MZmine 2 Example Parameters

Mass Detection

Parameter	Value
Retention time	0.40 - 22.0 min
MS level	1
Polarity	+/-
Spectrum type	Any
Mass detector	Centroid
Noise level	10000

Chromatogram Builder

Parameter	Value
Retention time	0.40 - 22.0 min
MS level	1
Polarity	+/-
Min time span (min)	0.05
Min height	100000
m/z tolerance	0.005 m/z or 10.0 ppm

Chromatogram Deconvolution

Parameter	Value
Algorithm	Local minimum search
Chromatographic threshold	0.02
Search minimum in RT range (min)	0.05
Minimum relative height	0.02
Minimum absolute height	500000
Min ratio of peak top/edge	3
Peak duration range (min)	0.05 - 1.50

Isotopic Peaks Groups

Parameter	Value
m/z tolerance	0.005 m/z or 10.0 ppm
Retention time tolerance	0.05 absolute (min)
Maximum charge	2
Representative isotope	Most intense

Join Aligner

Parameter	Value
m/z tolerance	0.005 m/z or 10.0 ppm
Weight for m/z	20
Retention time tolerance	0.1 absolute min
Weight for RT	20
Requier same charge state	no
Require same ID	no
Compare isotope pattern	no

Same RT and m/z Range Gap Filler

Parameter	Value
m/z tolerance	0.005 m/z or 10.0 ppm

Peak List Rows Filter

Parameter	Value
Minimum peaks in a row	0.75
Minimum peaks in an isotope pattern	2

Export to CSV File

Parameter	Value
Field separator	,
Export row ID	yes
Export row m/z	yes
Export row retention time	yes
Export row comment	yes
Export row number of detected peaks	yes
All identity elements	yes
Peak statues	yes
Peak m/z	yes
Peak RT	yes
Peak height	yes
Peak area	yes
Peak charge	yes
Peak FWHM	yes

Note: These parameters represent a suitable starting point for lipid analysis for the QE HF and should be systematically optimized for users' specific LC-MS/MS setup.