

Supplementary Figure S1:

Extracted-ion chromatogram (XIC) from LC-MS/MS analysis of sample S2\_C22. Upside illustrates XIC for 71 MRMs of acylcarnitines and amino acids, downside shows XIC for glutamic acid and its stable isotope-labeled glutamic acid-d5

Supplementary Table S1:

Paired t-test for metabolites in QC samples, comparison between three replicates in two days

Supplementary Table S2:

Mann-Whitney U test comparison between RRMS and healthy control groups,  $p < 0.05$  marked as green

Supplementary Figure S2:

Variance distribution between principal components in PCA

Supplementary Table S3:

Clinical data of the RRMS and HC groups

Supplementary Table S4:

Mass-spectrometry method parameters for analysis amino acids and acylcarnitines in MRM mode established on AB Sciex API 6500 QTRAP

Supplementary Figure S3:

Repeated (N=20) 5-fold cross-validation model on training subset (n=34). A. Dependence of AUC for random forest models with different number of trees from the selected number of randomly chosen metabolites. B. Dependence of AUC for random forest models based on preselected metabolites from the number of trees.