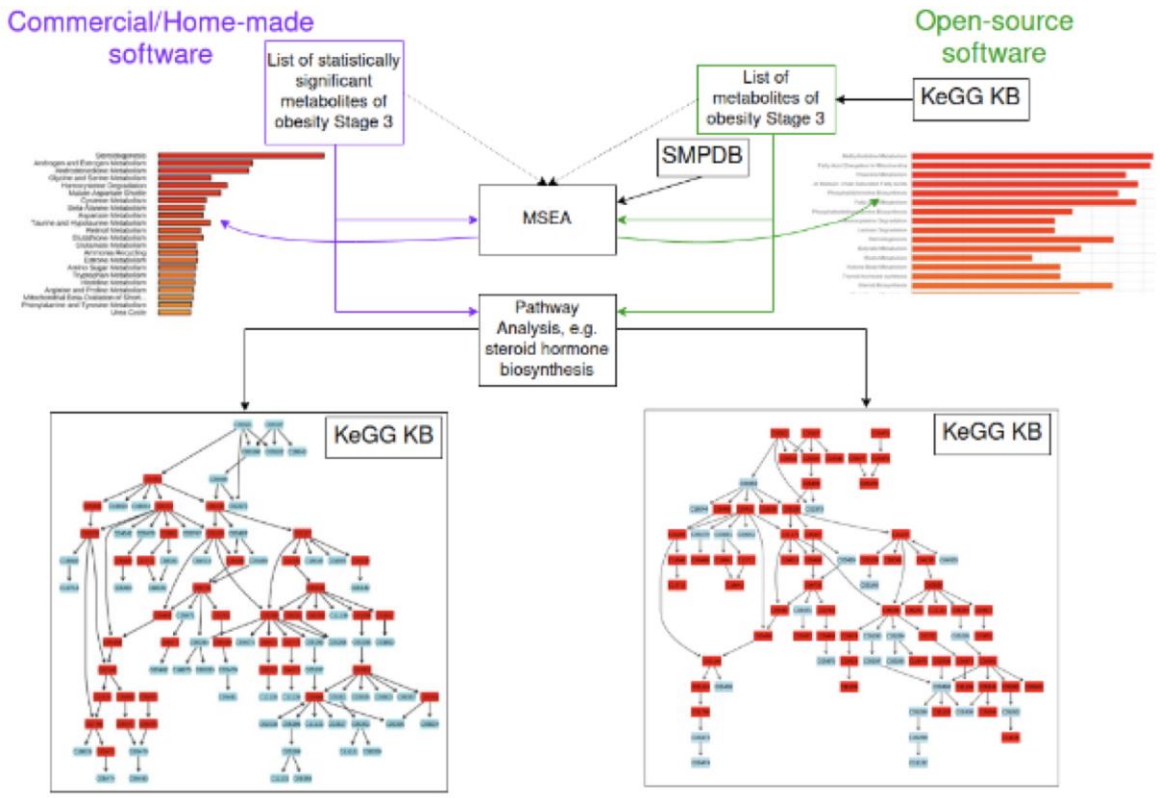

Figure S1. The scheme of algorithms for processing mass-spectrometric data of direct infusion. Utilizing the commercial program COMPASS DataAnalysis in junction with MatLab interactive development environment is shown on the left (purple). On the right (green) — open-source R packages: MSnbase, MALDIquant, MetaboAnalystR::Mummichog.