Table S1. Main findings and evidence from metabolites associated with food (higher levels of metabolites are associated with higher levels of food item consumption/dietary pattern adherence unless otherwise specified).

Metabolite	Food Item/Dietary Pattern
TMAO	Meat products [1]; omnivorous diet [2]; seafood [3]; Nordic diet [3]; low glycemic load diet [4]; low dairy intake [5]; a pattern that is high in meat, refined bread, and butter and low in vegetables, whole-meal bread, and fruits (cluster 3) [6]; low-fat diet [7,8]; and a diet that is most concordant with the WHO healthy eating guidelines [9]
Dimethylamine	Omnivorous diet [2]; a diet that is most concordant with the WHO healthy eating guidelines [9]
2,6-dihydroxybenzoic acid	High-fiber diet [10]
2-aminophenol sulfate	High-fiber diet [10]
Hippuric acid	Dietary fiber intake [11]; tea consumption [3,12,13]; phytochemical diet [14]; Nordic diet [3]; a diet high in whole grains, fatty fish, and blueberries [15]; whole grain [15]
Hippurate	Low dairy consumption [5]; low-fat diet [8]; a diet that is most concordant with the WHO healthy eating guidelines [9]; low glycemic index diet [7]; a healthy cluster: higher intakes of breakfast cereals, low fat and skimmed milks, potatoes, fruit, fish, and fish dishes [16].
Kynurenate	Low glycemic load diet [4]
Valine	Protein intake [17]; high in potatoes, dairy products, and cornflakes intake dietary pattern [18]; fish eaters [19]; vegetarians [19]; Mediterranean diet [8].
Phenylalanine	Protein intake [17]; high-fat meal with whey protein isolate [20]; coffee consumption negatively associated with phenylalanine in men [21]; Western dietary pattern [22]; omnivorous diet [2];
Tyrosine	Protein intake [17]; fish eaters [19]; vegetarians [19]
Glutamine	Inversely associated with protein intake [17]
Tryptophan	High-fat meal with whey protein isolate [20]; fish eaters [19]; vegetarians [19]; a healthy cluster: higher intakes of breakfast cereals, low fat and skimmed milks, potatoes, fruit, fish, and fish dishes [16].
Kynurenine	High-fat meal with whey protein isolate [20]
Theobromine metabolites	Cocoa consumption [23]
Polyphenol metabolites	Cocoa consumption [23]; consumption of poly-phenol rich foods (coffee, tea, red wine, citrus fruit, apples, pears, and chocolate) [24]
Tartrate	Wine polyphenol consumption [25]
Hydroxyphenylvaleric	Flavan-3-ols from almond skin [26]
Hydroxyphenylpropionic	Flavan-3-ols from almond skin [26]
Hydroxyphenylacetic acids	Flavan-3-ols from almond skin [26]
Betonicine	High polyphenol orange juice [27]
Stachydrine	High polyphenol orange juice [27]
Methyl glucopyranoside	High polyphenol orange juice [27]
Dihydroferulic acid	High polyphenol orange juice [27]
Galactonate	High polyphenol orange juice [27]
Proline	Citrus intake [28,29], Mediterranean diet [8].
Betaine	Citrus intake [20,29]; a healthy cluster: higher intakes of breakfast cereals, low fat and skimmed milks, potatoes, fruit, fish, and fish dishes [16]
S-methyl-L-cysteine sulfoxide	Cruciferous vegetables intake [30]

Creatine	High-lycopene tomato sauce [31]; Mediterranean diet [8]; a diet that is least concordant with the WHO healthy eating guideline and has high intake of red meat [9]
Creatinine	High-lycopene tomato sauce [31]; high dairy consumption [5], Mediterranean diet [8]; an unhealthy cluster: higher intakes of chips/processed potatoes, meat products, savory snacks, and high-energy beverages [7]
Leucine	High-lycopene tomato sauce [31]; refined wheat bread [32]; Western dietary pattern [22]; high potatoes, dairy products, and cornflakes intake dietary pattern [18]; fish eaters [19]; vegetarians [19]; Mediterranean diet [8].
Choline	High-lycopene tomato sauce [31]
Methionine	High-lycopene tomato sauce [31]; high potatoes, dairy products, and cornflakes intake dietary pattern [18]; fish eaters [19]; vegetarians [19]
Acetate	High-lycopene tomato sauce [31]
Ascorbic acid	Normal-lycopene content tomato sauce [31]
Lactate	Normal-lycopene content tomato sauce [31]
Pyruvate	Normal-lycopene content tomato sauce [31]
Isoleucine	Normal-lycopene content tomato sauce [31]; refined wheat bread [32]; high potatoes, dairy products, and cornflakes intake dietary pattern [18]; Mediterranean diet [8].
Alanine	Normal-lycopene content tomato sauce [31]; low-fat diet [7]
Sphingomyelins	Coffee [33]
Acylcarnitines	Coffee (negative association with long- and medium chain acylcarnitines) [33], Western dietary pattern (positive association with short-chain acylcarnitines) [22], high butter intake and low margarine intake dietary pattern [18], hypocaloric diet (acylcarnitine C9) [17], meat intake (C0, C4, C5) [19], prudent pattern (medium- to long- chain) [22]
Diacylphosphatidylcholine	Coffee consumption (C32:1, negatively association) [21], dietary component: high poultry, fish, rice, vegetables, fruit, chocolate, flaked oat, cheese, milk, curds, and low meat and sausages [34]
Acylalkyl-phosphatidylcholines	Coffee consumption (positive associated with C34:3, C40:6, and C42:5 in women) [21], high butter intake and low margarine intake dietary pattern [18], dietary component: high poultry, fish, rice, vegetables, fruit, chocolate, flaked oat, cheese, milk, curds, and low meat and sausages [34]
Phosphatidylcholines	High red meat and fish, and low whole-grain bread and tea dietary pattern [18], hypocaloric diet (phosphatidylcholine-dyacil C38:6) [17], Mediterranean diet (P-18:1, 20:3) [35]
Methylxanthines	Coffee [36–38]
Methylated forms of hydroxycinnamates	Coffee [36–38]
Hydroxytyrosol	Olive oil consumption [39], phenolic content of food [40], alcohol consumption [39]
3-(3,5-dihydroxyphenyl)-1-propanoic acid sulfate	Whole-grain rye bread intake [41]
Enterolactone glucuronide	Whole-grain rye bread intake [41]
Azelaic acid	Whole-grain rye bread intake [41]
2-aminophenol sulfate	Whole-grain rye bread intake [41]
Lysophosphatidylcholine	Full-fat dairy [42], high butter intake and low margarine intake dietary pattern [18]
Lyso-platelet activating factor	Full-fat dairy [42]
Phospholipid fatty acids	Full-fat dairy [42]

Citrate	High dairy consumption [5], lactovegetarian diet [2], Mediterranean diet [8], a healthy cluster: higher intakes of breakfast cereals, low fat and skimmed milks, potatoes, fruit, fish and fish dishes [16]
Hexose	High red meat and fish, and low whole-grain bread and tea dietary pattern [18].
Hydroxy-sphingomyelin	High butter intake and low margarine intake dietary pattern [18]
Glycerophospholipids	Meat eaters [19]
Sphingolipids	Meat eaters [19]
Lysine	Fish eaters [19]; vegetarians [19]
p-Hydroxyphenylacetate	Vegetarian diet [19]
Methylhistidine	Omnivorous diet [2]; low-fat diet [8], a diet that is most concordant with the WHO healthy eating guidelines (1-methylhistidine and 3-methylhistidine) [9]
Phenylacetylglutamine	Vegetables [6]; high vegetables, fish, and whole-grain breads (cluster 1) [6];
O-acetylcarnitine	Red meat [6]; a pattern that is high in meat, refined bread, butter and low in vegetables, whole-meal bread, and fruits (cluster 3) [6], a diet that is least concordant with the WHO healthy eating guidelines and has high intake of red meat [9]
Glycine	High vegetables, fish, and whole-grain breads (cluster 1) [6], Mediterranean diet [8].
Acetoacetate	High vegetables, fish, and whole-grain breads (cluster 1) [6]
N,Ndimethylglycine	A pattern that is high in meat, refined bread, butter and low in vegetables, whole-meal bread, and fruits (cluster 3) [6].
Proline betaine	Citrus intake [14]
Sulforaphane	Phytochemical diet [14]
Genistein,	Phytochemical diet [14]
Daidzein	Phytochemical diet [14]
Equol	Phytochemical diet [14]
Glycitein	Phytochemical diet [14]
O-desmethylangolensin	Phytochemical diet [14]
Enterolactone	Phytochemical diet [14]
Trigonelline	Phytochemical diet [14]
Hydroquinone-glucuronide	Nordic diet [3]
3,4,5,6-tetrahydrohippurate	Nordic diet [3]
Glucuronidated alk(en)ylresorcinols	A diet high in whole grains, fatty fish, and bilberries [15]; whole-grain [15]
Furan fatty acids	A diet high in whole grains, fatty fish and bilberries [15]; fish intake [15]
Hydroxybutyrate	Mediterranean diet (3-hydroxybutyrate) [8]; very-low-carbohydrate diet (β-hydroxybutyrate) [7]; a healthy cluster: higher intakes of breakfast cereals, low fat and skimmed milks, potatoes, fruit, fish, and fish dishes (3-hydroxybutyrate) [16]
Cisaconitate	Mediterranean diet [8]
N-acetylglutamine	Mediterranean diet [8]
Oleic acids	Mediterranean diet [8]
Suberic acids	Mediterranean diet [8]
Histidine	Low-fat diet [8]
Carnosine	Low-fat diet [8]
Anserine	Low-fat diet [8]; a healthy cluster: higher intakes of breakfast cereals, low fat and skimmed milks, potatoes, fruit, fish, and fish dishes [16]
Xanthosine	Low-fat diet [8]
Nacetyl-S-methyl-cysteine-sulfoxide	Diet 1, which is most concordant with the WHO healthy eating guidelines [9]
Carnitine	A diet that is least concordant with the WHO healthy eating guidelines and has high intake of red meat [9]; very-low-carbohydrate diet [7]
Triacylglycerol	Low-fat diet (C54:5) [7]

Asparagine	Very-low-carbohydrate diet [7]
Cholesteryl esters	Very-low-carbohydrate diet [7]
Propionate	Very-low-carbohydrate diet [7]
Sorbitol	Very-low-carbohydrate diet [7]
4-pyridoxate	Low-fat diet [7]
Triacylglycerides (TG)	Low-fat diet (certain TGs) [7]; low glycemic index diet (certain TGs) [7]
Allantoin	Low-fat diet [7]
2-aminoadipate	Low-fat diet [7]
Serine	Low-fat diet [7]
Cytosine	Low glycemic index diet [7]
Hydroxyproline	Low glycemic index diet [7]
5-aminolevulinic acid	Low glycemic index diet [7]
Pipecolic acid	Low glycemic index diet [7]
N-phenylacetylglutamine	A healthy cluster: higher intakes of breakfast cereals, low fat and skimmed milks, potatoes, fruit, fish, and fish dishes [16]
2-aminoadipate	A healthy cluster: higher intakes of breakfast cereals, low fat and skimmed milks, potatoes, fruit, fish, and fish dishes [16]
Glycylproline	An unhealthy cluster: higher intakes of chips/processed potatoes, meat products, savory snacks, and high-energy beverages [7]
N-aceytalglutamate	An unhealthy cluster: higher intakes of chips/processed potatoes, meat products, savory snacks, and high-energy beverages [7]
Theophylline	An unhealthy cluster: higher intakes of chips/processed potatoes, meat products, savory snacks, and high-energy beverages [7]

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