

There are many estimated parameters (for example, the parameters of the G matrix are equal to $3422 \times 3422 / 2$), so, it is difficult to reflect the convergence of all parameters directly.

Principal Component Analysis (**PCA**) was used to get the first 10 principal components (**PC**) of the G matrix (> 98% total variance explained) to reflect its overall estimated parameters.

The results from three analyses in the three datasets (Average fat percentage [**AFP**] + milk MIR spectra, 3,302 individuals x 3422 traits; Average CH₄ [**ACH4**] + milk MIR spectra 3,302 individuals x 3422 traits; Average SCS [**ASCS**] + milk MIR spectra, 3,302 individuals x 3422 traits) through MegaLMM were shown, separately. Based on the reviewer's suggestion, the chain was made longer to check the convergence. The new chain included 1,00,000 iterations and the first 10,000 as burn-in.

PS: Please note the Y-axis range value.

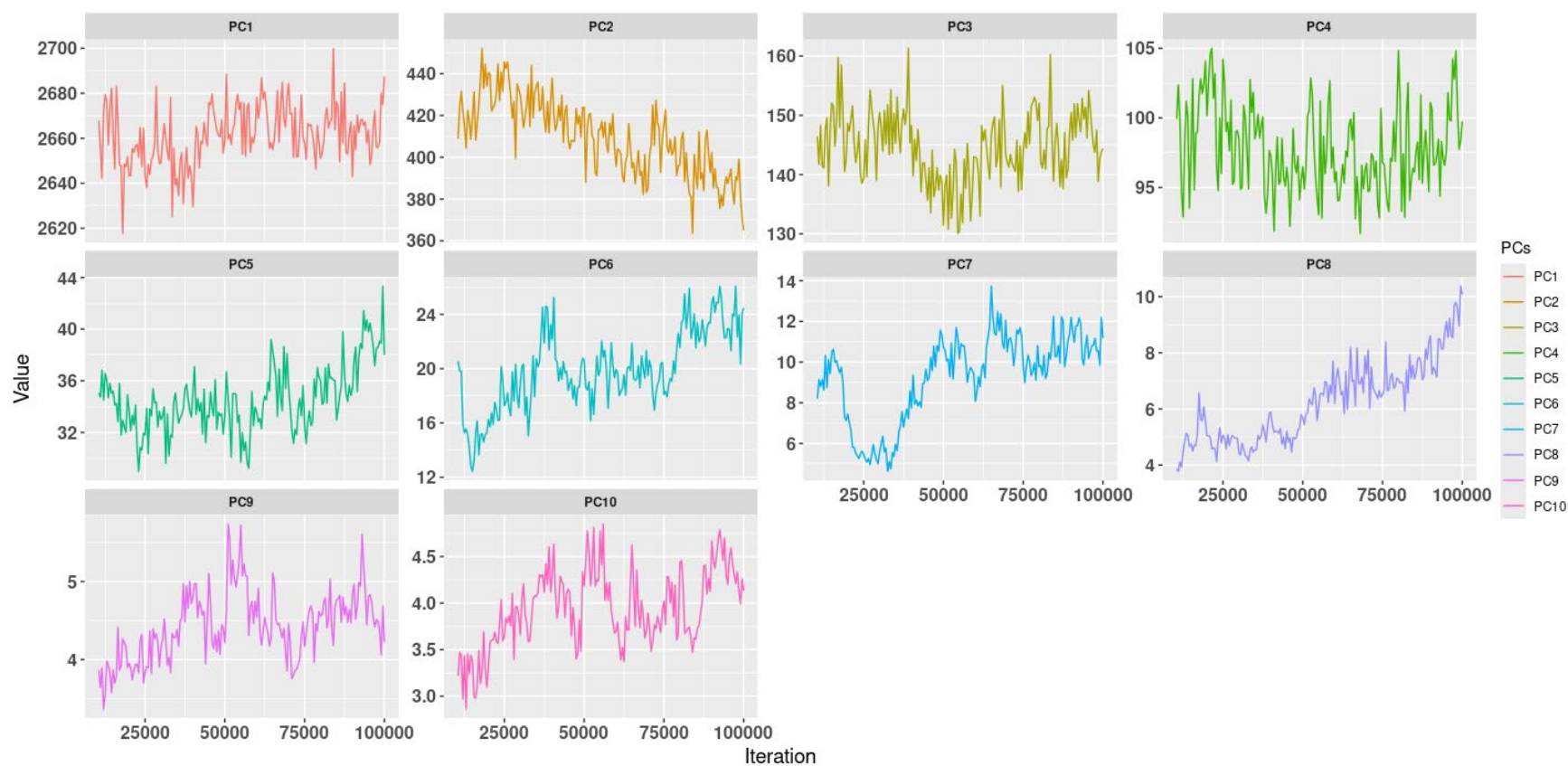


Figure S1. Example trace plot of the first 10 principal components (PC) on the saved MCMC samples for the G matrix of analysis in the **AFP** and **milk MIR spectra** dataset. The chain includes 100,000 iterations, and the first 10,000 are burn-in.

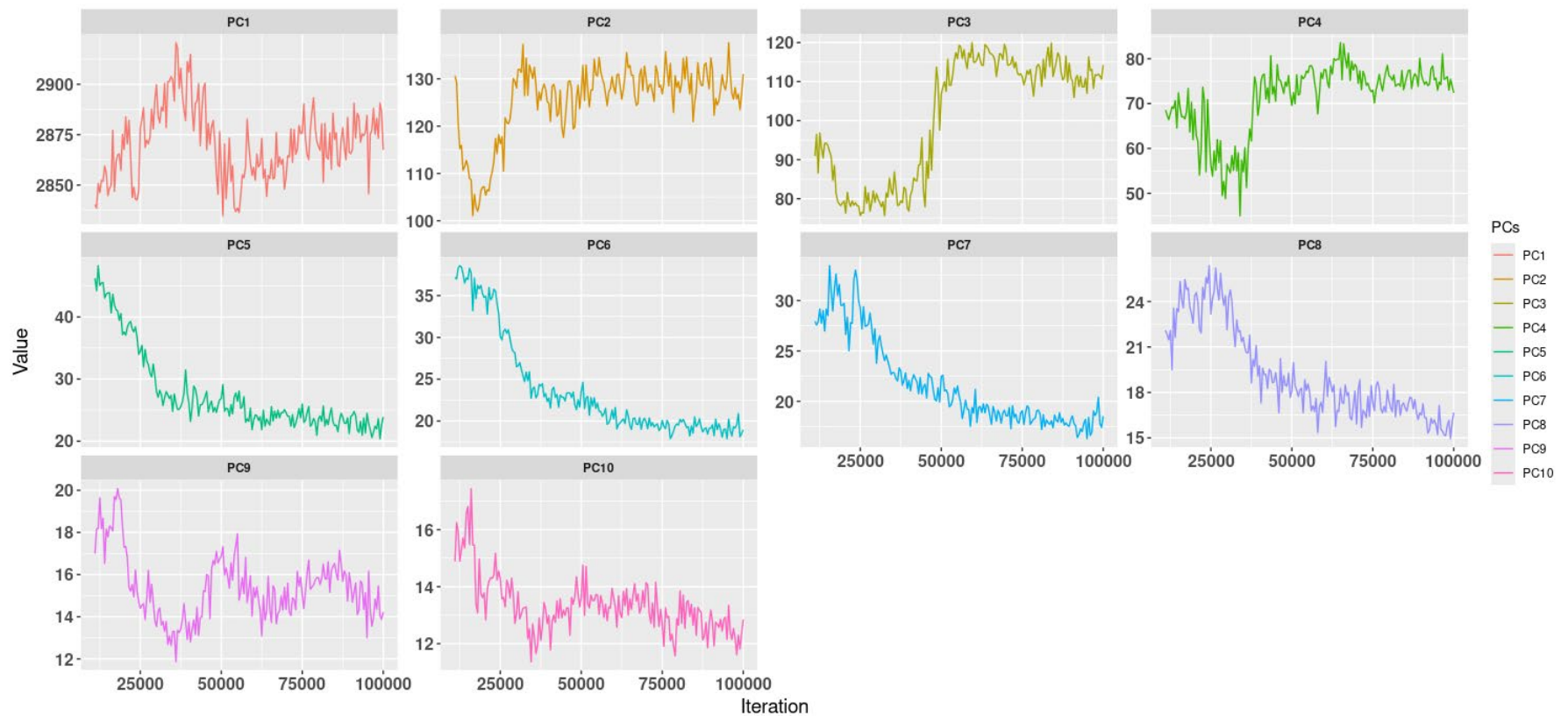


Figure S2. Example trace plot of the first 10 principal components (PC) on the saved MCMC samples for the G matrix of analysis in the **ACH4** and **milk MIR spectra** dataset. The chain includes 100,000 iterations, and the first 10,000 are burn-in.

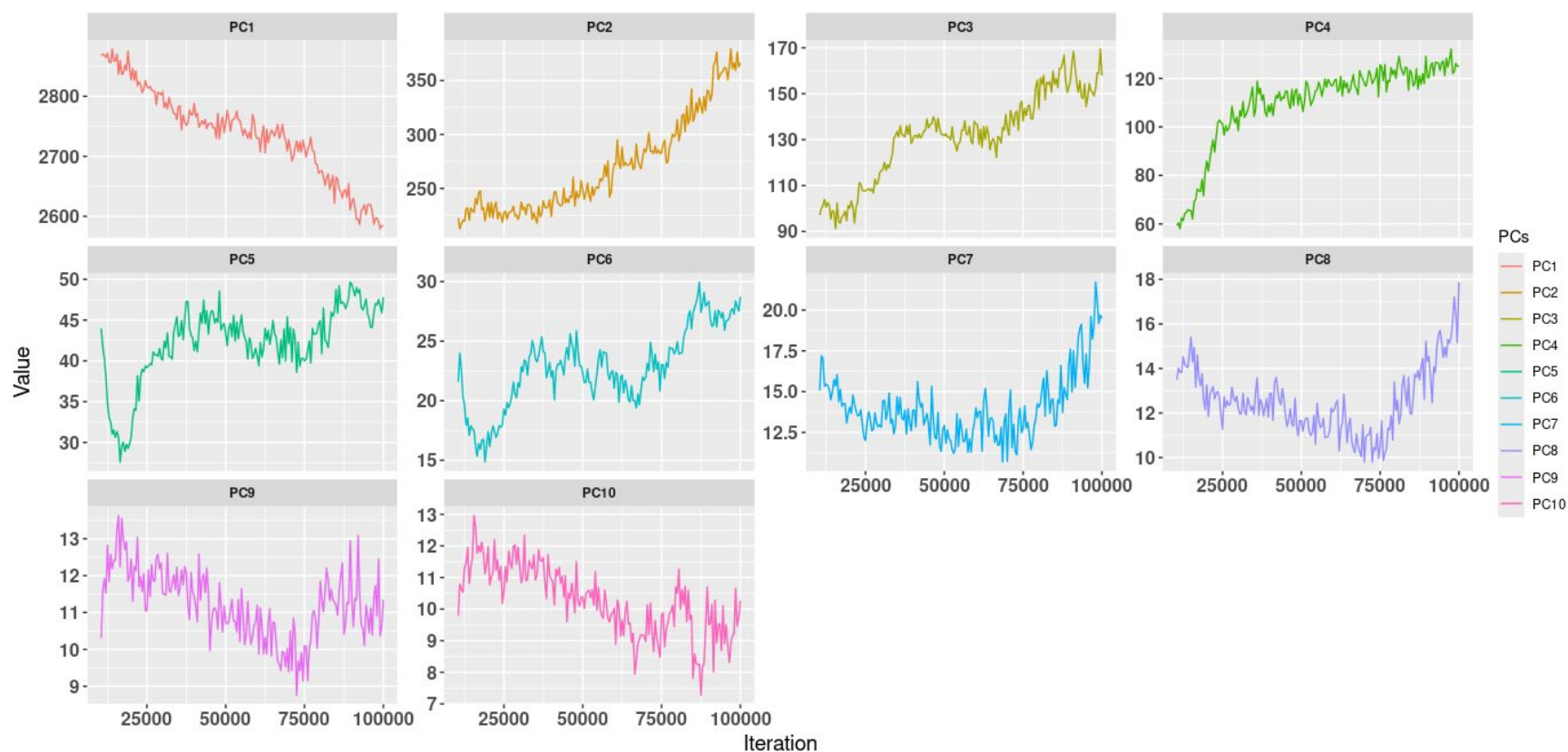


Figure S3. Example trace plot of the first 10 principal components (PC) on the saved MCMC samples for the G matrix of analysis in the **ASCS** and **milk MIR spectra** dataset. The chain includes 100,000 iterations, and the first 10,000 are burn-in.