

Experiment 166 data analysis protocol

Data analysis was performed using Find by Formula algorithm of the Agilent MassHunter Qualitative analysis software. Library for the analysis was constructed partially from the authentic standards and partially by creating “Known Unknowns” from mass spectral features consistently present in a large proportion of the samples. Molecular features were identified by Molecular Feature Extractor (Agilent MassHunter component) and processed using in-house software.