

Additoinal file 11: Detailed parameters used for XCMS analysis

Software:

XCMSOnline version: 0.0.84
XCMS version: 1.30.3

1. General parameters

Polarity: positive
retention time format: minutes

2. Feature detection

method: centWave
ppm: 5
snthr: 6
peakwidth: 5 60
mzdiff: 0.01
prefilter peaks: 3
prefilter intensity: 100
noise: 0

3. Retention time correction

method: obiwarp
profStep: 0.1

4. Alignment

method: density
bw: 20
mzwid: 0.015
minfrac: 0.7
minsamp: 1

5. FillPeaks

6. Diffreport

statistics.threshold.pvalue: 0.05
statistics.diffReport.value: into

7. Additional Plots & Statistics

8. Annotation (isotopes & adducts)

featureAnnotation.CAMERA.annotate: isotopes
featureAnnotation.CAMERA.mzabs: 0.015
featureAnnotation.CAMERA.ppm: 5
featureAnnotation.CAMERA.sigma: 6
featureAnnotation.CAMERA.perfwhm: 0.6
featureAnnotation.CAMERA.maxcharge: 3
featureAnnotation.CAMERA.maxiso 4
featureAnnotation.CAMERA.intensity into

9. Putative ID's (METLIN)

identification.METLIN.ppm: 5
identification.METLIN.adducts: " M+H, M+Na "