Title: Human odor and forensics. Optimization of a comprehensive two-dimensional gas chromatography method based on orthogonality: how not to choose between criteria.

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Human odor and forensics. Optimization of a comprehensive two-dimensional gas chromatography method based on orthogonality: how not to choose between criteria.

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Highlights:

- Comprehensive gas chromatography is relevant to analyze of human odor.
- 9 criteria were used to select an appropriate 2D analytical setup.
- Desirability functions were implemented to consider all criteria simultaneously.

Abstract:

The use of comprehensive two-dimensional gas chromatography coupled with mass spectrometry would be a real asset for the forensic profiling of human hand odor. This paper focuses on the optimization of a comprehensive gas chromatography method using a synthetic mixture of 80 compounds representative of human hand odor composition. In order to rank the candidate column sets, instead of using a unique criterion, we used a chemometric tool called desirability which is based on Derringer functions and enables to consider several criteria simultaneously and hence to get the best compromise. Nine criteria including six orthogonality criteria were used to evaluate the quality and the efficiency of the separation. The desirability analysis lead to a straightforward ranking and an accurate overview of the results in two situations, with an objective of routine analysis and without. In both cases, the DB-1MS×DB-1701 set was found to be best suited for the separation of the considered mixture, however with different gradients.

Keywords: