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| **Module** | **Parameters** |
| Raw data methods  >Mass detection | MS level: 2  Mass detector: Wavelet transform  >Noise level: 5.0E1  >Scale level: 1  >Wavelet window size: 100 % |
| Raw data methods  >Feature detection  >ADAP Chromatogram builder | MS level: 2  Min group size in # of scans: 5  Group intensity threshold: 5.0E1  Min highest intensity: 5.0E1  m/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 – 0.50  m/z center calculation: MEDIAN |
| Feature list methods  >Isotopes  >Isotopic peaks grouper | m/z tolerance: 0.015 m/z  Retention time tolerance: 0.5 absolute (min)  Maximum charge: 5  Representative isotope: Most intense |
| Feature list methods  >Export/Import  >Export to CSV file | Field separator: “,”  Export common elements:  >Export row m/z  >Export row retention time  Export data file elements:  >Peak height  >Peak charge |