

Supplementary Table 1. Group classification produced by hierarchical cluster analysis of data for plasma P

Group	Name	Retention index	Class	Subclass
Group 1	Glyoxylic acid-meto-TMS	986	Carboxylic acids and derivatives	Carboxylic acids
	Pyruvic acid-meto-TMS	1046	Keto acids and derivatives	Alpha-keto acids and derivatives
	Lactic acid-2TMS	1051	Hydroxy acids and derivatives	Alpha hydroxy acids and derivatives
	Alanine-2TMS	1095	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	Glycine-2TMS	1116	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	Glycerol-3TMS	1256	Organooxygen compounds	Carbohydrates and carbohydrate conjugates
	Isoleucine-2TMS	1281	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	Glyceric acid-3TMS	1312	Organooxygen compounds	Carbohydrates and carbohydrate conjugates
	Serine-3TMS	1343	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	Threonine-3TMS	1367	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	Creatinine-3TMS	1548	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	5-Dehydroquinic acid-meto-4TMS	1858	Hydroxy acids and derivatives	Alpha hydroxy acids and derivatives
	Glucosamine-5TMS(1)	1884	Organooxygen compounds	Carbohydrates and carbohydrate conjugates
Group 2	Paraxanthine-TMS	1993	Imidazopyrimidines	Purines and purine derivatives
	3-Aminopropanoic acid-2TMS	1185	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	2-Ketoisocaproic acid-meto-TMS(2)	1206	Keto acids and derivatives	Short-chain keto acids and derivatives
	Benzoic acid-TMS	1255	Benzene and substituted derivatives	Benzoic acids and derivatives
	2-Aminoethanol-3TMS	1255	Organonitrogen compounds	Amines
	Leucine-2TMS	1260	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	Proline-2TMS	1291	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	Decanoic acid-TMS	1453	Fatty Acyls	Fatty acids and conjugates
	Taurine-3TMS	1663	Organic sulfonic acids and derivatives	Organosulfonic acids and derivatives
	Glucose-meto-5TMS(2)	1882	Organooxygen compounds	Carbohydrates and carbohydrate conjugates
Group 3	2-Hydroxyisobutyric acid-2TMS	1052	Hydroxy acids and derivatives	Alpha hydroxy acids and derivatives
	Glycolic acid-2TMS	1069	Hydroxy acids and derivatives	Alpha hydroxy acids and derivatives
	2-Hydroxybutyric acid-2TMS	1117	Hydroxy acids and derivatives	Alpha hydroxy acids and derivatives
	3-Hydroxypropionic acid-2TMS	1135	Hydroxy acids and derivatives	Beta hydroxy acids and derivatives
	2-Hydroxyisovaleric acid-2TMS	1151	Fatty Acyls	Fatty acids and conjugates
	3-Hydroxybutyric acid-2TMS	1152	Hydroxy acids and derivatives	Beta hydroxy acids and derivatives
	Glycine-3TMS	1295	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	3-Aminopropanoic acid-3TMS	1416	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	Isocitric acid-4TMS	1793	Carboxylic acids and derivatives	Tricarboxylic acids and derivatives
	Ornithine-4TMS	1796	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	N-Acetylglutamine-3TMS	1898	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	Tryptophan-2TMS	2211	Indoles and derivatives	Indolyl carboxylic acids and derivatives
Group 4	Tryptophan-3TMS	2214	Indoles and derivatives	Indolyl carboxylic acids and derivatives
	Sarcosine-2TMS	1131	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	Urea-2TMS	1239	Organic carbonic acids and derivatives	Ureas
Group 5	2-Keto-isovaleric acid-meto-TMS	1102	Keto acids and derivatives	Short-chain keto acids and derivatives
	Oxalic acid-2TMS	1126	Carboxylic acids and derivatives	Dicarboxylic acids and derivatives
	3-Methyl-2-ketovaleric acid-meto-TMS(1)	1172	Keto acids and derivatives	Short-chain keto acids and derivatives
	3-Methyl-2-ketovaleric acid-meto-TMS(2)	1192	Keto acids and derivatives	Short-chain keto acids and derivatives
	Valine-2TMS	1204	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	Acetylglycine-TMS	1288	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	Fumaric acid-2TMS	1344	Carboxylic acids and derivatives	Dicarboxylic acids and derivatives
	Glutaric acid-2TMS	1397	Carboxylic acids and derivatives	Dicarboxylic acids and derivatives
	Threitol-4TMS	1471	Organooxygen compounds	Carbohydrates and carbohydrate conjugates
	Aspartic acid-3TMS	1503	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	3-Aminoglutaric acid-2TMS	1504	Non data	Non data
	4-Hydroxyproline-3TMS	1511	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	Methionine-2TMS	1513	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	5-Oxoproline-2TMS	1522	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	2-Ketoglutaric acid-meto-2TMS	1566	Keto acids and derivatives	Gamma-keto acids and derivatives
	Glutamic acid-3TMS	1603	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	Phenylalanine-2TMS	1623	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	Xylulose-meto-4TMS	1642	Organooxygen compounds	Carbohydrates and carbohydrate conjugates
	Glucose-meto-5TMS(1)	1861	Organooxygen compounds	Carbohydrates and carbohydrate conjugates
	4-Hydroxyphenyllactic acid-3TMS	1884	Phenylpropanoic acids	Not Available
	Glucuronic acid-meto-5TMS(1)	1902	Organooxygen compounds	Carbohydrates and carbohydrate conjugates
	Tyramine-3TMS	1909	Benzene and substituted derivatives	Phenethylamines
	Tyrosine-3TMS	1929	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	Galacturonic acid-meto-5TMS(2)	1931	Organooxygen compounds	Carbohydrates and carbohydrate conjugates
	N-Acetyl-Ornithine-4TMS	1952	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	Indol-3-acetic acid-2TMS	1974	Indoles and derivatives	Indolyl carboxylic acids and derivatives
	Inositol-6TMS	2058	Organooxygen compounds	Alcohols and polyols
	3-Indolepropionic acid-2TMS	2095	Indoles and derivatives	Indolyl carboxylic acids and derivatives

Group 6	2-Aminoisobutyric acid-2TMS	1135	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	Nonanoic acid-TMS	1357	Fatty Acyls	Fatty acids and conjugates
	Malic acid-3TMS	1472	Hydroxy acids and derivatives	Beta hydroxy acids and derivatives
	Glutamine-3TMS	1762	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	Mannose-meto-5TMS(1)	1849	Organooxygen compounds	Carbohydrates and carbohydrate conjugates
	Lysine-4TMS	1900	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	Palmitoleic acid-TMS	2026	Fatty Acyls	Fatty acids and conjugates
	Linoleic acid-TMS	2210	Fatty Acyls	Lineolic acids and derivatives
Group 7	Elaidic acid-TMS	2221	Fatty Acyls	Fatty acids and conjugates
	2-Aminobutyric acid-2TMS	1164	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	Isoleucine-TMS	1178	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	Serine-2TMS	1250	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	Octanoic acid-TMS	1260	Fatty Acyls	Fatty acids and conjugates
	Phosphoric acid-3TMS	1260	Non-metal oxoanionic compounds	Non-metal phosphates
	Succinic acid-2TMS	1307	Carboxylic acids and derivatives	Dicarboxylic acids and derivatives
	Cysteine-3TMS	1543	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	2-Hydroxyglutaric acid-3TMS	1556	Hydroxy acids and derivatives	Short-chain hydroxy acids and derivatives
	Lauric acid-TMS	1647	Fatty Acyls	Fatty acids and conjugates
	Ribose-meto-4TMS	1648	Organooxygen compounds	Carbohydrates and carbohydrate conjugates
	2-Deoxy-glucose-4TMS(1)	1698	Fatty Acyls	Fatty alcohols
	Sorbose-meto-5TMS(1)	1833	Organooxygen compounds	Carbohydrates and carbohydrate conjugates
Group 8	Oleic acid-TMS	2214	Fatty Acyls	Fatty acids and conjugates
	Myristic acid-TMS	1844	Fatty Acyls	Fatty acids and conjugates
Group 9	3-Hydroxyisovaleric acid-2TMS	1200	Fatty Acyls	Fatty acids and conjugates
	Ribulose-meto-4TMS	1646	Organooxygen compounds	Carbohydrates and carbohydrate conjugates
Group 10	meso-Erythritol-4TMS	1480	Organooxygen compounds	Carbohydrates and carbohydrate conjugates
	2-Isopropylmalic acid-3TMS	1560	Fatty Acyls	Fatty acids and conjugates
	Arabinose-meto-4TMS	1632	Organooxygen compounds	Carbohydrates and carbohydrate conjugates
	Arabitol-5TMS	1685	Organooxygen compounds	Carbohydrates and carbohydrate conjugates
	Citric acid-4TMS	1794	Carboxylic acids and derivatives	Tricarboxylic acids and derivatives
	Arginine-3TMS	1808	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	Psicose-meto-5TMS(1)	1819	Organooxygen compounds	Carbohydrates and carbohydrate conjugates
	1,5-Anhydro-glucitol-4TMS	1831	Organooxygen compounds	Carbohydrates and carbohydrate conjugates
	Fructose-meto-5TMS(2)	1844	Organooxygen compounds	Carbohydrates and carbohydrate conjugates
	Histidine-3TMS	1912	Carboxylic acids and derivatives	Amino acids, peptides, and analogues
	Glucuronic acid-meto-5TMS(2)	1920	Organooxygen compounds	Carbohydrates and carbohydrate conjugates
	1-Hexadecanol-TMS	1951	Fatty Acyls	Fatty alcohols
	Uric acid-4TMS	2082	Imidazopyrimidines	Purines and purine derivatives
	Margaric acid-TMS	2138	Fatty Acyls	Fatty acids and conjugates
	Sucrose-8TMS	2579	Organooxygen compounds	Carbohydrates and carbohydrate conjugates
Group 11	Palmitic acid-TMS	2040	Fatty Acyls	Fatty acids and conjugates
	Stearic acid-TMS	2238	Fatty Acyls	Fatty acids and conjugates
Group 12	Sorbitol-6TMS	1898	Organooxygen compounds	Carbohydrates and carbohydrate conjugates

In the group classification performed in Experiment A, the metabolites classified into each group are listed. For each metabolite, the retention index, class as chemical taxonomy, and subclass as chemical taxonomy are also listed. Class and subclass as chemical taxonomy are based on The Human Metabolome Database (<https://www.hmdb.ca/>).