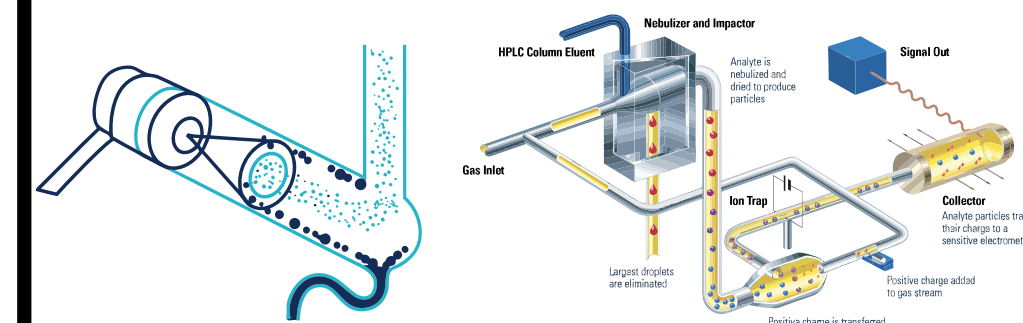
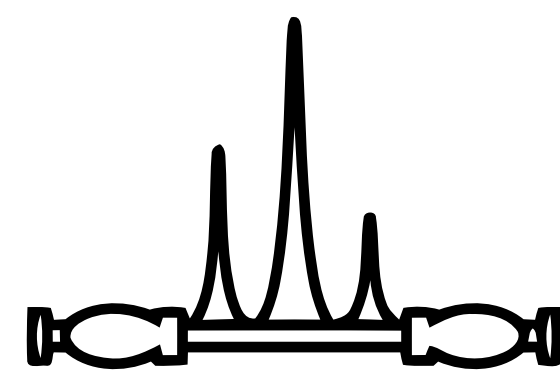
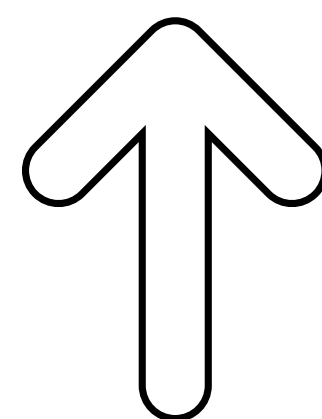


Input

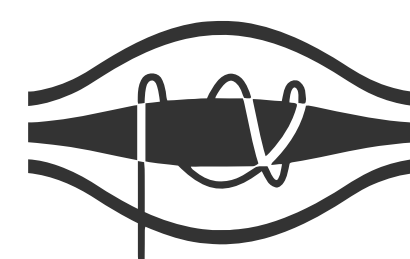
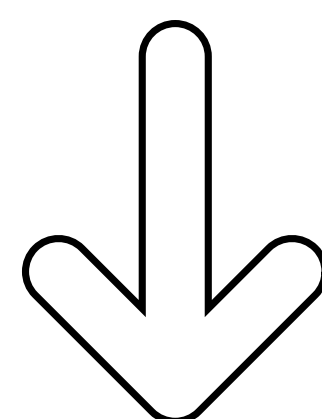
CAD



Universal detectors



Liquid chromatography

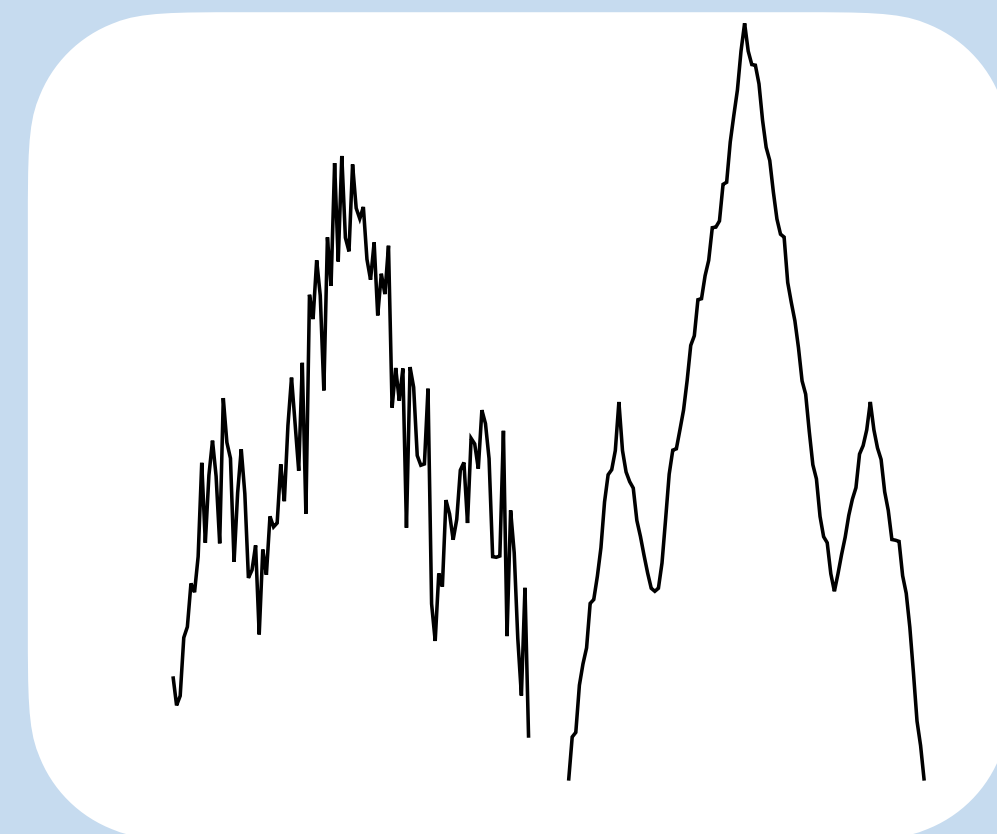


Mass spectrometry

MS

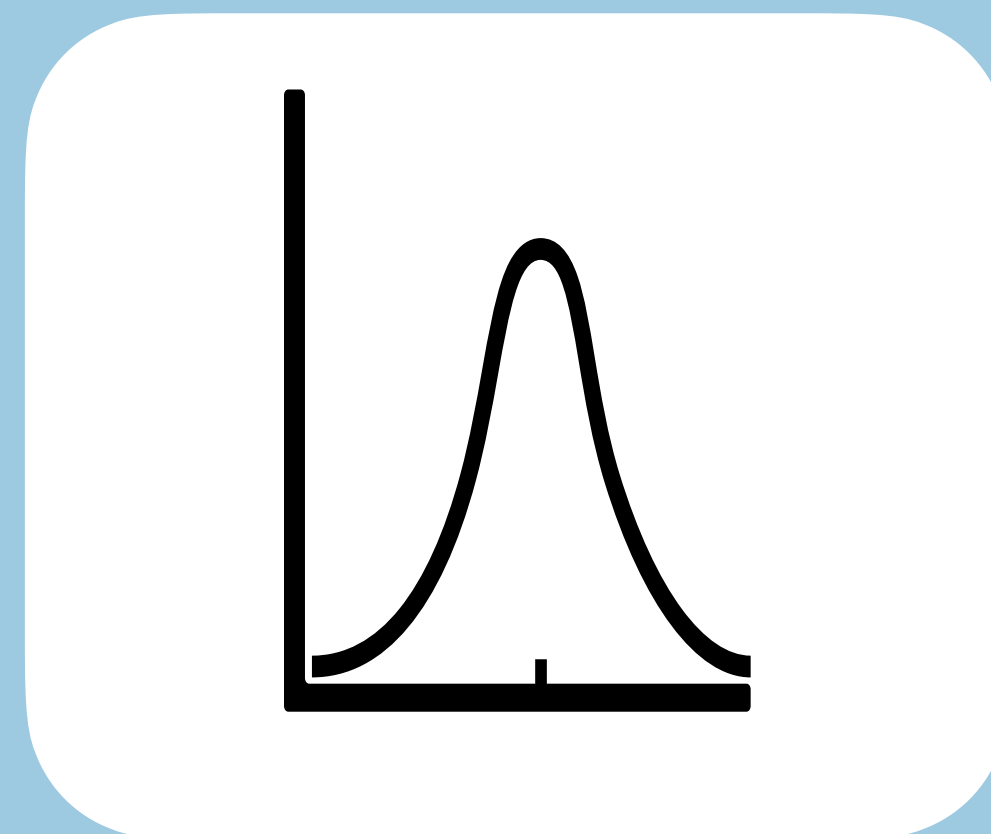
Process

Signal pre-processing



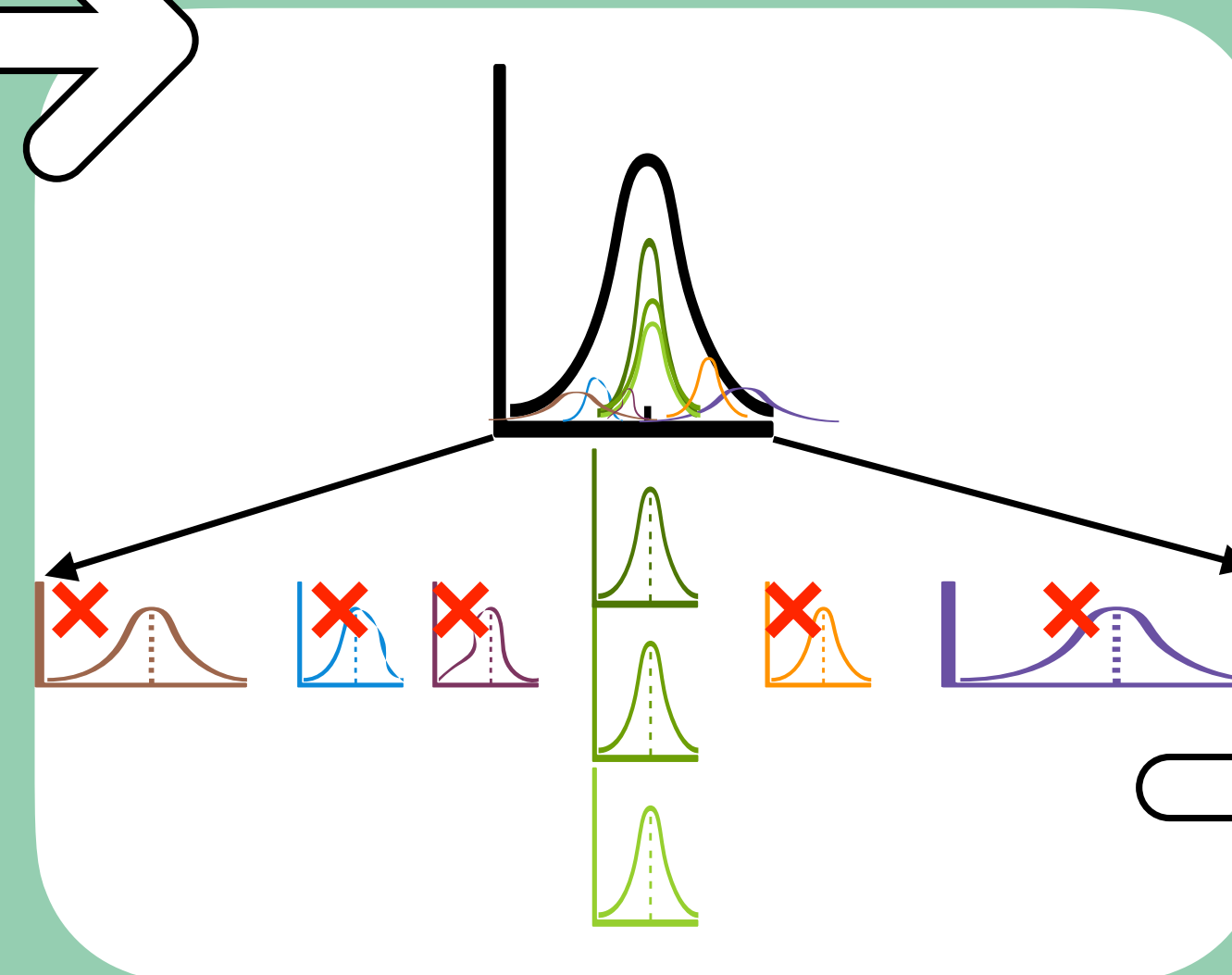
Detection improvement

Peaks extraction



Semi-quantitative integration

Peak-feature attribution

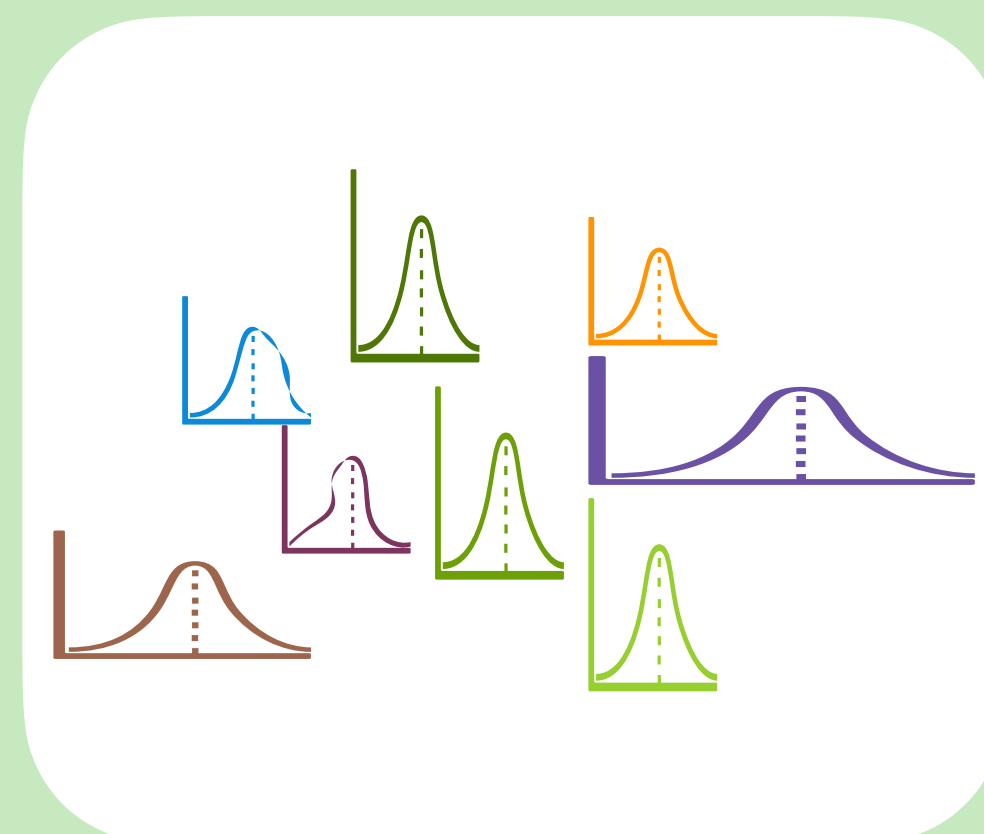


Peak shape similarity calculation

Combined qualitative and semi-quantitative information

Knowledge based prioritization

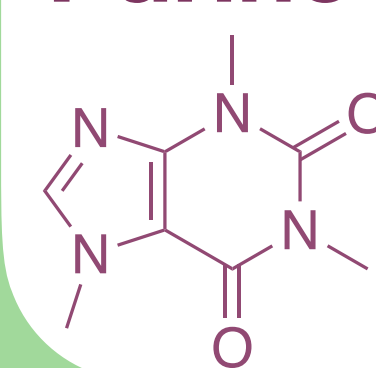
Features extraction



Clustering and Ion Identity Networking

Features annotation

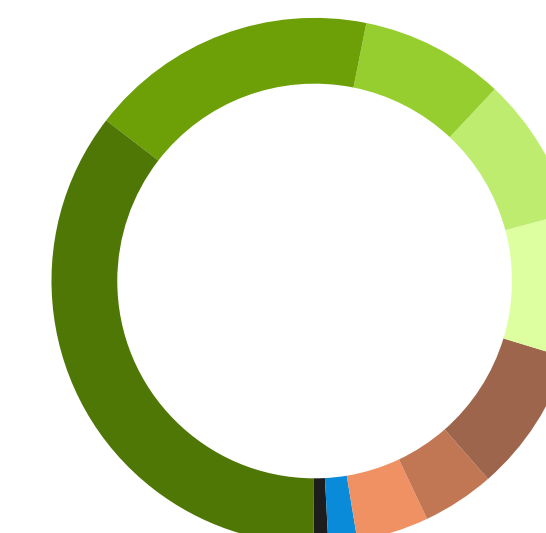
Alkaloids
Pseudoalkaloids
Purine alkaloids



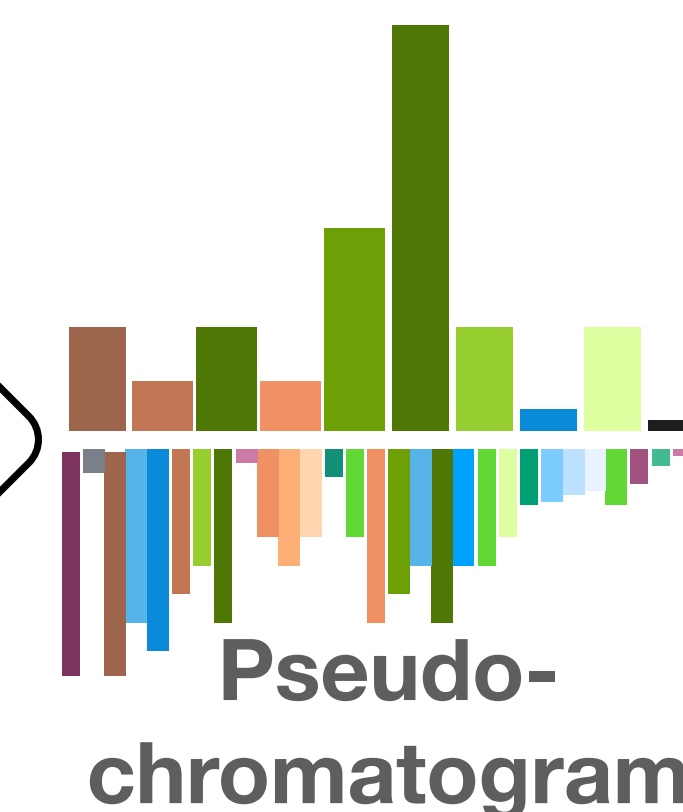
Confidence

Structural annotation and Compound class annotation

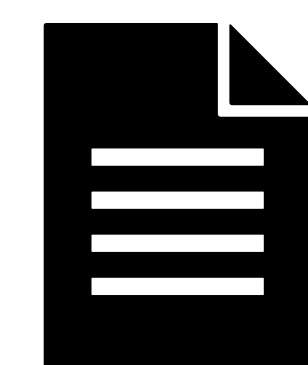
Output



Major metabolome



Pseudo-chromatogram



Automated report



Minor metabolome