

Supplementary Table 1

List of the measurable metabolites using the **Biocrates Absolute IDQ p180 kit**.

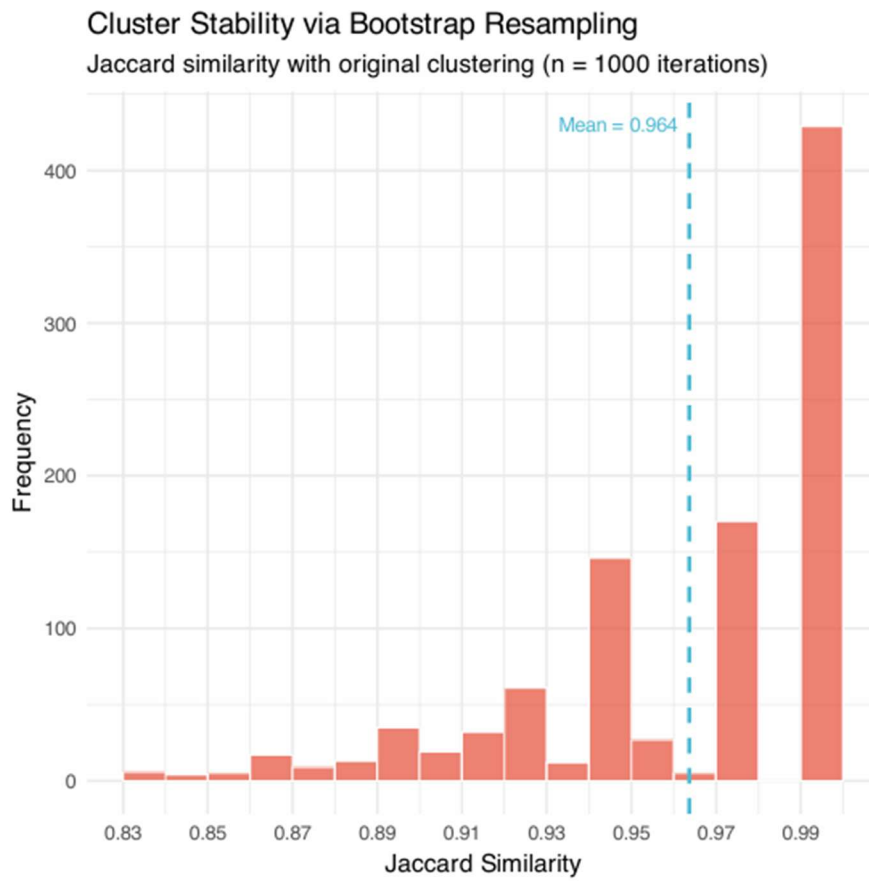
METABOLITE CLASS	N	RETAINED FOR ANALYSIS	NOT RETAINED FOR ANALYSIS
AMINO ACIDS	21	alanine, arginine, asparagine, citrulline, glutamine, glutamate, glycine, histidine, isoleucine, leucine, lysine, methionine, ornithine, phenylalanine, proline, serine, threonine, tryptophan, tyrosine, valine	aspartate
CARNITINE	1	C0	-
ACYLCARNITINE	39	C2, C3,	C3:1, C3-OH, C4, C4:1, C4-OH, C5, C5:1, C5:1-DC, C5-DC, C5-M-DC, C5-OH, C6, C6:1, C7-DC, C8, C9, C10, C10:1, C10:2, C12, C12-DC, C14, C14:1, C14:1-OH, C14:2, C14:2-OH, C16, C16:1, C16:1-OH, C16:2, C16:2-OH, C16-OH, C18, C18:1, C18:1-OH, C18:2, C12:1
BIOGENIC AMINES	19	Acetylornithine, asymmetric dimethylarginine, total dimethylarginine, alpha-aminoadipic acid, creatinine, kynurenine, methionine sulfoxide, hydroxyproline, spermidine, taurine	carnosine, histamine, nitrotyrosine, phenylethylamine, putrescine, sarcosine, serotonin, spermine
GLYCEROPHOSPHOLIPIDS: LYSO-PHOSPHATIDYLCHOLINES	14	lysoPC.a. C16:0, C16:1, C17:0, C18:0, C18:1, C18:2, C20:3, C20:4, C26:0, C26:1, C28:0, C28:1, C24:0	lysoPC.a. C14:0
GLYCEROPHOSPHOLIPIDS: DIACYL-PHOSPHATIDYLCHOLINES	38	PC.aa. C24:0, 28:1, C30:0, C30:2, C32:0, C32:1, C32:3, C34:1, C32:2, C34:2, C34:3, C34:4, C36:0, C36:1, C36:2, C36:3, C36:4, C36:5, C36:6, C38:0, C38:1, C38:3, C38:4, C38:5, C38:6, C40:3, C40:4, C40:5, C40:6, C42:0, C42:1, C42:2, C42:4, C42:5	PC.aa. C26:0, C42:6, C40:1, C40:2,
GLYCEROPHOSPHOLIPIDS: ACYL-ALKYL-PHOSPHATIDYLCHOLINE	38	PC.ae. C30:1, C30:2, C32:1, C32:2, C34:0, C34:1, C34:2, C34:3, C36:0, C36:1, C36:2, C36:3, C36:4, C36:5, C38:0, C38:1, C38:2, C38:3, C38:4, C38:5, C38:6, C40:1, C40:2, C40:3, C40:4, C40:5, C40:6, C42:2, C42:3, C42:4, C42:5, C44:3, C44:4, C44:5, C44:6	PC.ae. C30:0, C42:0, C42:1
SPHINGOLIPIDS	15	SM (OH) C14:1, SM C16:0, SM (OH) C16:1, SM C16:1, SM C18:0, SM C18:1, SM C20:2, SM (OH) C22:1, SM (OH) C22:2, SM C24:0, SM C24:1, SM (OH) C24:1, SM C26:0, SM C26:1	SM C22:3
MONOSACCHARIDE	1	sugar	-
TOTAL	186	130	56

Supplementary Table 2

Pairwise comparisons of baseline characteristics across metabolomic clusters

	Cluster 1 vs Cluster 2	Cluster 1 vs Cluster 3	Cluster 2 vs Cluster 3
ADMISSION CAUSE	0.472	0.760	0.723
DEMOGRAPHICS AND UNDERLYING DISEASES			
Sex, male, n (%)	0.716	0.494	0.235
Age, mean (IQR)	0.435	0.273	0.553
Arterial hypertension, n (%)	0.315	0.772	0.501
Diabetes Mellitus, n (%)	<0.001	<0.001	>0.999
Coronary artery disease, n (%)	0.685	>0.999	0.682
Other cardiovascular disease, n (%)	0.278	0.188	>0.999
Chronic lung disease, n (%)	0.691	0.701	0.225
Chronic kidney disease, n (%)	0.394	0.416	>0.999
Chronic liver failure, n (%)	0.538	>0.999	0.525
CHARACTERISTICS AT ICU ADMISSION			-
Anuria and/or RRT, n (%)	>0.999	0.489	0.361
Systolic arterial blood pressure (mmHg), mean (IQR)	>0.999	0.741	0.843
Diastolic arterial blood pressure (mmHg), mean (IQR)	0.911	0.601	0.597
Mean arterial blood pressure (mmHg), mean (IQR)	>0.999	0.543	0.655
Heart rate (bpm), mean (IQR)	0.577	0.790	0.908
Creatinine (mg/dL), mean (IQR)	0.219	0.693	0.186
Na ⁺ (mmol/L), mean (IQR)	0.936	0.923	0.766
K ⁺ (mmol/L), mean (IQR)	0.702	0.337	0.767
Cl ⁻ (mmol/L), mean (IQR)	0.185	0.480	0.298
Lactate, mean (IQR)	0.005	0.190	<0.001
pH, mean (IQR)	0.077	0.156	0.015
PaO ₂ (mmHg), mean (IQR)	0.279	0.454	0.051
PaCO ₂ (mmHg), mean (IQR)	0.265	0.149	0.008
HCO ₃ ⁻ (mmol/L), mean (IQR)	>0.999	0.596	0.572
Base Excess (mmol/L), mean (IQR)	0.127	0.921	0.073
SOFA score, mean (IQR)	0.821	0.049	0.035
APACHE II score, mean (IQR)	0.084	0.149	0.023
OUTCOMES			
ICU stay (d), mean (IQR)	0.655	0.257	0.727
Hospital stay (d), mean (IQR)	0.774	0.306	0.644
ICU mortality, n (%)	>0.999	0.072	0.073
Hospital mortality, n (%)	0.489	0.036	0.005

Supplementary Figure 1



Supplementary Figure 2

