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Other Chemical Constituents Isolated from *Solanum crinitum* Lam. (Solanaceae)

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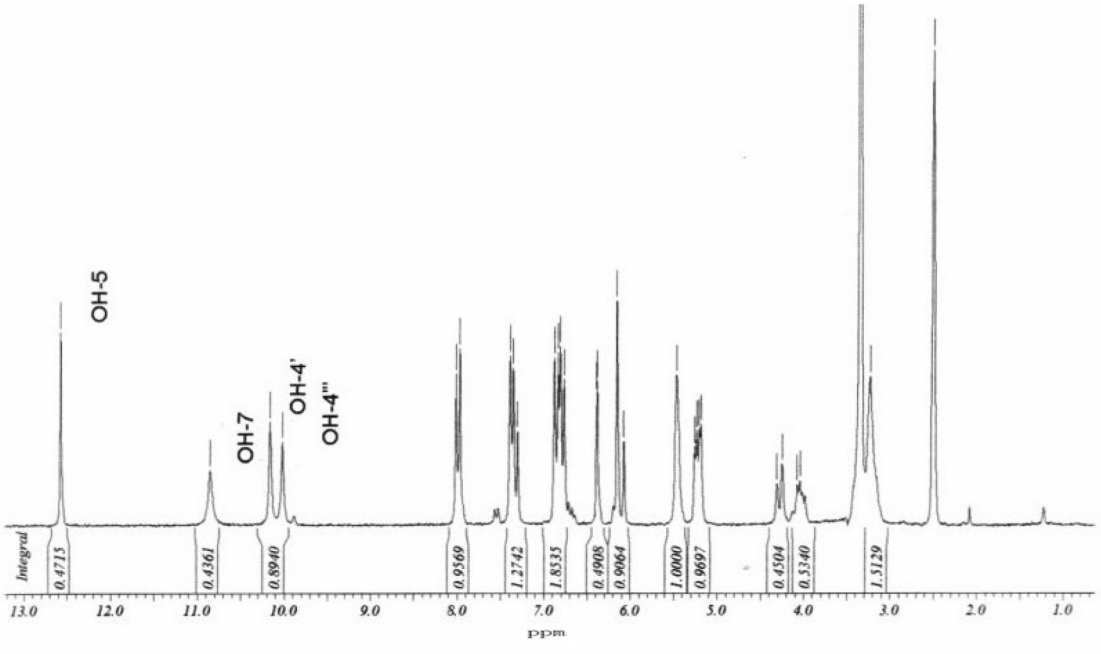

Figure S1. ^{1}H NMR spectrum of compound **1**.

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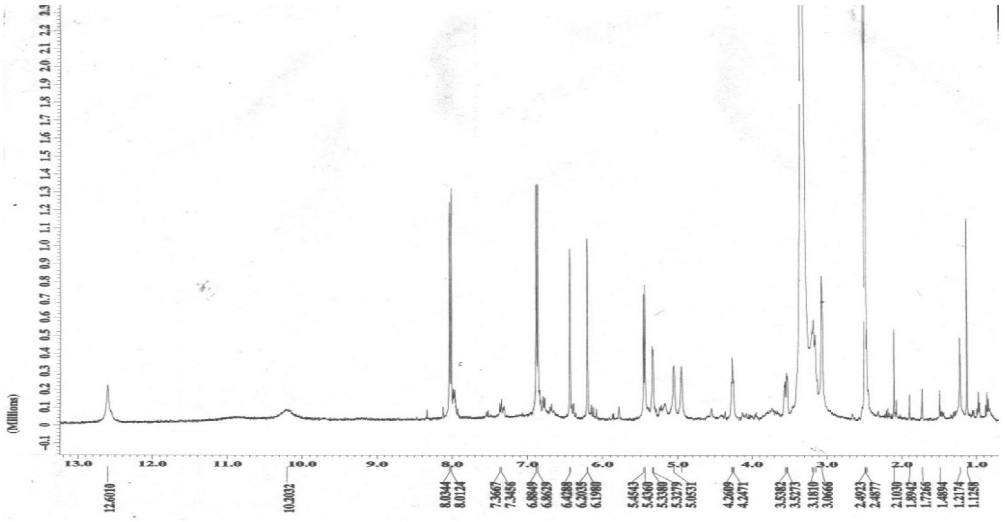

Figure S2. ^{1}H NMR spectrum of compound **2**.

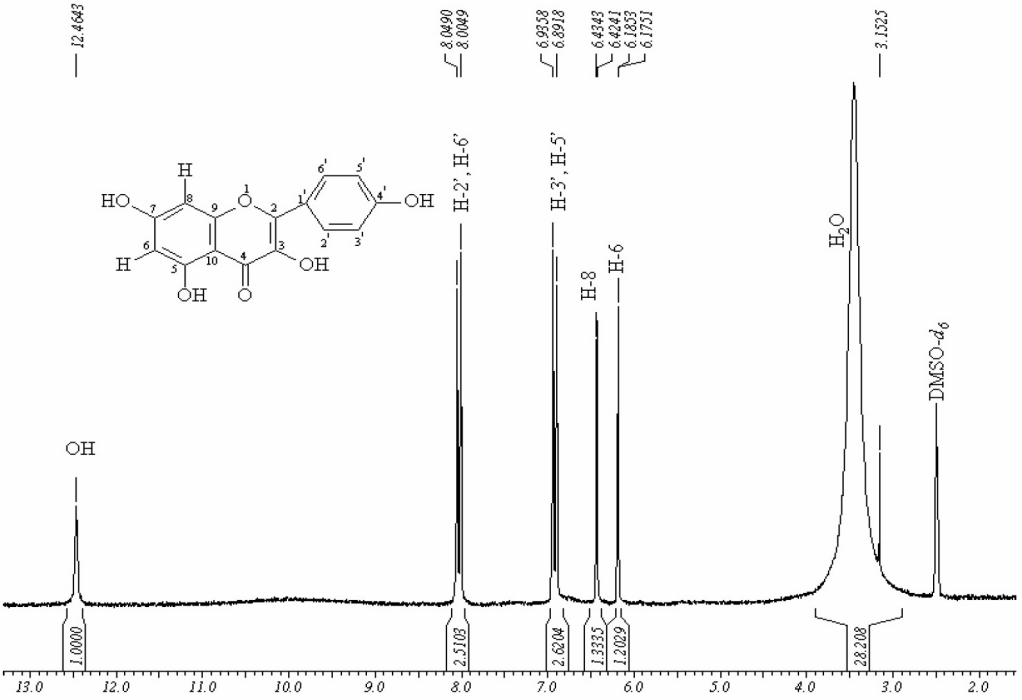

Figure S3. ^{1}H NMR spectrum of compound **3**.

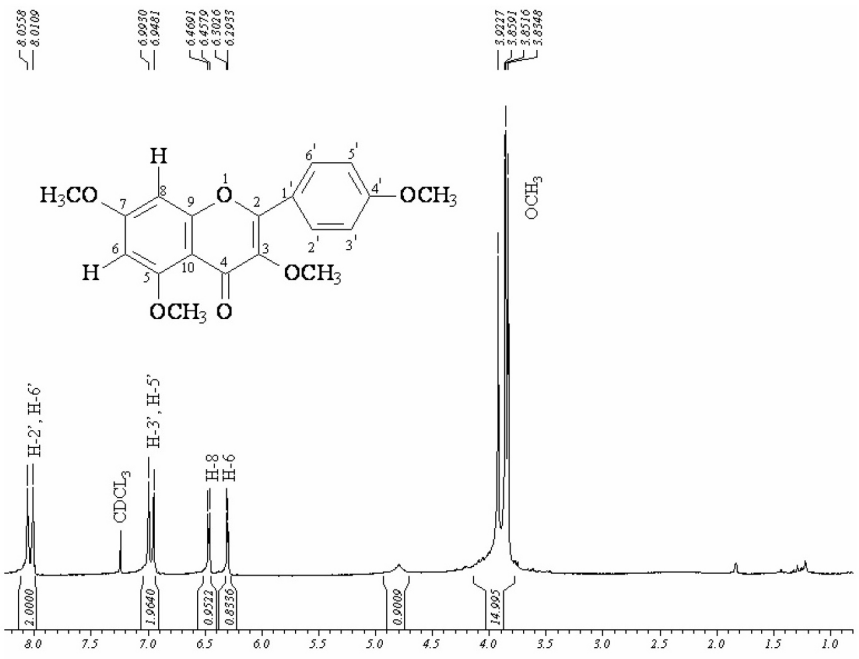

Figure S4. ^{13}C NMR spectrum of compound **4**.

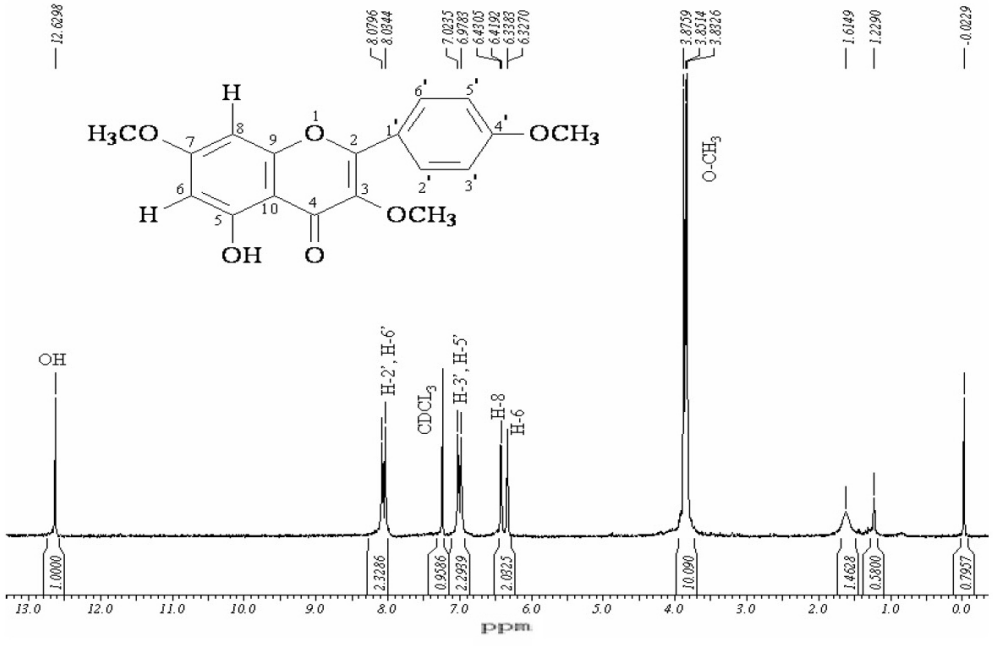

Figure S5. ^{1}H NMR spectrum of compound **5**.

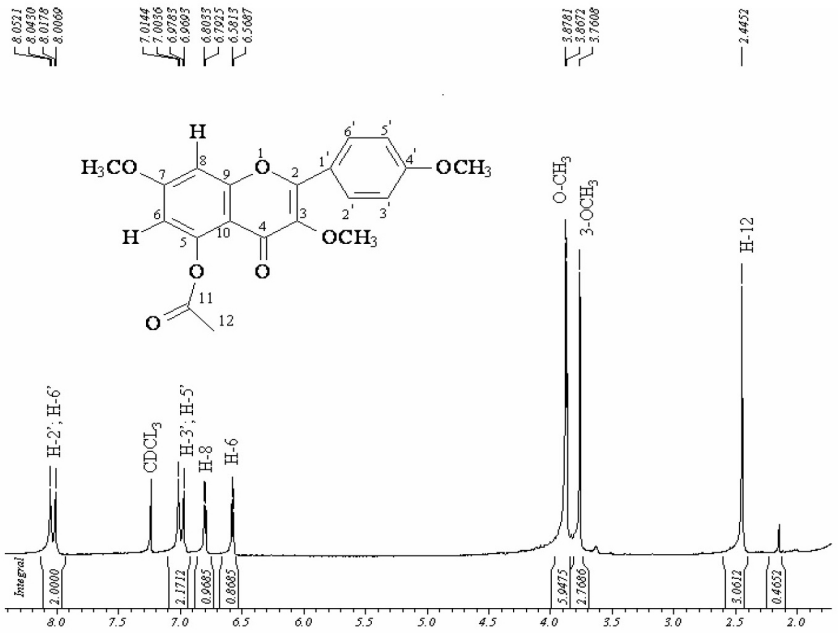

Figure S6. [1]H NMR spectrum of compound **6**.

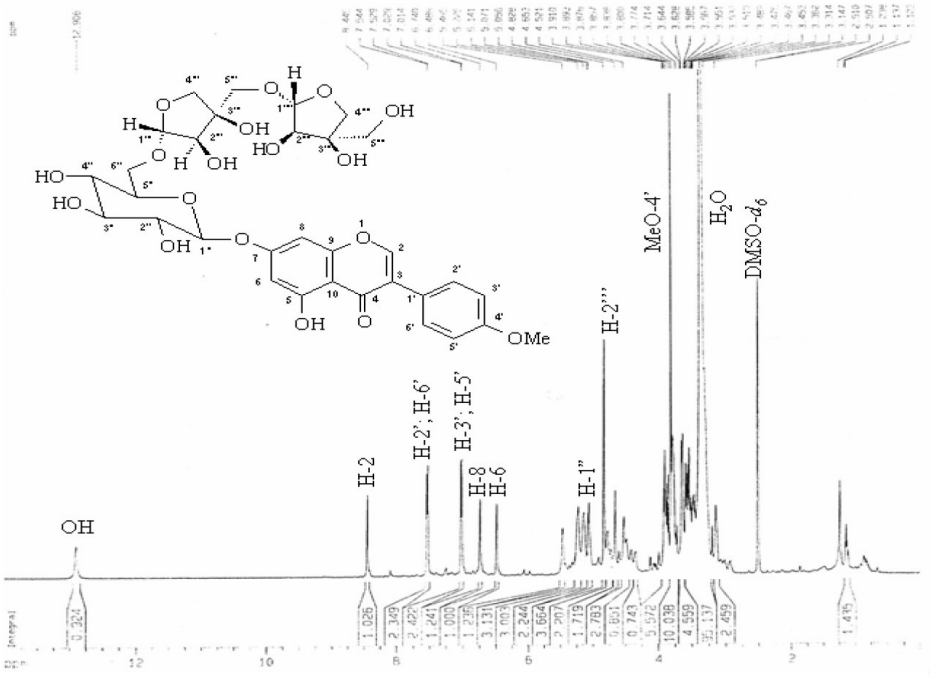

Figure S7. [1]H NMR (500 MHz) of compound **7**.

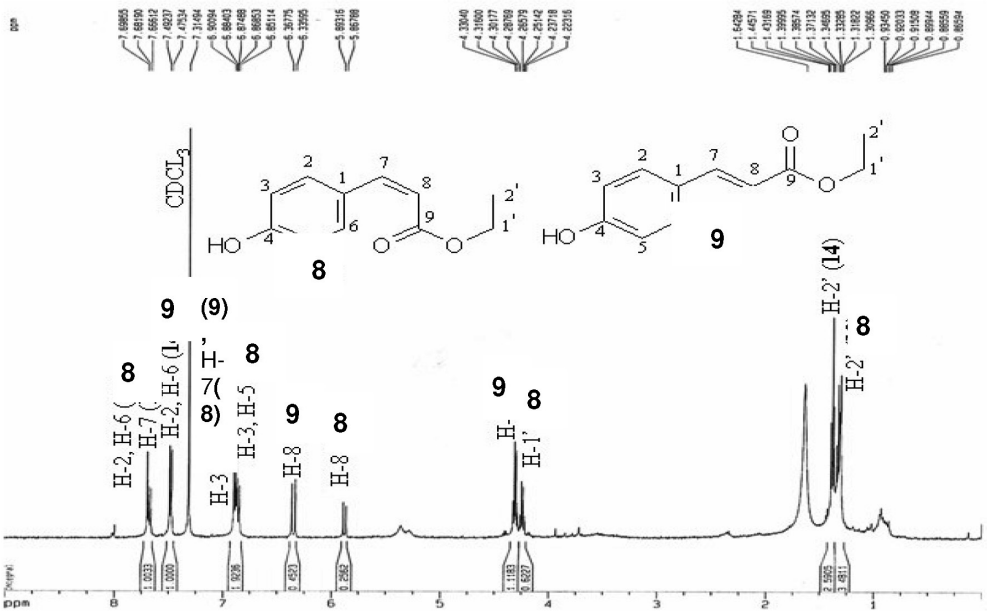

Figure S8. [1]H NMR spectrum(500 MHz) of compounds **8**+**9**.

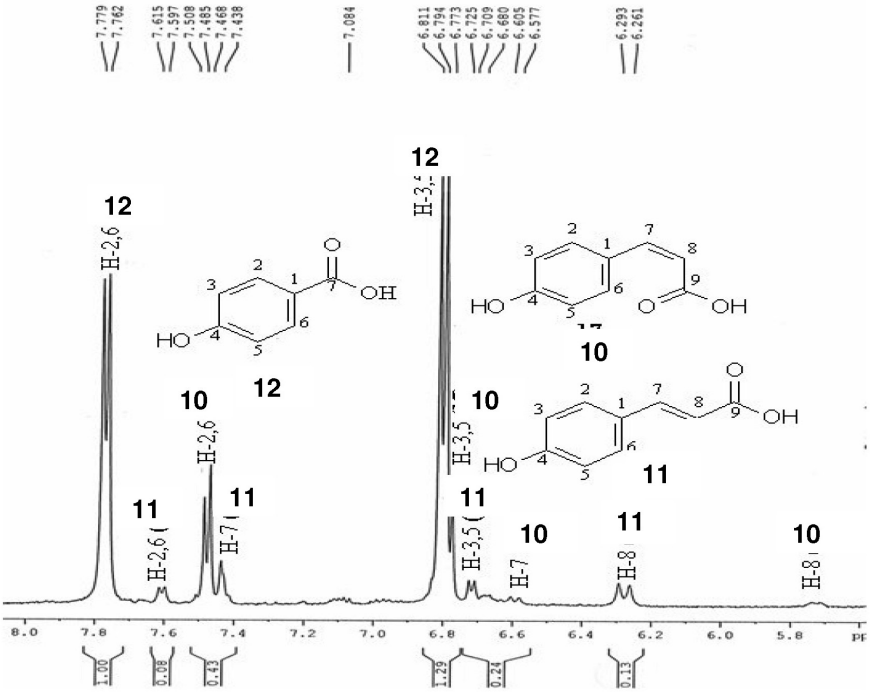

Figure S9. [1]H NMR spectrum (500 MHz) of compounds **10**+**11**+**12**.

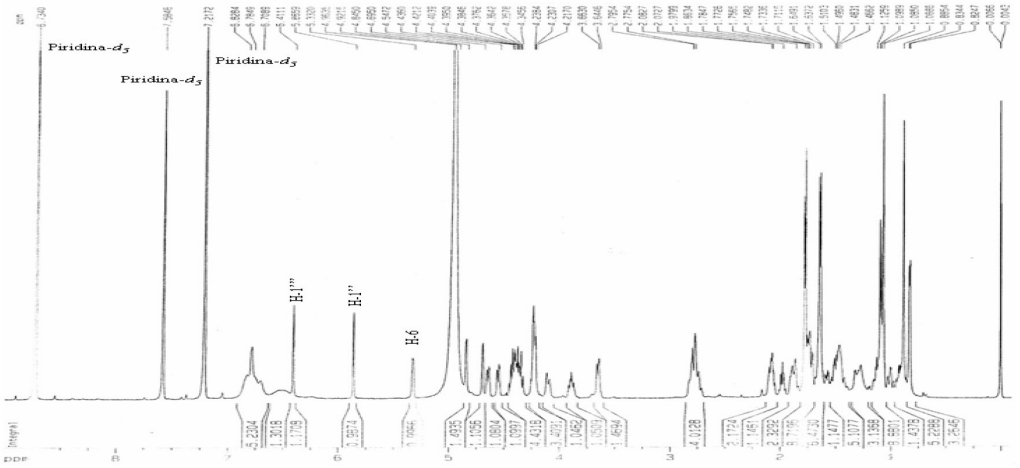

Figure S10. ^{1}H NMR spectrum (500 MHz, Pyridine-d_5) of the compound **13**.

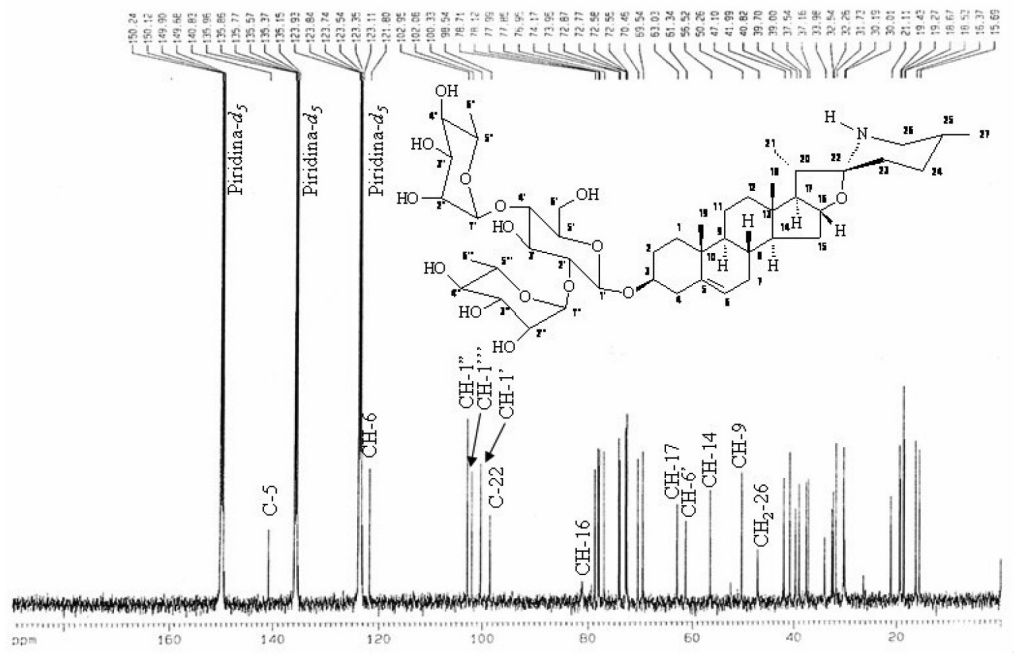

Figure S11. ^{13}C NMR (125 MHz) of compound **14**.

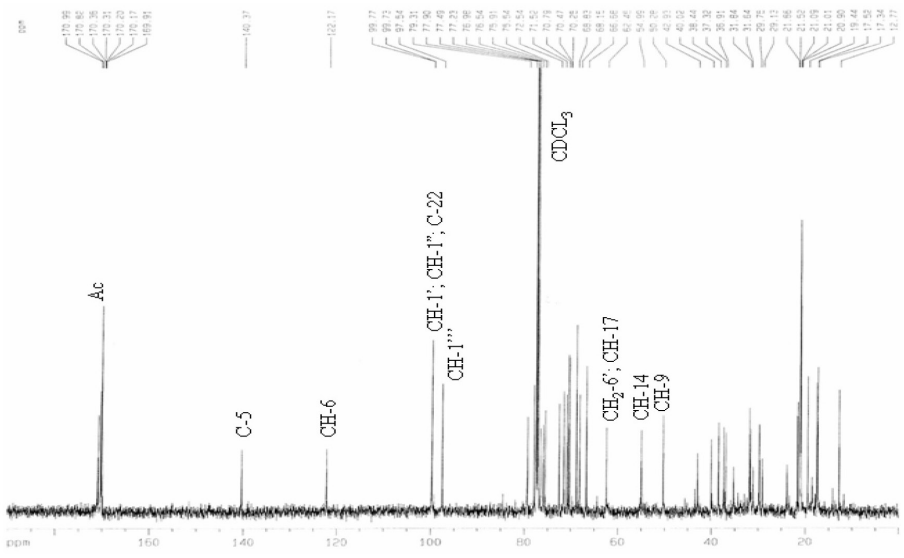

Figure S12. ^{13}C NMR spectrum (125 MHz) of compound **15.**

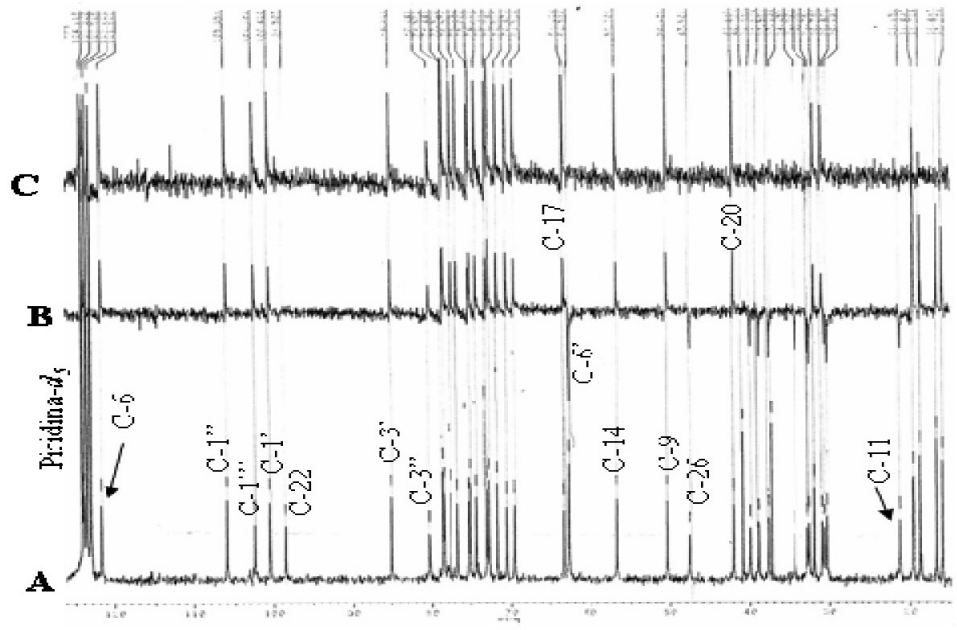

Figure S13. ^{13}C NMR spectrum BBD (A) and DEPT-135 ((B and C), 50 MHz, pyridine-d_6) of **16**.

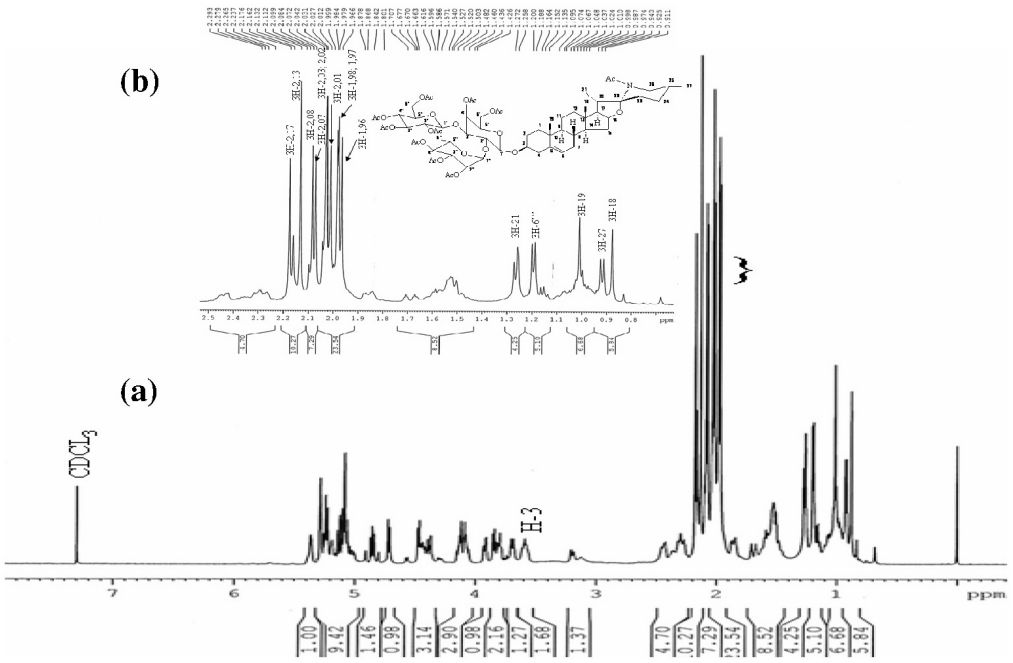

Figure S14. ^{1}H NMR spectrum (a) and expansion (b) (400 MHz, $CDCl_3$) of **17**.

Molecular Modeling

In order to compare the relative stabilities of the epimeric structures **13/14**, a molecular modeling study was implemented using the Spartan 06 for Linux program (Wavefunction, Inc.). Because the long chain attached to C-3 should only have a small influence on the relative stabilities, it was replaced by a methoxy group to reduce the computational cost for the calculations. The conformer distribution of the resulting alpha and beta epimer models (**13a** and **14a**) was determined with the Monte Carlo approach using the MMFF molecular mechanics force field. The most stable conformers of **13a** and **14a** were submitted to a previous energy minimization with the PM3 semi empirical method.[31] The PM3 optimized structures were then submitted to a complete energy minimization with the B3LYP/6-31G* DFT method. The B3LYP method was chosen because it usually yields results for many properties in close agreement with those obtained from MP calculations, and is more efficient than conventional *ab initio* correlated methods for larger-scale calculations. The possibility of existence of this epimer as a stable species was verified by a molecular modeling study at the DFT B3LYP/6-31G* level with models of both epimers. The β-epimer model at C-20 (**14a**) is less stable than the α-epimer one (**13a**), but the energy difference between both structures is only 4.85 kcal mol^{-1} (20.30 kJ mol^{-1}), as calculated with the B3LYP/6-31G* DFT method. Because of this small energy difference, the β-epimer is expected to exist in appreciable amount in an equilibrium mixture with the more stable α-epimer. The main reason for the lower stability of the β-epimer should be the proximity between the C-21 methyl group and carbons C-23 and C-18. The corresponding C-C distances, which are equal to 4.22 Å and 3.47 Å, respectively, in **13a**, are considerably shorter in **14a**, 3.43 Å and 2.98 Å, respectively. This closer proximity would raise more unfavorable steric interactions in **14a** than in **13a** (Figure S15).

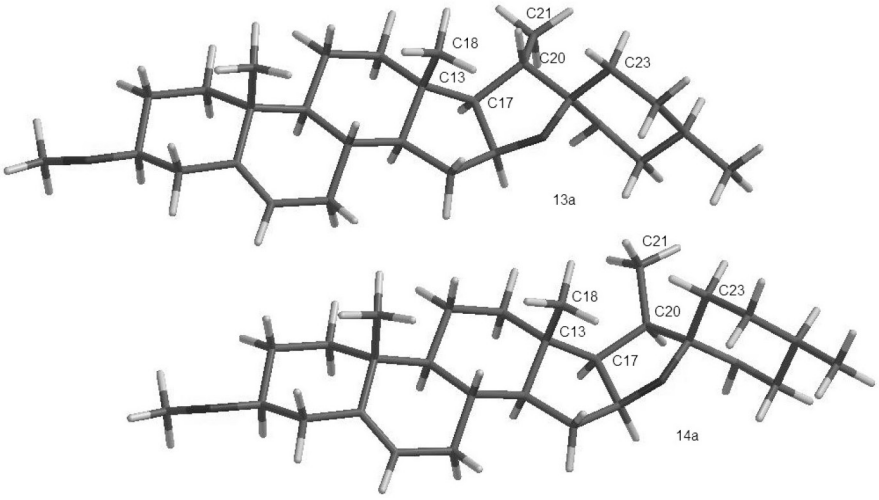

Figure S15. 3D representation of models **13a** and **14a** after optimization with the B3LYP/6-31G* DFT method.