

Phenotype-driven identification of modules in a hierarchical map of multifluid metabolic correlations

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Supporting Information S2: Explained variance of SHIP-TREND sub- and super-pathways

To enable the construction of a pathway-based correlation network, a single representative value per sample was defined as the first principal component of the metabolite concentrations in each sub-pathway (termed sub-pathway *eigenmetabolite*). 22% of the plasma, 34% of the urine, and 33% of the saliva sub-pathways comprise only one metabolite, and thus their representative value is equivalent to the concentration of that one metabolite. For the remaining sub-pathways, the *eigenmetabolite* explains more than 40% of the total sub-pathway variance in the majority of cases (69%, 57%, and 80% of plasma, urine, and saliva sub-pathways, respectively, Figure S2). This rather high degree of explained variance indicates that the predefined pathways mostly represent homogeneous groups of metabolites, and thus *eigenmetabolites* are reasonable statistical representatives of the pathways. Urine showed a lower number of *eigenmetabolites* explaining more than 40% variance than the other two fluids, suggesting a higher fraction of heterogeneous sub-pathways.

For super-pathways, we refrained from estimating a super-pathway GGM based on the super-pathway *eigenmetabolites* due to very high heterogeneity in some super-pathways. Only ‘Carbohydrate [plasma]’, ‘Carbohydrate [saliva]’, ‘Energy [saliva]’, and ‘Energy [urine]’ showed an explained variance of >40% in the first PC (Figure S2).

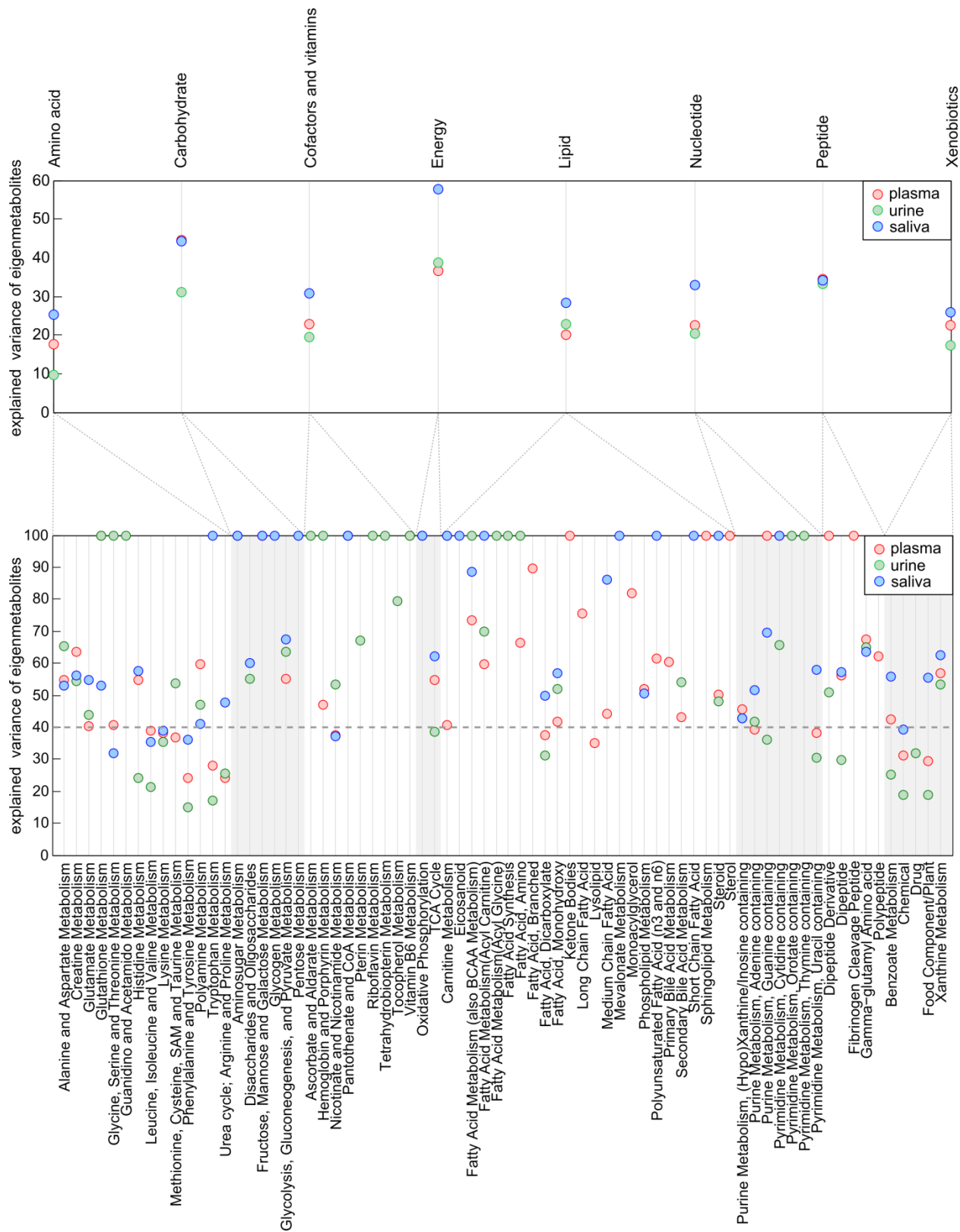
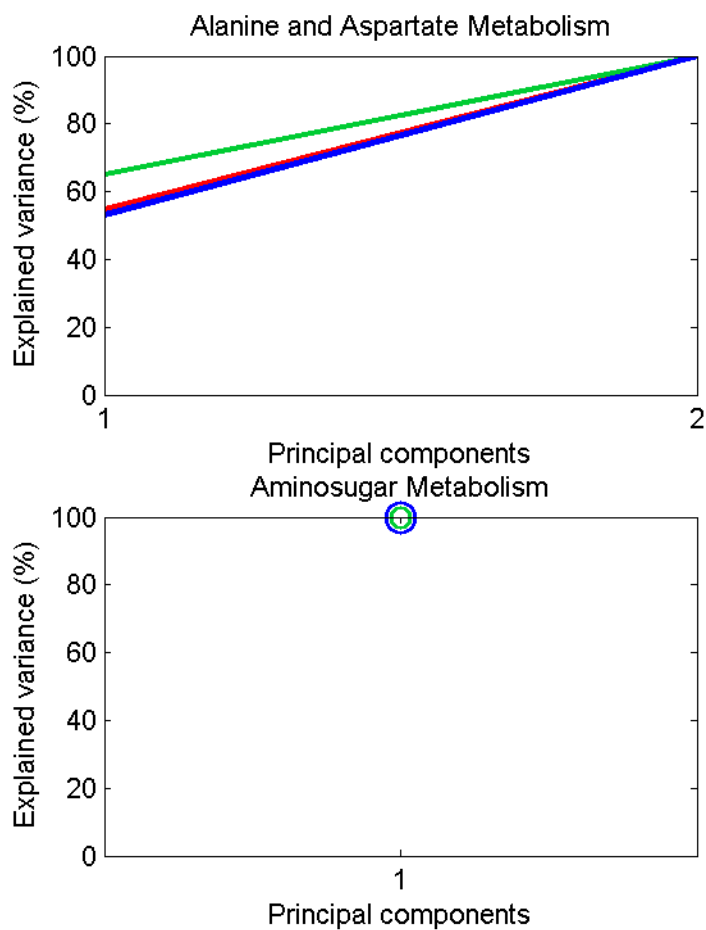
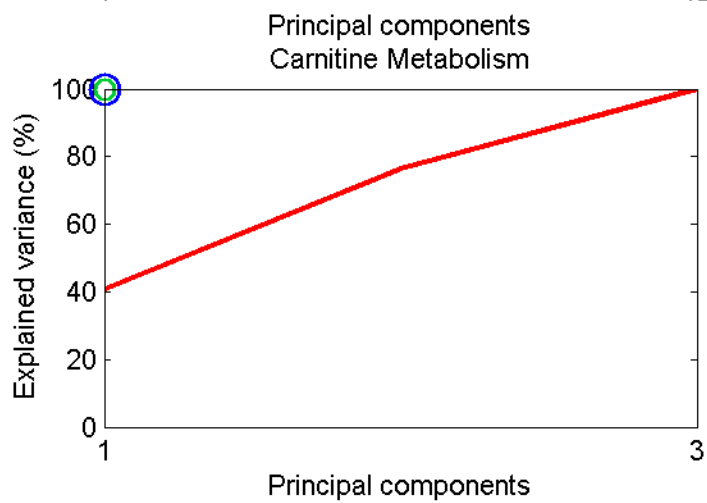
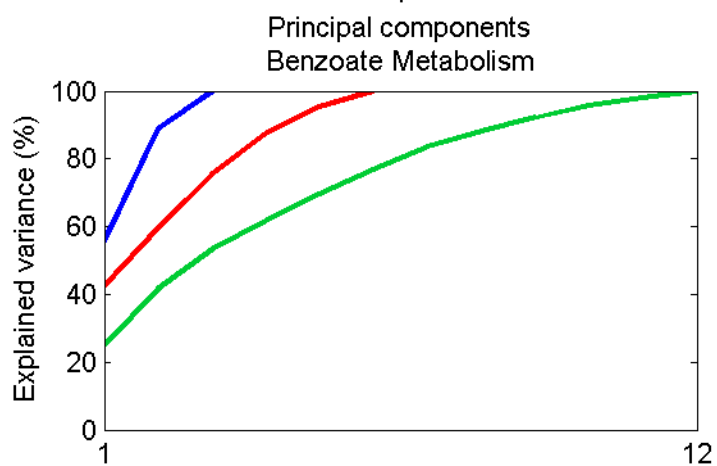
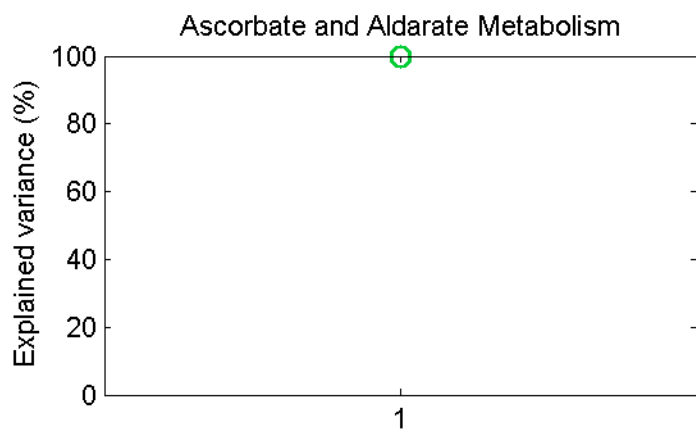


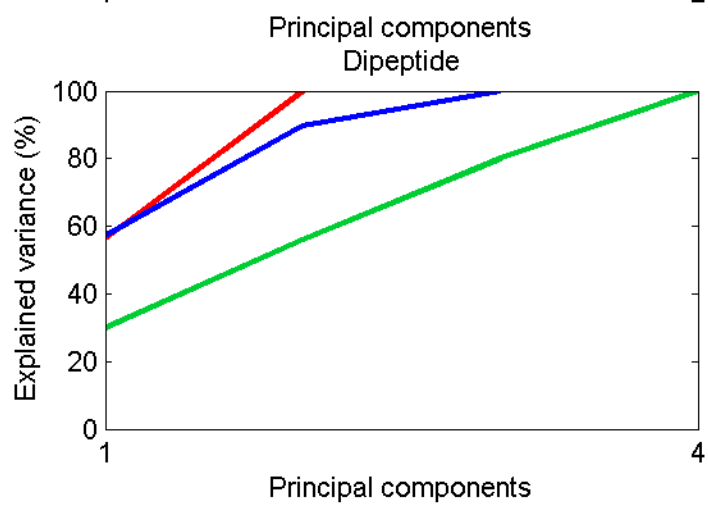
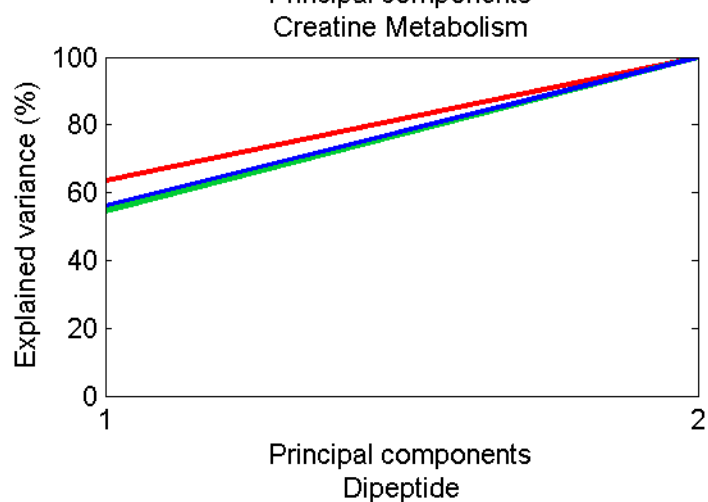
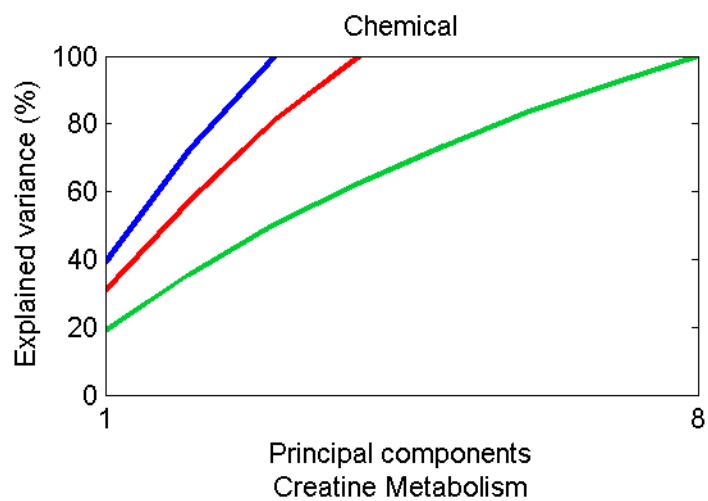
Figure S2. Explained variance of super- (top) and sub-pathway (bottom) eigenmetabolites.

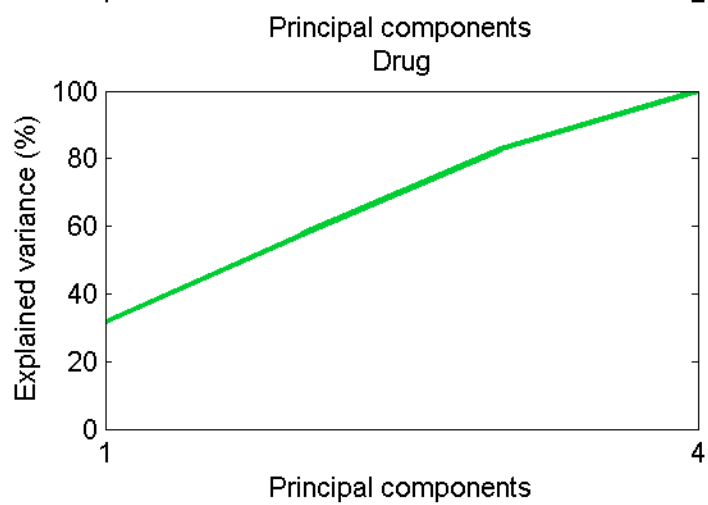
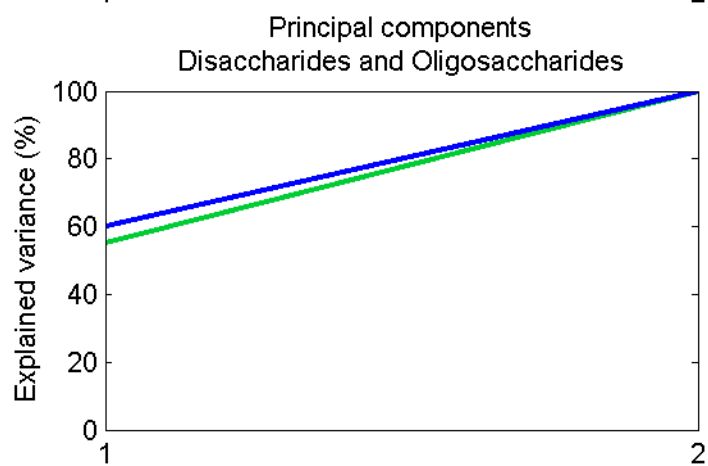
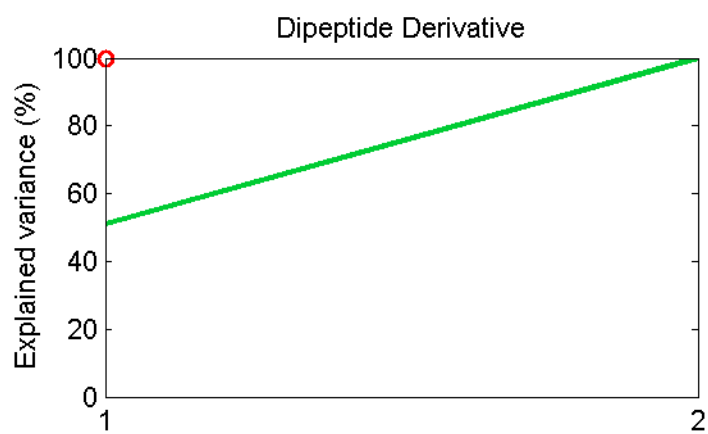
The following figures depict the cumulative explained variances of all principal components for each sub- and super-pathway in plasma (red), urine (green), and saliva (blue).

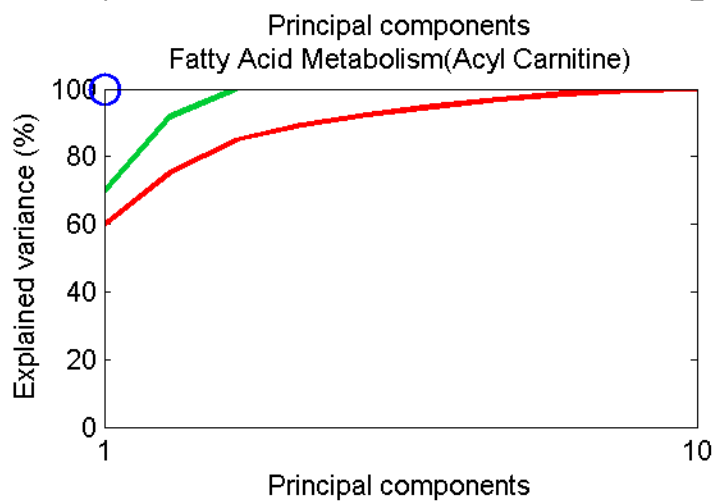
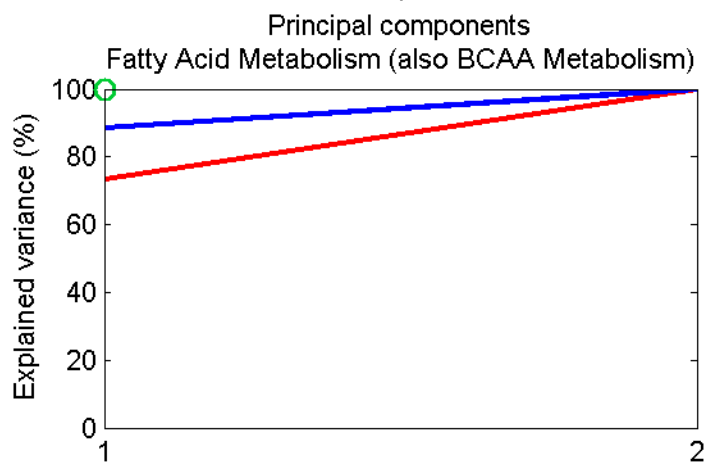
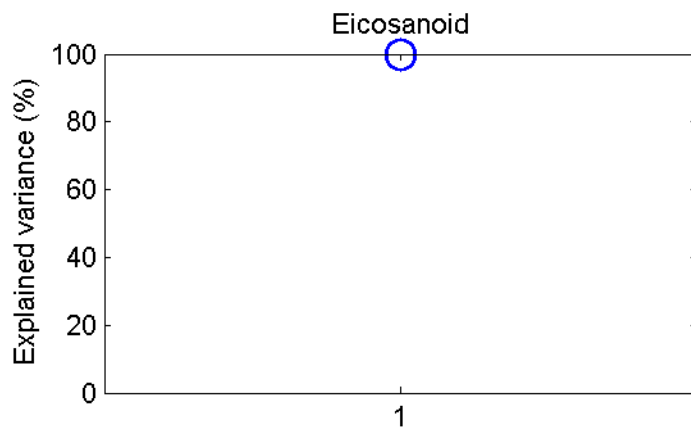
Sub-pathways

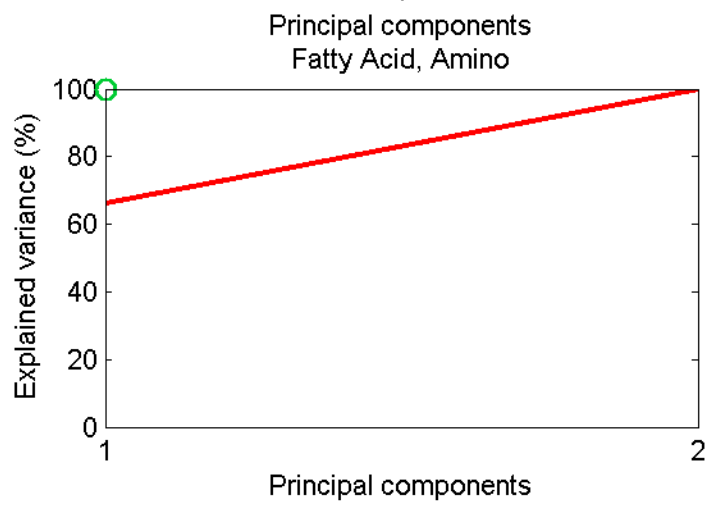
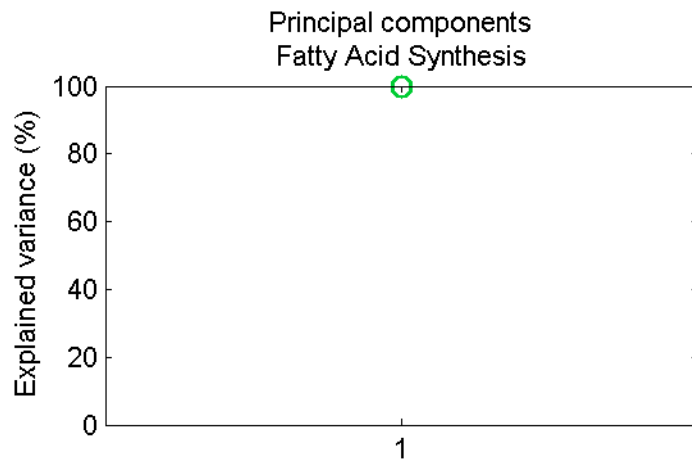
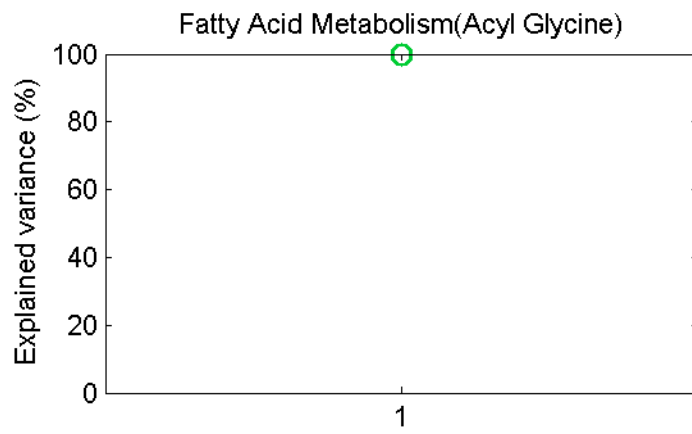


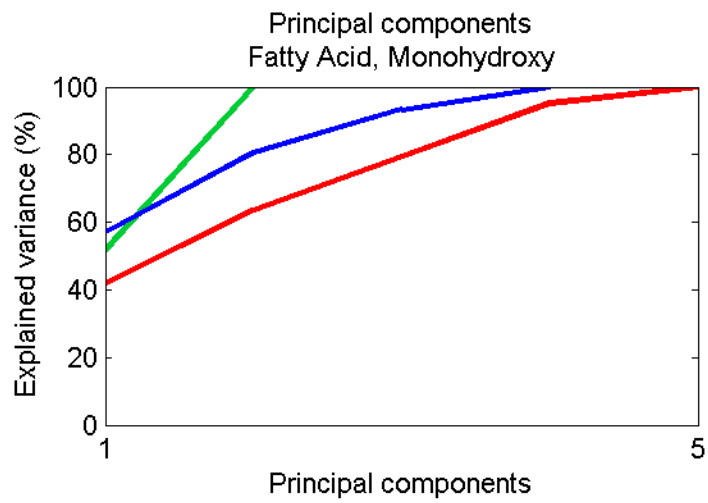
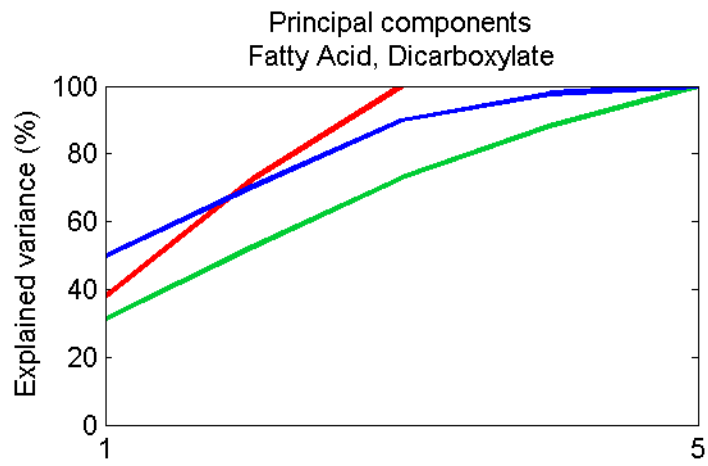
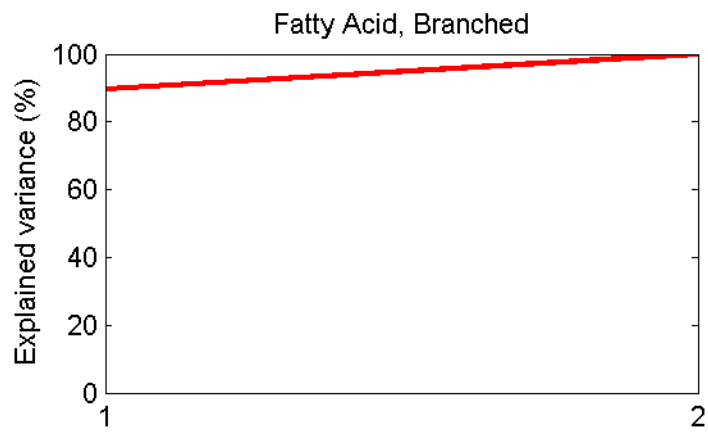


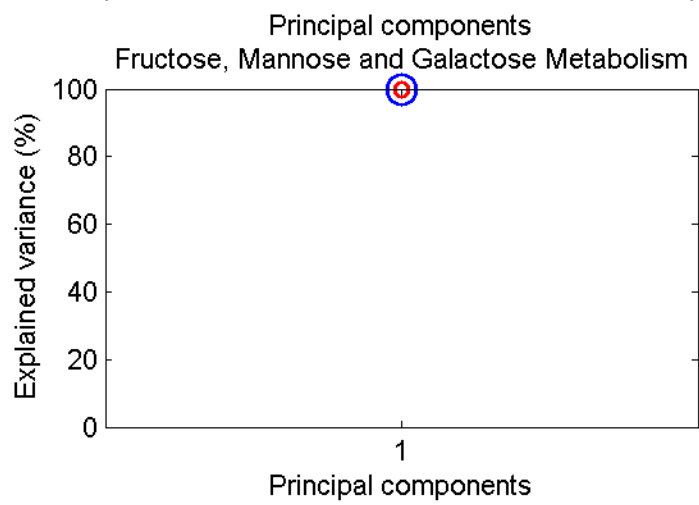
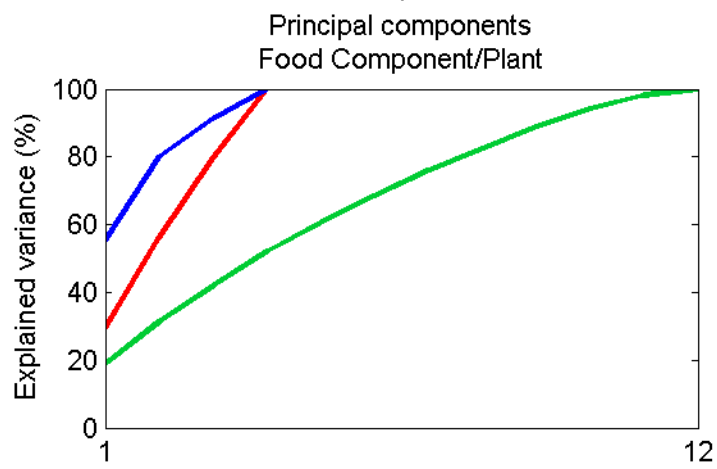
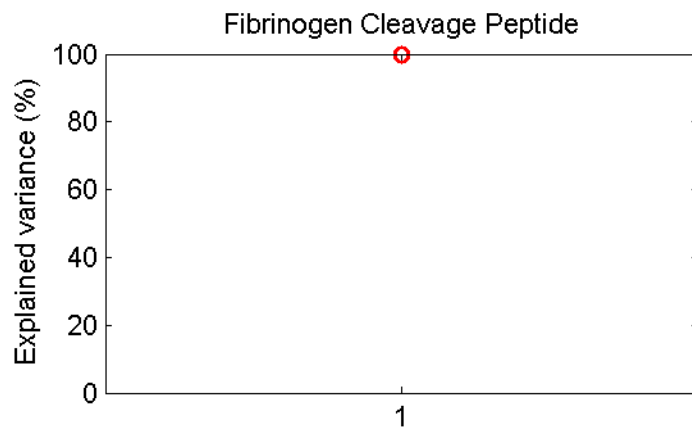


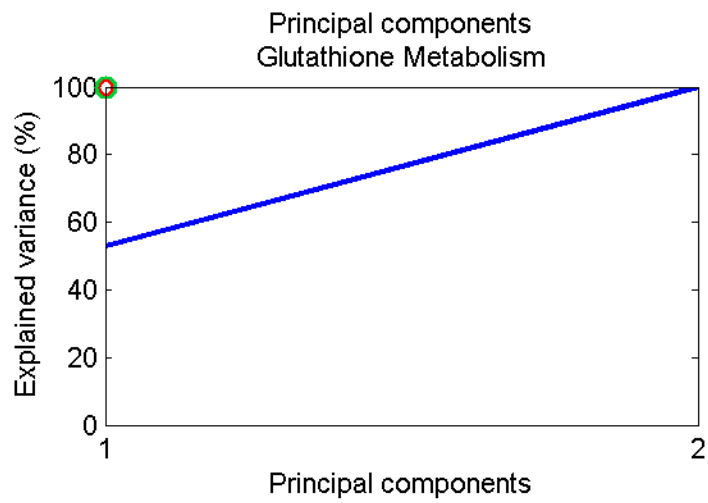
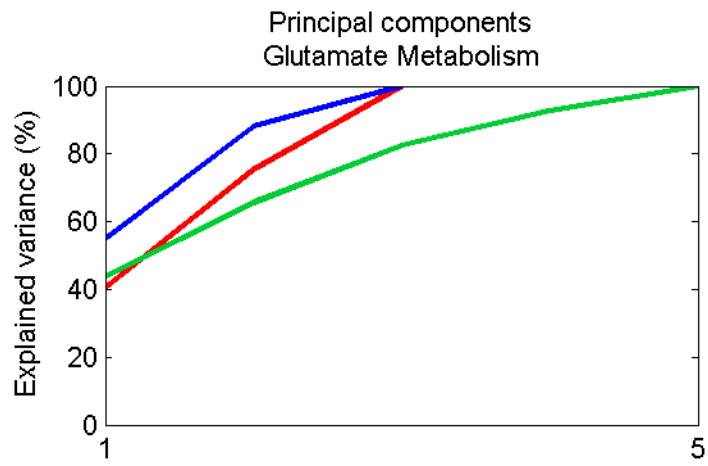
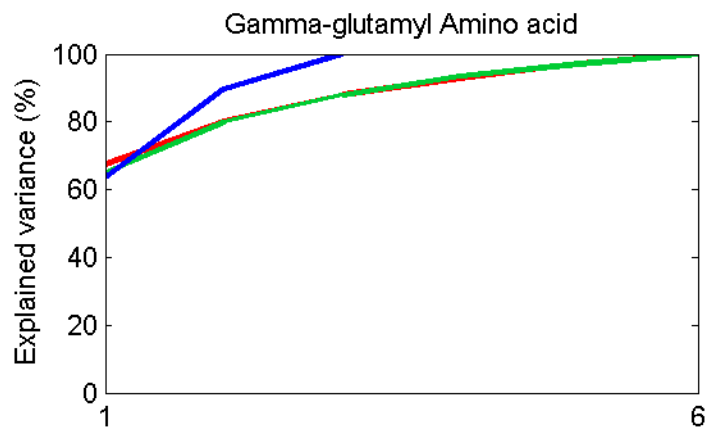


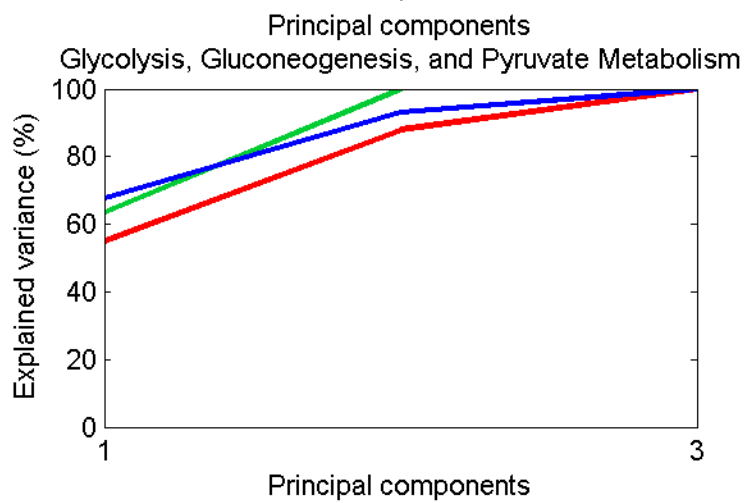
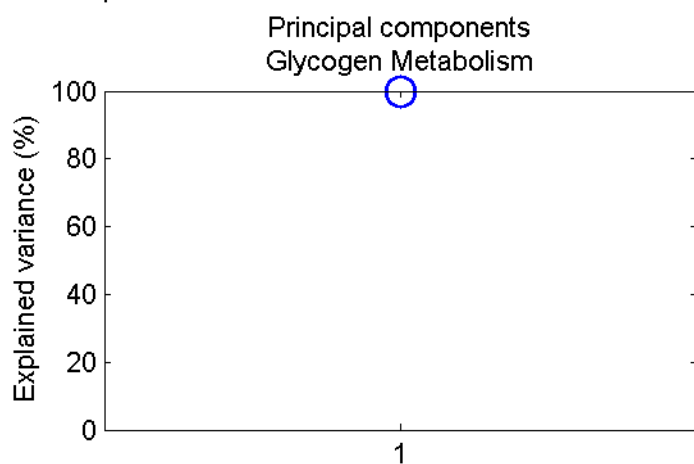
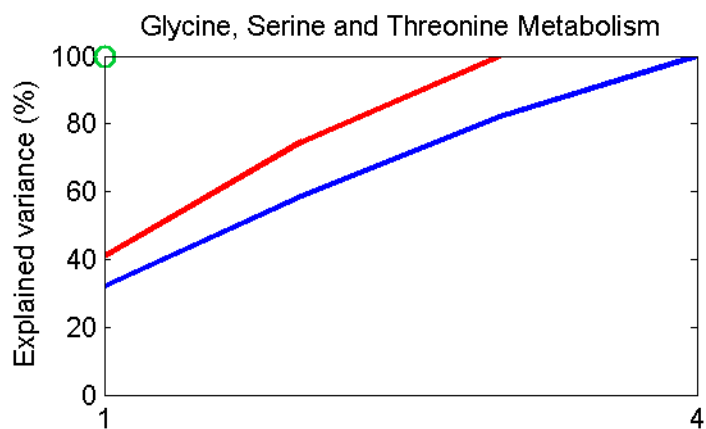


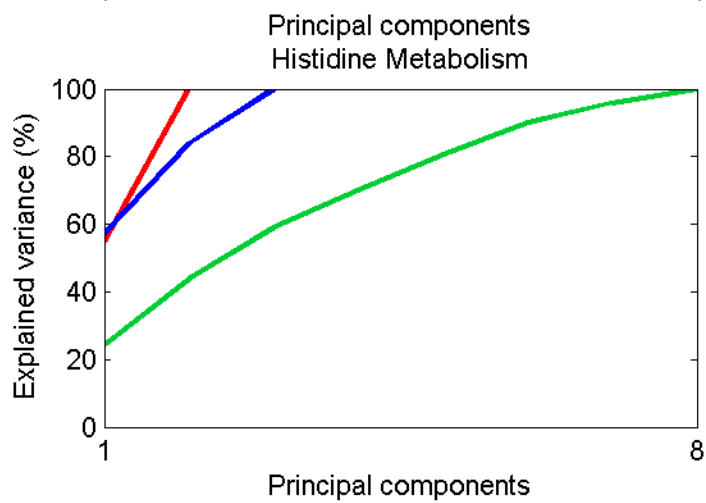
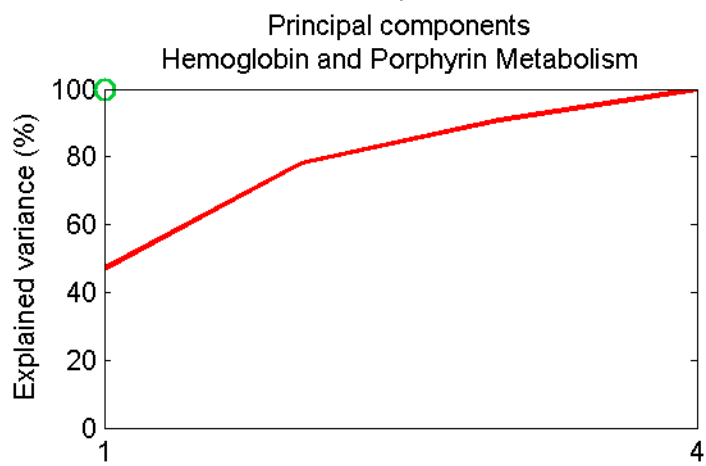
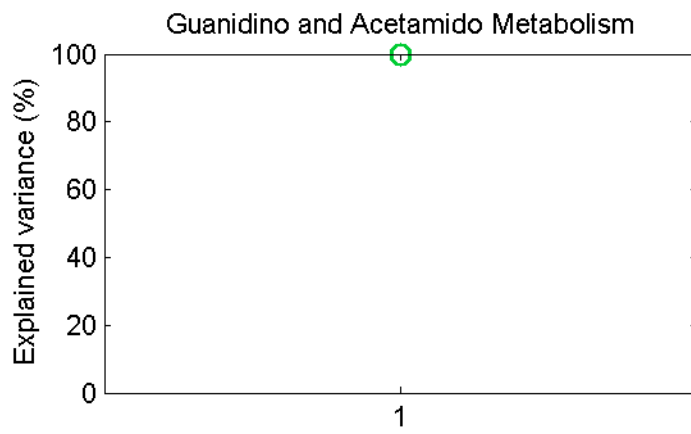


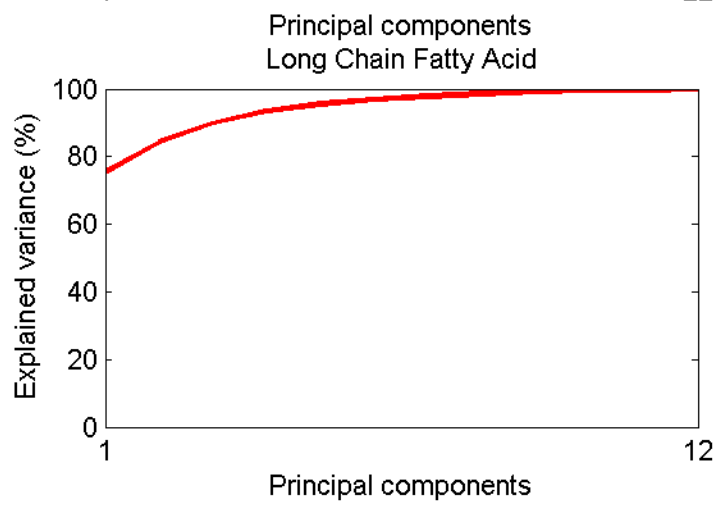
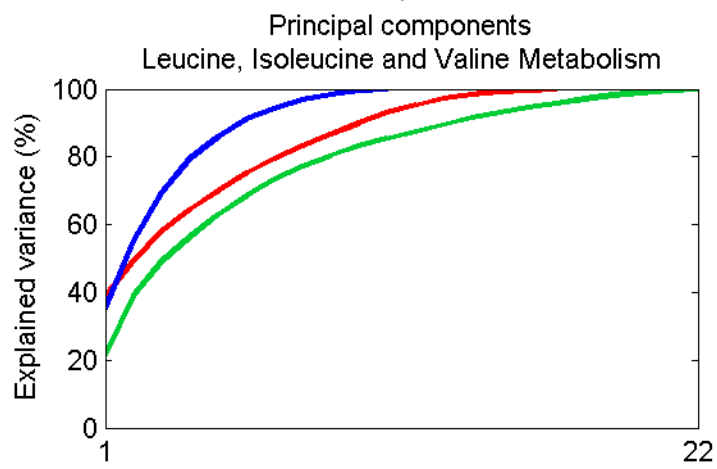
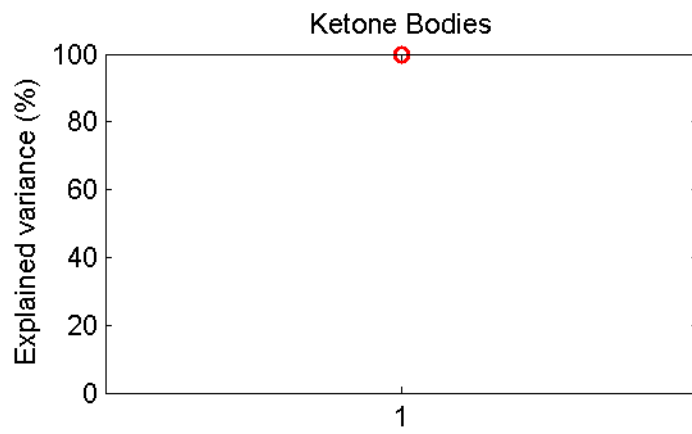


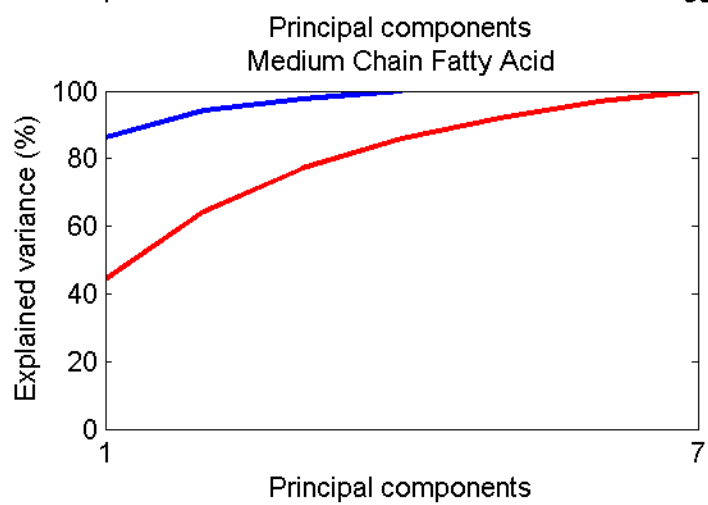
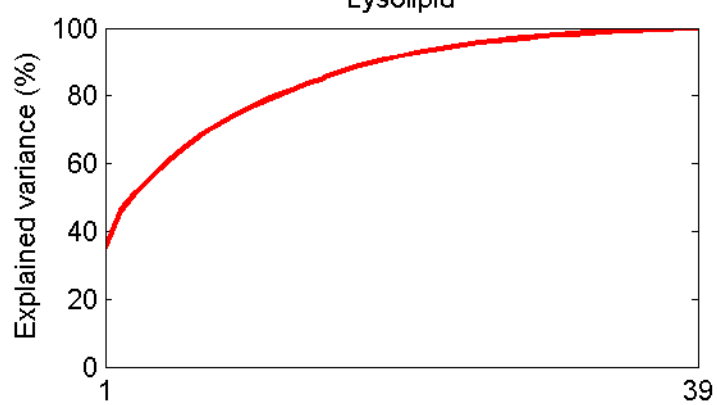
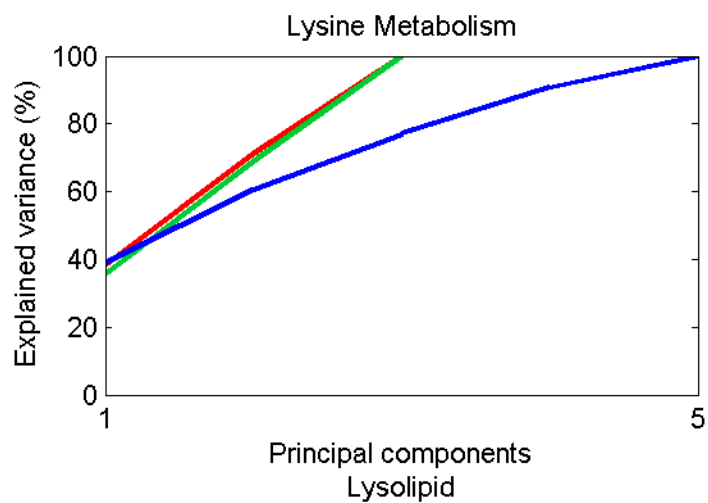


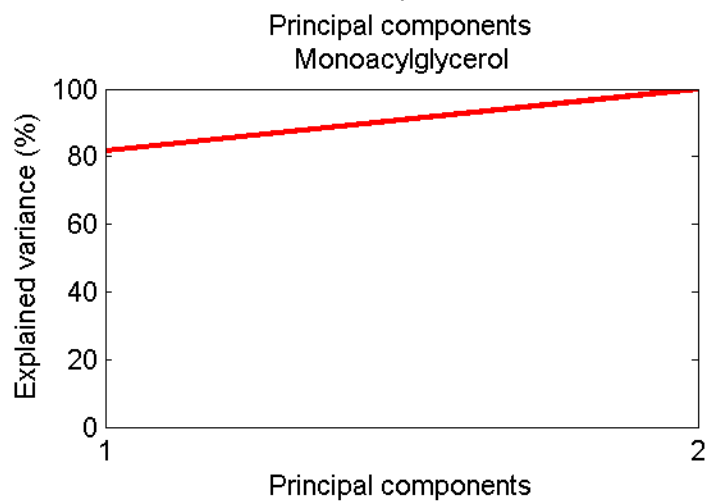
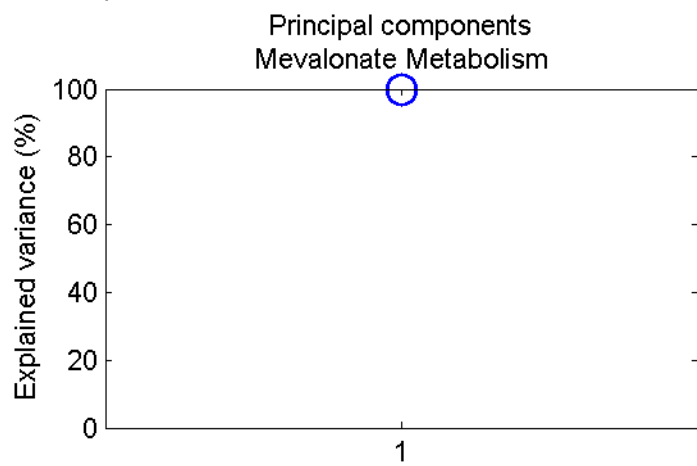
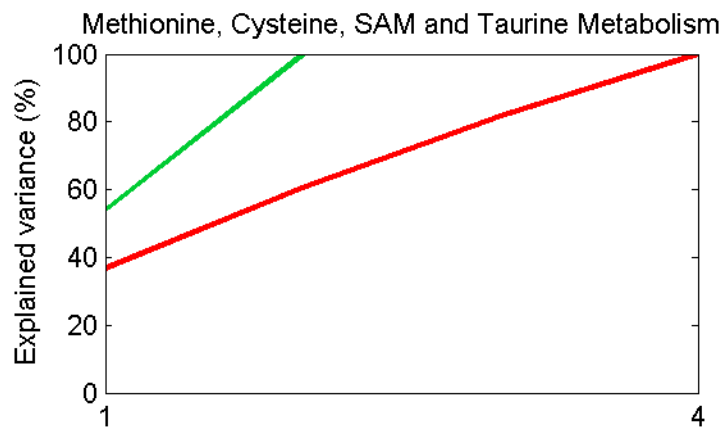


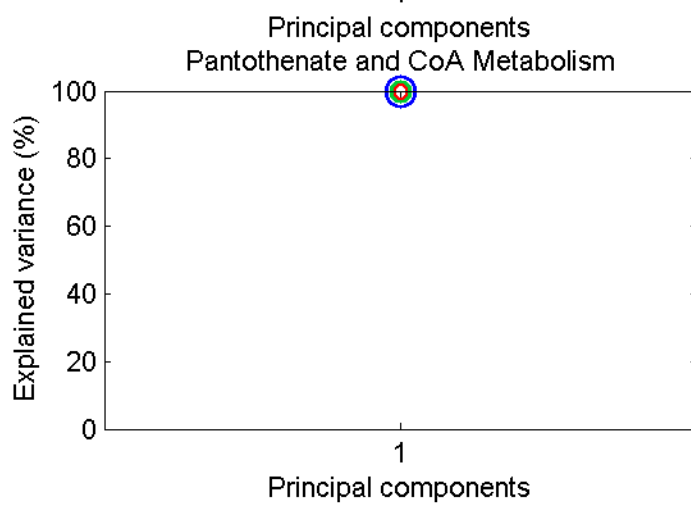
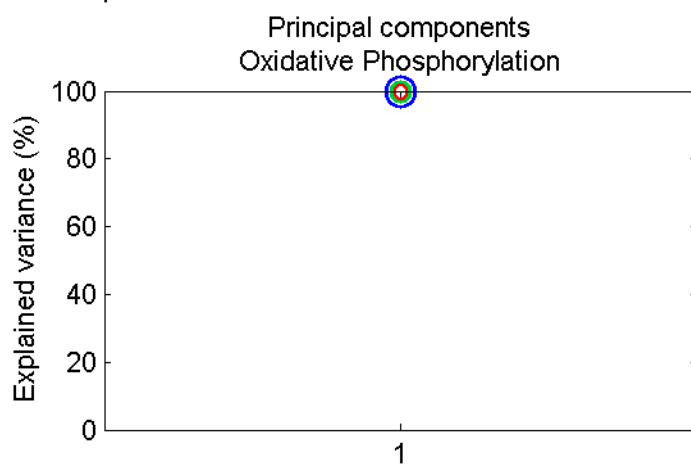
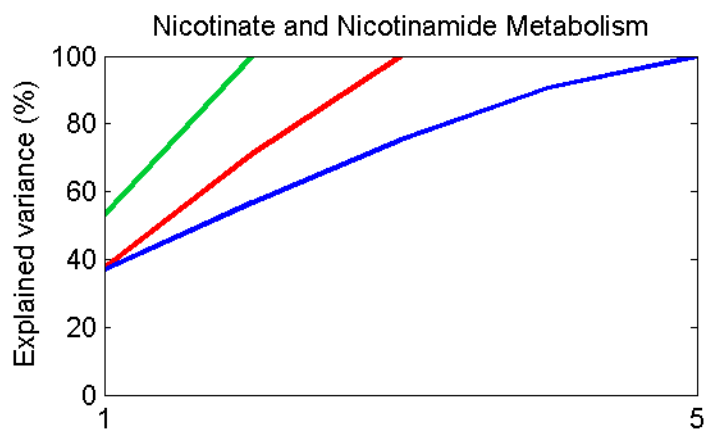


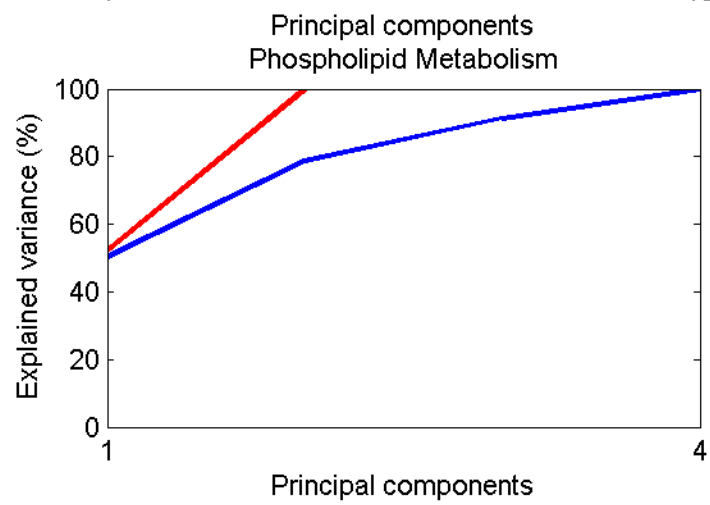
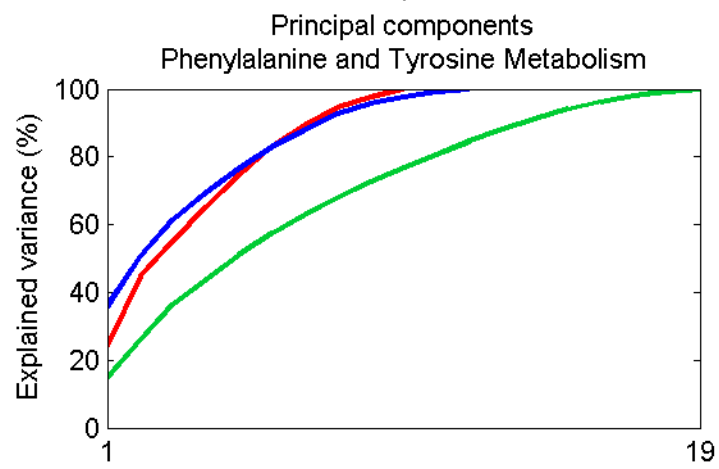
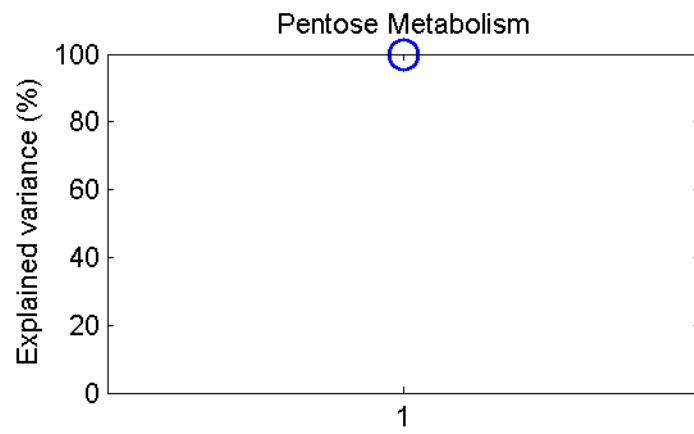


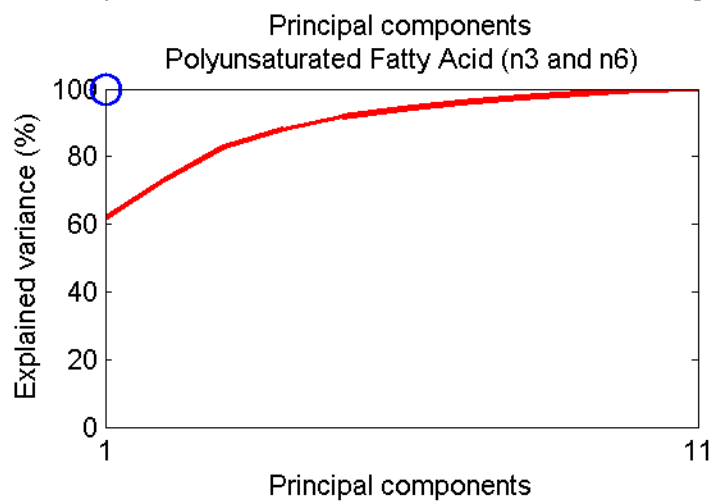
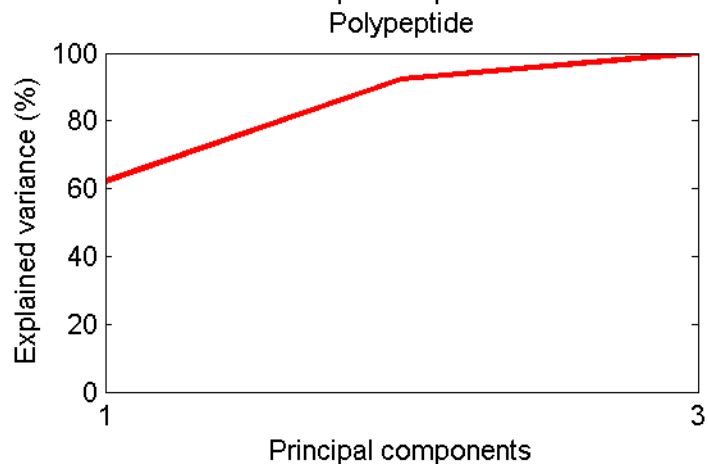
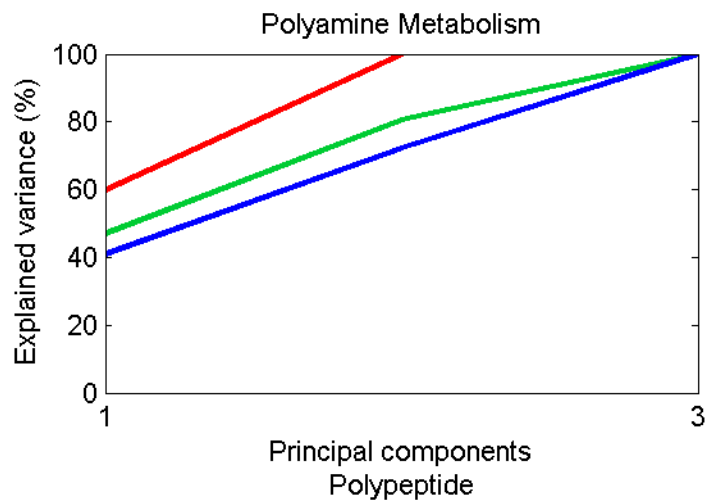


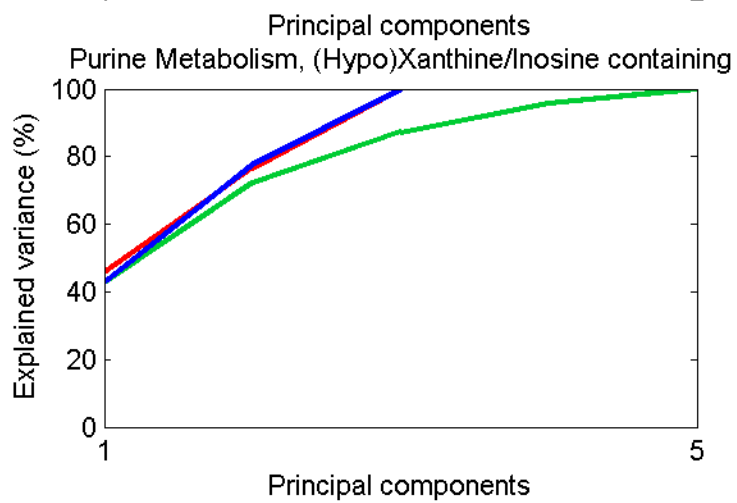
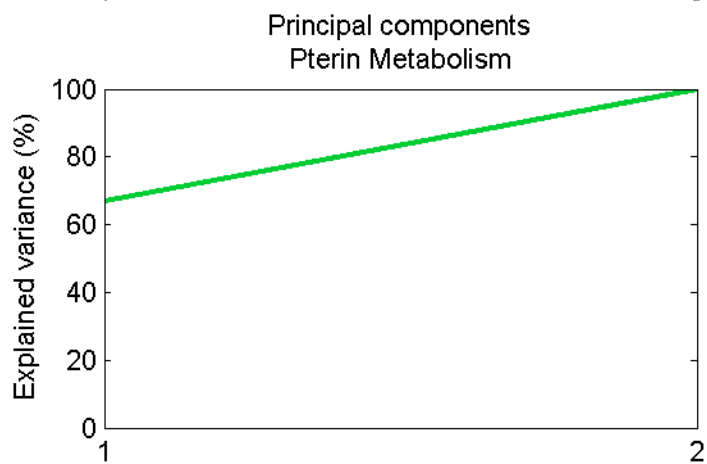
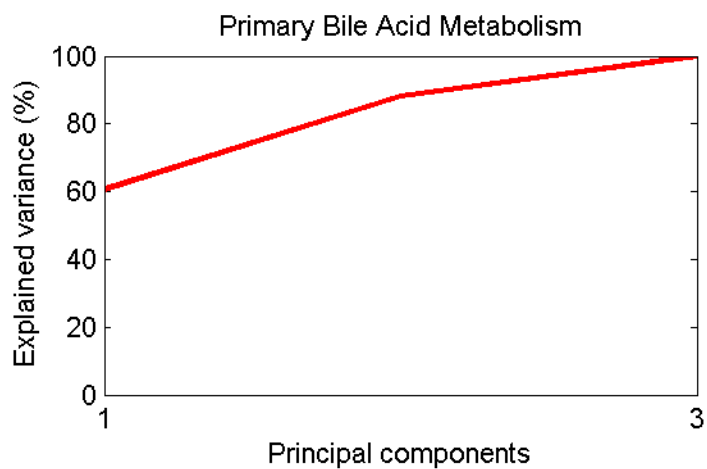


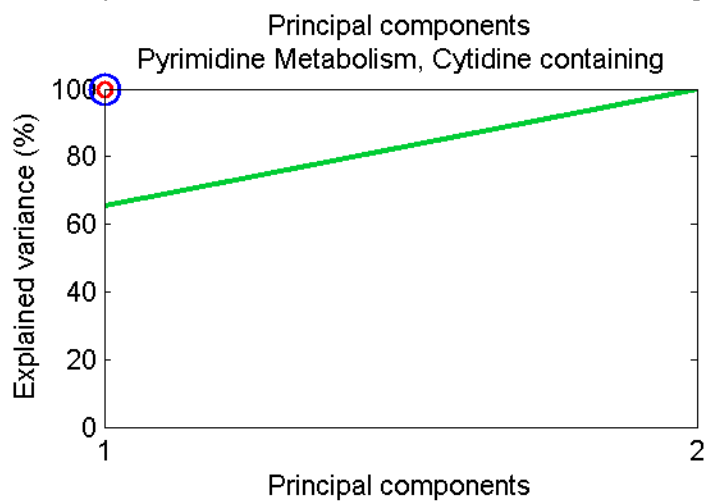
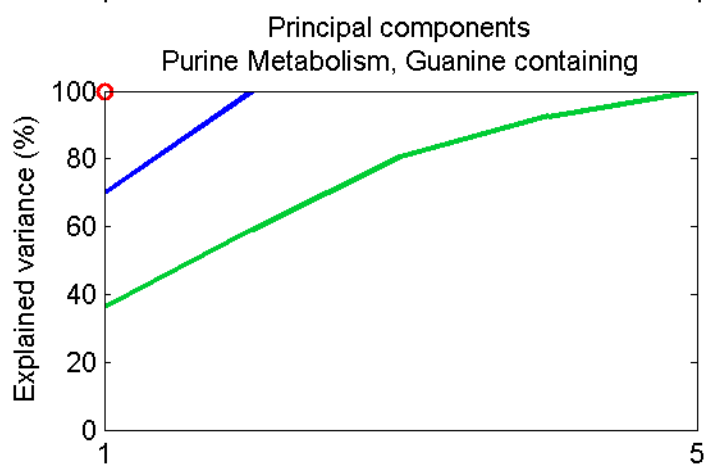
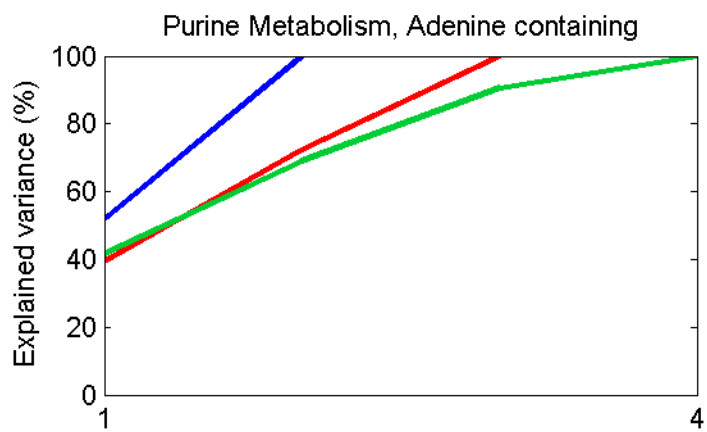


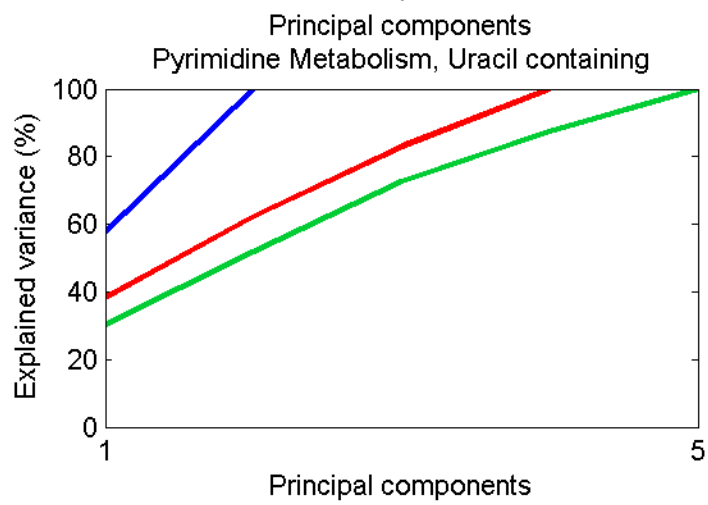
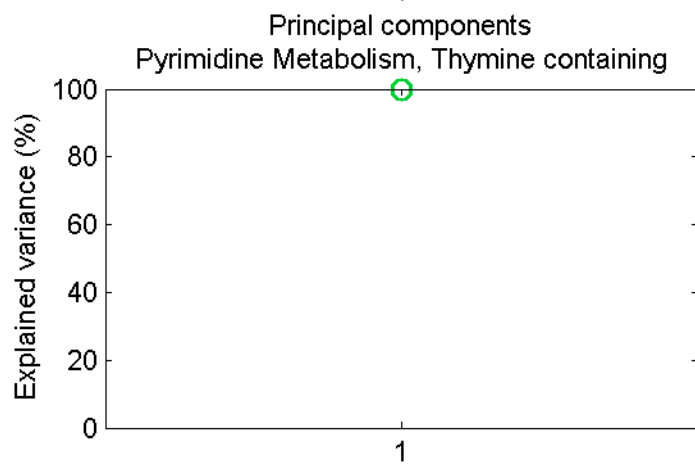
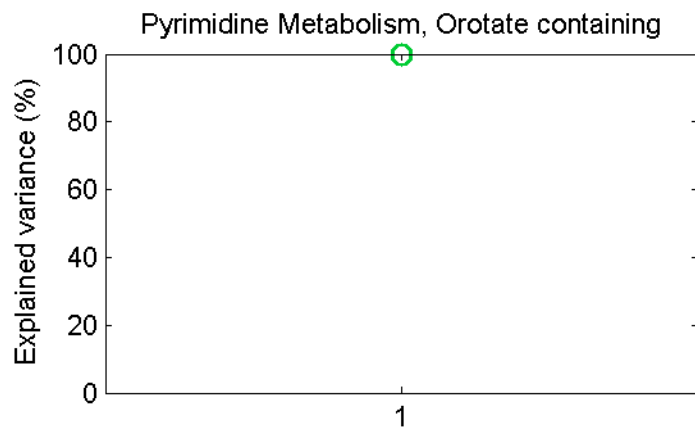


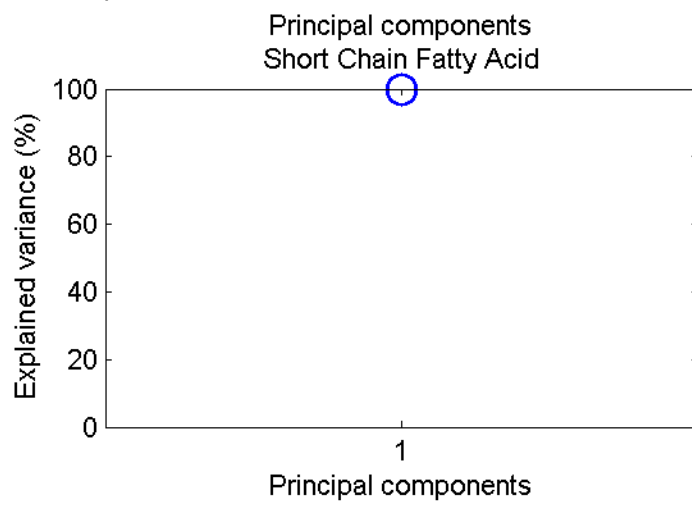
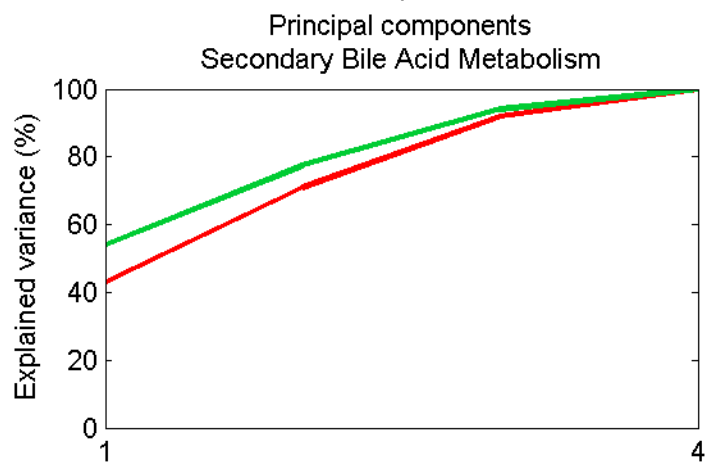
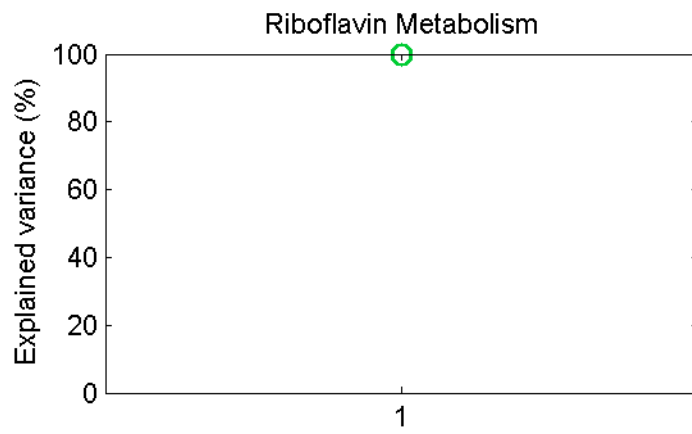


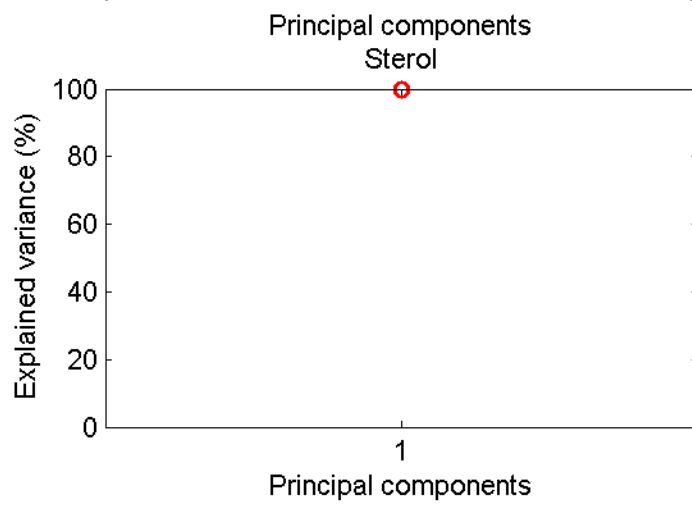
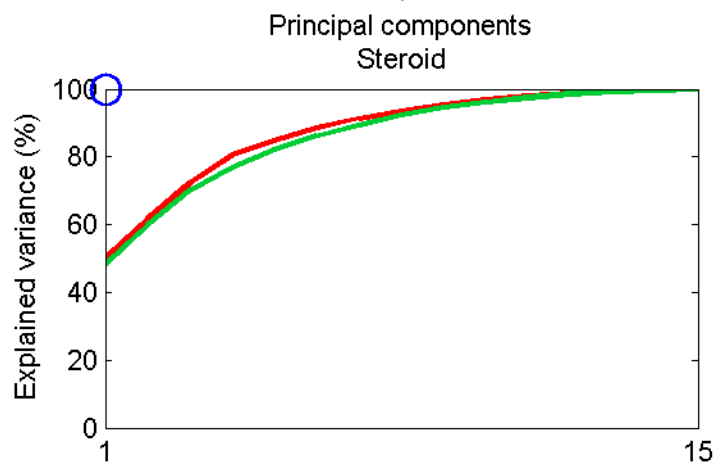
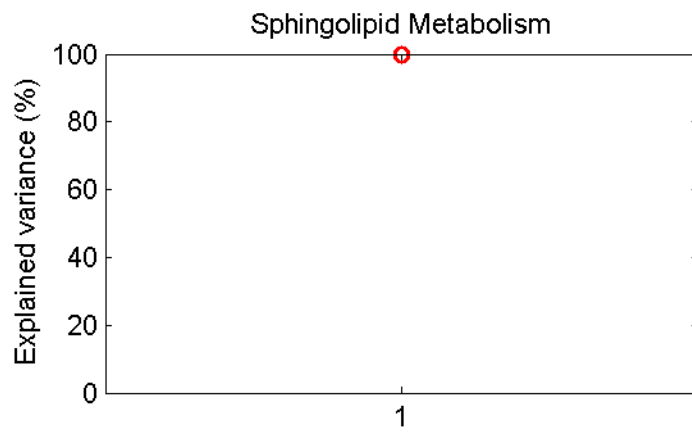


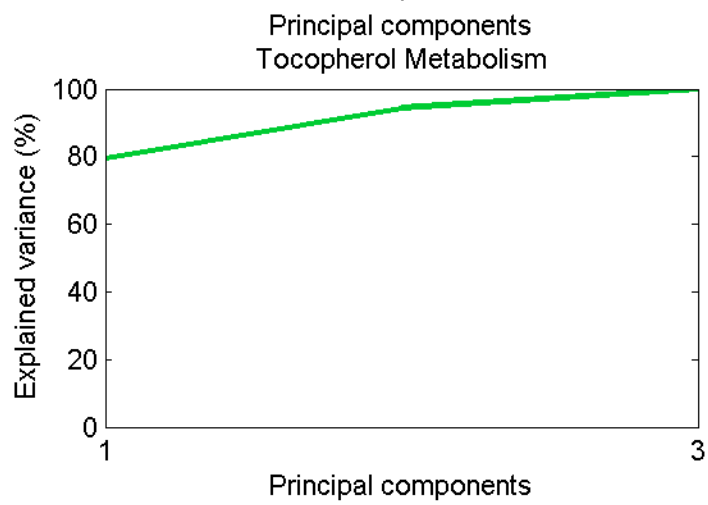
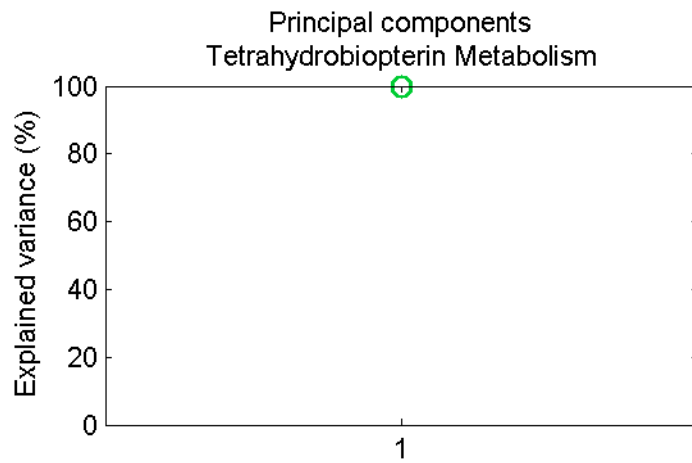
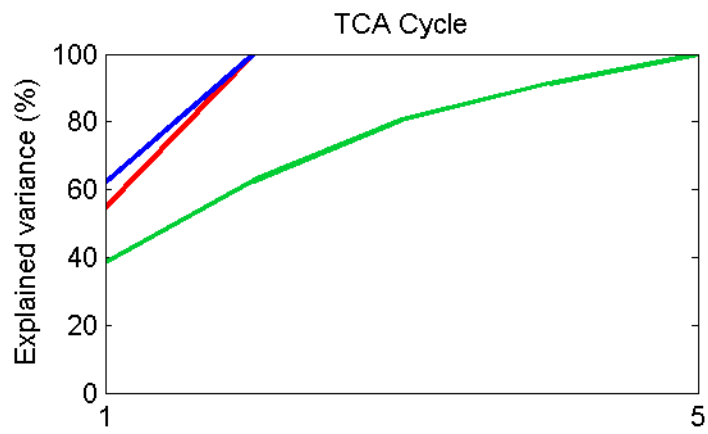


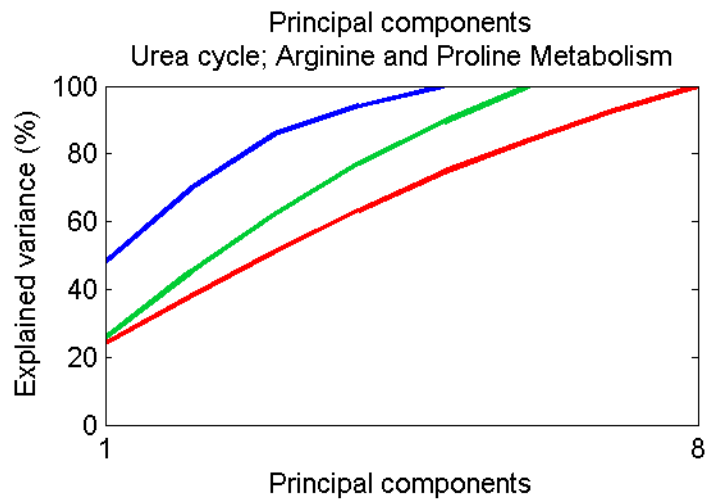
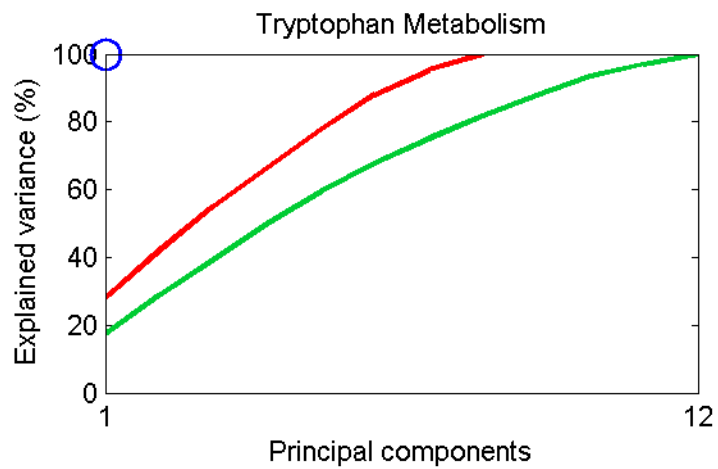


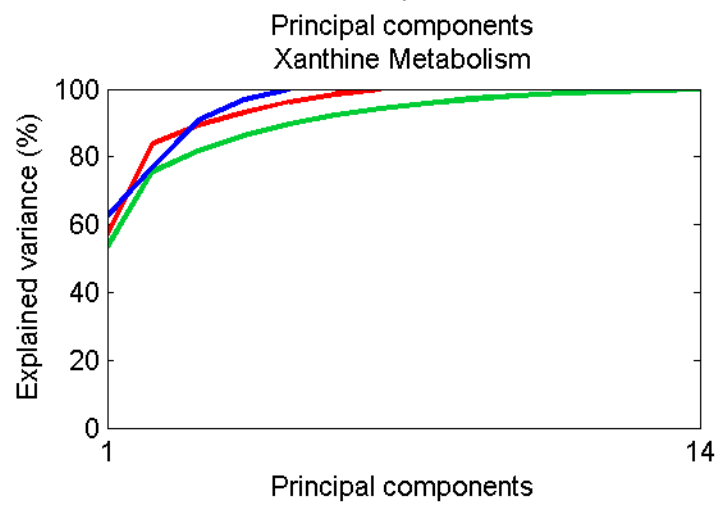
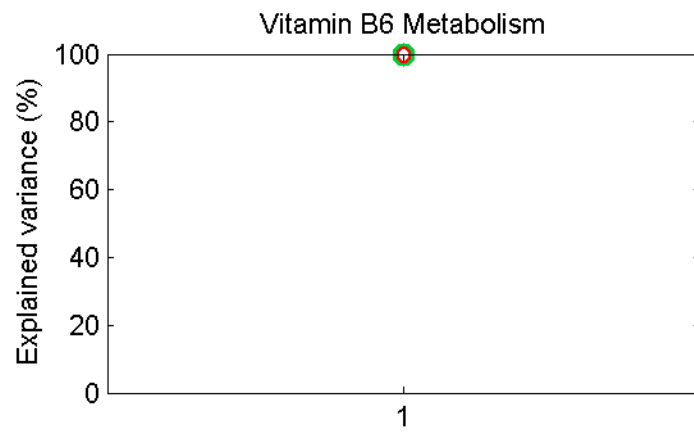












Super-pathways

