The Marine Sponge, *Diacarnus bismarckensis*, as a Source of Peroxiterpene Inhibitors of *Trypanosoma brucei*, the Causative Agent of Sleeping Sickness

Brent K. Rubio, Karen Tenney, Kean-Hooi Ang, Maha Abdulla, Michelle Arkin, James H. McKerrow, Phillip Crews.[*]

Department of Chemistry and Biochemistry and Institute for Marine Sciences, University of California Santa Cruz, Santa Cruz, California 95064, Sandler Center for Basic Research in Parasitic Disease, University of California San Francisco, San Francisco, CA 94143, and Small Molecule Discovery Center, University of California San Francisco, San Francisco, CA 94158

Table of Contents

Figure S1. ^{1}H NMR of (+)-muqubilone B (**1a**).

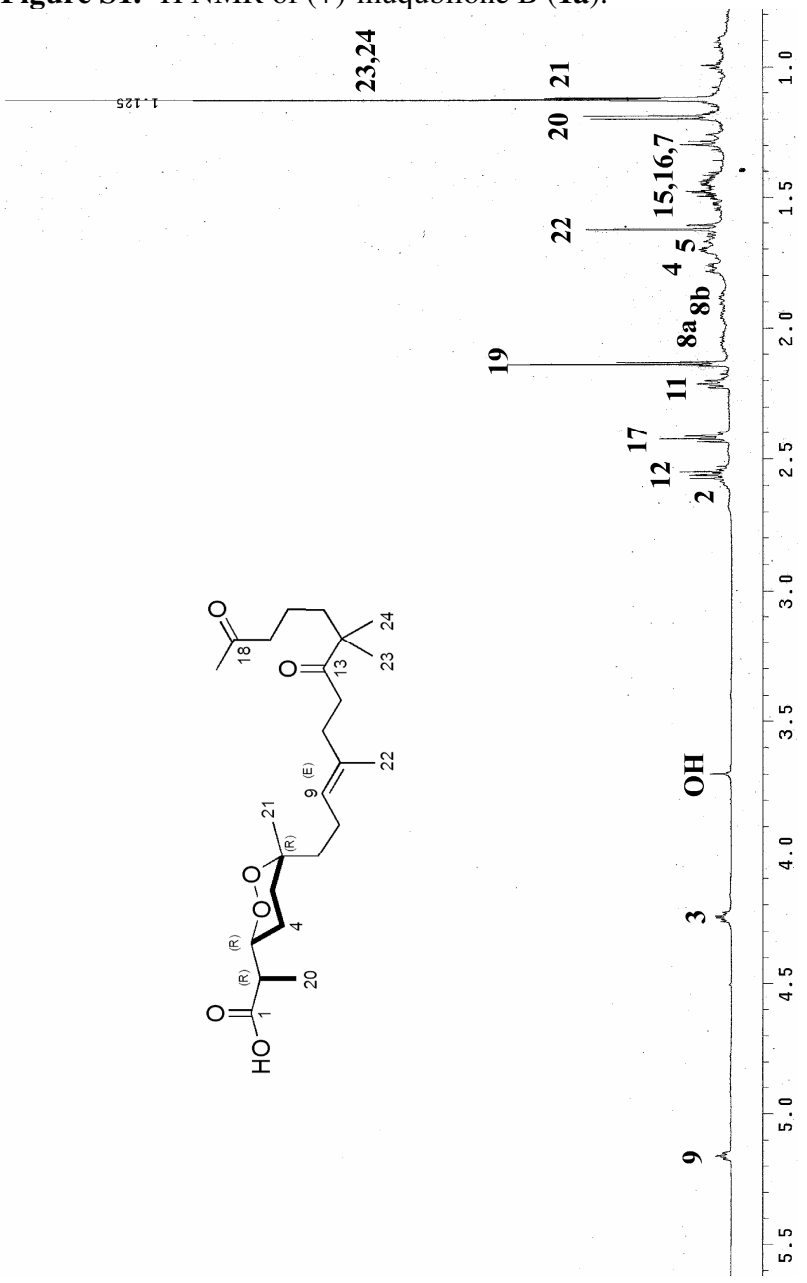


Figure S2. ^{13}C NMR of (+)-muqubilone B (**1a**).

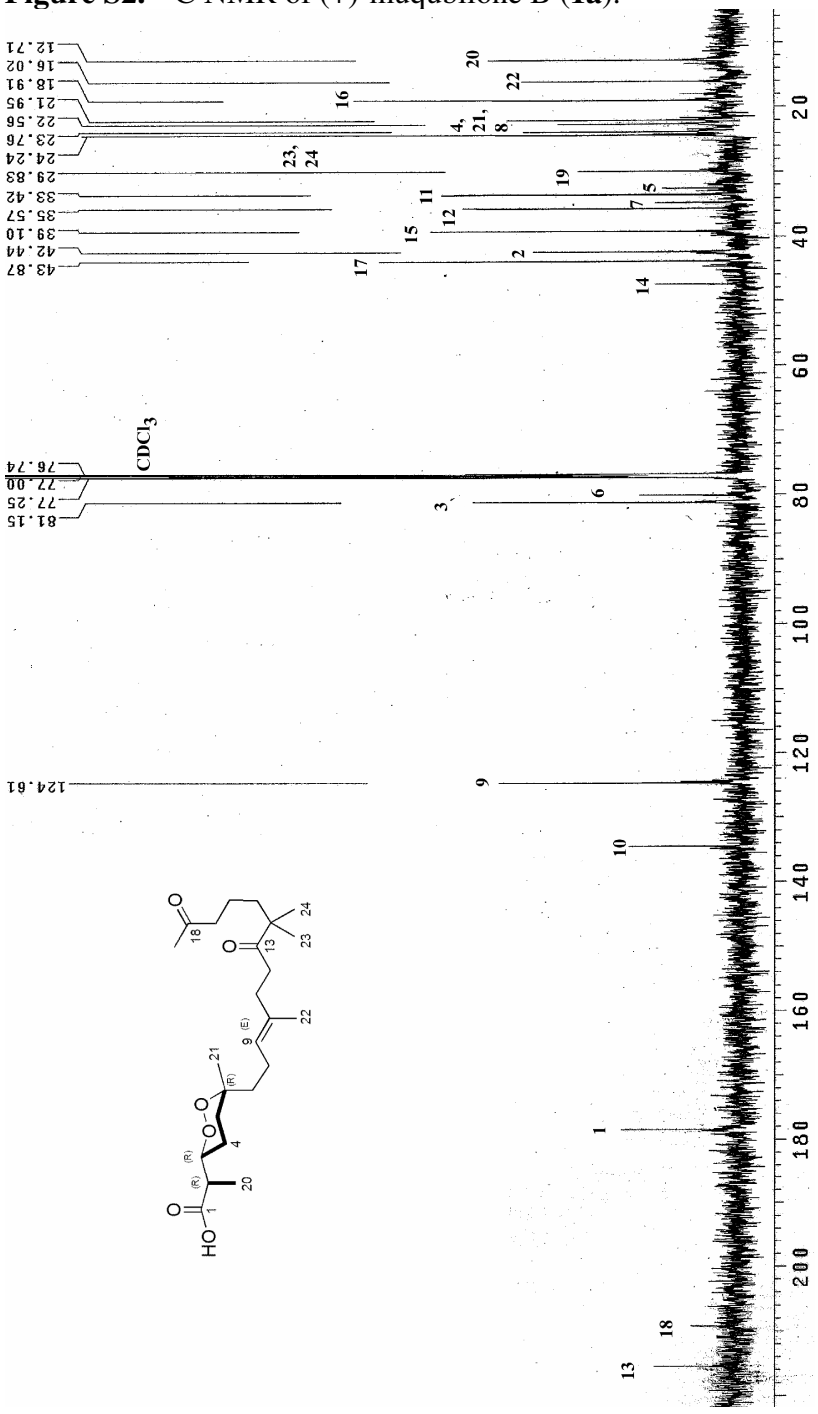


Figure S3. ESI-MS of (+)-muqubilone B (**1a**).

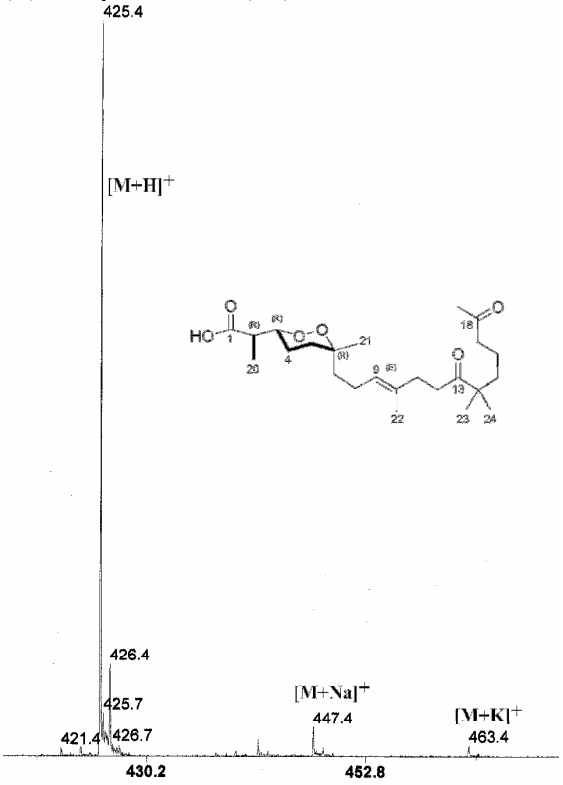


Figure S4. DEPT NMR of (+)-muqubilone B (**1a**).

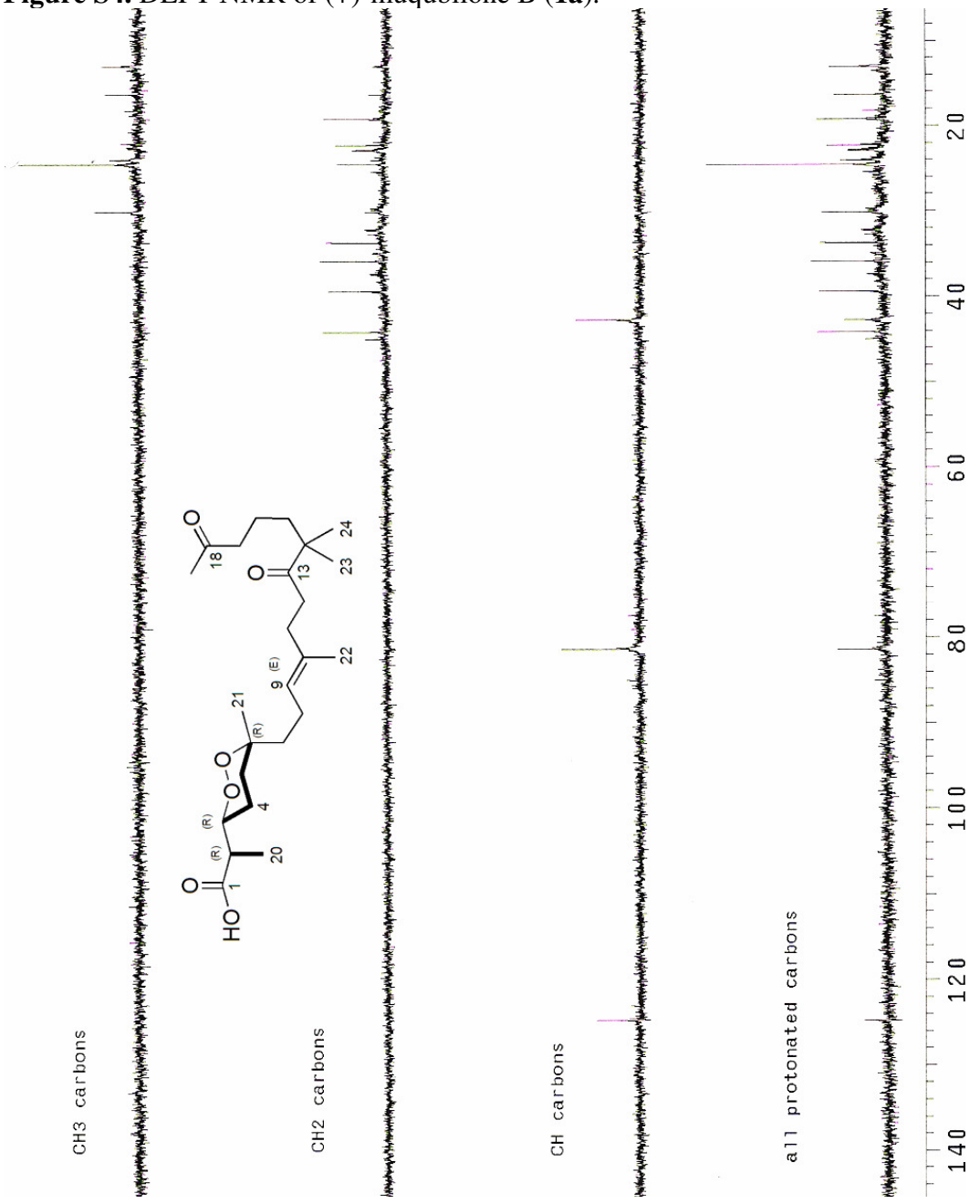


Figure S5. HSQC of (+)-muqubilone B (**1a**).

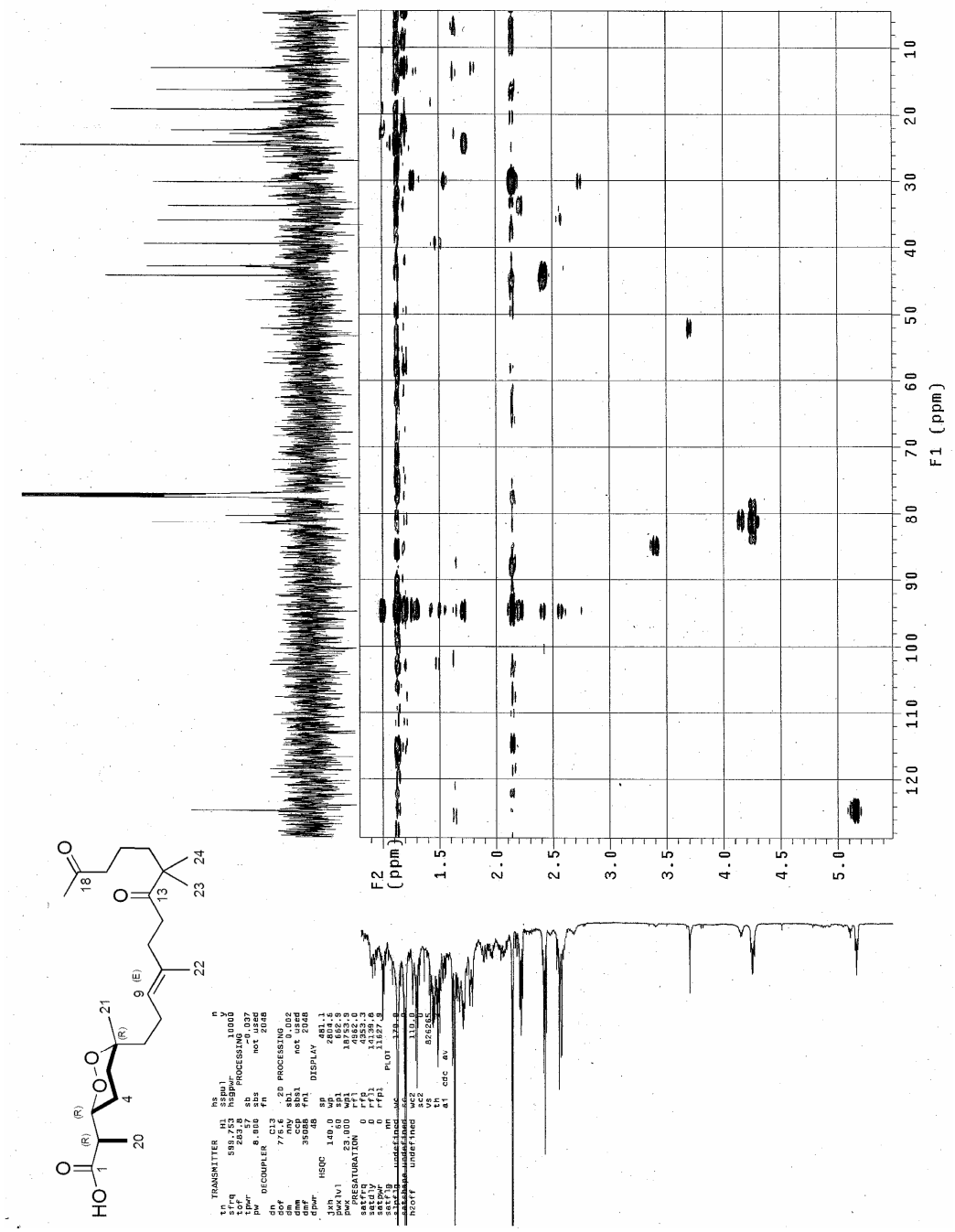


Figure S6. gHMBC of (+)-muqubilone B (**1a**).

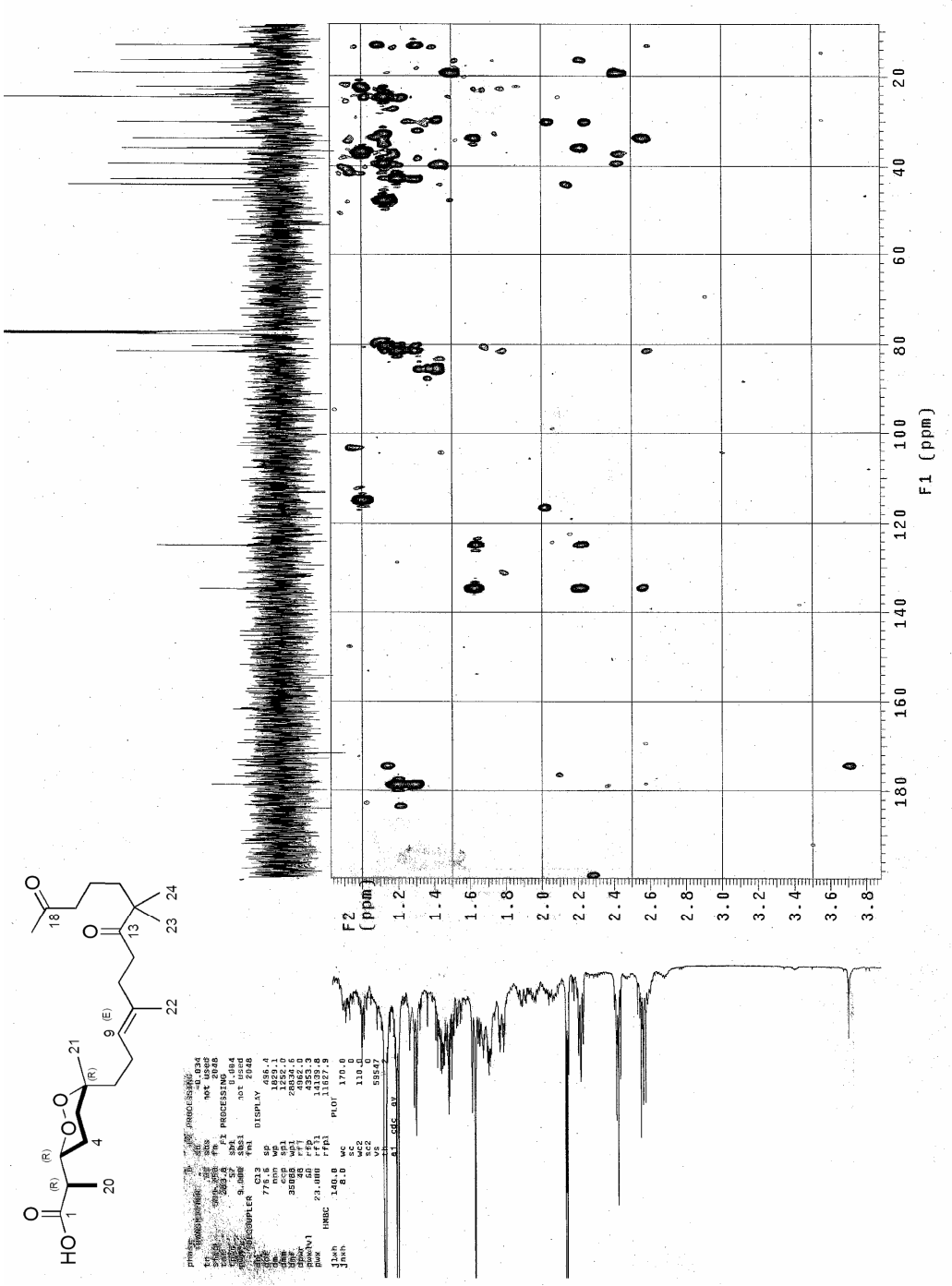


Figure S7. gCOSY of (+)-muqubilone B (**1a**).

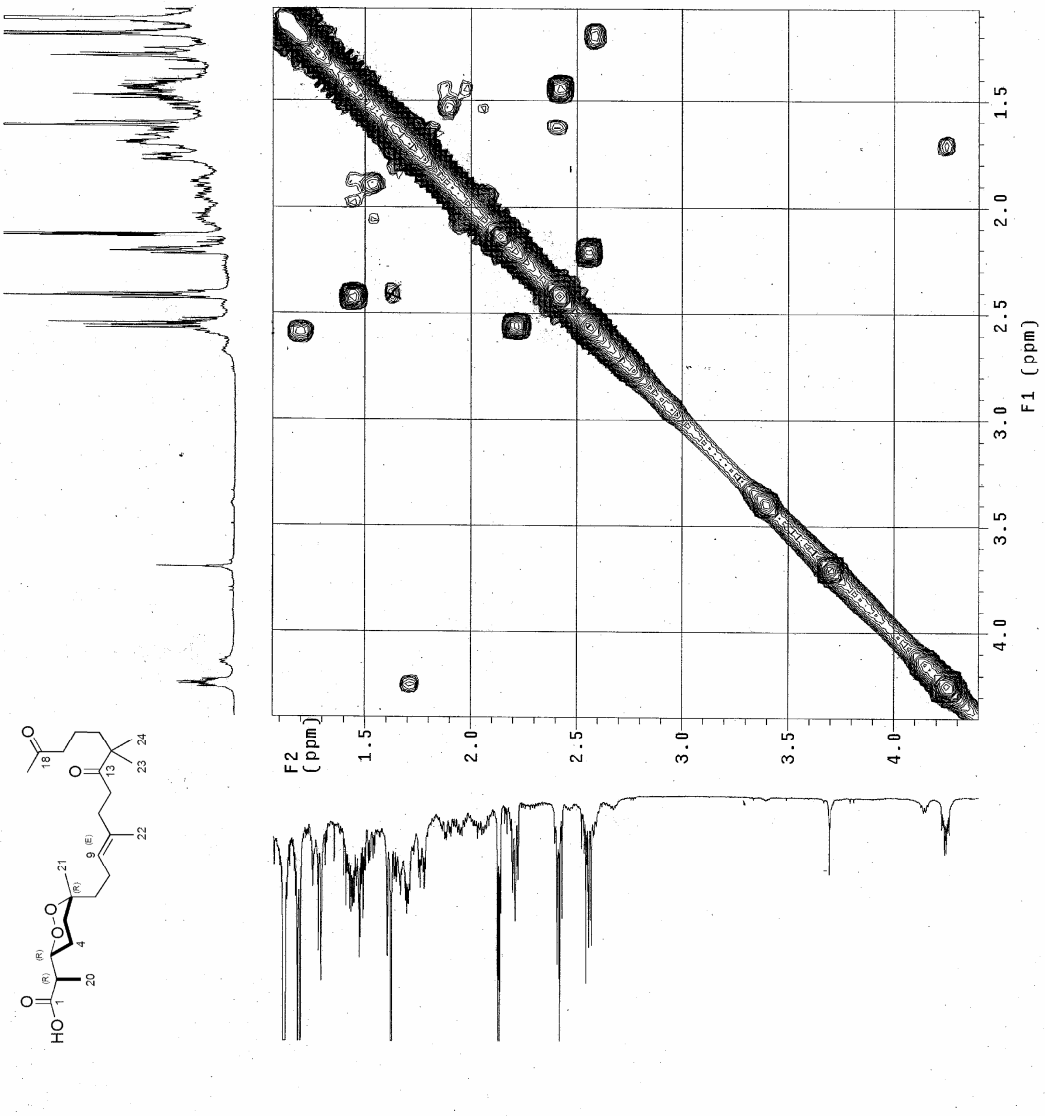


Figure S8. ^{1}H NMR of (+)-muqubilone B methyl ester (**1b**).

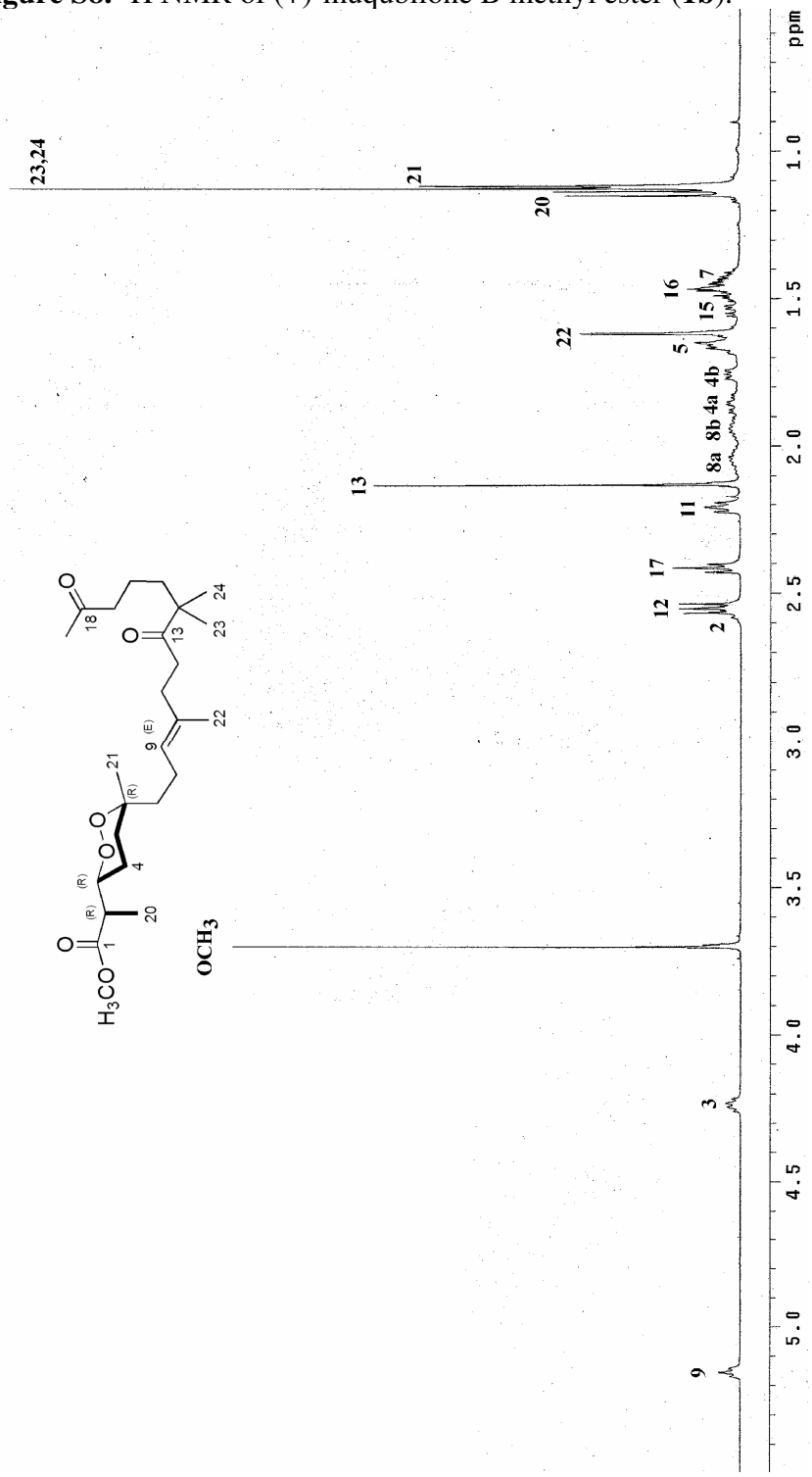


Figure S9. ^{13}C NMR of (+)-muqubilone B methyl ester (**1b**).

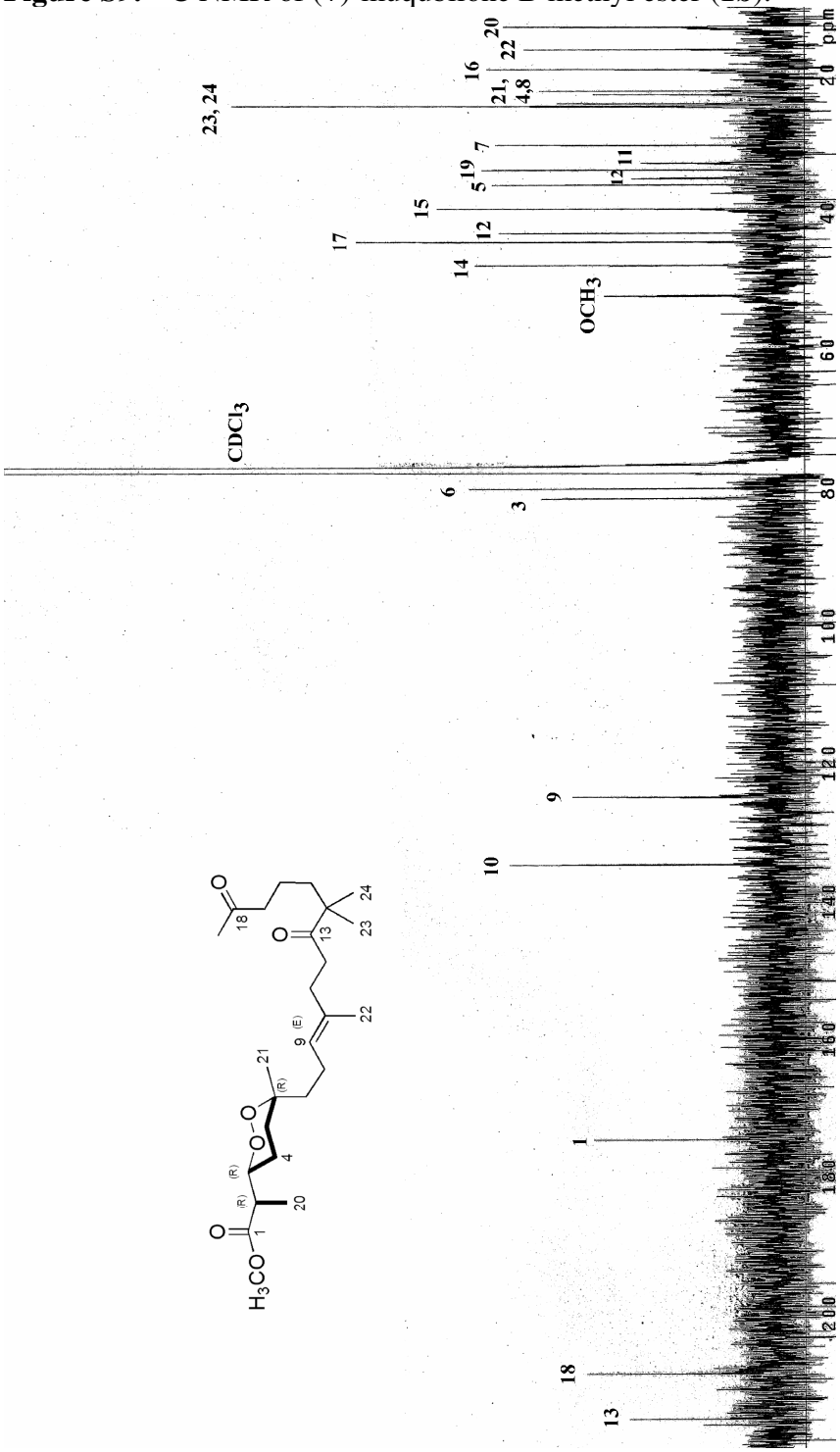


Figure S10. ESI-MS of (+)-muqubilone B methyl ester (**1b**).

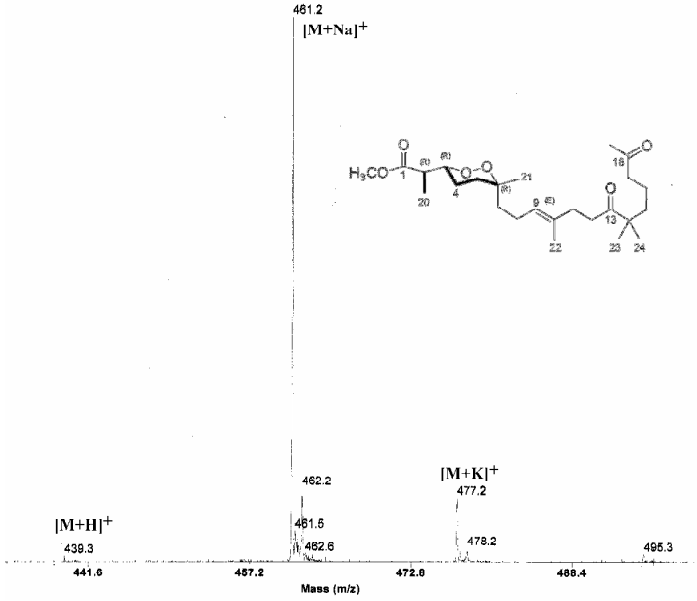


Figure S11. ^{1}H NMR of (+)-muqubilone B diol (**8**).

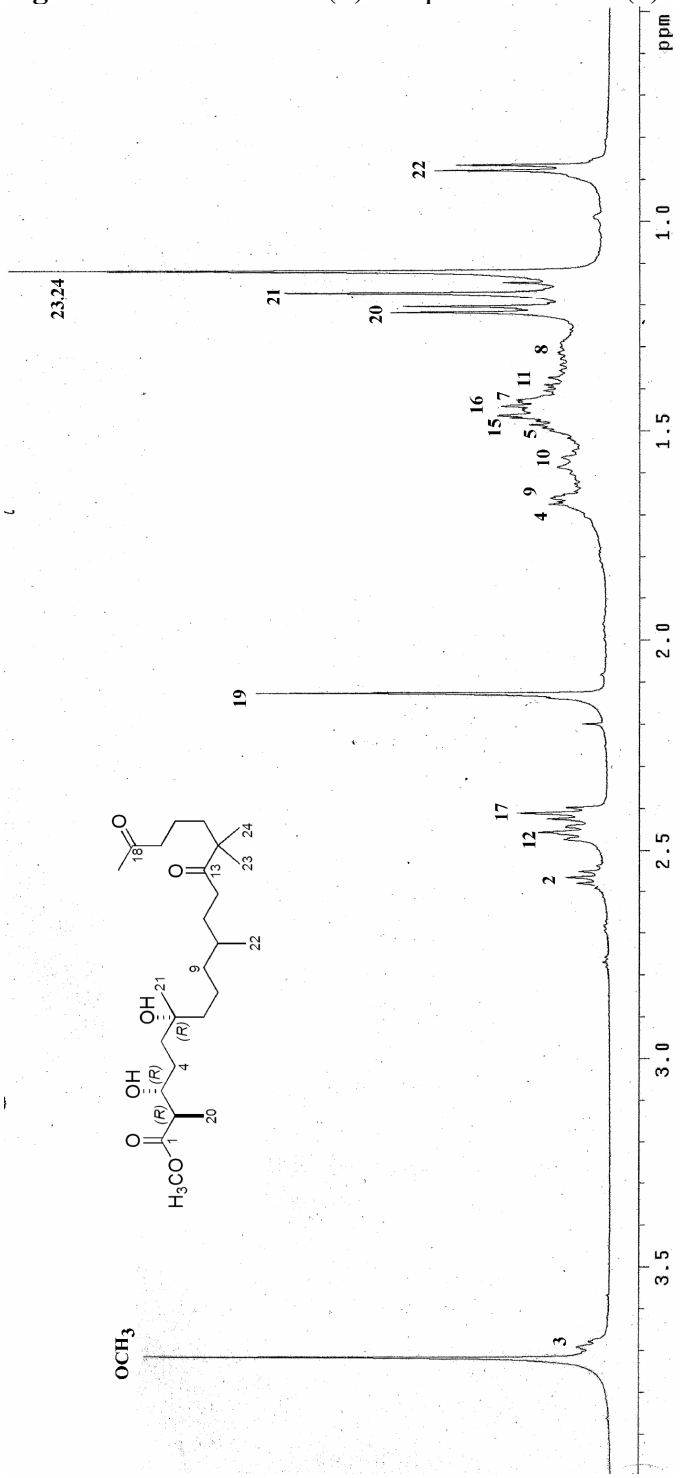


Figure S12. ^{13}C NMR of (+)-muqubilone B diol (**8**).

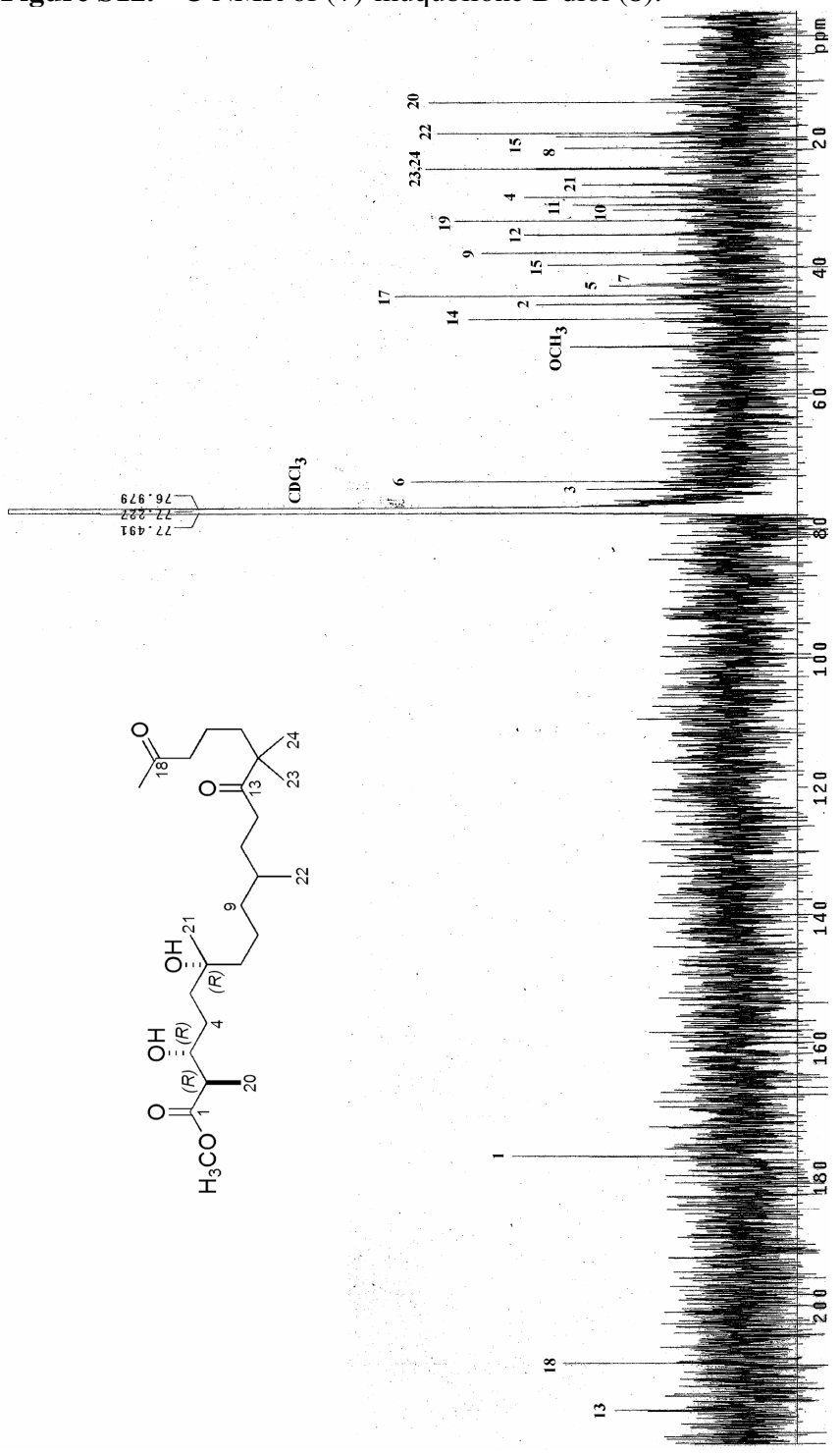


Figure S13. ESI-MS of (+)-muqubilone B diol (**8**).

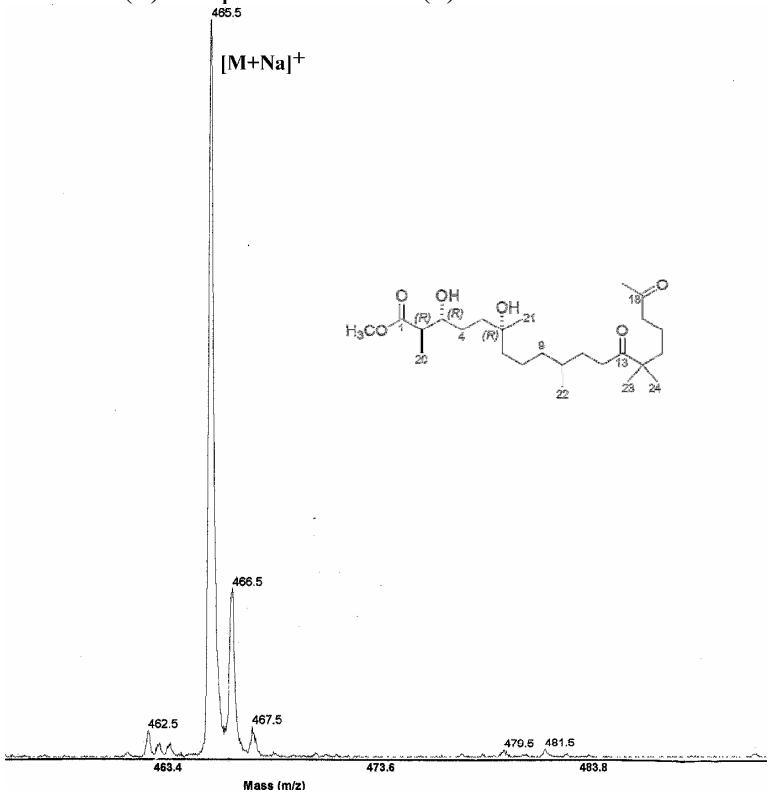


Figure S14. HSQC of (+)-muqubilone B diol (**8**).

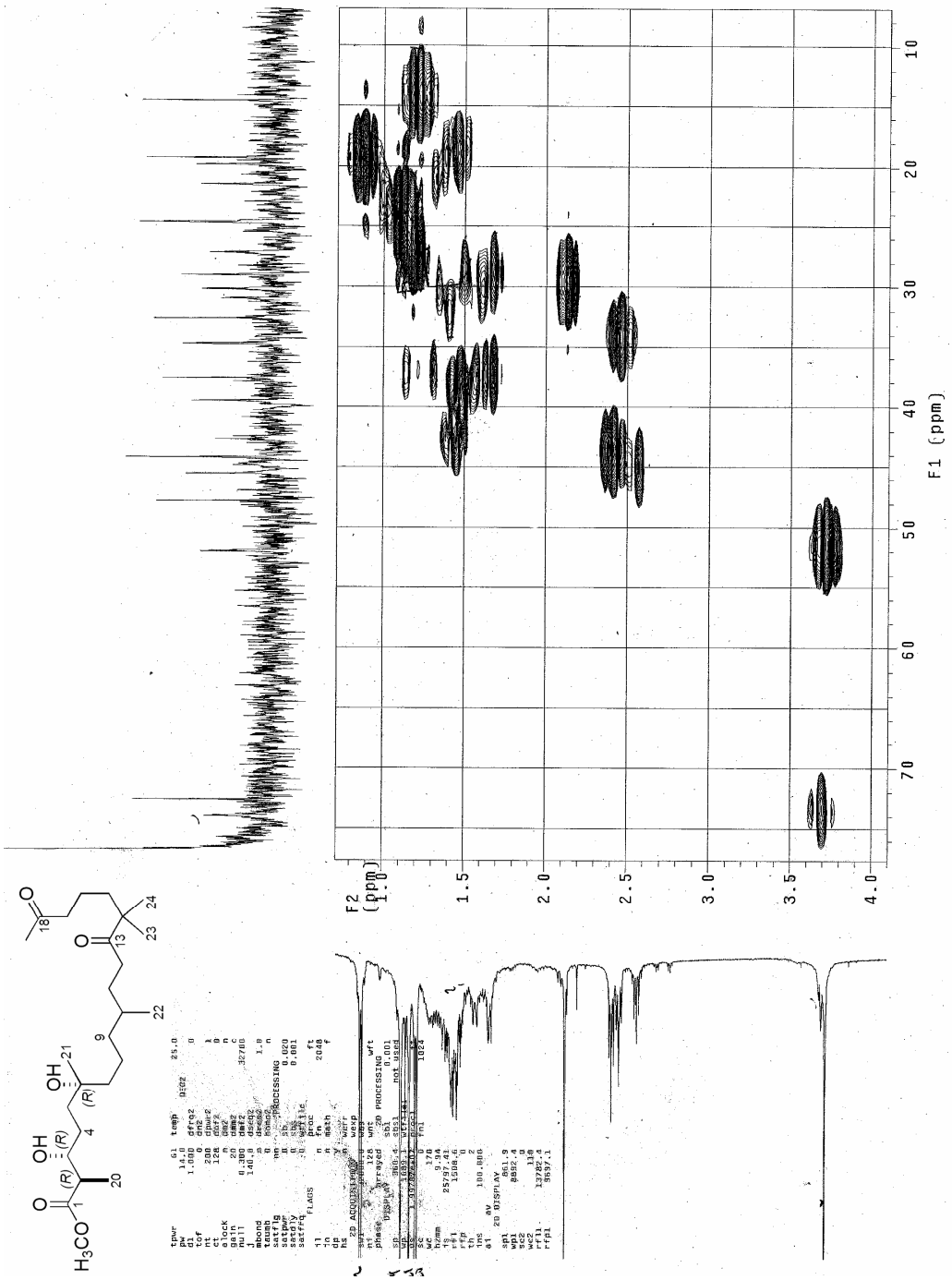


Figure S15. ^{1}H NMR of (+)-muqubilone B (*S*)-MTPA ester (**9a**)

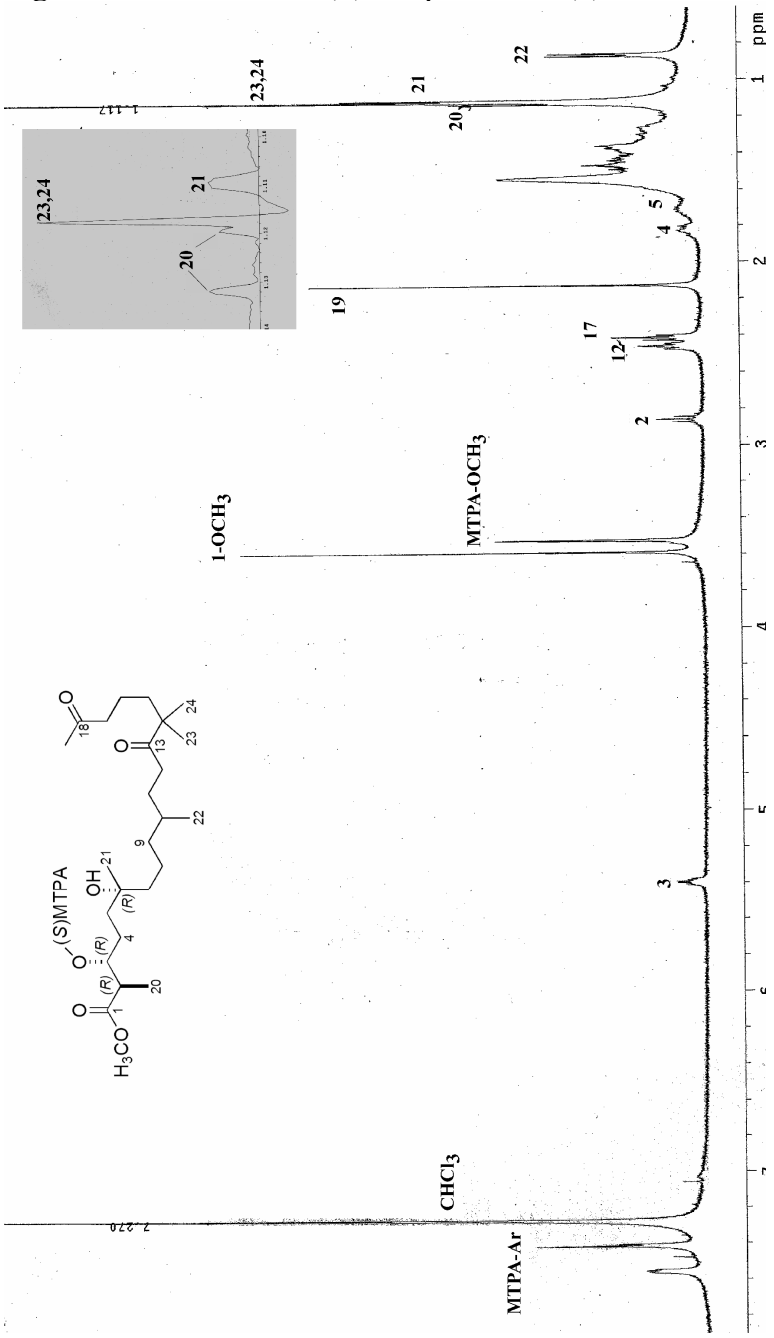


Figure S16. ESI-MS of (+)-muqubilone B (*S*)-MTPA ester (**9a**).

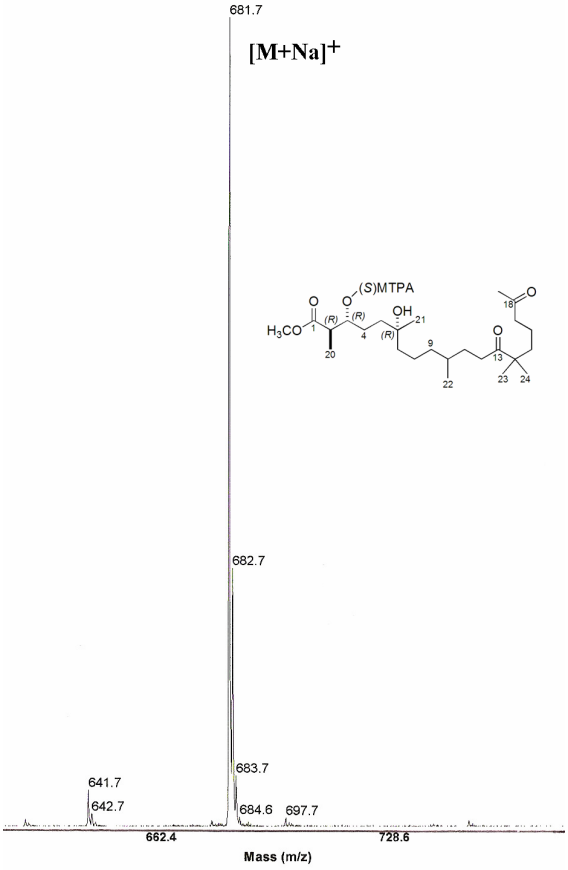


Figure S17. ^{1}H NMR of (+)-muqubilone B (*R*)-MTPA ester (**9b**).

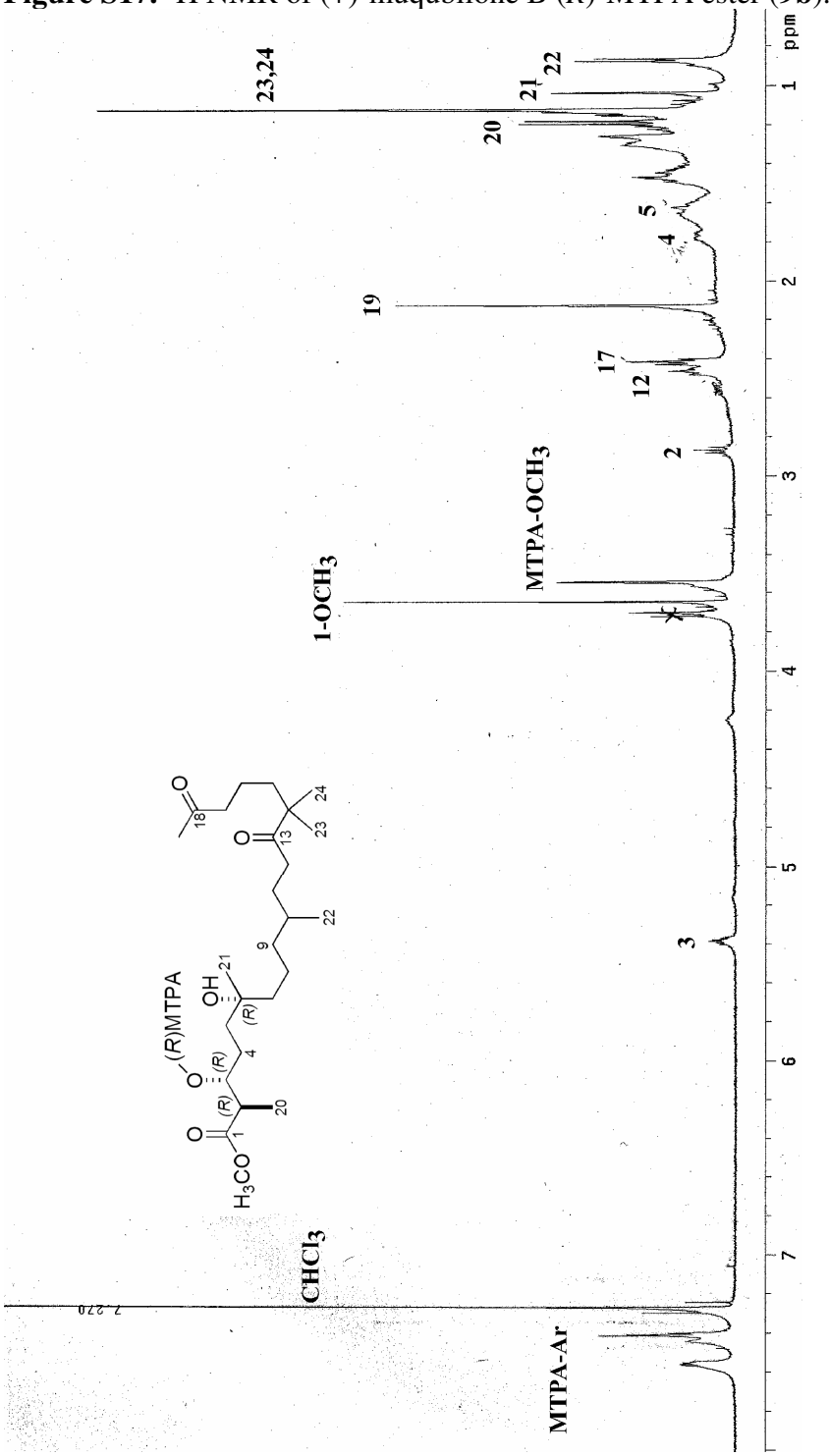


Figure S18. ESI-MS of (+)-muqubilone B (*R*)-MTPA ester (**9b**).

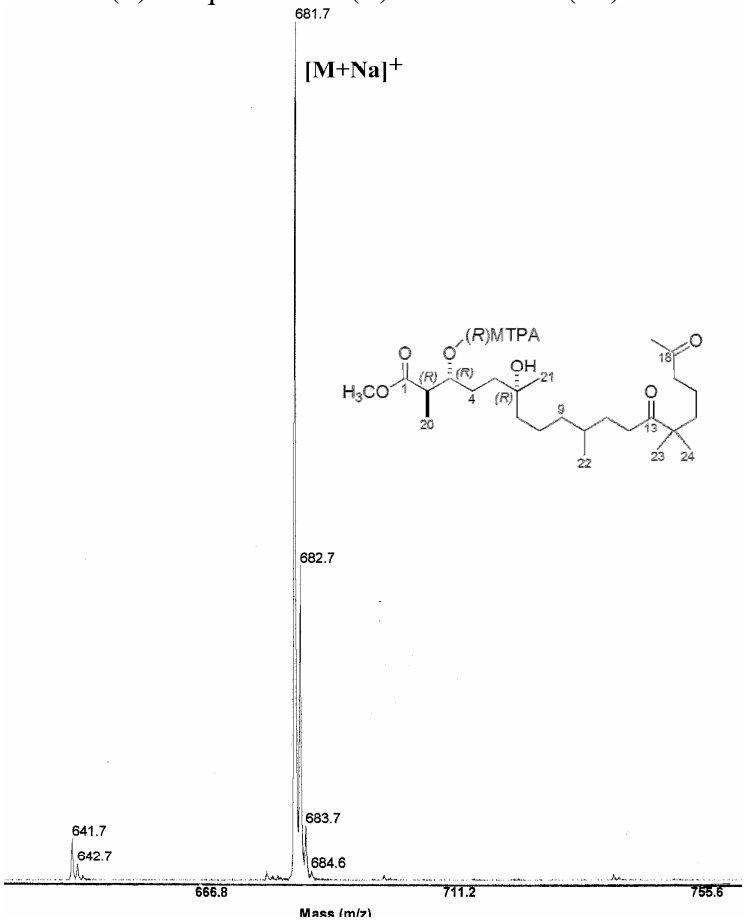


Figure S19. ^{1}H NMR of (-)-ent-muqubilone methyl ester (**3b**).

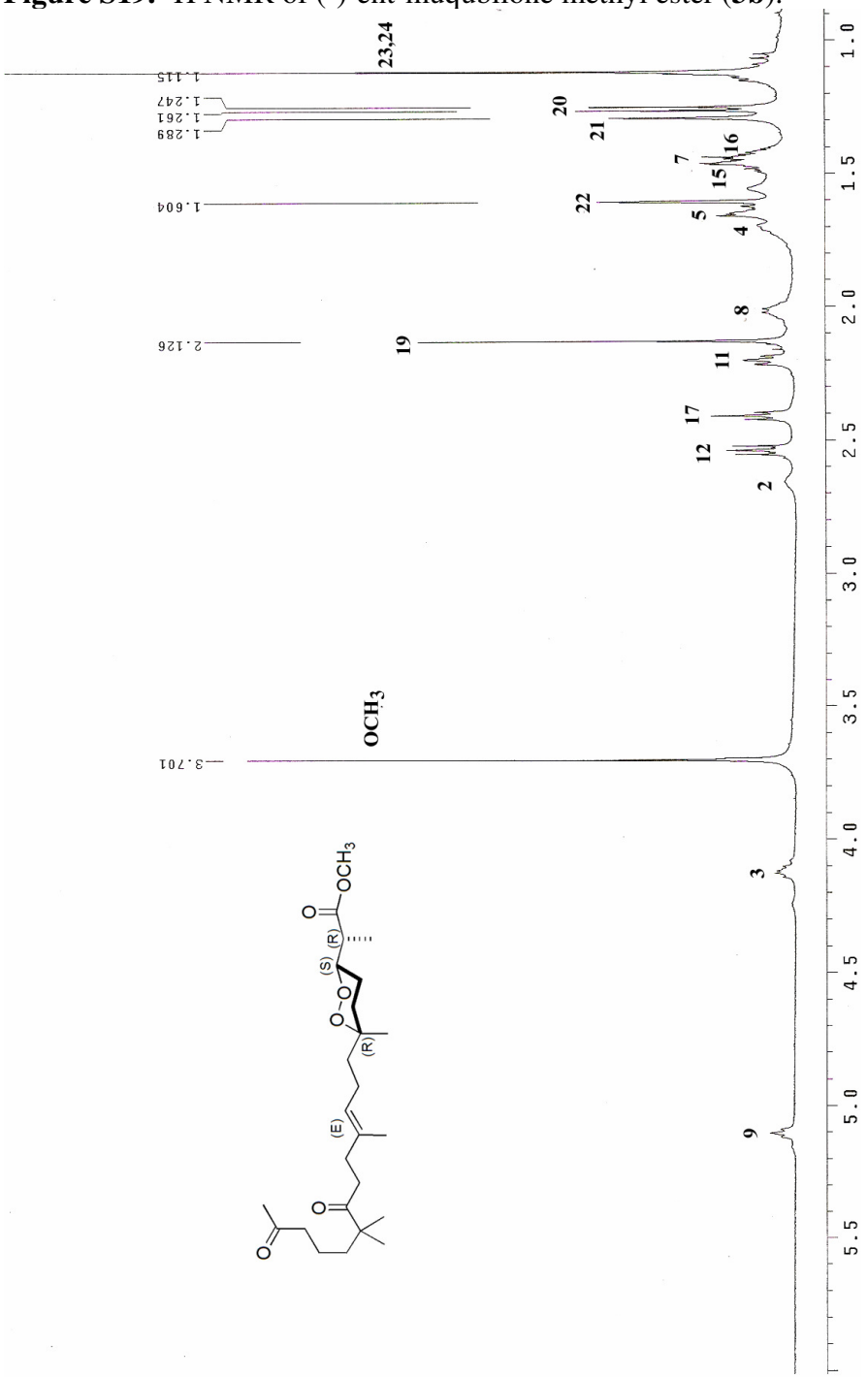


Figure S20. ^{13}C NMR of (-)-ent-muqubilone methyl ester (**3b**).

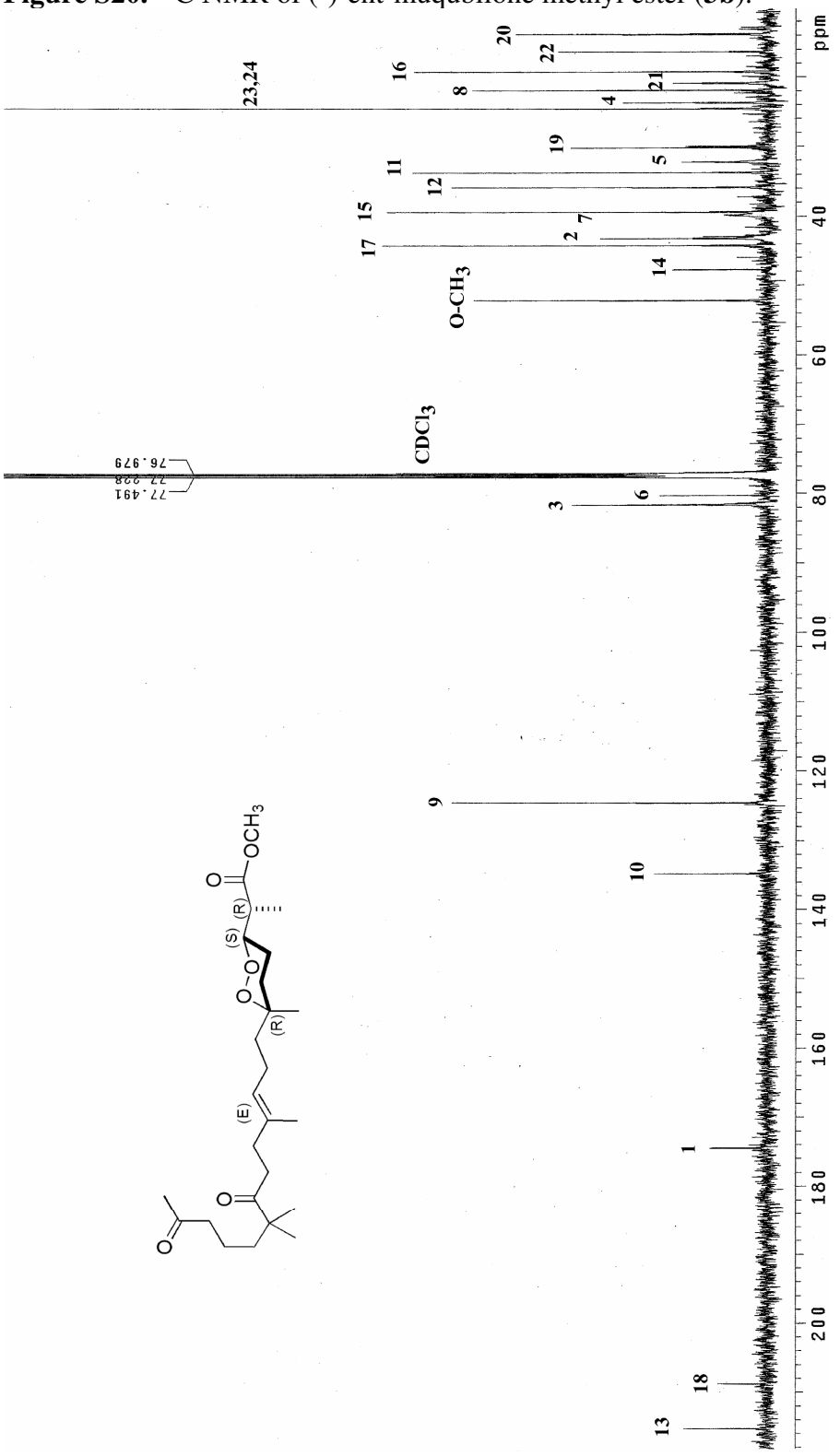


Figure S21. ESI-MS of (-)-ent-muqubilone methyl ester (**3b**).

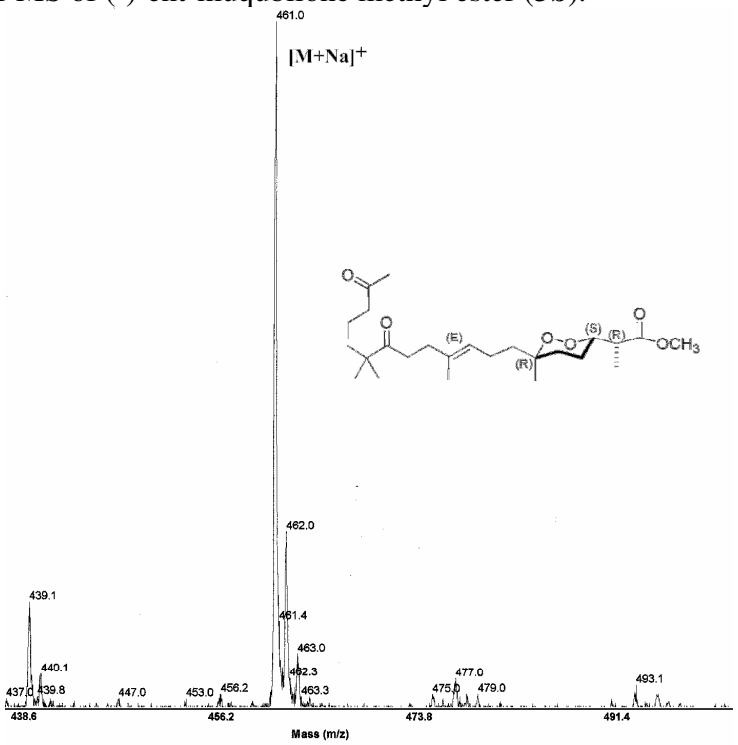


Figure S22. Above (top) and underwater (bottom) pictures of 03512.

Scheme S1. Isolation scheme for 03512.

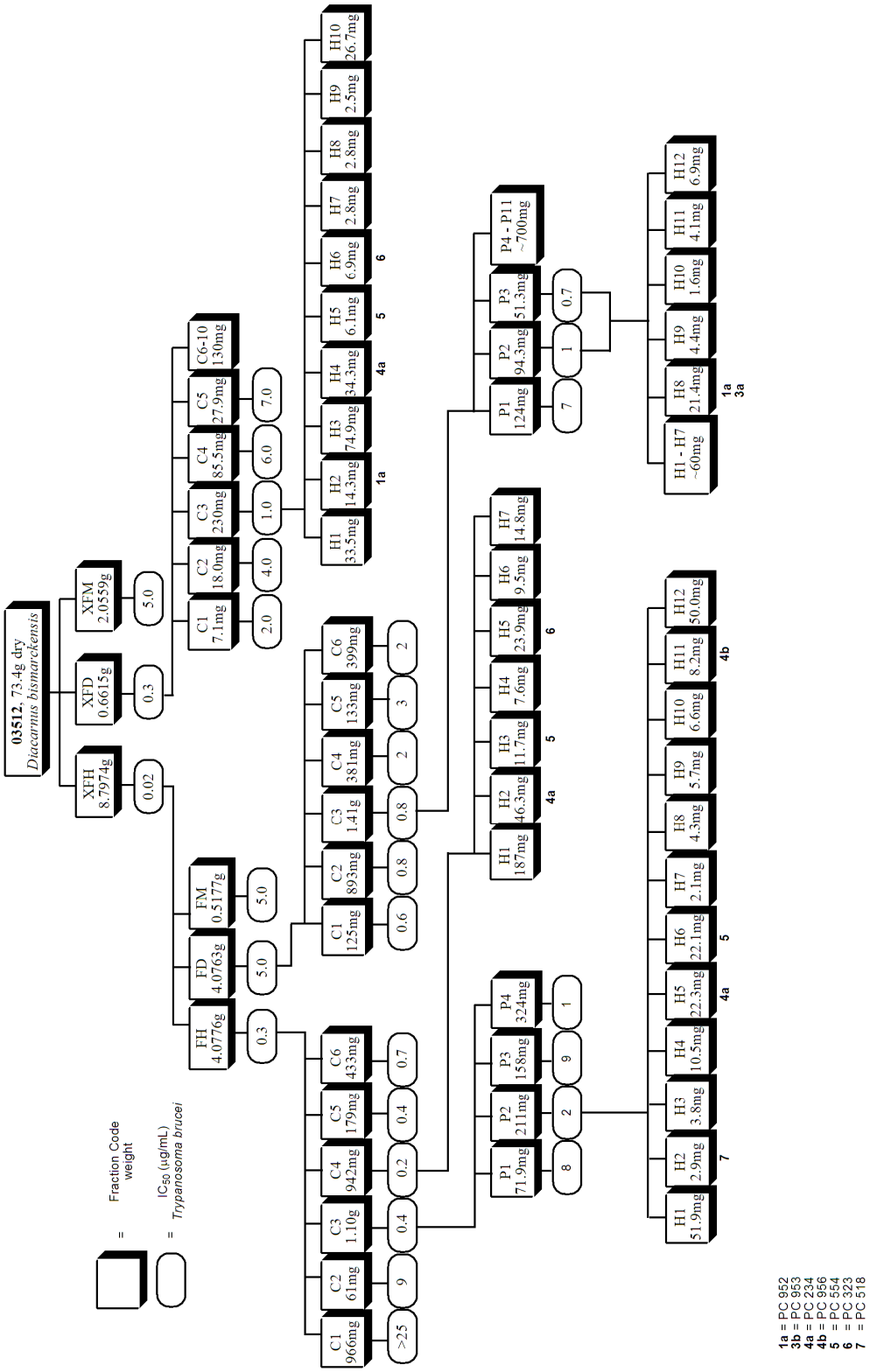
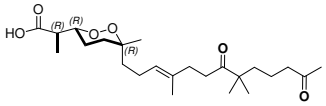
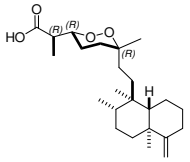
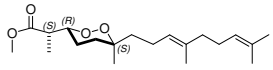
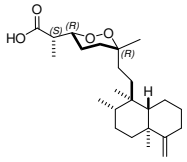
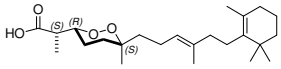
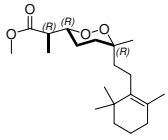
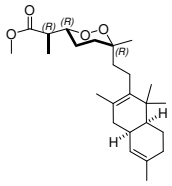
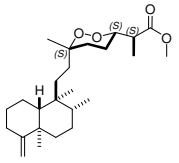
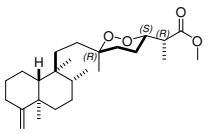
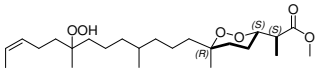
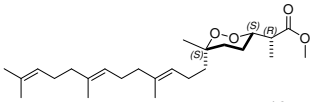
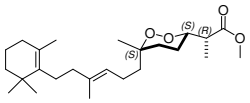
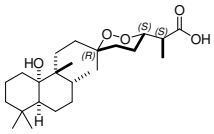
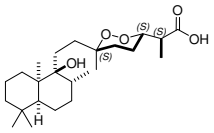
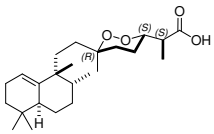
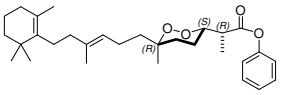


Table S1. Peroxiterpenes from Marine Sponges with Reported Optical Rotations and Absolute Stereochemistries Determined by Semi-Synthetic Methods

Compound	$[\alpha]_D$ (solvent)	Configuration 2	3	6
 (+)-muqubilone B	+60 ($CHCl_3$)	*R*	*R*	*R*
 (+)-sigmosceptrellin A[16,18]	+53 ($CHCl_3$)	*R*	*R*	*R*
 (+)-unnamed ester[18]	+52 ($CHCl_3$)	*S*	*R*	*S*
 (+)-sigmosceptrellin C[16,18]	+42 ($CHCl_3$)	*S*	*R*	*R*
 (+)-muqubilin[18, 23a]	+31 ($CHCl_3$)	*S*	*R*	*S*
 (+)-nuapapuin A[23b]	+62 ($CHCl_3$)	*R*	*R*	*R*
 (+)-trunculin A methyl ester[23f]	+158 ($CHCl_3$)	*R*	*R*	*R*
 (-)-ent-sigmosceptrellin A methyl ester[23e]	-57 ($CHCl_3$)	*S*	*S*	*S*

 (-)-sigmosceptrellin B methyl ester[16,18]	-61 ($CHCl_3$)	*R*	*S*	*R*
 (-)-sigmosceptrellin D methyl ester[23b]	-58 ($CHCl_3$)	*R*	*S*	*S*
 (-)-unnamed ester[18]	-60 ($CHCl_3$)	*S*	*S*	*R*
 (-)-unnamed ester[18]	-59 ($CHCl_3$)	*S*	*S*	*R*
 (-)-mycaperoxide A[23d]	-41 (acetone)	*R*	*S*	*S*
 (-)-mycaperoxide B[23d]	-41 (acetone)	*S*	*S*	*S*
 (-)-mycaperoxide H[23c]	-143 (acetone)	*R*	*S*	*S*
 (-)-unnamed ester[18]	-25 ($CHCl_3$)	*R*	*S*	*R*