

S3 Table. List of metabolites.

Cations	Sub class ^a	Anions	Sub class ^a	Abbreviations
Glycine	AA	Pyruvate	AKA	AA Amino acids, peptides, and analogs
Trimethylamine- <i>N</i> -oxide	AO	Lactate	AHA	AHA alpha-Hydroxy acids and derivatives
beta-Alanine	AA	2-Oxobutyrate	SKA	AKA alpha-Keto acids and derivatives
Alanine	AA	Malonate	DCA	ALK Alkaloids and derivatives
Sarcosine	AA	2-Hydroxybutyrate	AHA	ALC Alcohols and polyols
3-Aminoisobutyrate	AA	3-Hydroxybutyrate	BHA	AM Amines
2-Aminobutyrate	AA	Fumarate	DCA	AO Aminoxides
<i>N,N</i> -Dimethylglycine	AA	2-Oxoisopentanoate	SKA	ARX Arylsulfates
Choline	QA	Hexanoate	FAE	BA Benzoic acids and derivatives
Serine	AA	Succinate	DCA	BHA beta-Hydroxy acids and derivatives
Creatinine	AA	Isethionate	OSA	CHO Carbohydrates and carbohydrate conjugates
Proline	AA	5-Oxoproline	AA	CAB Carbonyl compounds
Guanidinoacetate	AA	Citraconate	FA	DCA Dicarboxylic acids and derivatives
Valine	AA	Ketoleicine	SKA	FA Fatty acids and conjugates
Betaine	AA	4-Acetylbutyrate	FA	FAE Fatty acid esters
Threonine	AA	Heptanoate	FA	GKA gamma-Keto acids and derivatives
Taurine	OSA	Glutarate	DCA	GP Glycerophosphates
Pipecolate	AA	Malate	BHA	GPC Glycerophosphocholines
Hydroxyproline	AA	Threonate	CHO	ICA Indolyl carboxylic acids and derivatives
Creatine	AA	Ethanolamine phosphate	PHE	LP Lipids and lipid-like molecules
Isoleucine	AA	Octanoate	FA	MP Methoxyphenols
Leucine	AA	2-Oxoglutarate	GKA	OSA Organosulfonic acids and derivatives
Asparagine	AA	Pelargonate	FA	PCA Pyridinecarboxylic acids and derivatives
Ornithine	AA	Terephthalate	BA	PHE Phosphate esters
Aspartate	AA	Urate	PR	PYN Pyrimidine nucleosides
Hypoxanthine	PR	Glycerophosphate	GP	PR Purines and purine derivatives
1-Methylnicotinamide	PCA	Decanoate	FA	QA Quaternary ammonium salts
Trigonelline	AL	trans-Aconitate	TCA	SKA Short-chain keto acids and derivatives
Proline betaine	AA	cis-Aconitate	TCA	TCA Tricarboxylic acids and derivatives
gamma-Butyrobetaine	FA	<i>N</i> -Acetylaspartate	AA	
Glutamine	AA	Hippurate	BA	
Lysine	AA	Homovanillate	MP	
Glutamic acid	AA	Azelate	FA	
Methionine	AA	Isocitrate	TCA	
Triethanolamine	AM	Citrate	TCA	
Histidine	AA	Quinate	ALC	
alpha-Amino adipate	AA	Glucuronate	CHO	
Carnitine	QA	Cysteine- <i>S</i> -sulfate	AA	
Phenylalanine	AA	Galactarate	CHO	
3-Methylhistidine	AA	3-Indoxyl sulfate	ARX	
Arginine	AA			
Guanidinosuccinate	AA			
Indole-3-acetate	ICA			
Citrulline	AA			
Tyrosine	AA			
Symmetric Dimethylarginine	AA			
Asymmetric Dimethylarginine	AA			
o-Acetylcarnitine	LP			
Tryptophan	AA			
Kynurenine	CAB			
Cysteineglutathione disulfide	AA			
Cystine	AA			
Uridine	PYN			
Glycerophosphorylcholine	GPC			

^a Ref.) The Human Metabolome Database (<http://www.hmdb.ca>)