

Supplement:**Table 1****List of analyzed metabolites**

Acylcarnitines (41)		
C0	Carnitine	quantitative
C2	Acetylcarnitine	quantitative
C3	Propionylcarnitine	quantitative
C3:1	Propenoylcarnitine	semi-quantitative
C3-OH	Hydroxypropionylcarnitine	semi-quantitative
C4	Butyrylcarnitine / Isobutyrylcarnitine	quantitative
C4:1	Butenoylcarnitine	semi-quantitative
C4-OH (C3-DC)	Hydroxybutyrylcarnitine (Malonylcarnitine)	semi-quantitative
C5	Valerylcarnitine / Isovalerylcarnitine / Methylbutyrylcarnitine	quantitative
C5:1	Tiglylcarnitine / Methylcrotonylcarnitine	semi-quantitative
C5:1-DC	Glutaconylcarnitine / Mesoconylcarnitine	semi-quantitative
C5-DC (C6-OH)	Glutaryl carnitine (Hydroxyhexanoylcarnitine)	semi-quantitative
C5-M-DC	Methylglutaryl carnitine	semi-quantitative
C5-OH (C3-DC-M)	Hydroxyvaleryl- / -isovaleryl- / -methylbutyrylcarnitine (Methylmalonylcarnitine)	semi-quantitative
C6 (C4:1-DC)	Hexanoylcarnitine (Fumaryl carnitine)	semi-quantitative
C6:1	Hexenoylcarnitine	semi-quantitative
C7-DC	Pimelylcarnitine	semi-quantitative
C8	Octanoylcarnitine	quantitative
C8:1	Octenoylcarnitine	semi-quantitative
C9	Nonanoylcarnitine	semi-quantitative
C10	Decanoylcarnitine	quantitative
C10:1	Decenoylcarnitine	semi-quantitative
C10:2	Decadienylcarnitine	semi-quantitative
C12	Dodecanoylcarnitine	quantitative
C12:1	Dodecenoylcarnitine	semi-quantitative
C12-DC	Dodecanedioylcarnitine	semi-quantitative
C14	Tetradecanoylcarnitine	quantitative
C14:1	Tetradecenoylcarnitine	semi-quantitative
C14:1-OH	Hydroxytetradecenoylcarnitine	semi-quantitative
C14:2	Tetradecadienylcarnitine	semi-quantitative
C14:2-OH	Hydroxytetradecadienylcarnitine	semi-quantitative
C16	Hexadecanoylcarnitine	quantitative
C16:1	Hexadecenoylcarnitine	semi-quantitative
C16:1-OH	Hydroxyhexadecenoylcarnitine	semi-quantitative
C16:2	Hexadecadienylcarnitine	semi-quantitative
C16:2-OH	Hydroxyhexadecadienylcarnitine	semi-quantitative
C16-OH	Hydroxyhexadecanoylcarnitine	semi-quantitative
C18	Octadecanoylcarnitine	quantitative
C18:1	Octadecenoylcarnitine	semi-quantitative
C18:1-OH	Hydroxyoctadecenoylcarnitine	semi-quantitative
C18:2	Octadecadienylcarnitine	semi-quantitative

Amino acids (21)		Bile acids (17)	
Alanine	quantitative	Cholic acid	quantitative
Arginine	quantitative	Chenodeoxycholic acid	quantitative
Asparagine	quantitative	Deoxycholic acid	quantitative
Aspartic acid	quantitative	Glycocholic acid	quantitative
Citrulline	quantitative	Glycochenodeoxycholic acid	quantitative
Glutamine	quantitative	Glycodeoxycholic acid	quantitative
Glutamic acid	quantitative	Glycolithocholic acid	quantitative
Glycine	quantitative	Glycolithocholic acid sulfate	quantitative
Histidine	quantitative	Glycoursodeoxycholic acid	quantitative
Isoleucine	quantitative	Lithocholic acid	quantitative
Leucine	quantitative	Taurocholic acid	quantitative
Lysine	semi-quantitative	Taurochenodeoxycholic acid	quantitative
Methionine	quantitative	Taurodeoxycholic acid	quantitative
Ornithine	quantitative	Taurolithocholic acid	quantitative
Phenylalanine	quantitative	Taurolithocholic acid sulfate	quantitative
Proline	quantitative	Tauroursodeoxycholic acid	quantitative
Serine	quantitative	Ursodeoxycholic acid	quantitative
Threonine	quantitative		
Tryptophan	quantitative	Eicosanoids and other Oxidation Products of Polyunsaturated Fatty acids (PUFA's)* (17)	
Tyrosine	quantitative	Leukotriene B4	quantitative
Valine	quantitative	Thromboxane B2	quantitative
		Leukotriene D4	quantitative
Biogenic Amines and Polyamines (14)		Prostaglandin E2	quantitative
Asymmetric dimethylarginine	quantitative	8-iso-Prostaglandin F2 α	quantitative
Symmetric dimethylarginine	quantitative	Prostaglandin F2 α	quantitative
Total dimethylarginine	quantitative	6-keto-Prostaglandin F1 α	quantitative
Histamine	quantitative	Prostaglandin D2	quantitative
Methionine-sulfoxide	quantitative	9S-HODE	quantitative
Kynurenine	quantitative	13S-HODE	quantitative
Hydroxykynurenine	quantitative	14(15)-EpETE	quantitative
Putrescine	quantitative	12S-HETE	quantitative
Spermidine	semi-quantitative	15S-HETE	quantitative
Spermine	semi-quantitative	15S-HpETE	quantitative
Serotonin	semi-quantitative	5S-HpETE	quantitative
Phenylethylamine	quantitative	Arachidonic acid	quantitative
Nitrotyrosine	quantitative	Docosahexaenoic acid	quantitative
Creatinine	quantitative		

Energy Metabolism (17)	
3-Phosphoglycerate	semi-quantitative
α -Ketoglutaric acid	quantitative
Adenosine-5'-monophosphate	semi-quantitative
Arginine	quantitative
Aspartate	quantitative
3'-5'-cyclic Adenosine monophosphate	semi-quantitative
Dihydroxyacetonephosphate + 3-Phosphoglyceraldehyde	semi-quantitative

Fumarate	quantitative
Glutamate	quantitative
Hexose (e.g. Glucose)	quantitative
Hexosephosphate (e.g. Glucose-1-phosphate + Glucose-6-phosphate + Fructose-6-phosphate)	quantitative
Lactate	quantitative
Pentosephosphate (e.g. Ribose-5-phosphate + Ribulose-5-phosphate)	semi-quantitative
Phosphoenolpyruvate	semi-quantitative
Pyruvate + Oxaloacetate	quantitative
Succinate	quantitative
Tetrosephosphate (e.g. Erythrose-4-phosphate)	semi-quantitative

Glycerophospholipids* (92)			
PC aa C24:0	semi-quantitative	PC ae C34:3	semi-quantitative
PC aa C26:0	semi-quantitative	PC ae C36:0	semi-quantitative
PC aa C28:1	semi-quantitative	PC ae C36:1	semi-quantitative
PC aa C30:0	semi-quantitative	PC ae C36:2	semi-quantitative
PC aa C30:2	semi-quantitative	PC ae C36:3	semi-quantitative
PC aa C32:0	semi-quantitative	PC ae C36:4	semi-quantitative
PC aa C32:1	semi-quantitative	PC ae C36:5	semi-quantitative
PC aa C32:2	semi-quantitative	PC ae C38:0	semi-quantitative
PC aa C32:3	semi-quantitative	PC ae C38:1	semi-quantitative
PC aa C34:1	semi-quantitative	PC ae C38:2	semi-quantitative
PC aa C34:2	semi-quantitative	PC ae C38:3	semi-quantitative
PC aa C34:3	semi-quantitative	PC ae C38:4	semi-quantitative
PC aa C34:4	semi-quantitative	PC ae C38:5	semi-quantitative
PC aa C36:0	semi-quantitative	PC ae C38:6	semi-quantitative
PC aa C36:1	semi-quantitative	PC ae C40:0	semi-quantitative
PC aa C36:2	semi-quantitative	PC ae C40:1	semi-quantitative
PC aa C36:3	semi-quantitative	PC ae C40:2	semi-quantitative
PC aa C36:4	semi-quantitative	PC ae C40:3	semi-quantitative
PC aa C36:5	semi-quantitative	PC ae C40:4	semi-quantitative
PC aa C36:6	semi-quantitative	PC ae C40:5	semi-quantitative
PC aa C38:0	semi-quantitative	PC ae C40:6	semi-quantitative
PC aa C38:1	semi-quantitative	PC ae C42:0	semi-quantitative
PC aa C38:3	semi-quantitative	PC ae C42:1	semi-quantitative
PC aa C38:4	semi-quantitative	PC ae C42:2	semi-quantitative
PC aa C38:5	semi-quantitative	PC ae C42:3	semi-quantitative
PC aa C38:6	semi-quantitative	PC ae C42:4	semi-quantitative
PC aa C40:1	semi-quantitative	PC ae C42:5	semi-quantitative
PC aa C40:2	semi-quantitative	PC ae C44:3	semi-quantitative
PC aa C40:3	semi-quantitative	PC ae C44:4	semi-quantitative
PC aa C40:4	semi-quantitative	PC ae C44:5	semi-quantitative
PC aa C40:5	semi-quantitative	PC ae C44:6	semi-quantitative
PC aa C40:6	semi-quantitative	lysoPC a C6:0	semi-quantitative
PC aa C42:0	semi-quantitative	lysoPC a C14:0	semi-quantitative
PC aa C42:1	semi-quantitative	lysoPC a C16:0	semi-quantitative
PC aa C42:2	semi-quantitative	lysoPC a C16:1	semi-quantitative

PC aa C42:4	semi-quantitative	lysoPC a C17:0	semi-quantitative
PC aa C42:5	semi-quantitative	lysoPC a C18:0	semi-quantitative
PC aa C42:6	semi-quantitative	lysoPC a C18:1	semi-quantitative
PC ae C30:0	semi-quantitative	lysoPC a C18:2	semi-quantitative
PC ae C30:1	semi-quantitative	lysoPC a C20:3	semi-quantitative
PC ae C30:2	semi-quantitative	lysoPC a C20:4	semi-quantitative
PC ae C32:1	semi-quantitative	lysoPC a C24:0	semi-quantitative
PC ae C32:2	semi-quantitative	lysoPC a C26:0	semi-quantitative
PC ae C34:0	semi-quantitative	lysoPC a C26:1	semi-quantitative
PC ae C34:1	semi-quantitative	lysoPC a C28:0	semi-quantitative
PC ae C34:2	semi-quantitative	lysoPC a C28:1	semi-quantitative

Oxysterols (16)	
22-R-Hydroxycholesterol	quantitative
24-S-Hydroxycholesterol	quantitative
25-Hydroxycholesterol	quantitative
27-Hydroxycholesterol	quantitative
22S-Hydroxycholesterol	quantitative
24,25-Epoxycholesterol	quantitative
7 α -Hydroxycholesterol	quantitative
7-Ketcholesterol	quantitative
5 β ,6 β -Epoxycholesterol	quantitative
5 α ,6 α -Epoxycholesterol	quantitative
4 β -Hydroxycholesterol	quantitative
Desmosterol	quantitative
7-Dehydrocholesterol	quantitative
Cholestenone	quantitative
Lanosterol	semi-quantitative
24-Dihydrolanosterol	quantitative

Sphingolipids (Sphingomyelins)* (15)	
SM (OH) C14:1	semi-quantitative
SM C16:0	semi-quantitative
SM C16:1	semi-quantitative
SM (OH) C16:1	semi-quantitative
SM C18:0	semi-quantitative
SM C18:1	semi-quantitative
SM C20:2	semi-quantitative
SM C22:3	semi-quantitative
SM (OH) C22:1	semi-quantitative
SM (OH) C22:2	semi-quantitative
SM C24:0	semi-quantitative
SM C24:1	semi-quantitative
SM (OH) C24:1	semi-quantitative
SM C26:0	semi-quantitative
SM C26:1	semi-quantitative

*) validated analytical method (FDA guidance for industry)

Analysed ratio`s

Definition	Numerator	Denominator
Orn/Cit	Ornithine	Citrulline
Orn/Arg	Ornithine	Arginine
Cit/Arg	Citrulline	Arginine
Glu/Gln	Glutamate	Glutamine
Asp/Asn	Aspartic acid	Asparagine
Ala/Lys	Alanine	Lysine
Phe/Tyr	Phenylalanine	Tyrosine
Serotonin/Trp	Serotonin	Tryptophane
Kyn/Trp	Kynurenine	Tryptophane
Kyn/OHKyn	Kynurenine	Hydrokynurenine
Putrescine/Orn	Putrescine	Ornithine
Spermine/Spermidine	Spermine	Spermidine
SDMA/ADMA	Symmetric dimethylarginine	Asymmetric dimethylarginine
Met-SO/Met	Methionine-Sulfoxide	Methionine
Ala/BCAA	Alanine	G.M. of Valine, Isoleucine and Leucine
Gly/BCAA	Glycine	G.M. of Valine, Isoleucine and Leucine
SumLyso	G.M. of 15 LysoPC	
SumPC+Lyso	G.M. of 92 LysoPC and PC	
SumPC	G.M. of 77 PC	
SumSM	G.M. of 15 SM	
SumSMOH/SumSM	G.M. of 5 SM(OH) G.M. of palmitoylcarnitine and stearyl carnitine	G.M. of 10 SM Carnitine (free)
C16+C18/C0		
SumMUFA	G.M. of 26 mono-unsaturated lipids	
SumPUFA	G.M. of 82 poly-unsaturated lipids	
SumSFA	G.M. of 25 saturated lipids	
PUFA/SFA	G.M. of 82 poly-unsaturated lipids	G.M. of 25 saturated lipids
PUFA/MUFA	G.M. of 82 poly-unsaturated lipids	G.M. of 26 mono-unsaturated lipids
MUFA/SFA	G.M. of 26 mono-unsaturated lipids	G.M. of 25 saturated lipids