

Figure A1. Putative identification for the Unknown_19.53 labelled compound based on mass isotopomer distribution similarity. The relative mass isotopomers are described as bars with 95% confidence intervals and numbers, with the compound name, the selected *m/z* (ion), the coefficient of determination (*R*²) and the sum of absolute mass isotopomer abundances (*S*) described. The numbers by the connecting lines indicate the similarity calculated using the Canberra distance measure.

