

Supplemental Table S3 – The *AbsoluteIDQ® p180* kit by Biocrates AG Life Sciences with all of the analytes and their standard nomenclature.

Amino acids (21)			
Ala	Alanine	Lys	Lysine
Arg	Arginine	Met	Methionine
Asn	Asparagine	Orn	Ornithine
Asp	Aspartate	Phe	Phenylalanine
Cit	Citrulline	Pro	Proline
Glu	Glutamate	Ser	Serine
Gln	Glutamine	Thr	Threonine
Gly	Glycine	Trp	Tryptophan
His	Histidine	Tyr	Tyrosine
Ile	Isoleucine	Val	Valine
Leu	Leucine		

Biogenic amines (21)			
Ac-Orn	Acetylornithine	Met-SO	Methionine sulfoxide
alpha-AAA	alpha-Aminoadipic acid	Nitro-Tyr ¹	Nitrotyrosine
ADMA	Asymmetric dimethylarginine	PEA	Phenylethylamine
Carnosine	Carnosine	Putrescine	Putrescine
Creatinine	Creatinine	Sarcosine	Sarcosine
DOPA	Dihydroxyphenylalanine	Serotonin	Serotonin
Dopamine	Dopamine	Spermidine	Spermidine
Histamine	Histamine	Spermine	Spermine
c4-OH-Pro	<i>cis</i> -4-Hydroxyproline	SDMA	Symmetric dimethylarginine
t4-OH-Pro	<i>trans</i> -4-Hydroxyproline	Taurine	Taurine
Kynurenine	Kynurenine		

Acylcarnitines (40)			
C0	Carnitine	C5-DC (C6-OH)	Glutaryl carnitine (Hydroxyhexanoyl carnitine)
C2	Acetyl carnitine	C5-M-DC	Methylglutaryl carnitine
C3	Propionyl carnitine	C5-OH (C3-DC-M)	Hydroxyvaleryl carnitine (Methylmalonyl carnitine)
C3-OH	Hydroxypropionyl carnitine	C5:1	Tiglyl carnitine
C3:1	Propenoyl carnitine	C5:1-DC	Glutaconyl carnitine
C4	Butyryl carnitine	C6 (C4:1-DC)	Hexanoyl carnitine (Fumaryl carnitine)
C4-OH (C3-DC)	Hydroxybutyryl carnitine (Malonyl carnitine)	C6:1	Hexenoyl carnitine
C4:1	Butenyl carnitine	C7-DC	Pimeloyl carnitine
C5	Valeryl carnitine	C8	Octanoyl carnitine
C9	Nonayl carnitine	C14:2-OH	Hydroxytetradecadienyl carnitine
C10	Decanoyl carnitine	C16	Hexadecanoyl carnitine
C10:1	Decenoyl carnitine	C16-OH	Hydroxyhexadecanoyl carnitine
C10:2	Decadienyl carnitine	C16:1	Hexadecenoyl carnitine
C12	Dodecanoyl carnitine	C16:1-OH	Hydroxyhexadecenoyl carnitine
C12-DC	Dodecanedioyl carnitine	C16:2	Hexadecadienyl carnitine
C12:1	Dodecenoyl carnitine	C16:2-OH	Hydroxyhexadecadienyl carnitine
C14	Tetradecanoyl carnitine	C18	Octadecanoyl carnitine
C14:1	Tetradecenoyl carnitine	C18:1	Octadecenoyl carnitine
C14:1-OH	Hydroxytetradecenoyl carnitine	C18:1-OH	Hydroxyoctadecenoyl carnitine
C14:2	Tetradecadienyl carnitine	C18:2	Octadecadienyl carnitine

Glycerophospholipids (90)			
lysoPC a C14:0	PC aa C34:1	PC aa C42:0	PC ae C38:2
lysoPC a C16:0	PC aa C34:2	PC aa C42:1	PC ae C38:3
lysoPC a C16:1	PC aa C34:3	PC aa C42:2	PC ae C38:4
lysoPC a C17:0	PC aa C34:4	PC aa C42:4	PC ae C38:5
lysoPC a C18:0	PC aa C36:0	PC aa C42:5	PC ae C38:6
lysoPC a C18:1	PC aa C36:1	PC aa C42:6	PC ae C40:1
lysoPC a C18:2	PC aa C36:2	PC ae C30:0	PC ae C40:2
lysoPC a C20:3	PC aa C36:3	PC ae C30:1	PC ae C40:3
lysoPC a C20:4	PC aa C36:4	PC ae C30:2	PC ae C40:4
lysoPC a C24:0	PC aa C36:5	PC ae C32:1	PC ae C40:5
lysoPC a C26:0	PC aa C36:6	PC ae C32:2	PC ae C40:6
lysoPC a C26:1	PC aa C38:0	PC ae C34:0	PC ae C42:0
lysoPC a C28:0	PC aa C38:1 ²	PC ae C34:1	PC ae C42:1
lysoPC a C28:1	PC aa C38:3	PC ae C34:2	PC ae C42:2
PC aa C24:0	PC aa C38:4	PC ae C34:3	PC ae C42:3
PC aa C26:0	PC aa C38:5	PC ae C36:0	PC ae C42:4
PC aa C28:1	PC aa C38:6	PC ae C36:1	PC ae C42:5
PC aa C30:0	PC aa C40:1	PC ae C36:2	PC ae C44:3
PC aa C30:2 ²	PC aa C40:2	PC ae C36:3	PC ae C44:4
PC aa C32:0	PC aa C40:3	PC ae C36:4	PC ae C44:5
PC aa C32:1	PC aa C40:4	PC ae C36:5	PC ae C44:6
PC aa C32:2	PC aa C40:5	PC ae C38:0	
PC aa C32:3	PC aa C40:6	PC ae C38:1	

Sphingomyelins (15)			
SM (OH) C14:1	SM C18:0	SM (OH) C22:2	SM (OH) C24:1
SM C16:0	SM C18:1	SM C22:3 ²	SM C26:0
SM C16:1	SM C20:2	SM C24:0	SM C26:1
SM (OH) C16:1	SM (OH) C22:1	SM C24:1	

Monosaccharides (1)			
H1	Hexoses (including glucose)		