

Food Flavor Reproduction in Mass Spectral Space by Removing Odorless Compounds

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Food flavor consists of both odor and odorless compounds. Odorless compounds interfere with the analysis of odor reproduction recipes. In this study, odorless compounds were identified using gas chromatography (GC) data, followed by the mass spectrum synthesis without them. Then, the mass spectrum of each food sample was approximated with a small set of odor of odor-component mass spectra. Figure 1 shows the recipe generation method based on non-negative matrix factorization (NMF) and non-negative least squares (NNLS). Totally 20 food samples were used to extract 12 odor components. Table 1 shows the sensory evaluation results of approximated odors, indicating that removing odorless compounds from the dataset improves the accuracy of odor reproduction recipes.

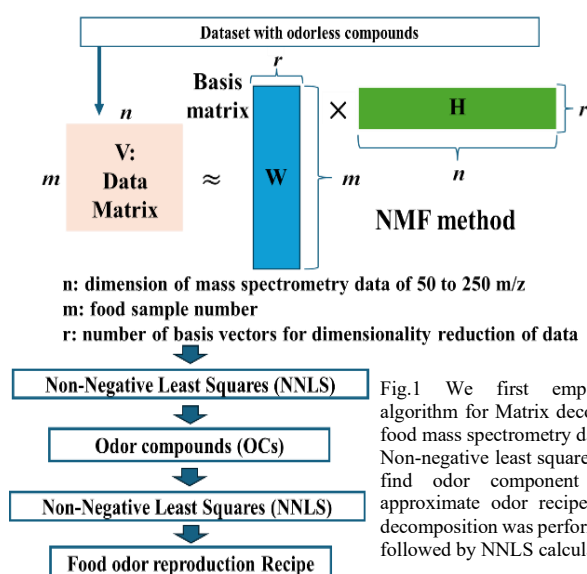


Table.1 Triangle test results(Comparison between datasets containing and excluding odorless compounds) Approximation is better if success rate is close to chance level (33%)

Triangle test Value : Success rate (odor approximation rate)			
$r=12$ (r is the number of odor components)	No.5 Walnut	No.6 Vanilla	No.15 milk
Previous method(with odorless)	80% (68%)	60% (63.5%)	50% (62%)
Improved method (without odorless)	30% (75.5%)	20% (74.3%)	80% (62.6%)

Fig.1 We first employed NMF algorithm for Matrix decomposition of food mass spectrometry data. Non-negative least squares was used to find odor component recipe and approximate odor recipe. The matrix decomposition was performed by NMF, followed by NNLS calculation.

References

1. Hanqing Zhao, Dani Prasetyawan, Takamichi Nakamoto, Exploration of Flavor Sample for Odor Reproduction In Mass Spectrum Space, IEEE Sensors 2024,6464.
2. Hanqing Zhao, Takamichi Nakamoto, Food-flavor Odor Reproduction in Mass Spectral Space Considering Odorless Compounds, IEEJ Sensor Symposium, 2025, L-331.
3. Hanqing Zhao, Takamichi Nakamoto, Food Flavor Reproduction in Mass Spectral Space with Reduced Interference from Odorless Compounds, ISOEN 2026