Structural and stereochemical elucidation of complex organic molecules with GIAO NMR calculations

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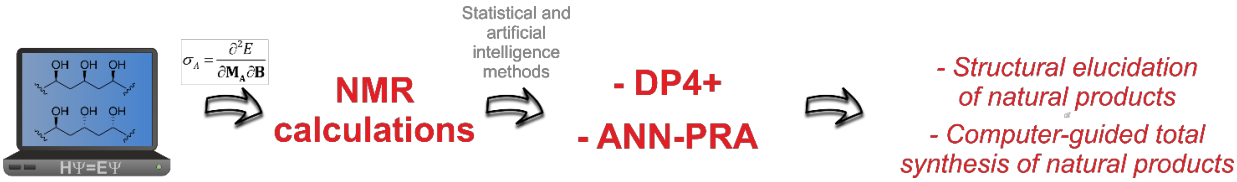

Nuclear magnetic resonance (NMR) is undoubtedly the most important spectroscopic technique for the structural elucidation of natural and synthetic products. However, even with the advent of increasingly sophisticated spectrometers and new pulse sequences, numerous structures are incorrectly assigned. This is evident in the hundreds of structural revisions that have been published in recent decades, most of which are detected after the total synthesis of the originally proposed structure.[1]

High levels of precision and accuracy in the prediction of magnetic properties of molecules (tensors, coupling constants) can be achieved by the use of computational methods based on quantum chemistry.[2] Hence, these methods represent valuable tools to facilitate the determination of the tridimensional structure of a wide variety of organic molecules, and have been widely spread in structural organic chemistry.

Our research group has made important contributions in this area.[3-6] On the one hand, we have developed an improved probability to determine the most probable structure of complex molecules when only one set of experimental data is available (DP4 + method).[4a,b] Alternatively, we developed a novel validation method combining NMR calculations with pattern recognition analysis via artificial neural networks (ANN-PRA).[4c-d] Moreover, the tools developed have been extensively used in the structural elucidation process of natural and synthetic products.[5,6]

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