What can we learn from the ultra-high resolving power of comprehensive two-dimensional gas chromatography for essential oil analysis?

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In the two decades that comprehensive two-dimensional gas chromatography (GCxGC) has been available, we have learned much about the operation of GCxGC, and the different separations that can be achieved for various sample types with different coupled column phases; it seems that every study reveals new knowledge about samples. The opportunity provided by GCxGC methods cannot be overstated. It is simply a matter of taking full advantage of this opportunity. The role of MDGC and GCxGC to provide very high separation power (1) is well recognised, but as pointed out in this reference, it is more than just good separations. There is a real underlying value that access to much greater resolution provides, but also in the manner of the 2D separations that are demonstrated. For instance, a chiral column as ^{1}D generates peaks for chiral components that adopt specific locations in 2D space (2). This helps identify compounds, but also allows much better – cleaner – separations of enantiomers, free from overlap. However, if enantiomer separation is not complete in ^{1}D, this can lead to difficulties in quantification of isomer abundances (3). We can use fast MDGC, or GCxGC with partial summation of modulated peaks for this problem, as described for terpinene-4-ol. The 2D space provides a fertile opportunity to relate peak position to the fundamental property of retention indices, and we have developed approaches to acquire *I* values in both dimensions (^{1}I and ^{2}I) of the experiment. This proved to be useful to assist in screening mass spectrometry data for saffron essential oil (4), giving better assurance of identification. The value of integrating MDGC with GCxGC is well demonstrated by using these methods for olfactometry. The latter method gives an overall profile of sample composition, whilst the former method allows target regions to be heart-cut to a long second column, with dual olfactometry and MS detection, suitable of odour-active compound detection. This has been used for coffee, wine, orange juice, banana liquor, and herb analysis (5). Finally, the discovery aspect of submitting essential oils, such as eucalypt or agarwood oils, to GCxGC-accTOFMS (6), provides a unique ability to ask critical questions about both minor and major components in the sample, and to consider both the source of such compounds in an oil, and also the increased secondary metabolite coverage which simply gives researchers an expanded pool of compounds upon which to draw conclusions. We are just starting to address the complexities that such an identification poses.

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