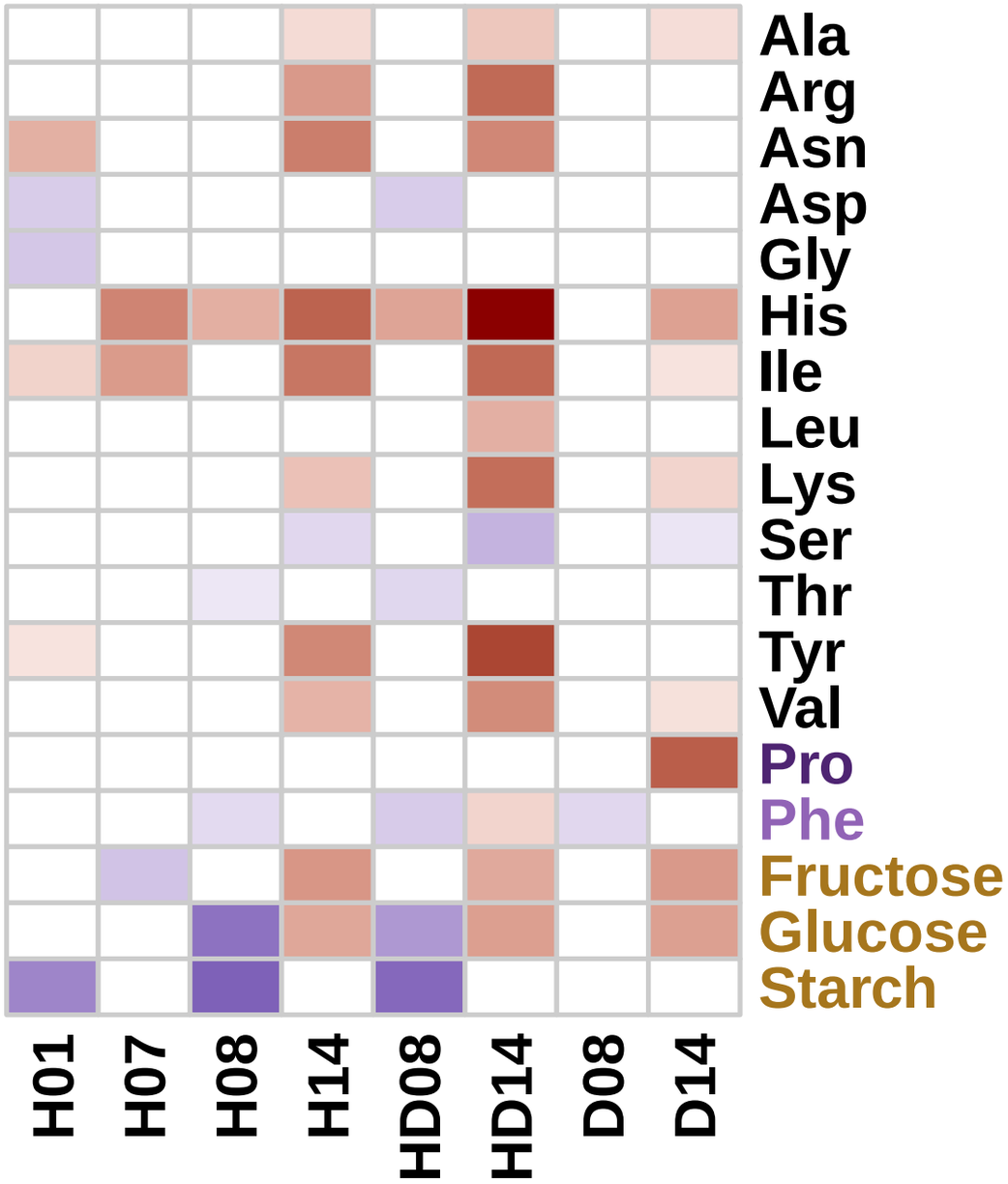metabolomics