Supplementary Information

Cyperane and Eudesmane-Type Sesquiterpenoids from the Chinese Liverwort and Their Anti-Diabetic Nephropathy Potential

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**Theory and Calculation Details.**

The calculations were performed by the Gaussian 03 program package\(^1\) The semi-empirical AM1 method\(^2\) and a DFT approach\(^3\) B3LYP/6-31G* were employed to scan the potential energy surface (PES). The geometries of all ground-state conformations obtained were further optimized at the B3LYP/6-31G* level at 298.15 K, followed by calculations of their harmonic frequency analysis to confirm these minima and thence calculations of room-temperature free energies.

Time-dependent density functional theory (TDDFT)\(^4\) at the same level was used to calculate the electronic excitation energies and rotational strengths in gas phase for the first 30 states. The rotatory strengths were summed and energetically weighted following the Boltzmann statistics and the final ECD spectra were then simulated by overlapping Gaussian functions according to the following equation\(^5\)

\[
\Delta \epsilon(E) = \frac{1}{2.296 \times 10^{-19}} \frac{1}{\sigma \sqrt{\pi}} \times \sum_i \Delta E_i R_i e^{-\left((E-E_i)/\sigma\right)^2}
\]

Where \(\sigma\) is the width of the band at 1/e height, while \(\Delta E_i\) and \(R_i\) are the excitation energies and rotatory strengths for transition, respectively. \(\sigma = 0.1\) eV and \(R_{vel}\) were used.
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