

Supplementary information

New Bromo- and Iodo-hydroxylactones with Two Methyl Groups Obtained by Biotransformation of Bicyclic Halolactones

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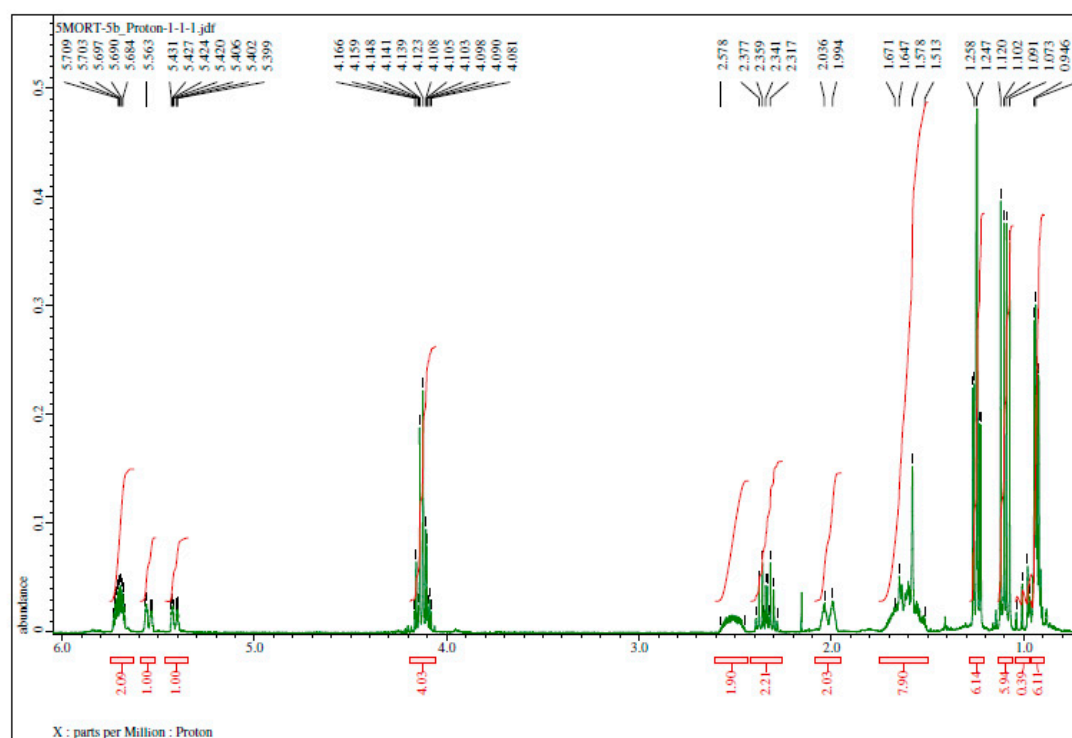


Figure S1. ¹H NMR (400 MHz, CDCl₃) spectrum of ester 2.

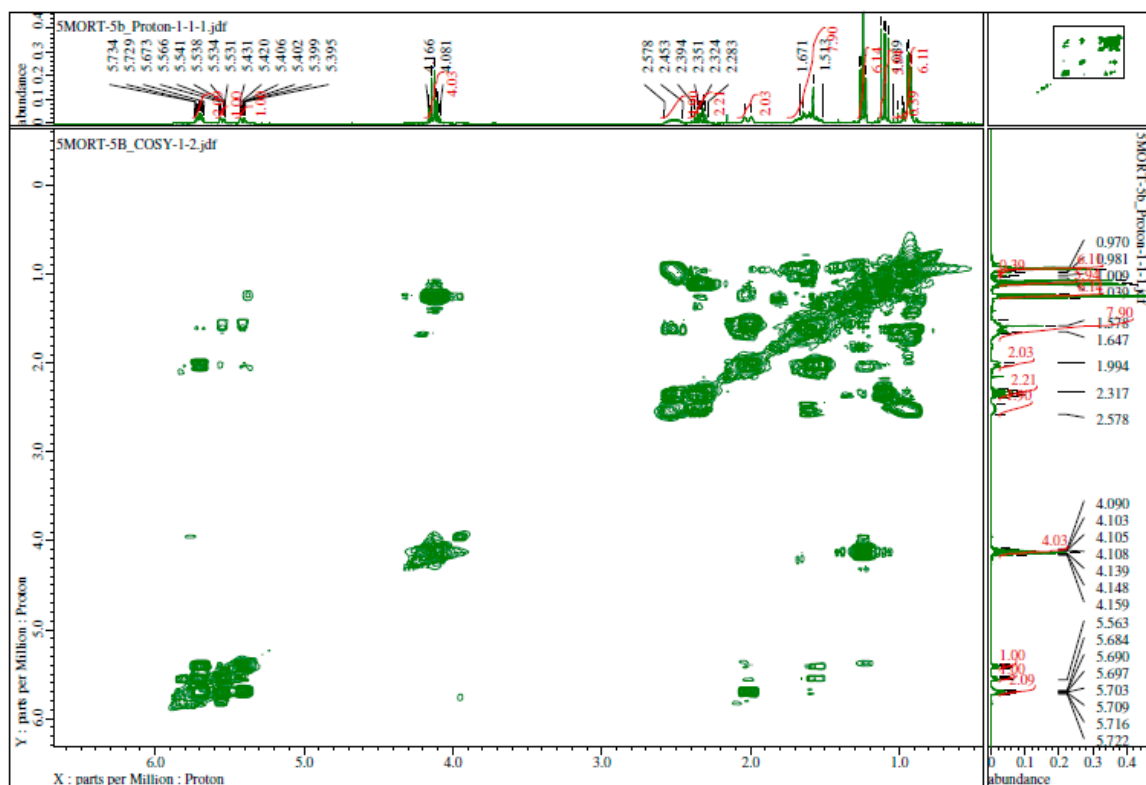


Figure S2. COSY (100 MHz, CDCl₃) spectrum of ester 2.

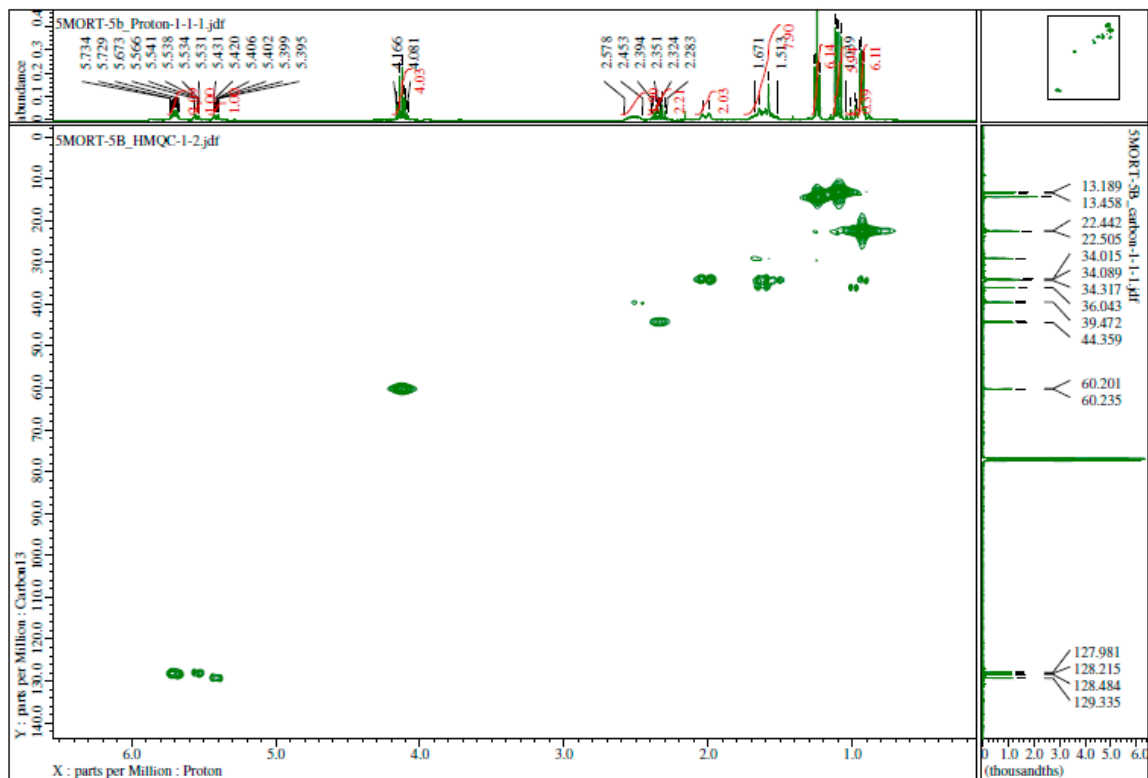


Figure S3. HMQC (100 MHz, CDCl₃) spectrum of ester 2.

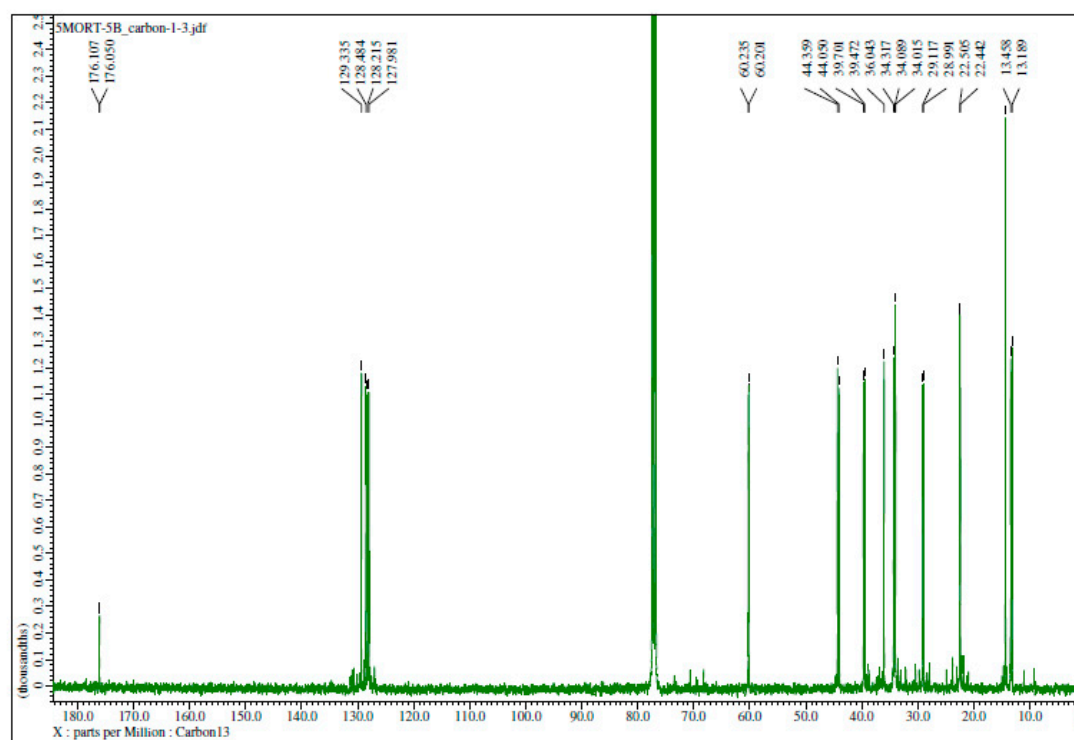


Figure S4. ^{13}C NMR (100 MHz, CDCl_3) spectrum of ester 2.

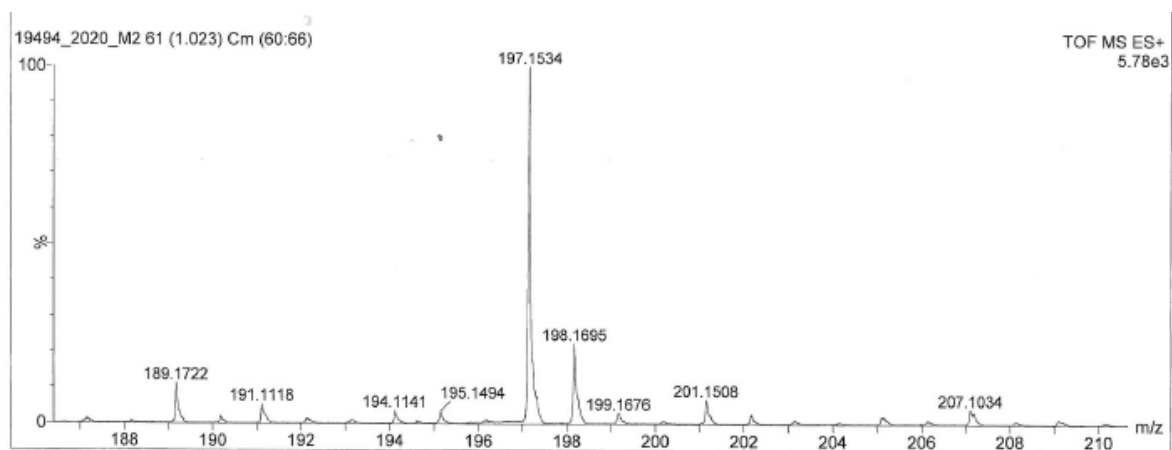


Figure S5. HRMS spectrum of ester 2.

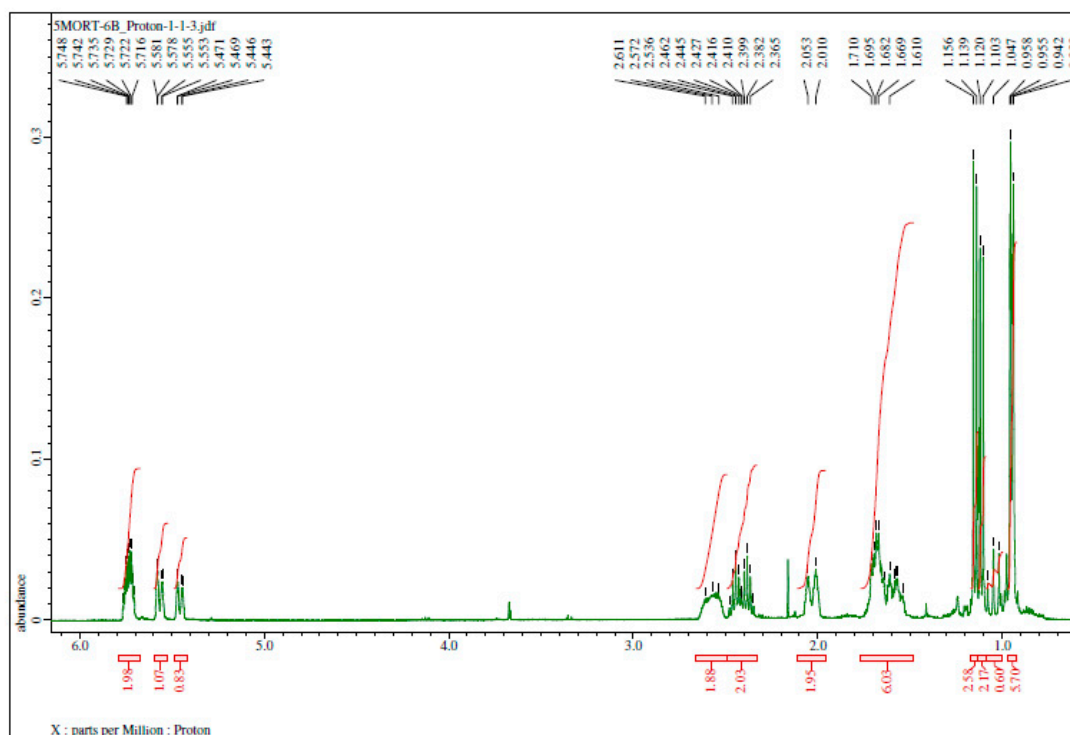


Figure S6. ^1H NMR (400 MHz, CDCl_3) spectrum of acid 3.

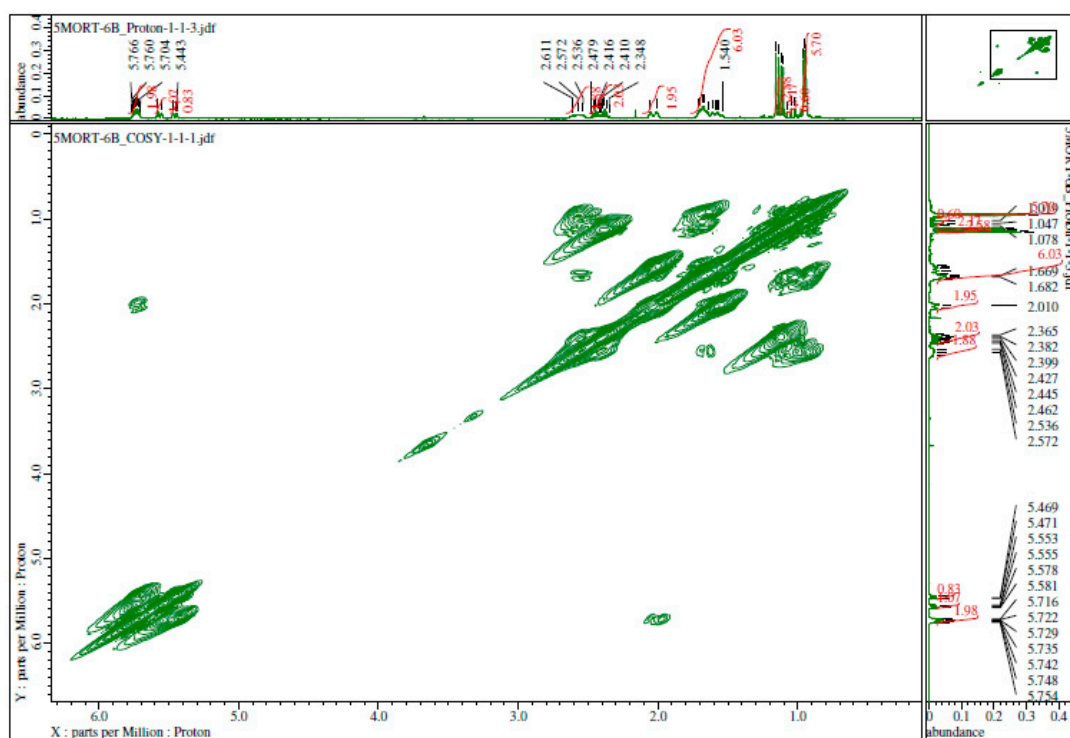


Figure S7. COSY (100 MHz, CDCl_3) spectrum of acid 3.

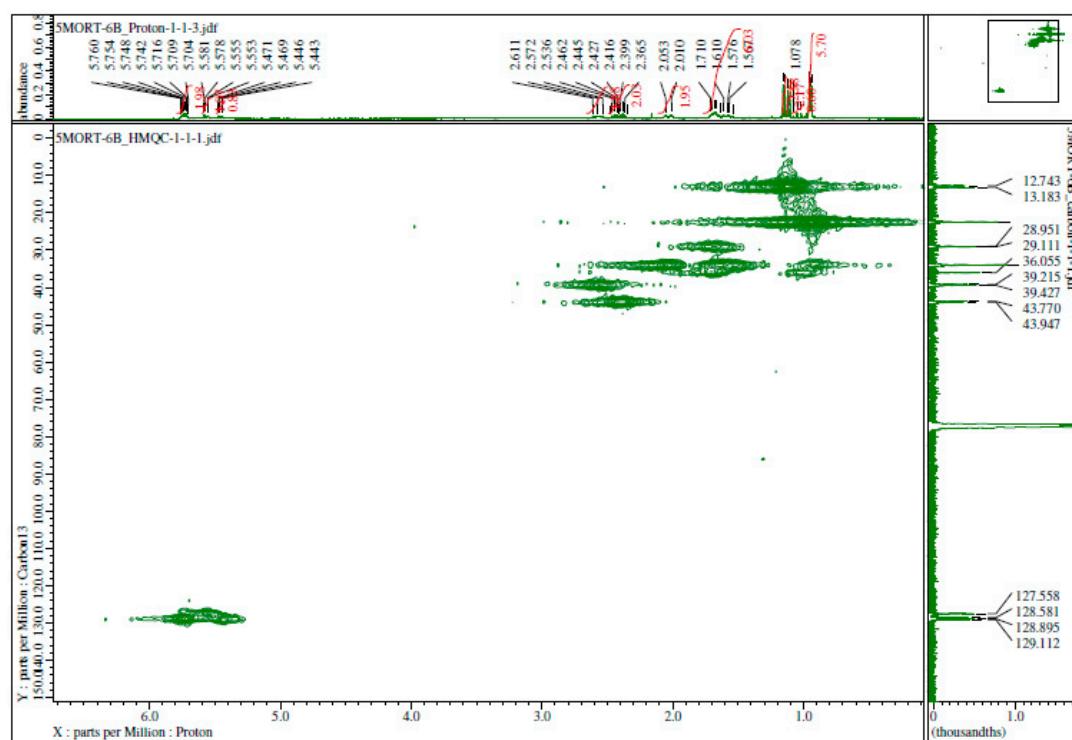


Figure S8. HMQC (100 MHz, CDCl₃) spectrum of acid 3.

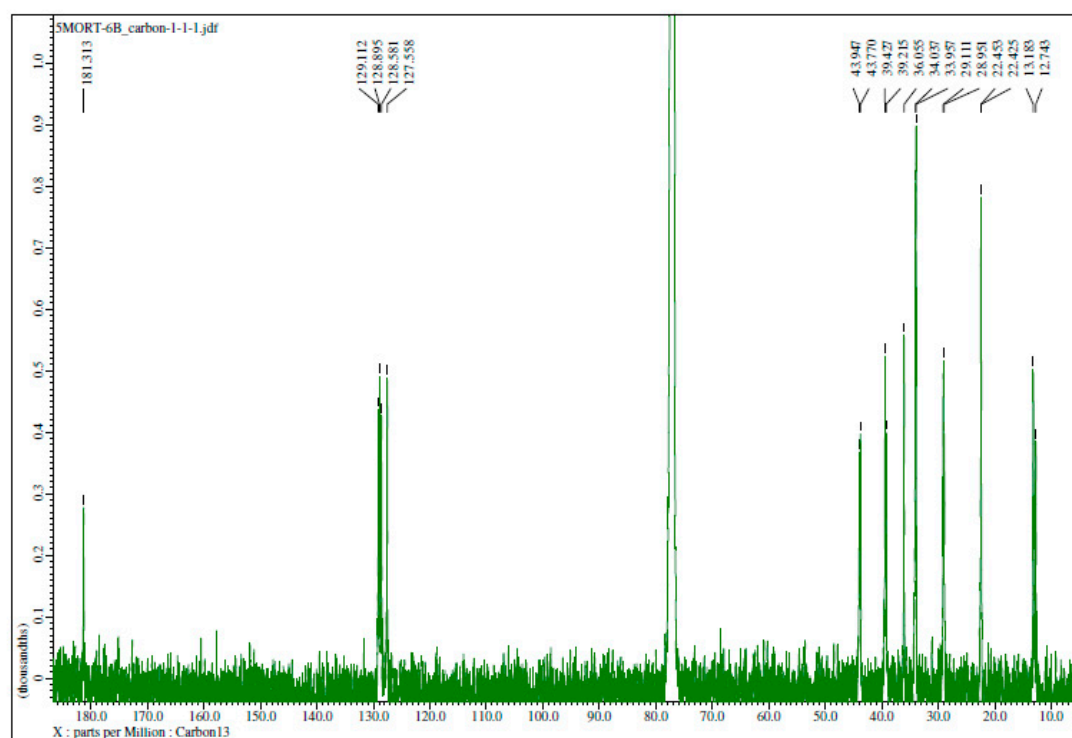


Figure S9. ¹³C NMR (100 MHz, CDCl₃) spectrum of acid 3.

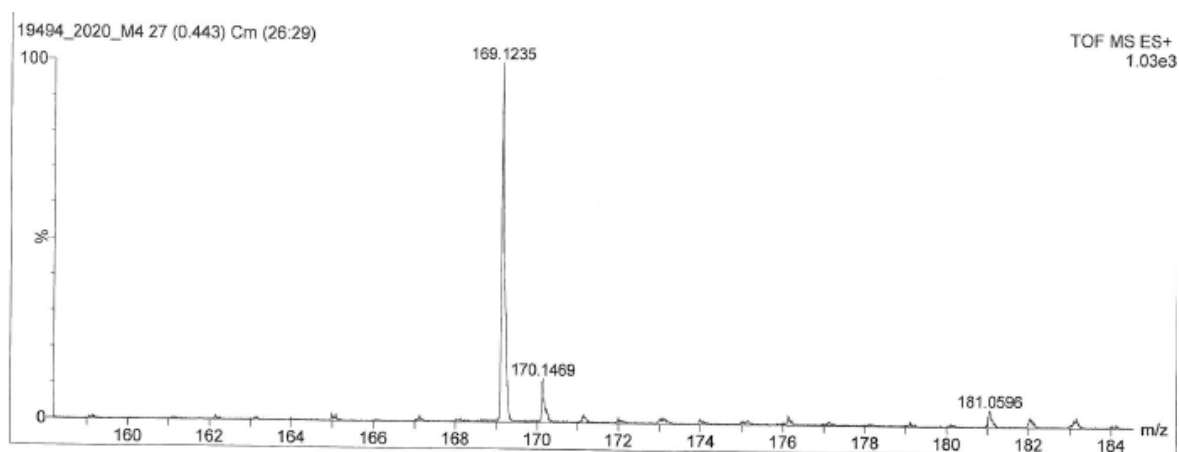


Figure S10. HRMS spectrum of acid 3.

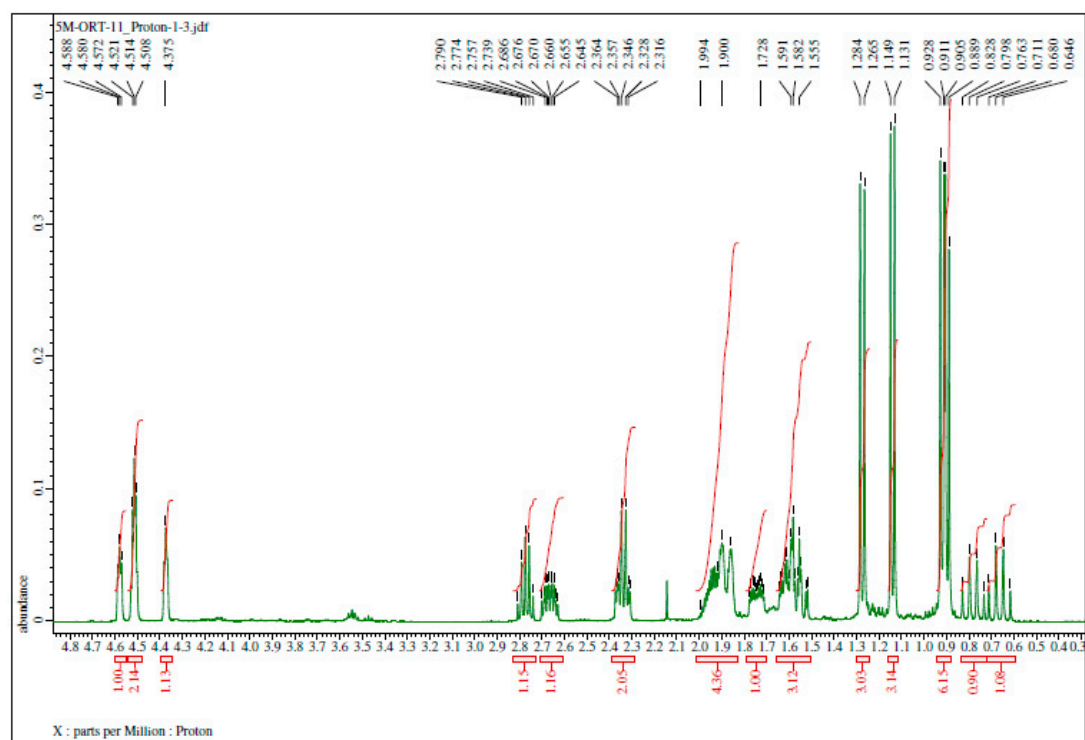


Figure S11. ^1H NMR (400 MHz, CDCl_3) spectrum of chlorolactone 4.

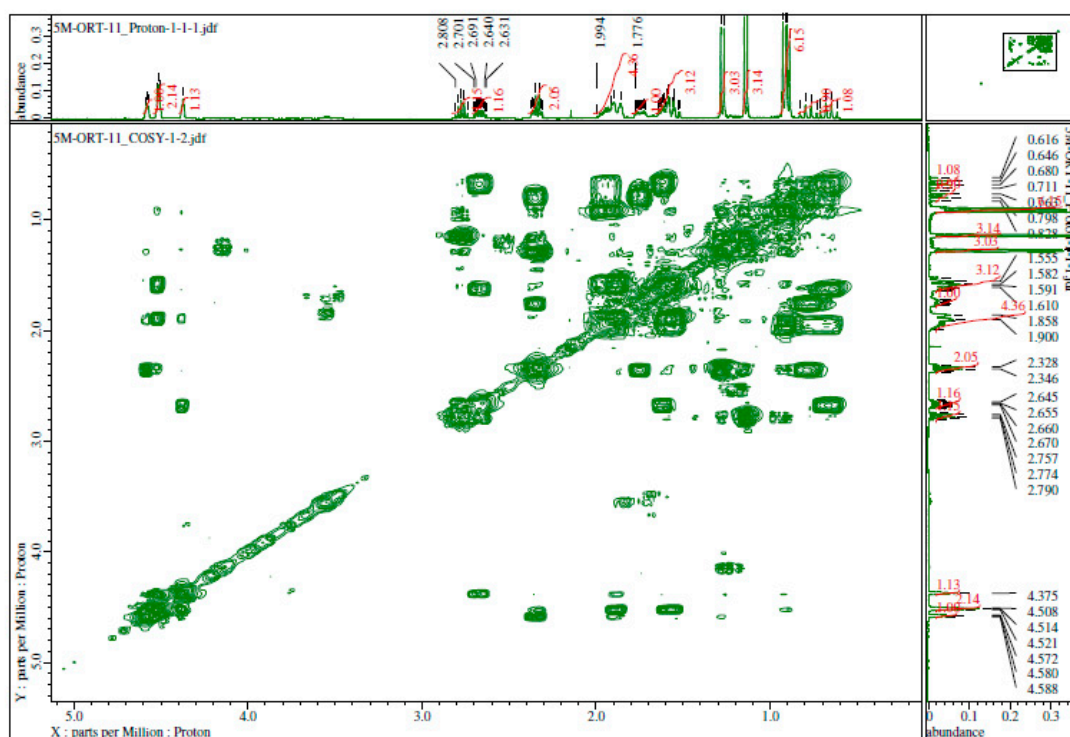


Figure S12. COSY (100 MHz, CDCl₃) spectrum of chlorolactone 4.

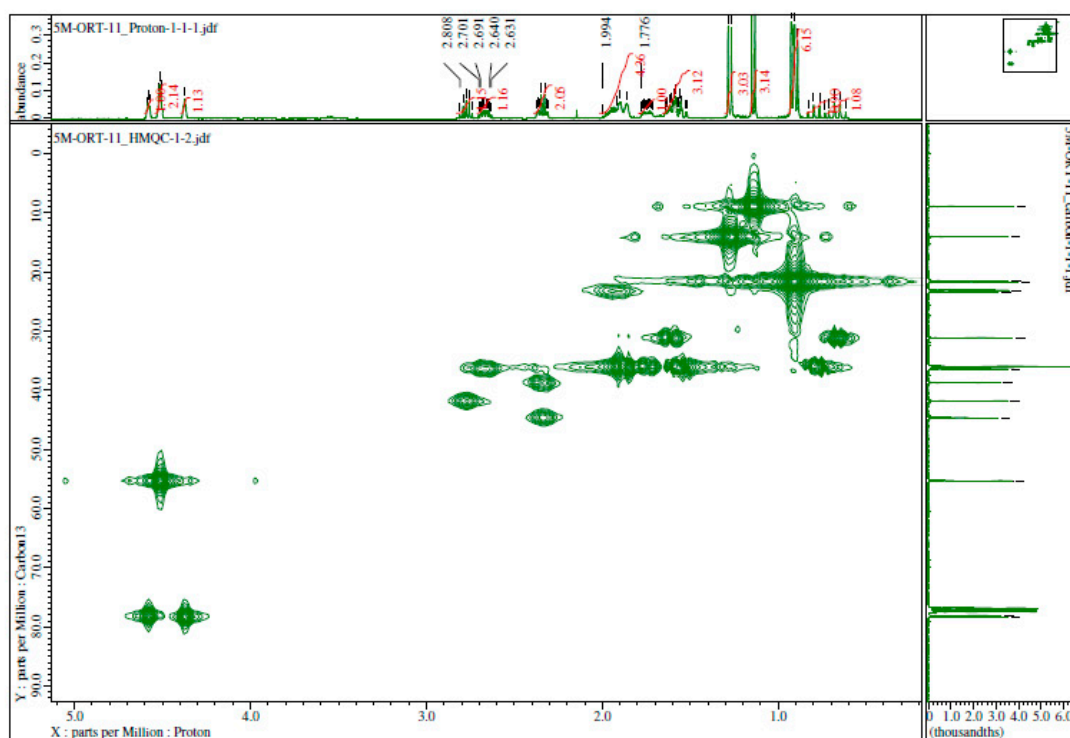


Figure S13. HMQC (100 MHz, CDCl₃) spectrum of chlorolactone 4.

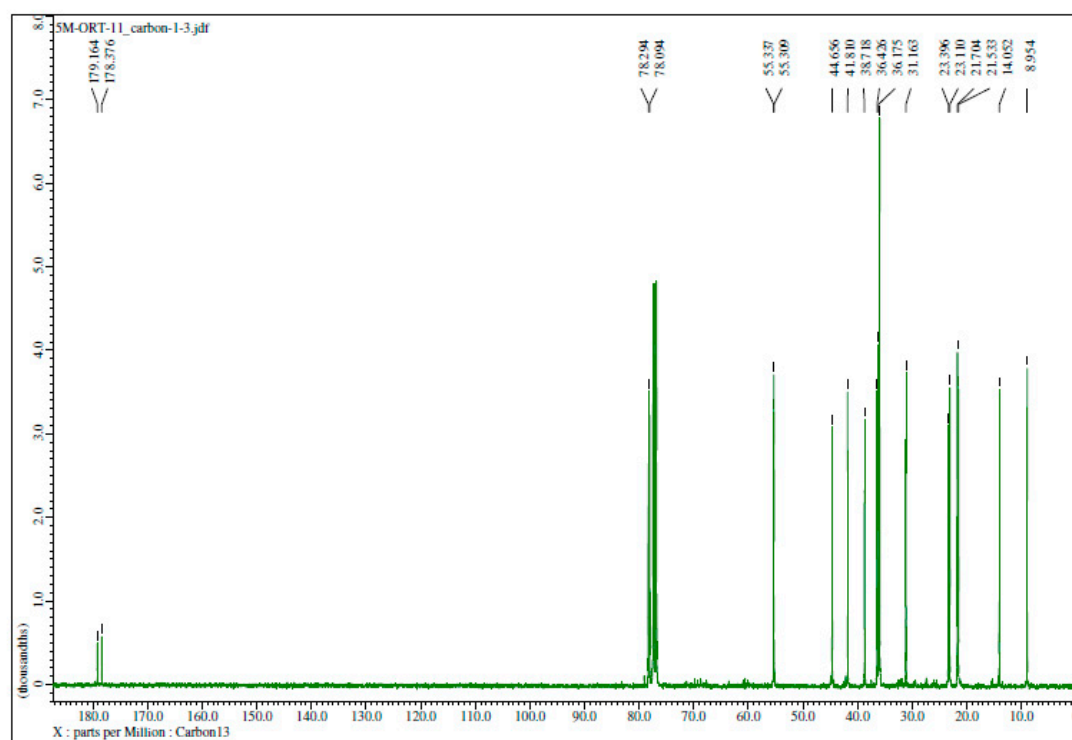


Figure S14. ¹³C NMR (100 MHz, CDCl₃) spectrum of chlorolactone 4.

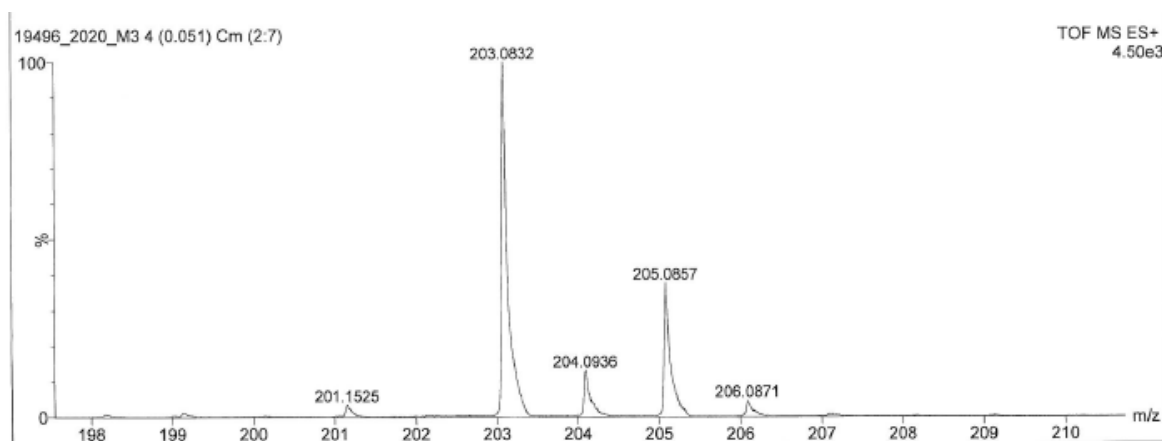


Figure S15. HRMS spectrum chlorolactone 4.

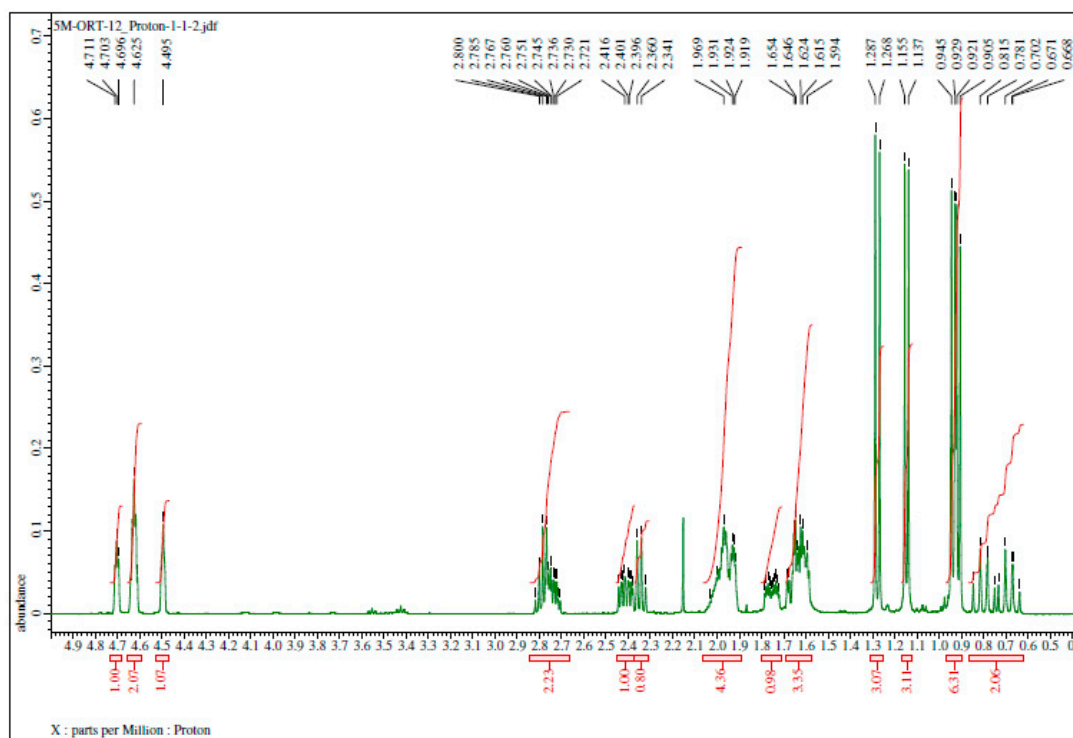


Figure S16. ^1H NMR (400 MHz, CDCl_3) spectrum of bromolactone 5.

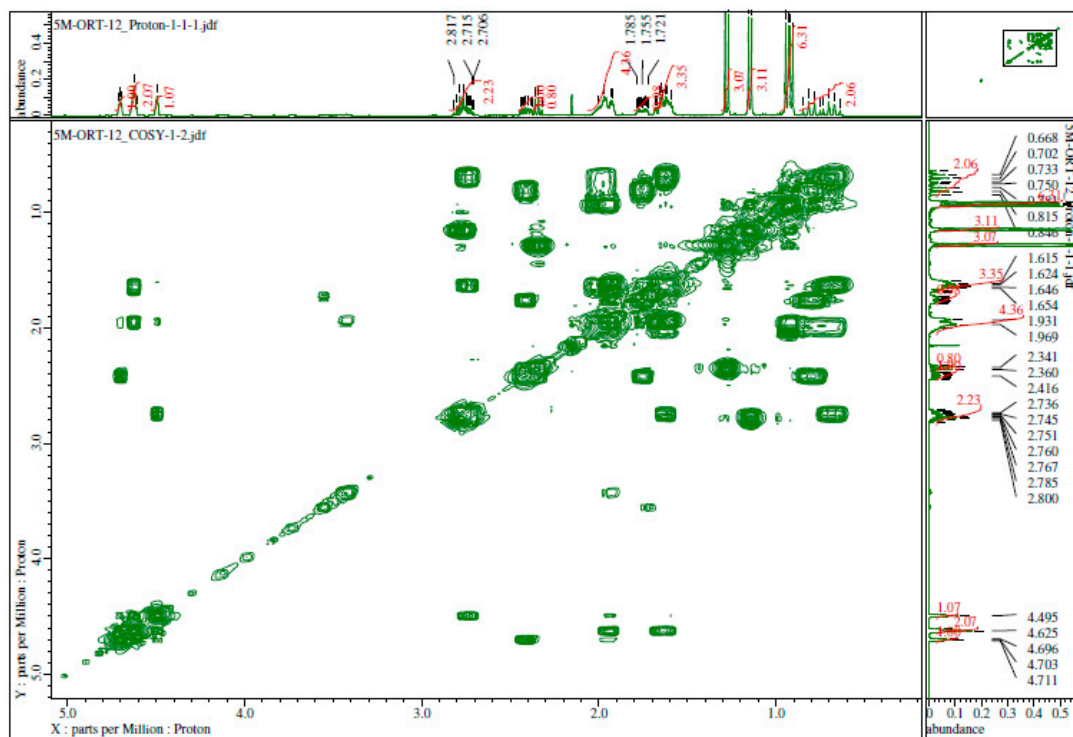


Figure S17. COSY (100 MHz, CDCl_3) spectrum of bromolactone 5.

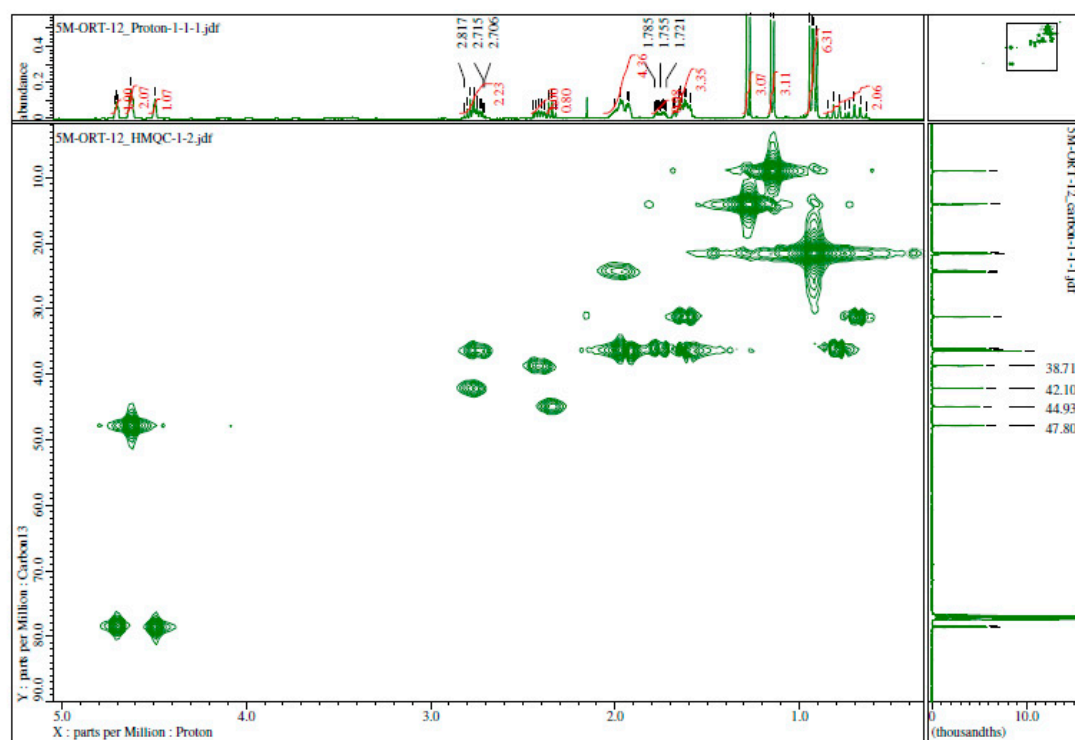


Figure S18. HMQC (100 MHz, CDCl₃) spectrum of bromolactone 5.

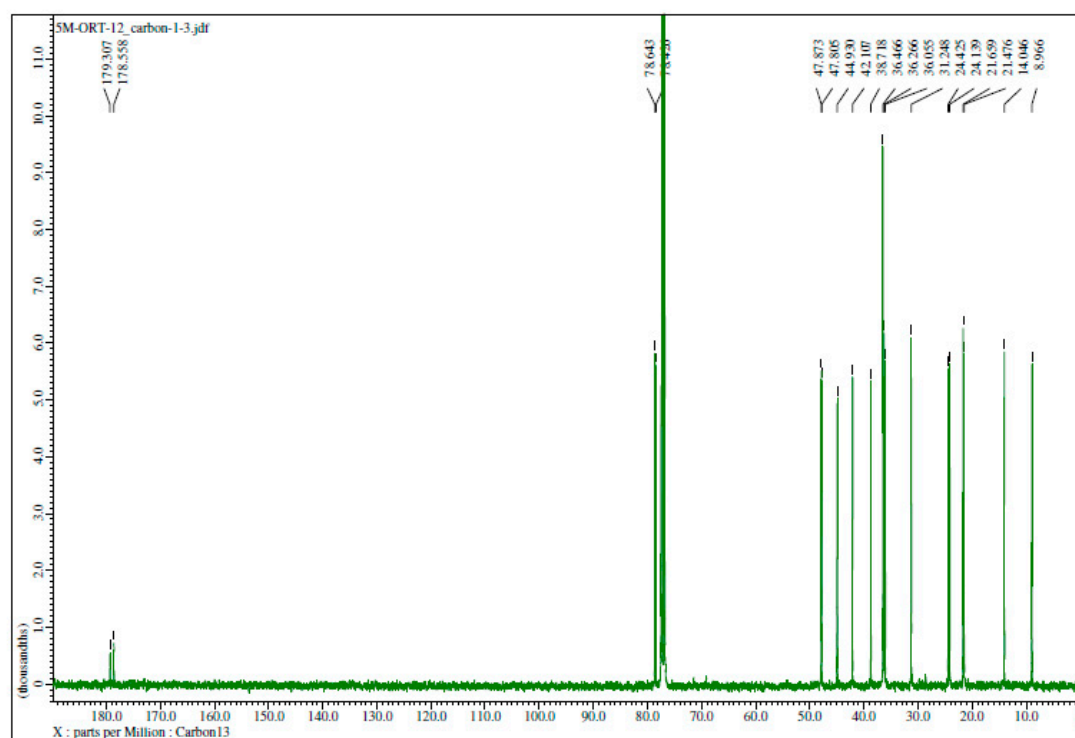


Figure S19. ¹³C NMR (100 MHz, CDCl₃) spectrum bromolactone 5.

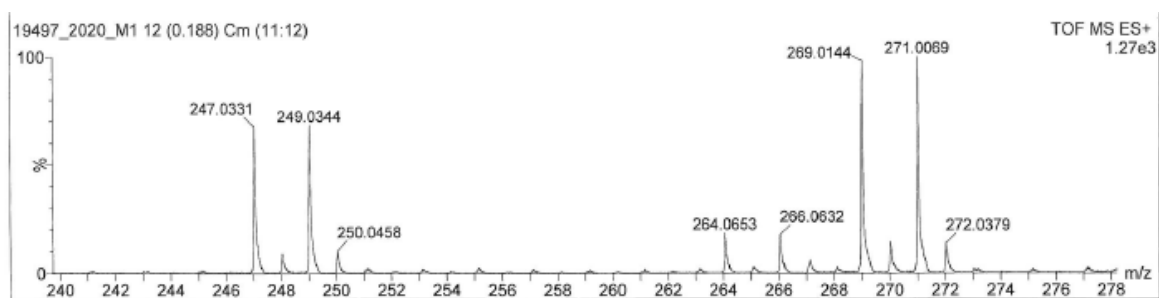


Figure S20. HRMS spectrum bromolactone 5.

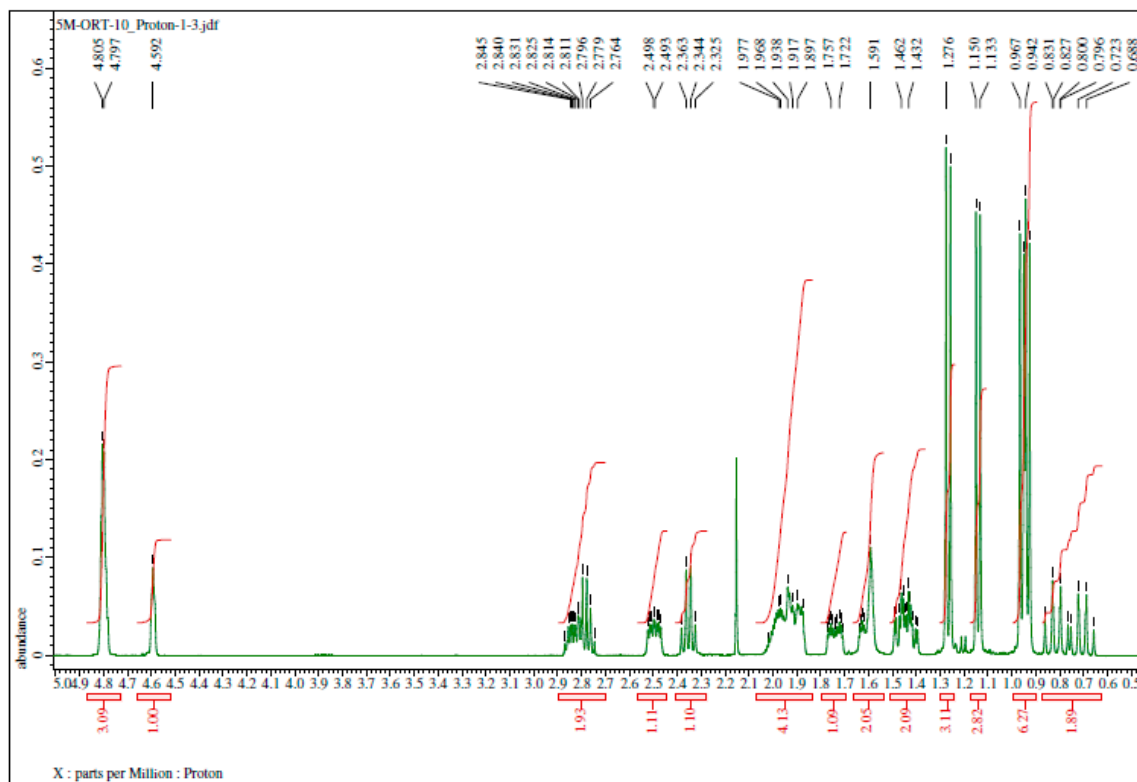


Figure S21. ^1H NMR (400 MHz, CDCl_3) spectrum of iodolactone 6.

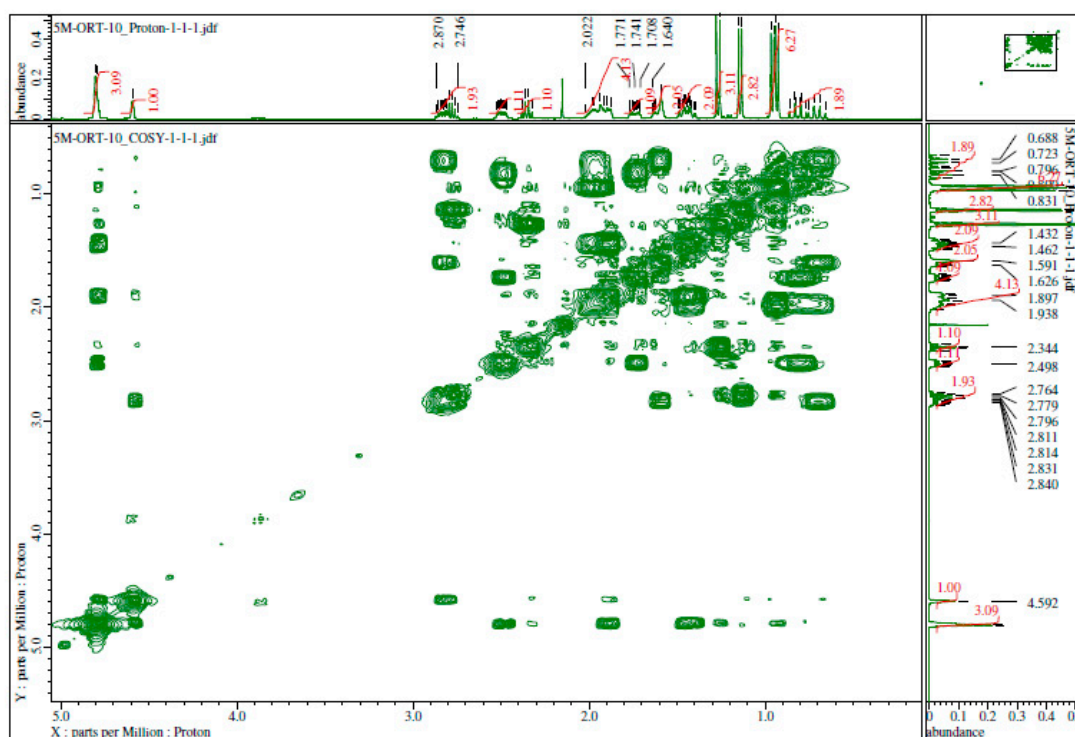


Figure S22. COSY (100 MHz, CDCl₃) spectrum of iodolactone 6.

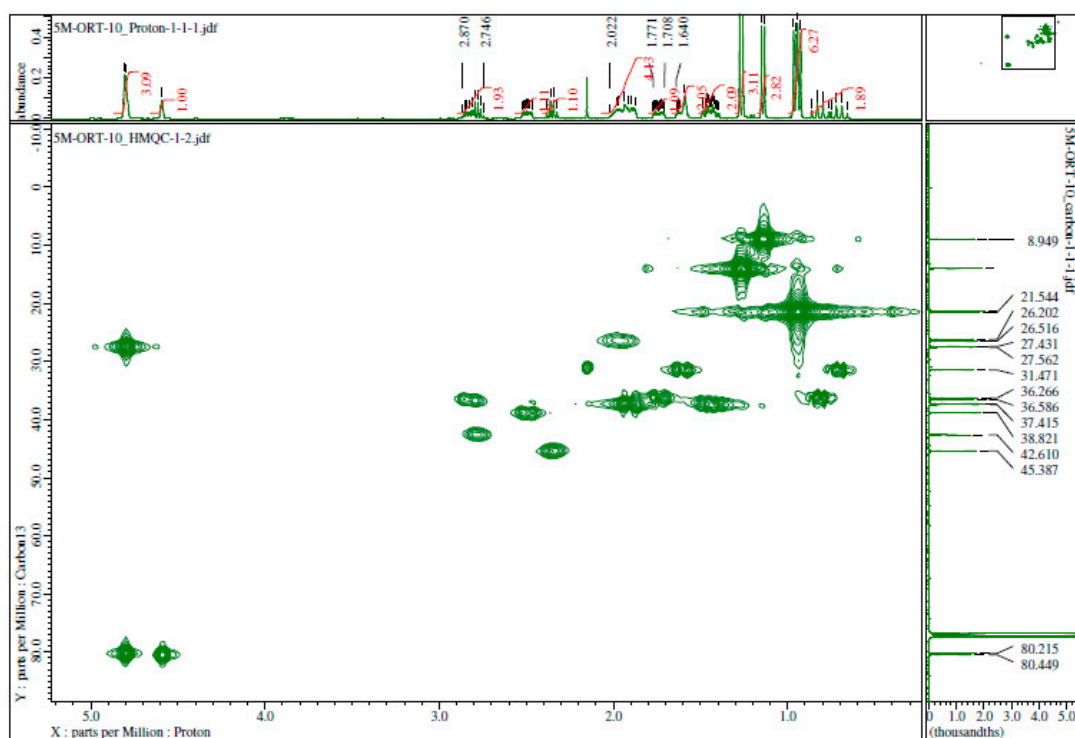


Figure S23. HMQC (100 MHz, CDCl₃) spectrum of iodolactone 6.

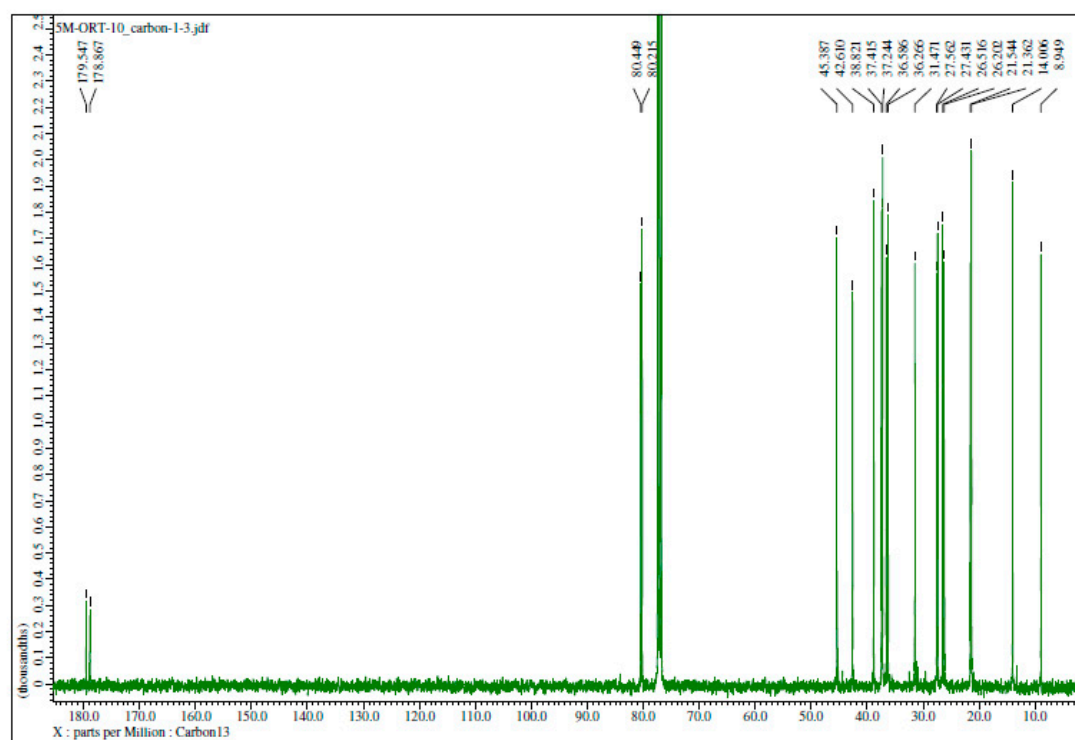


Figure S24. ^{13}C NMR (100 MHz, CDCl_3) spectrum of iodolactone 6.

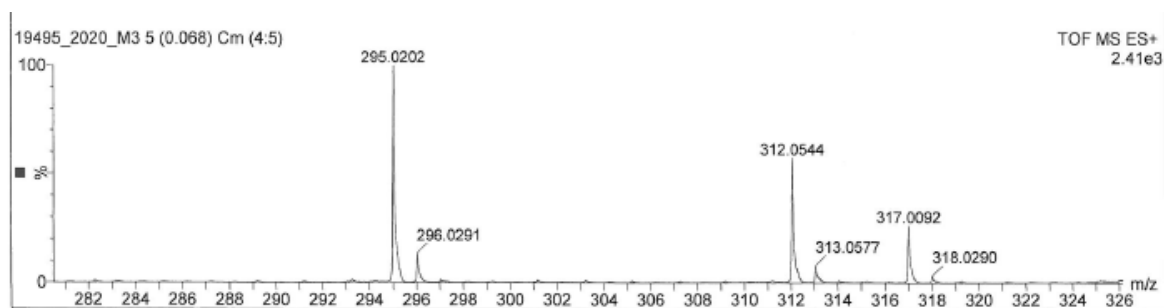


Figure S25. HRMS spectrum of iodolactone 6.

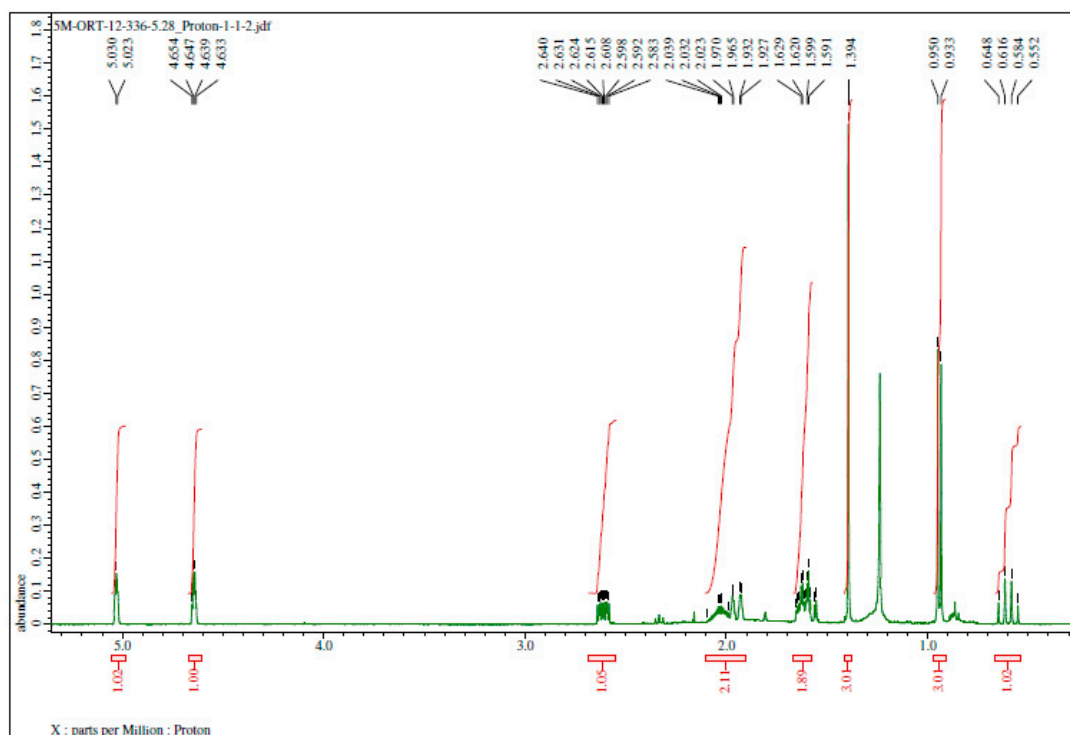


Figure S26. ^1H NMR (400 MHz, CDCl_3) spectrum of bromo-hydroxylactone 7.

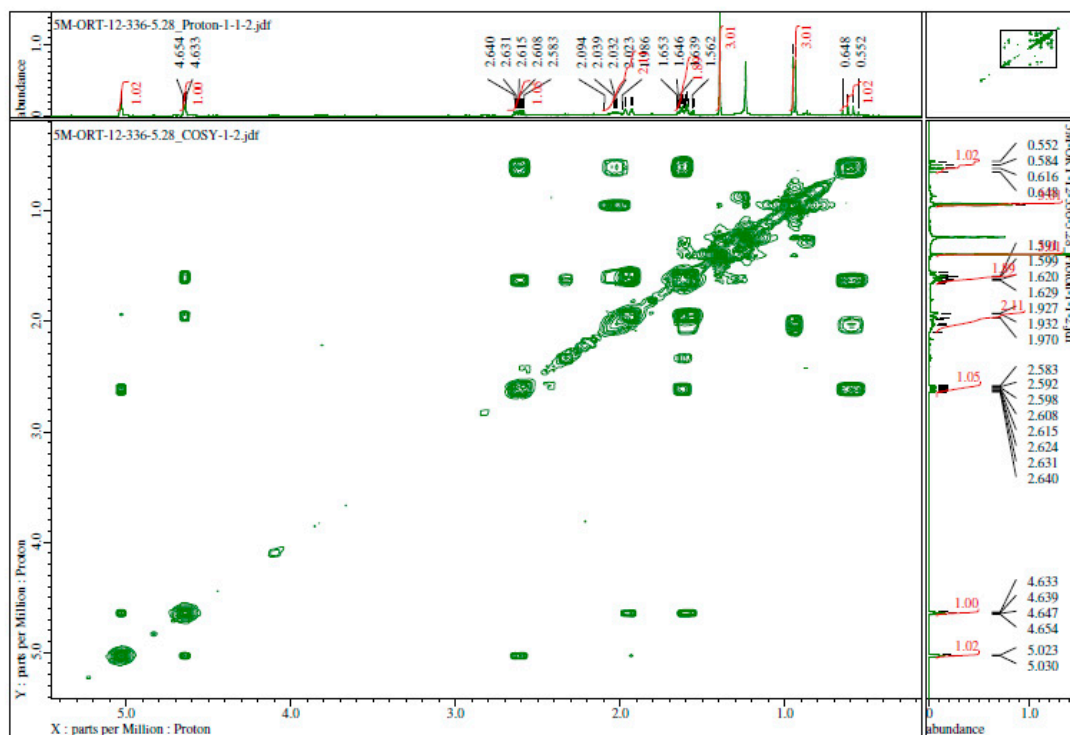


Figure S27. COSY (100 MHz, CDCl_3) spectrum of bromo-hydroxylactone 7.

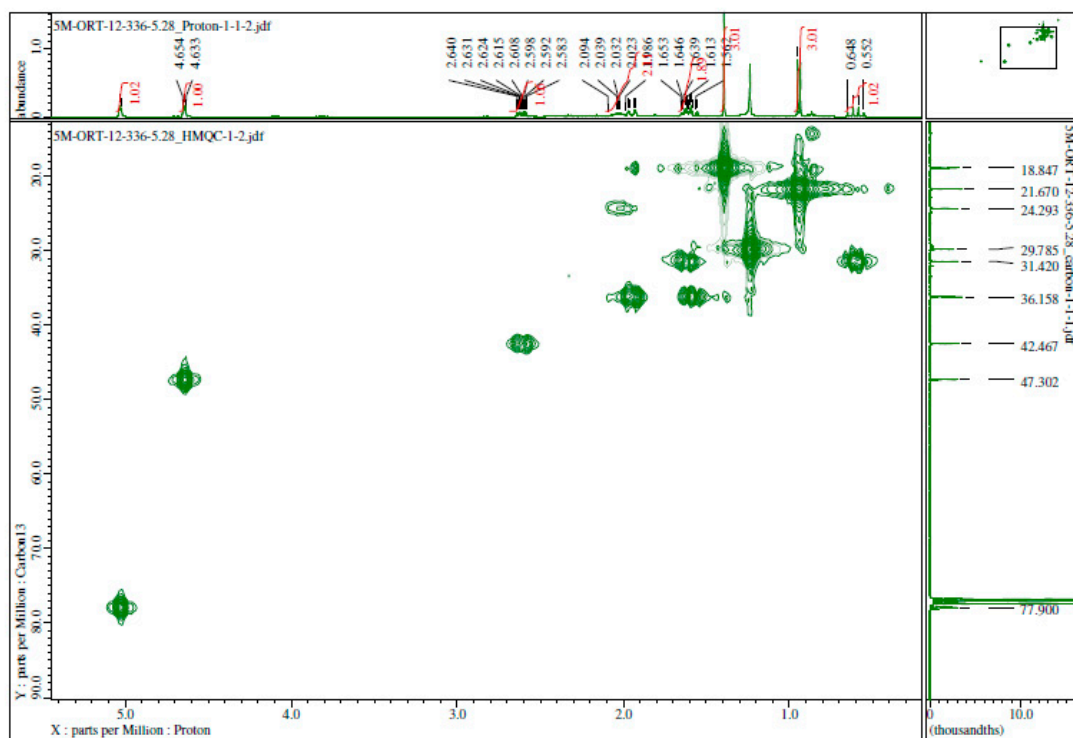


Figure S28. HMQC (100 MHz, CDCl₃) spectrum of bromo-hydroxylactone 7.

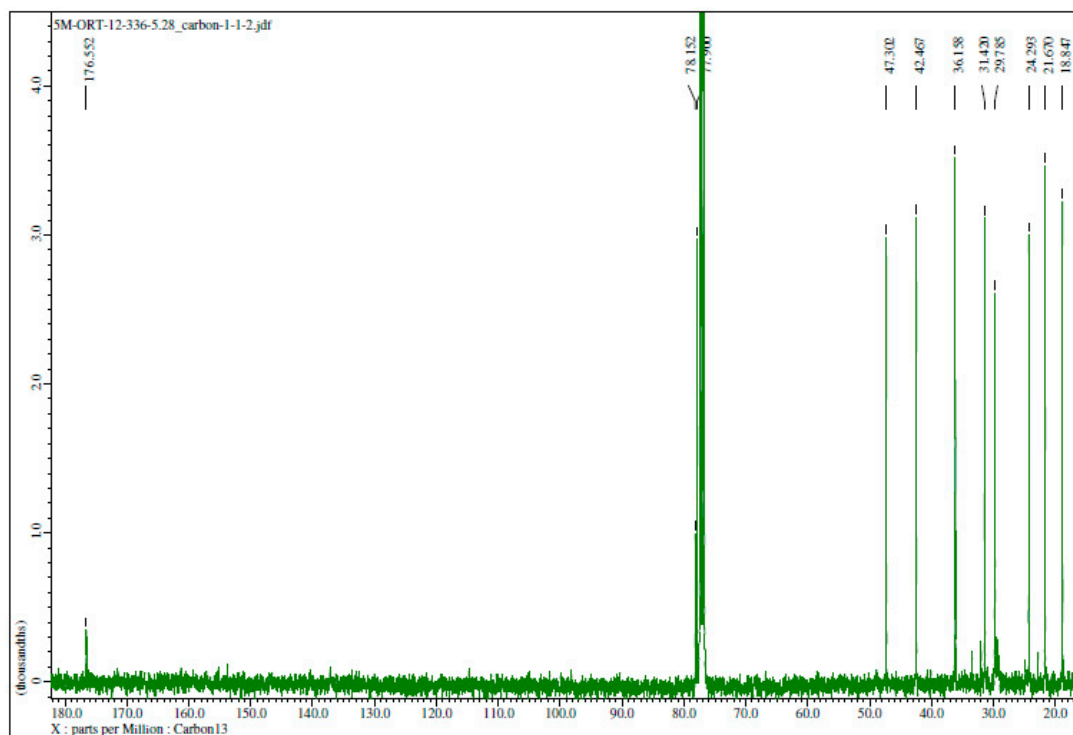


Figure S29. ¹³C NMR (100 MHz, CDCl₃) spectrum of bromo-hydroxylactone 7.

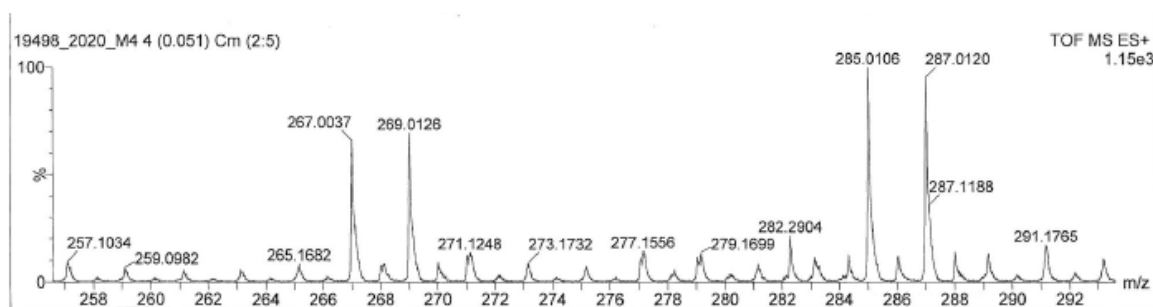


Figure S30. HRMS spectrum of bromo-hydroxylactone 7.

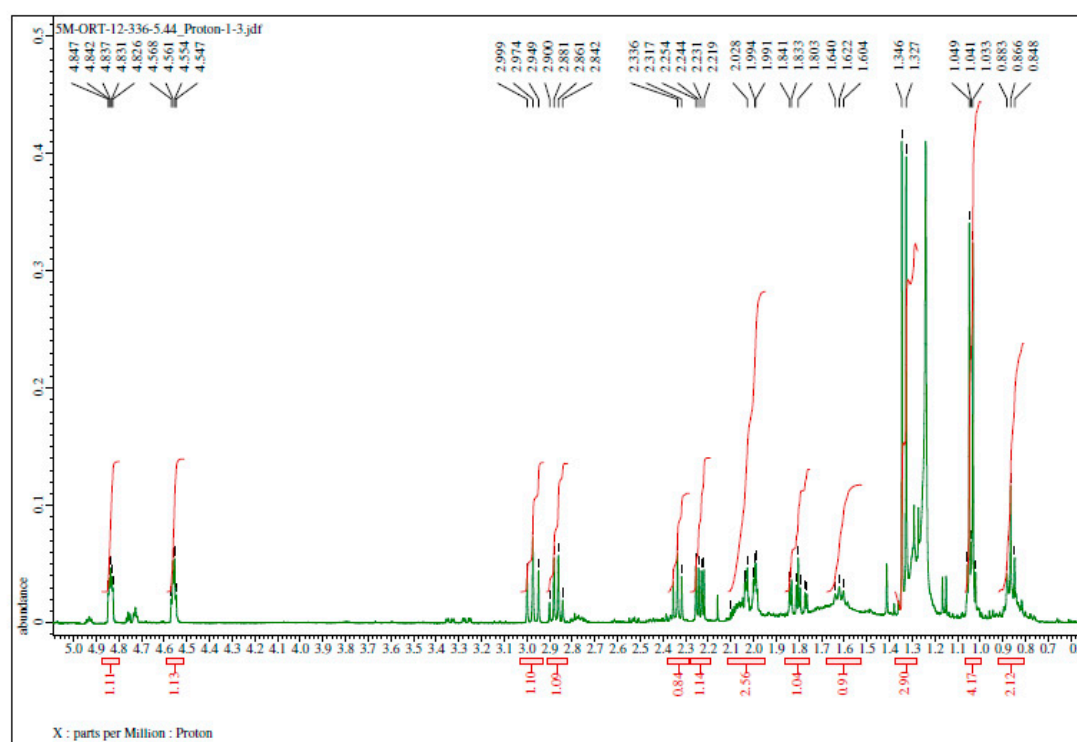


Figure S31. ^1H NMR (400 MHz, CDCl_3) spectrum of bromo-hydroxylactone 8.

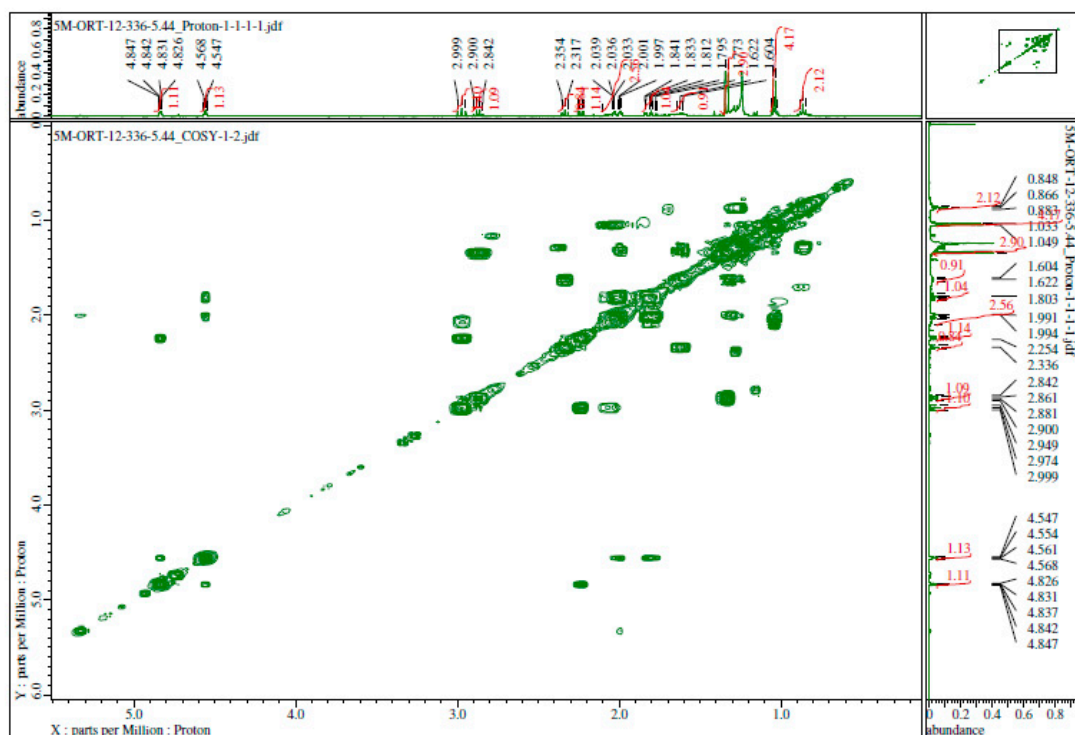


Figure S32. COSY (100 MHz, CDCl₃) spectrum of bromo-hydroxylactone 8.

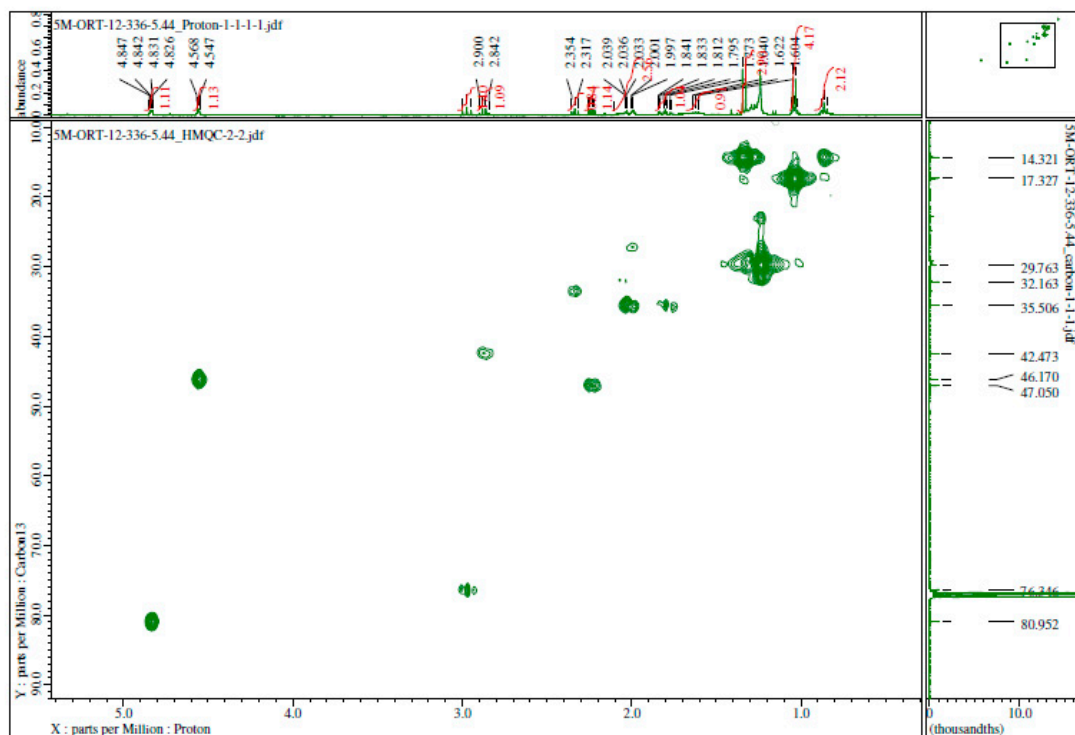


Figure S33. HMQC (100 MHz, CDCl₃) spectrum of bromo-hydroxylactone 8.

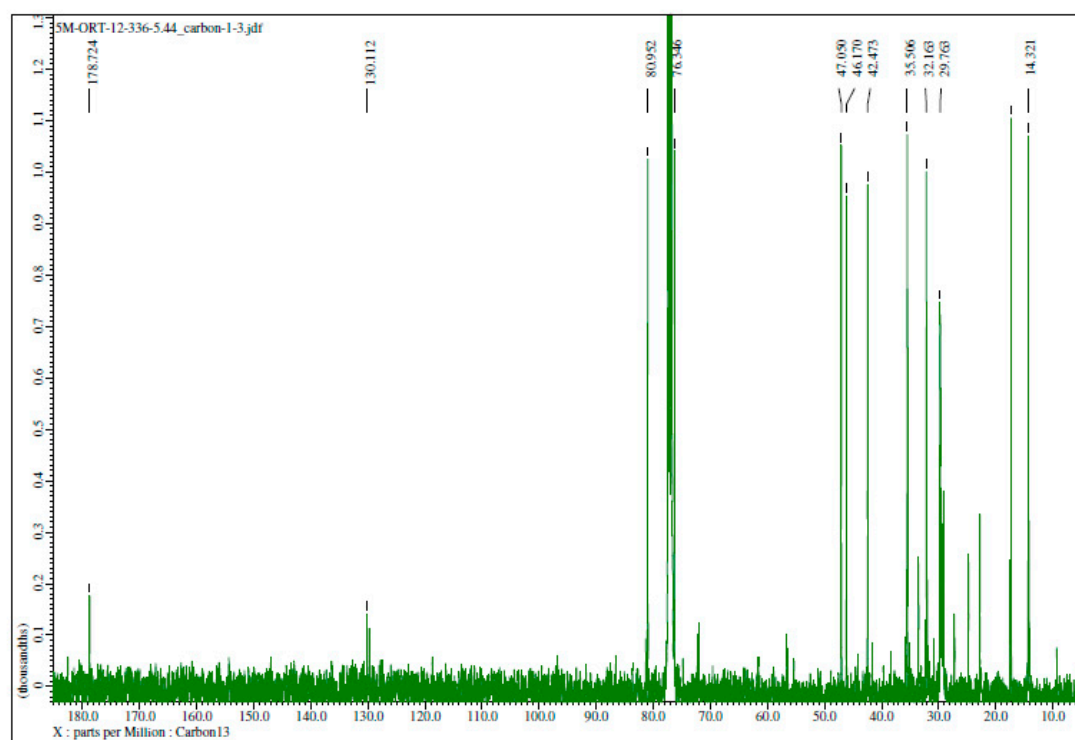


Figure S34. ^{13}C NMR (100 MHz, CDCl_3) spectrum of bromo-hydroxylactone 8.

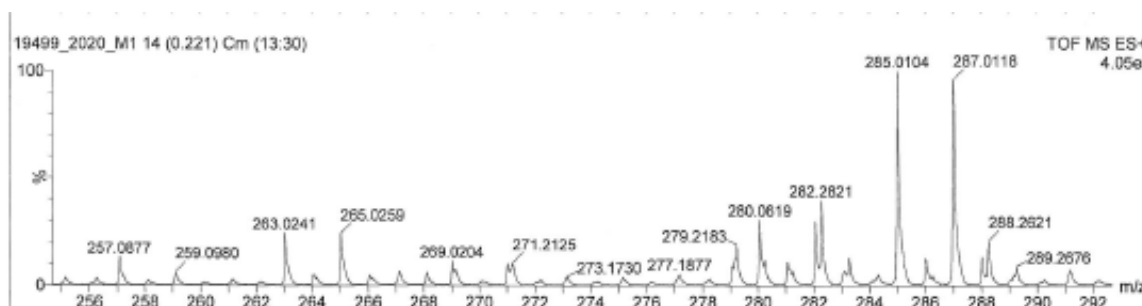


Figure S35. HRMS spectrum of bromo-hydroxylactone 8.

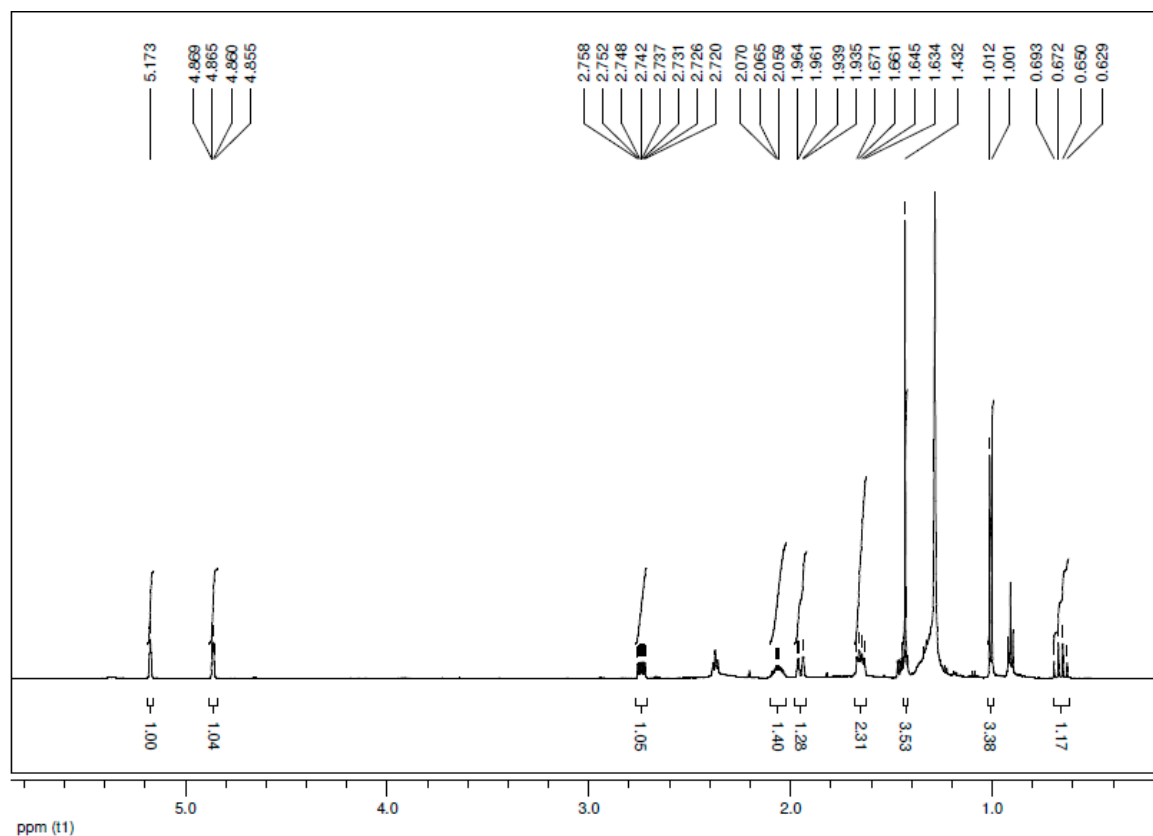


Figure S36. ^1H NMR (600 MHz, CDCl_3) spectrum of iodo-hydroxylactone 9.

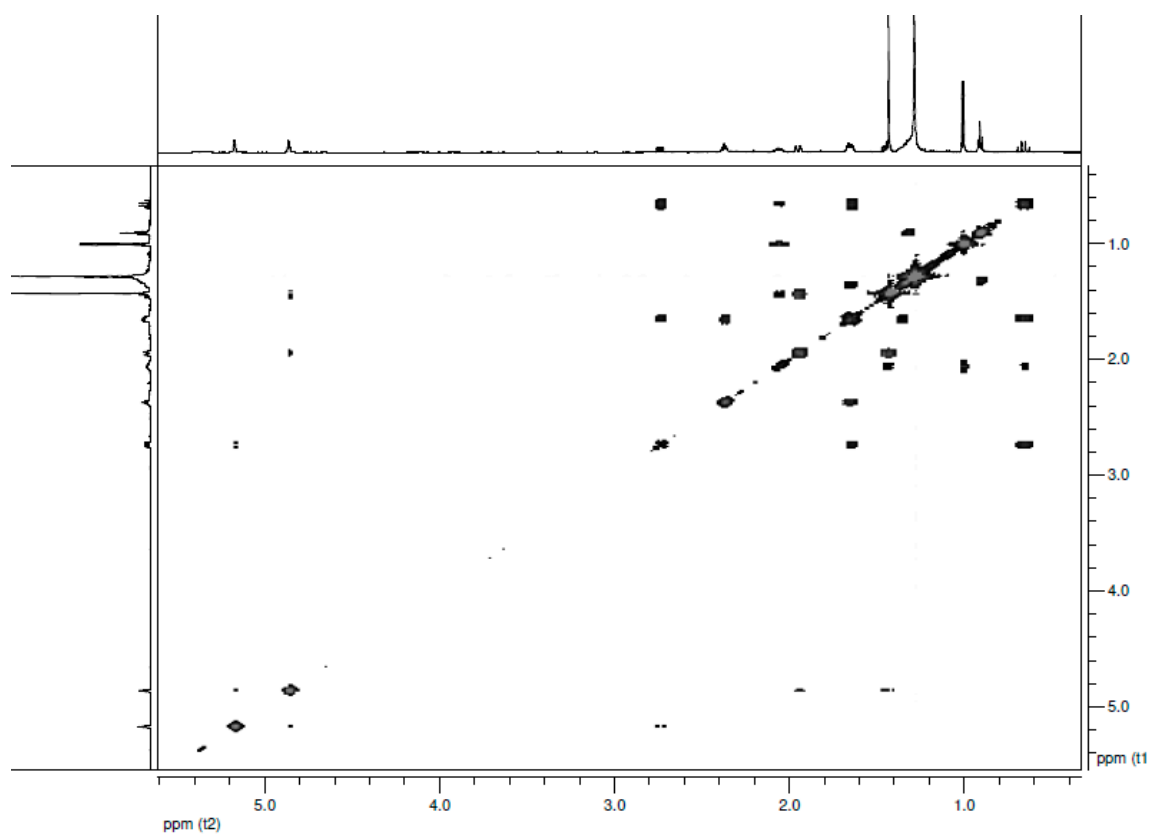


Figure S37. COSY (151 MHz, CDCl_3) spectrum of iodo-hydroxylactone 9.

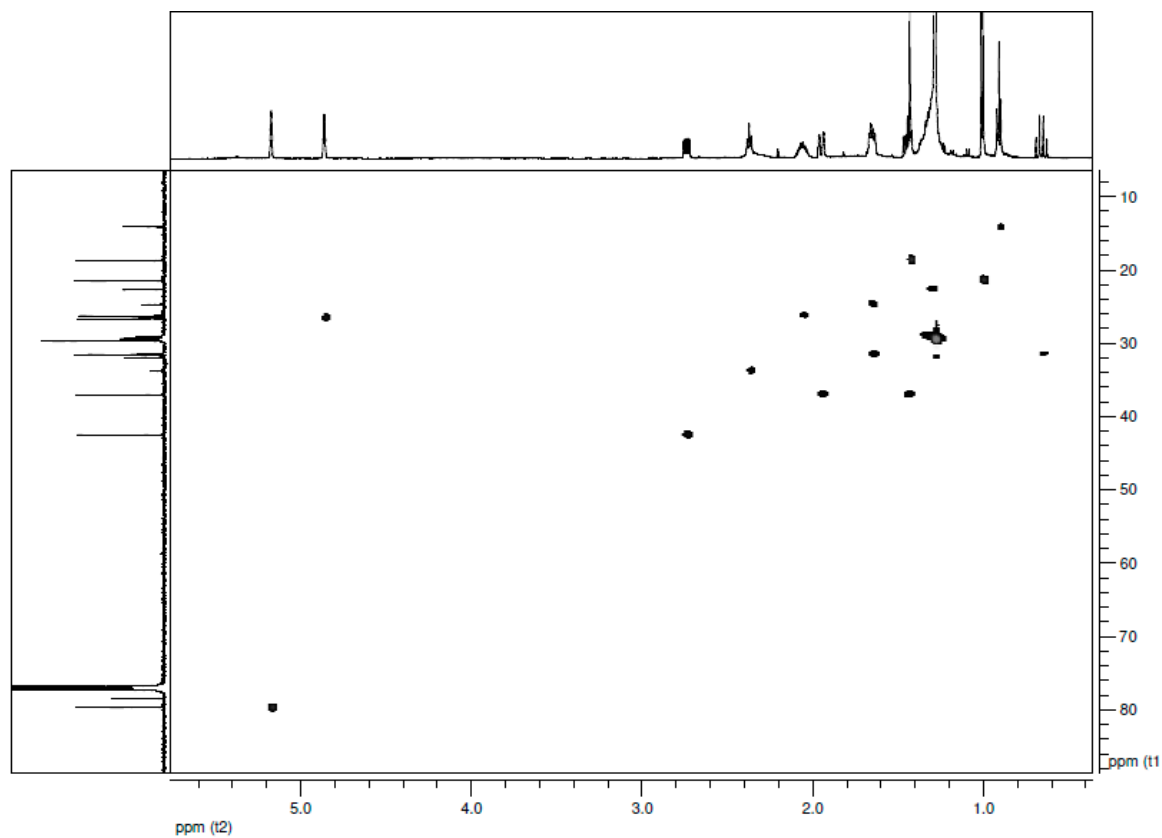


Figure S38. HMOC (151 MHz, CDCl₃) spectrum of iodo-hydroxylactone 9.

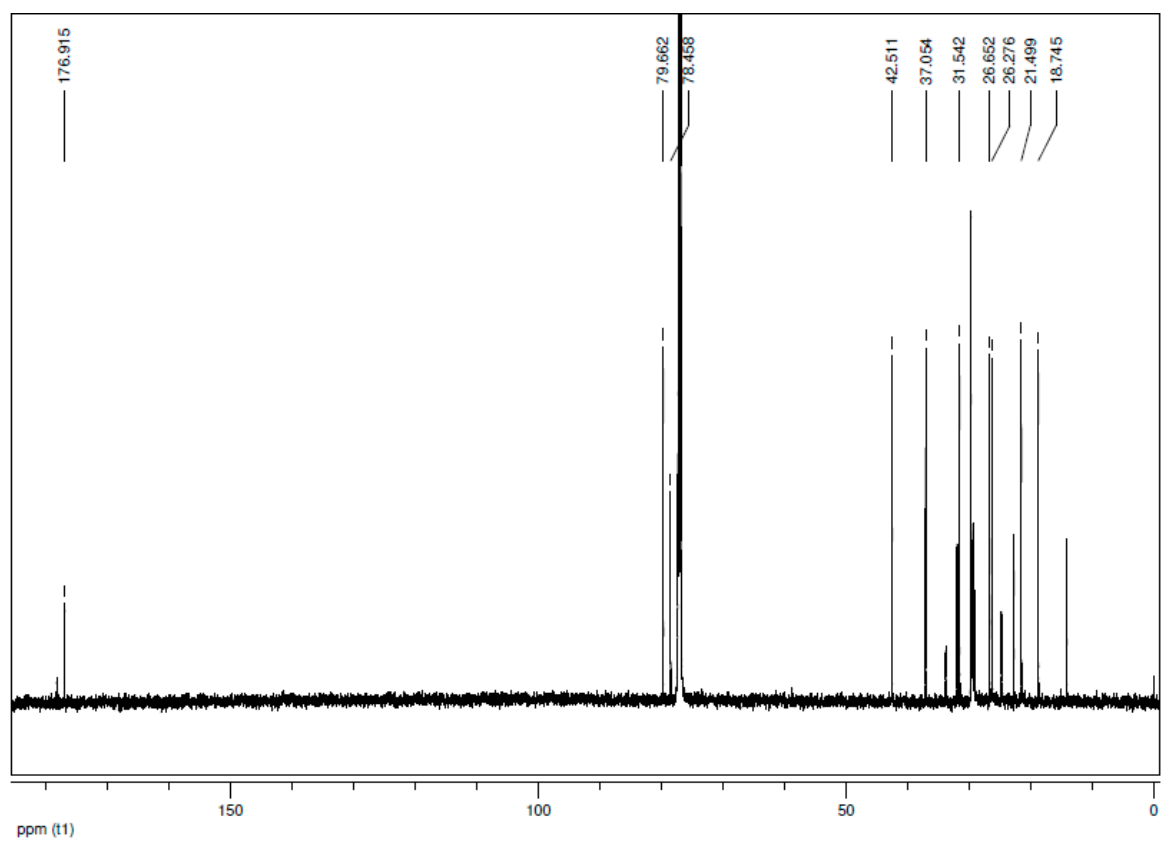


Figure S39. ¹³C NMR (151 MHz, CDCl₃) spectrum of iodo-hydroxylactone 9.

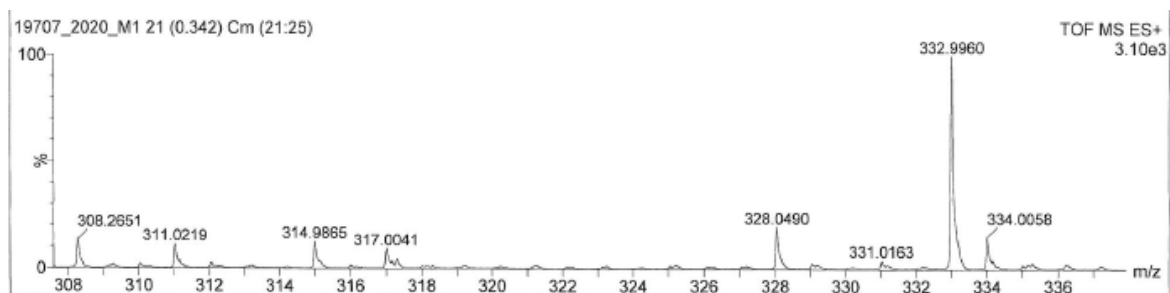
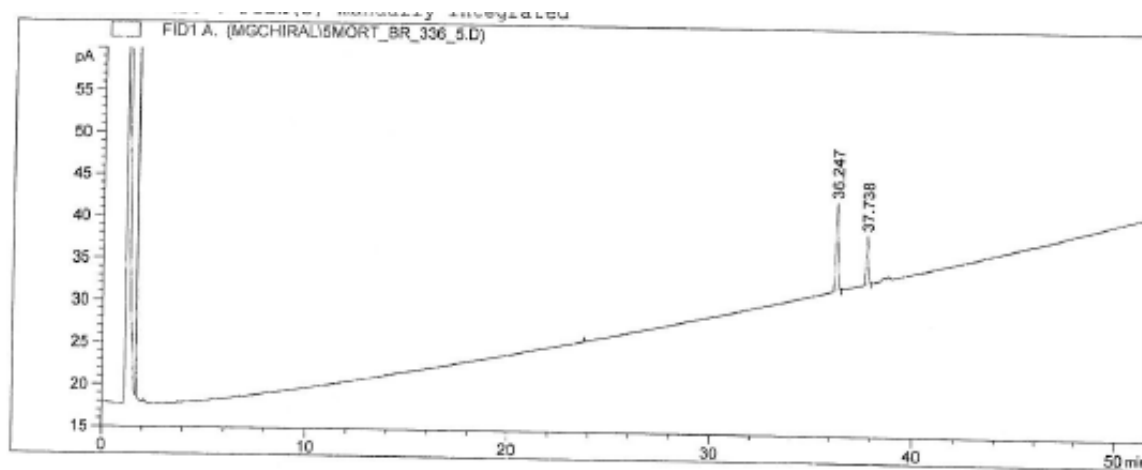
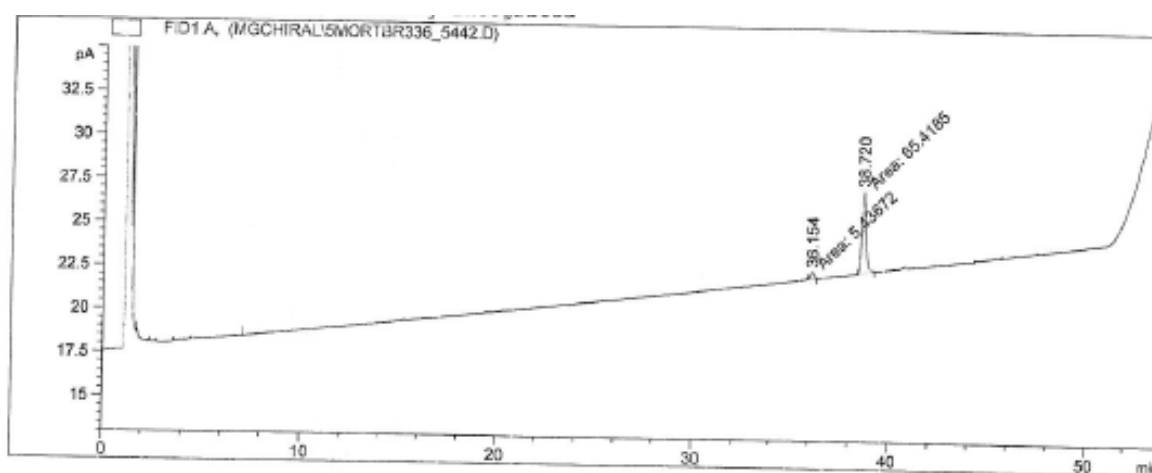


Figure S40. HRMS spectrum of iodo-hydroxylactone 9.



Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	36.247	BB	0.1159	89.71286	10.36830	66.19652
2	37.738	BB	0.1059	45.81219	5.63316	33.80348

Figure S41. Chiral chromatogram of bromo-hydroxylactone 7.



Peak #	RetTime [min]	Type	Width [min]	Area [pA*s]	Height [pA]	Area %
1	36.154	MM	0.2172	5.43672	4.17211e-1	7.67300
2	38.720	MM	0.2331	65.41850	4.67829	92.32700

Figure S42. Chiral chromatogram of bromo-hydroxylactone 8.

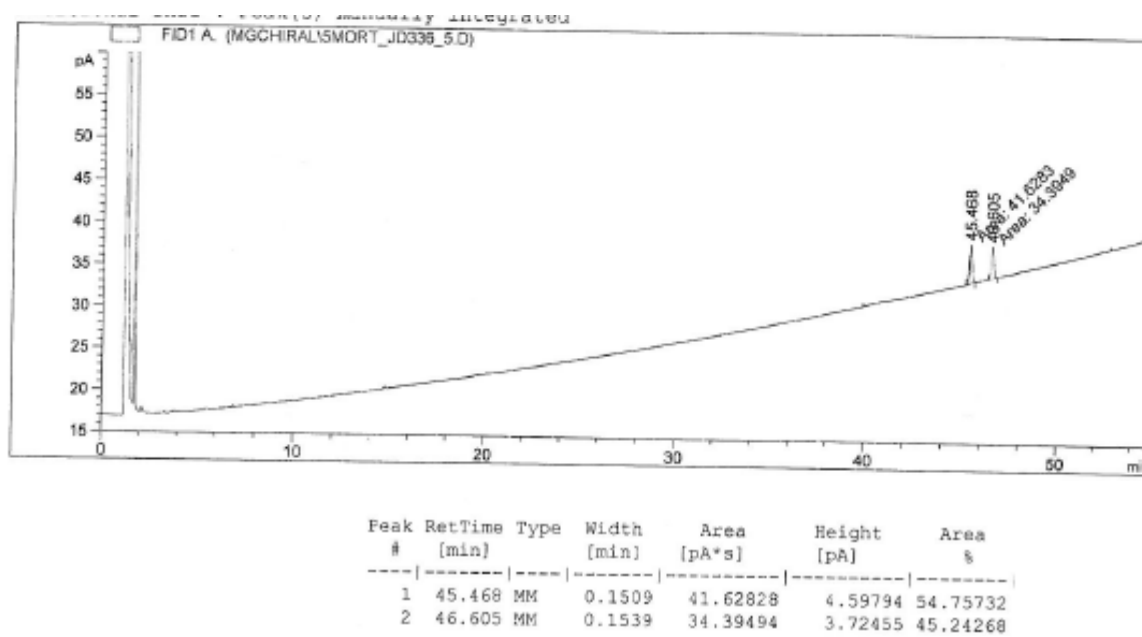


Figure S43. Chiral chromatogram of iodo-hydroxylactone **9**.