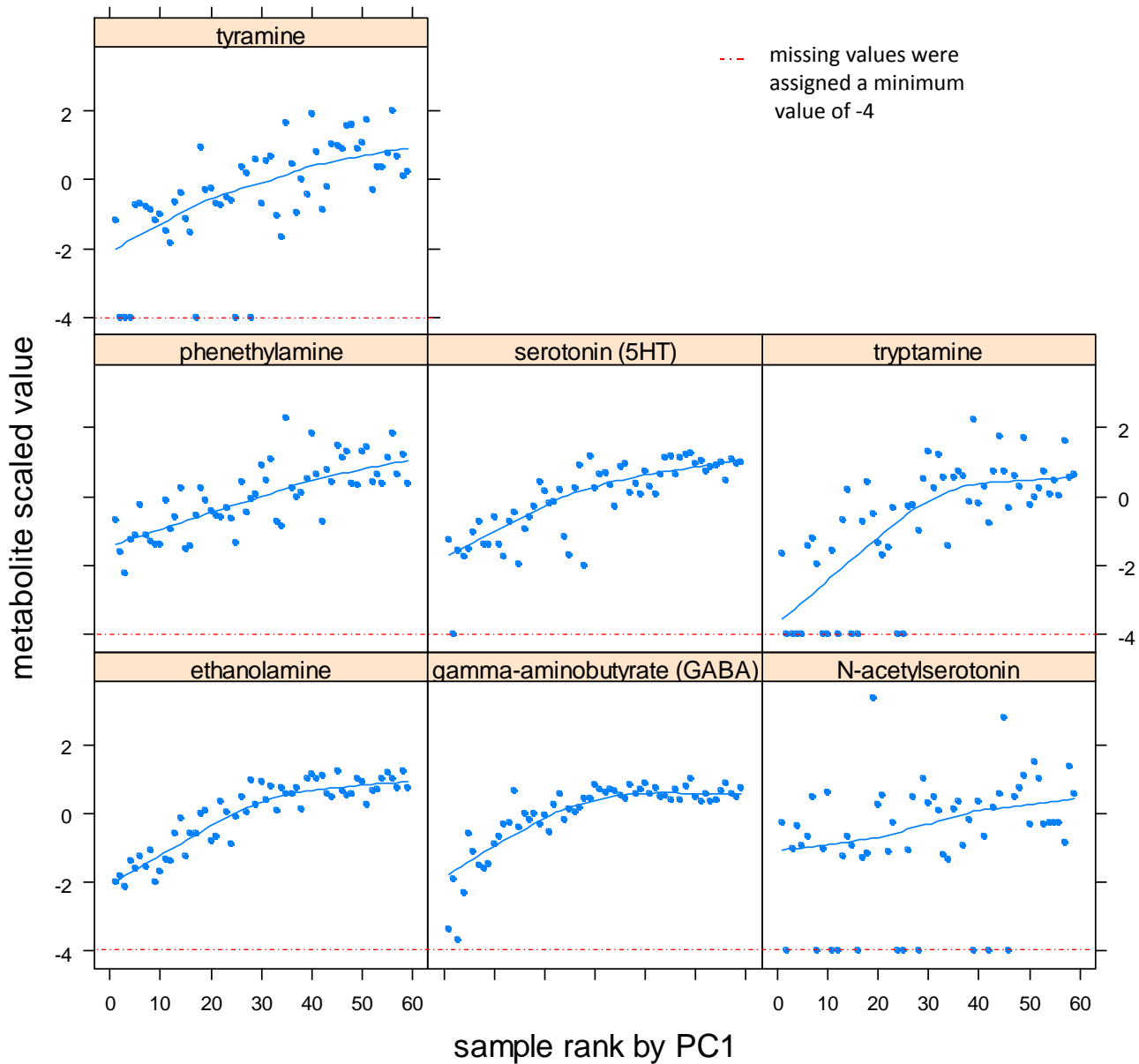


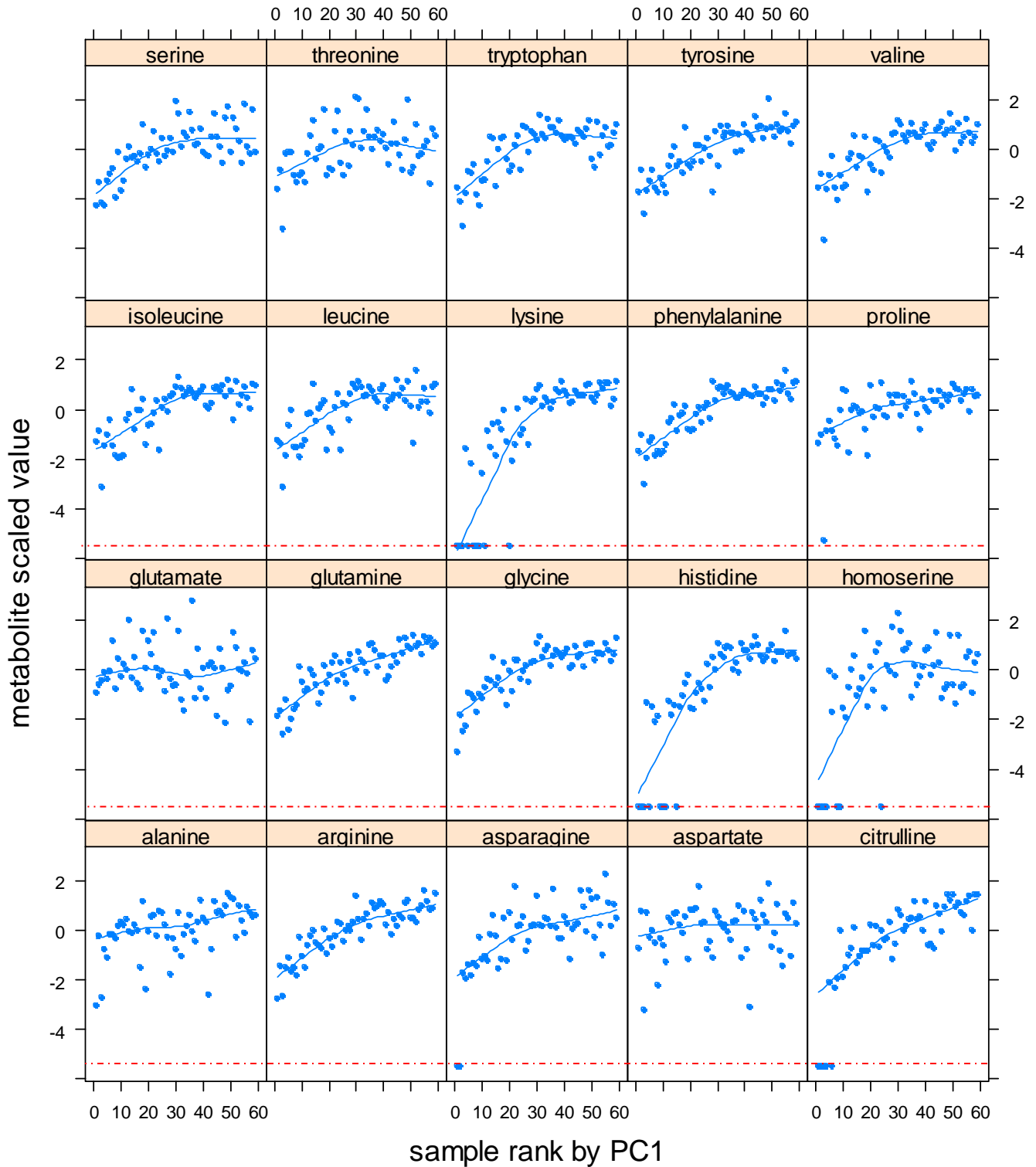
Additional file 4. Abundance profiles of standardized metabolite levels along DS2-mature samples arranged by increasing PC1 scores. Shown within their respective classes

primary amines

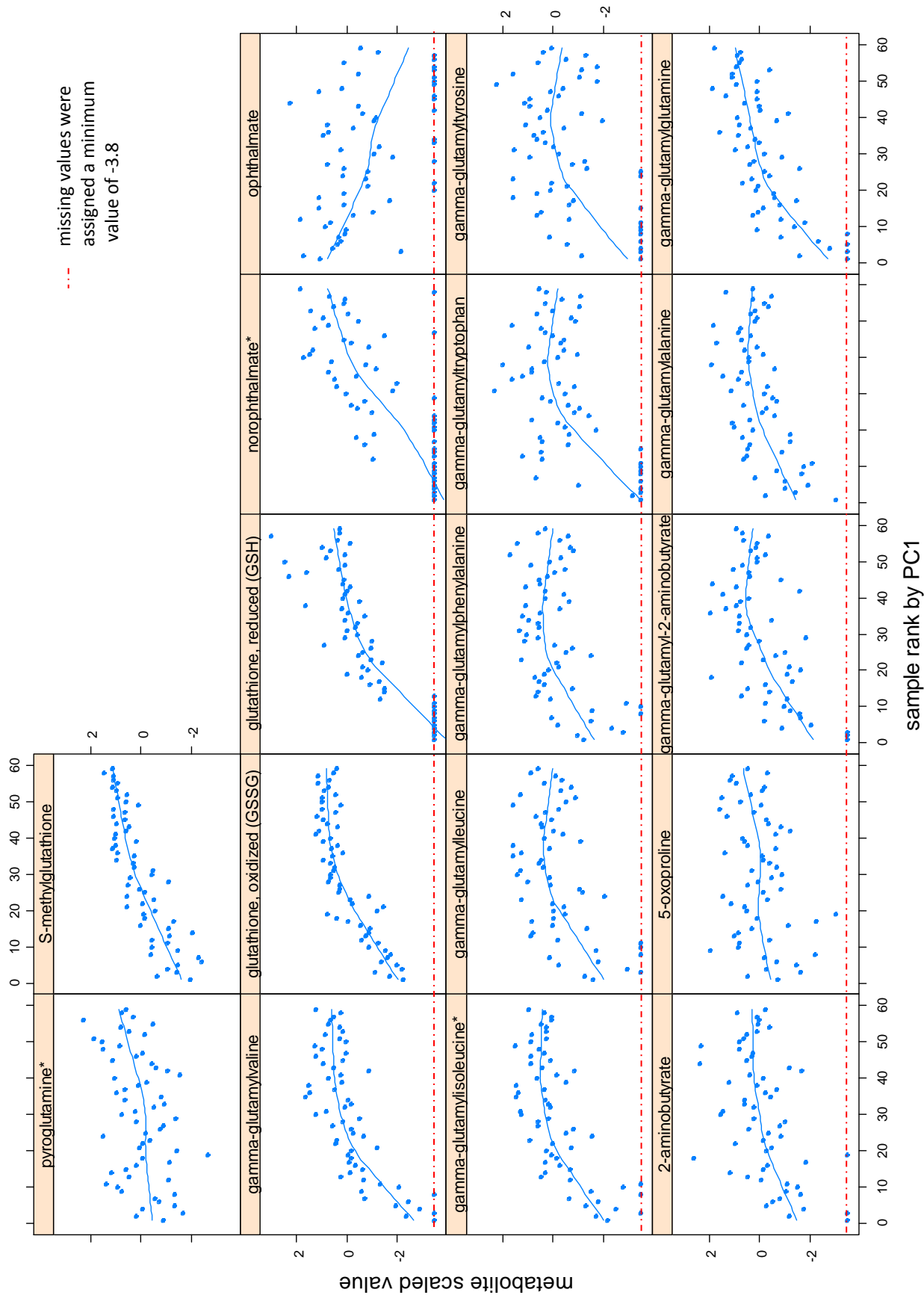


--- missing values were assigned a minimum value of -5.8

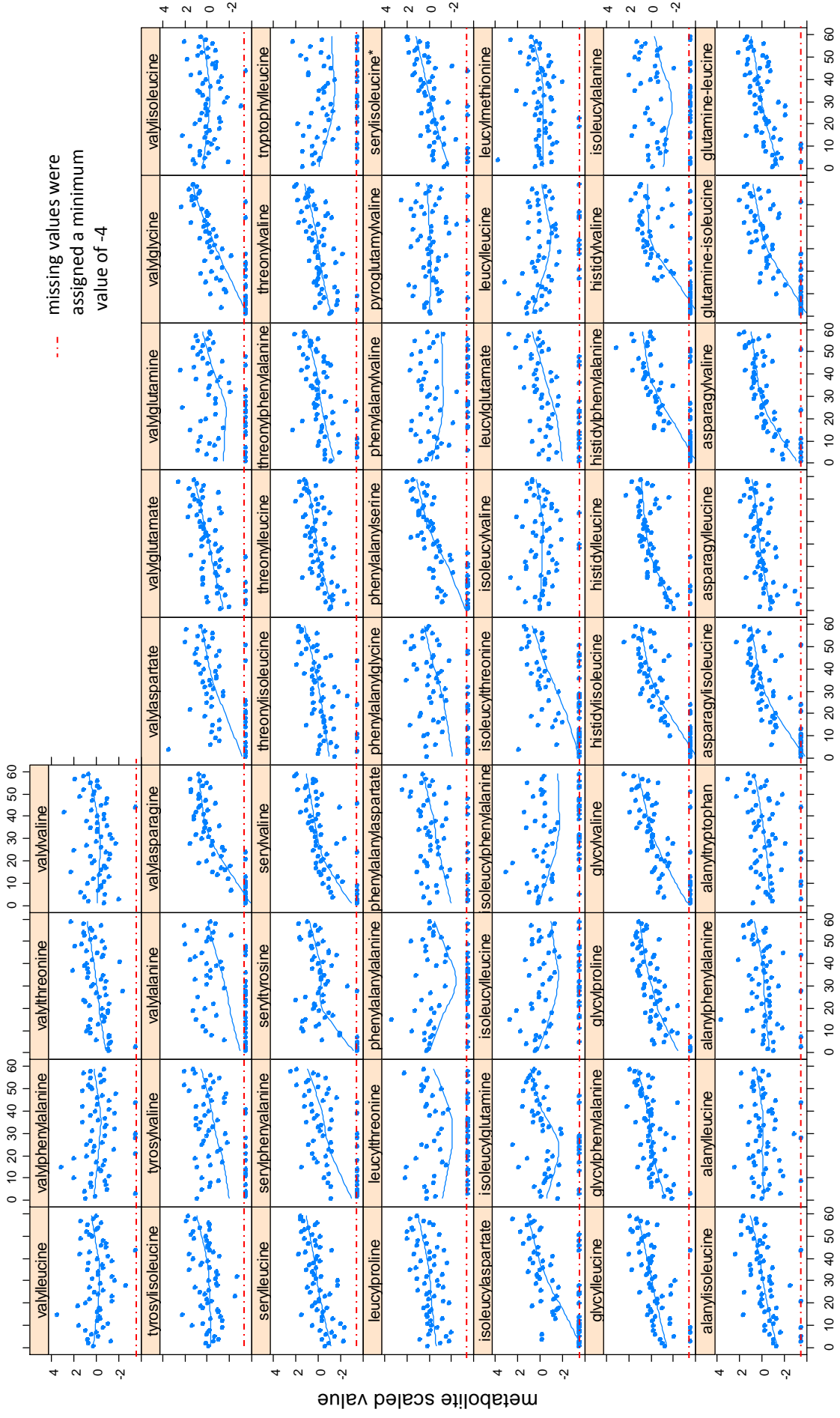
amino acids



glutathione cycle and glutathione metabolism



dipeptides

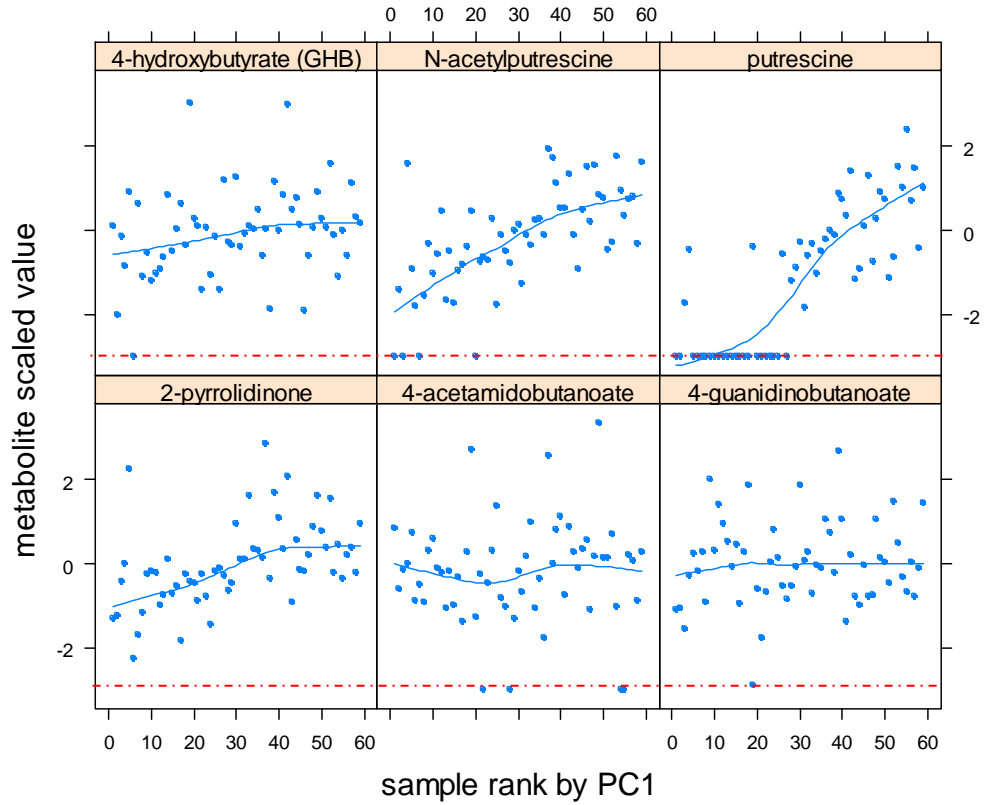


--- missing values were assigned a minimum value of -4

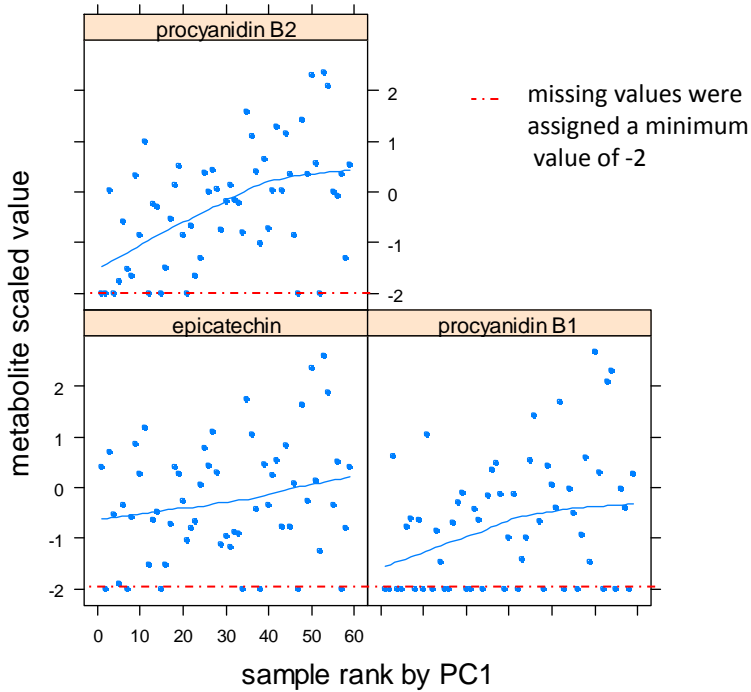
sample rank by PC1

--- missing values were assigned a minimum value of -3

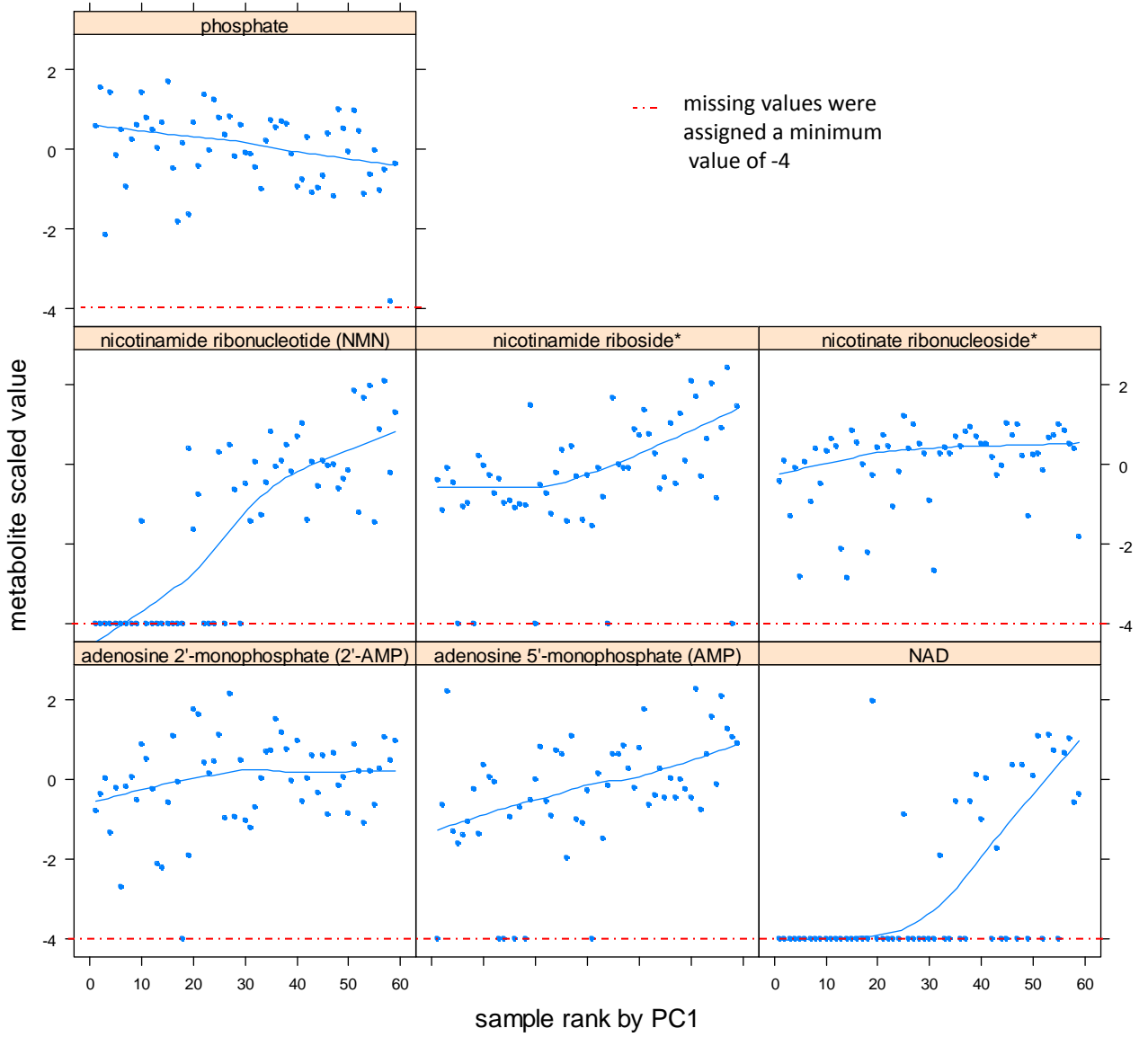
polyamines and polyamine degradation



tannins

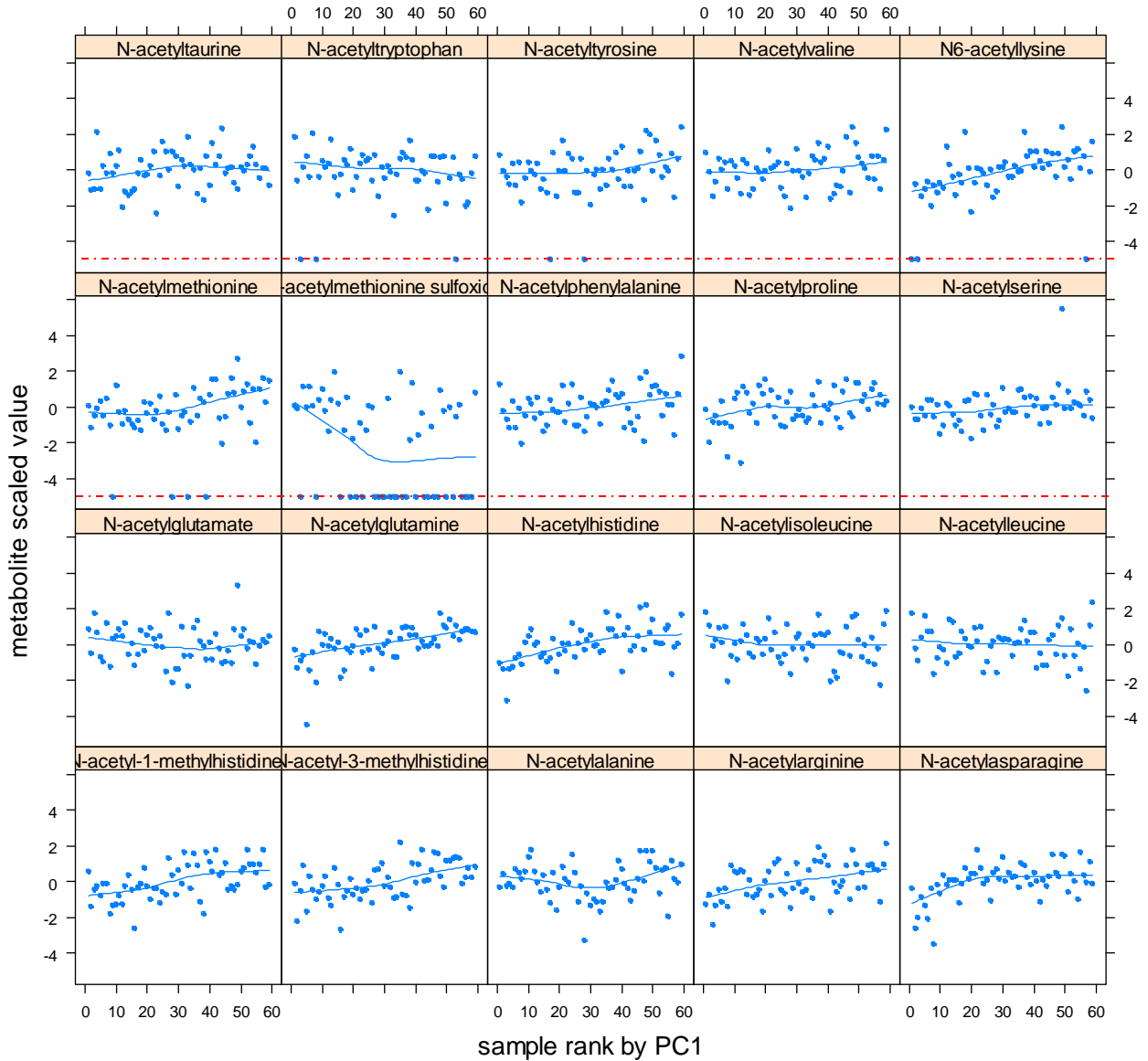


energy metabolism



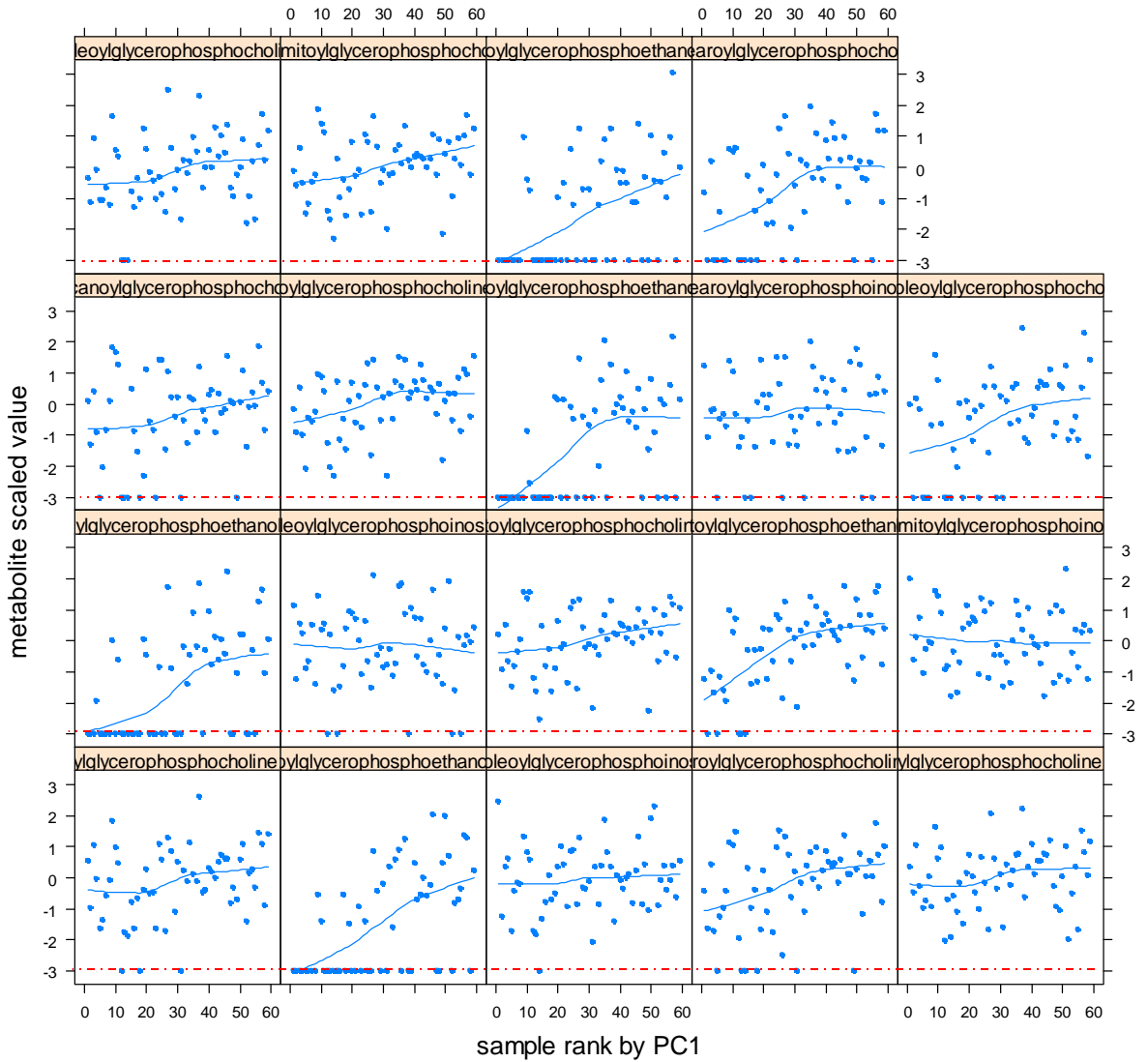
--- missing values were assigned a minimum value of -5

acetylated amino acids

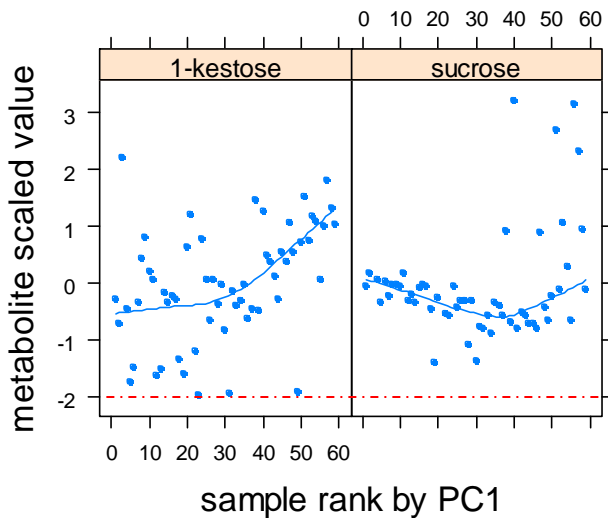


lysophospholipids

--- missing values were assigned a minimum value of -3

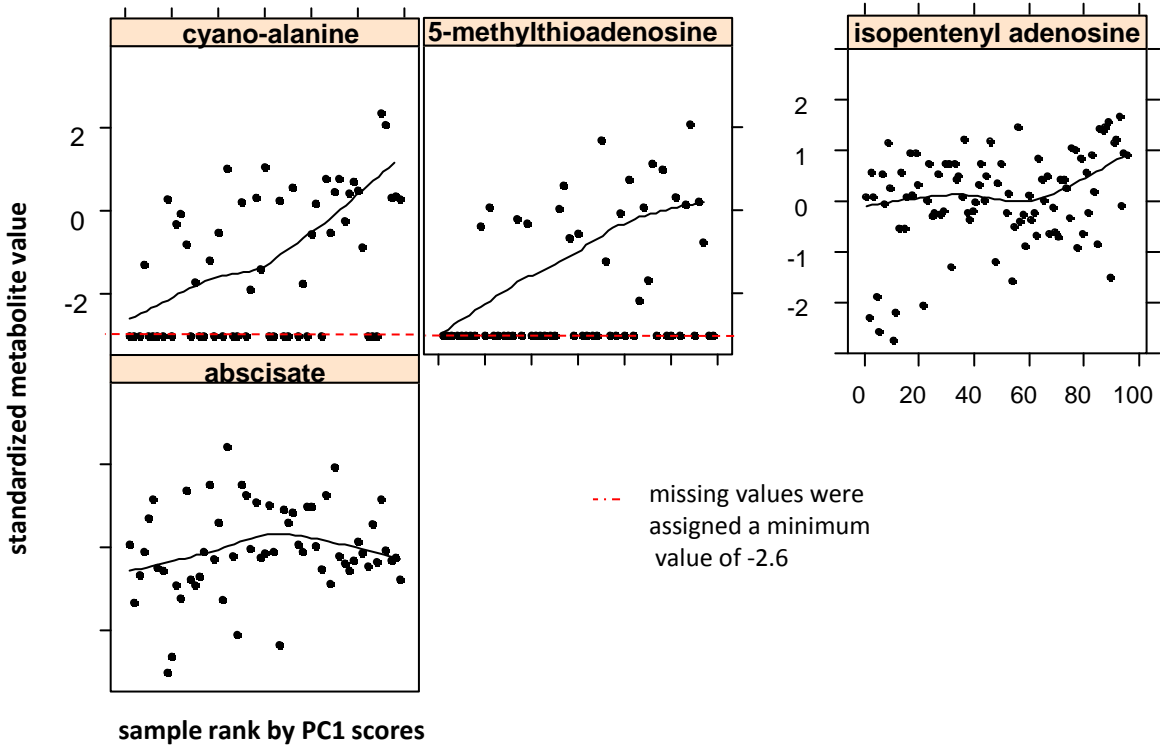


non-reducing sugars



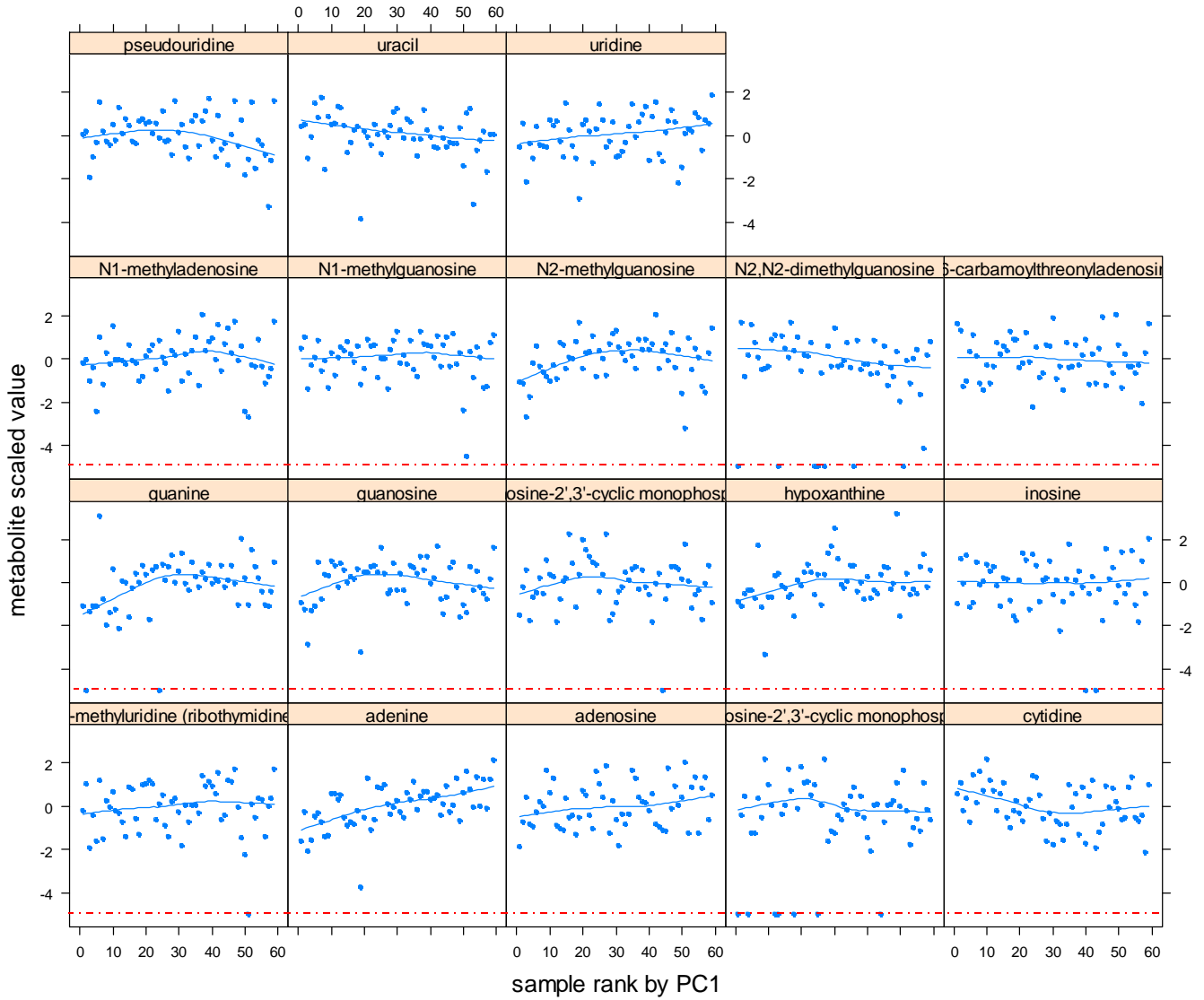
--- missing values were assigned a minimum value of -2

hormones



--- missing values were assigned a minimum value of -5

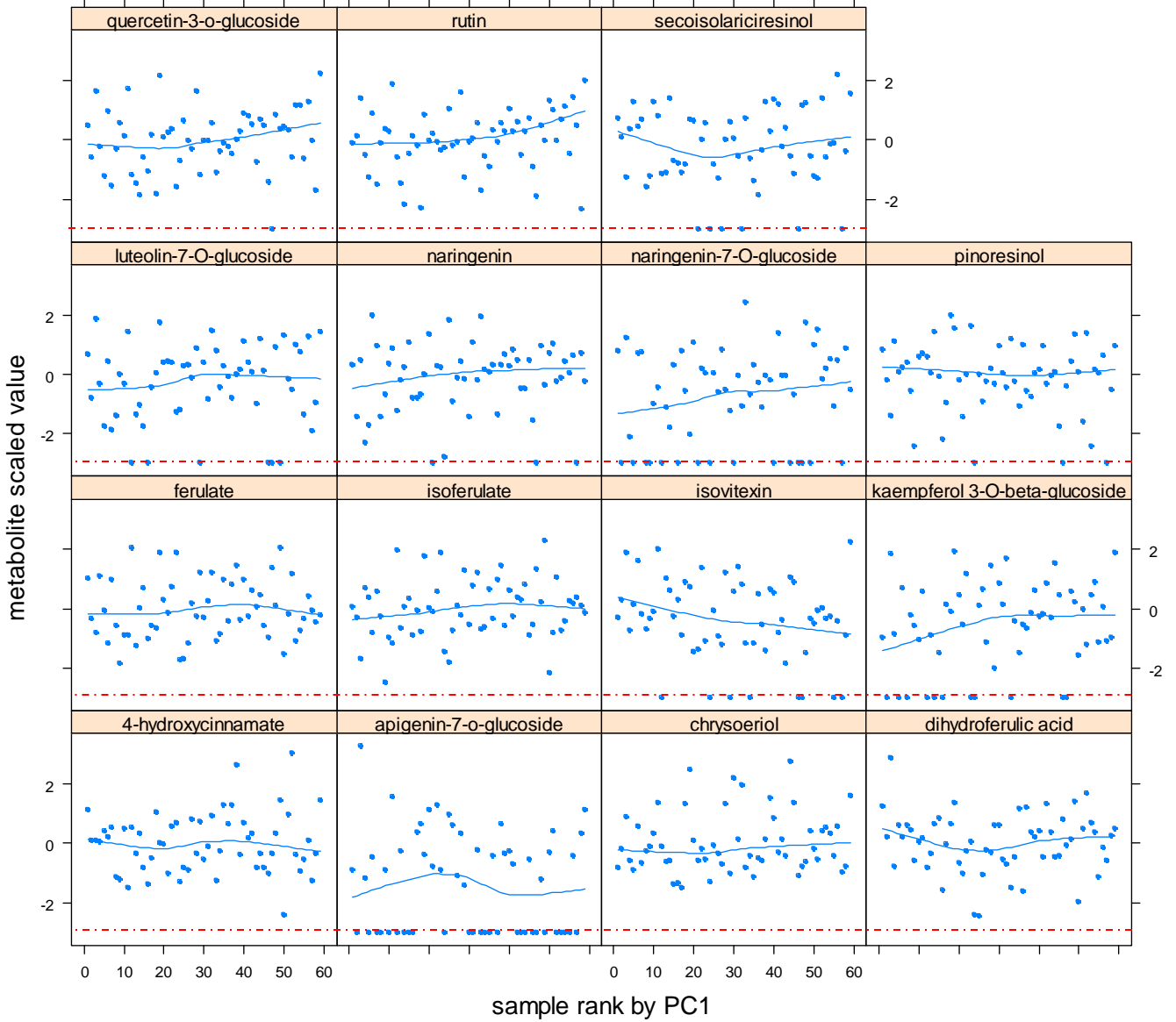
nucleic acid and tRNA nucleosides



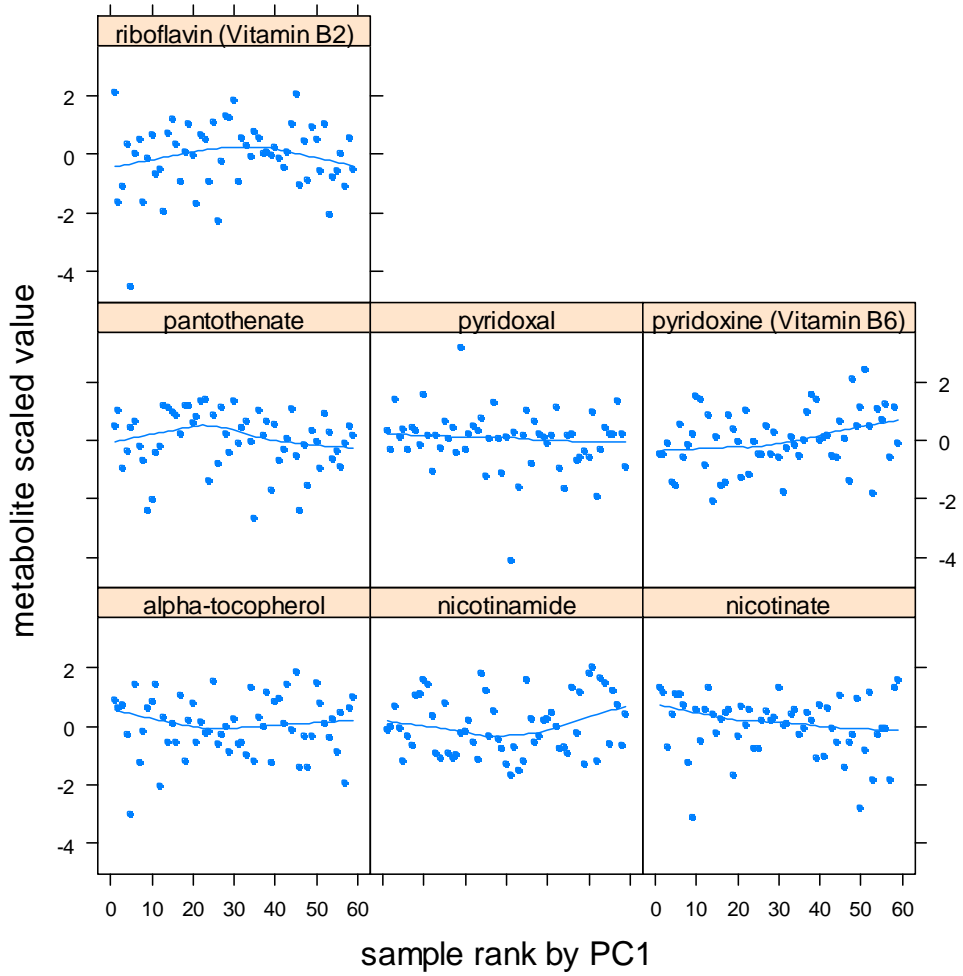
--- missing values were assigned a minimum value of -3

general phenylpropanoid pathway

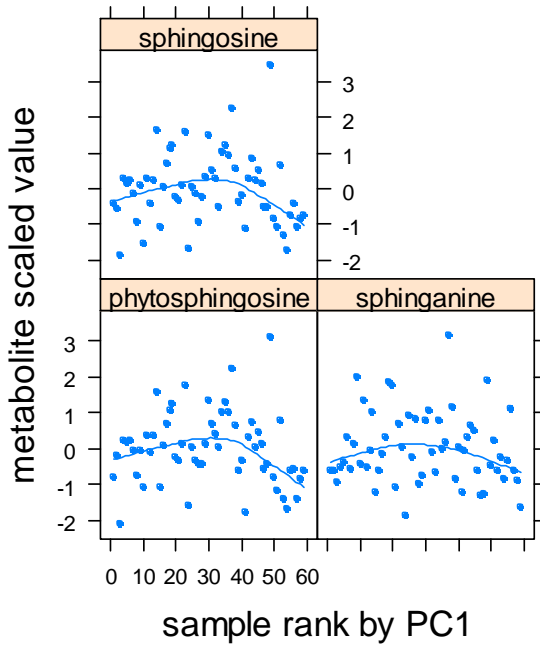
0 10 20 30 40 50 60



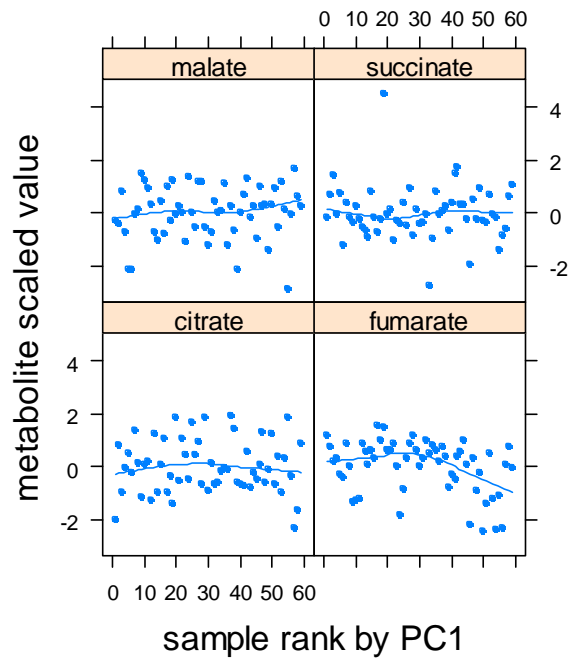
vitamins



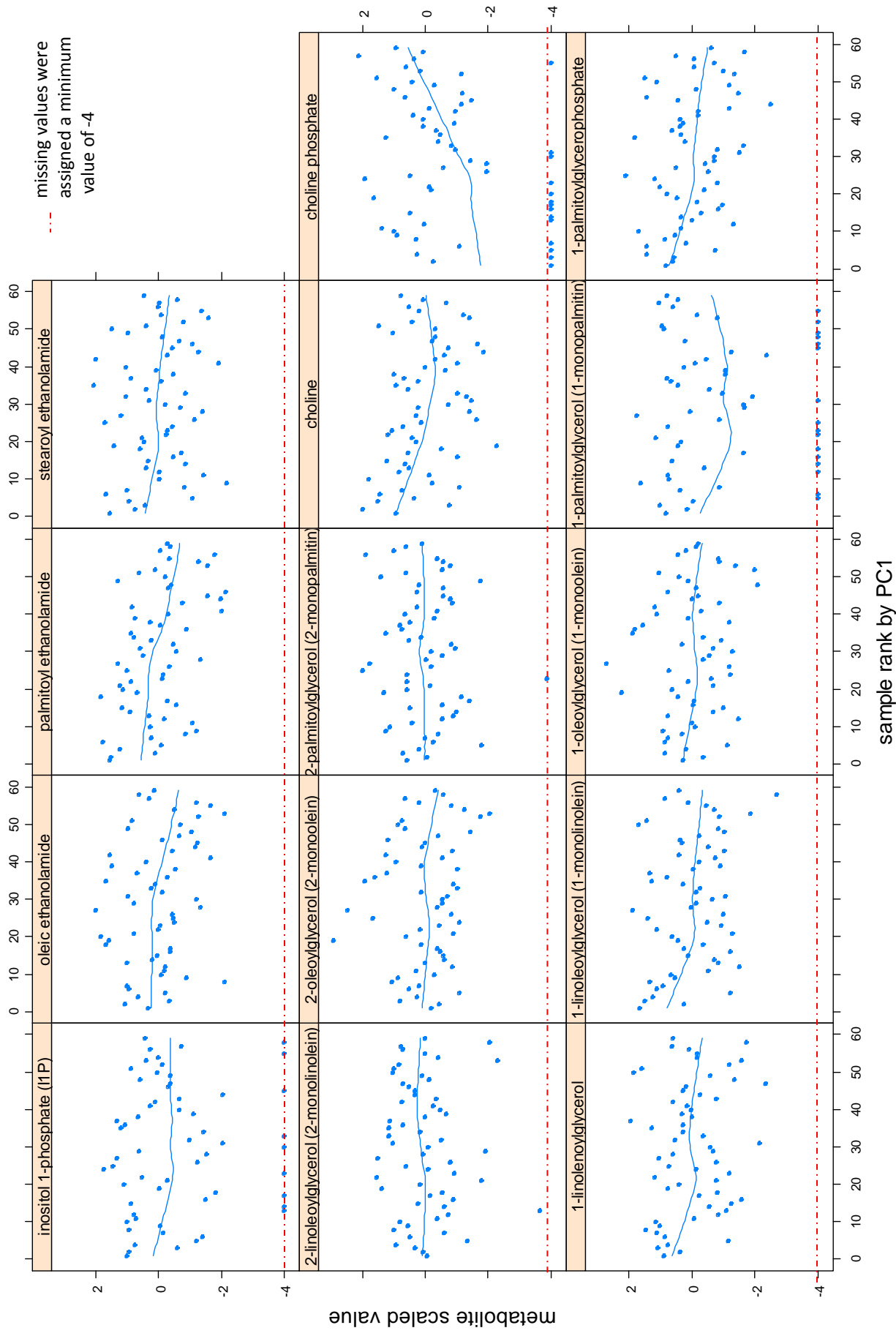
sphingoid bases



TCA

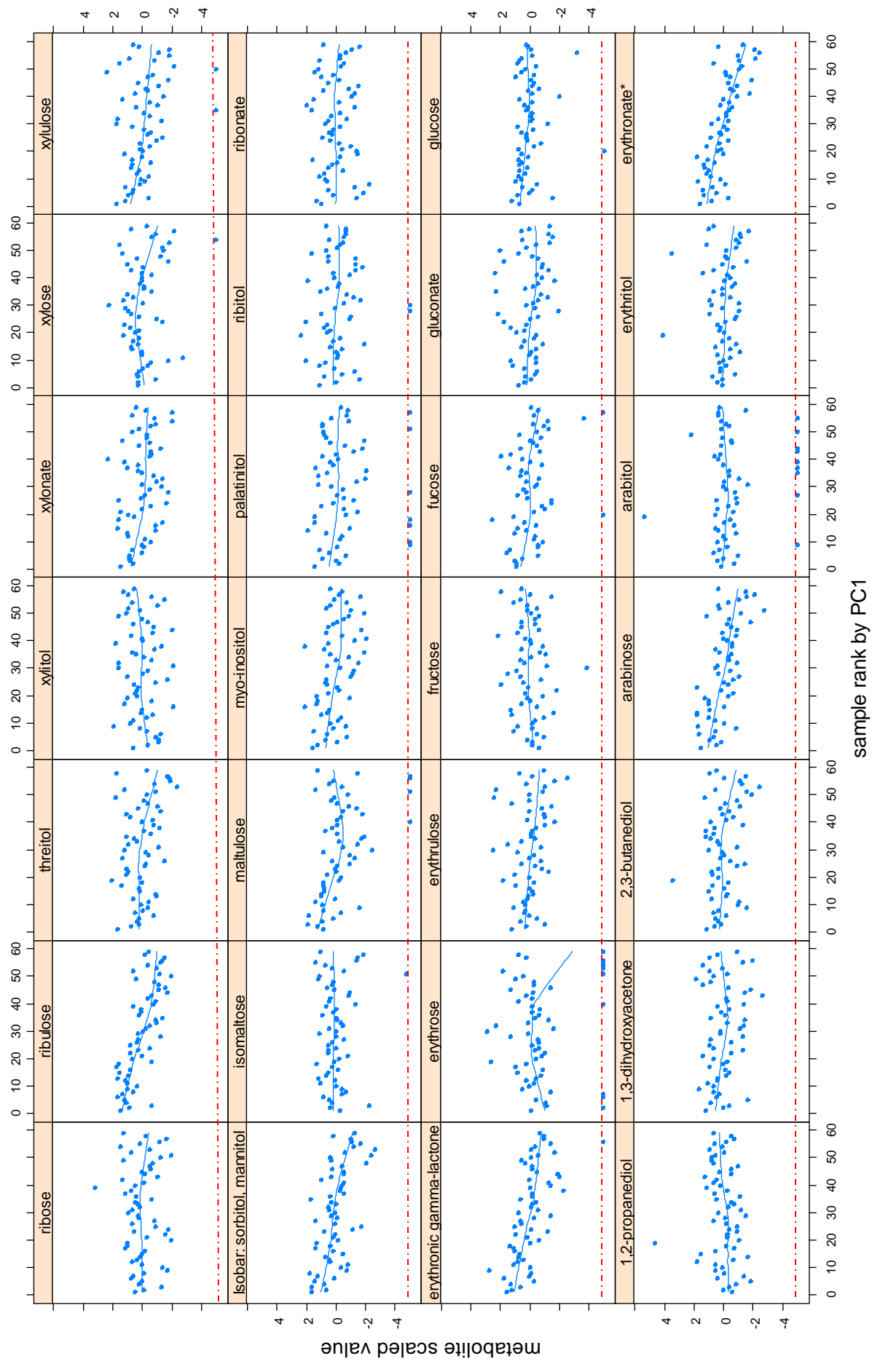


lysophospholipid degradation



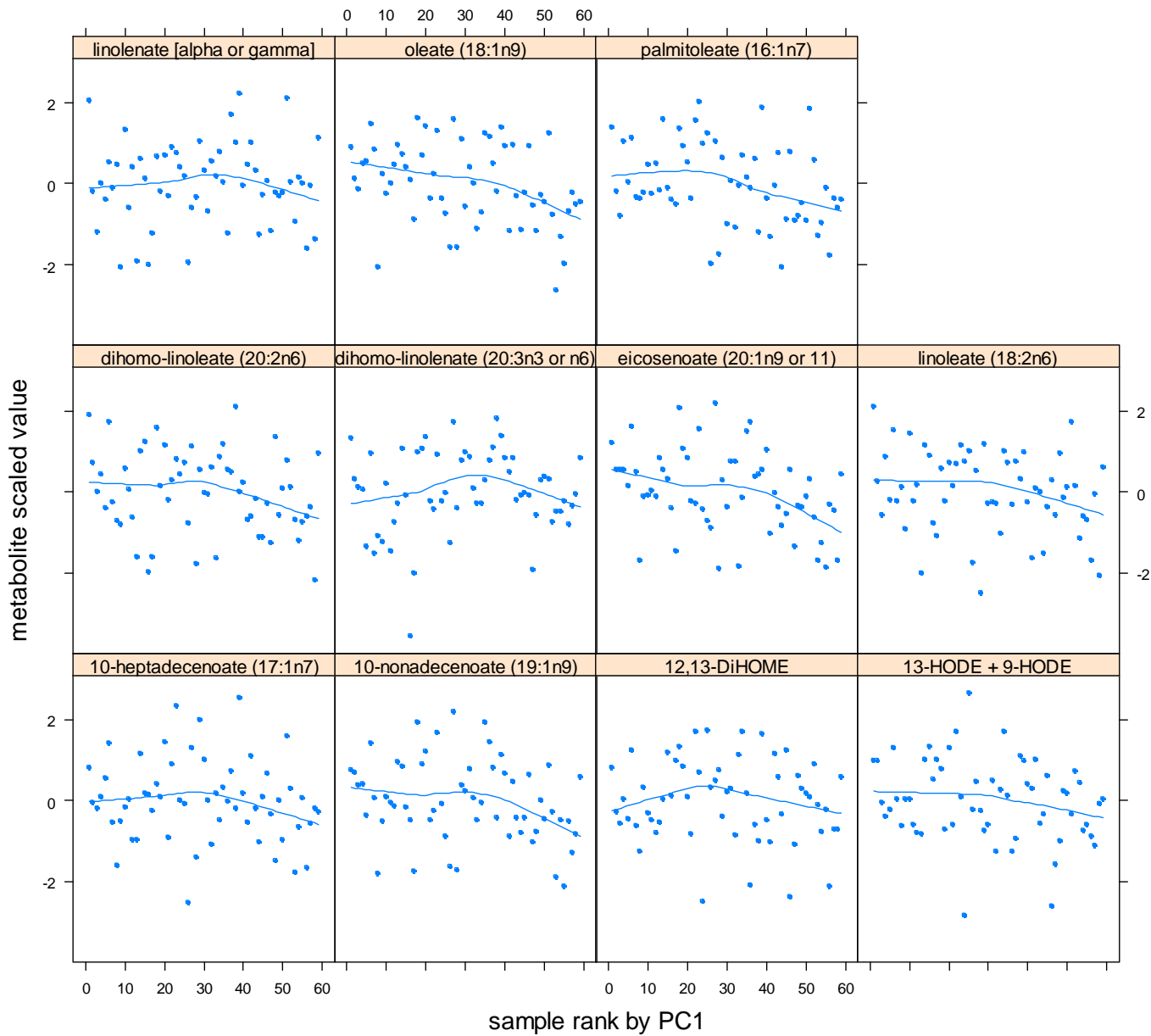
--- missing values were assigned a minimum value of -4.5

reducing sugars and derivative lactones, acids and alcohols



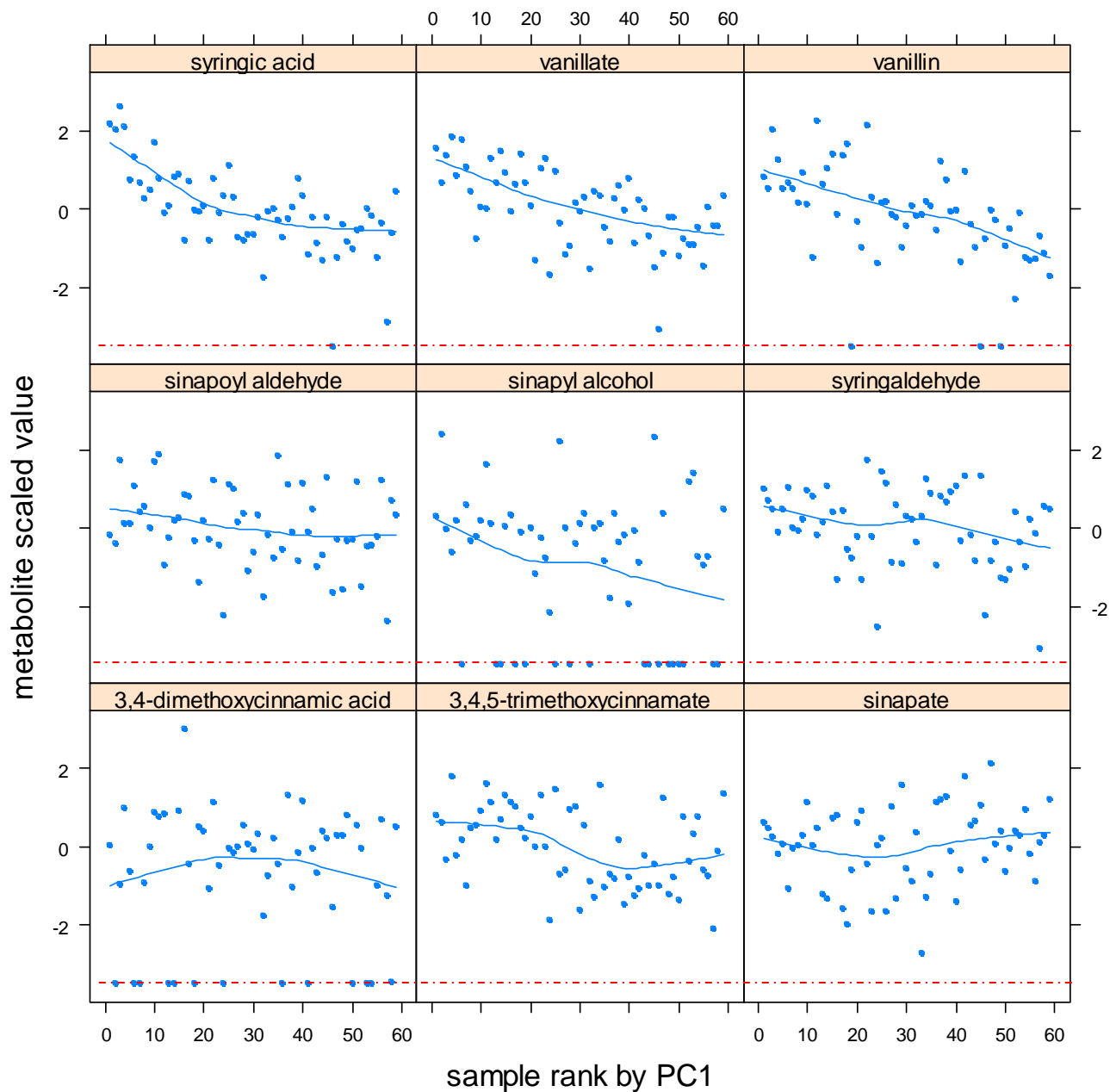
sample rank by PC1

unsaturated fatty acids and oxylipins



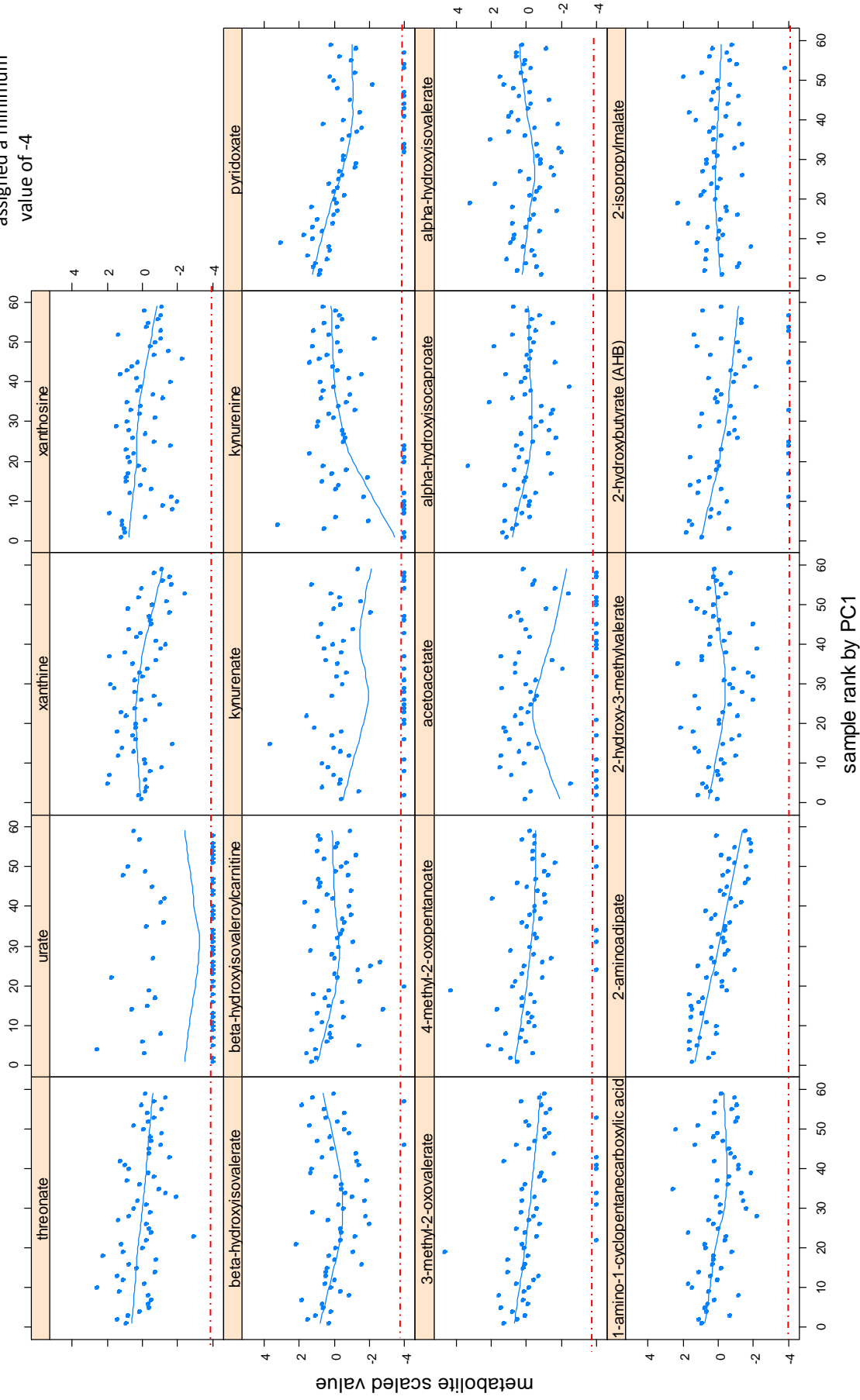
--- missing values were assigned a minimum value of -4

polymethoxycinnamates, derivative hydroxybenzoates and VOCs

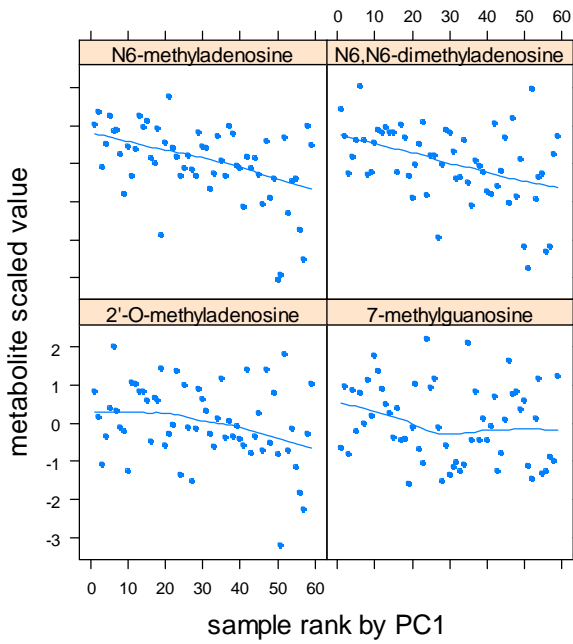


degradation activity and amino acid VOCs

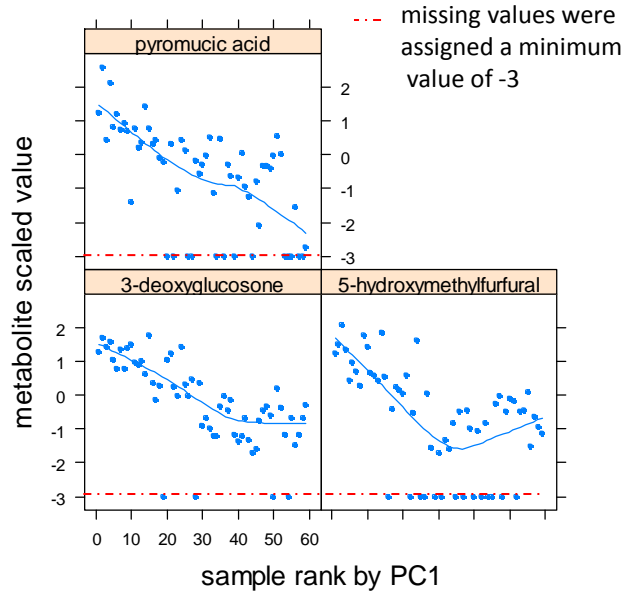
--- missing values were assigned a minimum value of -4



rRNA nucleosides



sugar dehydration



glycolysis

