

Metabolomic Analysis Services

List of metabolites identified and quantified by TMIC analytical services

Direct Flow Injection Mass Spectrometry (DI-MS)		
HMDB #	Metabolites	Classification
HMDB03357	Acetylnornithine	Biogenic amines
HMDB01539	Asymmetric dimethylarginine	Biogenic amines
HMDB03334	Symmetric dimethylarginine	Biogenic amines
	total dimethylarginine	Biogenic amines
	alpha-Aminoadipic acid	Biogenic amines
HMDB00033	Carnosine	Biogenic amines
HMDB00562	Creatinine	Biogenic amines
HMDB00181	Dopa	Biogenic amines
HMDB00073	Dopamine	Biogenic amines
HMDB00870	Histamine	Biogenic amines
HMDB00684	Kynurenine	Biogenic amines
	Methioninesulfoxide	Biogenic amines
	Nitrotyrosine	Biogenic amines
	Hydroxyproline	Biogenic amines
HMDB12275	Phenylethylamine	Biogenic amines
HMDB01414	Putrescine	Biogenic amines
HMDB00271	Sarcosine	Biogenic amines
HMDB00259	Serotonin	Biogenic amines
HMDB01257	Spermidine	Biogenic amines
HMDB01256	Spermine	Biogenic amines
HMDB00251	Taurine	Biogenic amines
HMDB00161	Alanine	Amino Acids
HMDB00517	Arginine	Amino Acids
HMDB00168	Asparagine	Amino Acids
HMDB00191	Aspartate	Amino Acids
HMDB00904	Citrulline	Amino Acids
HMDB03339	Glutamate	Amino Acids

HMDB00641	Glutamine	Amino Acids
HMDB00123	Glycine	Amino Acids
HMDB00177	Histidine	Amino Acids
HMDB00172	Isoleucine	Amino Acids
HMDB00687	Leucine	Amino Acids
HMDB00182	Lysine	Amino Acids
HMDB00696	Methionine	Amino Acids
HMDB00214	Ornithine	Amino Acids
HMDB00159	Phenylalanine	Amino Acids
HMDB00162	Proline	Amino Acids
HMDB00187	Serine	Amino Acids
HMDB00167	Threonine	Amino Acids
HMDB00929	Tryptophan	Amino Acids
HMDB00158	Tyrosine	Amino Acids
HMDB00883	Valine	Amino Acids
	C0 (Carnitine)	Acylcarnitines
	C10 (Decanoylcarnitine)	Acylcarnitines
	C10:1 (Decenoylcarnitine)	Acylcarnitines
	C10:2 (decadienylcarnitine)	Acylcarnitines
	C12 (dodecanoylcarnitine)	Acylcarnitines
	C12:1 (Dodecenoylcarnitine)	Acylcarnitines
	C12-DC (dodecanedioylcarnitine)	Acylcarnitines
	C14 (tetradecanoylcarnitine)	Acylcarnitines
	C14:1 (tetradecenoyl carnitine)	Acylcarnitines
	C14:1-OH (Hydroxytetradecenoyl carnitine)	Acylcarnitines
	C14:2 (Tetradecadienylcarnitine)	Acylcarnitines
	C14:2-OH (hydroxytetradecadienylcarnitine)	Acylcarnitines
	C16 (Hexadecanoylcarnitine)	Acylcarnitines
	C16:1 (Hexadecenoylcarnitine)	Acylcarnitines

	C16:1-OH (Hydroxyhexadecenoylcarnitine)	Acylcarnitines
	C16:2 (Hexadecadienylcarnitine)	Acylcarnitines
	C16:2-OH (hydroxyhexadecadienylcarnitine)	Acylcarnitines
	C16-OH (hydroxyhexadecanoylcarnitine)	Acylcarnitines
	C18 (Octadecanoylcarnitine)	Acylcarnitines
	C18:1 (Octadecenoylcarnitine)	Acylcarnitines
	C18:1-OH (Hydroxyoctadecenoylcarnitine)	Acylcarnitines
	C18:2 (Octadecadienylcarnitine)	Acylcarnitines
	C2 (Acetylcarnitine)	Acylcarnitines
	C3 (Propionylcarnitine)	Acylcarnitines
	C3:1 (Propenoylcarnitine)	Acylcarnitines
	C3-OH (hydroxyPropionylcarnitine)	Acylcarnitines
	C4 (butyrylcarnitine)	Acylcarnitines
	C4-OH (C3-DC) (Hydroxybutyrylcarnitine)	Acylcarnitines
	C4:1 (Butenylcarnitine)	Acylcarnitines
	C5 (Valerylcarnitine)	Acylcarnitines
	C5-DC (C6-OH)(Glutaryl carnitine)	Acylcarnitines
	C5-M-DC (methylglutaryl carnitine)	Acylcarnitines
	C5-OH (C3-DC-M) (hydroxyvalerylcarnitine)	Acylcarnitines
	C5:1 (Tiglylcarnitine)	Acylcarnitines
	C5:1-DC (Glutaconylcarnitine)	Acylcarnitines
	C6 (C4:1-DC) (Hexanoylcarnitine)	Acylcarnitines
	C6:1 (Hexenoylcarnitine)	Acylcarnitines
	C7-DC (pimelylcarnitine)	Acylcarnitines
	C8 (Octanoylcarnitine)	Acylcarnitines
	C9 (Nonaylcarnitine)	Acylcarnitines
HMDB00143	Hexose	Carbohydrates
	lysoPC a C14:0	Phospholipids
	lysoPC a C16:0	Phospholipids
	lysoPC a C16:1	Phospholipids
	lysoPC a C17:0	Phospholipids
	lysoPC a C18:0	Phospholipids
	lysoPC a C18:1	Phospholipids
	lysoPC a C18:2	Phospholipids
	lysoPC a C20:3	Phospholipids
	lysoPC a C20:4	Phospholipids
	lysoPC a C24:0	Phospholipids
	lysoPC a C26:0	Phospholipids
	lysoPC a C26:1	Phospholipids
	lysoPC a C28:0	Phospholipids
	lysoPC a C28:1	Phospholipids
	PC aa C24:0	Phospholipids
	PC aa C26:0	Phospholipids
	PC aa C28:1	Phospholipids
	PC aa C30:0	Phospholipids
	PC aa C30:2	Phospholipids

	PC aa C32:0	Phospholipids
	PC aa C32:1	Phospholipids
	PC aa C32:2	Phospholipids
	PC aa C32:3	Phospholipids
	PC aa C34:1	Phospholipids
	PC aa C34:2	Phospholipids
	PC aa C34:3	Phospholipids
	PC aa C34:4	Phospholipids
	PC aa C36:0	Phospholipids
	PC aa C36:1	Phospholipids
	PC aa C36:2	Phospholipids
	PC aa C36:3	Phospholipids
	PC aa C36:4	Phospholipids
	PC aa C36:5	Phospholipids
	PC aa C36:6	Phospholipids
	PC aa C38:0	Phospholipids
	PC aa C38:1	Phospholipids
	PC aa C38:3	Phospholipids
	PC aa C38:4	Phospholipids
	PC aa C38:5	Phospholipids
	PC aa C38:6	Phospholipids
	PC aa C40:1	Phospholipids
	PC aa C40:2	Phospholipids
	PC aa C40:3	Phospholipids
	PC aa C40:4	Phospholipids
	PC aa C40:5	Phospholipids
	PC aa C40:6	Phospholipids
	PC aa C42:0	Phospholipids
	PC aa C42:1	Phospholipids
	PC aa C42:2	Phospholipids
	PC aa C42:4	Phospholipids
	PC aa C42:5	Phospholipids
	PC aa C42:6	Phospholipids
	PC ae C30:0	Phospholipids
	PC ae C30:1	Phospholipids
	PC ae C32:1	Phospholipids
	PC ae C32:2	Phospholipids
	PC ae C34:0	Phospholipids
	PC ae C34:1	Phospholipids
	PC ae C34:2	Phospholipids
	PC ae C34:3	Phospholipids
	PC ae C36:0	Phospholipids
	PC ae C36:1	Phospholipids
	PC ae C36:2	Phospholipids
	PC ae C36:3	Phospholipids

	PC ae C36:4	Phospholipids
	PC ae C36:5	Phospholipids
	PC ae C38:0	Phospholipids
	PC ae C38:1	Phospholipids
	PC ae C38:2	Phospholipids
	PC ae C38:3	Phospholipids
	PC ae C38:4	Phospholipids
	PC ae C38:5	Phospholipids
	PC ae C38:6	Phospholipids
	PC ae C40:1	Phospholipids
	PC ae C40:2	Phospholipids
	PC ae C40:3	Phospholipids
	PC ae C40:4	Phospholipids
	PC ae C40:5	Phospholipids
	PC ae C40:6	Phospholipids
	PC ae C42:0	Phospholipids
	PC ae C42:1	Phospholipids
	PC ae C42:2	Phospholipids
	PC ae C42:3	Phospholipids
	PC ae C42:4	Phospholipids
	PC ae C42:5	Phospholipids
	PC ae C44:3	Phospholipids
	PC ae C44:4	Phospholipids
	PC ae C44:5	Phospholipids
	PC ae C44:6	Phospholipids
	SM (OH) C14:1	Sphingolipids
	SM (OH) C16:1	Sphingolipids
	SM (OH) C22:1	Sphingolipids
	SM (OH) C22:2	Sphingolipids
	SM (OH) C24:1	Sphingolipids
	SM C16:0	Sphingolipids
	SM C16:1	Sphingolipids
	SM C18:0	Sphingolipids
	SM C18:1	Sphingolipids
	SM C20:2	Sphingolipids
	SM C22:3	Sphingolipids
	SM C24:0	Sphingolipids
	SM C24:1	Sphingolipids
	SM C26:0	Sphingolipids
	SM C26:1	Sphingolipids

HMDB01857	1,3-Dimethyluric acid
HMDB03331	1-Methyladenosine
HMDB00001	1-Methylhistidine
HMDB00699	1-Methylnicotinamide
HMDB00439	2-Furoylglycine
HMDB00317	2-Hydroxy-3-methylpentanoic acid
HMDB00008	2-Hydroxybutyric acid
HMDB00694	2-Hydroxyglutaric acid
HMDB00005	2-Ketobutyric acid
HMDB00354	2-Methyl-3-hydroxybutyric acid
HMDB00408	2-Methyl-3-ketovaleric acid
HMDB00339	2-Methylbutyrylglycine
HMDB11659	2-Methylerythritol
HMDB00422	2-Methylglutaric acid
HMDB03911	3-Aminoisobutanoic acid
HMDB00357	3-Hydroxybutyric acid
HMDB06116	3-Hydroxyhippuric acid
HMDB00754	3-Hydroxyisovaleric acid
HMDB00355	3-Hydroxymethylglutaric acid
HMDB00440	3-Hydroxyphenylacetic acid
HMDB00491	3-Methyl-2-oxovaleric acid
HMDB00555	3-Methyladipic acid
HMDB00522	3-Methylglutaconic acid
HMDB00479	3-Methylhistidine
HMDB01886	3-Methylxanthine
HMDB00112	4-Aminobutyric acid
HMDB01867	4-Aminohippuric acid
HMDB02453	4-Deoxythreonic acid
HMDB29306	4-Ethylphenol
HMDB00500	4-Hydroxybenzoic acid
HMDB00710	4-Hydroxybutyric acid
HMDB13678	4-Hydroxyhippuric acid
MSEA0510	4-Hydroxyphenyllactic acid
HMDB00017	4-Pyridoxic acid
HMDB00076	5,6-Dihydrouracil
HMDB01149	5-Aminolevulinic acid
HMDB03355	5-Aminopentanoic acid
HMDB01991	7-Methylxanthine
HMDB00990	Acetaldehyde
HMDB01859	Acetaminophen
HMDB10316	Acetaminophen glucuronide
HMDB59911	Acetaminophen sulfate
HMDB00042	Acetic acid
HMDB00060	Acetoacetic acid
HMDB01659	Acetone
HMDB00201	Acetyl-L-carnitine
HMDB00034	Adenine

Quantitative NMR Spectroscopy

HMDB	Metabolites
HMDB00002	1,3-Diaminopropane

HMDB00050	Adenosine
HMDB00448	Adipic acid
HMDB01341	ADP
HMDB00462	Allantoin
HMDB00510	Alpha-Amino adipic acid
HMDB00452	Alpha-Aminobutyric acid
HMDB00729	Alpha-Hydroxyisobutyric acid
HMDB00019	Alpha-Ketoisovaleric acid
HMDB00194	Anserine
HMDB01851	Arabinitol
HMDB00044	Ascorbic acid
HMDB01539	Asymmetric dimethylarginine
HMDB00784	Azelaic acid
HMDB01870	Benzoic acid
HMDB00056	Beta-Alanine
HMDB00043	Betaine
HMDB00039	Butyric acid
HMDB01847	Caffeine
HMDB00033	Carnosine
HMDB00097	Choline
HMDB00567	Cinnamic acid
HMDB00072	Cis-Aconitic acid
HMDB00634	Citraconic acid
HMDB00426	Citramalic acid
HMDB00094	Citric acid
HMDB00064	Creatine
HMDB00562	Creatinine
HMDB00630	Cytosine
HMDB01264	Dehydroascorbic acid
HMDB00143	D-Galactose
HMDB00122	D-Glucose
HMDB00079	Dihydrothymine
HMDB04983	Dimethyl sulfone
HMDB00087	Dimethylamine
HMDB00092	Dimethylglycine
HMDB04136	D-Threitol
HMDB02917	D-Xylitol
HMDB00098	D-Xylose
HMDB02994	Erythritol
HMDB00108	Ethanol
HMDB00149	Ethanolamine
HMDB10325	Ethyl glucuronide
HMDB00622	Ethylmalonic acid
HMDB00142	Formic acid
HMDB00134	Fumaric acid
HMDB00663	Glucaric acid
HMDB00625	Gluconic acid
HMDB00127	Glucuronic acid
HMDB00620	Glutaconic acid

HMDB00661	Glutaric acid
HMDB00139	Glyceric acid
HMDB00131	Glycerol
HMDB00123	Glycine
HMDB00115	Glycolic acid
HMDB00128	Guanidoacetic acid
HMDB00714	Hippuric acid
HMDB00679	Homocitrulline
HMDB00130	Homogentisic acid
HMDB00118	Homovanillic acid
HMDB02643	HPPHA
HMDB00725	Hydroxyproline
HMDB00700	Hydroxypropionic acid
HMDB00157	Hypoxanthine
HMDB00197	Indoleacetic acid
HMDB00682	Indoxyl sulfate
HMDB00195	Inosine
HMDB01873	Isobutyric acid
HMDB00193	Isocitric acid
HMDB00718	Isovaleric acid
HMDB00678	Isovalerylglycine
HMDB00715	Kynurenic acid
HMDB00684	Kynurenine
HMDB00186	Lactose
HMDB00161	L-Alanine
HMDB00646	L-Arabinose
HMDB00517	L-Arginine
HMDB00168	L-Asparagine
HMDB00191	L-Aspartic acid
HMDB00062	L-Carnitine
HMDB00099	L-Cystathionine
HMDB00574	L-Cysteine
HMDB00192	L-Cystine
HMDB00640	Levoglucosan
HMDB00720	Levulinic acid
HMDB00174	L-Fucose
HMDB00148	L-Glutamic acid
HMDB00641	L-Glutamine
HMDB00177	L-Histidine
HMDB00172	L-Isoleucine
HMDB00190	L-Lactic acid
HMDB00687	L-Leucine
HMDB00182	L-Lysine
HMDB00696	L-Methionine
HMDB00159	L-Phenylalanine
HMDB00187	L-Serine
HMDB00167	L-Threonine
HMDB00929	L-Tryptophan
HMDB00158	L-Tyrosine

HMDB00883	L-Valine
HMDB00176	Maleic acid
HMDB00691	Malonic acid
HMDB00163	Maltose
HMDB00703	Mandelic acid
HMDB00765	Mannitol
HMDB01875	Methanol
HMDB00164	Methylamine
HMDB00752	Methylglutaric acid
HMDB01522	Methylguanidine
HMDB00202	Methylmalonic acid
HMDB01844	Methylsuccinic acid
HMDB00858	Monomethyl glutaric acid
HMDB01878	m-Thymol
HMDB00211	Myoinositol
HMDB00812	N-Acetylaspartic acid
HMDB00230	N-Acetylneuraminic acid
HMDB02064	N-Acetylputrescine
HMDB03646	N-Methylhydantoin
HMDB00669	o-Hydroxyphenylacetic acid
HMDB00208	Oxoglutaric acid
HMDB00786	Oxypurinol
HMDB00210	Pantothenic acid
HMDB11635	p-Cresol sulfate
HMDB00228	Phenol
HMDB00209	Phenylacetic acid
HMDB06344	Phenylacetylglutamine
HMDB01587	Phenylglyoxylic acid
HMDB01565	Phosphorylcholine
HMDB00020	p-Hydroxyphenylacetic acid
HMDB02243	Picolinic acid
HMDB00857	Pimelic acid
HMDB04827	Proline-betaine
HMDB01881	Propylene glycol
HMDB00767	Pseudouridine
HMDB00957	Pyrocatechol
HMDB00267	Pyroglutamic acid
HMDB00243	Pyruvic acid
HMDB00232	Quinolinic acid
HMDB00271	Sarcosine
HMDB06088	Scyllitol
HMDB00792	Sebacic acid
HMDB00247	Sorbitol
HMDB00893	Suberic acid
HMDB00254	Succinic acid
HMDB00635	Succinylacetone
HMDB00258	Sucrose
HMDB02432	Sumiki' s acid
HMDB03334	Symmetric dimethylarginine

HMDB02085	Syringic acid
HMDB00956	Tartaric acid
HMDB00251	Taurine
HMDB00943	Threonic acid
HMDB00273	Thymidine
HMDB00958	Trans-Aconitic acid
HMDB00954	Trans-Ferulic acid
HMDB00875	Trigonelline
HMDB00906	Trimethylamine
HMDB00925	Trimethylamine N-oxide
HMDB00300	Uracil
HMDB00294	Urea
HMDB00484	Vanillic acid
HMDB00291	Vanillylmandelic acid

Quantitative NMR Spectroscopy (Urine)

HMDB	Metabolites	Occurance
HMDB00001	1-Methylhistidine	100
HMDB00439	2-Furoylglycine	100
HMDB00317	2-Hydroxy-3-methylpentanoic acid	100
HMDB00694	2-Hydroxyglutaric acid	100
HMDB00005	2-Ketobutyric acid	100
HMD B03911	3-Aminoisobutanoic acid	100
HMDB00754	3-Hydroxyisovaleric acid	100
HMDB00479	3-Methylhistidine	100
HMDB01886	3-Methylxanthine	100
HMDB02453	4-Deoxythreonic acid	100
HMDB00710	4-Hydroxybutyric acid	100
HMDB13678	4-Hydroxyhippuric acid	100
HMDB00042	Acetic acid	100
HMDB00060	Acetoacetic acid	100
HMDB01659	Acetone	100
HMDB00201	Acetyl-L-carnitine	100
HMDB00462	Allantoin	100
HMDB00729	Alpha-Hydroxyisobutyric acid	100
HMDB00194	Anserine	100
HMDB01851	Arabinitol	100
HMDB01539	Asymmetric dimethylarginine	100
HMDB00043	Betaine	100
HMDB00097	Choline	100
HMDB00072	Cis-Aconitic acid	100
HMDB00094	Citric acid	100
HMDB00064	Creatine	100
HMDB00562	Creatinine	100
HMDB00143	D-Galactose	100
HMDB00122	D-Glucose	100
HMDB04983	Dimethyl sulfone	100

HMDB00087	Dimethylamine	100
HMDB00092	Dimethylglycine	100
HMDB04136	D-Threitol	100
HMDB02994	Erythritol	100
HMDB00149	Ethanolamine	100
HMDB00142	Formic acid	100
HMDB00625	Gluconic acid	100
HMDB00139	Glyceric acid	100
HMDB00131	Glycerol	100
HMDB00123	Glycine	100
HMDB00115	Glycolic acid	100
HMDB00128	Guanidoacetic acid	100
HMDB00714	Hippuric acid	100
HMDB00118	Homovanillic acid	100
HMDB02643	HPPHA	100
HMDB00157	Hypoxanthine	100
HMDB00197	Indoleacetic acid	100
HMDB00682	Indoxyl sulfate	100
HMDB00161	L-Alanine	100
HMDB00646	L-Arabinose	100
HMDB00062	L-Carnitine	100
HMDB00574	L-Cysteine	100
HMDB00192	L-Cystine	100
HMDB00148	L-Glutamic acid	100
HMDB00641	L-Glutamine	100
HMDB00177	L-Histidine	100
HMDB00172	L-Isoleucine	100
HMDB00190	L-Lactic acid	100
HMDB00687	L-Leucine	100
HMDB00182	L-Lysine	100
HMDB00159	L-Phenylalanine	100
HMDB00187	L-Serine	100
HMDB00167	L-Threonine	100
HMDB00929	L-Tryptophan	100
HMDB00158	L-Tyrosine	100
HMDB00883	L-Valine	100
HMDB01875	Methanol	100
HMDB00164	Methylamine	100
HMDB01844	Methylsuccinic acid	100
HMDB00211	Myoinositol	100
HMDB00812	N-Acetylaspartic acid	100
HMDB00230	N-Acetylneuraminic acid	100
HMDB00208	Oxoglutaric acid	100
HMDB00210	Pantothenic acid	100
HMDB06344	Phenylacetylglutamine	100
HMDB00020	p-Hydroxyphenylacetic acid	100
HMDB04827	Proline-betaine	100
HMDB01881	Propylene glycol	100
HMDB00767	Pseudouridine	100

HMDB00957	Pyrocatechol	100
HMDB00267	Pyroglutamic acid	100
HMDB00243	Pyruvic acid	100
HMDB00232	Quinolinic acid	100
HMDB00247	Sorbitol	100
HMDB00258	Sucrose	100
HMDB03334	Symmetric dimethylarginine	100
HMDB00251	Taurine	100
HMDB00943	Threonic acid	100
HMDB00875	Trigonelline	100
HMDB00925	Trimethylamine N-oxide	100
HMDB00300	Uracil	100
HMDB00294	Urea	100
HMDB00354	2-Methyl-3-hydroxybutyric	95
HMDB00017	4-Pyridoxic	95
HMDB01149	5-Aminolevulinic acid	95
HMDB00452	Alpha-Aminobutyric acid	95
HMDB02917	D-Xylitol	95
HMDB00622	Ethylmalonic acid	95
HMDB01873	Isobutyric acid	95
HMDB00517	L-Arginine	95
HMDB00168	L-Asparagine	95
HMDB00191	L-Aspartic acid	95
HMDB00765	Mannitol	95
HMDB01522	Methylguanidine	95
HMDB00202	Methylmalonic acid	95
HMDB00228	Phenol	95
HMDB00484	Vanillic acid	95
HMDB00440	3-Hydroxyphenylacetic acid	91
HMDB00491	3-Methyl-2-oxovaleric acid	91
HMDB00448	Adipic acid	91
HMDB00033	Carnosine	91
HMDB00426	Citramalic acid	91
HMDB00098	D-Xylose	91
HMDB00679	Homocitrulline	91
HMDB00678	Isovalerylglycine	91
HMDB00186	Lactose	91
HMDB00174	L-Fucose	91
HMDB00669	o-Hydroxyphenylacetic acid	91
HMDB11635	P-Cresol sulfate	91
HMDB00254	Succinic acid	91
HMDB00555	3-Methyladipic acid	86
HMDB01867	4-Aminohippuric acid	86
HMDB01870	Benzoic acid	86
HMDB00718	Isovaleric acid	86
HMDB01878	m-Thymol	86
HMDB00906	Trimethylamine	86
HMDB03331	1-Methyladenosine	82
HMDB00663	Glucaric acid	82

HMDB00700	Hydroxypropionic acid	82
HMDB00099	L-Cystathionine	82
HMDB00956	Tartaric acid	82
HMDB00699	1-Methylnicotinamide	77
HMDB00008	2-Hydroxybutyric acid	77
HMDB00357	3-Hydroxybutyric acid	77
HMDB00500	4-Hydroxybenzoic acid	77
HMDB01341	ADP	77
HMDB00039	Butyric acid	77
HMDB00127	Glucuronic acid	77
HMDB00691	Malonic acid	77
HMDB00857	Pimelic acid	77
HMDB00271	Sarcosine	77
HMDB00510	Alpha-Aminoadipic acid	73
HMDB00634	Citraconic acid	73
HMDB00163	Maltose	73
HMDB01857	1,3-Dimethyluric acid	68
HMDB00355	3-Hydroxymethylglutaric acid	68
HMDB00076	5,6-Dihydrouracil	68
HMDB00056	Beta-Alanine	68
HMDB00620	Glutaconic acid	68
HMDB00193	Isocitric acid	68
HMDB00858	Monomethylglutaric acid	68
HMDB06088	Scyllitol	68
HMDB00784	Azelaic acid	64
HMDB00079	Dihydrothymine	64
HMDB00715	Kynurenic acid	64
HMDB00720	Levulinic acid	64
HMDB00725	Hydroxyproline	55
HMDB03646	N-Methylhydantoin	55
HMDB00958	Trans-Aconitic acid	55
HMDB00755	4-Hydroxyphenyllactic acid	50
HMDB00019	Alpha-Ketoisovaleric acid	50
HMDB00134	Fumaric acid	50
HMDB00195	Inosine	50
HMDB00786	Oxypurinol	50
HMDB00422	2-Methylglutaric acid	45
HMDB00034	Adenine	45
HMDB00050	Adenosine	45
HMDB00130	Homogentisic acid	45
HMDB00696	L-Methionine	41
HMDB01565	Phosphorylcholine	41
HMDB00630	Cytosine	36
HMDB00635	Succinylacetone	36
HMDB00273	Thymidine	36
HMDB00339	2-Methylbutyrylglycine	32
HMDB06116	3-Hydroxyhippuric acid	32
HMDB00990	Acetaldehyde	32
HMDB01264	Dehydroascorbic acid	32

HMDB02064	N-Acetylputrescine	32
HMDB00893	Suberic acid	32
HMDB00640	Levogluconan	27
HMDB00684	Kynurenine	23
HMDB00522	3-Methylglutaconic acid	22
HMDB00408	2-Methyl-3-ketovaleric acid	18
HMDB29306	4-Ethylphenol	18
HMDB00661	Glutaric acid	18
HMDB02243	Picolinic acid	18
HMDB11659	2-Methylerythritol	14
HMDB00044	Ascorbic acid	14
HMDB00176	Maleic acid	14
HMDB00112	4-Aminobutyric acid	9
HMDB01991	7-Methylxanthine	9
HMDB00567	Cinnamic acid	9
HMDB00703	Mandelic acid	9
HMDB00752	Methylglutaric acid	9
HMDB00291	Vanillylmandelic acid	9
HMDB00002	1,3-Diaminopropane	5
HMDB03355	5-Aminopentanoic acid	5
HMDB01859	Acetaminophen	5
HMDB10316	Acetaminophen glucuronide	5
HMDB59911	Acetaminophen sulfate	5
HMDB00108	Ethanol	5
HMDB10325	Ethyl glucuronide	5
HMDB00209	Phenylacetic acid	5
HMDB01587	Phenylglyoxylic acid	5
HMDB00792	Sebacic acid	5
HMDB02432	Sumiki's acid	5
HMDB02085	Syringic acid	5
HMDB00954	Trans-Ferulic acid	5
HMDB01847	Caffeine	0.33

Quantitative GC-MS

HMDB	Metabolites
HMDB00650	2-aminobutyric acid
HMDB00008	2-Hydroxybutyrate
HMDB00729	2-Hydroxyisobutyrate
HMDB01863	2-hydroxyvalerate
HMDB02176	2-Methylbutanoic acid
HMDB00223	2-Oxobutanedioic acid
HMDB00442	3-Hydroxybutyrate
HMDB02453	4-Deoxythreonic acid
	6-O-alpha-D-glucopyranosyl-D-Fructose
HMDB00161	Alanine
HMDB01147	Aminomalonic acid
HMDB00646	Arabinose
HMDB00191	Aspartate

HMDB01870	Benzoic acid
HMDB00067	Cholesterol
HMDB00094	Citrate
HMDB00192	Cystine/Cysteine
HMDB03603	Decanoic acid
HMDB00613	Erythronic acid
HMDB00660	Fructose
HMDB00134	Fumaric acid
HMDB00143	Galactose
HMDB00625	Gluconate
HMDB00150	Gluconic acid lactone
HMDB00122	Glucose
HMDB00148	Glutamate
HMDB00641	Glutamine
HMDB00131	Glycerol
HMDB00123	Glycine
HMDB00177	Histidine
HMDB00725	Hydroxyproline
HMDB01873	Isobutyrate
HMDB00172	Isoleucine
HMDB00190	Lactate
HMDB00638	Lauric acid
HMDB00687	Leucine
HMDB00673	Linoleic acid
HMDB00156	Malate
HMDB00691	Malonate
HMDB00163	Maltose
HMDB00696	Methionine
HMDB00634	Methylmaleic acid
HMDB00202	Methylmalonate
HMDB00211	myo-Inositol
HMDB00806	Myristic acid
HMDB00215	N-acetyl-D-glucosamine
HMDB00532	N-Acetylglycine
HMDB01488	Nicotinic acid
HMDB00446	N- β -Acetyl-L-Lysine
HMDB00207	Oleic acid
HMDB02329	Oxalate
HMDB00208	Oxoglutarate
HMDB12328	Palmitelaidic acid
HMDB00220	Palmitic acid
HMDB00159	Phenylalanine
HMDB00162	Proline
HMDB00283	Ribose
HMDB01895	Salicylic acid
HMDB00187	Serine
HMDB00827	Stearic acid
HMDB00254	Succinate

HMDB00258	Sucrose
HMDB00956	Tartaric acid
HMDB00943	Threonic acid
HMDB00167	Threonine
HMDB00929	Tryptophan
HMDB00158	Tyrosine
HMDB00289	Urate
HMDB00294	Urea
HMDB00883	Valine

Quantitative GC-MS/MS (EI, PCI, NCI available)	
HMDB	Metabolites
HMDB00650	2-aminobutyric acid
HMDB00008	2-Hydroxybutyrate
HMDB00729	2-Hydroxyisobutyrate
HMDB01863	2-hydroxyvalerate
HMDB02176	2-Methylbutanoic acid
HMDB00223	2-Oxobutanedioic acid
HMDB00442	3-Hydroxybutyrate
HMDB02453	4-Deoxythreonic acid
	6-O-alpha-D-glucopyranosyl-D-Fructose
HMDB00161	Alanine
HMDB01147	Aminomalonic acid
HMDB00646	Arabinose
HMDB00191	Aspartate
HMDB01870	Benzoic acid
HMDB00067	Cholesterol
HMDB00094	Citrate
HMDB00192	Cystine/Cysteine
HMDB03603	Decanoic acid
HMDB00613	Erythronic acid
HMDB00660	Fructose
HMDB00134	Fumaric acid
HMDB00143	Galactose
HMDB00625	Gluconate
HMDB00150	Gluconic acid lactone
HMDB00122	Glucose
HMDB00148	Glutamate
HMDB00641	Glutamine
HMDB00131	Glycerol
HMDB00123	Glycine
HMDB00177	Histidine
HMDB00725	Hydroxyproline
HMDB01873	Isobutyrate
HMDB00172	Isoleucine
HMDB00190	Lactate
HMDB00638	Lauric acid

HMDB00687	Leucine
HMDB00673	Linoleic acid
HMDB00156	Malate
HMDB00691	Malonate
HMDB00163	Maltose
HMDB00696	Methionine
HMDB00634	Methylmaleic acid
HMDB00202	Methylmalonate
HMDB00211	myo-Inositol
HMDB00806	Myristic acid
HMDB00215	N-acetyl-D-glucosamine
HMDB00532	N-Acetylglycine
HMDB01488	Nicotinic acid
HMDB00446	N- ϵ -Acetyl-L-Lysine
HMDB00207	Oleic acid
HMDB02329	Oxalate
HMDB00208	Oxoglutarate
HMDB12328	Palmitelaidic acid
HMDB00220	Palmitic acid
HMDB00159	Phenylalanine
HMDB00162	Proline
HMDB00283	Ribose
HMDB01895	Salicylic acid
HMDB00187	Serine
HMDB00827	Stearic acid
HMDB00254	Succinate
HMDB00258	Sucrose
HMDB00956	Tartaric acid
HMDB00943	Threonic acid
HMDB00167	Threonine
HMDB00929	Tryptophan
HMDB00158	Tyrosine
HMDB00289	Urate
HMDB00294	Urea
HMDB00883	Valine

HMDB10214	19,20-DiHDEPA
	D4-9-HODE
HMDB10223	9-HODE
	9-HOTrE
HMDB06940	9-HpODE
HMDB61708	13-HODE
HMDB03871	13-HpODE
HMDB04668	13-KODE
	D8-5-HETE
HMDB03876	15-HETE
HMDB04679	8-HETE
HMDB11134	5-HETE

Vitamin Analysis - Water soluble

HMDB	Metabolites
HMDB00235	Thiamine (B1)
HMDB00244	Riboflavin (B2)
HMDB01488	Niacin (B3)
HMDB01406	Niacinamide (B3-amide)
HMDB00210	Pantothenic acid (B5)
HMDB00239	Pyridoxine (B6)
HMDB00030	Biotin (B7)
HMDB00121	Folic acid (B9)
HMDB00607	Cyanocobalamin (B12)

Vitamin Analysis - Fat soluble

HMDB	Metabolites
HMDB00305	Retinol (A)
HMDB00876	Vit D3
HMDB00900	Ergocalciferol (D2)
HMDB03550	25OH Vit D3
HMDB01893	Alpha-tocopherol (E)
HMDB00097	Choline

Oxylipins Analysis

HMDB	Metabolites
	D4-PGF2 α
	PGF2 α
	13,14-dihydro PGF2 α
	PGF1 α
	PGF3 α
	D8-12-HETE
HMDB04682	11-HETE
HMDB06111	12-HETE
HMDB10202	12(S)-HEPE
HMDB13620	19(20)-EpDPE

Endogenous vitamins and vitamin-like compounds analysis

HMDB	Metabolites
HMDB01358	Retinal (Vitamin A)
HMDB01852	Retinoic acid (Vitamin A)
HMDB00305	Retinol (Vitamin A)
HMDB00900	Vitamin D2
HMDB00876	Vitamin D3
	1-OH vitamin D2
	1-OH vitamin D3
HMDB01893	α -Tocopherol(Vitamin E)
HMDB06327	α -Tocotrienol(Vitamin E)
HMDB06335	β -Tocopherol(Vitamin E)
	β -Tocotrienol(Vitamin E)

HMDB01492	γ -Tocopherol(Vitamin E)
HMDB12958	γ -Tocotrienol(Vitamin E)
HMDB02902	δ -Tocopherol(Vitamin E)
HMDB30008	δ -Tocotrienol(Vitamin E)
HMDB03555	Vitamin K1(Vitamin K1)
HMDB30017	Vitamin K2(Vitamin K2)
HMDB00235	Thiamine (Vitamin B1)
HMDB02666	Thiamine monophosphate (Vitamin B1)
HMDB01372	Thiamine pyrophosphate (Vitamin B1)
HMDB00607	Cyanocobalamin(Vitamin B12)
HMDB00244	Riboflavin(Vitamin B2)
HMDB01520	Riboflavin 5' -monophosphate (Vitamin B2 phosphate)
HMDB01406	Nicotinamide(Vitamin B3)
HMDB00210	Pantothenic acid (Vitamin B5)
HMDB01545	Pyridoxal (Vitamin B6)
	Pyridoxal phosphate (Vitamin B6)
HMDB01431	Pyridoxamine (Vitamin B6)
HMDB00239	Pyridoxine (Vitamin B6)
HMDB00030	Biotin (Vitamin B7 also as B8 or H)
HMDB00121	Folic acid (Vitamin B9)
HMDB00097	Choline (Vitamin B-like)
HMDB01392	4-Aminobenzoic acid (Vitamin B-like compound)
HMDB14312	Lipoic acid (Vitamin B-like compound)
HMDB00044	Ascorbic acid (Vitamin C)

Bile acids analysis (I)

HMDB	Metabolites
HMDB00619	Cholic acid
HMDB00626	Deoxycholic acid
HMDB00761	Lithocholic acid
HMDB00505	Allocholic acid
HMDB00518	Chenodeoxycholic acid
	Dehydrocholic acid
HMDB00328	12-Ketolithocholic acid
	Dehydrolithocholic acid
HMDB00391	7-Ketodeoxycholic acid
HMDB00467	7-Ketolithocholic acid
	Alloisolithocholic acid
	Apocholic acid
	Hyodeoxycholic acid
HMDB00811	Murocholic acid
HMDB00946	Ursodeoxycholic acid
	Dioxolithocholic acid
HMDB00717	Isolithocholic acid
HMDB02536	Isodeoxycholic acid
HMDB00400	12-Ketochenodeoxycholic acid
	Nordeoxycholic acid

HMDB00502	3-Oxocholeic acid
	6,7-Diketolithocholic acid
HMDB00506	α -Muricholic acid
HMDB00415	β -Muricholic acid
HMDB00760	λ -Muricholic acid (hyocholic acid)
HMDB00364	ω -Muricholic acid
HMDB00917	Ursocholic Acid
	Noursodeoxycholic acid
	Norcholic acid
HMDB02159	DHCA
	THCA
HMDB00637	Glycochenodeoxycholic acid
HMDB00138	Glycocholic acid
	Glycodehydrocholic acid
HMDB00631	Glycodeoxycholic Acid
	Glycohyodeoxycholic acid
HMDB00708	Glycoursodeoxycholic acid
HMDB00698	Glycolithocholic acid
	Glycohyocholic acid
HMDB00896	Taurodeoxycholic Acid
HMDB00951	Taurochenodeoxycholic acid
HMDB00036	Taurocholic Acid
	Taurodehydrocholic acid
	Taurohyodeoxycholic acid
HMDB00722	Tauroolithocholic acid
HMDB00874	Tauroursodeoxycholic Acid
	Taurohyocholic acid
	Tauro- α -muricholic acid
HMDB00932	Tauro- β -muricholic acid
	Tauro- ω -muricholic acid

Bile acids analysis (II)

HMDB	Metabolites
HMDB00619	Cholic acid
HMDB00626	Deoxycholic acid
HMDB00761	Lithocholic acid
HMDB00505	Allocholic acid
HMDB00518	Chenodeoxycholic acid
	Dehydrocholic acid
HMDB00328	12-Ketolithocholic acid
	Dehydrolithocholic acid
HMDB00391	7-Ketodeoxycholic acid
HMDB00467	7-Ketolithocholic acid
	Alloisolithocholic acid
	Apocholic acid
	Hyodeoxycholic acid

HMDB00811	Murocholic acid
HMDB00946	Ursodeoxycholic acid
	Dioxolithocholic acid
HMDB00717	Isolithocholic acid
HMDB02536	Isodeoxycholic acid
HMDB00400	12-Ketochenodeoxycholic acid
	Nordeoxycholic acid
HMDB00502	3-Oxocholeic acid
	6,7-Diketolithocholic acid
HMDB00506	α -Muricholic acid
HMDB00415	β -Muricholic acid
HMDB00760	λ -Muricholic acid (hyocholic acid)
HMDB00364	ω -Muricholic acid
HMDB00917	Ursocholic Acid
	Norursodeoxycholic acid
	Norcholic acid
HMDB02159	DHCA
	THCA
HMDB00637	Glycochenodeoxycholic acid
HMDB00138	Glycocholic acid
	Glycodehydrocholic acid
HMDB00631	Glycodeoxycholic Acid
	Glycohyodeoxycholic acid
HMDB00708	Glycoursodeoxycholic acid
HMDB00698	Glycolithocholic acid
	Glycohyocholic acid
HMDB00896	Taurodeoxycholic Acid
HMDB00951	Taurochenodeoxycholic acid
HMDB00036	Taurocholic Acid
	Taurodehydrocholic acid
	Taurohyodeoxycholic acid
HMDB00722	Taurolithocholic acid
HMDB00874	Tauroursodeoxycholic Acid
	Taurohyocholic acid
	Tauro- α -muricholic acid
HMDB00932	Tauro- β -muricholic acid
	Tauro- ω -muricholic acid
HMDB02513	Lithocholic acid-3-glucuronide
	Lithocholic acid-24-glucuronide
HMDB02596	Deoxycholic acid - 3- glucuronide
	Chenodeoxycholic acid-3-glucuronide
	Chenodeoxycholic acid 24- β -D-glucuronide
HMDB00907	Lithocholic acid 3-sulfate
HMDB02504	Deoxycholic acid 3-sulfate
	Cholic acid 3-sulfate
HMDB02639	Glycolithocholic acid 3-sulfate
HMDB02497	Glycochenodeoxycholic acid 3-sulfate
	Glycodeoxycholic acid 3-sulfate

	Glycocholic acid 3-sulfate
HMDB02580	Taurolithocholic acid 3-sulfate
HMDB02486	Taurochenodeoxycholic acid 3-sulfate
	Taurodeoxycholic acid 3-sulfate
	Tauroursodeoxycholic acid 3-sulfate

Bile acids analysis (III)

HMDB	Metabolites
	Cholic acid
	Chenodeoxycholic acid
	Deoxycholic acid
	Glycocholic acid
	Glycochenodeoxycholic acid
	Glycodeoxycholic acid
	Glycolithocholic acid
	Glycoursodeoxycholic acid
	Hyodeoxycholic acid
	Lithocholic acid
	Alpha-muricholic acid
	Beta-muricholic acid
	Omega-muricholic acid
	Taurocholic acid
	Taurochenodeoxycholic acid
	Taurodeoxycholic acid
	Taurolithocholic acid
	Tauromuricholic acid (alpha + beta)
	Tauroursodeoxycholic acid
	Ursodeoxycholic acid

Organic acids analysis (GC-MS)

HMDB	Metabolites
HMDB00930	(E)-Cinnamic acid
HMDB00197	1H-Indole-3-acetic acid
HMDB01123	2-amino-benzoic acid
HMDB00439	2-Furoylglycine
HMDB01987	2-Hydroxy-2-methylbutyric acid
HMDB01895	2-Hydroxybenzoic acid (salicylic acid)
HMDB00694	2-Hydroxyglutaric Acid
HMDB00407	2-Hydroxyisovaleric Acid
HMDB02285	2-Indolecarboxylic acid
HMDB01844	2-Methylsuccinic acid
HMDB00375	3-(3-Hydroxyphenyl)propanoic acid
HMDB00423	3,4-Dihydroxyhydrocinnamic acid
HMDB01336	3,4-Dihydroxyphenylacetic acid
HMDB00423	3,4-dihydroxy-Phenylpropanoic acid
HMDB00357	3-hydroxybutyric acid

HMDB00754	3-Hydroxyisovaleric acid	HMDB00893	Suberic acid
HMDB00355	3-Hydroxymethylglutaric acid	HMDB00254	Succinic acid
HMDB00555	3-Methyladipic acid	HMDB02432	Sumiki' s acid
HMDB00522	3-methylglutaconic acid	HMDB00958	trans-Aconitic acid
HMDB02453	4-Deoxythreonate	HMDB00954	trans-Ferulic acid
HMDB13678	4-hydroxyhippuric Acid	HMDB00291	Vanillylmandelic acid
HMDB00763	5-Hydroxyindoleacetic acid	HMDB00360	2,4-dihydroxybutanoic acid
HMDB00448	Adipic acid	HMDB04812	2,5-furandicarboxylic acid
HMDB00729	alpha-Hydroxylsobutyric acid	HMDB00396	2-ethyl-3-hydroxypropionic acid
HMDB00784	Azelaic acid	HMDB00317	2-hydroxy-3-methylvaleric acid
HMDB00764	Benzenepropanoic acid	HMDB00321	2-hydroxyadipic acid
HMDB01870	Benzoic acid	HMDB00008	2-hydroxybutyric acid
HMDB00700	beta-Lactate	HMDB01863	2-hydroxyvaleric acid
HMDB00094	Citric Acid	HMDB00426	2-methylmalic acid
HMDB00638	Dodecanoic acid (Lauric acid)	HMDB00491	2-oxo-3-methylvaleric acid
HMDB00622	Ethylmalonic acid	HMDB00225	2-oxoadipic acid
HMDB00134	Fumaric Acid	HMDB06544	2-oxobutanoic acid
HMDB00620	Glutaconic Acid	HMDB00019	2-oxoisovaleric acid
HMDB00661	Glutaric acid	HMDB01865	2-oxovaleric acid
HMDB00115	glycolic acid	HMDB00913	3(4-OH-3-MO-phenyl)lactic acid
HMDB00220	Hexadecanoic acid (Palmitic acid)	HMDB02441	3,3-dimethylglutaric acid
HMDB00714	Hippuric acid	HMDB00337	3,4-dihydroxybutanoic acid
HMDB00118	Homovanillic acid	HMDB00354	3-hydroxy-2-methylbutyric acid
HMDB02643	HPPHA	HMDB00355	3-hydroxy-3-methylglutaric acid
HMDB00755	Hydroxyphenyllactic acid	HMDB00428	3-hydroxyglutaric acid
HMDB00671	Indolelactic acid	HMDB00023	3-hydroxyisobutyric acid
HMDB00715	Kynurenic acid	HMDB00440	3-hydroxyphenylacetic acid
HMDB00190	Lactic acid	HMDB00700	3-hydroxypropionic acid
HMDB00720	Levulinic acid	HMDB00752	3-methylglutaric acid
HMDB00156	L-Malic acid	HMDB00779	3-phenyllactic acid
HMDB00691	Malonic acid	HMDB00710	4-hydroxybutyric acid
HMDB01713	m-Coumaric acid	HMDB00882	4-hydroxymandelic acid
HMDB00634	Methylmaleic acid (citraconic acid)	HMDB00707	4-hydroxyphenylpyruvic acid
HMDB00202	Methylmalonic acid	HMDB00525	5-hydroxyhexanoic acid
HMDB06116	m-Hydroxyhippuric acid	HMDB00060	acetoacetic acid
HMDB00440	m-Hydroxyphenylacetic acid	HMDB00808	butyrylglycine
HMDB00827	Octadecanoic acid (Stearic acid)	HMDB00623	dodecanedioic acid
HMDB00669	o-Hydroxyphenylacetic acid	HMDB00139	glyceric acid
HMDB00208	Oxoglutaric acid	HMDB00119	glyoxylic acid
HMDB00821	Phenaceturic acid	HMDB00130	Homogentisic acid
HMDB00209	phenylacetic acid	HMDB03320	indole-3-carboxylic acid
HMDB02142	Phosphoric acid	HMDB60484	indole-3-pyruvic acid
HMDB00500	p-Hydroxybenzoic acid	HMDB00193	isocitric acid
HMDB00020	p-Hydroxyphenylacetic acid	HMDB00678	isovalerylglycine
HMDB00857	Pimelic acid	HMDB00176	maleic acid
HMDB00267	Pyroglutamic acid	HMDB00379	methylcitric acid
HMDB00243	Pyruvic acid	HMDB00634	methylmaleic acid
HMDB00232	Quinolinic acid	HMDB06024	Mevalonolactone
HMDB00792	Sebacic acid	HMDB00812	N-acetylaspatic acid

HMDB00866	N-acetyltyrosine
HMDB00226	orotic acid
HMDB02329	oxalic acid
HMDB00223	oxaloacetic acid
HMDB00860	phenylpropionylglycine
HMDB00783	Propionylglycine
HMDB00953	suberylglycine
HMDB00635	succinylacetone
HMDB00956	tartaric acid
HMDB01889	theophylline
HMDB00959	tiglylglycine
HMDB00300	uracil
HMDB01877	valproic acid
HMDB00484	vanillic acid

	CL(74:8)
	CL(74:9)
	CL(74:10)
	CL(76:10)
	CL(76:11)
	CL(76:12)
	CL(78:11)
	CL(78:12)
	CL(78:13)
	CL(78:14)
	CL(80:14)
	CL(80:15)
	CL(80:16)

Catecholamines analysis	
HMDB	Metabolites
HMDB01336	3,4-dihydroxyphenylacetic acid
HMDB00609	3,4-dihydroxyphenylalanine
HMDB00318	3,4-dihydroxyphenyl(ethylene)glycol
HMDB00073	Dopamine
HMDB00068	Epinephrine
HMDB04063	Metanephrine
HMDB00216	Norepinephrine
HMDB00819	Normetanephrine
HMDB00159	L-phenylalanine
HMDB12275	Phenylethylamine
HMDB00306	Tyramine
HMDB00158	L-tyrosine

Lipidomics for sphingolipid biosynthesis and metabolism	
HMDB	Metabolites
	Sphingosine
	Sphingosine-1-phosphate (S1P)
	Ceramide (d18:1/2:0)
	Ceramide (d18:1/4:0)
	Ceramide (d18:1/6:0)
	Ceramide (d18:1/8:0)
	Ceramide (d18:1/10:0)
	Ceramide (d18:1/12:0)
	Ceramide (d18:1/14:0)
	Ceramide (d18:1/16:0)
	Ceramide (d18:1/18:0)
	Ceramide (d18:1/18:1)
	Ceramide (d18:1/20:0)
	Ceramide (d18:1/22:0)
	Ceramide (d18:1/24:0)
	Ceramide (d18:1/24:1)
	SM (02:0)
	SM (06:0)
	SM (12:0)
	SM (12:0) dihydro
	SM (16:0)
	SM (17:0)
	SM (18:0)
	SM (18:1)
	SM (24:0)

Lipidomics for cardiolipins	
HMDB	Metabolites
	CL(54:6)
	CL(68:2)
	CL(68:3)
	CL(68:4)
	CL(68:5)
	CL(68:6)
	CL(68:7)
	CL(70:4)
	CL(70:5)
	CL(70:6)
	CL(70:7)
	CL(70:8)
	CL(72:7)
	CL(72:8)
	CL(72:9)

Low-MW sugars analysis	
HMDB	Metabolites
HMDB00122	Glucose
HMDB00169	Mannose
HMDB00660	Fructose
HMDB00143	Galactose
HMDB00283	Ribose

HMDB00098	Xylose
HMDB03371	Ribulose
HMDB01644	Xylulose
HMDB29942	Arabinose
HMDB00849	Rhamnose
HMDB00174	Fucose
	Lactose
HMDB00163	Maltose
HMDB00055	Cellobiose

Aldehydes analysis

HMDB	Metabolites
HMDB06112	Malondialdehyde (MDA)
HMDB41822	Acrolein
	4-HHE
	4-HNE
	Crotonaldehyde
	C2 Aldehyde
	C3 Aldehyde
	C4 Aldehyde
	C5 Aldehyde
	C6 Aldehyde
	C7 Aldehyde
	C8 Aldehyde
	10 Aldehyde

Oxysterols analysis

HMDB	Metabolites
HMDB00063	Cortisol
HMDB01547	Corticosterone
	6 β -OH cortisol
HMDB00067	Cholesterol
HMDB06119	7-OH cholesterol
HMDB01419	24-OH cholesterol
	17-OH cholesterol

Deoxynucleotide triphosphates (dNTPs) analysis

HMDB	Metabolites
HMDB01532	Deoxyadenosine triphosphate (dATP)
HMDB01342	Deoxythymidine triphosphate (dTTP)
HMDB00998	Deoxycytidine triphosphate (dCTP)
HMDB01440	Deoxyguanosine triphosphate (dGTP)
	Cyclic-di-adenosine monophosphate (c-di-AMP)

Polyphenol Analysis

HMDB	Metabolites
HMDB05807	Gallic acid

HMDB02780	Catechin
HMDB01964	Caffeic acid
HMDB02085	Syringic acid
HMDB02035	p-coumaric acid
HMDB00954	Ferulic acid
HMDB32616	Sinapic acid
HMDB01218	Coumarin
HMDB00567	Cinnamic acid
HMDB02927	Naringin
HMDB05801	Kaempferol
HMDB02899	Ellagic acid
HMDB05794	Quercetin
HMDB05800	Luteolin
HMDB02655	Isorhamnetin

Nucleoside/Nucleotide Analysis

HMDB	Metabolites
HMDB00902	NAD+
HMDB01487	NADH
HMDB00217	NADP+
HMDB00221	NADPH
HMDB00538	ATP
HMDB01341	ADP
HMDB14839	AMP
HMDB01273	GTP
HMDB01201	GDP

Thiol Analysis

HMDB	Metabolites
HMDB00574	Cysteine
HMDB00078	Cysteinylglycine
HMDB28816	Glutamylcysteine
HMDB02991	Cysteamine
HMDB00742	Homocysteine
HMDB00125	Glutathione
HMDB01890	Acetylcysteine

Carotenoid Analysis

HMDB	Metabolites
HMDB03101	Violaxanthin
HMDB03233	Lutein
HMDB02789	Zeaxanthin
HMDB03154	Canthaxanthin
	Cryptoxanthin
HMDB00561	b-Carotene

Acyl CoAs Analysis

HMDB	2.9167 in
HMDB01206	Acetyl CoA

HMDB03571	Lauroyl CoA
HMDB01521	Myristoyl CoA
HMDB01338	Palmitoyl CoA
HMDB01114	Stearoyl CoA
HMDB01322	Oleoyl CoA

Metal Analysis (Metalloids)

HMDB	Metabolites	Classification
HMDB01247	Aluminum	Metal
HMDB04118	Antimony	Metal
HMDB02290	Arsenic	Metal
HMDB04142	Barium	Metal
HMDB02386	Boron	Metal
HMDB00464	Calcium	Metal
HMDB13672	Cerium	Metal
HMDB13669	Cesium	Metal
HMDB00599	Chromium	Metal
HMDB00608	Cobalt	Metal
HMDB00657	Copper	Metal
HMDB01478	Gallium	Metal
HMDB02501	Germanium	Metal
HMDB29201	Hafnium	Metal
HMDB00692	Iron	Metal
HMDB13711	Lanthanum	Metal
HMDB04628	Lead	Metal
HMDB05949	Lithium	Metal
HMDB00547	Magnesium	Metal
HMDB01333	Manganese	Metal
HMDB01302	Molybdenum	Metal
HMDB13715	Neodymium	Metal
HMDB02457	Nickel	Metal
	Niobium	Metal
HMDB13670	Paladium	Metal
HMDB01315	Phosphorous	Metal
HMDB13671	Platinum	Metal
HMDB00586	Potassium	Metal
HMDB01327	Rubidium	Metal
HMDB01349	Selenium	Metal
HMDB04226	Sodium	Metal
HMDB03642	Strontium	Metal
HMDB01854	Tellurium	Metal
HMDB13724	Thallium	Metal
HMDB01960	Tin	Metal
HMDB01966	Titanium	Metal
HMDB01989	Tungsten	Metal
HMDB02503	Vanadium	Metal
HMDB13667	Yttrium	Metal
HMDB15532	Zinc	Metal
HMDB01475	Zirconium	Metal

Meat Biomarkers

HMDB	Metabolites
HMDB00062	L-Carnitine
HMDB00177	L-Histidine
HMDB00201	O-Acetylcarnitine
HMDB00251	Taurine
HMDB00925	Trimethylamine N-oxide
HMDB00001	ω-Methylhistidine
HMDB00479	τ-Methylhistidine

High-value Disease Biomarker Profiling

HMDB	Metabolites
	Asymmetric dimethylarginine
	Beta-hydroxybutyrate
	Betaine
	Choline
	Creatinine
	Glucose
	Glutamate
	Glutamine
	Lactate
	Leucine
	Methionine
	Phenylalanine
	Serine
	Taurine
	TMAO
	Tryptophan
	Tyrosine
	Aldosterone
	Amino adipic acid
	Carnosine
	Estradiol
	Folate
	Homocysteine
	HPHPA
	Indoxylsulfate
	Neopterin
	Pyruvic acid
	Testosterone
	Uric Acid
	Vitamin D

One-carbon metabolism

HMDB	Metabolites
HMDB00043	Betaine
HMDB00121	Folate

HMDB03339	Glutamate
HMDB00123	Glycine
HMDB00742	Homocysteine
HMDB00696	L-methionine
HMDB01185	S-adenosylmethionine
HMDB00187	L-serine
HMDB01846	Tetrahydrofolate
HMDB00607	Vitamin B12

Central carbon metabolism

HMDB	Metabolites
	Succinic acid
	Fumaric acid
	Glycolic acid
	Lactic acid
	Pyruvic acid
	Oxaloacetate
	Malic acid
	Citric acid
	α -Ketoglutaric acid
	DL- α -OH-glutaric acid
	Isocitric acid
	cAMP
	NAD+
	NADH
	NADP+
	NADPH
	ATP
	ADP
	AMP
	GTP
	GDP
	ADP-glucose
	UDP-glucose
	UDP
	Glucose-1-P
	Glucose-6-P
	Fructose-1-P
	Fructose-6-P
	Mannose-6-P
	Mannose-1-P
	Galactose-1-P
	Galactose-6-P
	Ribose-5-P
	Xylose-5-P
	Erythrose-4-P
	Ribulose-5P
	Sedoheptulose-7P

	Glucose 1,6-bisP
	Fructose-1,6-bisP
	Glyceraldehyde 3-P
	Dihydroxyacetone-P (DHAP)
	Phosphoenolpyruvate (PEP)
	6-Phosphogluconate
	3-P-glycerate/2-P-glycerate
	Glycerol-3-P
	Acetyl-P
	Malonyl-CoA
	Succinyl-CoA
	Acetyl-CoA
	Glucose

Amino acid metabolism/urea cycle metabolism

HMDB	Metabolites
HMDB00479	3-Methyl-L-histidine
HMDB00099	Cystathionine
HMDB00517	L-Arginine
HMDB00033	L-Carnosine
HMDB00679	L-Homocitrulline
HMDB00172	L-Isoleucine
HMDB00687	L-Leucine
HMDB01645	L-Norleucine
HMDB13716	L-Norvaline
HMDB00214	L-Ornithine
HMDB00159	L-Phenylalanine
HMDB00162	L-Proline
HMDB00929	L-Tryptophan
HMDB00883	L-Valine
	L- α -Amino-n-butyric acid
HMDB00123	L-Glycine
HMDB00161	L-Alanine
HMDB00168	L-Asparagine
HMDB00191	L-Aspartic acid
HMDB00904	L-Citrulline
	L-Cystine
HMDB03339	L-Glutamic acid
HMDB00641	L-Glutamine
HMDB00177	L-Histidine
	L-Homocystine
HMDB00182	L-Lysine
HMDB00696	L-Methionine
HMDB00187	L-Serine
HMDB00167	L-Threonine
HMDB00158	L-Tyrosine
HMDB00271	Sarcosine

HMDB00251	Taurine
	γ -Amino-n-butyric acid
	1-Methyl-L-histidine
	3-Bromotyrosine
	3-Chlorotyrosine
	3-Nitrotyrosine
	4-Hydroxyl-L-proline
	Agmatine
	Asymmetricdimethylarginine
	Cadaverine
	Dopamine
	Epinephrine (adrenaline)
	Histamine
	Melatonin
	N-methyl-4-hydroxyproline
	Norepinephrine
	Phenethylamine
	Putrescine
HMDB00259	Serotonin
HMDB01257	Spermidine
HMDB01256	Spermine
	Symmetricdimethylarginine
	Tyramine
	δ -Hydroxylysine
HMDB00294	Urea

Fatty acid metabolism - short- to long-chain fatty acids and acyl-carnitines analysis

HMDB	Metabolites	Classification
	Acetoacetic acid	Fatty acid
	β -hydroxybutyric acid	Fatty acid
	Malonic acid	Fatty acid
	Acetic acid	Fatty acid
	Propionic acid	Fatty acid
	Butyric acid	Fatty acid
	Isobutyric acid	Fatty acid
	Valeric acid	Fatty acid
	2-Methyl butyric acid	Fatty acid
	Isovaleric acid	Fatty acid
	Caproic acid	Fatty acid
	3-Metyl valeric acid	Fatty acid
	Hexanoic acid	Fatty acid
	Heptanoic acid	Fatty acid
	Octanoic acid	Fatty acid
	Decanoic acid	Fatty acid

	Dodecanoic acid	Fatty acid
	Myristic acid	Fatty acid
	Palmitic acid	Fatty acid
	Stearic acid	Fatty acid
HMDB02212	Arachidic acid (eicosanoic acid)	Fatty acid
	Behenic acid	Fatty acid
HMDB02003	Lignoceric acid	Fatty acid
	Palmitoleic acid	Fatty acid
	Petroselinic acid	Fatty acid
	Oleic acid	Fatty acid
	Elaidic acid	Fatty acid
HMDB00673	Linoleic acid	Fatty acid
HMDB01388	Linolenic acid	Fatty acid
HMDB01043	Arachidonic acid	Fatty acid
	Erucic acid	Fatty acid
	cis-4,7,3,6,9-Docosahexaenoic acid	Fatty acid
HMDB02368	Nervonic acid	Fatty acid
	C0 Carnitine	Acylcarnitine
	C2 Carnitine	Acylcarnitine
	C3 Carnitine	Acylcarnitine
	C4 Carnitine	Acylcarnitine
	C5-iso carnitine	Acylcarnitine
	C05-DC Glutaryl carnitine	Acylcarnitine
	C6 Carnitine	Acylcarnitine
	C8 Carnitine	Acylcarnitine
	C10 Carnitine	Acylcarnitine
	C10:1 Carnitine	Acylcarnitine
	C12 Carnitine	Acylcarnitine
	C14 Carnitine	Acylcarnitine
	C14:1 Carnitine	Acylcarnitine
	C16 Carnitine	Acylcarnitine
	C16-OH Carnitine	Acylcarnitine
	C18 Carnitine	Acylcarnitine
	C18:1 Carnitine	Acylcarnitine
	C18:2 Carnitine	Acylcarnitine
	C18-OH Carnitine	Acylcarnitine
	C20 Carnitine	Acylcarnitine
	C20:4 Carnitine	Acylcarnitine