Supporting information for

Isolation, Characterization and Antiproliferative Activities of Eudesmanolide Derivatives

from the Flowers of *Inula japonica*
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![13C NMR spectrum of compound 3](image)

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Beginning with the conformation of each compound obtained from the corresponding NOESY spectrum and Chem3D modeling, conformational searches were carried out first through MOE software\(^1\) and conformers were selected for geometry optimizations. Geometry optimizations and reoptimizations at the B3LYP/6-31+G(d) level were finished using Gaussian 09 package.\(^2\) TDDFT ECD calculations\(^3-5\) for the optimized conformers were performed at the CAM-B3LYP/SVP level with a CPCM solvent model in acetonitrile, and the calculated ECD spectra of different conformers were simulated with a half bandwidth of \(\sim 0.4\) eV. The ECD curves were extracted by SpecDis 1.62 software.\(^6\) The overall ECD curves of all the compounds were weighted by Boltzmann distribution after UV correction.

REFERENCES:


(2) Gaussian 09, revision B, 01; Gaussian Inc.: Wallingford, CT, USA, 2010.

