Predicting Odor Mixture Character from Chemical Structure

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Most smells, whether in food, perfume, or the environment, are complex mixtures of many odor molecules. A principled framework for modeling natural mixtures has been considered intractable because mixtures are widely assumed to generate nonlinear perceptual interactions that mirror nonlinear responses at the receptor and neural levels. We quantified perceptual interactions across 432 mixtures composed of 144 component odorants using a trained human panel, and nearly all mixtures were explained by a linear average of their component quality profiles. Within this linear modeling framework, averaging component profiles predicted mixture perception significantly better than the previous state-of-the-art and approached the ceiling set by measurement noise. Even mixtures previously reported to exhibit emergence were equally well predicted. Finally, to test how well linear models can reproduce complex food percepts we collected descriptive ratings for 24 foods alongside their published Sensomics-based reconstructions (GC-MS analysis followed by sensory testing). For 18 of 24 foods, mixtures designed by the linear model matched the aroma of the target food more closely than the Sensomics reconstructions. These results demonstrate that odor components combine predictably to reproduce complex food aromas, extending the validity of linear mixture models from simple laboratory mixtures to real food systems. Just as additive color mixing enabled colorimetry, linear mixing in olfaction opens the door to quantitative odorimetry, allowing mixtures to be predicted, reconstructed, and optimized computationally.