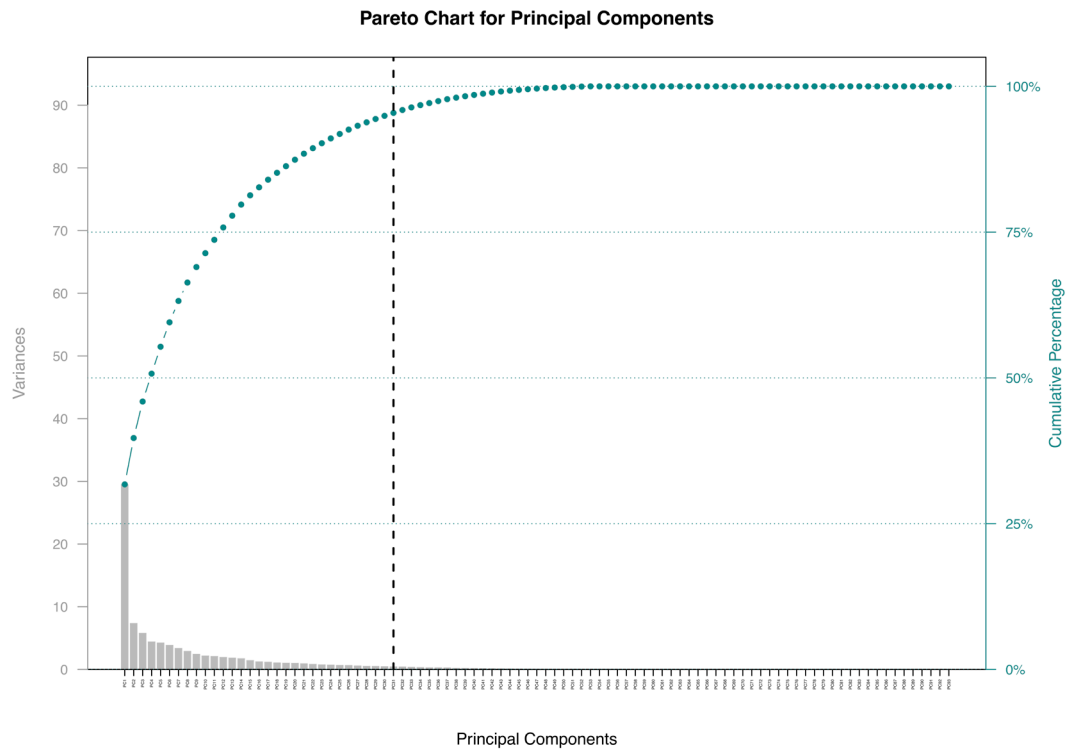




**Supplementary Figure 2:** Pareto chart from principal components analyses of the metabolite data.



**Note:** the dashed vertical line indicates the number of principal components explaining  $\geq 95\%$  of the variance within the metabolite data analysed.