MZmine v 2.33

Method	Parameter	Value
Mass Detection	MS1	1.80E+05
	MS2	1.00E+03
Chromatogram Builder	Min time span (min)	0.01
	Min height	5.40E+05
	m/z tolerance (ppm)	1.00E+01
	Filter	MS1
Chromatogram Deconvolution - Local Minimum Search	Chromatographic Threshold	5%
	Search minimum in RT range	0.10 min
	Min relative height	15%
	Min absolute height	3.00E+05
	Min ratio of peak top/edge	2
	Peak duration range	0.01-1.5min
	m/z range for MS2 scan pairing	0.01
	RT range for MS2 scan pairing	0.1min
Isotopic Peaks Grouper	*m/z* tolerance (ppm)	1.00E-02
	Retention time tolerance (min)	0.05
	Max charge	3
	Representative isotope	Lowest *m/z*
	Monotonic shape	Yes
Join Aligner	*m/z* tolerance (ppm)	10
	Weight for *m/z*	5
	Weight for RT	1
	Retention time tolerance (min)	0.5
Peaks List Row Filter	Retention time (min)	0.2-12.51
	Min peaks per row	empty (leave unchecked)
	Keep only peaks with MS2 scan (GNPS)	yes
Gap Filling Peak Finder*	Intensity tolerance (%)	75
	m/z tolerance (ppm)	1.00E+01
	m/z tolerance (*m/z*)	1.00E-06
	Retention time tolerance (min)	0.3
	RT correction	yes