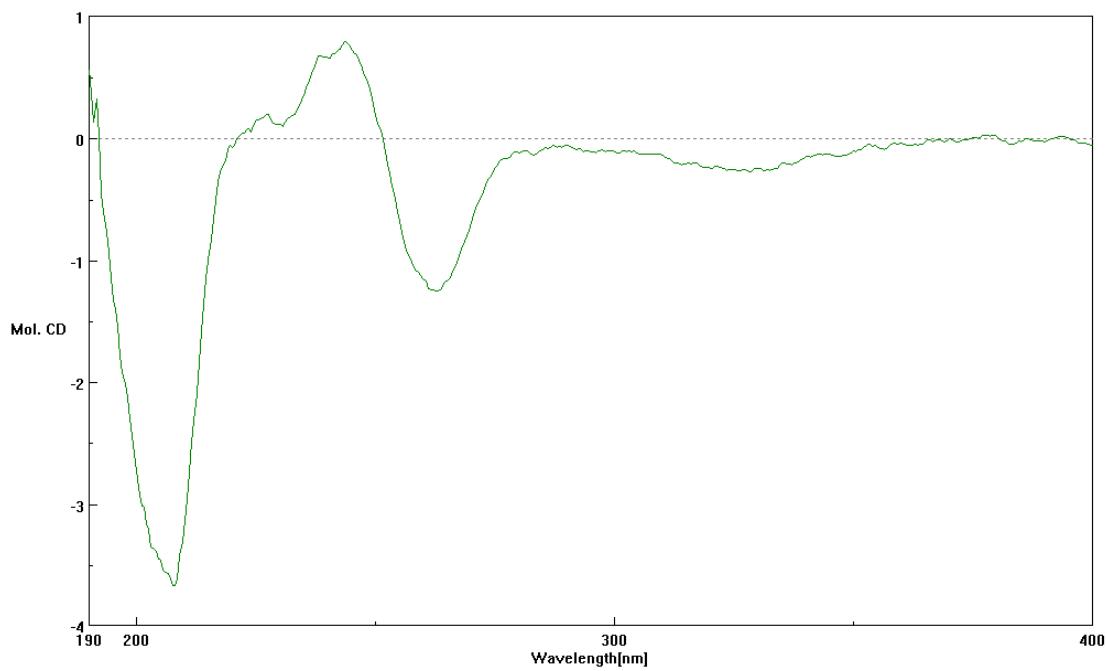
S103. Experimental ECD spectrum of **13** in MeCN



S104. Experimental ECD spectrum of **14** in MeCN



S105. Experimental ECD spectrum of **15** in MeCN



S106. Experimental ECD spectrum of **16** in MeCN