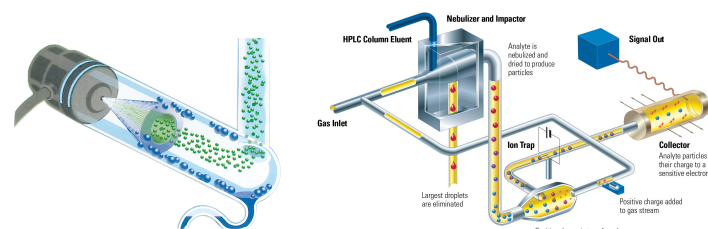
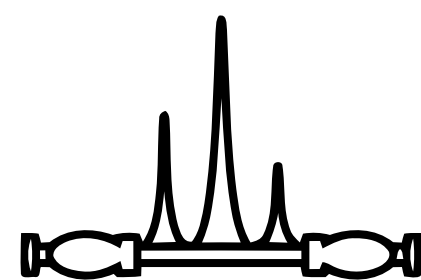
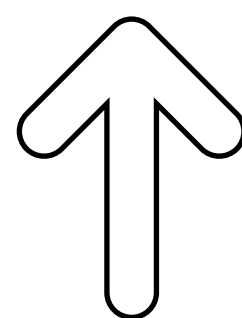


Input

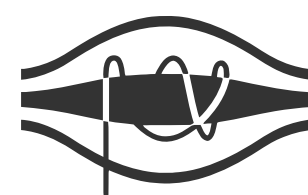
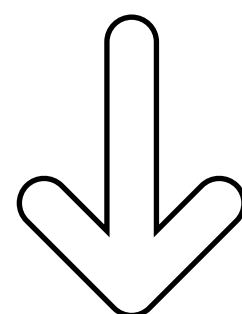
CAD



Universal detectors



Liquid chromatography

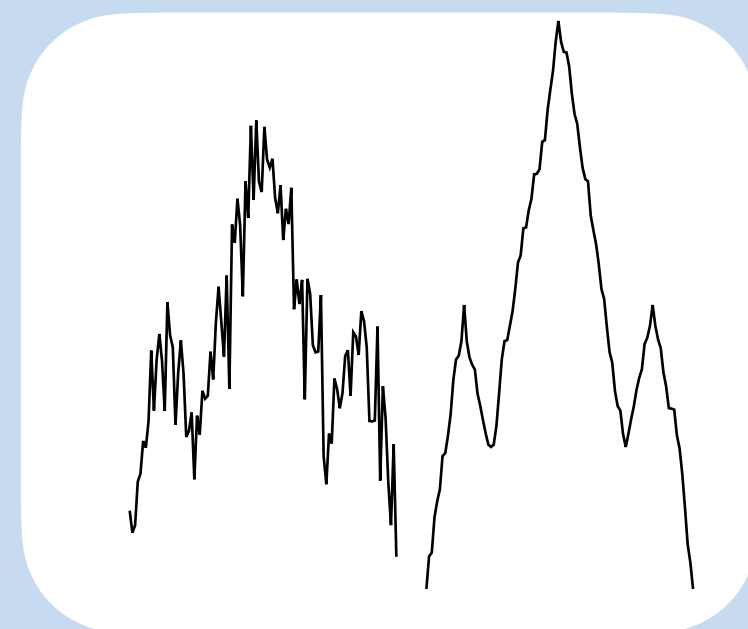


Mass spectrometry

MS

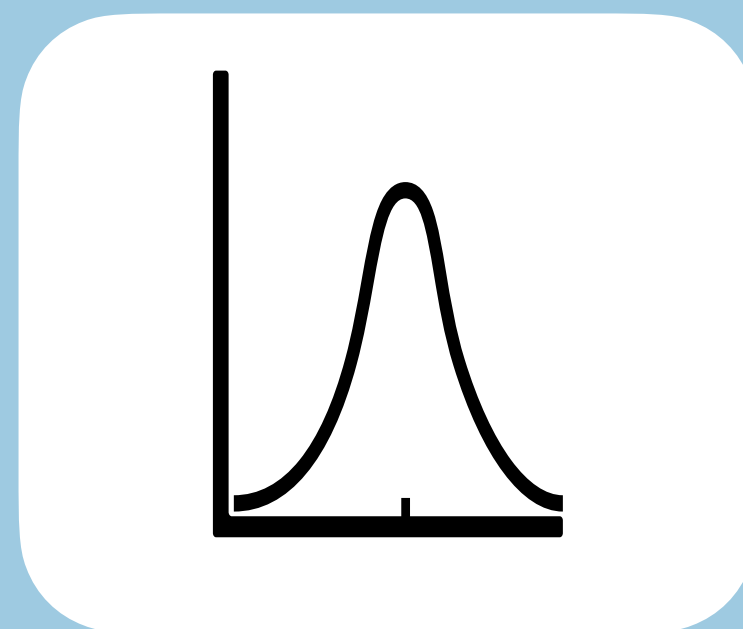
Process

Signal pre-processing



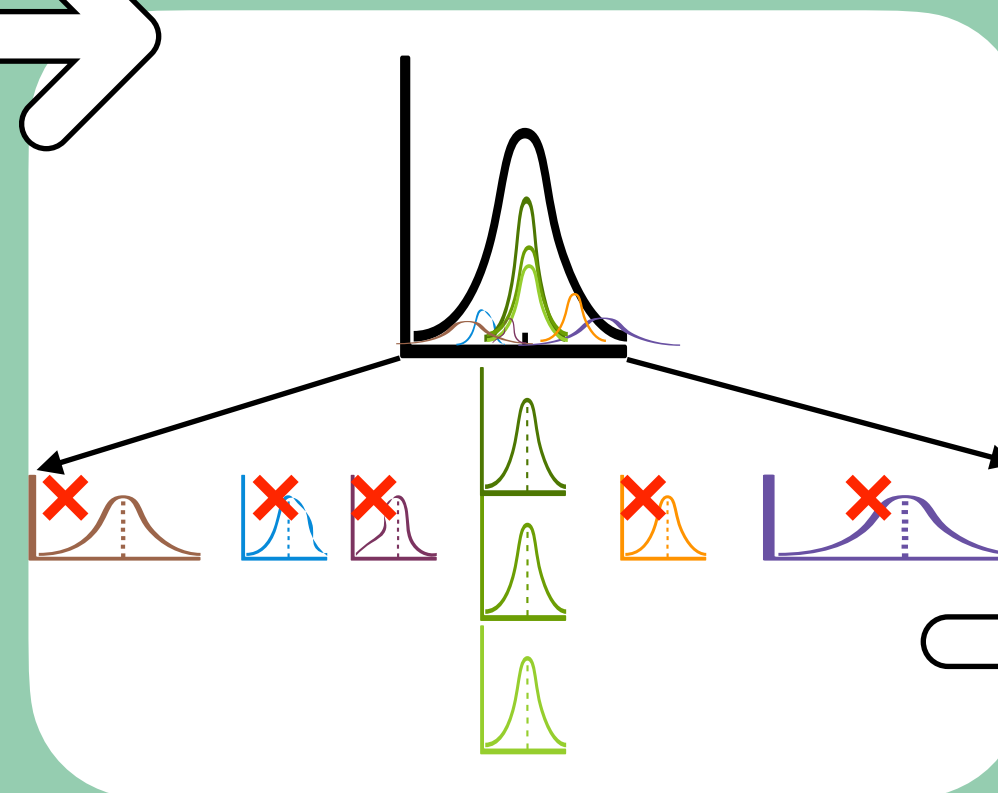
Detection improvement

Peaks extraction



Semi-quantitative integration

Peak-feature attribution

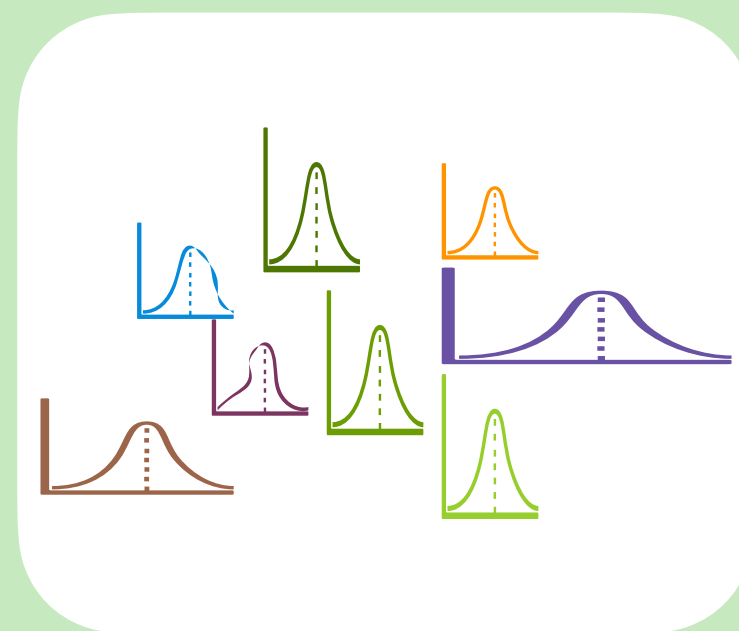


Peak shape similarity calculation

Combined qualitative and semi-quantitative information

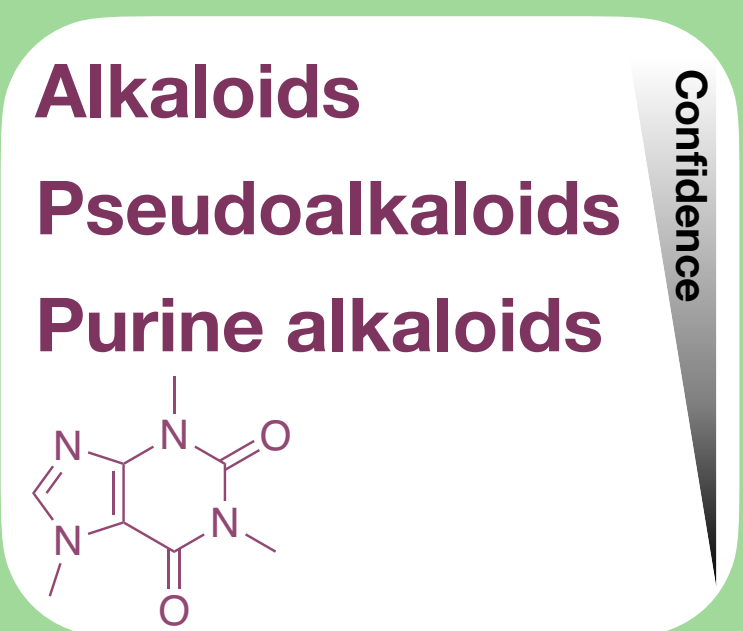
Knowledge based prioritization

Features extraction



Clustering and Ion Identity Networking

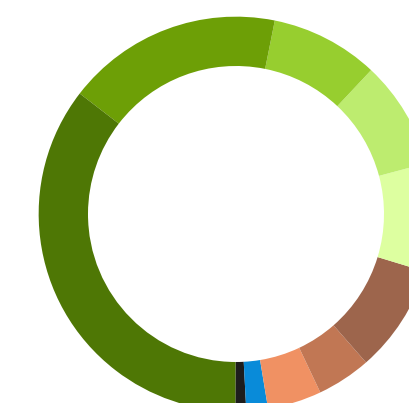
Features annotation



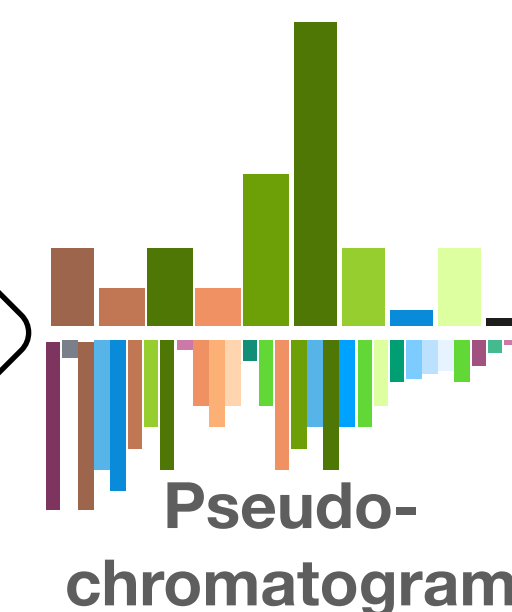
Confidence

Structural annotation and Compound class annotation

Output



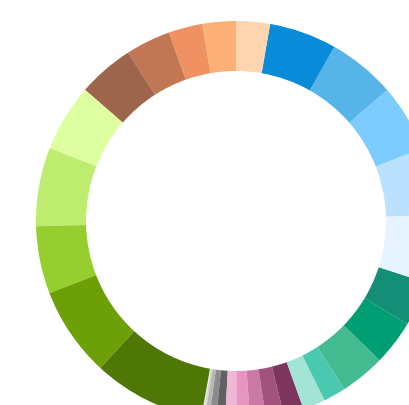
Major metabolome



Pseudo-chromatogram



Automated report



Minor metabolome