Example of computed NMR spectra being used to identify complex organic structures.\textsuperscript{1}

An alkaloid isolated from the custard apple tree was assigned the structure 1 and christened with the name samoquasine A.\textsuperscript{2} Two years later, the authors determined that samoquasine A was actually identical to perlolidine 2.\textsuperscript{3} Independent synthesis of the compound with structure 1 showed that its properties were not identical to that of samoquasine A.\textsuperscript{4,5} The properties of perlolidine were then found to differ from that of samoquasine A,\textsuperscript{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 Wipf decided to compute the $^{13}$C 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.

Source: http://comporgchem.com/blog/?p=108