

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

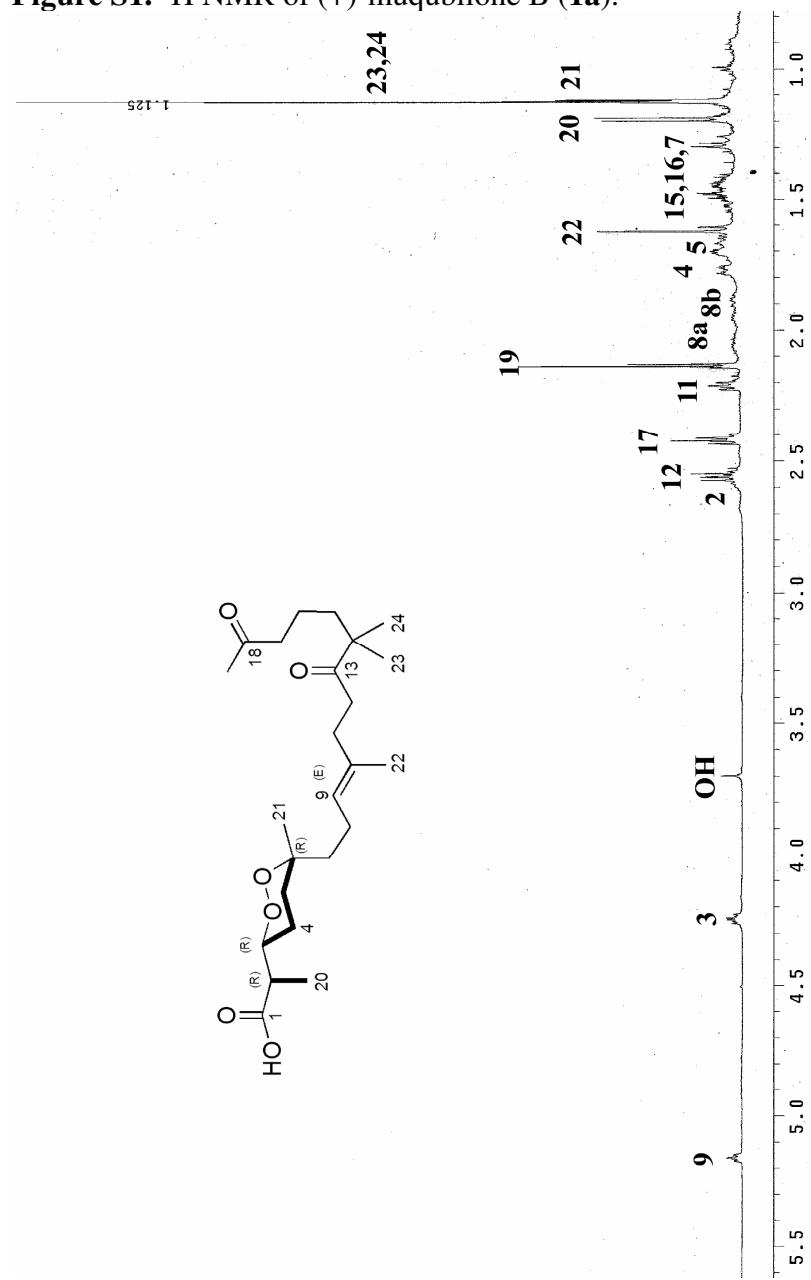
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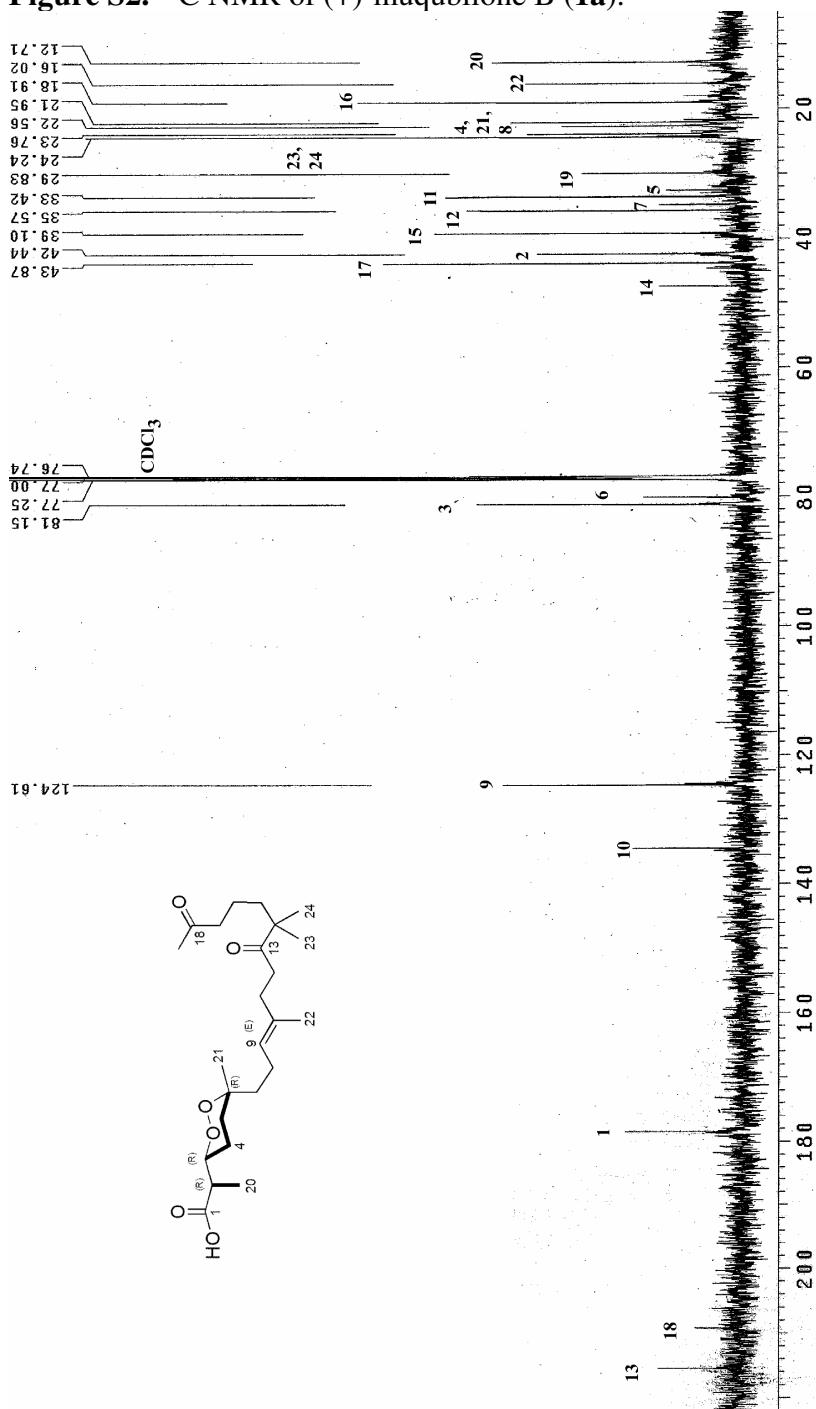
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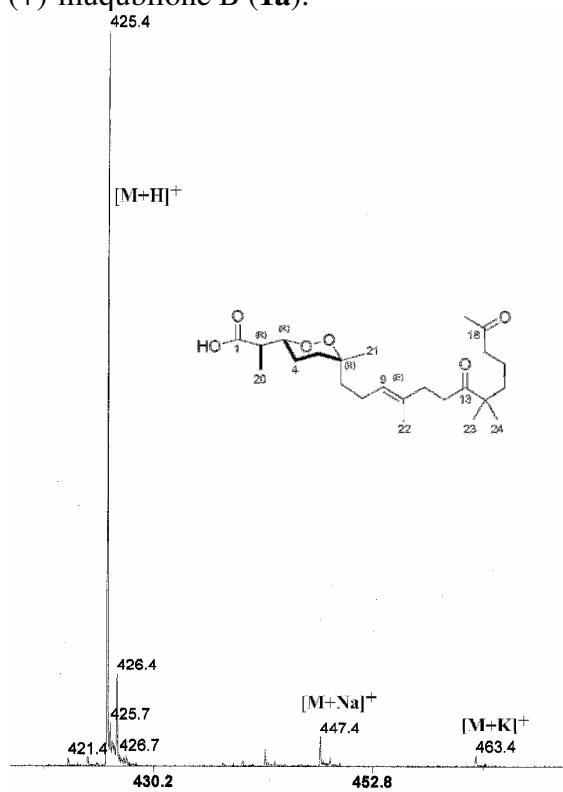
**Figure S1.**  $^1\text{H}$  NMR of (+)-muquibilone B (**1a**).



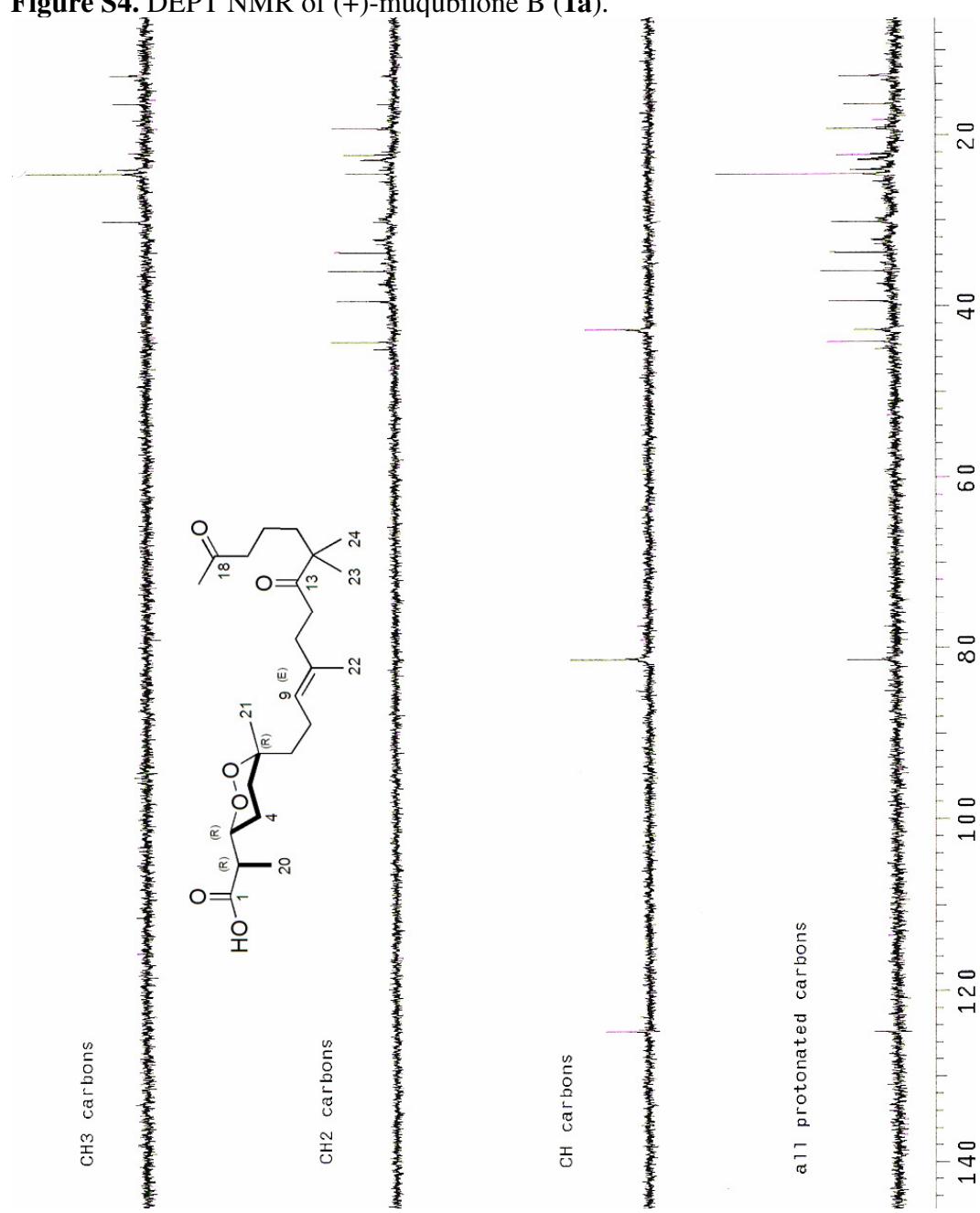
**Figure S2.**  $^{13}\text{C}$  NMR of (+)-muquibilone B (**1a**).



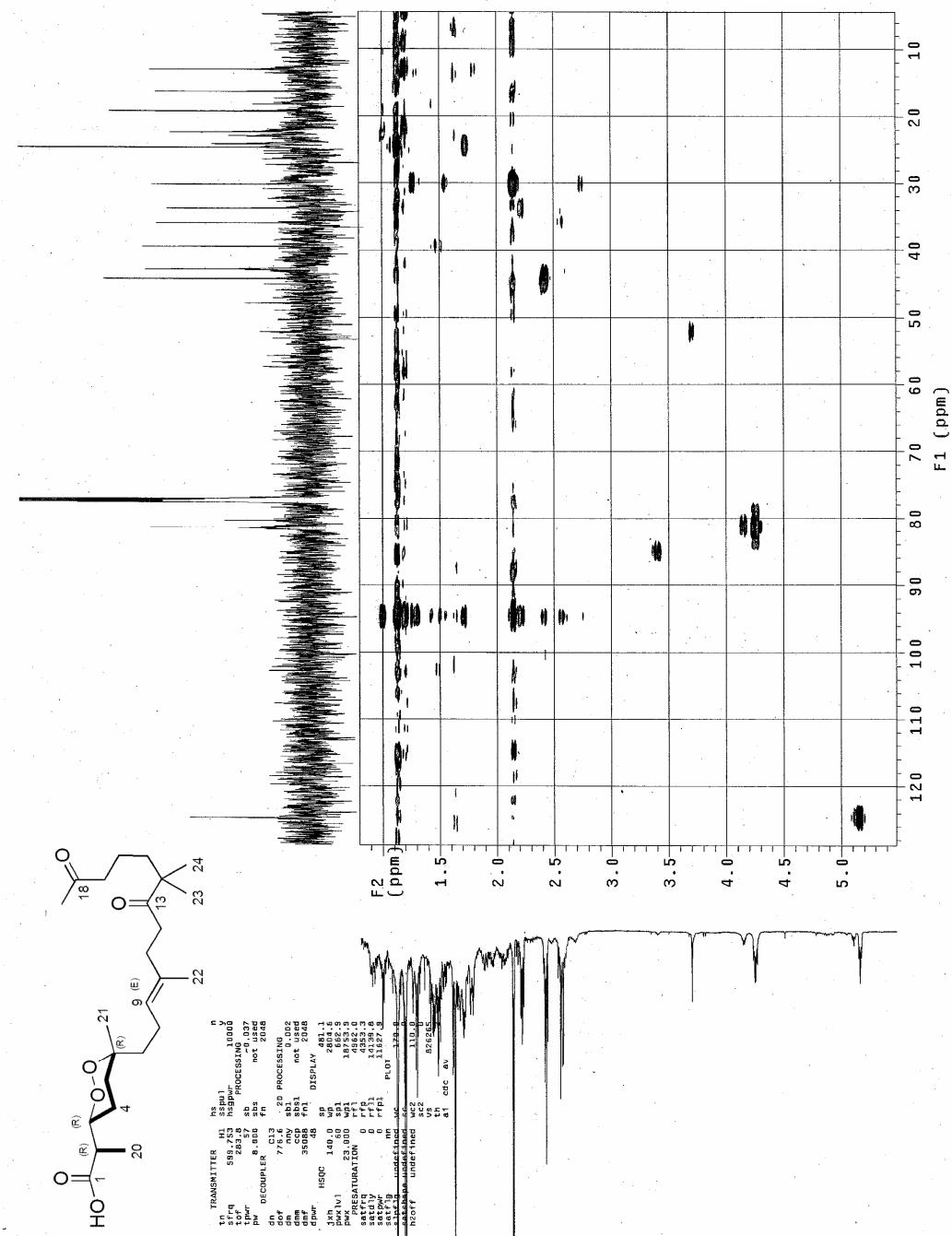
**Figure S3.** ESI-MS of (+)-muquibilone B (**1a**).



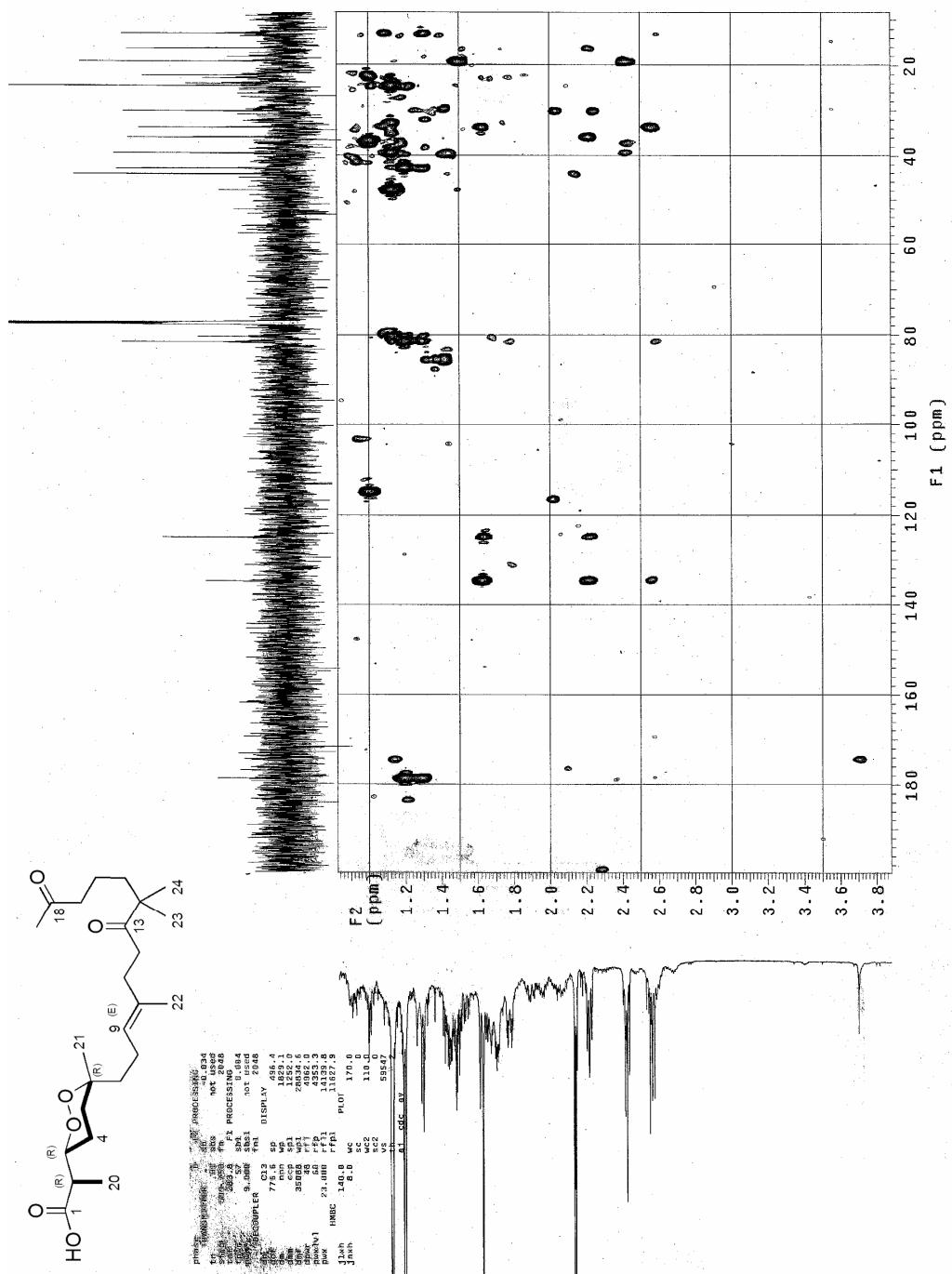
**Figure S4.** DEPT NMR of (+)-muquibilone B (**1a**).



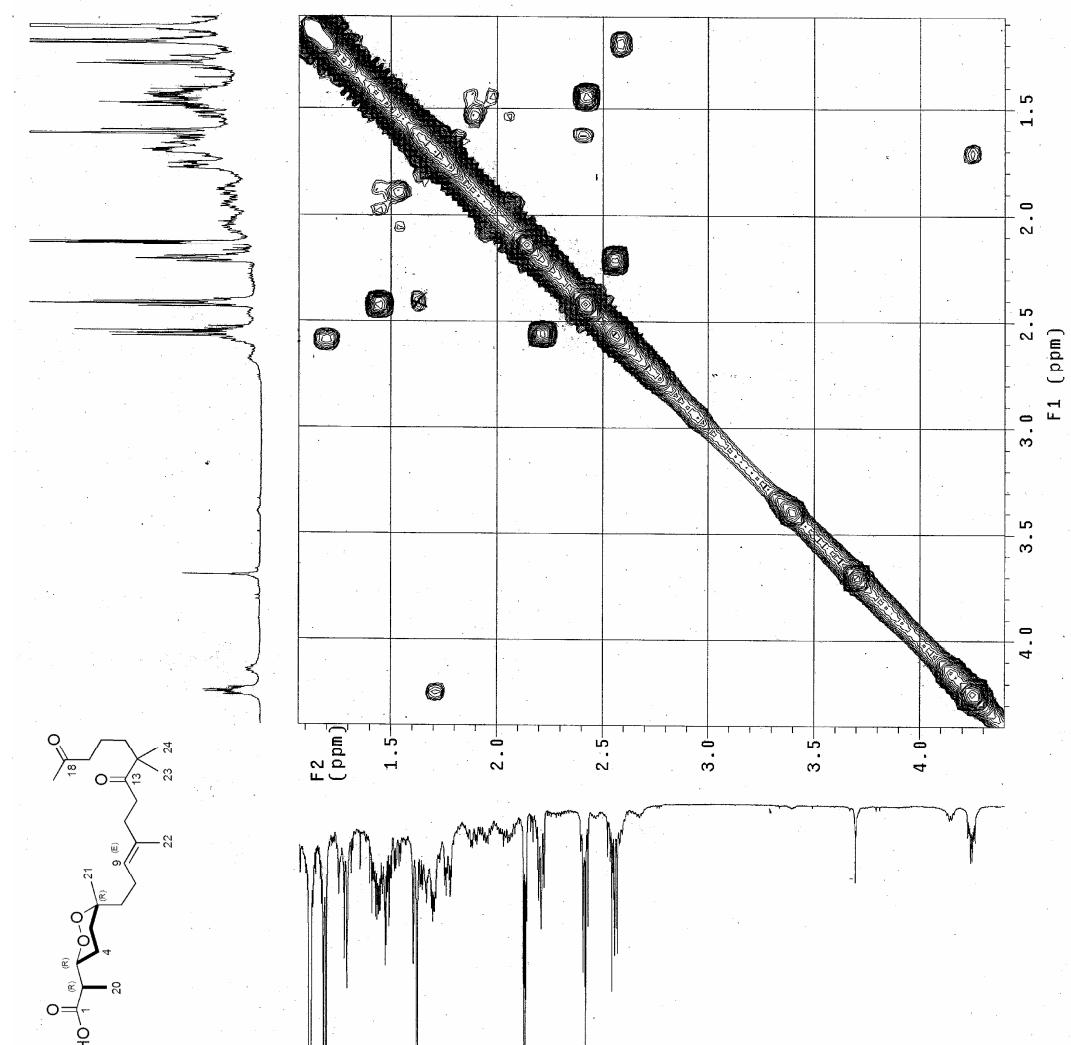
**Figure S5.** HSQC of (+)-muquibilone B (**1a**).



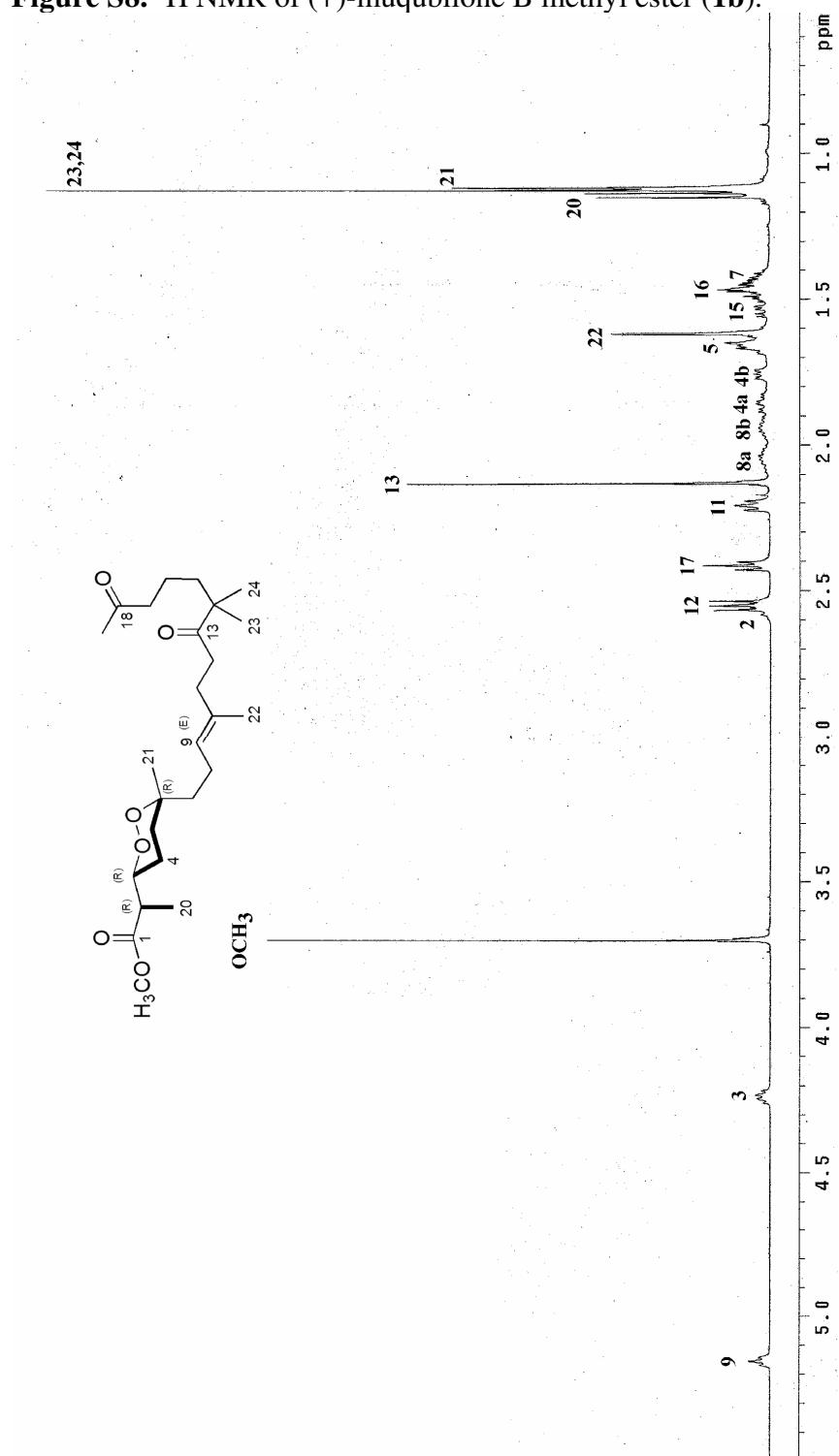
**Figure S6.** gHMBC of (+)-muquibilone B (**1a**).



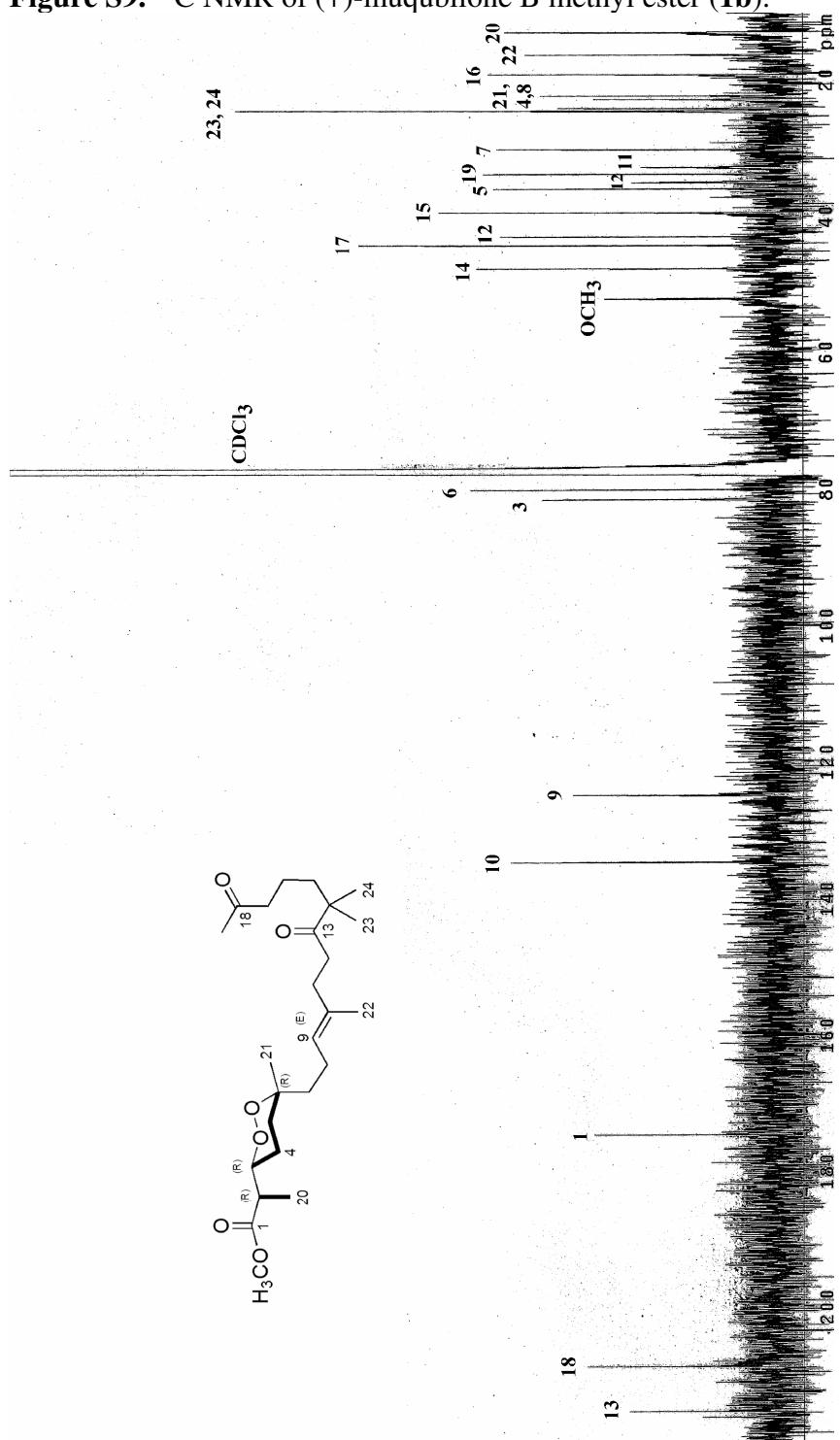
**Figure S7.** gCOSY of (+)-muqubilone B (**1a**).



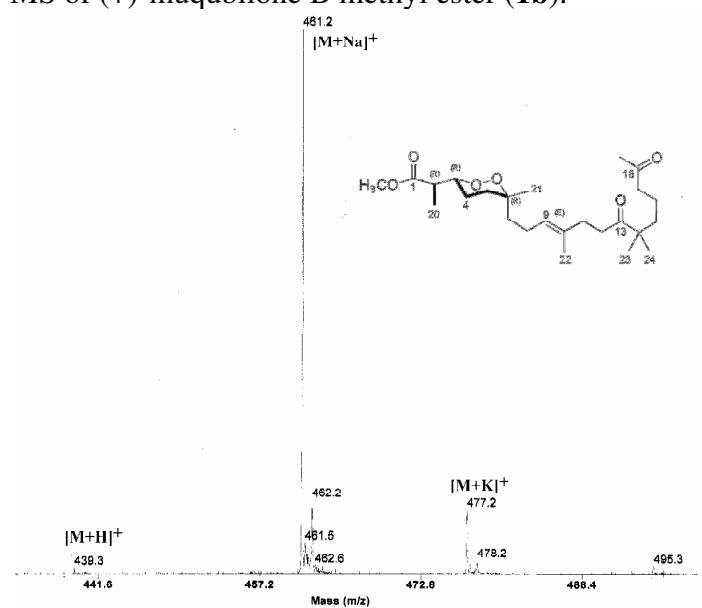
**Figure S8.**  $^1\text{H}$  NMR of (+)-muquibilone B methyl ester (**1b**).



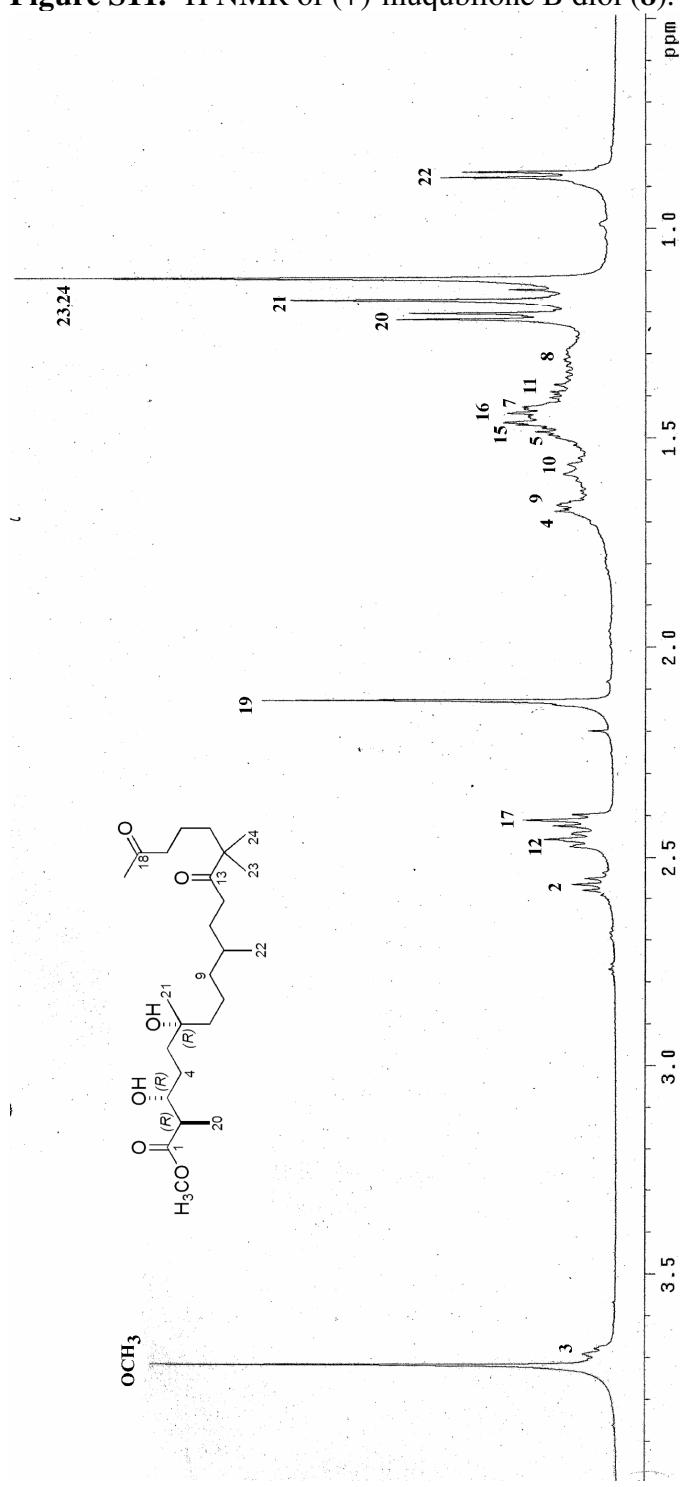
**Figure S9.**  $^{13}\text{C}$  NMR of (+)-muquibilone B methyl ester (**1b**).



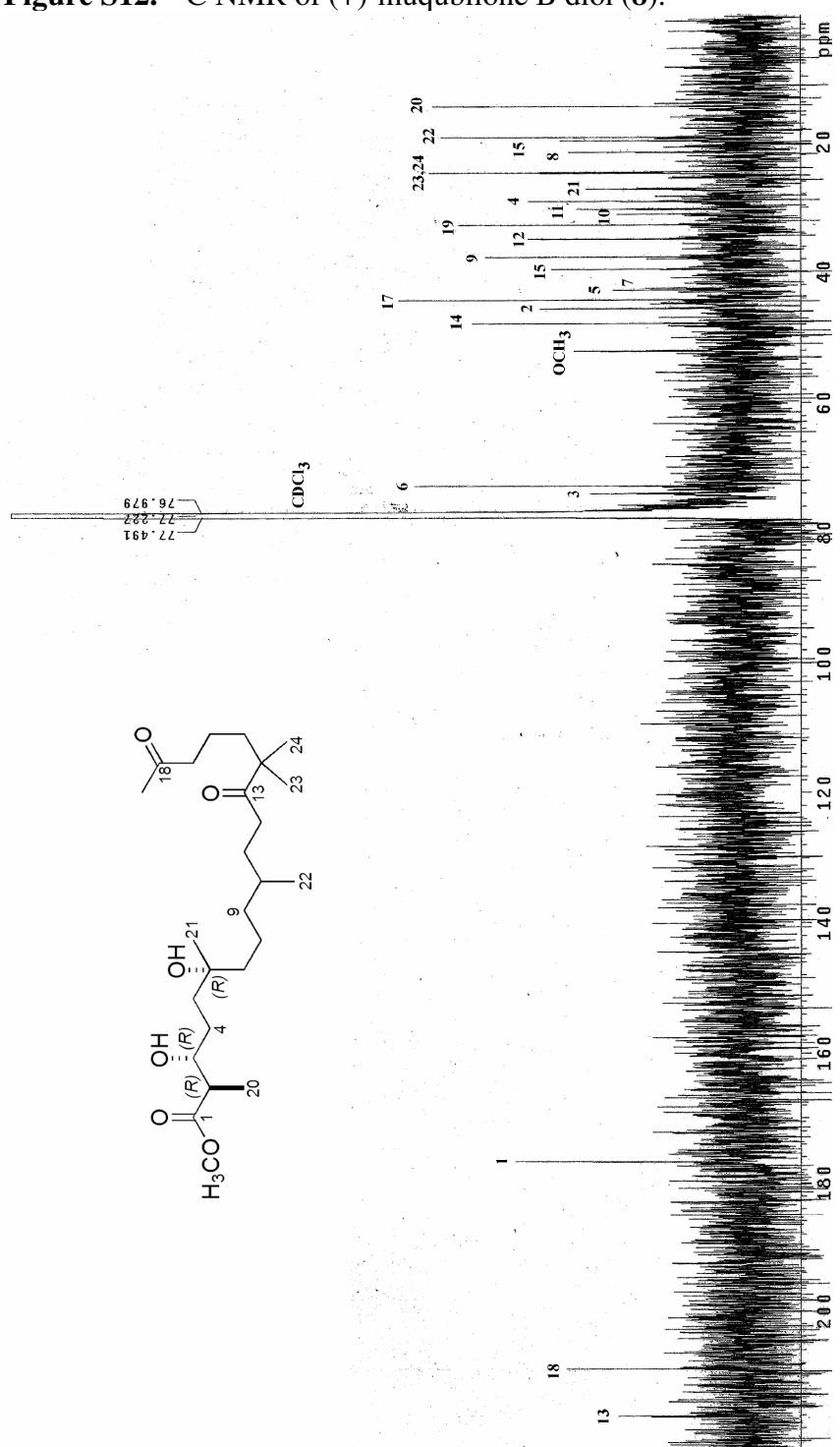
**Figure S10.** ESI-MS of (+)-muquibilone B methyl ester (**1b**).



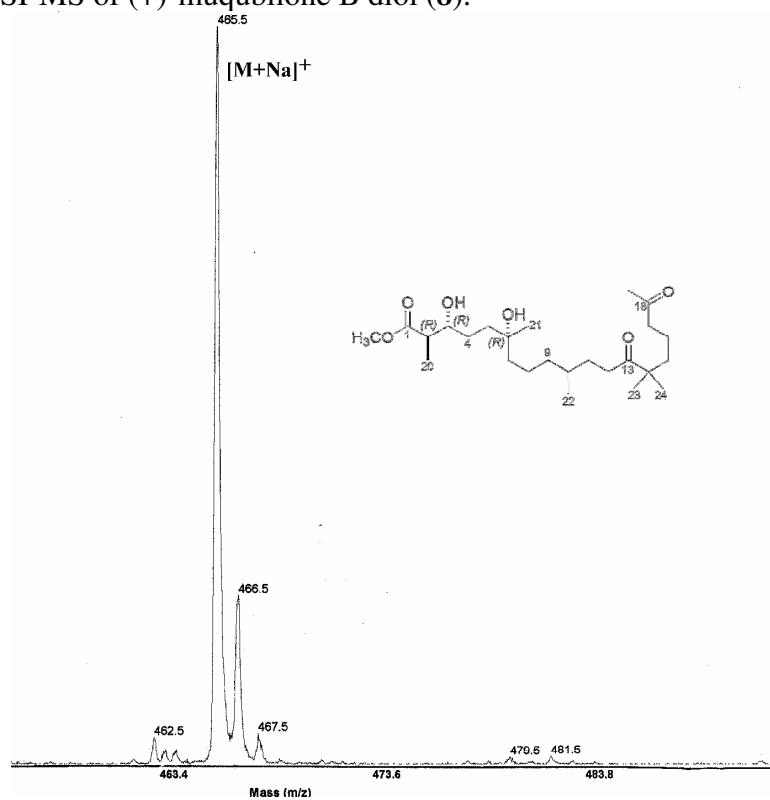
**Figure S11.**  $^1\text{H}$  NMR of (+)-muquibilone B diol (**8**).



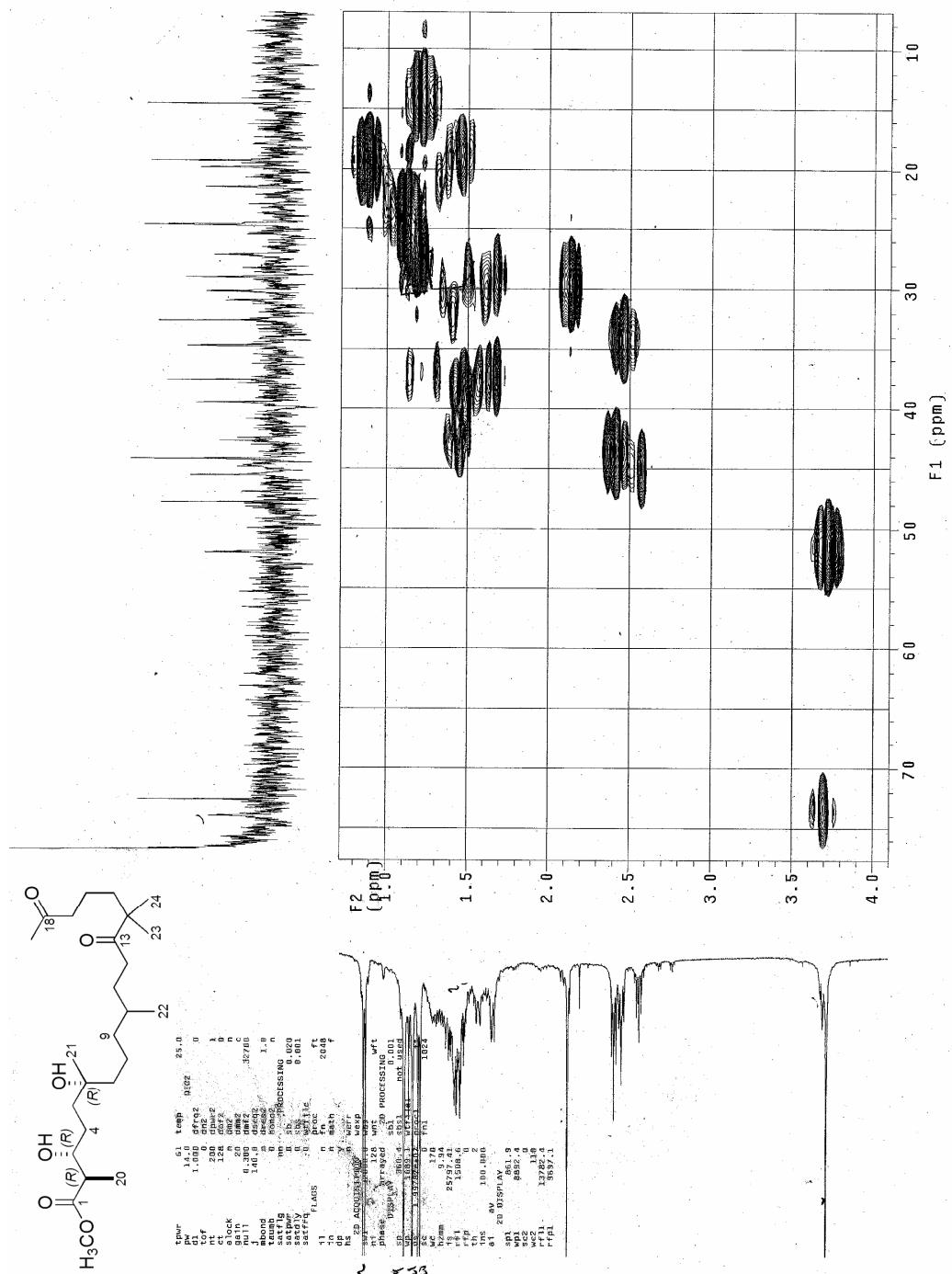
**Figure S12.**  $^{13}\text{C}$  NMR of (+)-muquibilone B diol (**8**).



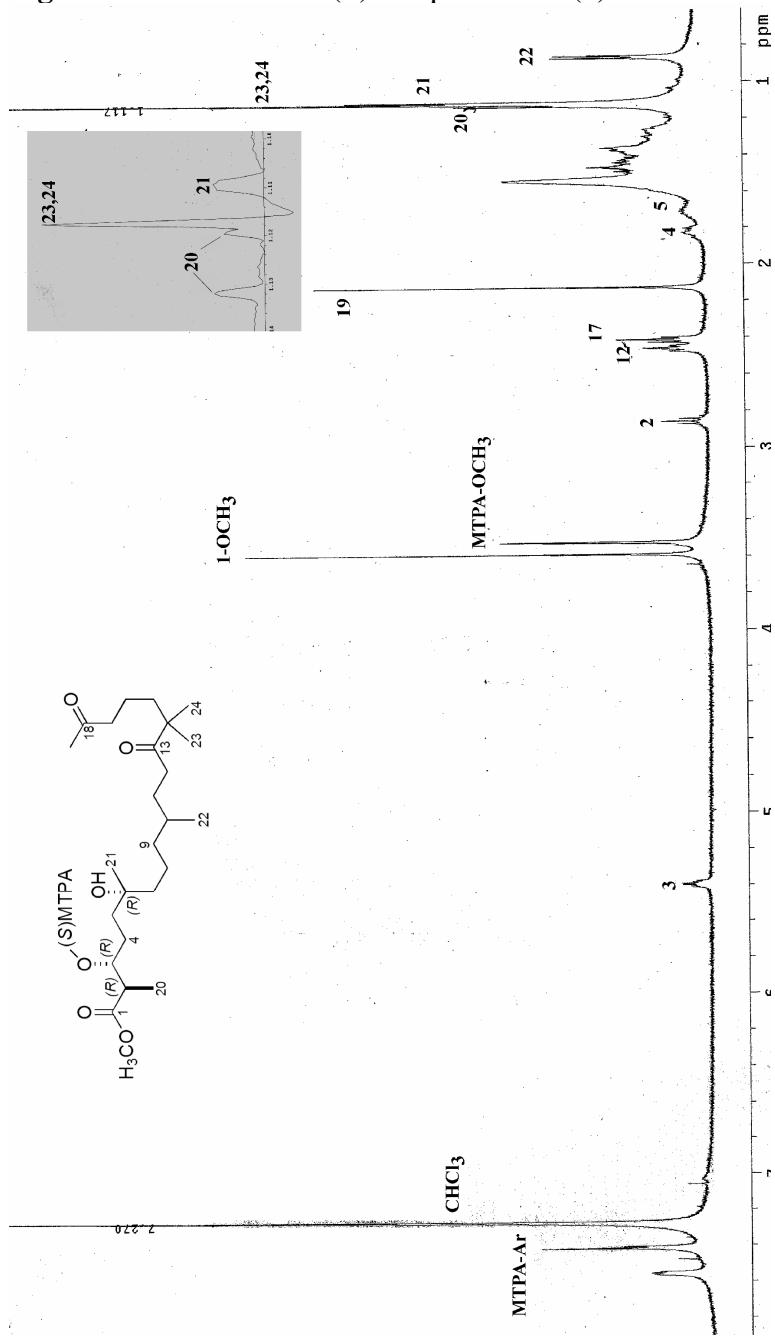
**Figure S13.** ESI-MS of (+)-muquibilone B diol (**8**).



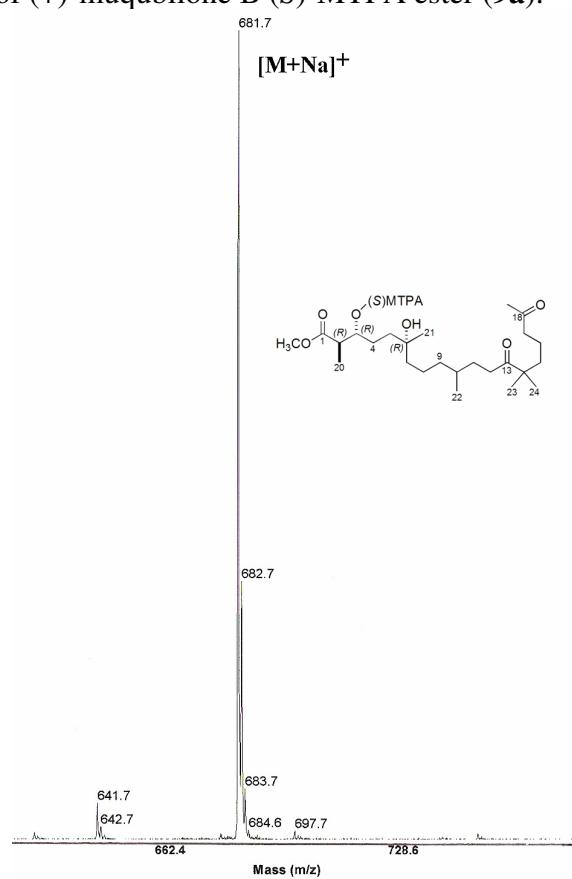
**Figure S14.** HSQC of (+)-muqubilone B diol (**8**).



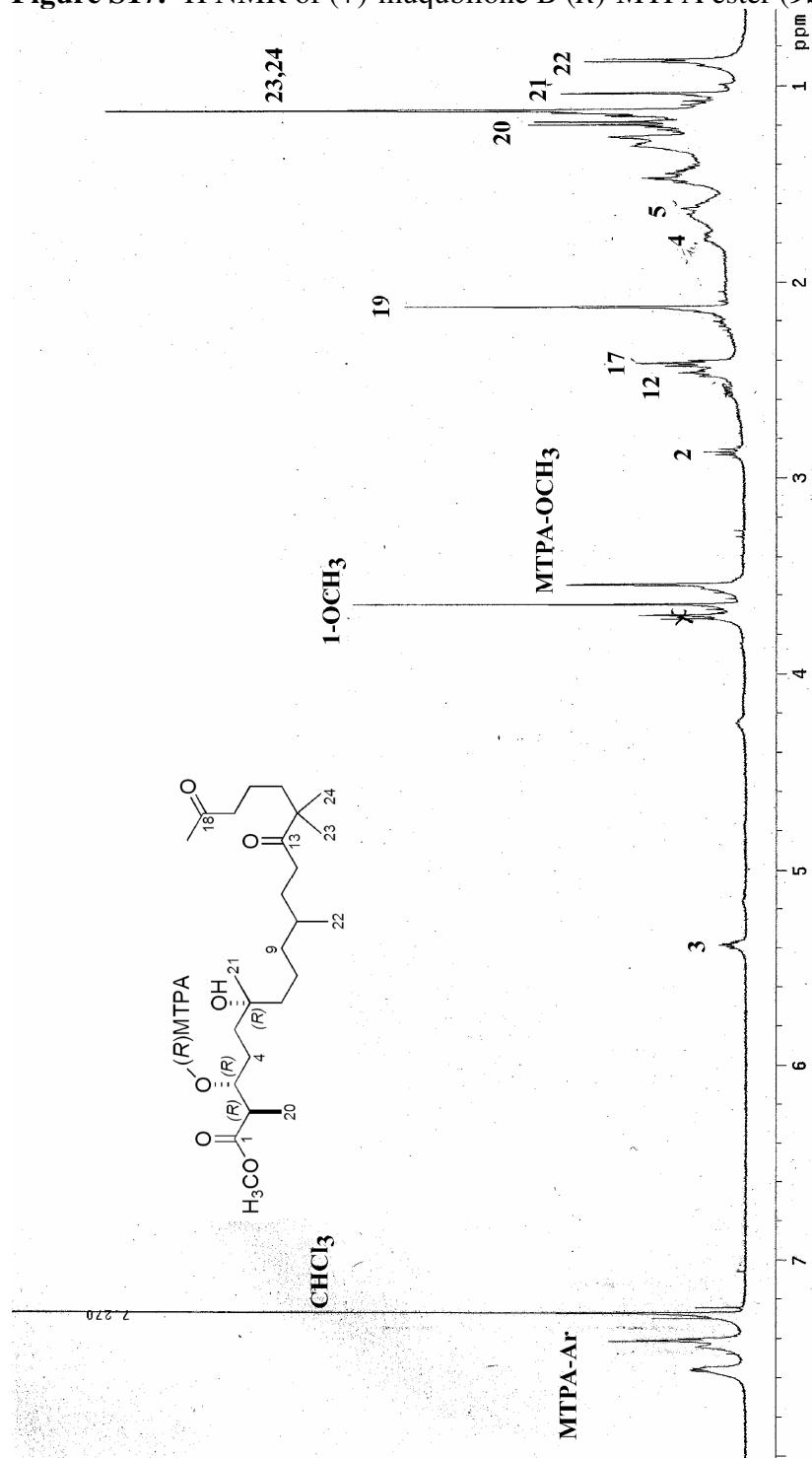
**Figure S15.**  $^1\text{H}$  NMR of (+)-muqubilone B (*S*)-MTPA ester (**9a**)



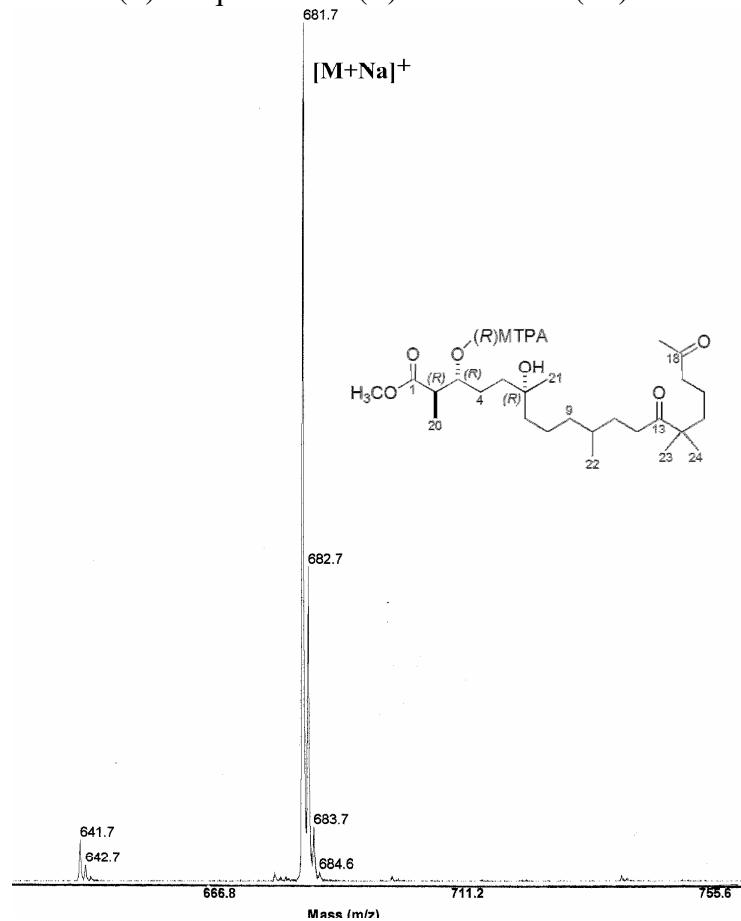
**Figure S16.** ESI-MS of (+)-muquibilone B (*S*)-MTPA ester (**9a**).



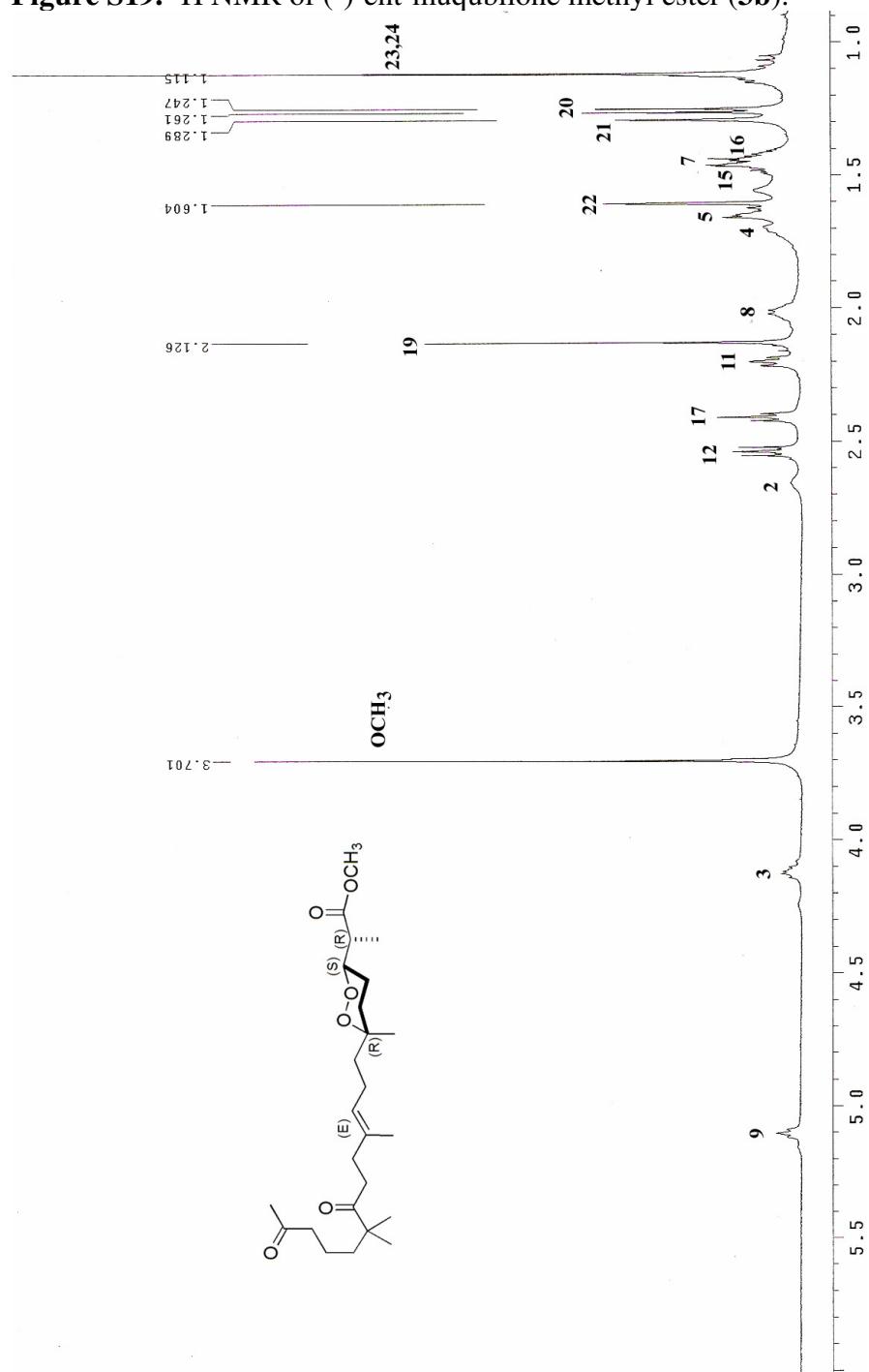
**Figure S17.**  $^1\text{H}$  NMR of (+)-muquibilone B (*R*)-MTPA ester (**9b**).



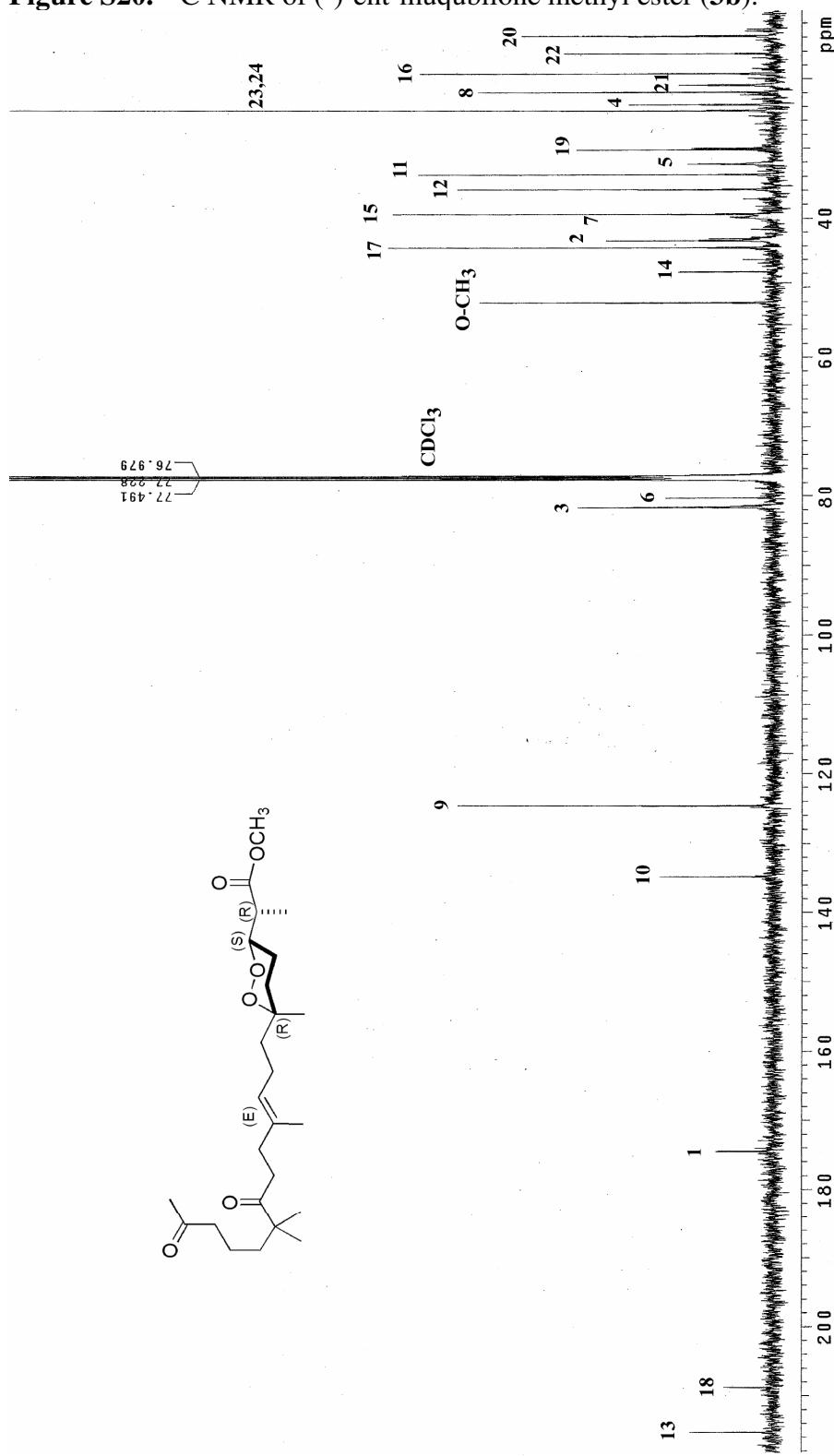
**Figure S18.** ESI-MS of (+)-muquibilone B (*R*)-MTPA ester (**9b**).



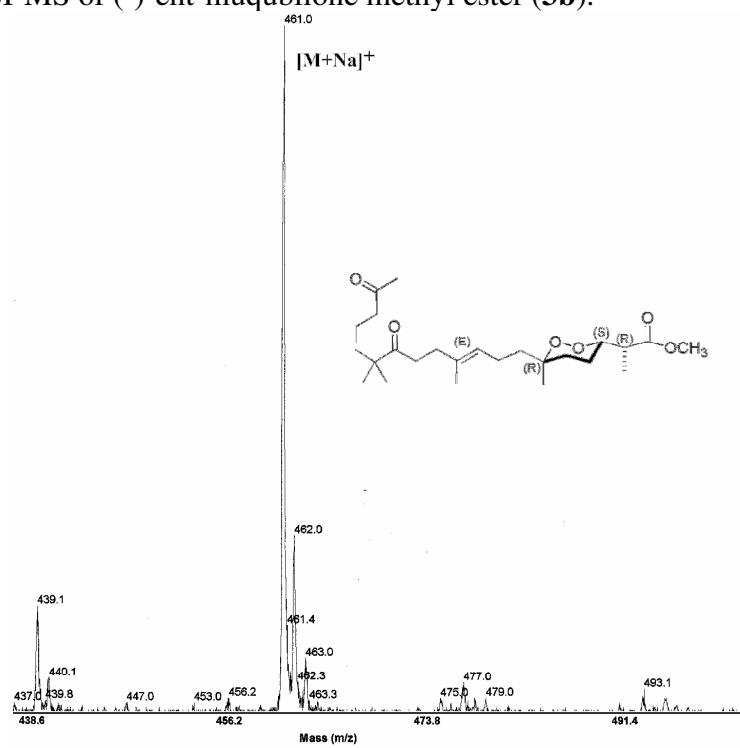
**Figure S19.**  $^1\text{H}$  NMR of (-)-ent-muquabilone methyl ester (**3b**).



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



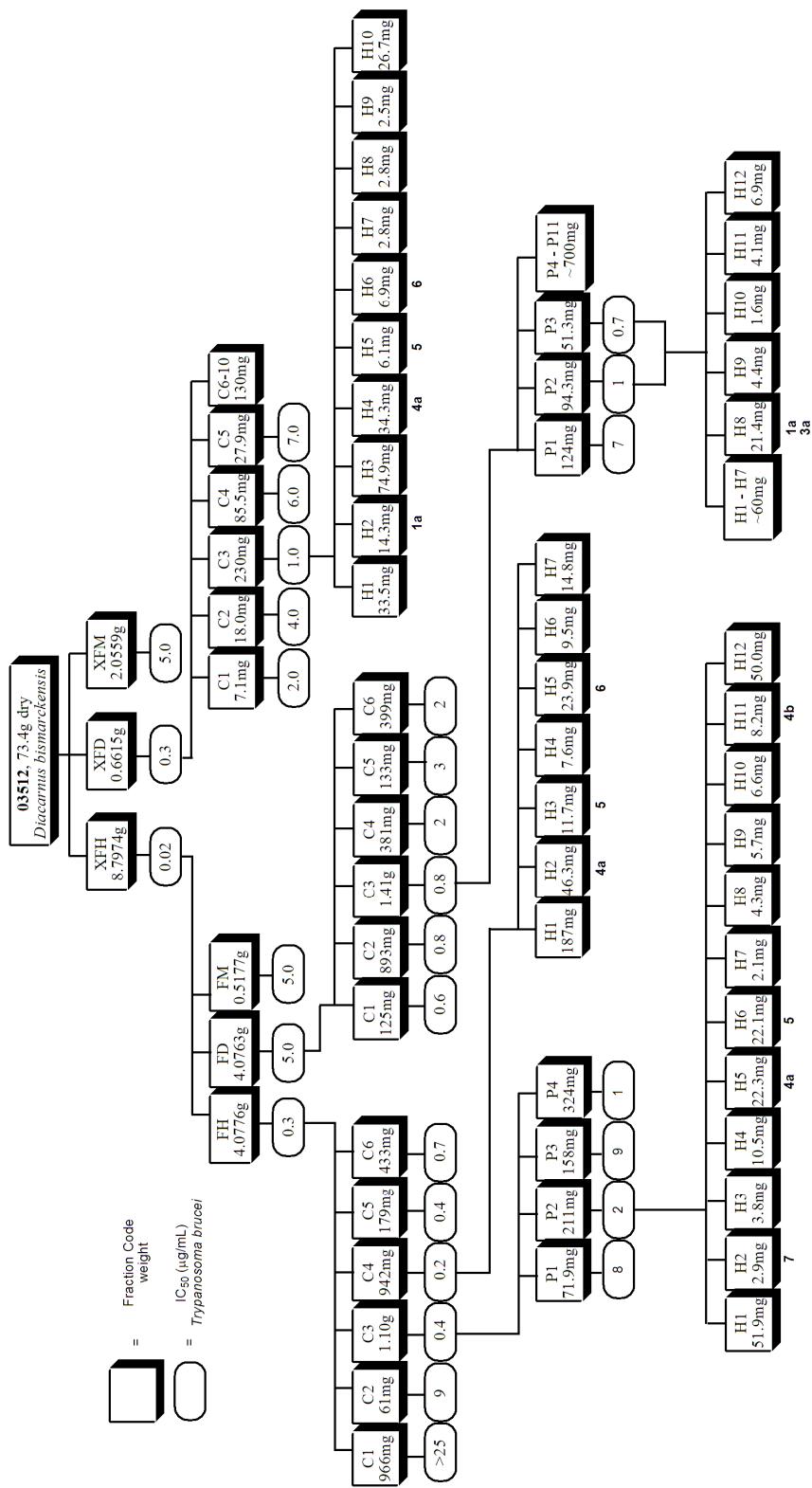
**Figure S21.** ESI-MS of (-)-ent-muquobilone methyl ester (**3b**).



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

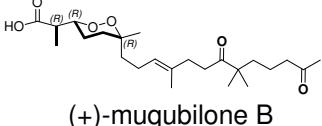
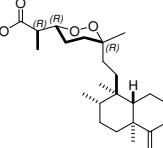
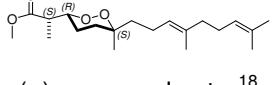
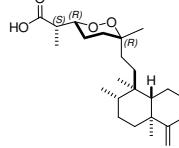
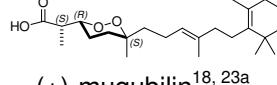
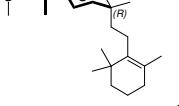
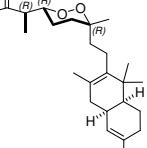
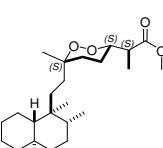


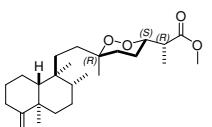
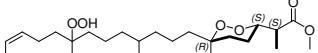
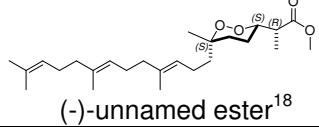
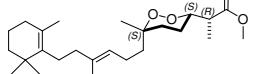
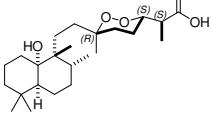
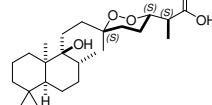
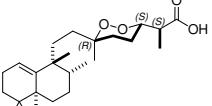
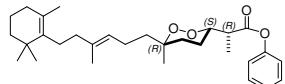
**Scheme S1.** Isolation scheme for 03512.



1a = PC 952  
 3b = PC 953  
 4a = PC 234  
 4b = PC 956  
 5 = PC 554  
 6 = PC 322  
 7 = PC 518

**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
 <b>(+)-muquibilone B</b>	+60 (CHCl <sub>3</sub> )	R	R	R
 <b>(+)-sigmosceptrellin A<sup>16,18</sup></b>	+53 (CHCl <sub>3</sub> )	R	R	R
 <b>(+)-unnamed ester<sup>18</sup></b>	+52 (CHCl <sub>3</sub> )	S	R	S
 <b>(+)-sigmosceptrellin C<sup>16,18</sup></b>	+42 (CHCl <sub>3</sub> )	S	R	R
 <b>(+)-muquibilin<sup>18, 23a</sup></b>	+31 (CHCl <sub>3</sub> )	S	R	S
 <b>(+)-nuapapuin A<sup>23b</sup></b>	+62 (CHCl <sub>3</sub> )	R	R	R
 <b>(+)-trunculin A methyl ester<sup>23f</sup></b>	+158 (CHCl <sub>3</sub> )	R	R	R
 <b>(-)-ent-sigmosceptrellin A methyl ester<sup>23e</sup></b>	-57 (CHCl <sub>3</sub> )	S	S	S

	(S)	(R)	(S)	(R)
	-61 (CHCl <sub>3</sub> )	R	S	R
(-)-sigmosceptrellin B methyl ester <sup>16,18</sup>				
	-58 (CHCl <sub>3</sub> )	R	S	S
(-)-sigmosceptrellin D methyl ester <sup>23b</sup>				
	-60 (CHCl <sub>3</sub> )	S	S	R
(-)-unnamed ester <sup>18</sup>				
	-59 (CHCl <sub>3</sub> )	S	S	R
(-)-unnamed ester <sup>18</sup>				
	-41 (acetone)	R	S	S
(-)-mycaperoxide A <sup>23d</sup>				
	-41 (acetone)	S	S	S
(-)-mycaperoxide B <sup>23d</sup>				
	-143 (acetone)	R	S	S
(-)-mycaperoxide H <sup>23c</sup>				
	-25 (CHCl <sub>3</sub> )	R	S	R
(-)-unnamed ester <sup>18</sup>				