

Supporting information for

Antroxazole A, an oxazole-containing chamigrane dimer from the fungus *Antrodiella albocinnamomea* with immunosuppressive activity

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Figure S1. ¹H NMR spectrum for antroxazole A (1)

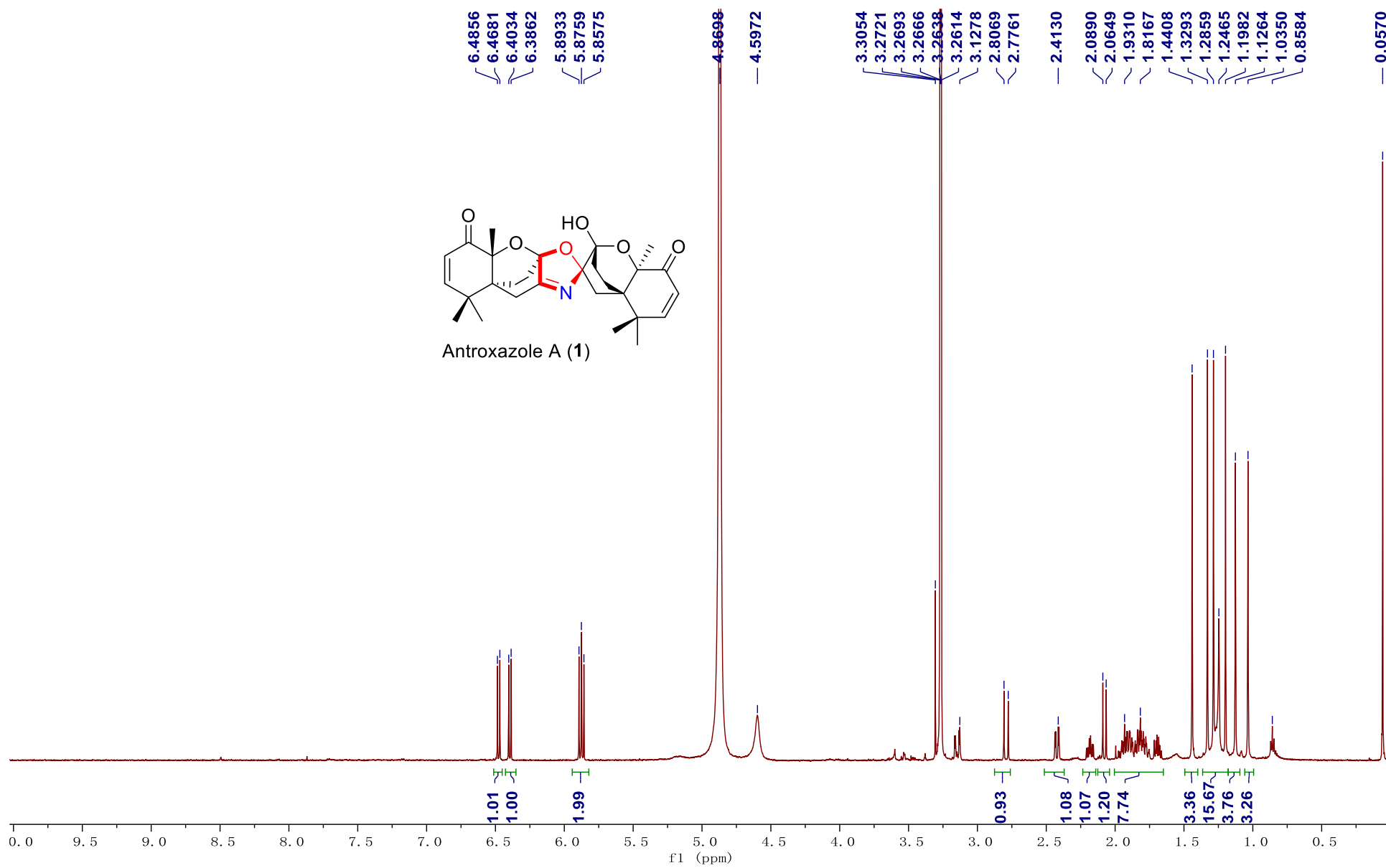


Figure S2. ^{13}C and DEPT NMR spectra for antroxazole A (1)

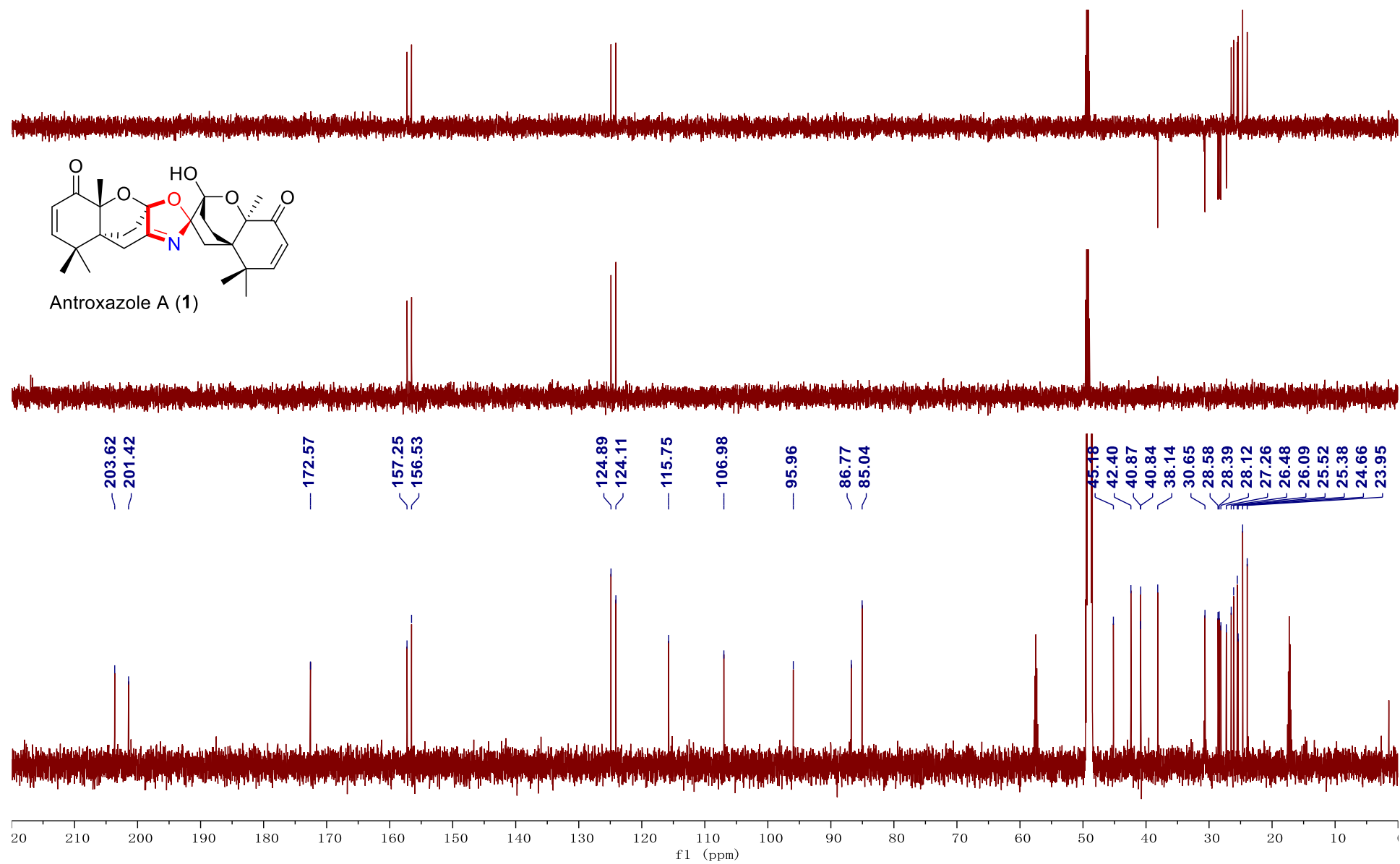


Figure S3. HSQC spectrum for antroxazole A (1)

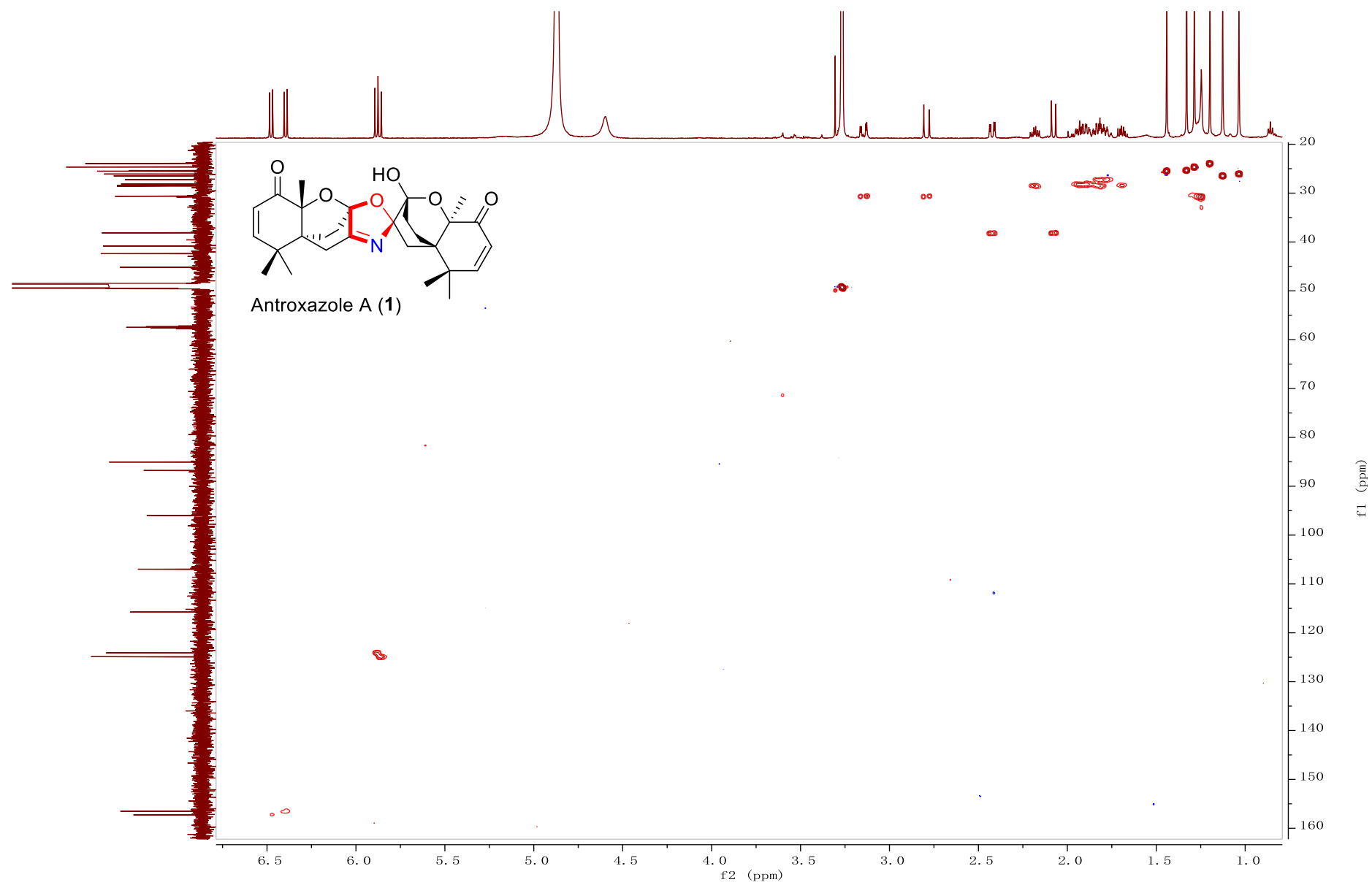


Figure S4. HMBC spectrum for antroxazole A (1)

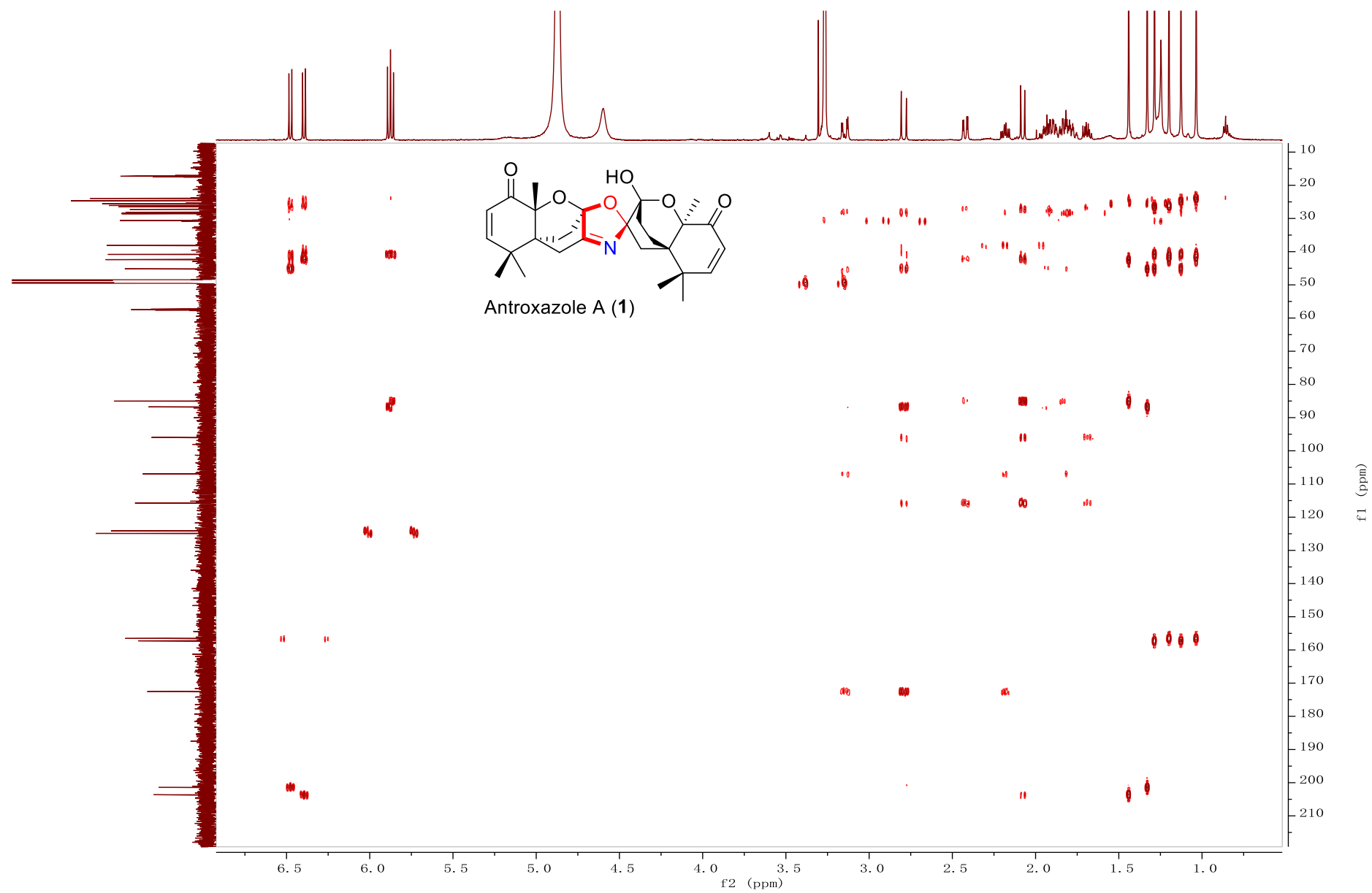


Figure S5. ^1H - ^1H COSY spectrum for antroxazole A (1)

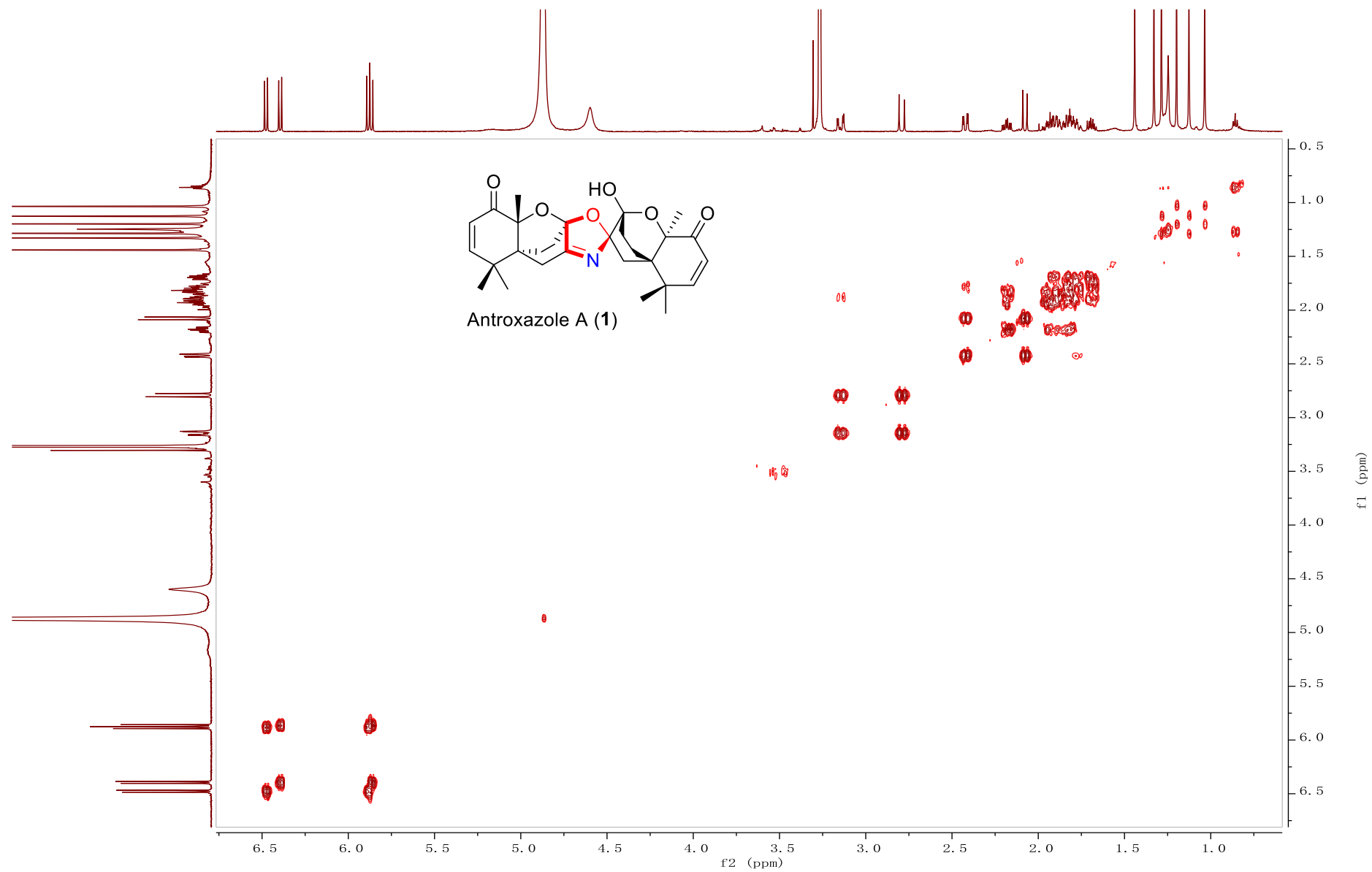


Figure S6. ROESY spectrum for antroxazole A (1)

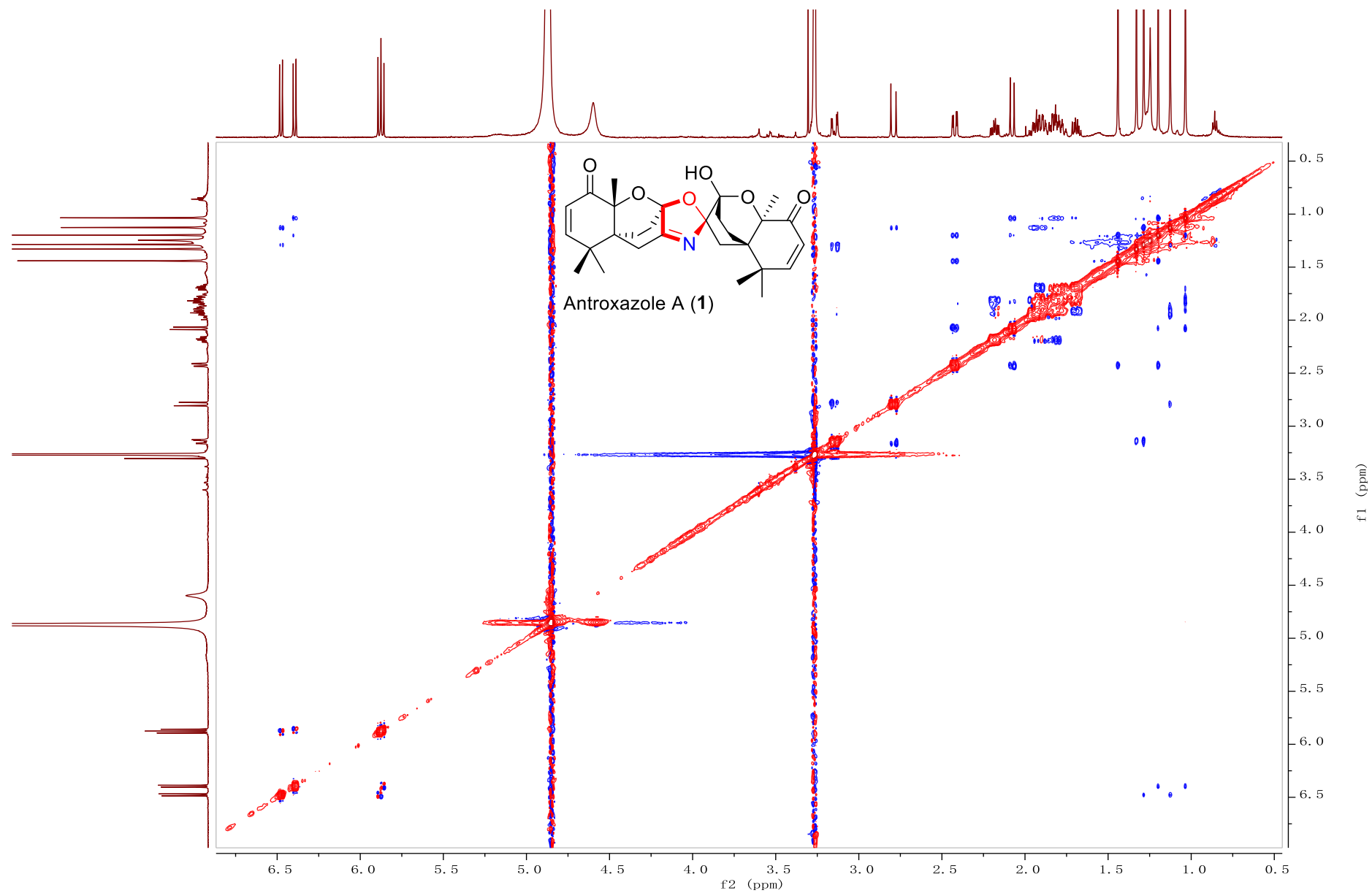
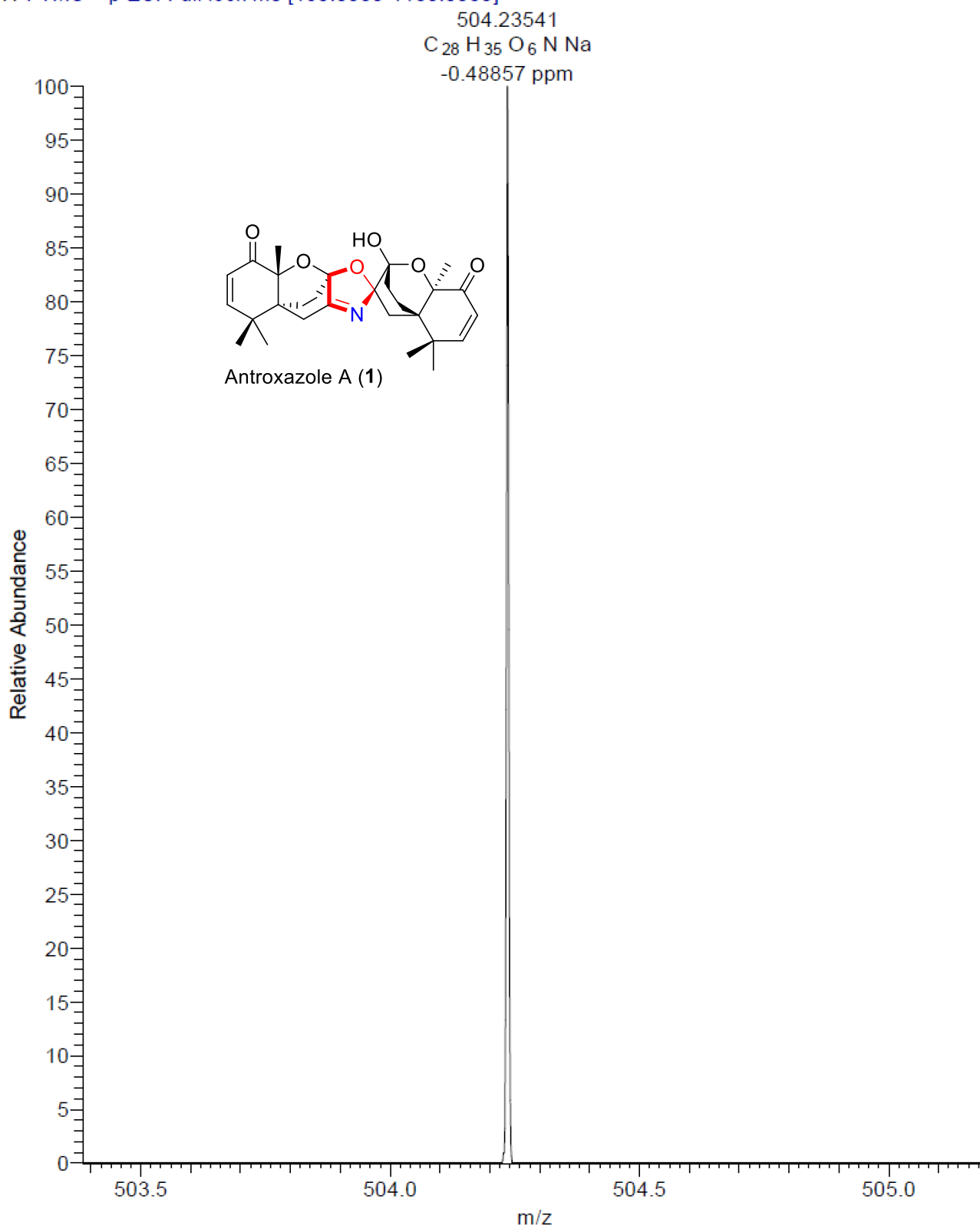


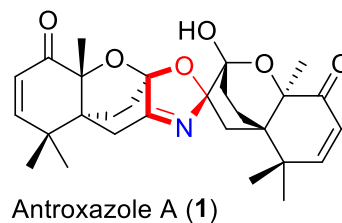
Figure S7. HRESIMS for antroxazole A (1)

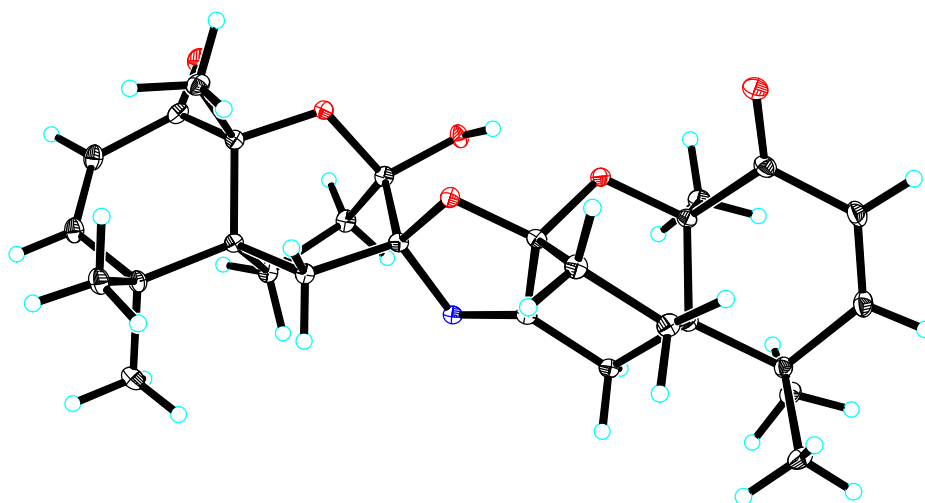
LYA-64 #13 RT: 0.17 AV: 1 NL: 4.95E8
T: FTMS + p ESI Full lock ms [150.0000-1100.0000]



Crystal data and structure refinement for antroxazole A (1).

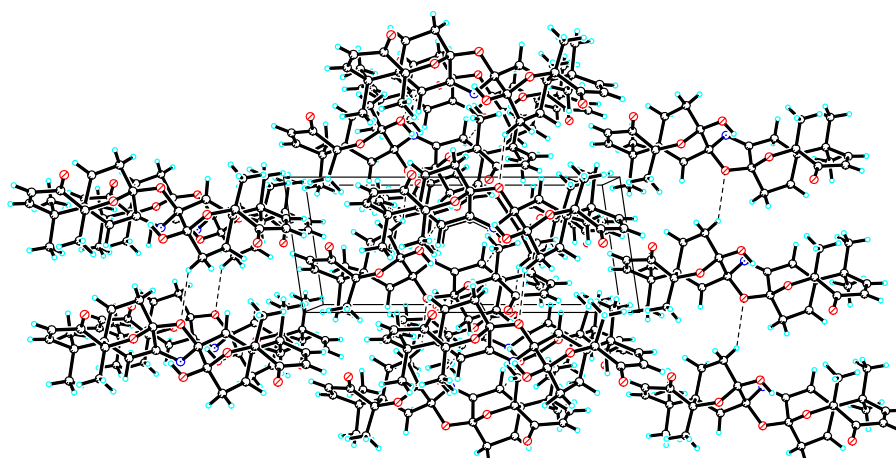
Identification code	global
Empirical formula	C ₂₈ H ₃₅ N O ₆
Formula weight	481.57
Temperature	100(2) K
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	P 1 21 1
Unit cell dimensions	a = 6.3881(4) Å α = 90°. b = 11.9470(7) Å β = 98.325(3)°. c = 15.7014(9) Å γ = 90°.
Volume	1185.68(12) Å ³
Z	2
Density (calculated)	1.349 Mg/m ³
Absorption coefficient	0.765 mm ⁻¹
F(000)	516
Crystal size	0.900 x 0.120 x 0.040 mm ³
Theta range for data collection	2.84 to 72.22°.
Index ranges	-5 ≤ h ≤ 7, -14 ≤ k ≤ 14, -19 ≤ l ≤ 19
Reflections collected	19093
Independent reflections	4663 [R(int) = 0.1013]
Completeness to theta = 72.22°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.97 and 0.74
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	4663 / 1 / 323
Goodness-of-fit on F ²	1.046
Final R indices [I > 2σ(I)]	R1 = 0.0402, wR2 = 0.0930
R indices (all data)	R1 = 0.0476, wR2 = 0.0973
Absolute structure parameter	-0.10(11)
Largest diff. peak and hole	0.321 and -0.209 e.Å ⁻³





View of a molecule of antroxazole A (**1**) with the atom-labelling scheme.

Displacement ellipsoids are drawn at the 30% probability level.



View of the pack drawing of antroxazole A (**1**).

Hydrogen-bonds are shown as dashed lines.