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| **Module** | **Parameters** |
| Raw data methods>Mass detection | MS level: 2Mass detector: Wavelet transform>Noise level: 5.0E1>Scale level: 1>Wavelet window size: 100 % |
| Raw data methods>Feature detection>ADAP Chromatogram builder | MS level: 2Min group size in # of scans: 5Group intensity threshold: 5.0E1Min highest intensity: 5.0E1m/z tolerance: 0.2 m/z |
| Feature list methods>Feature detection>Chromatogram deconvolution | Algorithm: Wavelets (ADAP)>S/N threshold: 1>S/N estimator: Intensity window SN>min feature height: 10>coefficient/area threshold: 0.5>Peak duration range: 0.00 – 100.00>RT wavelet range: 0.00 – 0.50m/z center calculation: MEDIAN |
| Feature list methods>Isotopes>Isotopic peaks grouper | m/z tolerance: 0.015 m/zRetention time tolerance: 0.5 absolute (min)Maximum charge: 5Representative isotope: Most intense |
| Feature list methods>Export/Import>Export to CSV file | Field separator: “,”Export common elements:>Export row m/z>Export row retention timeExport data file elements:>Peak height>Peak charge |