

List of metabolites

Aldehydes			
4-hydroxybenzaldehyde		Glyoxylic acid	
4-Hydroxynonenal		trans-2-Hexenal	
Alkaloids and derivatives			
Allantoin	Caffeine	Piperine	Trigonelline
Phenolic acids			
2-Hydroxyphenylacetic acid		Avenanthramide A	
3,4-Dihydroxybutyric acid		Ferulic acid	
3,4-Dihydroxyphenylacetic acid		Ferulic acid 4-glucuronide	
3,5-dihydroxybenzoic acid		o-coumaric acid	
3-Hydroxyphenylacetic acid		p-coumaric acid	
4-Hydroxybenzoic acid		Syringic acid	
4-Hydroxyphenylacetic acid		Vanillactic acid	
4-Pyridoxic acid		Vanillic acid	
Bile acids			
Chenodeoxycholic acid		Muricholic acid	
Cholic acid		taurochenodeoxycholic acid	
Deoxycholic acid		taurocholic acid	
Glycochenodeoxycholic acid		Taurodeoxycholic acid	
Glycocholic acid		Taurolithocholic acid	
Glycodeoxycholic acid		Taurolithocholic acid 3-sulfate	
Glycolithocholic acid		Tauromuricholic acid	
Hyodeoxycholic acid		Tauroursodeoxycholic acid	
Lithocholic acid		Ursodeoxycholic acid	
Biogenic amines			
1,3-Diaminopropane		N1-Acetylspermidine	
3-Methoxytyramine		N1-Acetylspermine	
Agmatine		N-Acetylputrescine	
Cadaverine		Phenylethylamine	
Creatinine		Putrescine	
Diacetylspermine		Spermidine	
Dimethylamine		Spermine	
Ethanolamine		TMAO	
Histamine		Trimethylamine	
Methylamine		Tyramine	
Catecholamines			
DOPA		Hydroxytyrosol	
Dopamine		Metanephrine	
Dopamine-3-O-sulfate		Norepinephrine	
Epinephrine			

List of metabolites

Amino acids and derivatives	
2-Aminopimelic acid	Methionine
2-Methylbutyrylglycine	Methionine sulfoxide
3-Aminobutyric acid	Methylhistidine
3-Aminoisobutyric acid	N1-Acetyl-Lysine
3-Hydroxyhippuric acid	N1-Acetyl-Lysine + N6-Acetyl-Lysine
3-MethoxyTyrosine	N2-Acetyl-Orn
4-Oxo-L-Proline	N-Acetyl-Alanine
5-Aminolevulinic acid	N-Acetyl-Arginine
5-Aminovaleric acid	N-Acetyl-Asparagine
5-Hydroxylysine	N-Acetyl-Aspartic acid
5-Oxoproline	N-Acetyl-Glutamic acid
AABA	N-Acetyl-Glutamine
ADMA	N-Acetyl-Glycine
Alanine	N-Acetyl-Histidine
Alliin	N-Acetyl-Isoleucine
alpha-Aminoadipic acid	N-Acetyl-Leucine
Arginine	N-Acetyl-Methionine
Asparagine	N-Acetyl-Proline
Aspartate	N-Acetyl-Serine
beta-Alanine	N-Acetyl-Tyrosine
Beta-Leucine	N-Acetyl-Valine
cis-4-Hydroxyproline	Nicotinuric acid
Citrulline	Nitro-Tyrosine
Cystathionine	N-Methyl-Aspartic acid
Dimethylglycine	Ornithine
Ectonie	Phenylacetylglutamine
Ergothioneine	Phenylalanine
Formiminoglutamic acid	p-Hydroxyhippuric acid
GABA	Proline
Glutamate	Proline betaine
Glutamine	S-Allylcysteine
Glycine	Sarcosine
Histidine	Serine
Homoarginine	S-phenylmercapturic acid
Homocitrulline	Threonine
Homocysteine	Tiglylglycine
Isoleucine	trans-4-Hydroxyproline
Leucine	Tyrosine
Lysine	Valine

List of metabolites

Indole Derivatives	
1H-Indole-4-carboxaldehyde	indole-3-carboxaldehyde
3-Indoleacetic acid	Indole-3-carboxylic acid
5,6-Dimethoxyindole-2-Carboxylic acid	Indole-3-propionic acid
5-Hydroxyindoleacetic acid	Indolelactic acid
Indole	Indoxyl glucoside
Indole-3-acetamide	Indoxyl glucuronide
Ketone and Keto acids	
2-Ketobutyric acid	alpha-Ketoglutaric acid
2-oxoadipic acid	alpha-Ketoisovaleric acid
2-oxoisocaproic acid	beta-Hydroxypyruvic acid
3-Hydroxybutyric acid	Phenylpyruvic acid
3-Methyl-2-oxovaleric acid	Pyruvic acid
Acetoacetic acid	
Nucleo Bases and Nucleosides	
1,3-Dimethyluric acid	Deoxyinosine
1-Methylguanosine	Deoxyuridine
1-Methylinosine	Guanidine
1-Methyluric acid	Guanine
3-Methyladenine	Guanosine
5-Methyluridine	Hypoxanthine
7-Methylguanine	Inosine
Adenine	Theobromine
Adenosine	Thymidine
ADMA+SDMA	Thymine
Cyclic AMP	Total MethylXanthine
Cytidine	Uracil
Cytosine	Uric acid
Deoxyadenosine	Uridine
Deoxycytidine	Xanthine
Deoxyguanosine	Xanthosine
Others	
4-Coumaryl alcohol	Sulforaphane
4-Hydroxybenzophenone	Triclocarban
4-Methylcatechol	Urea
Homovanillyl alcohol	Urolithin B
Nudifloramide	
Steroids and Hormones	
Abscisic acid	Solanidine
Estrone sulfate	Solanine

List of metabolites

Fatty acids and derivatives

2-Hydroxy-2-methylbutyric acid	Erucic acid
2-Hydroxy-3-methylvaleric acid+2-hydroxy-4-methylpentanoic acid	Fumaric acid
2-Hydroxybutyric acid	gamma-Linolenic acid
2-Hydroxyisobutyric acid	Glutaconic acid
2-Hydroxyisovaleric acid	Glutaric acid
2-hydroxymethylbutanoic acid	Heptanoic acid
2-Isopropylmalic acid	Homovanillic acid
2-Methylglutaric acid	Isovaleric acid
2-oxovaleric acid	Itaconic acid
3-(3-Hydroxyphenyl)-3-hydroxypropanoic acid	Lactic acid
3-Hydroxy propionic acid	Linoleic acid
3-Hydroxyglutaric acid	Malic acid
3-Hydroxyhexanedioic acid	Malonic acid
3-Hydroxyisobutyric acid	Margaric acid
3-Hydroxyisovaleric acid	Methylmalonic acid
3-Hydroxypentanoic acid	methylsuccinic acid
3-Hydroxysebacic acid	Myristic acid
3-Methylglutaconic acid	Palmitic acid
3-Methylglutaric acid	Palmitoleic acid
3-Methylvaleric acid	Pelargonic acid
4-Acetamidobutyric acid	Pentadecylic acid
4-Hydroxybutyric acid	Phytanic acid
Adipic acid	Pimelic acid
alpha-linolenic acid	Pristanic acid
Azelaic acid	Propionic acid
Behenic acid	Suberic acid
Butyric acid + Isobutyric acid	Succinic acid
Capric acid	Tartaric acid
Caproic acid	Tridecylic acid
Caprylic acid	Undecylenic acid
cis-8,11,14-Eicosatrienoic acid	Undecylic acid
Citraconic acid	Valeric acid
Docosahexaenoic acid	

Polyphenol and Isoflavones

Capsaicin	Hesperetin
Cyanidin-3-Glucoside	Naringenin
Daidzein	Phloretin
Dihydroisoferulic acid	Resveratrol
Genistein	

List of metabolites

Sulfates			
4-Ethylphenyl sulfate		p-Cresol sulfate	
Ferulic acid 4-Sulfate		Taurine	
Indoxyl sulfate			
Sugars, Sugarand acids and Sugar alcohols			
3-Deoxyglucosone		Lactose	
D-Psicose		Maltose	
Ethyl glucuronide		Mannose	
Fructose		N-acetylgalactosamine+n-Acetylglucosamine	
Fucose		Pentose (Arabinose+Ribose+Xylose+Xylulose)	
Gluconic acid+Galactonic acid		Pinitol	
Glucose		quinic acid	
Glucuronic acid		Ribonic acid+Xylonic acid	
L-Iduronic acid			
Organic acids			
2,5-Furandicarboxylic acid		Guanidoacetic acid	
2-hydroxyglutaric acid		Hippuric acid	
3-Carboxy-4-methyl-5-propyl-2-furanpropionic acid		Hydrocinnamic acid+2-Phenylpropionic acid	
3-Methyladipic acid		Imidazoleacetic acid	
4-Hydroxyphenylpyruvic acid		Isocitric acid	
Anthranilic acid		Maleic acid	
Argininic acid		Mandelic acid	
Benzoic acid		Monobutyl-Phthalate	
Betaine		N-Acetylneuraminic acid	
Caffeic acid		Orotic acid	
Cinnabarinic acid		Phenylacetic acid	
cis-Aconitic acid		Pipecolic acid	
Citramalic acid		Quinaldic acid	
Citric acid		Quinoline-4-carboxylic acid	
Creatine		Salicylic acid	
Erythronic acid		Shikimic acid	
Ethylmalonic acid		Threonic acid	
Glyceric acid		Ureidopropionic acid	
Glycolic acid		Urocanic acid	
Guanidinopropionic acid			
Drugs, pollutants, food additives and toxic compounds			
Butyl Paraben	Ethylparaben	Ibuprofen	Cotinine

List of metabolites

Trp-Kyn Pathway Metabolites

5-Methoxytryptamine	Picolinic acid
Kynurenic acid	Quinolinic acid
Kynurenine	Serotonin
N-Acetyl-Tryptophan	Trp
N'-FormylKynurenine	Tryptamine

Vitamins and Derivatives

1-Methylnicotinamide	Nicotinic acid
Choline	Pantothenic acid
Nicotinamide ribotide	α -Tocopherol

Acylcarnitines

Benzoylcarnitine	C0	C10	C10:1
C10:1-2OH	C10:2	C10:3	C10:3:DC
C10:DC-OH	C10-2OH	C11:1	C11:2
C11:3	C11:DC	C12	C12:1
C12:3	C12:4	C12-2OH	C12DC
C13	C13:1	C13:2	C13:3
C13:4	C14	C14:1	C14:1OH
C14:2	C14:2OH	C14:3	C14:3OH
C14:DC	C14DC	C16	C16:1
C16:1OH	C16:2	C16:2OH	C16:3
C16:4	C16:5	C16DC	C16OH
C18	C18:1	C18:1OH	C18:2
C2	C3	C3:1	C3OH
C4	C4:1	C4OH	C5
C5:1	C5:1DC	C5DC	C5MDC
C5OH	C6	C6:1	C6:2
C6:3	C7:1	C7:2	C7DC
C8	C8:1	C8:2	C8:DC
C9	C9:1	C9:1:DC	C9:2
C9:3	C9:4	C9:5	C9:DC
C9-2OH	Phenylacetylcarnitine	Phenylbutyrylcarnitine	Phenylvalerylcarnitine

Cholesterol esters

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

List of metabolites

Dipeptides			
Anserine	Aspartylleucine		Carnosine
Cyclo(L-Pro-L-Val)	enterolactone		Glycyl-Glycine
Glycylleucine	Glycylvaline		Phenylalanylglycine
Phosphatidylcholines			
LysoPC a C14:0	LysoPC a C16:0	LysoPC a C16:1	LysoPC a C17:0
LysoPC a C18:0	LysoPC a C18:1	LysoPC a C18:2	LysoPC a C20:3
LysoPC a C20:4	LysoPC a C24:0	LysoPC a C26:0	LysoPC a C26:1
LysoPC a C28:0	LysoPC a C28:1	PC aa C24:0	PC aa C26:0
PC aa C28:1	PC aa C30:0	PC aa C32:0	PC aa C32:1
PC aa C32:2	PC aa C32:3	PC aa C34:1	PC aa C34:2
PC aa C34:3	PC aa C34:4	PC aa C36:0	PC aa C36:1
PC aa C36:2	PC aa C36:3	PC aa C36:4	PC aa C36:5
PC aa C36:6	PC aa C38:0	PC aa C38:1	PC aa C38:3
PC aa C38:4	PC aa C38:5	PC aa C38:6	PC aa C40:1
PC aa C40:2	PC aa C40:3	PC aa C40:4	PC aa C40:5
PC aa C40:6	PC aa C42:0	PC aa C42:1	PC aa C42:2
PC aa C42:4	PC aa C42:5	PC aa C42:6	PC ae C30:0
PC ae C30:1	PC ae C30:2	PC ae C32:1	PC ae C32:2
PC ae C34:0	PC ae C34:1	PC ae C34:2	PC ae C34:3
PC ae C36:0	PC ae C36:1	PC ae C36:2	PC ae C36:3
PC ae C36:4	PC ae C36:5	PC ae C38:0	PC ae C38:1
PC ae C38:2	PC ae C38:3	PC ae C38:4	PC ae C38:5
PC ae C38:6	PC ae C40:1	PC ae C40:2	PC ae C40:3
PC ae C40:4	PC ae C40:5	PC ae C40:6	PC ae C42:0
PC ae C42:1	PC ae C42:2	PC ae C42:3	PC ae C42:4
PC ae C42:5	PC ae C44:3	PC ae C44:4	PC ae C44:5
PC ae C44:6			
Sphingomyelins			
SM C16:0	SM C16:1	SM C18:0	SM C18:1
SM C20:2	SM C24:0	SM C24:1	SM C26:0
SM C26:1	SM(OH) C14:1	SM(OH) C16:1	SM(OH) C22:1
SM(OH) C22:2	SM(OH) C24:1		
Ceramides			
Cer(d16:1/18:0)	Cer(d16:1/20:0)	Cer(d16:1/22:0)	Cer(d16:1/24:0)
Cer(d18:0/20:0)	Cer(d18:0/22:0)	Cer(d18:0/24:0)	Cer(d18:0/24:1)
Cer(d18:1/16:0)	Cer(d18:1/18:0)	Cer(d18:1/22:0)	Cer(d18:1/23:0)
Cer(d18:1/24:0)	Cer(d18:1/24:1)	Cer(d18:1/25:0)	Cer(d18:2/22:0)
Cer(d18:2/24:0)	Cer(d18:2/24:1)		

List of metabolites

Hexylceramides					
Hex2Cer(d18:1/14:0)		Hex2Cer(d18:1/16:0)		Hex2Cer(d18:1/18:0)	
Hex2Cer(d18:1/22:0)		Hex2Cer(d18:1/24:0)		Hex2Cer(d18:1/24:1)	
Hex3Cer(d18:1/18:0)		Hex3Cer(d18:1/24:1)		Hex3Cer(d18:1_22:0)	
HexCer(d18:1/16:0)		HexCer(d18:1/18:0)		HexCer(d18:1/18:1)	
HexCer(d18:1/22:0)		HexCer(d18:1/23:0)		HexCer(d18:1/24:0)	
HexCer(d18:1/26:0)		HexCer(d18:1/26:1)		HexCer(d18:2/16:0)	
HexCer(d18:2/20:0)		HexCer(d18:2/22:0)		HexCer(d18:2/23:0)	
HexCer(d18:2/24:0)					
Diacylglycerols					
DAG(14:0_14:0)	DAG(14:0_15:0)	DAG(14:0_16:0)	DAG(14:0_16:1)	DAG(14:0_17:0)	DAG(14:0_18:0)
DAG(14:0_18:1)	DAG(14:0_18:2)	DAG(14:0_18:3)	DAG(14:0_19:0)	DAG(14:0_20:0)	DAG(14:0_20:1)
DAG(14:0_20:2)	DAG(14:0_20:3)	DAG(14:0_20:4)	DAG(14:0_20:5)	DAG(14:0_22:4)	DAG(14:0_22:5)
DAG(14:0_22:6)	DAG(15:0_15:0)	DAG(15:0_16:0)	DAG(15:0_16:1)	DAG(15:0_17:0)	DAG(15:0_18:0)
DAG(15:0_18:1)	DAG(15:0_18:2)	DAG(15:0_18:3)	DAG(15:0_19:0)	DAG(15:0_20:0)	DAG(15:0_20:1)
DAG(15:0_20:2)	DAG(15:0_20:3)	DAG(15:0_20:4)	DAG(15:0_20:5)	DAG(15:0_22:4)	DAG(15:0_22:5)
DAG(15:0_22:6)	DAG(16:0_16:0)	DAG(16:0_16:1)	DAG(16:0_17:0)	DAG(16:0_18:0)	DAG(16:0_18:1)
DAG(16:0_18:2)	DAG(16:0_18:3)	DAG(16:0_19:0)	DAG(16:0_20:0)	DAG(16:0_20:1)	DAG(16:0_20:2)
DAG(16:0_20:3)	DAG(16:0_20:4)	DAG(16:0_20:5)	DAG(16:0_22:4)	DAG(16:0_22:5)	DAG(16:0_22:6)
DAG(16:1_16:1)	DAG(16:1_17:0)	DAG(16:1_18:0)	DAG(16:1_18:1)	DAG(16:1_18:2)	DAG(16:1_18:3)
DAG(16:1_19:0)	DAG(16:1_20:0)	DAG(16:1_20:1)	DAG(16:1_20:2)	DAG(16:1_20:3)	DAG(16:1_20:4)
DAG(16:1_20:5)	DAG(16:1_22:4)	DAG(16:1_22:5)	DAG(16:1_22:6)	DAG(17:0_17:0)	DAG(17:0_18:0)
DAG(17:0_18:1)	DAG(17:0_18:2)	DAG(17:0_18:3)	DAG(17:0_19:0)	DAG(17:0_20:0)	DAG(17:0_20:1)
DAG(17:0_20:2)	DAG(17:0_20:3)	DAG(17:0_20:4)	DAG(17:0_20:5)	DAG(17:0_22:4)	DAG(17:0_22:5)
DAG(17:0_22:6)	DAG(18:0_18:0)	DAG(18:0_18:1)	DAG(18:0_18:2)	DAG(18:0_18:3)	DAG(18:0_19:0)
DAG(18:0_20:0)	DAG(18:0_20:1)	DAG(18:0_20:2)	DAG(18:0_20:3)	DAG(18:0_20:4)	DAG(18:0_20:5)
DAG(18:0_22:4)	DAG(18:0_22:5)	DAG(18:0_22:6)	DAG(18:1_18:1)	DAG(18:1_18:2)	DAG(18:1_18:3)
DAG(18:1_19:0)	DAG(18:1_20:0)	DAG(18:1_20:1)	DAG(18:1_20:2)	DAG(18:1_20:3)	DAG(18:1_20:4)
DAG(18:1_20:5)	DAG(18:1_22:4)	DAG(18:1_22:5)	DAG(18:1_22:6)	DAG(18:2_18:2)	DAG(18:2_18:3)
DAG(18:2_19:0)	DAG(18:2_20:0)	DAG(18:2_20:1)	DAG(18:2_20:2)	DAG(18:2_20:3)	DAG(18:2_20:4)
DAG(18:2_20:5)	DAG(18:2_22:4)	DAG(18:2_22:5)	DAG(18:2_22:6)	DAG(18:3_18:3)	DAG(18:3_19:0)
DAG(18:3_20:0)	DAG(18:3_20:1)	DAG(18:3_20:2)	DAG(18:3_20:3)	DAG(18:3_20:4)	DAG(18:3_20:5)
DAG(18:3_22:4)	DAG(18:3_22:5)	DAG(18:3_22:6)	DAG(19:0_19:0)	DAG(19:0_20:0)	DAG(19:0_20:1)
DAG(19:0_20:2)	DAG(19:0_20:3)	DAG(19:0_20:4)	DAG(19:0_20:5)	DAG(19:0_22:4)	DAG(19:0_22:5)
DAG(19:0_22:6)	DAG(20:0_20:0)	DAG(20:0_20:1)	DAG(20:0_20:2)	DAG(20:0_20:3)	DAG(20:0_20:4)
DAG(20:0_20:5)	DAG(20:0_22:4)	DAG(20:0_22:5)	DAG(20:0_22:6)	DAG(20:1_20:1)	DAG(20:1_20:2)
DAG(20:1_20:3)	DAG(20:1_20:4)	DAG(20:1_20:5)	DAG(20:1_22:4)	DAG(20:1_22:5)	DAG(20:1_22:6)
DAG(20:2_20:2)	DAG(20:2_20:3)	DAG(20:2_20:4)	DAG(20:2_20:5)	DAG(20:2_22:4)	DAG(20:2_22:5)
DAG(20:2_22:6)	DAG(20:3_20:3)	DAG(20:3_20:4)	DAG(20:3_20:5)	DAG(20:3_22:4)	DAG(20:3_22:5)
DAG(20:3_22:6)	DAG(20:4_20:4)	DAG(20:4_20:5)	DAG(20:4_22:4)	DAG(20:4_22:5)	DAG(20:4_22:6)
DAG(20:5_20:5)	DAG(20:5_22:4)	DAG(20:5_22:5)	DAG(20:5_22:6)	DAG(22:4_22:4)	DAG(22:4_22:5)
DAG(22:4_22:6)	DAG(22:5_22:5)	DAG(22:5_22:6)	DAG(22:6_22:6)		

List of metabolites

Triacylglycerols			
TAG(40:0_FA14:0)	TAG(40:0_FA16:0)	TAG(42:0_FA14:0)	TAG(42:0_FA16:0)
TAG(42:1_FA14:0)	TAG(42:1_FA16:0)	TAG(42:1_FA16:1)	TAG(42:1_FA18:1)
TAG(42:2_FA18:2)	TAG(44:0_FA14:0)	TAG(44:0_FA16:0)	TAG(44:0_FA18:0)
TAG(44:1_FA14:0)	TAG(44:1_FA16:0)	TAG(44:1_FA16:1)	TAG(44:1_FA18:1)
TAG(44:2_FA14:0)	TAG(44:2_FA16:0)	TAG(44:2_FA16:1)	TAG(44:2_FA18:1)
TAG(44:2_FA18:2)	TAG(44:3_FA18:2)	TAG(45:0_FA14:0)	TAG(45:0_FA16:0)
TAG(45:1_FA16:0)	TAG(45:1_FA18:1)	TAG(46:0_FA14:0)	TAG(46:0_FA16:0)
TAG(46:0_FA18:0)	TAG(46:1_FA14:0)	TAG(46:1_FA16:0)	TAG(46:1_FA16:1)
TAG(46:1_FA18:0)	TAG(46:1_FA18:1)	TAG(46:2_FA14:0)	TAG(46:2_FA16:0)
TAG(46:2_FA16:1)	TAG(46:2_FA18:1)	TAG(46:2_FA18:2)	TAG(46:3_FA14:0)
TAG(46:3_FA16:0)	TAG(46:3_FA16:1)	TAG(46:3_FA18:1)	TAG(46:3_FA18:2)
TAG(46:3_FA18:3)	TAG(46:4_FA18:2)	TAG(47:0_FA14:0)	TAG(47:0_FA16:0)
TAG(47:0_FA17:0)	TAG(47:1_FA14:0)	TAG(47:1_FA16:0)	TAG(47:1_FA16:1)
TAG(47:1_FA17:0)	TAG(47:1_FA18:1)	TAG(47:2_FA14:0)	TAG(47:2_FA16:1)
TAG(47:2_FA18:1)	TAG(47:2_FA18:2)	TAG(48:0_FA14:0)	TAG(48:0_FA16:0)
TAG(48:0_FA18:0)	TAG(48:1_FA14:0)	TAG(48:1_FA16:0)	TAG(48:1_FA16:1)
TAG(48:1_FA18:0)	TAG(48:1_FA18:1)	TAG(48:2_FA14:0)	TAG(48:2_FA16:0)
TAG(48:2_FA16:1)	TAG(48:2_FA18:0)	TAG(48:2_FA18:1)	TAG(48:2_FA18:2)
TAG(48:3_FA14:0)	TAG(48:3_FA16:0)	TAG(48:3_FA16:1)	TAG(48:3_FA18:1)
TAG(48:3_FA18:2)	TAG(48:3_FA18:3)	TAG(48:4_FA14:0)	TAG(48:4_FA16:0)
TAG(48:4_FA16:1)	TAG(48:4_FA18:1)	TAG(48:4_FA18:2)	TAG(48:4_FA18:3)
TAG(48:4_FA20:4)	TAG(48:5_FA18:2)	TAG(48:5_FA18:3)	TAG(49:0_FA16:0)
TAG(49:0_FA17:0)	TAG(49:0_FA18:0)	TAG(49:1_FA14:0)	TAG(49:1_FA16:0)
TAG(49:1_FA16:1)	TAG(49:1_FA17:0)	TAG(49:1_FA18:1)	TAG(49:2_FA14:0)
TAG(49:2_FA16:0)	TAG(49:2_FA16:1)	TAG(49:2_FA17:0)	TAG(49:2_FA18:1)
TAG(49:2_FA18:2)	TAG(49:3_FA16:0)	TAG(49:3_FA16:1)	TAG(49:3_FA18:2)
TAG(49:3_FA18:3)	TAG(50:0_FA14:0)	TAG(50:0_FA16:0)	TAG(50:0_FA18:0)
TAG(50:1_FA14:0)	TAG(50:1_FA16:0)	TAG(50:1_FA16:1)	TAG(50:1_FA18:0)
TAG(50:1_FA18:1)	TAG(50:1_FA20:1)	TAG(50:2_FA14:0)	TAG(50:2_FA16:0)
TAG(50:2_FA16:1)	TAG(50:2_FA18:0)	TAG(50:2_FA18:1)	TAG(50:2_FA18:2)
TAG(50:2_FA20:2)	TAG(50:3_FA14:0)	TAG(50:3_FA16:0)	TAG(50:3_FA16:1)
TAG(50:3_FA18:0)	TAG(50:3_FA18:1)	TAG(50:3_FA18:2)	TAG(50:3_FA18:3)
TAG(50:3_FA20:3)	TAG(50:4_FA14:0)	TAG(50:4_FA16:0)	TAG(50:4_FA16:1)
TAG(50:4_FA18:1)	TAG(50:4_FA18:2)	TAG(50:4_FA18:3)	TAG(50:4_FA20:3)
TAG(50:4_FA20:4)	TAG(50:5_FA14:0)	TAG(50:5_FA16:0)	TAG(50:5_FA16:1)
TAG(50:5_FA18:1)	TAG(50:5_FA18:2)	TAG(50:5_FA18:3)	TAG(50:5_FA20:4)
TAG(50:5_FA20:5)	TAG(50:6_FA20:4)	TAG(51:0_FA16:0)	TAG(51:0_FA17:0)
TAG(51:0_FA18:0)	TAG(51:1_FA16:0)	TAG(51:1_FA17:0)	TAG(51:1_FA18:0)
TAG(51:1_FA18:1)	TAG(51:2_FA16:0)	TAG(51:2_FA16:1)	TAG(51:2_FA17:0)

List of metabolites

Triacylglycerols			
TAG(51:2_FA18:1)	TAG(51:2_FA18:2)	TAG(51:3_FA16:1)	TAG(51:3_FA17:0)
TAG(51:3_FA18:2)	TAG(51:3_FA18:3)	TAG(51:4_FA16:1)	TAG(51:4_FA18:2)
TAG(51:4_FA18:3)	TAG(51:4_FA20:4)	TAG(51:5_FA18:2)	TAG(51:5_FA18:3)
TAG(52:0_FA16:0)	TAG(52:0_FA18:0)	TAG(52:0_FA20:0)	TAG(52:1_FA16:0)
TAG(52:1_FA16:1)	TAG(52:1_FA18:0)	TAG(52:1_FA18:1)	TAG(52:1_FA20:0)
TAG(52:1_FA20:1)	TAG(52:2_FA14:0)	TAG(52:2_FA16:0)	TAG(52:2_FA16:1)
TAG(52:2_FA18:0)	TAG(52:2_FA18:1)	TAG(52:2_FA18:2)	TAG(52:2_FA20:0)
TAG(52:2_FA20:1)	TAG(52:2_FA20:2)	TAG(52:3_FA14:0)	TAG(52:3_FA16:0)
TAG(52:3_FA16:1)	TAG(52:3_FA18:0)	TAG(52:3_FA18:1)	TAG(52:3_FA18:2)
TAG(52:3_FA18:3)	TAG(52:3_FA20:0)	TAG(52:3_FA20:1)	TAG(52:3_FA20:2)
TAG(52:3_FA20:3)	TAG(52:4_FA14:0)	TAG(52:4_FA16:0)	TAG(52:4_FA16:1)
TAG(52:4_FA18:0)	TAG(52:4_FA18:1)	TAG(52:4_FA18:2)	TAG(52:4_FA18:3)
TAG(52:4_FA20:0)	TAG(52:4_FA20:2)	TAG(52:4_FA20:3)	TAG(52:4_FA20:4)
TAG(52:4_FA22:4)	TAG(52:5_FA14:0)	TAG(52:5_FA16:0)	TAG(52:5_FA16:1)
TAG(52:5_FA18:1)	TAG(52:5_FA18:2)	TAG(52:5_FA18:3)	TAG(52:5_FA20:3)
TAG(52:5_FA20:4)	TAG(52:5_FA20:5)	TAG(52:5_FA22:5)	TAG(52:6_FA14:0)
TAG(52:6_FA16:0)	TAG(52:6_FA16:1)	TAG(52:6_FA18:1)	TAG(52:6_FA18:2)
TAG(52:6_FA18:3)	TAG(52:6_FA20:4)	TAG(52:6_FA20:5)	TAG(52:6_FA22:6)
TAG(52:7_FA16:0)	TAG(52:7_FA18:1)	TAG(52:7_FA20:5)	TAG(52:7_FA22:6)
TAG(52:8_FA16:1)	TAG(52:8_FA18:2)	TAG(53:0_FA16:0)	TAG(53:1_FA16:0)
TAG(53:1_FA17:0)	TAG(53:1_FA18:0)	TAG(53:1_FA18:1)	TAG(53:2_FA16:0)
TAG(53:2_FA17:0)	TAG(53:2_FA18:1)	TAG(53:2_FA18:2)	TAG(53:3_FA16:0)
TAG(53:3_FA17:0)	TAG(53:3_FA18:2)	TAG(53:4_FA16:0)	TAG(53:4_FA17:0)
TAG(53:4_FA18:2)	TAG(53:4_FA18:3)	TAG(53:4_FA20:4)	TAG(53:5_FA20:4)
TAG(53:6_FA20:4)	TAG(54:0_FA16:0)	TAG(54:0_FA18:0)	TAG(54:1_FA16:0)
TAG(54:1_FA18:0)	TAG(54:1_FA18:1)	TAG(54:1_FA20:0)	TAG(54:1_FA20:1)
TAG(54:2_FA16:0)	TAG(54:2_FA18:0)	TAG(54:2_FA18:1)	TAG(54:2_FA18:2)
TAG(54:2_FA20:0)	TAG(54:2_FA20:1)	TAG(54:2_FA20:2)	TAG(54:3_FA16:0)
TAG(54:3_FA16:1)	TAG(54:3_FA18:0)	TAG(54:3_FA18:1)	TAG(54:3_FA18:2)
TAG(54:3_FA18:3)	TAG(54:3_FA20:1)	TAG(54:3_FA20:2)	TAG(54:3_FA20:3)
TAG(54:4_FA16:0)	TAG(54:4_FA16:1)	TAG(54:4_FA18:0)	TAG(54:4_FA18:1)
TAG(54:4_FA18:2)	TAG(54:4_FA18:3)	TAG(54:4_FA20:1)	TAG(54:4_FA20:2)
TAG(54:4_FA20:3)	TAG(54:4_FA20:4)	TAG(54:4_FA22:4)	TAG(54:5_FA16:0)
TAG(54:5_FA16:1)	TAG(54:5_FA18:0)	TAG(54:5_FA18:1)	TAG(54:5_FA18:2)
TAG(54:5_FA18:3)	TAG(54:5_FA20:2)	TAG(54:5_FA20:3)	TAG(54:5_FA20:4)
TAG(54:5_FA20:5)	TAG(54:5_FA22:4)	TAG(54:5_FA22:5)	TAG(54:6_FA16:0)
TAG(54:6_FA16:1)	TAG(54:6_FA18:1)	TAG(54:6_FA18:2)	TAG(54:6_FA18:3)
TAG(54:6_FA20:3)	TAG(54:6_FA20:4)	TAG(54:6_FA20:5)	TAG(54:6_FA22:5)
TAG(54:6_FA22:6)	TAG(54:7_FA16:1)	TAG(54:7_FA18:1)	TAG(54:7_FA18:2)

List of metabolites

Triacylglycerols			
TAG(54:7_FA18:3)	TAG(54:7_FA20:4)	TAG(54:7_FA20:5)	TAG(54:7_FA22:5)
TAG(54:7_FA22:6)	TAG(54:8_FA18:2)	TAG(54:8_FA18:3)	TAG(54:8_FA20:4)
TAG(54:8_FA20:5)	TAG(54:8_FA22:6)	TAG(55:1_FA16:0)	TAG(55:1_FA18:1)
TAG(55:2_FA18:1)	TAG(55:2_FA18:2)	TAG(55:3_FA18:1)	TAG(55:3_FA18:2)
TAG(55:4_FA18:1)	TAG(55:4_FA18:2)	TAG(55:5_FA18:1)	TAG(55:5_FA18:2)
TAG(55:5_FA20:4)	TAG(55:7_FA22:6)	TAG(56:1_FA16:0)	TAG(56:1_FA18:1)
TAG(56:10_FA18:2)	TAG(56:2_FA16:0)	TAG(56:2_FA18:0)	TAG(56:2_FA20:0)
TAG(56:2_FA20:1)	TAG(56:3_FA16:0)	TAG(56:3_FA18:0)	TAG(56:3_FA18:1)
TAG(56:3_FA18:2)	TAG(56:3_FA20:0)	TAG(56:3_FA20:1)	TAG(56:3_FA20:2)
TAG(56:4_FA16:0)	TAG(56:4_FA18:0)	TAG(56:4_FA18:1)	TAG(56:4_FA18:2)
TAG(56:4_FA20:1)	TAG(56:4_FA20:2)	TAG(56:4_FA20:3)	TAG(56:4_FA20:4)
TAG(56:4_FA22:4)	TAG(56:5_FA16:0)	TAG(56:5_FA18:0)	TAG(56:5_FA18:1)
TAG(56:5_FA18:2)	TAG(56:5_FA20:1)	TAG(56:5_FA20:2)	TAG(56:5_FA20:3)
TAG(56:5_FA20:4)	TAG(56:5_FA22:4)	TAG(56:5_FA22:5)	TAG(56:6_FA16:0)
TAG(56:6_FA18:0)	TAG(56:6_FA18:1)	TAG(56:6_FA18:2)	TAG(56:6_FA18:3)
TAG(56:6_FA20:2)	TAG(56:6_FA20:3)	TAG(56:6_FA20:4)	TAG(56:6_FA20:5)
TAG(56:6_FA22:4)	TAG(56:6_FA22:5)	TAG(56:6_FA22:6)	TAG(56:7_FA16:0)
TAG(56:7_FA16:1)	TAG(56:7_FA18:0)	TAG(56:7_FA18:1)	TAG(56:7_FA18:2)
TAG(56:7_FA18:3)	TAG(56:7_FA20:3)	TAG(56:7_FA20:4)	TAG(56:7_FA20:5)
TAG(56:7_FA22:4)	TAG(56:7_FA22:5)	TAG(56:7_FA22:6)	TAG(56:8_FA16:0)
TAG(56:8_FA16:1)	TAG(56:8_FA18:1)	TAG(56:8_FA18:2)	TAG(56:8_FA18:3)
TAG(56:8_FA20:4)	TAG(56:8_FA20:5)	TAG(56:8_FA22:5)	TAG(56:8_FA22:6)
TAG(56:9_FA18:3)	TAG(56:9_FA20:4)	TAG(56:9_FA20:5)	TAG(56:9_FA22:6)
TAG(57:10_FA22:6)	TAG(57:2_FA18:1)	TAG(57:3_FA18:2)	TAG(58:10_FA18:2)
TAG(58:10_FA20:4)	TAG(58:10_FA20:5)	TAG(58:10_FA22:5)	TAG(58:10_FA22:6)
TAG(58:2_FA18:1)	TAG(58:3_FA18:1)	TAG(58:5_FA18:1)	TAG(58:6_FA16:0)
TAG(58:6_FA18:0)	TAG(58:6_FA18:1)	TAG(58:6_FA20:4)	TAG(58:6_FA22:4)
TAG(58:6_FA22:5)	TAG(58:7_FA16:0)	TAG(58:7_FA18:0)	TAG(58:7_FA18:1)
TAG(58:7_FA18:2)	TAG(58:7_FA20:4)	TAG(58:7_FA22:4)	TAG(58:7_FA22:5)
TAG(58:7_FA22:6)	TAG(58:8_FA18:1)	TAG(58:8_FA18:2)	TAG(58:8_FA20:3)
TAG(58:8_FA20:4)	TAG(58:8_FA22:5)	TAG(58:8_FA22:6)	TAG(58:9_FA18:1)
TAG(58:9_FA18:2)	TAG(58:9_FA20:4)	TAG(58:9_FA22:5)	TAG(58:9_FA22:6)
TAG(60:10_FA22:5)	TAG(60:10_FA22:6)	TAG(60:11_FA22:5)	TAG(60:11_FA22:6)
TAG(60:12_FA22:6)			