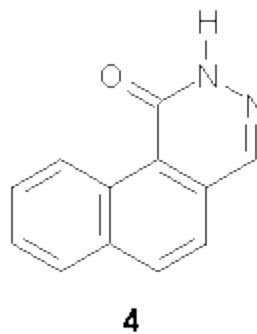
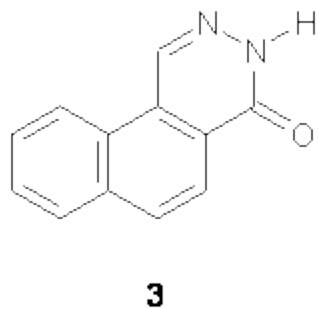
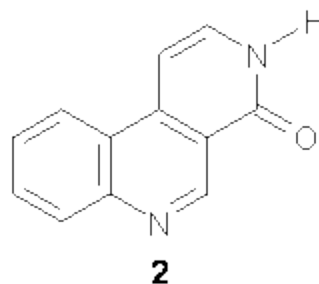
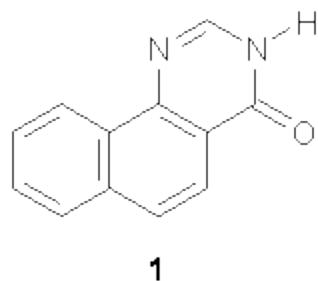


COMPUTED NMR SPECTRA TO IDENTIFY THE STRUCTURE OF SAMOQUASINE A

Example of computed NMR spectra being used to identify complex organic structures.¹

An alkaloid isolated from the custard apple tree was assigned the structure **1** and christened with the name samoquasine A.² Two years later, the authors determined that samoquasine A was actually identical to perlolidine **2**.³ Independent synthesis of the compound with structure **1** showed that its properties were not identical to that of samoquasine A.^{4,5} The properties of perlolidine were then found to differ from that of samoquasine A,⁴ leaving a void as to just what is the structure of samoquasine A.



Given that compounds **1** and the related compounds **3** and **4** had been prepared and their NMR spectra obtained, Timmons and Wipf¹ decided to compute the ¹³C NMR spectra of 48 related compounds at B3LYP/6-311+G(2d,p)//B3LYP/6-31G(d). The mean absolute difference between the computed and experimental chemical shifts for **1**, **3** and **4** are less than 2 ppm. Of the remaining 45 compounds, the one whose chemical shifts match best with that of samoquasine A is **2**, with a mean absolute deviation of 1.8 ppm. This agreement supports the contention that samoquasine A and perlolidine are in fact identical. The authors contend that the experimental data used to conjecture that they were not identical is in fact faulty.

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