

Supplementary Materials: Synthesis and Biotransformation of Bicyclic Unsaturated Lactones with Three or Four Methyl Groups

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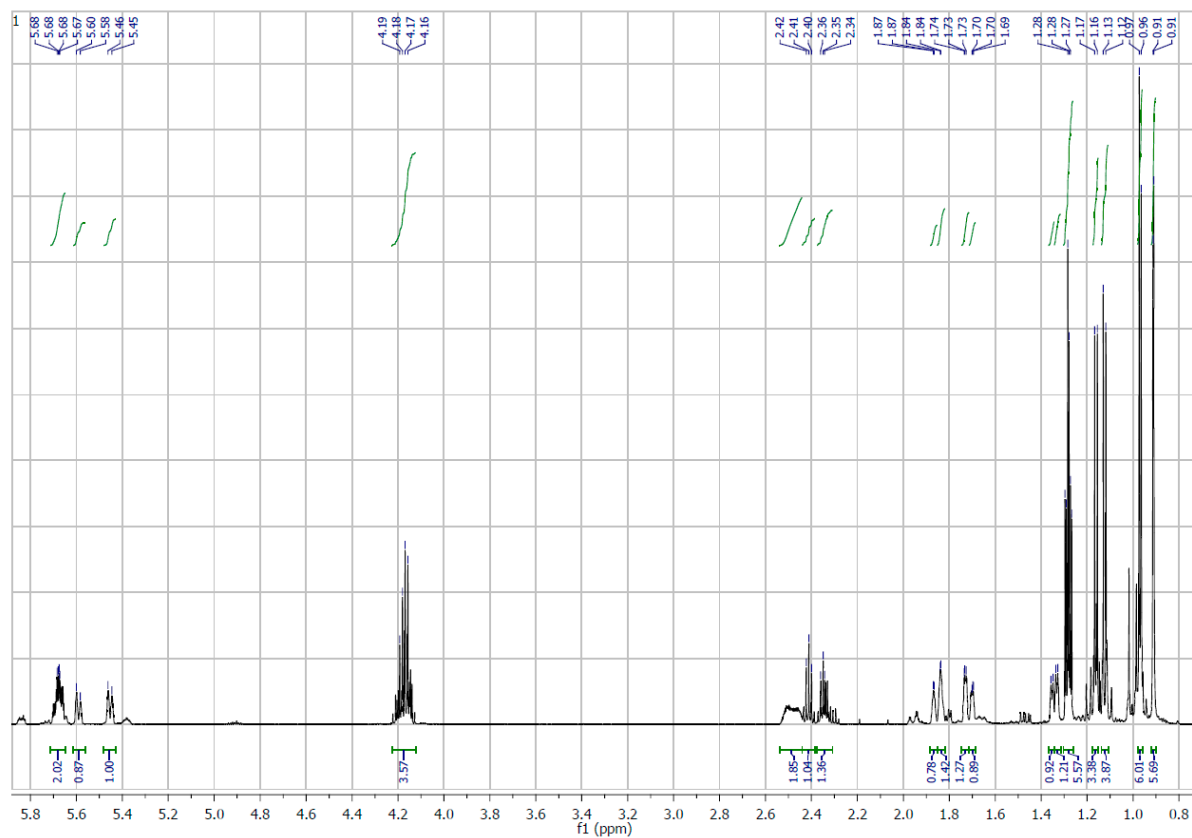


Figure S1. ¹H-NMR (600 MHz, CDCl₃) spectrum of ester 2a.

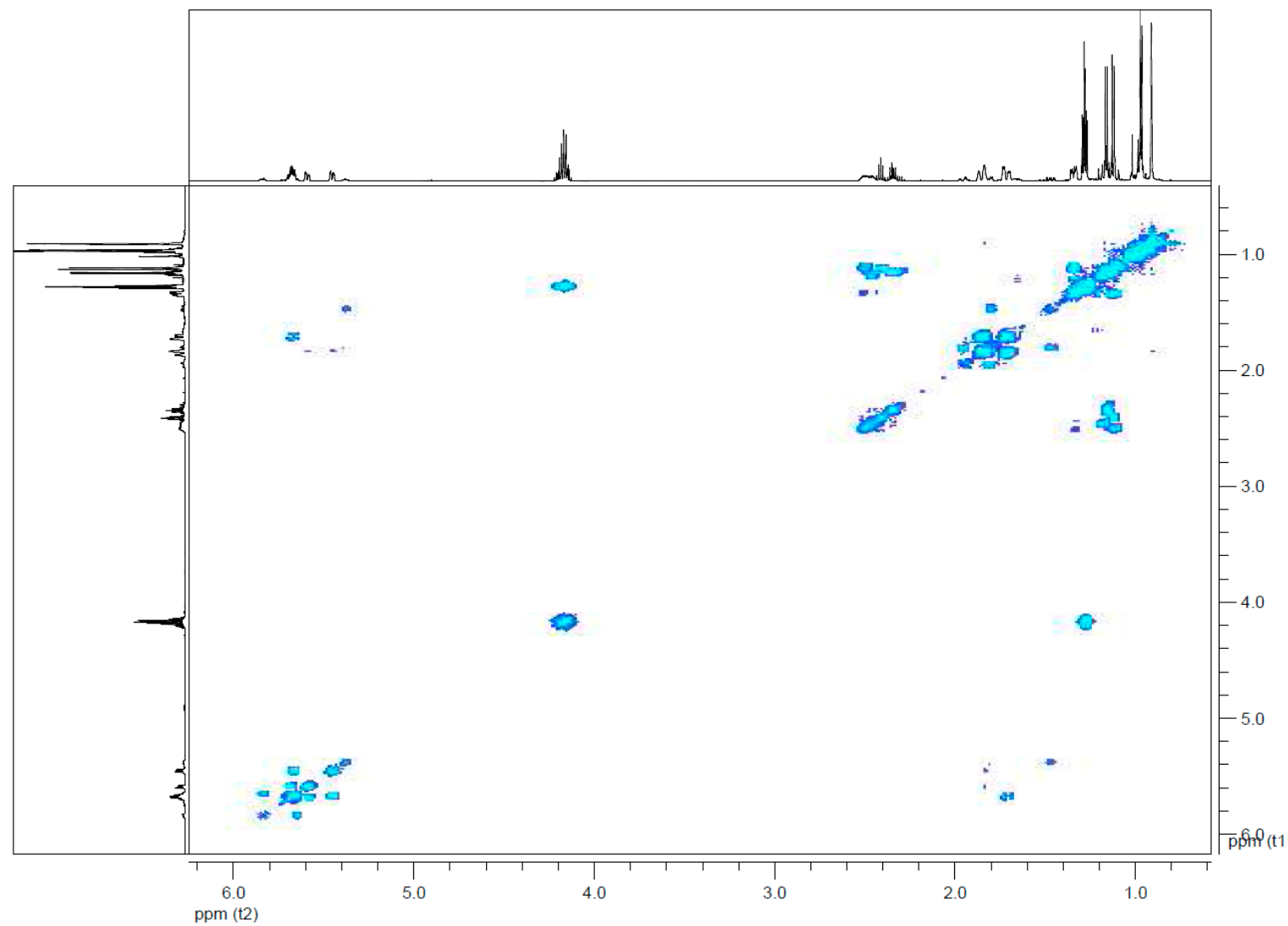


Figure S2. COSY (151 MHz, CDCl₃) spectrum of ester **2a**.

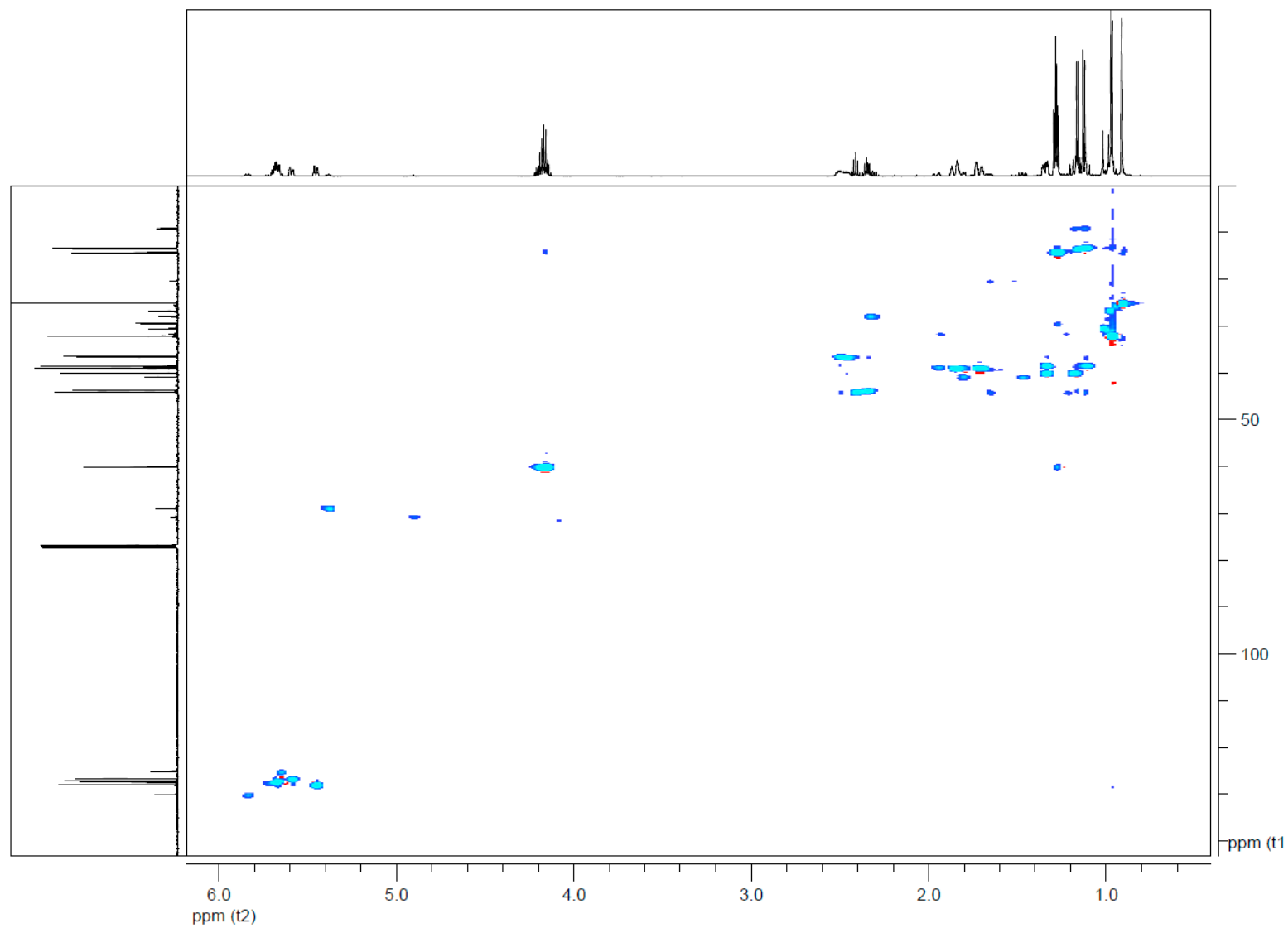


Figure S3. HMQC (151 MHz, CDCl_3) spectrum of ester 2a.

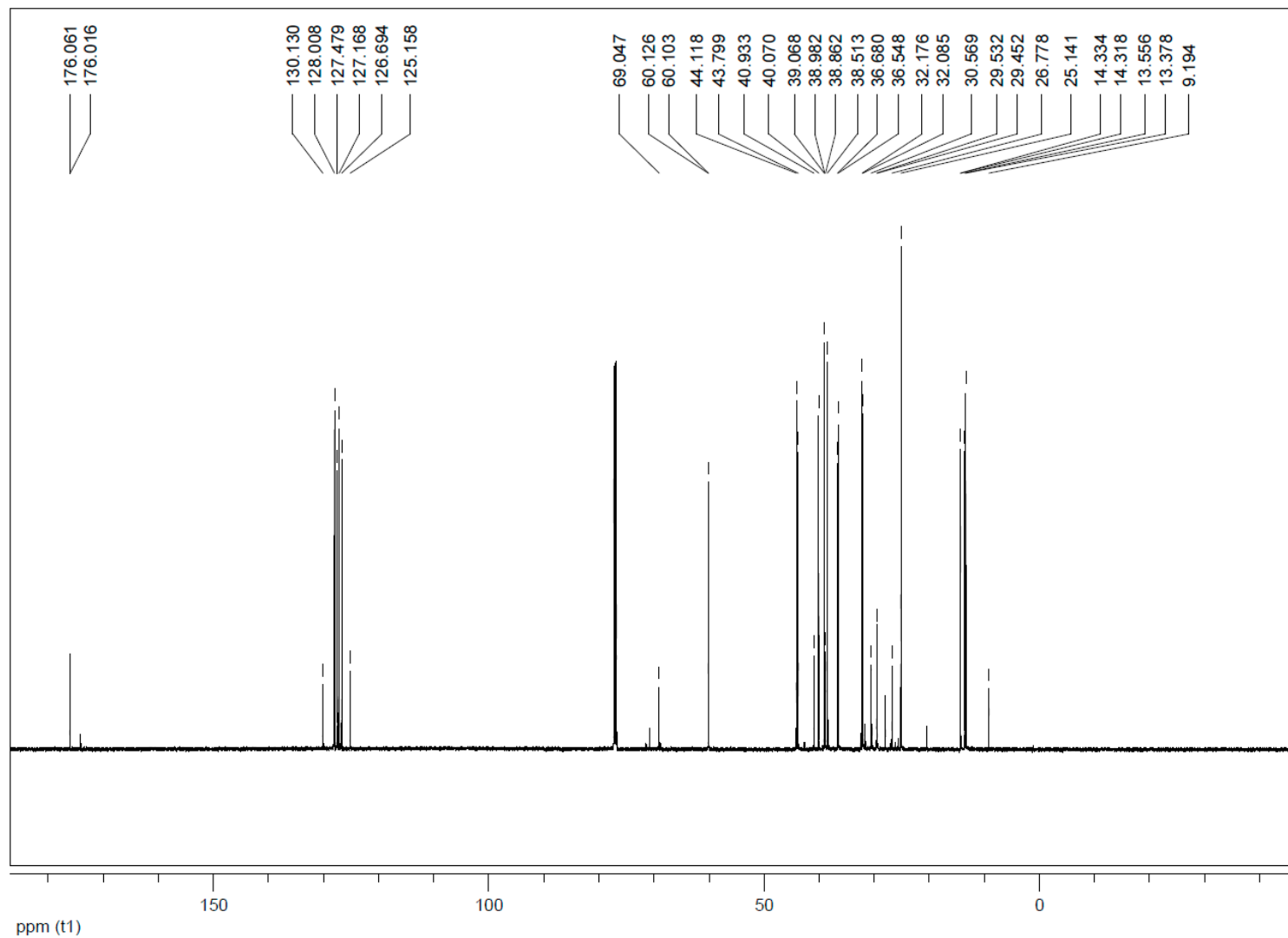


Figure S4. ^{13}C -NMR (151 MHz, CDCl_3) spectrum of ester 2a.

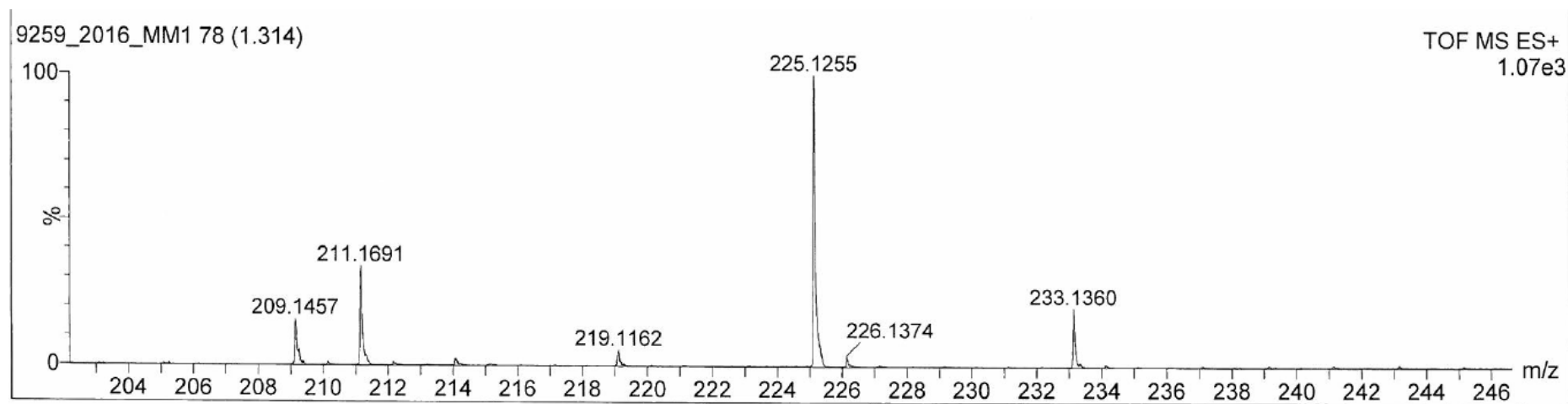


Figure S5. HRMS spectrum of ester 2a.

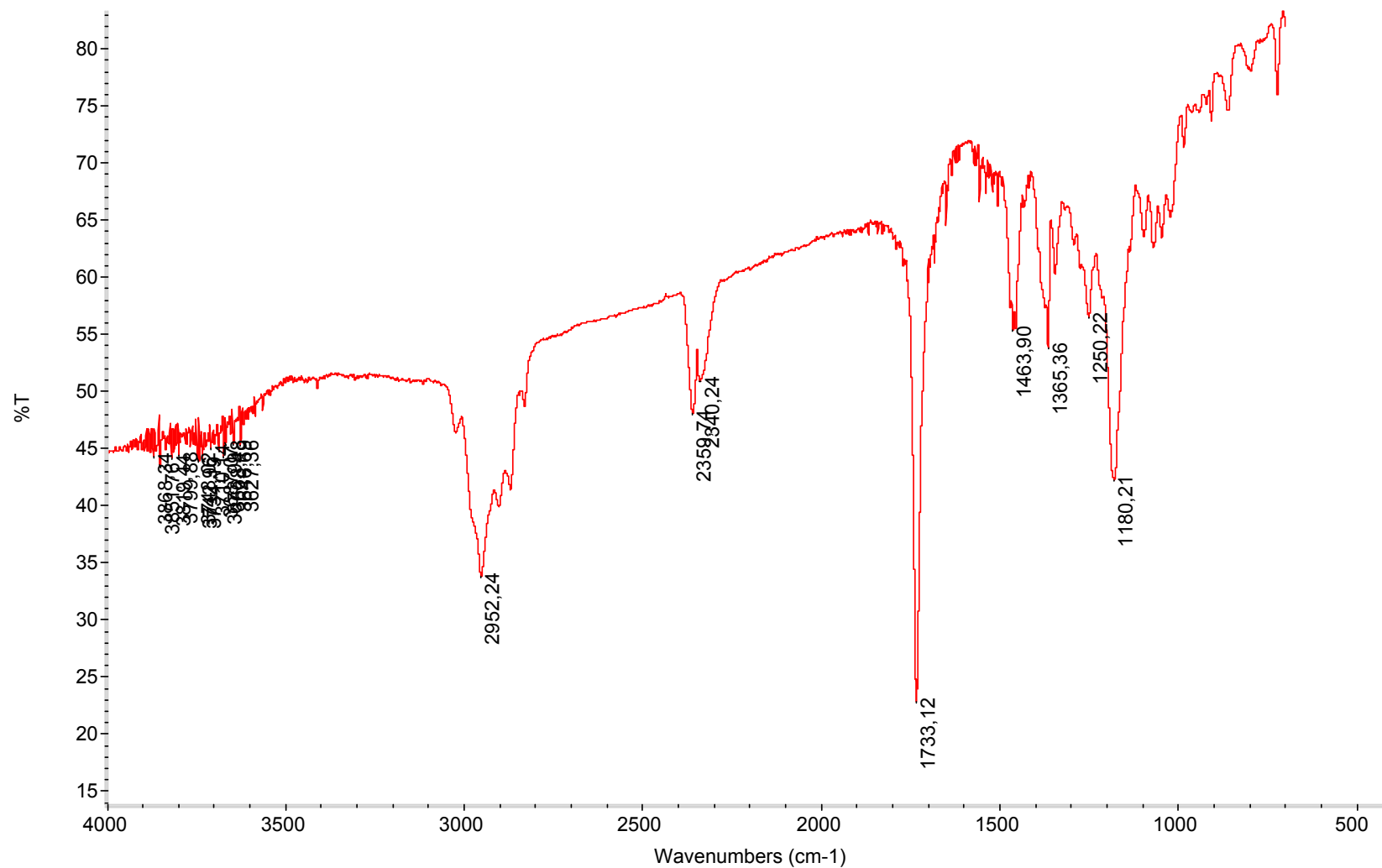
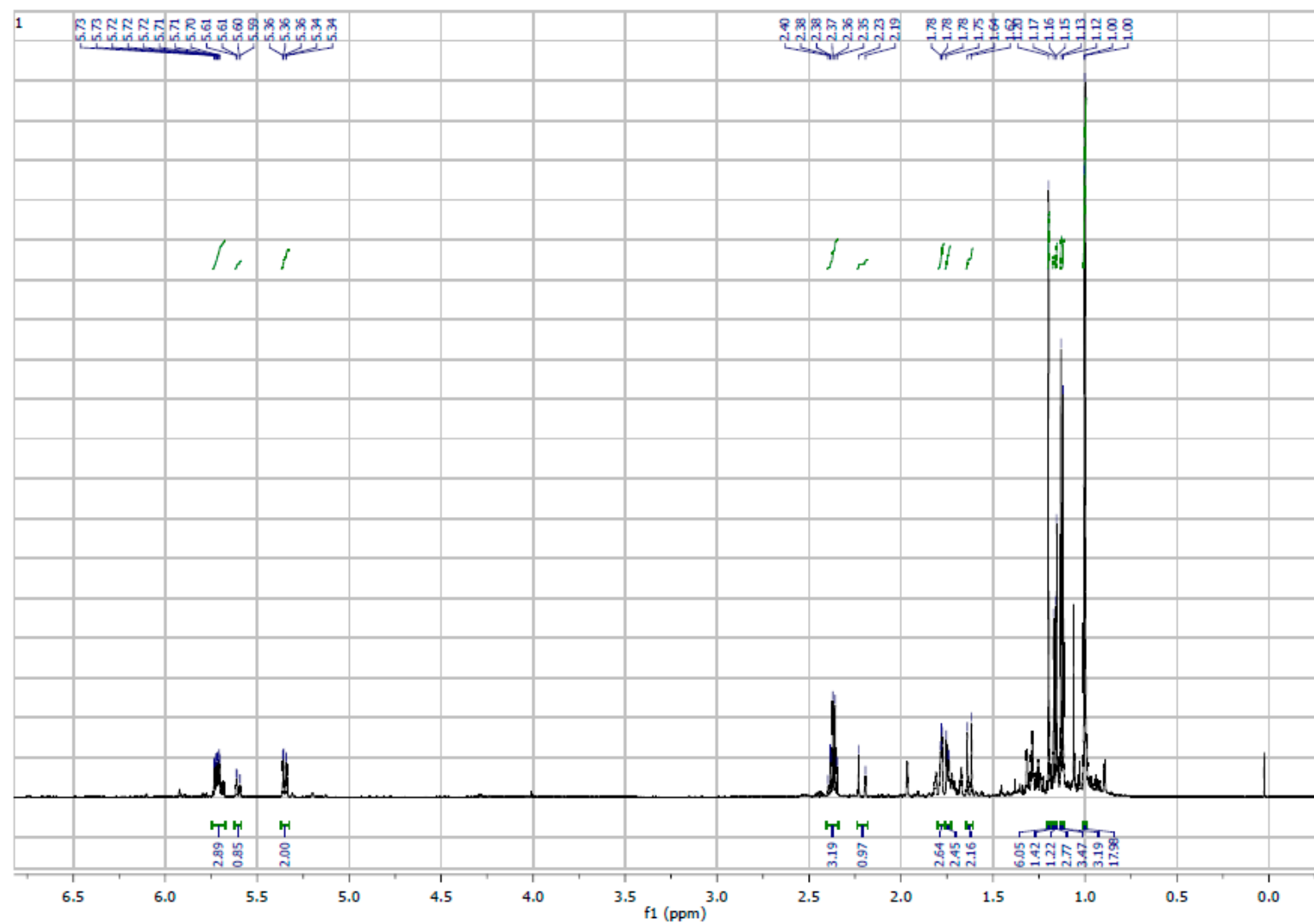


Figure S6. IR spectrum of ester 2a.

Figure S7. ¹H-NMR (600 MHz, CDCl₃) spectrum of acid 3a.

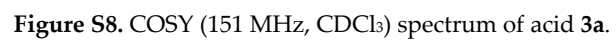


Figure S8. COSY (151 MHz, CDCl₃) spectrum of acid **3a**.

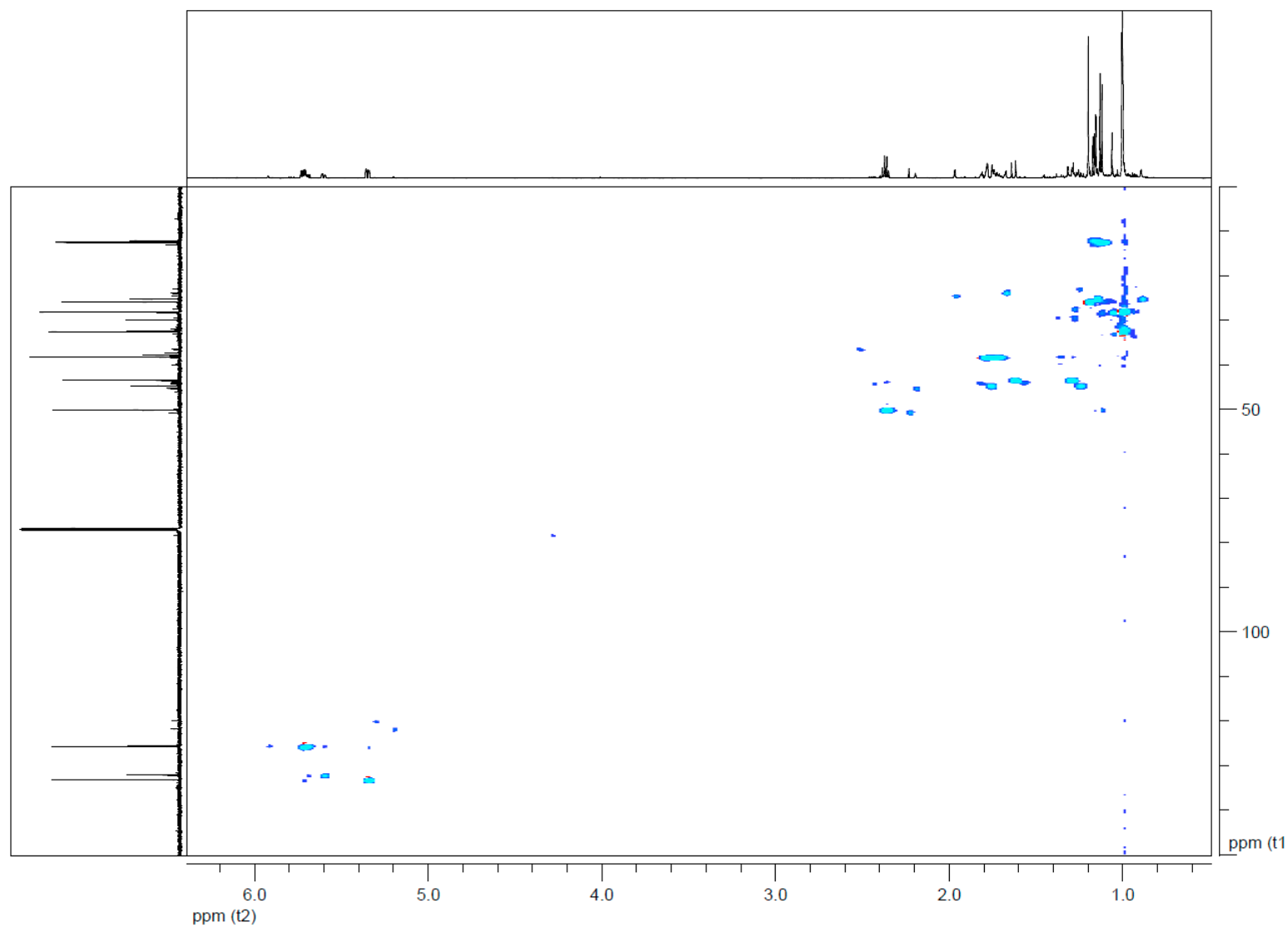


Figure S9. HMQC (151 MHz, CDCl₃) spectrum of acid 3a.

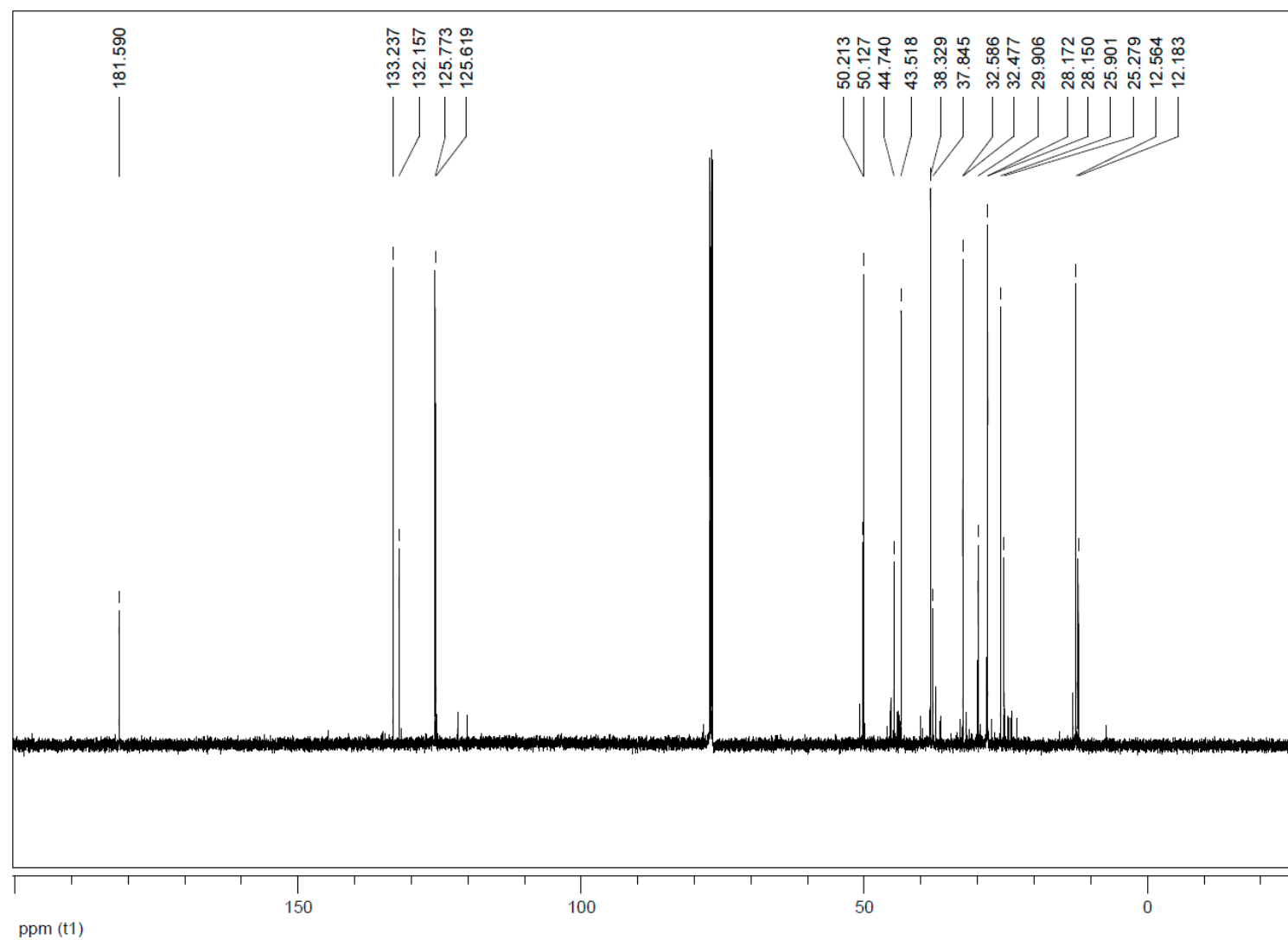


Figure S10. ^{13}C -NMR (151 MHz, CDCl_3) spectrum of acid **3a**.

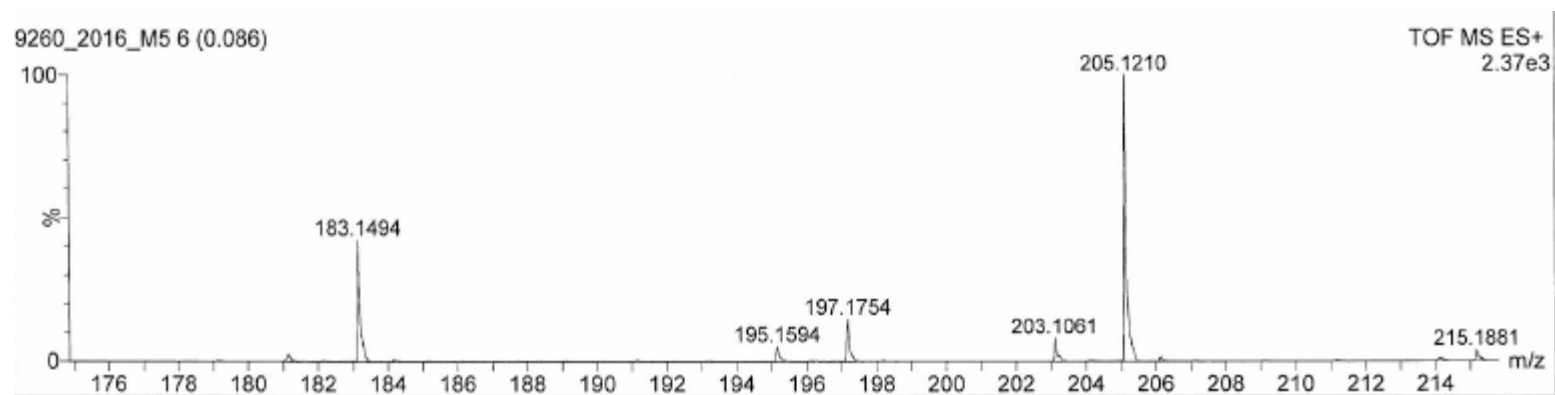


Figure S11. HRMS spectrum of acid 3a.

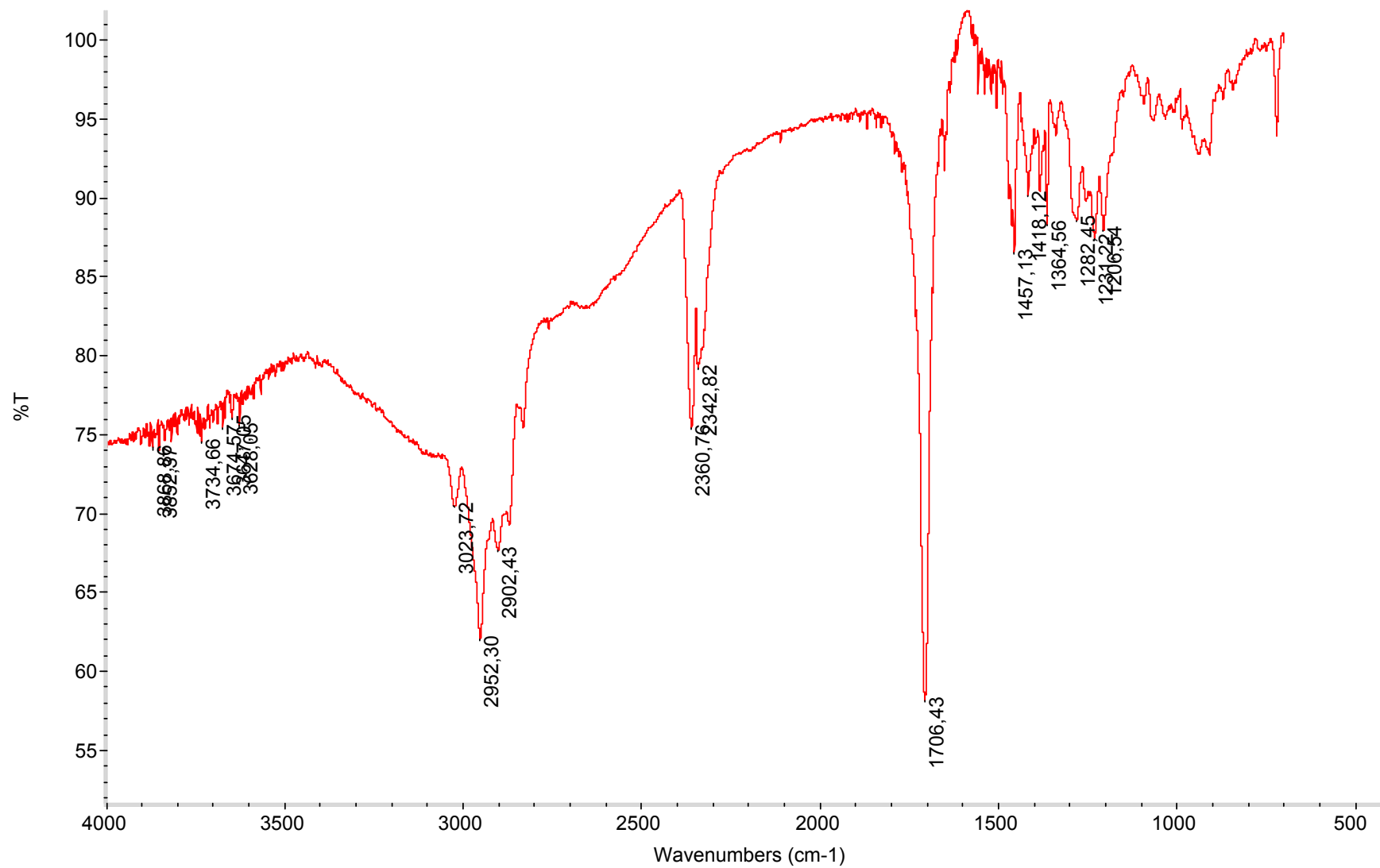


Figure S12. IR spectrum of acid 3a.

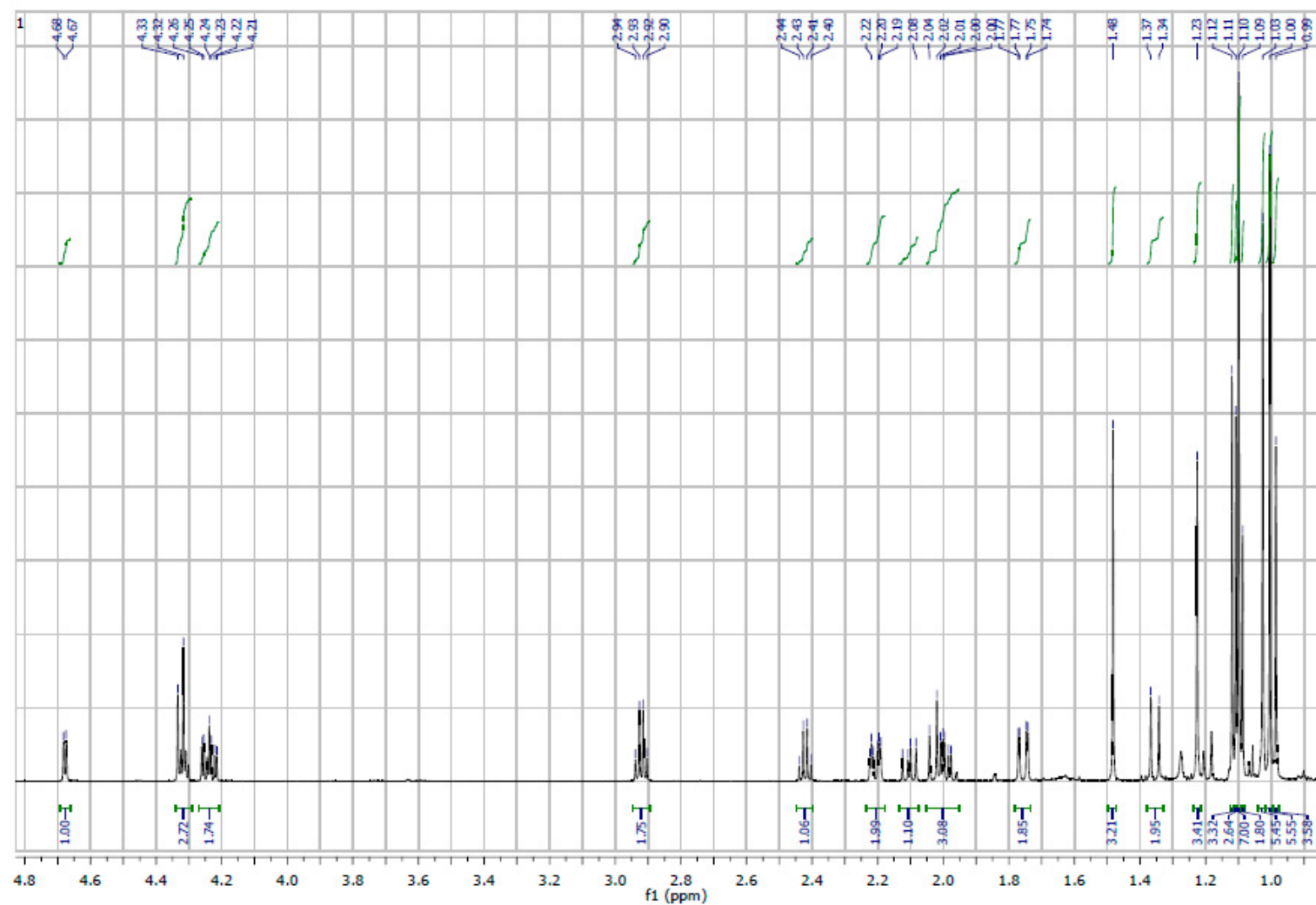


Figure S13. ^1H -NMR (600 MHz, CDCl_3) spectrum of iodolactone 4a.

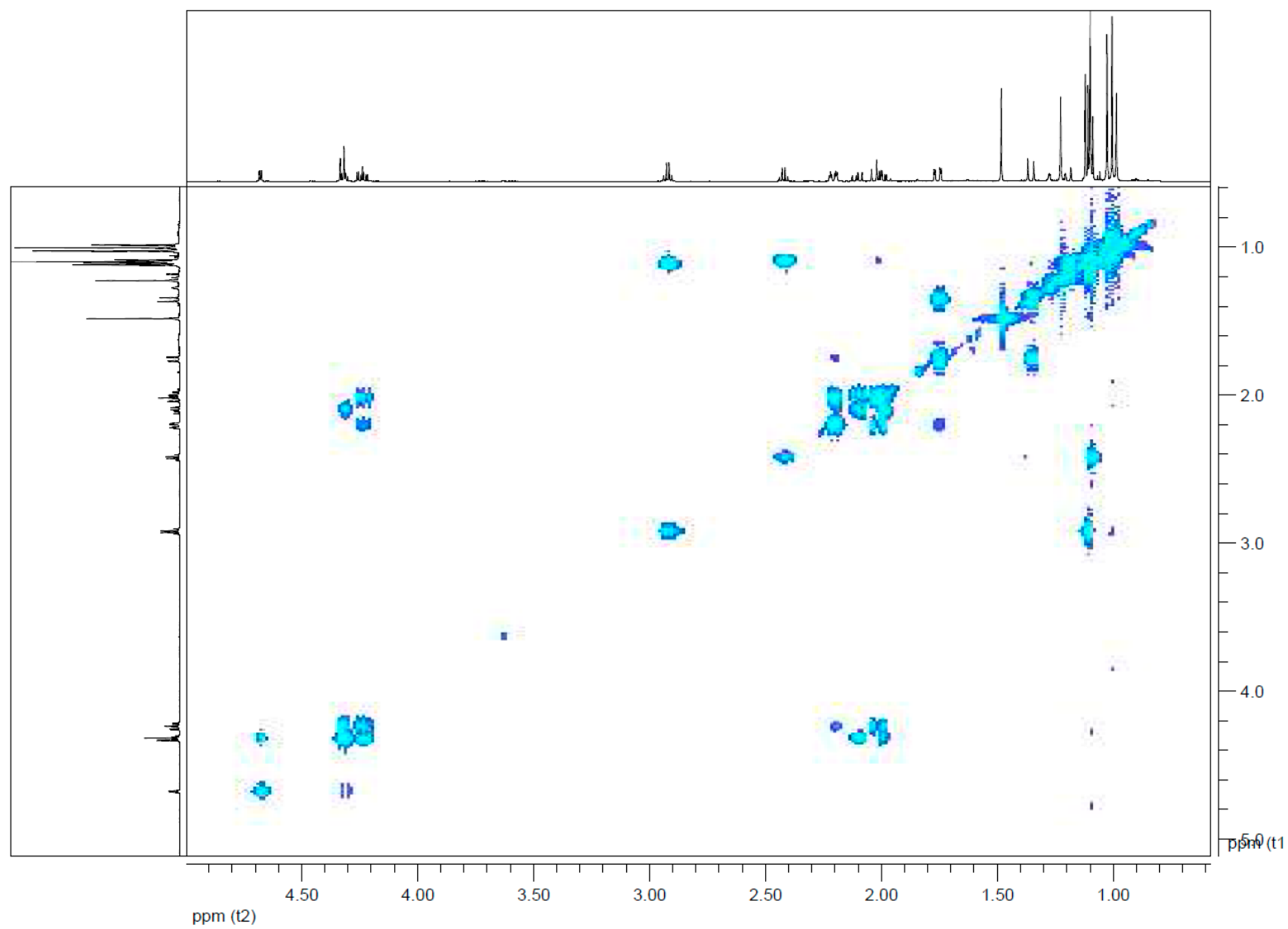


Figure S14. COSY (151 MHz, CDCl₃) spectrum of iodolactone 4a.

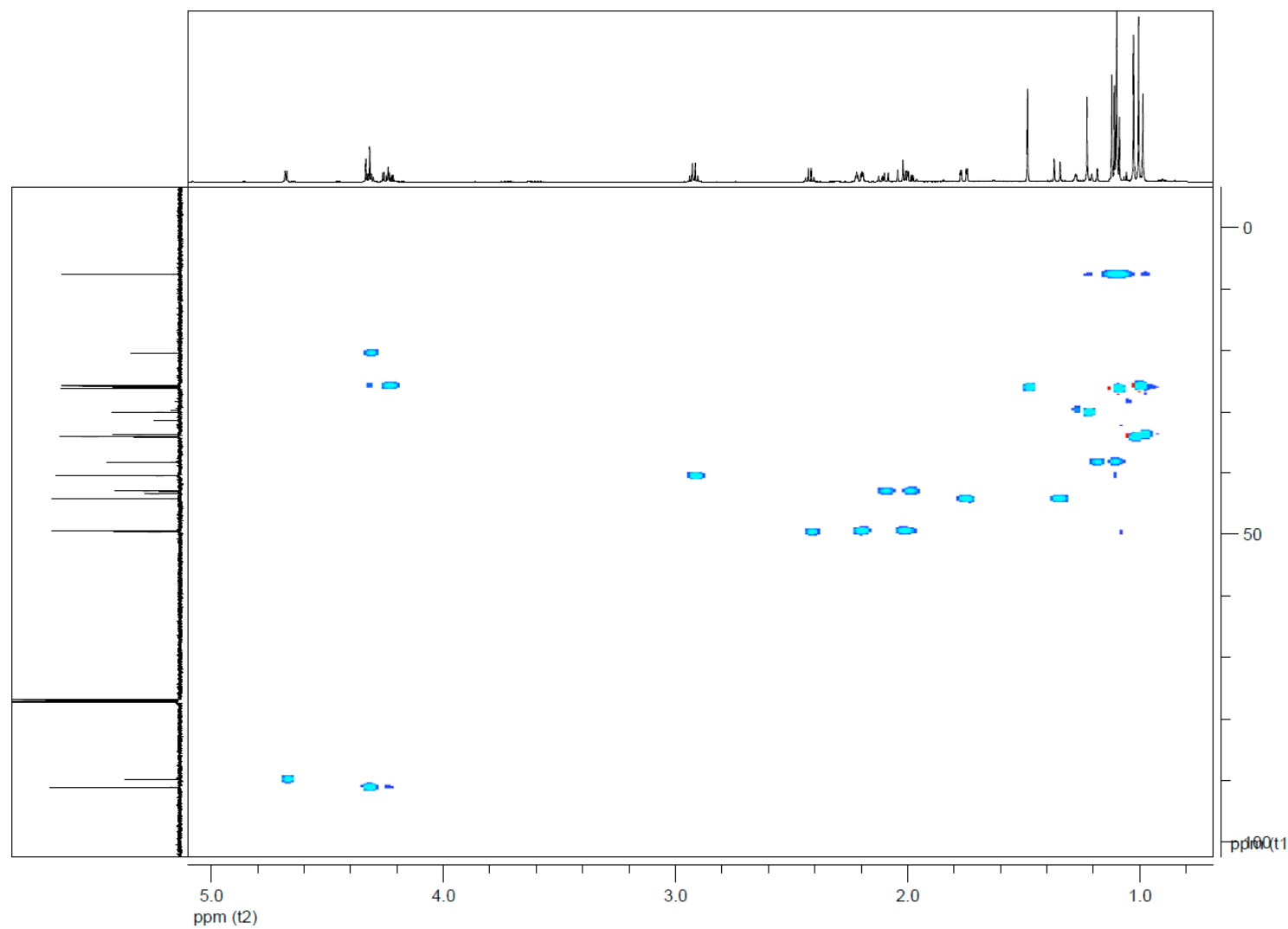


Figure S15. HMBC (151 MHz, CDCl_3) spectrum of iodolactone 4a.

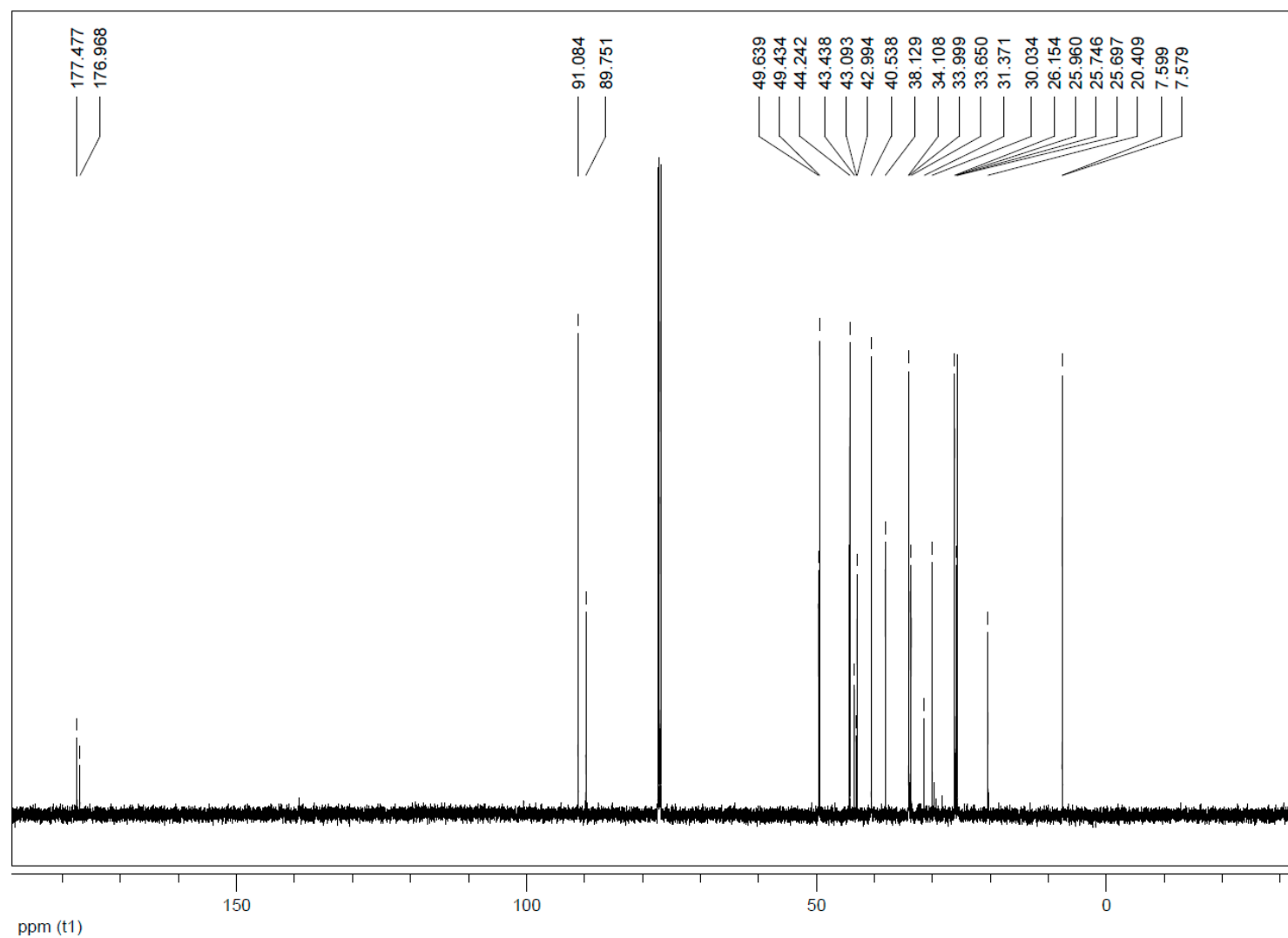


Figure S16. ¹³C-NMR (151 MHz, CDCl₃) spectrum of iodolactone **4a**.

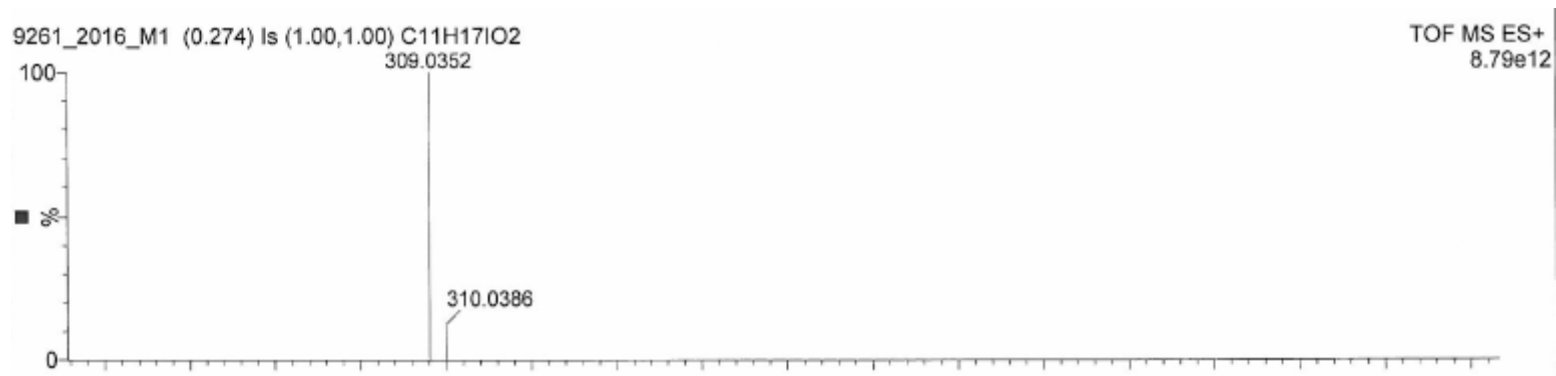


Figure S17. HRMS spectrum of iodolactone **4a**.

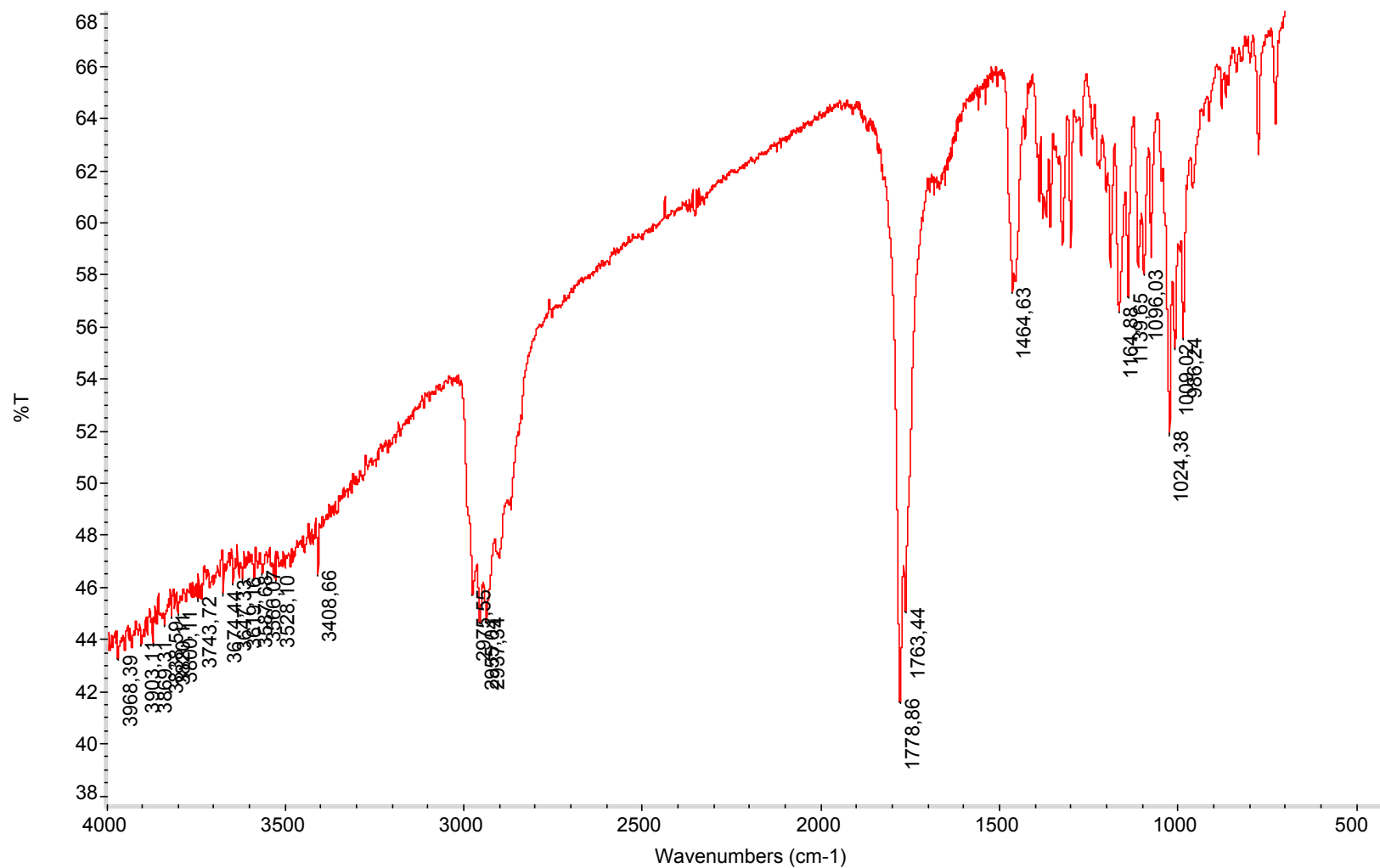


Figure S18. IR spectrum of iodolactone 4a.

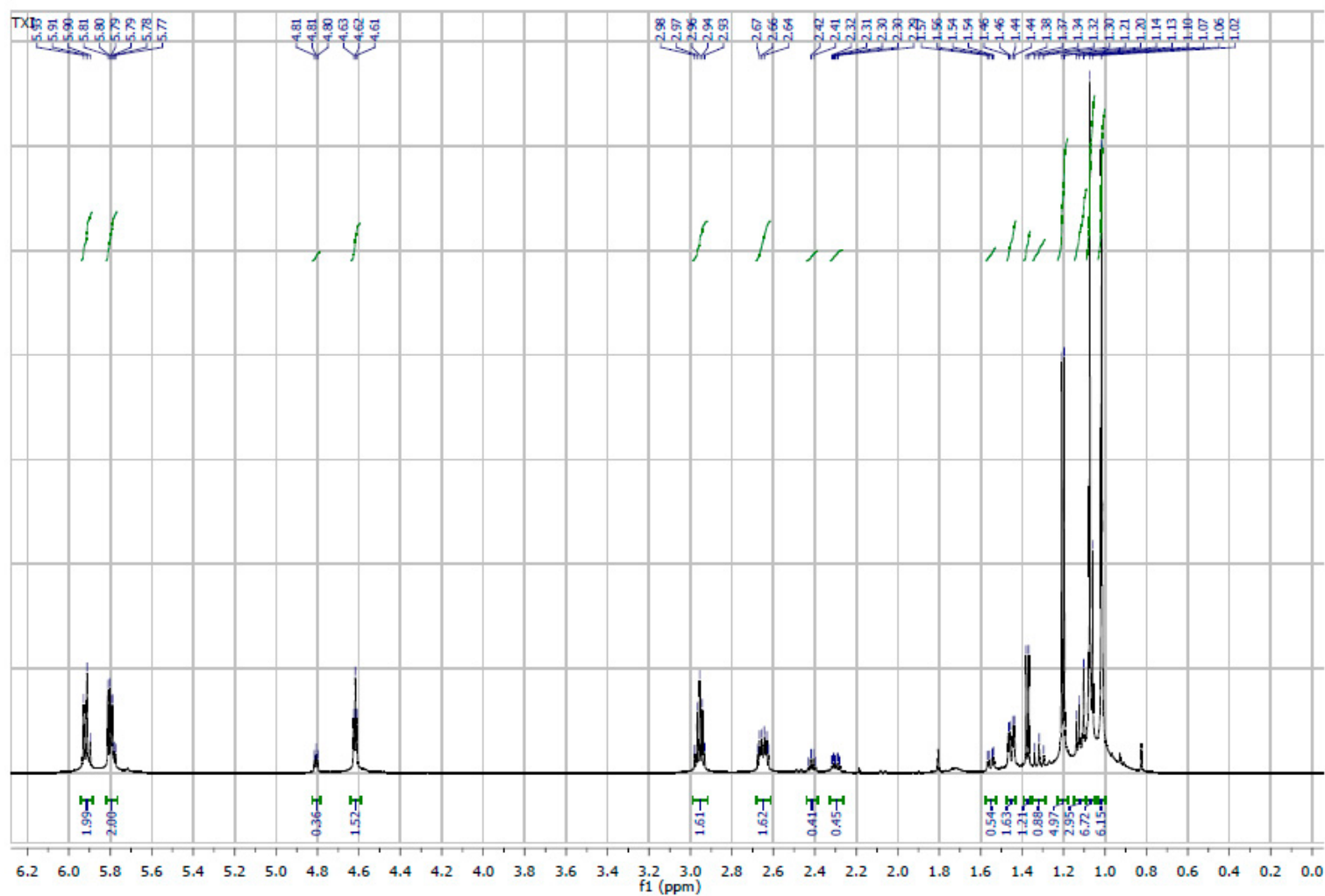


Figure S19. ¹H-NMR (600 MHz, CDCl₃) spectrum of unsaturated lactone 5a.

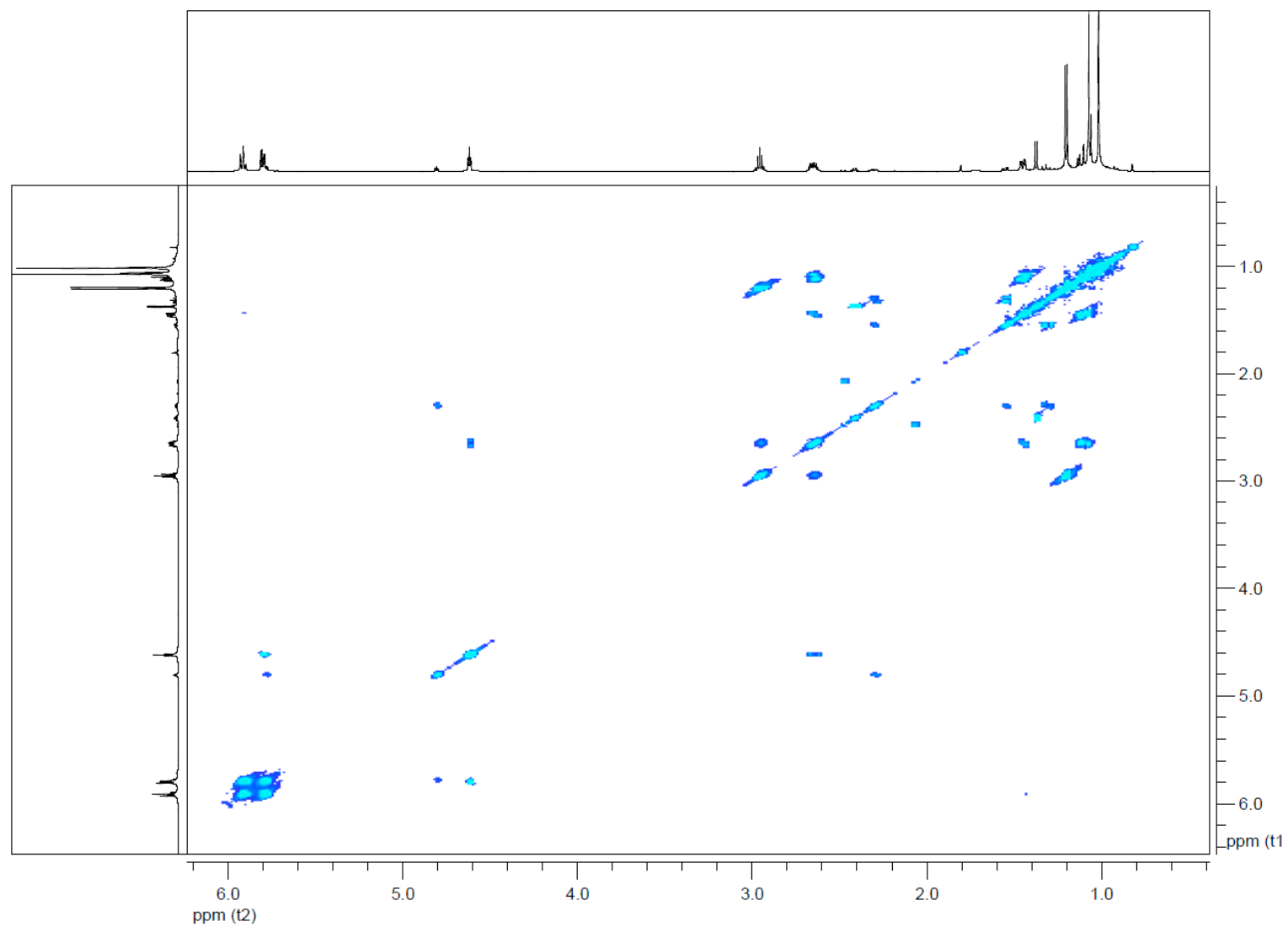


Figure S20. COSY (151 MHz, CDCl_3) spectrum of unsaturated lactone **5a**.

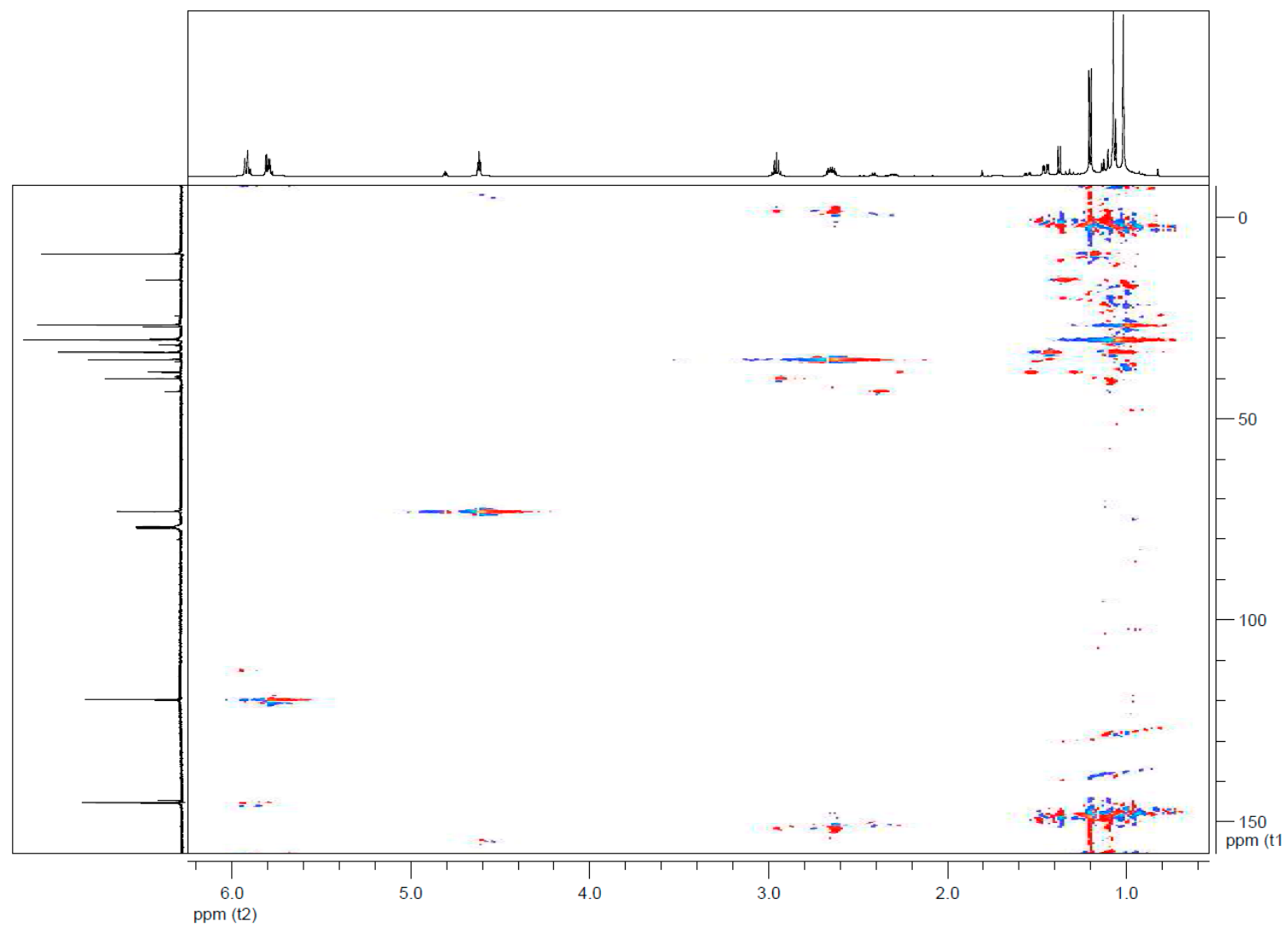


Figure S21. HMQC (151 MHz, CDCl_3) spectrum of unsaturated lactone 5a.

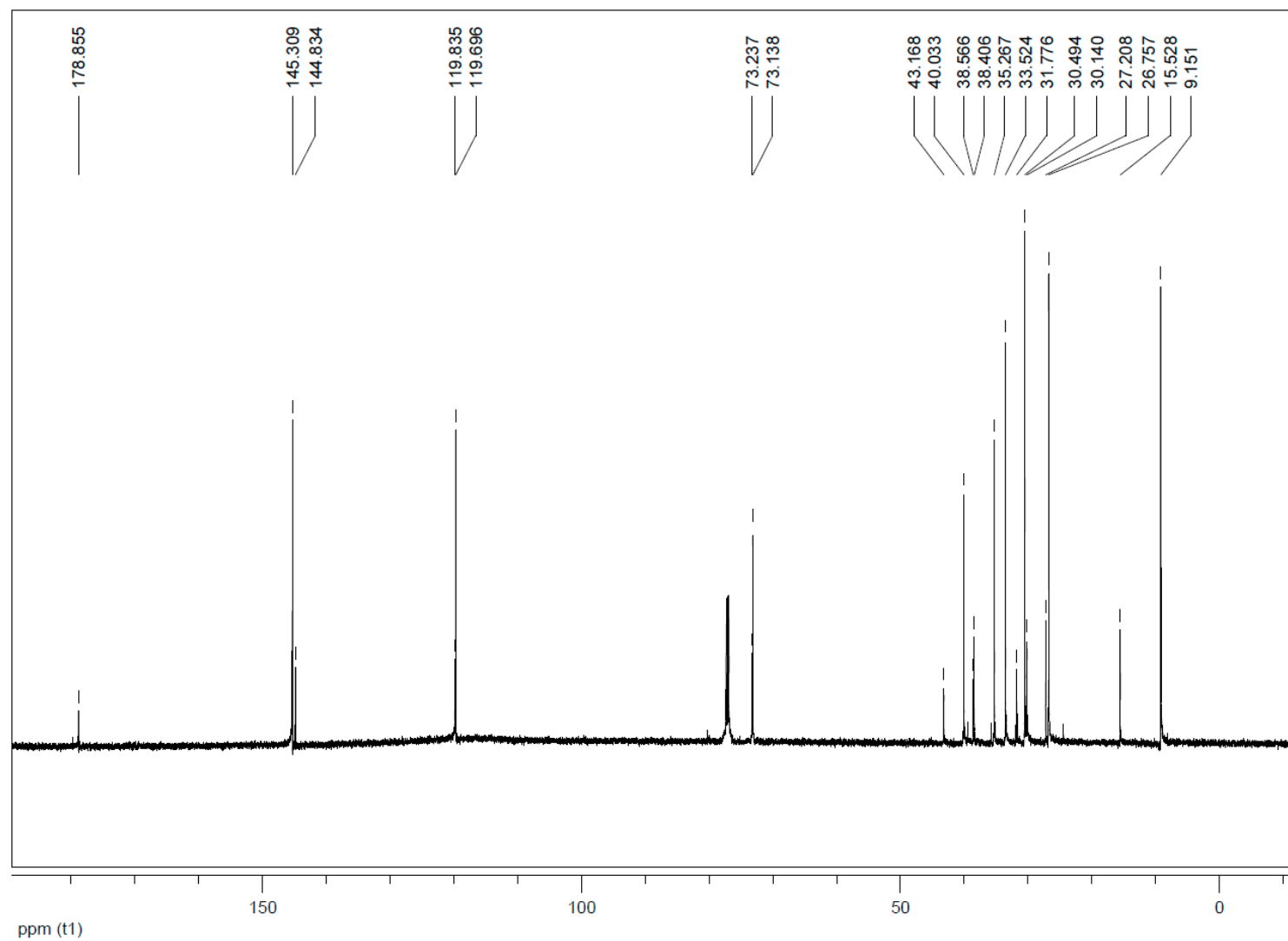


Figure S22. ^{13}C -NMR (151 MHz, CDCl_3) spectrum of unsaturated lactone **5a**.

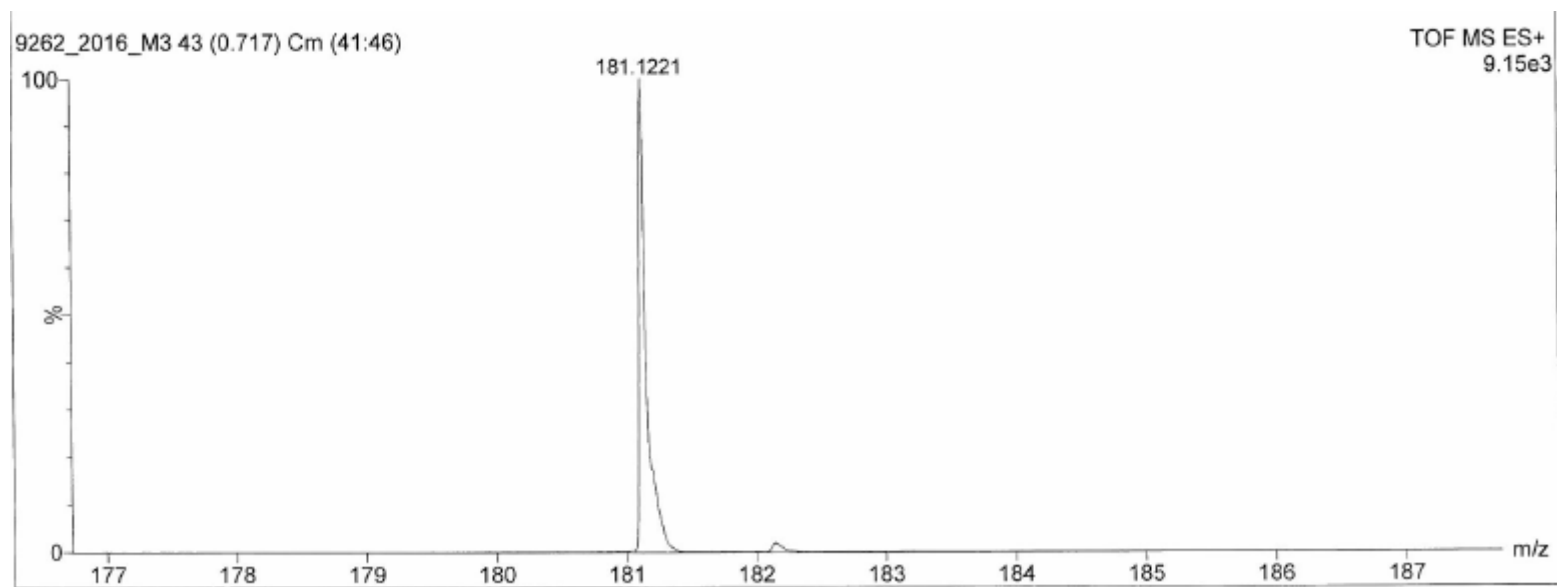


Figure S23. HRMS spectrum of unsaturated lactone 5a.

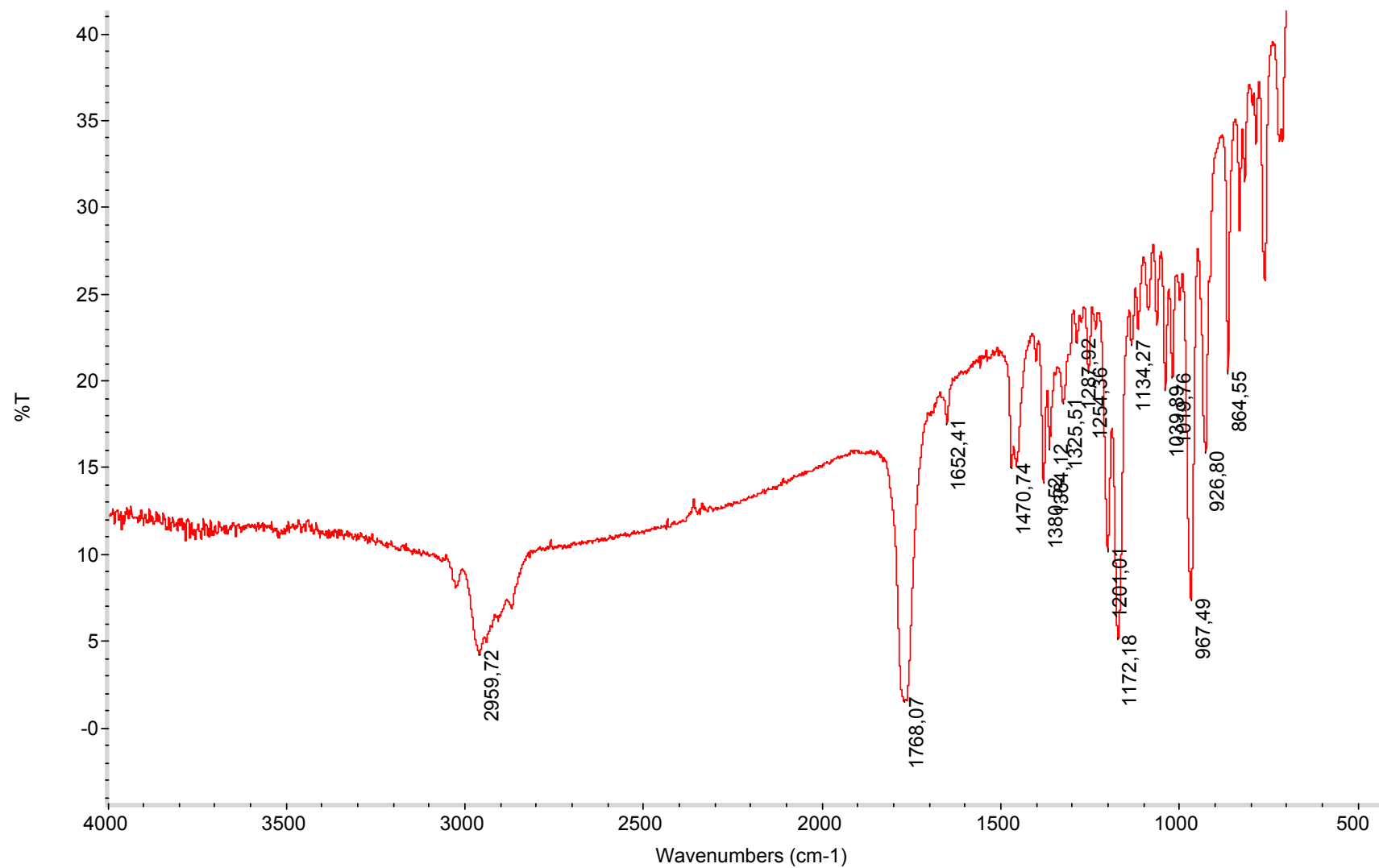


Figure S24. IR spectrum of unsaturated lactone 5a.

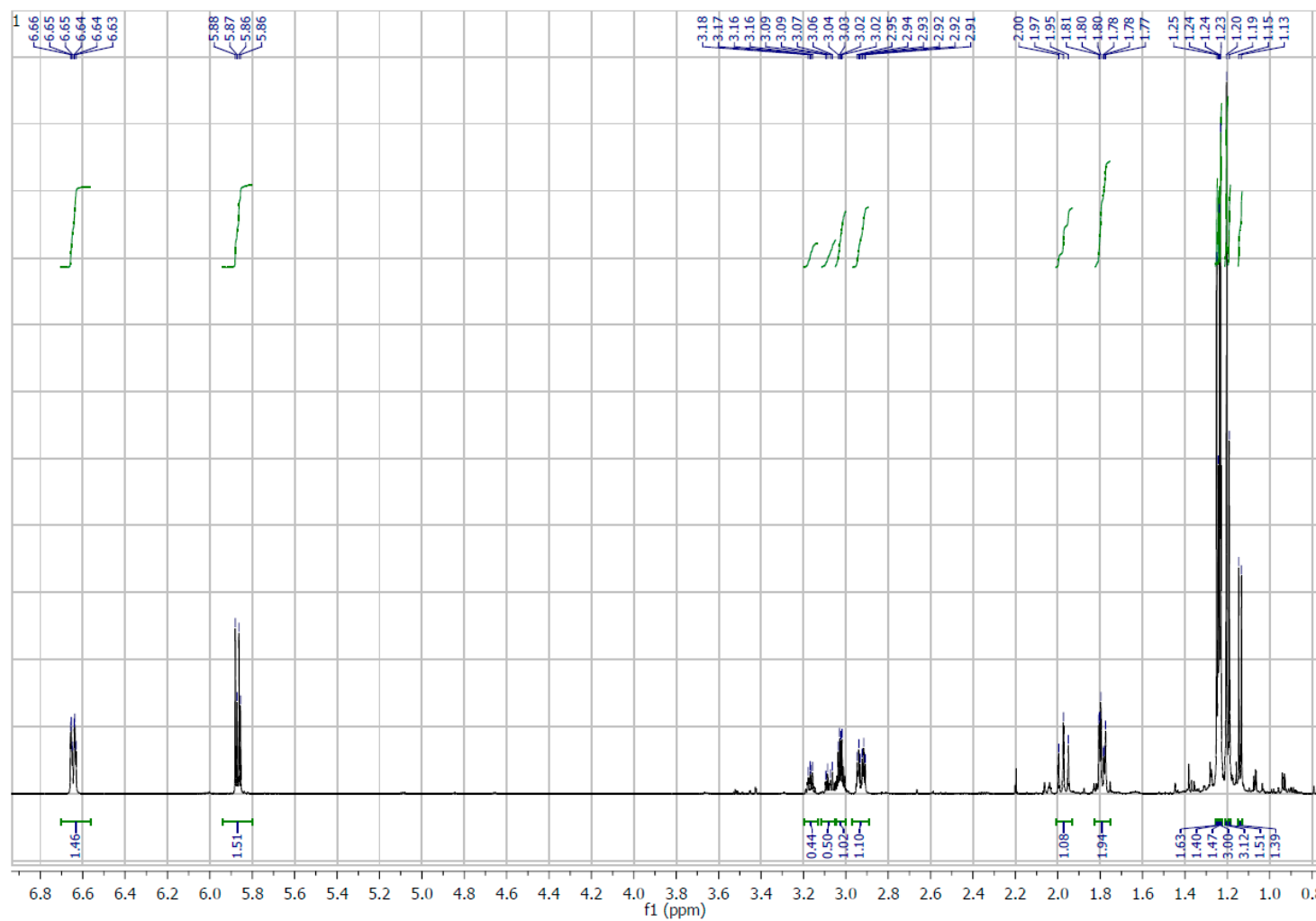


Figure S25. ¹H-NMR (600 MHz, CDCl₃) spectrum of hydroxylactone **6a**.

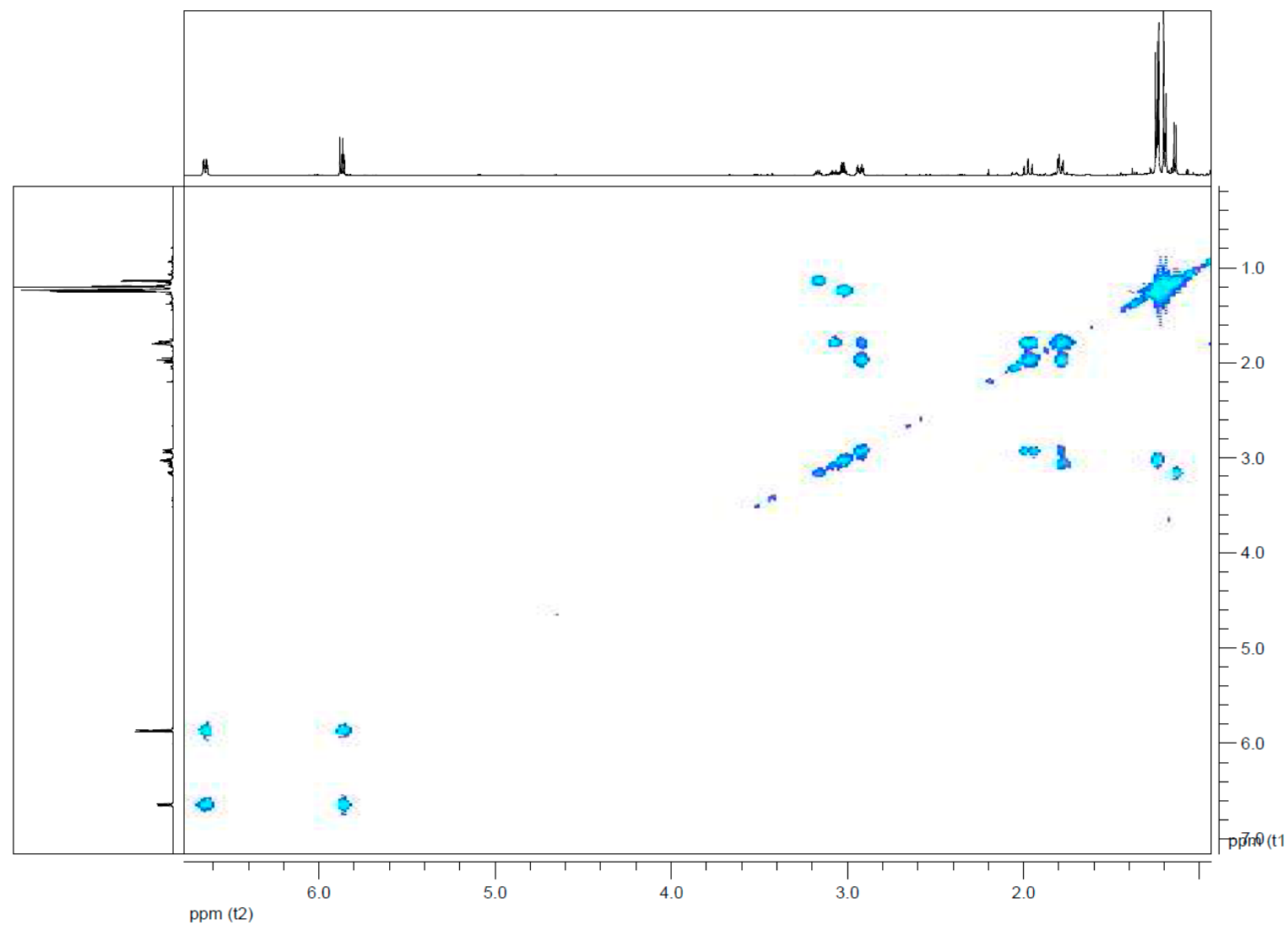


Figure S26. COSY (151 MHz, CDCl₃) spectrum of hydroxylactone **6a**.

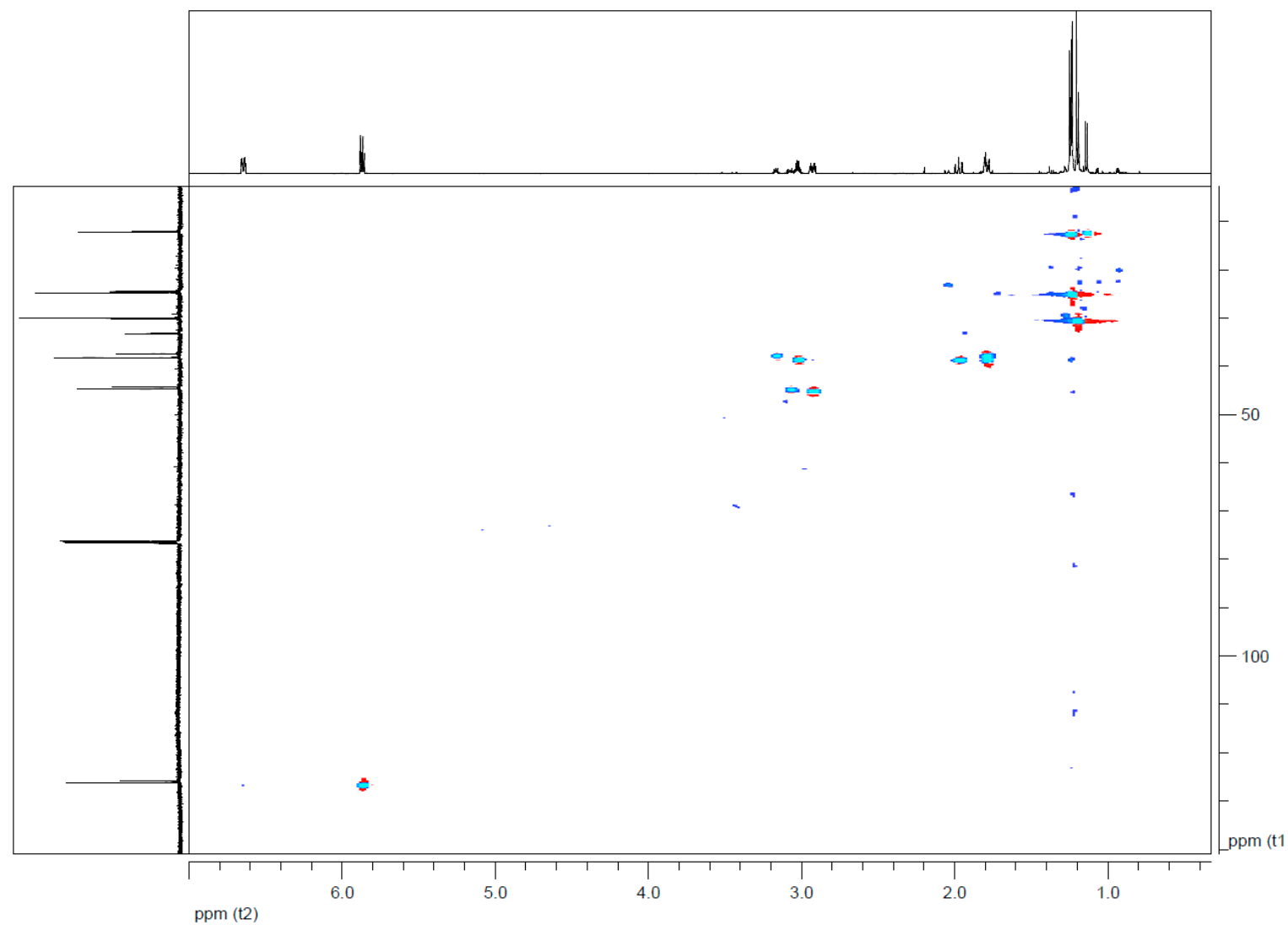


Figure S27. HMPC (151 MHz, CDCl₃) spectrum of hydroxylactone 6a.

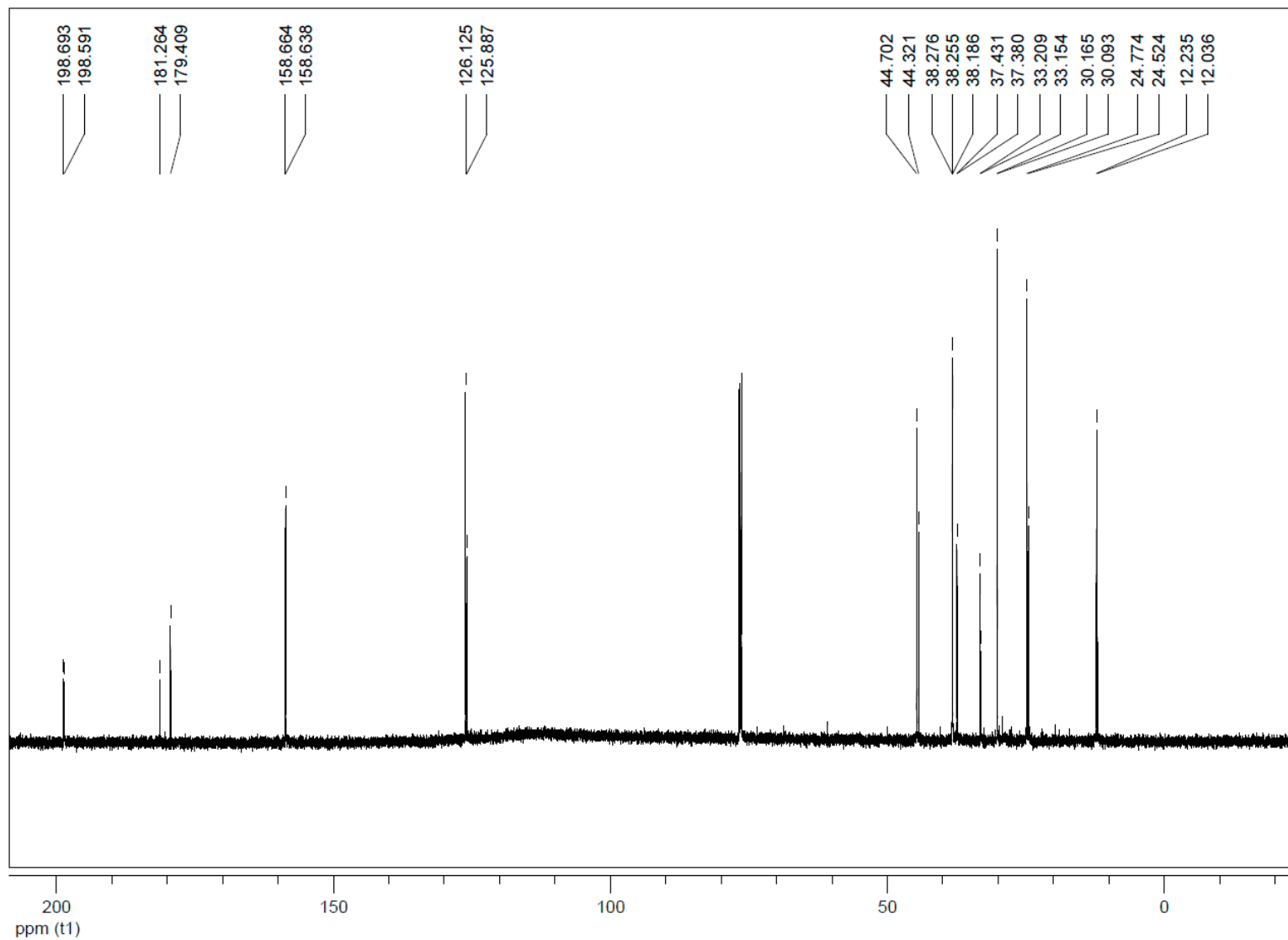


Figure S28. ^{13}C -NMR (151 MHz, CDCl_3) spectrum of hydroxylactone **6a**.

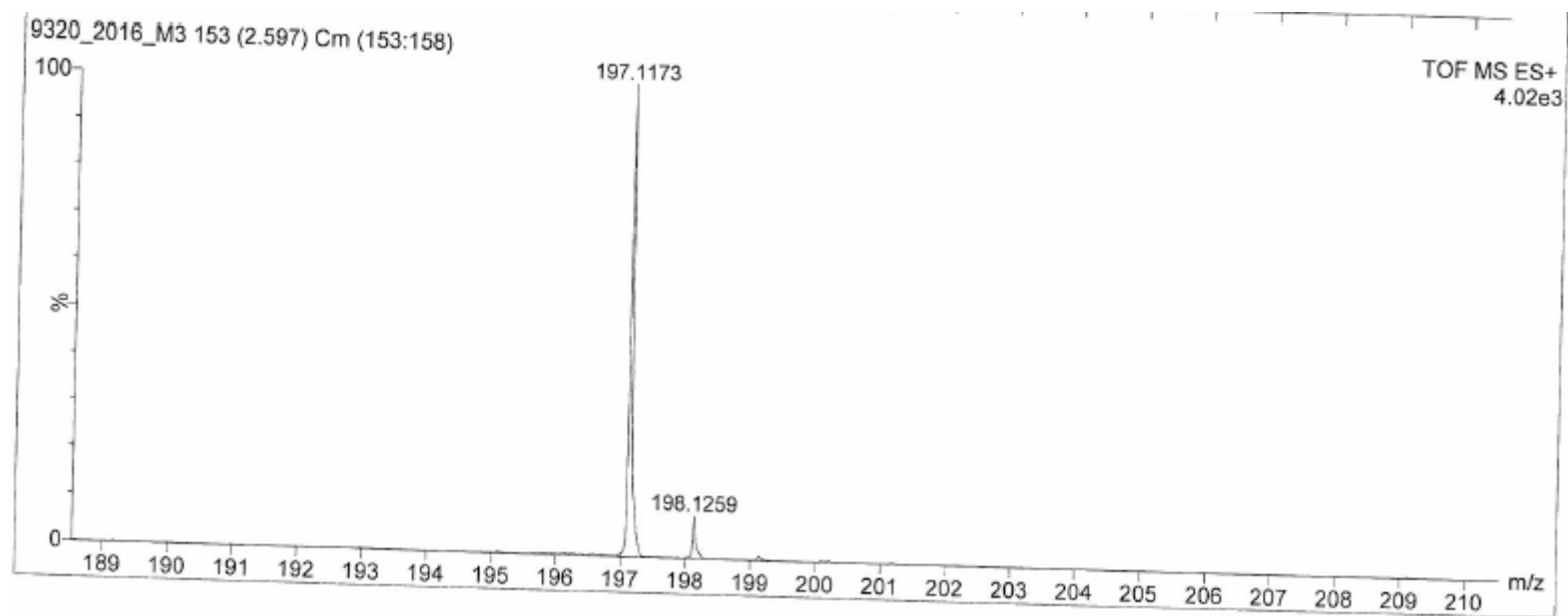


Figure S29. HRMS spectrum of hydroxylactone 6a.

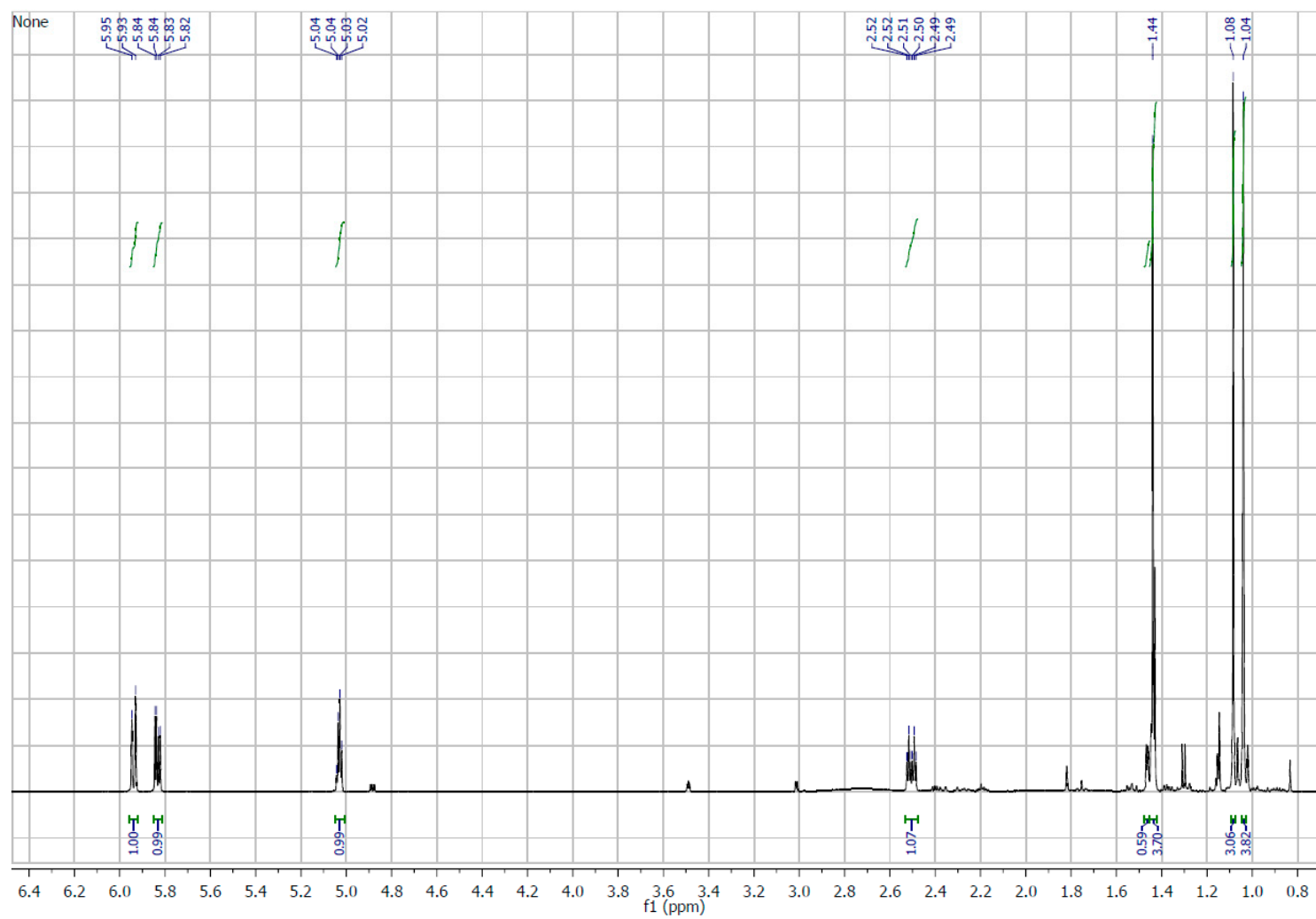


Figure S30. ¹H-NMR (600 MHz, CDCl₃) spectrum of hydroxylactone 7a.

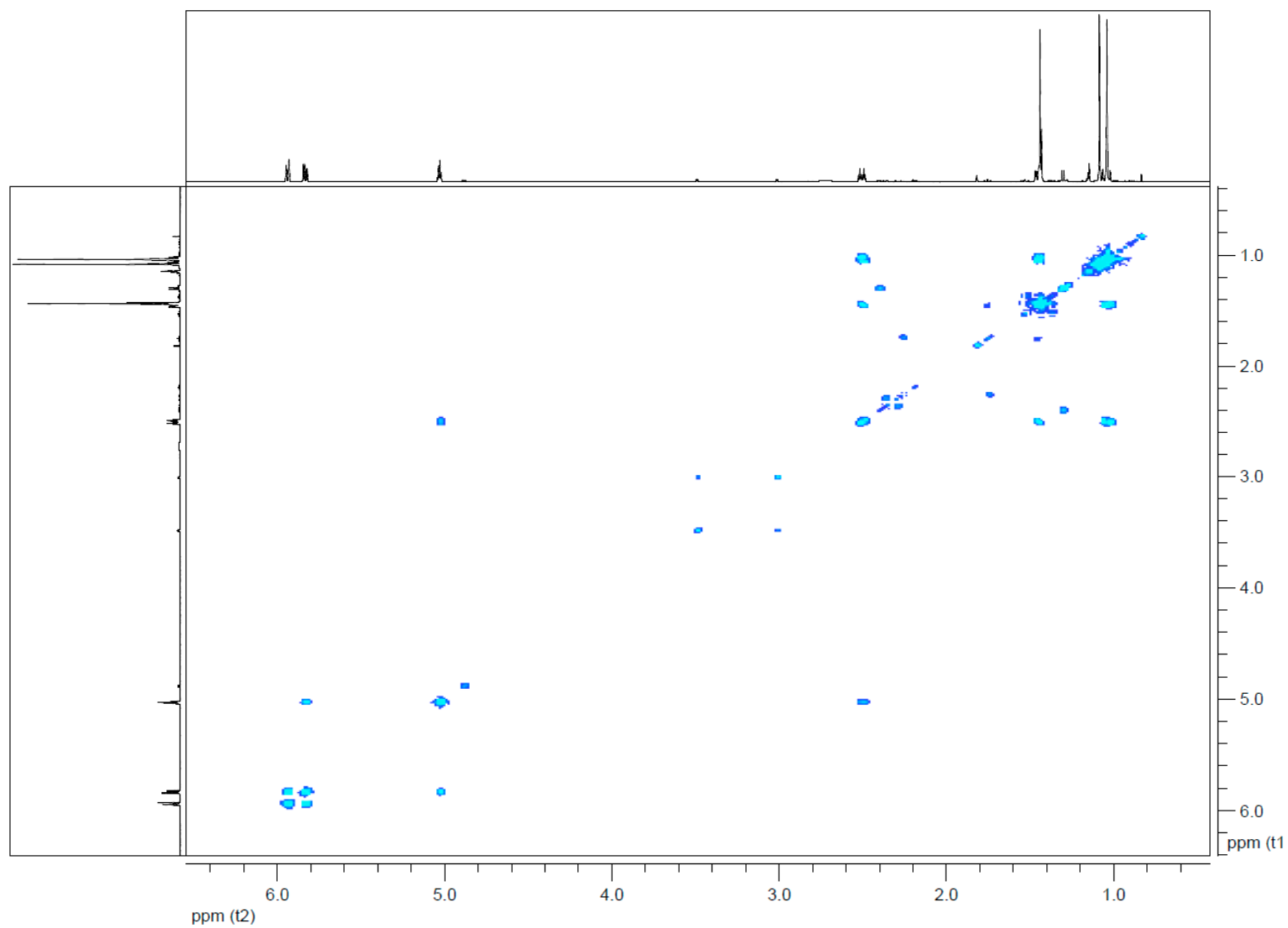


Figure S31. COSY (151 MHz, CDCl₃) spectrum of hydroxylactone **7a**.

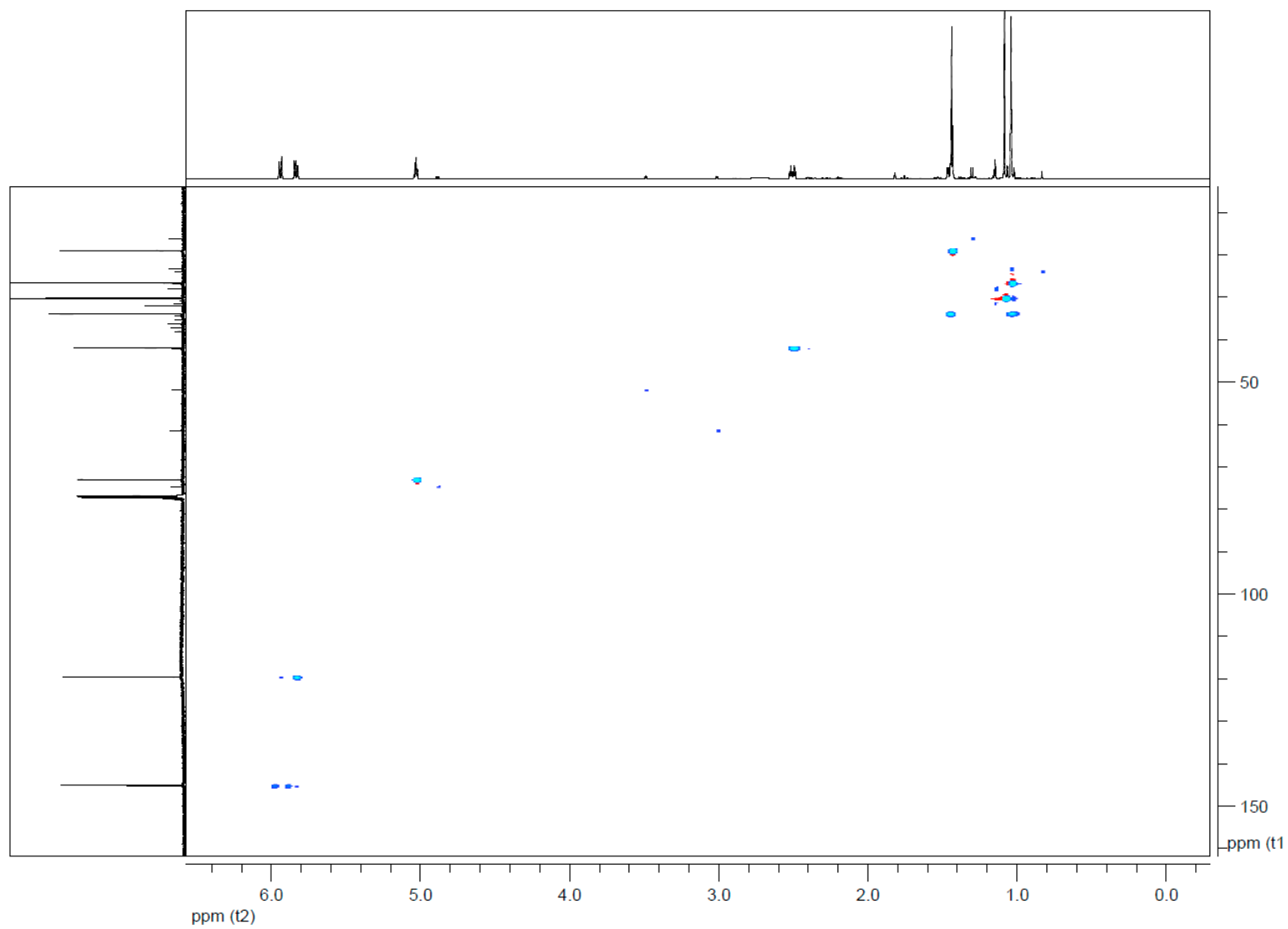


Figure S32. HMPC (151 MHz, CDCl_3) spectrum of hydroxylactone 7a.

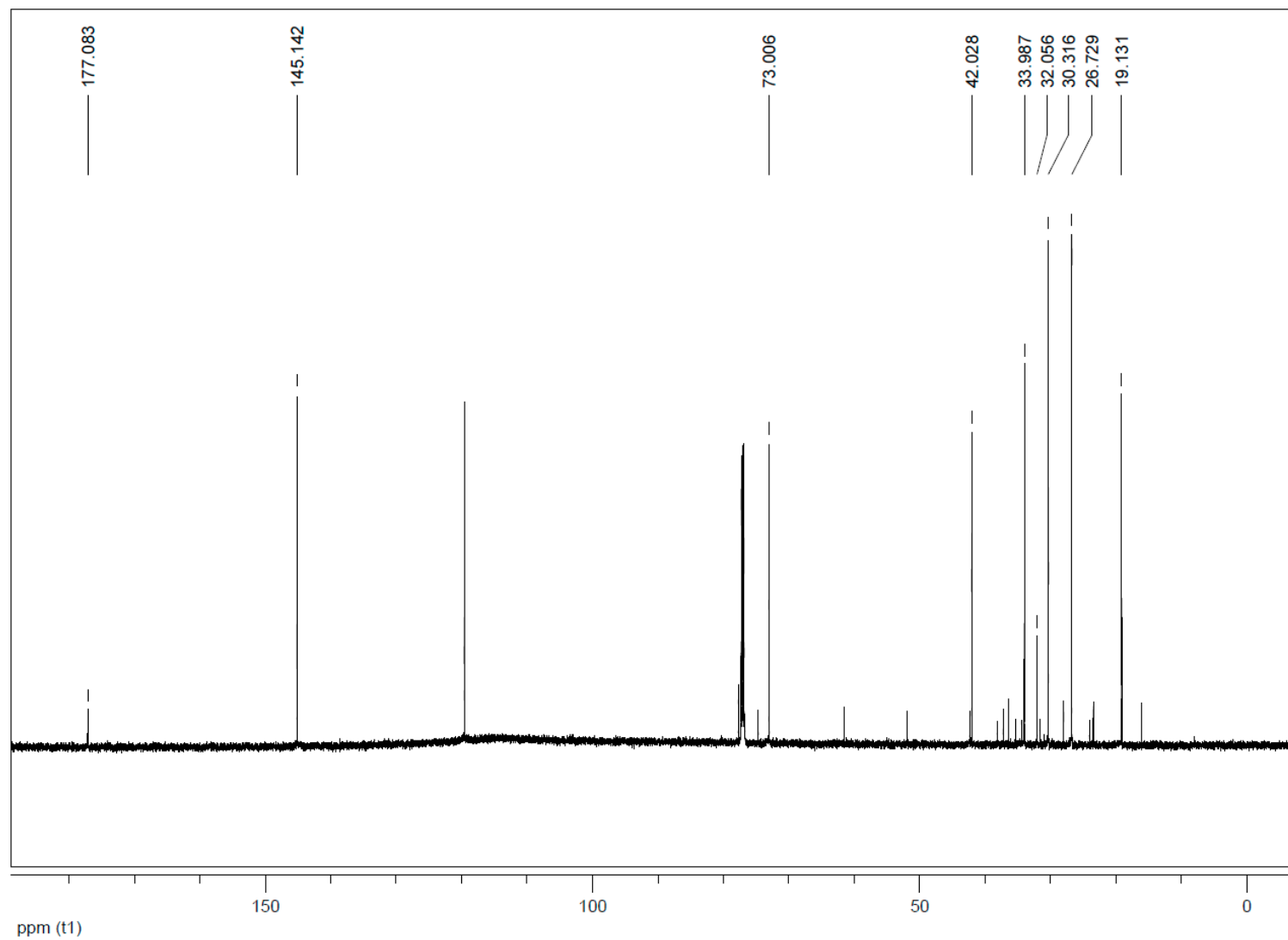


Figure S33. ^{13}C -NMR (151 MHz, CDCl_3) spectrum of hydroxylactone **7a**.

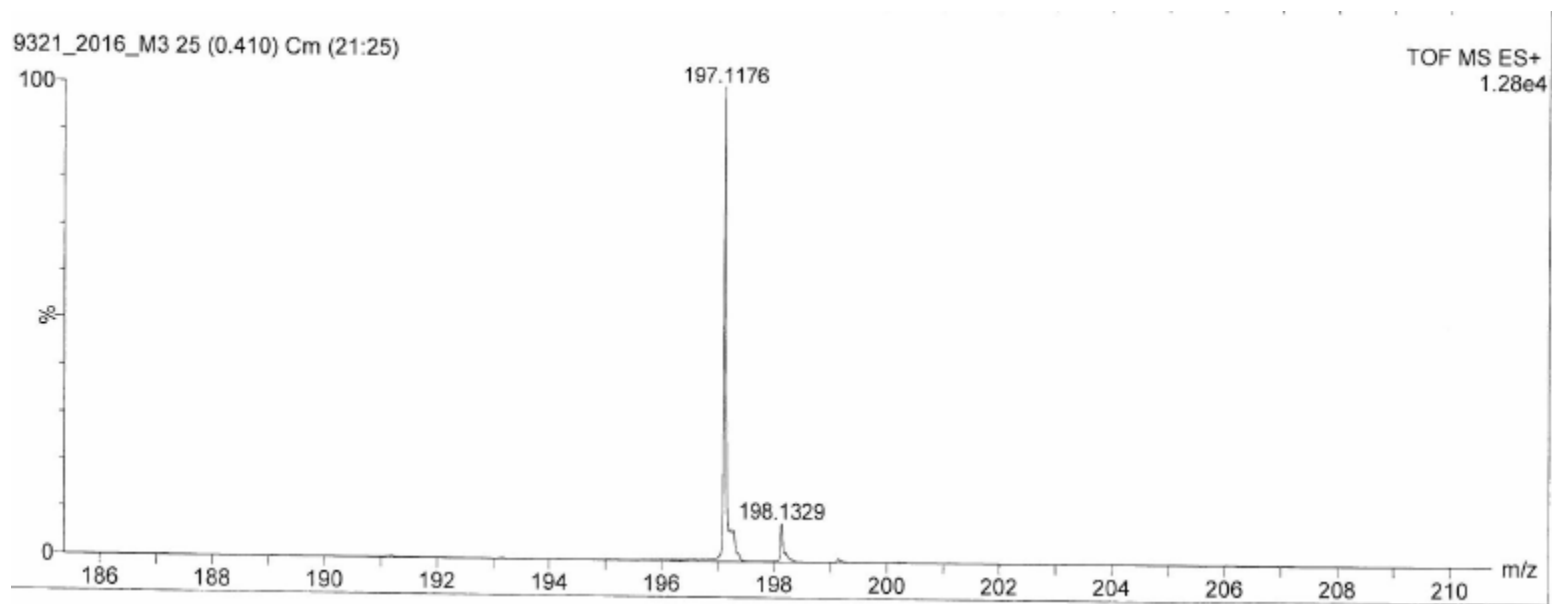


Figure S34. HRMS spectrum of hydroxylactone 7a.

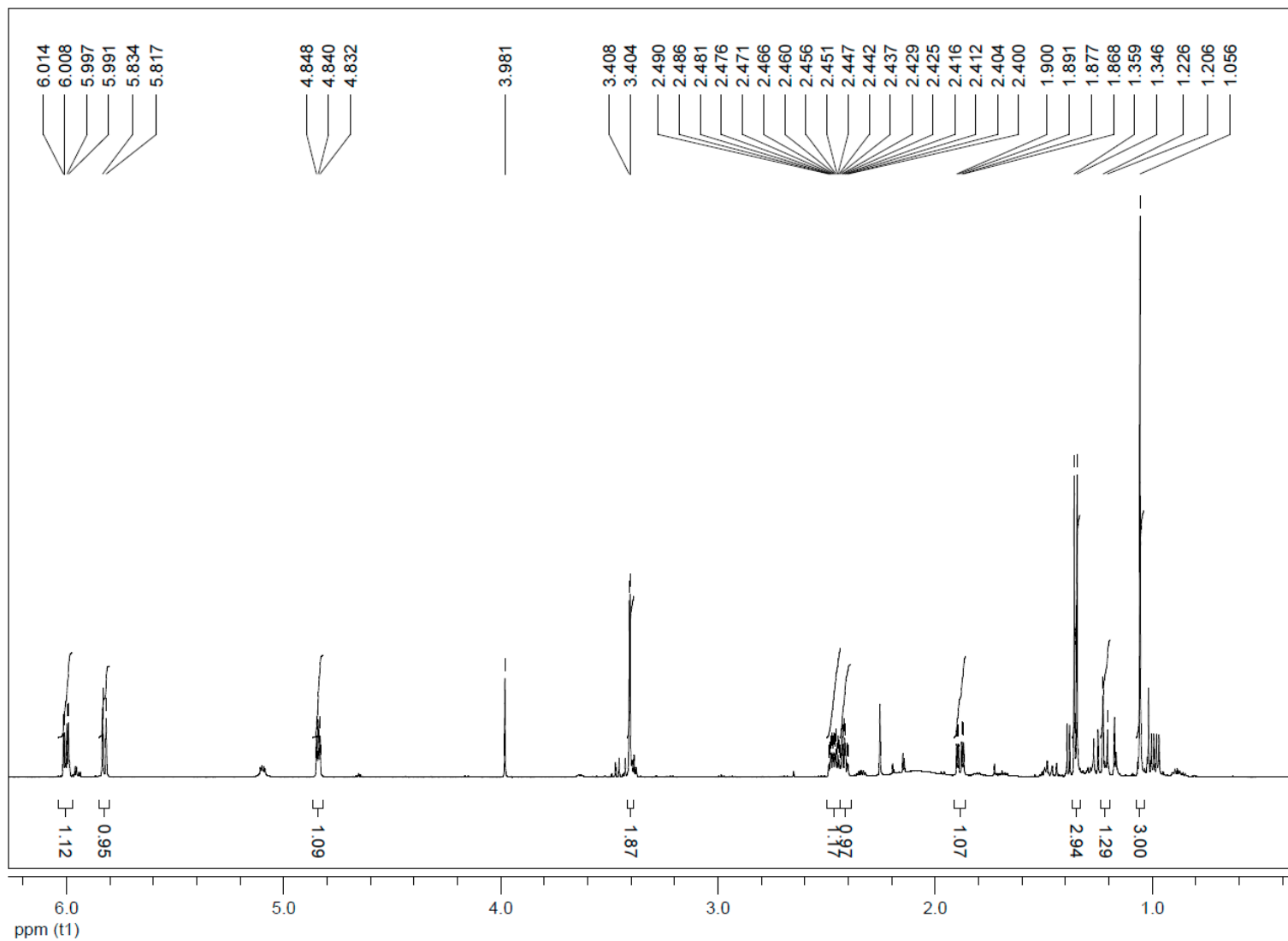


Figure S35. ^1H -NMR (600 MHz, CDCl_3) spectrum of hydroxylactone 8a.

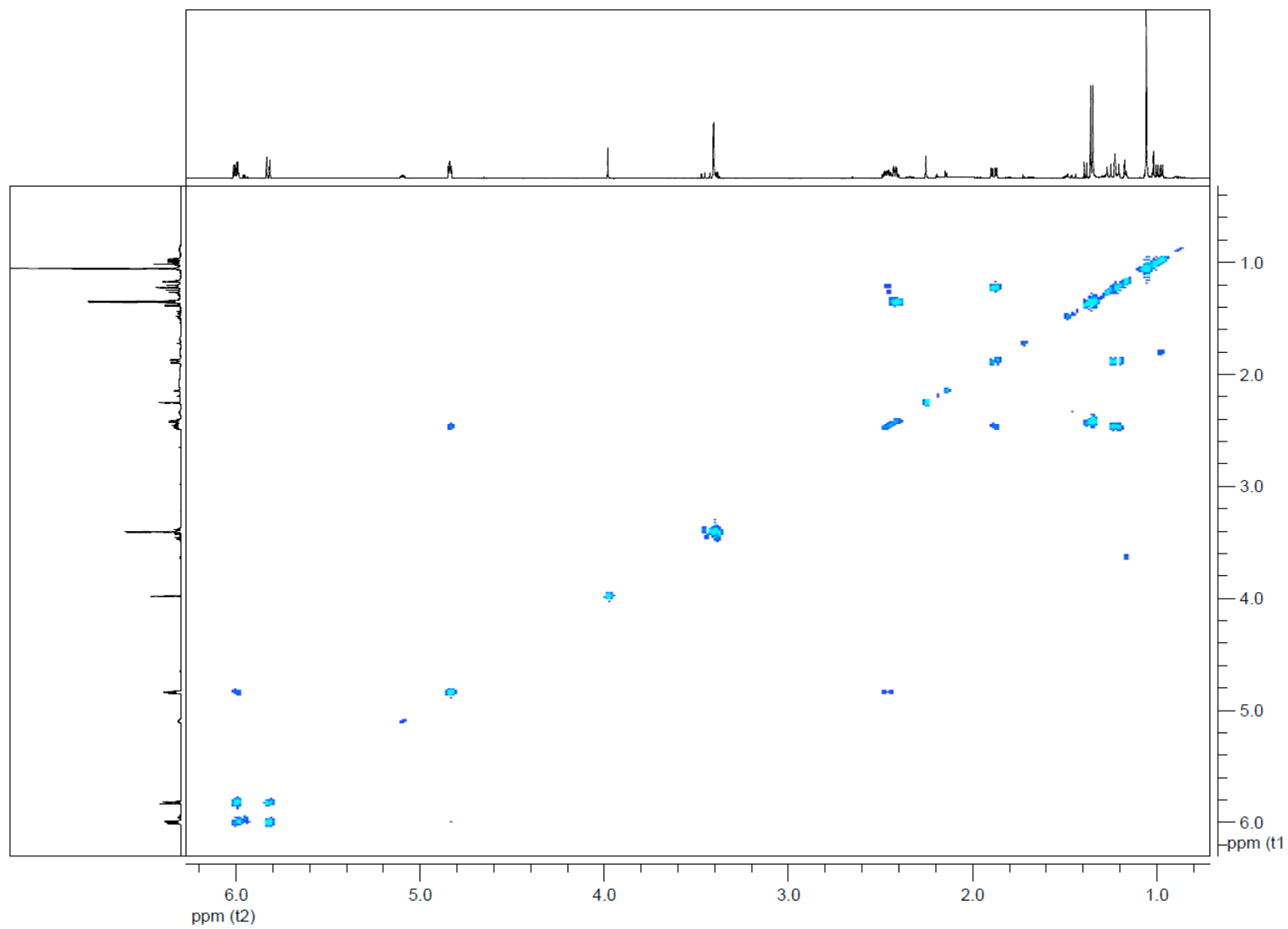


Figure S36. COSY (151 MHz, CDCl₃) spectrum of hydroxylactone **8a**.

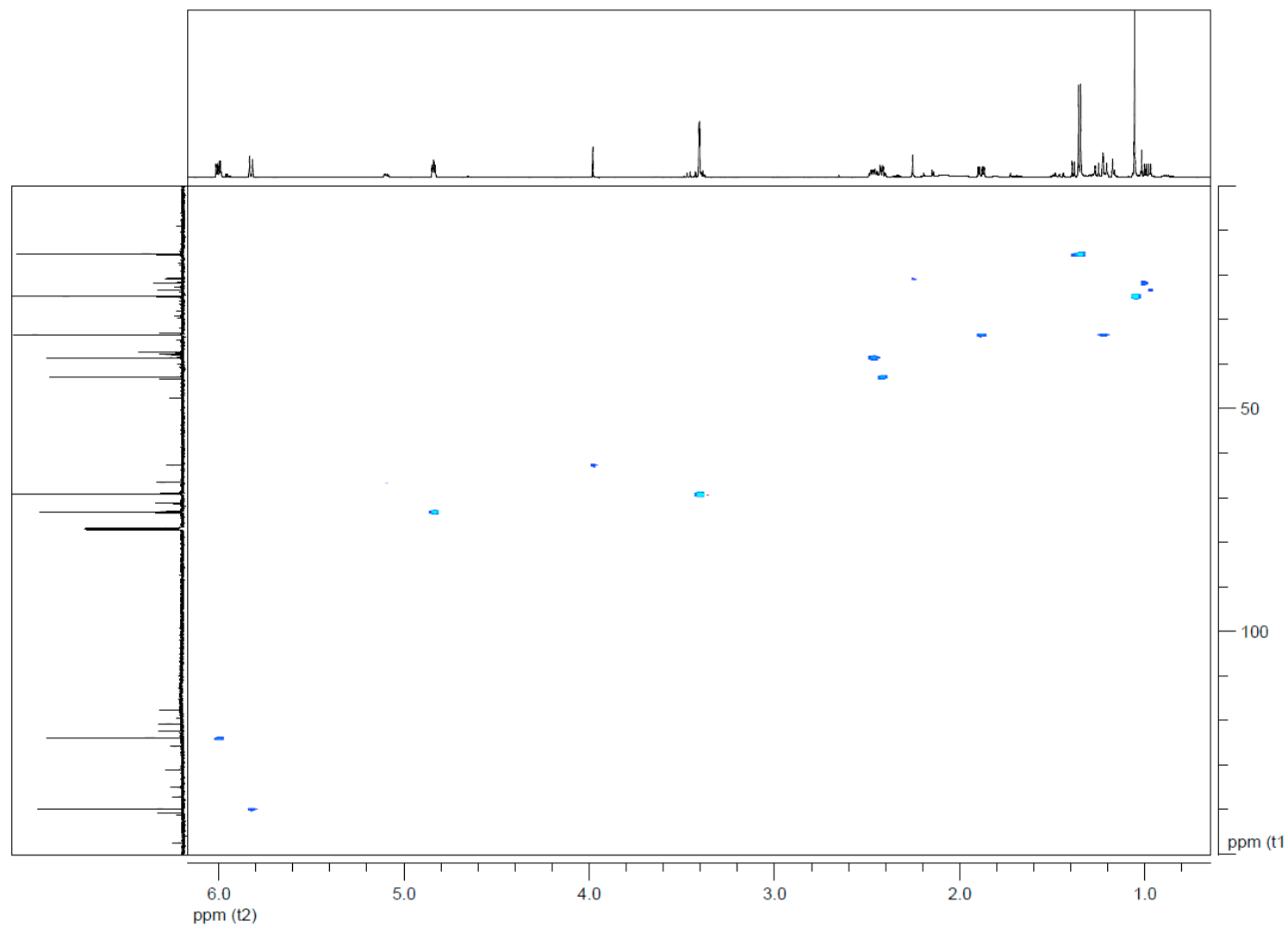


Figure S37. HMPC (151 MHz, CDCl₃) spectrum of hydroxylactone 8a.

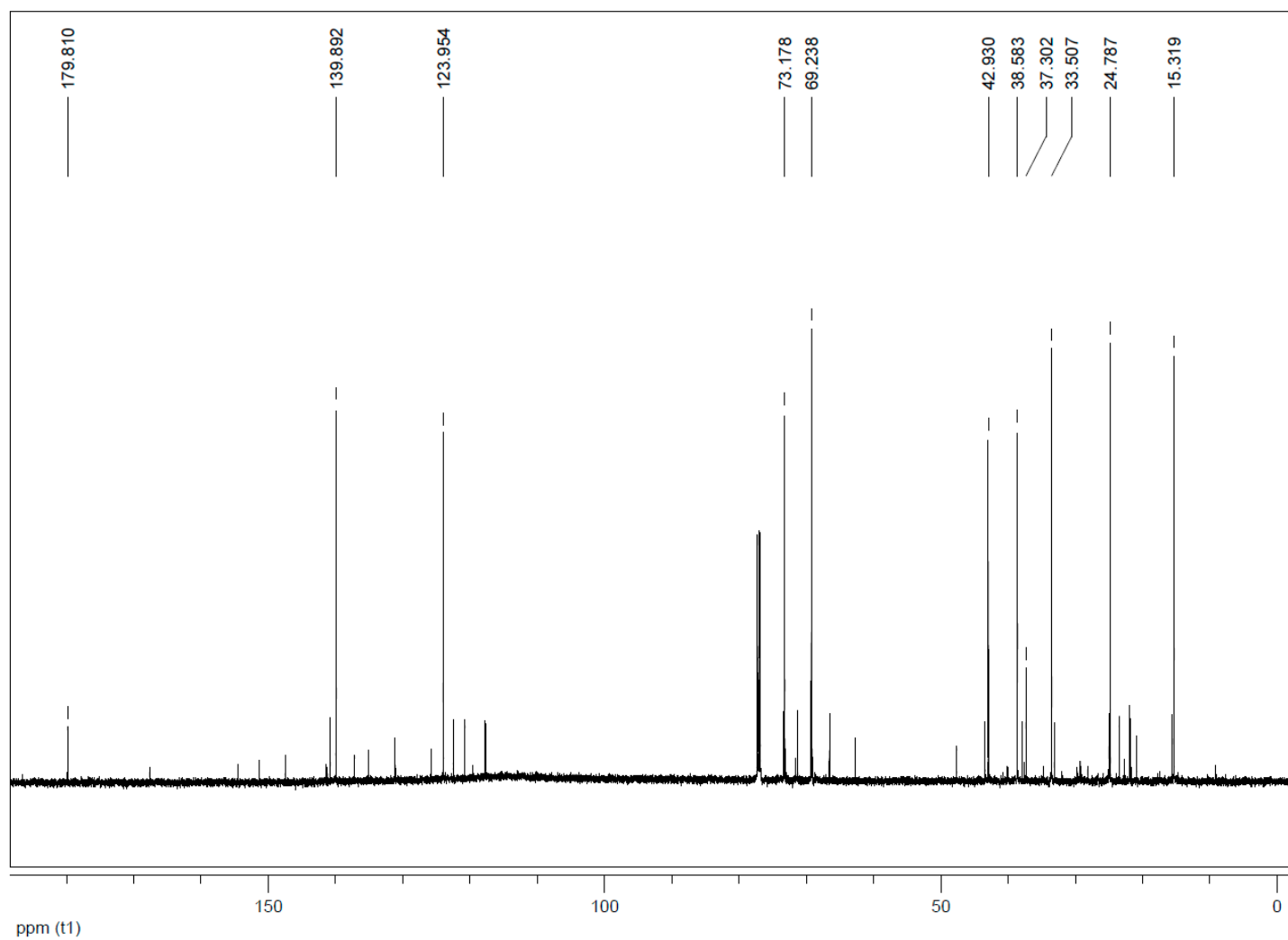


Figure S38. ^{13}C -NMR (151 MHz, CDCl_3) spectrum of hydroxylactone **8a**.

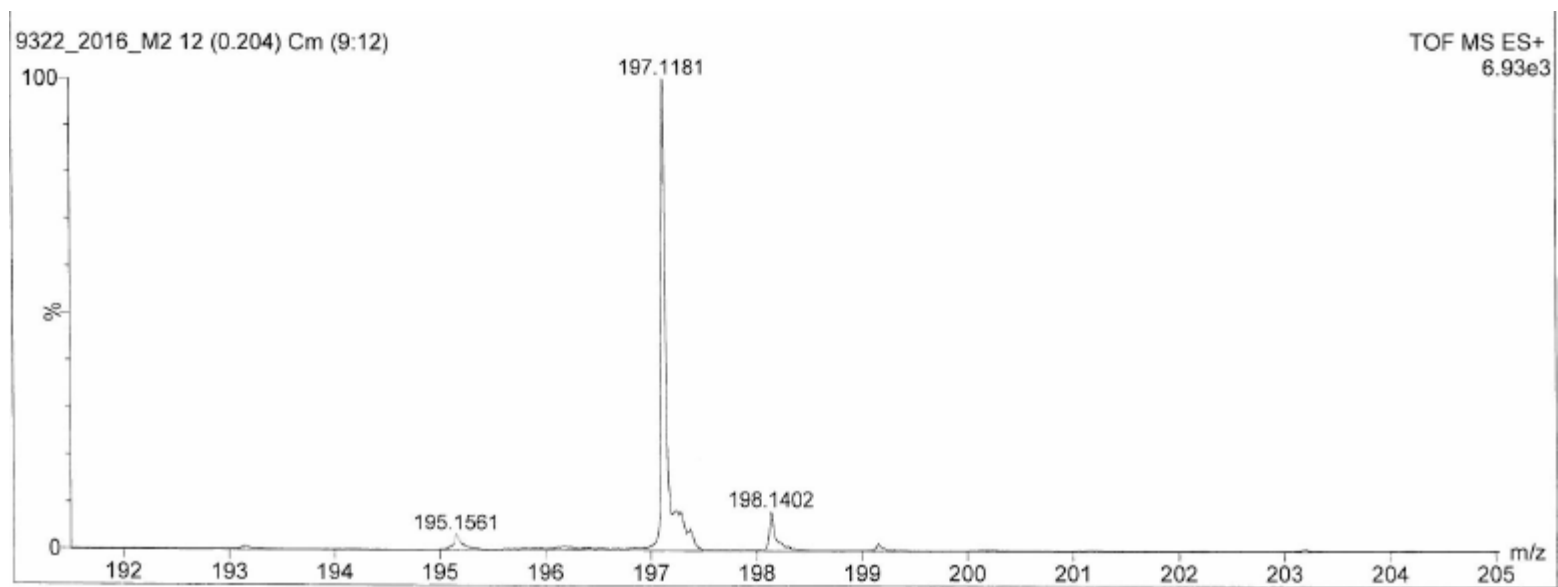


Figure S39. HRMS spectrum of hydroxylactone 8a.

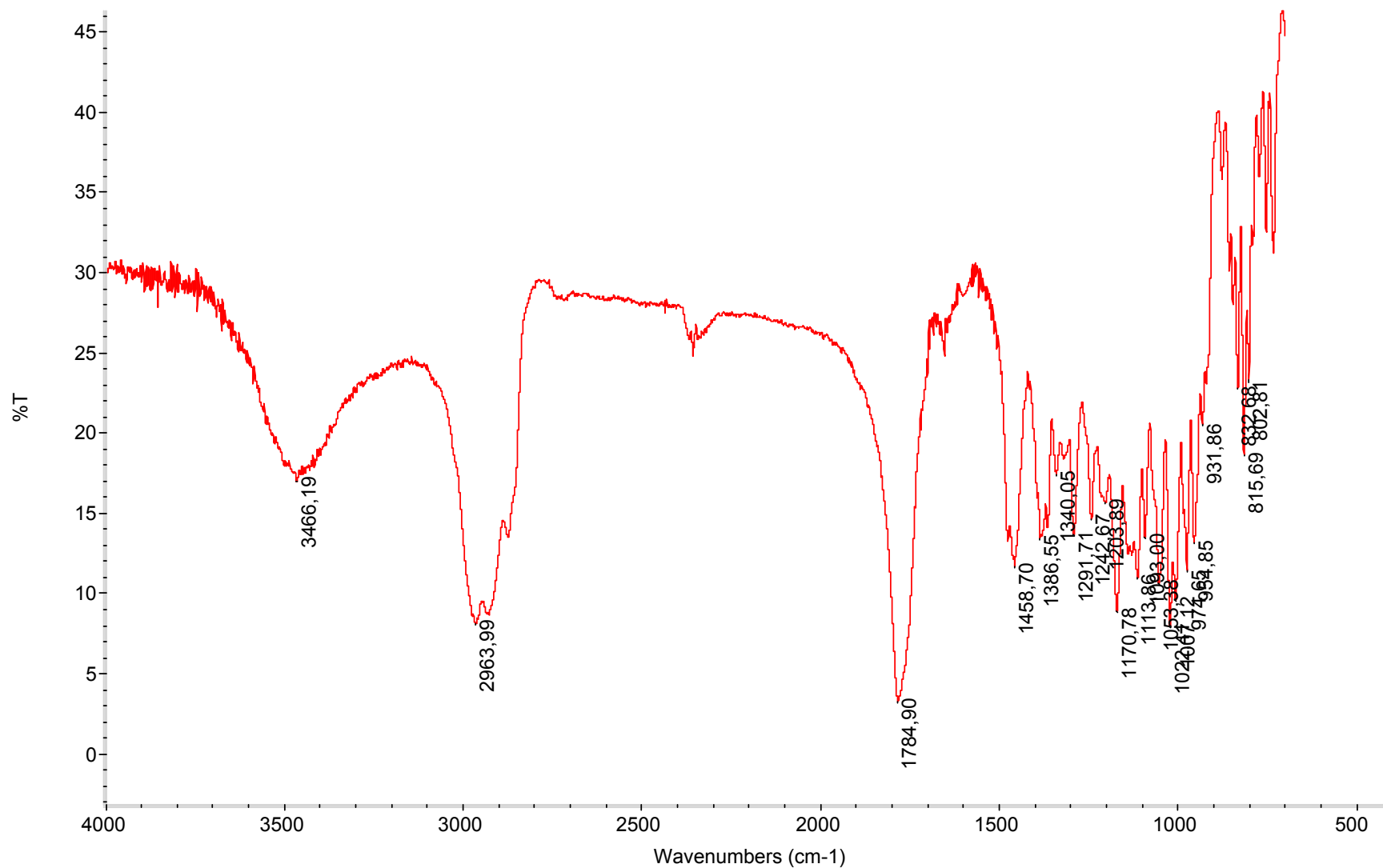


Figure S40. IR spectrum of hydroxylactone 8a.

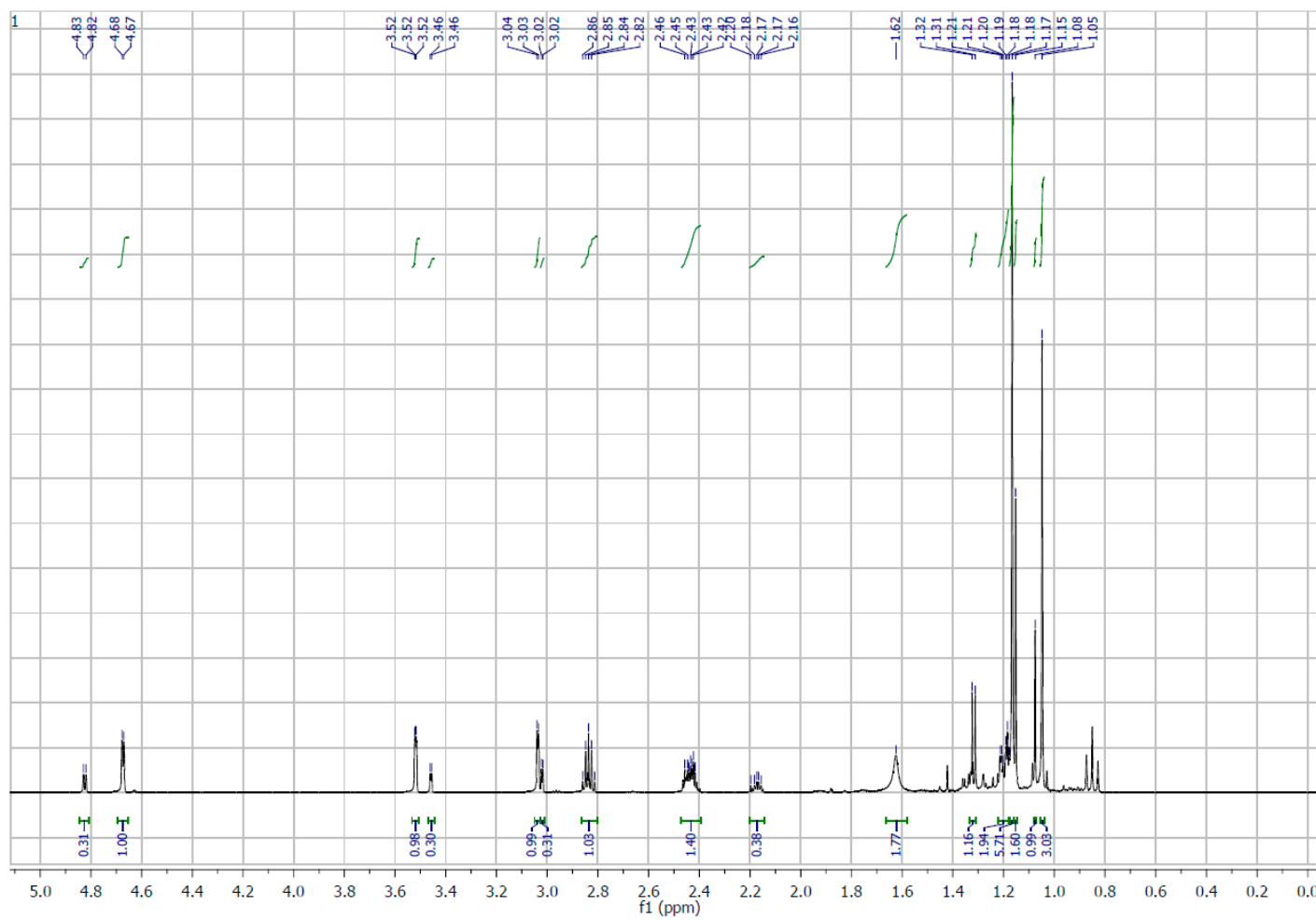


Figure S41. ¹H-NMR (600 MHz, CDCl₃) spectrum of epoxylactone **9a**.

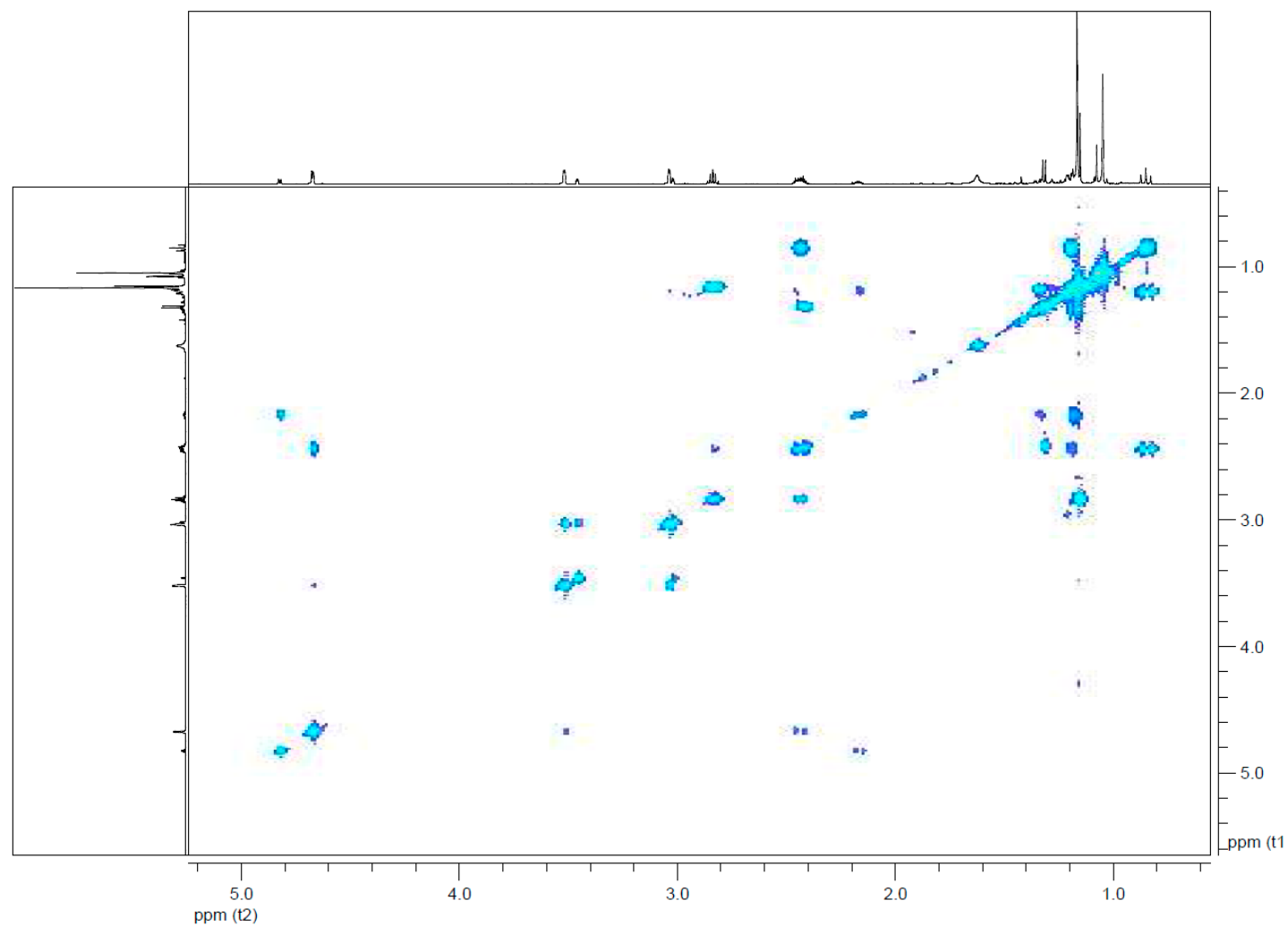


Figure S42. COSY (151 MHz, CDCl_3) spectrum of epoxylactone **9a**.

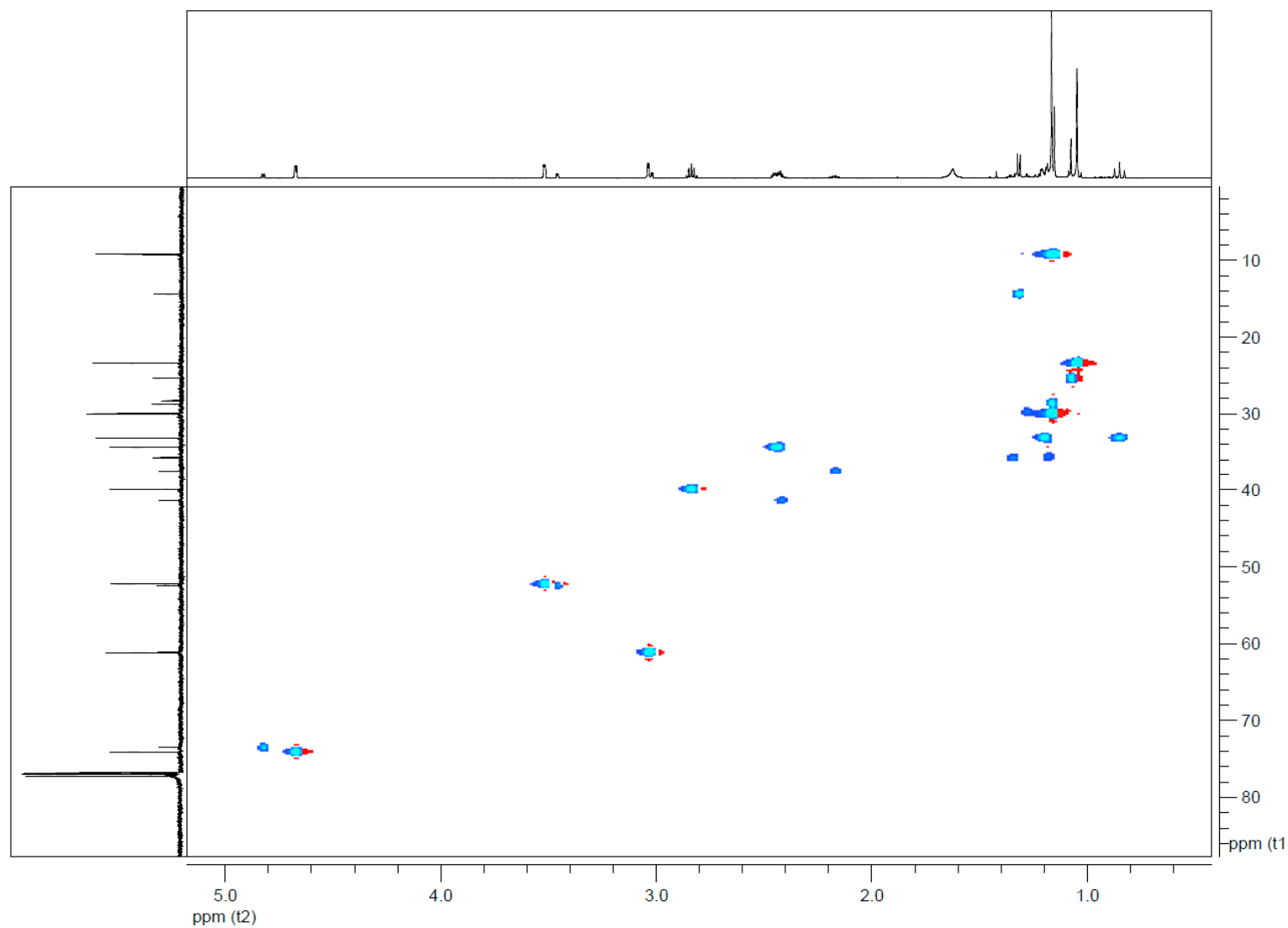


Figure S43. HMQC (151 MHz, CDCl_3) spectrum of epoxylactone 9a.

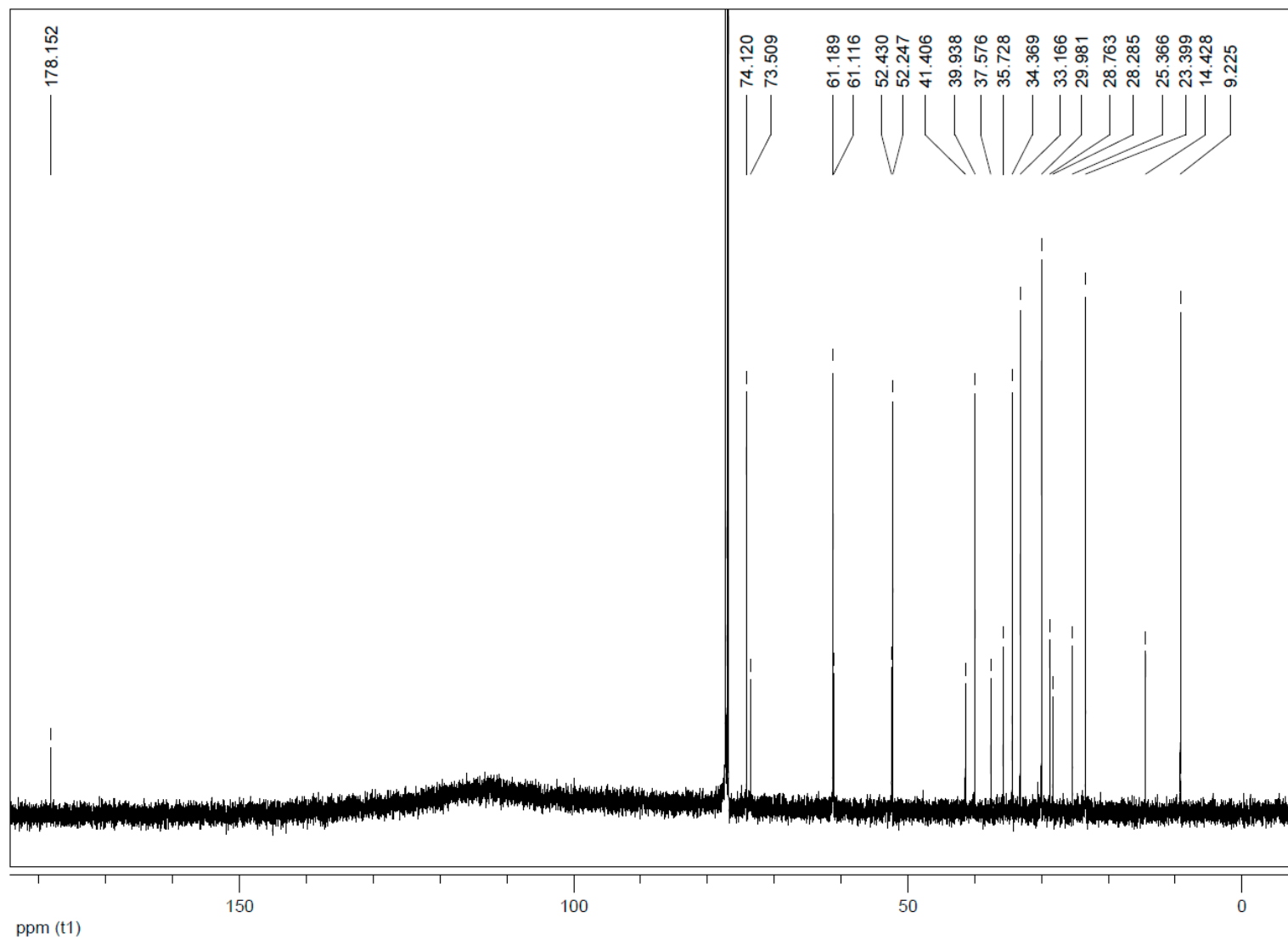


Figure S44. ¹³C-NMR (151 MHz, CDCl₃) spectrum of epoxylactone 9a.

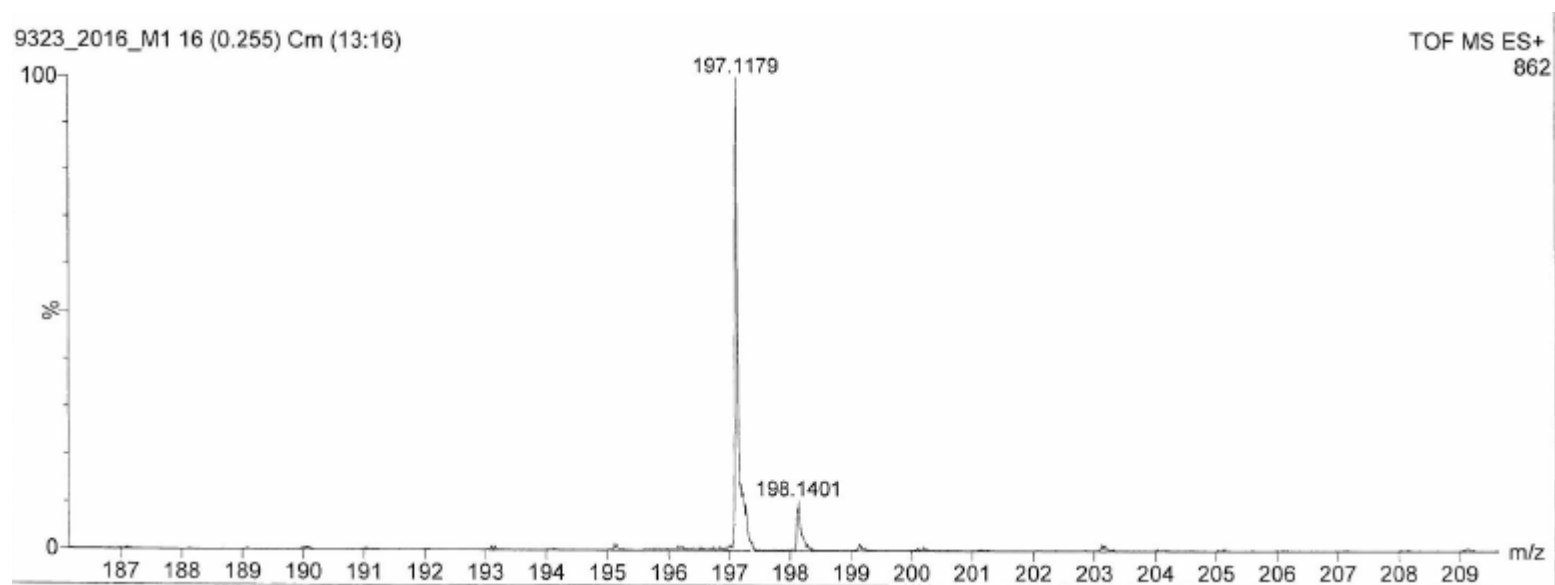


Figure S45. HRMS spectrum of epoxylactone 9a.

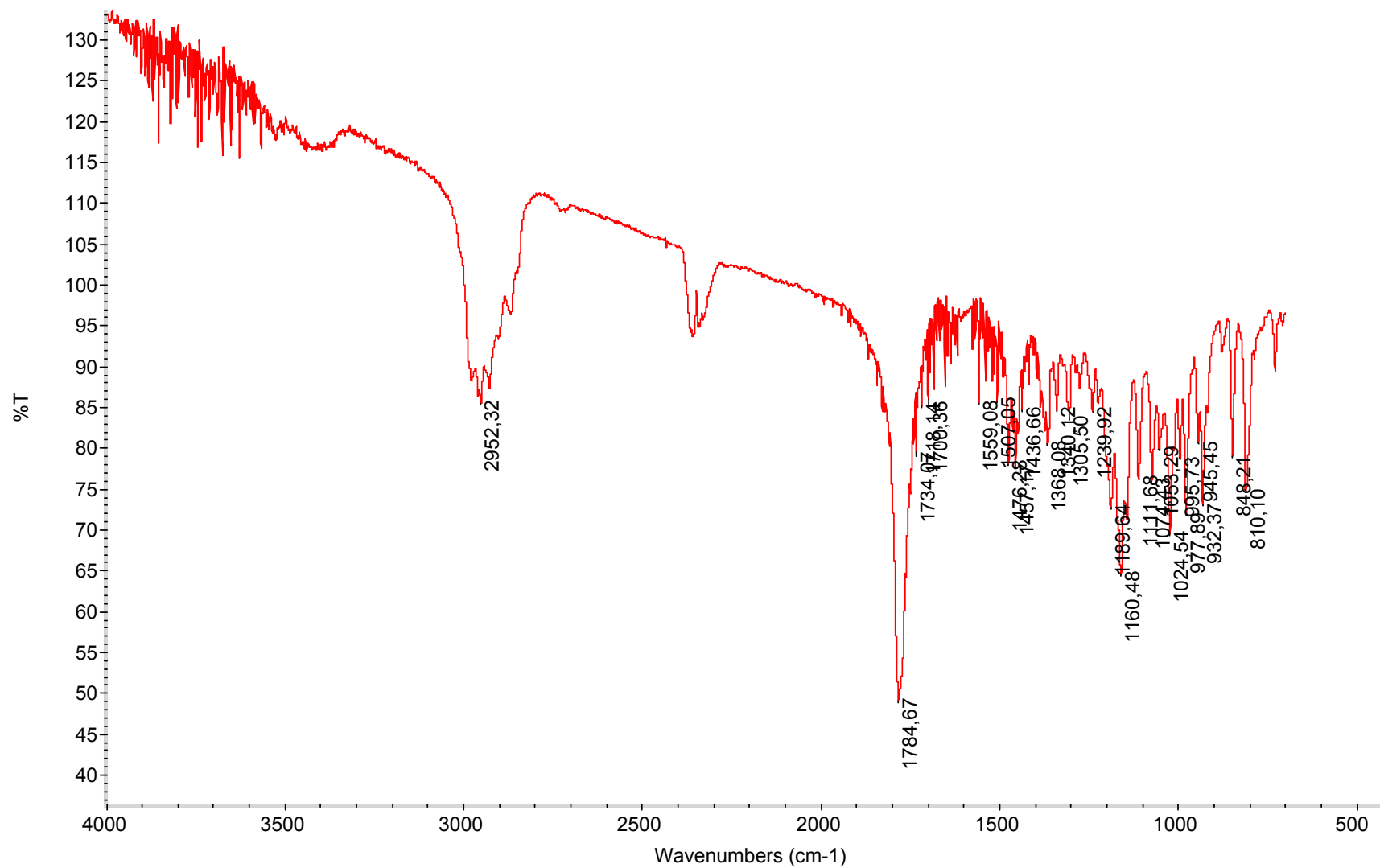
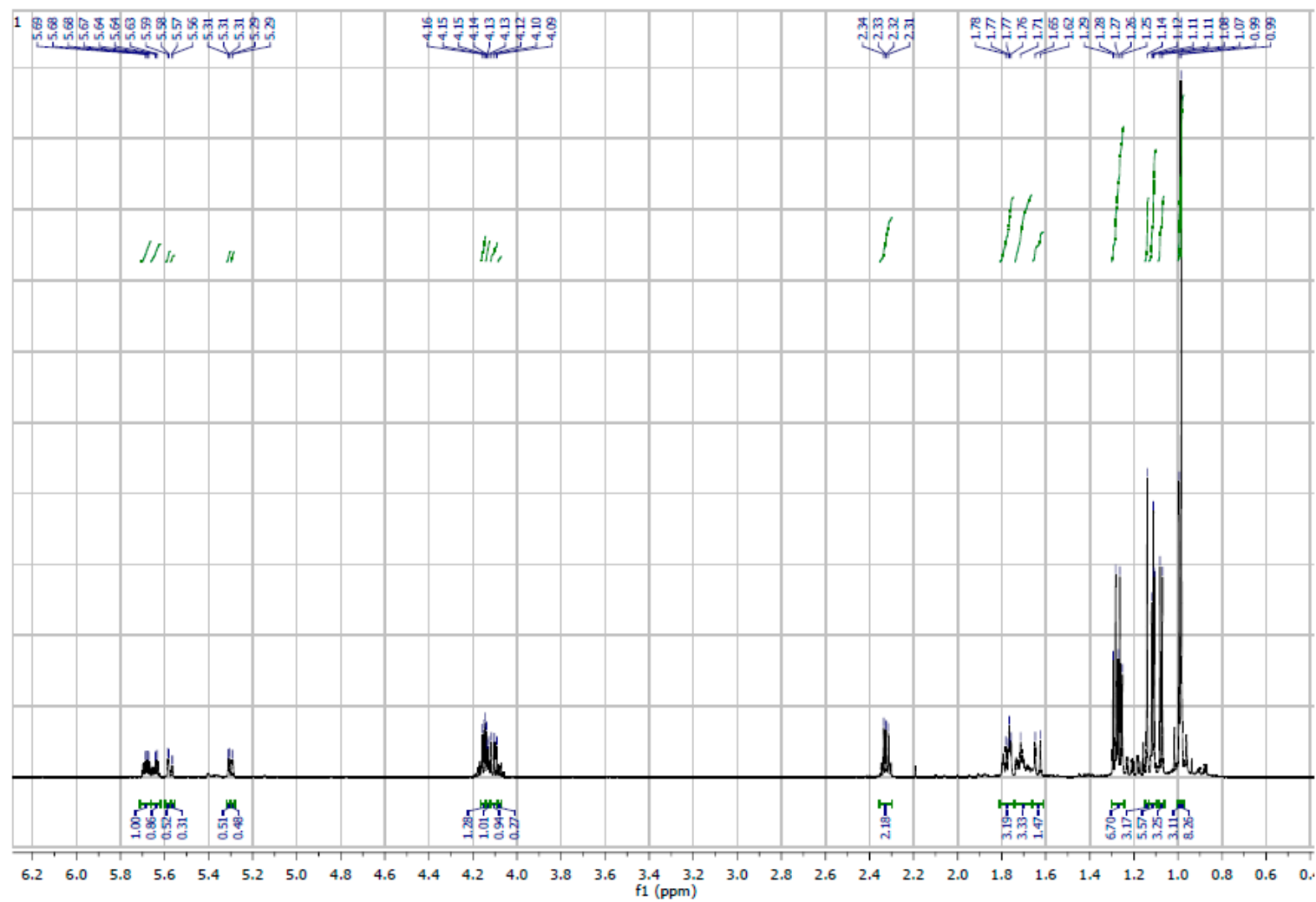


Figure S46. IR spectrum of epoxylactone 9a.

Figure S47. ¹H-NMR (600 MHz, CDCl₃) spectrum of ester **2b**.

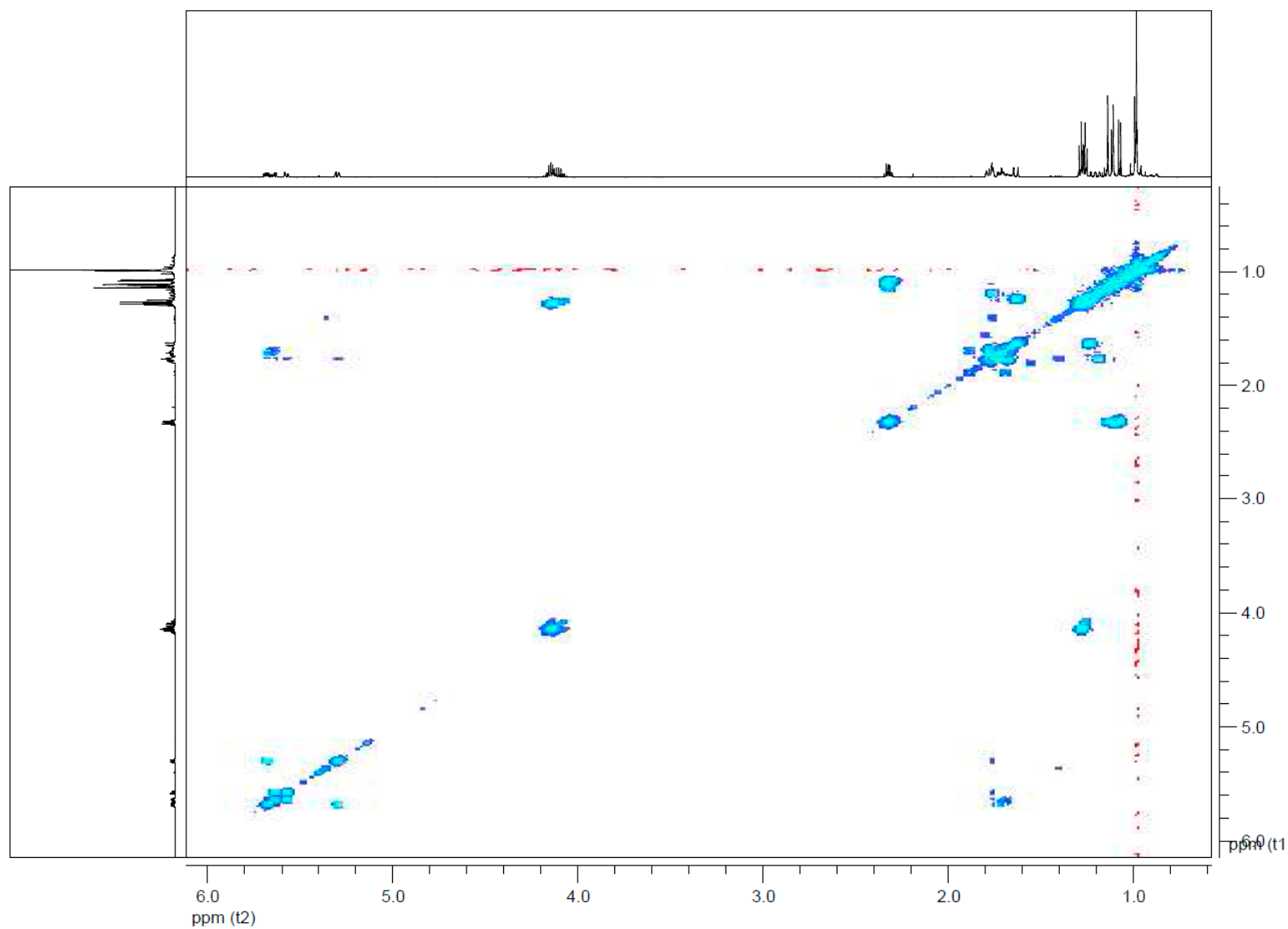


Figure S48. COSY (151 MHz, CDCl₃) spectrum of ester 2b.

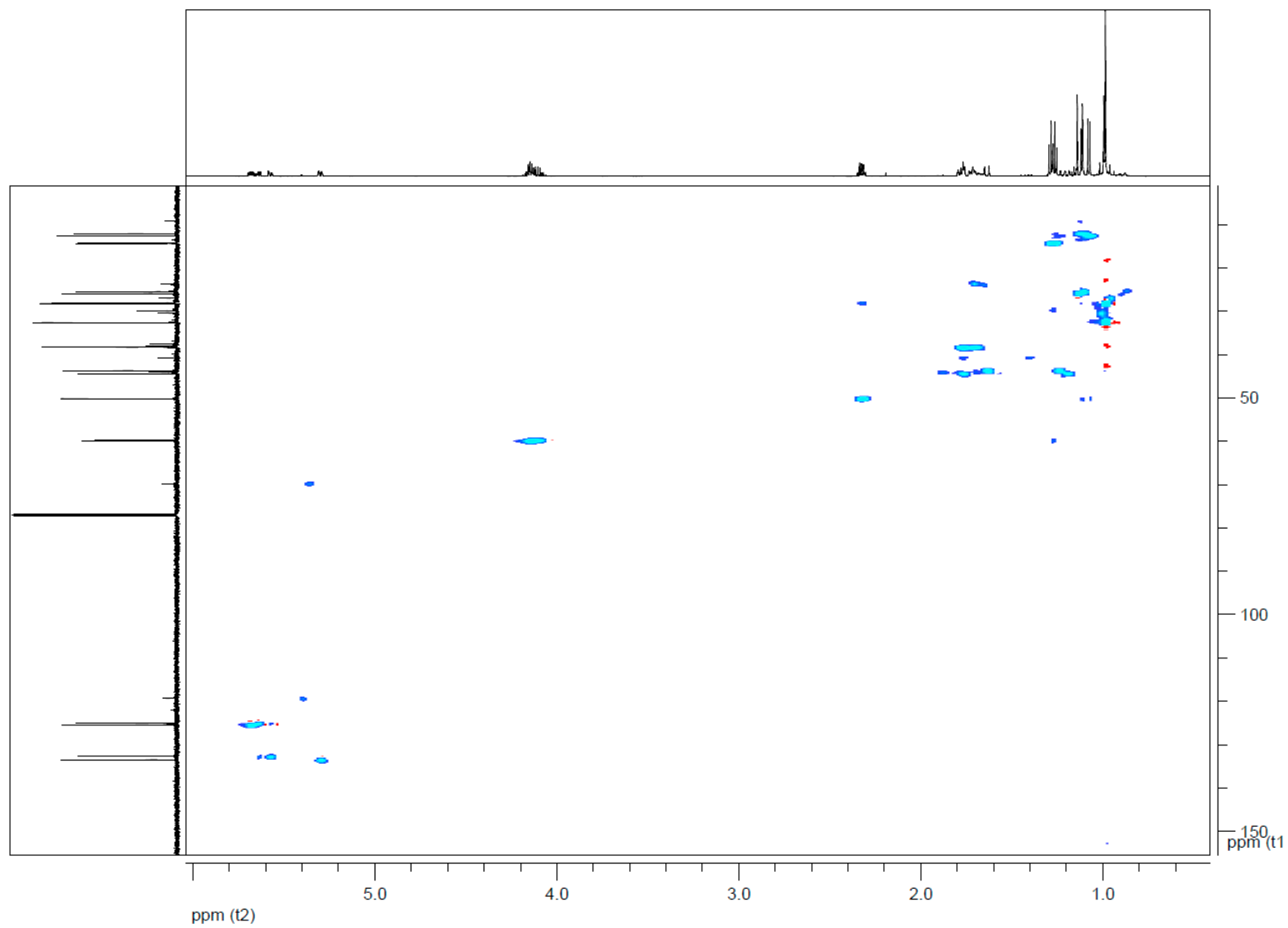


Figure S49. HMBC (151 MHz, CDCl_3) spectrum of ester **2b**.

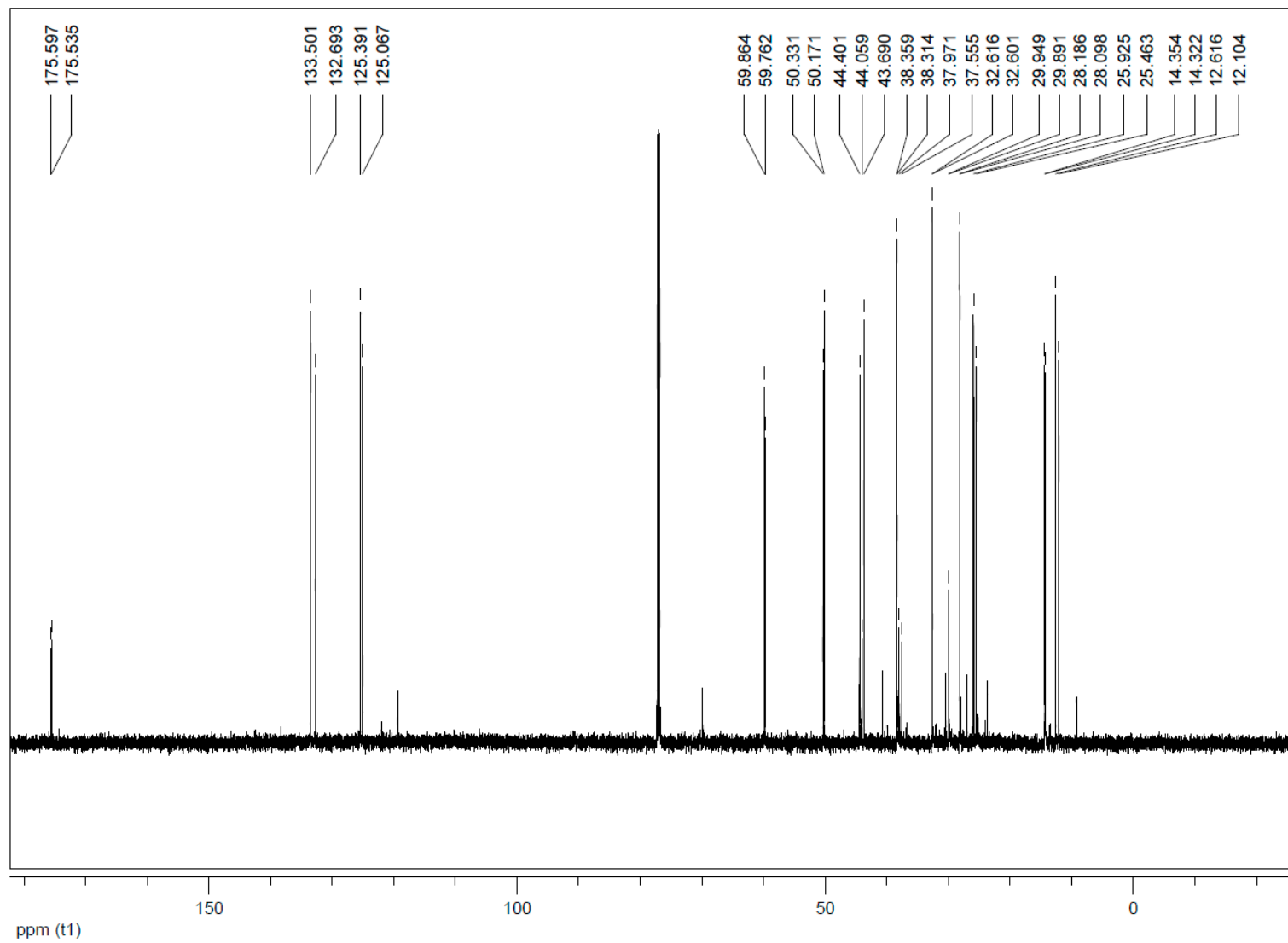


Figure S50. ¹³C-NMR (151 MHz, CDCl₃) spectrum of ester **2b**.

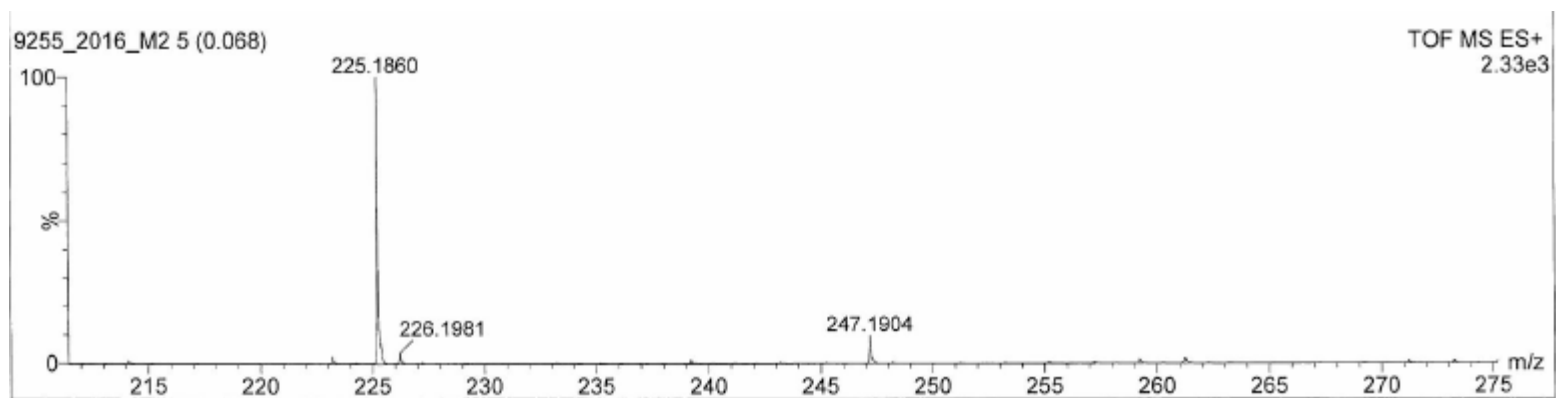


Figure S51. HRMS spectrum of ester **2b**.

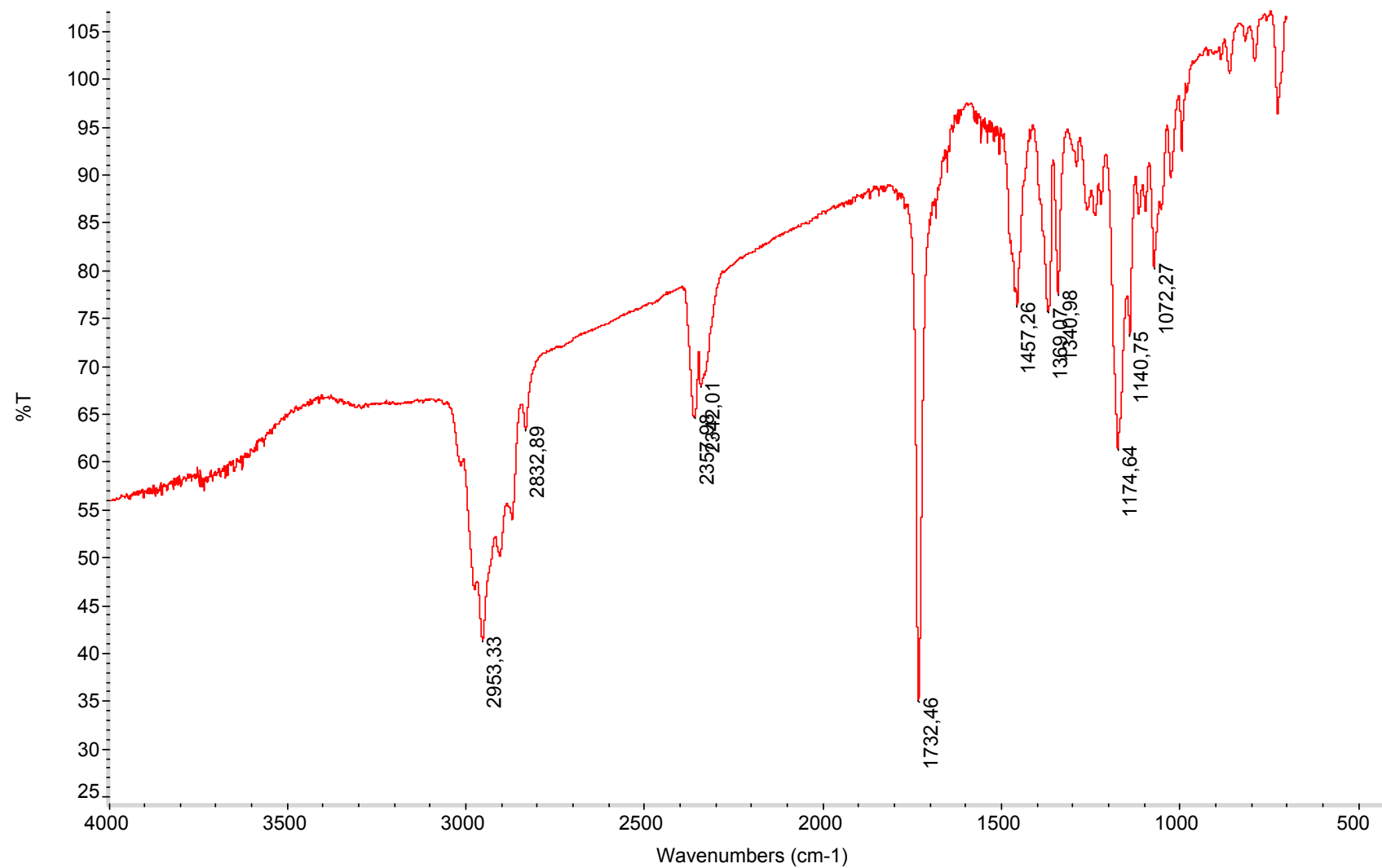


Figure S52. IR spectrum of ester **2b**.

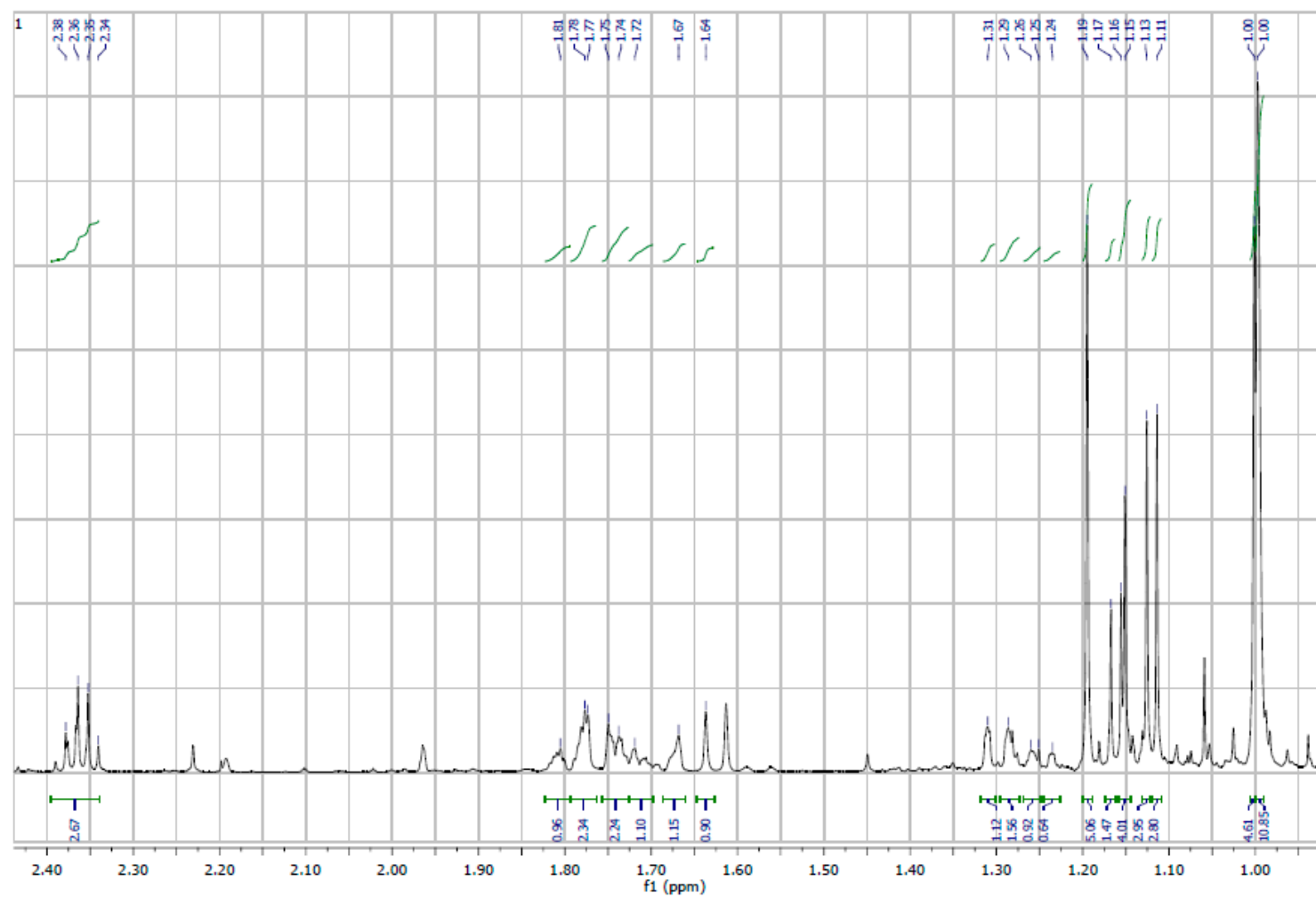


Figure S53. ^1H -NMR (600 MHz, CDCl_3) spectrum of acid **3b**.

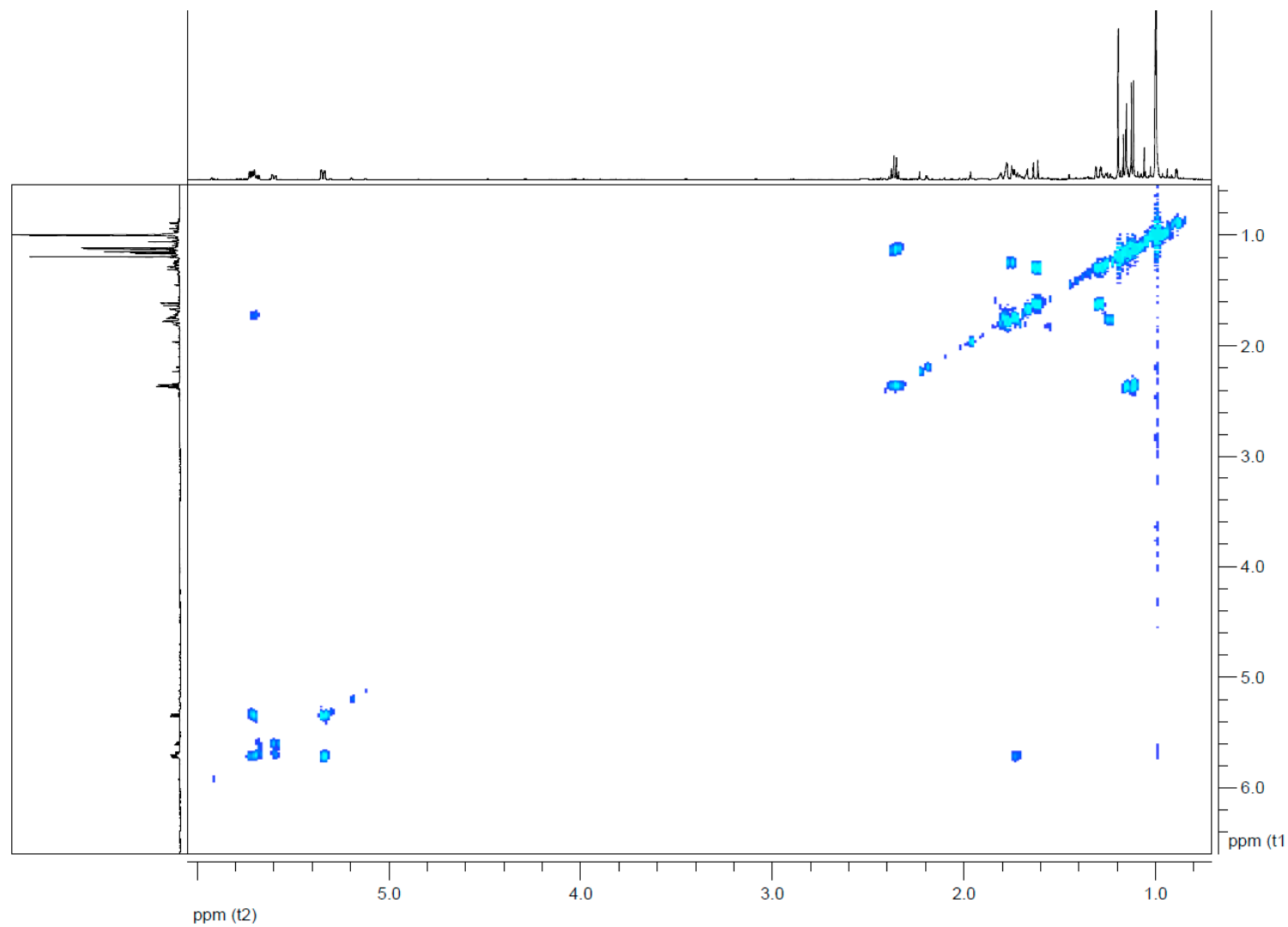


Figure S54. COSY (151 MHz, CDCl₃) spectrum of acid **3b**.

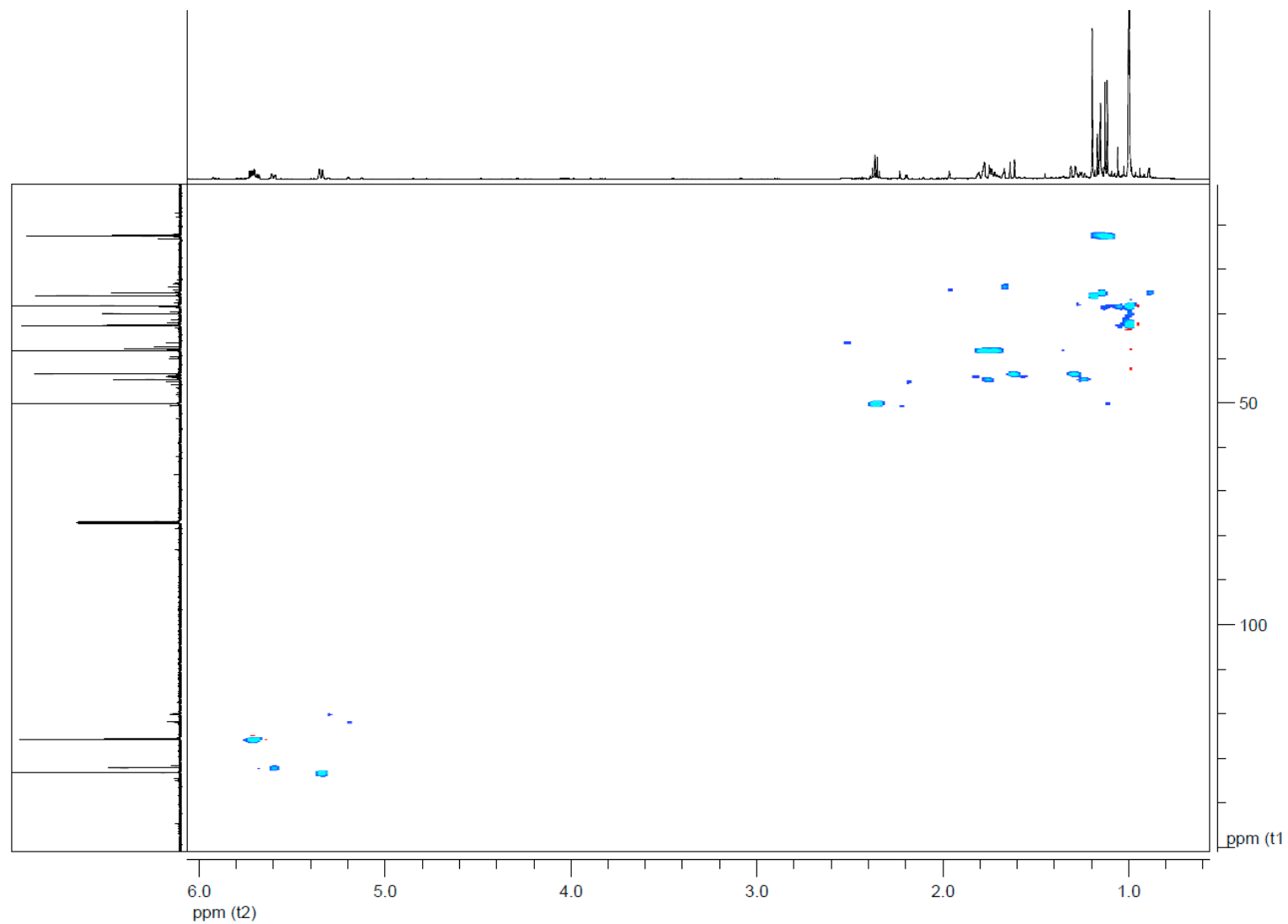


Figure S55. HMPC (151 MHz, CDCl₃) spectrum of acid 3b.

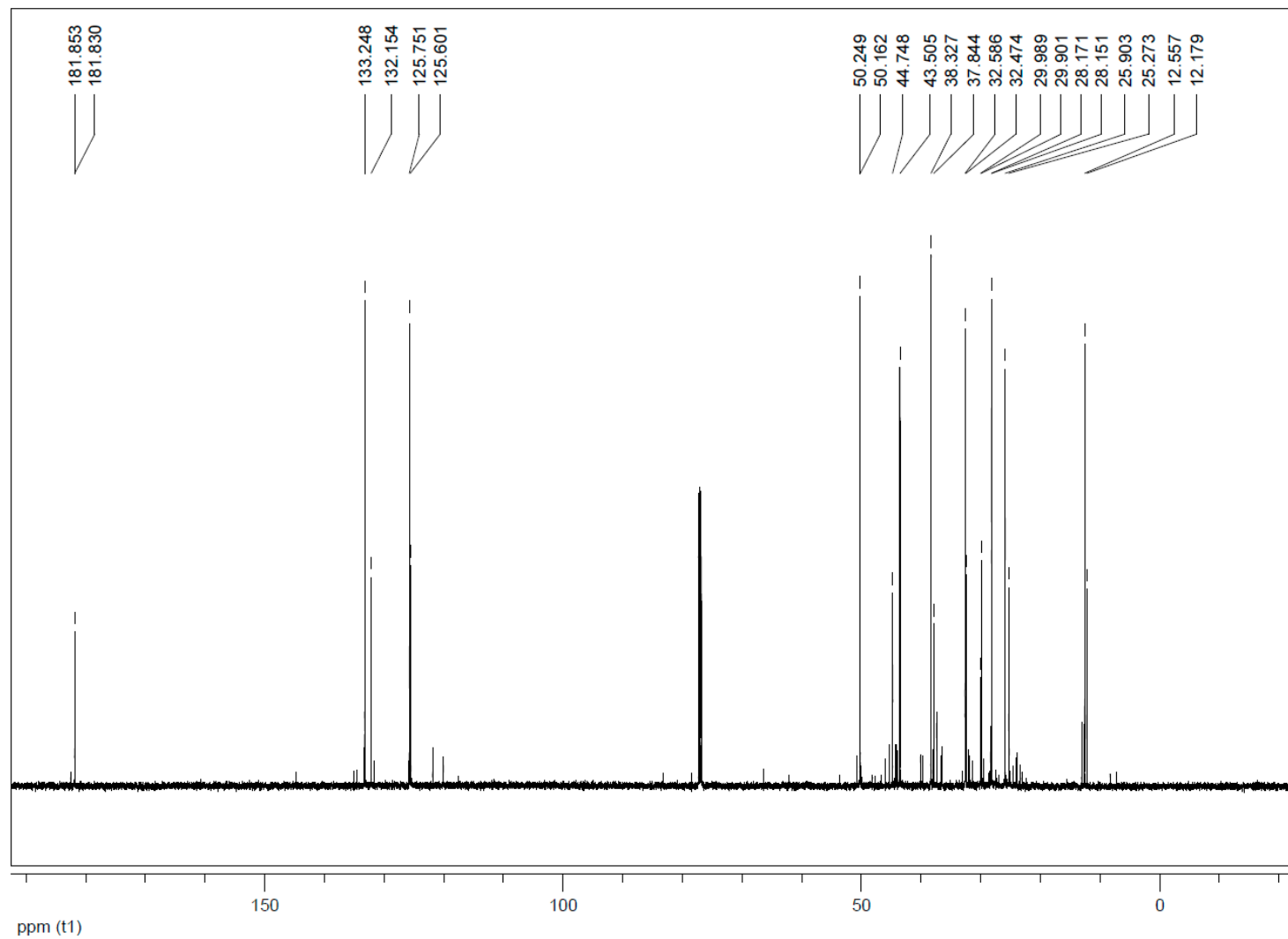


Figure S56. ¹³C-NMR (151 MHz, CDCl₃) spectrum of acid **3b**.

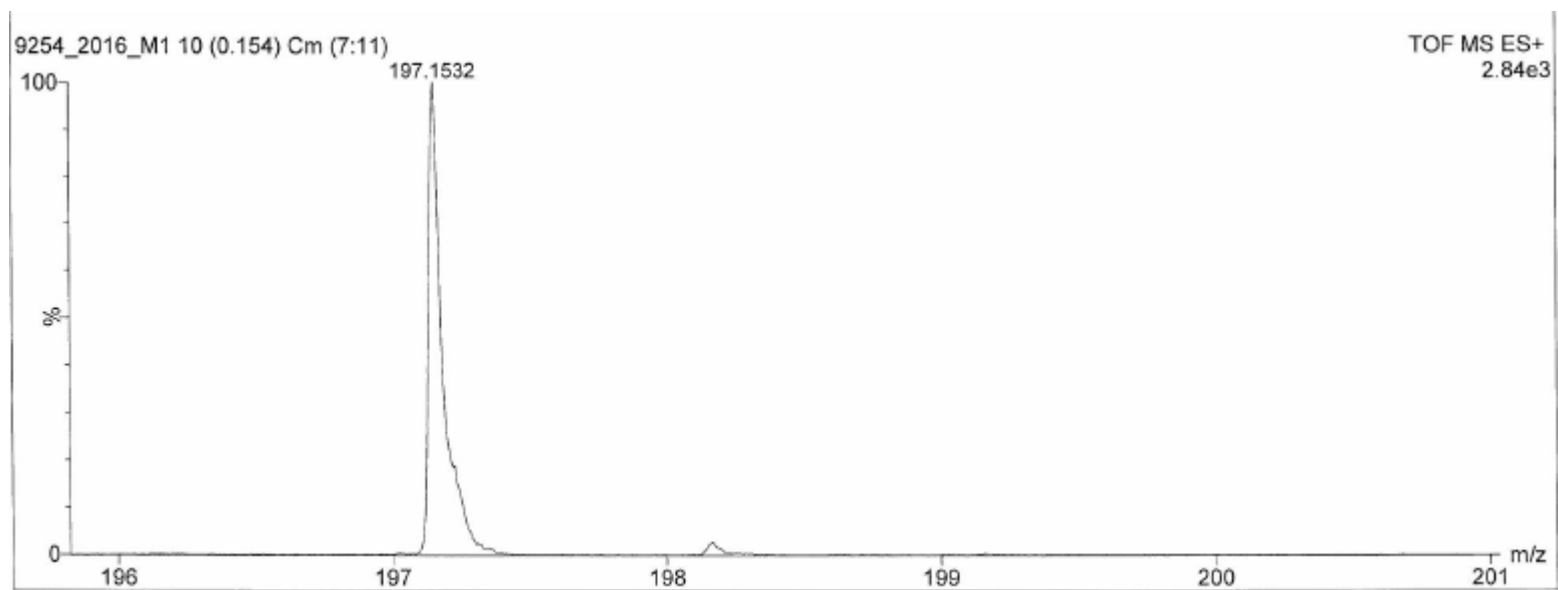


Figure S57. HRMS spectrum of acid 3b.

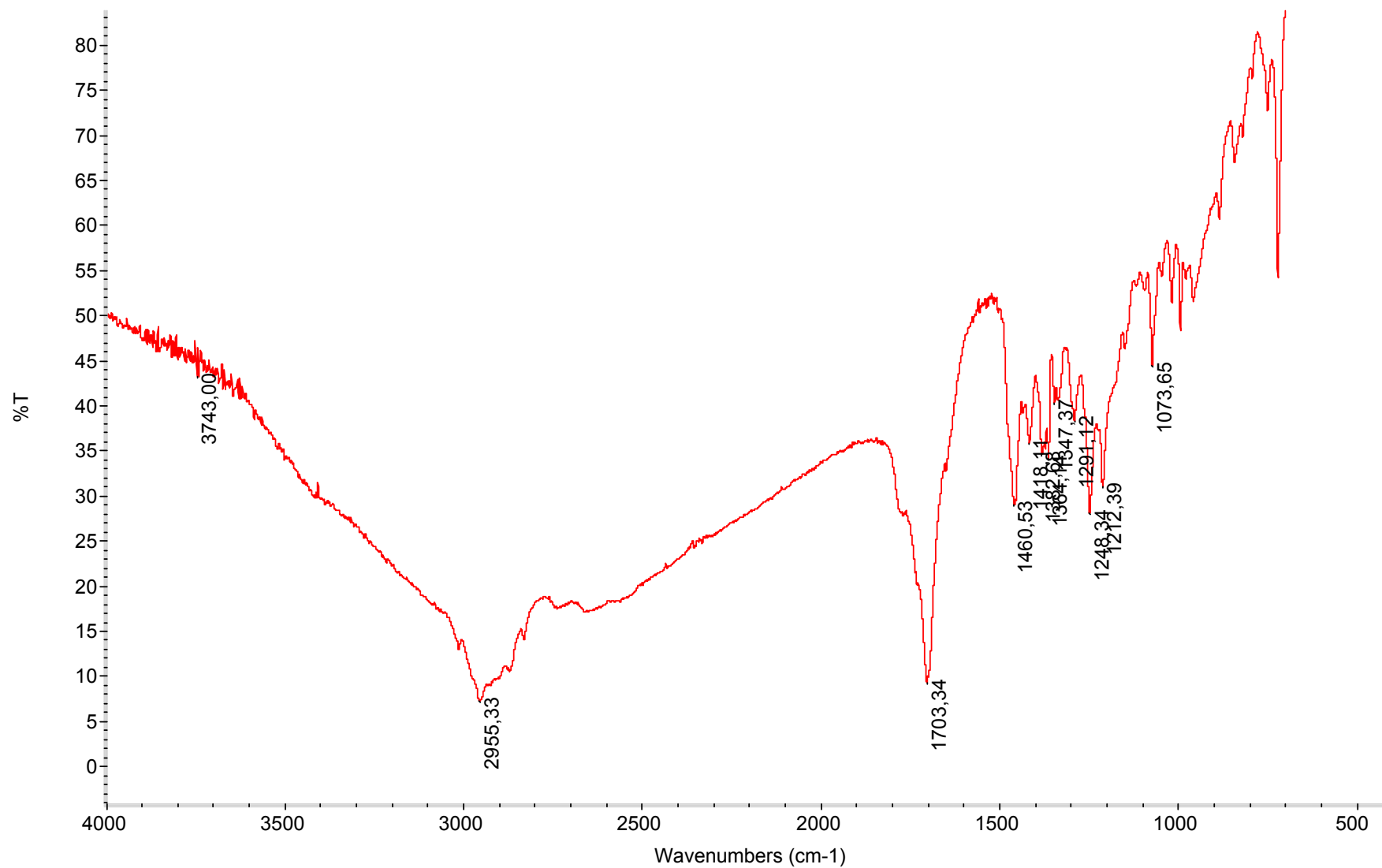


Figure S58. IR spectrum of acid 3b.

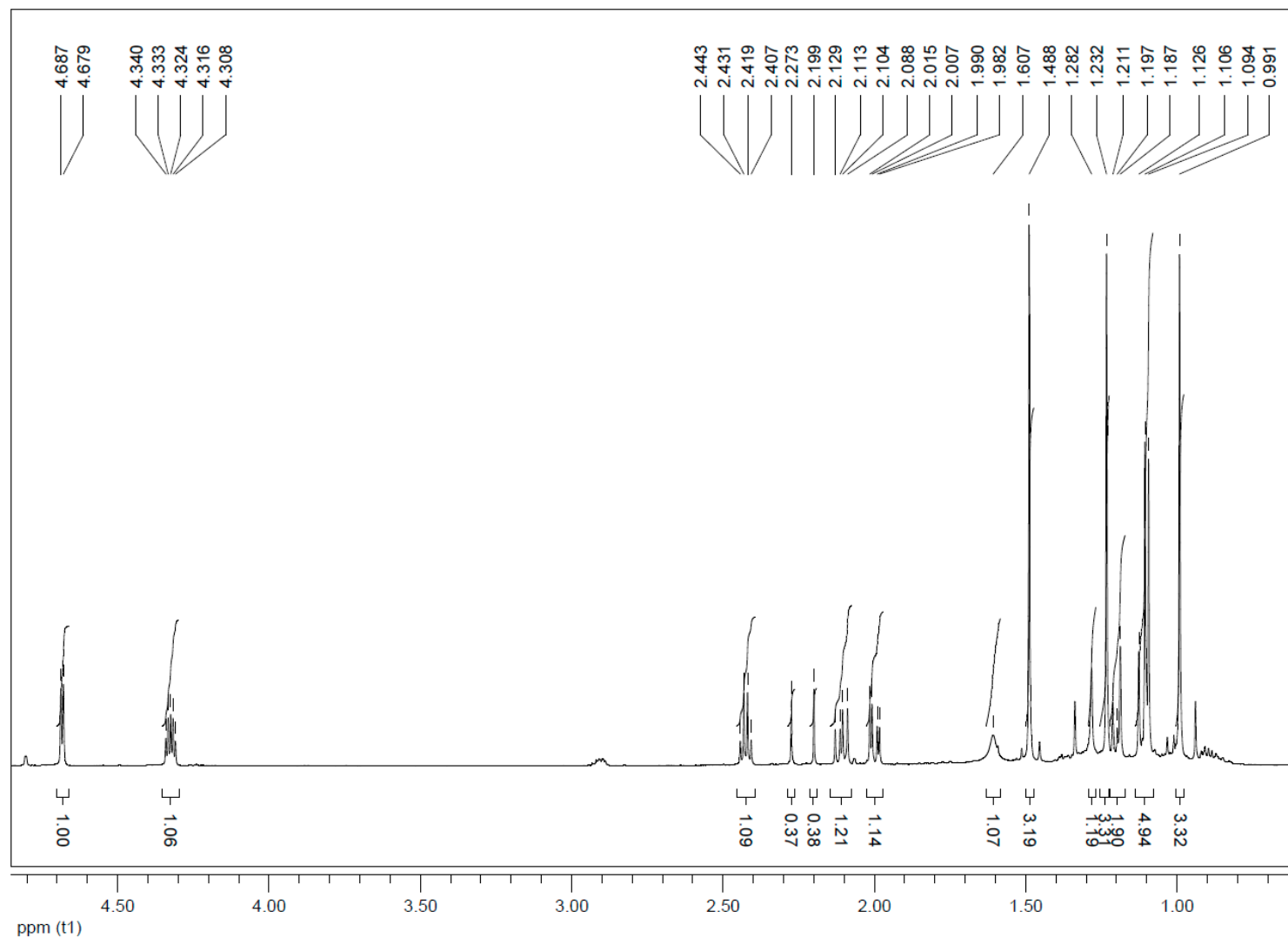


Figure S59. ¹H-NMR (600 MHz, CDCl₃) spectrum of iodolactone **4b-A**.

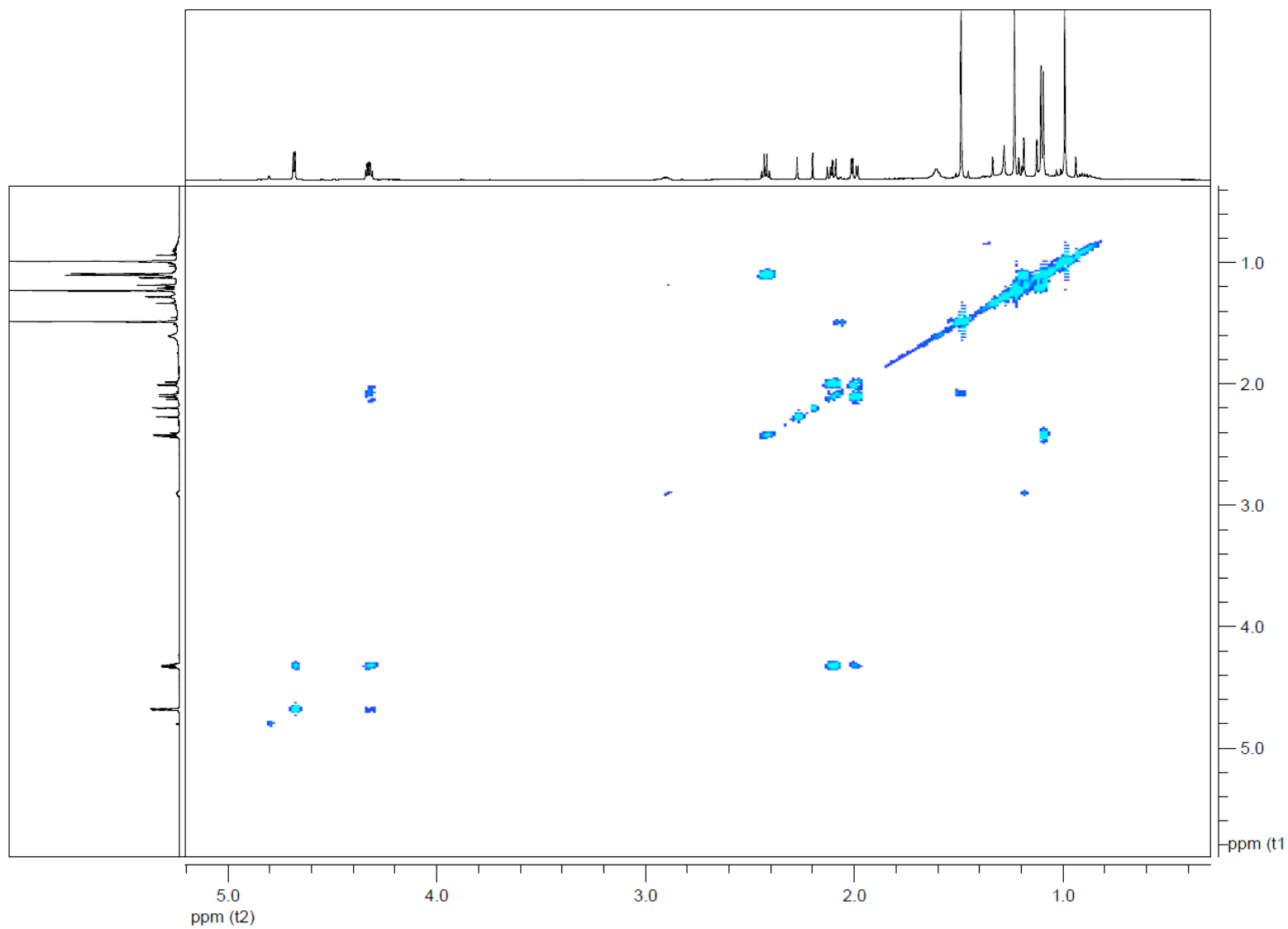


Figure S60. COSY (151 MHz, CDCl₃) spectrum of iodolactone **4b-A**.

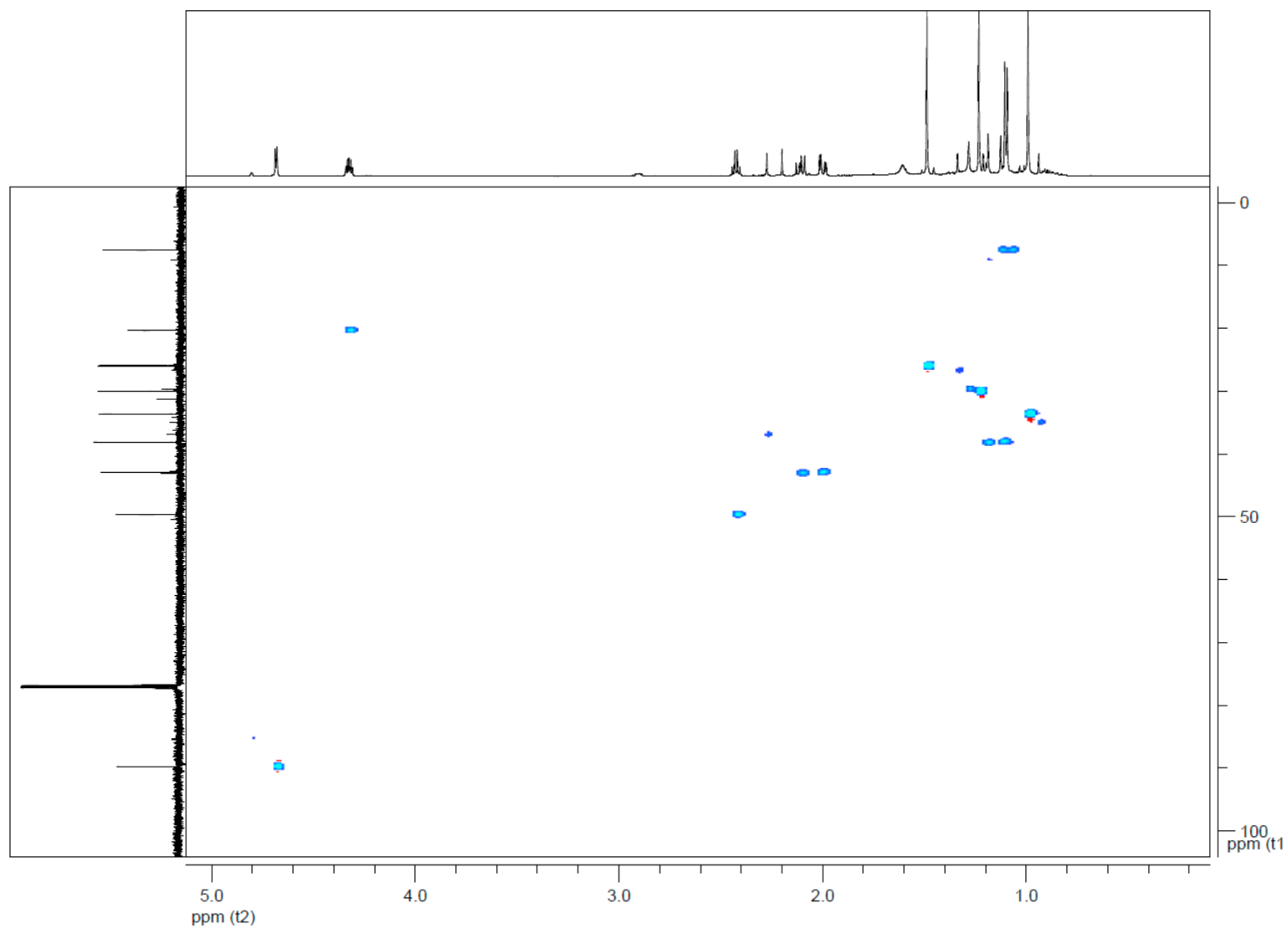


Figure S61. HMQC (151 MHz, CDCl₃) spectrum of iodolactone 4b-A.

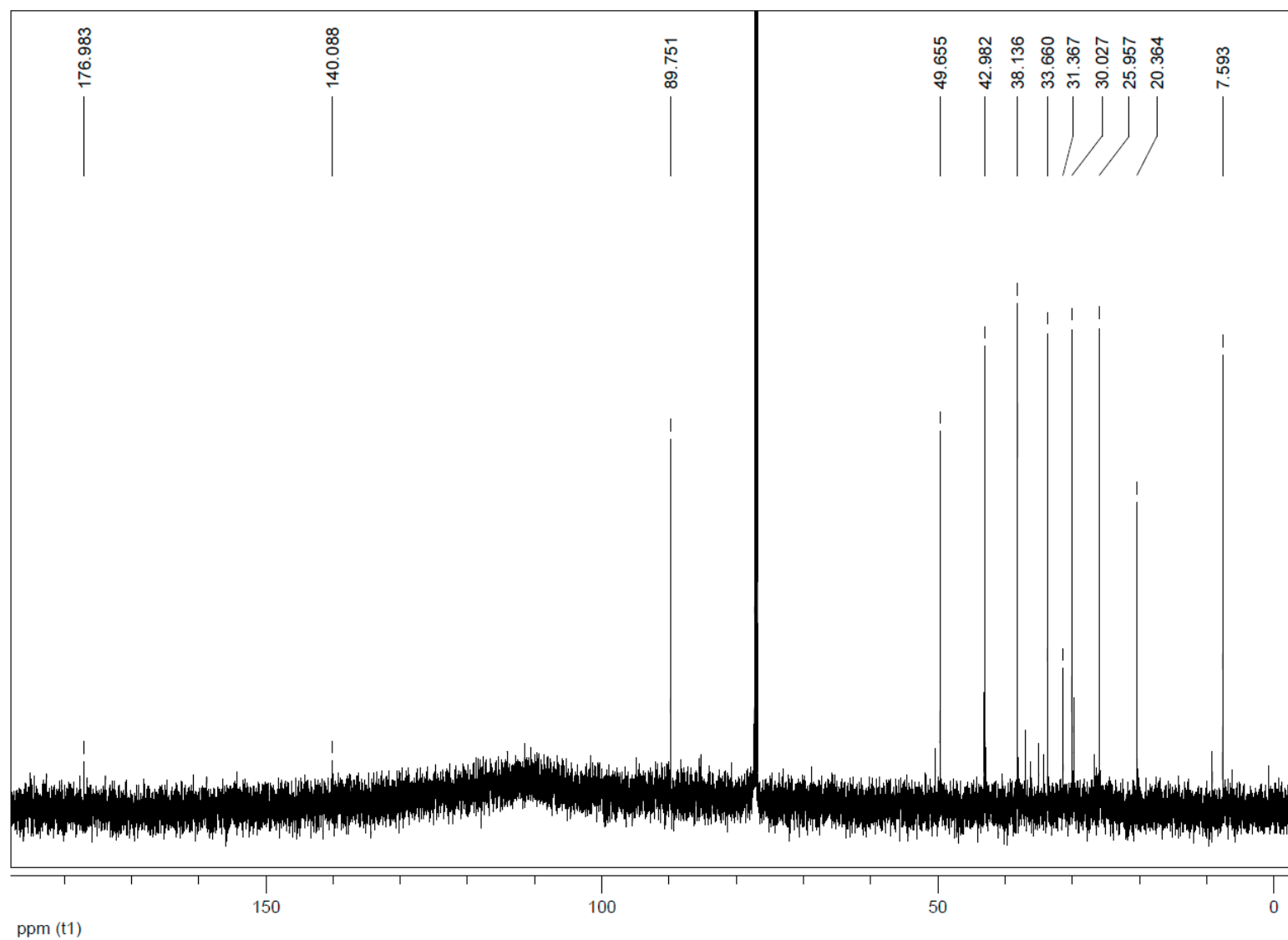


Figure S62. ^{13}C -NMR (151 MHz, CDCl_3) spectrum of iodolactone **4b-A**.

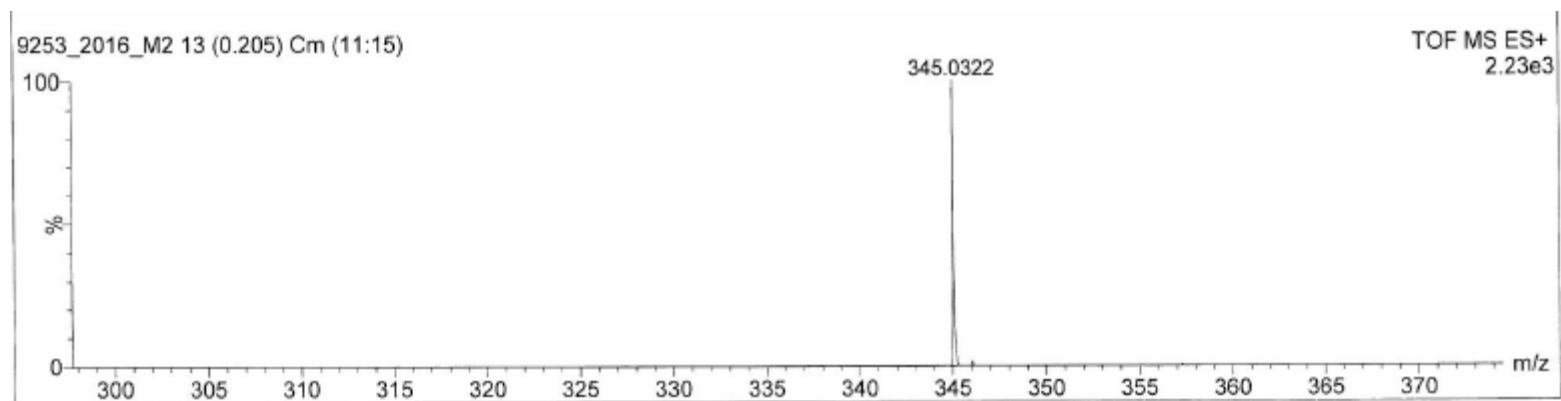


Figure S63. HRMS spectrum of iodolactone **4b-A**.

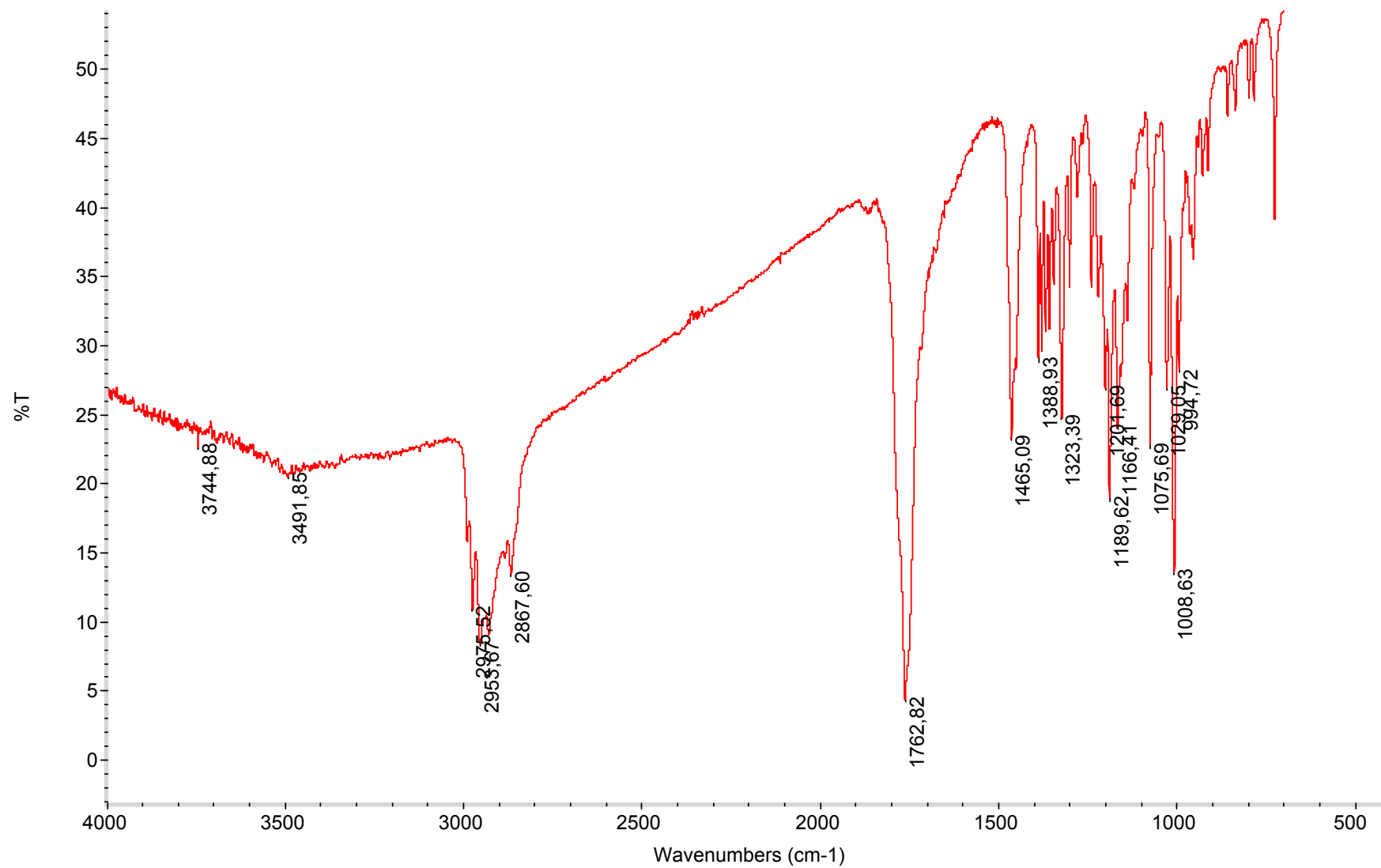


Figure S64. IR spectrum of iodolactone 4b-A.

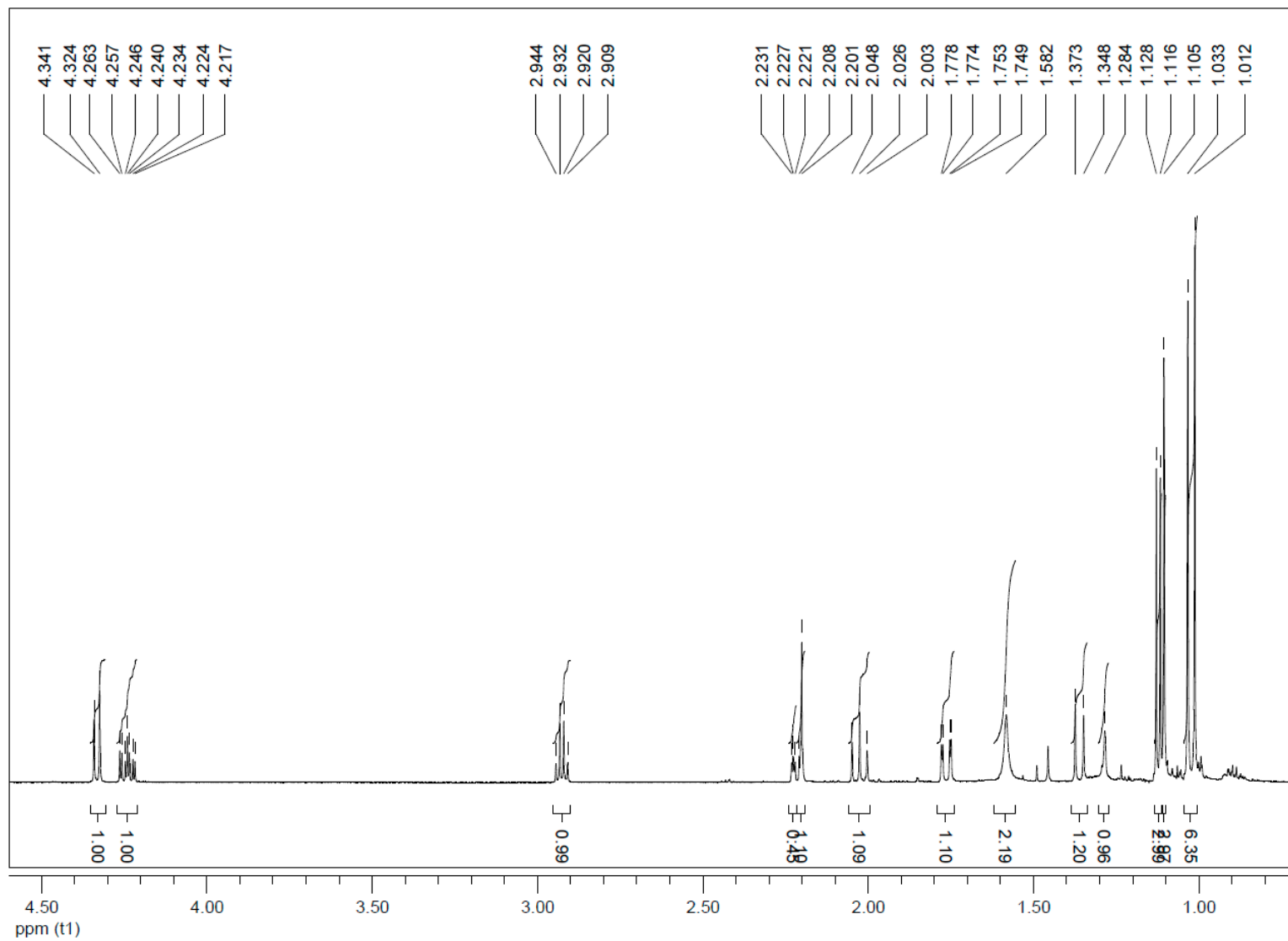


Figure S65. ¹H-NMR (600 MHz, CDCl₃) spectrum of iodolactone **4b-B**.

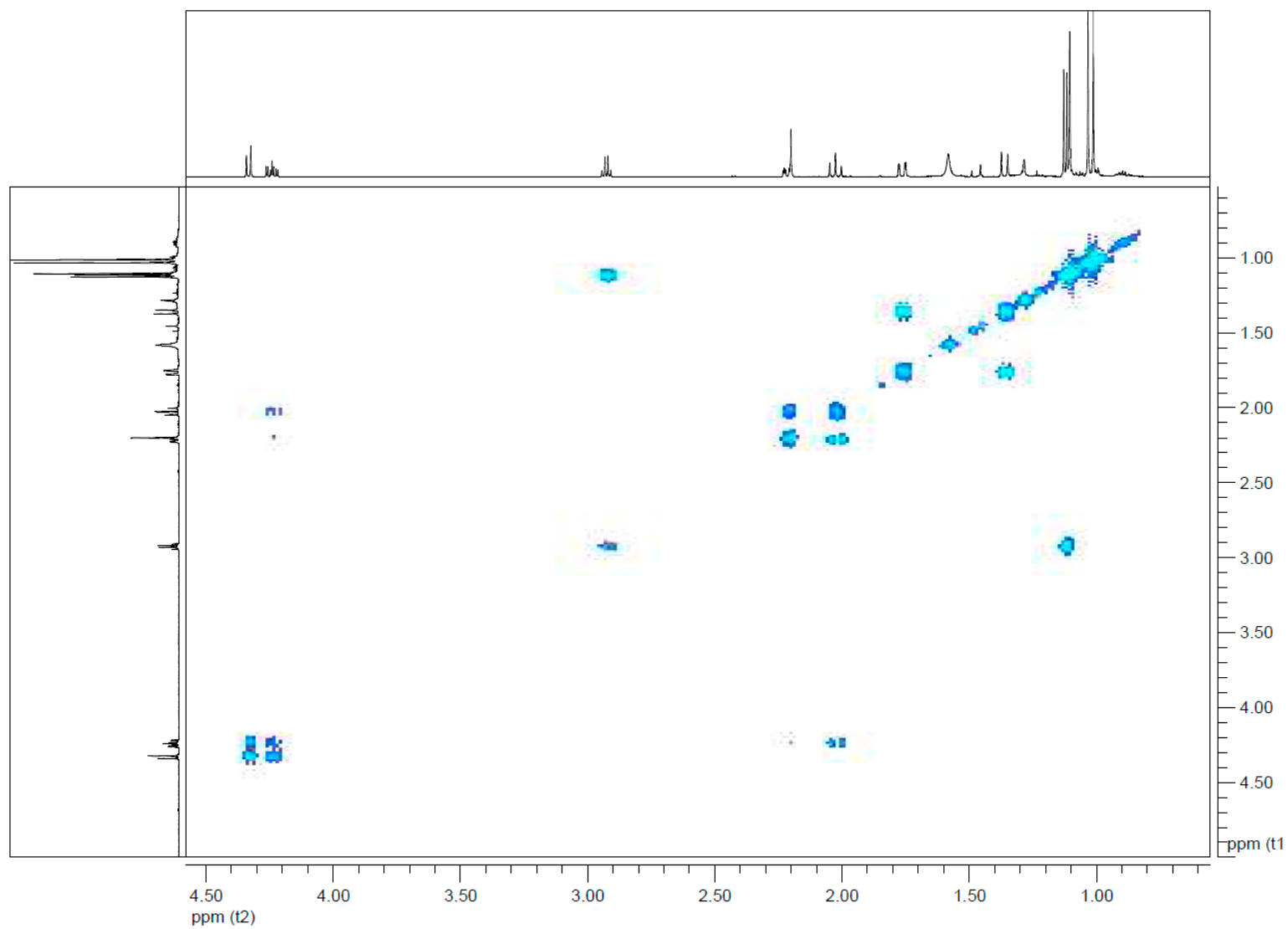


Figure S66. COSY (151 MHz, CDCl_3) spectrum of iodolactone **4b-B**.

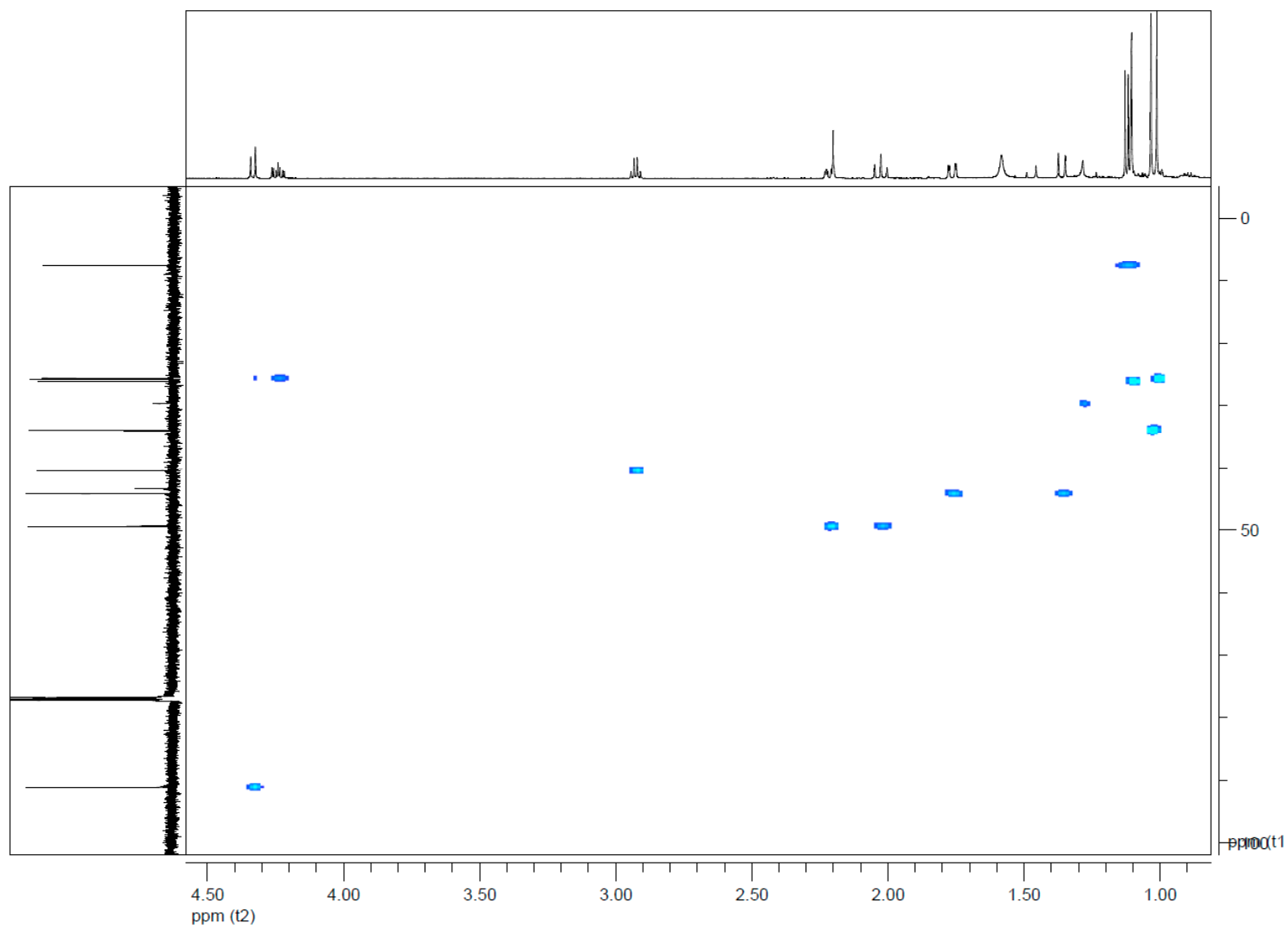


Figure S67. HMBC (151 MHz, CDCl₃) spectrum of iodolactone **4b-B**.

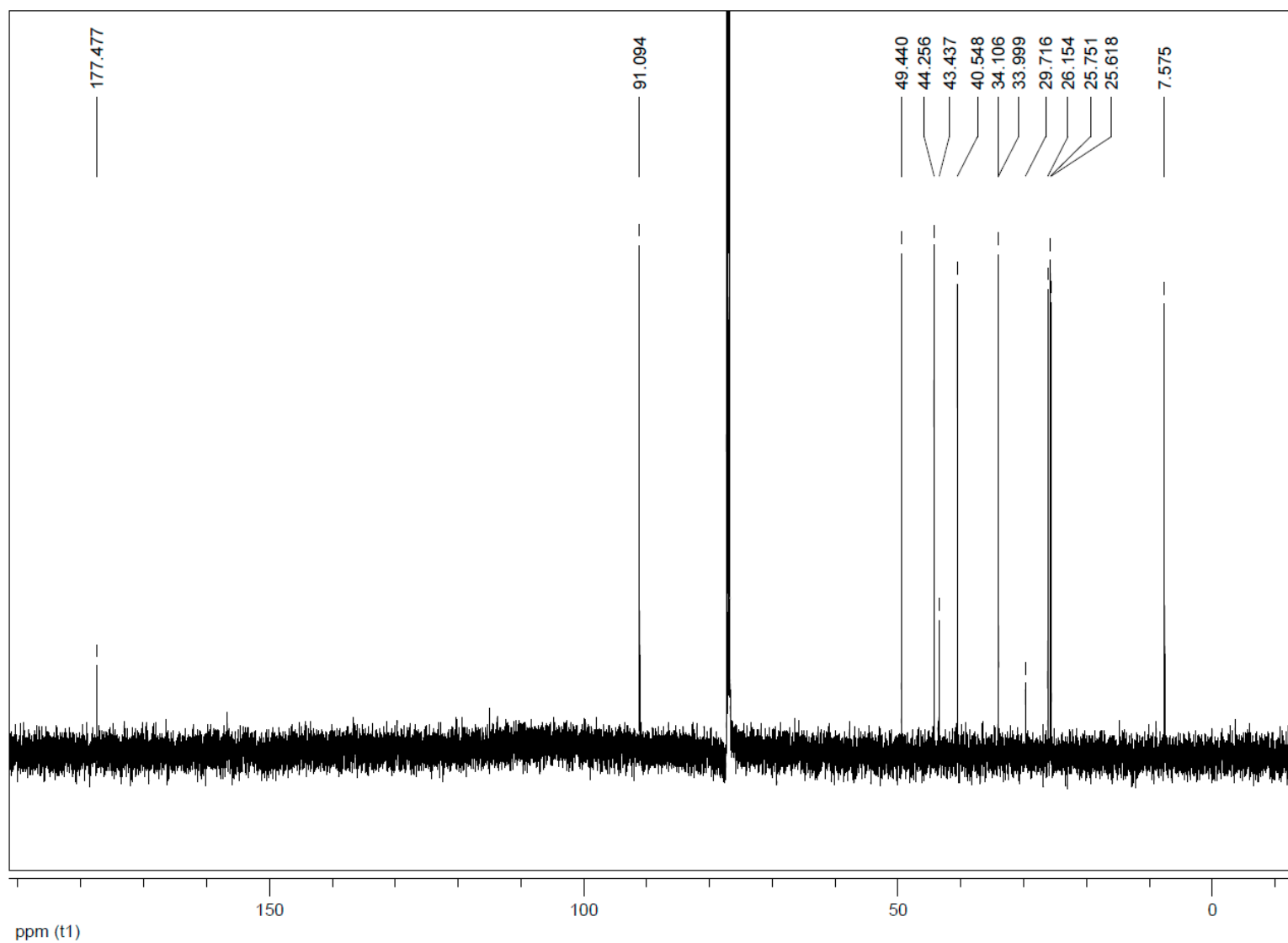


Figure S68. ^{13}C -NMR (151 MHz, CDCl_3) spectrum of iodolactone **4b-B**.

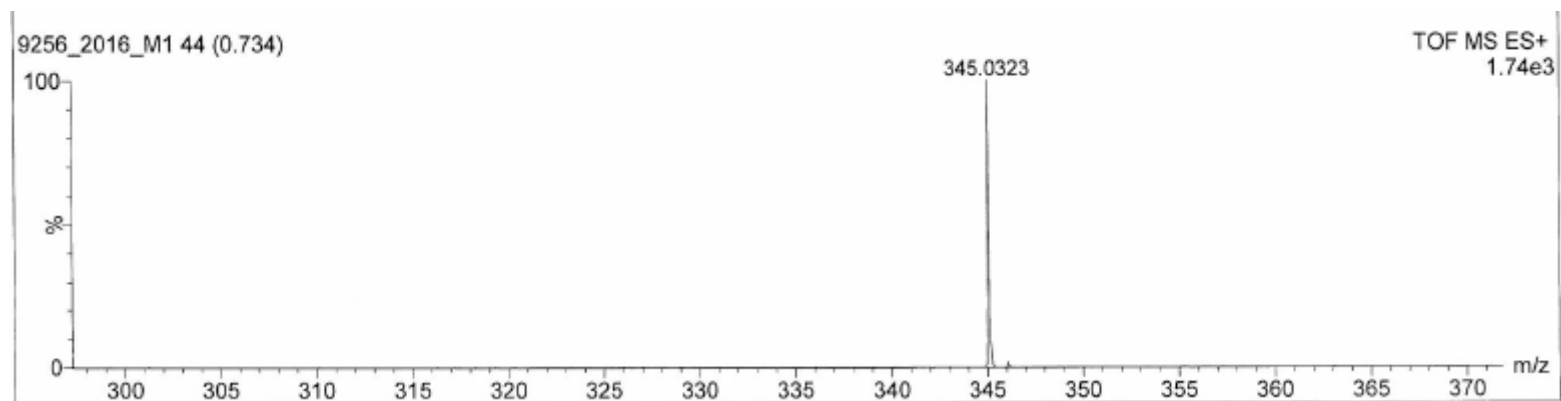


Figure S69. HRMS spectrum of iodolactone **4b-B**.

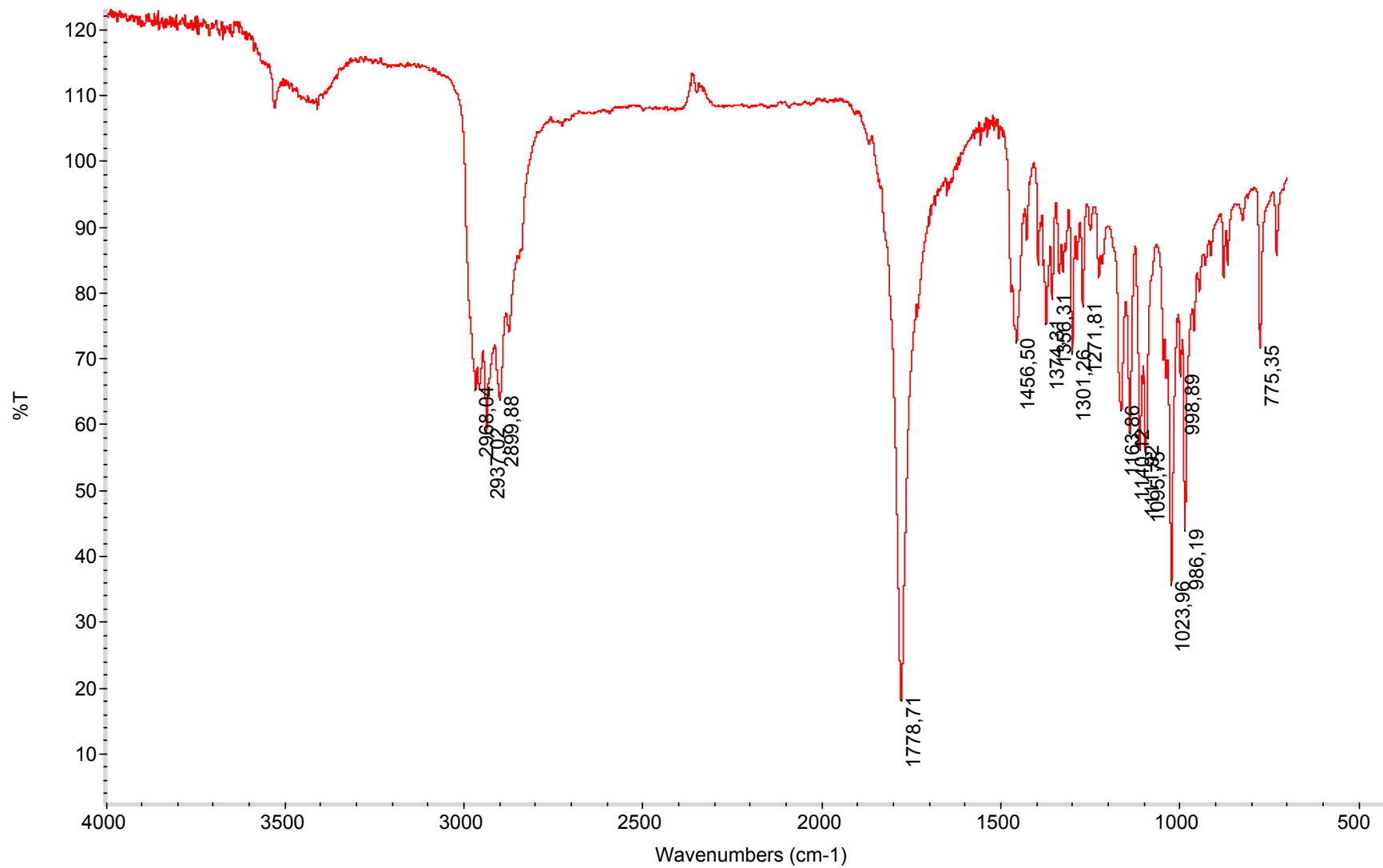


Figure S70. IR spectrum of iodolactone 4b-B.

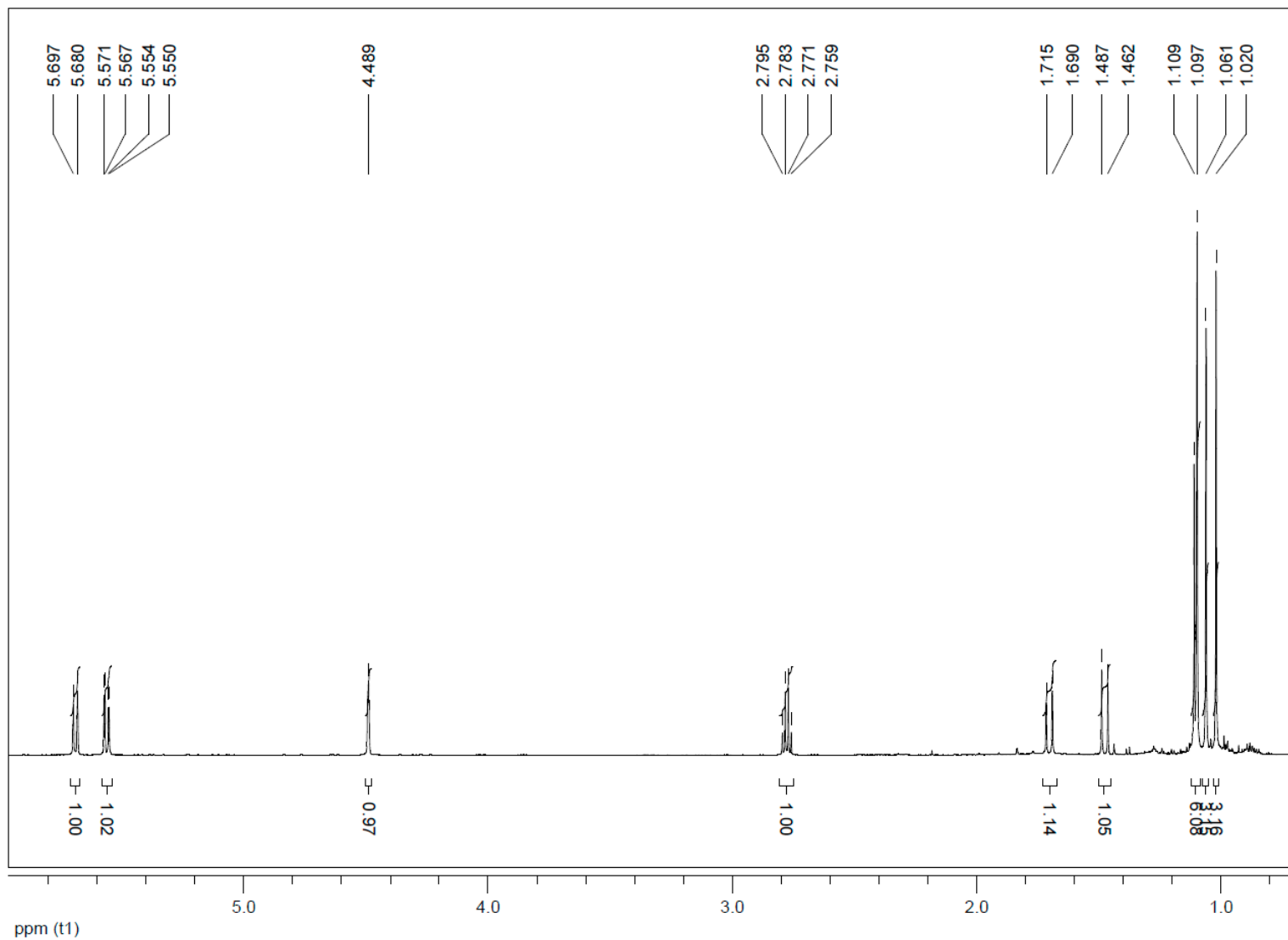


Figure S71. ¹H-NMR (600 MHz, CDCl₃) spectrum of unsaturated lactone **5b-A**.

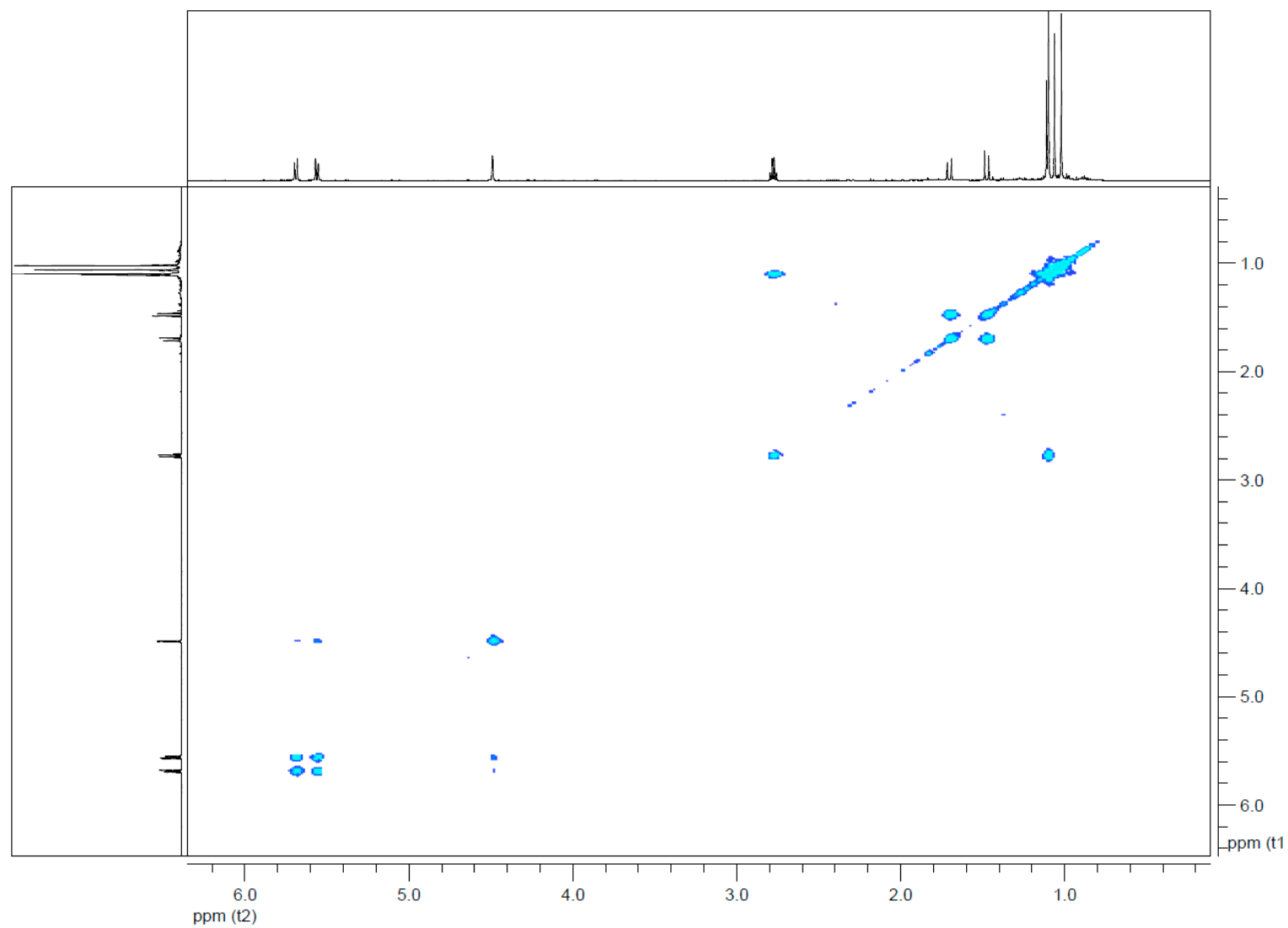


Figure S72. COSY (151 MHz, CDCl₃) spectrum of unsaturated lactone **5b-A**.

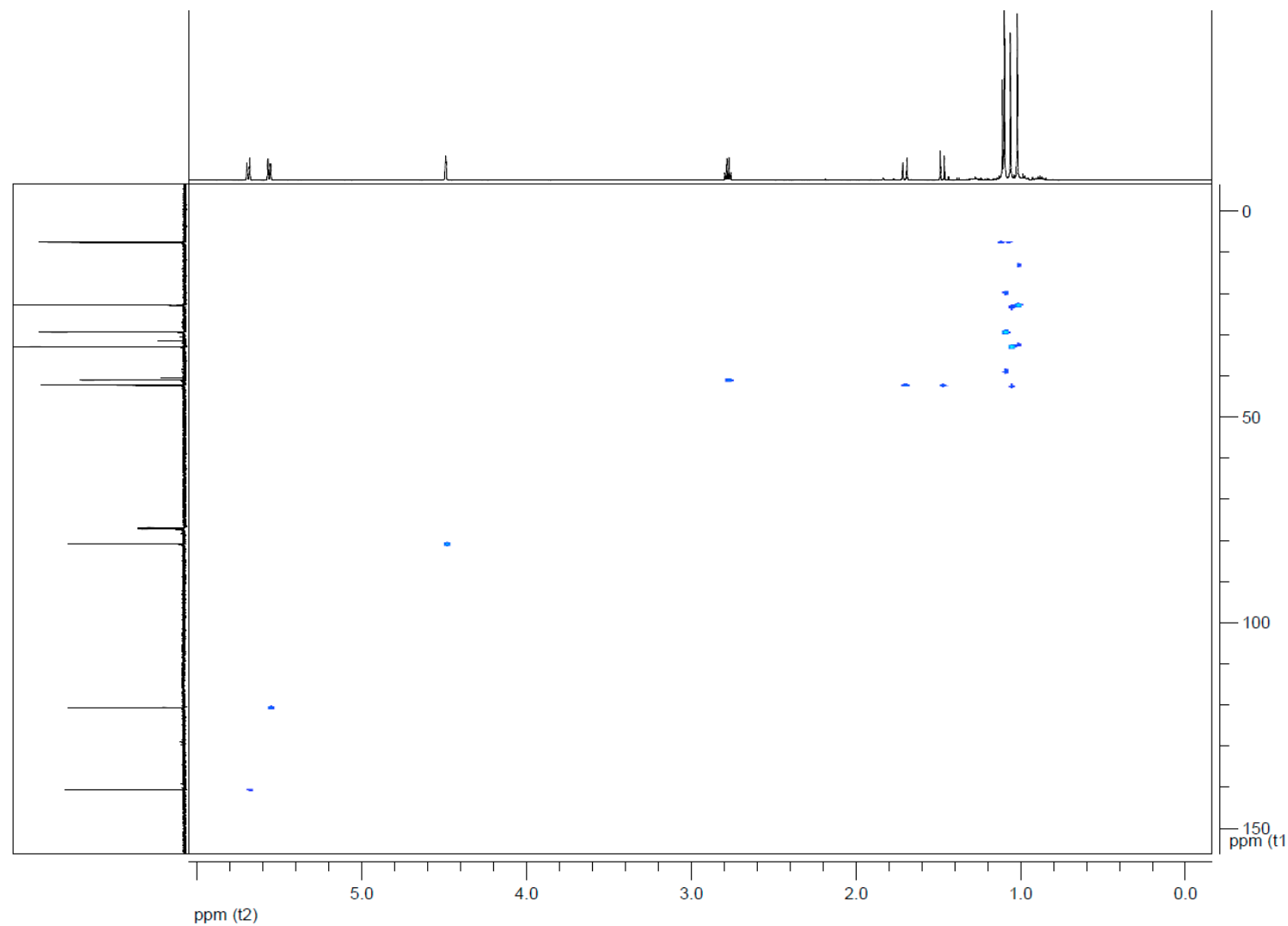


Figure S73. HMOC (151 MHz, CDCl₃) spectrum of unsaturated lactone **5b-A**.

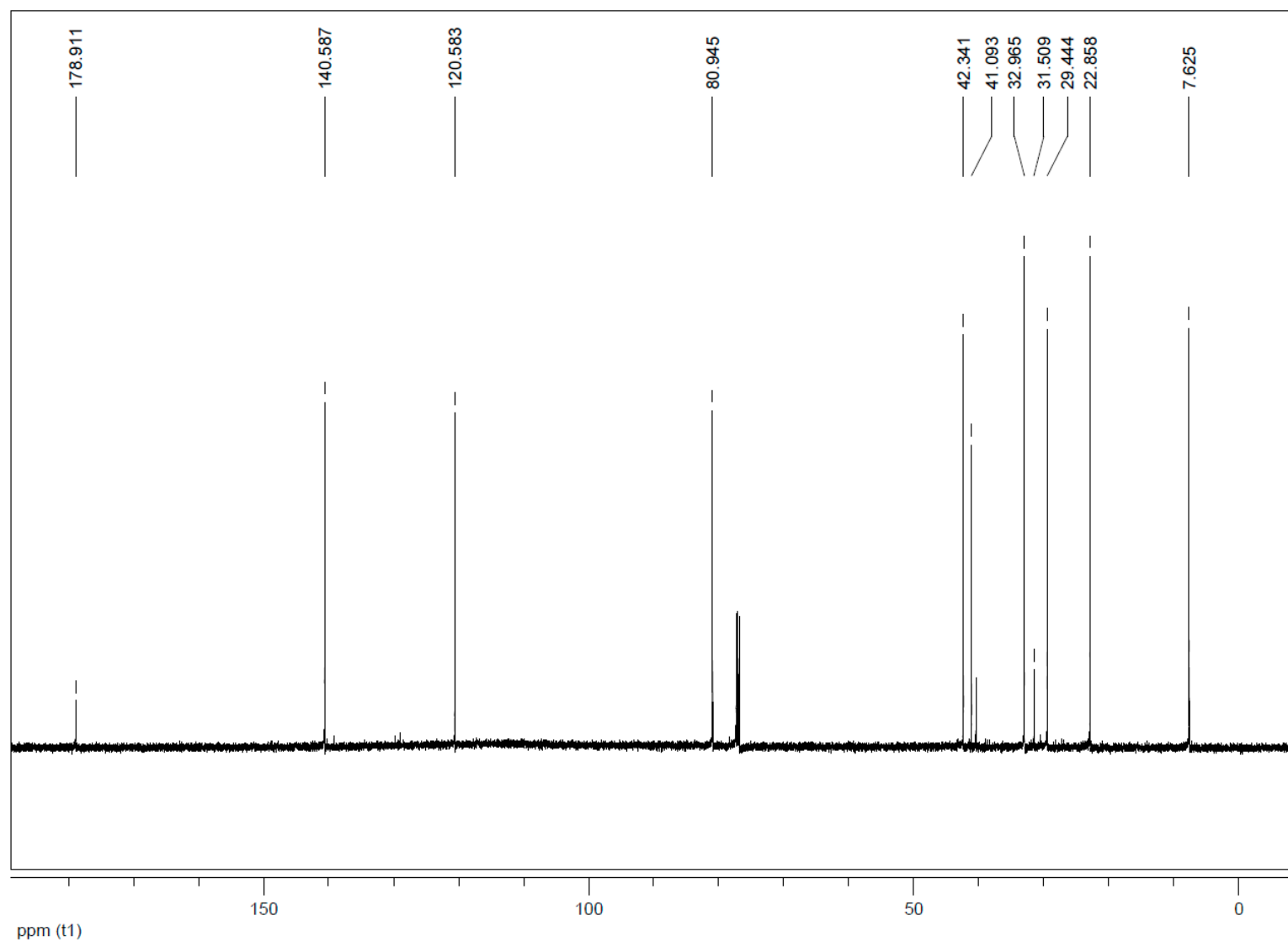


Figure S74. ^{13}C -NMR (151 MHz, CDCl_3) spectrum of unsaturated lactone **5b-A**.

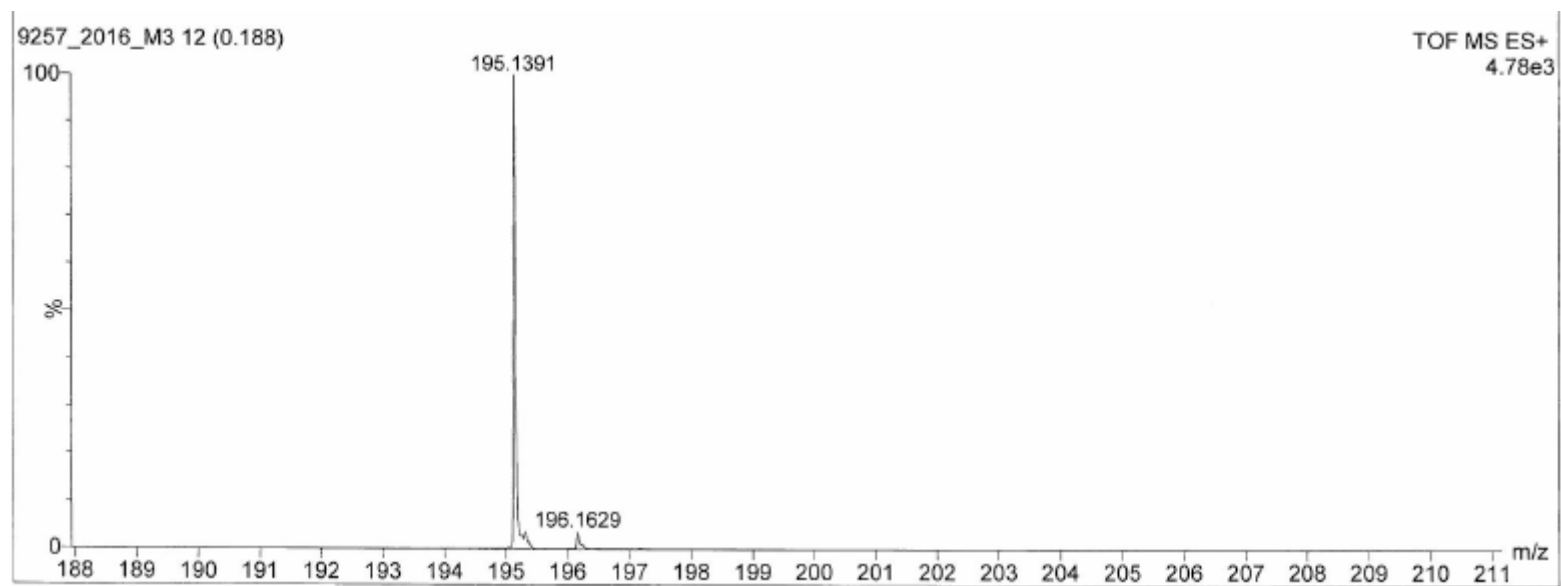


Figure S75. HRMS spectrum of unsaturated lactone **5b-A**.

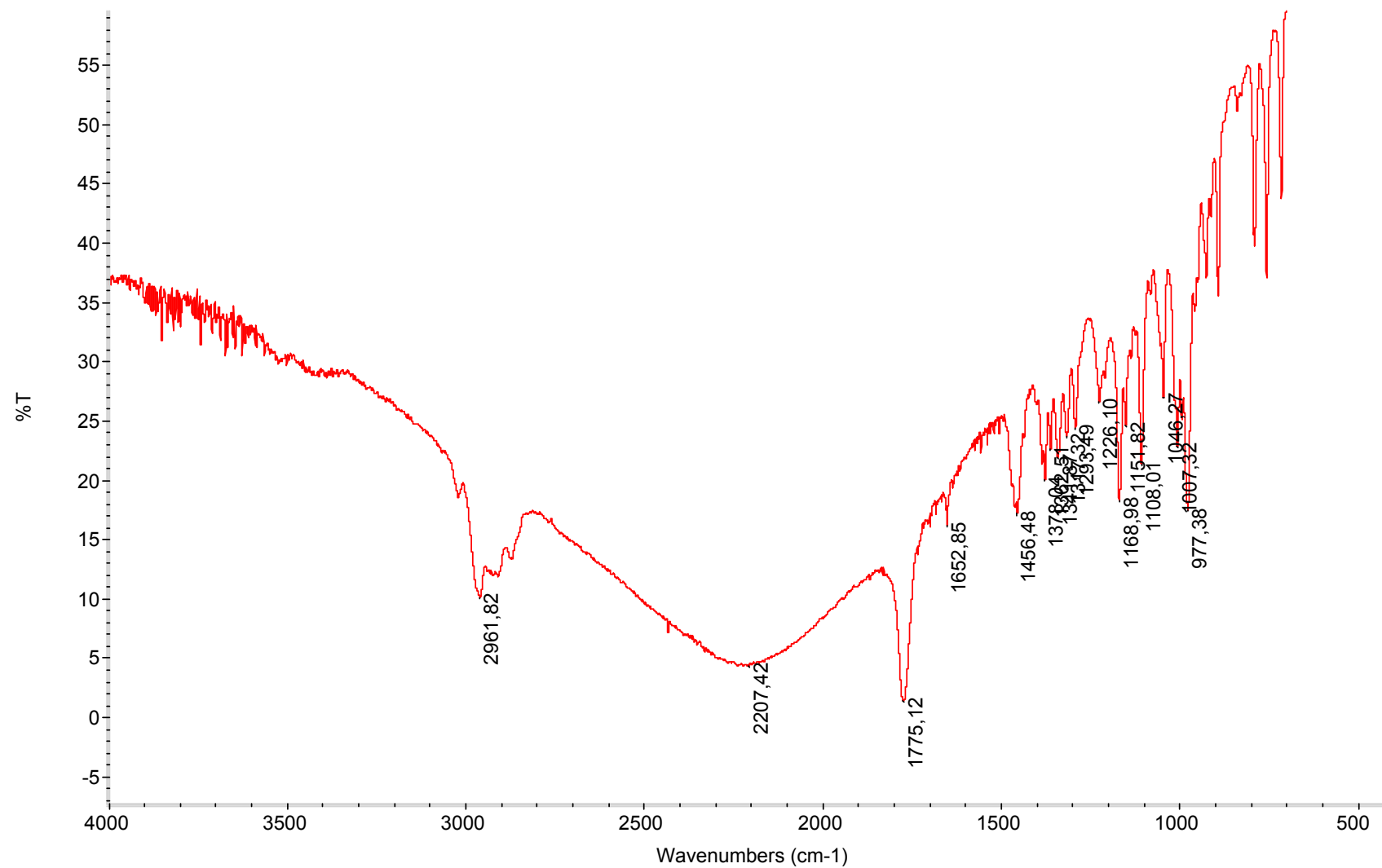


Figure S76. IR spectrum of unsaturated lactone **5b-A**.

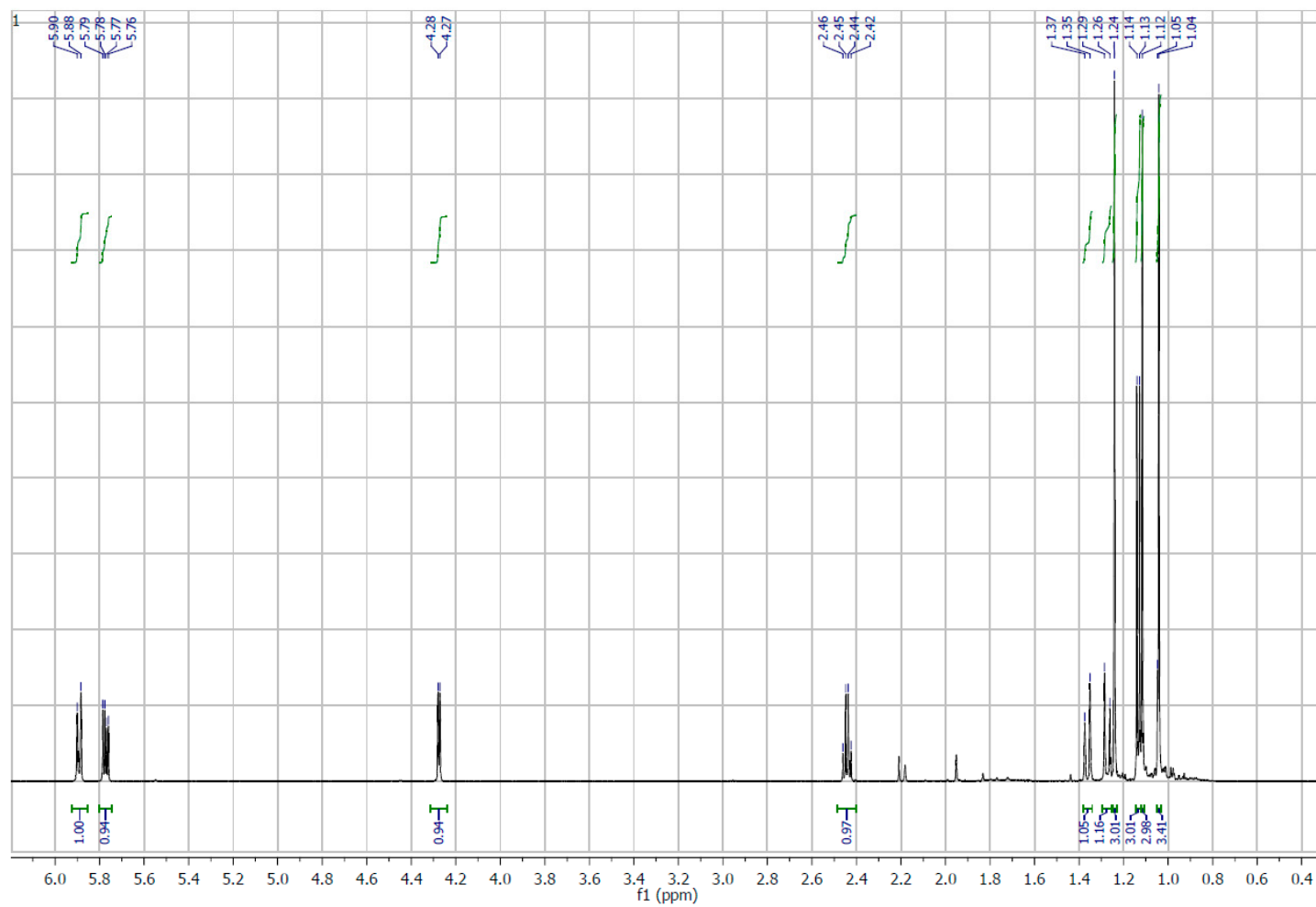


Figure S77. ¹H-NMR (600 MHz, CDCl₃) spectrum of unsaturated lactone **5b-B**.

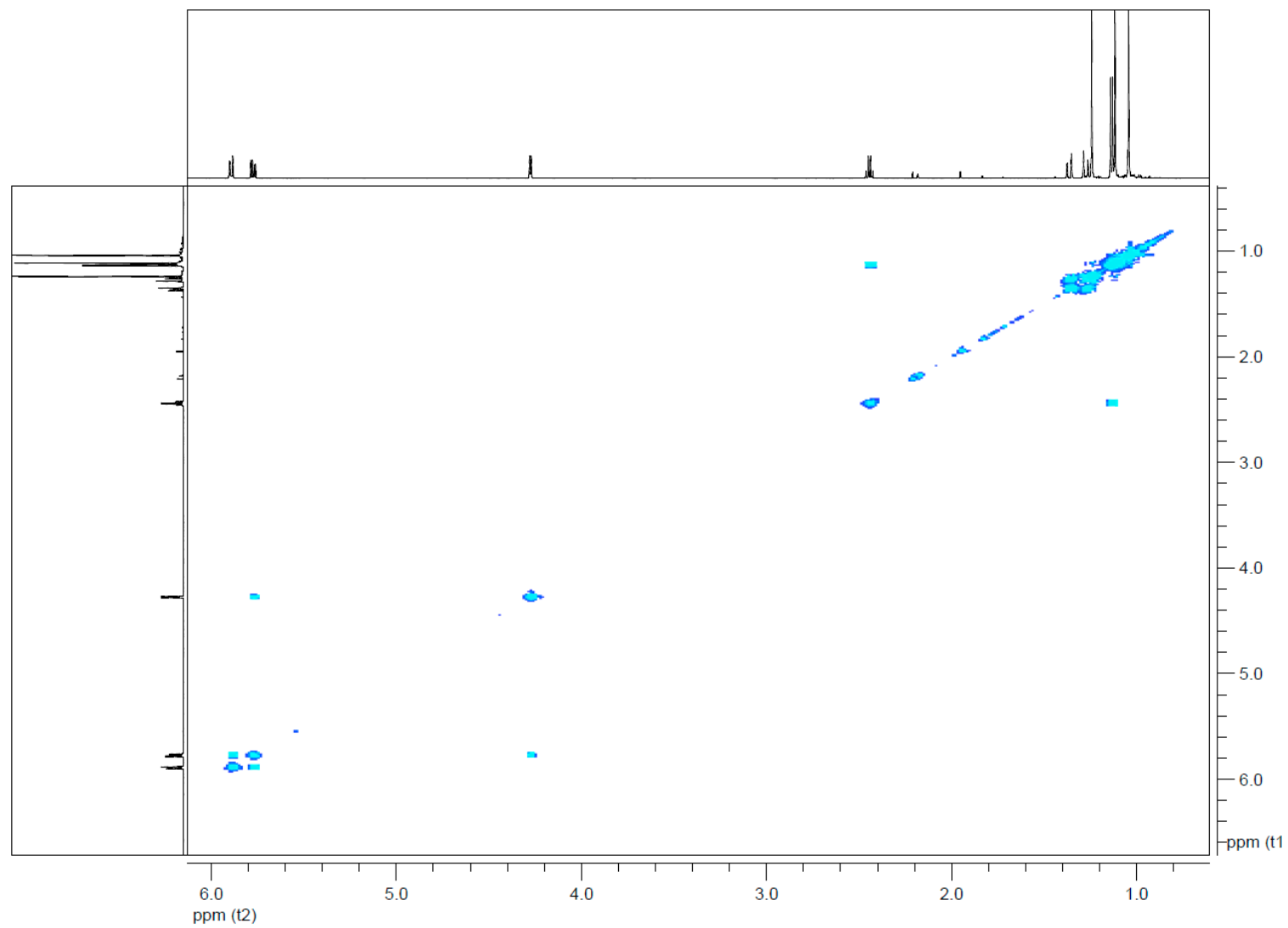


Figure S78. COSY (151 MHz, CDCl₃) spectrum of unsaturated lactone **5b-B**.

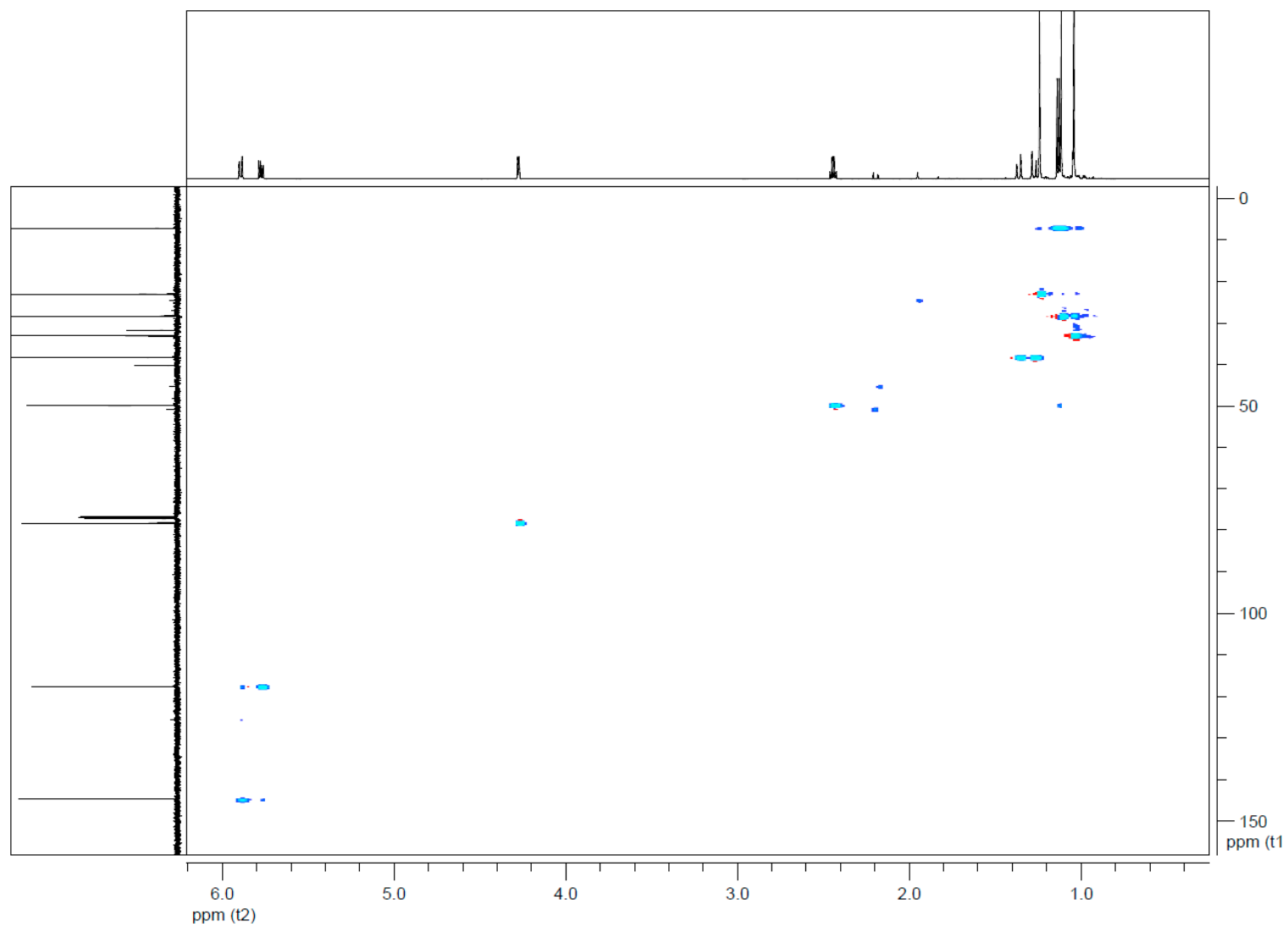


Figure S79. HMPC (151 MHz, CDCl₃) spectrum of unsaturated lactone **5b-B**.

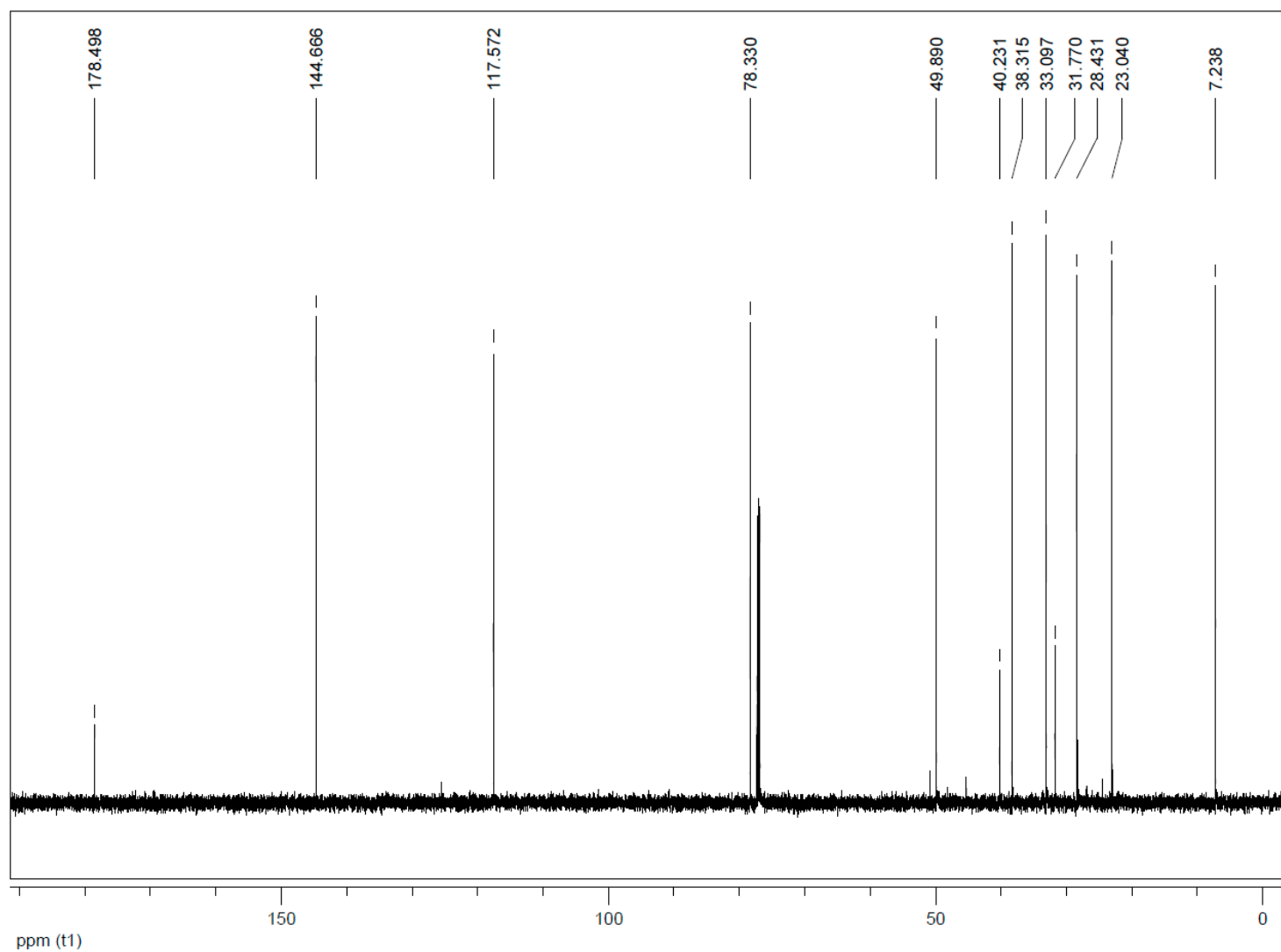


Figure S80. ^{13}C -NMR (151 MHz, CDCl_3) spectrum of unsaturated lactone **5b-B**.

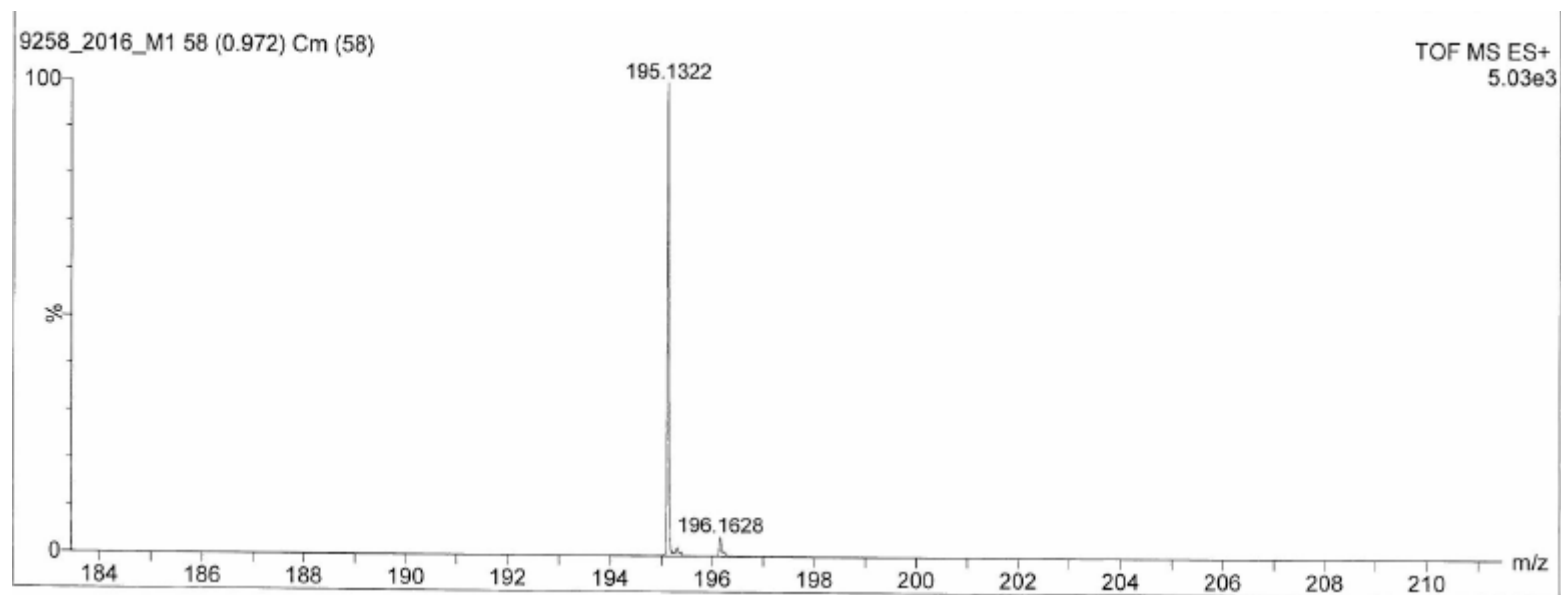


Figure S81. HRMS spectrum of unsaturated lactone **5b-B**.

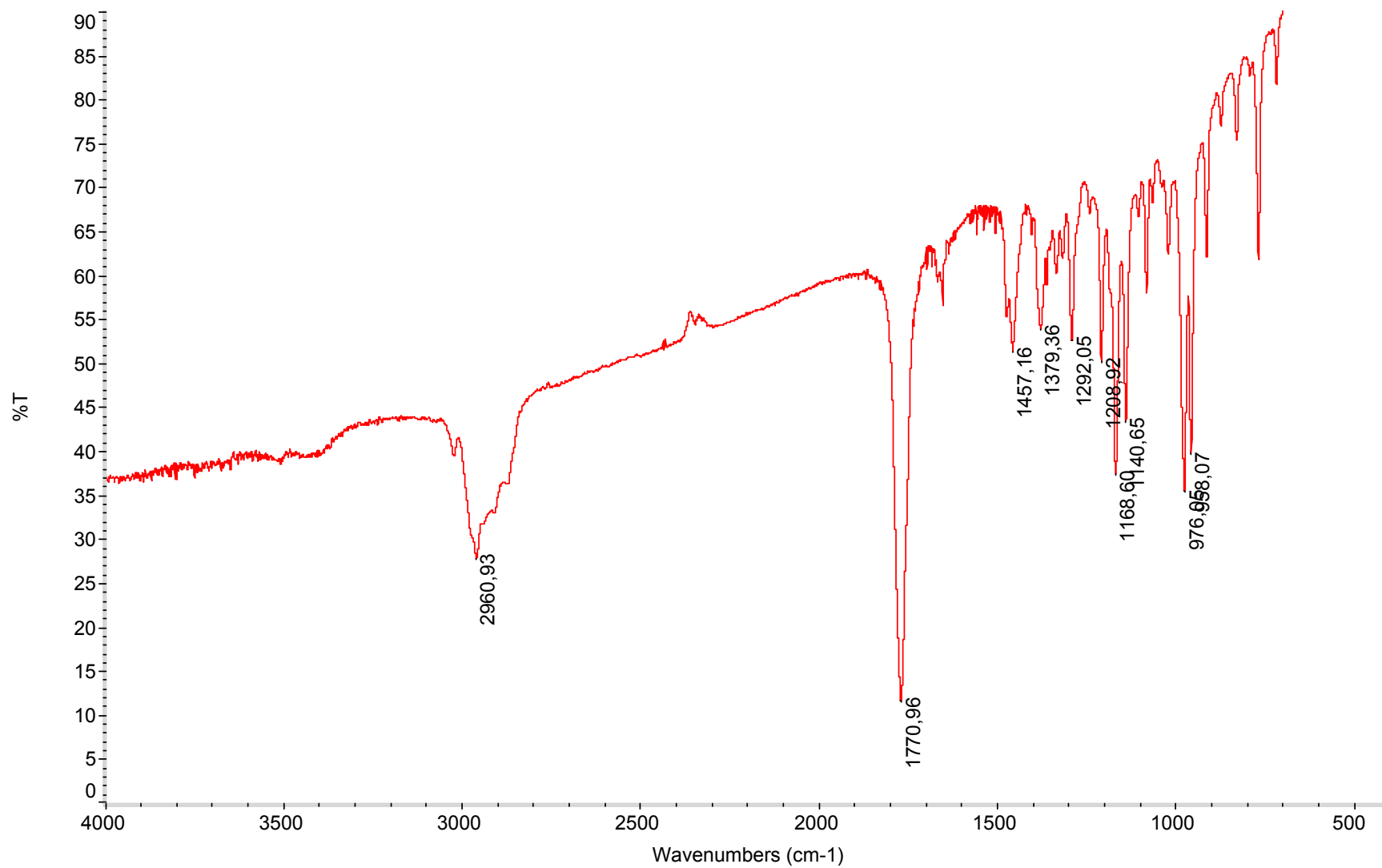


Figure S82. IR spectrum of unsaturated lactone 5b-B.

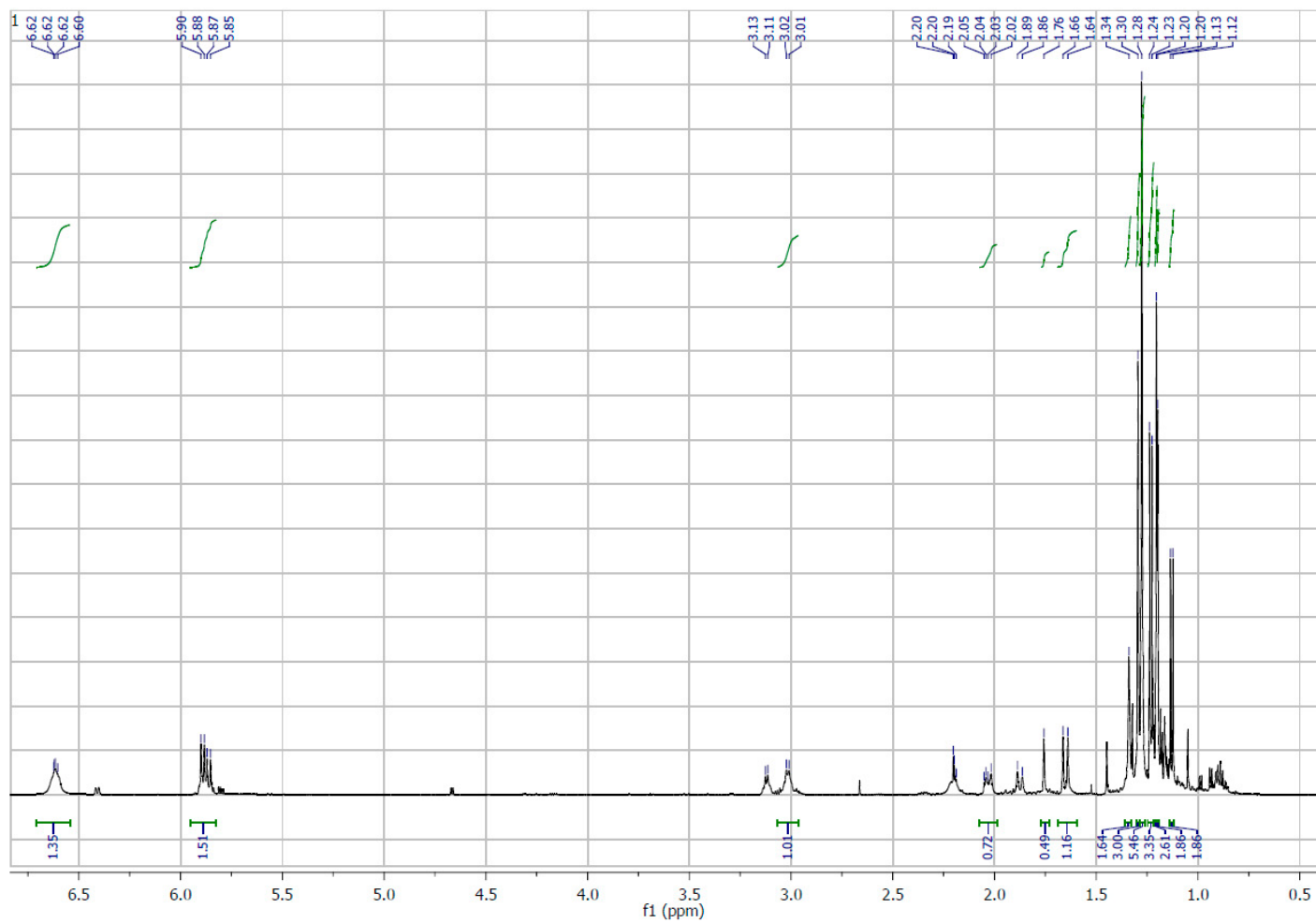


Figure S83. ¹H-NMR (600 MHz, CDCl₃) spectrum of hydroxylactone **6b**.

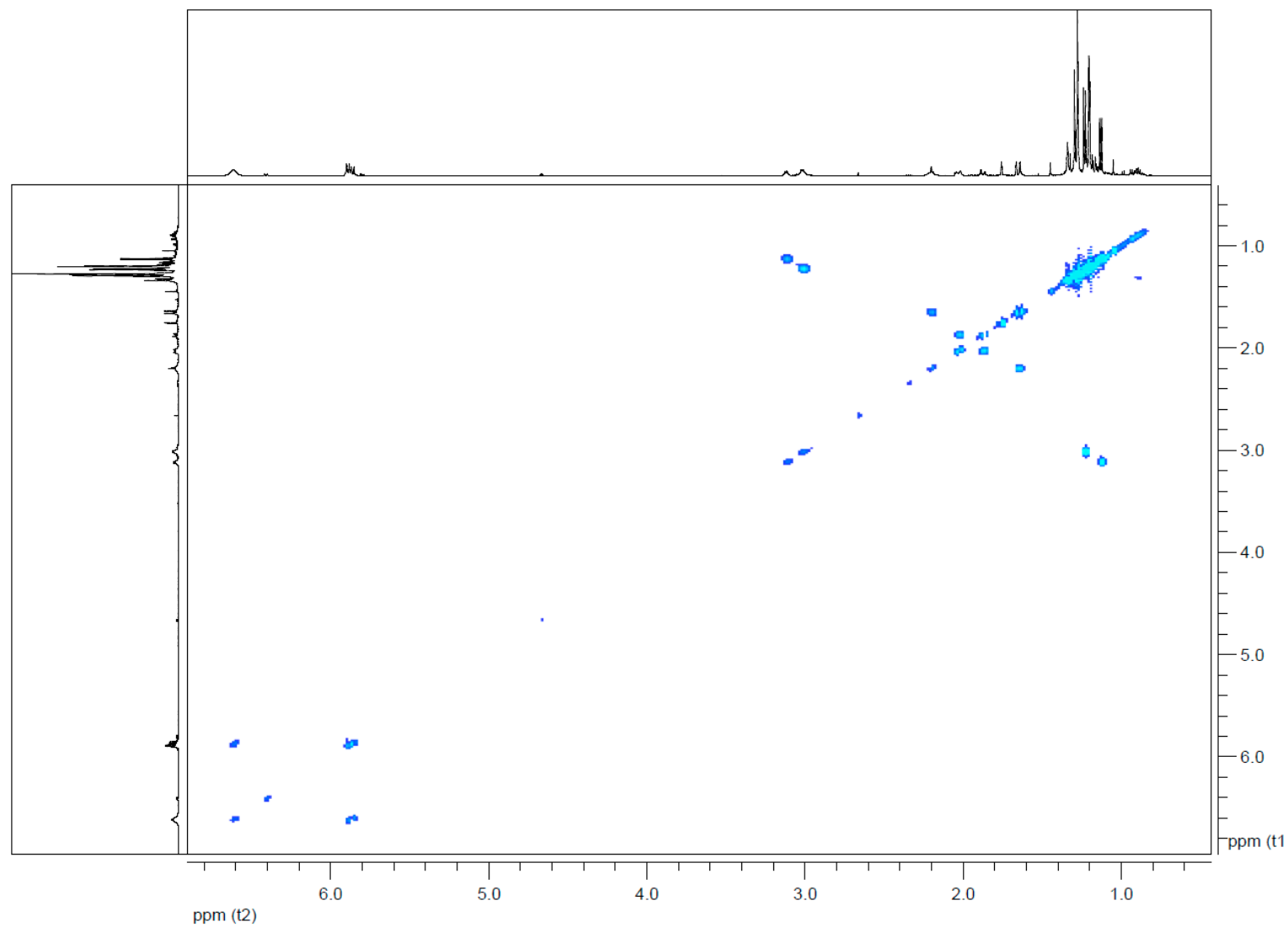


Figure S84. COSY (151 MHz, CDCl_3) spectrum of hydroxylactone **6b**.

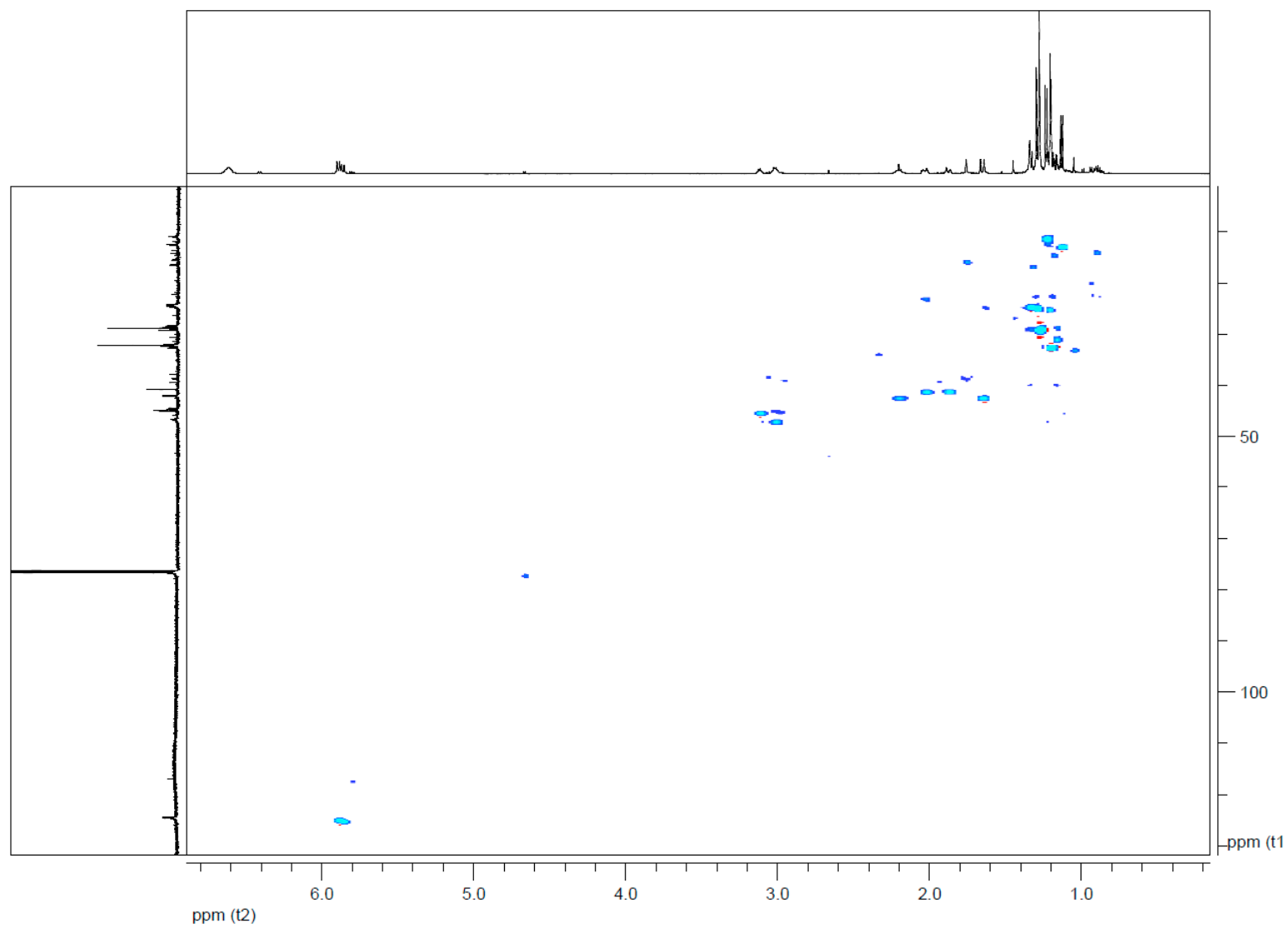


Figure S85. HMBC (151 MHz, CDCl_3) spectrum of hydroxylactone **6b**.

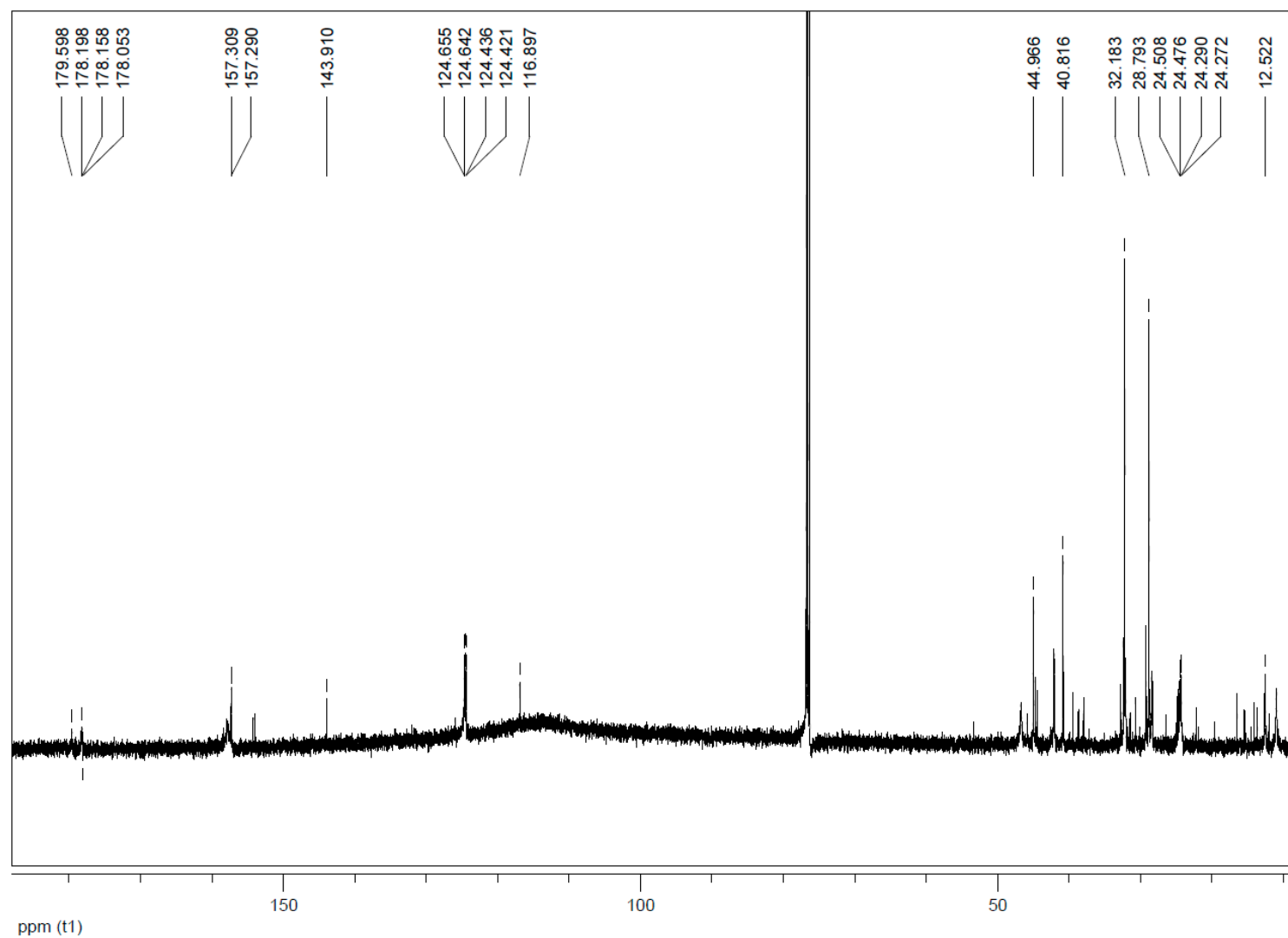


Figure S86. ¹³C-NMR (151 MHz, CDCl₃) spectrum of hydroxylactone **6b**.

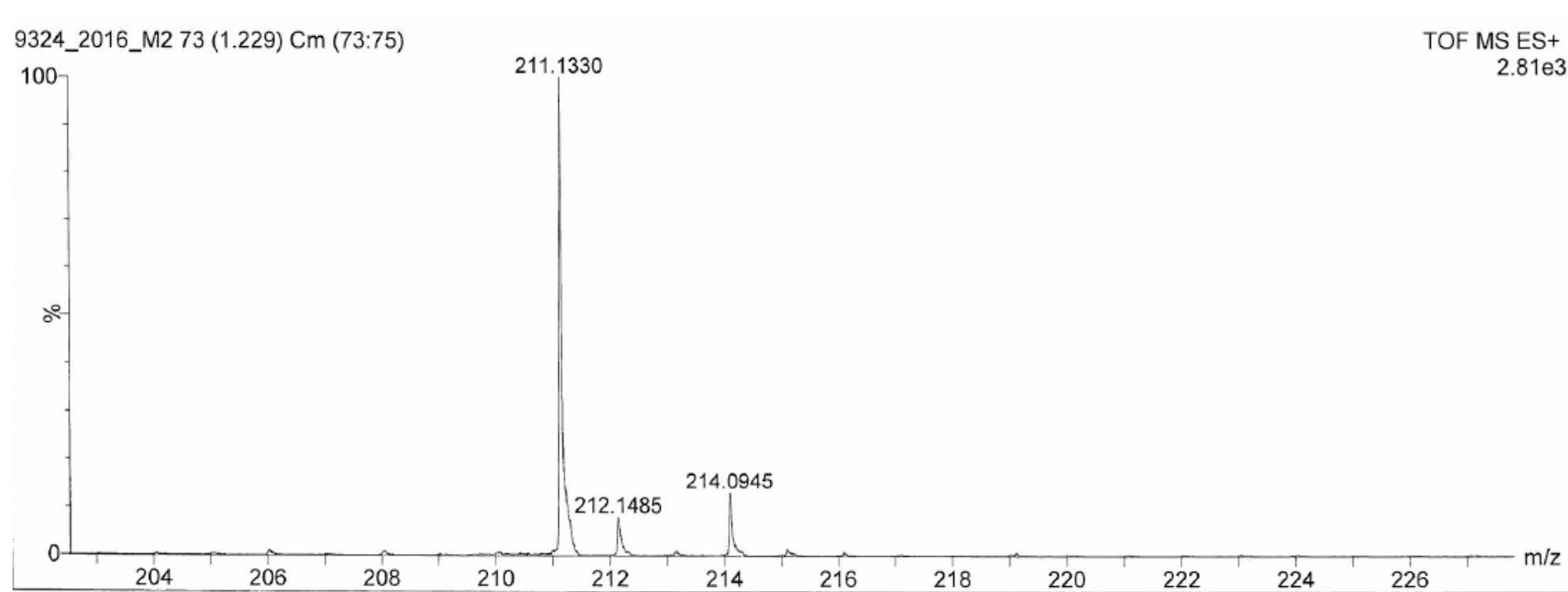


Figure S87. HRMS spectrum of hydroxylactone **6b**.

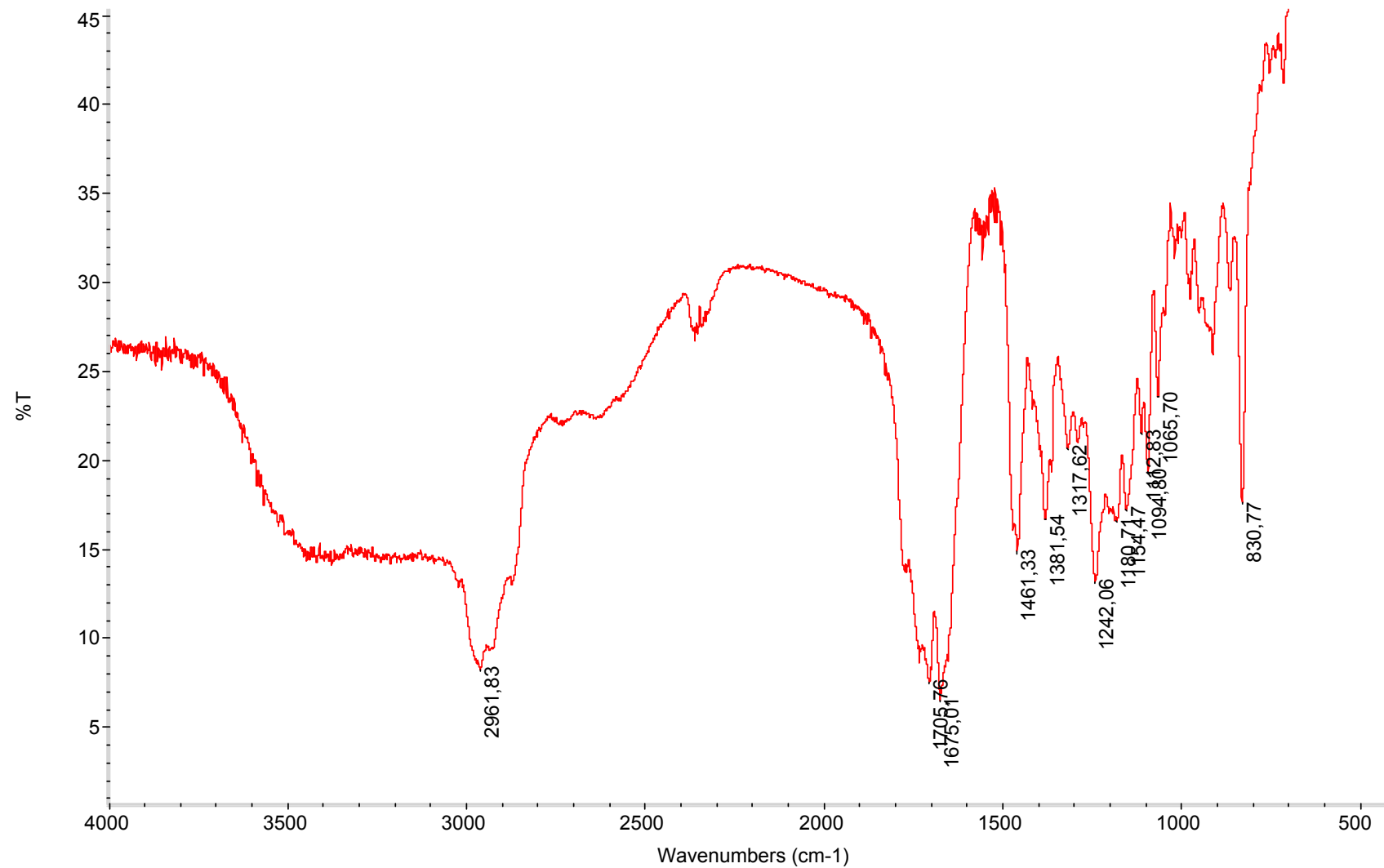


Figure S88. IR spectrum of hydroxylactone **6b**.

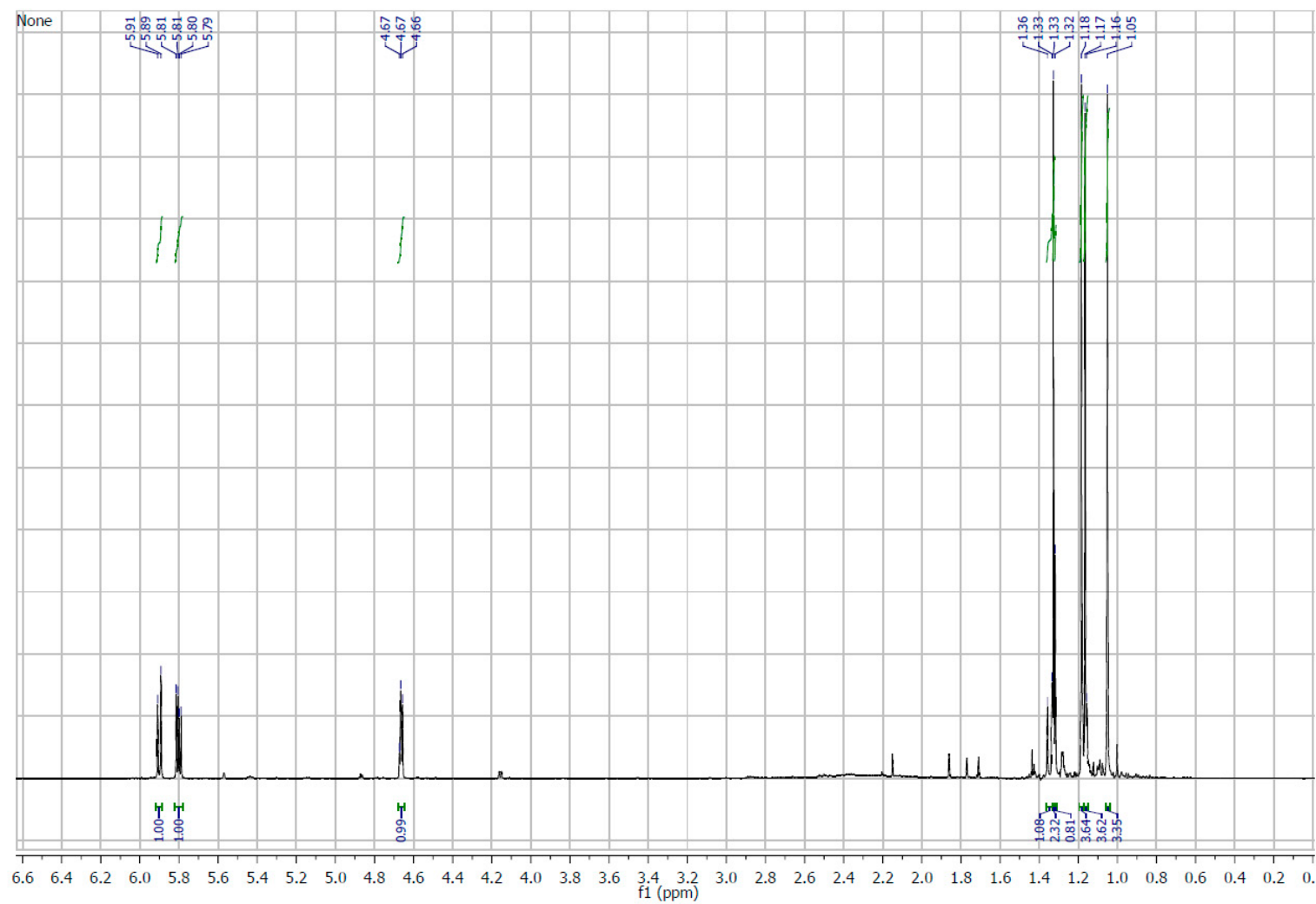


Figure S89. ¹H-NMR (600 MHz, CDCl₃) spectrum of hydroxylactone **7b**.

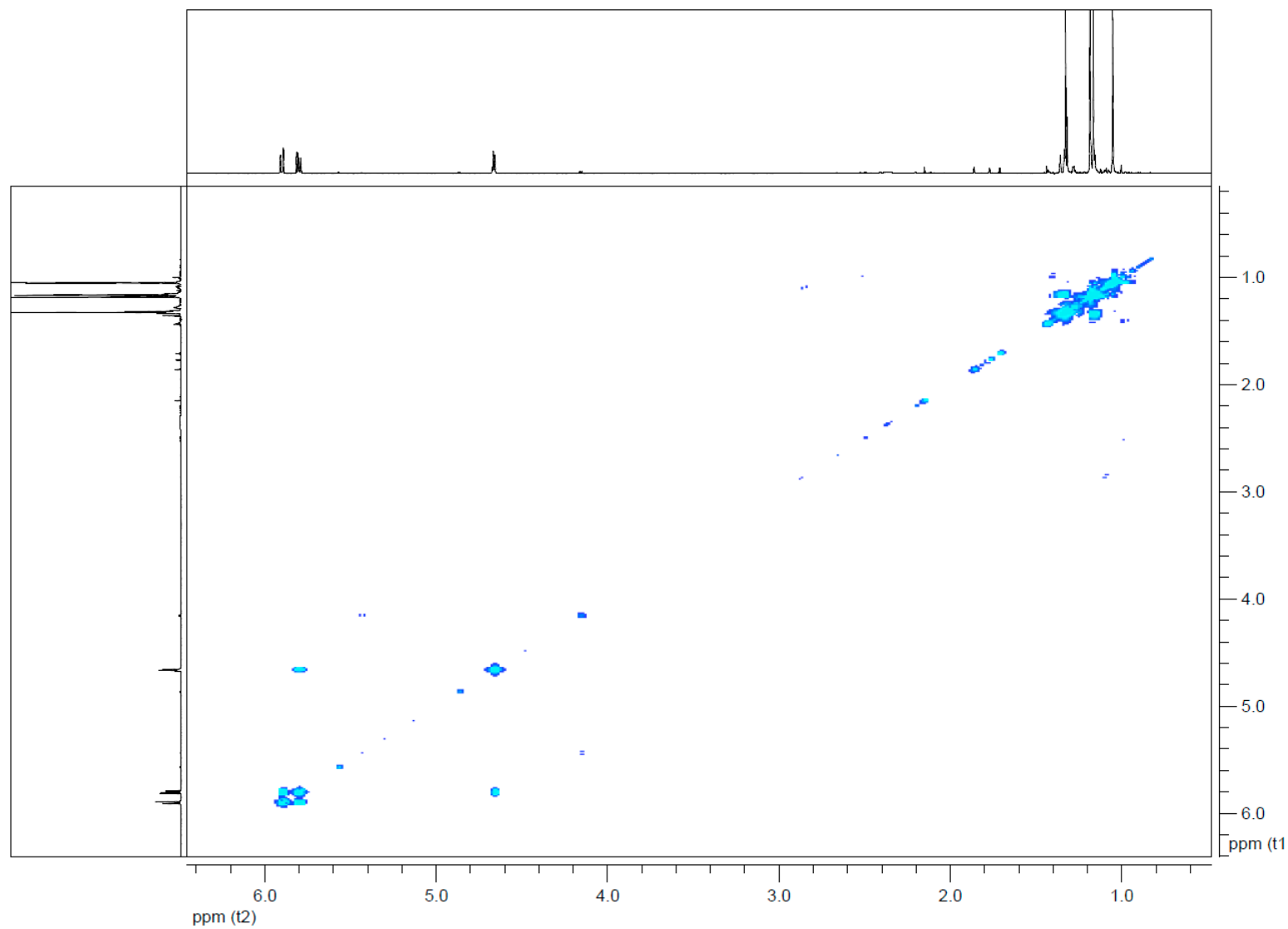


Figure S90. COSY (151 MHz, CDCl_3) spectrum of hydroxylactone **7b**.

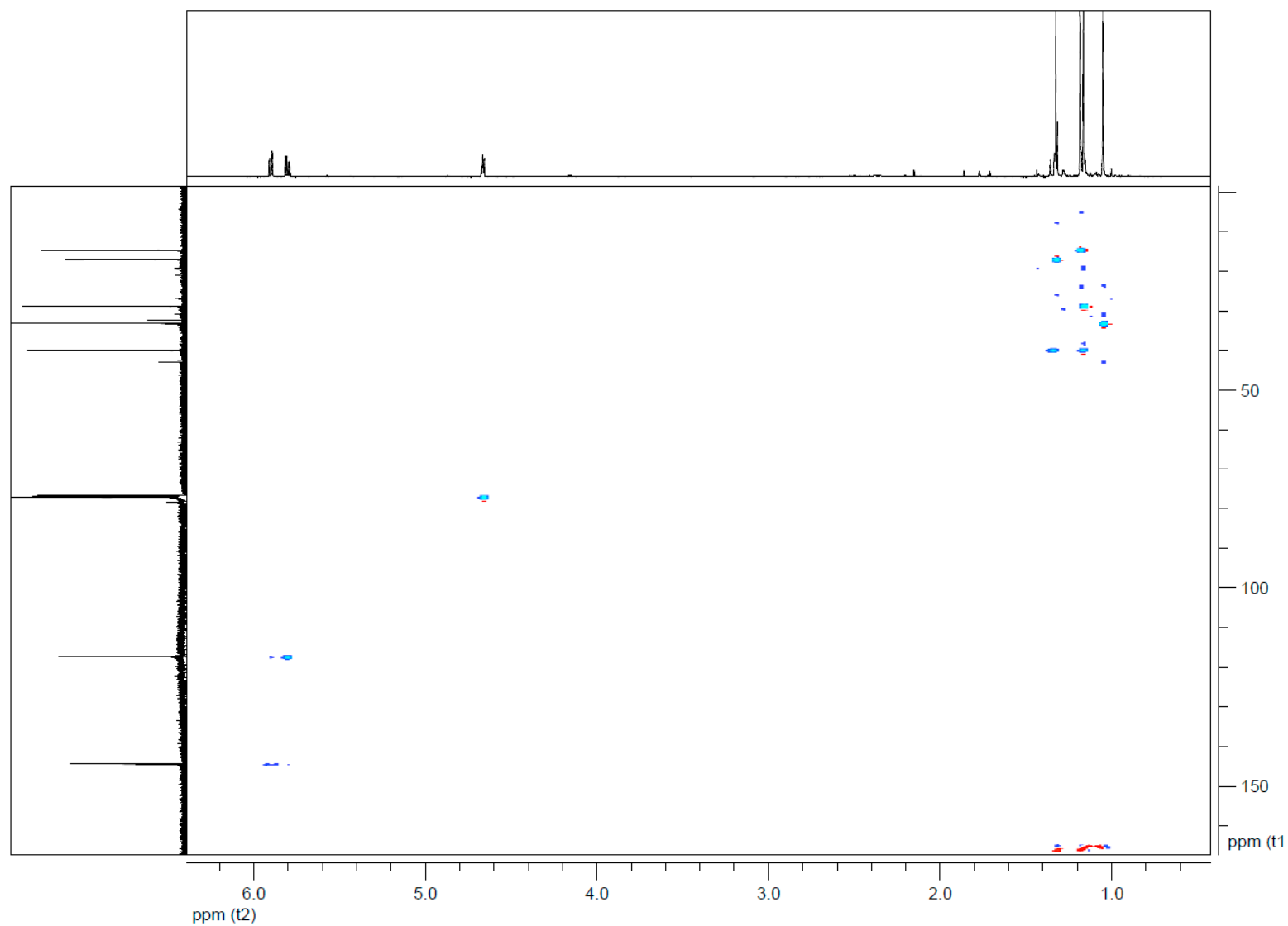


Figure S91. HMPC (151 MHz, CDCl_3) spectrum of hydroxylactone 7b.

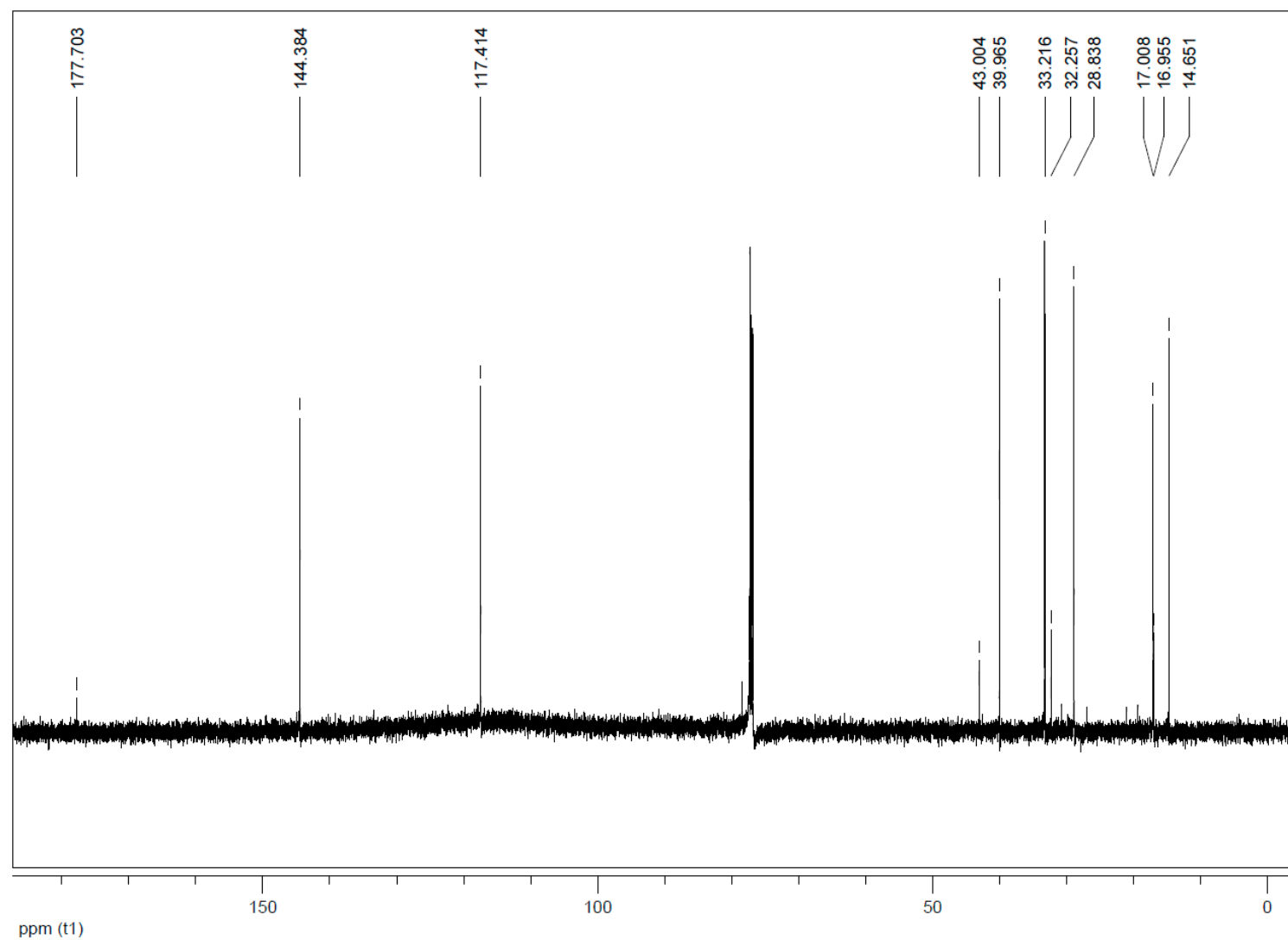


Figure S92. ^{13}C -NMR (151 MHz, CDCl_3) spectrum of hydroxylactone **7b**.

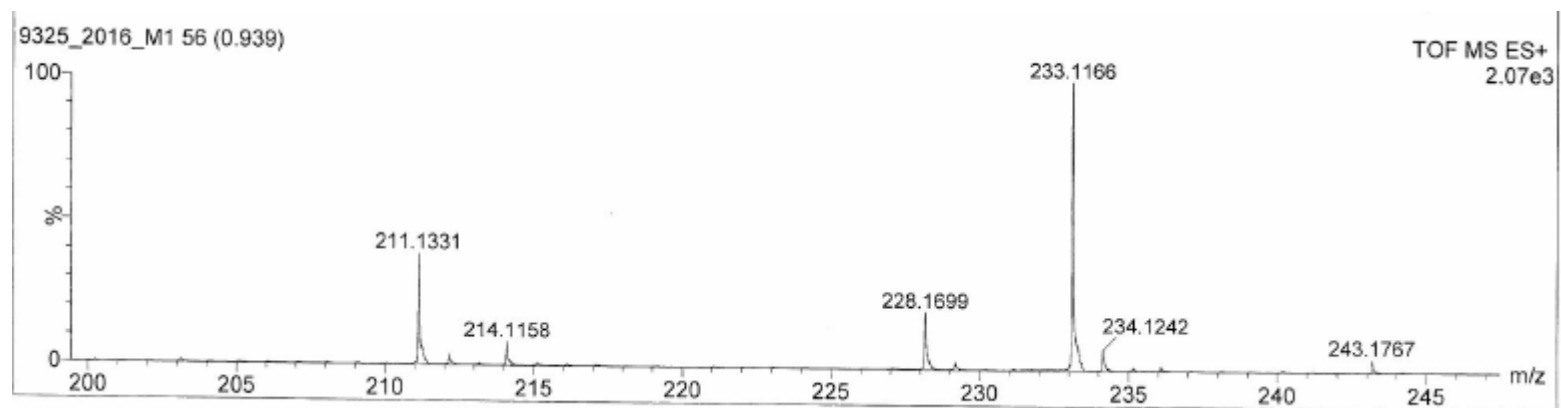


Figure S93. HRMS spectrum of hydroxylactone **7b**.

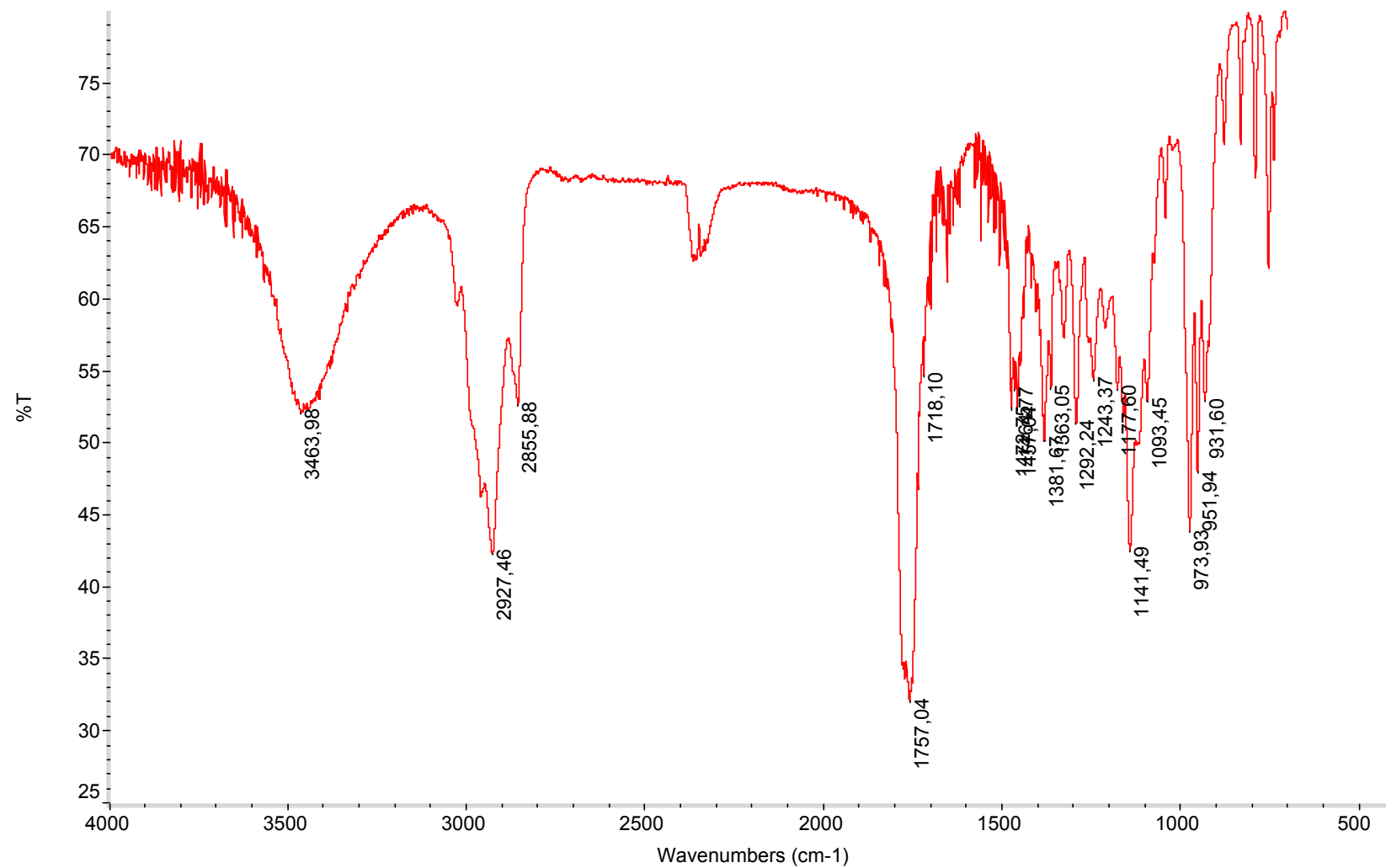


Figure S94. IR spectrum of hydroxylactone 7b.

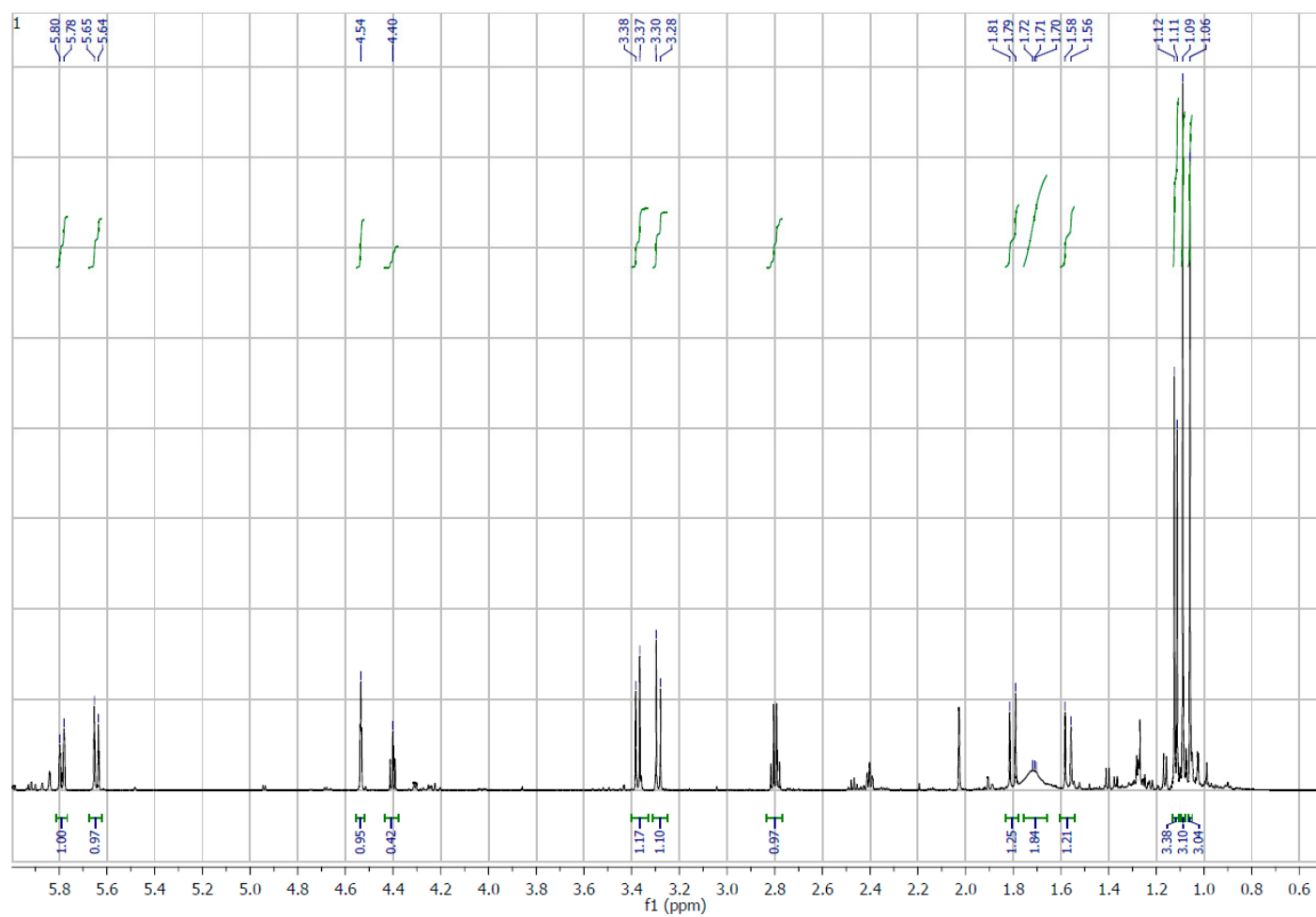


Figure S95. ¹H-NMR (600 MHz, CDCl₃) spectrum of hydroxylactone **8b**.

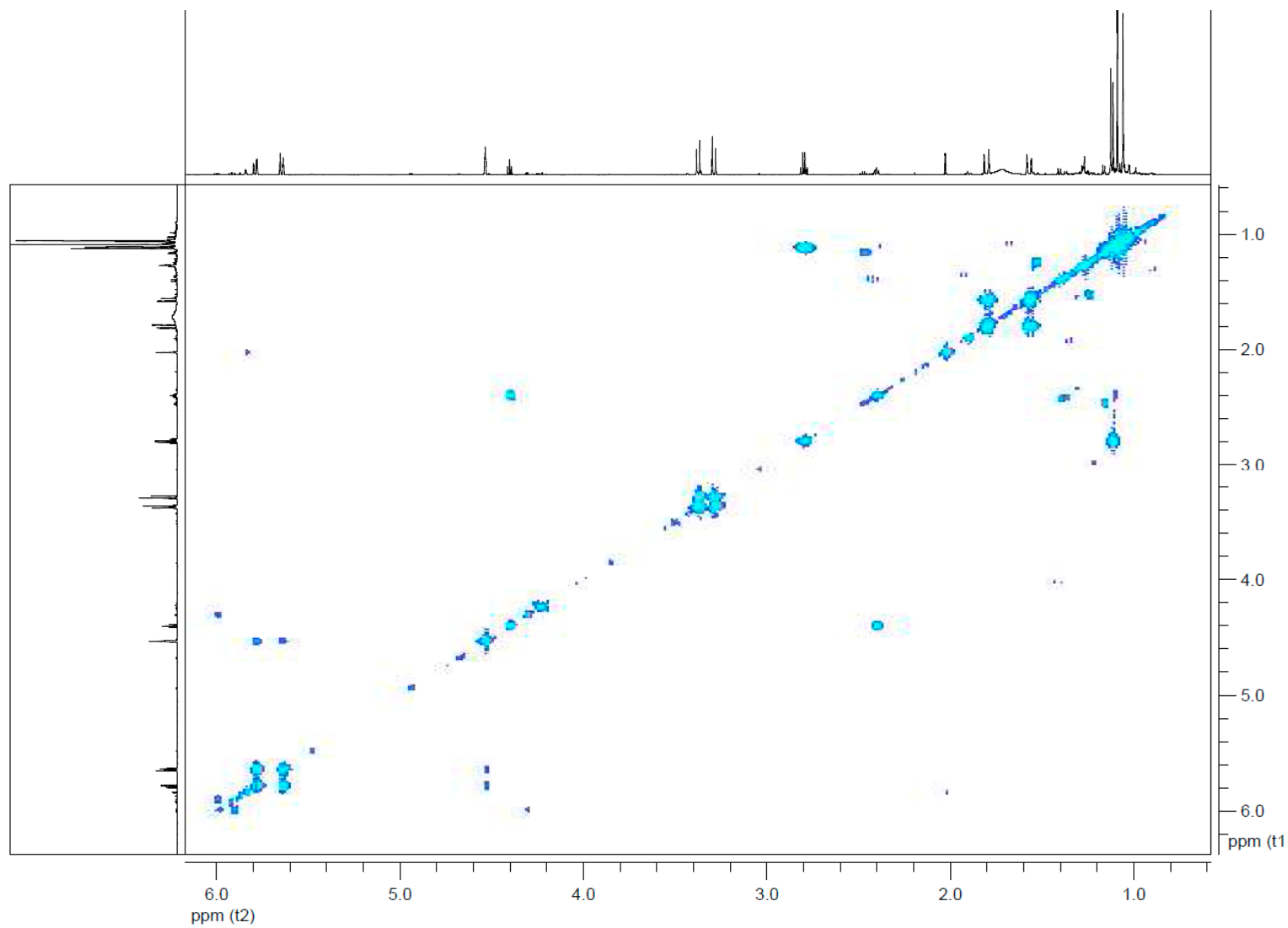


Figure S96. COSY (151 MHz, CDCl₃) spectrum of hydroxylactone **8b**.

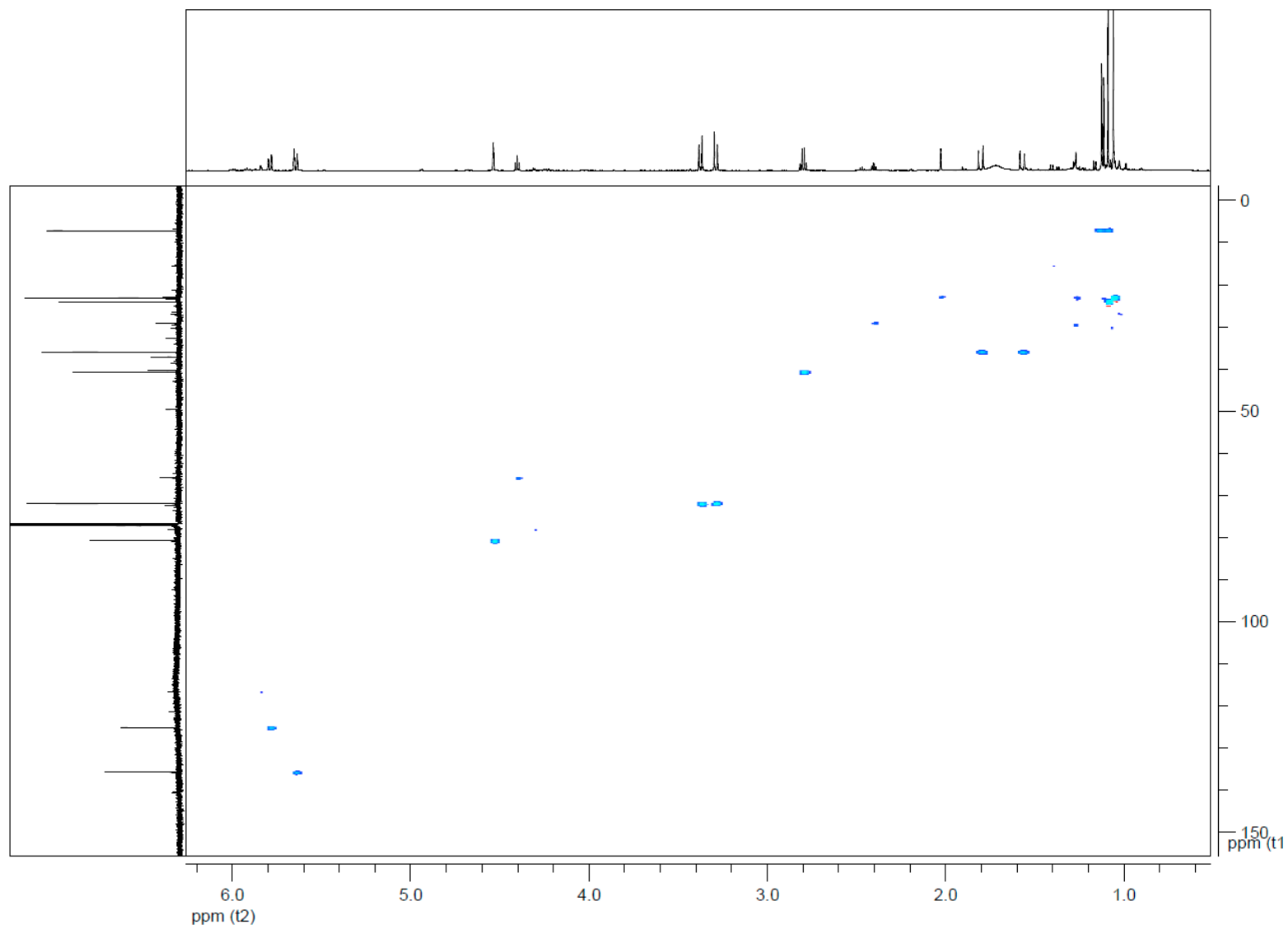


Figure S97. HMPC (151 MHz, CDCl₃) spectrum of hydroxylactone 8b.

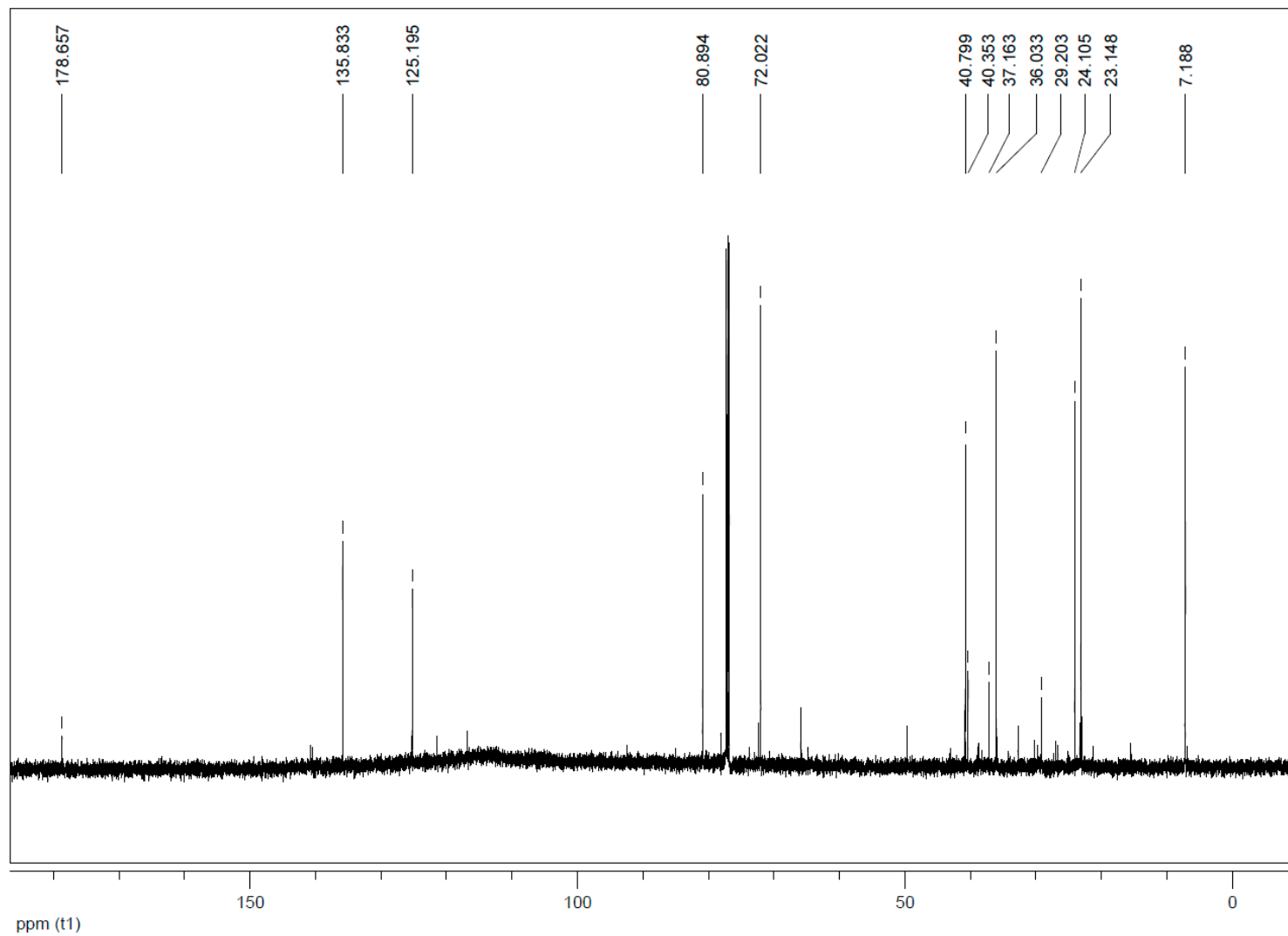


Figure S98. ^{13}C -NMR (151 MHz, CDCl_3) spectrum of hydroxylactone **8b**.

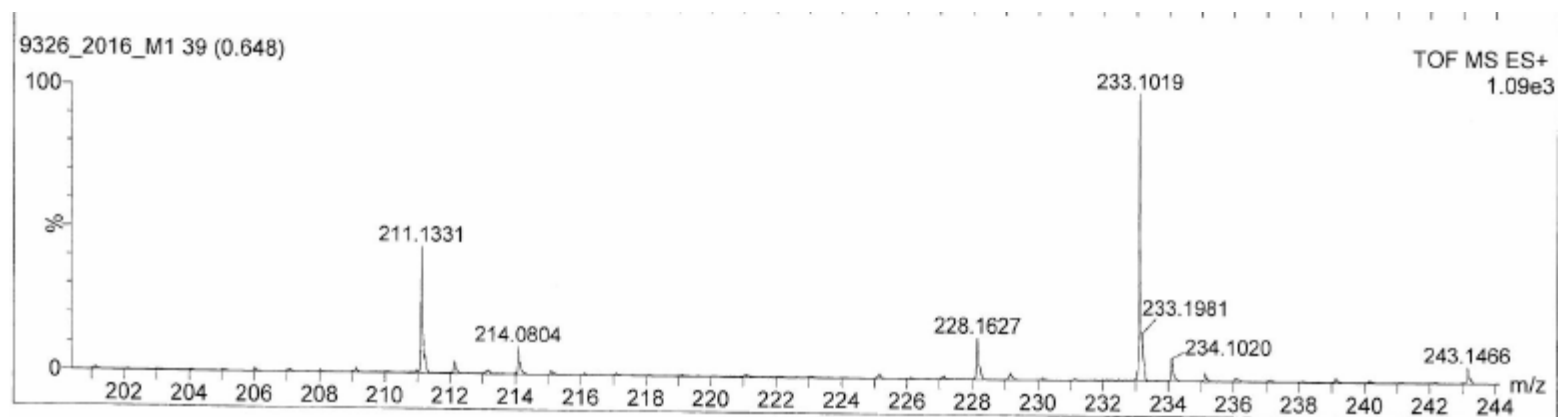


Figure S99. HRMS spectrum of hydroxylactone **8b**.

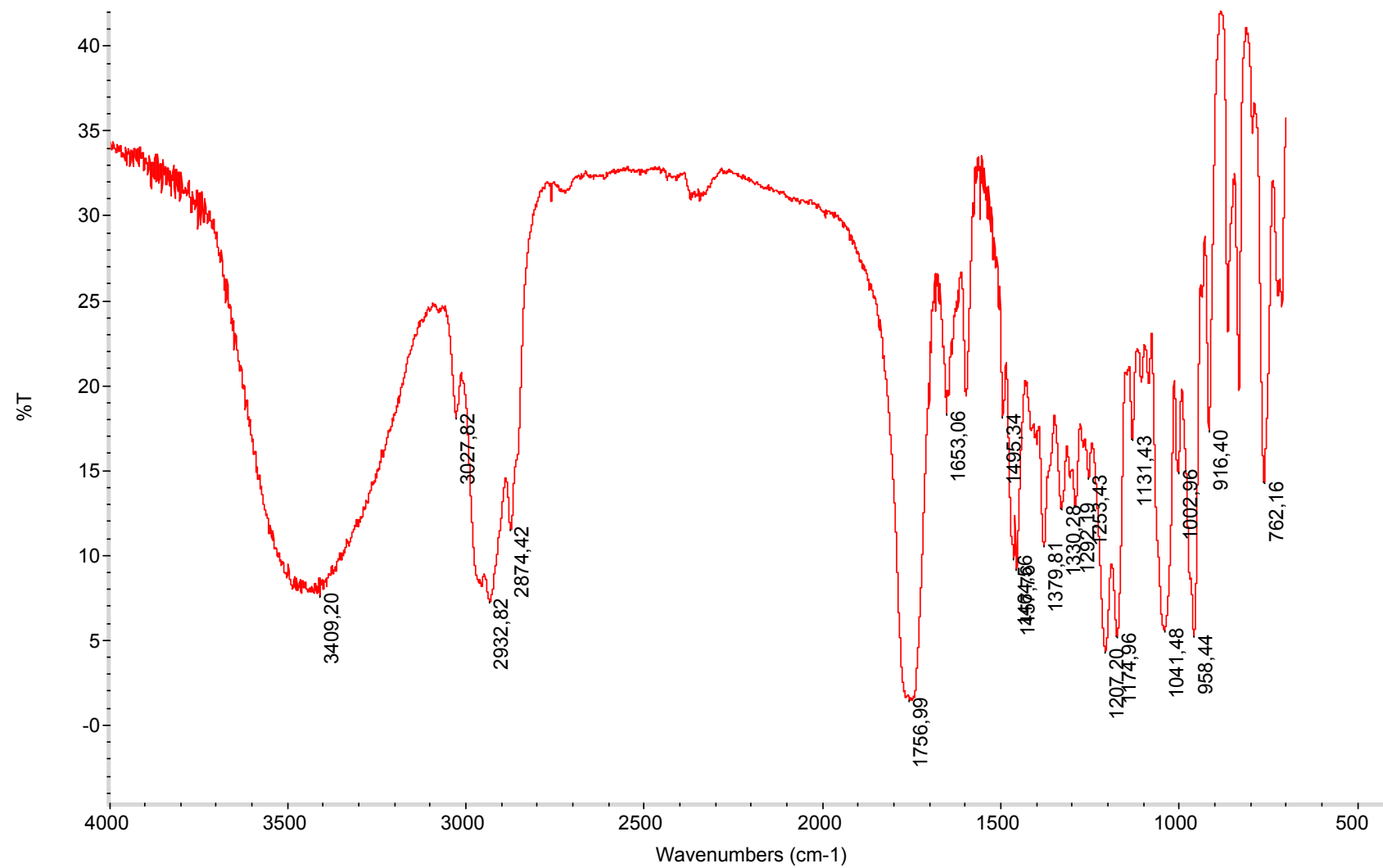


Figure S100. IR spectrum of hydroxylactone 8b.

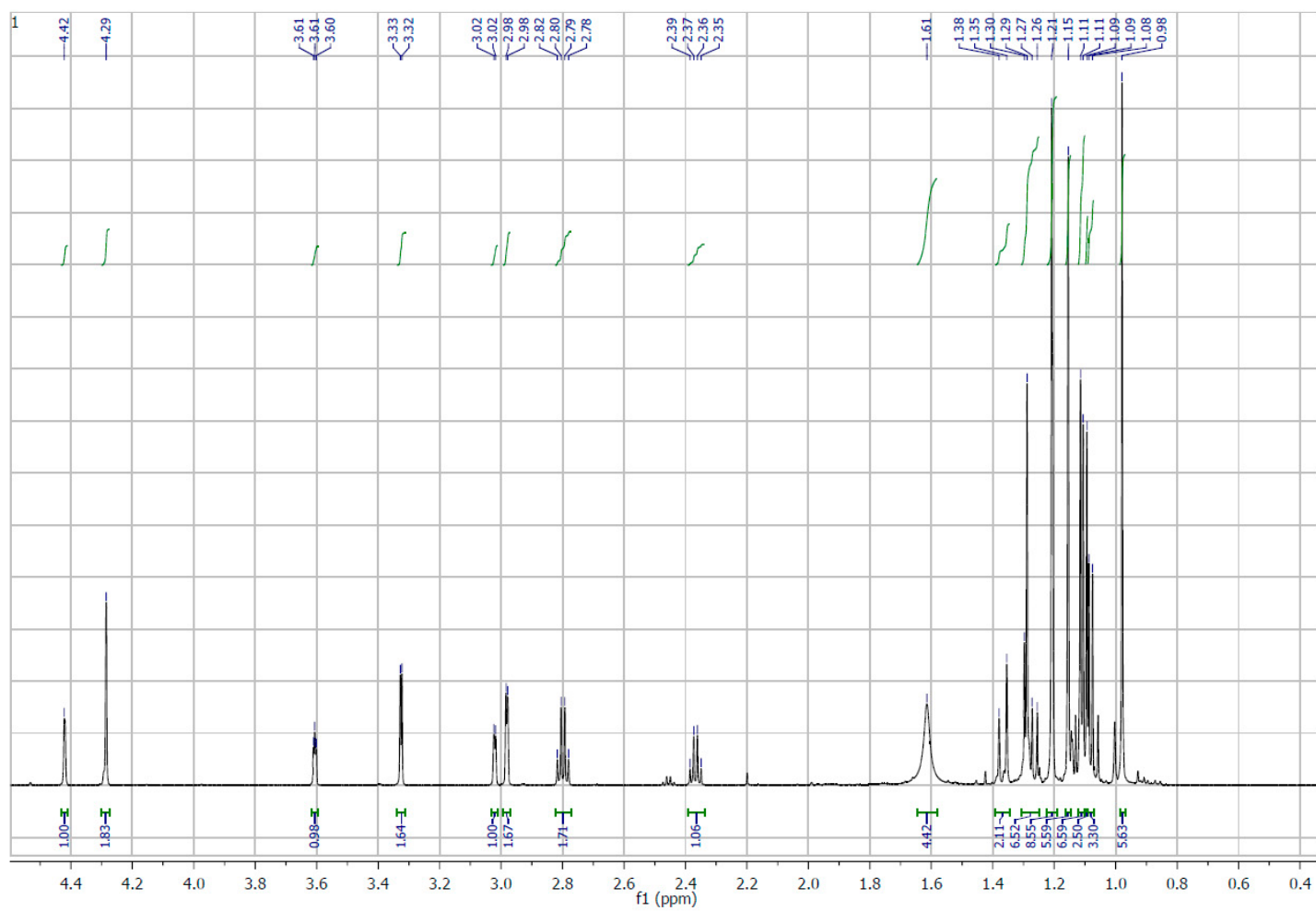


Figure S101. ^1H -NMR (600 MHz, CDCl_3) spectrum of epoxylactone **9b**.

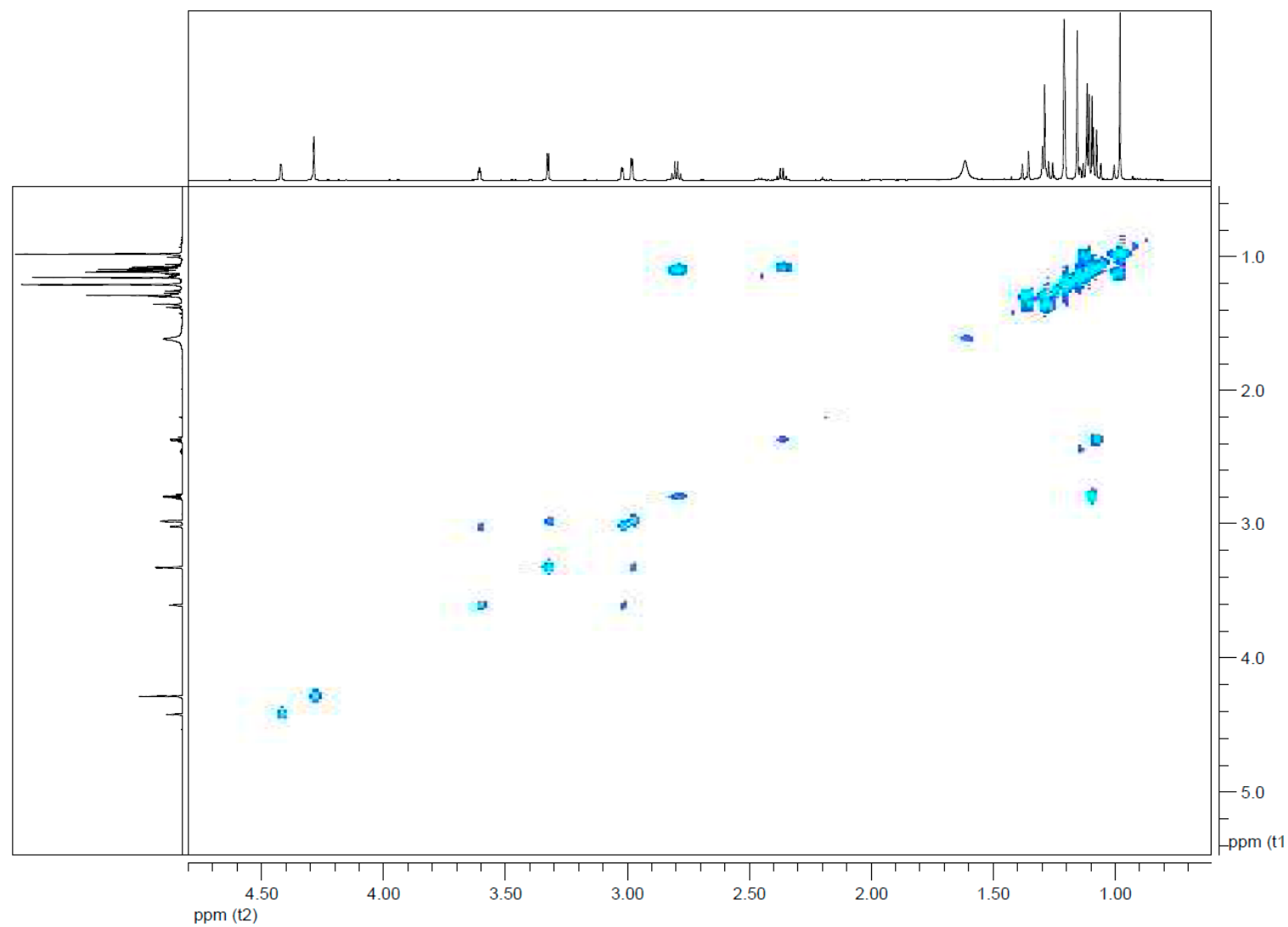


Figure S102. COSY (151 MHz, CDCl_3) spectrum of epoxylactone **9b**.

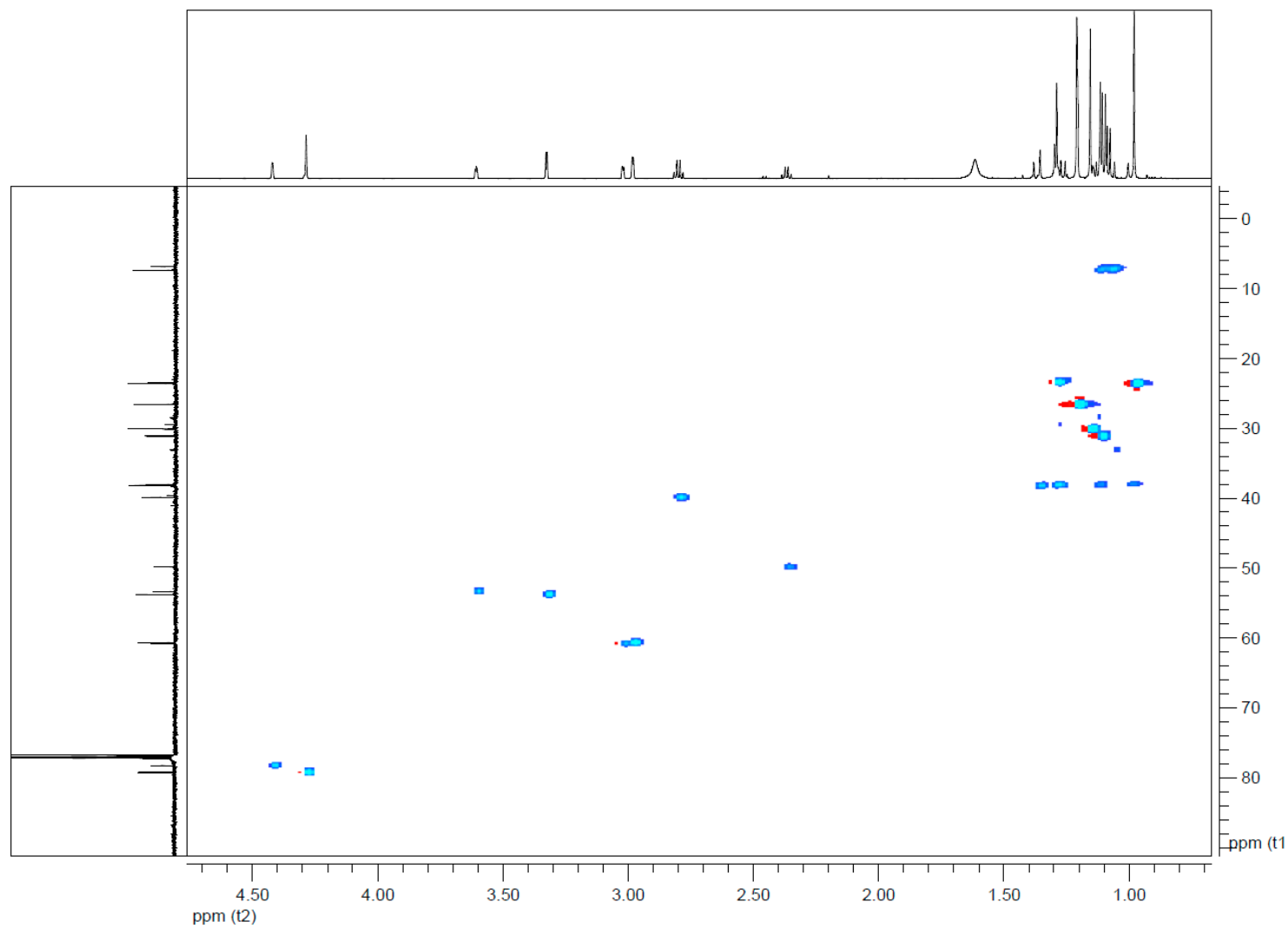


Figure S103. HMBC (151 MHz, CDCl_3) spectrum of epoxylactone **9b**.

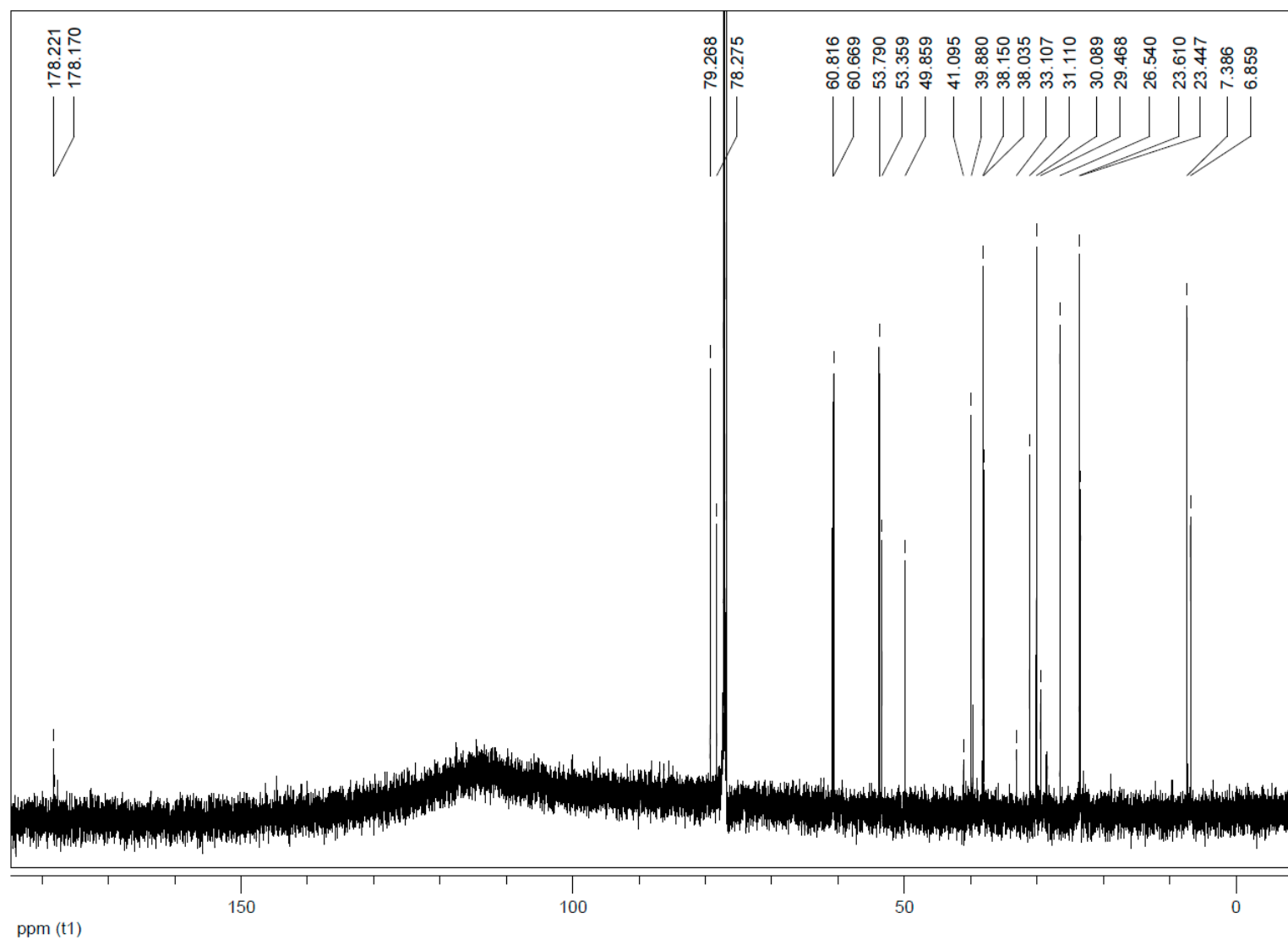


Figure S104. ¹³C-NMR (151 MHz, CDCl₃) spectrum of epoxylactone **9b**.

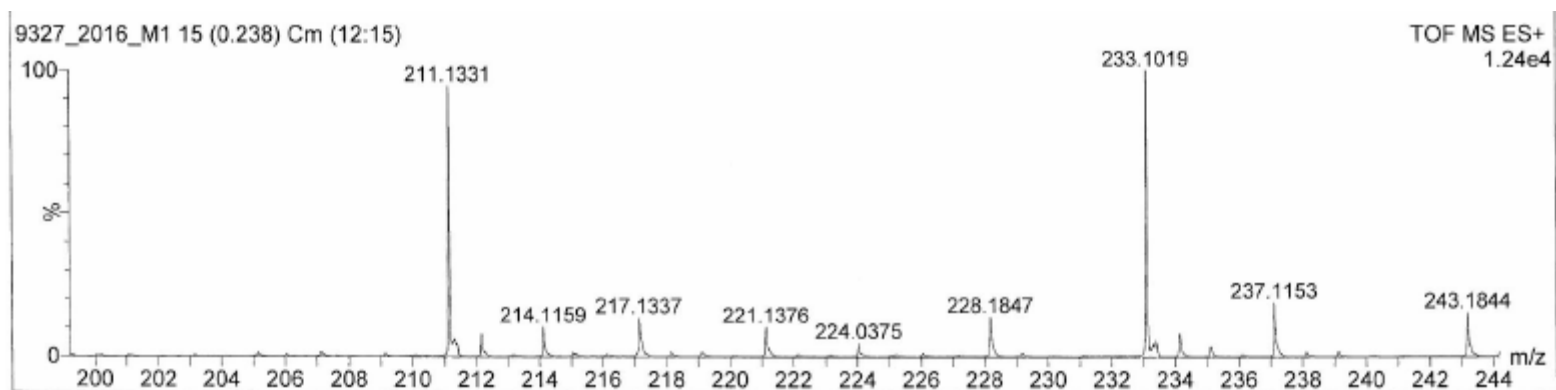


Figure S105. HRMS spectrum of epoxylactone **9b**.

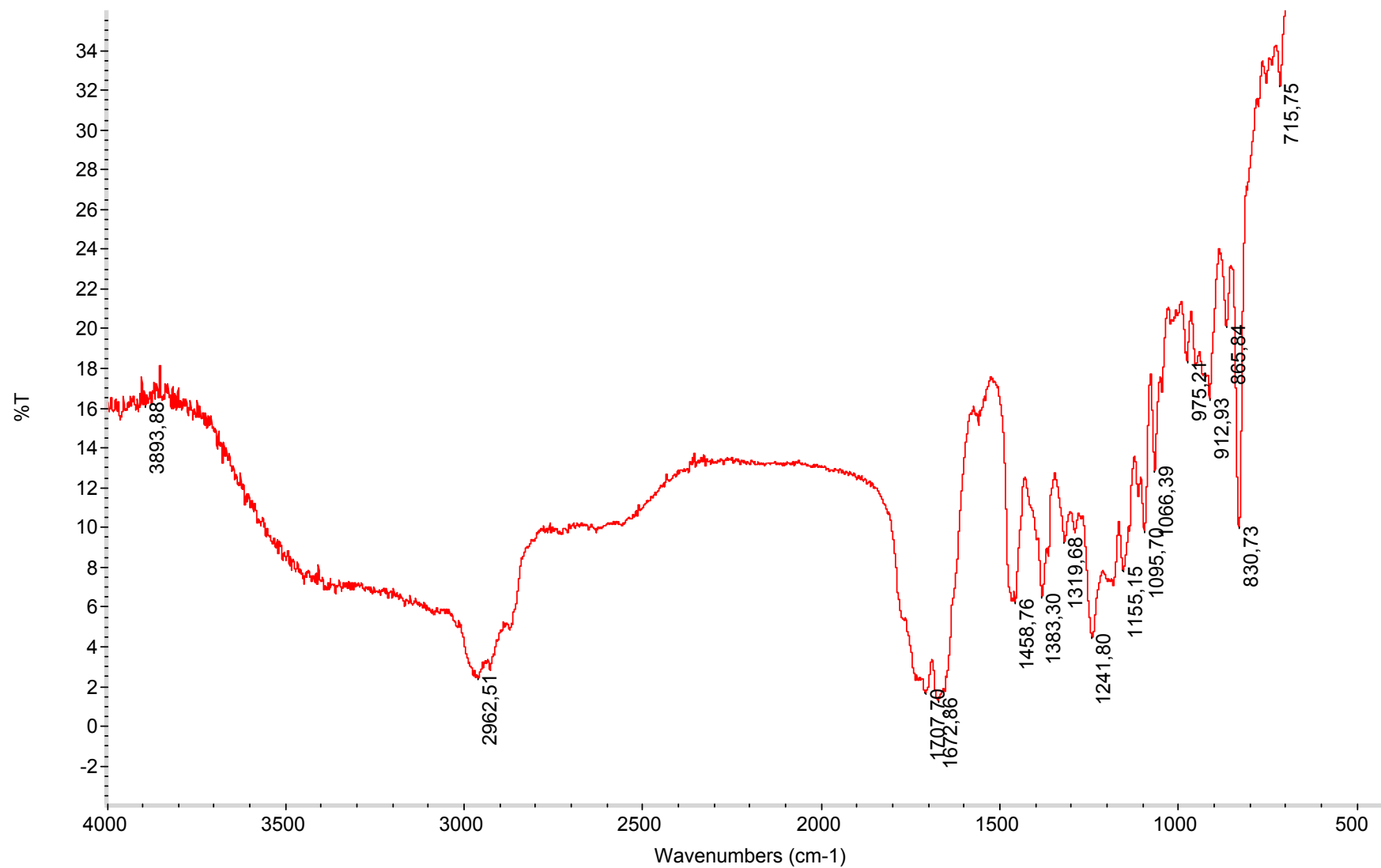


Figure S106. IR spectrum of epoxylactone 9b.

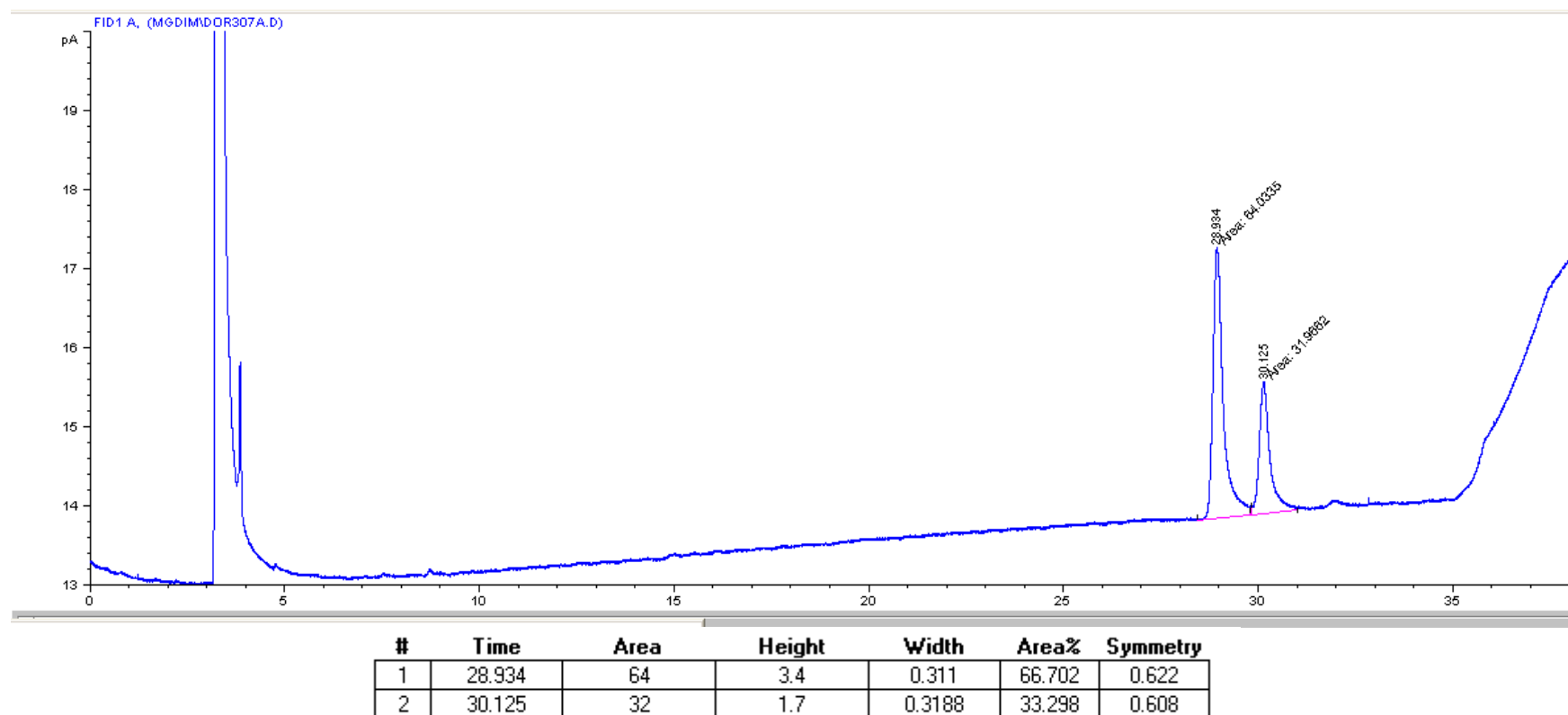


Figure S107. Chiral chromatogram of lactone **7a** (*P. vermiculatum* AM30).

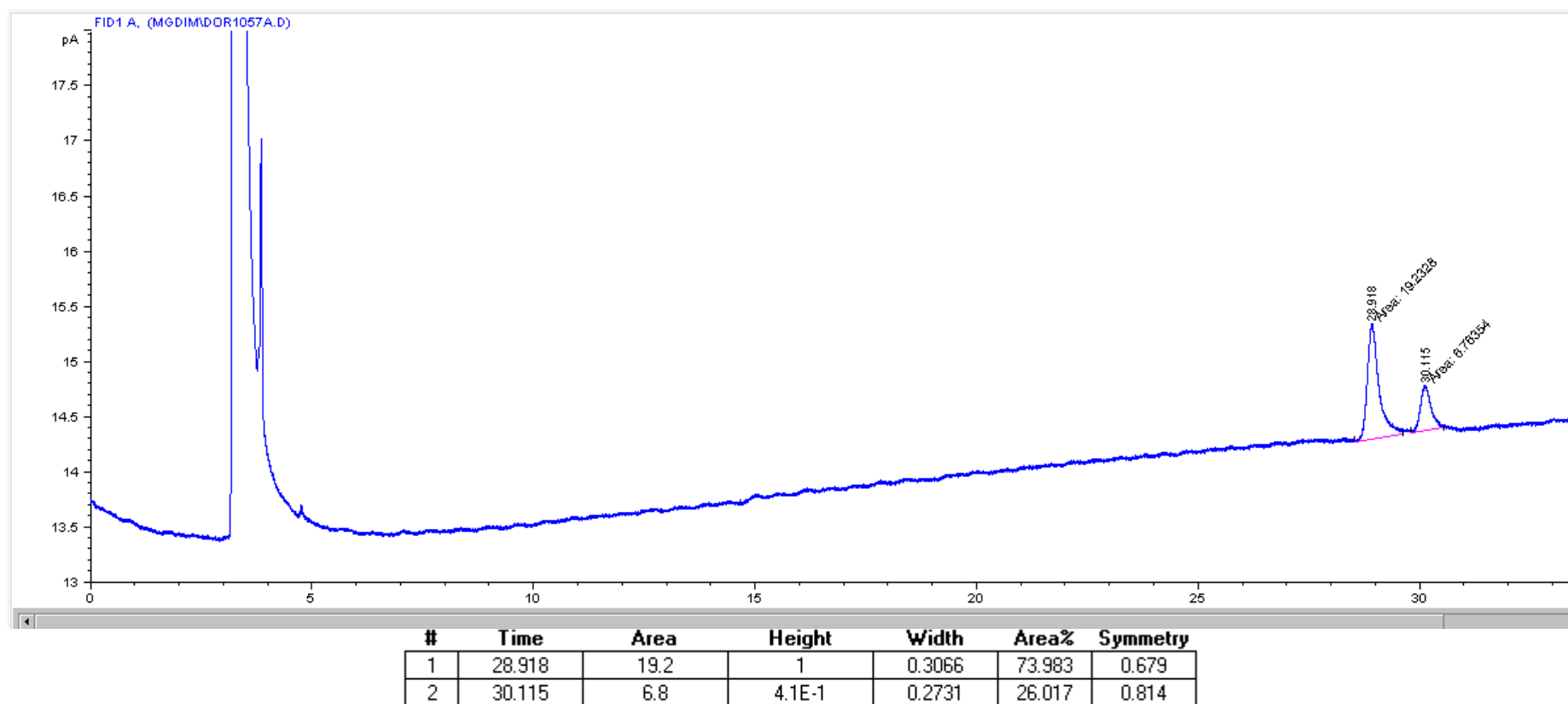


Figure S108. Chiral chromatogram of lactone **7a** (*S. racemosum* AM105).

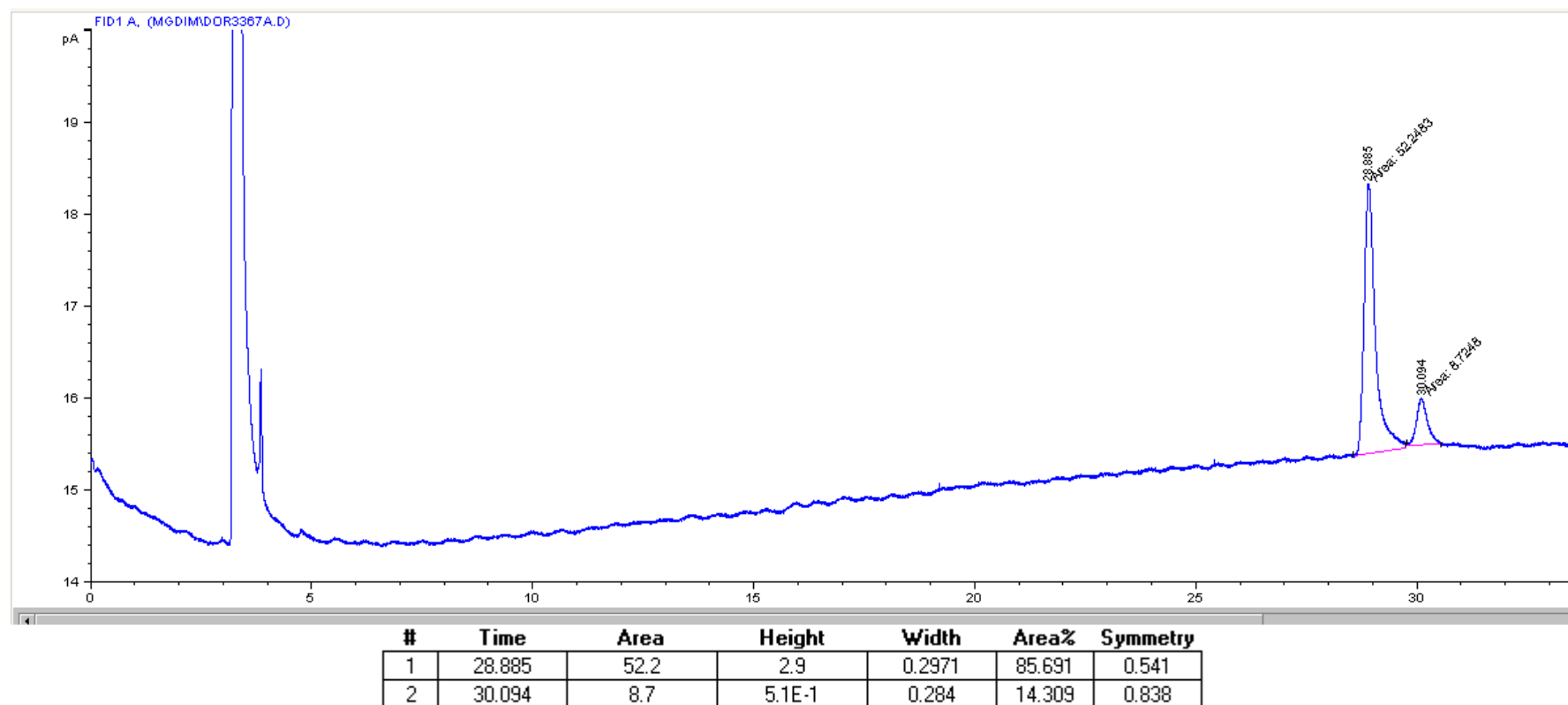


Figure S109. Chiral chromatogram of lactone **7a** (*A. cylindrospora* AM336).

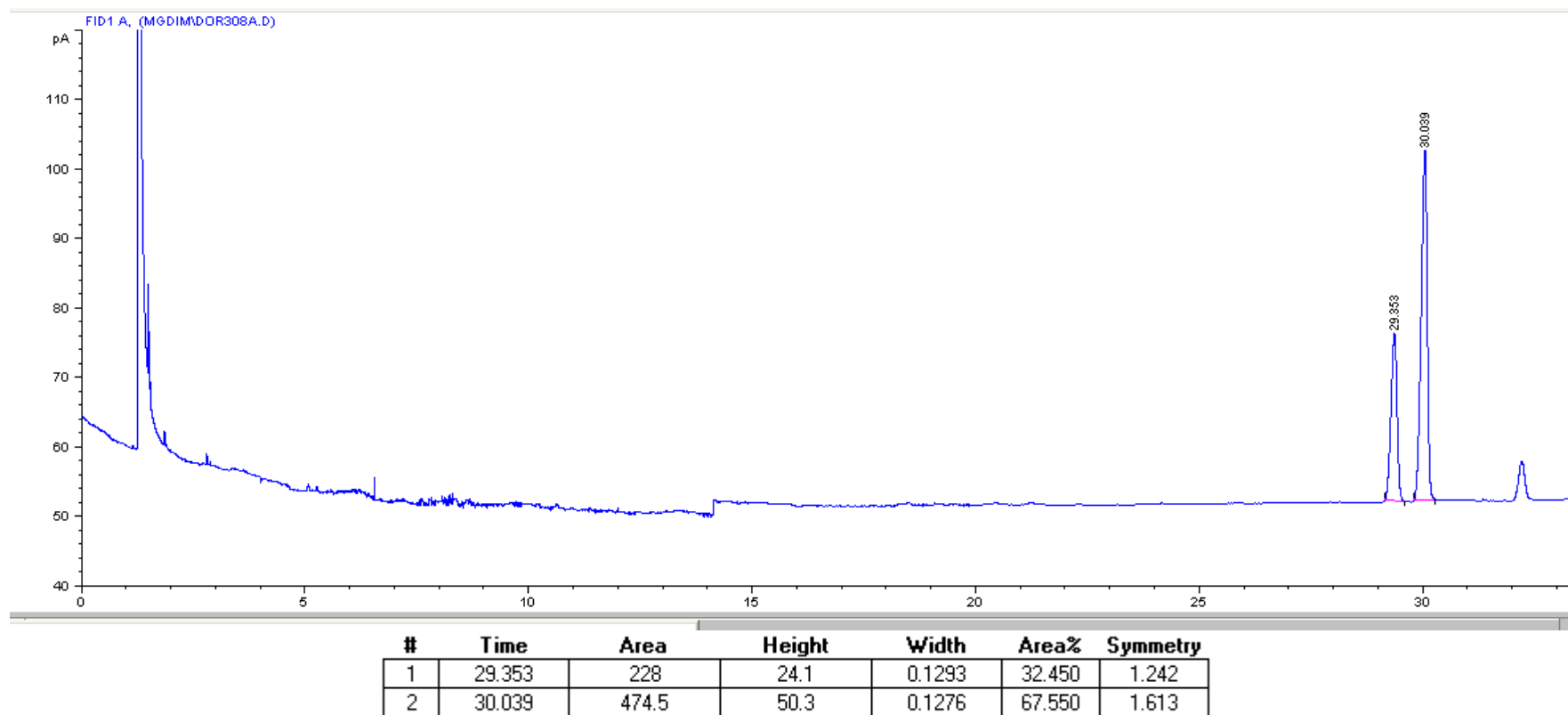
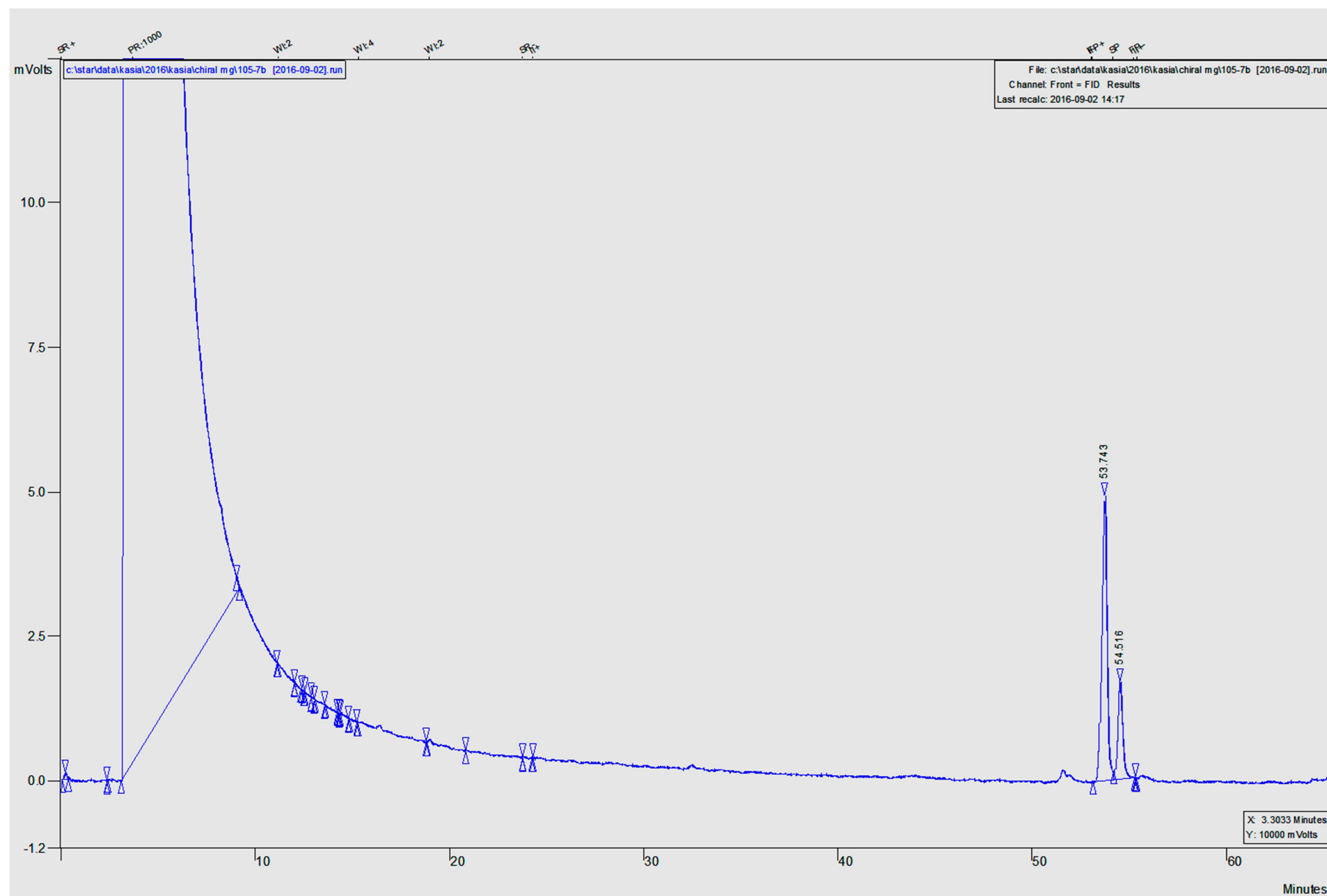


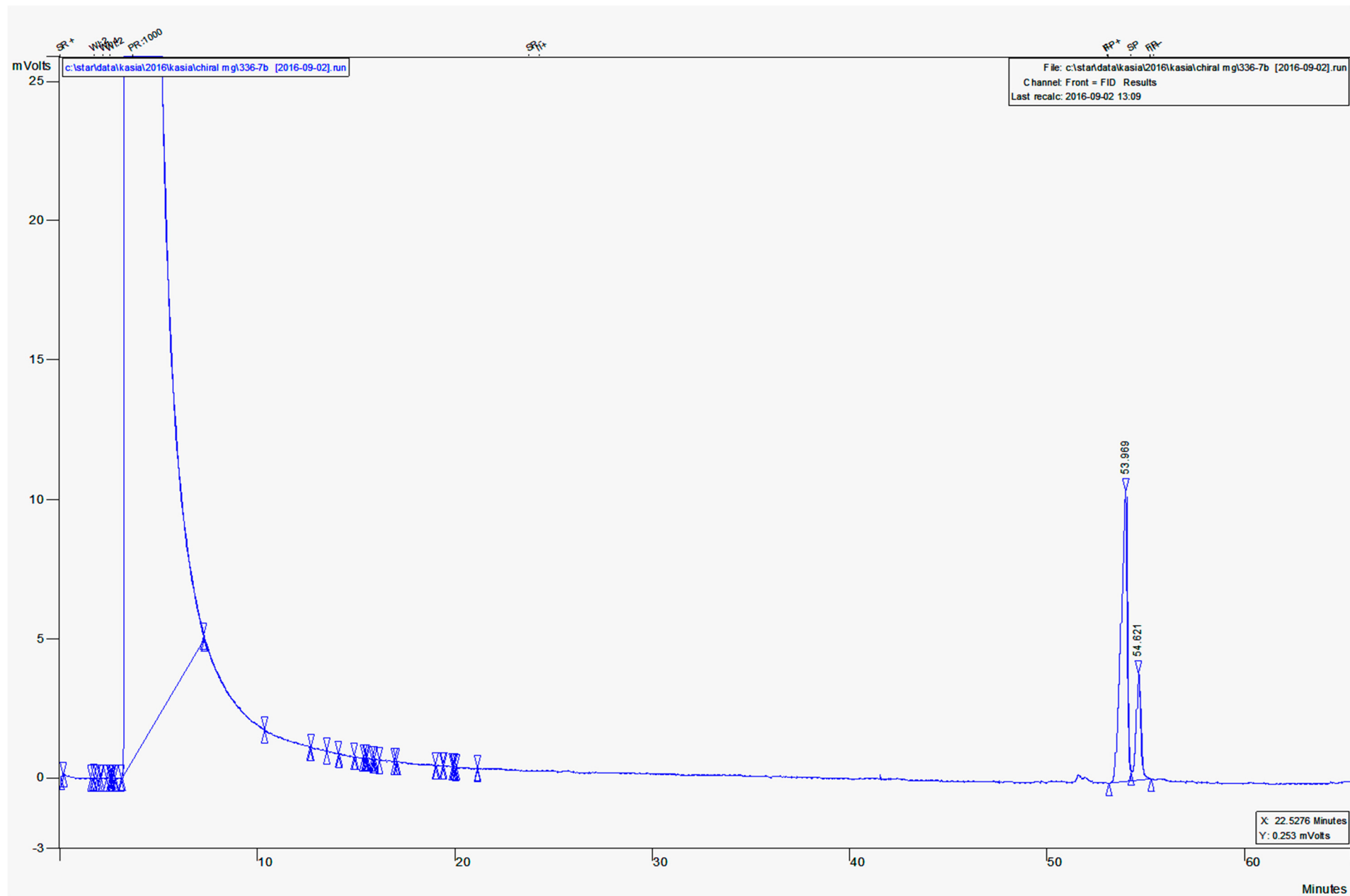
Figure S110. Chiral chromatogram of lactone **8a** (*P. vermiculatum* AM30).



Peak No.	Peak Name	Ret. Result ()	Time (min)	Offset (min)	Width Area (counts)	Sep. 1/2 Code (sec)	Status Codes
1		75.4178	53.743	0.000	93428	BV 0.0	
2		24.5822	54.516	0.000	30452	VB 14.7	
Totals:		100.0000		0.000	123880		

Total Unidentified Counts : 123880 counts

Figure S111. Chiral chromatogram of lactone **7b** (*S. racemosum* AM105).



Peak No.	Peak Name	Ret. Result ()	Time (min)	Offset (min)	Width Area (counts)	Sep. 1/2 Code (sec)	Status Codes
1		78.6297	53.969	0.000	238261	BV 0.0	
2		21.3703	54.621	0.000	64755	VB 14.1	
Totals:		100.0000		0.000	303016		
Total Unidentified Counts:				303016 counts			

Figure S112. Chiral chromatogram of lactone **7b** (*A. cylindrospora* AM336).

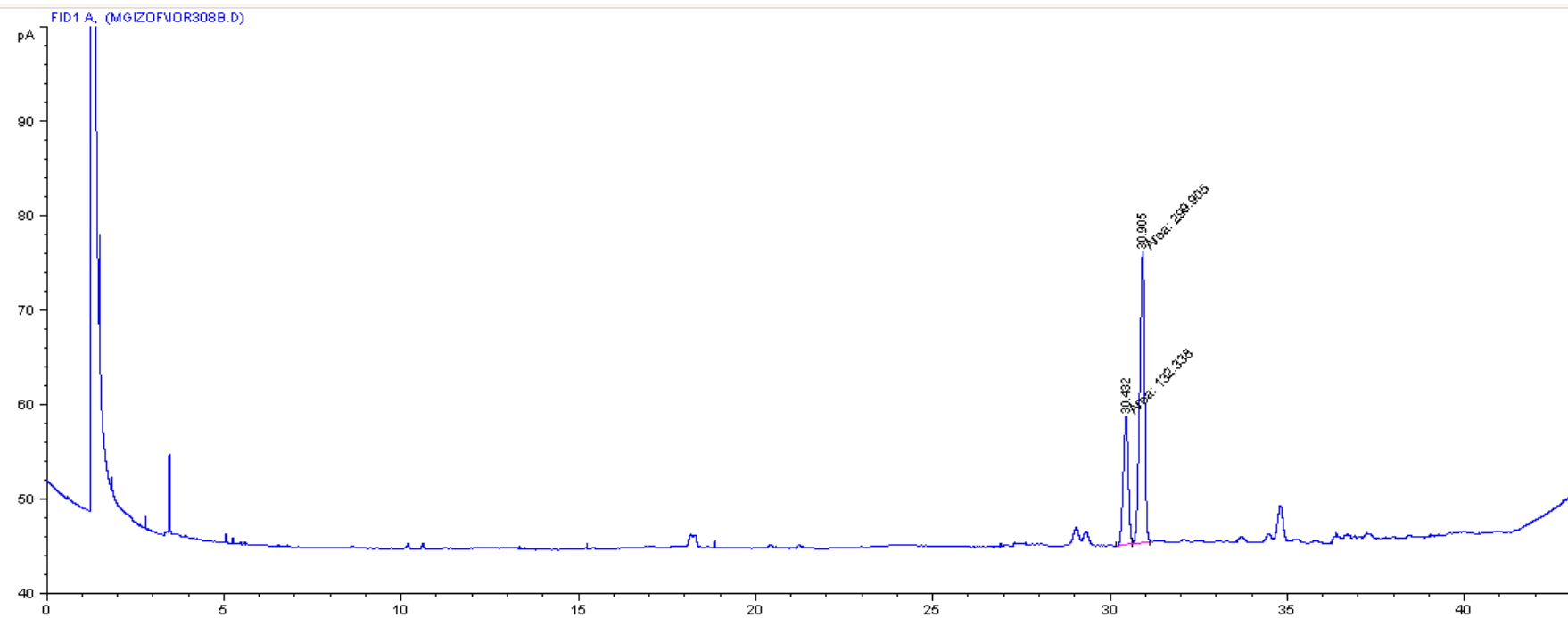


Figure S113. Chiral chromatogram of lactone **8b** (*P. vermiculatum* AM30).