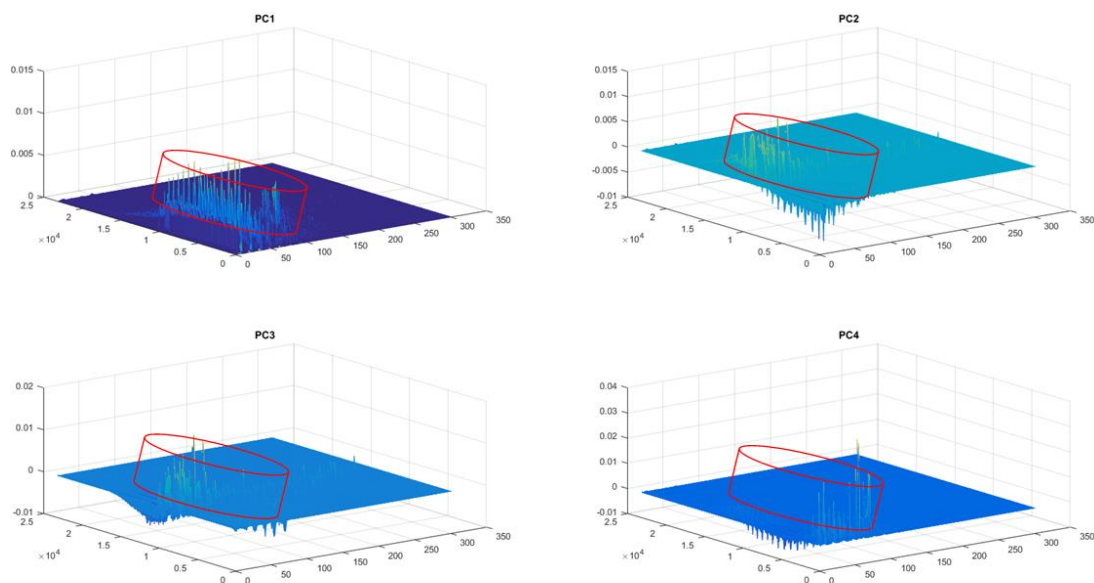Fig. 1   (Supporting information)

Figure S1. Principal components loadings for the first four principal components of the MPCA model. The red cylinder indicates those variables that have high loadings in these four principal components. These variables are those which are used for variable selection for the PARAFAC model.
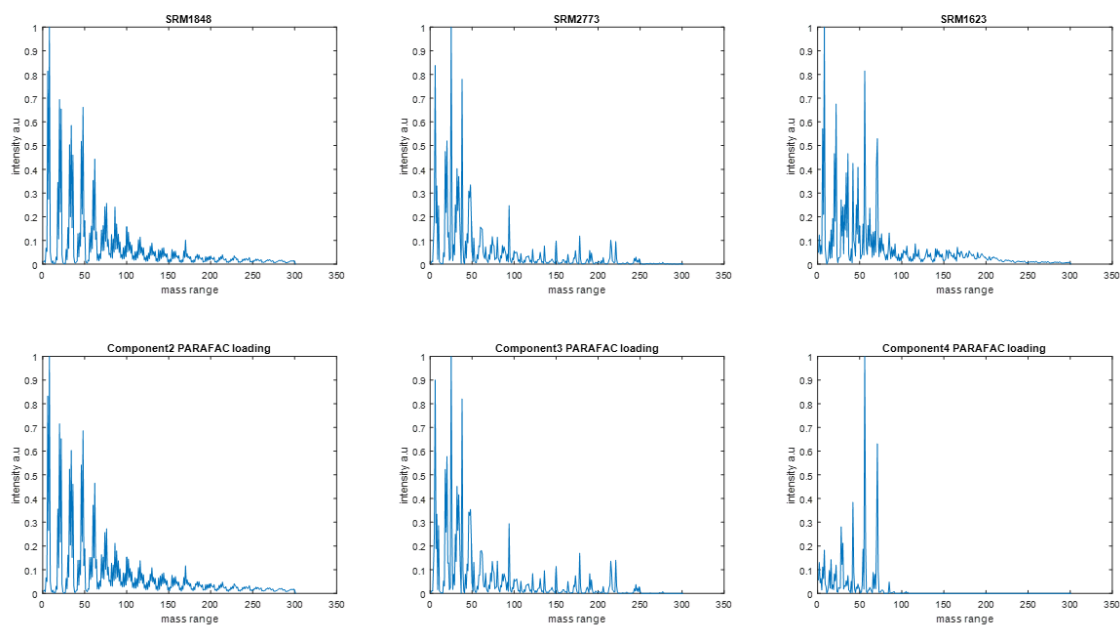
Fig. 2   (Supporting information)

Figure S2. Mass spectral loadings for the 2nd through 4th factors in the four-factor PARAFAC model compared with mass spectra for substances that are representative class members.

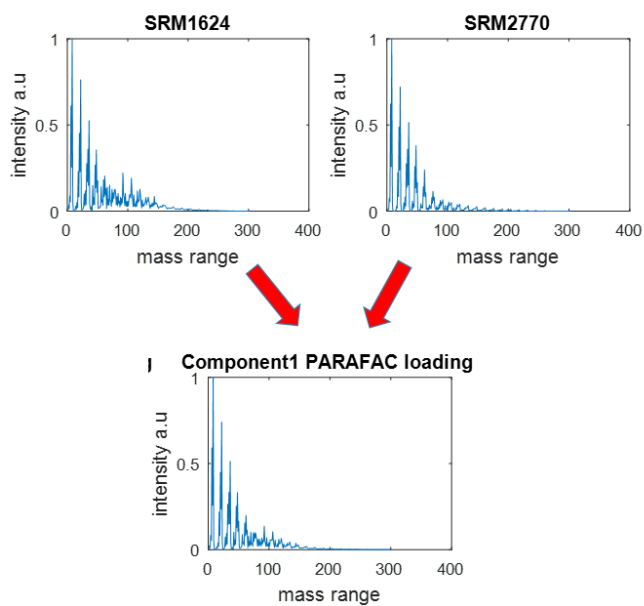Fig. 3   (Supporting information)

Figure S3. Mass spectral loadings for the first factor in the four-factor PARAFAC model compared with the total ion chromatograms for SRM 2770 and SRM 1624d.
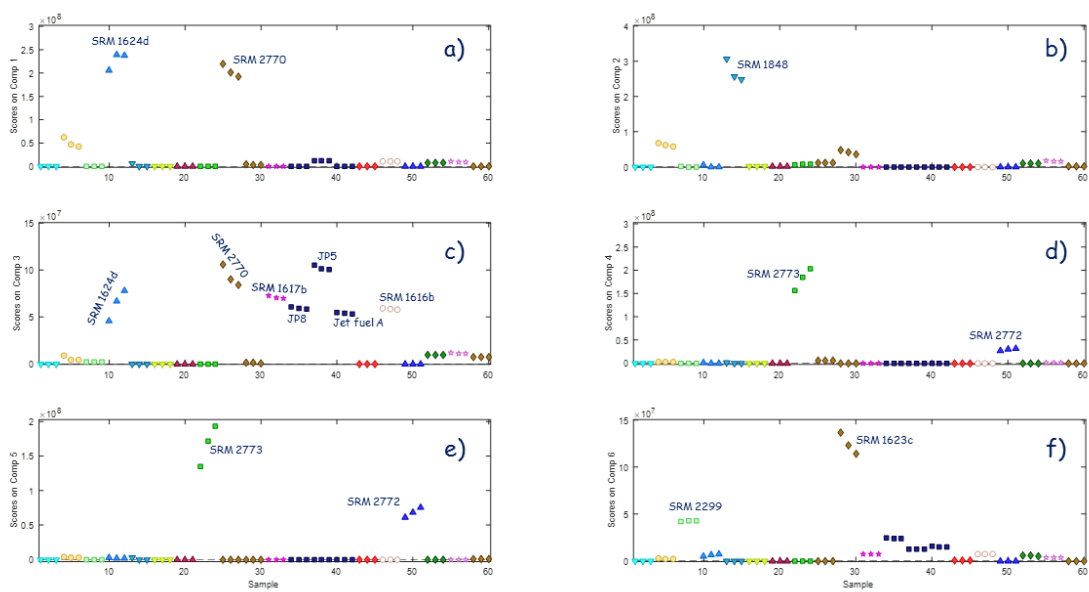
Fig. 4   (Supporting information)

Figure S4. PARAFAC scores for the all factors in the six-factor PARAFAC model.