Absolute Configuration of a New Alkaloid

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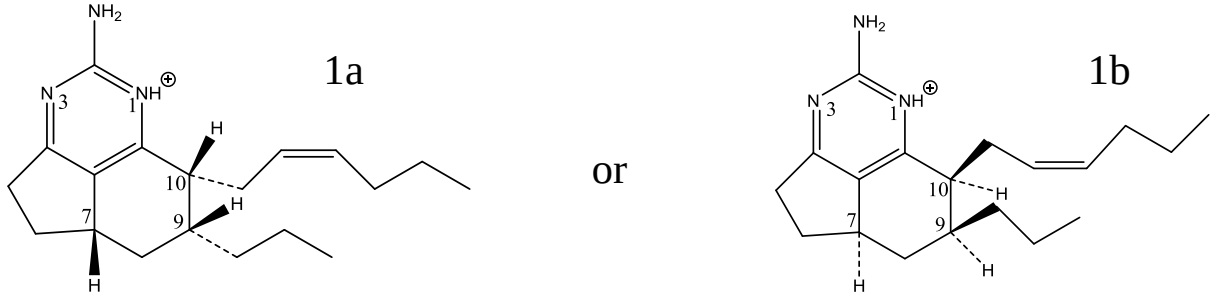
The tricyclic guanidine alkaloid (1) was isolated from a Madagascar marine sponge Biemna laboutei. Its structure was elucidated by NMR including 2D techniques. The purpose of this work was to assign the absolute stereostructure of this molecule: 7S,9R,10R (1a) or 7R,9S,10S (1b).



The conformations were optimized using the density functional method ωB97XD/6-31+G(d,p) [1] in vacuum and in methanol. Smd continuum model was used to simulate solvent effect [2].

UV and electronic circular dichroism (ECD) spectra were calculated for the most energetically minimum structures at the TD/ωB97XD/6-31++G(d,p) level. Then these spectra were weighted according to Boltzmann statistics and the results were compared to experimental UV and ECD spectra measured in methanol. The comparison of theoretical and experimental spectra suggested that 7S,9R,10R enantiomer (1a) was present in *Biemna laboutei* sponge.

References

1. J. D. Chai, M. Head-Gordon, Physical Chemistry Chemical Physics, 10, 2008, 6615-6620.
2. A. V. Marenich, C. J. Cramer and D. G. Truhlar, Journal of Physical Chemistry B, 113, 2009, 6378-6396.