|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Table S2**. MarkerLynx XS processing parameters  |  |  |  |  |
|  |  |  |  |  |  |  |
| Retention time range  | 0.7-12.0 min |  |  |  |  |  |
| Mass range | 100-1800 m/z |  |  |  |  |  |
| Mass tolerance  |  0.02 Da |  |  |  |  |  |
| Xic window | 0.02 Da |  |  |  |  |  |
| Apex Track Peak Parameters | Automatic |  |  |  |  |  |
| Apply Smoothing | Yes |  |  |  |  |  |
| Mass window | 0.02 Da |  |  |  |  |  |
| Retention time window | 0.2 Minutes |  |  |  |  |  |
| Noise elimination level | 10 |  |  |  |  |  |
| Deisotope data | Yes |  |  |  |  |  |
|  |  |  |  |  |  |  |
| Features discovered | 502 |  |  |  |  |  |
|  |  |  |  |  |  |  |
| Statistical analyses (PCA and OPLS-DA) were performed with Pareto scaling of the dataset |