

CHEMICAL STRUCTURES AND CYTOTOXIC ACTIVITIES OF THE CONSTITUENTS ISOLATED FROM *CITRUS SPHAEROCARPA*.

**Takuya Muraoka,^a Daisuke Imahori,^{a*} Rina Miyagi,^a Tomoe Ohta,^b Tatsusada
Yoshida,^b Hiroyuki Tanaka^{a*}**

^aFaculty of Pharmaceutical Sciences, Sanyo-Onoda City University, 1-1-1
Daigaku-dori, Yamaguchi 756-0884, Japan.

^bFaculty of Pharmaceutical Sciences, Nagasaki International University, 2825-7
Huis Ten Bosch-Cho, Sasebo, Nagasaki 859-3298, Japan.

E-mail address: imahori@rs.socu.ac.jp (D.I.), htanaka@rs.socu.ac.jp (H.T.)

List of Supporting Information

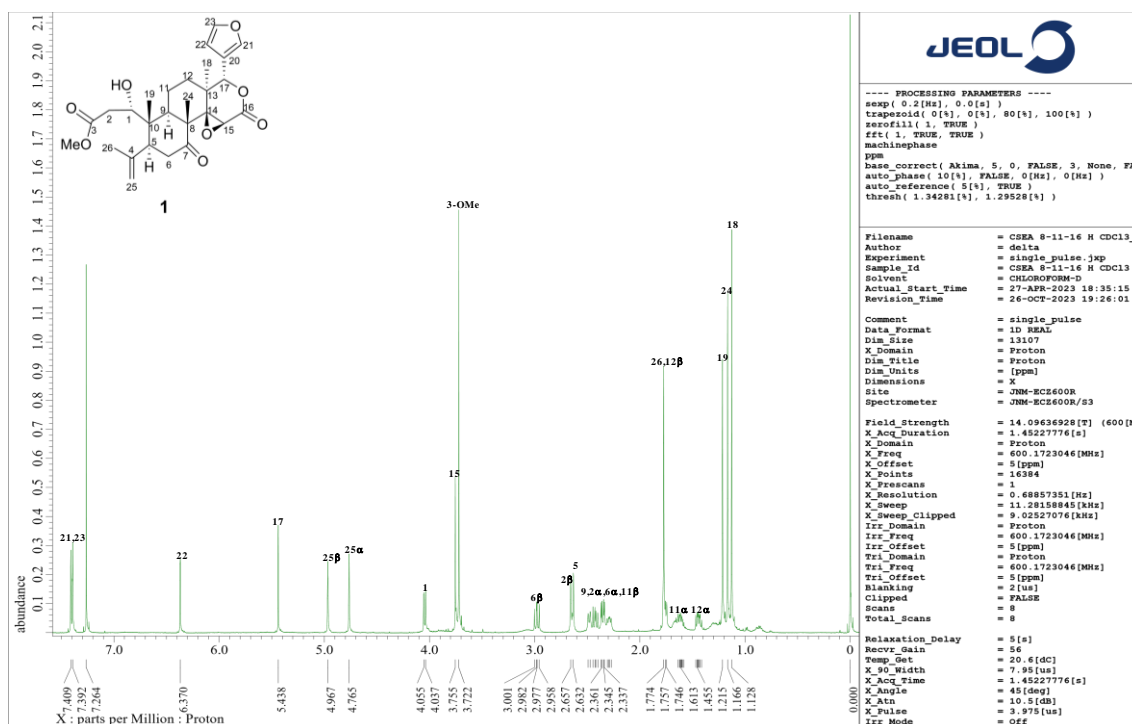
Figure S1. ¹H, ¹³C and 2D NMR spectra of sphaerocarpain I (**1**).

Figure S2. ¹H, ¹³C and 2D NMR spectra of sphaerocarpain II (**5**).

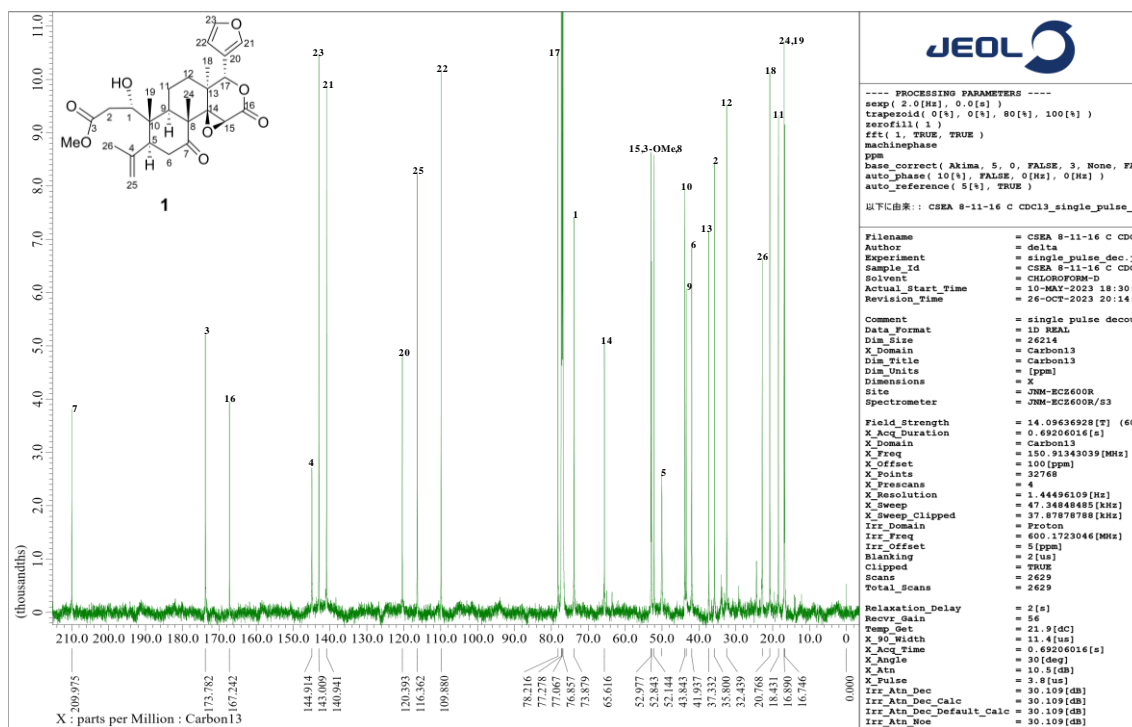
Figure S3. Optimized geometries, the minimum value of frequency, relative enthalpies including the ZPE correction, and Boltzmann distributions of conformers of sphaerocarpain I (**1**).

Figure S4. Optimized geometries, the minimum value of frequency, relative enthalpies including the ZPE correction, and Boltzmann distributions of conformers of sphaerocarpain II (**5**).

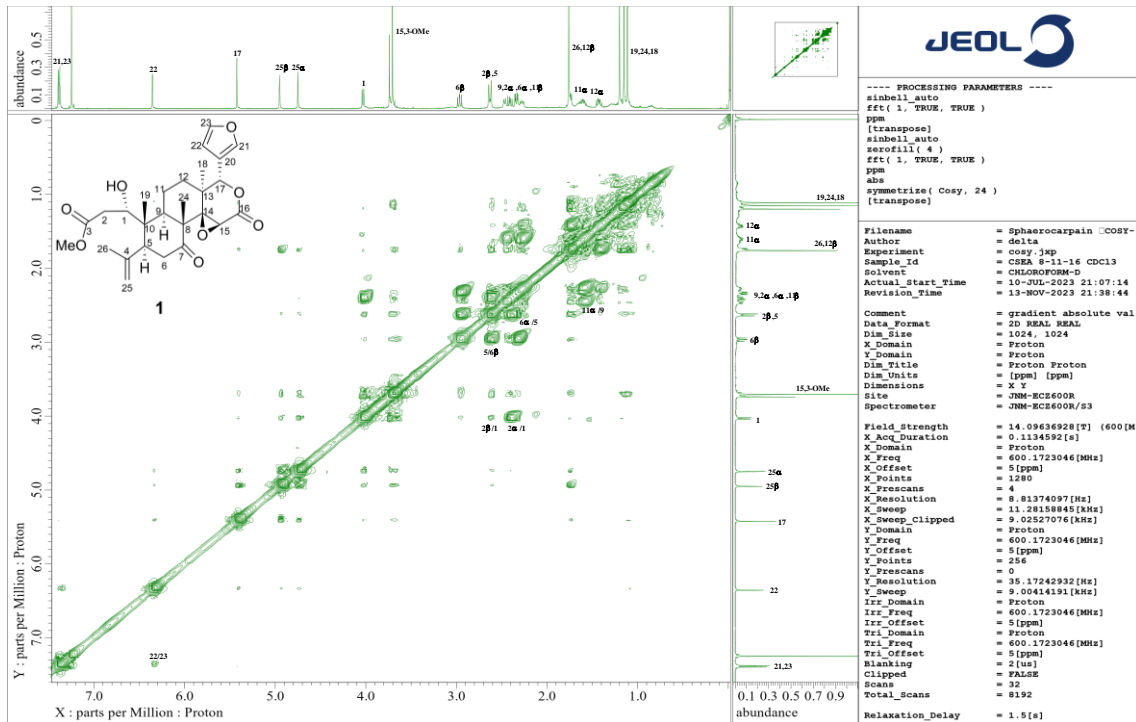
Figure S1. ^1H , ^{13}C and 2D NMR spectra of sphaerocarpain I (1).



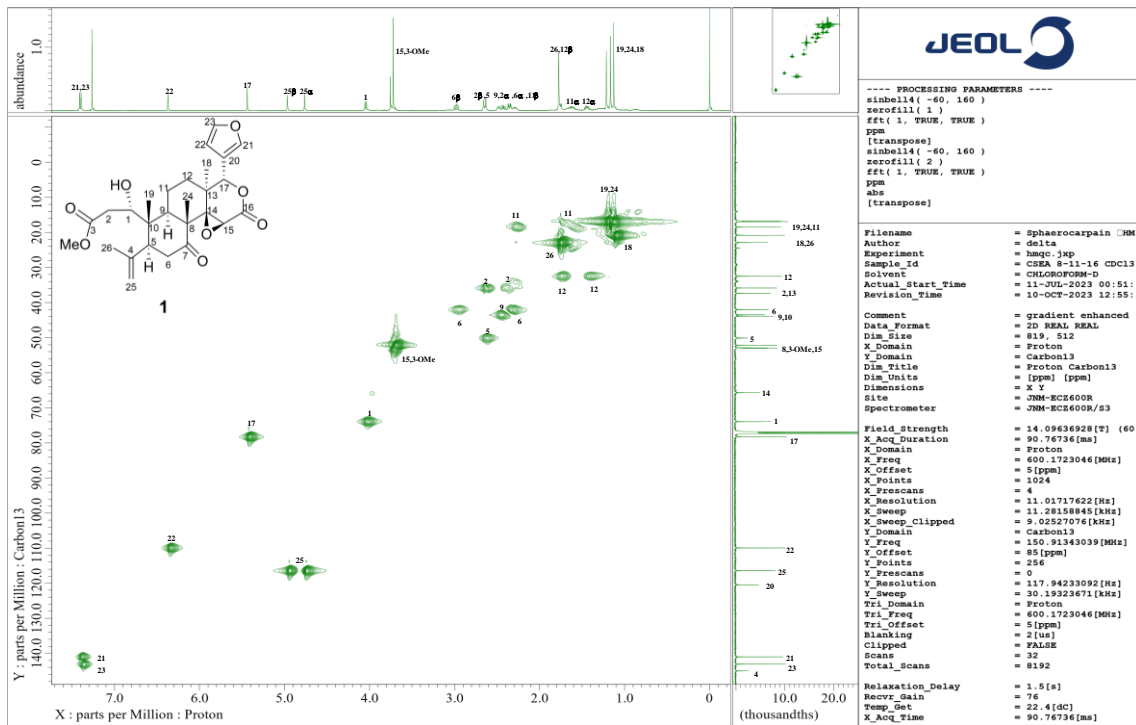
^1H NMR spectrum of 1



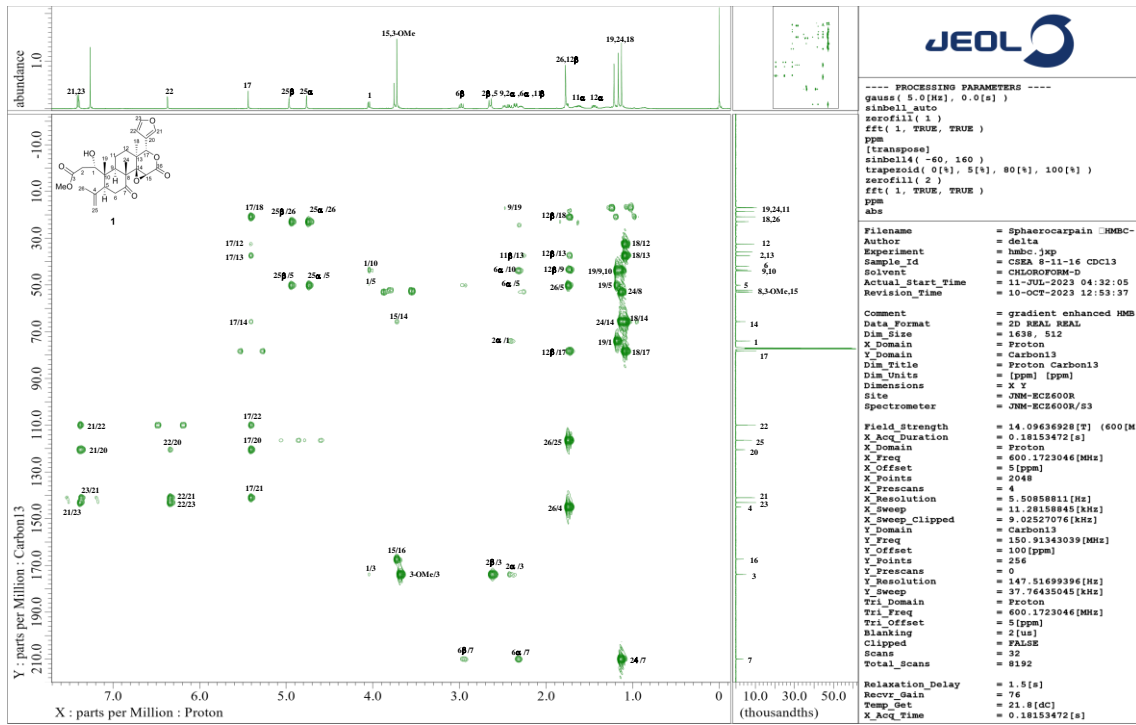
^{13}C NMR spectrum of 1



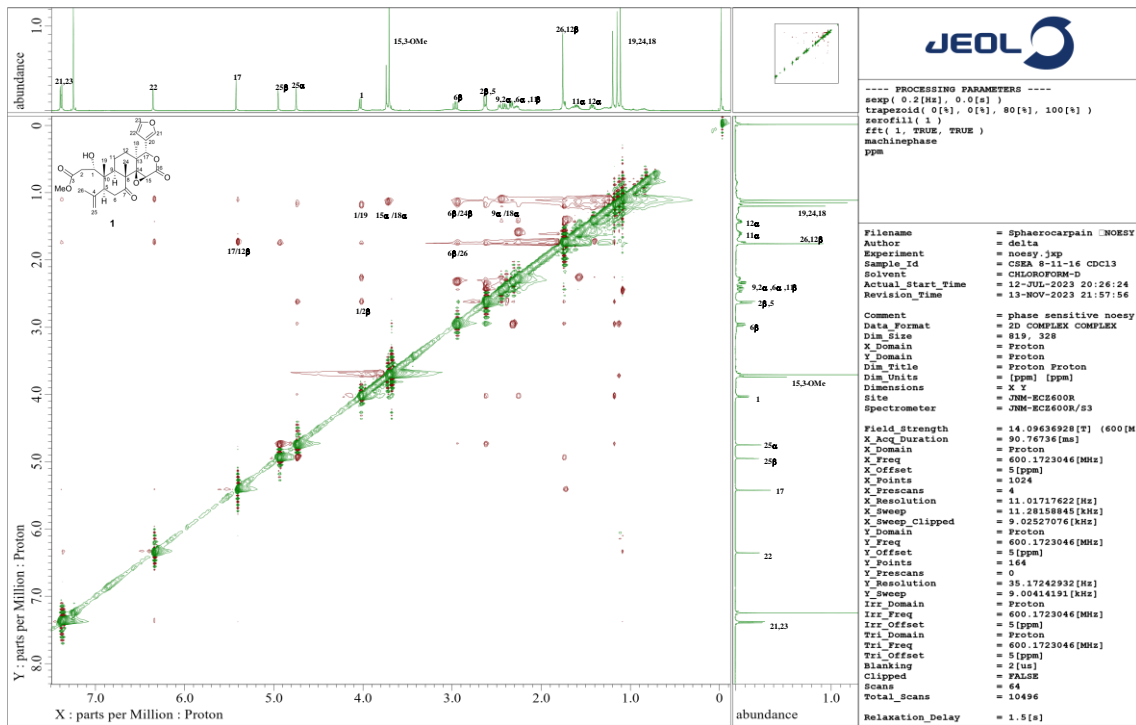
COSY spectrum of 1



HMQC spectrum of 1

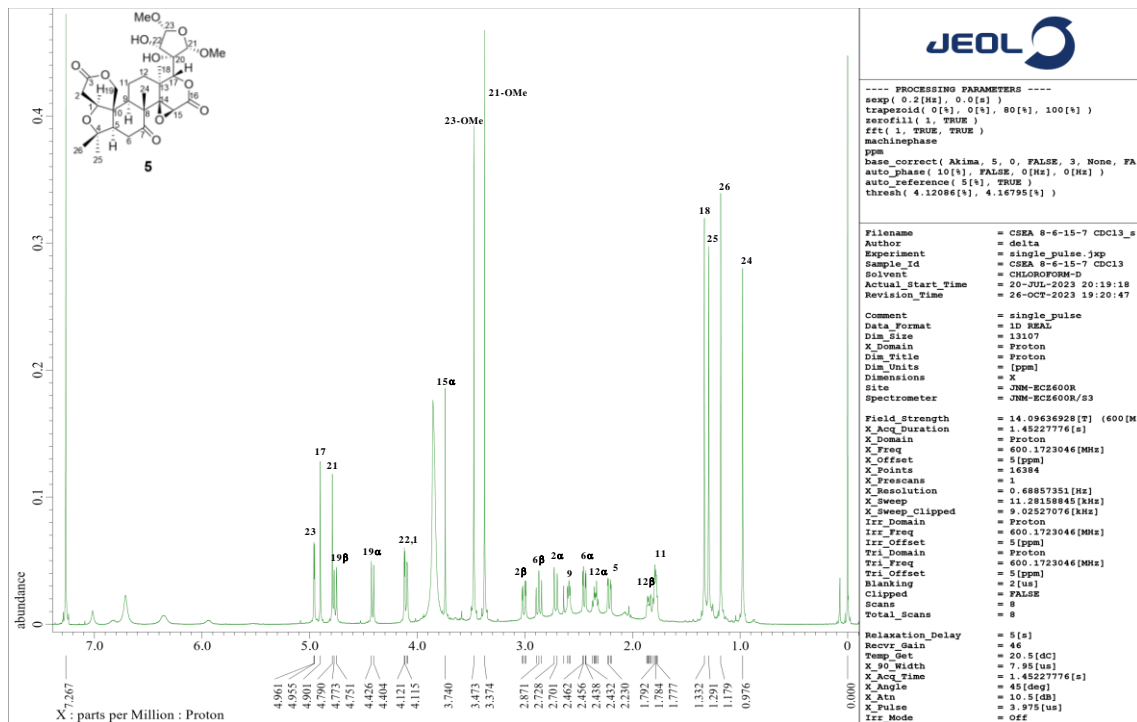


HMBC spectrum of **1**

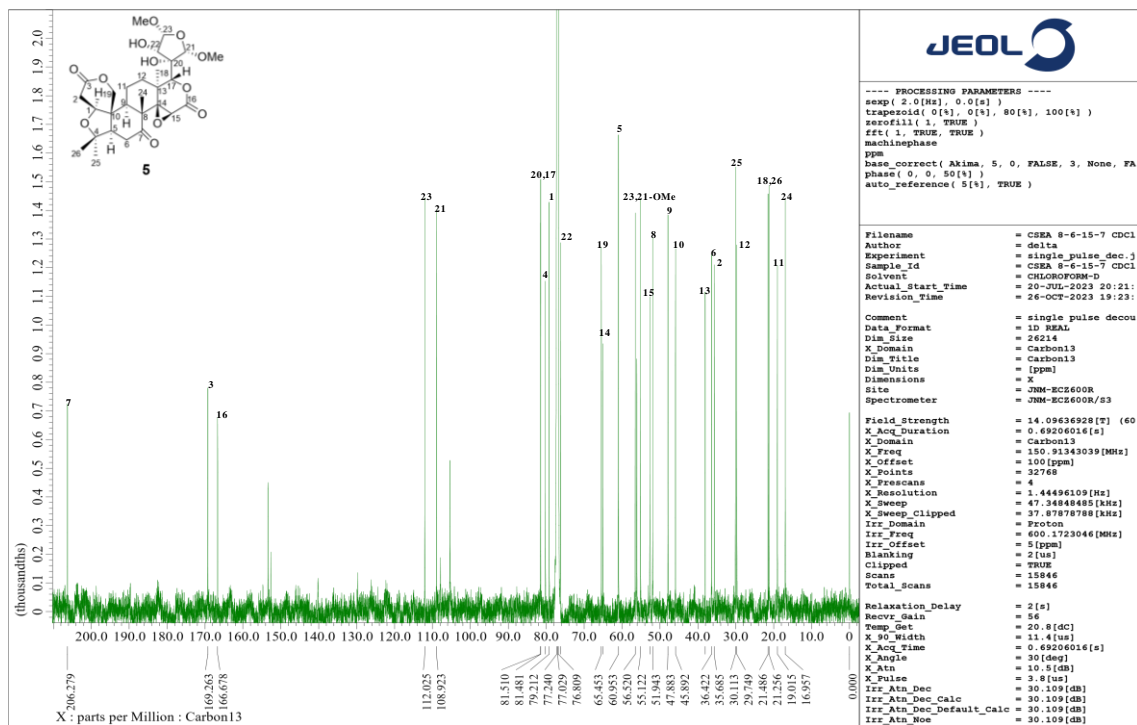


NOESY spectrum of **1**

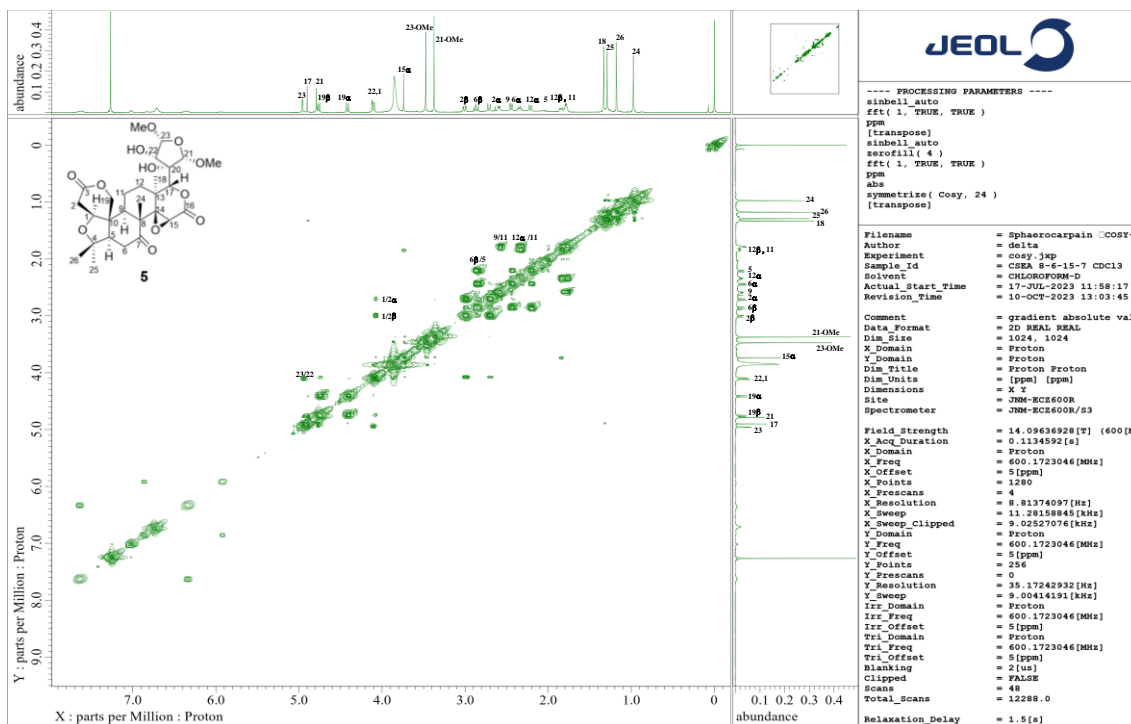
Figure S2. ¹H and ¹³C NMR spectra of sphaerocarpain II (5).



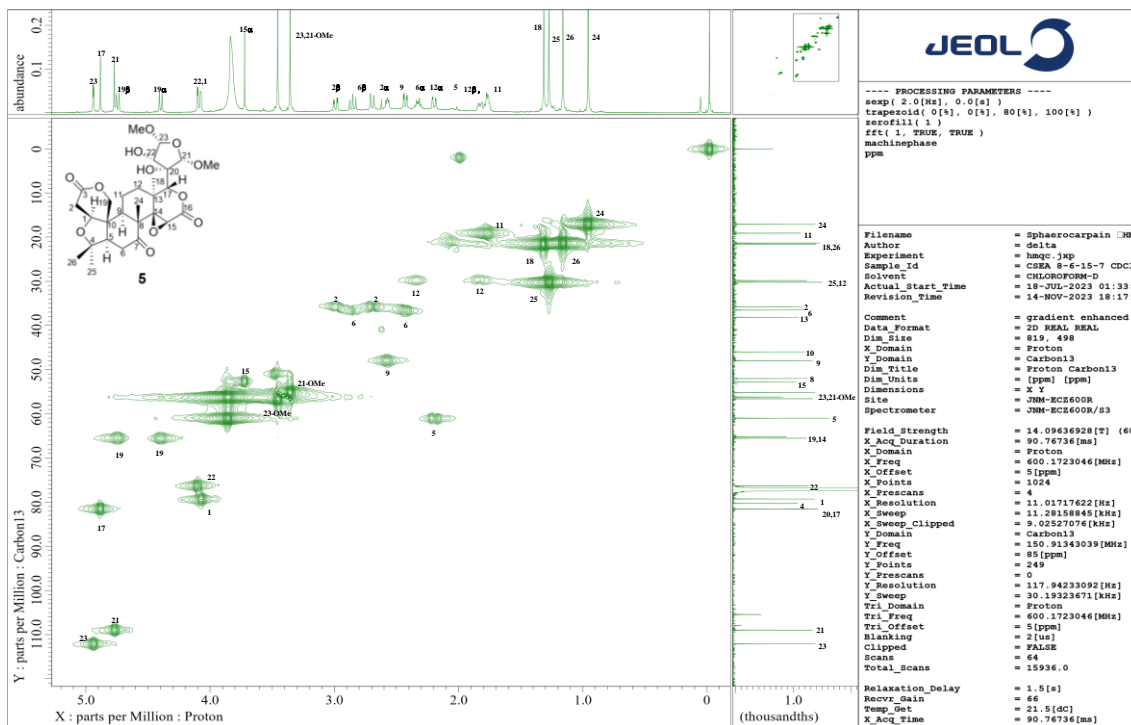
¹H NMR spectrum of 5



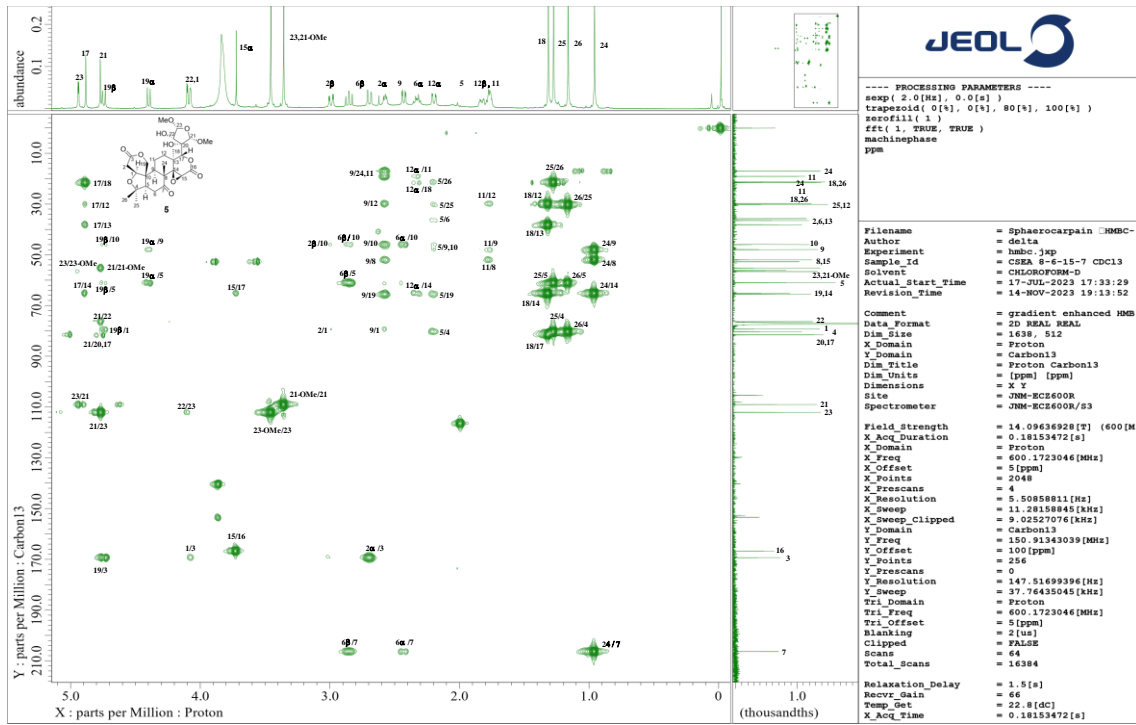
¹³C NMR spectrum of 5



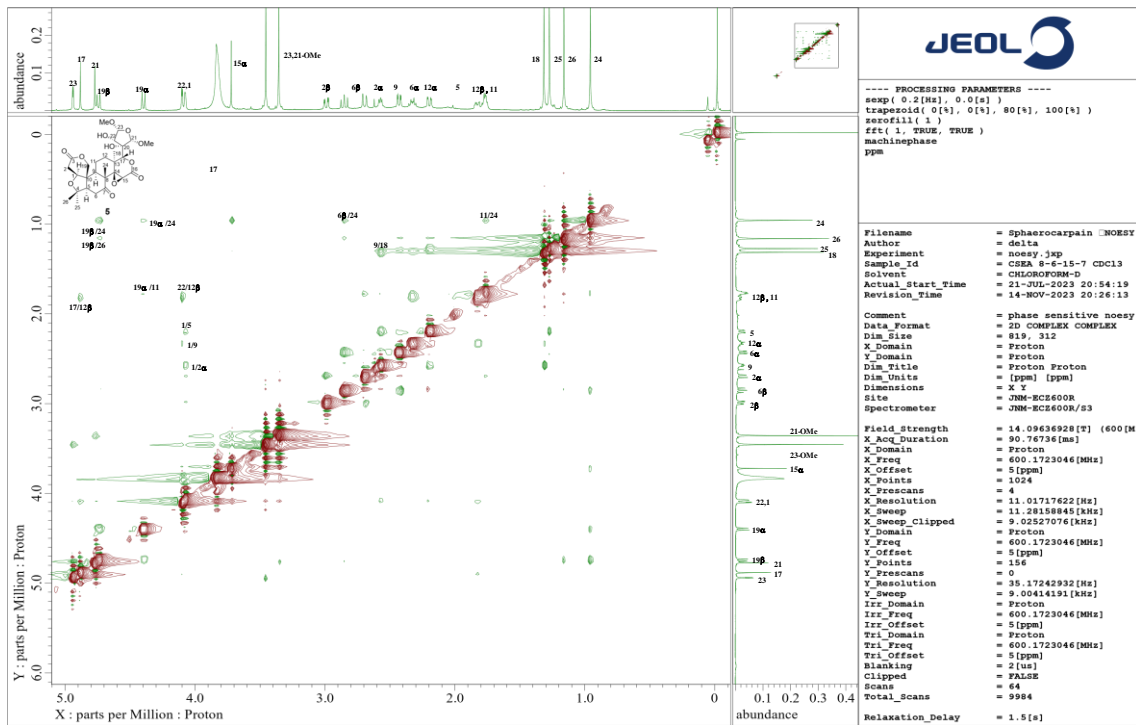
COSY spectrum of 5



HMQC spectrum of 5



HMBC spectrum of 5



NOESY spectrum of 5

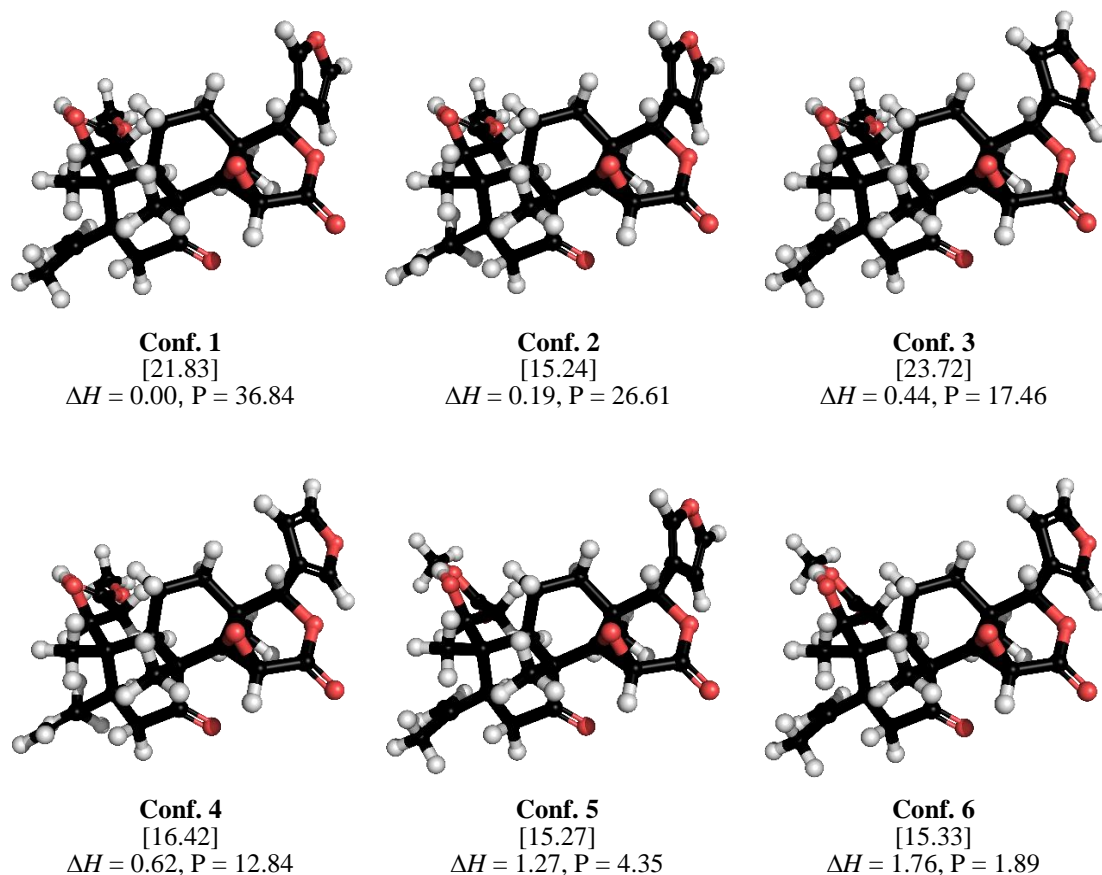


Figure S3. The optimized structures of six conformers of sphaerocarpain I (**1**) with the minimum value of frequency [in brackets, cm⁻¹], relative enthalpies including the ZPE correction (ΔH , kcal/mol), and Boltzmann distribution (P, %), at 298.15 K, calculated at the ω B97X-D/def2-TZVP level in MeOH.

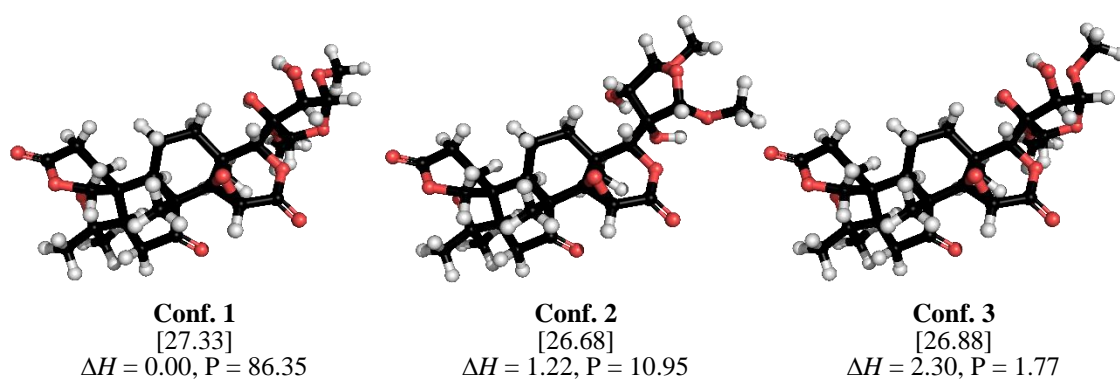


Figure S4. The optimized structures of three conformers of sphaerocarpain II (**5**) with the minimum value of frequency [in brackets, cm⁻¹], relative enthalpies including the ZPE correction (ΔH , kcal/mol), and Boltzmann distribution (P, %), at 298.15 K, calculated at the ω B97X-D/def2-TZVP level in MeOH.