

# Supplementary Information

## Variable-Temperature NMR and Conformational Analysis of Oenothien B

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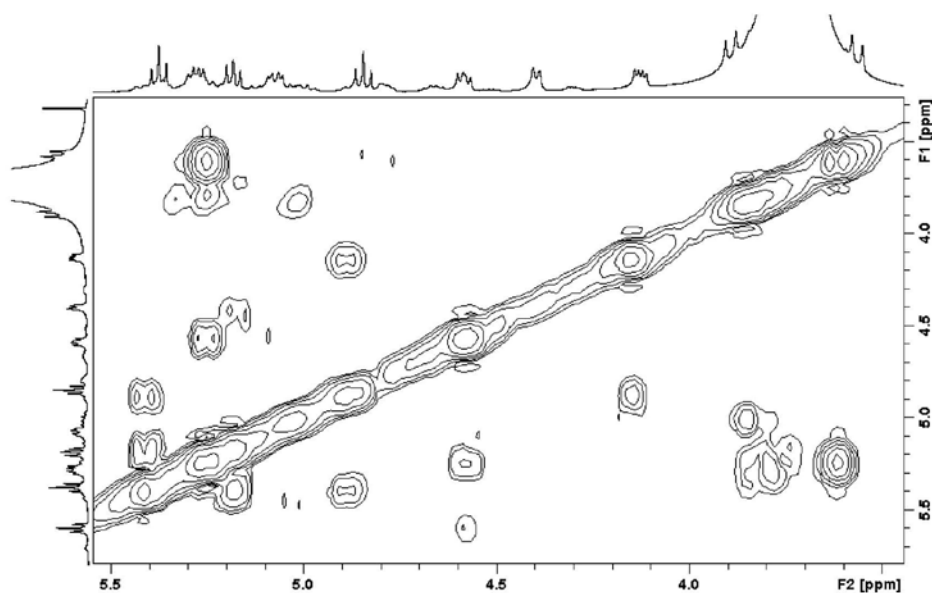


Figure S1. Expansion of the  $^1\text{H}$ - $^1\text{H}$  correlation map from COSY NMR experiment of oenothien B (acetone- $d_6$  +  $\text{D}_2\text{O}$ ,  $-20^\circ\text{C}$ , 500 MHz).

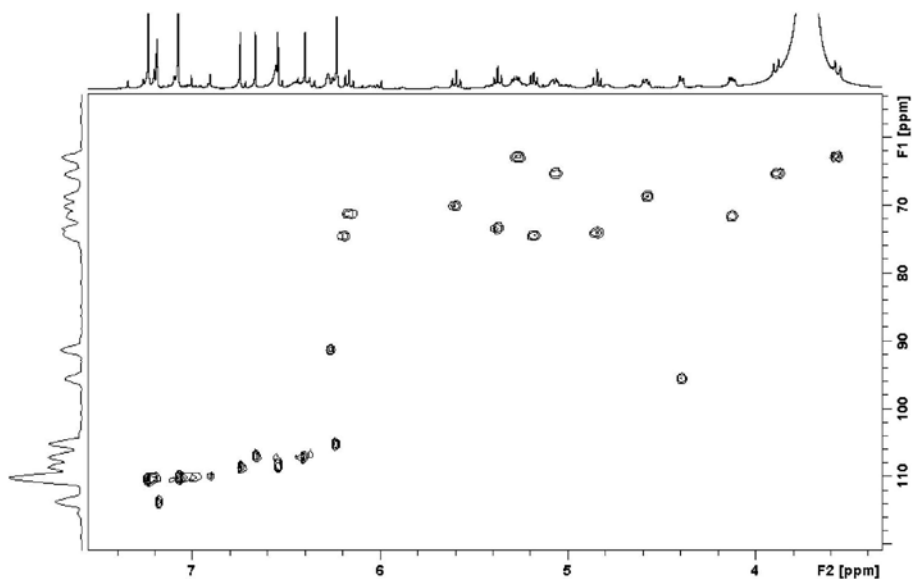
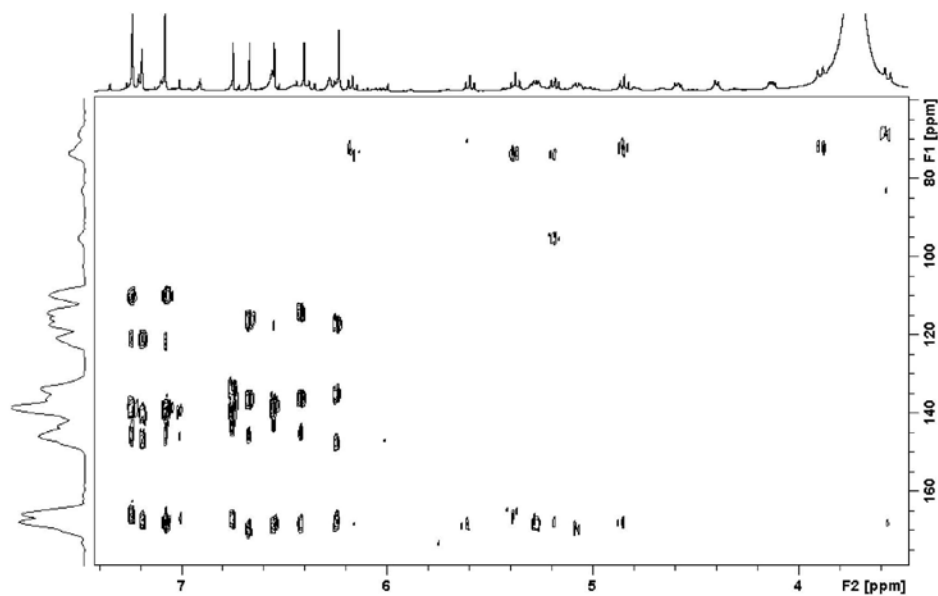
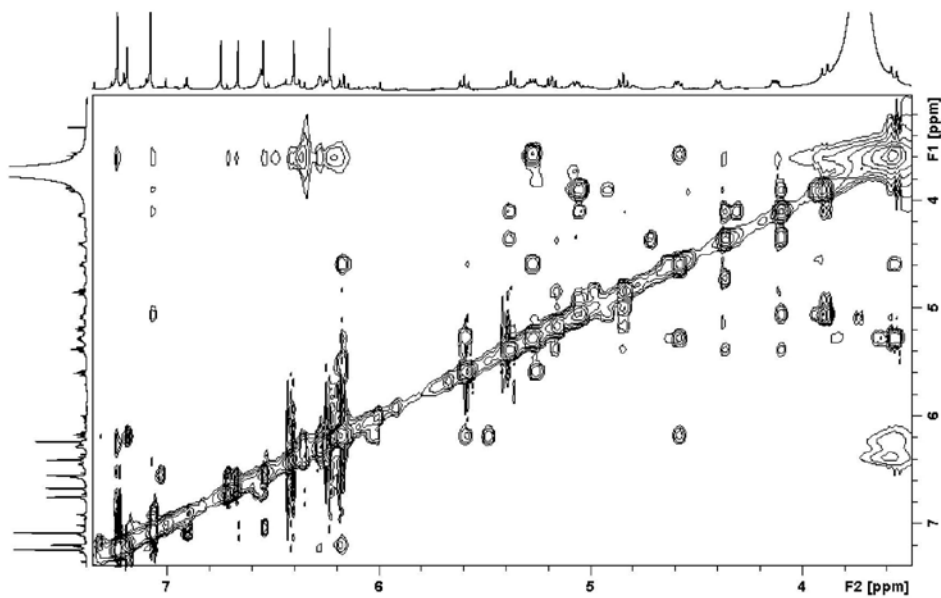


Figure S2. Expansion of the  $^1\text{H}$ - $^{13}\text{C}$  direct correlation map from HSQC NMR experiment of oenothien B (acetone- $d_6$  +  $\text{D}_2\text{O}$ ,  $-20^\circ\text{C}$ , 500 and 125 MHz).

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**Figure S3.** Expansion of the  $^1\text{H}$ - $^{13}\text{C}$  long-range correlation map from HMBC NMR experiment of oenothien B (acetone- $d_6$  +  $\text{D}_2\text{O}$ ,  $-20^\circ\text{C}$ , 500 and 125 MHz,  $J_{\text{CH}} = 10$  Hz).



**Figure S4.** Expansion of the  $^1\text{H}$ - $^1\text{H}$  correlation map from NOESY NMR experiment of oenothien B (acetone- $d_6$  +  $\text{D}_2\text{O}$ ,  $-20^\circ\text{C}$ , 500 MHz).

**Table S1.**  $^1\text{H}$ - $^{13}\text{C}$  direct and long-range correlation data for oenothain B (acetone- $d_6$  +  $\text{D}_2\text{O}$ ,  $-20\text{ }^\circ\text{C}$ , 500 and 125 MHz)

No.	$^1\text{H}$ - $^{13}\text{C}$ direct correlation		$^1\text{H}$ - $^{13}\text{C}$ long-range correlations
	$\delta_{\text{H}}$ (ppm)	$\delta_{\text{C}}$ (ppm)	
Glucose I			
1	6.28	91.2	–
2	6.18	74.4	C-3 <sub>I</sub>
3	6.16	71.2	C-2 <sub>I</sub> , C-7 <sub>I</sub> <sup>''</sup> <sub>G</sub>
4	5.59	70.1	C-3 <sub>I</sub> , C-5 <sub>I</sub> , C-7 <sub>I</sub> <sup>'</sup> <sub>A</sub>
5	4.58	68.6	–
6	3.56, 5.27	62.8	C-5 <sub>I</sub> , C-7 <sub>I</sub> <sup>'</sup> <sub>B</sub>
Glucose II			
1	4.40	95.5	–
2	5.18	74.4	C-1 <sub>II</sub> , C-4 <sub>II</sub> , C-7 <sub>I</sub> <sup>'</sup> <sub>C</sub>
3	5.38	73.4	C-4 <sub>II</sub> , C-7 <sub>I</sub> <sup>''</sup> <sub>G</sub>
4	4.84	73.9	C-5 <sub>II</sub> , C-7 <sub>I</sub> <sup>'</sup> <sub>B</sub>
5	4.13	71.6	–
6	3.89, 5.07	65.2	C-5 <sub>II</sub> , C-7 <sub>I</sub> <sup>'</sup> <sub>A</sub>
Valoneoyl (ring A)			
6 <sup>'</sup>	6.40	107.1	C-2 <sub>A</sub> <sup>'</sup> , C-4 <sub>A</sub> <sup>'</sup> , C-5 <sub>A</sub> <sup>'</sup> , C-7 <sub>A</sub> <sup>'</sup>
Valoneoyl (ring B)			
6 <sup>'</sup>	6.23	105.1	C-2 <sub>B</sub> <sup>'</sup> , C-4 <sub>B</sub> <sup>'</sup> , C-5 <sub>B</sub> <sup>'</sup> , C-7 <sub>B</sub> <sup>'</sup>
Valoneoyl (ring C)			
6 <sup>'</sup>	6.75	108.6	C-2 <sub>C</sub> <sup>'</sup> , C-4 <sub>C</sub> <sup>'</sup> , C-5 <sub>C</sub> <sup>'</sup> , C-7 <sub>C</sub> <sup>'</sup>
Valoneoyl (ring A')			
6 <sup>'</sup>	6.67	106.8	C-2 <sub>A</sub> <sup>'</sup> , C-4 <sub>A</sub> <sup>'</sup> , C-5 <sub>A</sub> <sup>'</sup> , C-7 <sub>A</sub> <sup>'</sup>
Valoneoyl (ring B')			
6 <sup>'</sup>	7.19	113.6	C-2 <sub>B</sub> <sup>'</sup> , C-4 <sub>B</sub> <sup>'</sup> , C-5 <sub>B</sub> <sup>'</sup> , C-7 <sub>B</sub> <sup>'</sup>
Valoneoyl (ring C')			
6 <sup>'</sup>	6.55	108.3	C-2 <sub>C</sub> <sup>'</sup> , C-4 <sub>C</sub> <sup>'</sup> , C-5 <sub>C</sub> <sup>'</sup> , C-7 <sub>C</sub> <sup>'</sup>
Galloyl G			
2 <sup>''</sup> , 6 <sup>''</sup>	7.23	110.3	C-1 <sub>G</sub> <sup>''</sup> , C-3 <sub>G</sub> <sup>''</sup> , C-4 <sub>G</sub> <sup>''</sup> , C-5 <sub>G</sub> <sup>''</sup> , C-7 <sub>G</sub> <sup>''</sup>
Galloyl G'			
2 <sup>''</sup> , 6 <sup>''</sup>	7.08	110.1	C-1 <sub>G</sub> <sup>''</sup> , C-3 <sub>G</sub> <sup>''</sup> , C-4 <sub>G</sub> <sup>''</sup> , C-5 <sub>G</sub> <sup>''</sup> , C-7 <sub>G</sub> <sup>''</sup>