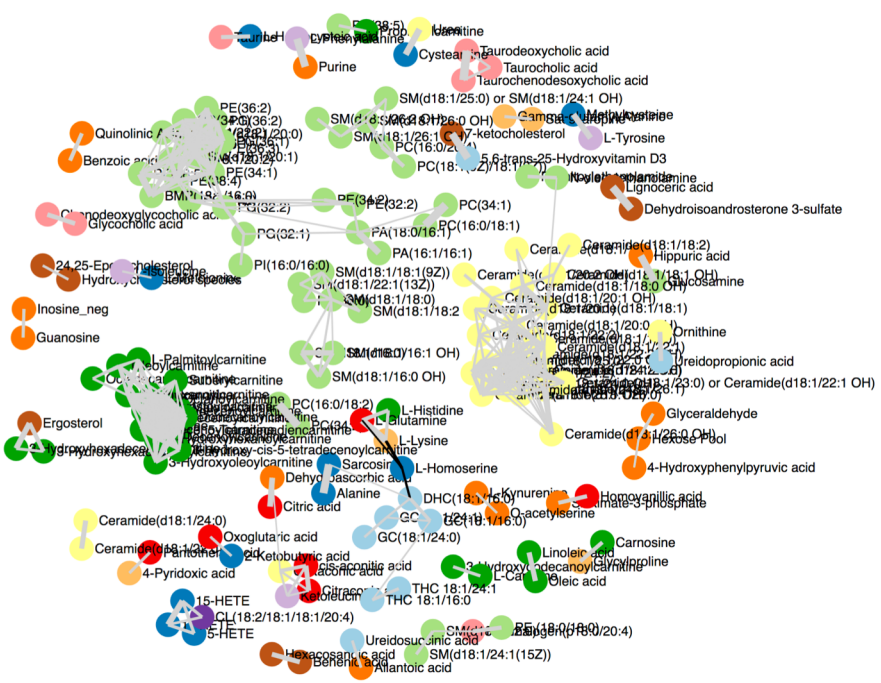
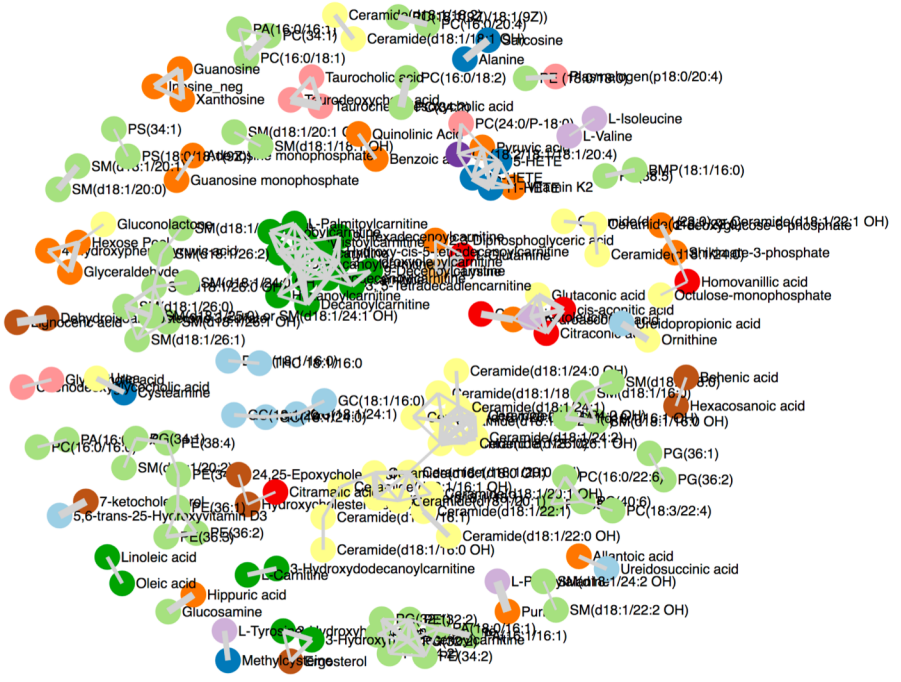
Figure S3.

A


Purine
Taurodeoxycholic acid
Taurocholic acid
Taurochenodesoxycholic acid
SM(d18:1/25:0) or SM(d18:1/24:1 OH)
L-Tyrosine
7-ketocholesterol
5,6-trans-25-Hydroxyvitamin D3
Lignoceric acid
Dehydroisoandrosterone 3-sulfate
Glycocholic acid
PC(34:1)
PC(16:0/18:1)
PA(18:0/16:1)
PA(16:1/16:1)
PI(16:0/16:0)
SM(d18:1/18:1(9Z))
SM(d18:1/22:1(13Z))
SM(d18:1/18:0)
SM(d18:1/18:2
Ceramide(d18:1/18:2)
Hippuric acid
Glycosamine
Ornithine
Ureidopropionic acid
SM(d18:1/16:1 OH)
SM(d18:1/16:0 OH)
Inosine_neg
Guanosine
L-Palmitoylcarnitine
Ergosterol
L-Histidine
L-Glutamine
L-Lysine
Sarcosine
L-Homoserine
Glyceraldehyde
4-Hydroxyphenylpyruvic acid
Dehydroascorbic acid
Alanine
Citric acid
Homovanillic acid
Ceramide(d18:1/24:0)
Oxoglutaric acid
Carnosine
4-Pyridoxic acid
Linoleic acid
Oleic acid
15-HETE
5-HETE
Ureidosuccinic acid
Hexacosanoic acid
Behenic acid
SM(d18:1/24:1(15Z))
Allantoic acid

B


Guanosine
Inosine_neg
Xanthosine
Alanine
PC(16:0/18:1)
PC(16:0/18:2)
PS(34:1)
Quinolinic Acid
L-Isoleucine
L-Valine
Pyruvic acid
Benzoic acid
Guanosine monophosphate
Gluconolactone
Hexose Pool
Glyceraldehyde
Homovanillic acid
Octulose-monophosphate
Glutaconic acid
cis-aconitic acid
Citraconic acid
Ornithine
Lignoceric acid
Cysteamine
Behenic acid
Hexacosanoic acid
PC(38:4)
PG(36:1)
PG(36:2)
PC(16:0/22:6,
PC(18:3/22:4)
24,25-Epoxycholesterol
Citramalic acid
7-ketocholesterol
5,6-trans-25-Hydroxyvitamin D3
Linoleic acid
Oleic acid
Hippuric acid
Glucosamine
Allantoic acid
Ureidosuccinic acid
Ergosterol