

## **Integrative Plasma Metabolic and Lipidomic Modelling of SARS-CoV-2 Infection in Relation to Clinical Severity and Early Mortality Prediction**

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**Key words:** COVID-19, SARS-CoV-2, NMR spectroscopy, mass spectrometry, plasma IVDr, metabolic phenotyping, diagnostic modeling, lipoproteins, lipids, mortality prediction, patient stratification.

**Acknowledgements:** We thank the support provided by the Department of Industry, Tourism and Trade of the Government of the Autonomous Community of the Basque Country (Elkartek BG2019) and the Agencia Estatal de Investigación (Spain) for grant RTI2018-101269-B-I00. We thank The Spinnaker Health Research Foundation, WA, The McCusker Foundation, WA, The Western Australian State Government, and the MRFF (grant number 2014349) for funding the Australian National Phenome Centre for this and related work. We thank the Department of Jobs, Tourism, Science and Innovation, Government of Western Australian Premier's Fellowship for funding EH; and ARC Laureate Fellowship funding for EH. We also would like to acknowledge the Western Australian Covid Research Response team (<https://research-au.net/covid-research-response/>). JW thanks Ministerio de Ciencia, Tecnología e Innovación (Minciencias), Ministerio de Educación Nacional, Ministerio de Industria, Comercio y Turismo e ICETEX (792–2017) 2a Convocatoria Ecosistema Científico - Colombia Científica para la Financiación de Proyectos de I + D + i), World Bank and Vicerrectoría de Investigaciones, Pontificia Universidad Javeriana, Bogotá, Colombia (contract no. FP44842 - 221-2018).

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**Table S1 - Full cohort demographic data for the control samples and SARS-CoV-2 positive patients.**

	<b>Controls (n=89)</b>	<b>SARS-CoV- 2 Positive (+) Group B severity (n=18)</b>	<b>SARS-CoV- 2 Positive (+) Group C severity (n=139)</b>	<b>SARS-CoV- 2 Positive (+) Group D severity (n=92)</b>	<b>SARS-CoV- 2 Positive (+) Group E severity (n=57)</b>
Sex, Male	43 (48.31%)	5 (27.78%)	56 (40.29%)	44 (47.83%)	33 (57.89%)
Age, years [SD]	48.00 [±11.95]	62.00 [±18.13]	68.00 [±18.21]	71.00 [±17.22]	75.00 [±13.46]
BMI, kg/m <sup>2</sup> [SD]	23.81 [±4.57]	-	-	-	-
Pre-diabetic/ diabetic	-	3 (16.67%)	29 (20.86%)	24 (26.09%)	19 (33.33%)
Hypertension	-	5 (27.78%)	48 (34.53%)	50 (54.35%)	33 (57.89%)
Cardiovascular disease	-	3 (16.67%)	33 (23.74%)	29 (31.52%)	21 (36.84%)
Cerebrovascular disease	-	2 (11.11%)	16 (11.51%)	9 (9.78%)	10 (17.54%)
Chronic Renal Disease	-	0	8 (5.76%)	9 (9.78%)	6 (10.53%)
Chronic liver disease	-	0	2 (1.44%)	1 (1.09%)	2 (3.51%)
Patients who died of SARS-CoV-2	-	0	0	0	32 (56.14%)

### **Quantification of Plasma Lipoproteins, Lipids and the low molecular weight metabolites**

Plasma lipoproteins – A total of 112 lipoprotein parameters were quantified based on 1D NMR experiments as part of Bruker's IVDr experiment suite for blood plasma. This approach is termed Bruker's IVDr lipoprotein class and subclass Analysis (B.I.-LISA™) and lipid analytes include cholesterol, free cholesterol, phospholipids, triglycerides, apolipoproteins A1/A2/B100 and ratio B100/A1, in total plasma concentration and resolved for main lipoprotein classes and subclasses. Main classes of plasma-lipoproteins were defined as: high-density lipoprotein (HDL, density 1.063–1.210 kg/L), intermediate-density lipoprotein (IDL, density 1.006–1.019 kg/L) low-density lipoprotein (LDL, density 1.09–1.63 kg/L) and very low-density lipoprotein (VLDL, 0.950–1.006 kg/L). The main lipoprotein classes HDL, LDL, VLDL were further divided into different lipoprotein sub-classes: (LDL-1: 1.019–1.031 kg/L, LDL-2: 1.031–1.034 kg/L, LDL-3: 1.034–1.037 kg/L, LDL-4: 1.037–1.040 kg/L, LDL-5: 1.040–1.044 kg/L, LDL-6: 1.044–1.063 kg/L), and

the HDL sub-fractions into four density classes (HDL-1 1.063–1.100 kg/L, HDL-2 1.100–1.125 kg/L, HDL-3 1.125–1.175 kg/L, and HDL-4 1.175–1.210 kg/L), the VLDL sub-fractions divided into 5 density classes.

**Table S2- Annotation of the keys used by the Bruker IVDr Lipoprotein Subclass Analysis (B.I.-LISA™) method.** Abbreviations: LDL – low-density lipoprotein; HDL – high-density lipoprotein; VLDL – very low-density lipoprotein; IDL – intermediate-density lipoprotein.

Key	Class/subclass	Compound	Concentration unit
TPTG	Total Plasma	Triglycerides	mg/dL
TPCH	Total Plasma	Cholesterol	mg/dL
LDCH	LDL	Cholesterol	mg/dL
HDCH	HDL	Cholesterol	mg/dL
TPA1	Total Plasma	Apolipoprotein-A1	mg/dL
TPA2	Total Plasma	Apolipoprotein-A2	mg/dL
TPAB	Total Plasma	Apolipoprotein-B100	mg/dL
LDHD	Ratio LDL and HDL Cholesterol	LDL Cholesterol / HDL Cholesterol	-/-
ABA1	Ratio of Apolipoproteins A1 and B100	Apolipoprotein-A1 / Apolipoprotein-B100	-/-
TBPN	Apolipoprotein-B100 particles	carrying Particle Number	nmol/L
VLPN	VLDL	Particle Number	nmol/L
IDPN	IDL	Particle Number	nmol/L
LDPN	LDL	Particle Number	nmol/L
L1PN	LDL-1	Particle Number	nmol/L
L2PN	LDL-2	Particle Number	nmol/L
L3PN	LDL-3	Particle Number	nmol/L
L4PN	LDL-4	Particle Number	nmol/L
L5PN	LDL-5	Particle Number	nmol/L
L6PN	LDL-6	Particle Number	nmol/L
VLTG	VLDL Class	Triglycerides	mg/dL
IDTG	IDL Class	Triglycerides	mg/dL
LDTG	LDL Class	Triglycerides	mg/dL
HDTG	HDL Class	Triglycerides	mg/dL
VLCH	VLDL Class	Cholesterol	mg/dL
IDCH	IDL Class	Cholesterol	mg/dL
LDCH	LDL Class	Cholesterol	mg/dL
HDCH	HDL Class	Cholesterol	mg/dL
VLFC	VLDL Class	Free Cholesterol	mg/dL
IDFC	IDL Class	Free Cholesterol	mg/dL
LDFC	LDL Class	Free Cholesterol	mg/dL
HDFC	HDL Class	Free Cholesterol	mg/dL
VLPL	VLDL Class	Phospholipids	mg/dL
IDPL	IDL Class	Phospholipids	mg/dL
LDPL	LDL Class	Phospholipids	mg/dL
HDPL	HDL Class	Phospholipids	mg/dL

HDA1 HDL Class	Apolipoprotein-A1	mg/dL
HDA2 HDL Class	Apolipoprotein-A2	mg/dL
VLAB VLDL Class	Apolipoprotein-B100	mg/dL
IDAB IDL Class	Apolipoprotein-B100	mg/dL
LDAB LDL Class	Apolipoprotein-B100	mg/dL
V1TG VLDL-1 Subclass	Triglycerides	mg/dL
V2TG VLDL-2 Subclass	Triglycerides	mg/dL
V3TG VLDL-3 Subclass	Triglycerides	mg/dL
V4TG VLDL-4 Subclass	Triglycerides	mg/dL
V5TG VLDL-5 Subclass	Triglycerides	mg/dL
V1CH VLDL-1 Subclass	Cholesterol	mg/dL
V2CH VLDL-2 Subclass	Cholesterol	mg/dL
V3CH VLDL-3 Subclass	Cholesterol	mg/dL
V4CH VLDL-4 Subclass	Cholesterol	mg/dL
V5CH VLDL-5 Subclass	Cholesterol	mg/dL
V1FC VLDL-1 Subclass	Free Cholesterol	mg/dL
V2FC VLDL-2 Subclass	Free Cholesterol	mg/dL
V3FC VLDL-3 Subclass	Free Cholesterol	mg/dL
V4FC VLDL-4 Subclass	Free Cholesterol	mg/dL
V5FC VLDL-5 Subclass	Free Cholesterol	mg/dL
V1PL VLDL-1 Subclass	Phospholipids	mg/dL
V2PL VLDL-2 Subclass	Phospholipids	mg/dL
V3PL VLDL-3 Subclass	Phospholipids	mg/dL
V4PL VLDL-4 Subclass	Phospholipids	mg/dL
V5PL VLDL-5 Subclass	Phospholipids	mg/dL
L1TG LDL-1 Subclass	Triglycerides	mg/dL
L2TG LDL-2 Subclass	Triglycerides	mg/dL
L3TG LDL-3 Subclass	Triglycerides	mg/dL
L4TG LDL-4 Subclass	Triglycerides	mg/dL
L5TG LDL-5 Subclass	Triglycerides	mg/dL
L6TG LDL-6 Subclass	Triglycerides	mg/dL
L1CH LDL-1 Subclass	Cholesterol	mg/dL
L2CH LDL-2 Subclass	Cholesterol	mg/dL
L3CH LDL-3 Subclass	Cholesterol	mg/dL
L4CH LDL-4 Subclass	Cholesterol	mg/dL
L5CH LDL-5 Subclass	Cholesterol	mg/dL
L6CH LDL-6 Subclass	Cholesterol	mg/dL
L1FC LDL-1 Subclass	Free apoHDA Cholesterol	mg/dL
L2FC LDL-2 Subclass	Free Cholesterol	mg/dL
L3FC LDL-3 Subclass	Free Cholesterol	mg/dL
L4FC LDL-4 Subclass	Free Cholesterol	mg/dL
L5FC LDL-5 Subclass	Free Cholesterol	mg/dL
L6FC LDL-6 Subclass	Free Cholesterol	mg/dL
L1PL LDL-1 Subclass	Phospholipids	mg/dL
L2PL LDL-2 Subclass	Phospholipids	mg/dL

L3PL	LDL-3 Subclass	Phospholipids	mg/dL
L4PL	LDL-4 Subclass	Phospholipids	mg/dL
L5PL	LDL-5 Subclass	Phospholipids	mg/dL
L6PL	LDL-6 Subclass	Phospholipids	mg/dL
L1AB	LDL-1 Subclass	Apolipoprotein-B100	mg/dL
L2AB	LDL-2 Subclass	Apolipoprotein-B100	mg/dL
L3AB	LDL-3 Subclass	Apolipoprotein-B100	mg/dL
L4AB	LDL-4 Subclass	Apolipoprotein-B100	mg/dL
L5AB	LDL-5 Subclass	Apolipoprotein-B100	mg/dL
L6AB	LDL-6 Subclass	Apolipoprotein-B100	mg/dL
H1TG	HDL-1 Subclass	Triglycerides	mg/dL
H2TG	HDL-2 Subclass	Triglycerides	mg/dL
H3TG	HDL-3 Subclass	Triglycerides	mg/dL
H4TG	HDL-4 Subclass	Triglycerides	mg/dL
H1CH	HDL-1 Subclass	Cholesterol	mg/dL
H2CH	HDL-2 Subclass	Cholesterol	mg/dL
H3CH	HDL-3 Subclass	Cholesterol	mg/dL
H4CH	HDL-4 Subclass	Cholesterol	mg/dL
H1FC	HDL-1 Subclass	Free Cholesterol	mg/dL
H2FC	HDL-2 Subclass	Free Cholesterol	mg/dL
H3FC	HDL-3 Subclass	Free Cholesterol	mg/dL
H4FC	HDL-4 Subclass	Free Cholesterol	mg/dL
H1PL	HDL-1 Subclass	Phospholipids	mg/dL
H2PL	HDL-2 Subclass	Phospholipids	mg/dL
H3PL	HDL-3 Subclass	Phospholipids	mg/dL
H4PL	HDL-4 Subclass	Phospholipids	mg/dL
H1A1	HDL-1 Subclass	Apolipoprotein-A1	mg/dL
H2A1	HDL-2 Subclass	Apolipoprotein-A1	mg/dL
H3A1	HDL-3 Subclass	Apolipoprotein-A1	mg/dL
H4A1	HDL-4 Subclass	Apolipoprotein-A1	mg/dL
H1A2	HDL-1 Subclass	Apolipoprotein-A2	mg/dL
H2A2	HDL-2 Subclass	Apolipoprotein-A2	mg/dL
H3A2	HDL-3 Subclass	Apolipoprotein-A2	mg/dL
H4A2	HDL-4 Subclass	Apolipoprotein-A2	mg/dL

**Table S3 - Annotation of the low molecular weight metabolites. Those in *italics* were quantified by NMR, while the remaining were quantified by LC-MS.**

<b>Abbreviations in models</b>	<b>Metabolite</b>	<b>Concentration unit</b>
<i>Acetic acid</i>	<i>Acetic acid</i>	<i>mmol/L</i>
<i>Acetoacetic acid</i>	<i>Acetoacetic acid</i>	<i>mmol/L</i>
<i>Acetone</i>	<i>Acetone</i>	<i>mmol/L</i>
<i>Citric acid</i>	<i>Citric acid</i>	<i>mmol/L</i>
<i>Creatine</i>	<i>Creatine</i>	<i>mmol/L</i>
<i>Creatinine</i>	<i>Creatinine</i>	<i>mmol/L</i>
<i>Formic acid</i>	<i>Formic acid</i>	<i>mmol/L</i>

Glucose	Glucose	mmol/L
D-3-hydroxybutyric acid	D-3-hydroxybutyric acid	mmol/L
Lactic acid	Lactic acid	mmol/L
Pyruvic acid	Pyruvic acid	mmol/L
Tryptophan	Tryptophan	μmol/L
3-Hydroxykynurenine	3-Hydroxykynurenine	μmol/L
3-Hydroxyanthranilic acid	3-Hydroxyanthranilic acid	μmol/L
Kynurenic acid	Kynurenic acid	μmol/L
Quinolinic acid	Quinolinic acid	μmol/L
Picolinic acid	Picolinic acid	μmol/L
Xanthurenic acid	Xanthurenic acid	μmol/L
Kynurenine	Kynurenine	μmol/L
Indole-3-acetic acid	Indole-3-acetic acid	μmol/L
5-Hydroxyindole acetic acid	5-Hydroxyindole acetic acid	μmol/L
Neopterin	Neopterin	μmol/L
Serotonin	Serotonin	μmol/L
1-methylhistidine	1-methylhistidine	μmol/L
3-methylhistidine	3-methylhistidine	μmol/L
Alanine	Alanine	μmol/L
Alpha aminobutyric acid	Alpha aminobutyric acid	μmol/L
Arginine	Arginine	μmol/L
Aspartic acid	Aspartic acid	μmol/L
Citrulline	Citrulline	μmol/L
Glutamic acid	Glutamic acid	μmol/L
Glutamine	Glutamine	μmol/L
Histidine	Histidine	μmol/L
Isoleucine	Isoleucine	μmol/L
Leucine	Leucine	μmol/L
Lysine	Lysine	μmol/L
Methionine	Methionine	μmol/L
Ornithine	Ornithine	μmol/L
Phenylalanine	Phenylalanine	μmol/L
Proline	Proline	μmol/L
Serine	Serine	μmol/L
Taurine	Taurine	μmol/L
Threonine	Threonine	μmol/L
Tyrosine	Tyrosine	μmol/L
Valine	Valine	μmol/L
Lac.pyr	Lactate/pyruvate	-/-
Kynurenine/tryptophan	Kynurenine/tryptophan	-/-
3-hydroxykynurenine/tryptophan	3-hydroxykynurenine/tryptophan	-/-
Kynurenic acid/tryptophan	Kynurenic acid/tryptophan	-/-
Neopterin/tryptophan	Neopterin/tryptophan	-/-
Serotonin/tryptophan	Serotonin/tryptophan	-/-
Quinolinic acid/tryptophan	Quinolinic acid/tryptophan	-/-
Fisher's ratio	Fisher's ratio	-/-

Branched AA/taurine	Branched chain amino acids/aromatic -/- amino acids
Asp...glu...asn...gln	Asp:Glu/Asn:Gln -/-

**Table S4 - Annotation of the lipids**

Abbreviation	Subclasses	Concentration unit
CE	Cholesterol esters	μmol/L
CER	Ceramides	μmol/L
DAG	Diacylglycerides	μmol/L
DCER	Dihydroceramides	μmol/L
FFA	Free fatty acids	μmol/L
HCER	Hexosylceramides	μmol/L
LCER	Lactosylceramides	μmol/L
LPC	Lysophosphocholines	μmol/L
LPE	Lysophosphoethanolamines	μmol/L
LPG	Lysophosphoglycerols	μmol/L
LPI	Lysophosphoinositols	μmol/L
MAG	Monoacylglycerols	μmol/L
PC	Phosphocholines	μmol/L
PE	Phosphoethanolamines	μmol/L
PG	Phosphoglycerols	μmol/L
PI	Phosphoinositols	μmol/L
PS	Phosphoserines	μmol/L
SM	Sphingomyelins	μmol/L
TAG	Triacylglycerides	μmol/L

## Integrated Spectroscopy Modeling

**Table S5 - OPLS loadings, Cliff's delta and adjusted p-values of the combined model (low molecular weight metabolites, lipoproteins and lipids) for the comparison of the controls and SARS-CoV-2 positive patients.** Only metabolites with significant p-values are shown in the table.

Metabolite	OPLS loadings	Cliff's delta	Adjusted p value
Formic acid	0.063	1.00	1.18x10 <sup>-43</sup>
PC (18:2/18:2)	0.085	-0.94	4.48x10 <sup>-39</sup>
PE.O (16:0/20:4)	0.073	-0.94	4.48x10 <sup>-39</sup>
Asp:Glu/Asn:Gln	0.039	0.93	1.21x10 <sup>-38</sup>
Pyruvic acid	0.050	0.93	2.67x10 <sup>-38</sup>
PE.P (18:1/20:4)	0.076	-0.93	2.67x10 <sup>-38</sup>
PC (18:1/18:2)	0.085	-0.92	5.41x10 <sup>-38</sup>
H4CH	0.069	-0.92	8.87x10 <sup>-38</sup>
H4PL	0.071	-0.92	1.08x10 <sup>-37</sup>

PE.P (18:1/18:2)	0.082	-0.92	1.21x10 <sup>-37</sup>
PE.P (16:0/18:2)	0.082	-0.91	2.00x10 <sup>-37</sup>
PE.P (16:0/22:5)	0.073	-0.91	2.00x10 <sup>-37</sup>
PE.O (16:0/18:2)	0.074	-0.91	2.60x10 <sup>-37</sup>
PE.P (18:1/20:4)	0.077	-0.91	2.60x10 <sup>-37</sup>
LPC (18:2)	0.077	-0.91	8.25x10 <sup>-37</sup>
PE.P (18:0/18:2)	0.079	-0.90	8.25x10 <sup>-37</sup>
PE.P (18:0/22:5)	0.076	-0.90	2.27x10 <sup>-36</sup>
PE.P (16:0/20:4)	0.074	-0.90	3.76x10 <sup>-36</sup>
PC (18:2/20:3)	0.077	-0.90	3.86x10 <sup>-36</sup>
PC (18:2/20:2)	0.076	-0.89	5.52x10 <sup>-36</sup>
PE.P (18:2/18:2)	0.076	-0.88	4.01x10 <sup>-35</sup>
Lactate/pyruvate	0.046	-0.88	6.10x10 <sup>-35</sup>
PC (20:0/20:3)	0.075	-0.88	6.10x10 <sup>-35</sup>
PE.P (18:0/18:1)	0.077	-0.88	7.95x10 <sup>-35</sup>
HCER.d (18:0/18:0)	0.074	-0.88	8.72x10 <sup>-35</sup>
PE.O (16:0/20:1)	0.073	-0.88	9.46x10 <sup>-35</sup>
H4A1	0.067	-0.87	2.68x10 <sup>-34</sup>
PE.P (18:1/22:5)	0.074	-0.87	2.95x10 <sup>-34</sup>
PE.O (16:0/22:5)	0.072	-0.87	3.00x10 <sup>-34</sup>
PE.P (18:0/20:4)	0.073	-0.87	3.40x10 <sup>-34</sup>
PE.P (16:0/20:1)	0.077	-0.87	4.35x10 <sup>-34</sup>
PC (18:2/20:4)	0.079	-0.87	4.81x10 <sup>-34</sup>
H4A2	0.067	-0.86	6.21x10 <sup>-34</sup>
PE.P (16:0/18:3)	0.066	-0.86	6.21x10 <sup>-34</sup>
PC (18:0/20:1)	0.076	-0.86	6.96x10 <sup>-34</sup>
PE.O (18:0/22:5)	0.070	-0.86	6.96x10 <sup>-34</sup>
LPC (20:0)	0.075	-0.86	1.03x10 <sup>-33</sup>
PE.P (18:0/22:4)	0.069	-0.86	1.22x10 <sup>-33</sup>
PE.O (16:0/18:1)	0.067	-0.86	1.70x10 <sup>-33</sup>
PE.P (18:0/20:1)	0.074	-0.85	4.02x10 <sup>-33</sup>
PE.P (18:0/20:3)	0.073	-0.85	4.59x10 <sup>-33</sup>
PC (18:2/18:3)	0.063	-0.84	2.40x10 <sup>-32</sup>
PE.P (18:0/16:0)	0.075	-0.84	2.71x10 <sup>-32</sup>
PE.P (18:1/22:4)	0.062	-0.84	4.30x10 <sup>-32</sup>
PE.P (18:0/20:2)	0.074	-0.84	5.79x10 <sup>-32</sup>
PE.P (18:1/18:1)	0.063	-0.84	6.28x10 <sup>-32</sup>

HCER (22:0)	0.069	-0.83	8.56x10 <sup>-32</sup>
Glutamic acid	0.045	0.83	1.59x10 <sup>-31</sup>
HCER (26:0)	0.072	-0.83	1.59x10 <sup>-31</sup>
Glutamic acid	0.046	0.83	1.69x10 <sup>-31</sup>
HCER.d (18:0/22:0)	0.069	-0.83	2.01x10 <sup>-31</sup>
PE.P (18:0/18:0)	0.071	-0.83	3.79x10 <sup>-31</sup>
LDTG	0.048	0.83	4.06x10 <sup>-31</sup>
PC (20:0/18:1)	0.068	-0.82	4.58x10 <sup>-31</sup>
PI (18:1/18:1)	0.068	-0.82	7.43x10 <sup>-31</sup>
PI (20:0/18:2)	0.070	-0.82	1.04x10 <sup>-30</sup>
PE.O (18:0/22:4)	0.052	-0.81	2.46x10 <sup>-30</sup>
PC (18:2/22:6)	0.074	-0.81	3.22x10 <sup>-30</sup>
HCER.d (18:0/24:0)	0.069	-0.81	3.25x10 <sup>-30</sup>
SM (20:0)	0.064	-0.81	4.74x10 <sup>-30</sup>
HCER (24:0)	0.069	-0.81	5.28x10 <sup>-30</sup>
PE.P (16:0/22:4)	0.057	-0.81	5.45x10 <sup>-30</sup>
TPA2	0.065	-0.81	7.21x10 <sup>-30</sup>
CER (26:0)	0.072	-0.81	7.64x10 <sup>-30</sup>
PC (18:2/22:5)	0.072	-0.80	1.55x10 <sup>-29</sup>
LPI (20:3)	0.062	-0.80	1.73x10 <sup>-29</sup>
PE.P (18:1/20:1)	0.070	-0.80	3.81x10 <sup>-29</sup>
PC (14:0/18:2)	0.071	-0.79	7.22x10 <sup>-29</sup>
SM (24:0)	0.065	-0.79	8.74x10 <sup>-29</sup>
PE.P (18:1/16:0)	0.034	-0.79	1.98x10 <sup>-28</sup>
LPC (20:3)	0.069	-0.79	2.02x10 <sup>-28</sup>
PC (16:1/18:2)	0.068	-0.78	3.14x10 <sup>-28</sup>
PC (16:0/18:2)	0.071	-0.78	4.28x10 <sup>-28</sup>
PI (18:1/20:4)	0.069	-0.78	6.18x10 <sup>-28</sup>
PI (18:1/18:2)	0.067	-0.78	6.55x10 <sup>-28</sup>
H4FC	0.062	-0.78	6.60x10 <sup>-28</sup>
MAG (20:3)	0.015	0.78	7.44x10 <sup>-28</sup>
LPI (18:1)	0.058	-0.78	8.17x10 <sup>-28</sup>
PC (18:2/20:5)	0.057	-0.78	8.17x10 <sup>-28</sup>
LPC (18:1)	0.069	-0.77	3.10x10 <sup>-27</sup>
SM (26:0)	0.064	-0.77	3.17x10 <sup>-27</sup>
Aspartic acid	0.046	0.77	4.05x10 <sup>-27</sup>
DCER (24:0)	0.072	-0.77	4.09x10 <sup>-27</sup>

PI (18:0/20:3)	0.069	-0.77	4.09x10 <sup>-27</sup>
HDA2	0.063	-0.77	4.99x10 <sup>-27</sup>
PE.P (16:0/20:5)	0.060	-0.76	7.34x10 <sup>-27</sup>
PE.P (16:0/18:1)	0.063	-0.76	8.05x10 <sup>-27</sup>
HDA1	0.066	-0.76	1.29x10 <sup>-26</sup>
PC (18:1/20:3)	0.070	-0.75	3.20x10 <sup>-26</sup>
PE.O (16:0/22:4)	0.056	-0.75	3.59x10 <sup>-26</sup>
PC (14:0/20:4)	0.066	-0.75	4.26x10 <sup>-26</sup>
HCER (20:0)	0.059	-0.75	4.62x10 <sup>-26</sup>
PC (14:0/18:3)	0.050	-0.75	8.38x10 <sup>-26</sup>
LPC (18:3)	0.060	-0.75	8.78x10 <sup>-26</sup>
Neopterin/tryptophan	0.024	0.71	1.49x10 <sup>-25</sup>
MAG (20:4)	0.015	0.74	1.52x10 <sup>-25</sup>
TPA1	0.066	-0.74	1.68x10 <sup>-25</sup>
PC (18:2/16:1)	0.065	-0.74	1.68x10 <sup>-25</sup>
PC (16:0/20:1)	0.068	-0.74	1.69x10 <sup>-25</sup>
Fisher's ratio	0.046	-0.74	2.07x10 <sup>-25</sup>
PI (20:0/20:4)	0.065	-0.74	2.27x10 <sup>-25</sup>
PC (20:0/20:4)	0.067	-0.74	2.38x10 <sup>-25</sup>
PC (18:0/20:2)	0.069	-0.74	4.68x10 <sup>-25</sup>
PI (18:1/20:3)	0.063	-0.73	5.49x10 <sup>-25</sup>
LPI (18:2)	0.049	-0.73	5.56x10 <sup>-25</sup>
PC (14:0/22:6)	0.065	-0.73	1.10x10 <sup>-24</sup>
PC (18:0/18:2)	0.068	-0.73	1.44x10 <sup>-24</sup>
H3FC	0.062	-0.72	2.53x10 <sup>-24</sup>
Quinolinic acid/tryptophan	0.016	0.72	3.12x10 <sup>-24</sup>
PE.P (18:1/20:3)	0.062	-0.72	3.79x10 <sup>-24</sup>
PE.P (18:1/20:5)	0.055	-0.72	6.03x10 <sup>-24</sup>
PS (20:0/18:2)	0.065	-0.72	6.67x10 <sup>-24</sup>
LPC (20:2)	0.067	-0.72	7.30x10 <sup>-24</sup>
LPI (20:4)	0.048	-0.72	8.16x10 <sup>-24</sup>
PG (20:0/18:2)	0.056	-0.72	8.18x10 <sup>-24</sup>
PE.O (16:0/22:6)	0.055	-0.71	8.75x10 <sup>-24</sup>
CER (24:0)	0.066	-0.71	9.16x10 <sup>-24</sup>
DCER (26:0)	0.062	-0.71	1.48x10 <sup>-23</sup>
PI (18:2/18:2)	0.051	-0.71	1.49x10 <sup>-23</sup>
HCER (14:0)	0.057	-0.71	1.61x10 <sup>-23</sup>

HDCH	0.061	-0.71	2.04x10 <sup>-23</sup>
PC (18:1/20:1)	0.061	-0.71	2.39x10 <sup>-23</sup>
PS (18:0/18:0)	0.041	0.71	2.40x10 <sup>-23</sup>
PC (14:0/20:3)	0.062	-0.71	2.71x10 <sup>-23</sup>
LPE (18:2)	0.052	-0.70	4.36x10 <sup>-23</sup>
Phenylalanine	0.046	0.70	6.63x10 <sup>-23</sup>
H2TG	0.038	0.70	6.63x10 <sup>-23</sup>
PC (18:1/18:3)	0.049	-0.70	8.92x10 <sup>-23</sup>
CE (16:0)	0.060	-0.70	9.44x10 <sup>-23</sup>
H3CH	0.061	-0.70	1.18x10 <sup>-22</sup>
L4TG	0.042	0.70	1.27x10 <sup>-22</sup>
PE.P (16:0/20:3)	0.059	-0.69	1.75x10 <sup>-22</sup>
PE.P (16:0/16:1)	0.054	-0.69	1.99x10 <sup>-22</sup>
PE.P (18:1/20:2)	0.063	-0.69	2.55x10 <sup>-22</sup>
MAG (18:1)	0.015	0.69	2.81x10 <sup>-22</sup>
PC (14:0/18:1)	0.058	-0.68	6.84x10 <sup>-22</sup>
SM (14:0)	0.063	-0.68	7.59x10 <sup>-22</sup>
PC (20:0/22:5)	0.057	-0.68	2.20x10 <sup>-21</sup>
DCER (26:1)	0.060	-0.67	2.36x10 <sup>-21</sup>
HCER.d (18:0/20:0)	0.055	-0.67	2.36x10 <sup>-21</sup>
PI (18:0/20:4)	0.061	-0.67	2.36x10 <sup>-21</sup>
PC (14:0/20:5)	0.049	-0.67	3.20x10 <sup>-21</sup>
Histidine	0.046	-0.67	3.34x10 <sup>-21</sup>
CE (18:1)	0.057	-0.67	4.03x10 <sup>-21</sup>
PC (18:0/20:3)	0.063	-0.67	4.09x10 <sup>-21</sup>
PE.P (18:1/18:0)	0.055	-0.67	5.09x10 <sup>-21</sup>
LCER (24:0)	0.054	-0.67	5.37x10 <sup>-21</sup>
L1TG	0.037	0.67	5.50x10 <sup>-21</sup>
L5TG	0.041	0.67	5.69x10 <sup>-21</sup>
Quinolinic acid	0.020	0.67	6.90x10 <sup>-21</sup>
PC (18:1/22:4)	0.056	-0.66	1.00x10 <sup>-20</sup>
CE (18:3)	0.050	-0.66	1.11x10 <sup>-20</sup>
PS (18:0/20:4)	0.047	-0.66	1.29x10 <sup>-20</sup>
Neopterin	0.026	0.66	1.39x10 <sup>-20</sup>
CER (18:0)	0.036	0.66	2.41x10 <sup>-20</sup>
PC (14:0/14:0)	0.040	-0.66	2.90x10 <sup>-20</sup>
CE (14:0)	0.053	-0.65	3.66x10 <sup>-20</sup>

Citrulline	0.042	-0.65	4.91x10 <sup>-20</sup>
L2TG	0.041	0.65	5.56x10 <sup>-20</sup>
PC (14:0/22:5)	0.053	-0.65	5.69x10 <sup>-20</sup>
PC (16:0/18:0)	0.019	-0.65	6.19x10 <sup>-20</sup>
HDPL	0.058	-0.65	7.11x10 <sup>-20</sup>
LPE (20:3)	0.042	-0.65	9.47x10 <sup>-20</sup>
PE (18:2/16:1)	0.055	-0.65	1.24x10 <sup>-19</sup>
LPC (20:4)	0.057	-0.64	2.25x10 <sup>-19</sup>
LPC (22:5)	0.055	-0.64	3.79x10 <sup>-19</sup>
PC (16:0/20:3)	0.063	-0.64	4.08x10 <sup>-19</sup>
H3PL	0.055	-0.64	4.49x10 <sup>-19</sup>
H3A1	0.058	-0.63	7.57x10 <sup>-19</sup>
PG (20:0/20:3)	0.038	-0.63	8.70x10 <sup>-19</sup>
PE.P (18:0/20:5)	0.051	-0.63	1.12x10 <sup>-19</sup>
LCER.d (18:0/22:0)	0.052	-0.63	1.44x10 <sup>-18</sup>
PC (18:0/18:1)	0.049	-0.63	1.44x10 <sup>-18</sup>
CE (22:0)	0.053	-0.63	1.44x10 <sup>-18</sup>
PC (18:0/18:0)	0.050	-0.63	1.51x10 <sup>-18</sup>
PS (20:0/18:3)	0.049	-0.63	1.51x10 <sup>-18</sup>
LPC (18:0)	0.062	-0.62	1.87x10 <sup>-18</sup>
CE (24:0)	0.047	-0.62	2.09x10 <sup>-18</sup>
LPE (20:4)	0.045	-0.62	3.38x10 <sup>-18</sup>
LCER.d (18:0/24:0)	0.051	-0.62	3.52x10 <sup>-18</sup>
PS (20:0/20:4)	0.057	-0.62	4.75x10 <sup>-18</sup>
DCER (22:0)	0.052	-0.62	5.19x10 <sup>-18</sup>
PC (14:0/22:4)	0.049	-0.61	6.72x10 <sup>-18</sup>
PS (20:0/20:5)	0.047	-0.61	6.94x10 <sup>-18</sup>
PE.O (18:0/18:2)	0.039	-0.61	1.07x10 <sup>-17</sup>
VLPN	0.032	0.61	1.35x10 <sup>-17</sup>
VLAB	0.032	0.61	1.35x10 <sup>-17</sup>
ABA1	0.040	0.61	1.51x10 <sup>-17</sup>
LPC (22:4)	0.052	-0.61	1.57x10 <sup>-17</sup>
PG (18:0/18:2)	0.049	-0.60	2.60x10 <sup>-17</sup>
PC (18:1/22:6)	0.057	-0.60	2.78x10 <sup>-17</sup>
PC (18:0/22:4)	0.052	-0.60	3.27x10 <sup>-17</sup>
DCER (22:1)	0.050	-0.60	3.91x10 <sup>-17</sup>
V4TG	0.033	0.60	4.83x10 <sup>-17</sup>

PI (16:0/20:3)	0.053	-0.60	$5.15 \times 10^{-17}$
PI (18:0/20:2)	0.042	-0.59	$6.92 \times 10^{-17}$
LPE (18:1)	0.051	-0.59	$7.48 \times 10^{-17}$
PE (18:2/20:4)	0.054	-0.59	$1.03 \times 10^{-16}$
PE (18:2/18:2)	0.053	-0.59	$1.19 \times 10^{-16}$
Glutamine	0.037	-0.59	$1.27 \times 10^{-16}$
LPC (22:6)	0.050	-0.59	$1.40 \times 10^{-16}$
PG (18:0/18:1)	0.051	-0.59	$1.71 \times 10^{-16}$
SM (20:1)	0.050	-0.59	$1.91 \times 10^{-16}$
PC (16:0/20:4)	0.053	-0.59	$1.96 \times 10^{-16}$
PC (14:0/20:2)	0.051	-0.59	$2.07 \times 10^{-16}$
PC (18:1/18:1)	0.050	-0.58	$2.26 \times 10^{-16}$
LPE (18:3)	0.028	-0.58	$2.52 \times 10^{-16}$
PI (18:0/18:1)	0.050	-0.58	$3.01 \times 10^{-16}$
CE (18:0)	0.052	-0.58	$4.67 \times 10^{-16}$
SM (24:1)	0.051	-0.58	$5.75 \times 10^{-16}$
HCER.d (18:0/26:0)	0.045	-0.58	$5.78 \times 10^{-16}$
PG (18:1/16:1)	0.045	0.58	$6.63 \times 10^{-16}$
MAG (22:5)	0.013	0.58	$6.77 \times 10^{-16}$
V3TG	0.027	0.57	$1.40 \times 10^{-15}$
CE (20:2)	0.053	-0.57	$1.51 \times 10^{-15}$
PE.P (16:0/22:6)	0.050	-0.57	$1.51 \times 10^{-15}$
LPE (20:1)	0.049	-0.57	$1.91 \times 10^{-15}$
PI (16:0/20:4)	0.047	-0.56	$4.21 \times 10^{-15}$
PC (16:0/22:4)	-0.050	-0.56	$4.85 \times 10^{-15}$
V2FC	0.025	0.56	$5.15 \times 10^{-15}$
H1TG	0.027	0.55	$7.66 \times 10^{-15}$
PI (18:0/22:4)	0.049	-0.55	$1.04 \times 10^{-14}$
PG (20:0/20:5)	0.035	-0.55	$1.11 \times 10^{-14}$
LPE (20:2)	0.041	-0.55	$1.15 \times 10^{-14}$
LCER (14:0)	0.042	-0.55	$1.66 \times 10^{-14}$
CE (20:3)	0.053	-0.54	$2.30 \times 10^{-14}$
L6TG	0.035	0.54	$2.54 \times 10^{-14}$
HDFC	0.050	-0.54	$2.94 \times 10^{-14}$
LPC (20:5)	0.040	-0.54	$3.71 \times 10^{-14}$
Kynurenine/tryptophan	0.033	0.54	$3.84 \times 10^{-14}$
PS (20:0/22:6)	0.051	-0.54	$4.10 \times 10^{-14}$

SM (22:1)	0.044	-0.54	4.70x10 <sup>-14</sup>
PG (18:0/20:0)	0.036	0.54	4.80x10 <sup>-14</sup>
PC (18:2/20:1)	0.042	-0.53	1.08x10 <sup>-13</sup>
PE.O (18:0/20:4)	0.040	-0.53	1.13x10 <sup>-13</sup>
PC (16:0/20:5)	0.040	-0.53	1.18x10 <sup>-13</sup>
V3FC	0.024	0.53	1.42x10 <sup>-13</sup>
MAG (22:4)	0.014	0.53	1.51x10 <sup>-13</sup>
PI (20:0/16:1)	0.050	-0.53	1.52x10 <sup>-13</sup>
PC (16:0/14:0)	0.040	-0.53	1.57x10 <sup>-13</sup>
CE (20:1)	0.037	-0.52	2.48x10 <sup>-13</sup>
MAG (16:0)	0.012	0.52	2.88x10 <sup>-13</sup>
PI (16:0/18:1)	0.045	-0.52	3.00x10 <sup>-13</sup>
PC (16:1/18:1)	0.036	-0.52	3.29x10 <sup>-13</sup>
MAG (18:2)	0.013	0.52	5.34x10 <sup>-13</sup>
H2A1	0.048	-0.51	6.06x10 <sup>-13</sup>
LCER (16:0)	0.038	-0.51	8.86x10 <sup>-13</sup>
PG (18:1/18:2)	0.035	0.51	9.70x10 <sup>-13</sup>
PC (18:0/14:0)	0.044	-0.51	1.05x10 <sup>-12</sup>
PE.P (16:0/18:0)	0.044	-0.51	1.22x10 <sup>-12</sup>
Threonine	0.027	-0.51	1.24x10 <sup>-12</sup>
3-Hydroxykynurenine	0.022	0.47	1.42x10 <sup>-12</sup>
H3TG	0.024	0.51	1.53x10 <sup>-12</sup>
PG (20:0/20:1)	0.047	-0.51	1.58x10 <sup>-12</sup>
PC (16:0/22:6)	0.049	-0.51	1.61x10 <sup>-12</sup>
LPC (14:0)	0.046	-0.50	1.87x10 <sup>-12</sup>
PI (16:0/20:2)	0.047	-0.50	1.95x10 <sup>-12</sup>
Lactic acid	0.030	0.50	2.42x10 <sup>-12</sup>
PE (18:1/18:2)	0.036	-0.50	2.38x10 <sup>-12</sup>
HCER.d (18:0/26:1)	0.032	-0.50	2.45x10 <sup>-12</sup>
V4PL	0.031	0.50	2.96x10 <sup>-12</sup>
HCER (22:1)	-0.037	-0.50	2.95x10 <sup>-12</sup>
LPC (20:1)	0.051	-0.50	3.23x10 <sup>-12</sup>
PC (16:0/18:3)	0.026	-0.50	3.96x10 <sup>-12</sup>
PC (16:0/18:1)	0.040	-0.50	4.32x10 <sup>-12</sup>
H3A2	0.046	-0.49	6.54x10 <sup>-12</sup>
PI (18:0/20:0)	0.039	0.49	6.54x10 <sup>-12</sup>
PC (18:1/20:4)	0.046	-0.49	7.01x10 <sup>-12</sup>

V2TG	0.018	0.49	$7.88 \times 10^{-12}$
PE.P (18:1/22:6)	0.047	-0.49	$1.14 \times 10^{-11}$
TPCH	0.048	-0.48	$1.48 \times 10^{-11}$
CE (22:5)	0.043	-0.48	$1.51 \times 10^{-11}$
LCER (26:1)	0.041	-0.48	$1.85 \times 10^{-11}$
PS (20:0/22:5)	0.049	-0.48	$3.29 \times 10^{-11}$
MAG (16:1)	0.011	0.47	$5.62 \times 10^{-11}$
TPTG	0.013	0.47	$5.75 \times 10^{-11}$
Glucose	0.024	0.47	$5.94 \times 10^{-11}$
LCER (24:1)	0.037	-0.47	$5.94 \times 10^{-11}$
V3PL	0.025	0.47	$6.29 \times 10^{-11}$
Methionine	0.016	-0.47	$7.06 \times 10^{-11}$
HDTG	0.021	0.47	$7.51 \times 10^{-11}$
PE (18:1/18:3)	0.029	-0.46	$1.31 \times 10^{-10}$
L3TG	0.031	0.46	$1.52 \times 10^{-10}$
H1FC	0.043	-0.46	$1.71 \times 10^{-10}$
PC (16:0/20:2)	0.045	-0.46	$1.88 \times 10^{-10}$
MAG (22:6)	0.012	0.46	$2.04 \times 10^{-10}$
HCER (26:1)	0.036	-0.45	$2.71 \times 10^{-10}$
CE (20:0)	0.035	-0.45	$2.74 \times 10^{-10}$
PE.P (18:0/22:6)	0.042	-0.45	$3.55 \times 10^{-10}$
HCER.d (18:0/24:1)	0.034	-0.45	$3.99 \times 10^{-10}$
V5TG	0.024	0.45	$5.21 \times 10^{-10}$
HCER (18:0)	0.032	-0.44	$6.39 \times 10^{-10}$
PC (16:0/22:5)	0.042	-0.44	$7.67 \times 10^{-10}$
SM (18:1)	0.042	-0.44	$9.01 \times 10^{-10}$
SM (26:1)	0.035	-0.44	$1.00 \times 10^{-9}$
L4CH	0.041	-0.44	$1.26 \times 10^{-9}$
MAG (20:2)	0.011	0.43	$1.57 \times 10^{-9}$
H2FC	0.039	-0.43	$1.62 \times 10^{-9}$
L1CH	0.028	-0.43	$1.77 \times 10^{-9}$
PS (20:0/20:3)	0.040	-0.43	$1.82 \times 10^{-9}$
CE (20:5)	0.035	-0.43	$2.84 \times 10^{-9}$
Tryptophan	0.033	-0.42	$4.02 \times 10^{-9}$
V3CH	0.023	0.42	$4.15 \times 10^{-9}$
DAG (16:0/20:4)	0.008	0.42	$4.43 \times 10^{-9}$
LPE (16:1)	0.025	-0.42	$6.29 \times 10^{-9}$

PE.O (18:0/22:6)	0.037	-0.41	8.67x10 <sup>-9</sup>
CER (22:1)	0.022	0.41	9.89x10 <sup>-9</sup>
V4FC	0.026	0.41	1.21x10 <sup>-8</sup>
VLTG	0.010	0.41	1.34x10 <sup>-8</sup>
PE (18:0/22:6)	0.015	0.41	1.38x10 <sup>-8</sup>
PE (18:2/18:3)	0.020	-0.41	1.39x10 <sup>-8</sup>
LPE (22:4)	0.021	-0.41	1.41x10 <sup>-8</sup>
LPC (16:0)	0.046	-0.41	1.46x10 <sup>-8</sup>
V2PL	0.016	0.41	1.74x10 <sup>-8</sup>
Acetone	0.015	0.40	1.96x10 <sup>-8</sup>
LDCH	0.037	-0.40	2.88x10 <sup>-8</sup>
CER (14:0)	0.040	-0.40	3.99x10 <sup>-8</sup>
DAG (16:0/18:1)	0.007	0.40	4.05x10 <sup>-8</sup>
PE.P (16:0/16:0)	0.033	-0.39	5.80x10 <sup>-8</sup>
3-Hydroxybutyric acid	0.022	0.39	6.03x10 <sup>-8</sup>
FFA (24:0)	0.033	-0.39	6.05x10 <sup>-8</sup>
PI (18:1/16:1)	0.032	-0.39	7.33x10 <sup>-8</sup>
Kynurenic acid	0.011	-0.39	8.31x10 <sup>-8</sup>
LCER (18:1)	0.028	-0.39	8.90x10 <sup>-8</sup>
IDPN	0.025	0.39	8.98x10 <sup>-8</sup>
IDAB	0.025	0.39	9.00x10 <sup>-8</sup>
VLCH	0.016	0.39	9.20x10 <sup>-8</sup>
PC (18:1/20:5)	0.024	-0.39	9.86x10 <sup>-8</sup>
HCER (24:1)	0.032	-0.38	1.08x10 <sup>-7</sup>
PE (16:0/18:1)	0.012	0.38	1.09x10 <sup>-7</sup>
PS (20:0/22:4)	0.027	-0.38	1.16x10 <sup>-7</sup>
DCER (18:0)	0.025	0.38	1.17x10 <sup>-7</sup>
LPC (16:1)	0.035	-0.38	1.26x10 <sup>-7</sup>
LPG (18:1)	0.025	-0.38	1.34x10 <sup>-7</sup>
PE.P (18:0/16:1)	0.037	-0.38	1.84x10 <sup>-7</sup>
L4PL	0.037	-0.38	2.00x10 <sup>-7</sup>
PG (18:1/20:4)	0.028	0.38	2.18x10 <sup>-7</sup>
DAG (18:1/20:4)	0.011	0.37	2.43x10 <sup>-7</sup>
DAG (16:0/22:6)	0.008	0.37	2.46x10 <sup>-7</sup>
PS (18:0/18:1)	0.013	0.37	2.66x10 <sup>-7</sup>
TAG (55:5)_FA (20:4)	0.008	0.37	2.70x10 <sup>-7</sup>
3-Hydroxykynurenine	0.019	0.37	3.60x10 <sup>-7</sup>

V2CH	0.015	0.37	$3.84 \times 10^{-7}$
L4FC	0.037	-0.37	$4.70 \times 10^{-7}$
PE (18:0/22:4)	0.025	-0.36	$5.13 \times 10^{-7}$
PE (18:1/20:4)	0.031	-0.36	$5.47 \times 10^{-7}$
PI (16:0/22:4)	0.032	-0.36	$6.05 \times 10^{-7}$
MAG (18:0)	0.017	0.36	$7.02 \times 10^{-7}$
V4CH	0.025	0.36	$7.26 \times 10^{-7}$
LPE (22:5)	0.013	-0.36	$7.64 \times 10^{-7}$
L3CH	0.032	-0.36	$8.91 \times 10^{-7}$
PI (18:0/18:3)	0.023	-0.36	$8.99 \times 10^{-7}$
PI (16:0/18:2)	0.034	-0.35	$1.10 \times 10^{-6}$
PI (18:0/18:2)	0.036	-0.35	$1.35 \times 10^{-6}$
TAG (54:4)_FA (20:4)	0.010	0.35	$1.40 \times 10^{-6}$
TAG (54:5)_FA (20:4)	0.013	0.35	$1.53 \times 10^{-6}$
PC (18:1/22:5)	0.036	-0.35	$2.02 \times 10^{-6}$
LPE (16:0)	0.029	-0.34	$2.90 \times 10^{-6}$
PC (18:0/18:3)	0.011	-0.34	$2.99 \times 10^{-6}$
CER (20:1)	0.019	0.34	$3.23 \times 10^{-6}$
CER (22:0)	0.032	-0.34	$3.43 \times 10^{-6}$
DAG (16:0/18:2)	0.002	0.33	$4.63 \times 10^{-6}$
LCER (20:0)	0.027	-0.33	$5.13 \times 10^{-6}$
DAG (18:2/22:4)	0.007	0.33	$5.14 \times 10^{-6}$
HCER (16:0)	0.026	-0.33	$5.29 \times 10^{-6}$
CE (22:4)	0.026	-0.33	$5.39 \times 10^{-6}$
PG (20:0/22:5)	0.012	-0.33	$5.69 \times 10^{-6}$
TAG (54:5)_FA (16:0)	0.007	0.33	$5.91 \times 10^{-6}$
TAG (52:4)_FA (20:4)	0.006	0.32	$1.06 \times 10^{-5}$
PI (20:0/18:1)	0.022	-0.32	$1.10 \times 10^{-5}$
PE (18:1/20:3)	0.028	-0.32	$1.18 \times 10^{-5}$
TAG (56:6)_FA (18:0)	0.012	0.32	$1.23 \times 10^{-5}$
TAG (54:6)_FA (20:4)	0.008	0.32	$1.25 \times 10^{-5}$
TAG (56:5)_FA (20:4)	0.014	0.32	$1.30 \times 10^{-5}$
VLFC	0.011	0.32	$1.44 \times 10^{-5}$
TAG (54:6)_FA (16:0)	0.004	0.31	$1.98 \times 10^{-5}$
IDTG	0.003	0.31	$2.54 \times 10^{-5}$
CER (20:0)	0.013	0.31	$2.56 \times 10^{-5}$
DAG (18:1/22:4)	0.007	0.31	$2.68 \times 10^{-5}$

DAG (16:0/16:0)	0.004	0.31	2.78x10 <sup>-5</sup>
V1TG	0.001	0.31	2.89x10 <sup>-5</sup>
LDPL	0.029	-0.31	2.91x10 <sup>-5</sup>
DAG (18:2/20:4)	0.006	0.31	2.93x10 <sup>-5</sup>
TAG (54:4)_FA (22:4)	0.002	0.30	3.57x10 <sup>-5</sup>
TAG (56:5)_FA (18:0)	0.012	0.30	3.77x10 <sup>-5</sup>
PI (16:0/18:0)	0.027	-0.30	4.40x10 <sup>-5</sup>
TAG (58:7)_FA (18:0)	0.006	0.30	4.43x10 <sup>-5</sup>
PG (18:1/20:2)	0.027	-0.30	4.77x10 <sup>-5</sup>
CE (16:1)	0.024	-0.30	5.97x10 <sup>-5</sup>
PC (16:0/16:1)	0.023	-0.29	6.60x10 <sup>-5</sup>
SM (18:0)	0.024	-0.29	6.88x10 <sup>-5</sup>
TAG (56:4)_FA (20:4)	0.009	0.29	6.88x10 <sup>-5</sup>
DAG (18:1/22:6)	0.008	0.29	8.08x10 <sup>-5</sup>
H2A2	0.029	-0.29	8.36x10 <sup>-5</sup>
TAG (58:6)_FA (18:0)	0.003	0.29	8.82x10 <sup>-5</sup>
PI (18:0/20:5)	0.014	-0.29	9.04x10 <sup>-5</sup>
DAG (16:0/20:5)	0.004	0.29	1.05x10 <sup>-4</sup>
CER (24:1)	0.009	0.29	1.09x10 <sup>-4</sup>
Citric acid	0.020	0.28	1.10x10 <sup>-4</sup>
L3PL	0.026	-0.28	1.19x10 <sup>-4</sup>
DAG (16:0/22:5)	0.005	0.28	1.21x10 <sup>-4</sup>
TAG (54:5)_FA (22:5)	0.003	0.28	1.29x10 <sup>-4</sup>
Asparagine	0.010	-0.28	1.34x10 <sup>-4</sup>
MAG (14:0)	0.008	0.28	1.43x10 <sup>-4</sup>
PG (18:2/16:1)	0.028	0.28	1.59x10 <sup>-4</sup>
H2CH	0.031	-0.28	1.59x10 <sup>-4</sup>
FFA (20:4)	0.008	0.28	1.59x10 <sup>-4</sup>
PI (18:0/22:5)	0.030	-0.28	1.61x10 <sup>-4</sup>
V1PL	0.001	0.28	1.72x10 <sup>-4</sup>
VLPL	0.009	0.28	1.92x10 <sup>-4</sup>
LDLC	0.027	-0.27	2.18x10 <sup>-4</sup>
PG (20:0/20:4)	0.011	-0.27	2.24x10 <sup>-4</sup>
PS (20:0/16:1)	0.015	-0.27	2.42x10 <sup>-4</sup>
L1FC	0.018	-0.27	2.53x10 <sup>-4</sup>
TAG (53:5)_FA (20:4)	0.002	0.27	2.74x10 <sup>-4</sup>
DAG (18:0/18:1)	0.004	0.27	2.89x10 <sup>-4</sup>

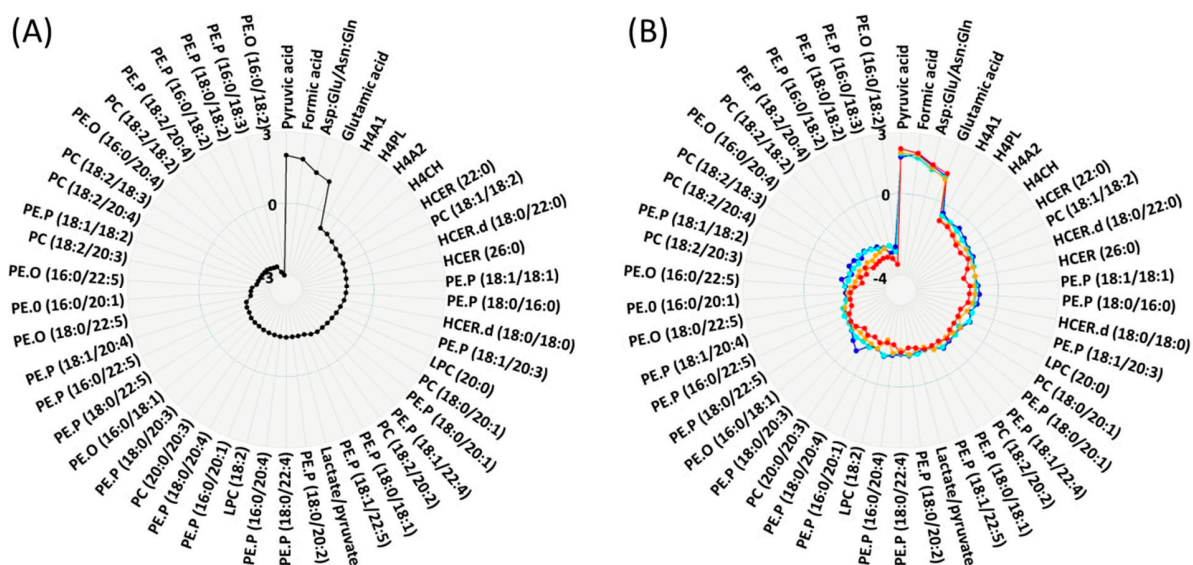
TAG (58:8)_FA (20:3)	0.030	-0.27	3.20x10 <sup>-4</sup>
Indole-3-acetic acid	0.008	-0.26	3.63x10 <sup>-4</sup>
TAG (56:6)_FA (20:4)	0.006	0.26	3.66x10 <sup>-4</sup>
L4PN	0.028	-0.26	4.34x10 <sup>-4</sup>
IDCH	0.014	0.26	4.34x10 <sup>-4</sup>
L1PL	0.013	-0.26	4.34x10 <sup>-4</sup>
L4AB	0.028	-0.26	4.34x10 <sup>-4</sup>
CER (16:0)	0.013	0.26	4.43x10 <sup>-4</sup>
MAG (18:3)	0.010	0.26	4.63x10 <sup>-4</sup>
DAG (16:0/16:1)	0.001	0.26	4.74x10 <sup>-4</sup>
CE (22:2)	0.023	-0.26	5.08x10 <sup>-4</sup>
Kynurenine	0.021	0.25	6.21x10 <sup>-4</sup>
PE (16:0/20:5)	0.020	-0.25	6.29x10 <sup>-4</sup>
CE (22:6)	0.028	-0.25	6.33x10 <sup>-4</sup>
PI (16:0_22:6)	0.025	-0.25	6.34x10 <sup>-4</sup>
TAG (58:6)_FA (22:4)	0.004	0.25	7.31x10 <sup>-4</sup>
Creatine	0.015	0.25	7.31x10 <sup>-4</sup>
TAG (51:1)_FA (18:1)	0.001	0.25	8.20x10 <sup>-4</sup>
DAG (18:1/18:1)	0.004	0.25	8.28x10 <sup>-4</sup>
DAG (16:1/20:4)	0.004	0.25	8.99x10 <sup>-4</sup>
L2CH	0.016	-0.24	1.10x10 <sup>-3</sup>
TAG (50:1)_FA (18:1)	0.006	0.24	1.21x10 <sup>-3</sup>
TAG (51:1)_FA (17:0)	0.000	0.24	1.21x10 <sup>-3</sup>
TAG (54:3)_FA (18:0)	0.005	0.24	1.36x10 <sup>-3</sup>
L3FC	0.024	-0.24	1.43x10 <sup>-3</sup>
DAG (18:0/18:2)	0.000	0.24	1.53x10 <sup>-3</sup>
DAG (16:1/18:2)	0.000	0.24	1.63x10 <sup>-3</sup>
TAG (51:1)_FA (16:0)	0.001	0.23	1.78x10 <sup>-3</sup>
TAG (56:5)_FA (22:4)	0.002	0.23	1.79x10 <sup>-3</sup>
TAG (54:8)_FA (18:3)	0.012	-0.23	1.80x10 <sup>-3</sup>
TAG (51:2)_FA (17:0)	0.001	0.23	1.82x10 <sup>-3</sup>
PE.O (18:0/18:1)	0.015	0.23	1.96x10 <sup>-3</sup>
TAG (50:2)_FA (16:0)	0.004	0.23	2.29x10 <sup>-3</sup>
LPE (18:0)	0.029	-0.23	2.35x10 <sup>-3</sup>
TAG (58:6)_FA (18:1)	0.003	0.23	2.44x10 <sup>-3</sup>
TAG (56:6)_FA (22:4)	0.000	0.23	2.53x10 <sup>-3</sup>
TAG (53:3)_FA (17:0)	0.002	0.23	2.59x10 <sup>-3</sup>

PE (18:0/20:0)	0.031	-0.23	2.69x10 <sup>-3</sup>
TAG (51:4)_FA (20:4)	0.002	0.23	2.70x10 <sup>-3</sup>
PI (18:0/22:6)	0.025	-0.23	2.71x10 <sup>-3</sup>
IDFC	0.011	0.22	2.82x10 <sup>-3</sup>
TAG (50:2)_FA (18:2)	0.000	0.22	2.86x10 <sup>-3</sup>
TAG (58:6)_FA (22:5)	0.001	0.22	2.89x10 <sup>-3</sup>
DCER (20:0)	0.013	-0.22	3.09x10 <sup>-3</sup>
TAG (49:0)_FA (16:0)	0.000	0.22	3.09x10 <sup>-3</sup>
TAG (53:1)_FA (18:1)	0.000	0.22	3.09x10 <sup>-3</sup>
TAG (49:0)_FA (17:0)	0.002	0.22	3.19x10 <sup>-3</sup>
TAG (53:2)_FA (17:0)	0.001	0.22	3.20x10 <sup>-3</sup>
DAG (16:1/18:0)	0.003	0.22	3.39x10 <sup>-3</sup>
TAG (56:4)_FA (22:4)	0.000	0.22	3.44x10 <sup>-3</sup>
TAG (56:6)_FA (18:1)	0.001	0.22	3.73x10 <sup>-3</sup>
TAG (50:1)_FA (16:0)	0.004	0.22	3.75x10 <sup>-3</sup>
PC (18:0/16:1)	0.016	-0.22	4.20x10 <sup>-3</sup>
TAG (52:2)_FA (18:0)	0.002	0.22	4.22x10 <sup>-3</sup>
TAG (54:2)_FA (18:0)	0.004	0.22	4.22x10 <sup>-3</sup>
Isoleucine	0.011	-0.22	4.39x10 <sup>-3</sup>
TAG (53:2)_FA (18:1)	0.000	0.22	4.39x10 <sup>-3</sup>
DAG (18:0/18:3)	0.000	0.22	4.39x10 <sup>-3</sup>
TAG (48:5)_FA (18:3)	0.021	-0.21	4.43x10 <sup>-3</sup>
TAG (52:2)_FA (16:1)	0.001	0.21	4.82x10 <sup>-3</sup>
LCER (18:0)	0.018	-0.21	4.82x10 <sup>-3</sup>
TAG (51:2)_FA (18:2)	0.005	0.21	4.83x10 <sup>-3</sup>
TAG (58:8)_FA (18:1)	0.005	0.21	5.48x10 <sup>-3</sup>
PS (18:0/20:0)	0.019	0.21	5.63x10 <sup>-3</sup>
TAG (52:3)_FA (18:0)	0.000	0.21	6.00x10 <sup>-3</sup>
TAG (48:1)_FA (16:1)	0.001	0.21	6.48x10 <sup>-3</sup>
PG (20:0/16:1)	0.003	-0.21	6.58x10 <sup>-3</sup>
SM (22:0)	0.005	-0.21	6.84x10 <sup>-3</sup>
TAG (53:1)_FA (17:0)	0.001	0.20	7.18x10 <sup>-3</sup>
TAG (56:8)_FA (16:0)	0.003	0.20	7.91x10 <sup>-3</sup>
FFA (22:6)	0.012	-0.20	8.06x10 <sup>-3</sup>
TAG (56:5)_FA (16:0)	0.000	0.20	8.06x10 <sup>-3</sup>
FFA (20:1)	0.011	0.20	8.41x10 <sup>-3</sup>
TAG (50:2)_FA (16:1)	0.003	0.20	9.09x10 <sup>-3</sup>

DAG (18:2/22:5)	0.004	0.20	9.37x10 <sup>-3</sup>
PG (18:2/18:2)	0.001	-0.20	9.51x10 <sup>-3</sup>
PG (16:0/18:2)	0.031	-0.20	9.56x10 <sup>-3</sup>
HCER (20:1)	0.015	-0.20	9.93x10 <sup>-3</sup>
TAG (58:7)_FA (18:1)	0.002	0.20	9.93x10 <sup>-3</sup>
TAG (56:7)_FA (20:3)	0.025	-0.20	9.98x10 <sup>-3</sup>
TAG (52:1)_FA (18:1)	0.003	0.20	1.00x10 <sup>-2</sup>
TAG (51:1)_FA (18:0)	0.001	0.20	1.03x10 <sup>-2</sup>
PE (18:0/18:2)	0.020	-0.20	1.05x10 <sup>-2</sup>
TAG (53:1)_FA (18:0)	0.000	0.20	1.05x10 <sup>-2</sup>
TAG (52:3)_FA (20:0)	0.001	0.20	1.05x10 <sup>-2</sup>
PC (18:1/20:2)	0.022	-0.19	1.07x10 <sup>-2</sup>
TAG (56:6)_FA (16:0)	0.002	0.19	1.10x10 <sup>-2</sup>
TAG (56:6)_FA (20:3)	0.025	-0.19	1.10x10 <sup>-2</sup>
TAG (56:7)_FA (20:4)	0.001	0.19	1.15x10 <sup>-2</sup>
TAG (54:3)_FA (18:1)	0.002	0.19	1.21x10 <sup>-2</sup>
DAG (16:1/22:6)	0.003	0.19	1.23x10 <sup>-2</sup>
PI (16:0/22:5)	0.022	-0.19	1.26x10 <sup>-2</sup>
TAG (56:6)_FA (22:6)	0.002	0.19	1.27x10 <sup>-2</sup>
TAG (54:4)_FA (18:0)	0.000	0.19	1.27x10 <sup>-2</sup>
PI (18:0/18:0)	0.015	-0.19	1.31x10 <sup>-2</sup>
TAG (49:1)_FA (18:1)	0.004	0.19	1.32x10 <sup>-2</sup>
PE (18:0/20:1)	0.021	-0.19	1.32x10 <sup>-2</sup>
TAG (56:2)_FA (20:0)	0.016	-0.19	1.32x10 <sup>-2</sup>
TAG (52:1)_FA (16:0)	0.003	0.19	1.36x10 <sup>-2</sup>
PE (18:1/18:1)	0.007	0.19	1.40x10 <sup>-2</sup>
TAG (53:2)_FA (18:2)	0.004	0.19	1.43x10 <sup>-2</sup>
PG (20:0/18:1)	0.007	-0.19	1.43x10 <sup>-2</sup>
TAG (50:4)_FA (20:3)	0.020	-0.19	1.54x10 <sup>-2</sup>
TAG (54:2)_FA (18:1)	0.002	0.18	1.61x10 <sup>-2</sup>
TAG (49:1)_FA (16:1)	0.002	0.18	1.64x10 <sup>-2</sup>
LDHD	0.011	0.18	1.66x10 <sup>-2</sup>
TAG (51:2)_FA (18:1)	0.003	0.18	1.73x10 <sup>-2</sup>
TAG (56:3)_FA (20:0)	0.019	-0.18	1.73x10 <sup>-2</sup>
TAG (48:0)_FA (16:0)	0.000	0.18	1.82x10 <sup>-2</sup>
TAG (48:4)_FA (18:3)	0.019	-0.18	1.82x10 <sup>-2</sup>
PE (18:0/20:4)	0.002	0.18	1.84x10 <sup>-2</sup>

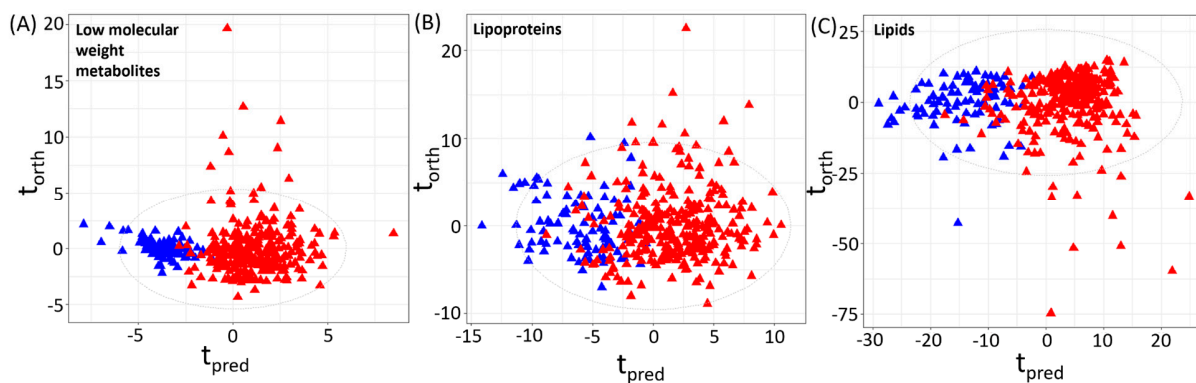
TAG (52:1)_FA (18:0)	0.004	0.18	1.84x10 <sup>-2</sup>
TAG (54:3)_FA (18:2)	0.003	0.18	1.84x10 <sup>-2</sup>
TAG (51:2)_FA (16:0)	0.004	0.18	1.87x10 <sup>-2</sup>
TAG (54:6)_FA (18:3)	0.021	-0.18	1.91x10 <sup>-2</sup>
TAG (56:9)_FA (18:3)	0.013	-0.18	1.91x10 <sup>-2</sup>
TAG (58:7)_FA (22:4)	0.001	0.18	1.91x10 <sup>-2</sup>
V5FC	0.007	-0.18	1.92x10 <sup>-2</sup>
TPAB	0.004	0.18	1.93x10 <sup>-2</sup>
TBPN	0.004	0.18	1.93x10 <sup>-2</sup>
LCER.d (18:0/20:0)	0.015	-0.18	1.95x10 <sup>-2</sup>
TAG (55:3)_FA (18:1)	0.000	0.18	1.97x10 <sup>-2</sup>
TAG (51:2)_FA (16:1)	0.002	0.18	1.97x10 <sup>-2</sup>
TAG (58:9)_FA (18:1)	0.000	0.18	2.00x10 <sup>-2</sup>
TAG (56:7)_FA (22:6)	0.002	0.18	2.03x10 <sup>-2</sup>
TAG (49:1)_FA (16:0)	0.005	0.18	2.05x10 <sup>-2</sup>
TAG (51:0)_FA (16:0)	0.001	0.18	2.06x10 <sup>-2</sup>
PE (16:0/18:3)	0.008	-0.18	2.08x10 <sup>-2</sup>
V5CH	0.009	0.18	2.13x10 <sup>-2</sup>
TAG (53:4)_FA (20:4)	0.001	0.18	2.16x10 <sup>-2</sup>
TAG (53:3)_FA (18:2)	0.006	0.18	2.17x10 <sup>-2</sup>
Valine	0.006	-0.18	2.19x10 <sup>-2</sup>
LPE (22:6)	0.013	-0.18	2.25x10 <sup>-2</sup>
TAG (52:5)_FA (20:5)	0.001	0.17	2.27x10 <sup>-2</sup>
TAG (58:7)_FA (22:6)	0.001	0.17	2.29x10 <sup>-2</sup>
Lysine	0.006	-0.17	2.31x10 <sup>-2</sup>
TAG (54:5)_FA (22:4)	0.003	0.17	2.33x10 <sup>-2</sup>
TAG (52:2)_FA (18:2)	0.003	0.17	2.33x10 <sup>-2</sup>
TAG (53:2)_FA (16:0)	0.002	0.17	2.33x10 <sup>-2</sup>
TAG (47:0)_FA (16:0)	0.003	0.17	2.35x10 <sup>-2</sup>
TAG (51:0)_FA (17:0)	0.002	0.17	2.35x10 <sup>-2</sup>
DAG (16:0/18:0)	0.002	0.17	2.48x10 <sup>-2</sup>
TAG (52:5)_FA (20:4)	0.004	0.17	2.55x10 <sup>-2</sup>
TAG (52:5)_FA (20:3)	0.023	-0.17	2.56x10 <sup>-2</sup>
DAG (16:0/18:3)	0.003	0.17	2.61x10 <sup>-2</sup>
TAG (51:0)_FA (18:0)	0.002	0.17	2.61x10 <sup>-2</sup>
L2PL	0.009	-0.17	2.63x10 <sup>-2</sup>
TAG (58:8)_FA (22:6)	0.002	0.17	2.63x10 <sup>-2</sup>

PG (18:1/20:3)	0.019	0.17	$2.65 \times 10^{-2}$
TAG (58:8)_FA (20:4)	0.001	0.17	$2.82 \times 10^{-2}$
TAG (58:7)_FA (18:2)	0.004	0.17	$2.90 \times 10^{-2}$
V5PL	0.008	0.17	$3.05 \times 10^{-2}$
TAG (52:3)_FA (18:1)	0.000	0.17	$3.19 \times 10^{-2}$
TAG (50:5)_FA (18:3)	0.019	-0.16	$3.24 \times 10^{-2}$
TAG (54:7)_FA (18:3)	0.017	-0.16	$3.28 \times 10^{-2}$
TAG (53:4)_FA (17:0)	0.004	0.16	$3.34 \times 10^{-2}$
DAG (18:1/20:1)	0.002	0.16	$3.44 \times 10^{-2}$
TAG (56:7)_FA (18:1)	0.002	0.16	$3.47 \times 10^{-2}$
TAG (52:3)_FA (16:1)	0.002	0.16	$3.60 \times 10^{-2}$
PC (18:0/22:5)	0.002	0.16	$3.63 \times 10^{-2}$
L2FC	0.010	-0.16	$3.65 \times 10^{-2}$
TAG (49:2)_FA (18:2)	0.006	0.16	$3.69 \times 10^{-2}$
TAG (53:6)_FA (20:4)	0.006	0.16	$3.76 \times 10^{-2}$
Creatinine	0.018	0.16	$3.77 \times 10^{-2}$
TAG (50:5)_FA (14:0)	0.019	-0.16	$3.83 \times 10^{-2}$
TAG (50:3)_FA (16:0)	0.003	0.16	$4.01 \times 10^{-2}$
TAG (50:1)_FA (16:1)	0.002	0.16	$4.09 \times 10^{-2}$
V1CH	0.003	0.16	$4.13 \times 10^{-2}$
TAG (58:10)_FA (20:5)	0.006	-0.16	$4.13 \times 10^{-2}$
L5CH	0.018	-0.16	$4.32 \times 10^{-2}$
TAG (49:2)_FA (16:0)	0.006	0.16	$4.38 \times 10^{-2}$
TAG (51:3)_FA (17:0)	0.003	0.16	$4.37 \times 10^{-2}$
TAG (54:4)_FA (18:1)	0.002	0.16	$4.38 \times 10^{-2}$
H1CH	0.023	-0.16	$4.40 \times 10^{-2}$
TAG (54:8)_FA (18:2)	0.009	-0.16	$4.49 \times 10^{-2}$
PE (18:1/22:6)	0.003	0.16	$4.52 \times 10^{-2}$
PE (18:1/20:1)	0.016	-0.16	$4.53 \times 10^{-2}$
DAG (18:0/22:6)	0.002	0.15	$4.61 \times 10^{-2}$
TAG (49:0)_FA (18:0)	0.000	0.15	$4.65 \times 10^{-2}$
TAG (56:7)_FA (16:0)	0.004	0.15	$4.72 \times 10^{-2}$
Ornithine	0.010	0.15	$4.73 \times 10^{-2}$
PS (18:1/18:2)	0.001	0.15	$4.75 \times 10^{-2}$

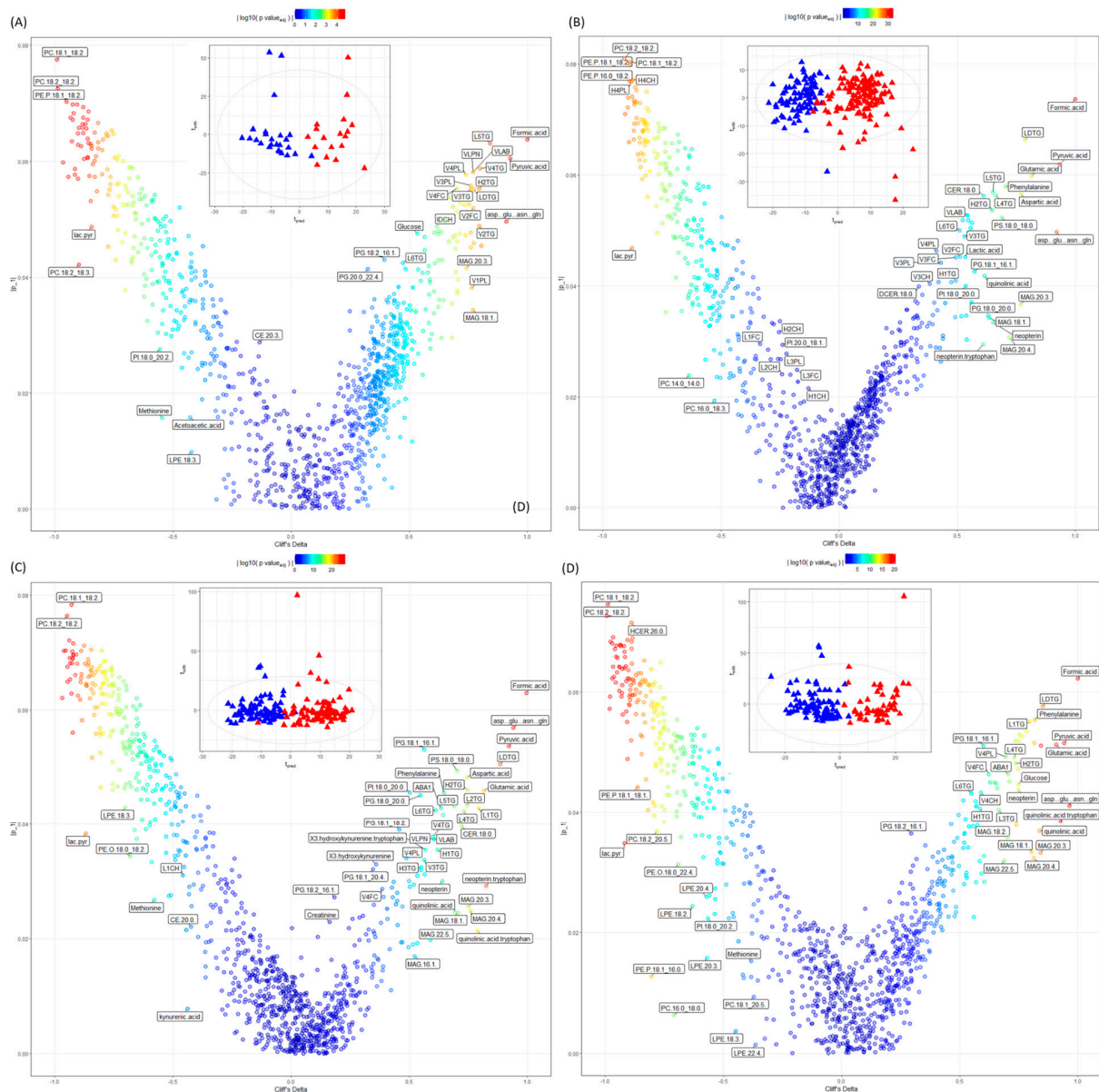


**Figure S1** - (A) Radar plot showing the log<sub>2</sub> fold change of the top 50 metabolites, lipoproteins and lipids with the most significant p-values for the control versus SARS-CoV-2 positive patients. (B) Radar plot showing the log<sub>2</sub> fold change of the top 50 metabolites, lipoproteins and lipids with the most significant p-values for the control versus SARS-CoV-2 positive model but coloured by severity class. Control vs group B severity log<sub>2</sub> fold change (blue), Control vs group C severity log<sub>2</sub> fold change (cyan), Control vs group D severity log<sub>2</sub> fold change (orange), Control vs group E severity log<sub>2</sub> fold change (red). The radar plots are ordered by fold change.





**Figure S3 – O-PLS-DA scores plots of the low molecular weight metabolites, lipoproteins and lipids.** (A) O-PLS-DA of control samples (blue triangles) and SARS-CoV-2 positive patients (red triangles) for the low molecular weight metabolites,  $R^2X=0.12$ , AUROC=1.00. (B) O-PLS-DA of control samples (blue triangles) and SARS-CoV-2 positive patients (red triangles) for the NMR derived lipoproteins,  $R^2X=0.26$ , AUROC=0.95. (C) O-PLS-DA of control samples (blue triangles) and SARS-CoV-2 positive patients (red triangles) for the MS derived lipids,  $R^2X=0.17$ , AUROC=0.98.



**Figure S4 - Orthogonal Partial Least Squared (O-PLS-DA) and eruption plots between controls and SARS-CoV-2 positive patients of each severity group for the four Integrated assays.** (A) Eruption plot of the controls vs group B severity group with the O-PLS-DA of controls (blue triangles) and SARS-CoV-2 group B severity patients (red triangles) ( $R^2X=0.21$ , AUROC=0.99) inset. (B) Eruption plot of the controls vs group C severity group with the O-PLS-DA of controls (blue triangles) and SARS-CoV-2 group B severity patients (red triangles) ( $R^2X=0.12$ , AUROC=0.99) inset. (C) Eruption plot of the controls vs group D severity group with the O-PLS-DA of controls (blue triangles) and SARS-CoV-2 group B severity patients (red triangles) ( $R^2X=0.20$ , AUROC=0.99) inset. (D) Eruption plot of the controls vs group E severity group with the O-PLS-DA of controls (blue triangles) and SARS-CoV-2 group B severity patients (red triangles) ( $R^2X=0.22$ , AUROC=1.00) inset.

**Table S6 - OPLS loadings, Cliff's delta and adjusted p-values of all the assays combined for the comparison of the controls and SARS-CoV-2 positive patients in severity class B. Only the 50 most significant metabolites are shown.**

Metabolite	OPLS loadings	Cliff's delta	Adjusted p-value
Formic acid	0.064	1.00	1.59x10 <sup>-5</sup>
PC (18:1/18:2)	0.078	-0.99	1.59x10 <sup>-5</sup>
PC (18:2/18:2)	0.073	-0.99	1.59x10 <sup>-5</sup>
PE.O (16:0/18:2)	0.060	-0.96	2.37x10 <sup>-5</sup>
PE.P (18:1/18:2)	0.070	-0.95	2.85x10 <sup>-5</sup>
Pyruvic acid	0.061	0.93	2.86x10 <sup>-5</sup>
LPC (18:2)	0.057	-0.94	2.86x10 <sup>-5</sup>
PE.P (16:0/18:2)	0.070	-0.92	2.86x10 <sup>-5</sup>
PE.P (18:0/18:2)	0.068	-0.93	2.86x10 <sup>-5</sup>
PE.P (18:0/20:1)	0.067	-0.92	2.86x10 <sup>-5</sup>
PE.P (18:2/20:4)	0.063	-0.93	2.86x10 <sup>-5</sup>
HCER.d (18:0/18:0)	0.068	-0.92	2.92x10 <sup>-5</sup>
PE.O (16:0/20:4)	0.059	-0.92	2.92x10 <sup>-5</sup>
PE.P (16:0/18:3)	0.058	-0.92	2.92x10 <sup>-5</sup>
Asp:Glu/Asn/Gln	0.050	0.91	3.09x10 <sup>-5</sup>
PC (18:2/20:2)	0.057	-0.90	3.16x10 <sup>-5</sup>
PE.O (18:0/22:5)	0.065	-0.90	3.16x10 <sup>-5</sup>
PE.P (18:1/20:1)	0.070	-0.91	3.16x10 <sup>-5</sup>
PE.P (18:0/20:4)	0.063	-0.90	3.16x10 <sup>-5</sup>
PC (18:2/18:3)	0.042	-0.90	3.25x10 <sup>-5</sup>
PC (18:2/20:4)	0.066	-0.90	3.25x10 <sup>-5</sup>
HCER (22:0)	0.063	-0.89	3.99x10 <sup>-5</sup>
PC (16:0/18:2)	0.066	-0.88	4.15x10 <sup>-5</sup>
PE.O (16:0/20:1)	0.066	-0.88	4.15x10 <sup>-5</sup>
PC (20:0/20:4)	0.065	-0.88	4.18x10 <sup>-5</sup>
PE.P (18:0/18:1)	0.068	-0.88	4.18x10 <sup>-5</sup>
PE.P (18:1/22:5)	0.069	-0.88	4.18x10 <sup>-5</sup>
PE.O (18:0/22:4)	0.060	-0.88	4.56x10 <sup>-5</sup>
H4CH	0.066	-0.87	4.99x10 <sup>-5</sup>
PC (18:0/20:1)	0.066	-0.87	5.44x10 <sup>-5</sup>
PE.O (16:0/18:1)	0.061	-0.86	5.44x10 <sup>-5</sup>
PE.P (16:0/22:5)	0.067	-0.86	5.44x10 <sup>-5</sup>
PE.P (18:0/20:4)	0.061	-0.86	5.44x10 <sup>-5</sup>

PE.P (18:1/22:4)	0.064	-0.86	5.44x10 <sup>-5</sup>
PE.P (18:0/22:5)	0.069	-0.86	5.80x10 <sup>-5</sup>
PE.P (18:2/18:2)	0.063	-0.86	5.80x10 <sup>-5</sup>
PE.O (16:0/22:5)	0.057	-0.85	6.38x10 <sup>-5</sup>
PE.O (16:0/22:6)	0.053	-0.85	6.83x10 <sup>-5</sup>
PE.P (18:0/22:4)	0.063	-0.85	6.83x10 <sup>-5</sup>
Lactate/pyruvate	0.049	-0.84	7.15x10 <sup>-5</sup>
PC (20:0/18:1)	0.062	-0.84	7.15x10 <sup>-5</sup>
PE.P (18:0/18:0)	0.063	-0.84	7.15x10 <sup>-5</sup>
L5TG	0.063	0.84	7.41x10 <sup>-5</sup>
PE.P (16:0/20:4)	0.059	-0.84	7.69x10 <sup>-5</sup>
HCER.d (18:0/22:0)	0.060	-0.83	9.13x10 <sup>-5</sup>
PE.P (16:0/20:1)	0.065	-0.83	9.13x10 <sup>-5</sup>
PE.P (18:1/16:0)	0.057	-0.83	9.13x10 <sup>-5</sup>
PE.P (18:0/16:0)	0.061	-0.83	1.01x10 <sup>-4</sup>
PC (20:0/20:3)	0.055	-0.82	1.11x10 <sup>-4</sup>
H4PL	0.063	-0.82	1.17x10 <sup>-4</sup>

**Table S7 - OPLS loadings, Cliff's delta and adjusted p-values of all the assays combined for the comparison of the controls and SARS-CoV-2 positive patients in severity class C.** Only the 50 most significant metabolites are shown.

Metabolite	OPLS loadings	Cliff's delta	Adjusted p-value
Formic acid	0.074	1.00	4.47x10 <sup>-34</sup>
Pyruvic acid	0.062	0.93	8.99x10 <sup>-30</sup>
Asp:Glu/Asn:Gln	0.050	0.92	4.05x10 <sup>-29</sup>
PC (18:2/18:2)	0.081	-0.91	1.28x10 <sup>-28</sup>
PE.O (16:0/20:4)	0.071	-0.91	1.66x10 <sup>-28</sup>
PE.O (16:0/18:2)	0.072	-0.89	8.50x10 <sup>-28</sup>
PE.P (18:2/20:4)	0.074	-0.89	8.50x10 <sup>-28</sup>
PE.P (16:0/22:5)	0.066	-0.89	1.31x10 <sup>-27</sup>
PE.P (16:0/18:2)	0.077	-0.89	1.49x10 <sup>-27</sup>
PE.P (18:1/18:2)	0.080	-0.89	1.49x10 <sup>-27</sup>
PC (18:1/18:2)	0.080	-0.88	1.88x10 <sup>-27</sup>
H4PL	0.077	-0.88	3.71x10 <sup>-27</sup>
Lactate/pyruvate	0.047	-0.88	4.94x10 <sup>-27</sup>
PE.P (18:0/18:2)	0.074	-0.88	4.94x10 <sup>-27</sup>

H4CH	0.077	-0.87	$5.88 \times 10^{-27}$
HCER.d (18:0/18:0)	0.073	-0.87	$1.24 \times 10^{-26}$
PE.O (16:0/18:1)	0.066	-0.87	$1.24 \times 10^{-26}$
PE.O (16:0/20:1)	0.068	-0.87	$1.24 \times 10^{-26}$
PE.P (18:0/18:1)	0.073	-0.87	$1.47 \times 10^{-26}$
PE.P (18:0/22:5)	0.069	-0.87	$1.47 \times 10^{-26}$
PE.P (18:0/20:4)	0.073	-0.87	$1.54 \times 10^{-26}$
PC (18:2/20:2)	0.076	-0.86	$2.12 \times 10^{-26}$
PE.P (16:0/20:1)	0.073	-0.86	$3.91 \times 10^{-26}$
LPC (18:2)	0.075	-0.86	$4.11 \times 10^{-26}$
PC (18:2/20:3)	0.070	-0.86	$4.22 \times 10^{-26}$
PE.P (16:0/20:4)	0.069	-0.85	$7.46 \times 10^{-26}$
PE.O (18:0/22:5)	0.064	-0.85	$7.52 \times 10^{-26}$
PC (20:0/20:3)	0.067	-0.84	$2.15 \times 10^{-25}$
PE.P (18:0/22:4)	0.063	-0.84	$2.15 \times 10^{-25}$
PE.P (18:2/18:2)	0.073	-0.84	$2.54 \times 10^{-25}$
PC (18:0/20:1)	0.066	-0.84	$2.68 \times 10^{-25}$
PE.O (18:0/22:4)	0.061	-0.84	$2.72 \times 10^{-25}$
PE.P (18:0/20:1)	0.070	-0.84	$4.69 \times 10^{-25}$
LPI (18:1)	0.064	-0.84	$4.87 \times 10^{-25}$
LPI (18:2)	0.059	-0.83	$6.88 \times 10^{-25}$
PE.P (18:1/22:5)	0.068	-0.83	$9.11 \times 10^{-25}$
HCER (26:0)	0.068	-0.83	$1.15 \times 10^{-24}$
PE.P (18:0/20:3)	0.068	-0.83	$1.20 \times 10^{-24}$
PE.P (16:0/18:3)	0.064	-0.83	$1.36 \times 10^{-24}$
PE.P (18:0/20:4)	0.069	-0.83	$1.97 \times 10^{-24}$
PE.O (16:0/22:5)	0.066	-0.82	$2.14 \times 10^{-24}$
PE.P (18:0/20:2)	0.070	-0.82	$2.14 \times 10^{-24}$
HCER (22:0)	0.066	-0.82	$2.54 \times 10^{-24}$
HCER.d (18:0/22:0)	0.065	-0.82	$2.54 \times 10^{-24}$
LPI (20:3)	0.063	-0.82	$2.65 \times 10^{-24}$
PE.P (18:0/18:0)	0.070	-0.82	$2.65 \times 10^{-24}$
PC (20:0/18:1)	0.060	-0.82	$4.46 \times 10^{-24}$
PE.P (18:1/18:1)	0.069	-0.82	$4.56 \times 10^{-24}$
PC (18:2/20:4)	0.068	-0.82	$5.19 \times 10^{-24}$
LPC (20:0)	0.075	-0.82	$6.05 \times 10^{-24}$

**Table S8 - OPLS loadings, Cliff's delta and adjusted p-values of all the assays combined for the comparison of the controls and SARS-CoV-2 positive patients in severity class D. Only the 50 most significant metabolites are shown.**

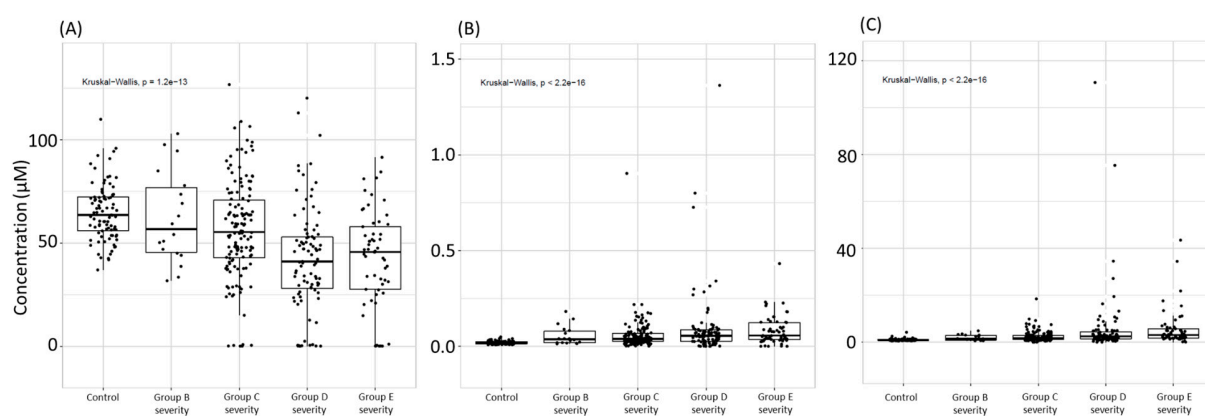
Metabolite	OPLS loadings	Cliff's delta	Adjusted p-value
Formic acid	0.063	1.00	5.46x10 <sup>-28</sup>
PE.O (16:0/20:4)	0.062	-0.97	1.14x10 <sup>-26</sup>
H4CH	0.070	-0.96	1.89x10 <sup>-26</sup>
H4PL	0.070	-0.95	4.13x10 <sup>-26</sup>
PC (18:2/18:2)	0.076	-0.95	5.90x10 <sup>-26</sup>
PE.P (18:1/20:4)	0.068	-0.95	5.90x10 <sup>-26</sup>
PE.P (18:2/20:4)	0.065	-0.95	5.90x10 <sup>-26</sup>
Asp:Glu/Asn:Gln	0.057	0.94	1.04x10 <sup>-25</sup>
PE.P (18:1/18:2)	0.072	-0.94	1.04x10 <sup>-25</sup>
LPC (18:2)	0.069	-0.94	1.27x10 <sup>-25</sup>
PE.P (16:0/20:4)	0.065	-0.94	1.41x10 <sup>-25</sup>
PE.P (16:0/22:5)	0.068	-0.94	1.41x10 <sup>-25</sup>
PC (18:1/18:2)	0.078	-0.93	2.41x10 <sup>-25</sup>
PE.O (16:0/18:2)	0.063	-0.93	2.53x10 <sup>-25</sup>
H4A2	0.068	-0.93	3.02x10 <sup>-25</sup>
PC (18:2/20:2)	0.069	-0.93	3.02x10 <sup>-25</sup>
H4A1	0.070	-0.93	3.12x10 <sup>-25</sup>
PE.P (18:0/18:2)	0.069	-0.92	3.65x10 <sup>-25</sup>
PC (18:2/18:3)	0.056	-0.92	3.91x10 <sup>-25</sup>
PE.P (16:0/18:2)	0.072	-0.92	4.20x10 <sup>-25</sup>
PE.P (18:0/22:5)	0.070	-0.92	4.26x10 <sup>-25</sup>
Pyruvic acid	0.054	0.92	4.96x10 <sup>-25</sup>
PC (18:2/20:3)	0.070	-0.92	4.96x10 <sup>-25</sup>
PE.P (18:2/18:2)	0.066	-0.91	1.08x10 <sup>-24</sup>
LPC (20:0)	0.070	-0.91	1.59x10 <sup>-24</sup>
PE.P (18:1/22:5)	0.068	-0.91	2.88x10 <sup>-24</sup>
PE.O (16:0/22:5)	0.063	-0.90	4.36x10 <sup>-24</sup>
PE.O (16:0/18:1)	0.062	-0.89	1.31x10 <sup>-23</sup>
PE.O (18:0/22:5)	0.065	-0.89	1.55x10 <sup>-23</sup>
PE.P (18:0/20:4)	0.066	-0.89	1.69x10 <sup>-23</sup>
PE.P (18:0/18:1)	0.070	-0.89	1.73x10 <sup>-23</sup>
PC (20:0/20:3)	0.066	-0.89	1.89x10 <sup>-23</sup>
Neopterin/tryptophan	0.029	0.82	1.93x10 <sup>-23</sup>

PE.P (16:0/18:3)	0.058	-0.89	2.32x10 <sup>-23</sup>
LDTG	0.051	0.88	2.94x10 <sup>-23</sup>
PC (18:2/20:4)	0.071	-0.88	7.29x10 <sup>-23</sup>
HCER.d (18:0/18:0)	0.068	-0.87	9.77x10 <sup>-23</sup>
Lactate/pyruvate	0.038	-0.87	1.70x10 <sup>-22</sup>
PE.O (16:0/20:1)	0.065	-0.87	1.91x10 <sup>-22</sup>
PI (20:0/18:2)	0.064	-0.87	2.09x10 <sup>-22</sup>
PE.P (18:1/22:4)	0.064	-0.87	2.23x10 <sup>-22</sup>
LPC (20:3)	0.068	-0.86	3.99x10 <sup>-22</sup>
PE.P (16:0/20:1)	0.069	-0.86	3.99x10 <sup>-22</sup>
PE.P (18:0/16:0)	0.068	-0.86	5.19x10 <sup>-22</sup>
PE.P (18:0/22:4)	0.066	-0.86	5.53x10 <sup>-22</sup>
PI (18:1/18:1)	0.062	-0.85	1.04x10 <sup>-21</sup>
TPA2	0.066	-0.85	1.05x10 <sup>-21</sup>
H4FC	0.067	-0.85	1.41x10 <sup>-21</sup>
PE.P (18:0/20:3)	0.064	-0.85	1.55x10 <sup>-21</sup>
SM (24:0)	0.067	-0.85	1.55x10 <sup>-21</sup>

**Table S9 - OPLS loadings, Cliff's delta and adjusted p-values of all the assays combined for the comparison of the controls and SARS-CoV-2 positive patients in severity class E. Only the 50 most significant metabolites are shown.**

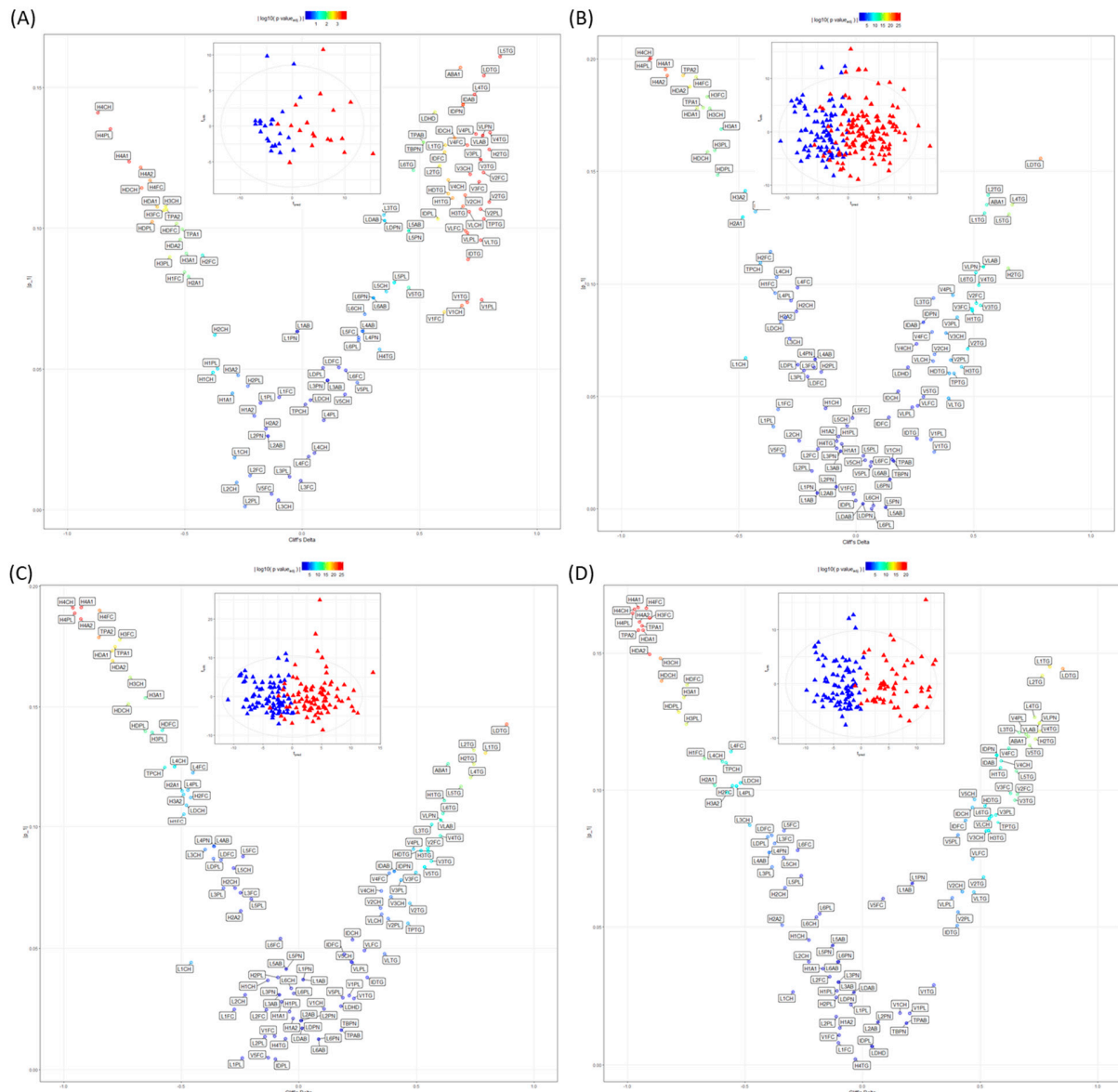
Metabolite	OPLS loadings	Cliff's delta	Adjusted p-value
Formic acid	0.064	1.00	2.50x10 <sup>-21</sup>
PC (18:1/18:2)	0.075	-0.99	2.67x10 <sup>-21</sup>
PC (18:2/18:2)	0.073	-0.99	2.67x10 <sup>-21</sup>
PE.O (16:0/20:4)	0.057	-0.98	3.92x10 <sup>-21</sup>
PE.P (18:2/20:4)	0.059	-0.98	3.92x10 <sup>-21</sup>
H4PL	0.068	-0.98	4.16x10 <sup>-21</sup>
H4CH	0.068	-0.97	7.25x10 <sup>-21</sup>
PC (20:0/20:3)	0.062	-0.97	7.25x10 <sup>-21</sup>
PC (18:2/20:3)	0.064	-0.97	8.31x10 <sup>-21</sup>
PC (18:2/20:4)	0.069	-0.97	8.31x10 <sup>-21</sup>
Asp:Glu/Asn:Gln	0.041	0.97	8.65x10 <sup>-21</sup>
PE.P (18:1/20:4)	0.063	-0.96	2.50x10 <sup>-21</sup>
PE.P (16:0/18:2)	0.067	-0.96	1.26x10 <sup>-20</sup>
LPC (18:2)	0.062	-0.96	1.73x10 <sup>-20</sup>

TPA2	0.066	-0.95	1.81x10 <sup>-20</sup>
H4A1	0.068	-0.95	1.81x10 <sup>-20</sup>
PE.P (16:0/22:5)	0.063	-0.95	2.28x10 <sup>-20</sup>
H4A2	0.066	0.95	2.62x10 <sup>-20</sup>
Neopterin/tryptophan	0.051	0.84	4.83x10 <sup>-20</sup>
Pyruvic acid	0.052	0.94	4.93x10 <sup>-20</sup>
PE.P (18:1/18:2)	0.064	-0.94	4.93x10 <sup>-20</sup>
PE.P (16:0/20:4)	0.060	-0.94	5.06x10 <sup>-20</sup>
TPA1	0.068	-0.94	5.63x10 <sup>-20</sup>
PE.P (18:0/22:5)	0.064	-0.94	5.63x10 <sup>-20</sup>
PC (18:0/20:1)	0.068	-0.94	7.36x10 <sup>-20</sup>
HDA1	0.068	-0.93	8.26x10 <sup>-20</sup>
PE.P (18:2/18:2)	0.059	-0.93	1.00x10 <sup>-20</sup>
PE.P (18:0/20:3)	0.060	-0.93	1.17x10 <sup>-19</sup>
PE.P (18:0/20:4)	0.061	-0.93	1.17x10 <sup>-19</sup>
Quinolinic acid/tryptophan	0.038	0.93	1.19x10 <sup>-19</sup>
PE.P (18:0/18:2)	0.064	-0.93	1.19x10 <sup>-19</sup>
PE.O (16:0/22:5)	0.056	-0.93	1.29x10 <sup>-19</sup>
H4FC	0.068	-0.92	2.37x10 <sup>-19</sup>
PC (18:2/22:5)	0.064	-0.92	2.60x10 <sup>-19</sup>
HCER (22:0)	0.067	-0.92	2.62x10 <sup>-19</sup>
Lactate/pyruvate	0.035	-0.92	2.75x10 <sup>-19</sup>
HCER.d (18:0/22:0)	0.066	-0.92	3.11x10 <sup>-19</sup>
LPC (20:0)	0.064	-0.91	3.80x10 <sup>-19</sup>
PE.P (18:0/22:4)	0.062	-0.91	4.47x10 <sup>-19</sup>
PI (20:0/18:2)	0.057	-0.91	4.70x10 <sup>-19</sup>
Glutamic acid	0.051	0.91	5.54x10 <sup>-19</sup>
PE.O (16:0/18:2)	0.055	-0.91	6.52x10 <sup>-19</sup>
PE.P (16:0/18:3)	0.049	-0.91	6.86x10 <sup>-19</sup>
H3FC	0.069	-0.91	7.32x10 <sup>-19</sup>
HDA2	0.062	-0.91	7.33x10 <sup>-19</sup>
PE.P (16:0/20:1)	0.064	-0.90	9.68x10 <sup>-19</sup>
PC (18:2/22:6)	0.062	-0.90	1.06x10 <sup>-18</sup>
PC (18:2/20:2)	0.058	-0.90	1.12x10 <sup>-18</sup>
PE.O (16:0/20:1)	0.059	-0.90	1.37x10 <sup>-18</sup>
PE.P (18:1/22:4)	0.058	-0.90	1.50x10 <sup>-18</sup>

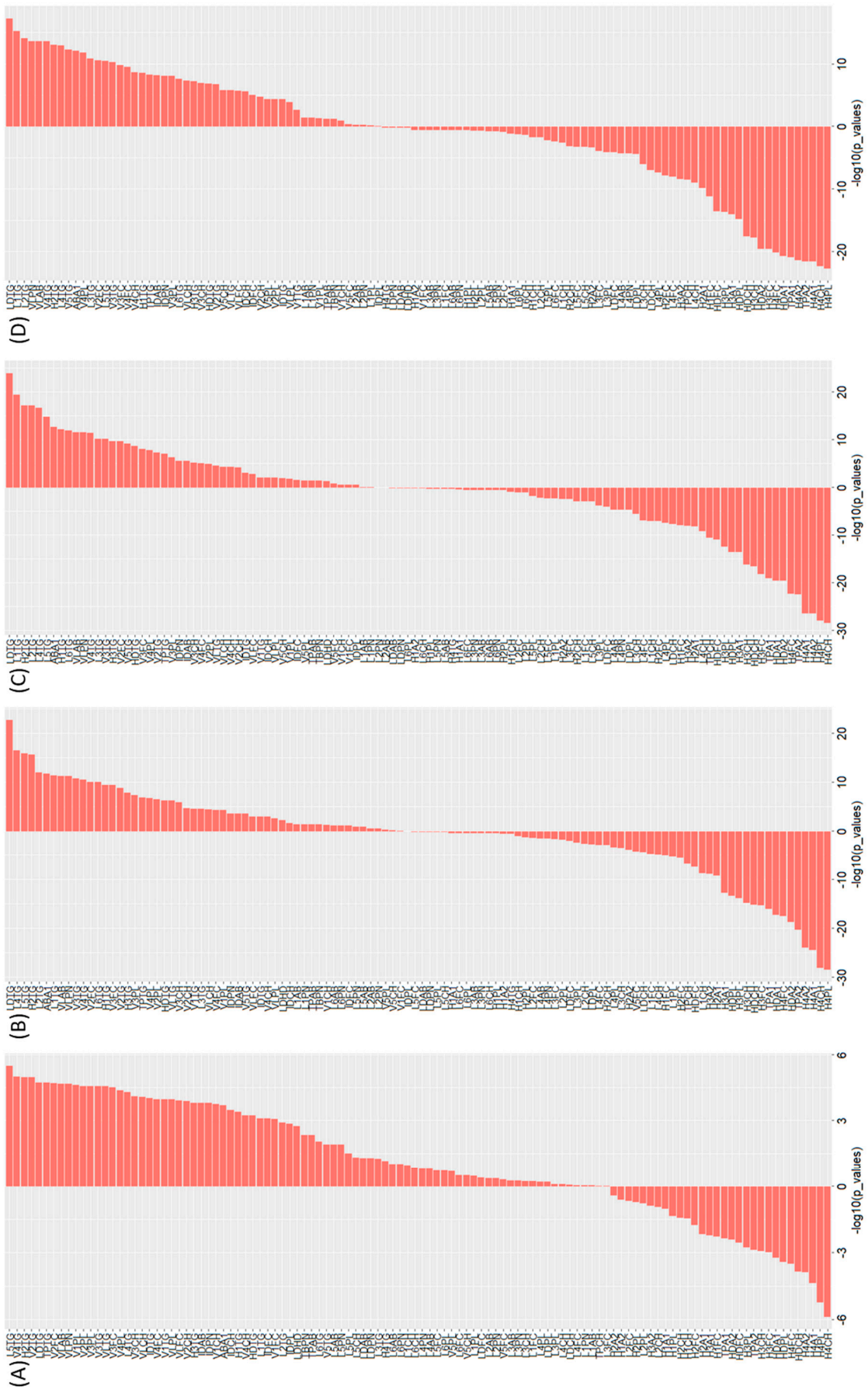


**Figure S5 – Concentrations of metabolites for the controls and each severity class. (A) tryptophan, (B) neopterin and (C) quinolinic acid.**

## Section 4 - Severity group modeling



**Figure S6 - Orthogonal Partial Least Squared (O-PLS-DA) and eruption plots between controls and SARS-CoV-2 positive patients of each severity group for the lipoproteins.** (A) Eruption plot of the controls vs group B severity group with the O-PLS-DA of controls (blue triangles) and SARS-CoV-2 group B severity patients (red triangles) ( $R_2X=0.39$ , AUROC=0.91) inset. (B) Eruption plot of the controls vs group C severity group with the O-PLS-DA of controls (blue triangles) and SARS-CoV-2 group C severity patients (red triangles) ( $R_2X=0.27$ , AUROC=0.95) inset. (C) Eruption plot of the controls vs group D severity group with the O-PLS-DA of controls (blue triangles) and SARS-CoV-2 group D severity patients (red triangles) ( $R_2X=0.29$ , AUROC=0.97) inset. (D) Eruption plot of the controls vs group E severity group with the O-PLS-DA of controls (blue triangles) and SARS-CoV-2 group E severity patients (red triangles) ( $R_2X=0.36$ , AUROC=1.00) inset. Eruption plots are formed from the Cliff's delta (abscissa) and O-PLS-DA loadings (ordinate). Coloured by significance.



**Figure S6 -  $-\log_{10}$  (p-values) between controls and SARS-CoV-2 positive patients of each severity group for the lipoproteins.** (A) Controls vs group B severity. (B) Controls vs Group C severity. (D) Controls vs Group D severity. (E) Controls vs Group E severity.

**Table S10 - OPLS loadings, Cliff's delta and adjusted p-values of the lipoproteins for the comparison of the controls and SARS-CoV-2 positive patients in severity class B.** Only metabolites with significant p-values are shown in the table.

Metabolite	OPLS loadings	Cliff's delta	Adjusted p-value
H4CH	0.141	-0.87	$1.57 \times 10^{-4}$
L5TG	0.161	0.84	$1.73 \times 10^{-4}$
TPTG	0.103	0.77	$1.79 \times 10^{-4}$
VLPN	0.133	0.77	$1.79 \times 10^{-4}$
VLTG	0.096	0.76	$1.79 \times 10^{-4}$
LDTG	0.154	0.77	$1.79 \times 10^{-4}$
VLAB	0.133	0.77	$1.79 \times 10^{-4}$
V2TG	0.109	0.80	$1.79 \times 10^{-4}$
V3TG	0.124	0.76	$1.79 \times 10^{-4}$
V4TG	0.134	0.80	$1.79 \times 10^{-4}$
V2FC	0.120	0.77	$1.79 \times 10^{-4}$
V1PL	0.075	0.76	$1.79 \times 10^{-4}$
V2PL	0.107	0.76	$1.79 \times 10^{-4}$
V3PL	0.124	0.76	$1.79 \times 10^{-4}$
H2TG	0.128	0.80	$1.79 \times 10^{-4}$
H4PL	0.135	-0.82	$1.79 \times 10^{-4}$
V3FC	0.117	0.75	$1.97 \times 10^{-4}$
V4PL	0.133	0.74	$2.58 \times 10^{-4}$
H4A1	0.124	-0.74	$2.58 \times 10^{-4}$
L4TG	0.148	0.73	$2.72 \times 10^{-4}$
V3CH	0.119	0.72	$3.93 \times 10^{-4}$
VLCH	0.106	0.71	$4.17 \times 10^{-4}$
IDTG	0.089	0.71	$4.32 \times 10^{-4}$
VLPL	0.098	0.70	$4.32 \times 10^{-4}$
V1TG	0.074	0.70	$4.32 \times 10^{-4}$
V4FC	0.130	0.70	$4.32 \times 10^{-4}$
VLFC	0.099	0.70	$4.84 \times 10^{-4}$
V2CH	0.112	0.69	$4.91 \times 10^{-4}$
HDCH	0.114	-0.68	$5.09 \times 10^{-4}$

IDPN	0.114	0.68	5.09x10 <sup>-4</sup>
IDAB	0.144	0.68	5.09x10 <sup>-4</sup>
H3TG	0.108	0.68	5.09x10 <sup>-4</sup>
H4A2	0.122	-0.69	5.09x10 <sup>-4</sup>
V1CH	0.073	0.68	5.45x10 <sup>-4</sup>
ABA1	0.157	0.67	6.08x10 <sup>-4</sup>
IDCH	0.132	0.65	9.85x10 <sup>-4</sup>
H4FC	0.117	-0.65	9.85x10 <sup>-4</sup>
HDPL	0.102	-0.64	1.13x10 <sup>-3</sup>
H1TG	0.111	0.64	1.13x10 <sup>-3</sup>
HDTG	0.112	0.62	1.55x10 <sup>-3</sup>
V4CH	0.117	0.62	1.55x10 <sup>-3</sup>
HDA1	0.108	-0.62	1.66x10 <sup>-3</sup>
L1TG	0.130	0.61	1.94x10 <sup>-3</sup>
IDFC	0.127	0.61	1.98x10 <sup>-3</sup>
V1FC	0.070	0.60	2.02x10 <sup>-3</sup>
H3FC	0.106	-0.59	2.69x10 <sup>-3</sup>
L2TG	0.122	0.58	2.87x10 <sup>-3</sup>
H3CH	0.108	-0.58	2.94x10 <sup>-3</sup>
TPA2	0.107	-0.58	3.07x10 <sup>-3</sup>
IDPL	0.103	0.58	3.07x10 <sup>-3</sup>
LDHD	0.141	0.56	3.81x10 <sup>-3</sup>
H3PL	0.090	-0.56	3.81x10 <sup>-3</sup>
HDFC	0.102	-0.54	6.36x10 <sup>-3</sup>
HDA2	0.096	-0.52	8.24x10 <sup>-3</sup>
TPAB	0.131	0.52	8.59x10 <sup>-3</sup>
TBPN	0.131	0.52	8.59x10 <sup>-3</sup>
TPA1	0.100	-0.51	9.12x10 <sup>-3</sup>
H1FC	0.084	-0.50	1.04x10 <sup>-2</sup>
H3A1	0.091	-0.49	1.19x10 <sup>-2</sup>
H2A1	0.083	-0.48	1.36x10 <sup>-2</sup>
L6TG	0.121	0.47	1.60x10 <sup>-2</sup>
L5PN	0.099	0.45	2.11x10 <sup>-2</sup>
V5TG	0.079	0.45	2.11x10 <sup>-2</sup>
L5AB	0.099	0.45	2.11x10 <sup>-2</sup>
H2FC	0.090	-0.42	3.22x10 <sup>-2</sup>

**Table S11 - OPLS loadings, Cliff's delta and adjusted p-values of the lipoproteins for the comparison of the controls and SARS-CoV-2 positive patients in severity class C. Only metabolites with significant p-values are shown in the table.**

Metabolite	OPLS loadings	Cliff's delta	Adjusted p-value
H4CH	0.200	-0.87	$4.77 \times 10^{-27}$
H4PL	0.195	-0.88	$4.77 \times 10^{-27}$
H4A1	0.195	-0.81	$1.72 \times 10^{-23}$
H4A2	0.193	-0.81	$3.19 \times 10^{-23}$
LDTG	0.156	0.79	$3.29 \times 10^{-23}$
TPA2	0.193	-0.74	$1.24 \times 10^{-19}$
HDA2	0.188	-0.71	$3.22 \times 10^{-18}$
H4FC	0.192	-0.68	$4.81 \times 10^{-17}$
HDA1	0.178	-0.68	$8.30 \times 10^{-17}$
L4TG	0.135	0.66	$3.07 \times 10^{-16}$
TPA1	0.178	-0.65	$1.05 \times 10^{-15}$
L5TG	0.131	0.65	$1.05 \times 10^{-15}$
H2TG	0.107	0.65	$1.52 \times 10^{-15}$
H3FC	0.183	-0.64	$4.79 \times 10^{-15}$
HDCH	0.159	-0.63	$5.62 \times 10^{-15}$
H3CH	0.178	-0.62	$1.44 \times 10^{-14}$
H3PL	0.159	-0.60	$1.15 \times 10^{-13}$
HDPL	0.148	-0.59	$3.56 \times 10^{-13}$
H3A1	0.169	-0.58	$1.36 \times 10^{-12}$
L2TG	0.139	0.56	$4.71 \times 10^{-12}$
ABA1	0.135	0.56	$7.45 \times 10^{-12}$
L1TG	0.131	0.55	$1.83 \times 10^{-11}$
VLPN	0.108	0.54	$2.31 \times 10^{-11}$
VLAB	0.108	0.54	$2.31 \times 10^{-11}$
V3TG	0.090	0.53	$6.74 \times 10^{-11}$
V4TG	0.099	0.52	$1.29 \times 10^{-10}$
V2FC	0.091	0.51	$3.20 \times 10^{-10}$
L6TG	0.105	0.51	$3.64 \times 10^{-10}$
V3FC	0.089	0.49	$1.25 \times 10^{-9}$
H1TG	0.088	0.49	$1.25 \times 10^{-9}$
H2A1	0.130	-0.48	$2.77 \times 10^{-9}$
V2TG	0.071	0.47	$5.31 \times 10^{-9}$
H3A2	0.141	-0.47	$6.35 \times 10^{-9}$

L1CH	0.067	-0.47	6.99x10 <sup>-9</sup>
H3TG	0.063	0.45	3.72x10 <sup>-8</sup>
V3PL	0.085	0.43	1.29x10 <sup>-7</sup>
HDFC	0.132	-0.43	1.42x10 <sup>-7</sup>
TPTG	0.060	0.42	3.60x10 <sup>-7</sup>
V4PL	0.095	0.41	4.48x10 <sup>-7</sup>
TPCH	0.109	-0.41	5.74x10 <sup>-7</sup>
V2PL	0.066	0.40	8.18x10 <sup>-7</sup>
HDTG	0.060	0.40	1.26x10 <sup>-6</sup>
VLTG	0.049	0.39	1.39x10 <sup>-6</sup>
V3CH	0.078	0.38	2.77x10 <sup>-6</sup>
H2FC	0.114	-0.36	8.54x10 <sup>-6</sup>
L1PL	0.037	-0.35	1.71x10 <sup>-5</sup>
H1FC	0.096	-0.34	2.75x10 <sup>-5</sup>
L4CH	0.103	-0.34	3.61x10 <sup>-5</sup>
V2CH	0.069	0.33	4.82x10 <sup>-5</sup>
L1FC	0.044	-0.33	4.85x10 <sup>-5</sup>
V1TG	0.025	0.33	5.22x10 <sup>-5</sup>
L3TG	0.094	0.33	6.05x10 <sup>-5</sup>
VLCH	0.066	0.33	6.44x10 <sup>-5</sup>
V4FC	0.079	0.32	8.42x10 <sup>-5</sup>
LDCH	0.083	-0.32	9.33x10 <sup>-5</sup>
V1PL	0.031	0.32	9.91x10 <sup>-5</sup>
V5FC	0.024	-0.31	1.24x10 <sup>-4</sup>
H2A2	0.085	-0.30	2.41x10 <sup>-4</sup>
IDPN	0.083	0.29	5.12x10 <sup>-4</sup>
IDAB	0.083	0.29	5.13x10 <sup>-4</sup>
V5TG	0.050	0.29	5.13x10 <sup>-4</sup>
L3CH	0.076	-0.28	5.40x10 <sup>-4</sup>
L4PL	0.093	-0.28	7.32x10 <sup>-4</sup>
VLFC	0.046	0.26	1.56x10 <sup>-3</sup>
IDTG	0.031	0.26	1.67x10 <sup>-3</sup>
V4CH	0.073	0.26	1.85x10 <sup>-3</sup>
H2CH	0.088	-0.25	2.02x10 <sup>-3</sup>
L4FC	0.098	-0.25	2.38x10 <sup>-3</sup>
LDPL	0.064	-0.25	2.58x10 <sup>-3</sup>
L2CH	0.030	-0.24	3.33x10 <sup>-3</sup>

VLPL	0.045	0.24	$3.70 \times 10^{-3}$
L3PL	0.062	-0.22	$7.06 \times 10^{-3}$
LDHD	0.063	0.22	$7.59 \times 10^{-3}$
LDFC	0.059	-0.21	$1.30 \times 10^{-2}$
L2PL	0.017	-0.19	$2.40 \times 10^{-2}$
L3FC	0.063	-0.18	$3.35 \times 10^{-2}$
IDCH	0.052	0.18	$3.37 \times 10^{-2}$
L4PN	0.067	-0.17	$3.75 \times 10^{-2}$
L4AB	0.066	-0.17	$3.75 \times 10^{-2}$
L1PN	0.007	-0.17	$4.79 \times 10^{-2}$
L1AB	0.007	-0.17	$4.79 \times 10^{-2}$

**Table S12 - OPLS loadings, Cliff's delta and adjusted p-values of the lipoproteins for the comparison of the controls and SARS-CoV-2 positive patients in severity class D.** Only metabolites with significant p-values are shown in the table.

Metabolite	OPLS loadings	Cliff's delta	Adjusted p-value
H4CH	0.191	-0.96	$6.16 \times 10^{-27}$
H4PL	0.189	-0.95	$8.95 \times 10^{-27}$
H4A1	0.191	-0.93	$1.44 \times 10^{-25}$
H4A2	0.186	-0.93	$1.44 \times 10^{-25}$
LDTG	0.143	0.88	$2.23 \times 10^{-23}$
TPA2	0.179	-0.85	$8.89 \times 10^{-22}$
H4FC	0.190	-0.85	$1.05 \times 10^{-21}$
HDA1	0.173	-0.79	$3.96 \times 10^{-19}$
HDA2	0.169	-0.79	$3.96 \times 10^{-19}$
L1TG	0.131	0.79	$3.96 \times 10^{-19}$
TPA1	0.175	-0.78	$1.02 \times 10^{-18}$
H3FC	0.178	-0.76	$7.79 \times 10^{-18}$
H2TG	0.126	0.74	$4.40 \times 10^{-17}$
L2TG	0.132	0.74	$4.46 \times 10^{-17}$
L4TG	0.121	0.73	$1.53 \times 10^{-16}$
HDCH	0.151	-0.73	$2.40 \times 10^{-16}$
H3CH	0.162	-0.72	$5.26 \times 10^{-16}$
L5TG	0.117	0.69	$7.42 \times 10^{-15}$
H3A1	0.154	-0.66	$1.83 \times 10^{-13}$

HDPL	0.140	-0.65	$1.94 \times 10^{-13}$
ABA1	0.126	0.63	$9.32 \times 10^{-13}$
H3PL	0.139	-0.62	$2.01 \times 10^{-12}$
H1TG	0.111	0.62	$3.20 \times 10^{-12}$
L6TG	0.106	0.61	$5.25 \times 10^{-12}$
VLPN	0.103	0.60	$1.01 \times 10^{-11}$
VLAB	0.103	0.60	$1.01 \times 10^{-11}$
V4TG	0.096	0.60	$1.19 \times 10^{-11}$
HDFC	0.140	-0.58	$5.71 \times 10^{-11}$
TPCH	0.125	-0.57	$1.28 \times 10^{-10}$
L3TG	0.101	0.57	$1.92 \times 10^{-10}$
V3TG	0.086	0.56	$2.03 \times 10^{-10}$
H3TG	0.090	0.55	$5.73 \times 10^{-10}$
V2FC	0.091	0.55	$6.11 \times 10^{-10}$
V5TG	0.083	0.53	$1.72 \times 10^{-9}$
L4CH	0.125	-0.53	$2.58 \times 10^{-9}$
HDTG	0.090	0.52	$5.28 \times 10^{-9}$
V3FC	0.081	0.50	$2.15 \times 10^{-8}$
H2A1	0.115	-0.50	$2.20 \times 10^{-8}$
H3A2	0.114	-0.49	$3.34 \times 10^{-8}$
H1FC	0.106	-0.49	$3.53 \times 10^{-8}$
V4PL	0.091	0.49	$4.21 \times 10^{-8}$
LDCH	0.109	-0.48	$7.00 \times 10^{-8}$
L4PL	0.116	-0.47	$1.09 \times 10^{-7}$
V2TG	0.068	0.47	$1.09 \times 10^{-7}$
TPTG	0.060	0.46	$1.70 \times 10^{-7}$
H2FC	0.112	-0.46	$2.27 \times 10^{-7}$
L1CH	0.044	-0.46	$2.48 \times 10^{-7}$
L4FC	0.123	-0.45	$3.27 \times 10^{-7}$
V3PL	0.078	0.43	$1.03 \times 10^{-6}$
IDPN	0.082	0.41	$5.58 \times 10^{-6}$
IDAB	0.082	0.40	$5.58 \times 10^{-6}$
L3CH	0.091	-0.40	$7.83 \times 10^{-6}$
V3CH	0.071	0.39	$1.15 \times 10^{-5}$
V4FC	0.081	0.38	$1.61 \times 10^{-5}$
V2PL	0.062	0.38	$2.12 \times 10^{-5}$
VLTG	0.048	0.36	$4.51 \times 10^{-5}$

LDPL	0.087	-0.36	4.81x10 <sup>-5</sup>
L4PN	0.092	-0.36	5.16x10 <sup>-5</sup>
L4AB	0.092	-0.36	5.16x10 <sup>-5</sup>
VLCH	0.064	0.35	8.33x10 <sup>-5</sup>
V4CH	0.074	0.35	8.76x10 <sup>-5</sup>
V2CH	0.067	0.35	9.56x10 <sup>-5</sup>
LDFC	0.086	-0.33	2.08x10 <sup>-4</sup>
L3PL	0.075	-0.32	3.46x10 <sup>-4</sup>
IDTG	0.038	0.29	1.27x10 <sup>-3</sup>
VLFC	0.049	0.28	2.00x10 <sup>-3</sup>
L5CH	0.083	-0.28	2.05x10 <sup>-3</sup>
L1FC	0.025	-0.28	2.27x10 <sup>-3</sup>
H2CH	0.075	-0.27	2.56x10 <sup>-3</sup>
L3FC	0.073	-0.25	6.16x10 <sup>-3</sup>
H2A2	0.065	-0.25	6.30x10 <sup>-3</sup>
L1PL	0.005	-0.24	8.14x10 <sup>-3</sup>
L5FC	0.088	-0.24	8.65x10 <sup>-3</sup>
V1TG	0.029	0.23	1.00x10 <sup>-2</sup>
L2CH	0.031	-0.23	1.16x10 <sup>-2</sup>
IDCH	0.054	0.23	1.17x10 <sup>-2</sup>
VLPL	0.044	0.23	1.21x10 <sup>-2</sup>
V5CH	0.044	0.22	1.40x10 <sup>-2</sup>
V1PL	0.031	0.21	1.82x10 <sup>-2</sup>
L5PL	0.070	-0.20	2.61x10 <sup>-2</sup>
IDFC	0.048	0.19	3.52x10 <sup>-2</sup>
V5PL	0.030	0.19	4.21x10 <sup>-2</sup>
TPAB	0.016	0.18	4.73x10 <sup>-2</sup>
TBPN	0.016	0.18	4.73x10 <sup>-2</sup>

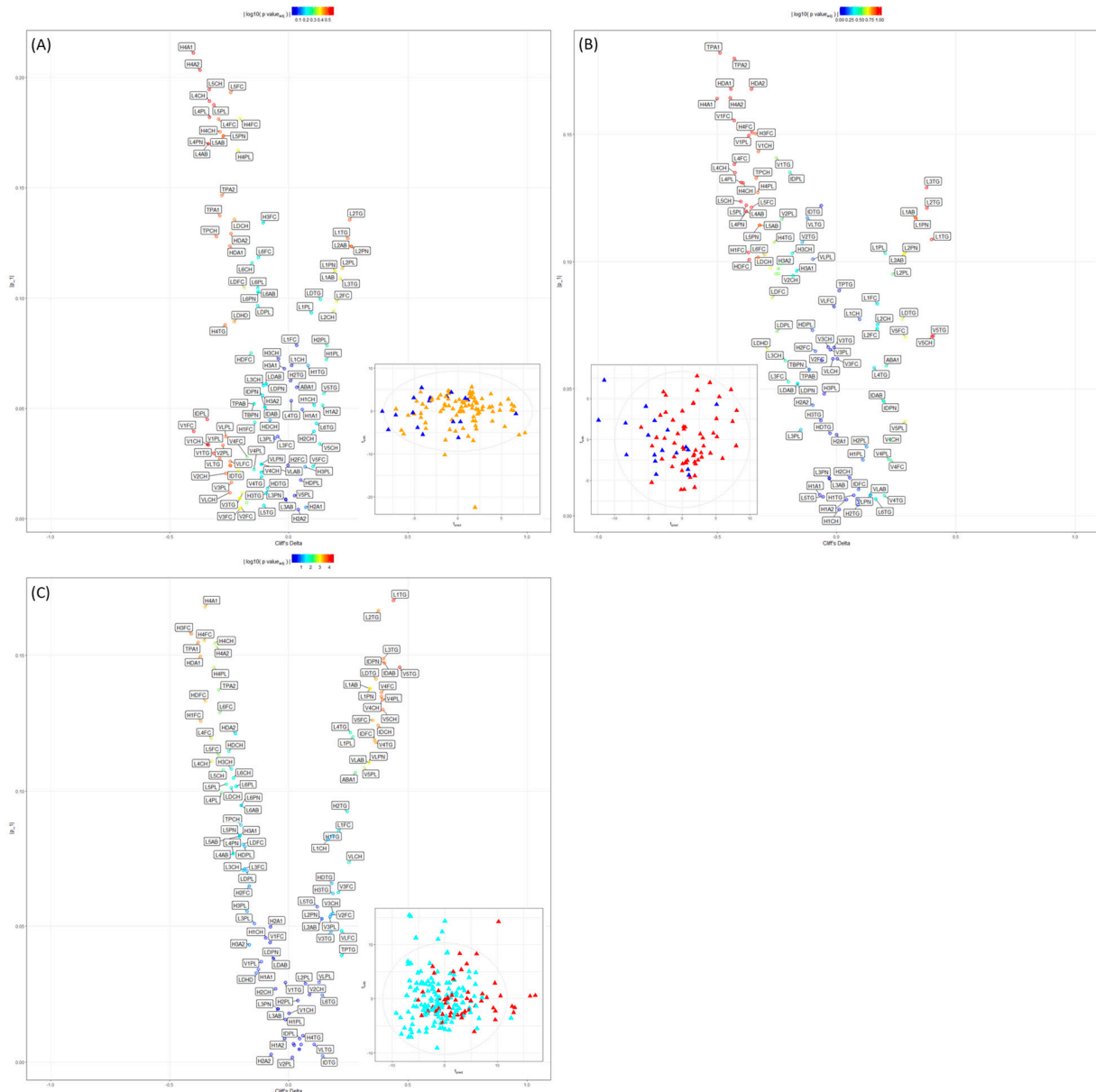
**Table S13 - OPLS loadings, Cliff's delta and adjusted p-values of the lipoproteins for the comparison of the controls and SARS-CoV-2 positive patients in severity class E.** Only metabolites with significant p-values are shown in the table.

Metabolite	OPLS loadings	Cliff's delta	Adjusted p-value
H4PL	0.165	-0.98	2.70x10 <sup>-21</sup>
H4CH	0.166	-0.97	3.01x10 <sup>-21</sup>
TPA2	0.158	-0.95	7.83x10 <sup>-21</sup>

H4A1	0.167	-0.95	$7.83 \times 10^{-21}$
H4A2	0.161	-0.95	$1.02 \times 10^{-20}$
TPA1	0.160	-0.94	$2.39 \times 10^{-20}$
HDA1	0.158	-0.93	$3.32 \times 10^{-20}$
H4FC	0.166	-0.92	$1.06 \times 10^{-19}$
HDA2	0.150	-0.91	$3.57 \times 10^{-19}$
H3FC	0.163	-0.91	$3.57 \times 10^{-19}$
H3CH	0.148	-0.86	$2.11 \times 10^{-17}$
HDCH	0.140	-0.86	$3.02 \times 10^{-17}$
LDTG	0.144	0.85	$4.11 \times 10^{-17}$
L1TG	0.145	0.80	$4.36 \times 10^{-15}$
HDPL	0.129	-0.78	$1.36 \times 10^{-14}$
L2TG	0.142	0.76	$5.23 \times 10^{-14}$
H3A1	0.134	-0.76	$6.97 \times 10^{-14}$
VLPN	0.124	0.75	$1.16 \times 10^{-13}$
VLAB	0.124	0.75	$1.16 \times 10^{-13}$
V4TG	0.121	0.75	$1.16 \times 10^{-13}$
H3PL	0.124	-0.75	$1.31 \times 10^{-13}$
HDFC	0.138	-0.75	$1.47 \times 10^{-13}$
H2TG	0.119	0.74	$3.52 \times 10^{-13}$
L4TG	0.127	0.73	$4.65 \times 10^{-13}$
V5TG	0.116	0.71	$2.18 \times 10^{-12}$
ABA1	0.120	0.70	$3.23 \times 10^{-12}$
V4PL	0.120	0.70	$6.23 \times 10^{-12}$
H1FC	0.112	-0.67	$2.92 \times 10^{-11}$
L3TG	0.121	0.67	$4.92 \times 10^{-11}$
V2FC	0.098	0.66	$8.04 \times 10^{-11}$
L5TG	0.107	0.65	$9.96 \times 10^{-11}$
V3TG	0.096	0.65	$1.55 \times 10^{-10}$
V3FC	0.099	0.63	$5.03 \times 10^{-10}$
H2A1	0.102	-0.63	$5.03 \times 10^{-10}$
V4FC	0.115	0.62	$7.93 \times 10^{-10}$
L4CH	0.110	-0.60	$3.78 \times 10^{-9}$
V4CH	0.111	0.59	$6.08 \times 10^{-9}$
H1TG	0.108	0.59	$7.39 \times 10^{-9}$
TPCH	0.110	-0.58	$9.54 \times 10^{-9}$
TPTG	0.088	0.58	$1.34 \times 10^{-8}$

H3A2	0.099	-0.58	1.34x10 <sup>-8</sup>
IDAB	0.113	0.57	1.70x10 <sup>-8</sup>
IDPN	0.113	0.57	1.74x10 <sup>-8</sup>
V3PL	0.091	0.57	2.04x10 <sup>-8</sup>
L4FC	0.114	-0.56	2.94x10 <sup>-8</sup>
H2FC	0.102	-0.55	4.38x10 <sup>-8</sup>
L6TG	0.091	0.55	5.66x10 <sup>-8</sup>
VLCH	0.090	0.54	9.94x10 <sup>-8</sup>
L4PL	0.101	-0.54	1.10x10 <sup>-7</sup>
H3TG	0.085	0.54	1.10x10 <sup>-7</sup>
V3CH	0.085	0.52	2.06x10 <sup>-7</sup>
LDCH	0.103	-0.52	2.59x10 <sup>-7</sup>
HDTG	0.094	0.52	2.60x10 <sup>-7</sup>
V2TG	0.068	0.52	3.31x10 <sup>-7</sup>
L3CH	0.087	-0.48	2.18x10 <sup>-6</sup>
V5CH	0.097	0.48	2.62x10 <sup>-6</sup>
VLTG	0.063	0.47	2.97x10 <sup>-6</sup>
VLFC	0.075	0.47	3.75x10 <sup>-6</sup>
IDCH	0.094	0.47	3.91x10 <sup>-6</sup>
IDFC	0.089	0.44	1.55x10 <sup>-5</sup>
V2CH	0.063	0.42	2.86x10 <sup>-5</sup>
V2PL	0.055	0.41	6.40x10 <sup>-5</sup>
V5PL	0.083	0.41	6.40x10 <sup>-5</sup>
IDTG	0.050	0.40	7.17x10 <sup>-5</sup>
IDPL	0.083	-0.40	7.19x10 <sup>-5</sup>
L4PN	0.077	-0.40	9.02x10 <sup>-5</sup>
L4AB	0.077	-0.40	9.02x10 <sup>-5</sup>
LDFC	0.083	-0.39	1.37x10 <sup>-4</sup>
L3PL	0.072	-0.39	1.41x10 <sup>-4</sup>
VLPL	0.061	0.38	1.69x10 <sup>-4</sup>
L3FC	0.080	-0.37	2.18x10 <sup>-4</sup>
H2A2	0.051	-0.34	7.86x10 <sup>-4</sup>
L5CH	0.075	-0.34	9.84x10 <sup>-4</sup>
L5FC	0.085	-0.33	1.02x10 <sup>-3</sup>
H2CH	0.064	-0.33	1.21x10 <sup>-3</sup>
V1TG	0.029	0.30	3.04x10 <sup>-3</sup>
L1CH	0.026	-0.30	3.84x10 <sup>-3</sup>

L6FC	0.078	-0.28	$6.97 \times 10^{-3}$
L5PL	0.069	-0.26	$1.10 \times 10^{-2}$
L2CH	0.037	-0.23	$2.76 \times 10^{-2}$
H1CH	0.045	-0.23	$2.76 \times 10^{-2}$
L1PN	0.066	0.21	$4.32 \times 10^{-2}$
L1AB	0.066	0.21	$4.32 \times 10^{-2}$



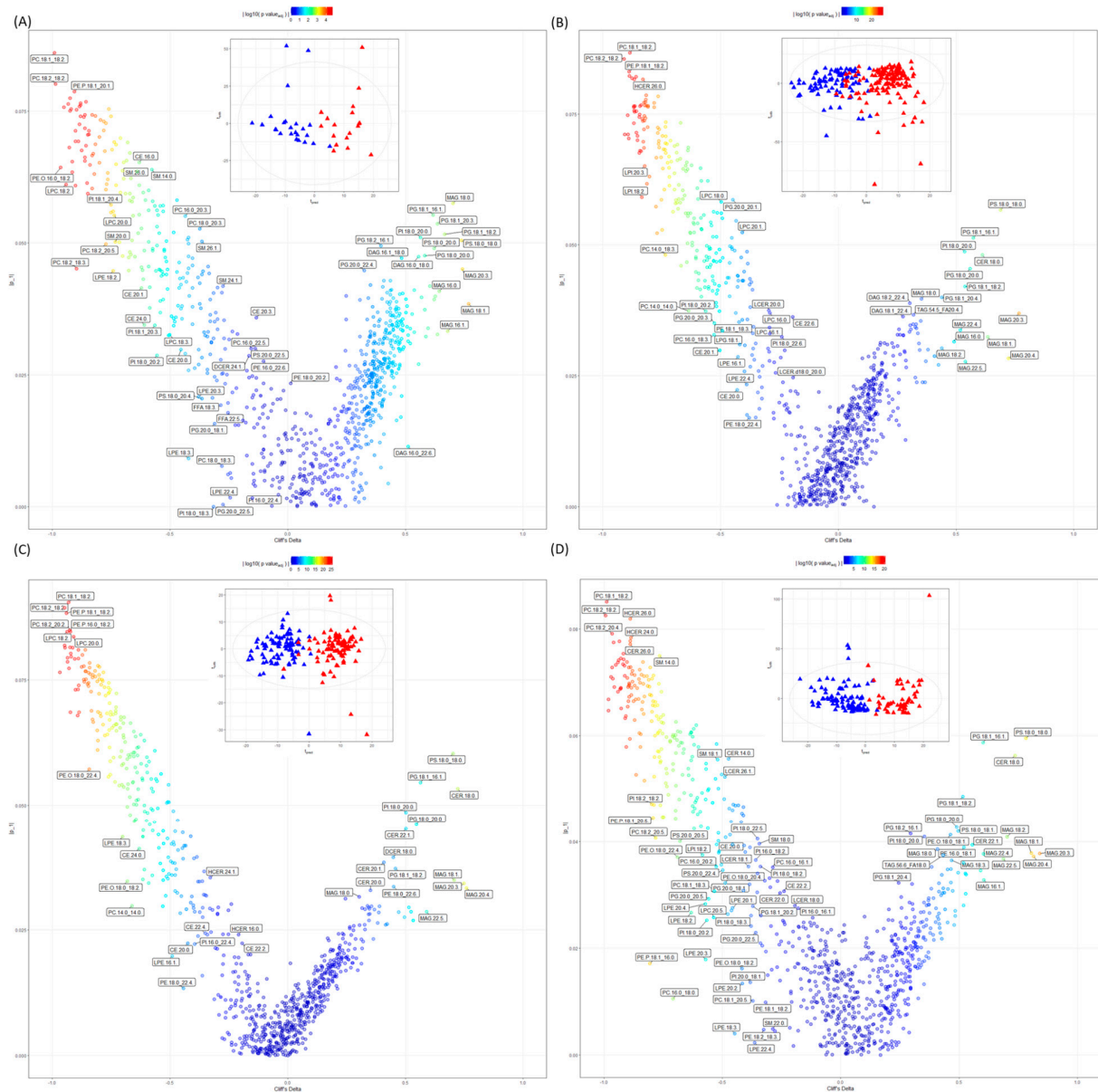
**Figure S8 - Orthogonal Partial Least Squared (O-PLS-DA) and eruption plots between different severity classes of SARS-CoV-2 positive patients for the lipoproteins. (A) O-PLS-DA SARS-CoV-2 severity group B (blue) and SARS-CoV-2 severity group D (orange) ( $R^2X=0.18$ ,  $AUROC=0.64$ ) and eruption plot. (B) O-PLS-DA SARS-CoV-2 severity group B**

(blue) and SARS-CoV-2 severity group E (red) ( $R_2X=0.21$ , AUROC=0.70) and eruption plot. (C) O-PLS-DA SARS-CoV-2 severity group C (cyan) and SARS-CoV-2 severity group E (red) ( $R_2X=0.28$ , AUROC=0.72) and eruption plot. Significant models could not be produced for severity group B vs C, group C vs D or D vs E.

**Table S14 - OPLS loadings, Cliff's delta and adjusted p-values of the lipoproteins for the comparison of severity class C and E.** Only metabolites with significant p-values are shown in the table.

Metabolite	OPLS loadings	Cliff's delta	Adjusted p-value
V5TG	0.146	0.47	$3.50 \times 10^{-5}$
L1TG	0.170	0.44	$7.69 \times 10^{-5}$
IDPN	0.147	0.40	$2.00 \times 10^{-4}$
IDAB	0.147	0.40	$2.00 \times 10^{-4}$
V5CH	0.130	0.40	$2.00 \times 10^{-4}$
V4PL	0.134	0.40	$2.00 \times 10^{-4}$
L3TG	0.149	0.40	$2.00 \times 10^{-4}$
H3FC	0.158	-0.41	$2.00 \times 10^{-4}$
V4CH	0.135	0.39	$2.20 \times 10^{-4}$
V4FC	0.136	0.39	$2.20 \times 10^{-4}$
TPA1	0.155	-0.38	$3.08 \times 10^{-4}$
L2TG	0.166	0.38	$3.26 \times 10^{-4}$
IDCH	0.124	0.37	$3.40 \times 10^{-4}$
HDA1	0.150	-0.37	$3.58 \times 10^{-4}$
H1FC	0.126	-0.37	$3.65 \times 10^{-4}$
LDTG	0.141	0.37	$4.20 \times 10^{-4}$
V4TG	0.118	0.36	$4.20 \times 10^{-4}$
V5FC	0.126	0.35	$4.57 \times 10^{-4}$
IDFC	0.119	0.36	$4.58 \times 10^{-4}$
H4FC	0.156	-0.35	$5.42 \times 10^{-4}$
H4A1	0.168	-0.35	$6.02 \times 10^{-4}$
HDFC	0.133	-0.35	$6.15 \times 10^{-4}$
L1PN	0.138	0.34	$8.71 \times 10^{-4}$
L1AB	0.138	0.34	$9.64 \times 10^{-4}$
VLPN	0.110	0.34	$9.64 \times 10^{-4}$
VLAB	0.110	0.34	$9.64 \times 10^{-4}$
L4FC	0.119	-0.33	$1.46 \times 10^{-3}$
L4CH	0.111	-0.32	$1.53 \times 10^{-3}$
V5PL	0.109	0.32	$1.91 \times 10^{-3}$
H4PL	0.146	-0.31	$2.08 \times 10^{-3}$
H4CH	0.154	-0.31	$2.39 \times 10^{-3}$

H4A2	0.153	-0.30	$3.07 \times 10^{-3}$
TPA2	0.137	-0.29	$4.04 \times 10^{-3}$
L5FC	0.113	-0.29	$4.04 \times 10^{-3}$
L6FC	0.129	-0.29	$4.70 \times 10^{-3}$
L4PL	0.099	-0.28	$5.81 \times 10^{-3}$
ABA1	0.107	0.28	$6.27 \times 10^{-3}$
L5CH	0.108	-0.27	$7.41 \times 10^{-3}$
L1PL	0.120	0.27	$8.88 \times 10^{-3}$
L5PL	0.103	-0.26	$1.09 \times 10^{-2}$
L4TG	0.121	0.26	$1.26 \times 10^{-2}$
HDCH	0.115	-0.25	$1.49 \times 10^{-2}$
VLCH	0.073	0.25	$1.49 \times 10^{-2}$
H2TG	0.092	0.24	$1.87 \times 10^{-2}$
LDCH	0.101	-0.24	$1.98 \times 10^{-2}$
H3CH	0.108	-0.24	$2.00 \times 10^{-2}$
L4PN	0.077	-0.23	$2.47 \times 10^{-2}$
L4AB	0.077	-0.23	$2.47 \times 10^{-2}$
L6CH	0.105	-0.23	$2.51 \times 10^{-2}$
HDA2	0.121	-0.22	$3.07 \times 10^{-2}$
TPTG	0.039	0.22	$3.14 \times 10^{-2}$
VLFC	0.048	0.22	$3.14 \times 10^{-2}$
L6PL	0.102	-0.22	$3.14 \times 10^{-2}$
L1FC	0.085	0.21	$4.35 \times 10^{-2}$
L5PN	0.083	-0.21	$4.56 \times 10^{-2}$
V3FC	0.062	0.21	$4.56 \times 10^{-2}$
L5AB	0.083	-0.21	$4.56 \times 10^{-2}$
H3A1	0.083	-0.20	$4.81 \times 10^{-2}$



**Figure S9 - Orthogonal Partial Least Squared (O-PLS-DA) and eruption plots between controls and SARS-CoV-2 positive patients of each severity group for the Lipids.** (A) Eruption plot of the controls vs group B severity group with the O-PLS-DA of controls (blue triangles) and SARS-CoV-2 group B severity patients (red triangles) ( $R^2X=0.22$ , AUROC=0.98) inset. (B) Eruption plot of the controls vs group C severity group with the O-PLS-DA of controls (blue triangles) and SARS-CoV-2 group C severity patients (red triangles) ( $R^2X=0.18$ , AUROC=0.97) inset. (C) Eruption plot of the controls vs group D severity group with the O-PLS-DA of controls (blue triangles) and SARS-CoV-2 group D severity patients (red triangles) ( $R^2X=0.12$ , AUROC=0.99) inset. (D) Eruption plot of the controls vs group E severity group with the O-PLS-DA of controls (blue triangles) and SARS-CoV-2 group E severity patients (red triangles) ( $R^2X=0.21$ , AUROC=0.99) inset.

**Table S15 - OPLS loadings, Cliff's delta and adjusted p-values of the lipids for the comparison of the controls and SARS-CoV-2 positive patients in severity class B.** Only the 50 most significant adjusted p-values are shown.

Metabolite	OPLS loadings	Cliff's delta	Adjusted p-value
PC (18:1/18:2)	0.086	-0.99	2.00x10 <sup>-5</sup>
PC (18:2/18:2)	0.080	-0.99	2.00x10 <sup>-5</sup>
PE.O (16:0/18:2)	0.064	-0.96	2.65x10 <sup>-5</sup>
HCER.d (18:0/18:0)	0.075	-0.92	2.85x10 <sup>-5</sup>
LPC (18:2)	0.061	-0.94	2.85x10 <sup>-5</sup>
PE.O (16:0/20:4)	0.063	-0.92	2.85x10 <sup>-5</sup>
PE.P (16:0/18:2)	0.077	-0.92	2.85x10 <sup>-5</sup>
PE.P (16:0/18:3)	0.065	-0.92	2.85x10 <sup>-5</sup>
PE.P (18:0/18:2)	0.076	-0.93	2.85x10 <sup>-5</sup>
PE.P (18:0/20:1)	0.075	-0.92	2.85x10 <sup>-5</sup>
PE.P (18:1/18:2)	0.076	-0.95	2.85x10 <sup>-5</sup>
PE.P (18:2/20:4)	0.068	-0.93	2.85x10 <sup>-5</sup>
PC (18:2/20:2)	0.061	-0.90	3.14x10 <sup>-5</sup>
PE.O (18:0/22:5)	0.071	-0.90	3.14x10 <sup>-5</sup>
PE.P (18:1/20:1)	0.079	-0.91	3.14x10 <sup>-5</sup>
PE.P (18:1/20:4)	0.069	-0.90	3.14x10 <sup>-5</sup>
PC (18:2/18:3)	0.045	-0.90	3.17x10 <sup>-5</sup>
PC (18:2/20:4)	0.075	-0.90	3.17x10 <sup>-5</sup>
HCER (22:0)	0.069	-0.89	3.87x10 <sup>-5</sup>
PC (16:0/18:2)	0.076	-0.88	3.93x10 <sup>-5</sup>
PC (20:0/20:4)	0.074	-0.88	3.93x10 <sup>-5</sup>
PE.O (16:0/20:1)	0.073	-0.88	3.93x10 <sup>-5</sup>
PE.P (18:0/18:1)	0.077	-0.88	3.93x10 <sup>-5</sup>
PE.P (18:1/22:5)	0.076	-0.88	3.93x10 <sup>-5</sup>
PE.O (18:0/22:4)	0.068	-0.88	4.28x10 <sup>-5</sup>
PC (18:0/20:1)	0.074	-0.87	5.16x10 <sup>-5</sup>
PE.O (16:0/18:1)	0.066	-0.86	5.16x10 <sup>-5</sup>
PE.P (16:0/22:5)	0.074	-0.86	5.16x10 <sup>-5</sup>
PE.P (18:0/20:4)	0.066	-0.86	5.16x10 <sup>-5</sup>
PE.P (18:1/22:4)	0.072	-0.86	5.16x10 <sup>-5</sup>
PE.P (18:0/22:5)	0.068	-0.86	5.46x10 <sup>-5</sup>
PE.P (18:2/18:2)	0.068	-0.86	5.46x10 <sup>-5</sup>
PE.O (16:0/22:5)	0.061	-0.85	5.98x10 <sup>-5</sup>

PE.O (16:0/22:6)	0.059	-0.85	6.36x10 <sup>-5</sup>
PE.P (18:0/22:4)	0.071	-0.85	6.36x10 <sup>-5</sup>
PC (20:0/18:1)	0.071	-0.84	6.79x10 <sup>-5</sup>
PE.P (18:0/18:0)	0.071	-0.84	6.79x10 <sup>-5</sup>
PE.P (16:0/20:4)	0.065	-0.84	7.45x10 <sup>-5</sup>
HCER.d (18:0/22:0)	0.067	-0.83	8.76x10 <sup>-5</sup>
PE.P (16:0/20:1)	0.074	-0.83	8.76x10 <sup>-5</sup>
PE.P (18:1/16:0)	0.060	-0.83	8.76x10 <sup>-5</sup>
PE.P (18:0/16:0)	0.067	-0.83	9.62x10 <sup>-5</sup>
PC (20:0/20:3)	0.063	-0.82	1.06x10 <sup>-4</sup>
PC (18:2/20:3)	0.069	-0.82	1.14x10 <sup>-4</sup>
PE.P (18:1/18:1)	0.074	-0.82	1.14x10 <sup>-4</sup>
PC (18:2/22:6)	0.065	-0.80	1.72x10 <sup>-4</sup>
PE.P (18:0/20:2)	0.070	-0.80	1.72x10 <sup>-4</sup>
PC (16:0/20:1)	0.073	-0.80	1.89x10 <sup>-4</sup>
HCER.d (18:0/24:0)	0.073	-0.78	2.55x10 <sup>-4</sup>
PE.P (16:0/18:1)	0.071	-0.78	2.55x10 <sup>-4</sup>

**Table S16 - OPLS loadings, Cliff's delta and adjusted p-values of the lipids for the comparison of the controls and SARS-CoV-2 positive patients in severity class C.** Only the 50 most significant adjusted p-values are shown.

Metabolite	OPLS loadings	Cliff's delta	Adjusted p-value
PC (18:2/18:2)	0.086	-0.91	3.47x10 <sup>-28</sup>
PE.O (16:0/20:4)	0.071	-0.91	3.47x10 <sup>-28</sup>
PE.O (16:0/18:2)	0.075	-0.89	1.24x10 <sup>-27</sup>
PE.P (18:2/20:4)	0.071	-0.89	1.24x10 <sup>-27</sup>
PE.P (16:0/22:5)	0.070	-0.89	1.75x10 <sup>-27</sup>
PE.P (16:0/18:2)	0.082	-0.89	1.78x10 <sup>-27</sup>
PE.P (18:1/18:2)	0.083	-0.89	1.78x10 <sup>-27</sup>
PC (18:1/18:2)	0.087	-0.88	2.16x10 <sup>-27</sup>
PE.P (18:0/18:2)	0.082	-0.88	6.43x10 <sup>-27</sup>
HCER.d (18:0/18:0)	0.076	-0.87	1.56x10 <sup>-26</sup>
PE.O (16:0/18:1)	0.073	-0.87	1.56x10 <sup>-26</sup>
PE.O (16:0/20:1)	0.076	-0.87	1.56x10 <sup>-26</sup>
PE.P (18:0/18:1)	0.082	-0.87	1.76x10 <sup>-26</sup>

PE.P (18:0/22:5)	0.076	-0.87	1.76x10 <sup>-26</sup>
PE.P (18:1/20:4)	0.075	-0.87	1.80x10 <sup>-26</sup>
PC (18:2/20:2)	0.076	-0.86	2.43x10 <sup>-26</sup>
PE.P (16:0/20:1)	0.082	-0.86	4.43x10 <sup>-26</sup>
LPC (18:2)	0.076	-0.86	4.58x10 <sup>-26</sup>
PC (18:2/20:3)	0.071	-0.86	4.64x10 <sup>-26</sup>
PE.O (18:0/22:5)	0.070	-0.85	8.09x10 <sup>-26</sup>
PE.P (16:0/20:4)	0.071	-0.85	8.09x10 <sup>-26</sup>
PC (20:0/20:3)	0.074	-0.84	2.26x10 <sup>-25</sup>
PE.P (18:0/22:4)	0.068	-0.84	2.26x10 <sup>-25</sup>
PE.P (18:2/18:2)	0.075	-0.84	2.65x10 <sup>-25</sup>
PC (18:0/20:1)	0.076	-0.84	2.78x10 <sup>-25</sup>
PE.O (18:0/22:4)	0.068	-0.84	2.80x10 <sup>-25</sup>
PE.P (18:0/20:1)	0.077	-0.84	4.80x10 <sup>-25</sup>
LPI (18:1)	0.068	-0.84	4.94x10 <sup>-25</sup>
LPI (18:2)	0.059	-0.83	6.95x10 <sup>-25</sup>
PE.P (18:1/22:5)	0.074	-0.83	9.14x10 <sup>-25</sup>
HCER (26:0)	0.082	-0.83	1.15x10 <sup>-24</sup>
PE.P (18:0/20:3)	0.074	-0.83	1.19x10 <sup>-24</sup>
PE.P (16:0/18:3)	0.070	-0.83	1.35x10 <sup>-24</sup>
PE.P (18:0/20:4)	0.072	-0.83	1.94x10 <sup>-24</sup>
PE.O (16:0/22:5)	0.069	-0.82	2.09x10 <sup>-24</sup>
PE.P (18:0/20:2)	0.077	-0.82	2.09x10 <sup>-24</sup>
HCER (22:0)	0.075	-0.82	2.46x10 <sup>-24</sup>
HCER.d (18:0/22:0)	0.074	-0.82	2.46x10 <sup>-24</sup>
LPI (20:3)	0.065	-0.82	2.55x10 <sup>-24</sup>
PE.P (18:0/18:0)	0.077	-0.82	2.55x10 <sup>-24</sup>
PC (20:0/18:1)	0.074	-0.82	4.27x10 <sup>-24</sup>
PE.P (18:1/18:1)	0.077	-0.82	4.36x10 <sup>-24</sup>
PC (18:2/20:4)	0.078	-0.82	4.95x10 <sup>-24</sup>
LPC (20:0)	0.079	-0.82	5.75x10 <sup>-24</sup>
HCER.d (18:0/24:0)	0.077	-0.81	7.44x10 <sup>-24</sup>
PE.P (18:1/22:4)	0.062	-0.81	8.83x10 <sup>-24</sup>
PI (18:1/18:1)	0.072	-0.81	1.22x10 <sup>-23</sup>
PE.P (18:0/16:0)	0.076	-0.81	1.33x10 <sup>-23</sup>
HCER (24:0)	0.077	-0.81	1.48x10 <sup>-23</sup>
PC (18:2/18:3)	0.063	-0.80	3.23x10 <sup>-23</sup>

**Table S17 - OPLS loadings, Cliff's delta and adjusted p-values of the lipids for the comparison of the controls and SARS-CoV-2 positive patients in severity class D. Only the 50 most significant adjusted p-values are shown.**

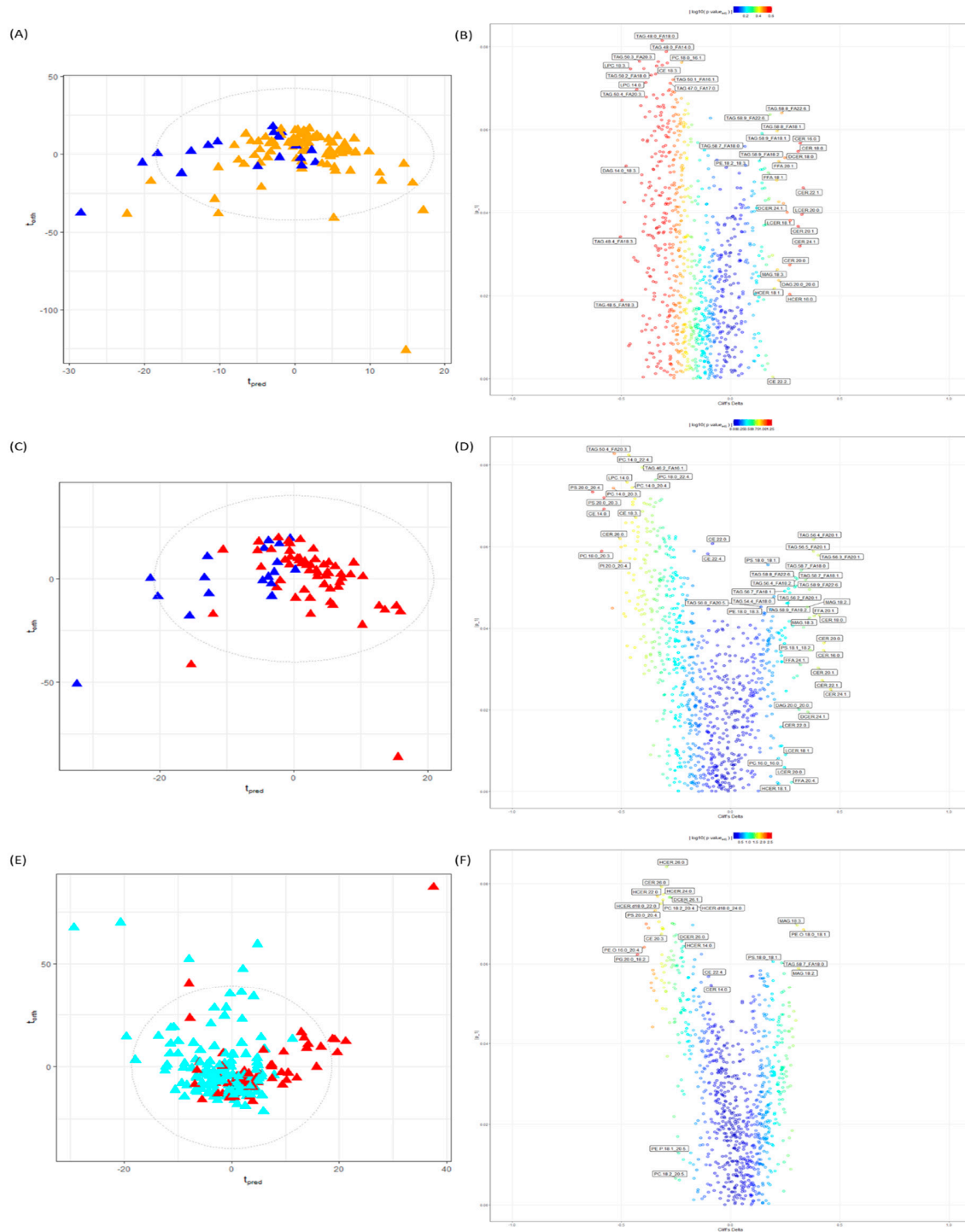
Metabolite	OPLS loadings	Cliff's delta	Adjusted p-value
PE.O (16:0/20:4)	0.077	-0.97	1.91x10 <sup>-26</sup>
PC (18:2/18:2)	0.089	-0.95	8.63x10 <sup>-26</sup>
PE.P (18:1/20:4)	0.082	-0.95	8.63x10 <sup>-26</sup>
PE.P (18:2/20:4)	0.081	-0.95	8.63x10 <sup>-26</sup>
PE.P (18:1/18:2)	0.088	-0.94	1.56x10 <sup>-25</sup>
LPC (18:2)	0.085	-0.94	1.76x10 <sup>-25</sup>
PE.P (16:0/20:4)	0.079	-0.94	1.76x10 <sup>-25</sup>
PE.P (16:0/22:5)	0.079	-0.94	1.76x10 <sup>-25</sup>
PC (18:1/18:2)	0.090	-0.93	2.91x10 <sup>-25</sup>
PE.O (16:0/18:2)	0.077	-0.93	2.97x10 <sup>-25</sup>
PC (18:1/20:2)	0.085	-0.93	3.67x10 <sup>-25</sup>
PE.P (18:0/18:2)	0.081	-0.92	4.58x10 <sup>-25</sup>
PC (18:2/18:3)	0.069	-0.92	4.78x10 <sup>-25</sup>
PE.P (16:0/18:2)	0.085	-0.92	4.98x10 <sup>-25</sup>
PE.P (18:0/22:5)	0.080	-0.92	4.98x10 <sup>-25</sup>
PC (18:2/20:3)	0.080	-0.92	5.97x10 <sup>-25</sup>
PE.P (18:2/18:2)	0.081	-0.91	1.28x10 <sup>-24</sup>
LPC (20:0)	0.084	-0.91	1.85x10 <sup>-24</sup>
PE.P (18:1/22:5)	0.079	-0.91	3.30x10 <sup>-24</sup>
PE.O (16:0/22:5)	0.073	-0.90	4.92x10 <sup>-24</sup>
PE.O (16:0/18:1)	0.068	-0.89	1.46x10 <sup>-23</sup>
PE.O (18:0/22:5)	0.073	-0.89	1.71x10 <sup>-23</sup>
PE.P (18:0/20:4)	0.079	-0.89	1.84x10 <sup>-23</sup>
PE.P (18:0/18:1)	0.081	-0.89	1.87x10 <sup>-23</sup>
PC (20:0/20:3)	0.074	-0.89	2.02x10 <sup>-23</sup>
PE.P (16:0/18:3)	0.069	-0.89	2.54x10 <sup>-23</sup>
PC (18:2/20:4)	0.078	-0.88	8.13x10 <sup>-23</sup>
HCER.d (18:0/18:0)	0.080	-0.87	1.08x10 <sup>-22</sup>
PE.O (16:0/20:1)	0.075	-0.87	2.15x10 <sup>-22</sup>
PI (20:0/18:2)	0.078	-0.87	2.33x10 <sup>-22</sup>
PE.P (18:1/22:4)	0.075	-0.87	2.46x10 <sup>-22</sup>
LPC (20:3)	0.077	-0.86	4.35x10 <sup>-22</sup>
PE.P (16:0/20:1)	0.081	-0.86	4.35x10 <sup>-22</sup>

PE.P (18:0/16:0)	0.077	-0.86	5.62x10 <sup>-22</sup>
PE.P (18:0/22:4)	0.075	-0.86	5.95x10 <sup>-22</sup>
PI (18:1/18:1)	0.074	-0.85	1.11x10 <sup>-21</sup>
PE.P (18:0/20:3)	0.074	-0.85	1.70x10 <sup>-21</sup>
SM (24:0)	0.076	-0.85	1.70x10 <sup>-21</sup>
PC (18:0/20:1)	0.074	-0.85	1.91x10 <sup>-21</sup>
PE.O (18:0/22:4)	0.057	-0.84	2.61x10 <sup>-21</sup>
PE.P (18:1/18:1)	0.078	-0.84	2.77x10 <sup>-21</sup>
PE.P (18:0/20:1)	0.077	-0.84	3.03x10 <sup>-21</sup>
PE.P (18:0/18:0)	0.076	-0.84	4.02x10 <sup>-21</sup>
PE.P (16:0/22:4)	0.073	-0.84	5.05x10 <sup>-21</sup>
LPI (20:3)	0.069	-0.83	6.35x10 <sup>-21</sup>
PE.P (18:0/20:2)	0.075	-0.83	1.05x10 <sup>-20</sup>
LPC (18:3)	0.067	-0.83	1.09x10 <sup>-20</sup>
LPC (18:1)	0.076	-0.83	1.16x10 <sup>-20</sup>
SM (20:0)	0.067	-0.83	1.34x10 <sup>-20</sup>
PC (18:2/22:6)	0.077	-0.82	3.24x10 <sup>-20</sup>

**Table S18 - OPLS loadings, Cliff's delta and adjusted p-values of the lipids for the comparison of the controls and SARS-CoV-2 positive patients in severity class E.** Only the 50 most significant adjusted p values are shown.

Metabolite	OPLS loadings	Cliff's delta	Adjusted p-value
PC (18:1/18:2)	0.085	-0.99	3.35x10 <sup>-21</sup>
PC (18:2/18:2)	0.082	-0.99	3.35x10 <sup>-21</sup>
PE.O (16:0/20:4)	0.065	-0.98	4.10x10 <sup>-21</sup>
PE.P (18:2/20:4)	0.067	-0.98	4.10x10 <sup>-21</sup>
PC (20:0/20:3)	0.071	-0.97	9.70x10 <sup>-21</sup>
PC (18:2/20:3)	0.073	-0.97	9.93x10 <sup>-21</sup>
PC (18:2/20:4)	0.079	-0.97	9.93x10 <sup>-21</sup>
PE.P (18:1/20:4)	0.071	-0.96	1.19x10 <sup>-20</sup>
PE.P (16:0/18:2)	0.077	-0.96	1.52x10 <sup>-20</sup>
LPC (18:2)	0.069	-0.96	2.03x10 <sup>-20</sup>
PE.P (16:0/22:5)	0.073	-0.95	2.95x10 <sup>-20</sup>
PE.P (18:1/18:2)	0.074	-0.94	6.91x10 <sup>-20</sup>
PE.P (16:0/20:4)	0.068	-0.94	7.16x10 <sup>-20</sup>

PE.P (18:0/22:5)	0.074	-0.94	$8.07 \times 10^{-20}$
PC (18:0/20:1)	0.078	-0.94	$1.03 \times 10^{-19}$
PE.P (18:2/18:2)	0.069	-0.93	$1.41 \times 10^{-19}$
PE.P (18:0/20:3)	0.069	-0.93	$1.58 \times 10^{-19}$
PE.P (18:0/20:4)	0.069	-0.93	$1.58 \times 10^{-19}$
PE.P (18:0/18:2)	0.074	-0.93	$1.62 \times 10^{-19}$
PE.O (16:0/22:5)	0.065	-0.93	$1.73 \times 10^{-19}$
HCER (22:0)	0.075	-0.92	$3.49 \times 10^{-19}$
PC (18:2/22:5)	0.073	-0.92	$3.49 \times 10^{-19}$
HCER.d (18:0/22:0)	0.074	-0.92	$4.19 \times 10^{-19}$
LPC (20:0)	0.073	-0.91	$5.04 \times 10^{-19}$
PE.P (18:0/22:4)	0.071	-0.91	$5.84 \times 10^{-19}$
PI (20:0/18:2)	0.063	-0.91	$6.05 \times 10^{-19}$
PE.O (16:0/18:2)	0.064	-0.91	$8.49 \times 10^{-19}$
PE.P (16:0/18:3)	0.058	-0.91	$8.82 \times 10^{-19}$
PE.P (16:0/20:1)	0.074	-0.90	$1.28 \times 10^{-18}$
PC (18:2/22:6)	0.071	-0.90	$1.39 \times 10^{-18}$
PC (18:2/20:2)	0.065	-0.90	$1.45 \times 10^{-18}$
PE.O (16:0/20:1)	0.069	-0.90	$1.75 \times 10^{-18}$
PE.P (18:1/22:4)	0.066	-0.90	$1.90 \times 10^{-18}$
PE.P (18:0/16:0)	0.073	-0.90	$2.14 \times 10^{-18}$
PE.P (18:1/22:5)	0.069	-0.89	$2.15 \times 10^{-18}$
PE.P (16:0/22:4)	0.067	-0.89	$2.17 \times 10^{-18}$
PE.P (18:0/20:1)	0.070	-0.89	$2.19 \times 10^{-18}$
HCER.d (18:0/18:0)	0.070	-0.89	$2.47 \times 10^{-18}$
SM (20:0)	0.059	-0.89	$2.90 \times 10^{-18}$
CER (26:0)	0.077	-0.89	$3.00 \times 10^{-18}$
HCER (26:0)	0.082	-0.89	$3.00 \times 10^{-18}$
HCER.d (18:0/24:0)	0.078	-0.89	$3.00 \times 10^{-18}$
SM (24:0)	0.073	-0.89	$3.28 \times 10^{-18}$
HCER (24:0)	0.078	-0.89	$3.99 \times 10^{-18}$
PE.P (18:0/20:2)	0.069	-0.89	$4.05 \times 10^{-18}$
PC (14:0/20:4)	0.068	-0.88	$4.26 \times 10^{-18}$
PI (18:1/20:4)	0.072	-0.88	$4.65 \times 10^{-18}$
PC (16:1/18:2)	0.070	-0.88	$6.09 \times 10^{-18}$
PE.P (18:0/18:1)	0.072	-0.88	$6.42 \times 10^{-18}$
PI (20:0/20:4)	0.066	-0.87	$9.72 \times 10^{-18}$



**Figure S10 - Orthogonal Partial Least Squared (O-PLS-DA) and eruption plots between different severity classes of SARS-CoV-2 positive patients for the lipids.** (A) O-PLS-DA SARS-CoV-2 severity group B (blue) and SARS-CoV-2 severity group D (orange) ( $R^2X=0.16$ ,  $AUROC=0.64$ ). (B) Eruption plot of severity group B vs severity group D. (C) O-

PLS-DA SARS-CoV-2 severity group B (blue) and SARS-CoV-2 severity group E (red) ( $R_2X=0.15$ , AUROC=0.79). (D) Eruption plot of severity group B vs severity group E. (E) O-PLS-DA SARS-CoV-2 severity group C (cyan) and SARS-CoV-2 severity group E (red) ( $R_2X=0.13$ , AUROC=0.72). Significant models could not be produced for severity group B vs C, group C vs D or D vs E.

**Table S19 - OPLS loadings, Cliff's delta and adjusted p-values of the lipids for the comparison of severity class B and E.** Only metabolites with significant p-values are shown in the table.

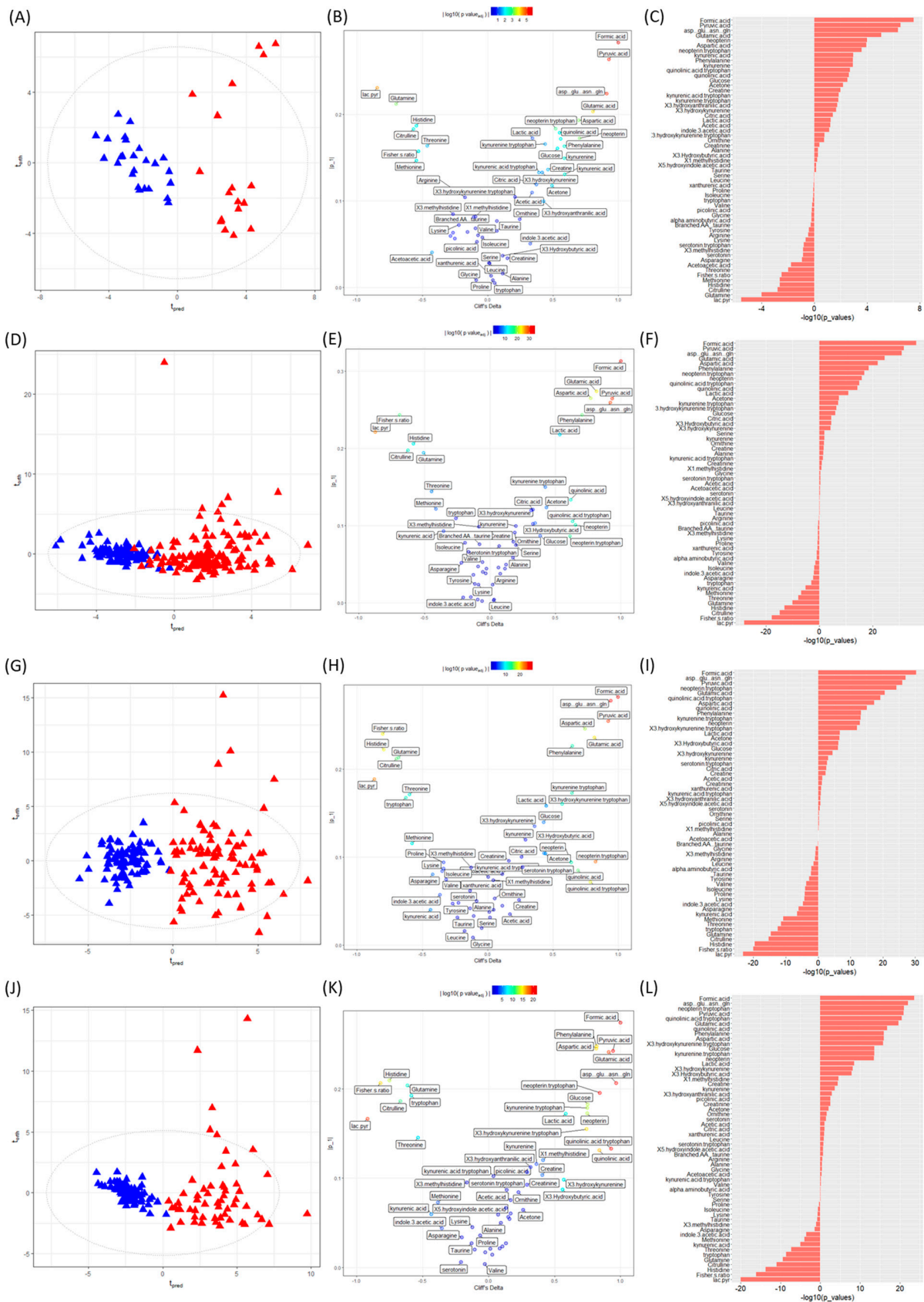
Lipid	OPLS loadings	Cliff's delta	Adjusted p-value
CE (14:0)	0.069	-0.58	$4.96 \times 10^{-2}$
PC (18:0/20:3)	0.059	-0.59	$4.96 \times 10^{-2}$
PS (20:0/20:3)	0.072	-0.58	$4.96 \times 10^{-2}$
PC (20:0/20:4)	0.073	-0.63	$4.96 \times 10^{-2}$

**Table S20 - OPLS loadings, Cliff's delta and adjusted p-values of the lipids for the comparison of severity class C and E.** Only metabolites with significant p-values are shown in the table.

Lipid	OPLS loadings	Cliff's delta	Adjusted p-value
PG (20:0/18:2)	0.062	-0.43	$2.39 \times 10^{-3}$
PE.O (16:0/20:4)	0.064	-0.40	$6.14 \times 10^{-3}$
PE.P (18:0/20:3)	0.070	-0.39	$6.18 \times 10^{-3}$
PI (20:0/20:4)	0.069	-0.38	$7.94 \times 10^{-3}$
PC (18:0/20:3)	0.054	-0.36	$9.36 \times 10^{-3}$
PE.P (16:0/20:3)	0.055	-0.36	$9.36 \times 10^{-3}$
PG (20:0/20:3)	0.044	-0.36	$9.83 \times 10^{-3}$
PS (20:0/22:6)	0.058	-0.36	$9.83 \times 10^{-3}$
PI (20:0/16:1)	0.058	-0.35	$9.99 \times 10^{-3}$
PI (20:0/18:2)	0.053	-0.35	$9.99 \times 10^{-3}$
PS (20:0/20:4)	0.073	-0.34	$1.21 \times 10^{-2}$
PE.P (18:1/20:3)	0.056	-0.34	$1.30 \times 10^{-2}$
PE (18:2/16:1)	0.051	-0.34	$1.33 \times 10^{-2}$
HCER (22:0)	0.077	-0.33	$1.46 \times 10^{-2}$
PE.O (18:0/18:1)	0.069	0.33	$1.46 \times 10^{-2}$
LPC (20:0)	0.071	-0.33	$1.68 \times 10^{-2}$
CE (16:0)	0.062	-0.31	$2.00 \times 10^{-2}$
CE (20:3)	0.067	-0.32	$2.00 \times 10^{-2}$
CER (26:0)	0.079	-0.32	$2.00 \times 10^{-2}$
HCER (24:0)	0.077	-0.31	$2.00 \times 10^{-2}$

HCER.d (18:0/22:0)	0.075	-0.32	2.00x10 <sup>-2</sup>
LPC (14:0)	0.069	-0.31	2.00x10 <sup>-2</sup>
LPC (16:0)	0.059	-0.31	2.00x10 <sup>-2</sup>
LPC (18:0)	0.069	-0.31	2.00x10 <sup>-2</sup>
MAG (18:2)	0.059	0.31	2.00x10 <sup>-2</sup>
PC (18:2/18:2)	0.069	-0.31	2.00x10 <sup>-2</sup>
PC (18:2/20:4)	0.076	-0.31	2.00x10 <sup>-2</sup>
PC (18:2/22:6)	0.060	-0.32	2.00x10 <sup>-2</sup>
PE.P (18:0/22:6)	0.049	-0.31	2.00x10 <sup>-2</sup>
SM (22:1)	0.056	-0.32	2.00x10 <sup>-2</sup>
MAG (18:3)	0.070	0.30	2.15x10 <sup>-2</sup>
PC (18:2/20:3)	0.054	-0.31	2.15x10 <sup>-2</sup>
PE.P (18:2/20:4)	0.058	-0.31	2.15x10 <sup>-2</sup>
PS (20:0/20:3)	0.055	-0.30	2.15x10 <sup>-2</sup>
PC (18:0/18:2)	0.060	-0.30	2.45x10 <sup>-2</sup>
TAG (56:3)_FA (20:1)	0.046	0.30	2.45x10 <sup>-2</sup>
PI (18:0/20:4)	0.049	-0.30	2.54x10 <sup>-2</sup>
SM (20:1)	0.053	-0.30	2.45x10 <sup>-2</sup>
PG (20:0/20:1)	0.053	-0.30	2.58x10 <sup>-2</sup>
HCER (26:0)	0.084	-0.29	2.77x10 <sup>-2</sup>
PC (14:0/22:6)	0.061	-0.29	2.83x10 <sup>-2</sup>
PG (20:0/18:1)	0.037	-0.29	2.94x10 <sup>-2</sup>
TAG (56:4)_FA (20:1)	0.048	0.29	2.94x10 <sup>-2</sup>
TAG (56:2)_FA (18:1)	0.042	0.28	3.37x10 <sup>-2</sup>
SM (24:0)	0.062	-0.28	3.42x10 <sup>-2</sup>
PE.P (16:0/22:6)	0.055	-0.28	3.45x10 <sup>-2</sup>
CER (16:0)	0.018	0.28	3.50x10 <sup>-2</sup>
HCER.d (18:0/24:0)	0.077	-0.28	3.50x10 <sup>-2</sup>
PC (16:0/22:6)	0.045	-0.28	3.55x10 <sup>-2</sup>
TAG (56:4)_FA (18:2)	0.044	0.28	3.55x10 <sup>-2</sup>
CER (24:1)	0.009	0.28	3.93x10 <sup>-2</sup>
DCER (26:1)	0.077	-0.28	3.93x10 <sup>-2</sup>
PE.P (18:0/20:4)	0.061	-0.28	3.93x10 <sup>-2</sup>
TAG (56:2)_FA (18:0)	0.035	0.28	3.93x10 <sup>-2</sup>
TAG (55:4)_FA (18:1)	0.030	0.27	4.15x10 <sup>-2</sup>
CER (20:0)	0.017	0.27	4.18x10 <sup>-2</sup>
FFA (20:1)	0.050	0.27	4.18x10 <sup>-2</sup>

HCER (20:0)	0.063	-0.27	$4.18 \times 10^{-2}$
MAG (18:1)	0.054	0.27	$4.18 \times 10^{-2}$
PC (18:1/20:4)	0.059	-0.27	$4.18 \times 10^{-2}$
PE (16:0/18:1)	0.047	0.27	$4.18 \times 10^{-2}$
TAG (54:3)_FA (18:0)	0.039	0.27	$4.18 \times 10^{-2}$
TAG (56:3)_FA (18:0)	0.043	0.27	$4.18 \times 10^{-2}$
TAG (56:7)_FA (18:1)	0.054	0.27	$4.18 \times 10^{-2}$
TAG (58:7)_FA (18:1)	0.049	0.27	$4.18 \times 10^{-2}$
PS (18:1/18:2)	0.050	0.27	$4.19 \times 10^{-2}$
PC (18:0/22:4)	0.070	-0.27	$4.28 \times 10^{-2}$
CE (22:5)	0.070	-0.26	$4.47 \times 10^{-2}$
TAG (58:3)_FA (18:1)	0.043	0.27	$4.47 \times 10^{-2}$
HCER.d (18:0/20:0)	0.060	-0.26	$4.48 \times 10^{-2}$
CER (22:1)	0.012	0.26	$4.54 \times 10^{-2}$
PE.P (18:1/20:4)	0.062	-0.26	$4.74 \times 10^{-2}$
TAG (55:3)_FA (18:1)	0.029	0.26	$4.74 \times 10^{-2}$
LPC (20:4)	0.054	-0.26	$4.84 \times 10^{-2}$
PE.P (16:0/20:4)	0.061	-0.26	$4.84 \times 10^{-3}$
PE.P (16:0/20:5)	0.022	-0.26	$4.84 \times 10^{-3}$
PC (14:0/20:4)	0.070	-0.30	$4.89 \times 10^{-3}$
PC (20:0/20:4)	0.067	-0.26	$4.89 \times 10^{-3}$
PC (18:0/20:2)	0.036	0.26	$4.89 \times 10^{-3}$
PE.P (18:2/18:2)	0.045	-0.26	$4.89 \times 10^{-3}$



**Figure S11 - Orthogonal Partial Least Squared (O-PLS-DA), eruption plots and  $-\log 10$  (p-values) between controls and SARS-CoV-2 positive patients of each severity group for the low molecular weight metabolites.** (A) O-PLS-DA of controls (blue triangles) and SARS-CoV-2 group B severity patients (red triangles) ( $R^2X=0.22$ , AUROC=0.98). (B) Eruption plot of the controls vs group B severity group. (C)  $-\log 10$  (p-values) of the controls vs group B severity group. (D) O-PLS-DA of controls (blue triangles) and SARS-CoV-2 group C severity patients (red triangles) ( $R^2X=0.15$ , AUROC=0.99). (E) Eruption plot of the controls vs group C severity group. (F)  $-\log 10$  (p-values) of the controls vs group C severity group. (G) O-PLS-DA of controls (blue triangles) and SARS-CoV-2 group D severity patients (red triangles) ( $R^2X=0.19$ , AUROC=1.00). (H) Eruption plot of the controls vs group D severity group. (I)  $-\log 10$  (p-values) of the controls vs group D severity group. (J) O-PLS-DA of controls (blue triangles) and SARS-CoV-2 group E severity patients (red triangles) ( $R^2X=0.21$ , AUROC=1.00). (K) Eruption plot of the controls vs group E severity group. (L)  $-\log 10$  (p-values) of the controls vs group E severity group. Eruption plots are formed from the Cliff's delta (abscissa) and O-PLS-DA loadings (ordinate). Coloured by significance.

**Table S21 - OPLS loadings, Cliff's delta and adjusted p-values of the low molecular weight metabolites for the comparison of the controls and SARS-CoV-2 positive patients in severity class B.** Only metabolites with significant p-values are shown in the table.

Metabolite	OPLS loadings	Cliff's delta	Adjusted p-value
Formic acid	0.283	1.00	$1.68 \times 10^{-6}$
Pyruvic acid	0.264	0.93	$8.01 \times 10^{-6}$
Asp/Glu:Asn/Gln	0.224	0.91	$8.50 \times 10^{-6}$
Lactate/pyruvate	0.231	-0.84	$4.14 \times 10^{-5}$
Glutamic acid	0.204	0.80	$9.52 \times 10^{-5}$
Neopterin	0.172	0.70	$7.91 \times 10^{-4}$
Aspartic acid	0.193	0.70	$7.91 \times 10^{-4}$
Glutamine	0.212	-0.70	$7.91 \times 10^{-4}$
Neopterin/tryptophan	0.184	0.52	$1.66 \times 10^{-3}$
Kynurenic acid	0.131	0.59	$5.49 \times 10^{-3}$
Kynurenine	0.149	0.47	$1.66 \times 10^{-3}$
Phenylalanine	0.163	0.59	$5.49 \times 10^{-3}$
Citrulline	0.183	-0.57	$7.13 \times 10^{-3}$
Quinolinic acid/tryptophan	0.172	0.56	$7.80 \times 10^{-3}$
Quinolinic acid	0.176	0.55	$8.25 \times 10^{-3}$
Histidine	0.187	-0.55	$8.25 \times 10^{-3}$
Methionine	0.147	-0.55	$8.25 \times 10^{-3}$
Glucose	0.161	0.53	$9.92 \times 10^{-3}$
Fisher's ratio	0.157	-0.53	$1.02 \times 10^{-2}$
Acetone	0.118	0.49	$1.84 \times 10^{-2}$
Creatine	0.135	0.46	$2.71 \times 10^{-2}$
Threonine	0.164	-0.46	$2.71 \times 10^{-2}$

Kynurenic acid/tryptophan	0.133	0.39	3.44x10 <sup>-2</sup>
Kynurenine/tryptophan	0.166	0.44	3.50x10 <sup>-2</sup>
Acetoacetic acid	0.040	-0.43	3.88x10 <sup>-2</sup>
3-hydroxyanthranilic acid	0.100	0.43	3.88x10 <sup>-2</sup>
3-hydroxykynurenine	0.133	0.42	4.49x10 <sup>-2</sup>

**Table S22 - OPLS loadings, Cliff's delta and adjusted p-values of the low molecular weight metabolites for the comparison of the controls and SARS-CoV-2 positive patients in severity class C.** Only metabolites with significant p-values are shown in the table.

Metabolite	OPLS loadings	Cliff's delta	Adjusted p-value
Formic acid	0.313	1.00	2.46x10 <sup>-35</sup>
Pyruvic acid	0.265	0.93	4.95x10 <sup>-31</sup>
Asp/Glu:Asn/Gln	0.259	0.92	2.23x10 <sup>-30</sup>
Lactate/pyruvate	0.221	-0.88	9.32x10 <sup>-28</sup>
Glutamic acid	0.274	0.81	3.79x10 <sup>-24</sup>
Aspartic acid	0.265	0.77	1.24x10 <sup>-21</sup>
Phenylalanine	0.243	0.70	2.64x10 <sup>-18</sup>
Fisher's ratio	0.243	-0.69	1.08x10 <sup>-17</sup>
Neopterin/tryptophan	0.086	0.61	8.43x10 <sup>-17</sup>
Neopterin	0.101	0.65	6.01x10 <sup>-16</sup>
Quinolinic acid/tryptophan	0.106	0.63	4.95x10 <sup>-15</sup>
Citrulline	0.197	-0.63	7.53x10 <sup>-15</sup>
Quinolinic acid	0.134	0.62	2.02x10 <sup>-14</sup>
Histidine	0.206	-0.59	3.70x10 <sup>-13</sup>
Lactic acid	0.218	0.53	3.92x10 <sup>-11</sup>
Glutamine	0.194	-0.51	3.95x10 <sup>-10</sup>
Threonine	0.144	-0.45	4.12x10 <sup>-8</sup>
Acetone	0.123	0.43	1.35x10 <sup>-7</sup>
Kynurenine/tryptophan	0.150	0.42	2.42x10 <sup>-7</sup>
Methionine	0.121	-0.41	4.40x10 <sup>-7</sup>
3-hydroxykynurenine/tryptophan	0.103	0.35	8.87x10 <sup>-7</sup>
Glucose	0.087	0.38	2.50x10 <sup>-6</sup>
Kynurenic acid	0.093	-0.35	1.55x10 <sup>-5</sup>
Citric acid	0.120	0.33	6.50x10 <sup>-5</sup>
3-Hydroxybutyric acid	0.102	0.33	6.85x10 <sup>-5</sup>
3-Hydroxykynurenine	0.120	0.31	1.45x10 <sup>-4</sup>
Tryptophan	0.109	-0.26	2.07x10 <sup>-3</sup>

Asparagine	0.052	-0.22	1.05x10 <sup>-2</sup>
Indole-3-acetic acid	0.007	-0.21	1.71x10 <sup>-2</sup>
Serine	0.075	0.20	2.17x10 <sup>-2</sup>
Kynurenine	0.099	0.20	2.28x10 <sup>-2</sup>
Isoleucine	0.078	-0.19	2.71x10 <sup>-2</sup>
Ornithine	0.091	0.19	2.89x10 <sup>-2</sup>
Creatine	0.079	0.18	4.08x10 <sup>-2</sup>
Alanine	0.058	0.18	4.22x10 <sup>-2</sup>

**Table S23 - OPLS loadings, Cliff's delta and adjusted p-values of the low molecular weight metabolites for the comparison of the controls and SARS-CoV-2 positive patients in severity class D.** Only metabolites with significant p-values are shown in the table.

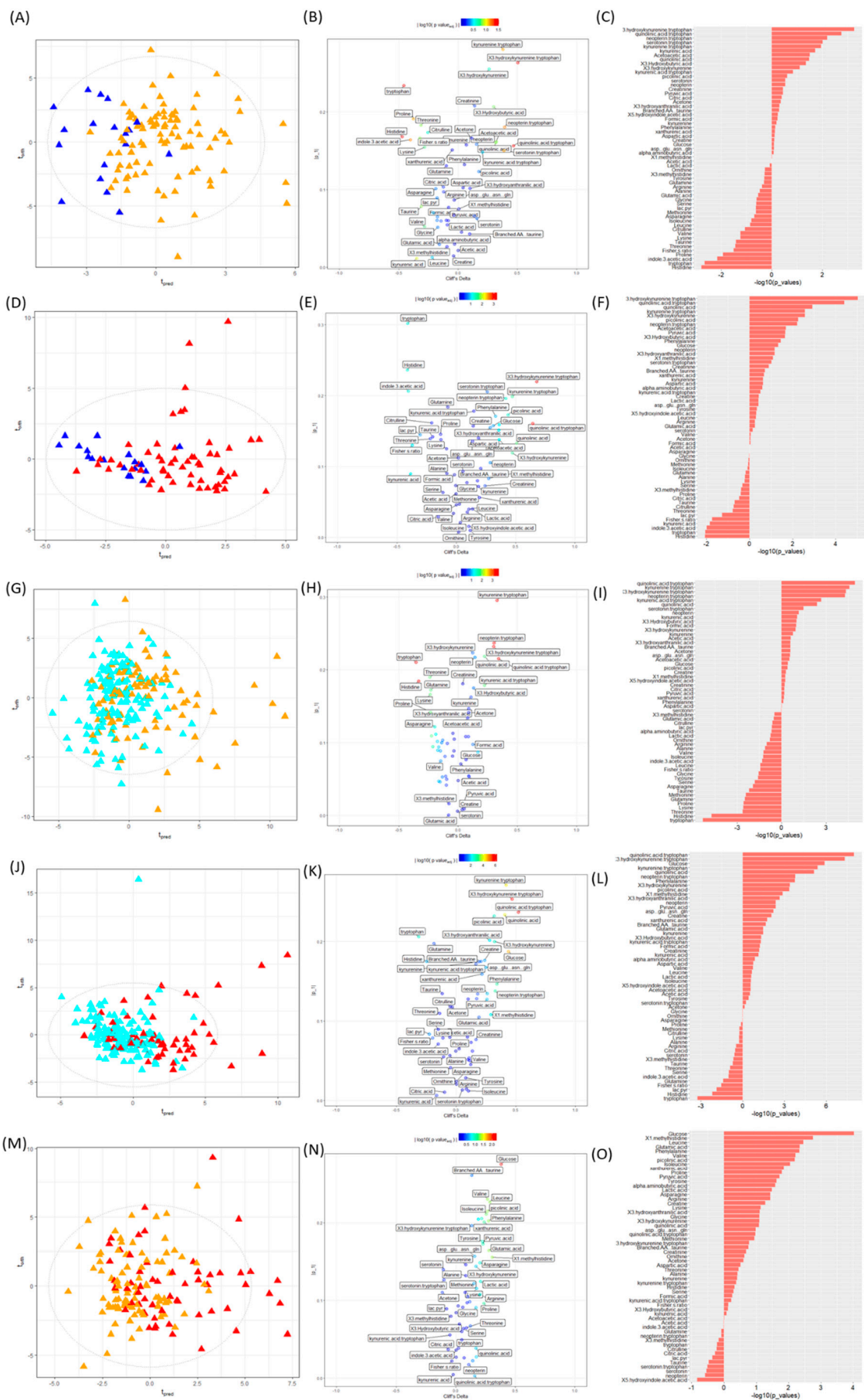
Metabolite	OPLS loadings	Cliff's delta	Adjusted p-value
Formic acid	0.282	1.00	3.01x10 <sup>-29</sup>
Asp/Glu:Asn/Gln	0.278	0.94	2.41x10 <sup>-26</sup>
Pyruvic acid	0.254	0.92	2.01x10 <sup>-25</sup>
Neopterin/tryptophan	0.095	0.82	8.77x10 <sup>-24</sup>
Lactate/pyruvate	0.189	-0.87	7.12x10 <sup>-23</sup>
Glutamic acid	0.236	0.82	2.67x10 <sup>-20</sup>
Fisher's ratio	0.240	-0.80	7.12x10 <sup>-20</sup>
Histidine	0.222	-0.80	1.72x10 <sup>-19</sup>
Quinolinic acid/tryptophan	0.072	0.79	3.62x10 <sup>-19</sup>
Aspartic acid	0.246	0.74	2.95x10 <sup>-17</sup>
Citrulline	0.212	-0.70	2.68x10 <sup>-15</sup>
Quinolinic acid	0.085	0.69	4.10x10 <sup>-15</sup>
Glutamine	0.213	-0.68	9.50x10 <sup>-15</sup>
Phenylalanine	0.227	0.65	2.36x10 <sup>-13</sup>
Kynurenine/tryptophan	0.173	0.64	2.82x10 <sup>-13</sup>
Neopterin	0.094	0.64	4.01x10 <sup>-13</sup>
Tryptophan	0.168	-0.63	1.04x10 <sup>-12</sup>
3-hydroxykynurenine/tryptophan	0.161	0.57	3.21x10 <sup>-12</sup>
Threonine	0.171	-0.60	1.08x10 <sup>-11</sup>
Methionine	0.116	-0.58	4.99x10 <sup>-11</sup>
Lactic acid	0.158	0.45	5.41x10 <sup>-7</sup>
Acetone	0.104	0.44	7.24x10 <sup>-7</sup>
Kynurenic acid	0.040	-0.44	8.95x10 <sup>-7</sup>
3-hydroxybutyric acid	0.105	0.43	1.33x10 <sup>-6</sup>

Glucose	0.140	0.43	1.59x10 <sup>-6</sup>
Asparagine	0.080	-0.42	2.19x10 <sup>-6</sup>
Indole-3-acetic acid	0.057	-0.36	4.73x10 <sup>-5</sup>
3-hydroxykynurenine	0.135	0.36	6.30x10 <sup>-5</sup>
Lysine	0.084	-0.35	1.03x10 <sup>-4</sup>
Proline	0.094	-0.34	1.54x10 <sup>-4</sup>
Isoleucine	0.087	-0.34	1.60x10 <sup>-4</sup>
Valine	0.075	-0.32	4.01x10 <sup>-4</sup>
Kynurenine	0.120	0.29	1.40x10 <sup>-3</sup>
Tyrosine	0.047	-0.27	3.02x10 <sup>-3</sup>
Serotonin/tryptophan	0.089	0.27	3.02x10 <sup>-3</sup>
Citric acid	0.100	0.26	4.09x10 <sup>-3</sup>
Creatine	0.052	0.24	8.30x10 <sup>-3</sup>
Taurine	0.032	-0.23	1.00x10 <sup>-2</sup>
Alpha-aminobutyric acid	0.048	-0.23	1.29x10 <sup>-2</sup>

**Table S24 - OPLS loadings, Cliff's delta and adjusted p-values of the low molecular weight metabolites for the comparison of the controls and SARS-CoV-2 positive patients in severity class E.** Only metabolites with significant p-values are shown in the table.

Metabolite	OPLS loadings	Cliff's delta	Adjusted p-value
Formic acid	0.274	1.00	1.38x10 <sup>-22</sup>
Asp/Glu:Asn/Gln	0.207	0.97	2.62x10 <sup>-21</sup>
Pyruvic acid	0.243	0.94	1.43x10 <sup>-20</sup>
Neopterin/tryptophan	0.196	0.84	1.43x10 <sup>-20</sup>
Quinolinic acid/tryptophan	0.133	0.93	3.93x10 <sup>-20</sup>
Lactate/pyruvate	0.167	-0.92	9.10x10 <sup>-20</sup>
Glutamic acid	0.242	0.91	1.79x10 <sup>-19</sup>
Quinolinic acid	0.131	0.84	1.04x10 <sup>-16</sup>
Fisher's ratio	0.207	-0.82	4.71x10 <sup>-16</sup>
Phenylalanine	0.248	0.82	5.29x10 <sup>-16</sup>
Aspartic acid	0.246	0.82	5.32x10 <sup>-16</sup>
3-hydroxykynurenine/tryptophan	0.155	0.74	6.96x10 <sup>-16</sup>
Histidine	0.210	-0.75	8.42x10 <sup>-14</sup>
Glucose	0.183	0.75	8.35x10 <sup>-12</sup>
Neopterin	0.173	0.75	1.01x10 <sup>-13</sup>
Kynurenine/tryptophan	0.179	0.75	1.01x10 <sup>-13</sup>
Citrulline	0.187	-0.67	3.78x10 <sup>-11</sup>

Glutamine	0.204	-0.61	$1.25 \times 10^{-9}$
Lactic acid	0.172	0.58	$7.98 \times 10^{-9}$
Tryptophan	0.192	-0.58	$7.98 \times 10^{-9}$
3-hydroxykynurenine	0.098	0.57	$1.82 \times 10^{-8}$
3-Hydroxybutyric acid	0.087	0.56	$3.21 \times 10^{-8}$
Threonine	0.145	-0.53	$1.31 \times 10^{-7}$
Kynurenic acid	0.060	-0.44	$2.81 \times 10^{-5}$
1-methylhistidine	0.120	0.41	$5.82 \times 10^{-5}$
Creatine	0.104	0.41	$8.15 \times 10^{-5}$
Methionine	0.073	-0.38	$2.02 \times 10^{-4}$
Kynurenine	0.116	0.36	$4.63 \times 10^{-4}$
Indole-3-acetic acid	0.044	-0.35	$6.06 \times 10^{-4}$
3-hydroxyanthranilic acid	0.112	0.32	$2.35 \times 10^{-3}$
Creatinine	0.093	0.29	$5.29 \times 10^{-3}$
Picolinic acid	0.107	0.29	$5.29 \times 10^{-3}$
Acetone	0.065	0.26	$1.32 \times 10^{-2}$
Ornithine	0.084	0.23	$3.55 \times 10^{-2}$



**Figure S12 - Orthogonal Partial Least Squared (O-PLS-DA), eruption plots and  $-\log 10$  (p-values) between different severity classes of SARS-CoV-2 positive patients for the low molecular weight metabolites.** (A) O-PLS-DA of SARS-CoV-2 severity group B (blue triangles) and SARS-CoV-2 severity group D (orange triangles) ( $R_2X=0.11$ , AUROC=0.76). (B) Eruption plot of group B vs group D. (C)  $-\log 10$  (p-values) of group B vs group D. (D) O-PLS-DA of SARS-CoV-2 severity group B (blue) and SARS-CoV-2 severity group E (red) ( $R_2X=0.09$ , AUROC=0.78). (E) Eruption plot of group B vs group E. (F)  $-\log 10$  (p-values) of group B vs group E. (G) O-PLS-DA of SARS-CoV-2 severity group C (cyan) and SARS-CoV-2 severity group D (orange) ( $R_2X=0.15$ , AUROC=0.65). (H) Eruption plot of group C vs group D. (I)  $-\log 10$  (p-values) of group C vs group D. (J) O-PLS-DA of SARS-CoV-2 severity group C (cyan) and SARS-CoV-2 severity group E (red) ( $R_2X=0.13$ , AUROC=0.74). (K) Eruption plot of group C vs group E. (L)  $-\log 10$  (p-values) of group C vs group E. (M) O-PLS-DA of SARS-CoV-2 severity group D (orange) and SARS-CoV-2 severity group E (red) ( $R_2X=0.12$ , AUROC=0.62). (N) Eruption plot of group D vs group E. (O)  $-\log 10$  (p-values) of group D vs group E. Comparison of severity group B vs severity group C produced no model (AUROC=0.58). Eruption plots are formed from the Cliff's delta (abscissa) and O-PLS-DA loadings (ordinate). Coloured by significance.

**Table S25 - OPLS loadings, Cliff's delta and adjusted p-values for the low molecular weight metabolites for the comparison of severity class B and D.** Only metabolites with significant p-values are shown in the table.

Metabolite	OPLS loadings	Cliff's delta	Adjusted p-value
3-hydroxykynurenine/tryptophan	0.263	0.50	$3.14 \times 10^{-2}$
Tryptophan	0.234	-0.46	$3.22 \times 10^{-2}$
Histidine	0.168	-0.47	$3.22 \times 10^{-2}$
Quinolinic acid/tryptophan	0.156	0.47	$3.22 \times 10^{-2}$

**Table S26 - OPLS loadings, Cliff's delta and adjusted p-values for the low molecular weight metabolites for the comparison of severity class B and E.** Only metabolites with significant p-values are shown in the table.

Metabolite	OPLS loadings	Cliff's delta	Adjusted p-value
3-hydroxykynurenine/tryptophan	0.220	0.68	$5.40 \times 10^{-4}$
Quinolinic acid/tryptophan	0.161	0.65	$1.14 \times 10^{-3}$
Quinolinic acid	0.133	0.51	$2.29 \times 10^{-2}$
3-hydroxykynurenine	0.119	0.47	$3.05 \times 10^{-2}$
Kynurenine/tryptophan	0.199	0.47	$3.05 \times 10^{-2}$

**Table S27 - OPLS loadings, Cliff's delta and adjusted p-values for the low molecular weight metabolites for the comparison of severity class C and D.** Only metabolites with significant p-values are shown in the table.

Metabolite	OPLS loadings	Cliff's delta	Adjusted p-value
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Tryptophan	0.232	-0.36	2.68x10 <sup>-4</sup>
Quinolinic acid/tryptophan	0.215	0.34	3.14x10 <sup>-4</sup>
Histidine	0.185	-0.33	3.46x10 <sup>-4</sup>
Kynurenine/tryptophan	0.296	0.33	3.73x10 <sup>-4</sup>
3-hydroxykynurenine/tryptophan	0.232	0.30	4.80x10 <sup>-4</sup>
Neopterin/tryptophan	0.237	0.30	4.80x10 <sup>-4</sup>
Lysine	0.166	-0.23	1.58x10 <sup>-2</sup>
Proline	0.142	-0.23	1.58x10 <sup>-2</sup>
Threonine	0.190	-0.24	1.58x10 <sup>-2</sup>
Kynurenic acid/tryptophan	0.179	0.22	1.58x10 <sup>-2</sup>
Glutamine	0.173	-0.23	1.68x10 <sup>-2</sup>
Quinolinic acid	0.219	0.22	1.78x10 <sup>-2</sup>
Methionine	0.109	-0.23	1.78x10 <sup>-2</sup>
Taurine	0.094	-0.21	2.60x10 <sup>-2</sup>
Asparagine	0.122	-0.20	4.35x10 <sup>-2</sup>

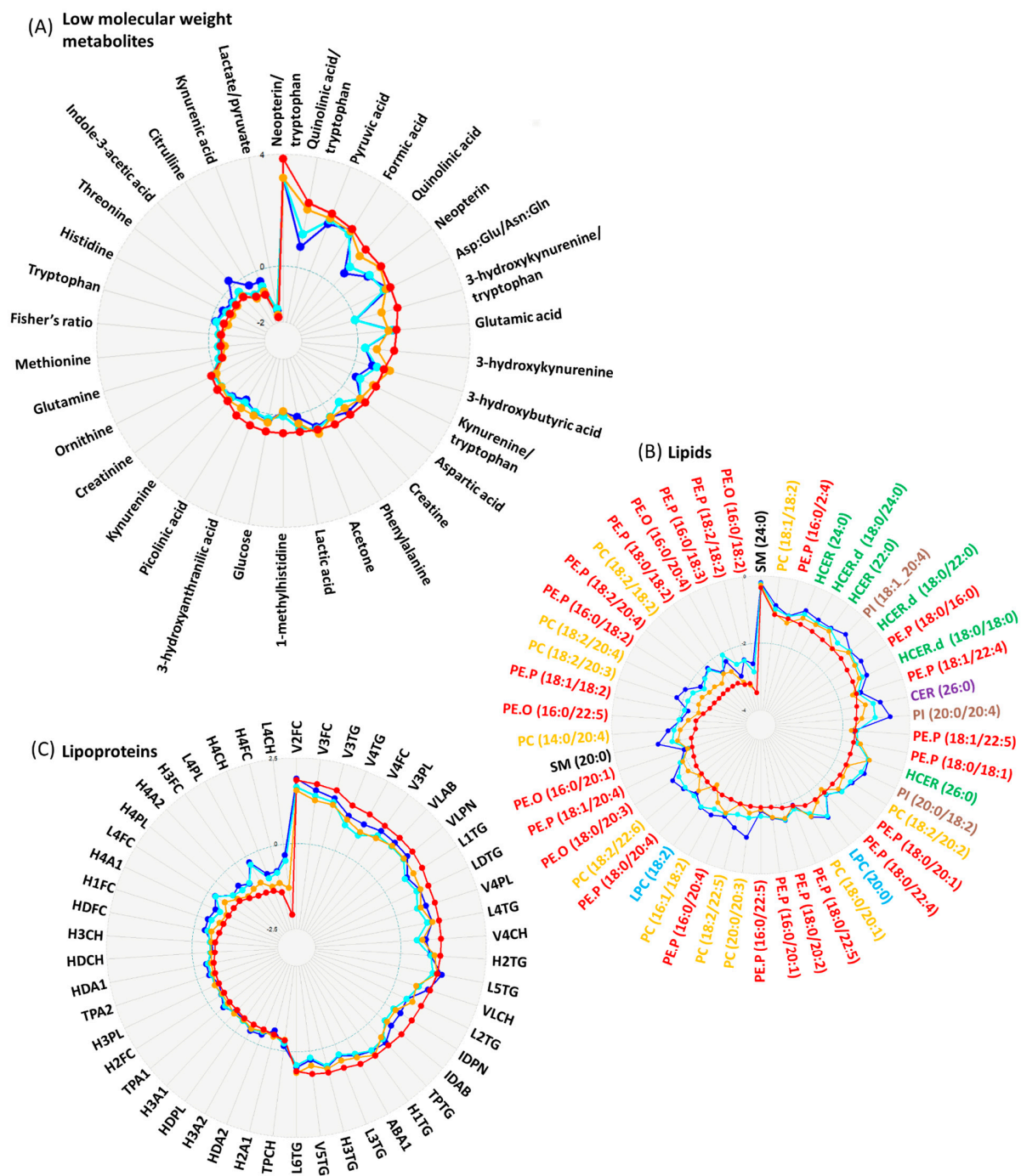
**Table S28 - OPLS loadings, Cliff's delta and adjusted p-values for the low molecular weight metabolites for the comparison of severity class C and E.** Only metabolites with significant p-values are shown in the table.

Metabolite	OPLS loadings	Cliff's delta	Adjusted p-value
Quinolinic acid/tryptophan	0.237	0.52	5.79x10 <sup>-7</sup>
3-hydroxykynurenine/tryptophan	0.253	0.47	1.34x10 <sup>-6</sup>
Glucose	0.187	0.44	2.52x10 <sup>-5</sup>
Kynurenine/tryptophan	0.271	0.42	5.88x10 <sup>-5</sup>
Quinolinic acid	0.234	0.41	8.53x10 <sup>-5</sup>
Phenylalanine	0.147	0.34	1.46x10 <sup>-3</sup>
Neopterin/tryptophan	0.138	0.33	1.46x10 <sup>-3</sup>
3-hydroxykynurenine	0.200	0.32	2.77x10 <sup>-3</sup>
Picolinic acid	0.232	0.32	2.77x10 <sup>-3</sup>
Tryptophan	0.206	-0.31	2.77x10 <sup>-3</sup>
1-methylhistidine	0.108	0.29	6.86x10 <sup>-3</sup>
3-hydroxyanthranilic acid	0.201	0.28	1.01x10 <sup>-2</sup>
Pyruvic acid	0.127	0.26	1.75x10 <sup>-2</sup>
Neopterin	0.135	0.26	1.75x10 <sup>-2</sup>
Asp/Glu:Asn/Gln	0.168	0.25	2.28x10 <sup>-2</sup>
Histidine	0.175	-0.25	2.33x10 <sup>-2</sup>
Creatine	0.176	0.24	2.82x10 <sup>-2</sup>

Lactate/pyruvate	0.084	-0.22	4.32x10 <sup>-2</sup>
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**Table S29 - OPLS loadings, Cliff's delta and adjusted p-values for the low molecular weight metabolites for the comparison of severity class D and E.** Only metabolites with significant p-values are shown in the table.

Metabolite	OPLS loadings	Cliff's delta	Adjusted p-value
Glucose	0.276	0.38	5.40x10 <sup>-3</sup>



**Figure S13– Radar plots showing the log<sub>2</sub> fold change between controls and SARS-CoV-2 severity group E patients of the most significant ( $p < 0.05$ ) metabolites, lipids and lipoproteins ordered by log<sub>2</sub> fold change. All radar plots are coloured in relation to fold change of each severity class in comparison to the controls. Controls vs group B (blue), controls vs group C severity (cyan), controls vs group D severity (orange) and controls vs group E severity (red). (A) Radar plot of the metabolites with a significant p-value from the controls vs group E severity model for the low molecular weight metabolites. (B) Radar plot of the top 50 most significant lipids from the controls vs group E severity model. (C) Radar plot of the top 50 most significant lipoproteins from the controls vs group E severity model.**

**Table S30 - Demographics for the severity group E patients who survived and who did not.**

<b>Patient</b>	<b>Sex</b>	<b>Age</b>	<b>Blood collection date</b>	<b>Date of death</b>	<b>Days between blood collection and death</b>
1	Male	73	01/04/2020	NA	
2	Female	75	01/04/2020	NA	
3	Male	65	01/04/2020	NA	
4	Female	74	01/04/2020	NA	
5	Female	68	01/04/2020	NA	
6	Male	77	01/04/2020	NA	
7	Male	77	01/04/2020	NA	
8	Male	73	01/04/2020	NA	
9	Male	73	01/04/2020	NA	
10	Male	72	01/04/2020	NA	
11	Female	72	01/04/2020	NA	
12	Female	66	01/04/2020	NA	
13	Male	76	01/04/2020	NA	
14	Female	70	01/04/2020	17/04/2020	16
15	Male	77	01/04/2020	14/04/2020	13
16	Male	77	01/04/2020	21/05/2020	50
17	Male	73	01/04/2020	28/04/2020	27
18	Male	73	01/04/2020	10/04/2020	9
19	Female	79	01/04/2020	02/05/2020	31
20	Female	75	01/04/2020	02/05/2020	31
21	Male	70	01/04/2020	01/06/2020	61
22	Female	68	07/04/2020	21/04/2020	14
23	Female	80	09/04/2020	unknown	-
24	Male	66	09/04/2020	17/04/2020	8
25	Female	79	09/04/2020	08/05/2020	29
26	Male	79	09/04/2020	03/05/2020	24

**Table S31 - OPLS loadings, Cliff's delta and adjusted p-values of the combined model (low molecular weight metabolites, lipoproteins and lipids) for the comparison group E severity patients comparing who survived and who died, samples were age matched. Only metabolites with significant p-values are shown in the table.**

Metabolite	OPLS loadings	Cliff's delta	Adjusted p-value
HCER (16:0)	0.057	0.92	$9.15 \times 10^{-3}$
HCER (20:0)	0.055	0.92	$9.15 \times 10^{-3}$
HCER (24:0)	0.063	0.91	$9.15 \times 10^{-3}$
HCER (24:1)	0.062	0.91	$9.15 \times 10^{-3}$
HCER (26:0)	0.061	0.95	$9.15 \times 10^{-3}$
HCER (26:1)	0.063	0.92	$9.15 \times 10^{-3}$
HCER.d (18:0/24:0)	0.063	0.91	$9.15 \times 10^{-3}$
HCER.d (18:0/24:1)	0.062	0.94	$9.15 \times 10^{-3}$
PE.O (18:0/18:1)	0.056	-0.98	$9.15 \times 10^{-3}$
PE.P (16:0/18:0)	0.053	-0.93	$9.15 \times 10^{-3}$
HCER (22:0)	0.063	0.89	$9.41 \times 10^{-3}$
HCER.d (18:0/22:0)	0.063	0.89	$9.41 \times 10^{-3}$
PE (16:0/18:1)	0.061	-0.88	$1.07 \times 10^{-2}$
TAG (54:1)_FA (16:0)	0.051	-0.87	$1.07 \times 10^{-2}$
TAG (54:1)_FA (20:0)	0.053	-0.87	$1.07 \times 10^{-2}$
TAG (56:1)_FA (16:0)	0.055	-0.87	$1.07 \times 10^{-2}$
H3FC	0.057	0.83	$1.19 \times 10^{-2}$
HCER (18:0)	0.052	0.83	$1.19 \times 10^{-2}$
PE (18:0/18:0)	0.059	-0.85	$1.19 \times 10^{-2}$
PE (18:0/18:1)	0.058	-0.83	$1.19 \times 10^{-2}$
PE (18:1/18:1)	0.059	-0.82	$1.19 \times 10^{-2}$
PE (18:1/18:3)	0.044	-0.82	$1.19 \times 10^{-2}$
PI (16:0/20:2)	0.040	-0.82	$1.19 \times 10^{-2}$
SM (26:0)	0.060	0.86	$1.19 \times 10^{-2}$
TAG (50:1)_FA (16:0)	0.053	-0.82	$1.19 \times 10^{-2}$
TAG (50:2)_FA (16:0)	0.048	-0.82	$1.19 \times 10^{-2}$
TAG (52:2)_FA (18:1)	0.055	-0.82	$1.19 \times 10^{-2}$
TAG (54:2)_FA (20:0)	0.036	-0.82	$1.19 \times 10^{-2}$
TAG (56:1)_FA (18:1)	0.053	-0.82	$1.19 \times 10^{-2}$
TAG (56:2)_FA (16:0)	0.054	-0.83	$1.19 \times 10^{-2}$
TAG (56:2)_FA (20:0)	0.053	-0.83	$1.19 \times 10^{-2}$
TAG (58:2)_FA (18:1)	0.038	-0.83	$1.19 \times 10^{-2}$

HCER.d (18:0/20:0)	0.050	0.81	$1.25 \times 10^{-2}$
PE (16:0/16:1)	0.050	-0.81	$1.25 \times 10^{-2}$
PE (16:0/18:2)	0.056	-0.81	$1.25 \times 10^{-2}$
PE (18:0/18:3)	0.048	-0.81	$1.25 \times 10^{-2}$
PG (18:1/18:1)	0.047	-0.81	$1.25 \times 10^{-2}$
HDCH	0.050	0.80	$1.30 \times 10^{-2}$
VLPN	0.050	-0.79	$1.30 \times 10^{-2}$
VLAB	0.050	-0.79	$1.30 \times 10^{-2}$
DAG (16:0/16:0)	0.040	-0.79	$1.30 \times 10^{-2}$
DAG (18:0/18:3)	0.038	-0.79	$1.30 \times 10^{-2}$
HCER (14:0)	0.049	0.79	$1.30 \times 10^{-2}$
MAG (18:3)	0.040	-0.79	$1.30 \times 10^{-2}$
PC (18:1/18:3)	0.048	-0.79	$1.30 \times 10^{-2}$
PI (18:0/18:3)	0.025	-0.80	$1.30 \times 10^{-2}$
TAG (50:1)_FA (18:1)	0.056	-0.79	$1.30 \times 10^{-2}$
TAG (51:2)_FA (16:0)	0.037	-0.80	$1.30 \times 10^{-2}$
TAG (52:1)_FA (18:1)	0.060	-0.79	$1.30 \times 10^{-2}$
TAG (55:1)_FA (16:0)	0.048	-0.80	$1.30 \times 10^{-2}$
TAG (55:1)_FA (18:1)	0.048	-0.80	$1.30 \times 10^{-2}$
TAG (56:3)_FA (16:0)	0.043	-0.80	$1.30 \times 10^{-2}$
MAG (18:1)	0.041	-0.78	$1.36 \times 10^{-2}$
PC (16:0/18:3)	0.044	-0.78	$1.36 \times 10^{-2}$
PC (18:0/20:4)	0.053	0.78	$1.36 \times 10^{-2}$
PE (16:0/18:3)	0.048	-0.78	$1.36 \times 10^{-2}$
TAG (51:1)_FA (16:0)	0.042	-0.78	$1.36 \times 10^{-2}$
TAG (52:4)_FA (16:0)	0.046	-0.78	$1.36 \times 10^{-2}$
TAG (53:0)_FA (16:0)	0.039	-0.78	$1.36 \times 10^{-2}$
TAG (58:3)_FA (18:1)	0.050	-0.78	$1.36 \times 10^{-2}$
L6FC	0.055	0.75	$1.51 \times 10^{-2}$
FFA (24:0)	0.041	-0.76	$1.51 \times 10^{-2}$
TAG (50:5)_FA (18:1)	0.035	-0.76	$1.54 \times 10^{-2}$
TAG (52:0)_FA (20:0)	0.042	-0.76	$1.54 \times 10^{-2}$
LPE (18:3)	0.041	-0.75	$1.66 \times 10^{-2}$
MAG (20:3)	0.040	-0.75	$1.66 \times 10^{-2}$
PC (18:1/18:1)	0.040	-0.75	$1.66 \times 10^{-2}$
SM (26:1)	0.043	0.75	$1.66 \times 10^{-2}$
TAG (52:3)_FA (18:3)	0.031	-0.75	$1.66 \times 10^{-2}$

TAG (54:0)_FA (16:0)	0.050	-0.75	1.66x10 <sup>-2</sup>
TAG (54:4)_FA (18:1)	0.053	-0.75	1.66x10 <sup>-2</sup>
DAG (16:0/18:0)	0.037	-0.74	1.72x10 <sup>-2</sup>
DAG (16:0/18:1)	0.047	-0.74	1.72x10 <sup>-2</sup>
LPE (18:1)	0.051	-0.74	1.72x10 <sup>-2</sup>
PC (20:0/20:4)	0.052	0.74	1.72x10 <sup>-2</sup>
PE (18:0/20:1)	0.047	-0.74	1.72x10 <sup>-2</sup>
TAG (51:1)_FA (18:1)	0.044	-0.74	1.72x10 <sup>-2</sup>
TAG (52:1)_FA (16:0)	0.057	-0.74	1.72x10 <sup>-2</sup>
TAG (52:2)_FA (20:0)	0.047	-0.74	1.72x10 <sup>-2</sup>
TAG (53:1)_FA (16:0)	0.038	-0.74	1.72x10 <sup>-2</sup>
TAG (54:2)_FA (16:0)	0.046	-0.74	1.72x10 <sup>-2</sup>
TAG (54:5)_FA (18:1)	0.051	-0.74	1.72x10 <sup>-2</sup>
V5TG	0.048	-0.73	1.79x10 <sup>-2</sup>
H1FC	0.054	0.73	1.79x10 <sup>-2</sup>
DCER (26:1)	0.055	0.73	1.79x10 <sup>-2</sup>
MAG (18:0)	0.036	-0.73	1.79x10 <sup>-2</sup>
PC (18:0/18:3)	0.035	-0.73	1.79x10 <sup>-2</sup>
PS (20:0/18:1)	0.041	-0.73	1.79x10 <sup>-2</sup>
TAG (51:1)_FA (17:0)	0.039	-0.73	1.79x10 <sup>-2</sup>
TAG (52:4)_FA (18:3)	0.039	-0.73	1.79x10 <sup>-2</sup>
TAG (54:4)_FA (18:3)	0.038	-0.73	1.79x10 <sup>-2</sup>
TAG (54:5)_FA (18:0)	0.035	-0.73	1.79x10 <sup>-2</sup>
TAG (54:6)_FA (18:1)	0.045	-0.73	1.79x10 <sup>-2</sup>
TAG (57:10)_FA (22:6)	0.034	-0.73	1.79x10 <sup>-2</sup>
TPTG	0.046	-0.72	1.84x10 <sup>-2</sup>
VLCH	0.043	-0.72	1.84x10 <sup>-2</sup>
V4FC	0.050	-0.72	1.84x10 <sup>-2</sup>
CE (16:0)	0.051	0.72	1.84x10 <sup>-2</sup>
DAG (16:0/18:3)	0.036	-0.72	1.84x10 <sup>-2</sup>
HCER.d (18:0/26:1)	0.048	0.72	1.84x10 <sup>-2</sup>
PE (18:1/20:1)	0.044	-0.72	1.84x10 <sup>-2</sup>
PS (18:0/18:1)	0.057	-0.72	1.84x10 <sup>-2</sup>
TAG (49:1)_FA (18:1)	0.032	-0.72	1.84x10 <sup>-2</sup>
TAG (50:3)_FA (18:3)	0.035	-0.72	1.84x10 <sup>-2</sup>
TAG (52:3)_FA (18:1)	0.052	-0.72	1.84x10 <sup>-2</sup>
TAG (52:7)_FA (18:1)	0.034	-0.72	1.84x10 <sup>-2</sup>

TAG (54:2)_FA (18:1)	0.054	-0.72	1.84x10 <sup>-2</sup>
TAG (55:5)_FA (18:1)	0.042	-0.72	1.84x10 <sup>-2</sup>
TAG (57:2)_FA (18:1)	0.051	-0.72	1.84x10 <sup>-2</sup>
Branched AA/Taurine	0.036	-0.70	1.94x10 <sup>-2</sup>
HDFC	0.053	0.70	1.94x10 <sup>-2</sup>
DAG (18:1/20:1)	0.051	-0.70	1.94x10 <sup>-2</sup>
SM (20:1)	0.048	0.70	1.94x10 <sup>-2</sup>
TAG (48:1)_FA (18:1)	0.040	-0.70	1.94x10 <sup>-2</sup>
TAG (50:4)_FA (16:0)	0.031	-0.70	1.94x10 <sup>-2</sup>
TAG (50:5)_FA (16:0)	0.033	-0.70	1.94x10 <sup>-2</sup>
TAG (52:6)_FA (16:0)	0.033	-0.70	1.94x10 <sup>-2</sup>
TAG (52:6)_FA (18:1)	0.035	-0.70	1.94x10 <sup>-2</sup>
TAG (53:1)_FA (18:1)	0.040	-0.70	1.94x10 <sup>-2</sup>
TAG (53:2)_FA (16:0)	0.044	-0.70	1.94x10 <sup>-2</sup>
TAG (54:2)_FA (20:1)	0.048	-0.70	1.94x10 <sup>-2</sup>
TAG (54:3)_FA (18:3)	0.032	-0.70	1.94x10 <sup>-2</sup>
TAG (54:7)_FA (18:1)	0.038	-0.70	1.94x10 <sup>-2</sup>
LDCH	0.054	0.69	2.04x10 <sup>-2</sup>
V4TG	0.043	-0.69	2.04x10 <sup>-2</sup>
MAG (20:2)	0.029	-0.69	2.04x10 <sup>-2</sup>
PE (16:0/22:5)	0.049	-0.69	2.04x10 <sup>-2</sup>
PE (18:0/18:2)	0.050	-0.69	2.04x10 <sup>-2</sup>
PE (18:1/18:2)	0.046	-0.69	2.04x10 <sup>-2</sup>
PI (16:0/20:3)	0.035	-0.69	2.04x10 <sup>-2</sup>
TAG (48:4)_FA (18:1)	0.042	-0.69	2.04x10 <sup>-2</sup>
TAG (49:0)_FA (16:0)	0.031	-0.69	2.04x10 <sup>-2</sup>
TAG (49:0)_FA (17:0)	0.030	-0.69	2.04x10 <sup>-2</sup>
TAG (49:1)_FA (16:0)	0.033	-0.69	2.04x10 <sup>-2</sup>
TAG (49:3)_FA (16:0)	0.023	-0.69	2.04x10 <sup>-2</sup>
TAG (51:2)_FA (17:0)	0.026	-0.69	2.04x10 <sup>-2</sup>
TAG (52:1)_FA (18:0)	0.055	-0.69	2.04x10 <sup>-2</sup>
TAG (52:3)_FA (18:2)	0.040	-0.69	2.04x10 <sup>-2</sup>
Taurine	0.033	0.68	2.18x10 <sup>-2</sup>
L6PN	0.046	0.68	2.18x10 <sup>-2</sup>
V2FC	0.041	-0.68	2.18x10 <sup>-2</sup>
V4PL	0.046	-0.68	2.18x10 <sup>-2</sup>
L6AB	0.046	0.68	2.18x10 <sup>-2</sup>

MAG (22:6)	0.032	-0.68	2.18x10 <sup>-2</sup>
PG (20:0/18:2)	0.052	0.68	2.18x10 <sup>-2</sup>
TAG (51:0)_FA (16:0)	0.034	-0.68	2.18x10 <sup>-2</sup>
TAG (52:1)_FA (20:0)	0.033	-0.68	2.18x10 <sup>-2</sup>
TAG (52:5)_FA (16:0)	0.037	-0.68	2.18x10 <sup>-2</sup>
TAG (53:2)_FA (17:0)	0.046	-0.68	2.18x10 <sup>-2</sup>
TAG (53:2)_FA (18:1)	0.050	-0.68	2.18x10 <sup>-2</sup>
TAG (54:5)_FA (18:3)	0.039	-0.68	2.18x10 <sup>-2</sup>
TAG (56:3)_FA (20:0)	0.047	-0.68	2.18x10 <sup>-2</sup>
H4FC	0.052	0.67	2.22x10 <sup>-2</sup>
IDTG	0.039	-0.67	2.31x10 <sup>-2</sup>
V3FC	0.040	-0.67	2.31x10 <sup>-2</sup>
CE (22:4)	0.049	0.67	2.31x10 <sup>-2</sup>
DAG (16:0/20:5)	0.024	-0.67	2.31x10 <sup>-2</sup>
LPE (18:2)	0.038	-0.67	2.31x10 <sup>-2</sup>
MAG (16:0)	0.037	-0.67	2.31x10 <sup>-2</sup>
MAG (18:2)	0.040	-0.67	2.31x10 <sup>-2</sup>
MAG (22:4)	0.037	-0.67	2.31x10 <sup>-2</sup>
PI (16:0/20:4)	0.036	-0.67	2.31x10 <sup>-2</sup>
TAG (48:4)_FA (16:0)	0.029	-0.67	2.31x10 <sup>-2</sup>
TAG (51:1)_FA (18:0)	0.029	-0.67	2.31x10 <sup>-2</sup>
TAG (51:2)_FA (16:1)	0.032	-0.67	2.31x10 <sup>-2</sup>
TAG (51:4)_FA (18:3)	0.025	-0.67	2.31x10 <sup>-2</sup>
TAG (53:4)_FA (16:0)	0.029	-0.67	2.31x10 <sup>-2</sup>
TAG (54:2)_FA (18:0)	0.055	-0.67	2.31x10 <sup>-2</sup>
L6CH	0.048	0.66	2.46x10 <sup>-2</sup>
H1CH	0.040	0.66	2.46x10 <sup>-2</sup>
DAG (18:0/18:1)	0.051	-0.66	2.46x10 <sup>-2</sup>
MAG (20:4)	0.036	-0.66	2.46x10 <sup>-2</sup>
PC (16:1/18:1)	0.037	-0.66	2.46x10 <sup>-2</sup>
PE (16:0/20:1)	0.050	-0.66	2.46x10 <sup>-2</sup>
PE (18:0/16:0)	0.045	-0.66	2.46x10 <sup>-2</sup>
PE (18:1/20:3)	0.046	-0.66	2.46x10 <sup>-2</sup>
PG (20:0/20:1)	0.047	0.66	2.46x10 <sup>-2</sup>
TAG (48:1)_FA (16:0)	0.039	-0.66	2.46x10 <sup>-2</sup>
TAG (49:1)_FA (16:1)	0.025	-0.66	2.46x10 <sup>-2</sup>
TAG (49:2)_FA (18:1)	0.027	-0.66	2.46x10 <sup>-2</sup>

TAG (50:2)_FA (18:1)	0.047	-0.66	2.46x10 <sup>-2</sup>
TAG (51:2)_FA (18:1)	0.043	-0.66	2.46x10 <sup>-2</sup>
TAG (52:5)_FA (22:5)	0.029	-0.66	2.46x10 <sup>-2</sup>
TAG (53:1)_FA (17:0)	0.036	-0.66	2.46x10 <sup>-2</sup>
TAG (54:4)_FA (16:0)	0.037	-0.66	2.46x10 <sup>-2</sup>
TAG (56:3)_FA (18:2)	0.040	-0.66	2.46x10 <sup>-2</sup>
$\alpha$ -aminobutyric acid	0.029	-0.64	2.46x10 <sup>-2</sup>
Isoleucine	0.023	-0.64	2.60x10 <sup>-2</sup>
DAG (18:1/20:5)	0.026	-0.64	2.60x10 <sup>-2</sup>
MAG (22:5)	0.037	-0.64	2.60x10 <sup>-2</sup>
PC (16:0/18:1)	0.037	-0.64	2.60x10 <sup>-2</sup>
PI (18:0/20:5)	0.023	-0.64	2.60x10 <sup>-2</sup>
PI (18:1/18:1)	0.031	-0.64	2.60x10 <sup>-2</sup>
TAG (46:3)_FA (16:0)	0.030	-0.64	2.60x10 <sup>-2</sup>
TAG (48:1)_FA (14:0)	0.036	-0.64	2.60x10 <sup>-2</sup>
TAG (48:2)_FA (16:0)	0.022	-0.64	2.60x10 <sup>-2</sup>
TAG (49:2)_FA (16:0)	0.022	-0.64	2.60x10 <sup>-2</sup>
TAG (50:0)_FA (18:0)	0.035	-0.64	2.60x10 <sup>-2</sup>
TAG (50:2)_FA (16:1)	0.043	-0.64	2.60x10 <sup>-2</sup>
TAG (52:0)_FA (16:0)	0.045	-0.64	2.60x10 <sup>-2</sup>
TAG (52:1)_FA (20:1)	0.039	-0.64	2.60x10 <sup>-2</sup>
TAG (52:2)_FA (20:2)	0.034	-0.64	2.60x10 <sup>-2</sup>
TAG (52:3)_FA (20:2)	0.025	-0.64	2.60x10 <sup>-2</sup>
TAG (53:1)_FA (18:0)	0.036	-0.64	2.60x10 <sup>-2</sup>
TAG (54:1)_FA (18:0)	0.053	-0.64	2.60x10 <sup>-2</sup>
TAG (54:1)_FA (18:1)	0.053	-0.64	2.60x10 <sup>-2</sup>
TAG (56:7)_FA (20:5)	0.032	-0.64	2.60x10 <sup>-2</sup>
VLFC	0.038	-0.63	2.70x10 <sup>-2</sup>
V5FC	0.042	-0.63	2.70x10 <sup>-2</sup>
H2TG	0.049	-0.63	2.70x10 <sup>-2</sup>
CE (20:3)	0.039	0.63	2.70x10 <sup>-2</sup>
DAG (14:0/18:3)	0.029	-0.63	2.70x10 <sup>-2</sup>
DAG (16:0/20:4)	0.033	-0.63	2.70x10 <sup>-2</sup>
DAG (18:0/18:2)	0.034	-0.63	2.70x10 <sup>-2</sup>
DAG (18:1/18:1)	0.043	-0.63	2.70x10 <sup>-2</sup>
PE (18:0/20:2)	0.047	-0.63	2.70x10 <sup>-2</sup>
PE.P (16:0/22:6)	0.034	0.63	2.70x10 <sup>-2</sup>

PE.P (18:0/20:4)	0.040	0.63	2.70x10 <sup>-2</sup>
PI (16:0/18:1)	0.041	-0.63	2.70x10 <sup>-2</sup>
TAG (47:1)_FA (16:0)	0.025	-0.63	2.70x10 <sup>-2</sup>
TAG (49:0)_FA (18:0)	0.024	-0.63	2.70x10 <sup>-2</sup>
TAG (49:3)_FA (18:3)	0.021	-0.63	2.70x10 <sup>-2</sup>
TAG (50:0)_FA (16:0)	0.041	-0.63	2.70x10 <sup>-2</sup>
TAG (50:3)_FA (16:0)	0.029	-0.63	2.70x10 <sup>-2</sup>
TAG (51:3)_FA (18:3)	0.023	-0.63	2.70x10 <sup>-2</sup>
TAG (52:7)_FA (16:0)	0.030	-0.63	2.70x10 <sup>-2</sup>
TAG (54:3)_FA (16:0)	0.036	-0.63	2.70x10 <sup>-2</sup>
TAG (54:3)_FA (18:1)	0.051	-0.63	2.70x10 <sup>-2</sup>
TAG (54:3)_FA (20:2)	0.038	-0.63	2.70x10 <sup>-2</sup>
TAG (54:8)_FA (18:2)	0.031	-0.63	2.70x10 <sup>-2</sup>
TAG (56:2)_FA (18:0)	0.044	-0.63	2.70x10 <sup>-2</sup>
TAG (56:4)_FA (16:0)	0.036	-0.63	2.70x10 <sup>-2</sup>
TAG (56:7)_FA (18:1)	0.041	-0.63	2.70x10 <sup>-2</sup>
Tyrosine	0.032	-0.62	2.90x10 <sup>-2</sup>
V5CH	0.042	-0.62	2.90x10 <sup>-2</sup>
L3FC	0.047	0.62	2.90x10 <sup>-2</sup>
CE (20:0)	0.046	0.62	2.90x10 <sup>-2</sup>
FFA (20:0)	0.038	-0.62	2.90x10 <sup>-2</sup>
LPE (20:1)	0.046	-0.62	2.90x10 <sup>-2</sup>
PC (14:0/18:1)	0.038	-0.62	2.90x10 <sup>-2</sup>
PC (18:1/20:2)	0.037	-0.62	2.90x10 <sup>-2</sup>
PC (18:2/18:3)	0.042	-0.62	2.90x10 <sup>-2</sup>
TAG (45:1)_FA (16:0)	0.025	-0.62	2.90x10 <sup>-2</sup>
TAG (48:1)_FA (16:1)	0.035	-0.62	2.90x10 <sup>-2</sup>
TAG (52:2)_FA (14:0)	0.028	-0.62	2.90x10 <sup>-2</sup>
TAG (52:3)_FA (20:3)	0.035	-0.62	2.90x10 <sup>-2</sup>
TAG (52:5)_FA (20:5)	0.030	-0.62	2.90x10 <sup>-2</sup>
TAG (53:4)_FA (18:3)	0.026	-0.62	2.90x10 <sup>-2</sup>
TAG (54:1)_FA (20:1)	0.041	-0.62	2.90x10 <sup>-2</sup>
TAG (54:2)_FA (20:2)	0.032	-0.62	2.90x10 <sup>-2</sup>
TAG (54:6)_FA (20:5)	0.031	-0.62	2.90x10 <sup>-2</sup>
TAG (55:2)_FA (18:2)	0.028	-0.62	2.90x10 <sup>-2</sup>
TAG (56:5)_FA (18:1)	0.044	-0.62	2.90x10 <sup>-2</sup>
LDFC	0.051	0.61	3.08x10 <sup>-2</sup>

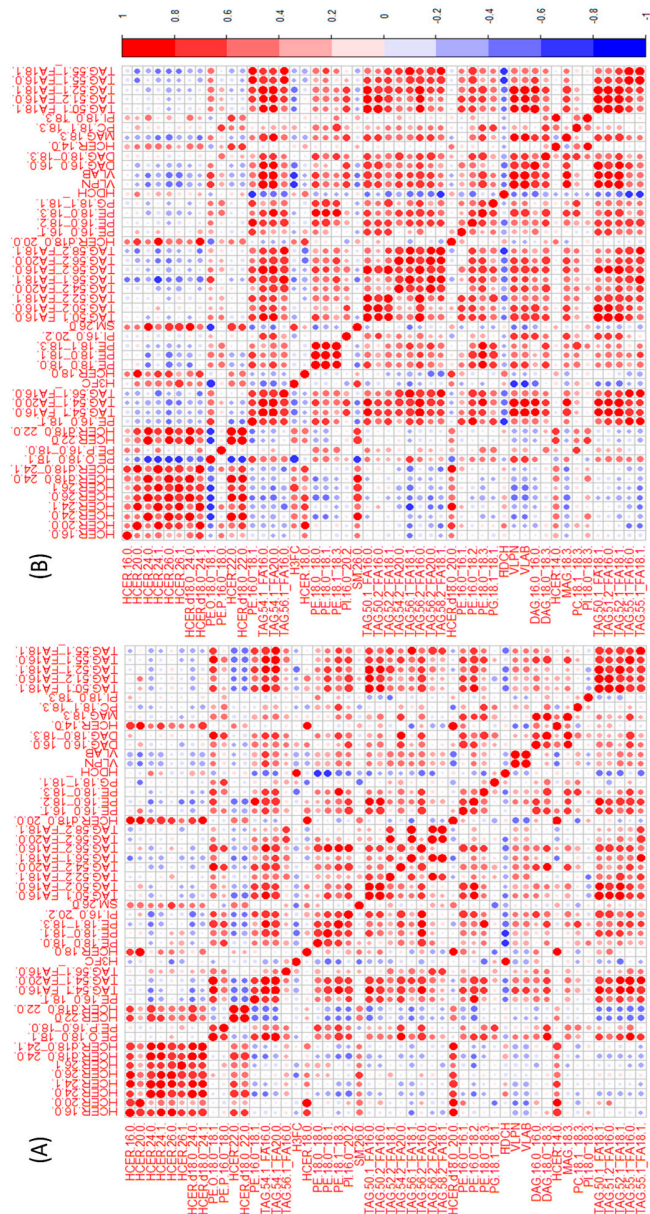
HDA1	0.045	0.61	$3.08 \times 10^{-2}$
V5PL	0.038	-0.61	$3.08 \times 10^{-2}$
L6PL	0.047	0.61	$3.08 \times 10^{-2}$
H4A1	0.045	0.61	$3.08 \times 10^{-2}$
DAG (16:1/18:0)	0.035	-0.61	$3.08 \times 10^{-2}$
DAG (18:2/18:3)	0.031	-0.61	$3.08 \times 10^{-2}$
PE (18:1/22:6)	0.047	-0.61	$3.08 \times 10^{-2}$
PE.P (16:0/16:1)	0.034	-0.61	$3.08 \times 10^{-2}$
PE.P (16:0/20:4)	0.042	0.61	$3.08 \times 10^{-2}$
PI (16:0/22:4)	0.019	-0.61	$3.08 \times 10^{-2}$
TAG (44:2)_FA (16:0)	0.020	-0.61	$3.08 \times 10^{-2}$
TAG (44:2)_FA (18:1)	0.025	-0.61	$3.08 \times 10^{-2}$
TAG (46:3)_FA (18:1)	0.024	-0.61	$3.08 \times 10^{-2}$
TAG (47:0)_FA (16:0)	0.025	-0.61	$3.08 \times 10^{-2}$
TAG (52:3)_FA (14:0)	0.024	-0.61	$3.08 \times 10^{-2}$
TAG (54:4)_FA (20:3)	0.036	-0.61	$3.08 \times 10^{-2}$
TAG (54:5)_FA (16:0)	0.041	-0.61	$3.08 \times 10^{-2}$
TAG (54:5)_FA (20:5)	0.029	-0.61	$3.08 \times 10^{-2}$
TAG (54:5)_FA (22:5)	0.033	-0.61	$3.08 \times 10^{-2}$
TAG (54:8)_FA (18:3)	0.035	-0.61	$3.08 \times 10^{-2}$
TAG (56:2)_FA (20:1)	0.047	-0.61	$3.08 \times 10^{-2}$
TAG (56:3)_FA (18:1)	0.049	-0.61	$3.08 \times 10^{-2}$
TAG (56:5)_FA (16:0)	0.033	-0.61	$3.08 \times 10^{-2}$
TPA1	0.047	0.60	$3.30 \times 10^{-2}$
LDPL	0.049	0.60	$3.30 \times 10^{-2}$
DAG (16:0/22:5)	0.029	-0.60	$3.30 \times 10^{-2}$
FFA (20:5)	0.024	-0.60	$3.30 \times 10^{-2}$
HCER.d (18:0/26:0)	0.036	0.60	$3.30 \times 10^{-2}$
PC (16:0/16:1)	0.035	-0.60	$3.30 \times 10^{-2}$
PE (16:0/20:3)	0.045	-0.60	$3.30 \times 10^{-2}$
PE (16:0/20:4)	0.048	-0.60	$3.30 \times 10^{-2}$
PE (18:0/22:5)	0.046	-0.60	$3.30 \times 10^{-2}$
PG (18:2/18:2)	0.028	-0.60	$3.30 \times 10^{-2}$
PI (16:0/22:5)	0.041	-0.60	$3.30 \times 10^{-2}$
PI (18:1/18:2)	0.030	-0.60	$3.30 \times 10^{-2}$
PS (20:0/18:3)	0.034	-0.60	$3.30 \times 10^{-2}$
SM (18:0)	0.032	0.60	$3.30 \times 10^{-2}$

SM (22:1)	0.046	0.60	$3.30 \times 10^{-2}$
TAG (48:0)_FA (16:0)	0.036	-0.60	$3.30 \times 10^{-2}$
TAG (48:2)_FA (14:0)	0.021	-0.60	$3.30 \times 10^{-2}$
TAG (48:3)_FA (18:3)	0.025	-0.60	$3.30 \times 10^{-2}$
TAG (51:0)_FA (18:0)	0.031	-0.60	$3.30 \times 10^{-2}$
TAG (51:3)_FA (17:0)	0.020	-0.60	$3.30 \times 10^{-2}$
TAG (54:3)_FA (20:3)	0.037	-0.60	$3.30 \times 10^{-2}$
TAG (56:3)_FA (18:0)	0.039	-0.60	$3.30 \times 10^{-2}$
TAG (56:3)_FA (20:2)	0.043	-0.60	$3.30 \times 10^{-2}$
TAG (56:4)_FA (22:4)	0.030	-0.60	$3.30 \times 10^{-2}$
CE (22:6)	0.048	0.59	$3.59 \times 10^{-2}$
DAG (18:1/20:2)	0.039	-0.59	$3.59 \times 10^{-2}$
DAG (18:2/20:5)	0.024	-0.59	$3.59 \times 10^{-2}$
PE.O (18:0/18:2)	0.038	-0.59	$3.59 \times 10^{-2}$
PE.P (18:1/20:4)	0.043	0.59	$3.59 \times 10^{-2}$
TAG (42:1)_FA (16:0)	0.021	-0.59	$3.59 \times 10^{-2}$
TAG (47:1)_FA (16:1)	0.023	-0.59	$3.59 \times 10^{-2}$
TAG (48:3)_FA (16:0)	0.018	-0.59	$3.59 \times 10^{-2}$
TAG (49:1)_FA (17:0)	0.026	-0.59	$3.59 \times 10^{-2}$
TAG (49:2)_FA (14:0)	0.023	-0.59	$3.59 \times 10^{-2}$
TAG (49:2)_FA (16:1)	0.023	-0.59	$3.59 \times 10^{-2}$
TAG (50:1)_FA (16:1)	0.031	-0.59	$3.59 \times 10^{-2}$
TAG (50:4)_FA (18:1)	0.032	-0.59	$3.59 \times 10^{-2}$
TAG (52:1)_FA (16:1)	0.034	-0.59	$3.59 \times 10^{-2}$
TAG (52:5)_FA (18:1)	0.035	-0.59	$3.59 \times 10^{-2}$
TAG (54:3)_FA (18:0)	0.047	-0.59	$3.59 \times 10^{-2}$
TAG (54:5)_FA (20:4)	0.038	-0.59	$3.59 \times 10^{-2}$
TAG (57:3)_FA (18:2)	0.034	-0.59	$3.59 \times 10^{-2}$
TAG (58:7)_FA (18:1)	0.038	-0.59	$3.59 \times 10^{-2}$
H3TG	0.047	-0.58	$3.83 \times 10^{-2}$
IDPN	0.044	-0.57	$3.90 \times 10^{-2}$
IDAB	0.044	-0.57	$3.90 \times 10^{-2}$
V3PL	0.036	-0.57	$3.90 \times 10^{-2}$
L1TG	0.044	-0.57	$3.90 \times 10^{-2}$
DAG (18:1/20:4)	0.031	-0.57	$3.90 \times 10^{-2}$
LPE (16:1)	0.038	-0.57	$3.90 \times 10^{-2}$
LPE (20:3)	0.037	-0.57	$3.90 \times 10^{-2}$

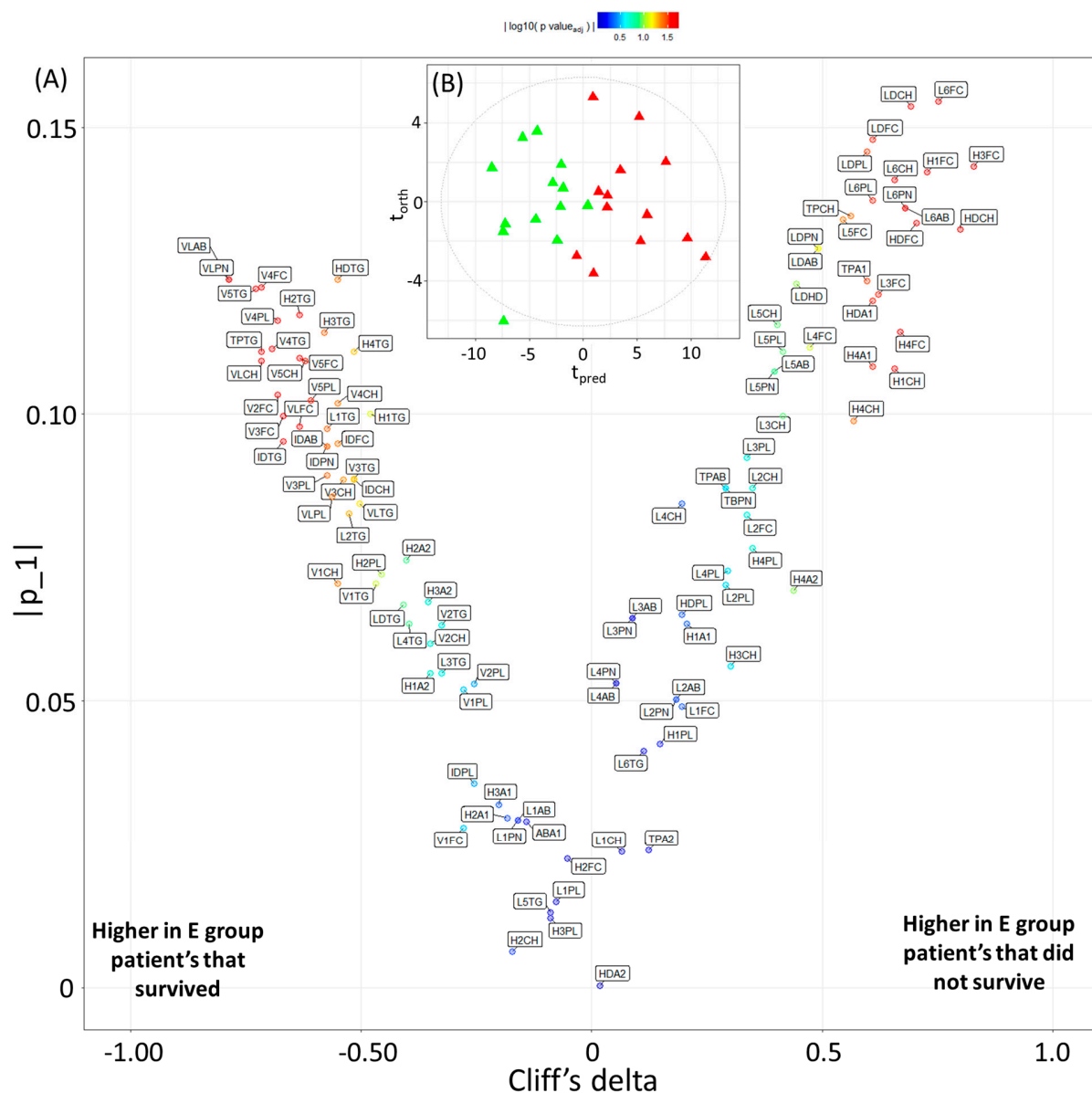
LPE (22:5)	0.043	-0.57	$3.90 \times 10^{-2}$
MAG (16:1)	0.038	-0.57	$3.90 \times 10^{-2}$
PE.P (18:1/22:6)	0.040	0.57	$3.90 \times 10^{-2}$
PI (18:0/18:1)	0.031	-0.57	$3.90 \times 10^{-2}$
PI (18:1/16:1)	0.036	-0.57	$3.90 \times 10^{-2}$
PI (18:1/20:3)	0.037	-0.57	$3.90 \times 10^{-2}$
TAG (46:0)_FA (14:0)	0.028	-0.57	$3.90 \times 10^{-2}$
TAG (50:1)_FA (20:1)	0.024	-0.57	$3.90 \times 10^{-2}$
TAG (50:2)_FA (18:2)	0.035	-0.57	$3.90 \times 10^{-2}$
TAG (51:0)_FA (17:0)	0.032	-0.57	$3.90 \times 10^{-2}$
TAG (53:3)_FA (17:0)	0.031	-0.57	$3.90 \times 10^{-2}$
TAG (54:4)_FA (20:4)	0.035	-0.57	$3.90 \times 10^{-2}$
H4CH	0.043	0.57	$4.15 \times 10^{-2}$
TPCH	0.046	0.56	$4.17 \times 10^{-2}$
VLPL	0.034	-0.56	$4.17 \times 10^{-2}$
DAG (18:0/22:6)	0.028	-0.56	$4.17 \times 10^{-2}$
DAG (18:1/22:4)	0.036	-0.56	$4.17 \times 10^{-2}$
DAG (18:1/22:6)	0.030	-0.56	$4.17 \times 10^{-2}$
LPC (18:3)	0.028	-0.56	$4.17 \times 10^{-2}$
PE (18:2/18:3)	0.037	-0.56	$4.17 \times 10^{-2}$
TAG (44:1)_FA (16:0)	0.022	-0.56	$4.17 \times 10^{-2}$
TAG (46:0)_FA (16:0)	0.028	-0.56	$4.17 \times 10^{-2}$
TAG (46:1)_FA (16:0)	0.022	-0.56	$4.17 \times 10^{-2}$
TAG (49:1)_FA (14:0)	0.025	-0.56	$4.17 \times 10^{-2}$
TAG (50:2)_FA (20:2)	0.023	-0.56	$4.17 \times 10^{-2}$
TAG (51:2)_FA (18:2)	0.022	-0.56	$4.17 \times 10^{-2}$
TAG (52:0)_FA (18:0)	0.042	-0.56	$4.17 \times 10^{-2}$
TAG (52:2)_FA (18:0)	0.042	-0.56	$4.17 \times 10^{-2}$
TAG (52:4)_FA (18:0)	0.028	-0.56	$4.17 \times 10^{-2}$
TAG (52:4)_FA (20:4)	0.035	-0.56	$4.17 \times 10^{-2}$
TAG (52:8)_FA (18:2)	0.032	-0.56	$4.17 \times 10^{-2}$
TAG (54:2)_FA (18:2)	0.034	-0.56	$4.17 \times 10^{-2}$
TAG (54:4)_FA (22:4)	0.030	-0.56	$4.17 \times 10^{-2}$
TAG (54:6)_FA (16:0)	0.034	-0.56	$4.17 \times 10^{-2}$
TAG (54:6)_FA (18:3)	0.027	-0.56	$4.17 \times 10^{-2}$
TAG (55:3)_FA (18:1)	0.047	-0.56	$4.17 \times 10^{-2}$
TAG (56:3)_FA (20:1)	0.047	-0.56	$4.17 \times 10^{-2}$

TAG (56:5)_FA (22:4)	0.032	-0.56	4.17x10 <sup>-2</sup>
TAG (56:8)_FA (18:1)	0.029	-0.56	4.17x10 <sup>-2</sup>
3-hydroxyanthranilic acid	0.031	-0.55	4.43x10 <sup>-2</sup>
HDTG	0.049	-0.55	4.43x10 <sup>-2</sup>
IDFC	0.043	-0.55	4.43x10 <sup>-2</sup>
V1CH	0.029	-0.55	4.43x10 <sup>-2</sup>
V4CH	0.041	-0.55	4.43x10 <sup>-2</sup>
CE (18:0)	0.039	0.55	4.43x10 <sup>-2</sup>
CE (20:1)	0.035	0.55	4.43x10 <sup>-2</sup>
CE (22:5)	0.044	0.55	4.43x10 <sup>-2</sup>
DAG (16:0/16:1)	0.034	-0.55	4.43x10 <sup>-2</sup>
DAG (18:1/22:5)	0.035	-0.55	4.43x10 <sup>-2</sup>
DCER (22:1)	0.024	-0.55	4.43x10 <sup>-2</sup>
LPE (16:0)	0.035	-0.55	4.43x10 <sup>-2</sup>
PE.O (16:0/20:4)	0.034	0.55	4.43x10 <sup>-2</sup>
PE.P (18:0/22:6)	0.037	0.55	4.43x10 <sup>-2</sup>
PE.P (18:1/18:0)	0.035	-0.55	4.43x10 <sup>-2</sup>
PI (18:1/20:4)	0.030	-0.55	4.43x10 <sup>-2</sup>
SM (24:1)	0.043	0.55	4.43x10 <sup>-2</sup>
TAG (46:2)_FA (16:0)	0.021	-0.55	4.43x10 <sup>-2</sup>
TAG (46:2)_FA (18:1)	0.025	-0.55	4.43x10 <sup>-2</sup>
TAG (47:2)_FA (18:1)	0.024	-0.55	4.43x10 <sup>-2</sup>
TAG (50:4)_FA (18:3)	0.025	-0.55	4.43x10 <sup>-2</sup>
TAG (52:2)_FA (20:1)	0.023	-0.55	4.43x10 <sup>-2</sup>
TAG (52:3)_FA (18:0)	0.032	-0.55	4.43x10 <sup>-2</sup>
TAG (53:2)_FA (18:2)	0.023	-0.55	4.43x10 <sup>-2</sup>
TAG (53:3)_FA (16:0)	0.031	-0.55	4.43x10 <sup>-2</sup>
TAG (55:2)_FA (18:1)	0.048	-0.55	4.43x10 <sup>-2</sup>
TAG (55:4)_FA (18:1)	0.046	-0.55	4.43x10 <sup>-2</sup>
TAG (56:4)_FA (18:0)	0.039	-0.55	4.43x10 <sup>-2</sup>
TAG (56:6)_FA (16:0)	0.033	-0.55	4.43x10 <sup>-2</sup>
TAG (56:6)_FA (18:1)	0.041	-0.55	4.43x10 <sup>-2</sup>
L5FC	0.046	0.54	4.56x10 <sup>-2</sup>
Acetone	0.008	0.53	4.66x10 <sup>-2</sup>
Glucose	0.031	-0.54	4.88x10 <sup>-2</sup>
Xanthurenic acid	0.029	-0.54	4.88x10 <sup>-2</sup>
V3CH	0.035	-0.54	4.88x10 <sup>-2</sup>

DAG (16:0/20:3)	0.032	-0.54	$4.88 \times 10^{-2}$
DCER (26:0)	0.044	0.54	$4.88 \times 10^{-2}$
LPE (22:4)	0.036	-0.54	$4.88 \times 10^{-2}$
PC (18:0/18:1)	0.036	-0.54	$4.88 \times 10^{-2}$
PE (18:0/20:3)	0.040	-0.54	$4.88 \times 10^{-2}$
PE (18:0/20:5)	0.031	-0.54	$4.88 \times 10^{-2}$
TAG (45:0)_FA (16:0)	0.023	-0.54	$4.88 \times 10^{-2}$
TAG (48:5)_FA (18:2)	0.031	-0.54	$4.88 \times 10^{-2}$
TAG (50:2)_FA (14:0)	0.040	-0.54	$4.88 \times 10^{-2}$
TAG (50:5)_FA (20:5)	0.028	-0.54	$4.88 \times 10^{-2}$
TAG (52:2)_FA (16:1)	0.041	-0.54	$4.80 \times 10^{-3}$
TAG (54:4)_FA (18:2)	0.036	-0.54	$4.81 \times 10^{-3}$
TAG (54:7)_FA (18:3)	0.028	-0.54	$4.89 \times 10^{-2}$



**Figure S14 - Correlation plot of the (A) survived model and (B) Did not survive model.** The top 50 metabolites are shown according to adjusted p-values.



**Figure S15 – Modeling COVID-19 mortality prediction using only the lipoproteins** (A) Eruption plot of the severity group E patients who survived vs the severity group E patients who died. (B) O-PLS-DA of severity group E patients who survived (green triangles) and severity group E patients who died (red triangles),  $R^2X=0.32$ ,  $AUROC=0.81$ . Cliff's delta, OPLS loadings values and the adjusted p values for this model can be found in table S30.

**Table S32 - OPLS loadings, Cliff's delta and adjusted p-values of lipoprotein model for the comparison group E severity patients comparing who survived and who died, samples were age matched.** Only metabolites with significant p-values are shown in the table.

Metabolite	OPLS loadings	Cliff's delta	Adjusted p-value
HDCH	0.132	0.80	1.82x10 <sup>-2</sup>
VLPN	0.123	-0.79	1.82x10 <sup>-2</sup>
VLAB	0.123	-0.79	1.82x10 <sup>-2</sup>
H3FC	0.143	0.83	1.82x10 <sup>-2</sup>
L6FC	0.154	0.75	1.98x10 <sup>-2</sup>
TPTG	0.111	-0.72	2.04x10 <sup>-2</sup>
LDCH	0.154	0.69	2.04x10 <sup>-2</sup>
L6PN	0.136	0.68	2.04x10 <sup>-2</sup>
VLCH	0.109	-0.72	2.04x10 <sup>-2</sup>
HDFC	0.133	0.70	2.04x10 <sup>-2</sup>
V4TG	0.111	-0.69	2.04x10 <sup>-2</sup>
V5TG	0.122	-0.73	2.04x10 <sup>-2</sup>
V2FC	0.103	-0.68	2.04x10 <sup>-2</sup>
V4FC	0.122	-0.72	2.04x10 <sup>-2</sup>
V4PL	0.116	-0.68	2.04x10 <sup>-2</sup>
L6AB	0.136	0.68	2.04x10 <sup>-2</sup>
H1FC	0.412	0.73	2.04x10 <sup>-2</sup>
H4FC	0.114	0.67	2.04x10 <sup>-2</sup>
IDTG	0.095	-0.67	2.11x10 <sup>-2</sup>
V3FC	0.100	-0.67	2.11x10 <sup>-2</sup>
L6CH	0.141	0.66	2.16x10 <sup>-2</sup>
H1CH	0.108	0.66	2.25x10 <sup>-2</sup>
VLFC	0.098	-0.63	2.72x10 <sup>-2</sup>
V5FC	0.110	-0.63	2.72x10 <sup>-2</sup>
H2TG	0.117	-0.63	2.72x10 <sup>-2</sup>
LDFC	0.148	0.61	2.89x10 <sup>-2</sup>
HDA1	0.120	0.61	2.89x10 <sup>-2</sup>
V5CH	0.109	-0.62	2.89x10 <sup>-2</sup>
V5PL	0.102	-0.61	2.89x10 <sup>-2</sup>
L3FC	0.121	0.62	2.89x10 <sup>-2</sup>
L6PL	0.137	0.61	2.89x10 <sup>-2</sup>
H4A1	0.108	0.61	2.89x10 <sup>-2</sup>
TPA1	0.123	0.60	3.16x10 <sup>-2</sup>

LDPL	0.146	0.60	$3.16 \times 10^{-2}$
IDPN	0.094	-0.57	$3.70 \times 10^{-2}$
IDAB	0.094	-0.57	$3.70 \times 10^{-2}$
V3PL	0.089	-0.57	$3.70 \times 10^{-2}$
L1TG	0.097	-0.57	$3.70 \times 10^{-2}$
H3TG	0.114	-0.58	$3.70 \times 10^{-2}$
H4CH	0.099	0.57	$3.85 \times 10^{-2}$
TPCH	0.134	0.56	$3.96 \times 10^{-2}$
VLPL	0.086	-0.56	$3.96 \times 10^{-2}$
HDTG	0.123	-0.55	$4.16 \times 10^{-2}$
IDFC	0.095	-0.55	$4.16 \times 10^{-2}$
V1CH	0.071	-0.55	$4.16 \times 10^{-2}$
V4CH	0.102	-0.55	$4.16 \times 10^{-2}$
L5FC	0.135	0.54	$4.20 \times 10^{-2}$
V3CH	0.089	-0.54	$4.58 \times 10^{-2}$

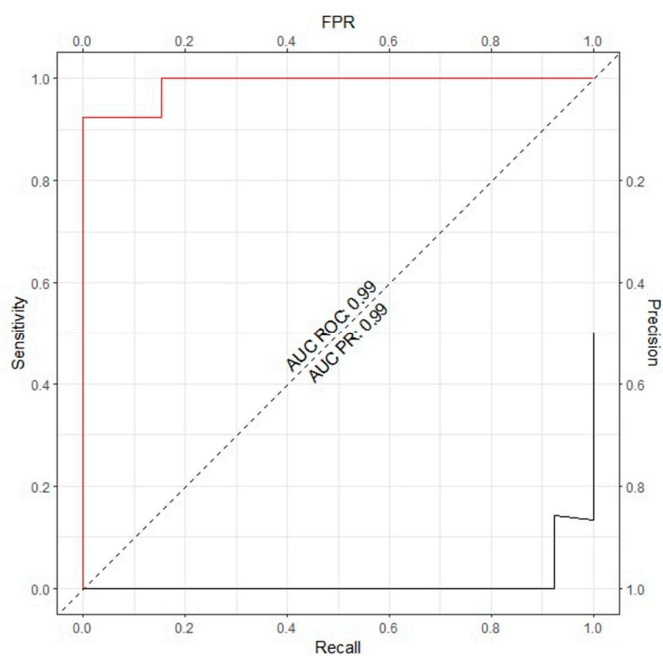


Figure S16 - AUROC showing prediction of mortality (AUCROC = 0.99) built using HCer 16:0 and PEO 18:0\_18:1