Oral Presentation

The Analysis of Essential Oils and Related Natural Products: Avoiding the Pitfalls

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Research in natural product chemistry often starts with an identification task. Until the early sixties, this was frequently achieved by isolating a quantity of pure substance, which was then converted by a variety of degradation and derivatization reactions into more readily analyzable molecules. These, or crystallized derivatives, could in turn be identified by comparison with known ones, e.g. with the help of elemental analysis and melting points . Today, a battery of advanced nondestructive spectroscopic methods exists for the expeditious assignment of structures to highly complex molecules isolated from nature in milligram or sub-milligram quantities. In the domain of flavour and fragrance related substances, this is mostly achieved by GC-MS, even though more sophisticated hyphenated techniques are becoming more popular. However, GC-MS in isolation practically always restricts identification to previously known substances. Misidentifications and gross errors are observed frequently when precautions are not taken to avoid biases or pitfalls generated by an excessive confidence in the data generated by this powerful instrumentation. Such drawbacks apply to both qualitative and quantitative analysis. Examples and strategies to avoid their occurrence will be presented.

As in the old days, the identification of new components in a natural mixture (either essential oil or solvent extract) still requires today the isolation of a sufficient amount of pure substance, and then to submit it to standard spectroscopic analysis in order to determine the molecular structure, ideally including absolute configuration. Among the many preparative separations which can be used, some techniques have sadly been abandoned or neglected over the years; such methods include high efficiency fractional distillation and preparative GC. The benefits of rejuvenating such techniques will be discussed, with examples.