Cyanolide A, a Glycosidic Macrolide with Potent Molluscicidal Activity from the Papua New Guinea Cyanobacterium *Lyngbya bouillonii*

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Figure S1. ^{1}H NMR spectrum of cyanolide A (**2**) (recorded in $CDCl_3$ at 600 MHz).

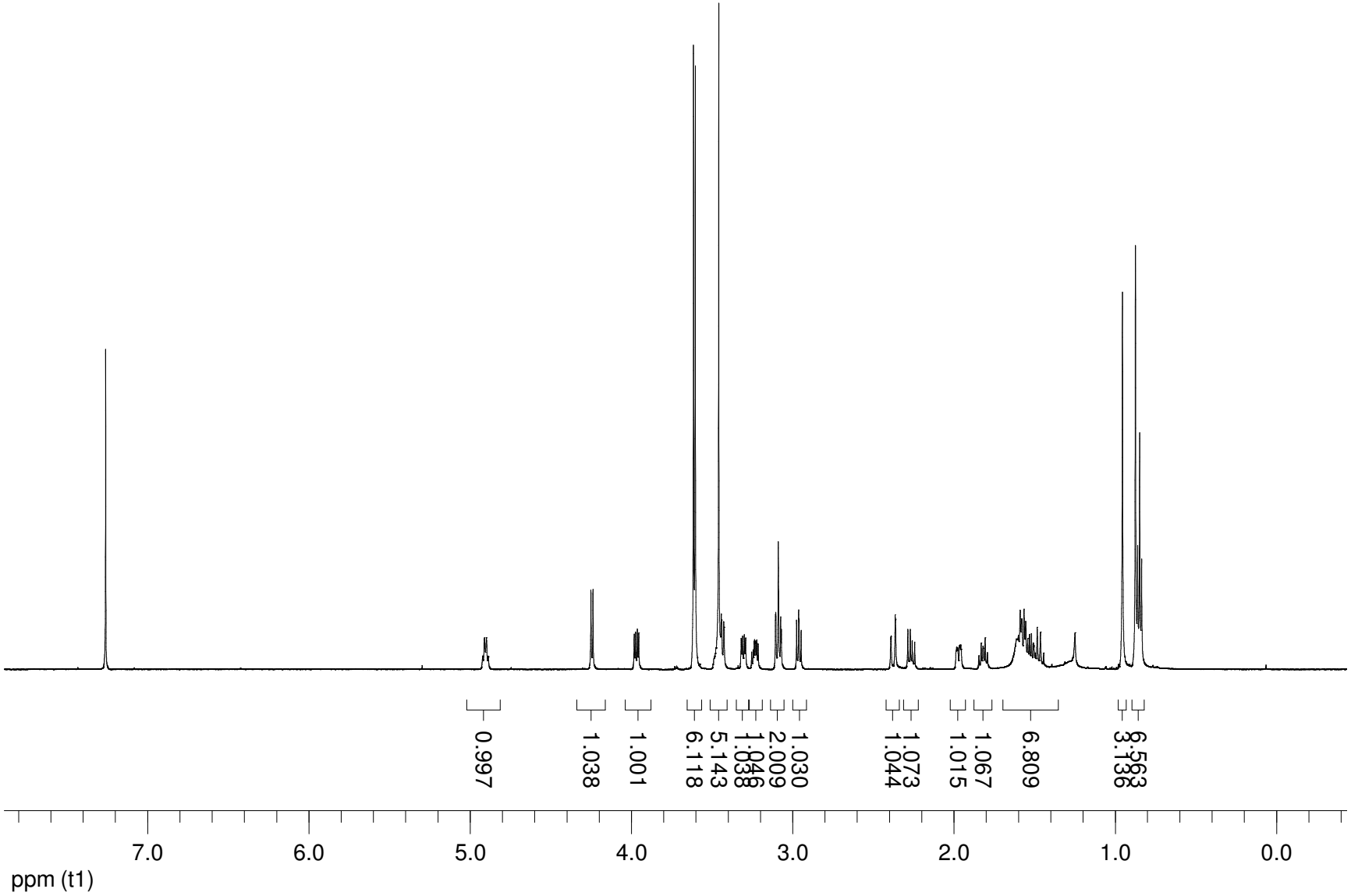


Figure S2. ^{13}C NMR spectrum of cyanolide A (**2**) (recorded in $CDCl_3$ at 150 MHz).

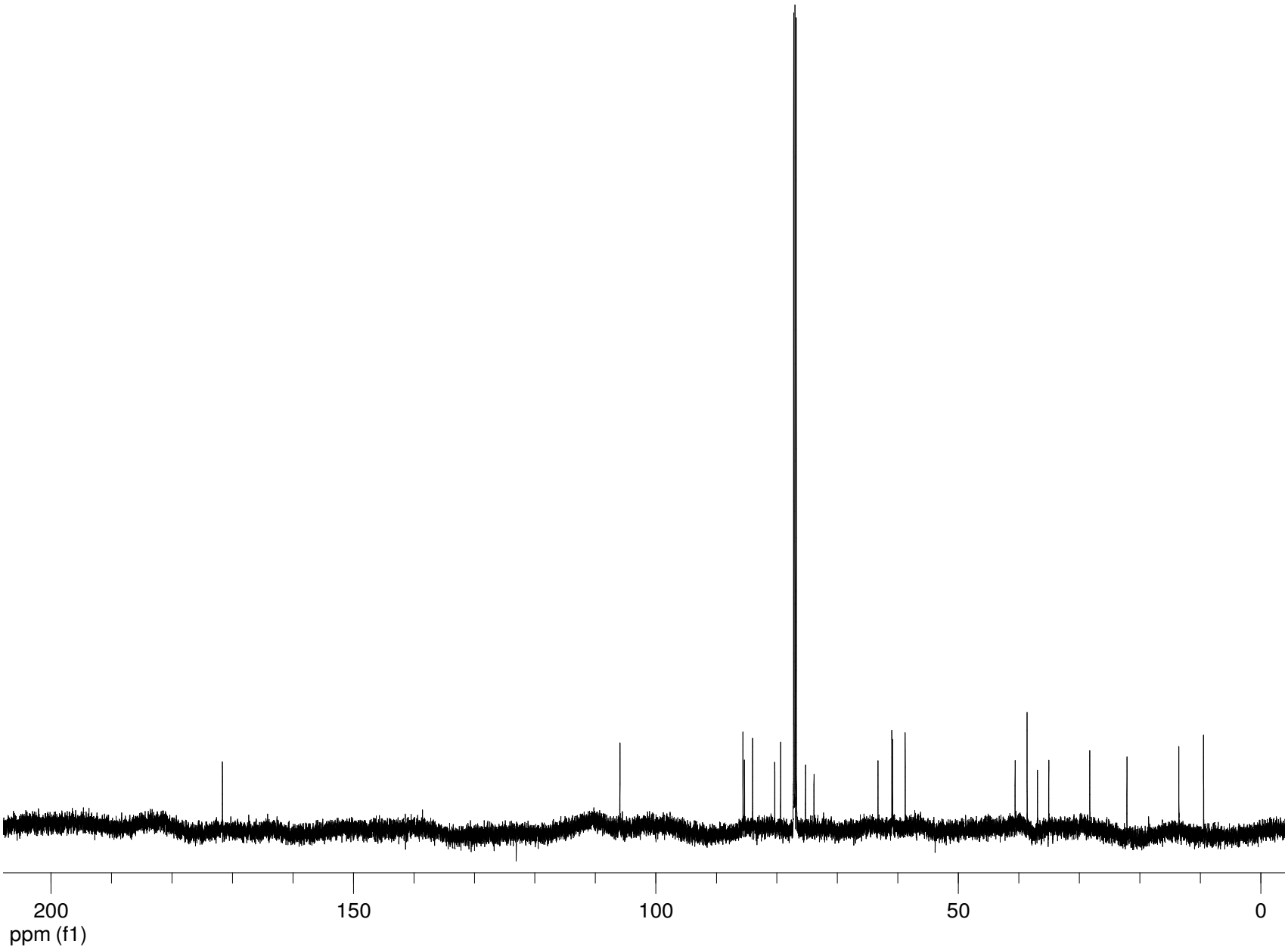


Figure S3. HMBC spectrum of cyanolide A (**2**) (recorded in $CDCl_3$ at 600 MHz).

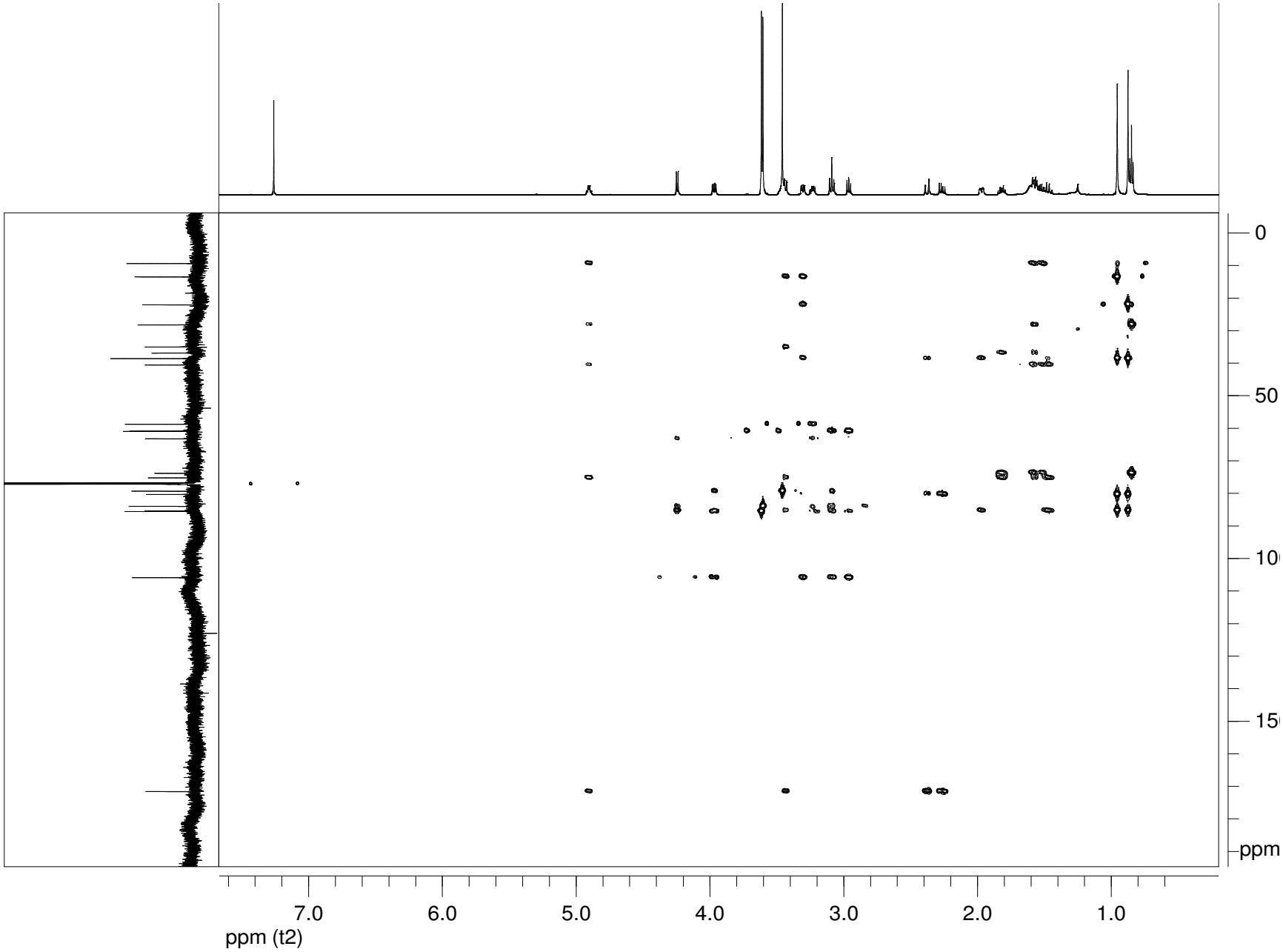


Figure S4. HSQC spectrum of cyanolide A (**2**) (recorded in $CDCl_3$ at 600 MHz).

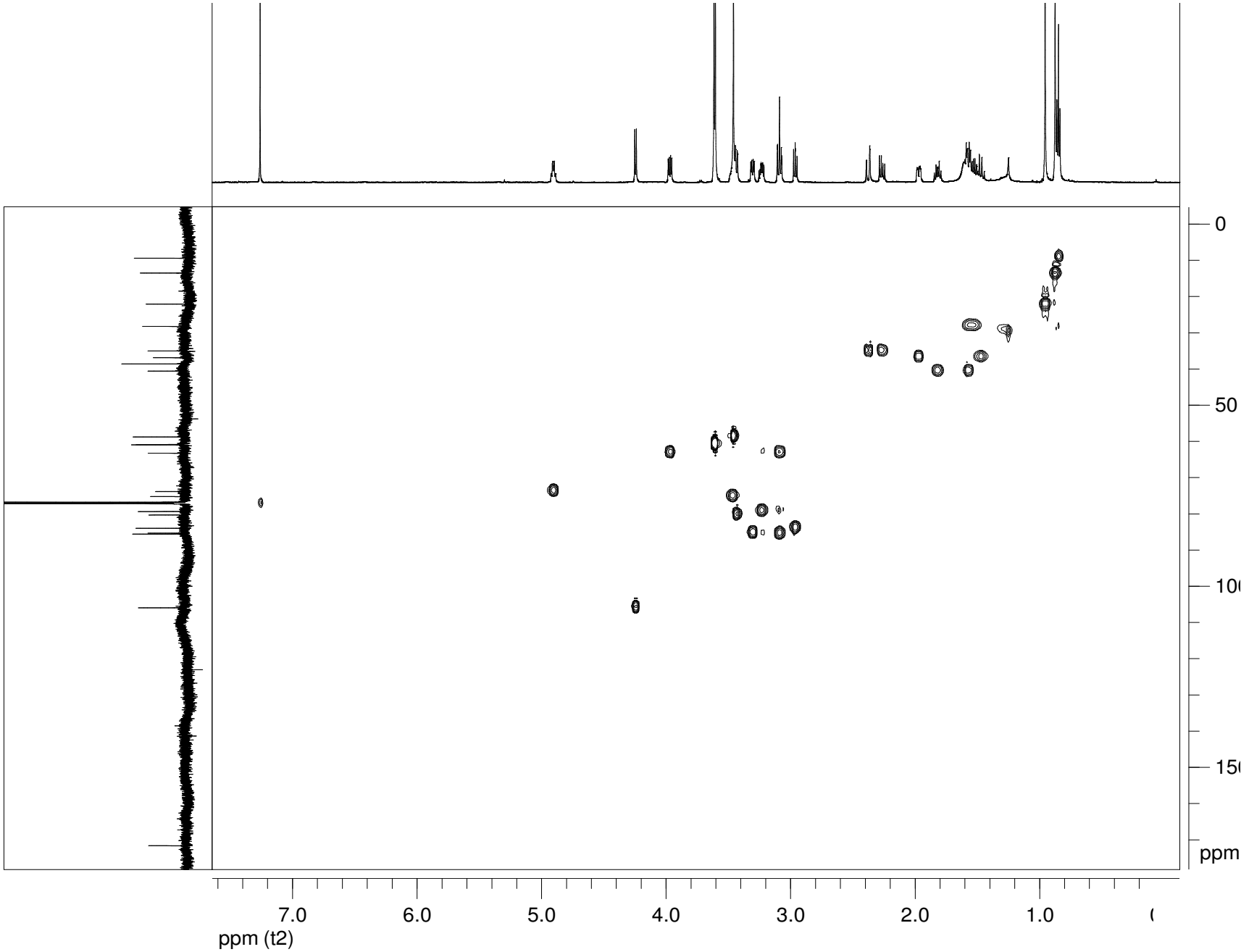


Figure S5. COSY spectrum of cyanolide A (**2**) (recorded in $CDCl_3$ at 600 MHz).

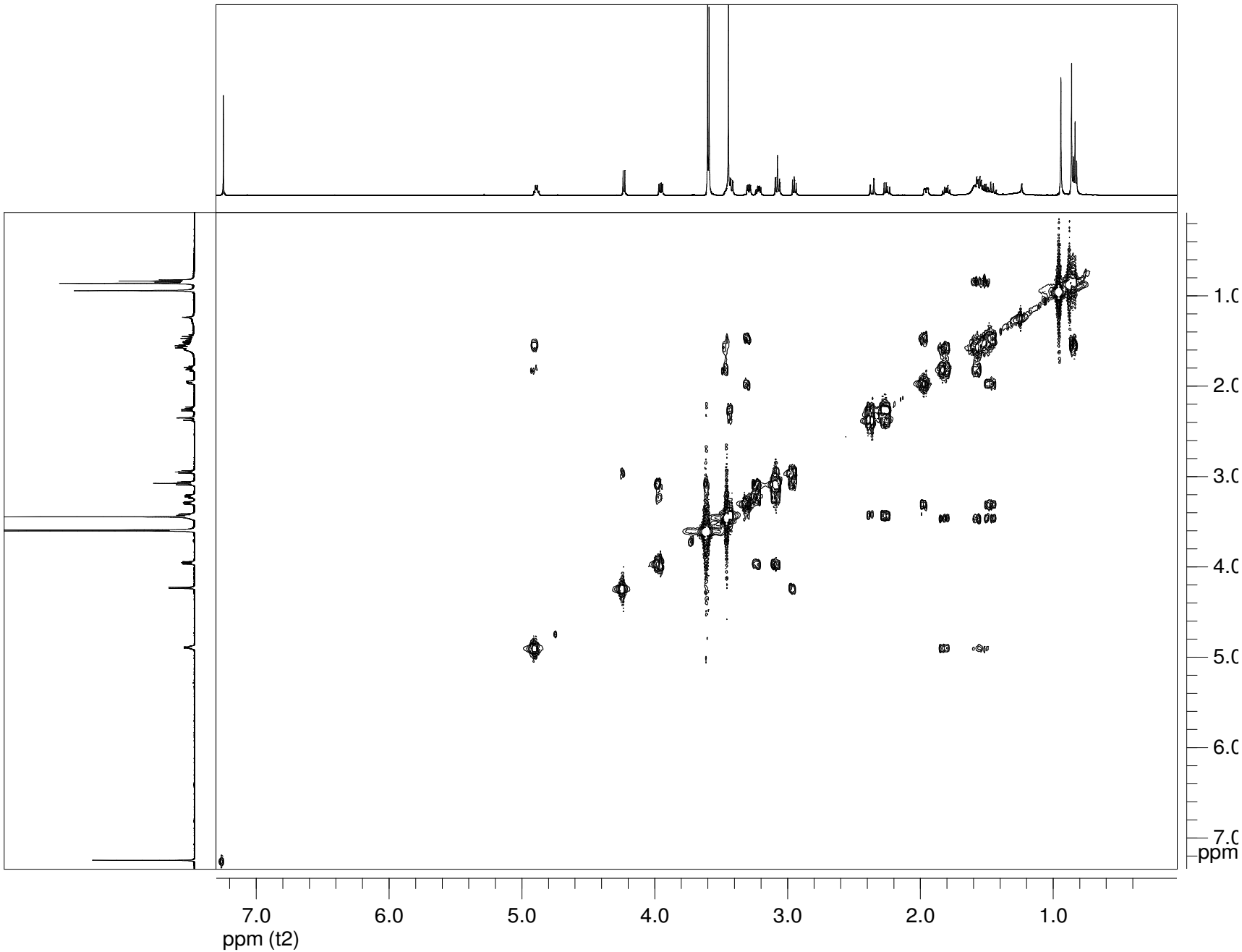


Figure S6. NOESY spectrum of cyanolide A (**2**) (recorded in $CDCl_3$ at 500 MHz).

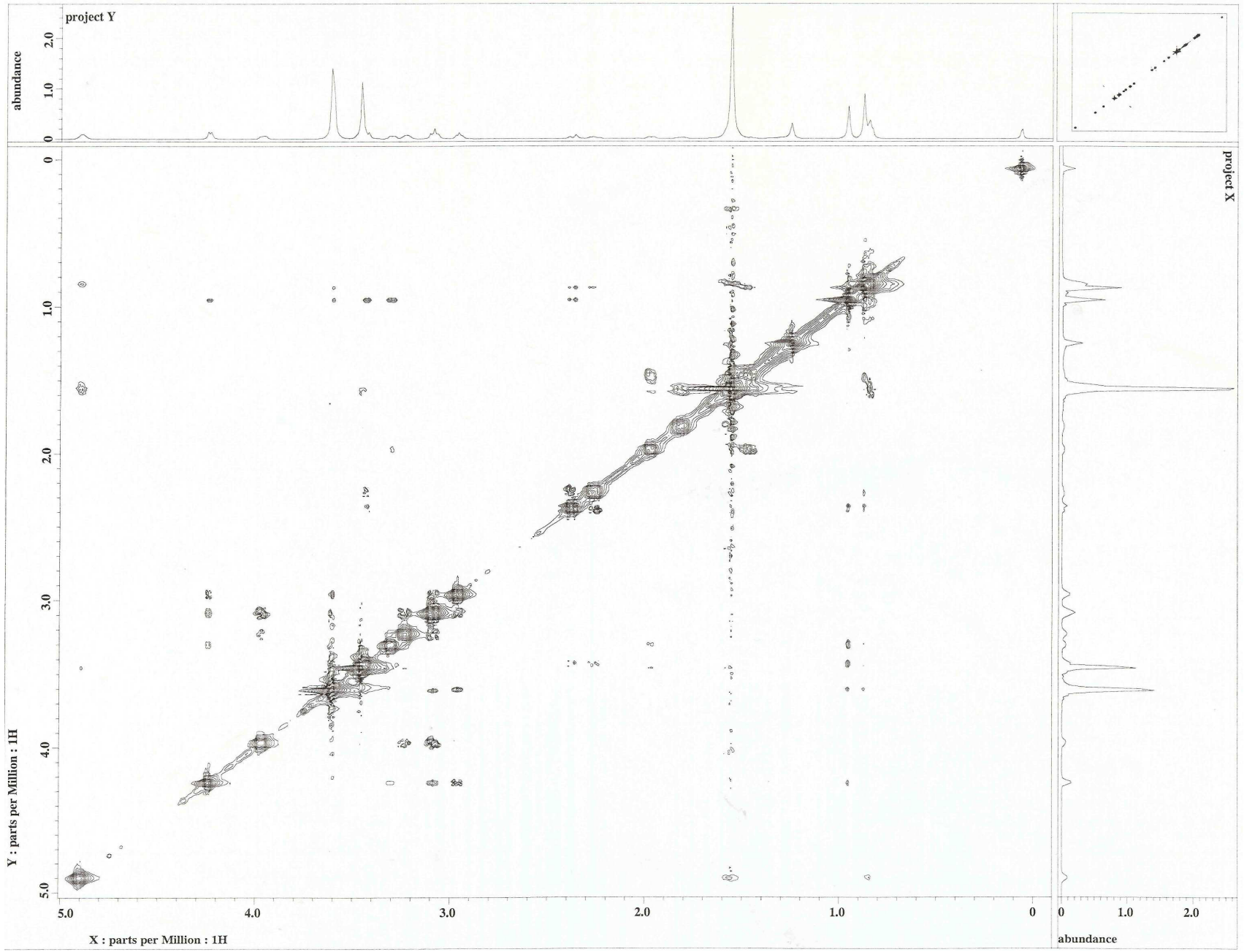
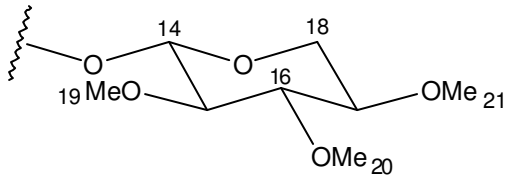


Table S1. ^{13}C NMR chemical shifts for the xylose moiety of clavosolides A-D (**3**-**6**) and cyanolide A (**2**).



#C	Clavosolides				Cyanolide A
	A (**3**)	B (**4**)	C (**5**)	D (**6**)	(**2**)
14	105.4	105.3	105.4	105.4	105.9
15	83.8	83.8	83.8	83.6	84.0
16	85.6	85.6	85.1	85.3	85.6
17	79.4	79.4	79.4	79.2	79.4
18	63.2	63.2	63.2	63.1	63.3
19	60.7	60.8	60.7	60.6	61.0
20	60.8	60.2	60.6	60.6	60.9
21	58.5	58.5	58.7	58.7	58.8

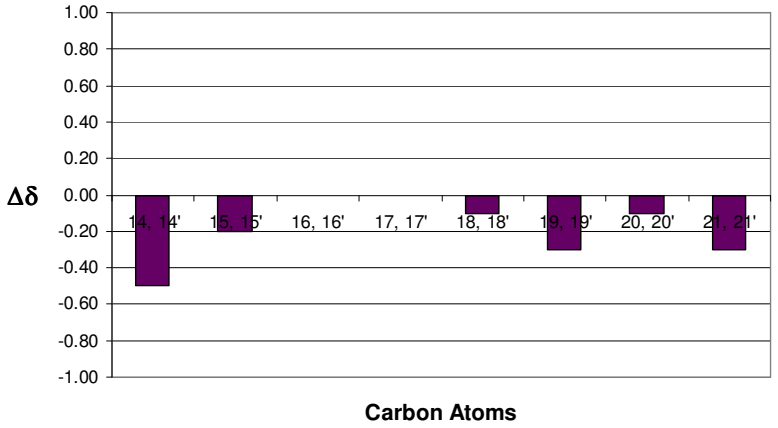


Figure S7. $\Delta\delta_C$ for the xylose moieties of clavosolide A (**3**) and cyanolide A (**2**).

Table S2. ^{1}H NMR chemical shifts, multiplicity and coupling constants for the xylose moiety of clavosolides A-D (**3**-**6**) and cyanolide A (**2**).

#C	Clavosolides				Cyanolide A (**2**)
	A (**3**)	B (**4**)	C (**5**)	D (**6**)	
14	4.27 (d, 8)	4.26 (d, 8)	4.24 (d, 8)	4.24 (d, 8)	4.24 (d, 8)
15	2.96 (t, 8)	2.96 (t, 8)	2.94 (dd, 9, 7)	2.93 (dd, 9, 8)	2.96 (dd, 9, 8)
16	3.12 (t, 8)	3.11 (t, 8)	3.07 (m)	3.06 (m)	3.089 (dd, 10, 9)
17	3.25 (td, 8, 5)	3.25 (td, 8, 5)	3.22 (m)	3.22 (ddd, 10, 10, 5)	3.23 (ddd, 10, 10, 5)
18	3.96 (dd, 11, 5)	3.96 (dd, 11, 5)	3.93 (dd, 12, 4)	3.92 (dd, 9, 5)	3.97 (dd, 11, 5)
	3.10 (dd, 11, 8)	3.10 (dd, 11, 8)	3.06 (m)	3.06 (m)	3.087 (dd, 11, 10)
19	3.57 (s)	3.58 (s)	3.56 (s)	3.56 (s)	3.60 (s)
20	3.62 (s)	3.62 (s)	3.59 (s)	3.59 (s)	3.61 (s)
21	3.47 (s)	3.47 (s)	3.44 (s)	3.44 (s)	3.46 (s)

Table S3. Specific rotation values of clavosolides A-D (**3**-**6**) and cyanolide A (**2**).

Compound	**$[\alpha]_D$**	**c (g/100 mL), $CHCl_3$**
Clavosolide A (**3**)	-48.5	1
Clavosolide B (**4**)	-41.0	0.5
Clavosolide C (**5**)	-20[a]	0.04
Clavosolide D (**6**)	-38.5[b]	0.65
Cyanolide A (**2**)	-59	0.6

[a]Reported in MeOH. [b]Measured from synthetic material.[18]

Figure S7. Low-resolution APCI MS spectrum of cyanolide A (**2**).

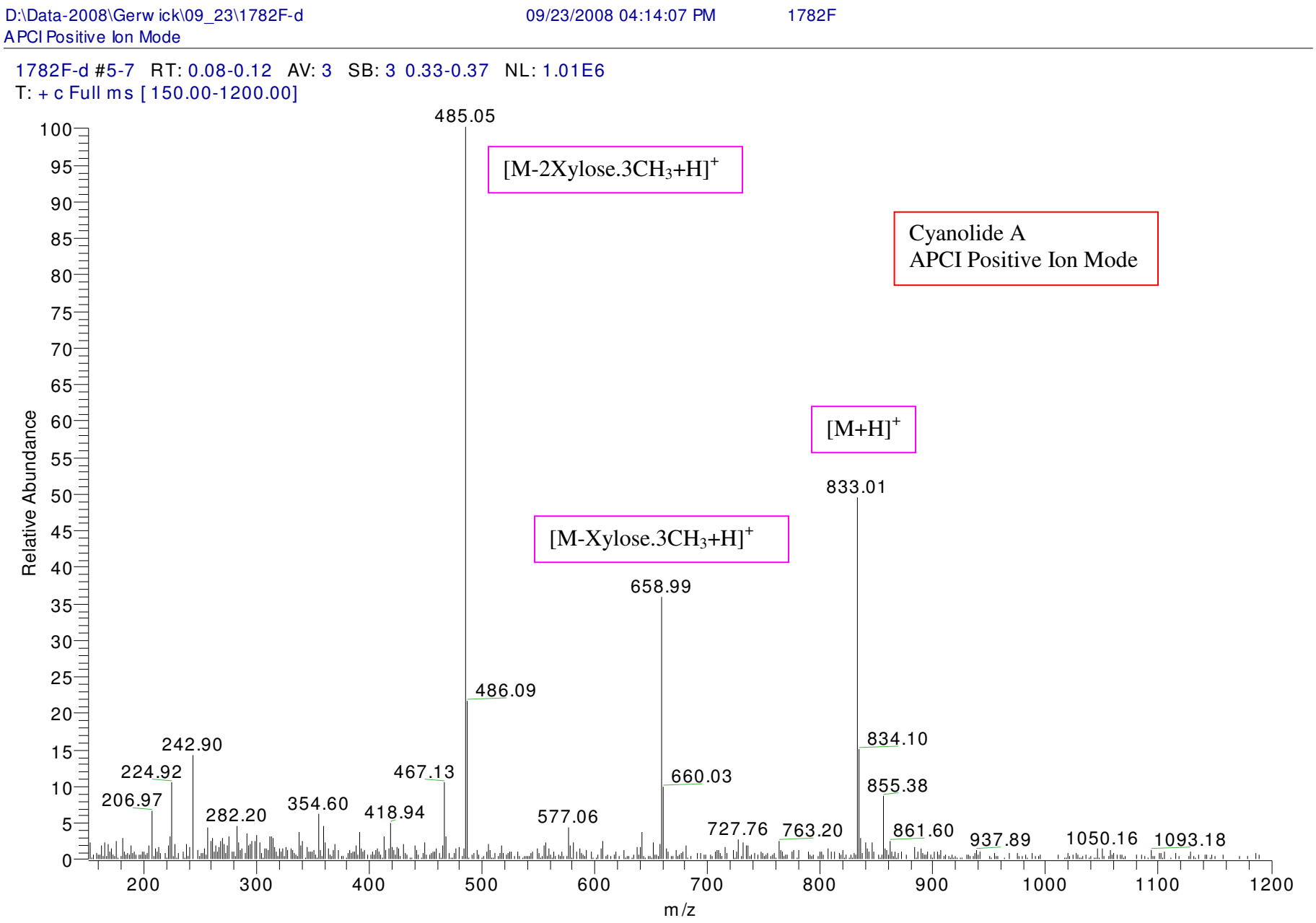


Figure S8. Low-resolution ESI MS spectrum of cyanolide A (**2**).

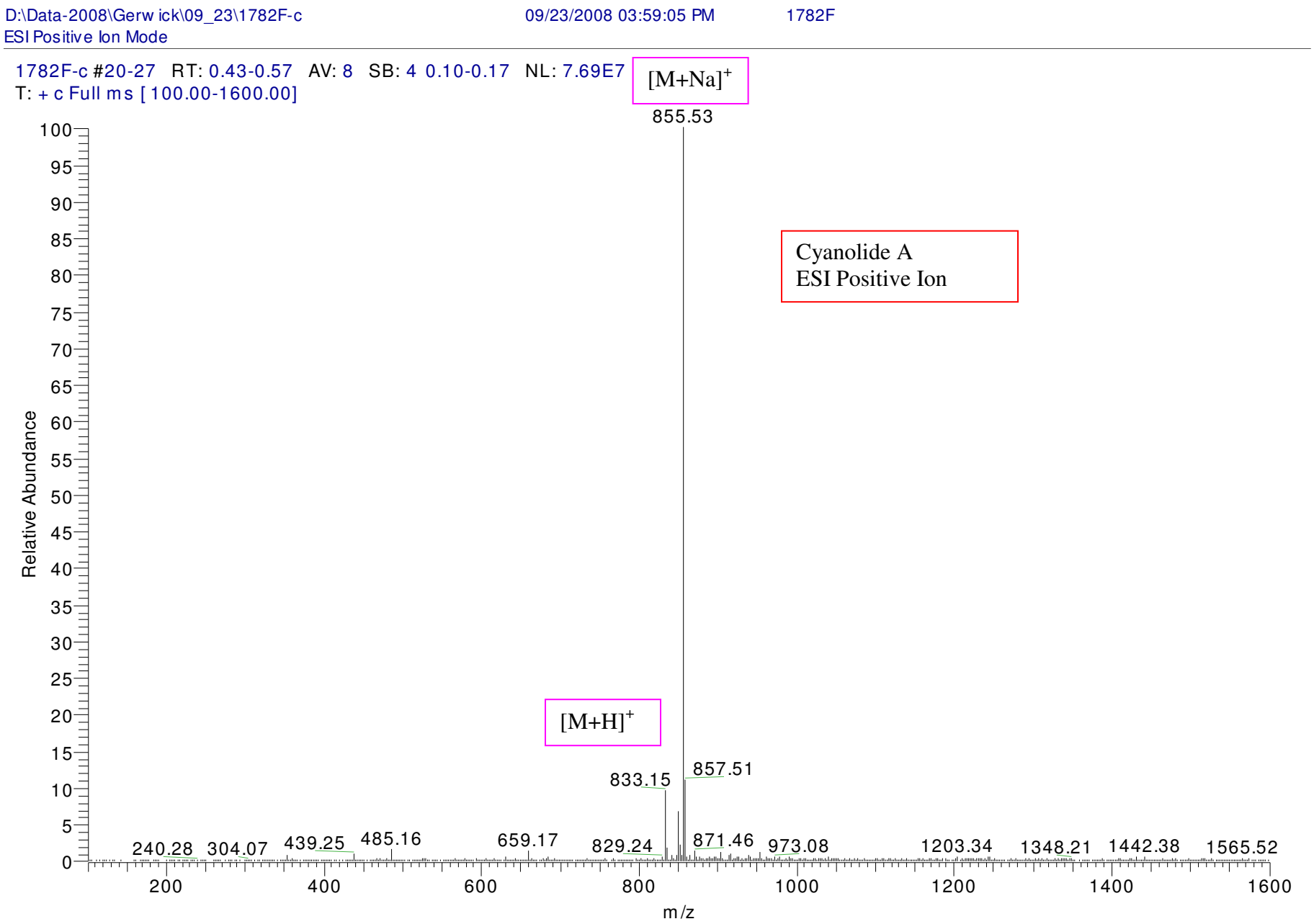
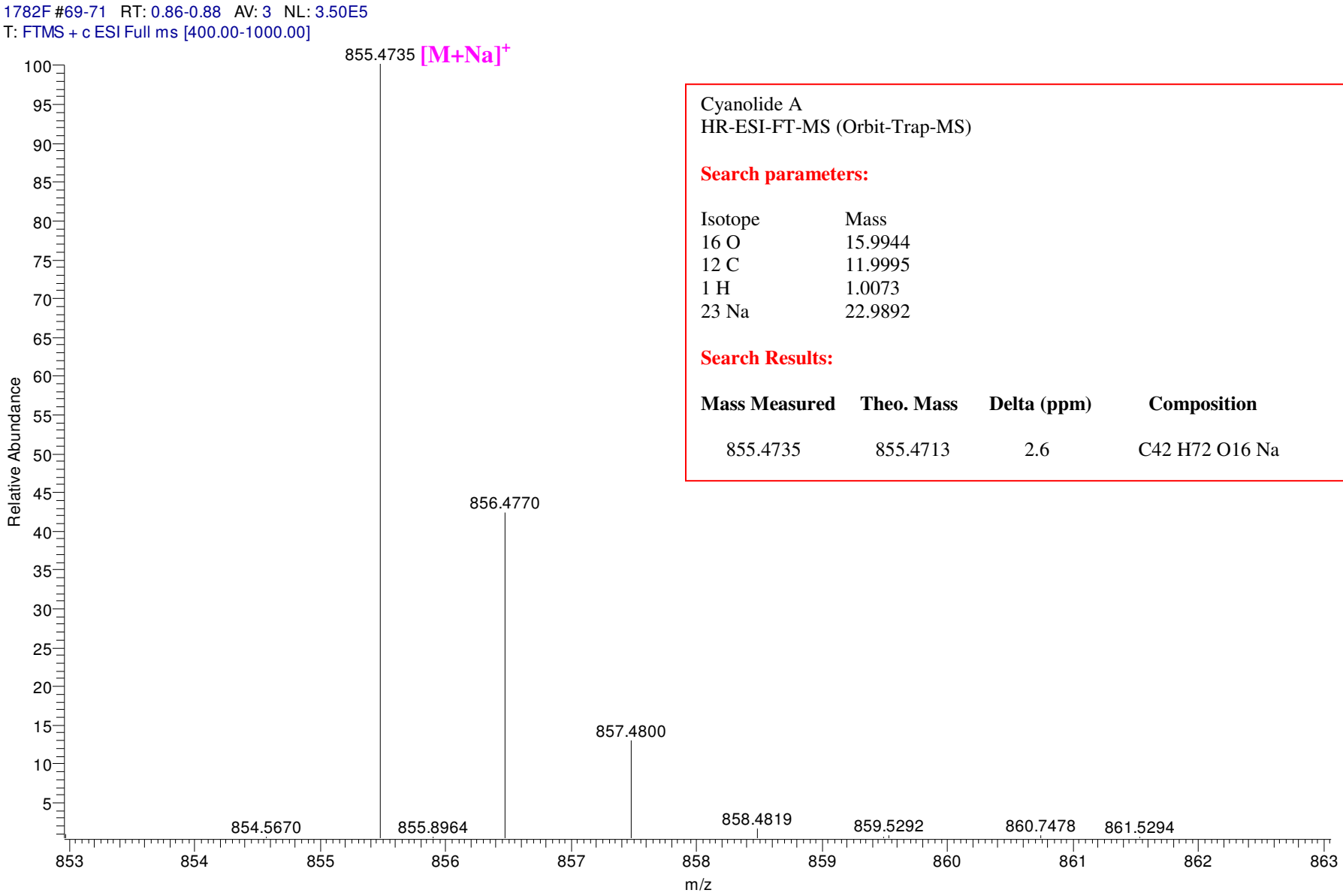


Figure S9. High-resolution ESI MS spectrum of cyanolide A (**2**).



Morphological characterization and taxonomic identification of PNG5-19-05-8

The cyanobacteria PNG5-19-05-8 was collected as a dark-reddish, non-gelatinous, mat-like colony found tenaciously attached to the surrounding corals. The colony was irregular and approximately 10 cm in diameter and 1 cm thick. Careful microscopic characterization revealed the algae to be composed of the cyanobacterial species *Lyngbya bouillonii* (Hoffmann et Demoulin).

The filaments of *L. bouillonii* were reddish, and straight or slightly waved and entangled into dense mats. The filaments were cylindrical, 23.8 µm (n = 3) wide, with distinct sheaths and were constricted at the cross-walls. The cells were disk-shaped but relatively long; 19.1 µm (n = 30) wide and 4.2 µm long (cell width/length ration = 0.2) with constrictions at their cross-walls. The terminal cells of the filaments were rounded and without calyptras.

Morphological characterizations were performed using an Olympus IX51 epifluorescent microscope (100x objective) equipped with an Olympus U-CMAD3 camera. Taxonomic identification of cyanobacterial species was performed in accordance with current phycological systems.[1,2]

References

(1) Hoffmann, L.; Demoulin, V. *Belg. J. Bot*. **1991**, *124*, 82-88.
(2) Komárek, J.; Anagnostidis, K. In *Susswasserflora von mitteleuropa*; Budel, B.; Krienitz, L.; Gartner, G.; Schagerl, M., Eds.; Elsevier GmbH: Munchen, 2005; Vol 19/2, pp. 627.