

Supporting Information

Pterolobirins A and B, Oxygen-bridged Cassane Diterpenoid Dimers from the Fruits of *Pterolobium macropterum*

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Supporting Information Available

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Table S1. X-ray crystallographic data for pterolobirin A (**1**)

Crystal habit	Rod, colorless
Crystal size [mm ³]	0.18×0.40×0.48
Empirical formula	C ₄₀ H ₅₆ O ₅
Formula weight	616.84
Crystal system	Orthorhombic
Space group	P2 ₁ 2 ₁ 2 ₁ (No. 19)
<i>a</i> [Å]	6.9234(2)
<i>b</i> [Å]	12.1772(3)
<i>c</i> [Å]	41.1985(9)
α [°]	90
β [°]	90
γ [°]	90
<i>V</i> [Å ³]	3473.4(2)
<i>Z</i>	4
ρ _{calcd} [Mg m ⁻³]	1.180
μ [mm ⁻¹]	0.593
<i>F</i> (000)	1344
<i>T</i> [K]	296(2)
Radiation [Å]	CuKα, 1.54178
θ _{max} (°)	68.35
Completeness to θ = 67.68 (%)	99.2
Reflns collected / unique / > 2σ(<i>I</i>)	21426, 6216, 5920
<i>R</i> _{int}	0.0386
Data / parameters	6216 / 413
Goodness on fit	1.045
<i>R</i> ₁ , ^a <i>wR</i> ₂ ^b [<i>I</i> > 2σ(<i>I</i>)]	0.0418, 0.1054
<i>R</i> ₁ , <i>wR</i> ₂ [all data]	0.0435, 0.1066
Δρ [e Å ⁻³]	-0.21, 0.14
Absolute structure parameter	-0.02(7)
CCDC	1864612

^a *R* = ∑|*F*_o| - |*F*_c|/∑|*F*_o|. ^b *wR* = ∑{*w*(*F*_o² - *F*_c²)²/∑*w*(*F*_o²)²}^{1/2}.

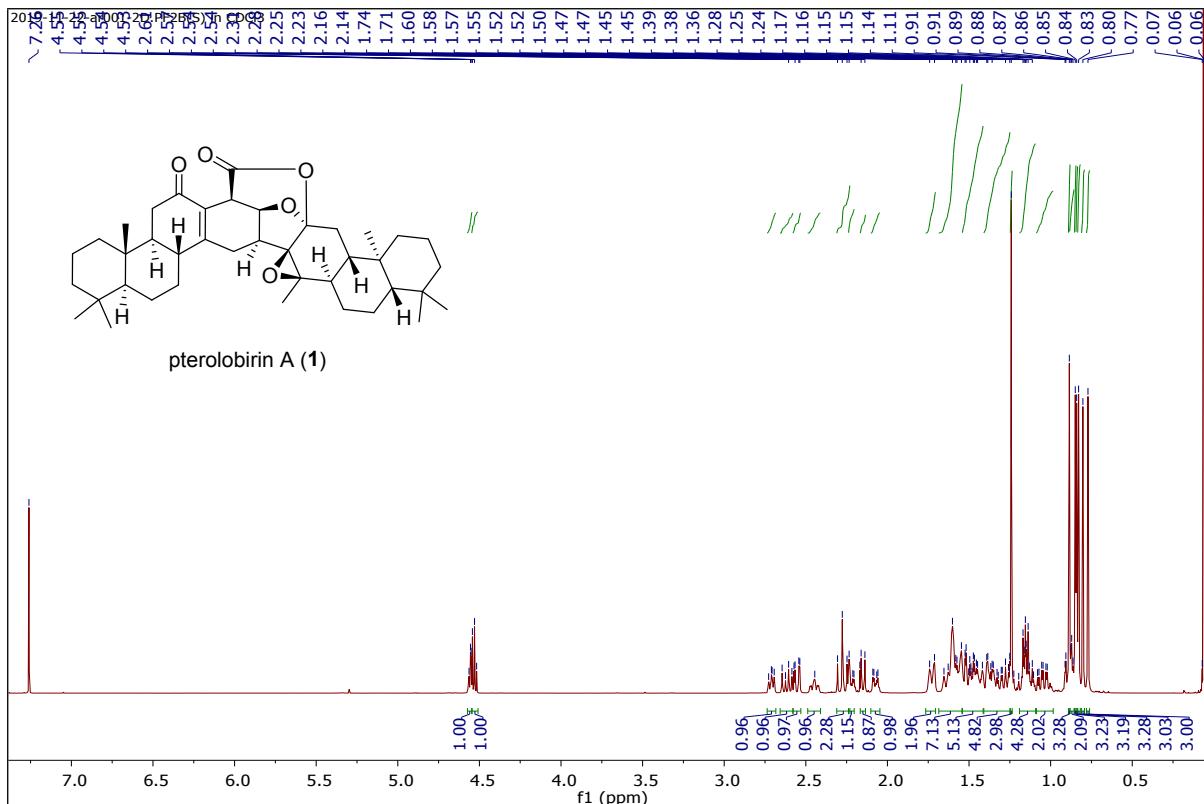


Figure S1. ^1H NMR spectrum (500 MHz, CDCl_3) of pterolobirin A (1)

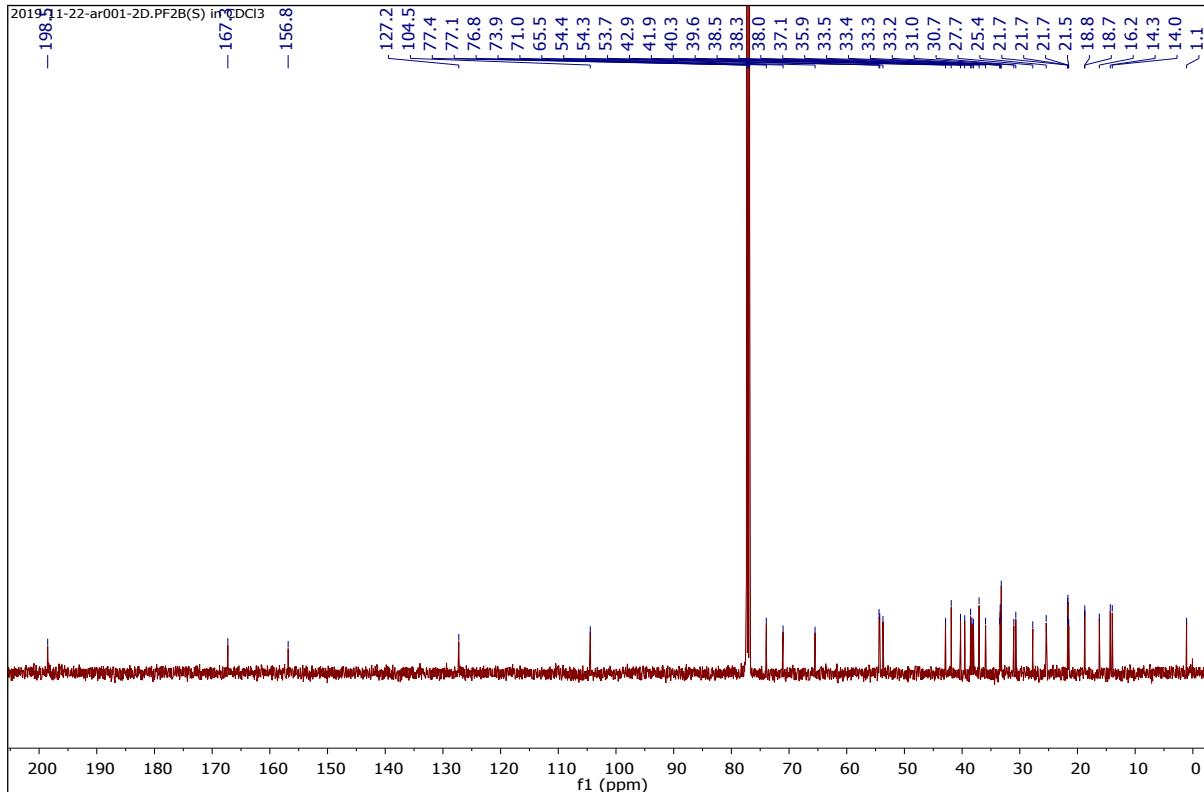


Figure S2. ^{13}C NMR spectrum (125 MHz, CDCl_3) of pterolobirin A (**1**)

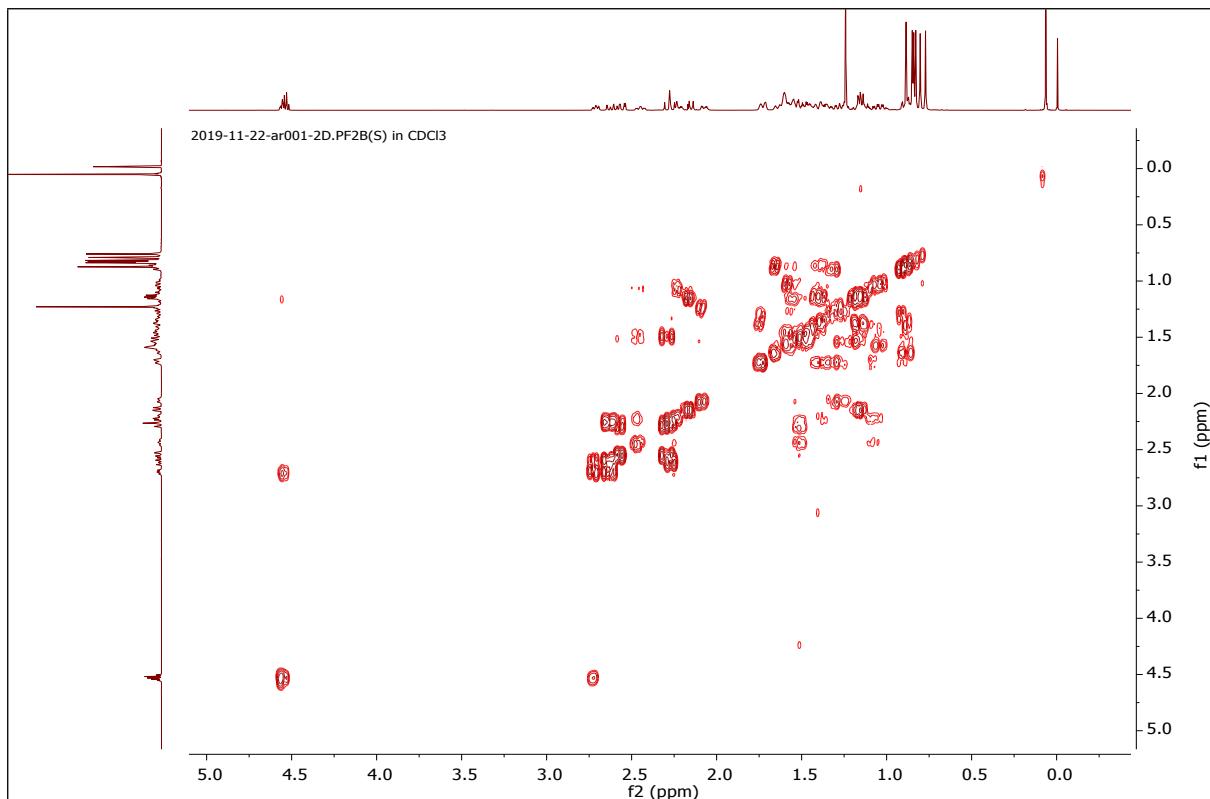


Figure S3. COSY spectrum of pterolobirin A (**1**)

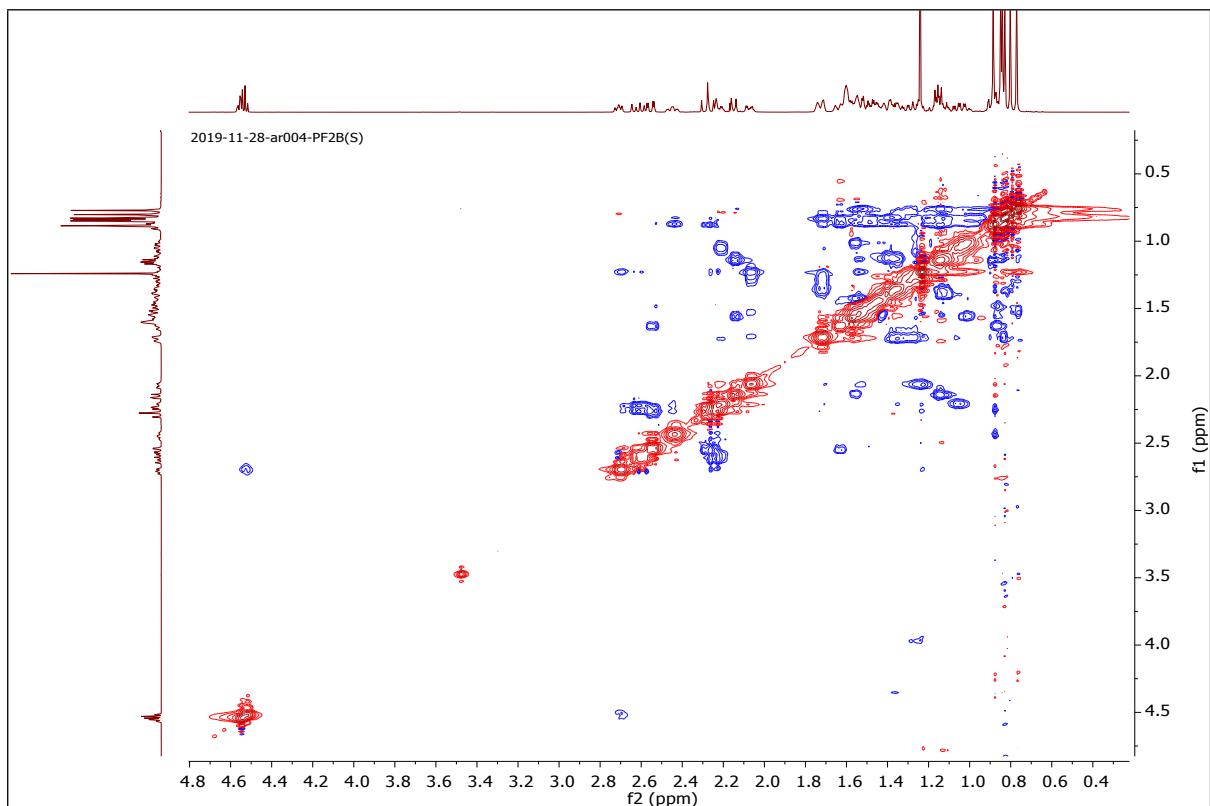


Figure S4. NOESY spectrum of pterolobirin A (**1**)

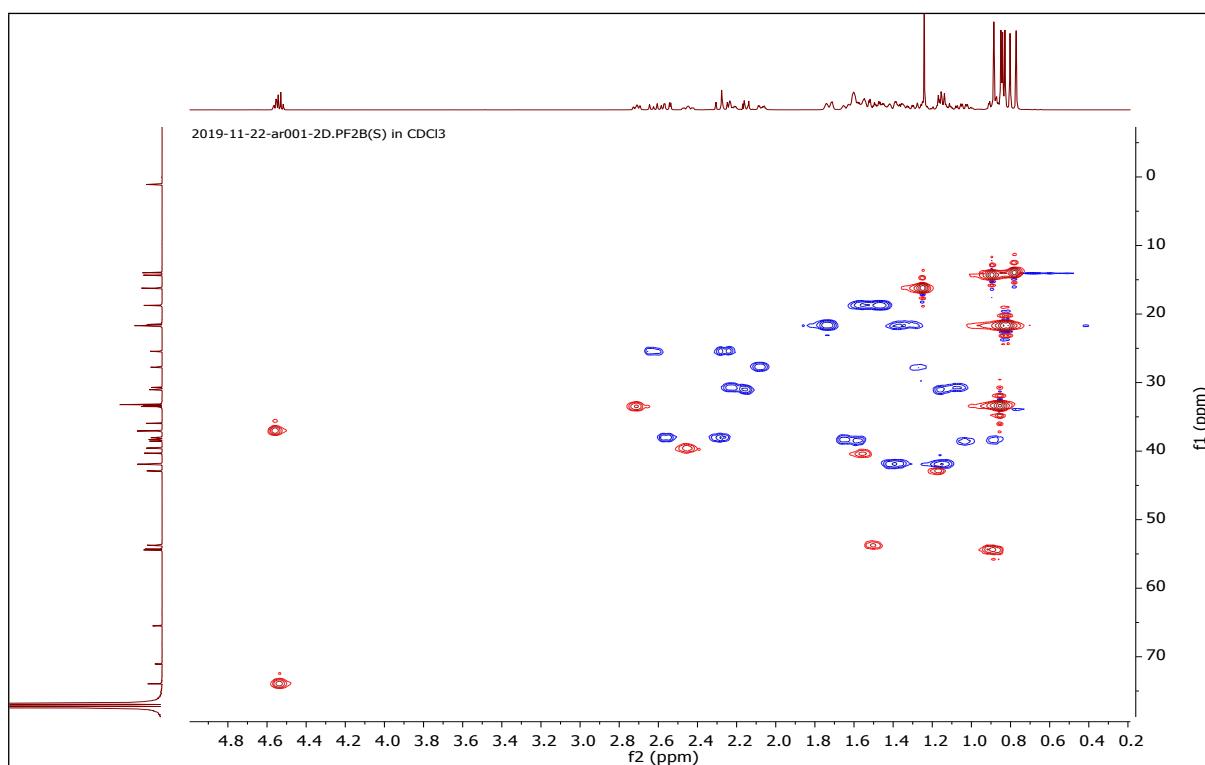


Figure S5. HSQC spectrum of pterolobirin A (**1**)

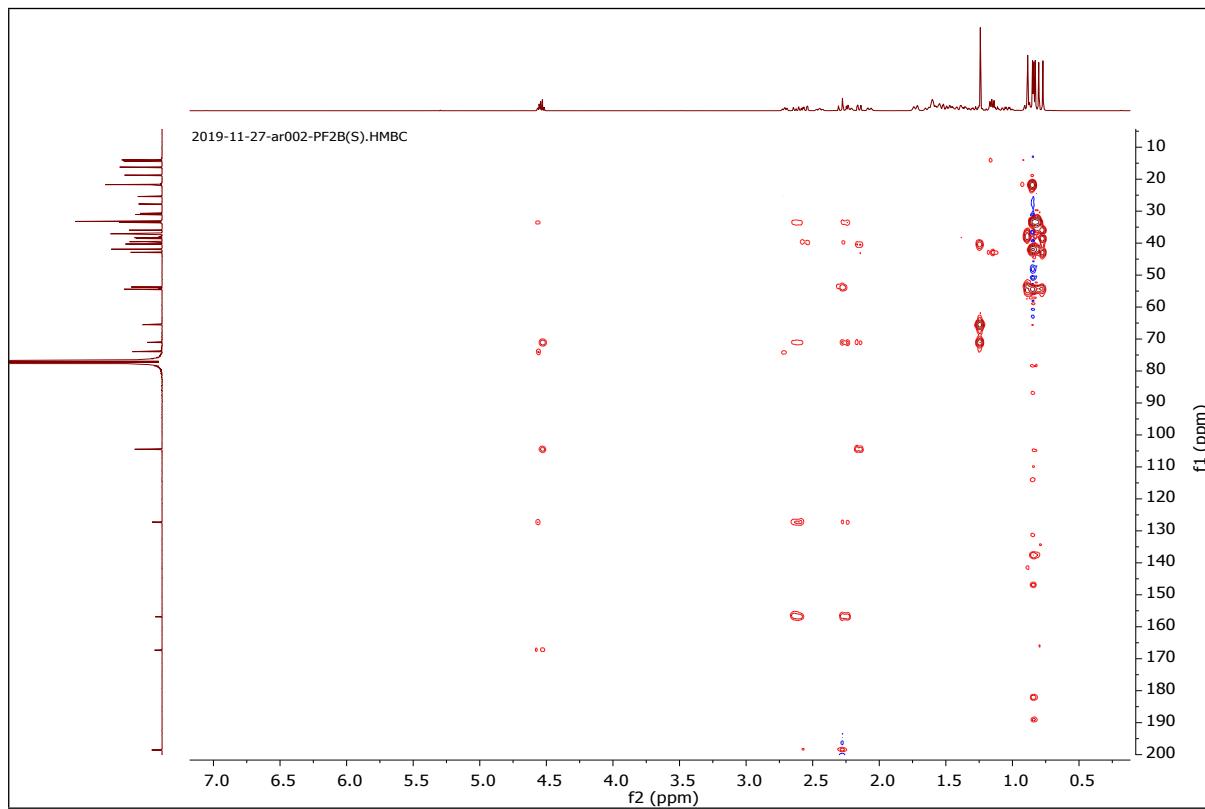


Figure S6. HMBC spectrum of pterolobirin A (**1**)

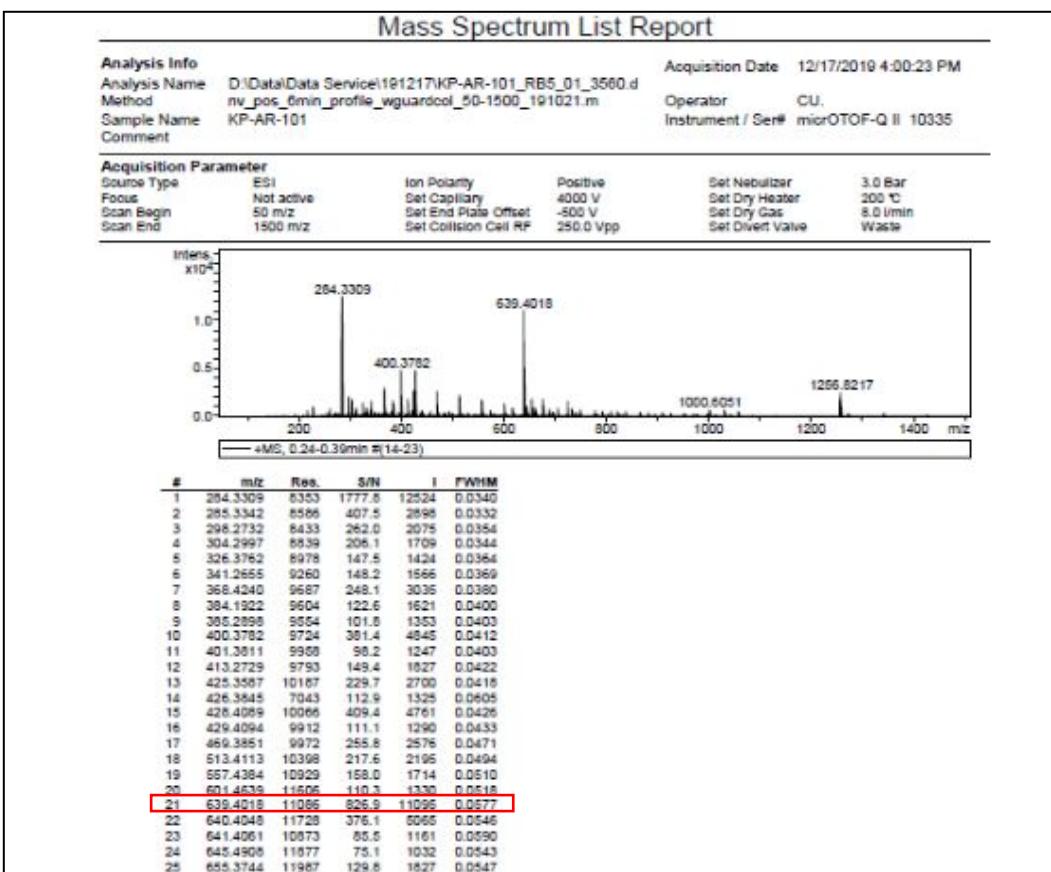


Figure S7. HRTOFMS spectrum of pterolobirin A (**1**)

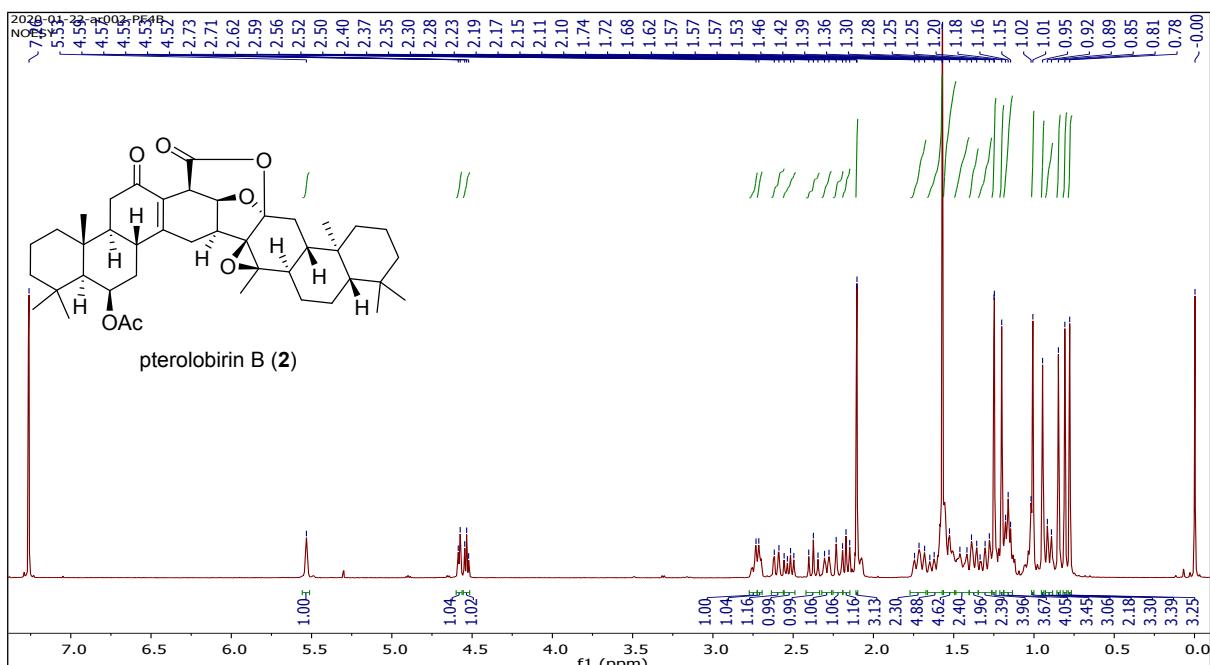


Figure S8. ^1H NMR spectrum (500 MHz, CDCl_3) of pterolobirin B (2)

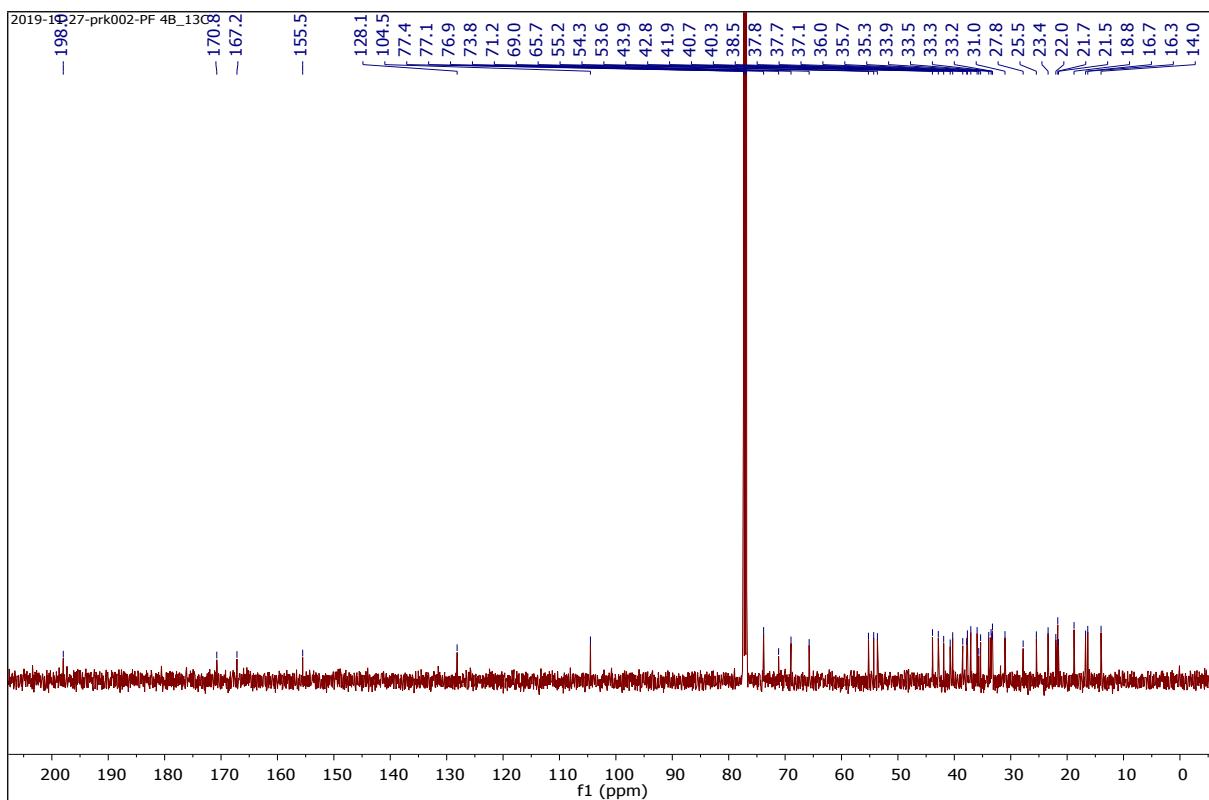


Figure S9. ¹³C NMR spectrum (125 MHz, CDCl₃) of pterolobirin B (2)

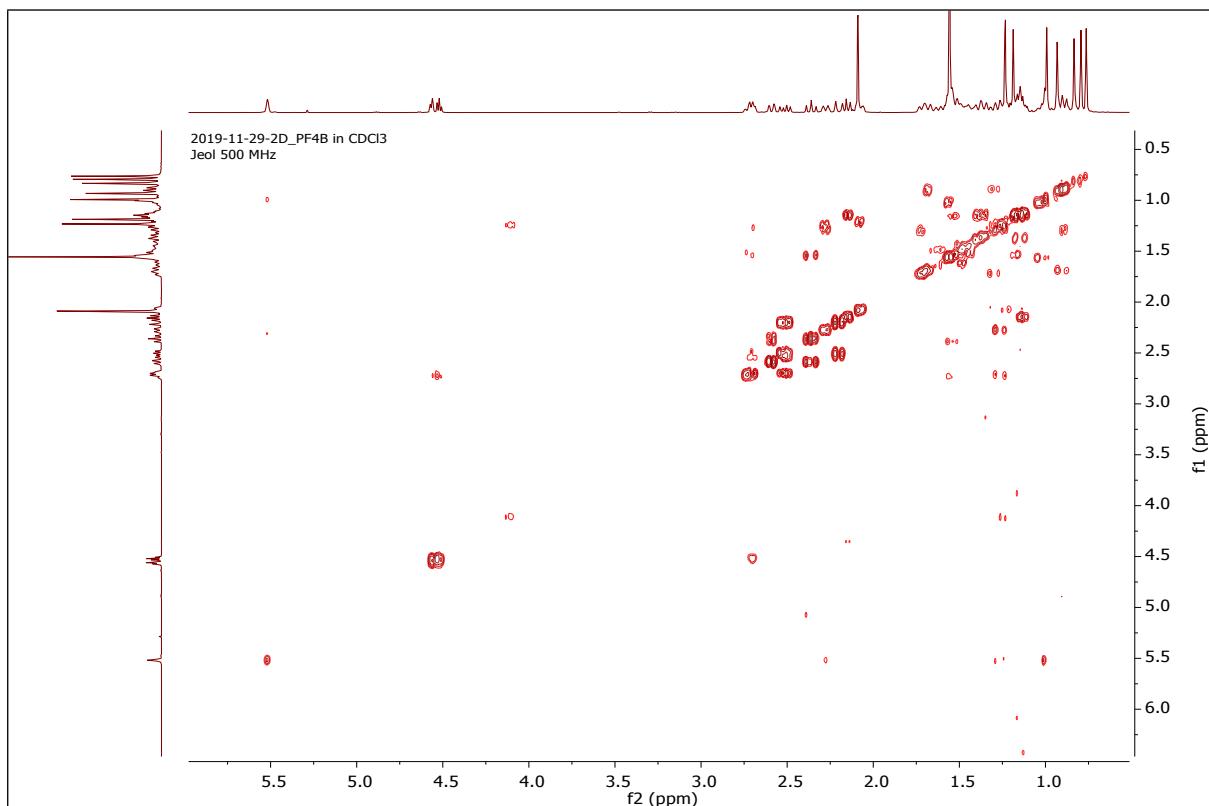


Figure S10. COSY spectrum of pterolobirin B (2)

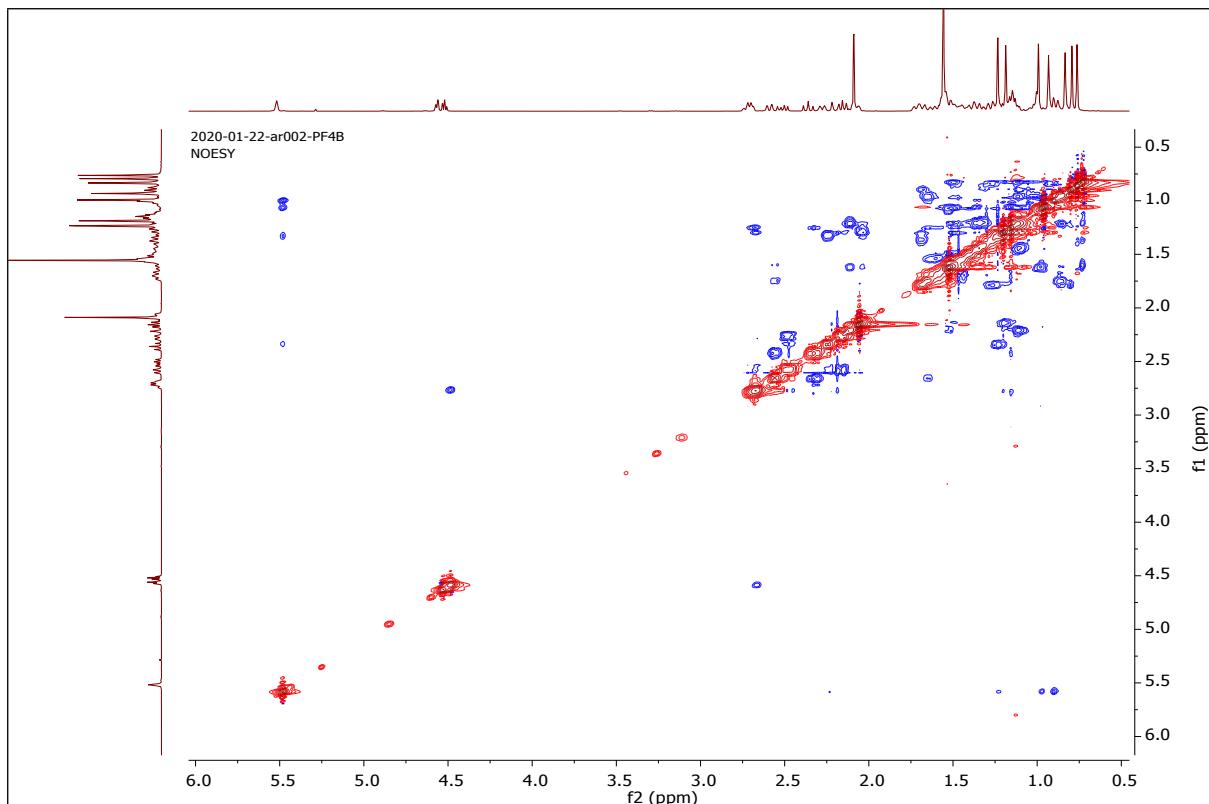


Figure S11. NOESY spectrum of pterolobirin B (2)

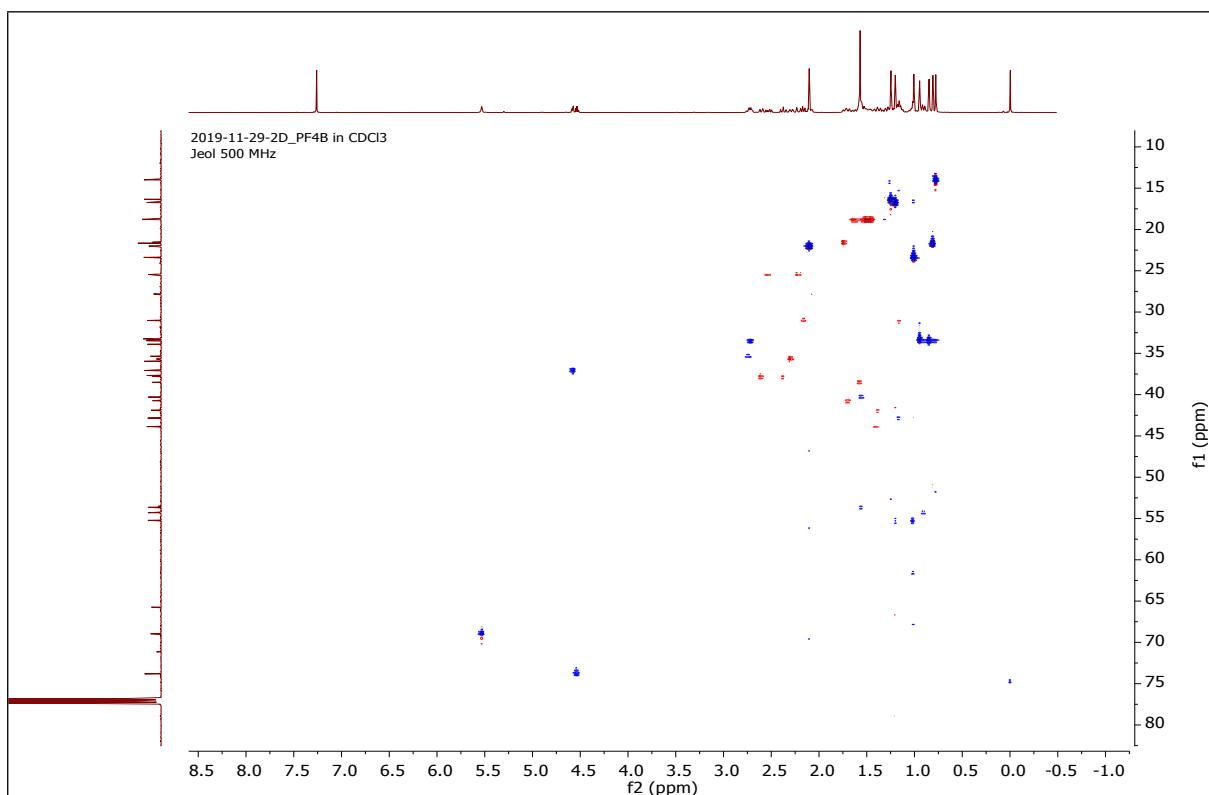


Figure S12. HSQC spectrum of pterolobirin B (2)

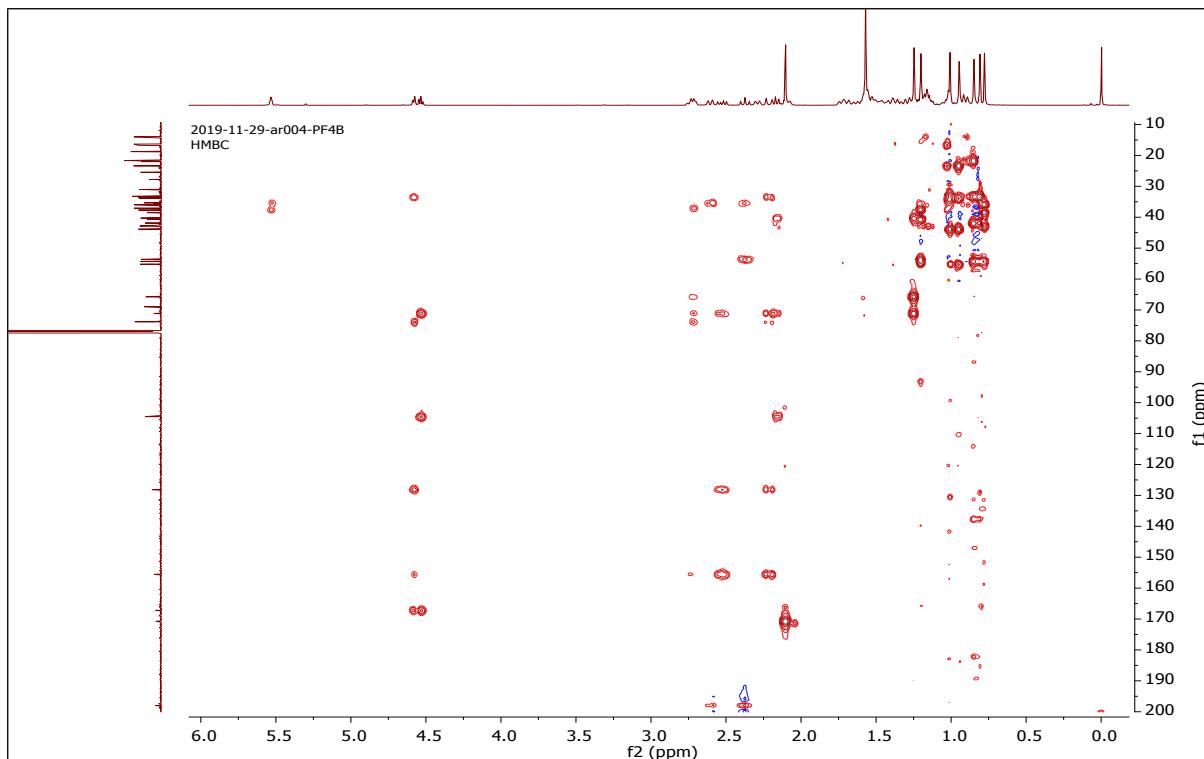


Figure S13. HMBC spectrum of pterolobirin B (2)

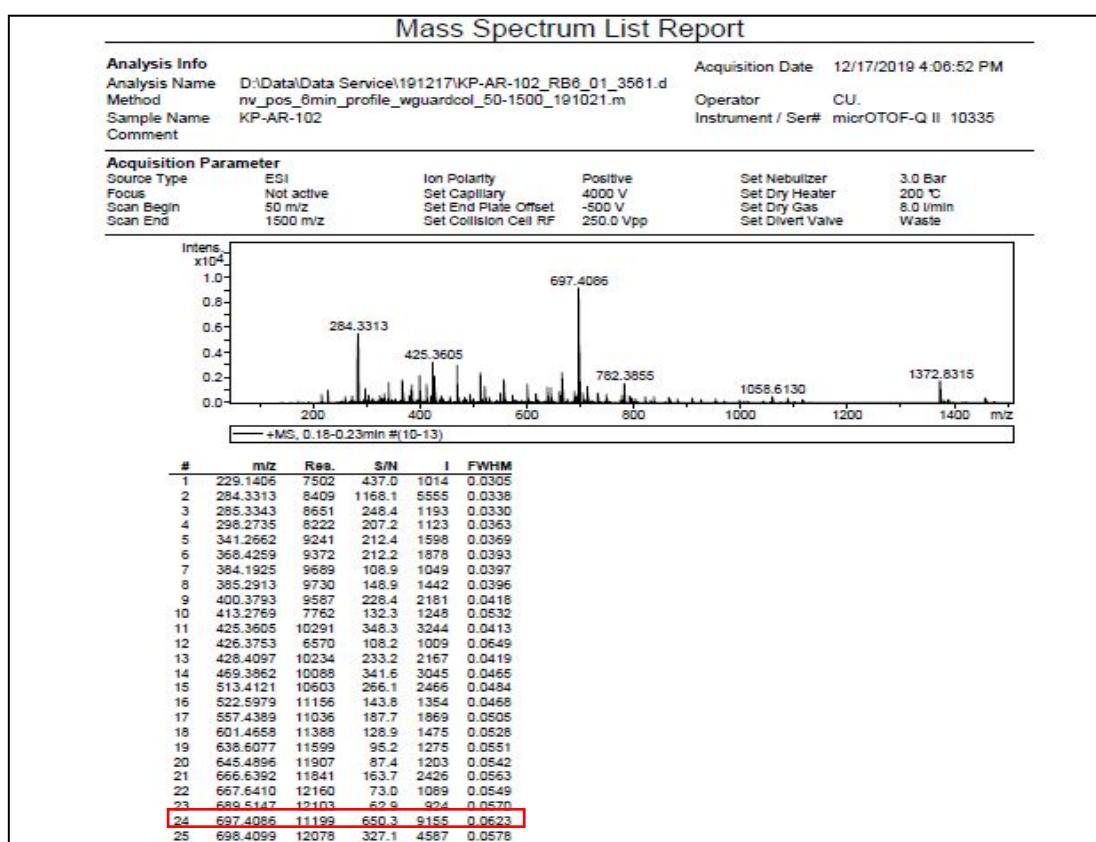


Figure S14. HRTOFMS spectrum of pterolobirin B (2)

