Extraction of pure odor

A method utilizing Independent Component Analysis (ICA) to extract pure odor separated from interference by unwanted compounds. As an example, extraction of pure odor data separated from preservatives (fixatives) which can cause contradiction in odorant analysis.
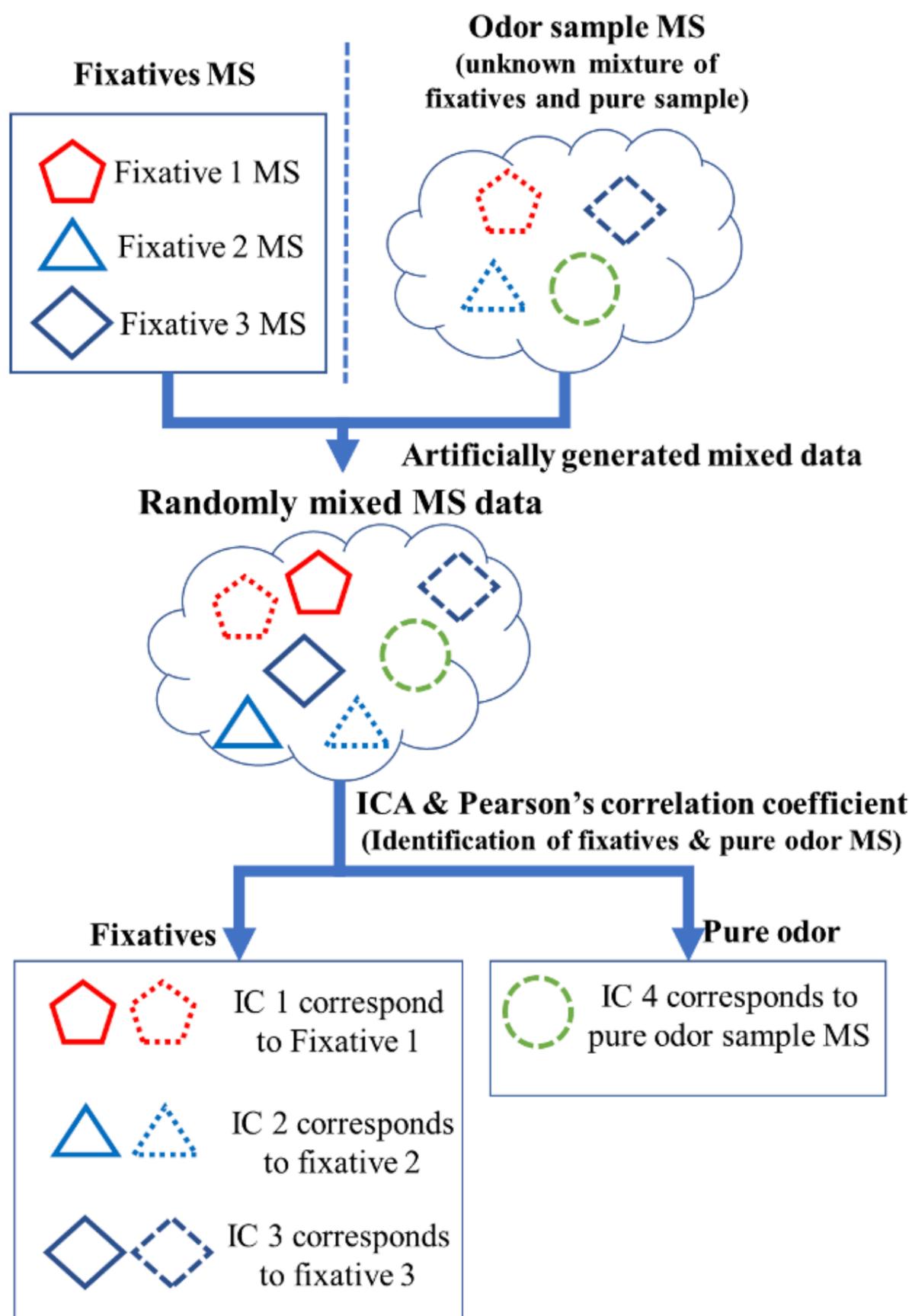

Figure 1.   Illustration of the extraction of pure odor using ICA in the study.

The procedure of the study is:

1. Gathering mass spectrum of odor sample.
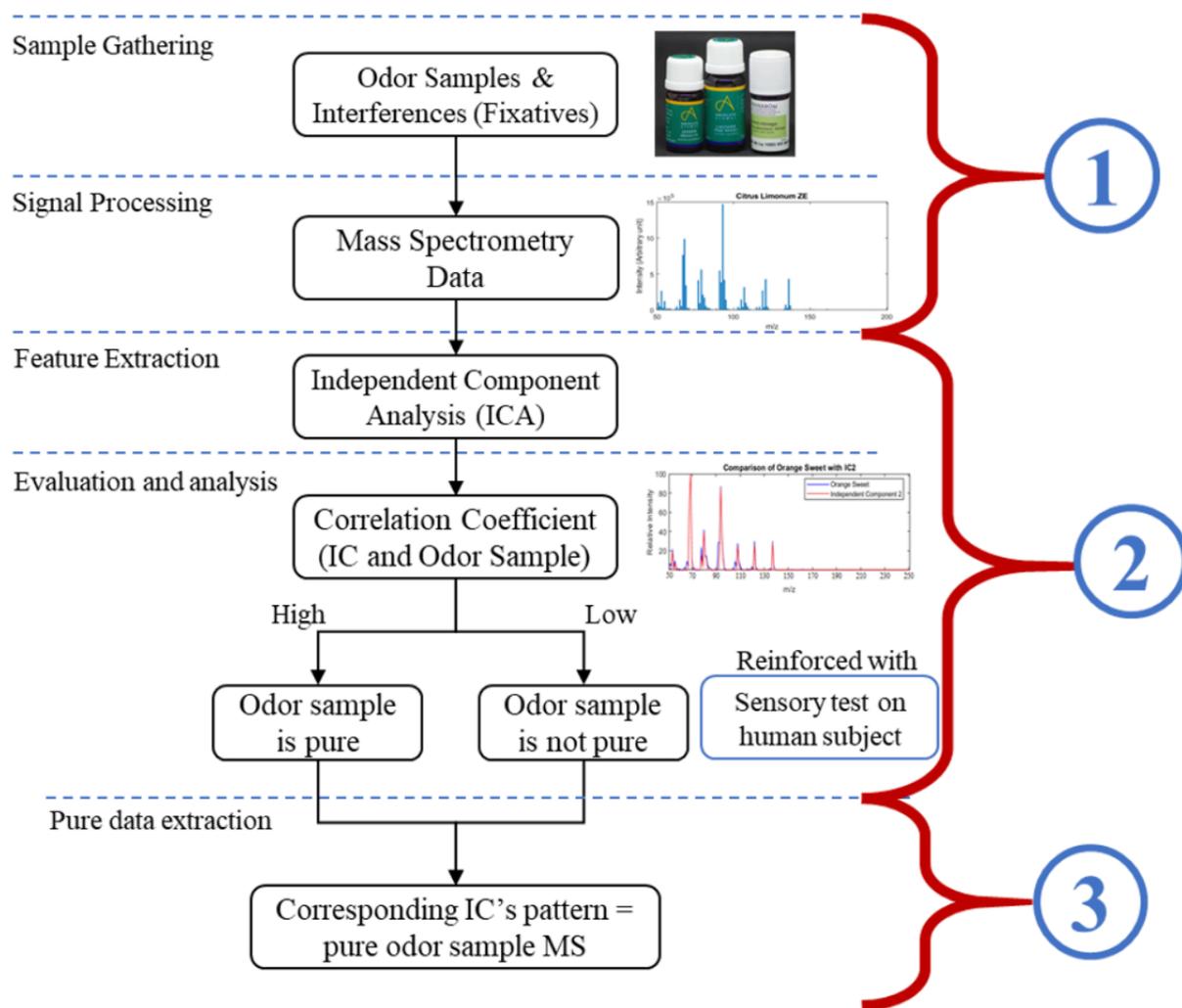2. Analyze using ICA.
3. Extract the pure odor.

Figure 2. The procedure of the study.

Basically, ICA cannot identify the independent components in order. Thus, we applied Pearson's correlation coefficient to identify each IC. Example of identification is shown below. We demonstrated that ICA allows extracting independent components corresponding to the pure original odor regardless of the presence of interferences with high correlation in the mass spectrum space.

Table 1. The correlation coefficient between original data and independent components (ICs) for orange sweet odor sample.
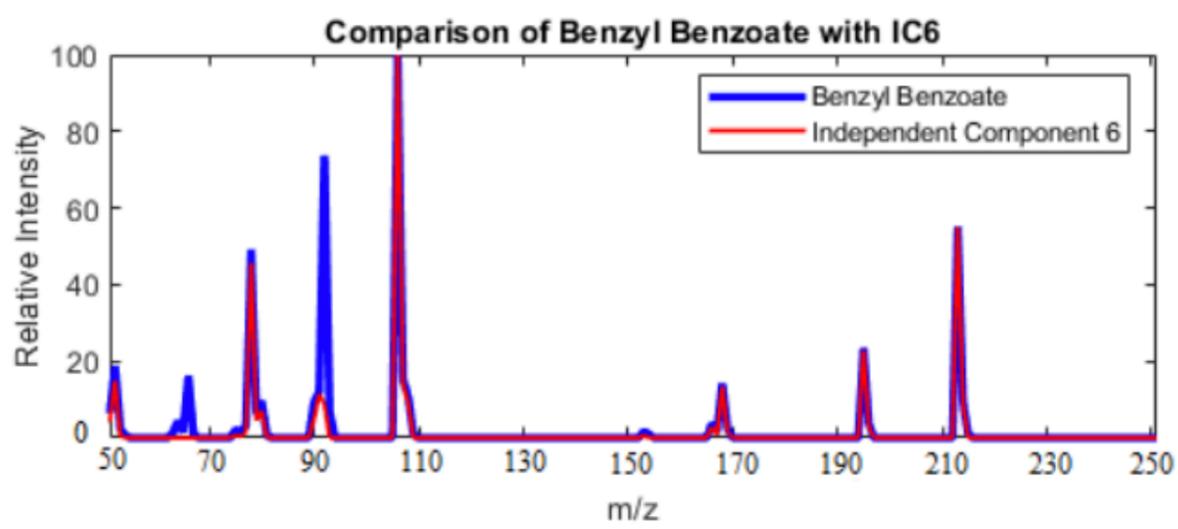
	IC 1	IC 2	IC 3	IC 4	IC 5	IC6
Orange sweet	0.19	0.98	0	0.01	0	0.07
Benzyl benzoate	0.51	0.01	0	0.01	0.01	0.86
Benzyl salicylate	0.99	0.03	0	0.01	0.01	0.06
Propylene glycol	0	0	0.1	0.99	0.05	0
Dipropylene glycol	0	0.01	0.99	0.02	0.03	0
Octanoic acid	0.01	0.01	0.02	0.1	0.99	0.01

Independent components

(a)

Comparison of Orange Sweet with IC2

(b)

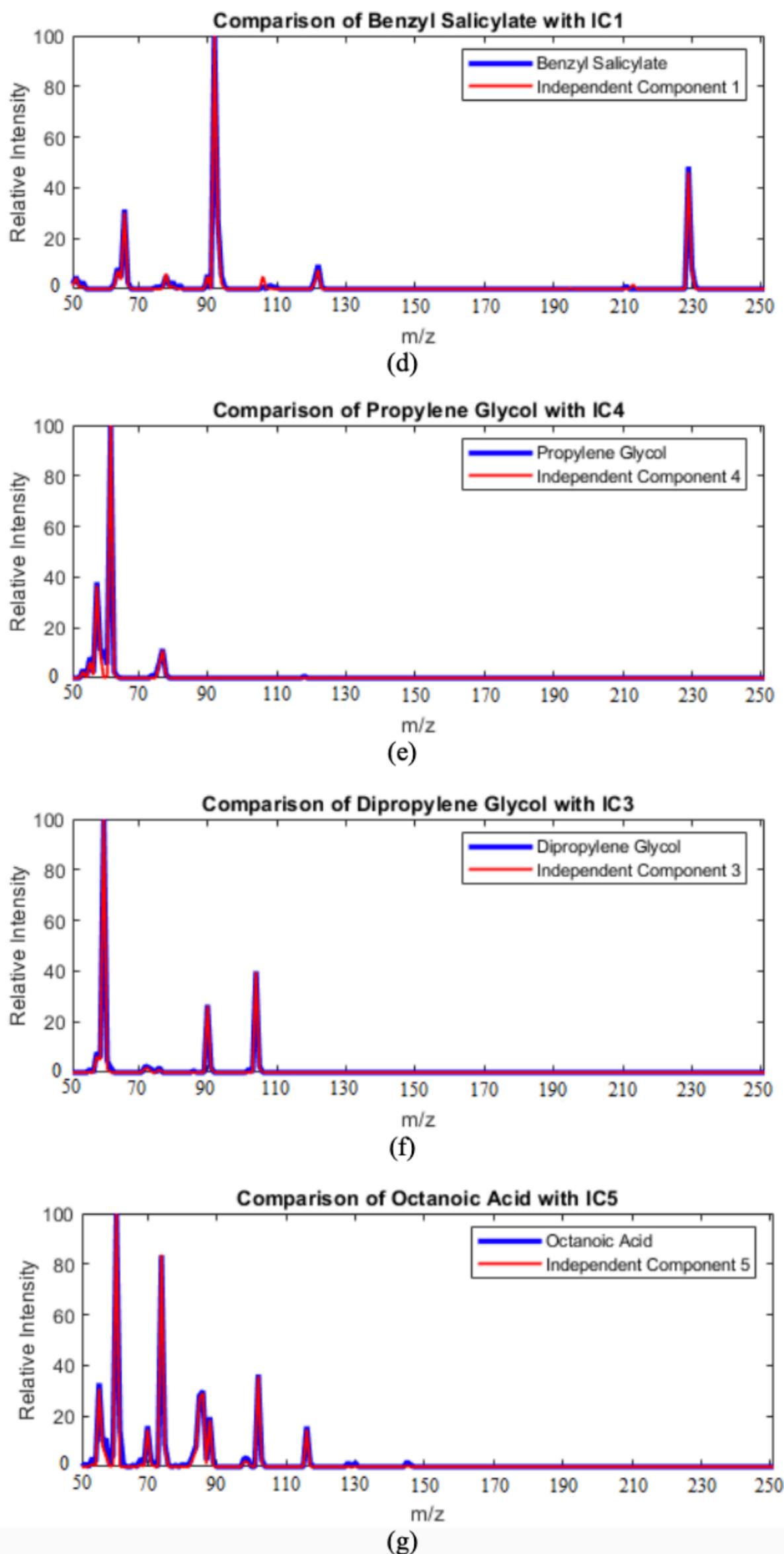

Comparison of Benzyl Benzoate with IC6
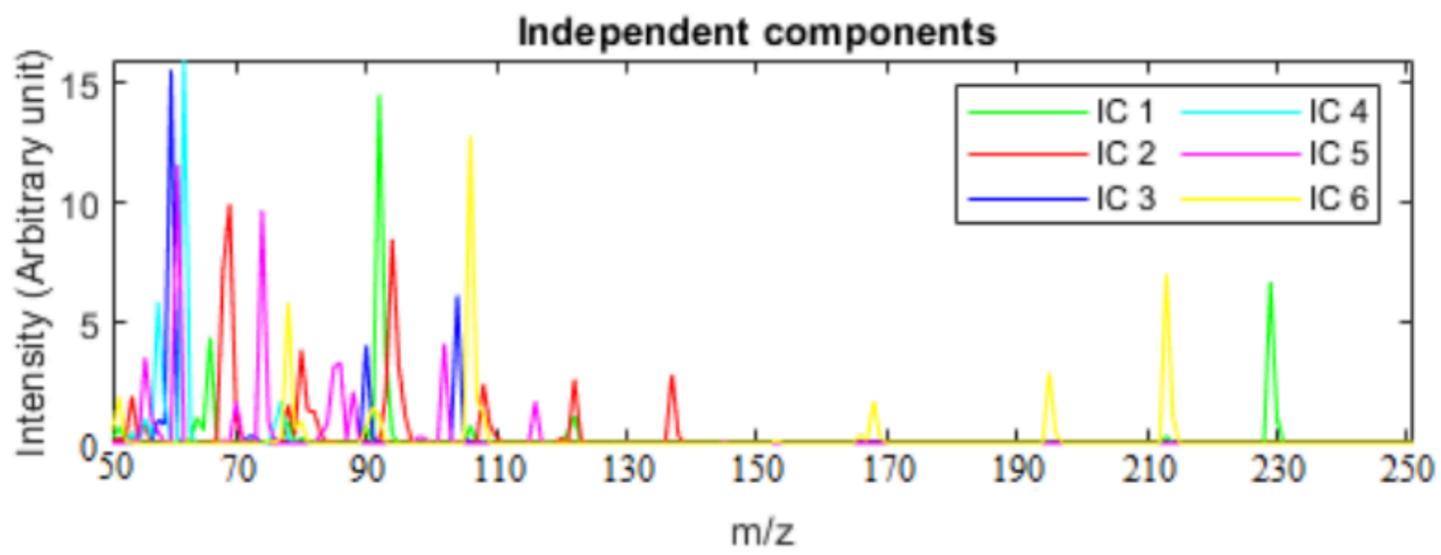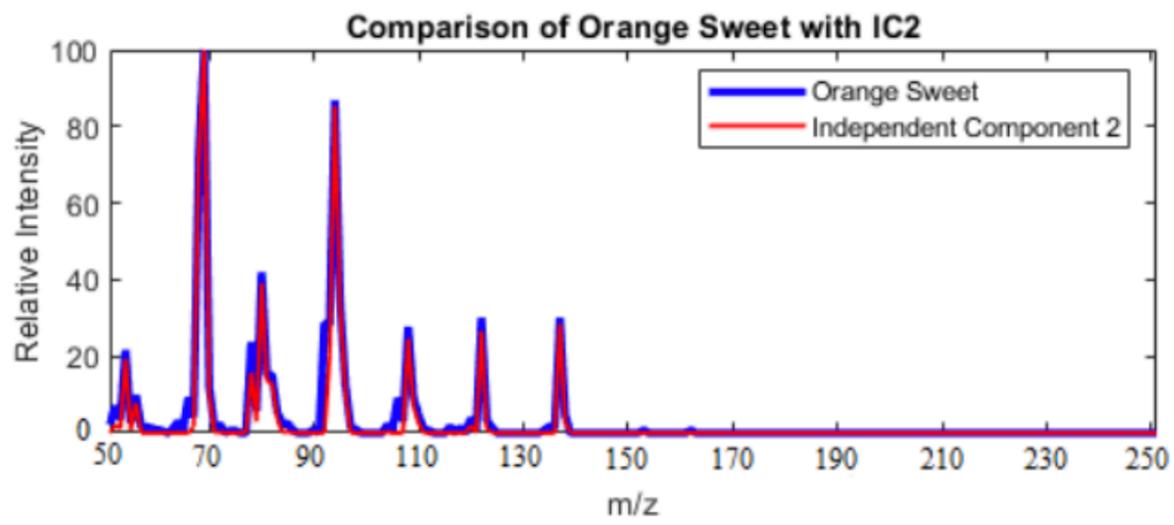
(c)

Figure 3. Mass spectra of independent components with their corresponding original data. (a) independent components obtained through ICA, (b) orange sweet with IC 2, (c) benzyl benzoate with IC 6, (d) benzyl salicylate with IC 1, (e) propylene glycol with IC 4, (f) dipropylene glycol with IC 3, (g) octanoic acid with IC 5.