Supporting Information


Cephalounei A, a New Cephalotaxus Alkaloid from the Powdered Stems of Cephalotaxus fortune Hook. f

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Figure S1. $^1$H NMR of compound 1 in CD$_3$OD (600 MHz)
Figure S2. $^{13}$C NMR of compound 1 in CD$_3$OD (150 MHz)

Figure S3. HMBC of compound 1 in CD$_3$OD
Figure S4. HSQC of compound 1 in CD$_3$OD

Figure S5. $^1$H–$^1$H COSY of compound 1 in CD$_3$OD
Figure S6. $^1$H–$^1$H ROESY of compound 1 in CD$_3$OD
Figure S7. IR of compound 1
Figure S8. HRESIMS of compound 1
**Figure S9.** UV of compound 1
Figure S10  Optical Rotation of compound 1

Figure S11.  low resolution mass spectrometry of compound 1
**S12: ECD computational details of compound 1 (Cephalounei A)**

A conformation searches based on molecular mechanics with MMFF94S force fields were performed for compound 1 which gave nine stable conformers [1-2]. Selected six conformers with distributions higher than 1% were further optimized by density functional theory method at the B3LYP/6-31G(d,p) level in Gaussian 09 program package [3], leading to two minimum geometries, which was further checked by frequency calculation and resulted in no imaginary frequencies. The ECD was calculated using TDDFT-B3LYP/6-311G(2d, p) of theory on B3LYP/6-31G(d, p) optimized geometry. The calculated ECD curve for 1 and weighted ECD were all generated using SpecDis 1.64 with $\sigma = 0.3$ ev, and UV shift 5 nm [4].

Two optimized conformers of 1(2R, 3S, 6S)

![Conformer 1](image1)

46.28% 37.12%

![Conformer 2](image2)

0.95% 0.95%

![Conformer 3](image3)

11.33% 3.38%

References:

