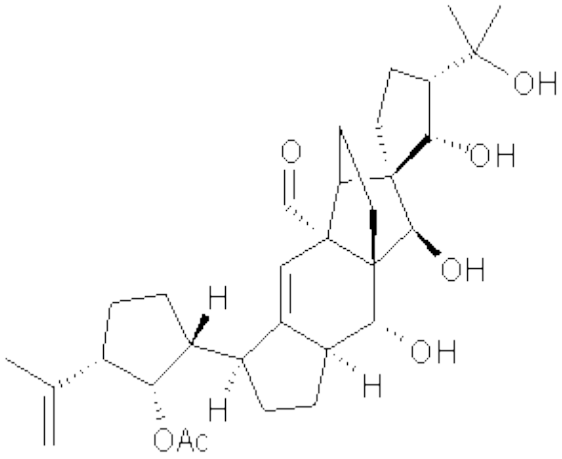
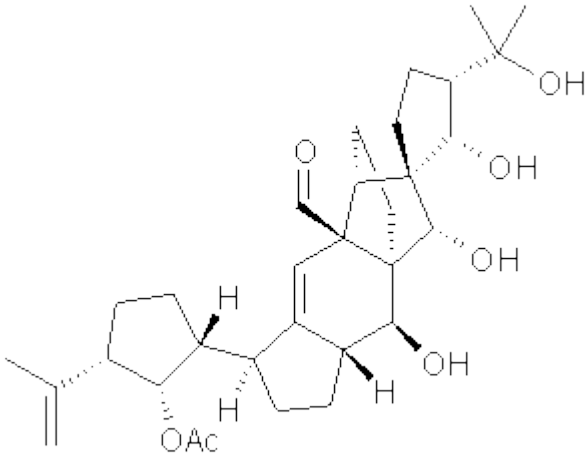
STRUCTURE OF VANNUSAL B

Saelli, Nicolaou, and Bagno point out in a recent article how the determination of the structure of vannusal B might have been guided by DFT computed ^{13}C NMR chemical shifts, had they been available.[1] The original structure was proposed in 1999 as **1**,[2] but was ultimately settled as **2** in 2010.[3]



1



2

The ^{13}C NMR chemical shifts of **1** and **2** and some other alternatives were computed at M06/pcS-2//B3LYP/6-31g(d,p), where the pcS-2 basis set[4] is one proposed by Jensen for computing chemical shifts. The computed chemical shifts of **1** poorly correlate with the experimental chemical shifts of vannusal B, with a low correlation coefficient of 0.9580 and a maximum error of 16.2 ppm.

On the other hand, the correlation between the computed chemical shifts of **2** with the experimental values is excellent (R^2=0.9948) and a maximum error of 3.0 ppm. Comparison of computed and experimental H-H coupling constants of model compounds of the “northeast” section of the molecule verified the correct structure is **2**.

Source: http://comporgchem.com/blog/?p=1551