Peak Detection Results Comparison (note: parameters not listed here are set with default value)

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| --- | --- | --- | --- | --- | --- |
| **Tool** | **Data** | **My parameter settings** | **Their parameter settings** | **My result** | **Their result** |
| XCMS | DCSM | version = 3.4.4 | version = 1.47.2 (modified) | 30,424 | 5,910 |
| ppm = 0.01 | mzTolerance = 0.01 |
| Peakwidth = (1.2, 36.0) | Peakwidth = (1.2, 36.0) |
| Noise = 100 | Noise = 100 |
| Prefilter = (1, 5000) | Prefilter = (1, 5000) |
| Integrate = 2 | Integrate = 2 |
| ADAP | Version = 2.38 | Version = 2.21 | 4,920 | 4,532 |
| **Mass detection** | |
| Noise level = 100 | Noise level = 100 |
| Scale level = 20 | Scale level = 20 |
| Wavelet window size = 50 | Wavelet window size = 50 |
| **ADAP chromatogram builder** | |
| Min group size = 4 | Min group size = 4 |
| Group intensity threshold = 500 | Group intensity threshold = 500 |
| Min highest intensity = 5,000 | Min highest intensity = 5,000 |
| m/z tolerance = 0.01 | m/z tolerance = 0.01 |
| **Chromatogram peak picking** | |
| S/N threshold = 10 | S/N threshold = 10 |
| Min feature height = 5,000 | Min feature height = 5,000 |
| Coefficient/area threshold = 120 | Coefficient/area threshold = 120 |
| Peak duration range = 0.01-0.60 | Peak duration range = 0.01-0.60 |
| mzMine 2 | Version = 2.38 | Version = 2.21 | 2,510 | 5,599 |
|  | Version = 2.21  (xcms version 1.48.0) | 4,031 |