

**Table S2. Molecular networking: MZmine 2 data-preprocessing parameters**

| Steps                        | Methods                         | Parameters                           | Values          |
|------------------------------|---------------------------------|--------------------------------------|-----------------|
| <b>Mass detection</b>        |                                 | Noise level MS1                      | 0               |
|                              |                                 | Noise level MS2                      | 0               |
| <b>chromatogram builder</b>  | ADAP                            | Minimum group size of scan           | 4               |
|                              |                                 | Group intensity threshold            | 3000            |
|                              |                                 | Minimum highest intensity            | 4000            |
|                              |                                 | m/z tolerance                        | 0.005 (20 ppm)  |
| <b>Deconvolution</b>         | ADAP Wavelets algorithm         | S/N threshold                        | 8               |
|                              |                                 | Minimum feature height               | 4000            |
|                              |                                 | Coefficient/area threshold           | 20              |
|                              |                                 | Peak duration range                  | 0.05 – 1 min    |
|                              |                                 | T <sub>R</sub> wavelet range         | 0.01 – 0.07 min |
| <b>MS2 scans paired</b>      |                                 | m/z tolerance                        | 0.02 Da         |
|                              |                                 | t <sub>R</sub> tolerance             | 0.3 min         |
| <b>Isotopologue grouping</b> | Isotopic peak grouper algorithm | m/z tolerance                        | 0.005 (20 ppm)  |
|                              |                                 | t <sub>R</sub> tolerance             | 0.2 min         |
| <b>Filtering</b>             | Feature list rows filter        | Retention time range                 | 1 – 14 min      |
|                              |                                 | <b>Keep only peaks with MS2 scan</b> |                 |
| <b>Peak alignment</b>        | Join aligner module             | m/z tolerance                        | 0.005 (20 ppm)  |
|                              |                                 | Weight for m/z                       | 2               |
|                              |                                 | t <sub>R</sub> tolerance             | 0.5 min         |
|                              |                                 | Weight for t <sub>R</sub>            | 1               |
| <b>Gap filled</b>            |                                 | m/z tolerance                        | 0.005 (20 ppm)  |
|                              |                                 | t <sub>R</sub> tolerance             | 0.5 min         |