

Figure S1. The calibration procedure used for visualization and quality control, including an overlay of all total ion chromatograms acquired before Rt. Calibration.

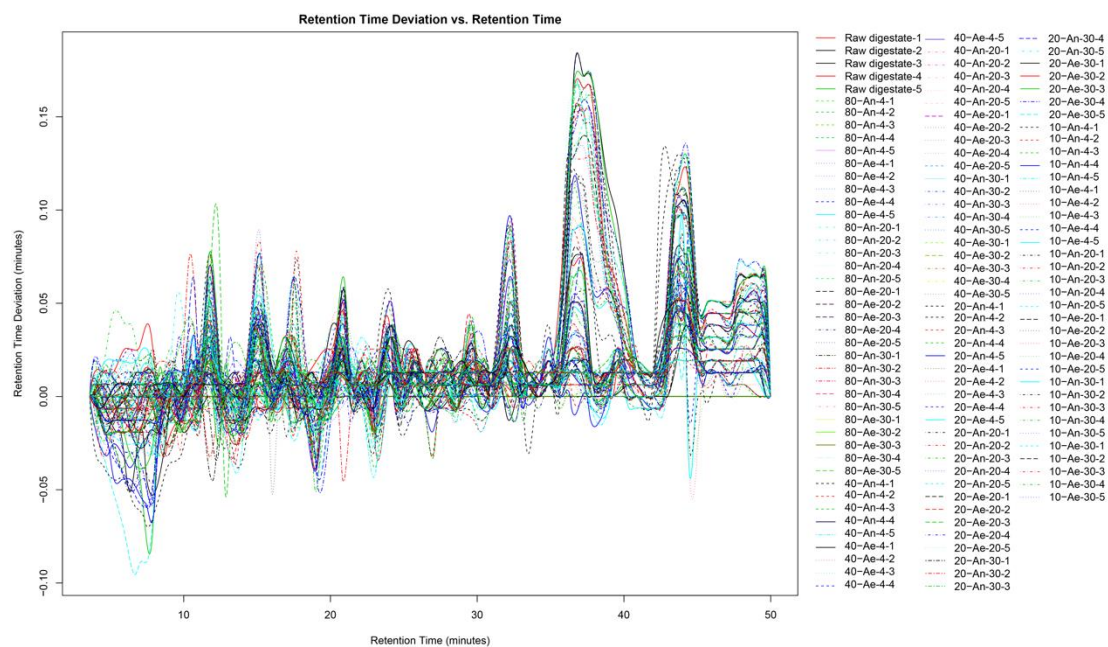


Figure S2. The calibration procedure used for visualization and quality control, including an overlay of all total ion chromatograms acquired after Rt. Calibration.

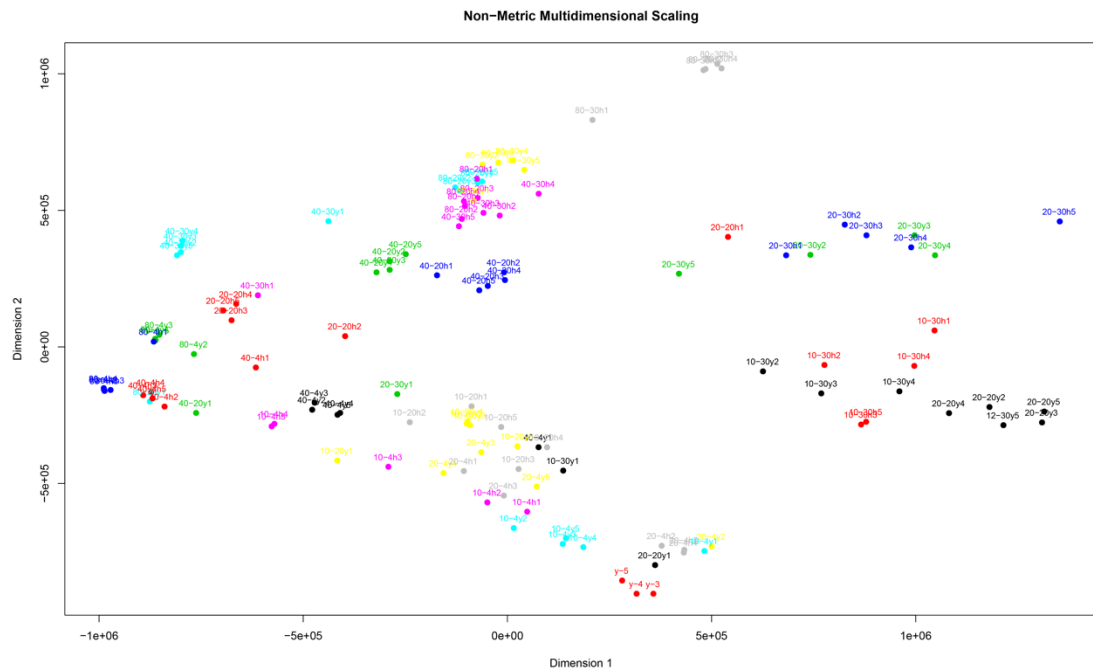


Figure S3. Non-Metric Multidimensional Scaling (NMDS) biplot.