

Omega-3 fatty acids correlate with gut microbiome diversity and production of N-carbamylglutamate in middle aged and elderly women

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Supplementary Table 1. List of faecal metabolites significantly associated to DHA circulating levels (FDR<0.05)adjusting for age, BMI and family relatedness.

Super Pathway	Sub pathway	Metabolite	BETA	SE	P	Q
Lipid	Polyunsaturated Fatty Acid (n3 and n6)	eicosapentaenoate (EPA; 20:5n3)	0.15	0.04	4.35×10^{-5}	0.01
Xenobiotics	Carbamylated aminoacid	N-carbamylglutamate	0.15	0.04	1.21×10^{-4}	0.02
Peptide	Dipeptide Derivative	anserine	0.13	0.04	5.39×10^{-4}	0.04

Supplementary Table 2. Associations between five measures of microbiome diversity and circulating levels of PUFA adjusting for age, BMI

fibre intake and family relatedness

	SHANNON DIVERSITY			CHAO1			OBSERVED SPECIES			Phylogenetic Diversity			SIMPSON		
	Beta	SE	P	Beta	SE	P	Beta	SE	P	Beta	SE	P	Beta	SE	P
DHA	0.13	0.04	0.002	0.12	0.04	0.003	0.14	0.04	0.001	0.12	0.04	0.01	0.09	0.04	0.02
FAW3	0.12	0.04	0.005	0.13	0.04	0.003	0.13	0.04	0.002	0.12	0.05	0.01	0.08	0.04	0.05
LA (18:2)	0.10	0.05	0.02	0.10	0.05	0.03	0.10	0.05	0.03	0.10	0.05	0.03	0.09	0.04	0.04
FAW6	0.09	0.04	0.02	0.10	0.04	0.01	0.10	0.04	0.01	0.10	0.04	0.02	0.08	0.04	0.05

DHA=22:6 docosahexaenoic acid;; FAW3= Omega-3 fatty acids; 18:2, LA= linoleic acid;; FAW6=omega-6 fatty acids

Supplementary Table 3. List of faecal metabolites measured using commercial metabolomic panel Metabolon Inc

Super-pathway	Sub-pathway	Metabolite name
Amino Acid	Alanine and Aspartate Metabolism	3-sulfo-L-alanine
Amino Acid	Alanine and Aspartate Metabolism	alanine
Amino Acid	Alanine and Aspartate Metabolism	asparagine
Amino Acid	Alanine and Aspartate Metabolism	aspartate
Amino Acid	Alanine and Aspartate Metabolism	N-acetylalanine
Amino Acid	Alanine and Aspartate Metabolism	N-acetylasparagine
Amino Acid	Alanine and Aspartate Metabolism	N-acetylaspartate (NAA)
Amino Acid	Alanine and Aspartate Metabolism	N-carbamoylalanine
Amino Acid	Alanine and Aspartate Metabolism	N-methylalanine
Amino Acid	Creatine Metabolism	creatine
Amino Acid	Creatine Metabolism	creatinine
Amino Acid	Creatine Metabolism	N-carbamoylsarcosine
Amino Acid	Glutamate Metabolism	carboxyethyl-GABA
Amino Acid	Glutamate Metabolism	gamma-aminobutyrate (GABA)
Amino Acid	Glutamate Metabolism	glutamate
Amino Acid	Glutamate Metabolism	glutamate, gamma-methyl ester
Amino Acid	Glutamate Metabolism	glutamine
Amino Acid	Glutamate Metabolism	N-acetylglutamate
Amino Acid	Glutamate Metabolism	N-acetylglutamine
Amino Acid	Glutamate Metabolism	N-methylglutamate
Amino Acid	Glutamate Metabolism	pyroglutamine*
Amino Acid	Glutamate Metabolism	S-1-pyrroline-5-carboxylate
Amino Acid	Glutathione Metabolism	5-oxoproline
Amino Acid	Glycine, Serine and Threonine Metabolism	allo-threonine
Amino Acid	Glycine, Serine and Threonine Metabolism	betaine
Amino Acid	Glycine, Serine and Threonine Metabolism	dimethylglycine
Amino Acid	Glycine, Serine and Threonine Metabolism	glycine
Amino Acid	Glycine, Serine and Threonine Metabolism	N-acetylglycine
Amino Acid	Glycine, Serine and Threonine Metabolism	N-acetyls erine
Amino Acid	Glycine, Serine and Threonine Metabolism	N-acetylthreonine
Amino Acid	Glycine, Serine and Threonine Metabolism	O-acetylhomoserine
Amino Acid	Glycine, Serine and Threonine Metabolism	serine
Amino Acid	Glycine, Serine and Threonine Metabolism	threonine
Amino Acid	Guanidino and Acetamido Metabolism	1-methylguanidine
Amino Acid	Guanidino and Acetamido Metabolism	4-guanidinobutanoate
Amino Acid	Histidine Metabolism	1-methylimidazoleacetate
Amino Acid	Histidine Metabolism	3-methylhistidine
Amino Acid	Histidine Metabolism	4-imidazoleacetate
Amino Acid	Histidine Metabolism	cis-urocanate
Amino Acid	Histidine Metabolism	formiminoglutamate
Amino Acid	Histidine Metabolism	histidine
Amino Acid	Histidine Metabolism	imidazole lactate

Amino Acid	Histidine Metabolism	imidazole propionate
Amino Acid	Histidine Metabolism	N-acetylhistidine
Amino Acid	Histidine Metabolism	trans-urocanate
Amino Acid	Leucine, Isoleucine and Valine Metabolism	2,3-dimethylsuccinate
Amino Acid	Leucine, Isoleucine and Valine Metabolism	2-hydroxy-3-methylvalerate
Amino Acid	Leucine, Isoleucine and Valine Metabolism	3-methyl-2-oxobutyrate
Amino Acid	Leucine, Isoleucine and Valine Metabolism	3-methyl-2-oxovalerate
Amino Acid	Leucine, Isoleucine and Valine Metabolism	4-methyl-2-oxopentanoate
Amino Acid	Leucine, Isoleucine and Valine Metabolism	alpha-hydroxyisocaproate
Amino Acid	Leucine, Isoleucine and Valine Metabolism	alpha-hydroxyisovalerate
Amino Acid	Leucine, Isoleucine and Valine Metabolism	ethylmalonate
Amino Acid	Leucine, Isoleucine and Valine Metabolism	isoleucine
Amino Acid	Leucine, Isoleucine and Valine Metabolism	isovalerate (C5)
Amino Acid	Leucine, Isoleucine and Valine Metabolism	isovalerylglycine
Amino Acid	Leucine, Isoleucine and Valine Metabolism	leucine
Amino Acid	Leucine, Isoleucine and Valine Metabolism	methylsuccinate
Amino Acid	Leucine, Isoleucine and Valine Metabolism	N-acetylisoleucine
Amino Acid	Leucine, Isoleucine and Valine Metabolism	N-acetylleucine
Amino Acid	Leucine, Isoleucine and Valine Metabolism	N-acetylvaline
Amino Acid	Leucine, Isoleucine and Valine Metabolism	valine
Amino Acid	Lysine Metabolism	2-aminoadipate
Amino Acid	Lysine Metabolism	5-aminovalerate
Amino Acid	Lysine Metabolism	6-oxopiperidine-2-carboxylic acid
Amino Acid	Lysine Metabolism	glutarate (pentanedioate)
Amino Acid	Lysine Metabolism	lysine
Amino Acid	Lysine Metabolism	N2,N6-diacetyllysine
Amino Acid	Lysine Metabolism	N2-acetyllysine
Amino Acid	Lysine Metabolism	N6,N6,N6-trimethyllysine
Amino Acid	Lysine Metabolism	N6-acetyllysine
Amino Acid	Lysine Metabolism	N6-carboxyethyllysine
Amino Acid	Lysine Metabolism	N6-formyllysine
Amino Acid	Lysine Metabolism	N-acetyl-cadaverine
Amino Acid	Lysine Metabolism	pipecolate
Amino Acid	Lysine Metabolism	saccharopine
Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	2-aminobutyrate
Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	2-hydroxybutyrate/2-hydroxyisobutyrate
Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	cysteine
Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	cysteine s-sulfate
Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	cysteine sulfinic acid
Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	cystine
Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	methionine
Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	methionine sulfoxide

	Metabolism	
Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	N-acetylcysteine
Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	N-acetylmethionine
Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	N-acetylmethionine sulfoxide
Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	N-formylmethionine
Amino Acid	Methionine, Cysteine, SAM and Taurine Metabolism	taurine
Amino Acid	Phenylalanine and Tyrosine Metabolism	(R)-salsolinol
Amino Acid	Phenylalanine and Tyrosine Metabolism	3-(3-hydroxyphenyl)propionate
Amino Acid	Phenylalanine and Tyrosine Metabolism	3-(4-hydroxyphenyl)lactate (HPLA)
Amino Acid	Phenylalanine and Tyrosine Metabolism	3-(4-hydroxyphenyl)propionate
Amino Acid	Phenylalanine and Tyrosine Metabolism	3-phenylpropionate (hydrocinnamate)
Amino Acid	Phenylalanine and Tyrosine Metabolism	4-hydroxycinnamate
Amino Acid	Phenylalanine and Tyrosine Metabolism	4-hydroxyphenylacetate
Amino Acid	Phenylalanine and Tyrosine Metabolism	4-hydroxyphenylpyruvate
Amino Acid	Phenylalanine and Tyrosine Metabolism	cis-4-hydroxycyclohexylacetic acid
Amino Acid	Phenylalanine and Tyrosine Metabolism	dihydrocaffeate
Amino Acid	Phenylalanine and Tyrosine Metabolism	N-acetylphenylalanine
Amino Acid	Phenylalanine and Tyrosine Metabolism	N-acetyltyrosine
Amino Acid	Phenylalanine and Tyrosine Metabolism	N-formylphenylalanine
Amino Acid	Phenylalanine and Tyrosine Metabolism	p-cresol
Amino Acid	Phenylalanine and Tyrosine Metabolism	p-cresol sulfate
Amino Acid	Phenylalanine and Tyrosine Metabolism	phenethylamine
Amino Acid	Phenylalanine and Tyrosine Metabolism	phenylacetate
Amino Acid	Phenylalanine and Tyrosine Metabolism	phenylalanine
Amino Acid	Phenylalanine and Tyrosine Metabolism	phenyllactate (PLA)
Amino Acid	Phenylalanine and Tyrosine Metabolism	phenylpyruvate
Amino Acid	Phenylalanine and Tyrosine Metabolism	tyramine
Amino Acid	Phenylalanine and Tyrosine Metabolism	tyrosine
Amino Acid	Phenylalanine and Tyrosine Metabolism	valerylphenylalanine
Amino Acid	Polyamine Metabolism	4-acetamidobutanoate
Amino Acid	Polyamine Metabolism	acisoga
Amino Acid	Polyamine Metabolism	N-acetylputrescine
Amino Acid	Polyamine Metabolism	spermidine
Amino Acid	Tryptophan Metabolism	2-aminophenol
Amino Acid	Tryptophan Metabolism	indole-3-carboxylic acid
Amino Acid	Tryptophan Metabolism	indoleacetate
Amino Acid	Tryptophan Metabolism	indolelactate
Amino Acid	Tryptophan Metabolism	indolepropionate
Amino Acid	Tryptophan Metabolism	kynurenate
Amino Acid	Tryptophan Metabolism	N-acetyltryptophan
Amino Acid	Tryptophan Metabolism	picolinate
Amino Acid	Tryptophan Metabolism	serotonin

Amino Acid	Tryptophan Metabolism	thioprolin
Amino Acid	Tryptophan Metabolism	tryptamin
Amino Acid	Tryptophan Metabolism	tryptophan
Amino Acid	Urea cycle; Arginine and Proline Metabolism	arginin
Amino Acid	Urea cycle; Arginine and Proline Metabolism	citrullin
Amino Acid	Urea cycle; Arginine and Proline Metabolism	dimethylarginin (ADMA + SDMA)
Amino Acid	Urea cycle; Arginine and Proline Metabolism	homocitrullin
Amino Acid	Urea cycle; Arginine and Proline Metabolism	hydroxyprolin
Amino Acid	Urea cycle; Arginine and Proline Metabolism	N-acetylarginin
Amino Acid	Urea cycle; Arginine and Proline Metabolism	N-acetylcitrullin
Amino Acid	Urea cycle; Arginine and Proline Metabolism	N-acetylprolin
Amino Acid	Urea cycle; Arginine and Proline Metabolism	N-alpha-acetylornithin
Amino Acid	Urea cycle; Arginine and Proline Metabolism	N-delta-acetylornithin
Amino Acid	Urea cycle; Arginine and Proline Metabolism	N-methylprolin
Amino Acid	Urea cycle; Arginine and Proline Metabolism	ornithin
Amino Acid	Urea cycle; Arginine and Proline Metabolism	prolin
Carbohydrate	Advanced Glycation End-product	N6-carboxymethyllysine
Carbohydrate	Aminosugar Metabolism	erythronat*
Carbohydrate	Aminosugar Metabolism	glucuronat
Carbohydrate	Aminosugar Metabolism	N-acetyl-beta-glucosaminylamin
Carbohydrate	Aminosugar Metabolism	N-acetylglucosamin/N-acetylgalactosamin
Carbohydrate	Aminosugar Metabolism	N-acetylglucosaminylasparagin
Carbohydrate	Aminosugar Metabolism	N-acetylmuramat
Carbohydrate	Aminosugar Metabolism	N-acetylneuraminat
Carbohydrate	Fructose, Mannose and Galactose Metabolism	fructose
Carbohydrate	Fructose, Mannose and Galactose Metabolism	galactonat
Carbohydrate	Fructose, Mannose and Galactose Metabolism	mannitol/sorbitol
Carbohydrate	Fructose, Mannose and Galactose Metabolism	mannose
Carbohydrate	Glycogen Metabolism	maltose
Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	glucose
Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	glycerat
Carbohydrate	Glycolysis, Gluconeogenesis, and Pyruvate Metabolism	lactat
Carbohydrate	Pentose Metabolism	2-deoxyribose
Carbohydrate	Pentose Metabolism	arabinose
Carbohydrate	Pentose Metabolism	arabitol/xylitol
Carbohydrate	Pentose Metabolism	arabonat/xylonat
Carbohydrate	Pentose Metabolism	fucose
Carbohydrate	Pentose Metabolism	ribitol
Carbohydrate	Pentose Metabolism	ribonat (ribonolacton)
Carbohydrate	Pentose Metabolism	ribulose/xylulose
Carbohydrate	Pentose Metabolism	sedoheptulose
Carbohydrate	Pentose Metabolism	xylose
Cofactors and Vitamins	Ascorbate and Aldarate Metabolism	threonat

Cofactors and Vitamins	Biotin Metabolism	biocytin
Cofactors and Vitamins	Biotin Metabolism	biotin
Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	bilirubin
Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	biliverdin
Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	D-urobilin
Cofactors and Vitamins	Hemoglobin and Porphyrin Metabolism	L-urobilin
Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	6-hydroxynicotinate
Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	nicotinamide
Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	nicotinamide riboside
Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	nicotinate
Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	nicotinate ribonucleoside
Cofactors and Vitamins	Nicotinate and Nicotinamide Metabolism	trigonelline (N'-methylnicotinate)
Cofactors and Vitamins	Pantothenate and CoA Metabolism	pantothenate (Vitamin B5)
Cofactors and Vitamins	Pterin Metabolism	pterin
Cofactors and Vitamins	Riboflavin Metabolism	riboflavin (Vitamin B2)
Cofactors and Vitamins	Thiamine Metabolism	5-(2-Hydroxyethyl)-4-methylthiazole
Cofactors and Vitamins	Thiamine Metabolism	thiamin (Vitamin B1)
Cofactors and Vitamins	Tocopherol Metabolism	alpha-tocopherol
Cofactors and Vitamins	Tocopherol Metabolism	alpha-tocotrienol
Cofactors and Vitamins	Tocopherol Metabolism	gamma-tocopherol/beta-tocopherol
Cofactors and Vitamins	Tocopherol Metabolism	gamma-tocotrienol
Cofactors and Vitamins	Vitamin B6 Metabolism	pyridoxal
Cofactors and Vitamins	Vitamin B6 Metabolism	pyridoxamine
Cofactors and Vitamins	Vitamin B6 Metabolism	pyridoxate
Cofactors and Vitamins	Vitamin B6 Metabolism	pyridoxine (Vitamin B6)
Energy	Oxidative Phosphorylation	phosphate
Energy	TCA Cycle	2-methylcitrate/homocitrate
Energy	TCA Cycle	alpha-ketoglutarate
Energy	TCA Cycle	citrate
Energy	TCA Cycle	fumarate

Energy	TCA Cycle	malate
Energy	TCA Cycle	succinate
Energy	TCA Cycle	tricarballylate
Lipid	Carnitine Metabolism	carnitine
Lipid	Carnitine Metabolism	deoxycarnitine
Lipid	Diacylglycerol	1-oleoyl-3-linoleoyl-glycerol (18:1/18:2)
Lipid	Diacylglycerol	1-palmitoyl-3-linoleoyl-glycerol (16:0/18:2)*
Lipid	Endocannabinoid	linoleoyl ethanolamide
Lipid	Endocannabinoid	oleoyl ethanolamide
Lipid	Endocannabinoid	palmitoyl ethanolamide
Lipid	Endocannabinoid	stearoyl ethanolamide
Lipid	Fatty Acid Metabolism (also BCAA Metabolism)	propionylglycine (C3)
Lipid	Fatty Acid Synthesis	malonate
Lipid	Fatty Acid, Amide	linoleamide (18:2n6)
Lipid	Fatty Acid, Branched	13-methylmyristate
Lipid	Fatty Acid, Branched	17-methylstearate
Lipid	Fatty Acid, Branched	methylpalmitate (15 or 2)
Lipid	Fatty Acid, Branched	pristanate
Lipid	Fatty Acid, Dicarboxylate	1,11-undecanedicarboxylate
Lipid	Fatty Acid, Dicarboxylate	2-hydroxyglutarate
Lipid	Fatty Acid, Dicarboxylate	3-carboxyadipate
Lipid	Fatty Acid, Dicarboxylate	3-methyladipate
Lipid	Fatty Acid, Dicarboxylate	3-methylglutarate/2-methylglutarate
Lipid	Fatty Acid, Dicarboxylate	adipate
Lipid	Fatty Acid, Dicarboxylate	azelate (nonanedioate; C9)
Lipid	Fatty Acid, Dicarboxylate	dimethylmalonic acid
Lipid	Fatty Acid, Dicarboxylate	dodecanedioate (C12)
Lipid	Fatty Acid, Dicarboxylate	hexadecanedioate (C16)
Lipid	Fatty Acid, Dicarboxylate	maleate
Lipid	Fatty Acid, Dicarboxylate	octadecanedioate (C18)
Lipid	Fatty Acid, Dicarboxylate	sebacate (decanedioate)
Lipid	Fatty Acid, Dicarboxylate	suberate (octanedioate)
Lipid	Fatty Acid, Dicarboxylate	undecanedioate
Lipid	Fatty Acid, Dihydroxy	12,13-DiHOME
Lipid	Fatty Acid, Dihydroxy	9,10-DiHOME
Lipid	Fatty Acid, Monohydroxy	10-hydroxystearate
Lipid	Fatty Acid, Monohydroxy	13-HODE + 9-HODE
Lipid	Fatty Acid, Monohydroxy	2-hydroxydecanoate
Lipid	Fatty Acid, Monohydroxy	2-hydroxypalmitate
Lipid	Fatty Acid, Monohydroxy	3-hydroxymyristate
Lipid	Fatty Acid, Monohydroxy	3-hydroxystearate
Lipid	Fatty Acid, Monohydroxy	5-hydroxyhexanoate
Lipid	Glycerolipid Metabolism	glycerol
Lipid	Glycerolipid Metabolism	glycerol 3-phosphate
Lipid	Glycerolipid Metabolism	glycerophosphoglycerol

Lipid	Inositol Metabolism	myo-inositol
Lipid	Ketone Bodies	3-hydroxybutyrate (BHBA)
Lipid	Long Chain Fatty Acid	10-heptadecenoate (17:1n7)
Lipid	Long Chain Fatty Acid	arachidate (20:0)
Lipid	Long Chain Fatty Acid	eicosenoate (20:1n9 or 1n11)
Lipid	Long Chain Fatty Acid	erucate (22:1n9)
Lipid	Long Chain Fatty Acid	margarate (17:0)
Lipid	Long Chain Fatty Acid	myristate (14:0)
Lipid	Long Chain Fatty Acid	myristoleate (14:1n5)
Lipid	Long Chain Fatty Acid	nonadecanoate (19:0)
Lipid	Long Chain Fatty Acid	oleate/vaccenate (18:1)
Lipid	Long Chain Fatty Acid	palmitate (16:0)
Lipid	Long Chain Fatty Acid	palmitoleate (16:1n7)
Lipid	Long Chain Fatty Acid	stearate (18:0)
Lipid	Lysolipid	1-palmitoyl-GPC (16:0)
Lipid	Lysolipid	1-palmitoyl-GPE (16:0)
Lipid	Lysolipid	1-palmitoyl-GPG (16:0)*
Lipid	Lysolipid	1-stearoyl-GPC (18:0)
Lipid	Lysolipid	1-stearoyl-GPE (18:0)
Lipid	Lysoplasmalogen	1-(1-enyl-stearoyl)-GPE (P-18:0)*
Lipid	Medium Chain Fatty Acid	5-dodecenoate (12:1n7)
Lipid	Medium Chain Fatty Acid	caprate (10:0)
Lipid	Medium Chain Fatty Acid	caproate (6:0)
Lipid	Medium Chain Fatty Acid	caprylate (8:0)
Lipid	Medium Chain Fatty Acid	heptanoate (7:0)
Lipid	Medium Chain Fatty Acid	laurate (12:0)
Lipid	Mevalonate Metabolism	3-hydroxy-3-methylglutarate
Lipid	Mevalonate Metabolism	mevalonate
Lipid	Monoacylglycerol	1-linoleoylglycerol (18:2)
Lipid	Monoacylglycerol	1-palmitoylglycerol (16:0)
Lipid	Phospholipid Metabolism	1-oleoyl-2-linoleoyl-GPC (18:1/18:2)*
Lipid	Phospholipid Metabolism	1-palmitoyl-2-linoleoyl-GPC (16:0/18:2)
Lipid	Phospholipid Metabolism	1-palmitoyl-2-oleoyl-GPC (16:0/18:1)
Lipid	Phospholipid Metabolism	choline
Lipid	Phospholipid Metabolism	glycerophosphoethanolamine
Lipid	Phospholipid Metabolism	glycerophosphoinositol*
Lipid	Phospholipid Metabolism	phosphocholine
Lipid	Phospholipid Metabolism	trimethylamine N-oxide
Lipid	Polyunsaturated Fatty Acid (n3 and n6)	arachidonate (20:4n6)
Lipid	Polyunsaturated Fatty Acid (n3 and n6)	dihomolinoleate (20:2n6)
Lipid	Polyunsaturated Fatty Acid (n3 and n6)	dihomolinolenate (20:3n3 or 3n6)
Lipid	Polyunsaturated Fatty Acid (n3 and n6)	docosadienoate (22:2n6)
Lipid	Polyunsaturated Fatty Acid (n3 and n6)	docosahexaenoate (DHA; 22:6n3)
Lipid	Polyunsaturated Fatty Acid (n3 and n6)	docosapentaenoate (DPA; 22:5n3)
Lipid	Polyunsaturated Fatty Acid (n3 and n6)	eicosapentaenoate (EPA; 20:5n3)

Lipid	Polyunsaturated Fatty Acid (n3 and n6)	linoleate (18:2n6)
Lipid	Polyunsaturated Fatty Acid (n3 and n6)	linolenate (18:3n3 or 3n6)
Lipid	Primary Bile Acid Metabolism	cholate
Lipid	Primary Bile Acid Metabolism	glycochenodeoxycholate
Lipid	Primary Bile Acid Metabolism	glycocholate
Lipid	Secondary Bile Acid Metabolism	3b-hydroxy-5-cholenoic acid
Lipid	Secondary Bile Acid Metabolism	6-oxolithocholate
Lipid	Secondary Bile Acid Metabolism	dehydrolithocholate
Lipid	Secondary Bile Acid Metabolism	deoxycholate
Lipid	Secondary Bile Acid Metabolism	glycodeoxycholate
Lipid	Secondary Bile Acid Metabolism	glycolithocholate sulfate*
Lipid	Secondary Bile Acid Metabolism	hyocholate
Lipid	Secondary Bile Acid Metabolism	lithocholate
Lipid	Short Chain Fatty Acid	valerate (5:0)
Lipid	Sphingolipid Metabolism	3-ketosphinganine
Lipid	Sphingolipid Metabolism	N-palmitoyl-sphinganine (d18:0/16:0)
Lipid	Sphingolipid Metabolism	N-palmitoyl-sphingosine (d18:1/16:0)
Lipid	Sphingolipid Metabolism	palmitoyl sphingomyelin (d18:1/16:0)
Lipid	Sphingolipid Metabolism	phytosphingosine
Lipid	Sphingolipid Metabolism	sphinganine
Lipid	Sphingolipid Metabolism	sphingosine
Lipid	Sterol	4-cholesten-3-one
Lipid	Sterol	beta-sitosterol
Lipid	Sterol	campesterol
Lipid	Sterol	cholesterol
Lipid	Sterol	coprostanol
Lipid	Sterol	lanosterol
Nucleotide	Purine and Pyrimidine Metabolism	methylphosphate
Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	2'-deoxyinosine
Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	hypoxanthine
Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	inosine
Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	urate
Nucleotide	Purine Metabolism, (Hypo)Xanthine/Inosine containing	xanthine
Nucleotide	Purine Metabolism, Adenine containing	1-methyladenine
Nucleotide	Purine Metabolism, Adenine containing	2'-deoxyadenosine
Nucleotide	Purine Metabolism, Adenine containing	adenine
Nucleotide	Purine Metabolism, Adenine containing	adenosine
Nucleotide	Purine Metabolism, Adenine containing	N6-dimethylallyladenine
Nucleotide	Purine Metabolism, Guanine containing	2'-deoxyguanosine
Nucleotide	Purine Metabolism, Guanine containing	7-methylguanine
Nucleotide	Purine Metabolism, Guanine containing	8-hydroxyguanine
Nucleotide	Purine Metabolism, Guanine containing	guanine
Nucleotide	Purine Metabolism, Guanine containing	guanosine

Nucleotide	Pyrimidine Metabolism, Cytidine containing	2'-deoxycytidine
Nucleotide	Pyrimidine Metabolism, Cytidine containing	cytidine
Nucleotide	Pyrimidine Metabolism, Cytidine containing	cytosine
Nucleotide	Pyrimidine Metabolism, Orotate containing	dihydroorotate
Nucleotide	Pyrimidine Metabolism, Orotate containing	N-carbamoylaspartate
Nucleotide	Pyrimidine Metabolism, Orotate containing	orotate
Nucleotide	Pyrimidine Metabolism, Thymine containing	thymidine
Nucleotide	Pyrimidine Metabolism, Thymine containing	thymine
Nucleotide	Pyrimidine Metabolism, Uracil containing	2'-deoxyuridine
Nucleotide	Pyrimidine Metabolism, Uracil containing	3-ureidopropionate
Nucleotide	Pyrimidine Metabolism, Uracil containing	4-ureidobutyrate
Nucleotide	Pyrimidine Metabolism, Uracil containing	5-methyluridine (ribothymidine)
Nucleotide	Pyrimidine Metabolism, Uracil containing	beta-alanine
Nucleotide	Pyrimidine Metabolism, Uracil containing	pseudouridine
Nucleotide	Pyrimidine Metabolism, Uracil containing	uracil
Nucleotide	Pyrimidine Metabolism, Uracil containing	uridine
Peptide	Dipeptide	alanylleucine
Peptide	Dipeptide	glycylisoleucine
Peptide	Dipeptide	glycylleucine
Peptide	Dipeptide	glycylvaline
Peptide	Dipeptide	isoleucylglycine
Peptide	Dipeptide	leucylalanine
Peptide	Dipeptide	leucylglutamine*
Peptide	Dipeptide	leucylglycine
Peptide	Dipeptide	phenylalanylalanine
Peptide	Dipeptide	phenylalanylglycine
Peptide	Dipeptide	threonylphenylalanine
Peptide	Dipeptide	tryptophylglycine
Peptide	Dipeptide	valylglutamine
Peptide	Dipeptide	valylglycine
Peptide	Dipeptide	valylleucine
Peptide	Dipeptide Derivative	anserine
Peptide	Gamma-glutamyl Amino Acid	gamma-glutamylalanine
Peptide	Gamma-glutamyl Amino Acid	gamma-glutamyl-epsilon-lysine
Peptide	Gamma-glutamyl Amino Acid	gamma-glutamylglutamate
Peptide	Gamma-glutamyl Amino Acid	gamma-glutamylglycine
Peptide	Gamma-glutamyl Amino Acid	gamma-glutamylisoleucine*
Peptide	Gamma-glutamyl Amino Acid	gamma-glutamylleucine
Peptide	Gamma-glutamyl Amino Acid	gamma-glutamylmethionine
Peptide	Gamma-glutamyl Amino Acid	gamma-glutamylphenylalanine
Peptide	Gamma-glutamyl Amino Acid	gamma-glutamyltyrosine
Xenobiotics	Benzoate Metabolism	2,4,6-trihydroxybenzoate
Xenobiotics	Benzoate Metabolism	3,4-dihydroxybenzoate
Xenobiotics	Benzoate Metabolism	benzoate
Xenobiotics	Chemical	1,3-propanediol
Xenobiotics	Chemical	2-oxo-1-pyrrolidinepropionate

Xenobiotics	Chemical	3-hydroxypyridine
Xenobiotics	Chemical	diethanolamine
Xenobiotics	Chemical	diglycerol
Xenobiotics	Chemical	ectoine
Xenobiotics	Chemical	N-methylpipercolate
Xenobiotics	Chemical	N-propionylmethionine
Xenobiotics	Chemical	succinimide
Xenobiotics	Chemical	sulfate*
Xenobiotics	Drug	N-carbamylglutamate
Xenobiotics	Food Component/Plant	1-methyl-beta-carboline-3-carboxylic acid
Xenobiotics	Food Component/Plant	2,3-dihydroxyisovalerate
Xenobiotics	Food Component/Plant	2-isopropylmalate
Xenobiotics	Food Component/Plant	2-keto-3-deoxy-gluconate
Xenobiotics	Food Component/Plant	2-oxindole-3-acetate
Xenobiotics	Food Component/Plant	2-piperidinone
Xenobiotics	Food Component/Plant	beta-guanidinopropanoate
Xenobiotics	Food Component/Plant	caffeate
Xenobiotics	Food Component/Plant	diaminopimelate
Xenobiotics	Food Component/Plant	dihydroferulic acid
Xenobiotics	Food Component/Plant	dipicolinate
Xenobiotics	Food Component/Plant	enterolactone
Xenobiotics	Food Component/Plant	erythrose
Xenobiotics	Food Component/Plant	ferulate
Xenobiotics	Food Component/Plant	galacturonate
Xenobiotics	Food Component/Plant	gluconate
Xenobiotics	Food Component/Plant	indolin-2-one
Xenobiotics	Food Component/Plant	levulinate (4-oxovalerate)
Xenobiotics	Food Component/Plant	nicotianamine
Xenobiotics	Food Component/Plant	pheophorbide A
Xenobiotics	Food Component/Plant	phytanate
Xenobiotics	Food Component/Plant	piperidine
Xenobiotics	Food Component/Plant	piperine
Xenobiotics	Food Component/Plant	pyrraline
Xenobiotics	Food Component/Plant	quinat
Xenobiotics	Food Component/Plant	sitostanol
Xenobiotics	Food Component/Plant	solanidine
Xenobiotics	Food Component/Plant	stachydrine
Xenobiotics	Food Component/Plant	tyrosol
Xenobiotics	Xanthine Metabolism	1,3,7-trimethylurate
Xenobiotics	Xanthine Metabolism	1,3-dimethylurate
Xenobiotics	Xanthine Metabolism	1,7-dimethylurate
Xenobiotics	Xanthine Metabolism	3,7-dimethylurate
Xenobiotics	Xanthine Metabolism	5-acetylamino-6-amino-3-methyluracil
Xenobiotics	Xanthine Metabolism	caffeine
Xenobiotics	Xanthine Metabolism	paraxanthine

Xenobiotics

Xanthine Metabolism

theophylline