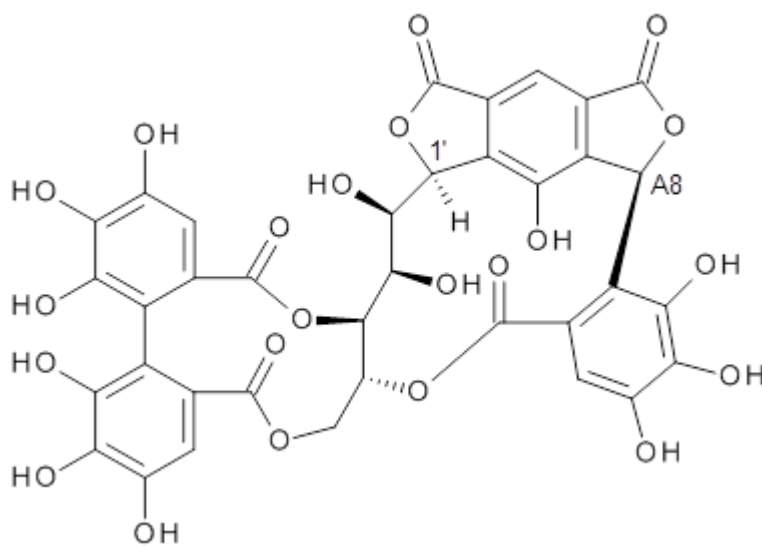


# STRUCTURE DETERMINATION: QUERCUSNIN A

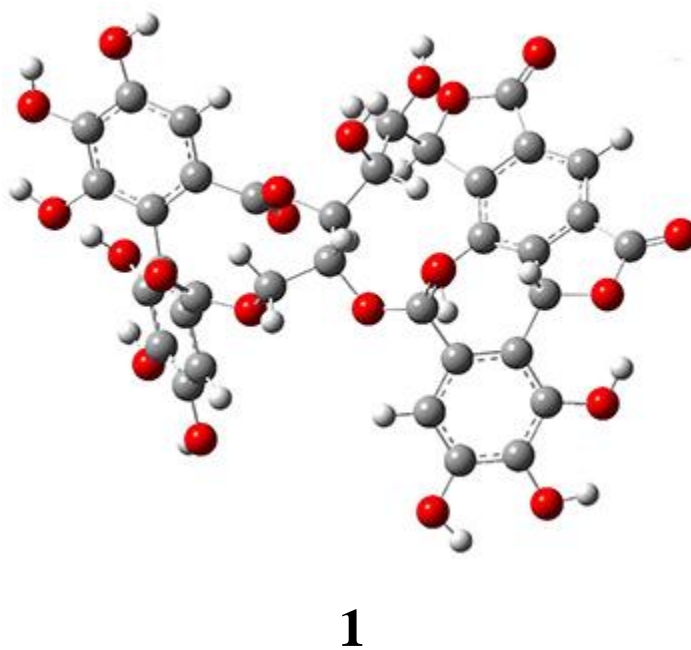
Here's another nice example of the use of computed NMR spectra to aid in structure identification. Quercusnin A was identified in an extract of dried sapwood from the oak tree *Quercus crispula*. The NMR spectrum along with structural comparison to the previously determined extract vescalagin, led the authors to the structure **1**.<sup>1</sup>



**1**

To aid in determining the absolute stereochemistry as centers 1' and A8, the authors employed a computational approach. Conformers of the four diastereomers (*RR*, *RS*, *SR*, *SS*) were optimized first with molecular mechanics, then the low energy conformers were reoptimized at AM1, and then finally all of the

conformers within 6 kcal mol<sup>-1</sup> of the lowest energy structure were reoptimized at PCM(acetone)/B3LYP/6-31G(d,p). The <sup>1</sup>H and <sup>13</sup>C NMR chemical shifts for all of the structures that contribute greater than 1% to the Boltzmann population were computed at PCM(acetone)mPW1PW91/6-311+G(2d,p)//B3LYP/6-31G(d,p). The DP4 probability (see this post) identified the (1'S,A8R) isomer with 100% probability for matching up with the experimental NMR spectrum. Additionally, the computed ECD spectrum matches nicely with the experimental spectra for this same stereoisomer. The lowest energy conformer of **1** is shown in Figure 1.



**Figure 1.** PCM(acetone)/B3LYP/6-31G(d,p) structure of the lowest energy conformer of **1**.

Source: <http://comporgchem.com/blog/?p=3042>