Odor reproduction of food samples

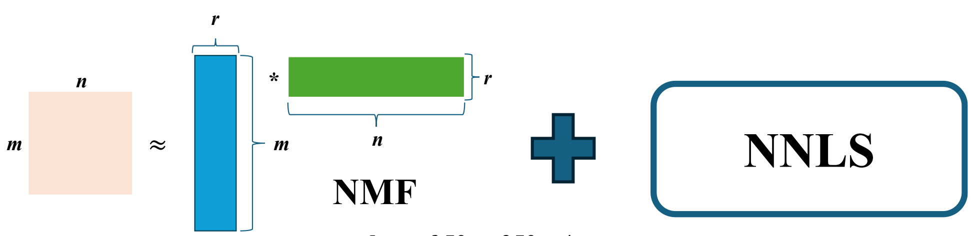
Sample Name	Sample Name	Sample Name	Sample Name
1. Acacia	26. Mushroom	51.Iodine	76.Peanuts
2. Aubepine	27. Hazelnut	52.Mercaptan	77.Coconut
3. Sweet Brier	28. Walnut	53.Sulfur	78.Chocolate
4. Geranium	29. Truffle	54.Vinegar	79.Cocoa
5. Peony	30. Anise	55.kyoho grapes	80.azuki bean
6. Rose	31. Cinnamon	56.Apricot	81.green tea
7. Linden	32. Clove	57.Kiwi fruit	82.black tea
8. Violet	33. Mint	58.Guava	83.Oolong Tea
9. Apricot	34. Pepper	59.Cherry	84.Matcha
10. Pineapple	35. Licorice	60.white peach	85.Cola
11. Banana	36. Thyme	61.Peach	86.Cider
12. Cassis	37. Oak	62.passion fruit	87.Cranberry
13. Cherry	38. Hay Cut	63.Mango	88.Lime
14. Lemon	39.Fern	64.Chestnut	89.Citrus sudachi
15. Quince	40.Pine	65.La France pear	90.Citrus sphaerocarpa
16. Strawberry	41.Vanilla	66.Melon	91.Baked sweet potato
17. Raspberry	42.Butter	67.Raspberry	92.Perilla
18. Muscat	43.Caramel	68.Framboise	93.Brandy
19. Orange	44.Honey	69.Lychee	94.Whisky
20. Pear	45.Green Pepper	70.Milk	95.Ginjo sake
21. Apple	46.Civet	71.Cheese	96.Rum
22. Plum	47.Musk	72.Yogurt	97.Prunus mume
23. Bitter Almond	48.Cork	73.fresh cream	98.cherry blossom
24. Cacao	49.Smoked	74.condensed milk	99.Honey
25. Coffee	50.Tar	75.almond	100.brown sugar

Fig.1 food flavor list

Food odors are a familiar part of our daily lives. In this study, we reproduced food odors using an MS(Mass spectrometry) dataset consisting of 100 food-flavor samples (Figure 1). The recipe analysis method used in this process is illustrated in Figure 2. By applying NMF, we obtained reconstructed MS data, and the approximated data were then used to analyze and explore recipes of odor components for odor reproduction.

Figure 3 presents an example of the original MS data, while Figure 4 shows the approximate MS data reconstructed using 20 odor components, successfully preserving the major informative peaks. Table 1 summarizes the correlation coefficients between the original and reconstructed MS data when using different numbers of odor components [1].

Figure 5 explores the odorless compounds present in food odors and how their interference with food-odor reproduction can be removed[2].



n: mass spectrometry data of 50 to 250 m/z
m: each food sample number
r: the number of basis vectors for dimensionality reduction of data

Fig.2 Non-negative least squares (NNLS) was used to find odor component recipes and approximate odor recipes. The matrix decomposition was performed by Non-negative Matrix Factorization (NMF), followed by NNLS calculation

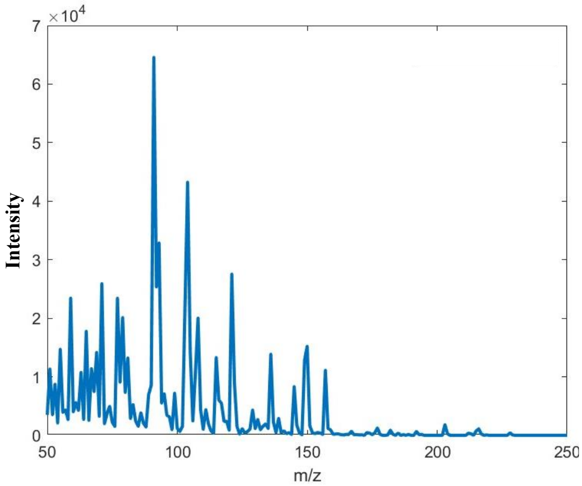


Fig.3.Example of food odor mass spectrometry data (Acacia)

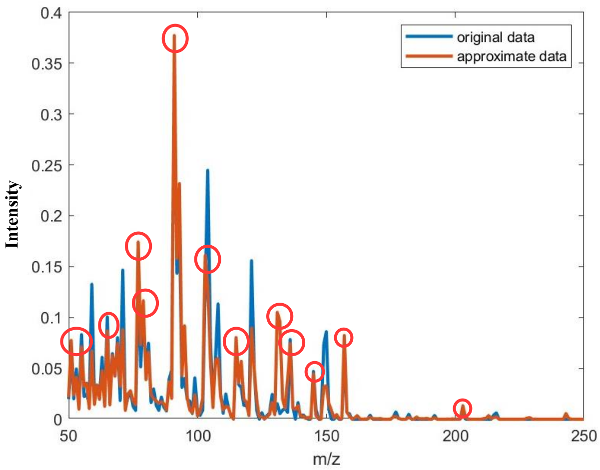


Fig.4. Example of sample fitting results for base vector when r=20. (Sample name: Acacia, category is flower)

Table.1. Evaluation of correlation coefficients from 10 to 100 basis vectors r (r : number of odor components)

r	10	20	30	40	50	60	70	80	90	100
NMF cc	0.83	0.899	0.93	0.96	0.97	0.98	0.98	0.99	0.99	0.99
NNLS cc	0.83	0.89	0.92	0.94	0.96	0.97	0.97	0.98	0.98	0.98

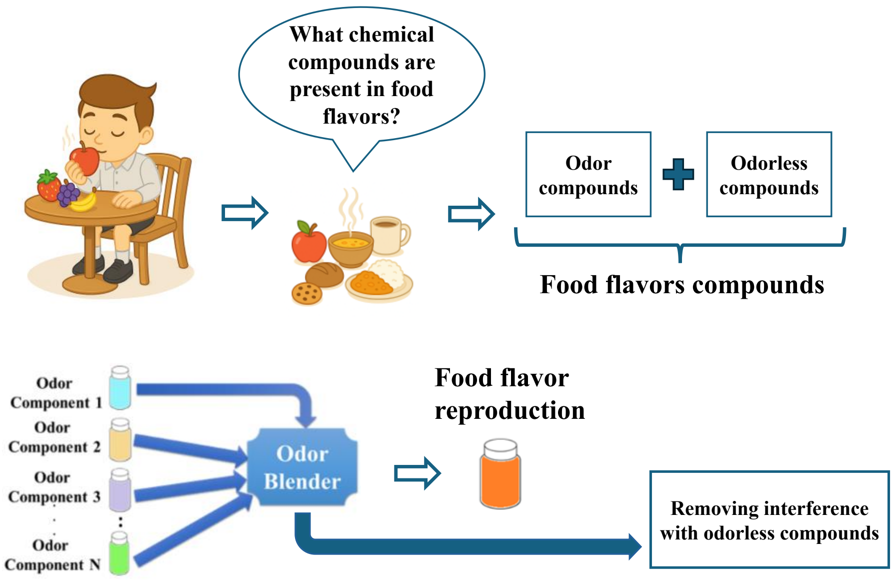


Fig.5. Analysis of interference from odorless compounds in food odor reproduction

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.