**Additional file 1**

Table S1: Algorithms and libraries used in Mass-Up.

| Task | Subtask | Algorithm | Library/Reference |
| --- | --- | --- | --- |
| Load data | Load mzXML |  | jmzReader 1.2.0 |
| Load mzML |  | jmzReader 1.2.0 |
| Load CSV |  | Own implementation |
| Preprocessing | Smoothing | Moving average window | MALDIquant 1.8 |
| Savitzky Golay | MALDIquant 1.8 |
| Baseline correction | SNIP | MALDIquant 1.8 |
| Convex Hull | MALDIquant 1.8 |
| Top Hat | MALDIquant 1.8 |
| Median | MALDIquant 1.8 |
| Normalization | Total Ion Current (TIC) | MALDIquant 1.8 |
| Probabilistic Quotient Normalization (PQN) | MALDIquant 1.8 |
| Median | MALDIquant 1.8 |
| Peak detection | Continuous Wavelet Transform (CWT) | MassSpecWavelet 2.12 |
| Signal-to-noise threshold | MALDIquant 1.8 |
| Peak matching | MALDIquant binPeaks function | MALDIquant 1.8 |
| Quality Control |  | Forward algorithm | Own implementation |
| Box-and-whiskers plotting | JFreeChart 1.0.13 |
| Biomarker Discovery | Intra-label |  | Own implementation |
| Inter-label | Chi-square test | Apache Commons Math 3.0 |
| Fisher exact test | Own implementation |
| Randomization test | Own implementation  Apache Commons Math 3.0 |
| Yates’ chi-squared test | Own implementation |
| Benjamini & Hochberg FDR correction | Own implementation |
| Clustering | Clustering computation | Agglomerative Hierarchical Clustering | Own implementation |
| Clustering visualization |  | JTreeView |
| Biclustering |  | Bimax | BicAT (Biclustering Analysis Toolbox) |
| BiBit | http://www.upo.es/eps/bigs/BiBit\_algorithm.html |
| Classification Analysis | Classifiers | Weka | Weka 3.6 |
| Principal Component Analysis | PCA computation | Weka | Weka 3.6 |
| PCA visualization |  | Jzy3d 0.9 |