

Supporting Information

Faecal metabolomic fingerprint after moderate consumption of red wine by healthy subjects

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Supporting Information Table

Table S1. Summary table of MZmine settings used in this work.

Mass detection	Chromatogram builder	Chromatogram deconvolution	Deisotoping
Mass detection = Centroid Noise level = 4×10^4 a.u	Min time span = 0.10 min Min height = 4×10^4 a.u m/z tolerance = 0.02 or 50 ppm	Peak recognition = Local minimum search Chromatographic threshold=20% Minimum relative height= 2% Minimum absolute height= 2×10^2 Minimum ratio of peak top/edge=2 Peak duration=0.1-2 min	m/z tolerance = 0.01 Rt tolerance = 0:00 Mono tonic shape Maximum charge = 2 Representative isotope = Most intense
Adduct search	Alignment (replicates)	Alignment (samples)	Exporting
Show all possible adducts Max. adduct peak height= 100%	RANSAC aligner: m/z tolerance = 0.05 m/z or 20 ppm Rt tolerance = 0.1 min Minimum number of common points= 90%	Join aligner: m/z tolerance= 0.05 m/z or 20ppm Weight for m/z= 80 Rt tolerance = 0.5 min Absolute Rt tolerance= 1:00	Export to CSV file Export MZmine ID, m/z, retention time, Peak area

Supporting Information Figure

Figure S1: Total ion chromatograms (TIC) from the pooled faecal sample analyzed applying four different gradients (A, B, C and D). Tables on the upper-left of each TIC representation show the programmed gradient in each case. Mean number of peaks (n=3 injections) found applying each gradient are also included on the right of each TIC. All these analysis were performed in the negative ion mode and with the same mobile phases composition (phase A: Water, 0.01% HCOOH (v/v); phase B: ACN, 0.01% HCOOH (v/v)).

Supplemental Figure 1.

