According to the review [1], around 1000 articles were published between 1990 and 2004 where originally determined structures were revised. The labor and other expenses used in structural misassignments and subsequent reassignments are thus roughly double the cost of getting the right answer at the start.

It has been shown [2,3] that application of modern Computer-Aided Structure Elucidation (CASE) systems [4] can usually help the chemist to avoid initial errors in structure identification. If nevertheless the researcher begins down the wrong track, the expert system can give a signal of caution. This is possible because molecular structure elucidation can be formally described as deducing all logical corollaries – without exclusions - from a system of statements (“axioms”) which ultimately form a particular axiomatic theory related to a current spectrum-structural problem [4]. These corollaries constitute all conceivable structures that meet the initial system of axioms. When structure elucidation of a new chemical compound is performed with assistance of expert systems, all axioms are expressed explicitly. Therefore it becomes possible to investigate dependence of the solution of a structural problem on any change in the initial data.

However, in many publications, the structure revision is performed on the basis of total chemical synthesis. Often, to disprove a wrong structure and confirm a new structural hypothesis, both structures – original and revised, at the least – are synthesized by researchers. Computational experiments with the aid of expert system ACD/Structure Elucidator Suite lead to the following conclusions: if the 1D and 2D NMR data used by a researcher for inferring an original (wrong) structure were entered into the CASE system, then most frequently the correct (revised) structure would be assigned as the most probable, while the wrong one would be rejected by the program.

As an example, we discuss a recently performed acremolin structure revision by total synthesis (Januar and Molinski [1]). The original (incorrect) structure was deduced by Julianti et al [2] from 1D and 2D NMR spectra. Januar and Molinski hypothesized the revised structure of acremolin and synthesized it in five steps. 1D and 2D NMR spectra of the product of synthesis coincided with those obtained for acremolin. A competing regioisomer structure whose possibility was also considered in [1] was rejected on the basis of $^1$H-$^{15}$N HMBC spectrum.

We posed two questions. First, which structures would be delivered by CASE if it were used from the very beginning? The initial NMR data ($^1$H, $^{13}$C and $^1$H-$^{13}$C HMBC) from [6] were entered into the program and the problem was solved in fully automatic mode. The resulting structural file contained all three structures – original, revised and the competing regioisomer. $^{13}$C chemical shift prediction
reliably selected the correct structure as the best and rejected both wrong ones – original and the competing regioisomer.

The second question was which structures can be generated from all theoretically possible $^1$H-$^{13}$C HMBC correlations corresponding to the original structure? The program instantly (0.06 s) produced four structures and reliably ranked them in the following order: revised structure and tautomer, original structure, competing regioisomer. The erroneous hypothesis was immediately called into question, and that arduous total synthesis becomes unnecessary.

Though the classic dictum “synthesis is the ultimate proof of structure” remains valid, it should be enhanced: before starting total synthesis for structure revision it is very desirable to take into account results delivered by a CASE system.