CHALLENGES IN DATA PROCESSING AND EVALUATION OF SCENT SAMPLES ANALYSED BY GC×GC-TOF

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THE AIM OF THIS STUDY

The aim of this contribution is to summarize the methods and procedures used in processing data obtained from the analyses of scent samples. The poster also demonstrates problems with the ChromaTOF software in processing raw data (version 5.51.06.0 and 5.55.41_BT by Leco).

DATA EVALUATION

Three types of approaches:

1) **DA_2DCHROM [3]** - automatic data alignment, anchor points → not successful on such dense data

2) **Kovats indexes** – 15 manually selected peaks as references in each chromatogram, retention indexes calculation for all other peaks
   → semi-automatic, not always successful, slightly subjective according to the person
   OUR CHOICE FOR MOST EXPERIMENTS

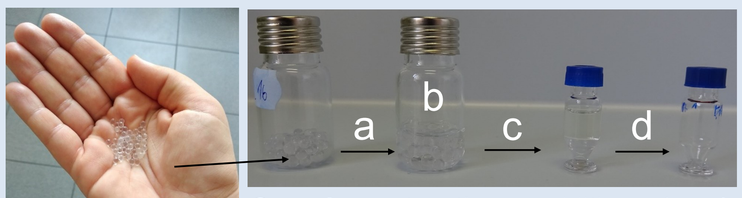
3) **Target peaks** – manually selected peaks (up to 300 per chromatogram)
   → successful, but very time-consuming, subjective
   USEFUL FOR CERTAIN EXPERIMENTS

CONCLUSIONS

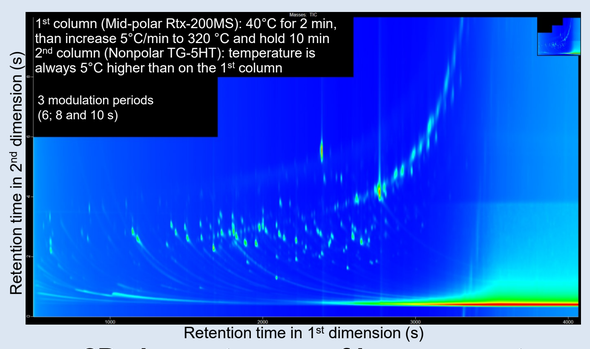
Data evaluation types 2 and 3 are unsuccessful for data acquired from the **BT-4D** GC×GC-MS. Evaluating repeatability when using a mixture of standards is not possible even when using the target approach (this could be done on a version for 4D-C type).

MATERIAL AND METHODS

According to the methodology [1], samples were collected from a volunteer palms using glass beads (3.6 mm; cleaned before sampling). Samples were then extracted into ethanol and evaporated. The extracts were dissolved in 70 µl of ethanol and analysed by comprehensive gas chromatography (GC×GC-MS, BT-4D, Leco). [2]



Sample extraction: addition 1 ml of ethanol (a), extraction (b), transferring the extract to a new vial (c) and evaporating. Steps a,b,c were repeated twice. Residue dissolving in 70 µl of ethanol (d).



2D chromatogram of human scent

DATA ERRORS (BY SOFTWARE)

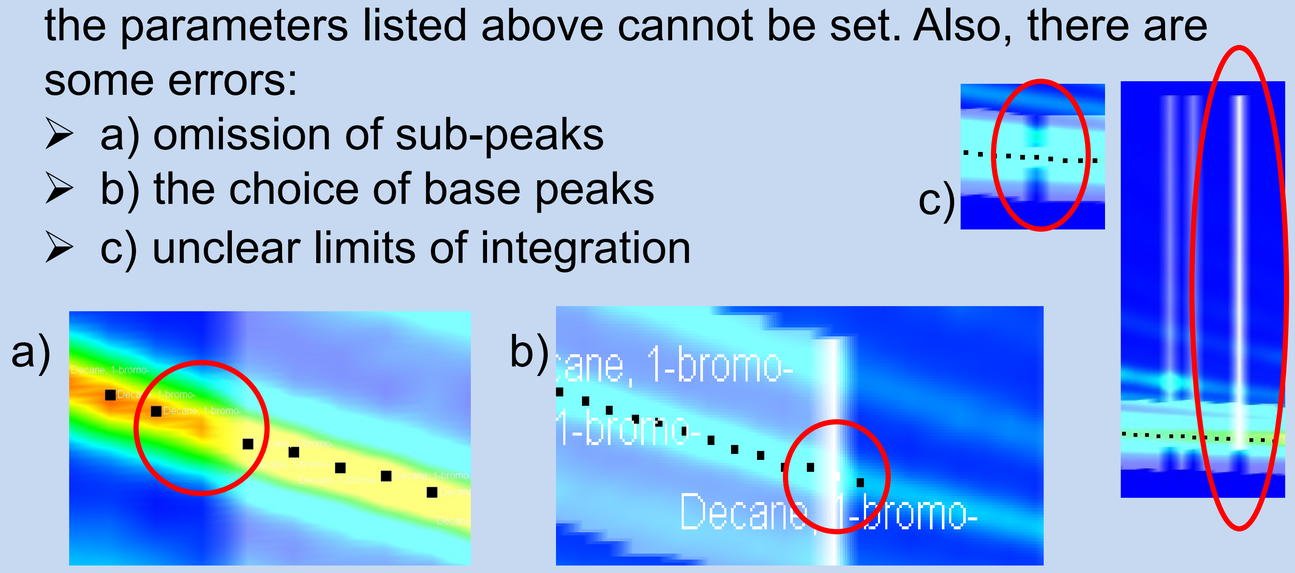
Data evaluation approaches are affected by the processing of raw data by ChromaTOF. In ChromaTOF version 4.72.0.0 (software version for GC×GC-MS, 4D-C, Leco), the user had more options to set parameters:

- min peak width;
- max retention time shift in the second dimension for sub-peak combination;
- the signal to noise ratio set before peak finding and integrate.

Also, after combining or un-combining of sub-peaks, the software does deconvolution again.

In newer ChromaTOF versions (5.51.06.0/5.55.41_BT for BT-4D), the parameters listed above cannot be set. Also, there are some errors:

- a) omission of sub-peaks
- b) the choice of base peaks
- c) unclear limits of integration



base peak is the 34th sub-peak

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