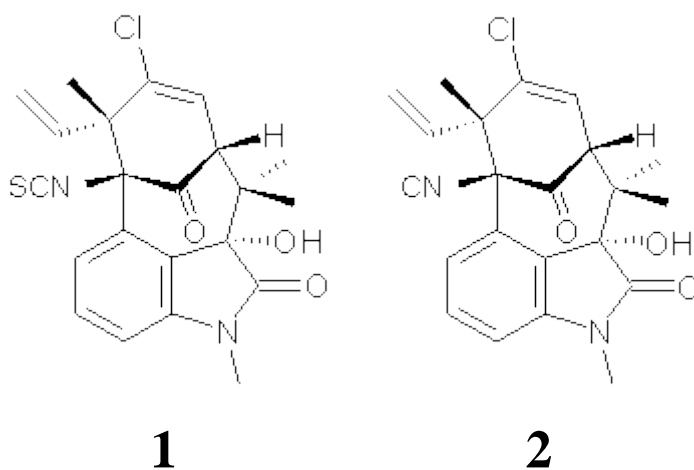


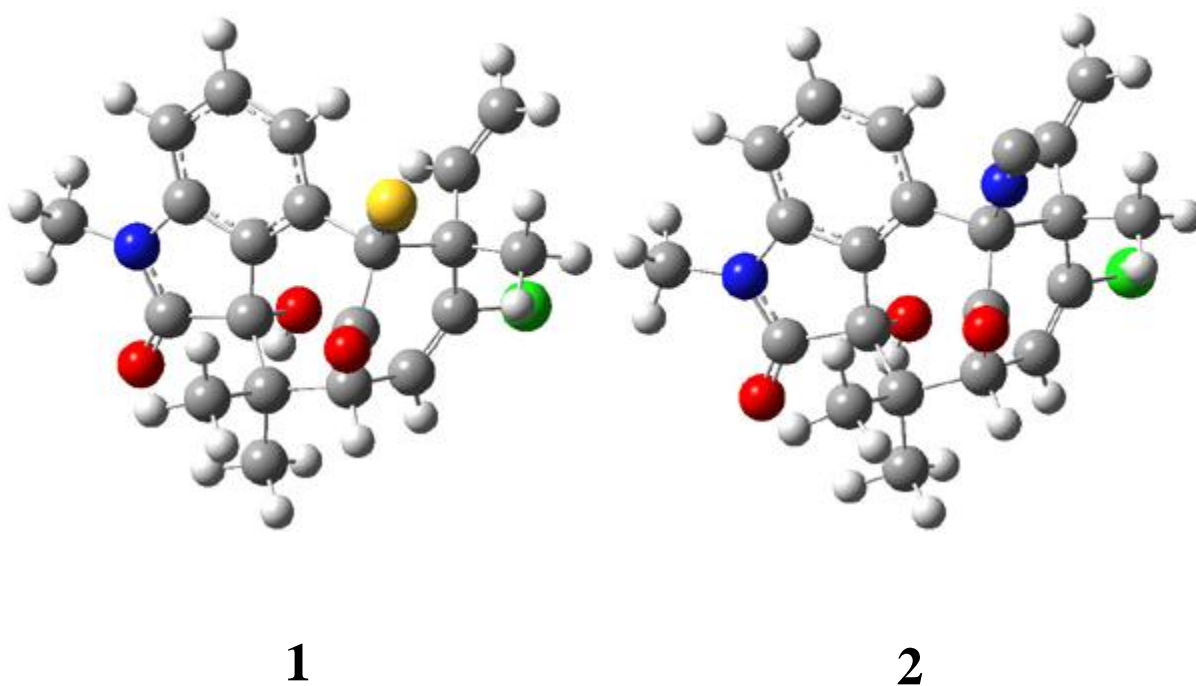
# WELWITINDOLINONES STRUCTURE

A quick note here on the use of computed NMR to determine stereochemical structure. The Garg group synthesized two “oxidized welwitindolines”, compounds **1** and **2**.<sup>1</sup> The relative stereochemistry at the C3 position (the carbon with the hydroxy group) was unknown.



Low energy gas-phase conformers of both epimers of **1** and **2** were optimized at B3LYP/6-31+G(d,p). (These computations were done by the Tantillo group.) See Figure 1 for the optimized lowest energy conformers. Using these geometries the NMR chemical shifts were computed at mPW1PW91/6-311+G(d,p) with implicit solvent (chloroform). The chemical shifts were Boltzmann-weighted and scaled according to the prescription (see this post) of Jain, Bally and Rablen.<sup>2</sup> The computed chemical shifts were then compared against the experimental NMR

spectra. For both **1** and **2**, the  $^{13}\text{C}$  NMR shifts could not readily distinguish the two epimers. However, the computed  $^1\text{H}$  chemical shifts for the *S* epimer of each compound was significantly in better agreement with the experimental values; the mean average deviation for the *S* epimer of **2** is 0.08 ppm but 0.36 ppm for the *R* epimer. As a check of these results, DP4 analysis<sup>3</sup> (see this post) of **2** indicated a 100% probability for the *S* epimer using only the proton chemical shifts or with the combination of proton and carbon data.



**Figure 1.** B3LYP/6-31+G(d,p) optimized geometries of the lowest energy conformations of **1** and **2**.

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