

Classification of metabolites

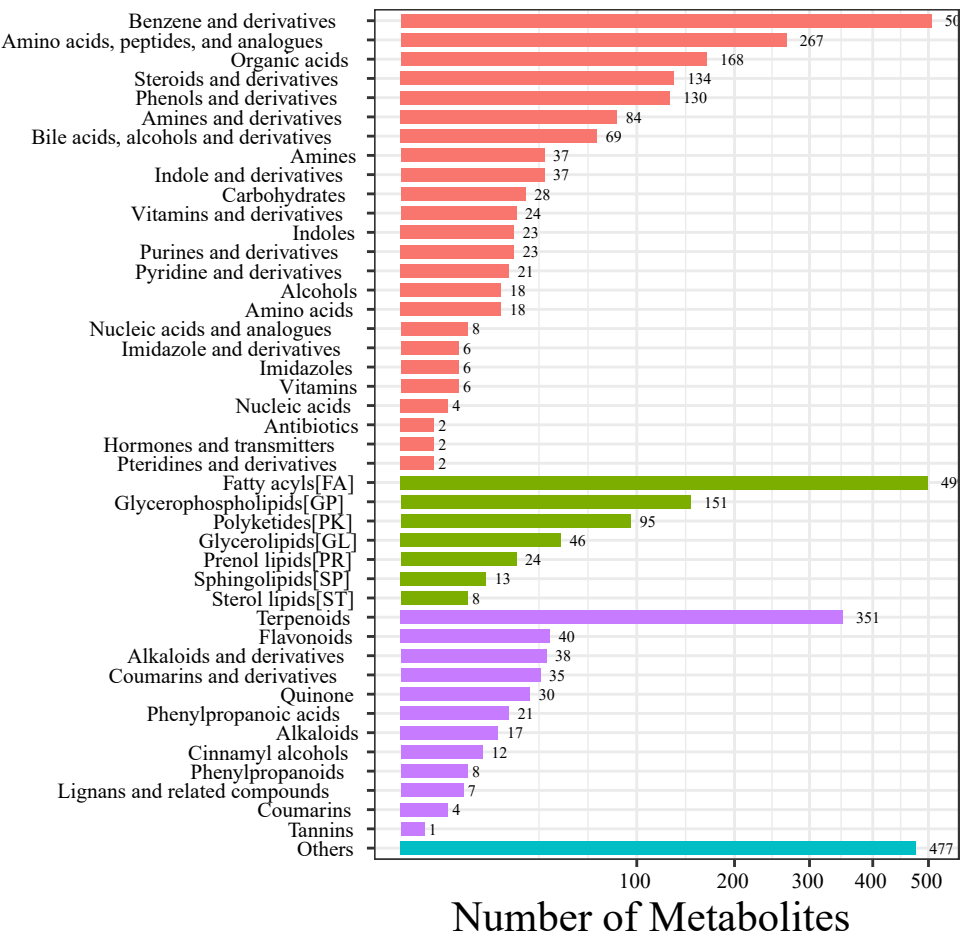
a

negative mode



b

positive mode

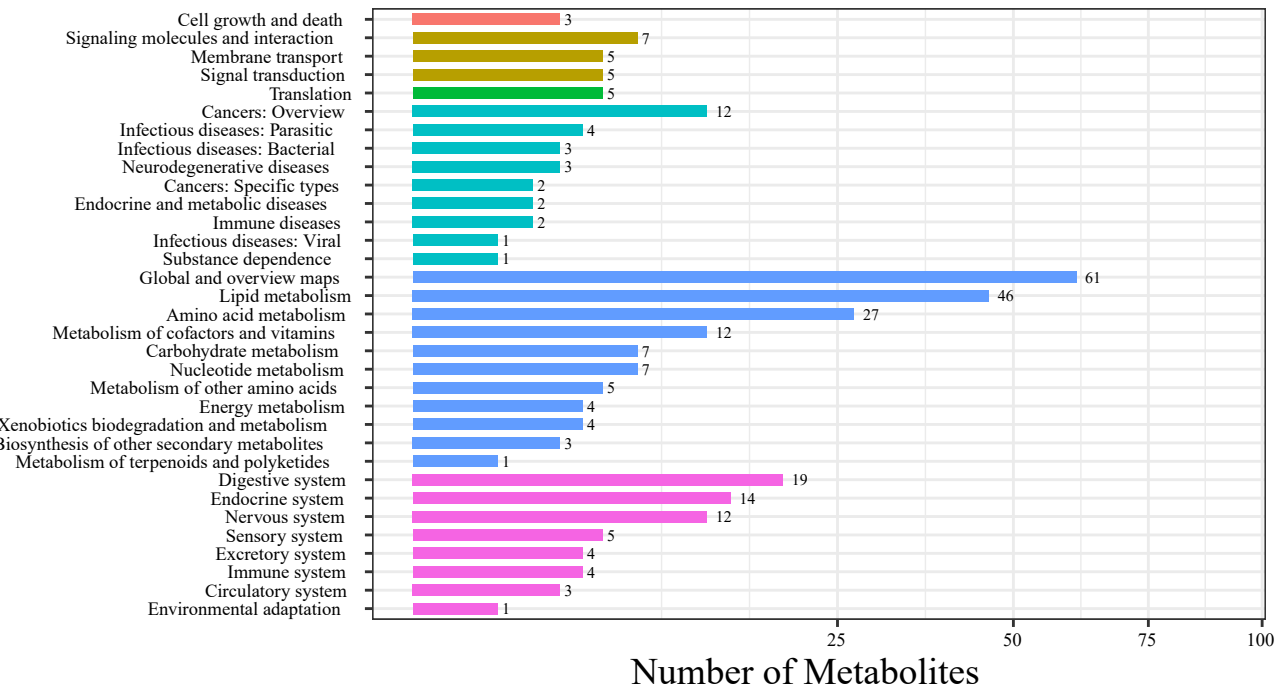


Compounds with biological roles
Lipids
Others
Phytochemical compounds

level identification of KEGG

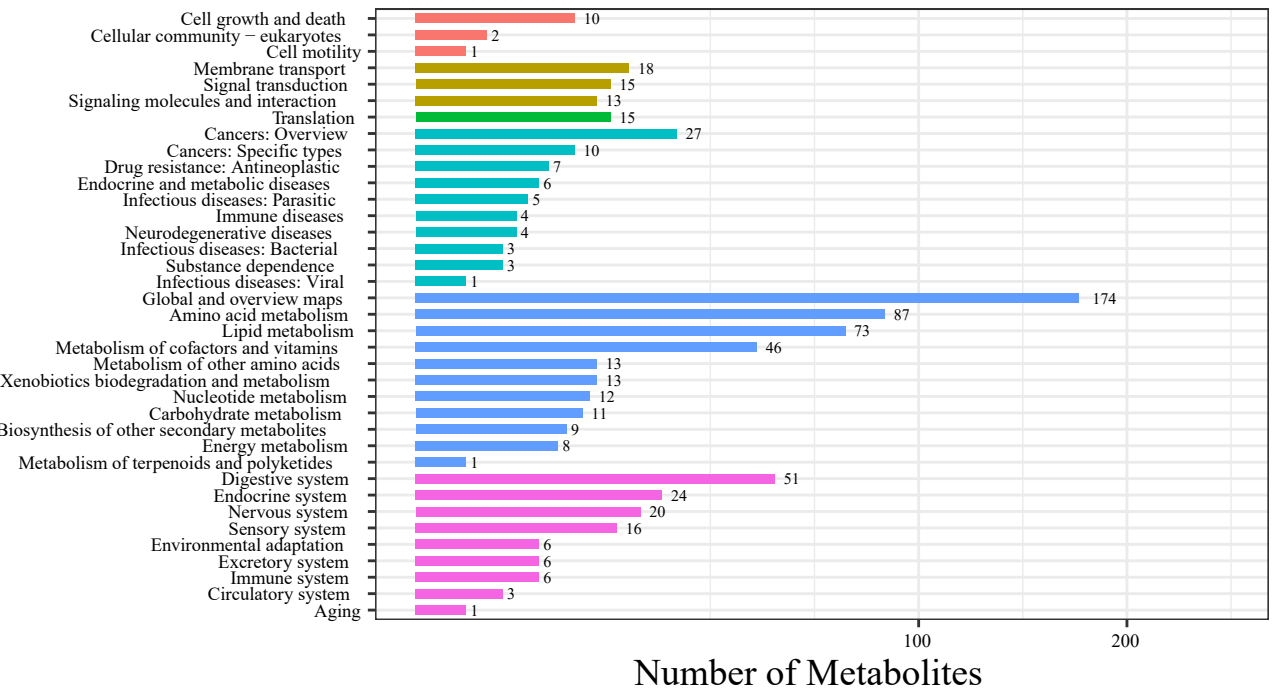
c

negative mode



d

positive mode



Cellular Processes
Environmental Information Processing
Genetic Information Processing
Human Diseases
Metabolism
Organismal Systems

Figure S9

(a-b) Classification of all metabolites annotated in ESI+ and ESI- mode.

(c-d) Identification of KEGG levels of all metabolites in ESI+ and ESI- mode.(level 1 and level 2)