**Supplementary Figure 1.** Flowchart for identification of metabolites that make up the red meat metabolite score in the trial. GPE, glycerophosphoethanolamine; GPC, glycerophosphocholine; IARC, International Agency for Research on Cancer; TMAO, trimethylamine N-oxide.
**Supplementary Figure 2.** The correlations between meat scores and 7day diet diary (7dDD) measured meat intake. A, the means and 95% confidence intervals (CI) of red meat consumption measured by (7dDD) in quintiles of the derived red meat metabolite score (139 metabolites) in the exploratory set in the EPIC-Norfolk study (n=11,432); B, the means and 95% CI of processed meat consumption measured by 7dDD in quintiles of the processed meat metabolite score (82 metabolites) in the exploratory set in the EPIC-Norfolk study (n=11,432); C, the means and 95% CI of poultry consumption measured by 7dDD in quintiles of the poultry metabolite score (139 metabolites) in the exploratory set in the EPIC-Norfolk study (n=11,432); D, the correlations matrix for consumption of types of meat (red meat, processed meat and poultry) measured by 7dDD and measured by derived metabolite scores in the validation set in the EPIC-Norfolk study (n=853).
Supplementary Figure 3. Plasma levels of selected metabolites after consumption of pork and tofu in the randomized cross-over trial. Metabolites that were positively associated with red meat consumption in both the EPIC-Norfolk and the randomized cross-over trial are shown. Fold-change and p-values are reported in Table 2.
| Compound                                | Chromatogram in plasma after tofu intake | Chromatogram in plasma after pork intake | Isotope pattern | Chromatograms in several plasma samples after pork intake |
|-----------------------------------------|------------------------------------------|------------------------------------------|----------------|-------------------------------------------------------------|
| Deoxycarnitine                          | ![Chromatogram](image1.png)              | ![Chromatogram](image2.png)              | ![Isotope pattern](image3.png) | ![Chromatograms](image4.png)                                |
| 1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4) | ![Chromatogram](image5.png)              | ![Chromatogram](image6.png)              | ![Isotope pattern](image7.png) | ![Chromatograms](image8.png)                                |
1-(1-enyl-stearoyl)-2-linoleoyl-GPC (P-18:0/18:2)

Stearoylcarnitine

**Supplementary Figure 4.** Chromatographic tracing of selected metabolites after consumption of pork vs. tofu in the intervention study. Column 2 and 3 show the chromatogram of a compound after tofu intake and pork intake separately in the same participant. Isotope pattern was used as one indicator of the peak quality. The vertical lines represent the detected intensities of compounds. The boxes show the expected peaks. The plots indicate that high intensity compounds usually match very well with the expected isotope pattern. Column 5 shows the chromatogram of a compound in several samples of plasma after pork intake. It shows the variability of peak shapes and intensities (the variation of intensity of metabolites is reported in the boxplots in Supplementary Figure 3).
**Supplementary Figure 5.** Heatmap of correlations between types of meat consumption and top-ranked metabolites (n=11) in the red meat metabolite score that validated in the intervention study: EPIC-Norfolk study (n=11,432). The single asterisk in metabolite name represents the metabolite was annotated based on in-silico predictions which indicates the compound has not been confirmed based on a standard but its identity is confident.
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**Supplementary Table 1.** The definition of non-communicable diseases outcomes in the exploratory analyses for the association between red meat metabolite score and health outcomes.

**Supplementary Table 2.** Overview of metabolites included for the red meat metabolite score. A single asterisk in metabolite name represents the compound has not been confirmed based on a standard but its identity is confident.

**Supplementary Table 3.** Overview of metabolites included for the processed meat metabolite score.

**Supplementary Table 4.** Overview of metabolites included for the poultry metabolite score.

**Supplementary Table 5.** The parameters of feature (metabolite) selection using bootstrapping enhanced elastic net regression.

**Supplementary Table 6.** The rank of metabolites in the red meat metabolite score ordered by selected times in the bootstrapping process.

**Supplementary Table 7.** The number of metabolites in each metabolite score and its explained variance.

**Supplementary Table 8.** Correlation matrix of top-ranked metabolites in the red meat metabolite score and identified in the RCT (n=11).

**Supplementary Table 9.** The missing rates of metabolites in the red meat metabolite score in the exploratory set (combination of batch 2 and batch 3) and subgroups of red meat consumers and non-consumers.
d randomized controlled dietary intervention. Chunxiao Li Online Supplementary Material

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Table 5. The rank of metabolites in the red meat metabolite score ordered by selected times in the bootstrapping process.

Table 6. The number of metabolites in each metabolite score and its explained variance of meat consumption using different thresholds in the exploratory and validation sets.

Table 7. The correlation matrix of top-ranked metabolites in the red meat metabolite score and identified in the RCT (n=11).

Table 8. The missing rates of metabolites in the red meat metabolite score in the exploratory set (combination of batch 2 and batch 3) and subgroups of red meat consumers and non-consumers.
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Supplementary Table 3. Overview of metabolites included for the processed meat metabolite score. A single asterisk in metabolite name represents the compound has not been confirmed based on a standard but its identity is confident.
| Name                                      | Definition                          | notes                                      |
|-------------------------------------------|-------------------------------------|--------------------------------------------|
| Incident cardiovasc. disease              | Incident coronary heart disease     | Incident cases were defined either by hospital admissions data or death certificate. |
|                                           | ICD-9 codes: 410-414; ICD-10 codes: I20-I25 |                                            |
|                                           | Incident cerebral stroke            | Incident cases were defined either by hospital admissions data or death certificate. |
|                                           | ICD-9 codes: 433-435; ICD-10 codes: I63, I65, I66 |                                            |
|                                           | Incident haemorrhagic stroke        | Incident cases were defined either by hospital admissions data or death certificate. |
|                                           | ICD-9 codes: 430-432; ICD-10 codes: I60-I62 |                                            |
|                                           | Incident atrial fibrillation        | Incident cases were defined either by hospital admissions data or death certificate. |
|                                           | ICD-9 codes: 427.3; ICD-10 codes: I48 |                                            |
|                                           | Incident heart failure              | Incident cases were defined either by hospital admissions data or death certificate. |
|                                           | ICD-9 codes: 428; ICD-10 codes: I50 |                                            |
| Incident liver disease                    | Incident liver disease              | Incident cases were defined either by hospital admissions data or death certificate. |
|                                           | ICD-10 codes: B15-19, C22, E83, E88, I85, K70, K72-76, R18, Z94 |                                            |
| Incident renal disease                    | Incident renal disease              | Incident cases were defined either by hospital admissions data or death certificate. |
|                                           | ICD-9 codes: 580-589, 593; ICD-10 codes: N00-N19, N25-N29 |                                            |
| Incident gastrointestinal cancer           | Incident colon cancer               | Incident cases were defined either by hospital admissions data or death certificate. |
|                                           | ICD-9 codes: 153.0-153.9; ICD-10 codes: C18 |                                            |
|                                           | Incident rectal cancer              | Incident cases were defined either by hospital admissions data or death certificate. |
|                                           | ICD-9 codes: 154.0-154.1, 159.0; ICD-10 codes: C19-C20 |                                            |
| Incident stomach cancer | ICD-9 codes: 151; ICD-10 codes: C16 | Incident cases were defined either by hospital admissions data or death certificate. |
|-------------------------|------------------------------------|----------------------------------------------------------------------------------|
| Incident fractures      | ICD-10 codes: S02, S12, S22, S32, S42, S52, S62, S72, S82, S92, S120-S122, S127-S129, S220-S225, S228, S229, S320-S3325, S327, S328, S520-S529, S620-S627, S720-S729, S820-S829, S920-S929, T02, T08, T10 | Incident cases were defined based on hospital admission data. |
| All-cause mortality     | All-cause mortality                | Mortality from all causes was defined from death certificates. |
### Prevalent cases for exclusion

| Condition                        | Definition                                                                                     |
|----------------------------------|-----------------------------------------------------------------------------------------------|
| Prevalent coronary heart disease | Defined by a self-reported history of either angina or myocardial infarction.                |
| Prevalent stroke                 | Defined based on a self-reported history of stroke (any kind) by a doctor.                    |
| Prevalent stroke                 | Defined based on a self-reported history of stroke (any kind) by a doctor.                    |
| Prevalent atrial fibrillation (AF)| Defined by self-reported intake of drugs that were used for treatment of AF in clinical practice at the time of the baseline survey (digitalis or vitamin K antagonists; PMID 25059930). |
| Prevalent heart failure          | Defined by self-reported intake of drugs that were recommended for treatment of heart failure, namely loop diuretics in combination with digitalis or angiotensin-converting enzyme inhibitors (PMID 21835284). |
| Prevalent liver disease          | Defined based on self-reported diagnosis of any liver disease by a doctor.                    |
| Prevalent kidney disease         | Defined as an eGFR < 50 ml/min/1.73m².                                                        |
| Prevalent cases                  | Defined based on a self-reported history of any cancer.                                       |
| Prevalent cases                  | Defined based on a self-reported history of any cancer.                                       |
Prevalent cases were defined based on a self-reported history of any cancer.

Prevalent cases were reported based on any reported fracture at baseline examinations.
| **BIOCHEMICAL** | **Overview of metabolites included for the red meat metabolite score** |
|----------------|----------------------------------------------------------------------|
| 1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)* | 1-(1-enyl-stearoyl)-2-arachidonoyl-GPC (P-18:0/20:4) |
| 1-margaroyl-2-oleoyl-GPC (17:0/18:1)* | trans-4-hydroxyproline |
| verapamil | trimethylamine N-oxide |
| X - 11381 | 1-(1-enyl-palmitoyl)-2-linoleoyl-GPC (P-16:0/18:2)* |
| 1-palmityl-GPC (O-16:0) | 1-palmitoyl-2-palmitoleoyl-GPC (16:0/16:1)* |
| creatinine | 17-methylstearate |
| ergothioneine | creatine |
| 10-heptadecenoate (17:1n7) | sphingomyelin (d18:1/15:0, d16:1/17:0)* |
| 1-palmityl-2-arachidonoyl-GPC (O-16:0/20:4)* | 1-(1-enyl-stearoyl)-2-linoleoyl-GPC (P-18:0/18:2)* |
| methionine sulfone | 1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)* |
| 1-docosapentaenoyl-GPC (22:5n3)* | deoxycarnitine |
| 3-carboxy-4-methyl-5-propyl-2-furanpropanoate (CMPF) | cholesterol |
| X - 02249 | N-acetylnorvaline |
| imidazole lactate | 2-hydroxyoctanoate |
| N-acetylcarnosine | 1-stearoyl-2-oleoyl-GPE (18:0/18:1) |
| choline | ranitidine |
| X - 21315 | X - 12731 |
| X - 18913 | 5-methyluridine (ribothymidine) |
| 1-oleoyl-GPI (18:1)* | alpha-hydroxyisocaproate |
| 4-vinylphenol sulfate | Salpha-androstan-3alpha,17beta-diol monosulfate (2) |
| N-palmitoyl-sphingosine (d18:1/16:0) | X - 24309 |
| gamma-glutamylvaline | andro steroid monosulfate (1)* |
| N-acetylglutamine | dodecanedioate |
| S-methylcysteine | X - 11483 |
| X - 24293 | |
| Compound                                               | Formula |
|--------------------------------------------------------|---------|
| 1-myristoylglycerol (14:0)                             | X - 21659 |
| 2-hydroxy-3-methylvalerate                             | X - 16580, X - 21442 |
| fructose                                               | X - 15492, X - 18779, X - 14662 |
| sphingosine                                             | X - 15492 |
| N-acetylputrescine                                      | X - 18779 |
| stearoylcarnitine                                      | X - 14662 |
| cysteine sulfinic acid                                 | X - 15492, X - 18779, X - 14662 |
| 4-vinylguaiacol sulfate                                | X - 23583 |
| serotonin                                              | X - 17145 |
| N-acetyl-1-methylhistidine*                             | X - 17145 |
| phenylacetate                                           | X - 11852 |
| guanosine                                               | X - 11852 |
| pantothete                                             | X - 11852 |
| propionylglycine                                       | X - 21821 |
| 4-hydroxyhippurate                                     | X - 12729, X - 13658, X - 11315 |
| vanillic alcohol sulfate                               | X - 13729, X - 23782, X - 23593 |
| methionine sulfoxide                                    | X - 13729, X - 23782, X - 23593 |
| carotene diol (2)                                      | X - 12212 |
| 13-HODE + 9-HODE                                        | X - 12212 |
| N-acetylaspartate (A)                                   | X - 12212 |
| taurocholate                                            | X - 12212 |
| homostachydrine*                                       | X - 12212 |
| cysteine                                               | X - 12212 |
| 5-hydroxylysine                                        | X - 12212 |
| 1-palmitoyl-2-palmitoyl-GPC (O-16:0/16:0)*              | X - 11849, X - 21286 |
| 2-linoleoylglycerol (18:2)                             | X - 11849, X - 21286 |
| phenol sulfate                                         | X - 11849, X - 21286 |
| glycerate                                               | X - 11849, X - 21286 |
| 1-arachidonoyl-GPA (20:4)                              | X - 11849, X - 21286 |
| 1-(1-enyl-palmitoyl)-2-myristoyl-GPC (P-16:0/14:0)*     | X - 11905 |
| 1-arachidonoyl-GPA (20:4)                              | X - 11905 |
propyl 4-hydroxybenzoate sulfate
X - 18914
X - 17676
furosemide
X - 18899
quine
1-(1-enyl-palmitoyl)-2-docosahexaenoyl-GPE (P-16:0/22:6)*
2-oxoarginine*
uridine
alanine
O-sulfo-L-tyrosine
1-methylimidazoleacetate
asparagine
4-acetylphenol sulfate
2-palmitoyl-GPC (16:0)*
3-aminoisobutyrate
4-hydroxyphenylpyruvate
1-(1-enyl-palmitoyl)-2-palmitoyl-GPC (P-16:0/16:0)*
betaine
1-stearoyl-2-arachidonoyl-GPI (18:0/20:4)
1-(1-enyl-stearoyl)-2-docosahexaenoyl-GPE (P-18:0/22:6)*
sphingomyelin (d18:1/20:1, d18:2/20:0)*
pseudouridine
1-(1-enyl-palmitoyl)-2-oleoyl-GPC (P-16:0/18:1)*
citrulline
pyroglutamine*
X - 13684
X - 09789
X - 14838
1-arachidonoyl-GPC (20:4n6)*
palmitoyl dihydro sphingomyelin (d18:0/16:0)*
X - 12511
docosahexaenoate (DHA; 22:6n3)
1-stearoyl-2-arachidonoyl-GPC (18:0/20:4)
glycine
sphingomyelin (d18:2/14:0, d18:1/14:1)*
1-pentadecanoyl-GPC (15:0)*
1-palmitoyl-2-linoleoyl-GPC (16:0/18:2)
X - 12442
triamterene
sphingomyelin (d18:1/14:0, d16:1/16:0)*
## Red Meat Metabolite Score

| Sub_pathway                                                                 | Super_pathway     |
|-----------------------------------------------------------------------------|-------------------|
| Plasmalogen                                                                 | Lipid             |
| Plasmalogen                                                                 | Lipid             |
| Phosphatidylcholine (PC)                                                   | Lipid             |
| Urea cycle; Arginine and Proline Metabolism                                | Amino Acid        |
| Drug                                                                        | Xenobiotics       |
| Unknown                                                                     | Unknown           |
| Phospholipid Metabolism                                                    | Lipid             |
| Plasmalogen                                                                 | Lipid             |
| Lysoplasmalogen                                                            | Lipid             |
| Phosphatidylcholine (PC)                                                   | Lipid             |
| Creatine Metabolism                                                        | Amino Acid        |
| Fatty Acid, Branched                                                       | Lipid             |
| Creatine Metabolism                                                        | Amino Acid        |
| Food Component/Plant                                                       | Xenobiotics       |
| Long Chain Fatty Acid                                                      | Lipid             |
| Sphingolipid Metabolism                                                    | Lipid             |
| Plasmalogen                                                                 | Lipid             |
| Plasmalogen                                                                 | Lipid             |
| Methionine, Cysteine, SAM and Taurine Metabolism                           | Amino Acid        |
| Lysophosphatidylcholine                                                    | Lipid             |
| Carnitine Metabolism                                                       | Lipid             |
| Fatty Acid, Dicarboxylate                                                  | Lipid             |
| Sterol                                                                      | Lipid             |
| Unknown                                                                     | Unknown           |
| Phenylalanine Metabolism                                                   | Amino Acid        |
| Histidine Metabolism                                                       | Amino Acid        |
| Fatty Acid, Monohydroxy                                                    | Lipid             |
| Dipeptide Derivative                                                       | Peptide           |
| Phosphatidylethanolamine (PE)                                               | Lipid             |
| Phospholipid Metabolism                                                    | Lipid             |
| Drug                                                                        | Xenobiotics       |
| Unknown                                                                     | Unknown           |
| Unknown                                                                     | Unknown           |
| Unknown                                                                     | Unknown           |
| Pyrimidine Metabolism, Uracil containing                                   | Nucleotide        |
| Lysophosphatidylcholine                                                    | Lipid             |
| Leucine, Isoleucine and Valine Metabolism                                  | Amino Acid        |
| Benzoate Metabolism                                                        | Xenobiotics       |
| Androgenic Steroids                                                        | Lipid             |
| Ceramides                                                                   | Lipid             |
| Unknown                                                                     | Unknown           |
| Gamma-glutamyl Amino Acid                                                  | Peptide           |
| Androgenic Steroids                                                        | Lipid             |
| Glutamate Metabolism                                                       | Amino Acid        |
| Fatty Acid, Dicarboxylate                                                  | Lipid             |
| Methionine, Cysteine, SAM and Taurine Metabolism                           | Amino Acid        |
| Unknown                                                                     | Unknown           |
| Unknown                                                                     | Unknown           |
Monoacylglycerol
Unknown
Leucine, Isoleucine and Valine Metabolism
Unknown
Unknown
Fructose, Mannose and Galactose Metabolism
Unknown
Unknown
Polyamine Metabolism
Unknown
Unknown
Methionine, Cysteine, SAM and Taurine Metabolism
Unknown
Unknown
Food Component/Plant
Unknown
Unknown
Tryptophan Metabolism
Unknown
Unknown
Phenylalanine Metabolism
Unknown
Unknown
Purine Metabolism, Guanine containing
Unknown
Unknown
Pantothete and CoA Metabolism
Unknown
Unknown
Fatty Acid Metabolism (also BCAA Metabolism)
Unknown
Unknown
Benzoate Metabolism
Unknown
Unknown
Fatty Acid, Monohydroxy
Unknown
Unknown
Alanine and Aspartate Metabolism
Unknown
Unknown
Primary Bile Acid Metabolism
Unknown
Unknown
Food Component/Plant
Unknown
Unknown
Methionine, Cysteine, SAM and Taurine Metabolism
Unknown
Unknown
Lysine Metabolism
Unknown
Unknown
Plasmalogen
Unknown
Unknown
Tyrosine Metabolism
Unknown
Unknown
Glycolysis, Gluconeogenesis, and Pyruvate Metabolism
Unknown
Unknown
Lysophospholipid
Unknown
Unknown
Plasmalogen
Unknown
Unknown
Tyrosine Metabolism
Unknown
Unknown
Glycolysis, Gluconeogenesis, and Pyruvate Metabolism
Unknown
Unknown
Lysophospholipid
Unknown
Unknown
Plasmalogen
Unknown
Unknown
Tyrosine Metabolism
Unknown
Unknown
Glycolysis, Gluconeogenesis, and Pyruvate Metabolism
Unknown
Unknown
Lysophospholipid
Unknown
Unknown
Plasmalogen
Unknown
Unknown
| Pathway                                                        | Type           |
|---------------------------------------------------------------|----------------|
| Benzoate Metabolism                                           | Xenobiotics    |
| Unknown                                                       | Unknown        |
| Unknown                                                       | Unknown        |
| Drug                                                          | Xenobiotics    |
| Unknown                                                       | Unknown        |
| Drug                                                          | Xenobiotics    |
| Plasmalogen                                                   | Lipid          |
| Urea cycle; Arginine and Proline Metabolism                  | Amino Acid     |
| Pyrimidine Metabolism, Uracil containing                      | Nucleotide     |
| Alanine and Aspartate Metabolism                              | Amino Acid     |
| Chemical                                                      | Xenobiotics    |
| Histidine Metabolism                                          | Amino Acid     |
| Alanine and Aspartate Metabolism                              | Amino Acid     |
| Drug                                                          | Xenobiotics    |
| Lysophospholipid                                              | Lipid          |
| Pyrimidine Metabolism, Thymine containing                     | Nucleotide     |
| Tyrosine Metabolism                                           | Amino Acid     |
| Plasmalogen                                                   | Lipid          |
| Glycine, Serine and Threonine Metabolism                      | Amino Acid     |
| Phosphatidylinositol (PI)                                     | Lipid          |
| Plasmalogen                                                   | Lipid          |
| Sphingolipid Metabolism                                       | Lipid          |
| Pyrimidine Metabolism, Uracil containing                      | Nucleotide     |
| Plasmalogen                                                   | Lipid          |
| Urea cycle; Arginine and Proline Metabolism                  | Amino Acid     |
| Glutamate Metabolism                                          | Amino Acid     |
| Unknown                                                       | Unknown        |
| Unknown                                                       | Unknown        |
| Unknown                                                       | Unknown        |
| Lysophospholipid                                              | Lipid          |
| Sphingolipid Metabolism                                       | Lipid          |
| Unknown                                                       | Unknown        |
| Polyunsaturated Fatty Acid (n3 and n6)                        | Lipid          |
| Phosphatidylcholine (PC)                                      | Lipid          |
| Glycine, Serine and Threonine Metabolism                      | Amino Acid     |
| Sphingolipid Metabolism                                       | Lipid          |
| Lysophospholipid                                              | Lipid          |
| Phosphatidylcholine (PC)                                      | Lipid          |
| Unknown                                                       | Unknown        |
| Drug                                                          | Xenobiotics    |
| Sphingolipid Metabolism                                       | Lipid          |
| PLATFORM               | Retention Index | MASS     | PubChem   | ChemSpider | HMBD_ID     |
|-----------------------|----------------|----------|-----------|------------|-------------|
| LC/MS Pos Late        | 2511           | 752.5589 | 9547058   | 7826008    | HMDB05779   |
| LC/MS Pos Late        | 2350           | 794.6058 |           | 24767528   |             |
| LC/MS Pos Late        | 2450           | 774.6007 |           | 24822423   |             |
| LC/MS Pos Early       | 1064           | 132.0655 | 5810      | 5605       | HMDB00725   |
| LC/MS Pos Late        | 945            | 455.2904 | 2520      | 2425       | HMDB01850   |
| LC/MS Neg             | 1118           | 184.0982 |           | 1113       | HMDB00925   |
| LC/MS Pos Late        | 2226           | 742.5745 |           | 24767486   | HMDB11211   |
| LC/MS Pos Late        | 1573           | 482.3605 | 3983      | 3845       |             |
| LC/MS Pos Late        | 2160           | 732.5538 |           | 6981       | HMDB07969   |
| LC/MS Pos Early       | 2055           | 114.0662 | 588       | 568        | HMDB00562   |
| LC/MS Pos Early       | 5993           | 297.2799 | 3083779   | 2340933    | HMDB37397   |
| LC/MS Pos Early       | 1947           | 132.0768 | 586       | 566        | HMDB00064   |
| LC/MS Pos Early       | 850            | 230.0958 | 3032311   | 2297320    | HMDB03045   |
| LC/MS Neg             | 5555           | 267.233  | 5312435   | 4471860    | HMDB60038   |
| LC/MS Pos Late        | 2082           | 689.5592 |           | 28532777   |             |
| LC/MS Pos Late        | 2183           | 768.5902 | 6443139   | 4947173    |             |
| LC/MS Pos Late        | 2461           | 770.6058 |           | 24767519   |             |
| LC/MS Pos Early       | 1250           | 182.0482 | 69961     | 63154      |             |
| LC/MS Neg             | 5958           | 644.3569 |           |            |             |
| LC/MS Pos Early       | 2052           | 146.1176 | 134       | 705        | HMDB01161   |
| LC/MS Neg             | 2840           | 239.0925 | 123979    | 110498     | HMDB611112  |
| LC/MS Pos Late        | 2707           | 369.3516 | 11025495  | 4937803    | HMDB00067   |
| LC/MS Neg             | 4012           | 267.1239 |           |            |             |
| LC/MS Neg             | 2597           | 206.0823 | 74839     | 67404      | HMDB00512   |
| LC/MS Pos Early       | 2040           | 157.0608 | 440129    | 389128     | HMDB02320   |
| LC/MS Neg             | 3736.8         | 159.1027 | 94180     | 84994      | HMDB02264   |
| LC/MS Pos Early       | 2141           | 269.1244 | 9903482   | 8079136    | HMDB12881   |
| LC/MS Pos Late        | 2858           | 746.5694 |           |            | HMDB08993   |
| LC/MS Pos Early       | 1961           | 104.107  | 305       | 149278     | HMDB00097   |
| LC/MS Pos Early       | 2910           | 315.1485 | 3001055   | 2272523    | HMDB01930   |
| LC/MS Neg             | 3698.1         | 240.9139 |           |            |             |
| LC/MS Neg             | 2040           | 238.9694 |           |            |             |
| LC/MS Neg             | 4538           | 185.1182 |           |            |             |
| LC/MS Neg             | 1778.1         | 257.0779 | 445408    | 393058     | HMDB00884   |
| LC/MS Neg             | 5599           | 597.3045 |           |            |             |
| LC/MS Neg             | 1840           | 131.0714 | 83697     | 75520      | HMDB00746   |
| LC/MS Neg             | 3320           | 199.0071 | 6426766   | 4932200    | HMDB04072   |
| LC/MS Neg             | 5080           | 371.1898 |           |            |             |
| LC/MS Pos Late        | 2893           | 538.5194 | 5283564   | 4446677    | HMDB04949   |
| LC/MS Neg             | 4430           | 321.148  |           |            |             |
| LC/MS Pos Early       | 2700           | 247.1289 | 7015683   |            | HMDB11172   |
| LC/MS Neg             | 3871           | 383.1534 |           |            | HMDB02759   |
| LC/MS Polar           | 2140           | 187.0724 | 182230    | 158492     | HMDB06029   |
| LC/MS Neg             | 2990           | 229.1445 | 12736     | 12213      | HMDB00623   |
| LC/MS Neg             | 880            | 134.0281 | 24417     | 22826      | HMDB02108   |
| LC/MS Neg             | 4449           | 505.2082 |           |            |             |
| LC/MS Pos Early       | 1189           | 226.1283 |           |            |             |
| Compound Type   | Retention Time | M/z Value | Intensity | Adduct | HMDB ID |
|----------------|----------------|-----------|-----------|--------|---------|
| LC/MS Neg      | 6353.3         | 227.2016  | 79050     |        | HMDB11561 |
| LC/MS Neg      | 3975           | 462.1768  |           |        |         |
| LC/MS Neg      | 1800           | 131.0714  | 164623    | 144317 | HMDB00317 |
| LC/MS Neg      | 2537           | 222.0791  |           |        |         |
| LC/MS Neg      | 3823           | 333.2077  |           |        |         |
| LC/MS Neg      | 2022.2         | 225.0616  | 5984      | 5764   | HMDB00660 |
| LC/MS Pos Early| 1393           | 300.2891  | 5353955   | 4510275| HMDB00252 |
| LC/MS Pos Early| 2230           | 131.1179  | 122356    | 109095 | HMDB02064 |
| LC/MS Pos Late | 1485           | 428.3734  | 6426855   | 21233653| HMDB00848 |
| LC/MS Pos Early| 597            | 154.0169  | 109       | 107    | HMDB00996 |
| LC/MS Neg      | 4678           | 541.2647  |           |        |         |
| LC/MS Neg      | 1969           | 209.0454  |           |        |         |
| LC/MS Neg      | 4336           | 263.6283  |           |        |         |
| LC/MS Neg      | 3354           | 229.0176  |           |        |         |
| LC/MS Pos Early| 1112           | 116.0707  |           |        |         |
| LC/MS Pos Early| 2550           | 177.1022  | 5202      | 5013   | HMDB00259 |
| LC/MS Pos Early| 2100           | 212.1028  |           |        |         |
| LC/MS Neg      | 3862           | 257.1761  |           |        |         |
| LC/MS Neg      | 2150           | 135.0452  | 999       | 10181341| HMDB00209 |
| LC/MS Neg      | 3277.6         | 232.9949  |           |        |         |
| LC/MS Pos Early| 1728           | 284.0999  | 6802      | 6544   | HMDB00133 |
| LC/MS Neg      | 1498.7         | 218.1034  | 6613      | 6361   | HMDB00210 |
| LC/MS Neg      | 960            | 130.051   | 98681     | 89122  | HMDB00783 |
| LC/MS Neg      | 2930           | 243.0783  |           |        |         |
| LC/MS Neg      | 1475           | 194.0459  | 151012    | 133104 | HMDB13678 |
| LC/MS Pos Early| 2021           | 227.9973  |           |        |         |
| LC/MS Neg      | 4643           | 253.0832  |           |        |         |
| LC/MS Neg      | 1157           | 128.0715  |           |        |         |
| LC/MS Neg      | 1808           | 233.0125  |           |        |         |
| LC/MS Neg      | 1745           | 241.9768  |           |        |         |
| LC/MS Pos Late | 1627           | 349.2732  |           |        |         |
| LC/MS Pos Early| 1531           | 191.1023  |           |        |         |
| LC/MS Pos Early| 1272           | 166.0533  | 158980    | 139840 | HMDB02005 |
| LC/MS Pos Late | 1916           | 568.428   |           |        |         |
| LC/MS Neg      | 3597.7         | 229.0179  |           |        |         |
| LC/MS Neg      | 5275           | 295.2283  | 43013     |        |         |
| LC/MS Polar    | 3143           | 174.0408  | 65065     | 58576  | HMDB00812 |
| LC/MS Neg      | 5150           | 514.2844  | 6675      |        | HMDB00036 |
| LC/MS Pos Early| 1750           | 158.1176  | 441447    | 390180 | HMDB33433 |
| LC/MS Pos Early| 1488           | 122.027   | 5862      | 5653   | HMDB00574 |
| LC/MS Pos Early| 2790           | 163.1077  | 1029      | 1002   | HMDB00450 |
| LC/MS Pos Late | 2400           | 720.5874  |           |        |         |
| LC/MS Neg      | 3215           | 266.0179  |           |        |         |
| LC/MS Neg      | 1550           | 164.0355  |           |        |         |
| LC/MS Neg      | 6250           | 279.2329  | 5365676   | 4517636| HMDB11538 |
| LC/MS Neg      | 2156           | 172.9914  | 74426     | 67018  | HMDB60015 |
| LC/MS Polar    | 2070.4         | 105.0193  | 752       | 732    | HMDB00139 |
| LC/MS Neg      | 5499           | 457.2361  |           |        |         |
| LC/MS Pos Late | 2220           | 690.5432  |           | 24767479|         |
| LC/MS Neg      | 4396.5         | 283.1919  |           |        |         |
| Method       | Retention Time | M/Z | Description | Exp M/Z | Intensity  | HMDB ID  |
|--------------|----------------|-----|-------------|---------|------------|----------|
| LC/MS Neg    | 3971           | 259.0282 |             |         |            |          |
| LC/MS Neg    | 4503           | 266.8889 |             |         |            |          |
| LC/MS Neg    | 1485           | 167.0468 |             |         |            |          |
| LC/MS Neg    | 3515           | 329.0004 | 3440        | 3322    | HMDB01933  |          |
| LC/MS Neg    | 3730           | 337.1427 |             |         |            |          |
| LC/MS Neg    | 3378           | 325.1911 | 2728270     | 2010267 |            |          |
| LC/MS Neg    | 2181           | 748.5276 | 5283497     | 4446616 |            |          |
| LC/MS Neg    | 1792           | 174.0872 |             |         |            |          |
| LC/MS Neg    | 1700           | 90.055  | 5950        | 5735    | HMDB00161  |          |
| LC/MS Neg    | 990            | 260.0234 | 514186      | 448617  |            |          |
| LC/MS Neg    | 2064           | 141.0691 | 75810       | 68319   | HMDB02820  |          |
| LC/MS Neg    | 1225           | 133.0608 | 6267        | 6031    | HMDB00168  |          |
| LC/MS Neg    | 2375           | 215.002 | 4684006     | 3872009 |            |          |
| LC/MS Neg    | 6215           | 570.3413 | 15061532    | 21403165 | HMDB61702  |          |
| LC/MS Pos Early | 2215     | 104.0706 | 64956       | 58481   | HMDB03911  |          |
| LC/MS Neg    | 1690.1         | 179.035 | 979         | 954     | HMDB00707  |          |
| LC/MS Pos Late | 2454     | 718.5745 | 11146967    | 9322076 | HMDB11206  |          |
| LC/MS Pos Early | 1064     | 118.0863 | 247         | 24219951173 | HMDB00043 |          |
| LC/MS Polar  | 870           | 885.5495 |            | 21403055 | HMDB09815  |          |
| LC/MS Pos Late | 2401   | 776.5589 |            | 24769278 |            |          |
| LC/MS Pos Late | 2383   | 757.6218 |            |         |            |          |
| LC/MS Polar  | 1929.3        | 243.0623 | 15047       | 21403010 | HMDB00767  |          |
| LC/MS Pos Late | 2443  | 744.5902 |            |         |            |          |
| LC/MS Pos Early | 1520   | 176.103  | 9750        | 810     | HMDB00904  |          |
| LC/MS Pos Early | 1900   | 129.0659 | 134508      | 118562  |            |          |
| LC/MS Pos Early | 1642   | 242.0147 |            |         |            |          |
| LC/MS Neg    | 2580.5        | 153.0197 |            |         |            |          |
| LC/MS Pos Early | 2000   | 141.0658 |            |         |            |          |
| LC/MS Pos Late | 1460  | 544.3398 | 21403155    |         | HMDB10395  |          |
| LC/MS Pos Late | 2290   | 705.5905 | 9939965     | 8115586 |            |          |
| LC/MS Neg    | 3943          | 200.1295 |            |         |            |          |
| LC/MS Neg    | 5525          | 327.233  | 445580      | 393183  | HMDB02183  |          |
| LC/MS Pos Late | 2300   | 810.6007 | 16219824    | 17347139 | HMDB08048  |          |
| LC/MS Pos Early | 1375   | 76.0393  | 750         | 730     | HMDB00123  |          |
| LC/MS Pos Late | 1860   | 673.5279 |            |         |            |          |
| LC/MS Pos Late | 1474   | 482.3241 |            |         |            |          |
| LC/MS Pos Late | 2160   | 758.5694 | 5287971     | 4450224 | HMDB07973  |          |
| LC/MS Neg    | 5315          | 223.1705 |            |         |            |          |
| LC/MS Pos Early | 3164   | 254.1149 | 5546        | 5345    | HMDB01940  |          |
| LC/MS Pos Late | 1998   | 675.5436 | 11433862    | 9608732 | HMDB12097  |          |
| Beta          |
|--------------|
| 3.042191689  |
| 2.765347928  |
| 2.750397493  |
| 2.671601458  |
| 2.527996234  |
| 2.295964511  |
| 2.175362291  |
| 1.98185332   |
| 1.701393093  |
| 1.611011761  |
| 1.543375225  |
| 1.453908261  |
| 1.42998924   |
| 1.375928552  |
| 1.375382929  |
| 1.277513016  |
| 1.134439109  |
| 1.055089182  |
| 1.047342526  |
| 0.980014078  |
| 0.918175572  |
| 0.910854355  |
| 0.897956826  |
| 0.897083604  |
| 0.87944214   |
| 0.843897259  |
| 0.83812825   |
| 0.796319988  |
| 0.773152806  |
| 0.759766967  |
| 0.734834682  |
| 0.707636712  |
| 0.699256636  |
| 0.691365505  |
| 0.676034864  |
| 0.664682329  |
| 0.657132414  |
| 0.598247936  |
| 0.576639993  |
| 0.570501005  |
| 0.560401864  |
| 0.518377223  |
| 0.514154942  |
| 0.503149611  |
| 0.501864662  |
| 0.490223091  |
| 0.47996596   |
| 0.475794977  |
-0.558706559
-0.566295401
-0.578491493
-0.603774044
-0.613365016
-0.625361328
-0.628028712
-0.633081233
-0.634500795
-0.635341432
-0.65191283
-0.653698092
-0.664624022
-0.668383385
-0.683171726
-0.73174674
-0.734782733
-0.756473805
-0.756659927
-0.759202352
-0.879504352
-0.964659423
-1.005850478
-1.046092941
-1.091709742
-1.125186336
-1.130031679
-1.155137021
-1.163263148
-1.191797205
-1.244759629
-1.322954594
-1.345452548
-1.383379048
-1.38689238
-1.459574406
-1.472994874
-1.590887566
-1.701358023
-1.878889307
-2.751450285
### Supplementary Table 3. Overview of metabolites included for the processed meat metabolite score

| BIOCHEMICAL                                    |
|------------------------------------------------|
| trans-4-hydroxyproline                        |
| 1-palmitoyl-2-arachidonoyl-GPC (O-16:0/20:4)*  |
| oleoylcarnitine (C18:1)                       |
| choline                                        |
| X - 11787                                      |
| 1-(1-enyl-stearyoyl)-2-arachidonoyl-GPE (P-18:0/20:4)* |
| 1-stearyoyl-2-linoleoyl-GPE (18:0/18:2)*       |
| isovalerylcarnitine (C5)                       |
| pregnen-diol disulfate C21H34O8S2*             |
| mannose                                        |
| N6,N6,N6-trimethyllysine                      |
| X - 24293                                      |
| 1-(1-enyl-oleoyl)-GPE (P-18:1)*                |
| o-cresol sulfate                              |
| 1-methylhistidine                             |
| X - 12798                                      |
| 5alpha-androstan-3alpha,17beta-diol monosulfate (2) |
| O-methylcatechol sulfate                      |
| beta-alanine                                   |
| 1,5-anhydroglucitol (1,5-AG)                   |
| 3-methylglutarylcaritnine (2)                  |
| 3-(4-hydroxyphenyl)lactate                     |
| X - 02269                                      |
| androstenediol (3alpha, 17alpha) monosulfate (3) |
| 1-oleoylglycerol (18:1)                        |
| X - 11852                                      |
| sarcosine                                      |
| X - 12830                                      |
| 1-(1-enyl-palmitoyl)-2-oleoyl-GPE (P-16:0/18:1)* |
| X - 02249                                      |
| X - 23997                                      |
| X - 21792                                      |
| X - 17337                                      |
| X - 11381                                      |
| X - 16649                                      |
| theanine                                       |
| X - 13431                                      |
| isoeugenol sulfate                            |
| galactote                                      |
| N-acetylhistidine                              |
| fumarate                                       |
| gamma-glutamyl-epsilon-lysine                 |
| X - 17189                                      |
| N-acetylpurbluecine                            |
| methionine sulfoxide                           |
estrone 3-sulfate
gamma-glutamylglycine
X - 21752
X - 11849
X - 12544
N-acetyllalliin
taurocholate
3-ureidopropiote
S-allylcysteine
asparagine
2-hydroxydecanoate
phenol sulfate
myo-inositol
2-arachidonoyl-GPC (20:4)*
X - 12739
methionine sulfone
cortisol
androstenediol (3beta,17beta) monosulfate (2)
X - 21442
tryptophan betaine
X - 18901
threonine
7-methylguanine
erythrote*
palmitoyl dihydrosphingomyelin (d18:0/16:0)*
N-acetyllalanine
1-methylnicotimide
nicotimide
1-methylimidazoleacetate
1-stearoyl-2-arachidonoyl-GPC (18:0/20:4)
1-palmityl-2-palmitoyl-GPC (O-16:0/16:0)*
X - 11315
S-methylcysteine
3-methylhistidine
trimethylamine N-oxide
N-trimethyl 5-aminovalerate
sphingomyelin (d18:2/14:0, d18:1/14:1)*
## Supplementary Table 3. Overview of metabolites included for the processed meat metabolite score

| Sub_pathway                                                                 | Super_pathway      | PLATFORM      |
|----------------------------------------------------------------------------|--------------------|---------------|
| Urea cycle; Arginine and Proline Metabolism                                | Amino Acid         | LC/MS Pos Early |
| Plasmalogen                                                                | Lipid              | LC/MS Pos Late |
| Fatty Acid Metabolism (Acyl Carnitine)                                     | Lipid              | LC/MS Pos Late |
| Phospholipid Metabolism                                                   | Lipid              | LC/MS Pos Late |
| Unknown                                                                    | Unknown            | LC/MS Pos Early |
| Plasmalogen                                                                | Lipid              | LC/MS Pos Late |
| Phosphatidylethanolamine (PE)                                              | Lipid              | LC/MS Pos Late |
| Leucine, Isoleucine and Valine Metabolism                                  | Amino Acid         | LC/MS Pos Early |
| Progestin Steroids                                                         | Lipid              | LC/MS Neg     |
| Fructose, Mannose and Galactose Metabolism                                 | Carbohydrate       | LC/MS Polar   |
| Lysine Metabolism                                                         | Amino Acid         | LC/MS Pos Early |
| Unknown                                                                    | Unknown            | LC/MS Pos Early |
| Lyso plasmalogen                                                           | Lipid              | LC/MS Pos Late |
| Benzoate Metabolism                                                        | Xenobiotics        | LC/MS Neg     |
| Histidine Metabolism                                                       | Amino Acid         | LC/MS Pos Early |
| Unknown                                                                    | Unknown            | LC/MS Pos Early |
| Androgenic Steroids                                                        | Lipid              | LC/MS Neg     |
| Benzoate Metabolism                                                        | Xenobiotics        | LC/MS Neg     |
| Pyrimidine Metabolism, Uracil containing                                   | Nucleotide         | LC/MS Pos Early |
| Glycolysis, Gluconeogenesis, and Pyruvate Metabolism                       | Carbohydrate       | LC/MS Neg     |
| Leucine, Isoleucine and Valine Metabolism                                  | Amino Acid         | LC/MS Pos Early |
| Tyrosine Metabolism                                                        | Amino Acid         | LC/MS Neg     |
| Unknown                                                                    | Unknown            | LC/MS Neg     |
| Androgenic Steroids                                                        | Lipid              | LC/MS Neg     |
| Monoacylglycerol                                                           | Lipid              | LC/MS Neg     |
| Unknown                                                                    | Unknown            | LC/MS Neg     |
| Glycine, Serine and Threonine Metabolism                                   | Amino Acid         | LC/MS Pos Early |
| Unknown                                                                    | Unknown            | LC/MS Neg     |
| Plasmalogen                                                                | Lipid              | LC/MS Pos Late |
| Unknown                                                                    | Unknown            | LC/MS Pos Late |
| Unknown                                                                    | Unknown            | LC/MS Pos Late |
| Unknown                                                                    | Unknown            | LC/MS Neg     |
| Unknown                                                                    | Unknown            | LC/MS Neg     |
| Food Component/Plant                                                       | Xenobiotics        | LC/MS Neg     |
| Unknown                                                                    | Unknown            | LC/MS Pos Late |
| Food Component/Plant                                                       | Xenobiotics        | LC/MS Neg     |
| Fructose, Mannose and Galactose Metabolism                                 | Carbohydrate       | LC/MS Polar   |
| Histidine Metabolism                                                       | Amino Acid         | LC/MS Pos Early |
| TCA Cycle                                                                  | Energy             | LC/MS Polar   |
| Gamma-glutamyl Amino Acid                                                  | Peptide            | LC/MS Pos Early |
| Unknown                                                                    | Unknown            | LC/MS Neg     |
| Polyamine Metabolism                                                       | Amino Acid         | LC/MS Pos Early |
| Methionine, Cysteine, SAM and Taurine Metabolism                           | Amino Acid         | LC/MS Pos Early |
| Metabolism                                      | Chemical Class | Mass Spectrometry Method |
|------------------------------------------------|----------------|--------------------------|
| Estrogenic Steroids                            | Lipid          | LC/MS Neg                |
| Gamma-glutamyl Amino Acid                      | Peptide        | LC/MS Pos Early          |
| Unknown                                        | Unknown        | LC/MS Neg                |
| Unknown                                        | Unknown        | LC/MS Neg                |
| Food Component/Plant                           | Xenobiotics    | LC/MS Neg                |
| Primary Bile Acid Metabolism                   | Lipid          | LC/MS Neg                |
| Pyrimidine Metabolism, Uracil containing       | Nucleotide     | LC/MS Pos Early          |
| Food Component/Plant                           | Xenobiotics    | LC/MS Pos Early          |
| Alanine and Aspartate Metabolism               | Amino Acid     | LC/MS Pos Early          |
| Fatty Acid, Monohydroxy                        | Lipid          | LC/MS Neg                |
| Tyrosine Metabolism                            | Amino Acid     | LC/MS Neg                |
| Inositol Metabolism                            | Lipid          | LC/MS Polar              |
| Lysophospholipid                               | Lipid          | LC/MS Neg                |
| Unknown                                        | Unknown        | LC/MS Neg                |
| Methionine, Cysteine, SAM and Taurine Metabolism| Amino Acid     | LC/MS Pos Early          |
| Corticosteroids                                | Lipid          | LC/MS Neg                |
| Androgenic Steroids                            | Lipid          | LC/MS Neg                |
| Unknown                                        | Unknown        | LC/MS Neg                |
| Tryptophan Metabolism                          | Amino Acid     | LC/MS Pos Early          |
| Unknown                                        | Unknown        | LC/MS Neg                |
| Glycine, Serine and Threonine Metabolism       | Amino Acid     | LC/MS Pos Early          |
| Purine Metabolism, Guanine containing          | Nucleotide     | LC/MS Pos Early          |
| Aminosugar Metabolism                          | Carbohydrate   | LC/MS Polar              |
| Sphingolipid Metabolism                        | Lipid          | LC/MS Pos Late           |
| Alanine and Aspartate Metabolism               | Amino Acid     | LC/MS Neg                |
| Nicotite and Nicotimide Metabolism             | Cofactors and Vitamins | LC/MS Pos Early |
| Nicotite and Nicotimide Metabolism             | Cofactors and Vitamins | LC/MS Pos Early |
| Histidine Metabolism                           | Amino Acid     | LC/MS Pos Early          |
| Phosphatidylcholine (PC)                       | Lipid          | LC/MS Pos Late           |
| Plasmalogen                                     | Lipid          | LC/MS Pos Late           |
| Unknown                                        | Unknown        | LC/MS Neg                |
| Methionine, Cysteine, SAM and Taurine Metabolism| Amino Acid     | LC/MS Neg                |
| Histidine Metabolism                           | Amino Acid     | LC/MS Neg                |
| Phospholipid Metabolism                        | Lipid          | LC/MS Pos Early          |
| Lysine Metabolism                              | Amino Acid     | LC/MS Pos Early          |
| Sphingolipid Metabolism                        | Lipid          | LC/MS Pos Late           |
| Retention_Index | MASS     | PubChem  | ChemSpider | HMDB_ID       | Beta     |
|-----------------|----------|----------|------------|----------------|---------|
| 1064            | 132.0655 | 5810     | 5605       | HMDB00725      | 2.712106182 |
| 2183            | 768.5902 | 6443139  | 4947173    |                | 2.386297619  |
| 1423            | 426.3578 | 6441392  |            | HMDB05065      | 1.060299314  |
| 1961            | 104.107  | 305      | 149278     | HMDB00097      | 0.909178486  |
| 2319            | 148.0968 |          |            |                | 0.902136385  |
| 2511            | 752.5589 | 9547058  | 7826008    | HMDB05779      | 0.858712564  |
| 2522            | 744.5538 | 9546749  | 7825699    | HMDB08994      | 0.824785693  |
| 3085            | 246.17   | 6426851  |            | HMDB00688      | 0.780659333  |
| 3868            | 238.0775 |          |            |                | 0.714854755  |
| 2200            | 225.0616 | 18950    | 141983     | HMDB00169      | 0.709813088  |
| 2825            | 189.1598 | 440120   | 140379     | HMDB01325      | 0.667682545  |
| 1189            | 226.1283 |          |            |                | 0.63113102   |
| 1566            | 464.3136 |          |            |                | 0.618170451  |
| 2796            | 187.0071 | 11615528 | 9790277    |                | 0.589318351  |
| 2755            | 170.0924 | 92105    | 83153      | HMDB00001      | 0.556717709  |
| 2011            | 240.1017 |          |            |                | 0.522097933  |
| 5080            | 371.1898 |          |            |                | 0.498809193  |
| 2344            | 203.002  | 22473    | 21078      | HMDB0013       | 0.49182115   |
| 1939            | 90.055   | 239      | 234        | HMDB00056      | 0.472851485  |
| 802             | 163.0612 | 64960    |            | HMDB02712      | 0.466526578  |
| 2675            | 290.1598 | 128145   | 113619     | HMDB00552      | 0.456034181  |
| 1379            | 181.0506 | 9378     | 9010       | HMDB00755      | 0.442029898  |
| 1525.4          | 255.0876 |          |            |                | 0.435946134  |
| 5180            | 369.1741 |          |            |                | 0.407322815  |
| 6500            | 281.2486 | 5283468  | 4446588    | HMDB11567      | 0.386304852  |
| 3277.6          | 232.9949 |          |            |                | 0.385331942  |
| 1280            | 90.055   | 1088     | 1057       | HMDB00271      | 0.381784472  |
| 3197            | 372.1128 |          |            |                | 0.377105915  |
| 2600            | 702.5432 |          |            | HMDB11342      | 0.372129887  |
| 4012            | 267.1239 |          |            |                | 0.365875875  |
| 1634            | 223.0745 |          |            |                | 0.360853658  |
| 1290            | 197.0827 |          |            |                | 0.360289185  |
| 1136            | 328.2476 |          |            |                | 0.338684853  |
| 1118            | 184.0982 |          |            |                | 0.332568551  |
| 3018            | 353.0346 |          |            |                | 0.298753205  |
| 1180            | 173.0932 | 439378   | 388498     | HMDB34365      | 0.221059256  |
| 1015            | 302.2322 |          |            |                | 0.201234964  |
| 3893            | 243.0333 |          |            |                | 0.19099696   |
| 3085            | 195.051  | 128869   | 114198     | HMDB00565      | -0.140135327 |
| 2065            | 198.0873 | 75619    | 68142      | HMDB32055      | -0.184676344 |
| 3084            | 115.0037 | 444972   | 10197150   | HMDB00134      | -0.189258967 |
| 2717            | 276.1554 | 7015684;7015685 | 5378717 | HMDB03869 | -0.236534217 |
| 2399            | 411.4896 |          |            |                | -0.257993375 |
| 2230            | 131.1179 | 122356   | 109095     | HMDB02064      | -0.2658603   |
| 1272            | 166.0533 | 158980   | 139840     | HMDB02005      | -0.301655882 |
|    |     |     |     |     |                  |
|----|-----|-----|-----|-----|------------------|
| 4417.3 | 349.1115 | 3001028 | 16740220 | HMDB01425 | -0.309126278 |
| 1535  | 205.0819  | 165527  | 145071  | HMDB11667 | -0.313947657 |
| 5090  | 621.3307  |        | -0.317160886 |
| 3215  | 266.0179  |        | -0.318950077 |
| 3166.9 | 209.0822  |        | -0.321926059 |
| 1467  | 218.0493  |        | -0.327826955 |
| 5150  | 514.2844  | 6675   | HMDB0036 | -0.333568025 |
| 875   | 133.0608  | 111    | 109    | HMDB0026  | -0.338106162 |
| 2690  | 162.0583  | 98280  | 88744  | HMDB34323 | -0.37301125 |
| 1225  | 133.0608  | 6267   | 6031   | HMDB00168 | -0.381107325 |
| 4840  | 187.134   | 21488  | 20195  |          | -0.39469837 |
| 2156  | 172.9914  | 74426  | 67018  | HMDB60015 | -0.419226077 |
| 3506.3 | 225.0616  | 892    | 10239179 | HMDB0021 | -0.428902312 |
| 5965  | 618.3413  | 21403158 | HMDB61699 | -0.43052056 |
| 2406  | 241.1195  |        |        |          | -0.484350261 |
| 1250  | 182.0482  | 69961  | 63154  |          | -0.514829225 |
| 4713.2 | 361.202   | 5754   | HMDB0063 | -0.516035894 |
| 4500  | 369.1741  |        |        |          | -0.53631549 |
| 3823  | 333.2077  |        |        |          | -0.543314794 |
| 2673  | 247.1441  | 442106 | HMDB61115 | -0.560502359 |
| 3800  | 211.0247  |        |        |          | -0.563198775 |
| 1514  | 120.0655  | 6288   | 6051   | HMDB00167 | -0.580069014 |
| 2175  | 166.0723  | 11361  | 10883  | HMDB00897 | -0.582891771 |
| 2186  | 135.0299  | 2781043 | 2061231 | HMDB00613 | -0.583402709 |
| 2290  | 705.5905  | 9939965 | 8115586 |          | -0.593952949 |
| 861.2 | 130.051   | 88064  | 79449  | HMDB00766 | -0.623925693 |
| 1940  | 137.0709  | 10129985 | 8305504 | HMDB00699 | -0.665002998 |
| 1942  | 123.0553  | 936    | 911    | HMDB01406 | -0.703684813 |
| 2064  | 141.0659  | 75810  | 68319  | HMDB02820 | -0.721353202 |
| 2300  | 810.6007  | 16219824 | 17347139 | HMDB08048 | -0.725572799 |
| 2400  | 720.5874  |        |        |          | -0.728891836 |
| 1157  | 128.0715  |        |        |          | -0.874234672 |
| 880   | 134.0281  | 24417  | 22826  | HMDB02108 | -0.896197351 |
| 906.3 | 168.0779  | 64969  | 58494  | HMDB00479 | -0.901212513 |
| 2100  | 76.0757   | 1145   | 1113   | HMDB00925 | -0.914916251 |
| 2186  | 160.1332  |        |        |          | -1.496211186 |
| 1860  | 673.5279  |        |        |          | -1.656381993 |
Supplementary Table 4. Overview of metabolites included for the poultry metabolite score

| METABOLITE | X - 23652 | X - 14838 | X - 11787 | X - 13835 | X - 11849 | X - 12127 | X - 21752 | X - 12739 | X - 21365 | X - 12100 | X - 13431 |
|------------|----------|----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| 1-(1-enyl-palmitoyl)-2-arachidonoyl-GPE (P-16:0/20:4)* | 3-methylhistidine | ibuprofen | serine | 1-(1-enyl-palmitoyl)-2-docosahexaenoyl-GPC (P-16:0/22:6)* | bilirubin (E,E)* | taurolithocholate 3-sulfate | kynurete | S-allylcysteine | valerate | N-acetyltryptophan | trans-4-hydroxyproline | N-acetyl-beta-alanine | 5alpha-pregn-3beta,20beta-diol monosulfate (1) | phosphate | lanthionine | uracil | sphingosine | N-acetyltaurine | X - 24309 | N-acetylglutamate | phenyllactate (PLA) | 1-margaroyl-2-linoleoyl-GPC (17:0/18:2)* | phenylacetate | N-acetylputrescine | 1-eicosenoyl-GPC (20:1)* | 3-methoxytyrosine | X - 13431 |
|------------|----------|----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
| 3-methylhistidine | ibuprofen | serine | 1-(1-enyl-palmitoyl)-2-docosahexaenoyl-GPC (P-16:0/22:6)* | bilirubin (E,E)* | taurolithocholate 3-sulfate | kynurete | S-allylcysteine | valerate | N-acetyltryptophan | trans-4-hydroxyproline | N-acetyl-beta-alanine | 5alpha-pregn-3beta,20beta-diol monosulfate (1) | phosphate | lanthionine | uracil | sphingosine | N-acetyltaurine | X - 24309 | N-acetylglutamate | phenyllactate (PLA) | 1-margaroyl-2-linoleoyl-GPC (17:0/18:2)* | phenylacetate | N-acetylputrescine | 1-eicosenoyl-GPC (20:1)* | 3-methoxytyrosine | X - 13431 |
| 1-margaroyl-2-linoleoyl-GPC (17:0/18:2)* | phenylacetate | N-acetylputrescine | 1-eicosenoyl-GPC (20:1)* | 3-methoxytyrosine | X - 12100 | N-acetylneuramite | 4-acetamidobutanoate | X - 13431 | pyroglutamine* |
methionine sulfone
sphingomyelin (d18:2/14:0, d18:1/14:1)*
1-(1-enyl-stearoyl)-2-arachidonoyl-GPC (P-18:0/20:4)
trimethylamine N-oxide
## Poultry metabolite score

| Sub_pathway                                      | Super_pathway      | PLATFORM         |
|-------------------------------------------------|--------------------|-----------------|
| Plasmalogen                                      | Lipid              | LC/MS Pos Late  |
| Histidine Metabolism                             | Amino Acid         | LC/MS Neg       |
| Unknown                                         | Unknown            | LC/MS Pos Early |
| Drug                                            | Xenobiotics        | LC/MS Neg       |
| Unknown                                         | Unknown            | LC/MS Pos Early |
| Glycine, Serine and Threonine Metabolism         | Amino Acid         | LC/MS Pos Early |
| Plasmalogen                                      | Lipid              | LC/MS Pos Late  |
| Unknown                                         | Unknown            | LC/MS Neg       |
| Hemoglobin and Porphyrin Metabolism             | Cofactors and Vitamins | LC/MS Pos Late |
| Secondary Bile Acid Metabolism                   | Lipid              | LC/MS Neg       |
| Tryptophan Metabolism                            | Amino Acid         | LC/MS Pos Early |
| Food Component/Plant                             | Xenobiotics        | LC/MS Pos Early |
| Short Chain Fatty Acid                           | Lipid              | LC/MS Neg       |
| Tryptophan Metabolism                            | Amino Acid         | LC/MS Pos Early |
| Urea cycle; Arginine and Proline Metabolism      | Amino Acid         | LC/MS Pos Early |
| Pyrimidine Metabolism, Uracil containing         | Nucleotide         | LC/MS Neg       |
| Progestin Steroids                               | Lipid              | LC/MS Neg       |
| Unknown                                         | Unknown            | LC/MS Neg       |
| Oxidative Phosphorylation                        | Energy             | LC/MS Pos Early |
| Chemical                                         | Xenobiotics        | LC/MS Pos Early |
| Pyrimidine Metabolism, Uracil containing         | Nucleotide         | LC/MS Polar     |
| Unknown                                         | Unknown            | LC/MS Pos Early |
| Sphingolipid Metabolism                          | Lipid              | LC/MS Pos Late  |
| Unknown                                         | Unknown            | LC/MS Neg       |
| Methionine, Cysteine, SAM and Taurine Metabolism | Amino Acid         | LC/MS Neg       |
| Unknown                                         | Unknown            | LC/MS Neg       |
| Lysine Metabolism                                | Amino Acid         | LC/MS Pos Early |
| Food Component/Plant                             | Xenobiotics        | LC/MS Neg       |
| Secondary Bile Acid Metabolism                   | Lipid              | LC/MS Neg       |
| Fatty Acid, Monohydroxy                          | Lipid              | LC/MS Neg       |
| TCA Cycle                                       | Energy             | LC/MS Neg       |
| Unknown                                         | Unknown            | LC/MS Neg       |
| Glutamate Metabolism                             | Amino Acid         | LC/MS Polar     |
| Phenylalanine Metabolism                         | Amino Acid         | LC/MS Neg       |
| Phosphatidylcholine (PC)                         | Lipid              | LC/MS Pos Late  |
| Phenylalanine Metabolism                         | Amino Acid         | LC/MS Neg       |
| Polyamine Metabolism                             | Amino Acid         | LC/MS Pos Early |
| Lysophospholipid                                 | Lipid              | LC/MS Pos Late  |
| Tyrosine Metabolism                              | Amino Acid         | LC/MS Pos Early |
| Unknown                                         | Unknown            | LC/MS Pos Early |
| Aminosugar Metabolism                            | Carbohydrate       | LC/MS Pos Early |
| Polyamine Metabolism                             | Amino Acid         | LC/MS Neg       |
| Unknown                                         | Unknown            | LC/MS Pos Late  |
| Glutamate Metabolism                             | Amino Acid         | LC/MS Pos Early |
| Metabolism                                      | Type       | MS Mode  |
|------------------------------------------------|------------|----------|
| Methionine, Cysteine, SAM and Taurine Metabolism| Amino Acid | LC/MS Pos Early |
| Sphingolipid Metabolism                        | Lipid      | LC/MS Pos Late   |
| Plasmalogen                                    | Lipid      | LC/MS Pos Late   |
| Phospholipid Metabolism                        | Lipid      | LC/MS Pos Early   |
| Retention_Index | MASS       | PubChem  | ChemSpider | HMBD_ID      | Beta       |
|-----------------|------------|----------|------------|---------------|------------|
| 2270            | 724.5276   | 24769238 | HMBD11352  | 2.99219766    |
| 906.3           | 168.0779   | 58494    | HMBD00479  | 2.484591916   |
| 1991            | 171.0761   | 24769238 | HMBD11352  | 2.208646224   |
| 2000            | 141.0658   | 24769238 | HMBD11352  | 2.001496418   |
| 4925            | 205.1234   | 3544     | HMBD01925  | 1.154806129   |
| 2319            | 148.0968   | 24769238 | HMBD11352  | 0.954141873   |
| 1239            | 106.0499   | 5736     | HMBD00187  | 0.83860118    |
| 2041            | 790.5745   | 68881    | HMBD00187  | 0.789095059   |
| 1017            | 169.0618   | 68881    | HMBD00187  | 0.717051018   |
| 1045            | 585.2708   | 4474753  | HMBD00187  | 0.687198377   |
| 5026.7          | 280.6221   | 389078   | HMBD02580  | 0.633456478   |
| 2385            | 190.0499   | 3712     | HMBD00715  | 0.589003219   |
| 2690            | 162.0583   | 88744    | HMBD34323  | 0.55961595    |
| 1718            | 101.0608   | 7701     | HMBD00892  | 0.46242741    |
| 2640            | 247.1077   | 610602   | HMBD13713  | 0.44524427    |
| 1064            | 132.0655   | 5605     | HMBD00725  | 0.442879819   |
| 773             | 130.051    | 68881    | HMBD00725  | 0.426923627   |
| 5180            | 399.2211   | 1141     | HMBD00300  | 0.204846929   |
| 3215            | 266.0179   | 1174     | HMBD00300  | -0.301430749  |
| 576             | 98.9842    | 1032     | HMBD01429  | 0.339295943   |
| 1730            | 209.0591   | 88959    | HMBD01429  | 0.28884462    |
| 1089.7          | 111.02     | 1141     | HMBD00300  | 0.204846929   |
| 2160            | 226.0817   | 0.0173   | HMBD00300  | -0.301430749  |
| 1393            | 300.2897   | 4510275  | HMBD00252  | -0.306766043  |
| 5090            | 621.3307   | 140553   | HMBD00252  | -0.318337893  |
| 800             | 166.018    | 159864   | HMBD00252  | -0.338861086  |
| 2406            | 241.1195   | 1174     | HMBD00252  | -0.356586457  |
| 2195            | 160.1333   | 0.0373   | HMBD00252  | -0.373315252  |
| 2304            | 253.1194   | 19980286 | HMBD33143  | -0.438483391  |
| 4750            | 254.6229   | 19980286 | HMBD33143  | -0.459264524  |
| 5275            | 295.2283   | 43013    | HMBD33143  | -0.48465637   |
| 615.6           | 133.0143   | 510      | HMBD00156  | -0.499875568  |
| 4430            | 321.148    | 510      | HMBD00156  | -0.54953697   |
| 3106            | 188.0564   | 1266066  | HMBD01138  | -0.550950624  |
| 2208            | 165.0557   | 3715     | HMBD00779  | -0.580365888  |
| 2242            | 772.5851   | 0.0373   | HMBD00779  | -0.586324184  |
| 2150            | 135.0452   | 10181341 | HMBD00209  | -0.615055956  |
| 2230            | 131.1179   | 109095   | HMBD02064  | -0.620669247  |
| 1630            | 550.3867   | 0.0373   | HMBD02064  | -0.626938841  |
| 2555            | 212.0917   | 8948     | HMBD01434  | -0.628345253  |
| 2650            | 221.0919   | 8948     | HMBD01434  | -0.657663085  |
| 660             | 310.1133   | 10292217 | HMBD00230  | -0.671371775  |
| 893.7           | 144.0666   | 17180    | HMBD03681  | -0.769661334  |
| 1015            | 302.2322   | 118562   | HMBD03681  | -0.877268869  |
| 1900            | 129.0659   | 134508   | HMBD03681  | -0.946378781  |
|     |       |       |       |                  |
|-----|-------|-------|-------|------------------|
| 1250| 182.0482 | 69961 | 63154 | -0.964208425     |
| 1860| 673.5279  |       |       | -1.094598248     |
| 2350| 794.6058  | 24767528 |       | -1.342151679     |
| 2100| 76.0757   | 1145 | 1113  | HMDB00925 -1.628258621 |
Supplementary Table 5. The parameters of feature (metabolite) selection using bootstrapping enhanced elastic net regression

| Bootstrap num | r²   | RMSE  | lambda | alpha |
|---------------|------|-------|--------|-------|
| 1             | 0.24 | 702.90| 0.21   | 0.85  |
| 2             | 0.25 | 706.76| 0.74   | 0.25  |
| 3             | 0.25 | 687.02| 0.23   | 0.7   |
| 4             | 0.26 | 691.75| 0.33   | 0.45  |
| 5             | 0.25 | 682.02| 0.19   | 0.85  |
| 6             | 0.25 | 702.46| 0.18   | 0.75  |
| 7             | 0.25 | 698.87| 0.19   | 0.85  |
| 8             | 0.25 | 695.39| 0.36   | 0.4   |
| 9             | 0.26 | 694.62| 0.69   | 0.2   |
| 10            | 0.24 | 690.44| 0.24   | 0.8   |
| 11            | 0.25 | 693.70| 0.32   | 0.5   |
| 12            | 0.24 | 684.82| 0.38   | 0.45  |
| 13            | 0.25 | 688.98| 0.31   | 0.5   |
| 14            | 0.25 | 689.96| 0.32   | 0.45  |
| 15            | 0.24 | 699.11| 1.16   | 0.15  |
| 16            | 0.24 | 693.72| 0.63   | 0.25  |
| 17            | 0.25 | 686.37| 0.46   | 0.35  |
| 18            | 0.25 | 697.92| 0.22   | 0.7   |
| 19            | 0.25 | 702.72| 0.23   | 0.7   |
| 20            | 0.24 | 701.10| 0.36   | 0.45  |
| 21            | 0.26 | 685.66| 0.20   | 0.65  |
| 22            | 0.25 | 688.44| 0.72   | 0.2   |
| 23            | 0.25 | 686.81| 0.31   | 0.45  |
| 24            | 0.24 | 713.05| 0.38   | 0.5   |
| 25            | 0.25 | 675.12| 0.54   | 0.3   |
| 26            | 0.25 | 682.93| 0.98   | 0.15  |
| 27            | 0.25 | 699.17| 1.10   | 0.15  |
| 28            | 0.25 | 696.77| 0.24   | 0.6   |
| 29            | 0.26 | 680.71| 0.18   | 0.8   |
| 30            | 0.24 | 694.90| 1.57   | 0.1   |
| 31            | 0.26 | 680.42| 0.14   | 0.85  |
| 32            | 0.25 | 690.38| 0.32   | 0.6   |
| 33            | 0.25 | 680.39| 0.97   | 0.15  |
| 34            | 0.25 | 683.73| 0.64   | 0.25  |
| 35            | 0.25 | 712.30| 0.21   | 0.75  |
| 36            | 0.23 | 699.04| 0.26   | 0.8   |
| 37            | 0.24 | 701.63| 0.54   | 0.3   |
| 38            | 0.25 | 682.38| 0.64   | 0.25  |
| 39            | 0.25 | 684.28| 0.20   | 0.85  |
| 40            | 0.23 | 684.52| 0.87   | 0.25  |
| 41            | 0.24 | 691.60| 0.39   | 0.45  |
| 42            | 0.23 | 704.75| 0.65   | 0.3   |
| 43            | 0.25 | 685.99| 0.32   | 0.55  |
| 44            | 0.26 | 700.42| 0.83   | 0.15  |
| 45            | 0.25 | 698.24| 0.21   | 0.7   |
|   |    |     |    |    |
|---|----|-----|----|----|
| 46| 0.24 | 682.10 | 0.26 | 0.6 |
| 47| 0.25 | 692.75 | 0.98 | 0.15 |
| 48| 0.25 | 688.66 | 0.20 | 0.75 |
| 49| 0.24 | 695.56 | 0.79 | 0.25 |
| 50| 0.24 | 696.55 | 0.24 | 0.75 |
| 51| 0.23 | 686.04 | 0.27 | 0.8 |
| 52| 0.25 | 701.35 | 1.48 | 0.1 |
| 53| 0.25 | 699.22 | 0.66 | 0.2 |
| 54| 0.25 | 683.09 | 0.41 | 0.4 |
| 55| 0.23 | 689.37 | 0.58 | 0.35 |
| 56| 0.24 | 697.67 | 0.56 | 0.35 |
| 57| 0.25 | 691.86 | 0.45 | 0.4 |
| 58| 0.24 | 701.39 | 0.66 | 0.3 |
| 59| 0.25 | 687.02 | 0.27 | 0.6 |
| 60| 0.25 | 699.87 | 0.19 | 0.7 |
| 61| 0.25 | 699.74 | 0.33 | 0.45 |
| 62| 0.23 | 702.22 | 0.38 | 0.5 |
| 63| 0.25 | 703.37 | 0.90 | 0.15 |
| 64| 0.24 | 700.47 | 0.22 | 0.9 |
| 65| 0.24 | 694.62 | 0.36 | 0.55 |
| 66| 0.25 | 711.04 | 0.49 | 0.3 |
| 67| 0.26 | 679.05 | 1.18 | 0.1 |
| 68| 0.25 | 685.34 | 0.65 | 0.25 |
| 69| 0.25 | 673.62 | 0.24 | 0.6 |
| 70| 0.24 | 683.88 | 1.28 | 0.15 |
| 71| 0.25 | 679.29 | 0.27 | 0.55 |
| 72| 0.24 | 696.13 | 0.27 | 0.8 |
| 73| 0.25 | 705.15 | 0.33 | 0.5 |
| 74| 0.25 | 677.07 | 0.29 | 0.55 |
| 75| 0.25 | 683.32 | 0.18 | 0.8 |
| 76| 0.24 | 695.14 | 0.35 | 0.5 |
| 77| 0.26 | 694.19 | 0.35 | 0.35 |
| 78| 0.24 | 693.71 | 0.23 | 0.7 |
| 79| 0.25 | 698.61 | 0.22 | 0.7 |
| 80| 0.24 | 692.05 | 0.32 | 0.55 |
| 81| 0.24 | 678.87 | 0.25 | 0.7 |
| 82| 0.24 | 690.60 | 0.26 | 0.65 |
| 83| 0.25 | 689.84 | 0.53 | 0.3 |
| 84| 0.25 | 686.18 | 0.23 | 0.7 |
| 85| 0.25 | 708.69 | 0.35 | 0.45 |
| 86| 0.24 | 686.04 | 0.33 | 0.6 |
| 87| 0.25 | 683.84 | 0.18 | 0.9 |
| 88| 0.25 | 680.07 | 0.26 | 0.55 |
| 89| 0.25 | 681.85 | 0.22 | 0.85 |
| 90| 0.24 | 694.26 | 0.89 | 0.2 |
| 91| 0.26 | 684.63 | 0.27 | 0.55 |
| 92| 0.24 | 674.10 | 0.26 | 0.7 |
|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 93 | 0.25 | 696.72 | 0.25 | 0.7 |
| 94 | 0.26 | 702.35 | 0.15 | 0.9 |
| 95 | 0.26 | 683.84 | 0.30 | 0.5 |
| 96 | 0.24 | 681.25 | 0.72 | 0.25 |
| 97 | 0.25 | 696.24 | 0.30 | 0.55 |
| 98 | 0.24 | 706.95 | 0.37 | 0.5 |
| 99 | 0.24 | 702.93 | 0.21 | 0.85 |
| 100 | 0.25 | 706.16 | 1.09 | 0.15 |
Supplementary Table 5. The parameters of feature (metabolite) selection using bootstrapping enhanced elastic net regression
Supplementary Table 6. The rank of metabolites in the red meat metabolite score ordered by selected times in the bootstrapping process

| biochemical          | super_pathway |
|----------------------|---------------|
| glycine              | Amino Acid    |
| cholesterol          | Lipid         |
| creatinine           | Amino Acid    |
| alanine              | Amino Acid    |
| 4-hydroxyphenylpyruvate | Amino Acid   |
| citrulline           | Amino Acid    |
| imidazole lactate    | Amino Acid    |
| sphingosine          | Lipid         |
| 1-palmityl-GPC (O-16:0) | Lipid    |
| alpha-hydroxyisocaproate | Amino Acid |
| creatine             | Amino Acid    |
| trans-4-hydroxyproline | Amino Acid  |
| 2-linoleoylglycerol (18:2) | Lipid     |
| andro steroid monosulfate C19H28O6S (1)* | Lipid |
| homostachydrine*     | Xenobiotics   |
| 1-arachidonoyl-GPC (20:4n6)* | Lipid |
| N-acetylglutamine    | Amino Acid    |
| N-acetylphenylalanine | Amino Acid   |
| 10-heptadecenoate (17:1n7) | Lipid |
| 1-myristoylglycerol (14:0) | Lipid     |
| 4-vinylphenol sulfate | Xenobiotics |
| deoxycarnitine       | Lipid         |
| 5alpha-androstan-3alpha,17beta-diol monosulfate (2) | Lipid |
| 1-docosapentaenoyl-GPC (22:5n3)* | Lipid |
| 1-pentadecanoyl-GPC (15:0)* | Lipid |
| ergothioneine        | Xenobiotics   |
| 17-methylstearate    | Lipid         |
| S-methylcysteine     | Amino Acid    |
| trimethylamine N-oxide | Lipid      |
| 1-stearyl-2-oleoyl-GPE (18:0/18:1) | Lipid |
| sphingomyelin (d18:1/14:0, d16:1/16:0)* | Lipid |
| verapamil            | Xenobiotics   |
| N-acetylcarnosine    | Peptide       |
| 4-acetylspheno sul fate | Xenobiotics |
| docosahexaenoate (DHA; 22:6n3) | Lipid |
| N-palmitoyl-sphingosine (d18:1/16:0) | Lipid |
| methionine sulfone   | Amino Acid    |
| X - 21286            | X             |
| 1-arachidonoyl-GPA (20:4) | Lipid    |
| X - 11381            | X             |
| X - 09789            | X             |
| X - 12212            | X             |
| X - 21315            | X             |
| X - 12511            | X             |
| X - 02249            | X             |
| X - 11849            | X             |
| X - 12729            | X             |
| X - 15492            | X             |
sphingomyelin (d18:2/14:0, d18:1/14:1)*
sphingomyelin (d18:1/20:1, d18:2/20:0)*
propyl 4-hydroxybenzoate sulfate
palmitoyl dihydrospingomyelin (d18:0/16:0)*
1-palmitoyl-2-palmitoleoyl-GPC (16:0/16:1)*
1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)*
1-margaroyl-2-oleoyl-GPC (17:0/18:1)*
1-(1-enyl-palmitoyl)-2-linoleoyl-GPC (P-16:0/18:2)*
1-(1-enyl-palmitoyl)-2-palmitoyl-GPC (P-16:0/16:0)*
1-palmityl-2-arachidonoyl-GPC (O-16:0/20:4)*
asparagine
3-aminoisobutyrate
cysteine
betaine
2-hydroxyoctanoate
propionylglycine
1-methylimidazoleacetate
pseudouridine
N-acetylputrescine
1-stearoyl-2-arachidonoyl-GPC (18:0/20:4)
pyroglutamine*
1-stearoyl-2-arachidonoyl-GPI (18:0/20:4)
serotonin
methionine sulfoxide
taurocholate
4-hydroxyhippurate
1-oleoyl-GPI (18:1)*
cysteine sulfenic acid
triamterene
X - 21442
vanillic alcohol sulfate
X - 11315
glycerate
N-acetylaspartate (NAA)
2-palmitoyl-GPC (16:0)*
1-palmitoyl-2-linoleoyl-GPC (16:0/18:2)
X - 23583
1-(1-enyl-palmitoyl)-2-oleoyl-GPC (P-16:0/18:1)*
13-HODE + 9-HODE
X - 18914
X - 11852
1-(1-enyl-stearoyl)-2-docosahexaenoyl-GPE (P-16:0/22:6)*
uridine
pantothenate
phenylacetate
stearoylcarnitine (C18)
X - 17145
3-carboxy-4-methyl-5-propyl-2-furanpropanoate (CMPF)
O-sulfo-L-tyrosine
fructose
X - 23593
guanosine
dodecanedioate
5-methyluridine (ribothymidine)
ranitidine
N-acetyl-1-methylhistidine*
1-palmitoyl-2-palmitoyl-GPC (O-16:0/16:0)*
furosemide
X - 11905
X - 14662
X - 13729
sphingomyelin (d17:1/16:0, d18:1/15:0, d16:1/17:0)*
1-(1-enyl-palmitoyl)-2-docosahexaenoyl-GPE (P-16:0/22:6)*
fumarate
myristoylcarnitine (C14)
sphingosine 1-phosphate
ibuprofen
glycocholenate sulfate*
1-dihomo-linolenoyl-GPC (20:3n3 or 6)*
5alpha-androstan-3alpha,17beta-diol disulfate
X - 12462
X - 23587

Amino Acid
Amino Acid
Lipid
Xenobiotics
Lipid
Xenobiotics
Amino Acid
X
Amino Acid
Carbohydrate
Amino Acid
Lipid
Amino Acid
Cofactors and Vitamins
Amino Acid
Lipid
X
Lipid
X
Lipid
Xenobiotics
Carbohydrate
X
Nucleotide
Lipid
Nucleotide
Xenobiotics
Amino Acid
Lipid
Xenobiotics
X
X
Lipid
Energy
Lipid
Lipid
Xenobiotics
Lipid
Lipid
Lipid
Lipid
X
X
orotate
erythritol
X - 21353
X - 12849
cystine
heptanoate (7:0)
tyramine O-sulfate
imidazole propionate
glycerol 3-phosphate
X - 24243
1-pentadecanoyl-2-linoleoyl-GPC (15:0/18:2)*

1-(1-enyl-palmitoyl)-2-arachidonoyl-GPE (P-16:0/20:4)*
benzoate
3-hydroxyaurate
pregnane-3-glucuronide
5-methylthioadenosine (MTA)
estrone 3-sulfate
stearoyl sphingomyelin (d18:1/18:0)
3-indoxyl sulfate
1-stearoyl-2-linoleoyl-GPC (18:0/18:2)*
maleate
N-acetylasparagine

naproxen
sphingomyelin (d18:2/16:0, d18:1/16:1)*
proline
3-methylhistidine
2-oleoylglycerol (18:1)
theanine
1-palmitoyl-2-arachidonoyl-GPE (16:0/20:4)*
erucate (22:1n9)
alpah-tocopherol
N-acetylleucine

X - 12101
X - 12127
X - 11441
X - 21319
X - 12170
X - 12026
X - 17677
X - 17299

X - 12101
Nucleotide
Xenobiotics
X

X

Amino Acid
Lipid
X

Amino Acid
Amino Acid
Lipid

X

Lipid
Xenobiotics
Lipid
Amino Acid
Lipid
Amino Acid
Lipid
Amino Acid

Xenobiotics
Lipid
Amino Acid

Xenobiotics
Lipid

Xenobiotics
Lipid

Cofactors and Vitamins
Amino Acid
X

X

Lipid
Lipid

Amino Acid

Xenobiotics
Lipid

Xenobiotics
Amino Acid
X

X

Amino Acid
Xenobiotics

Xenobiotics
Cofactors and Vitamins
X

X
gamma-CEHC
X - 15728
gulonate*
X - 23644
threonine
adrenate (22:4n6)
X - 11438
X - 12740
1-dihomo-linolenylglycerol (20:3)
taurodeoxycholate
gamma-glutamylhistidine
DSGEGDFXAEGGGVR*
bilirubin (E,E)*
eryonate*
2-methoxyresorcinol sulfate
X - 12472
ornithine
3-hydroxydecanoate
oxypurinol
3-hydroxycotinine glucuronide
X - 02269
X - 16570
X - 23196
kynurenine
3-phenylpropionate (hydrocinnamate)
hexanoylcarnitine (C6)
lidocaine
X - 16947
X - 21849
X - 12686
hpyotaurine
1-palmitoyl-2-docosahexaenoyl-GPE (16:0/22:6)*
dimethylarginine (SDMA + ADMA)
prolylglycine
X - 12798
pyrraline
caprate (10:0)
thymol sulfate
acetylcarnitine (C2)
cis-4-decenoylcarnitine (C10:1)
3-methyl-2-oxobutyrate
gluconate
maltose
oleoyl ethanolamide
X - 12306
X - 23680
1-palmitoyl-2-arachidonoyl-GPC (16:0/20:4n6)
1,3-dimethylurate
2-arachidonoyl-GPC (20:4)*
hydantoin-5-propionic acid
isovalerate
linoleate (18:2n6)
saccharin
homocitrulline
caprylate (8:0)
ferulic acid 4-sulfate
X - 18345
cystathionine
1-palmitoyl-2-oleoyl-GPE (16:0/18:1)
pyridoxate
2-aminobutyrate
X - 17185
X - 12844
X - 12206
X - 17367
X - 23590
N6,N6,N6-trimethyllysine
4-hydroxychlorothalonil
chenodeoxycholate
palmitoylcarnitine (C16)
X - 16649
N-acetylcitrulline
retinol (Vitamin A)
N-acetylglycine
2-hydroxypalmitate
hexadecanedioate
warfarin
X - 15674
isoursodeoxycholate
myo-inositol
X - 18249
X - 16071
urate
indolelactate
X - 21729
X - 11564
5,6-dihydrothymine
dimethylglycine
glycocholate
N-acetylneuraminate
N-acetyltreonine
glycohyocholate
X - 21668
umbelliferone sulfate
X - 12730
nonadecanoate (19:0)
hippurate
tartrionate (hydroxymalonate)
1-arachidonylglycerol (20:4)
lanthionine
beta-citrylglutamate
3-hydroxy-3-methylglutarate
carnitine
ethylmalonate
X - 11795
caffeine
sphinganine
salicylic glucuronide*
7-methylguanine
3-hydroxyquinine
5alpha-androstan-3beta,17beta-diol disulfate
atenolol
glutamate
 gamma-glutamylglutamine
glycochenodeoxycholate
7-methylxanthine
acisoga
pipecolate
4-hydroxyphenylacetate
alpha-hydroxyisovalerate
X - 23639
palmitic amide
glutarylcarnitine (C5-DC)
N-trimethyl 5-aminovalerate
X - 11491
X - 19455
1,3,7-trimethylurate
3-methyl catechol sulfate (1)
X - 18901
kynurenate
valine
glycerol
pro-hydroxy-pro
X - 12407
arabitol/xylitol
stearate (18:0)
X - 11540
indoleacetylglutamine
X - 12063
theophylline
orotidine
X - 21339
X - 11858
isocitrate
stachydrine
sphingomyelin (d18:1/18:1, d18:2/18:0)
X - 19141
X - 11540
X - 18901
kynurenate
valine
glycerol
pro-hydroxy-pro
X - 12407
arabitol/xylitol
stearate (18:0)
X - 11540
indoleacetylglutamine
X - 12063
theophylline
orotidine
X - 21339
X - 11858
isocitrate
stachydrine
sphingomyelin (d18:1/18:1, d18:2/18:0)
gamma-tocopherol/beta-tocopherol
alpha-ketoglutarate
suberate (octanedioate)
gamma-glutamylleucine
theobromine
threonate
myristoleate (14:1n5)
quinolinate
5-dodecanoate (12:1n7)
choline phosphate
androstenediol (3beta,17beta) disulfate (1)
omeprazole
X - 11452
p-cresol-glucuronide*
1-(1-enyl-palmitoyl)-2-arachidonoyl-GPC (P-16:0/20:4)*
ursodeoxycholate
xanthine
X - 17327
galactonate
andosterone sulfate
4-methylcatechol sulfate
X - 11444
isobutyrylcarnitine (C4)
5alpha-pregnan-3beta,20beta-diol monosulfate (1)
X - 11378
X - 11429
X - 21752
N-acetyltaurine
glucuronate
1-linolenoyl-GPC (18:3)*
3-(4-hydroxyphenyl)lactate
N-palmitoylglycine
1-myristoyl-GPC (14:0)
deoxycholate
dihomo-linolenate (20:3n3 or n6)
o-cresol sulfate
X - 12411
X - 23314
1-methylnicotinamide
N-acetyl-beta-alanine
cimetidine
X - 19183
1-palmitoyl-2-eicosapentaenoyl-GPC (16:0/20:5)*
1-(1-enyl-palmitoyl)-2-palmitoleoyl-GPC (P-16:0/16:1)*
sarcosine
1-palmitoleoyl-GPC (16:1)*
1-methylxanthine
1,7-dimethylurate
X - 21341
X - 12013
tartarate
oxalate (ethanedioate)
oleoylcarnitine (C18:1)
2-piperidinone
valerate
arachidonic acid (20:4n6)
1-palmitoylglycerol (16:0)
X - 17325
X - 14314
NA
androstenediol (3beta,17beta) monosulfate (1)
3-hydroxyhippurate
X - 07765
X - 14939
X - 21607
X - 23588
gamma-glutamyltyrosine
gamma-glutamylisoleucine*
C-glycosyltryptophan
nicotinamide
cortisone
2-amino-octanoate
guanidinoacetate
X - 21258
N-methylpyroglutamate
X - 12688
hydroquinone sulfate
isobutyrylglycine
eicosanoid
21-hydroxypregnenolone disulfate
X - 22379
4-guanidino-butanoate
2-arachidonoyl-GPE (20:4)*
3-(3-hydroxyphenyl)propionate
X - 16083
sphingomyelin (d18:1/22:1, d18:2/22:0, d16:1/24:1)*
maltose
hypoxanthine
2-hydroxyhippurate (salicylate)
1,2-dipalmitoyl-GPC (16:0/16:0)
4-methyl-2-oxopentanoate
1-docosahexaenoyl-GPC (22:6)*
1-arachidonoyl-GPC (20:0)
1-(1-ene-stearoyl)-2-oleoyl-GPE (P-18:0/18:1)
cotinine
N1-methyladenosine  
dihomo-linoleate (20:2n6)  
5alpha-pregnan-3beta,20alpha-diol disulfate  
N1-Methyl-2-pyridone-5-carboxamide  
X - 11843  
X - 12544  
dopamine 3-O-sulfate  
glutamine  
octanoylcarnitine (C8)  
1-linolenoylglycerol (18:3)  
tiglylcarnitine (C5:1-DC)  
glycerophosphoethanolamine  
succinimide  
X - 15503  
2-palmitoleoylglycerol (16:1)*  
phenylpyruvate  
sucrose  
thyroxine  
riboflavin  
glycodeoxycholate  
tauroliothiocholate 3-sulfate  
phosphate  
1-docosapentaenoyl-GPC (22:5n6)*  
desmethylnaproxen sulfate  
X - 17346  
1-palmitoleoylglycerol (16:1)*  
sphingomyelin (d18:2/24:1, d18:1/24:2)*  
histidine  
urea  
2-amino adipate  
azelate (nonanedioate)  
1-palmitoyl-GPA (16:0)  
ethyl glucuronide  
X - 16124  
X - 15469  
X - 21803  
X - 21807  
X - 12812  
X - 12221  
mannose  
X - 23297  
1-oleoylglycerol (18:1)  
glycolithocholate  
N-acetylhistidine  
N6-carbamoylthreonyladenosine  
catechol sulfate  
4-hydroxycoumarin  
1-dihomo-linolenoyl-GPE (20:3n3 or 6)*  
X - 12739  
X - 17269

N1-methyladenosine  
dihomo-linoleate (20:2n6)  
5alpha-pregnan-3beta,20alpha-diol disulfate  
N1-Methyl-2-pyridone-5-carboxamide  
X - 11843  
X - 12544  
dopamine 3-O-sulfate  
glutamine  
octanoylcarnitine (C8)  
1-linolenoylglycerol (18:3)  
tiglylcarnitine (C5:1-DC)  
glycerophosphoethanolamine  
succinimide  
X - 15503  
2-palmitoleoylglycerol (16:1)*  
phenylpyruvate  
sucrose  
thyroxine  
riboflavin  
glycodeoxycholate  
tauroliothiocholate 3-sulfate  
phosphate  
1-docosapentaenoyl-GPC (22:5n6)*  
desmethylnaproxen sulfate  
X - 17346  
1-palmitoleoylglycerol (16:1)*  
sphingomyelin (d18:2/24:1, d18:1/24:2)*  
histidine  
urea  
2-amino adipate  
azelate (nonanedioate)  
1-palmitoyl-GPA (16:0)  
ethyl glucuronide  
X - 16124  
X - 15469  
X - 21803  
X - 21807  
X - 12812  
X - 12221  
mannose  
X - 23297  
1-oleoylglycerol (18:1)  
glycolithocholate  
N-acetylhistidine  
N6-carbamoylthreonyladenosine  
catechol sulfate  
4-hydroxycoumarin  
1-dihomo-linolenoyl-GPE (20:3n3 or 6)*  
X - 12739  
X - 17269
4-hydroxyphenylacetylglutamine
5-oxoprolin
phenolphthalein beta-D-glucuronide
1-palmitoyl-GPE (16:0)
succinylcarnitine (C4-DC)
2-hydroxyibuprofen
X - 12847
X - 17690
1-(1-enyl-stearoyl)-2-oleoyl-GPC (P-18:0/18:1)
allantoin
4-acetamidobutanoate
malonate
cys-gly, oxidized
X - 11787
1-dihomo-linoleoyl-GPC (20:2)*
O-methylcatechol sulfate
methyl glucopyranoside (alpha + beta)
vanillylmandelate (VMA)
beta-hydroxyisovalerate
gentisate
taurolchenate sulfate
2,3-dihydroxyisovalerate
hydrochlorothiazide
X - 11442
X - 21470
X - 12846
X - 17469
X - 12822
X - 12410
glutarate (pentanedioate)
N-acetyltyrosine
gamma-glutamyl-epsilon-lysine
isovalerylglycine
1-eicosenoyl-GPC (20:1)*
gamma-glutamylmethionine
X - 21343
X - 17166
sulfate*
X - 21796
eugenol sulfate
1-margaroyl-2-linoleoyl-GPC (17:0/18:2)*
3-hydroxyisobutyrate
methyl indole-3-acetate
cortisol
biliverdin
2-hydroxystearate
sebacate (decanedioate)  
butyrylcarnitine (C4)  
1-arachidonoyl-GPI (20:4)*  
5-acetylamino-6-formylamino-3-methyluracil androstenediol (3beta,17beta) monosulfate (2)  
X - 21411  
X - 12830  
isoegenol sulfate  
X - 23739  
beta-alanine  
3-methoxytyrosine  
1,5-anhydroglucitol (1,5-AG)  
docosapentaenoate (n3 DPA; 22:5n3)  
N-acetyltryptophan  
hexanoylglycine  
p-cresol sulfate  
N-acetylserine  
chiro-inositol  
1-eicosapentaenoyl-GPC (20:5)*  
1-(1-enyl-oleoyl)-GPE (P-18:1)*  
mannitol/sorbitol  
X - 11850  
X - 12816  
etiocholanolone glucuronide  
X - 13737  
X - 12714  
gamma-glutamyl-alpha-lysine  
N-acetylvaline  
cholate  
3-methylxanthine  
1-palmitoyl-GPI (16:0)  
gamma-glutamylglutamate  
7-alpha-hydroxy-3-oxo-4-cholestenoate (7-Hoca)  
16a-hydroxy DHEA 3-sulfate  
2-aminophenol sulfate  
hexanoylglutamine  
X - 16946  
X - 11372  
X - 12701  
tryptophan  
uracil  
isoleucine  
succinate  
citrate  
5-hydroxyhexanoate  
caproate (6:0)  
X - 21736  
X - 22515  
X - 17357
| Substance                                                                 | Category   |
|--------------------------------------------------------------------------|------------|
| methyl-4-hydroxybenzoate sulfate                                         | Xenobiotics|
| X - 23369                                                               | X          |
| 1-(1-enyl-stearoyl)-2-docosahexaenoyl-GPC (P-18:0/22:6)*                 | Lipid      |
| aspartate                                                                | Amino Acid |
| N-acetyllalanine                                                         | Amino Acid |
| N-acetylmethionine                                                       | Amino Acid |
| 3-ureidopropionate                                                       | Nucleotide |
| N-acetylglutamate                                                        | Amino Acid |
| indoleacetate                                                            | Amino Acid |
| 1-methylhistidine                                                        | Amino Acid |
| glycolithocholate sulfate*                                               | Lipid      |
| N2,N2-dimethylguanosine                                                 | Nucleotide |
| 4-allylphenol sulfate                                                    | Xenobiotics|
| N-methylproline                                                         | Amino Acid |
| pregnenolone sulfate                                                    | Lipid      |
| 6-oxopiperidine-2-carboxylate                                           | Amino Acid |
| 3-hydroxybutyrylcarnitine (1)                                            | Lipid      |
| X - 21441                                                               | X          |
| X - 11299                                                               | X          |
| X - 12230                                                               | X          |
| X - 14658                                                               | X          |
| X - 16935                                                               | X          |
| X - 21792                                                               | X          |
| X - 12543                                                               | X          |
| X - 23729                                                               | X          |
| tyrosine                                                                | Amino Acid |
| lysine                                                                  | Amino Acid |
| phenyllactate (PLA)                                                     | Amino Acid |
| 1-palmitoyl-GPC (16:0)                                                  | Lipid      |
| N6-acetyllysine                                                         | Amino Acid |
| Salpha-androstan-3alpha,17beta-diol monosulfate (1)                     | Lipid      |
| Salpha-pregnan-3beta,20alpha-diol monosulfate (2)                       | Lipid      |
| 1-(1-enyl-palmitoyl)-GPE (P-16:0)*                                       | Lipid      |
| X - 11530                                                               | X          |
| X - 12007                                                               | X          |
| X - 21626                                                               | X          |
| linoleoylcholine*                                                       | Lipid      |
| arginine*                                                               | Amino Acid |
| X - 13431                                                               | X          |
| arabinonate/xylonate                                                    | Carbohydrate|
| dopamine 4-sulfate                                                      | Amino Acid |
| 2-acetamidophenol sulfate                                               | Xenobiotics|
| 1-stearyl-2-linoleoyl-GPE (18:0/18:2)*                                  | Lipid      |
| homoarginine                                                            | Amino Acid |
| phenylacetylglutamine                                                   | Peptide    |
| cysteinylglycine                                                         | Amino Acid |
| 4-acetaminophen sulfate                                                 | Xenobiotics|
| 1-(1-enyl-stearyl)-GPE (P-18:0)*                                        | Lipid      |
| N-delta-acetylornithine                                                 | Amino Acid |
| 2-aminoheptanoate                                                       | Lipid      |
1-docosahexaenoyl-GPE (22:6)*
N-acetyllalliiin
2-palmitoyl-GPE (16:0)*
desmethylnaproxen
X - 13866
X - 01911
3-methylglutaryl carnitine (2)
X - 14056
1,2,3-benzenetriol sulfate (1)
1-(1-enyl-palmitoyl)-2-oleoyl-GPE (P-16:0/18:1)*
phenylalanine
salicylate
3-hydroxy-2-ethylpropionate
gamma-glutamylphenylalanine
decanoylcarnitine (C10)
3,7-dimethylurate
isovaleryl carnitine (C5)
2-linoleoyl-GPE (18:2)*
5alpha-androstan-3beta,17alpha-diol disulfate
glycoursodeoxycholate
2-stearoyl-GPE (18:0)*
2-hydroxydecanoate
X - 15497
X - 11470
X - 11538
X - 11880
X - 12216
X - 12126
X - 12680
X - 13844
X - 17685
2-oleoyl-GPC (18:1)*
N-acetylkynurenine (2)
pyruvate
1-stearoyl-2-linoleoyl-GPI (18:0/18:2)
1-(1-enyl-palmitoyl)-2-docosahexaenoyl-GPC (P-16:0/22:6)*
arachidate (20:0)
serine
N-formylmethionine
4-acetamidophenylglucuronide
glycerophosphorylcholine (GPC)
1-linoleoylglycerol (18:2)
2-hydroxyacetaminophen sulfate*
3-(cystein-S-yl)acetaminophen*
1-docosahexaenoylglycerol (22:6)
cinnamoylglycine
3-(3-hydroxyphenyl)propionate sulfate
X - 11440
X - 12231
X - 12329
| Compound                                      | Category       |
|-----------------------------------------------|----------------|
| 1-palmitoyl-2-arachidonoyl-GPI (16:0/20:4)*   | Lipid          |
| arginine                                      | Amino Acid     |
| 3-methyl-2-oxovalerate                        | Amino Acid     |
| paraxanthine                                  | Xenobiotics    |
| taurochenodeoxycholate                        | Lipid          |
| 1-stearoyl-GPI (18:0)                         | Lipid          |
| N-(2-furoyl)glycine                           | Xenobiotics    |
| propionylcarnitine (C3)                       | Lipid          |
| gamma-glutamylthreonine                       | Peptide        |
| stearidonate (18:4n3)                         | Lipid          |
| 1-methylurate                                 | Xenobiotics    |
| 1-arachidonoyl-GPE (20:4n6)*                  | Lipid          |
| 1-oleoyl-GPE (18:1)                           | Lipid          |
| 1-linoleoyl-GPI (18:2)*                       | Lipid          |
| androstenediol (3beta,17beta) disulfate (2)   | Lipid          |
| cotinine N-oxide                              | Xenobiotics    |
| X - 15486                                     |                |
| X - 11478                                     |                |
| X - 12261                                     |                |
| X - 17351                                     |                |
| sphingomyelin (d18:1/20:0, d16:1/22:0)*       | Lipid          |
Supplementary Table 6. The rank of metabolites in the red meat metabolite score ordered by selected times in the bootstrapping process

| sub_pathway                                                                 | selected times |
|----------------------------------------------------------------------------|----------------|
| Glycine, Serine and Threonine Metabolism                                    | 100            |
| Sterol                                                                      | 100            |
| Creatine Metabolism                                                        | 100            |
| Alanine and Aspartate Metabolism                                           | 100            |
| Tyrosine Metabolism                                                        | 100            |
| Urea cycle; Arginine and Proline Metabolism                                | 100            |
| Histidine Metabolism                                                       | 100            |
| Sphingolipid Metabolism                                                    | 100            |
| Lysophosphalogen                                                            | 100            |
| Leucine, Isoleucine and Valine Metabolism                                   | 100            |
| Creatine Metabolism                                                        | 100            |
| Urea cycle; Arginine and Proline Metabolism                                | 100            |
| Monoacylglycerol                                                            | 100            |
| Androgenic Steroids                                                         | 100            |
| Food Component/Plant                                                        | 100            |
| Lysophospholipid                                                            | 100            |
| Glutamate Metabolism                                                       | 100            |
| Phenylalanine Metabolism                                                   | 100            |
| Long Chain Fatty Acid                                                       | 100            |
| Monoacylglycerol                                                            | 100            |
| Benzoate Metabolism                                                        | 100            |
| Carnitine Metabolism                                                       | 100            |
| Androgenic Steroids                                                         | 100            |
| Lysophospholipid                                                            | 100            |
| Lysophospholipid                                                            | 100            |
| Food Component/Plant                                                        | 100            |
| Fatty Acid, Branched                                                        | 100            |
| Methionine, Cysteine, SAM and Taurine Metabolism                           | 100            |
| Phospholipid Metabolism                                                    | 100            |
| Phosphatidylethanolamine (PE)                                               | 100            |
| Sphingolipid Metabolism                                                    | 100            |
| Drug                                                                        | 100            |
| Dipeptide Derivative                                                       | 100            |
| Drug                                                                        | 100            |
| Polyunsaturated Fatty Acid (n3 and n6)                                     | 100            |
| Ceramides                                                                   | 100            |
| Methionine, Cysteine, SAM and Taurine Metabolism                           | 100            |
| X                                                                            | 100            |
| Lysophospholipid                                                            | 100            |
| X                                                                            | 100            |
| X                                                                            | 100            |
| X                                                                            | 100            |
| X                                                                            | 100            |
| X                                                                            | 100            |
| X                                                                            | 100            |
| X                                                                            | 100            |
| X                                                                            | 100            |
| X                                                                            | 100            |
| X                                                                            | 100            |
| X                                                                            | 100            |
| X                                                                            | 100            |
| X                                                                            | 100            |
| X                                                                            | 100            |
Sphingolipid Metabolism 100
Urea cycle; Arginine and Proline Metabolism 100
Phosphatidylcholine (PC) 100
Phosphatidylcholine (PC) 100
Plasmalogen 100
Plasmalogen 100
Plasmalogen 100
Plasmalogen 100
Plasmalogen 100
Alanine and Aspartate Metabolism 99
Pyrimidine Metabolism, Thymine containing 99
Methionine, Cysteine, SAM and Taurine Metabolism 99
Glycine, Serine and Threonine Metabolism 99
Fatty Acid, Monohydroxy 99
Fatty Acid Metabolism (also BCAA Metabolism) 99
Histidine Metabolism 99
Pyrimidine Metabolism, Uracil containing 99
Polyamine Metabolism 99
Phosphatidylcholine (PC) 99
Glutamate Metabolism 99
Food Component/Plant 99
Food Component/Plant 99
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| Food Component/Plant                                | 87   |
| Methionine, Cysteine, SAM and Taurine Metabolism    | 87   |
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| Plasmalogen                                         | 85   |
| Benzoate Metabolism                                 | 84   |
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| Polyamine Metabolism                                | 83   |
| Estrogenic Steroids                                 | 83   |
| Sphingolipid Metabolism                             | 83   |
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| Urea cycle; Arginine and Proline Metabolism         | 80   |
| Histidine Metabolism                                | 80   |
| Monoacylglycerol                                    | 80   |
| Food Component/Plant                                | 80   |
| Phosphatidylethanolamine (PE)                       | 80   |
| Long Chain Fatty Acid                               | 79   |
| Tocopherol Metabolism                               | 79   |
| Leucine, Isoleucine and Valine Metabolism           | 79   |
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| Purine Metabolism, Adenine containing               | 78   |
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| Benzoate Metabolism                                 | 78   |
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X 62
X 61
X 61
X 61
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Purine Metabolism, Guanine containing
Drug
Androgenic Steroids
Drug
Glutamate Metabolism
Gamma-glutamyl Amino Acid
Primary Bile Acid Metabolism
Xanthine Metabolism
Polyamine Metabolism
Lysine Metabolism
Phenylalanine Metabolism
Leucine, Isoleucine and Valine Metabolism
X
Fatty Acid, Amide
Lysine Metabolism
Lysine Metabolism
X
X
Xanthine Metabolism
Benzoate Metabolism
X
Tryptophan Metabolism
Leucine, Isoleucine and Valine Metabolism
Glycerolipid Metabolism
Urea cycle; Arginine and Proline Metabolism
X
Pentose Metabolism
Long Chain Fatty Acid
X
Tryptophan Metabolism
X
Xanthine Metabolism
Pyrimidine Metabolism, Orotate containing
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X
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X
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X  25
X  25
X  25
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Lysophospholipid  20
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Polyunsaturated Fatty Acid (n3 and n6)
Progestin Steroids
Nicotinate and Nicotinamide Metabolism
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X
Tyrosine Metabolism
Glutamate Metabolism
Fatty Acid Metabolism (Acyl Carnitine)
Monoacylglycerol
Leucine, Isoleucine and Valine Metabolism
Phospholipid Metabolism
Chemical
X
Monoacylglycerol
Phenylalanine Metabolism
Disaccharides and Oligosaccharides
Tyrosine Metabolism
Pentose Metabolism
Secondary Bile Acid Metabolism
Secondary Bile Acid Metabolism
Oxidative Phosphorylation
Lysophospholipid
Drug
X
Monoacylglycerol
Sphingolipid Metabolism
Histidine Metabolism
Urea cycle; Arginine and Proline Metabolism
Lysine Metabolism
Fatty Acid, Dicarboxylate
Lysophospholipid
Chemical
X
X
X
X
Fructose, Mannose and Galactose Metabolism
X
Monoacylglycerol
Secondary Bile Acid Metabolism
Histidine Metabolism
Purine Metabolism, Adenine containing
Benzoate Metabolism
Drug
Lysophospholipid
X
X
Acetylated Peptides
Glutathione Metabolism
Chemical
Lysophospholipid
TCA Cycle
Drug
Plasmalogen
Purine Metabolism, (Hypo)Xanthine/Inosine containing
Polyamine Metabolism
Fatty Acid Synthesis
Glutathione Metabolism
Lysophospholipid
Benzoate Metabolism
Food Component/Plant
Tyrosine Metabolism
Leucine, Isoleucine and Valine Metabolism
Tyrosine Metabolism
Secondary Bile Acid Metabolism
Food Component/Plant
Drug
Leucine, Isoleucine and Valine Metabolism
Fatty Acid, Dicarboxylate
Tyrosine Metabolism
Gamma-glutamyl Amino Acid
Leucine, Isoleucine and Valine Metabolism
Lysophospholipid
Gamma-glutamyl Amino Acid
Chemical
Food Component/Plant
Phosphatidylcholine (PC)
Leucine, Isoleucine and Valine Metabolism
Food Component/Plant
Corticosteroids
Hemoglobin and Porphyrin Metabolism
Fatty Acid, Monohydroxy
| Pathway                                                                 | Score |
|------------------------------------------------------------------------|-------|
| Fatty Acid, Dicarboxylate                                              | 10    |
| Fatty Acid Metabolism (also BCAA Metabolism)                          | 10    |
| Lysophospholipid                                                       | 10    |
| X                                                                       | 10    |
| X                                                                       | 10    |
| Food Component/Plant                                                   | 10    |
| X                                                                       | 10    |
| Lysophospholipid                                                       | 9     |
| X                                                                       | 9     |
| X                                                                       | 9     |
| Pyrimidine Metabolism, Uracil containing                               | 9     |
| Tyrosine Metabolism                                                    | 9     |
| Glycolysis, Gluconeogenesis, and Pyruvate Metabolism                   | 9     |
| Polyunsaturated Fatty Acid (n3 and n6)                                 | 9     |
| Tryptophan Metabolism                                                  | 9     |
| Fatty Acid Metabolism (Acyl Glutamine)                                 | 9     |
| Benzoate Metabolism                                                    | 9     |
| Glycine, Serine and Threonine Metabolism                               | 9     |
| Inositol Metabolism                                                    | 9     |
| Lysophospholipid                                                       | 9     |
| Lysoplasmalogen                                                        | 9     |
| Fructose, Mannose and Galactose Metabolism                             | 9     |
| X                                                                       | 9     |
| X                                                                       | 9     |
| Androgenic Steroids                                                    | 9     |
| X                                                                       | 9     |
| X                                                                       | 9     |
| Gamma-glutamyl Amino Acid                                              | 9     |
| Leucine, Isoleucine and Valine Metabolism                              | 8     |
| Methionine, Cysteine, SAM and Taurine Metabolism                       | 8     |
| Primary Bile Acid Metabolism                                           | 8     |
| X                                                                       | 8     |
| X                                                                       | 8     |
| Sterol                                                                  | 8     |
| Androgenic Steroids                                                    | 8     |
| Chemical                                                                | 8     |
| Fatty Acid Metabolism (Acyl Glutamine)                                 | 8     |
| X                                                                       | 8     |
| X                                                                       | 8     |
| X                                                                       | 8     |
| Tryptophan Metabolism                                                  | 7     |
| Pyrimidine Metabolism, Uracil containing                               | 7     |
| Leucine, Isoleucine and Valine Metabolism                              | 7     |
| TCA Cycle                                                              | 7     |
| Fatty Acid, Monohydroxy                                                | 7     |
| Medium Chain Fatty Acid                                                | 7     |
| X                                                                       | 7     |
| X                                                                       | 7     |
| X                                                                       | 7     |
Benzoate Metabolism
Plasmalogen
Alanine and Aspartate Metabolism
Alanine and Aspartate Metabolism
Methionine, Cysteine, SAM and Taurine Metabolism
Pyrimidine Metabolism, Uracil containing
Glutamate Metabolism
Tryptophan Metabolism
Histidine Metabolism
Secondary Bile Acid Metabolism
Purine Metabolism, Guanine containing
Food Component/Plant
Urea cycle; Arginine and Proline Metabolism
Pregnenolone Steroids
Lysine Metabolism
Fatty Acid Metabolism (Acyl Carnitine)
Tyrosine Metabolism
Lysine Metabolism
Phenylalanine Metabolism
Lysophospholipid
Lysine Metabolism
Androgenic Steroids
Progestin Steroids
Lysoplasmalogen
X
X
X
X
X
X
X
X
X
Tyrosine Metabolism
Lysine Metabolism
Phenylalanine Metabolism
Lysophospholipid
Lysine Metabolism
Androgenic Steroids
Progestin Steroids
Lysoplasmalogen
X
X
Fatty Acid Metabolism (Acyl Choline)
Urea cycle; Arginine and Proline Metabolism
Pentose Metabolism
Tyrosine Metabolism
Drug
Phosphatidylethanolamine (PE)
Urea cycle; Arginine and Proline Metabolism
Acetylated Peptides
Glutathione Metabolism
Drug
Lysoplasmalogen
Urea cycle; Arginine and Proline Metabolism
Fatty Acid, Amino
| Metabolism and Pathways                                      | Count |
|-------------------------------------------------------------|-------|
| Lysophospholipid                                            | 4     |
| Food Component/Plant                                        | 4     |
| Lysophospholipid                                            | 4     |
| Drug                                                        | 4     |
| X                                                           | 4     |
| X                                                           | 4     |
| Leucine, Isoleucine and Valine Metabolism                   | 4     |
| Chemical                                                    | 4     |
| Plasmalogen                                                 | 4     |
| Phenylalanine Metabolism                                    | 3     |
| Drug                                                        | 3     |
| Leucine, Isoleucine and Valine Metabolism                   | 3     |
| Gamma-glutamyl Amino Acid                                   | 3     |
| Fatty Acid Metabolism(Acyl Carnitine)                       | 3     |
| Xanthine Metabolism                                         | 3     |
| Leucine, Isoleucine and Valine Metabolism                   | 3     |
| Lysophospholipid                                            | 3     |
| Androgenic Steroids                                         | 3     |
| Secondary Bile Acid Metabolism                              | 3     |
| Lysophospholipid                                            | 3     |
| Fatty Acid, Monohydroxy                                     | 3     |
| X                                                           | 3     |
| X                                                           | 3     |
| X                                                           | 3     |
| X                                                           | 3     |
| X                                                           | 3     |
| X                                                           | 3     |
| Lysophospholipid                                            | 3     |
| Tryptophan Metabolism                                       | 3     |
| Glycolysis, Gluconeogenesis, and Pyruvate Metabolism        | 3     |
| Phosphatidylinositol (PI)                                   | 3     |
| Plasmalogen                                                 | 3     |
| Long Chain Fatty Acid                                       | 2     |
| Glycine, Serine and Threonine Metabolism                    | 2     |
| Methionine, Cysteine, SAM and Taurine Metabolism            | 2     |
| Drug                                                        | 2     |
| Phospholipid Metabolism                                     | 2     |
| Monoacylglycerol                                            | 2     |
| Drug                                                        | 2     |
| Drug                                                        | 2     |
| Monoacylglycerol                                            | 2     |
| Food Component/Plant                                        | 2     |
| Benzoate Metabolism                                         | 2     |
| X                                                           | 2     |
| X                                                           | 2     |
| X                                                           | 2     |
| Metabolism                                      | Count |
|------------------------------------------------|-------|
| Phosphatidylinositol (PI)                      | 2     |
| Urea cycle; Arginine and Proline Metabolism    | 1     |
| Leucine, Isoleucine and Valine Metabolism      | 1     |
| Xanthine Metabolism                            | 1     |
| Primary Bile Acid Metabolism                   | 1     |
| Lysophospholipid                               | 1     |
| Food Component/Plant                            | 1     |
| Fatty Acid Metabolism (also BCAA Metabolism)   | 1     |
| Gamma-glutamyl Amino Acid                      | 1     |
| Polyunsaturated Fatty Acid (n3 and n6)         | 1     |
| Xanthine Metabolism                            | 1     |
| Lysophospholipid                               | 1     |
| Lysophospholipid                               | 1     |
| Lysophospholipid                               | 1     |
| Androgenic Steroids                             | 1     |
| Tobacco Metabolite                             | 1     |
| X                                              | 1     |
| X                                              | 1     |
| X                                              | 1     |
| X                                              | 1     |
| Sphingolipid Metabolism                        | 1     |
Supplementary Table 7. The number of metabolites in each metabolite score and its explained variance of meat consumption using different thresholds in the exploratory and validation sets.

| Threshold  | 95% | No. of metabolites in the score | $R^2_{\text{exploratory set}}$ | $R^2_{\text{validation set}}$ |
|------------|-----|--------------------------------|---------------------------------|--------------------------------|
| red meat   |     | 114                            | 0.23                            | 0.17                           |
| proc meat  |     | 62                             | 0.17                            | 0.16                           |
| poultry    |     | 41                             | 0.16                            | 0.13                           |
Supplementary Table 7. The number of metabolites in each metabolite score and its explained variance of meat consumption using different thresholds in the exploratory and validation sets

| 90%       | 80%       |
|-----------|-----------|
| No. of metabolites in the score | No. of metabolites in the score |
|           | $R^2_{\text{exploratory \_set}}$ | $R^2_{\text{validation \_set}}$ |           |           |
| 139       | 0.24      | 0.17      | 174       |
| 82        | 0.18      | 0.15      | 104       |
| 49        | 0.16      | 0.13      | 70        |
### Supplementary Table 7

The number of metabolites in each metabolite score and its explained variance of meat consumption using different thresholds in the exploratory and validation sets.

| R²_{exploratory_set} | R²_{validation_set} | No. of metabolites in the score | R²_{exploratory_set} |
|-----------------------|----------------------|---------------------------------|-----------------------|
| 0.24                  | 0.17                 | 300                             | 0.25                  |
| 0.18                  | 0.15                 | 175                             | 0.18                  |
| 0.17                  | 0.12                 | 126                             | 0.18                  |
| $R^2_{validation\_set}$ |   |
|-------------------------|---|
| 0.18                    |   |
| 0.14                    |   |
| 0.12                    |   |
Supplementary Table 8. Correlation matrix of top-ranked metabolites in the red meat metabolite score and identified in the trial

|                          | 1-palmityl-GPC (O-16:0) | creatine |
|--------------------------|-------------------------|----------|
| 1-palmityl-GPC (O-16:0)  | 0.07                    |          |
| creatine                 | 1                       | 0.07     |
| trans-4-hydroxyproline   | 0.07                    | 0.21     |
| stearoylcarnitine        | 0.05                    | -0.08    |
| deoxycarnitine           | 0.13                    | -0.22    |
| trimethylamine N-oxide   | 0                       | 0.14     |
| 1-(1-etyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)* | 0.27 | 0.21 |
| 1-(1-etyl-stearoyl)-2-arachidonoyl-GPC (P-18:0/20:4)    | 0.30       | 0.08     |
| 1-(1-etyl-palmitoyl)-2-linoleoyl-GPC (P-16:0/18:2)*     | 0.29       | 0.09     |
| 1-(1-etyl-stearoyl)-2-linoleoyl-GPC (P-18:0/18:2)*      | 0.25       | 0.13     |
| 1-palmityl-2-arachidonoyl-GPC (O-16:0/20:4)*             | 0.38       | 0.07     |
Supplementary Table 8. Correlation matrix of top-ranked metabolites in the red meat metabolite score and identified in the trial.

|                          | trans-4-hydroxy | stearoylcarnitine | deoxycarnitine | trimethyl | 1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)* | 1-(1-enyl-stearoyl)-2-arachidonoyl-GPC (P-18:0/20:4) | 1-(1-enyl-palmitoyl)-2-linoleoyl-GPC (P-16:0/18:2)* | 1-(1-enyl-stearoyl)-2-linoleoyl-GPC (P-18:0/18:2) |
|--------------------------|-----------------|-------------------|----------------|------------|-----------------------------------------------------|-----------------------------------------------------|-----------------------------------------------------|-----------------------------------------------------|
| trans-4-hydroxy          | 0.07            | 0.05              | 0.13           | 0.00       | 0.27                                                | 0.3                                                | 0.29                                                | 0.25                                                |
| stearoylcarnitine        | 0.21            | -0.08             | -0.22          | 0.14       | 0.21                                                | 0.08                                               | 0.09                                                | 0.13                                                |
| deoxycarnitine           | 0.1             | 0.21              | 0.14           | 0.25       | 0.13                                                | 0.1                                                | 0.1                                                 | 0.09                                                |
| trimethyl                | 0.07            | 0.05              | 0.13           | 0.00       | 0.27                                                | 0.3                                                | 0.29                                                | 0.25                                                |
| 1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)* | 0.21            | -0.08             | -0.22          | 0.14       | 0.21                                                | 0.08                                               | 0.09                                                | 0.13                                                |
| 1-(1-enyl-stearoyl)-2-arachidonoyl-GPC (P-18:0/20:4) | 1.00             | 0.27              | 0.04           | 0.25       | 0.17                                                | 0.12                                               | 0.17                                                | 0.17                                                |
| 1-(1-enyl-palmitoyl)-2-linoleoyl-GPC (P-16:0/18:2)* | 0.1             | 0.27              | 1.00           | 0.15       | 0.12                                                | 0.12                                               | 0.08                                                | 0.08                                                |
| 1-(1-enyl-stearoyl)-2-linoleoyl-GPC (P-18:0/18:2) | 0.14            | 0.04              | 0.15           | 1.00       | 0.08                                                | 0.06                                               | -0.02                                               | 0.03                                                |
| 1.00                     | 0.21            | 0.27              | 1.00           | 0.15       | 0.12                                                | 0.12                                               | 0.08                                                | 0.08                                                |
| 0.13                     | 0.25            | 0.25              | 0.12           | 0.08       | 1.00                                                | 0.68                                               | 0.41                                                | 0.38                                                |
| 0.17                     | 0.17            | 0.25              | 0.12           | 0.08       | -0.02                                               | 1.00                                                | 0.51                                                | 0.49                                                |
| 0.08                     | 0.25            | 0.25              | 0.12           | 0.08       | -0.02                                               | 0.41                                               | 0.51                                                | 1.00                                                |
| 0.41                     | 0.51            | 1.00              | 0.68           | 1.00       | 0.51                                                | 1.00                                                | 0.74                                                | 1.00                                                |
| 0.68                     | 0.74            | 1.00              | 0.41           | 0.51       | 0.51                                                | 1.00                                                | 0.74                                                | 1.00                                                |
| 0.74                     | 0.49            | 0.74              | 0.38           | 0.41       | 0.51                                                | 1.00                                                | 0.74                                                | 1.00                                                |
| 1.00                     | 0.09            | 0.17              | 0.08           | 0.38       | 0.49                                                | 0.74                                                | 1.00                                                | 1.00                                                |
| 0.17                     | 0.19            | 0.13              | 0.01           | 0.65       | 0.63                                                | 0.21                                                | 0.14                                                | 0.14                                                |
| 0.08                     | 0.38            | 0.19              | 0.01           | 0.65       | 0.63                                                | 0.21                                                | 0.14                                                | 0.14                                                |
| 0.03                     | 0.41            | 0.17              | 0.08           | 0.38       | 0.49                                                | 0.74                                                | 1.00                                                | 1.00                                                |
1-palmityl-2-arachidonoyl-GPC (O-16:0/20:4)*

|          |        |        |        |        |        |
|----------|--------|--------|--------|--------|--------|
|          | 0.38   | 0.07   | 0.18   | 0.19   | 0.13   |
|          | 0.01   | 0.65   | 0.63   | 0.21   | 0.14   |
|          | 1      |        |        |        |        |
| metabolites         | BIOCHEMICAL                                                                 | coef. In the score |
|---------------------|------------------------------------------------------------------------------|--------------------|
| s_M52475            | 1-(1-enyl-stearoyl)-2-arachidonoyl-GPE (P-18:0/20:4)*                       | 3.042              |
| s_M52613            | 1-(1-enyl-stearoyl)-2-arachidonoyl-GPC (P-18:0/20:4)                        | 2.765              |
| s_M52499            | 1-margaroyl-2-oleoyl-GPC (17:0/18:1)*                                       | 2.750              |
| s_M32306            | trans-4-hydroxyproline                                                      | 2.672              |
| s_M42990            | verapamil                                                                   | 2.528              |
| s_M46347            | X - 11381                                                                   | 2.296              |
| s_M40406            | trimethylamine N-oxide                                                      | 2.175              |
| s_M52682            | 1-(1-enyl-palmitoyl)-2-linoleoyl-GPC (P-16:0/18:2)*                         | 1.982              |
| s_M20458            | 1-palmitoyl-GPC (O-16:0)                                                    | 1.701              |
| s_M52470            | 1-palmitoyl-2-palmitoleoyl-GPC (16:0/16:1)*                                | 1.611              |
| s_M00513            | creatinine                                                                  | 1.543              |
| s_M38296            | 17-methylstearate                                                           | 1.454              |
| s_M27718            | creatine                                                                    | 1.430              |
| s_M37459            | ergothioneine                                                               | 1.376              |
| s_M33971            | 10-heptadecenoate (17:1n7)                                                  | 1.375              |
| s_M52433            | sphingomyelin (d18:1/15:0, d16:1/17:0)*                                     | 1.278              |
| s_M52718            | 1-palmitoyl-2-arachidonoyl-GPC (O-16:0/20:4)*                              | 1.134              |
| s_M52712            | 1-(1-enyl-stearoyl)-2-linoleoyl-GPC (P-18:0/18:2)*                          | 1.055              |
| s_M44878            | methionine sulfone                                                          | 1.047              |
| s_M37231            | 1-docosapentaenoyl-GPC (22:5n3)*                                            | 0.980              |
| s_M36747            | deoxyxarnitine                                                              | 0.918              |
| s_M31787            | 3-carboxy-4-methyl-5-propyl-2-furanproanoyate (CMPF)                         | 0.911              |
| s_M00063            | cholesterol                                                                 | 0.898              |
| s_M46500            | X - 02249                                                                   | 0.897              |
| s_M33950            | N-acetylphenylalanine                                                        | 0.879              |
| s_M15716            | imidazole lactate                                                           | 0.844              |
| s_M22036            | 2-hydroxyoctanoate                                                          | 0.838              |
| s_M43488            | N-acetylcarnosine                                                            | 0.796              |
| s_M42448            | 1-stearoyl-2-oleoyl-GPE (18:0/18:1)                                          | 0.773              |
| s_M15506            | choline                                                                     | 0.760              |
| s_M38595            | ranitidine                                                                  | 0.735              |
| s_M46359            | X - 21315                                                                   | 0.708              |
| s_M47938            | X - 12731                                                                   | 0.699              |
| s_M46695            | X - 18913                                                                   | 0.691              |
| s_M35136            | 5-methyluridine (ribothymidine)                                              | 0.676              |
| s_M36602            | 1-oleoyl-GPI (18:1)*                                                        | 0.665              |
| s_M22132            | alpha-hydroxyisocaproate                                                    | 0.657              |
| s_M36098            | 4-vinylphenol sulfate                                                       | 0.598              |
| s_M37185            | Salpha-androstan-3alpha,17beta-diol monosulfate (2)                         | 0.577              |
| s_M44877            | N-palmitoyl-sphingosine (d18:1/16:0)                                         | 0.571              |
| s_M52504            | X - 24309                                                                   | 0.560              |
| s_M43829            | gamma-glutamylvaline                                                        | 0.518              |
| s_M32827            | andro steroid monosulfate (1)*                                              | 0.514              |
| s_M33943            | N-acetylglutamine                                                           | 0.503              |
| Protein ID | Name                                | logP   |
|------------|-------------------------------------|--------|
| s_M32388   | dodecanedioate                       | 0.502  |
| s_M39592   | S-methylcysteine                    | 0.490  |
| s_M47650   | X - 11483                           | 0.480  |
| s_M52297   | X - 24293                           | 0.476  |
| s_M35625   | 1-myristoylglycerol (14:0)          | 0.475  |
| s_M46728   | X - 21659                           | 0.452  |
| s_M36746   | 2-hydroxy-3-methylvalerate          | 0.435  |
| s_M47804   | X - 16580                           | 0.426  |
| s_M46487   | X - 21442                           | 0.402  |
| s_M48195   | fructose                            | 0.397  |
| s_M17747   | sphingosine                          | 0.375  |
| s_M37496   | N-acetylputrescine                  | 0.367  |
| s_M34409   | stearoylcarnitine                   | 0.347  |
| s_M3743    | cysteine sulfonic acid              | 0.316  |
| s_M46662   | X - 15492                           | 0.313  |
| s_M46687   | X - 18779                           | 0.310  |
| s_M46656   | X - 14662                           | 0.288  |
| s_M48442   | 4-vinylguaiacol sulfate             | 0.274  |
| s_M49459   | X - 23583                           | 0.234  |
| s_M02342   | serotonin                           | 0.227  |
| s_M43255   | N-acetyl-1-methylhistidine*         | 0.221  |
| s_M4689    | X - 17145                           | -0.141 |
| s_M15958   | phenylacetate                       | -0.182 |
| s_M46521   | X - 11852                           | -0.200 |
| s_M01573   | guanosine                           | -0.223 |
| s_M01508   | pantothenate                        | -0.237 |
| s_M31932   | propionylglycine                    | -0.242 |
| s_M46998   | X - 21821                           | -0.249 |
| s_M35527   | 4-hydroxyhippurate                  | -0.308 |
| s_M46623   | X - 12729                           | -0.335 |
| s_M47664   | X - 13658                           | -0.343 |
| s_M49592   | X - 11315                           | -0.349 |
| s_M48733   | vanillic alcohol sulfate            | -0.383 |
| s_M47971   | X - 13729                           | -0.389 |
| s_M49681   | X - 23782                           | -0.404 |
| s_M49469   | X - 23593                           | -0.407 |
| s_M18374   | methionine sulfoxide                | -0.427 |
| s_M49647   | X - 23749                           | -0.435 |
| s_M46358   | X - 12212                           | -0.441 |
| s_M37752   | 13-HODE + 9-HODE                    | -0.447 |
| s_M22185   | N-acetylaspartate (NAA)              | -0.447 |
| s_M18497   | taurocholate                        | -0.455 |
| s_M33009   | homostachydrine*                    | -0.467 |
| s_M01868   | cysteine                            | -0.470 |
| s_M15685   | 5-hydroxylysine                     | -0.474 |
| s_M57332   | X - 24061                           | -0.507 |
| s_M46607   | X - 11849                           | -0.510 |
| s_M46295   | X - 21286                           | -0.516 |
| s_M32506   | 2-linoleoylglycerol (18:2)          | -0.529 |
| s_M32553   | phenol sulfate                      | -0.535 |
| Compound                                      | Ms Value | Retention Time |
|-----------------------------------------------|----------|----------------|
| glycerate                                     | s_M01572| -0.537         |
| 1-arachidonoyl-GPA (20:4)                     | s_M46325 | -0.539         |
| 1-(1-enyl-palmitoyl)-2-myristoyl-GPC (P-16:0/14:0)* | s_M52715 | -0.554         |
| X - 11905                                     | s_M46367 | -0.556         |
| propyl 4-hydroxybenzoate sulfate              | s_M48460 | -0.559         |
| X - 18914                                     | s_M46368 | -0.566         |
| X - 17676                                     | s_M46970 | -0.578         |
| furosemide                                    | s_M43009 | -0.604         |
| X - 18899                                     | s_M47670 | -0.613         |
| quinine                                       | s_M39767 | -0.625         |
| 1-(1-enyl-palmitoyl)-2-docosahexaenoyl-GPE (P-16:0/22:6)* | s_M52672 | -0.628         |
| X - 12339                                     | s_M47709 | -0.633         |
| uridine                                       | s_M00606 | -0.635         |
| alanine                                       | s_M01126 | -0.635         |
| O-sulfo-L-tyrosine                            | s_M45413 | -0.652         |
| 1-methylimidazoleacetate                      | s_M32350 | -0.654         |
| asparagine                                    | s_M00512 | -0.665         |
| 4-acetylphenol sulfate                        | s_M44620 | -0.668         |
| 2-palmitoyl-GPC (16:0)*                       | s_M35253 | -0.683         |
| 3-aminoisobutyrate                            | s_M01566 | -0.732         |
| 4-hydroxyphenylpyruvate                       | s_M01669 | -0.735         |
| 1-(1-enyl-palmitoyl)-2-palmitoyl-GPC (P-16:0/16:0)* | s_M52716 | -0.756         |
| betaine                                       | s_M03141 | -0.757         |
| 1-stearoyl-2-arachidonoyl-GPI (18:0/20:4)     | s_M52449 | -0.759         |
| 1-(1-enyl-stearoyl)-2-docosahexaenoyl-GPE (P-18:0/22:6)* | s_M52476 | -0.880         |
| sphingomyelin (d18:1/20:1, d18:2/20:0)*       | s_M48491 | -0.965         |
| pseudouridine                                 | s_M33442 | -1.006         |
| 1-(1-enyl-palmitoyl)-2-oleoyl-GPC (P-16:0/18:1)* | s_M52478 | -1.046         |
| citrulline                                    | s_M02132 | -1.092         |
| pyroglutamine*                                | s_M46225 | -1.125         |
| X - 13684                                     | s_M47790 | -1.130         |
| X - 09789                                     | s_M46355 | -1.155         |
| X - 14838                                     | s_M47787 | -1.163         |
| 1-arachidonoyl-GPC (20:4n6)*                  | s_M33228 | -1.192         |
| palmitoyl dihydro sphingomyelin (d18:0/16:0)*  | s_M52434 | -1.245         |
| X - 12511                                     | s_M46458 | -1.323         |
| docosahexaenoate (DHA; 22:6n3)                | s_M44675 | -1.345         |
| 1-stearoyl-2-arachidonoyl-GPC (18:0/20:4)     | s_M42450 | -1.383         |
| glycine                                       | s_M00058 | -1.387         |
| sphingomyelin (d18:2/14:0, d18:1/14:1)*       | s_M47154 | -1.460         |
| 1-pentadecanoyl-GPC (15:0)*                   | s_M37418 | -1.473         |
| 1-palmitoyl-2-linoleoyl-GPC (16:0/18:2)       | s_M42446 | -1.591         |
| X - 12442                                     | s_M46618 | -1.701         |
| triamterene                                   | s_M42593 | -1.879         |
| sphingomyelin (d18:1/14:0, d16:1/16:0)*       | s_M42463 | -2.751         |
| miss_rate_ | miss_rate_ | miss_rate_ | miss_rate_ | miss_rate_ | miss_rate_ | miss_rate_ |
|-----------|-----------|-----------|-----------|-----------|-----------|-----------|
|           | batch2    | batch3    | batch23   | redmeat_  | redmeat_  | redmeat_  |
|           | consumer  | nonconsumer | consumer  | nonconsumer | consumer  | nonconsumer |
| 0.000     | 0.000     | 0.000     | 0.000     | 0.000     | 0.000     | 0.000     |
| 0.002     | 0.001     | 0.002     | 0.001     | 0.002     | 0.001     | 0.001     |
| 0.000     | 0.000     | 0.000     | 0.000     | 0.000     | 0.000     | 0.000     |
| 0.001     | 0.000     | 0.001     | 0.001     | 0.001     | 0.000     | 0.000     |
| 0.004     | 0.000     | 0.002     | 0.004     | 0.002     | 0.000     | 0.000     |
| 0.000     | 0.000     | 0.000     | 0.000     | 0.000     | 0.000     | 0.000     |
| 0.001     | 0.001     | 0.001     | 0.001     | 0.004     | 0.000     | 0.001     |
| 0.000     | 0.000     | 0.000     | 0.000     | 0.000     | 0.000     | 0.000     |
| 0.063     | 0.009     | 0.036     | 0.062     | 0.068     | 0.008     | 0.008     |
| 0.000     | 0.000     | 0.000     | 0.000     | 0.000     | 0.000     | 0.000     |
| 0.000     | 0.000     | 0.000     | 0.000     | 0.000     | 0.000     | 0.000     |
| 0.000     | 0.000     | 0.000     | 0.000     | 0.000     | 0.000     | 0.000     |
| 0.024     | 0.001     | 0.013     | 0.023     | 0.031     | 0.001     | 0.000     |
| 0.001     | 0.000     | 0.000     | 0.000     | 0.000     | 0.000     | 0.000     |
| 0.011     | 0.000     | 0.005     | 0.010     | 0.010     | 0.000     | 0.000     |
| 0.000     | 0.000     | 0.000     | 0.000     | 0.000     | 0.000     | 0.000     |
| 0.000     | 0.000     | 0.000     | 0.000     | 0.000     | 0.000     | 0.000     |
| 0.002     | 0.000     | 0.001     | 0.002     | 0.002     | 0.000     | 0.000     |
| 0.001     | 0.000     | 0.000     | 0.000     | 0.001     | 0.000     | 0.000     |
| 0.005     | 0.011     | 0.008     | 0.004     | 0.006     | 0.012     | 0.005     |
| 0.001     | 0.000     | 0.000     | 0.000     | 0.000     | 0.000     | 0.000     |
| 0.007     | 0.016     | 0.012     | 0.006     | 0.011     | 0.015     | 0.015     |
| 0.060     | 0.080     | 0.070     | 0.056     | 0.076     | 0.075     | 0.117     |
| 0.008     | 0.000     | 0.004     | 0.006     | 0.015     | 0.000     | 0.000     |
| 0.000     | 0.000     | 0.000     | 0.000     | 0.000     | 0.000     | 0.000     |
| 0.983     | 0.978     | 0.980     | 0.983     | 0.983     | 0.977     | 0.981     |
| 0.505     | 0.613     | 0.559     | 0.498     | 0.544     | 0.606     | 0.646     |
| 0.317     | 0.318     | 0.317     | 0.310     | 0.386     | 0.313     | 0.366     |
| 0.012     | 0.012     | 0.012     | 0.010     | 0.023     | 0.011     | 0.012     |
| 0.003     | 0.000     | 0.002     | 0.002     | 0.005     | 0.000     | 0.000     |
| 0.001     | 0.002     | 0.002     | 0.001     | 0.000     | 0.002     | 0.003     |
| 0.011     | 0.000     | 0.005     | 0.010     | 0.011     | 0.000     | 0.000     |
| 0.001     | 0.000     | 0.001     | 0.000     | 0.001     | 0.000     | 0.000     |
| 0.575     | 0.571     | 0.573     | 0.567     | 0.655     | 0.565     | 0.636     |
| 0.001     | 0.000     | 0.001     | 0.000     | 0.002     | 0.000     | 0.000     |
| 0.006     | 0.003     | 0.004     | 0.006     | 0.006     | 0.002     | 0.007     |
| 0.013     | 0.001     | 0.007     | 0.010     | 0.024     | 0.000     | 0.001     |
| 0.088     | 0.199     | 0.144     | 0.085     | 0.088     | 0.196     | 0.218     |
| 0.052     | 0.090     | 0.071     | 0.050     | 0.058     | 0.089     | 0.091     |
