Amino Acids and Derivatives	
3-Aminoisobutyric acid (BAIBA)	N-Acetyl-Arginine (N-alpha-L-Acetyl-arginine)
3-Nitrotyrosine	N-Acetyl-Asparagine (Nα-Acetyl-L-asparagine)
4-Hydroxyhippuric acid	N-Acetyl-Aspartic acid
4-Hydroxyphenylacetic acid (p-Hydroxyphenylacetic acid, 4-HPAA)	N-Acetyl-Glutamic acid
5-Aminolevulinic Acid (5ALA)	N-Acetyl-Glutamine
5-Hydroxylysine	N-Acetyl-Glycine (Acetylglycine)
5-Oxoproline (Pyroglutamic acid)	N-Acetyl-Histidine
Alanine	N-Acetyl-Isoleucine
alpha-Aminoadipic acid (alpha-AAA)	N-Acetyl-Leucine
alpha-Aminobutyric acid (Butyrine, AABA)	N-Acetyl-Methionine
Arginine	N-Acetyl-proline
Asparagine (Asn)	N-Acetyl-Serine
Aspartic acid (Asp)	N-Acetyl-Tryptophan
Asymmetric dimethylarginine (ADMA)	N-Acetyl-Tyrosine
beta-Alanine	N-Acetyl-Valine
Betaine (Glycine Betaine)	N-Methyl-Aspartic acid
cis-4-Hydroxyproline	N1-Acetyl-Lysine (N-alpha-Acetyl-L-lysine)
Citrulline	N2-Acetyl-Ornithine (Acetylornithine)
Cystathionine (Cth)	N6-Acetyl-Lysine (N-epsilon-Acetyl-L-lysine)
Dimethylglycine	Ornithine
Gamma-Aminobutyric acid (GABA)	Phenylacetylglutamine
Glutamic acid (Glu)	Phenylalanine (Phe)
Glutamine (Gln)	Pipecolic acid (Homoproline)
Glycine (Gly)	Proline (Pro)
Histidine (His)	Sarcosine
Homoarginine	Serine
Homocitrulline	Symmetric dimethylarginine (SDMA)
Homocysteine (2-Amino-4-Mercaptobutyric Acid)	Taurine
Isoleucine (Ile)	Threonine (Thr)
Leucine (Leu)	Tiglylglycine
Lysine	trans-4-Hydroxyproline (Hyp)
Methionine (Met)	Tryptophan
Methionine sulfoxide (Met-SO)	Tyrosine (Tyr)
Methylhistidine	Valine
N-Acetyl-Alanine	

Biogenic Amines

1,3-Diaminopropane	N1-Acetylspermidine
3-Methoxytyramine	N1,N12-Diacetylspermine (Diacetylspermine)
Agmatine	Phenylethylamine (PEA)
Cadaverine	Putrescine
Creatinine	Serotonin (5-HT)
Dimethylamine	Spermidine
Ethanolamine	Spermine
Histamine	Trimethylamine (TMA)
Kynurenine	Trimethylamine N-oxide (TMAO)
Methylamine	Tyramine
N-Acetylputrescine	

Indole Derivatives

3-Indoleacetic acid (IAA)	Indole-3-propionic acid (IPA)
5-Hydroxyindoleacetic Acid (5-HIAA)	Indolelactic acid (Indole-3-lactic acid)
5-Methoxytryptamine	Indoxyl glucuronide
Indole	Indoxyl-β-D-glucoside (Indican)
Indole-3-acetamide	Tryptamine
Indole-3-carboxylic acid	

Nucleotides & Nucleosides

5-Methyluridine (Ribothymidine)	Deoxyuridine
7-Methylguanine	Guanine
Adenine	Guanosine
Adenosine	Hypoxanthine
Cyclic AMP (Adenosine 3',5'-cyclic monophosphate)	Inosine
Cytidine	Thymidine
Cytosine	Thymine
Deoxyadenosine	Uracil
Deoxycytidine	Uridine
Deoxyguanosine	Xanthine
Deoxyinosine	Xanthosine

Organic Acids

2-Hydroxy-2-methylbutyric acid	Glutaric Acid
2-hydroxy-3-methylvaleric acid (HMVA)	Glyceric acid
2-Hydroxybutyric acid	Guanidinopropionic acid (3-GPA)
2-hydroxyglutaric acid	Guanidoacetic acid (Glycocyamine)
2-Hydroxyisobutyric acid (MTBE)	Hippuric acid
2-Hydroxyisovaleric acid (2-Hydroxy-3-methylbutyric acid)	Homovanillic acid
2-Hydroxyphenylacetic acid (2-HPAA)	Isocitric acid
3-(3-hydroxyphenyl)-3-hydroxypropanoic acid (HPHPA)	Kynurenic acid
3-Carboxy-4-methyl-5-propyl-2-furanpropionic acid (CMPF)	Lactic acid
3-hydroxyisobutyric acid (3-HIBA)	Maleic acid
3-Hydroxyisovaleric acid	Malic acid
3-Hydroxyphenylacetic acid	Malonic acid
3-Methyladipic acid	Methylmalonic acid (Isosuccinic Acid)
3,4-Dihydroxybutyric acid	Orotic Acid
4-hydroxybenzoic acid (p-Salicylic acid)	Phenylacetic acid
4-Hydroxyphenylpyruvic acid (4-HPPA)	Picolinic acid (2-Picolinic acid/PICA)
Argininic acid	Quinaldic acid
Benzoic acid	Quinoline-4-carboxylic acid
Caffeic acid	Quinolinic acid
cis-Aconitic acid	Salicylic acid (2-Hydroxybenzoic acid)
Citric acid	Shikimic acid
Creatine	Succinic acid
Ethylmalonic acid	Tartaric acid
Fumaric acid	Threonic acid
Furan-2,5-dicarboxylic acid (FDCA)	Uric acid

Ketones & Keto acids

2-oxoadipic acid (Oxoadipic acid)	alpha-Ketoglutaric acid (2-Oxoglutaric acid)
2-Oxoisocaproic acid (Ketoleucine)	alpha-Ketoisovaleric acid (2-oxo-3-Methylbutyric acid)
3-Hydroxybutyric acid (beta-Hydroxybutyric acid)	Pyruvic acid (2-Oxopropanoic acid)
Acetoacetic acid	

Sulfates

4-Ethylphenyl sulfate	p-Cresol sulfate
Indoxyl sulfate	

Others

Allantoin
Nudifloramide (N1-Methyl-2-pyridone-5-carboxamide)
Urea

Short & Medium Chain Fatty Acids

Acetic Acid	Isovaleric acid
Butyric acid + Isobutyric acid	Propionic acid
Caproic acid	Valeric acid
Caprylic acid (Octanoic Acid)	

Vitamins & Derivatives

1-Methylnicotinamide
Choline
Nicotinamide ribotide (β-NMN)

Sugars

3-Deoxyglucosone (3-Deoxyfructose)
Glucose

Catecholamines

DOPA	Epinephrine
Dopamine	Norepinephrine

Dipeptides

Carnosine

Acylcarnitines	
C0	C18:1OH
C10	C18:2
C10:1	C2
C10:2	C3
C12	C3:1
C12:1	C3OH
C12DC	C4
C14	C4:1
C14:1	C4OH
C14:1OH	C5
C14:2	C5:1
C14:2OH	C5:1DC
C16	C5DC
C16:1	C5MDC
C16:1OH	C5OH
C16:2	C6
C16:2OH	C6:1
C16OH	C7DC
C18	C8
C18:1	C9

Lipids: Ceramides	
LacCer(d18:1/14:0)	GlcCer(d18:2/18:0)
Cer(d18:1/14:0)	Cer(d18:2/16:0)
Cer(d18:1/16:0)	GlcCer(d18:1/18:0)
LacCer(d18:1/16:0)	GlcCer(d18:2/20:0)
Cer(d16:1/18:0)	LacCer(d18:1/24:0)
Cer(d18:1/18:0)	GlcCer(d18:1/18:1)
Cer(d18:1/18:0(OH))	Cer(d18:2/18:0)
Cer(d18:1/18:1)	Cer(d18:2/18:1)
Cer(d16:1/18:0)	LacCer(d18:1/24:0)
LacCer(d18:1/18:0)	GlcCer(d18:2/22:0)
Cer(d16:1/20:0)	LacCer(d18:1/24:1)
Cer(d18:1/20:0(OH))	Cer(d18:2/20:0)
Trihexosylceramide(d18:1/20:0)	GlcCer(d16:1/24:0)
Cer(d16:1/20:0)	LacCer(d18:1/24:1)
LacCer(d18:1/20:0)	GlcCer(d18:2/23:0)
Cer(d16:1/22:0)	Trihexosylceramide(d18:1/16:0)
Cer(d18:1/22:0)	GlcCer(d18:1/20:0)
Cer(d16:1/22:0)	Trihexosylceramide(d18:1/16:0)
LacCer(d18:1/22:0)	GlcCer(d18:2/24:0)
Cer(d18:1/23:0)	GlcCer(d18:1/22:0)
Cer(d16:1/23:0)	Cer(d18:2/23:0)

Cer(d16:1/24:0)	Trihexosylceramide(d18:1/18:0)
Cer(d18:1/24:0)	GlcCer(d18:1/23:0)
Cer(d18:1/24:1)	GlcCer(d18:1/24:0)
Cer(d16:1/24:0)	Trihexosylceramide(d18:1/18:0)
Cer(d18:0/24:0)	GlcCer(d16:1/22:0)
Cer(d18:0/24:1)	GlcCer(d18:1/16:0)
Cer(d18:0/18:0(OH))	Cer(d18:1/20:0(OH))
Cer(d18:0/18:0)	Cer(d18:1/20:0)
Cer(d18:0/26:1(OH))	Cer(d18:1/26:1)
Cer(d18:0/26:1)	Cer(d18:2/14:0)
Cer(d18:0/20:0)	Trihexosylceramide(d18:1/24:1)
Cer(d18:0/20:0)	Trihexosylceramide(d18:1/24:1)
Cer(d18:0/22:0)	Trihexosylceramide(d18:1/22:0)
Cer(d18:1/25:0)	GlcCer(d18:1/24:1)
LacCer(d18:1/26:1)	Cer(d18:2/23:0)
Trihexosylceramide(d18:1/26:1)	GlcCer(d18:1/14:0)
Cer(d18:2/22:0)	GlcCer(d18:1/26:0)
Cer(d18:2/24:0)	GlcCer(d18:1/26:1)
Cer(d18:2/24:1)	GlcCer(d18:2/16:0)

Lipids: Cholesterol esters

CE(14:0)	CE(18:3)
CE(14:1)	CE(20:0)
CE(15:0)	CE(20:1)
CE(15:1)	CE(20:3)
CE(16:0)	CE(20:4)
CE(16:1)	CE(20:5)
CE(17:0)	CE(22:0)
CE(17:1)	CE(22:1)
CE(18:0)	CE(22:2)
CE(18:1)	CE(22:5)
CE(18:2)	CE(22:6)

Lipids: Diacylglycerols (DAG)

DG(14:0/14:0)	DG(18:1/18:1)
DG(14:0/18:1)	DG(18:1/18:3)
DG(14:0/18:2)	DG(18:1/20:3)
DG(14:0/20:0)	DG(18:1/20:4)
DG(14:1/18:1)	DG(17:0/18:1)
DG(14:1/20:2)	DG-O(16:0/20:4)
DG(16:0/20:3)	DG(18:3/18:3)
DG(16:0/20:4)	DG(21:0/22:6)
DG(16:0/16:0)	DG(18:1/18:2)
DG(16:0/16:1)	DG(18:3/20:2)
DG(16:0/18:1)	DG(18:2/18:4)

DG(16:0/18:2)	DG(22:1/22:2)
DG(16:0/20:0)	DG-O(14:0/18:2)
DG(16:1/18:0)	DG(17:0/17:1)
DG(16:1/18:1)	DG(18:1/22:6)
DG(16:1/18:2)	DG(18:2/18:2)
DG(16:1/20:0)	DG(18:2/18:3)
DG(18:0/20:4)	DG(18:1/22:5)
DG(18:1/18:4)	DG(18:0/20:0)
DG(18:1/20:0)	DG-O(16:0/18:1)
DG(18:1/20:1)	DG(18:2/20:0)
DG(18:1/20:2)	DG(18:2/20:4)

Lipids: Sphingomyelins	
SM(d18:1/16:0)	SM(d18:1/26:0)
SM(d18:1/16:1)	SM(d18:1/26:1)
SM(d18:1/18:0)	Hydroxysphingomyeline C14:1
SM(d18:1/18:1)	Hydroxysphingomyeline C16:1
SM(d18:1/20:2)	Hydroxysphingomyeline C22:1
SM(d18:1/24:0)	Hydroxysphingomyeline C22:2

Lipids: Sphingomyelins	
SM(d18:1/16:0)	SM(d18:1/26:0)
SM(d18:1/24:1)	Hydroxysphingomyeline C24:1

Lipids: Phosphatidylcholines	
PC(24:0)	PC(O-30:1)
PC(26:0)	PC(O-30:2)
PC(28:1)	PC(O-32:1)
PC(30:0)	PC(O-32:2)
PC(32:0)	PC(O-34:0)
PC(32:1)	PC(O-34:1)
PC(32:2)	PC(O-34:2)
PC(32:3)	PC(O-34:3)
PC(34:1)	PC(O-36:0)
PC(34:2)	PC(O-36:1)
PC(34:3)	PC(O-36:2)
PC(34:4)	PC(O-36:3)
PC(36:0)	PC(O-36:4)
PC(36:1)	PC(O-36:5)
PC(36:2)	PC(O-38:0)
PC(36:3)	PC(O-38:1)
PC(36:4)	PC(O-38:2)
PC(36:5)	PC(O-38:3)
PC(36:6)	PC(O-38:4)
PC(38:0)	PC(O-38:5)
PC(38:1)	PC(O-38:6)
PC(38:3)	PC(O-40:1)
PC(38:4)	PC(O-40:2)
PC(38:5)	PC(O-40:3)
PC(38:6)	PC(O-40:4)
PC(40:1)	PC(O-40:5)
PC(40:2)	PC(O-40:6)
PC(40:3)	PC(O-42:0)
PC(40:4)	PC(O-42:1)
PC(40:5)	PC(O-42:2)
PC(40:6)	PC(O-42:3)
PC(42:0)	PC(O-42:4)
PC(42:1)	PC(O-42:5)
PC(42:2)	PC(O-44:3)
PC(42:4)	PC(O-44:4)

PC(42:5)	PC(O-44:5)
PC(42:6)	PC(O-44:6)
PC(O-30:0)	

Lipids: Lysophosphatidylcholines

LysoPC(14:0/0:0)	LysoPC(20:3/0:0)
LysoPC(16:0/0:0)	LysoPC(20:4/0:0)
LysoPC(16:1/0:0)	LysoPC(24:0/0:0)
LysoPC(17:0/0:0)	LysoPC(26:0/0:0)
LysoPC(18:0/0:0)	LysoPC(26:1/0:0)
LysoPC(18:1/0:0)	LysoPC(28:0/0:0)
LysoPC(18:2/0:0)	LysoPC(28:1/0:0)

Lipids: Triacylglycerols (TAG)

TG(14:0_32:2)	TG(17:1_34:1)	TG(18:2_36:5)
TG(14:0_34:0)	TG(17:1_34:2)	TG(18:2_38:4)
TG(14:0_34:1)	TG(17:1_34:3)	TG(18:2_38:5)
TG(14:0_34:2)	TG(17:1_36:3)	TG(18:2_38:6)
TG(14:0_34:3)	TG(17:1_36:4)	TG(18:3_30:0)
TG(14:0_35:1)	TG(18:0_30:0)	TG(18:3_32:0)
TG(14:0_35:2)	TG(18:0_30:1)	TG(18:3_32:1)
TG(14:0_36:1)	TG(18:0_32:0)	TG(18:3_34:0)
TG(14:0_36:2)	TG(18:0_32:1)	TG(18:3_34:1)
TG(14:0_36:3)	TG(18:0_32:2)	TG(18:3_34:2)
TG(14:0_36:4)	TG(18:0_34:2)	TG(18:3_34:3)
TG(14:0_38:4)	TG(18:0_34:3)	TG(18:3_36:1)
TG(14:0_38:5)	TG(18:0_36:1)	TG(18:3_36:2)
TG(16:0_28:1)	TG(18:0_36:2)	TG(18:3_36:3)
TG(16:0_28:2)	TG(18:0_36:3)	TG(18:3_36:4)
TG(16:0_30:2)	TG(18:0_36:4)	TG(18:3_38:5)
TG(16:0_32:0)	TG(18:0_36:5)	TG(18:3_38:6)
TG(16:0_32:1)	TG(18:0_38:6)	TG(20:0_32:3)
TG(16:0_32:2)	TG(18:0_38:7)	TG(20:0_32:4)
TG(16:0_32:3)	TG(18:1_26:0)	TG(20:0_34:1)
TG(16:0_33:1)	TG(18:1_28:1)	TG(20:1_24:3)

TG(16:0_33:2)	TG(18:1_30:0)	TG(20:1_26:1)
TG(16:0_34:0)	TG(18:1_30:1)	TG(20:1_30:1)
TG(16:0_34:1)	TG(18:1_30:2)	TG(20:1_31:0)
TG(16:0_34:2)	TG(18:1_31:0)	TG(20:1_32:1)
TG(16:0_34:3)	TG(18:1_32:0)	TG(20:1_32:2)
TG(16:0_34:4)	TG(18:1_32:1)	TG(20:1_32:3)
TG(16:0_35:1)	TG(18:1_32:2)	TG(20:1_34:0)
TG(16:0_35:2)	TG(18:1_32:3)	TG(20:1_34:1)
TG(16:0_35:3)	TG(18:1_33:0)	TG(20:1_34:2)
TG(16:0_36:2)	TG(18:1_33:1)	TG(20:1_34:3)
TG(16:0_36:3)	TG(18:1_33:2)	TG(20:2_32:0)
TG(16:0_36:4)	TG(18:1_34:1)	TG(20:2_32:1)

Lipids: Triacylglycerols (TAG)

TG(16:0_36:5)	TG(18:1_34:2)	TG(20:2_34:1)
TG(16:0_36:6)	TG(18:1_34:3)	TG(20:2_34:2)
TG(16:0_37:3)	TG(18:1_34:4)	TG(20:2_34:3)
TG(16:0_38:1)	TG(18:1_35:2)	TG(20:3_32:0)
TG(16:0_38:2)	TG(18:1_35:3)	TG(20:3_32:1)
TG(16:0_38:3)	TG(18:1_36:0)	TG(20:3_32:2)
TG(16:0_38:4)	TG(18:1_36:1)	TG(20:3_34:0)
TG(16:0_38:5)	TG(18:1_36:2)	TG(20:3_34:1)
TG(16:0_38:6)	TG(18:1_36:3)	TG(20:3_34:2)
TG(16:0_38:7)	TG(18:1_36:4)	TG(20:3_34:3)
TG(16:0_40:6)	TG(18:1_36:5)	TG(20:3_36:3)
TG(16:0_40:7)	TG(18:1_36:6)	TG(20:3_36:4)
TG(16:0_40:8)	TG(18:1_38:5)	TG(20:4_30:0)
TG(16:1_28:0)	TG(18:1_38:6)	TG(20:4_32:0)
TG(16:1_30:1)	TG(18:1_38:7)	TG(20:4_32:1)
TG(16:1_32:0)	TG(18:2_28:0)	TG(20:4_32:2)
TG(16:1_32:1)	TG(18:2_30:0)	TG(20:4_34:0)
TG(16:1_32:2)	TG(18:2_30:1)	TG(20:4_34:1)
TG(16:1_33:1)	TG(18:2_31:0)	TG(20:4_34:2)
TG(16:1_34:0)	TG(18:2_32:0)	TG(20:4_34:3)
TG(16:1_34:1)	TG(18:2_32:1)	TG(20:4_36:2)
TG(16:1_34:2)	TG(18:2_32:2)	TG(20:4_36:3)
TG(16:1_34:3)	TG(18:2_33:0)	TG(20:4_36:4)
TG(16:1_36:1)	TG(18:2_33:1)	TG(20:5_34:0)
TG(16:1_36:2)	TG(18:2_33:2)	TG(20:5_34:1)
TG(16:1_36:3)	TG(18:2_34:0)	TG(20:5_34:2)
TG(16:1_36:4)	TG(18:2_34:1)	TG(20:5_36:2)
TG(16:1_36:5)	TG(18:2_34:2)	TG(20:5_36:3)
TG(16:1_38:3)	TG(18:2_34:3)	TG(22:4_34:2)
TG(16:1_38:4)	TG(18:2_34:4)	TG(22:5_32:0)
TG(16:1_38:5)	TG(18:2_35:1)	TG(22:5_32:1)
TG(17:0_32:1)	TG(18:2_35:2)	TG(22:5_34:1)
TG(17:0_34:1)	TG(18:2_35:3)	TG(22:5_34:2)
TG(17:0_34:2)	TG(18:2_36:0)	TG(22:6_32:0)
TG(17:0_34:3)	TG(18:2_36:1)	TG(22:6_32:1)
TG(17:0_36:3)	TG(18:2_36:2)	TG(22:6_34:1)
TG(17:0_36:4)	TG(18:2_36:3)	TG(22:6_34:2)
TG(17:1_32:1)	TG(18:2_36:4)	TG(14:0/39:3)
TG(17:1/36:5)	TG(17:2/38:6)	TG(20:4/36:5)
TG(17:1/38:5)	TG(17:2/38:7)	TG(22:0/32:4)
TG(17:1/38:6)	TG(18:1/33:3)	TG(22:1/32:5)
TG(17:1/38:7)	TG(18:3/33:2)	TG(22:2/32:4)
TG(17:2/34:2)	TG(18:3/35:2)	TG(22:3/30:2)
TG(17:2/34:3)	TG(20:2/34:4)	TG(22:4/32:0)
TG(17:2/36:2)	TG(20:2/36:5)	TG(22:4/32:2)

TG(17:2/36:3)	TG(20:3/36:5)	TG(22:5/34:3)
TG(17:2/36:4)	TG(20:4/33:2)	TG(22:6/34:3)
TG(17:2/38:5)	TG(20:4/35:3)	