

Supplementary Materials: Identification of a Novel Saxitoxin Analogue, 12 β -Deoxygonyautoxin 3, in the Cyanobacterium, *Anabaena circinalis* (TA04)

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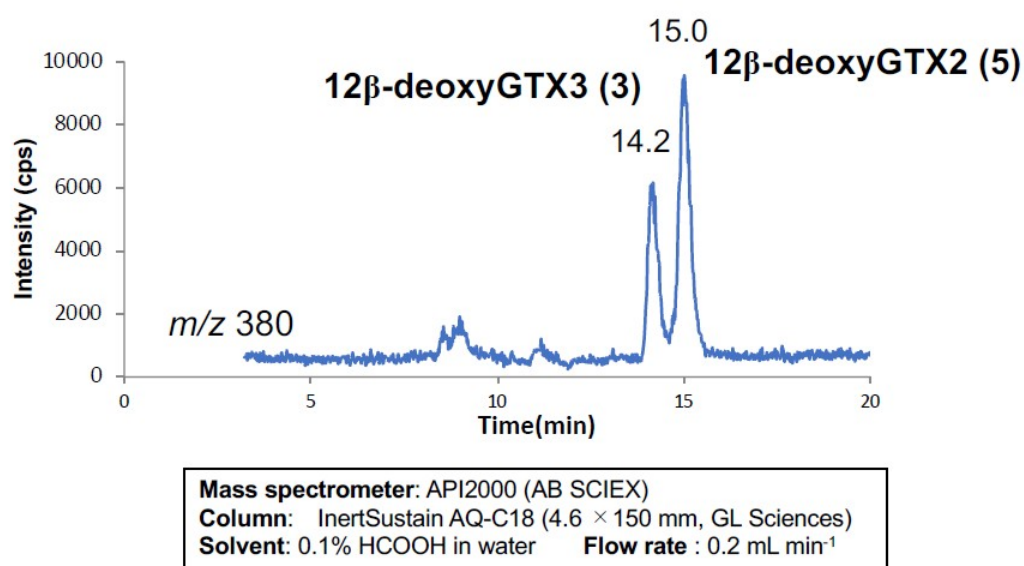


Figure S1. Separation of 3 and 5 using reverse-phase chromatography.

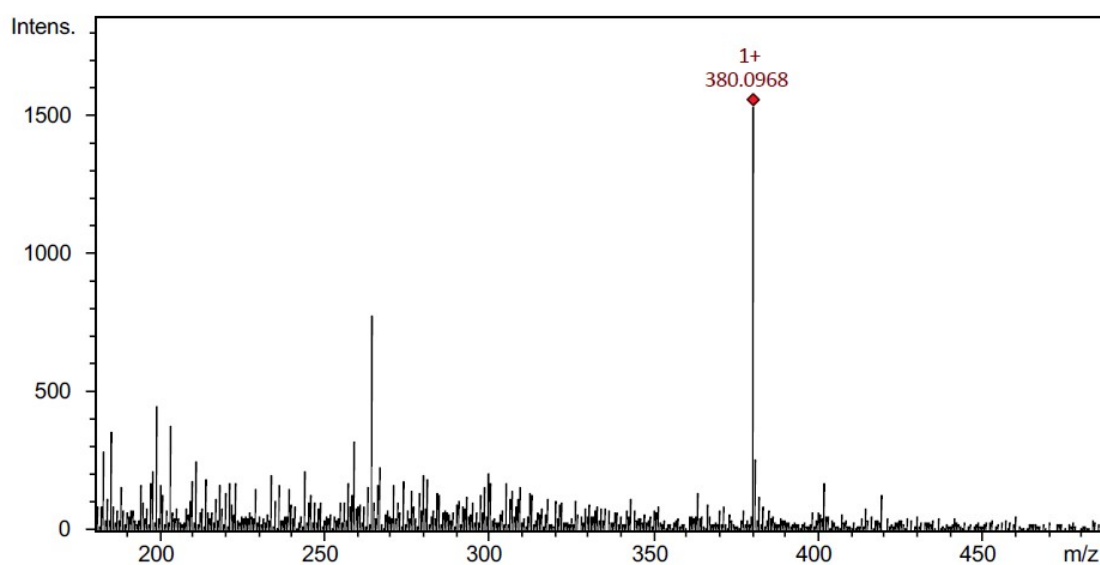


Figure S2. ESI-HRMS spectrum of synthetic 12 β -deoxyGTX3 (3) ([M+H]⁺, m/z 380.0968 C₁₀H₁₈N₇O₇S, Δ 3.9 ppm).

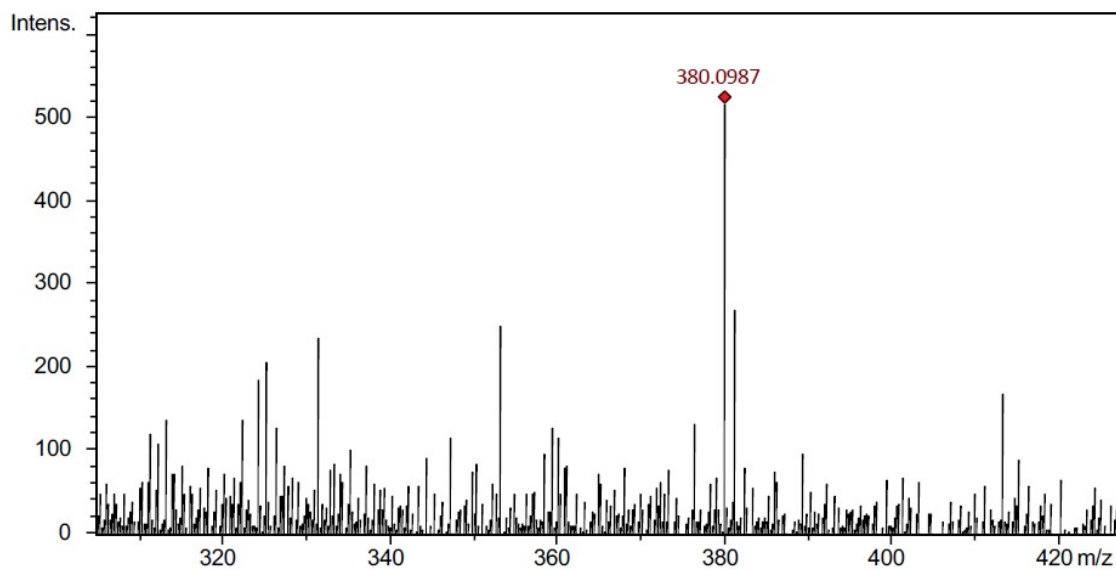


Figure S3. ESI-HRMS spectrum of synthetic 12 β -deoxyGTX2 (5). ($[M+H]^+$, m/z 380.0987 $C_{10}H_{18}N_7O_7S$, Δ 1.1 ppm)

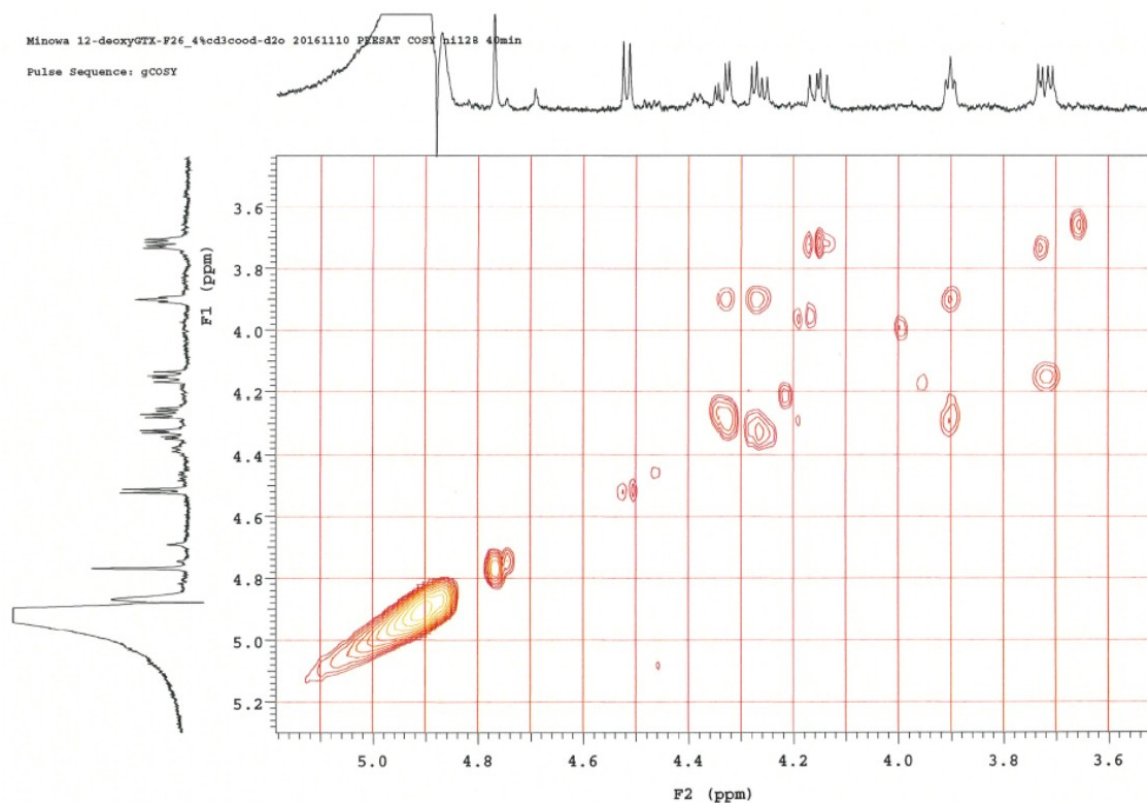


Figure S4. COSY spectrum of synthetic 12 β -deoxyGTX3 (3), 600 MHz, $CD_3COOD-D_2O$ (4:96, v/v).

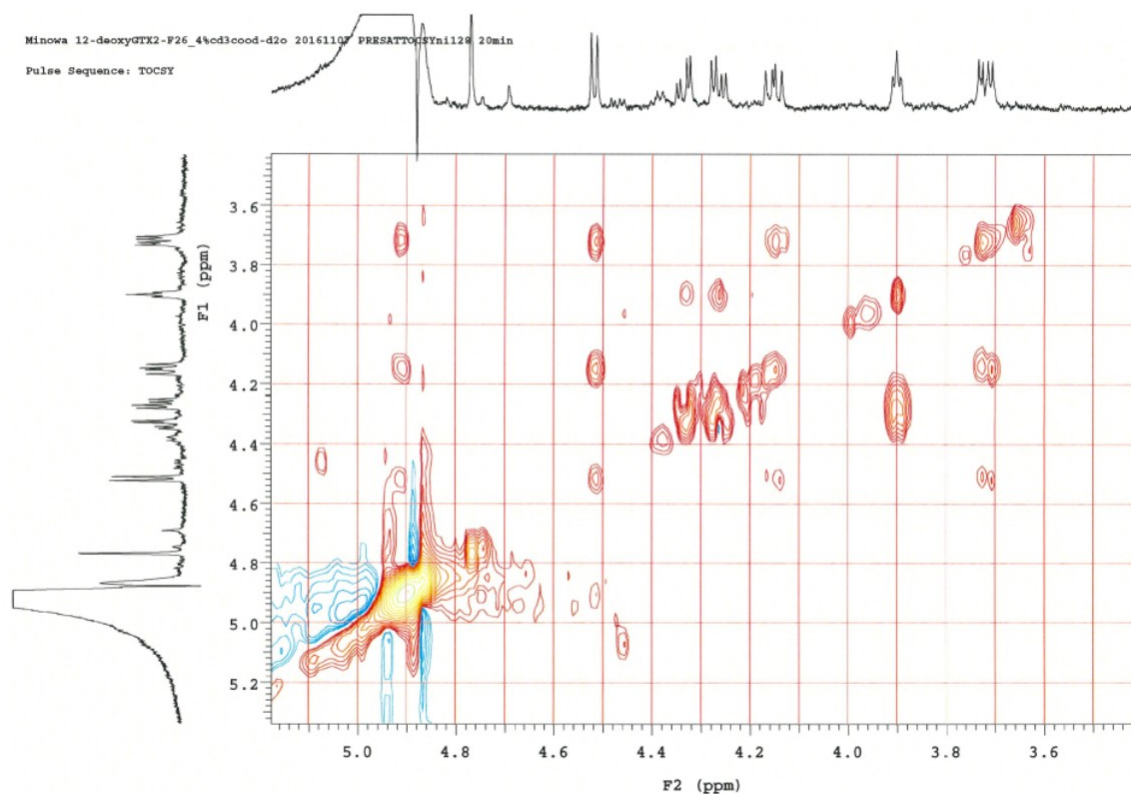


Figure S5. TOCSY spectrum of synthetic 12β-deoxyGTX3 (3), 600 MHz, CD₃COOD-D₂O (4:96, v/v)

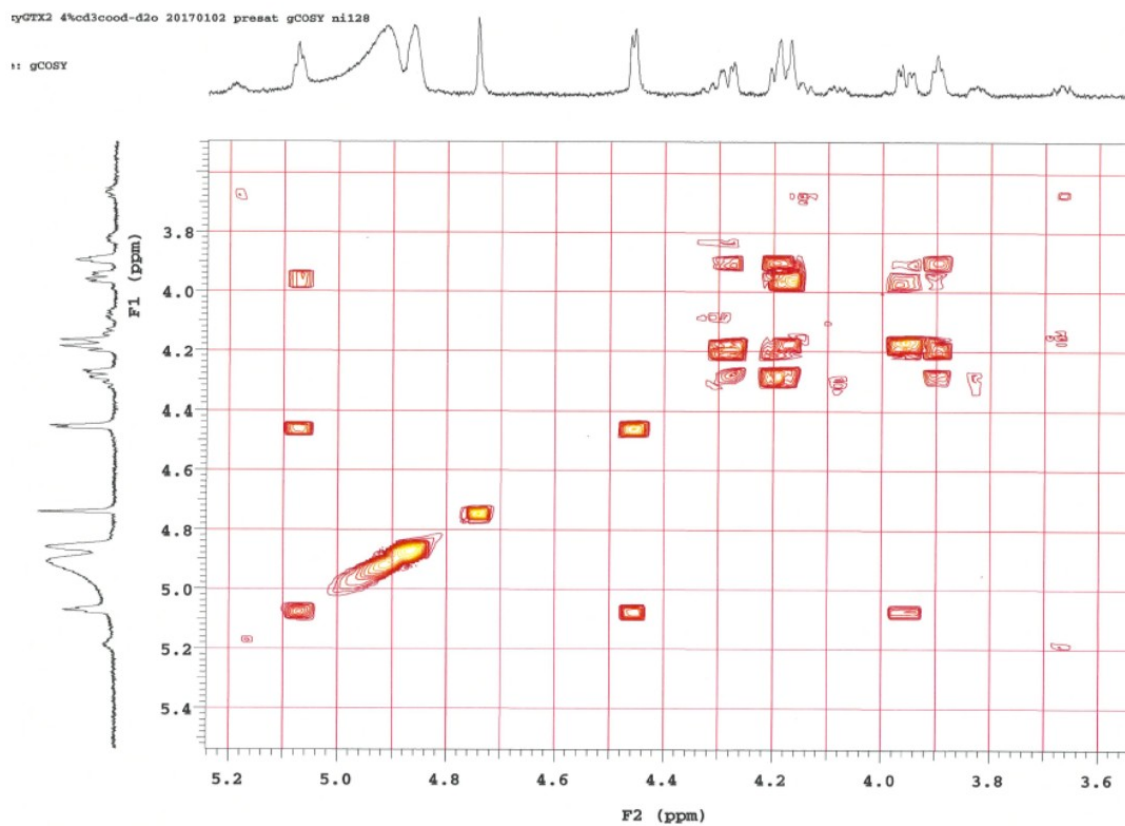


Figure S6. COSY spectrum of synthetic 12β-deoxyGTX2 (5), 600 MHz, CD₃COOD-D₂O (4:96, v/v).

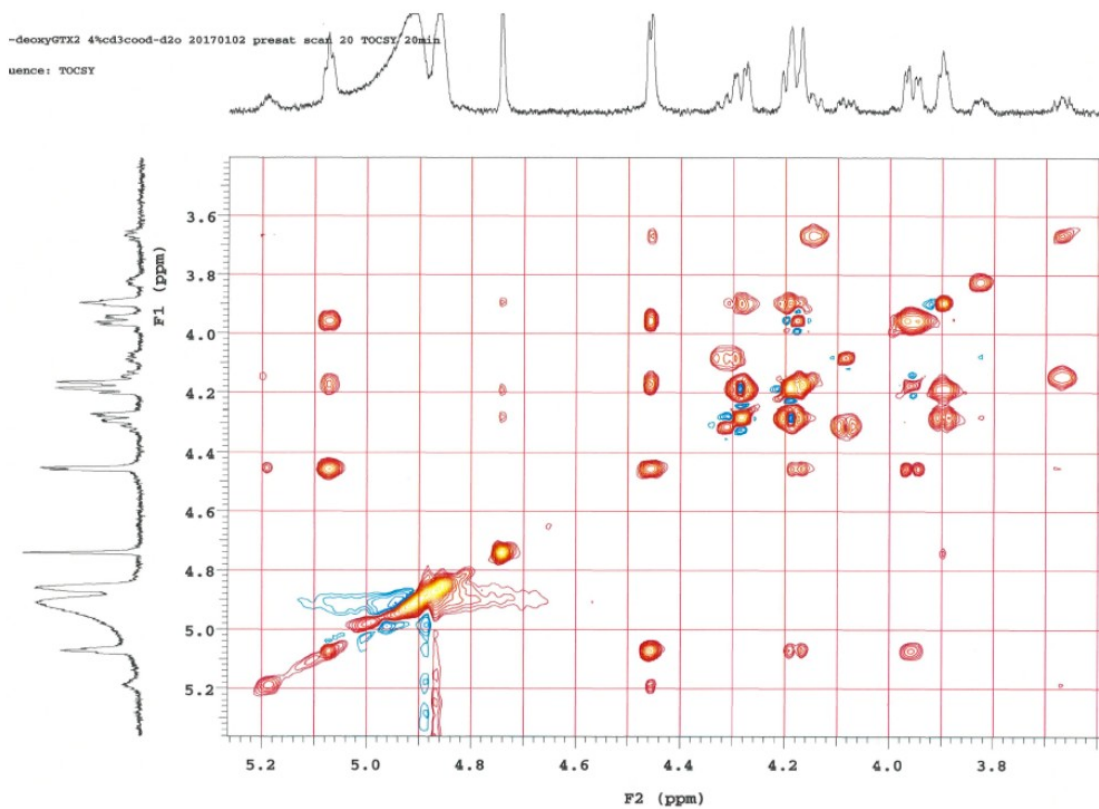


Figure S7. TOCSY spectrum of synthetic 12β-deoxyGTX2 (5), 600 MHz, CD₃COOD-D₂O (4:96, v/v).