

Metabolomic and lipidomic landscape of porcine kidney associated with kidney perfusion in heart beating donors and donors after cardiac death

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Supplementary Material

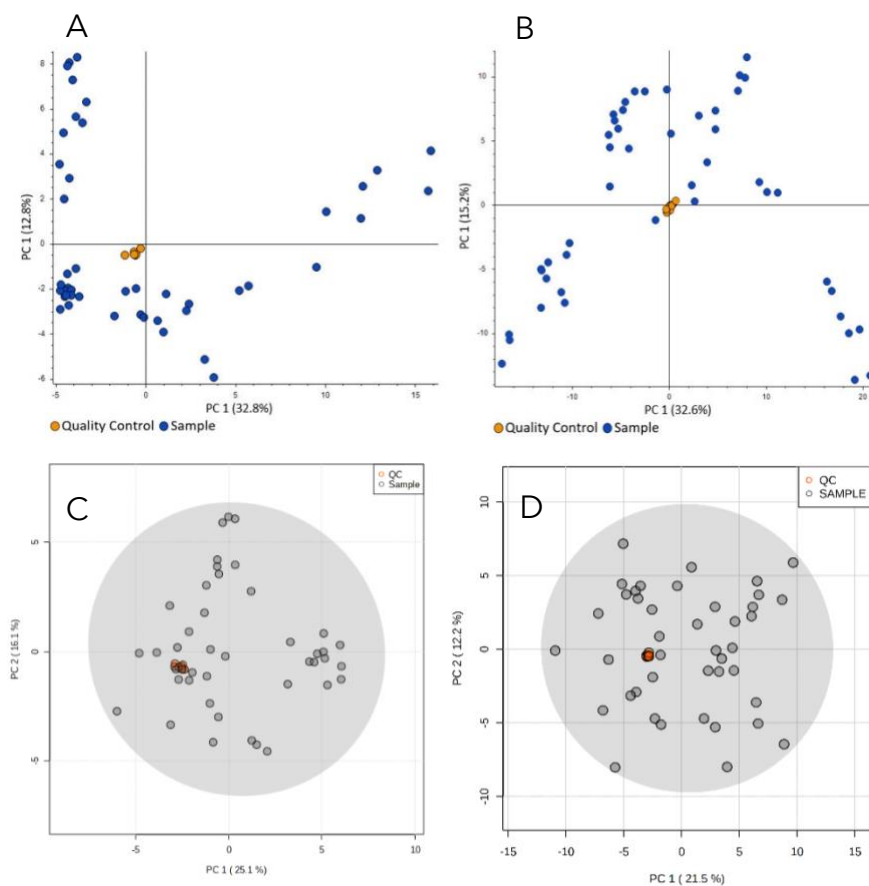


Fig. S1 Principal component analysis (PCA) score plots of all analyzed samples and extraction quality control (QC) samples. A- metabolomics, RP, positive ionization mode; B- metabolomics, RP, negative ionization mode; C- lipidomics, HILIC, positive ionization mode; D – lipidomic, RP, positive ionization mode;

Table S1. The list of metabolites identified with the use of MS/MS mode

Molecular Weight [u]	RT [min]	Name
positive ionization mode		
109.06421	1.818	2-amino-4-methylpyrimidine
131.05824	1.262	5-Aminolevulinic acid
145.05268	11.58	8-Hydroxyquinoline
203.11575	8.904	Acetylcarnitine
174.10035	1.51	Acetylorithine
246.10022	11.572	Acetyltryptophan
267.0965	7.452	Adenosine
347.06276	1.51	Adenosine monophosphate
89.04817	1.834	Alanine
202.13174	7.69	Alanyl-Leucine
161.06869	1.511	alpha-Aminoadipic acid
174.11161	1.931	Arginine
132.05339	1.252	Asparagine
133.0375	1.268	Aspartic acid
175.09561	1.435	Citrulline
131.06947	1.875	Creatine
240.02358	1.216	Cystine
315.27694	16.619	Dehydrophytosphingosine
267.09664	7.24	Deoxyguanosine
296.2349	16.964	Dimorphecolic acid
147.05303	1.413	Glutamic acid
146.06901	1.315	Glutamine
198.18576	22.404	Guanethidine
151.0493	3.737	Guanine
179.05828	9.63	Hippuric acid
155.06941	1.816	Histidine
136.03852	7.064	Hypoxanthin
156.05345	2.484	Imidazolelactic acid
131.09468	7.127	Leucine

146.10547	1.832	Lysine
126.06544	2.484	Melamine
149.05098	3.017	Methionine
165.0459	1.366	Methionine sulfoxide
281.11213	7.505	Methyladenosine
257.10258	1.272	Methylcytidine
169.08505	1.934	Methylhistidine
219.11051	1.514	Pantothenic acid
115.0635	1.505	Proline
143.09453	1.512	Proline
129.04257	1.511	Pyroglutamic acid
105.0429	1.259	Serine
281.27146	21.522	Sphingosine
119.05837	1.339	Threonine
126.04298	2.691	Thymine
204.08995	11.574	Tryptophan
244.06921	1.5	Uridine
138.04274	6.97	Urocanic acid
117.07907	2.41	Valine

negative ionization mode

195.05258	8.343	3-Hydroxyhippuric acid
207.08896	12.458	Acetylphenylalanine
246.10028	11.833	Acetyltryptophan
158.04289	1.235	Allantoin
138.04164	6.93	Aminonicotinic acid
133.03617	1.207	Aspartic acid
131.06815	1.833	Creatine
240.02358	1.159	Cystine
196.0576	1.117	Gluconic acid
180.06273	1.096	Glucose
147.05194	1.35	Glutamic acid
146.06794	1.252	Glutamine
465.30937	13.764	Glycocholic Acid

437.29105	18.422	Glycoursodeoxycholic acid
151.0483	3.722	Guanine
155.06828	1.756	Histidine
156.05237	2.426	Imidazolelactic acid
205.0732	11.808	Indolelactic acid
205.07328	12.086	Indolelactic acid
268.08096	7.067	Inosine
90.03009	1.438	Lactic acid
182.07823	1.098	Mannitol
262.04852	11.523	Mannitol-1-phosphate
193.07312	10.128	Methylhippuric acid
129.04104	1.349	Oxoproline
165.07795	8.856	Phenylalanine
368.16614	14.772	Testosterone sulfate
370.23588	12.907	Thromboxane B2
204.08919	11.521	Tryptophan
181.07305	7.237	Tyrosine
138.04168	7.8	Urocanic acid

RT – retention time

Table S2. The list of lipid species identified with the use of MS/MS mode

m/z	RT [min]	adduct	Lipid Species Shorthand
HILIC			
480.3448	8.13	+H	LPC P-16:0
494.3241	8.62	+H	LPC 16:1
522.3554	8.06	+H	LPC 18:1
522.3554	8.48	+H	LPC 18:1
524.3710	8.45	+H	LPC 18:0
544.3397	8.46	+H	LPC 20:4
566.3217		+Na	
696.4962	7.14	+H	PE P-34:4
700.5275	7.22	+H	PE P-34:2
702.5432	7.19	+H	PE P-34:1
722.5119	7.08	+H	PE P-36:5
724.5275	7.08	+H	PE P-36:4
746.5095		+Na	
728.5588	7.08	+H	PE P-36:2
740.5200	7.25	+Na	PE 34:1
744.5537	7.23	+H	PE 36:2
766.5357		+Na	
750.5432	7.01	+H	PE P-38:5
752.5564	7.00	+Na	PE O-36:2
752.5588	7.00	+H	PE P-38:4
774.5408		+Na	
764.5200	7.18	+Na	PE 36:3
764.5200	7.49	+Na	PE 36:3
766.5381	7.13	+H	PE 38:5
788.5200		+Na	
768.5513	7.13	+Na	PE 36:1
772.5251	6.97	+Na	PE O-38:6
774.5408	6.97	+Na	PE O-38:5
780.5901	6.87	+H	PE P-40:4

790.5357	7.13	+Na	PE 38:4
804.5513	6.06	+Na	PC 36:4
806.5670	6.48	+Na	PC 36:3
725.5592	7.78	+H	SM 36:4;O2
RP			
331.2842	4.77	+H	MG 16:0
376.3421	5.58	+NH4	MG 18:0
572.4884	10.66	+NH4	TG 30:0
586.5405	10.76	+NH4	DG 32:0
600.5197	10.59	+NH4	TG 32:0
605.4751		+Na	
612.5561	10.94	+NH4	DG 34:1
614.5718	11.35	+NH4	DG 34:0
628.5510	11.19	+NH4	TG 34:0
633.5064		+Na	
638.5718	11.09	+NH4	DG 36:2
656.5823	11.71	+NH4	TG 36:0
661.5377		+Na	
662.5718	11.10	+NH4	DG 38:4
666.6183	13.90	+NH4	CE 18:2
684.6136	12.17	+NH4	TG 38:0
689.5690		+Na	
712.6449	12.57	+NH4	TG 40:0
724.5275	9.45	+H	PE P-36:4
740.6762	12.93	+NH4	TG 42:0
771.6497	5.74	+H	TG 46:4
794.7232	13.33	+NH4	TG 46:1
796.7388	13.56	+NH4	TG 46:0
820.7388	13.41	+NH4	TG 48:2
822.7545	13.64	+NH4	TG 48:1
827.7099		+Na	
846.7545	13.48	+NH4	TG 50:3
848.7701	13.70	+NH4	TG 50:2

850.7858	13.90	+NH4	TG 50:1
862.7858	13.83	+NH4	TG 51:2
864.8014	14.02	+NH4	TG 51:1
872.7701	13.56	+NH4	TG 52:4
877.7255		+Na	
874.7858	13.75	+NH4	TG 52:3
879.7412		+Na	
876.8014	13.96	+NH4	TG 52:2
881.7568		+Na	
878.8171	14.14	+NH4	TG 52:1
896.7701	13.41	+NH4	TG 54:6
898.7858	13.63	+NH4	TG 54:5
903.7412		+Na	
900.8014	13.82	+NH4	TG 54:4
902.8171	14.00	+NH4	TG 54:3
907.7725		+Na	
904.8327	14.19	+NH4	TG 54:2
909.7881		+Na	

m/z – mass to charge ratio; RT – retention time

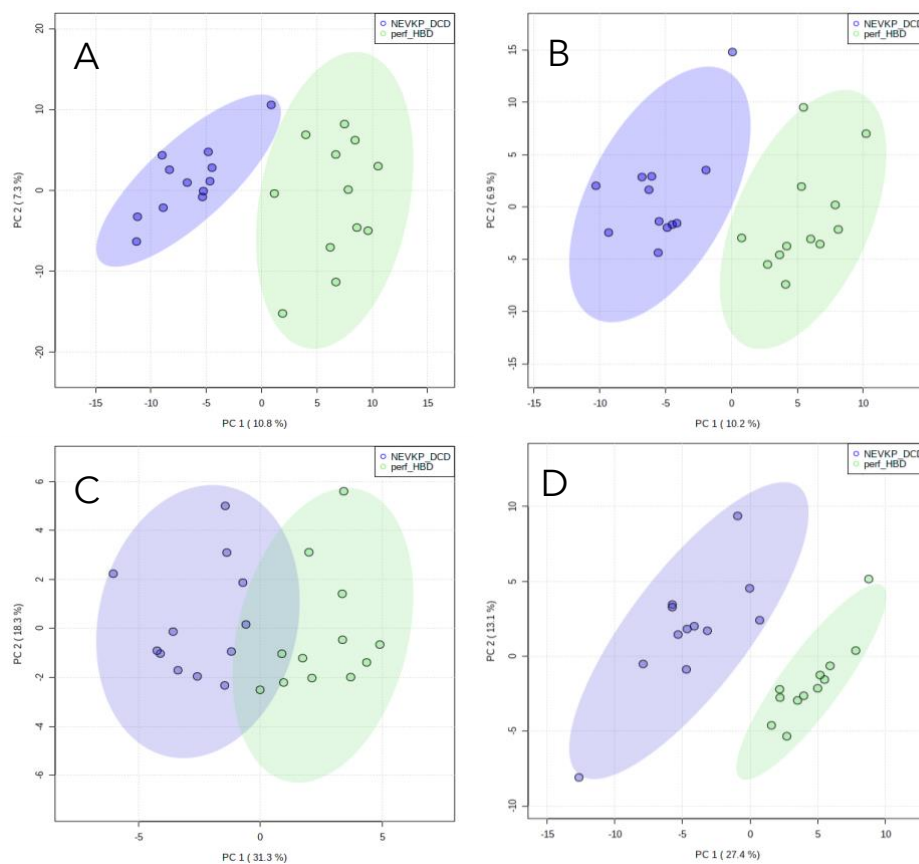


Fig. S2 PCA score plots showing separation between HBD and DCD perfusions. RP metabolomic analyses in positive (A) and negative (B) ionization modes, lipidomic analyses with HILIC (C) and RP (D) separations

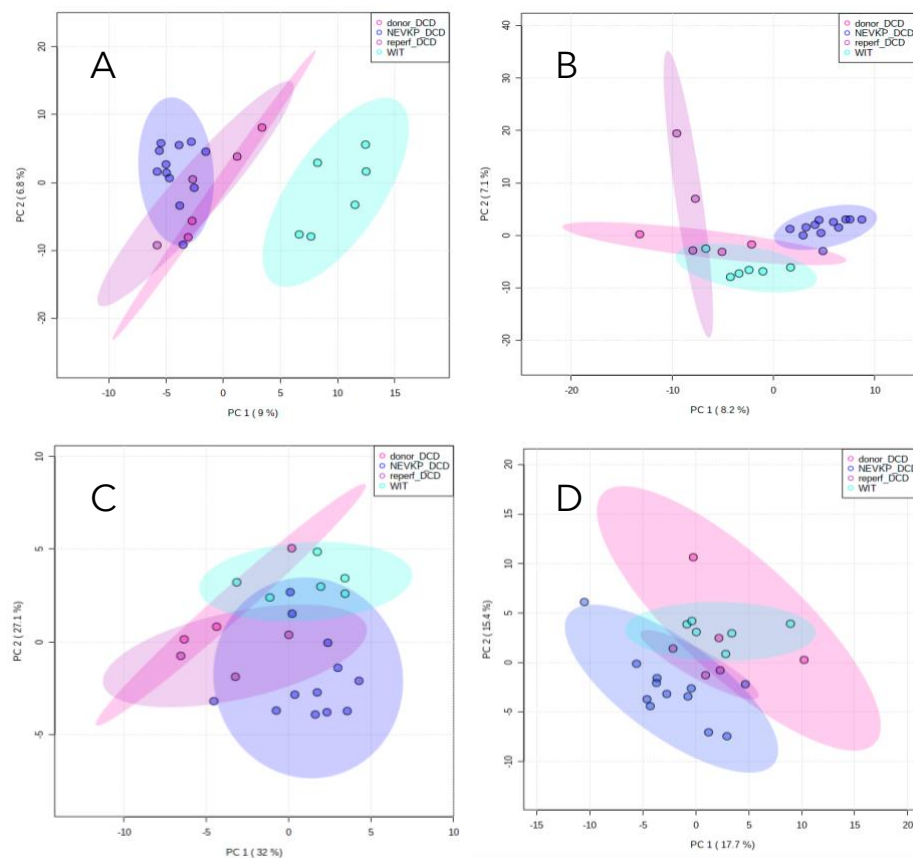


Fig. S3 PCA score plots of DCD metabolomic and lipidomic data. A – metabolomics, RP, positive ionization mode; B – metabolomics, RP, negative ionization mode; C – lipidomics, HILIC, positive ionization mode; D – lipidomics, RP, positive ionization mode

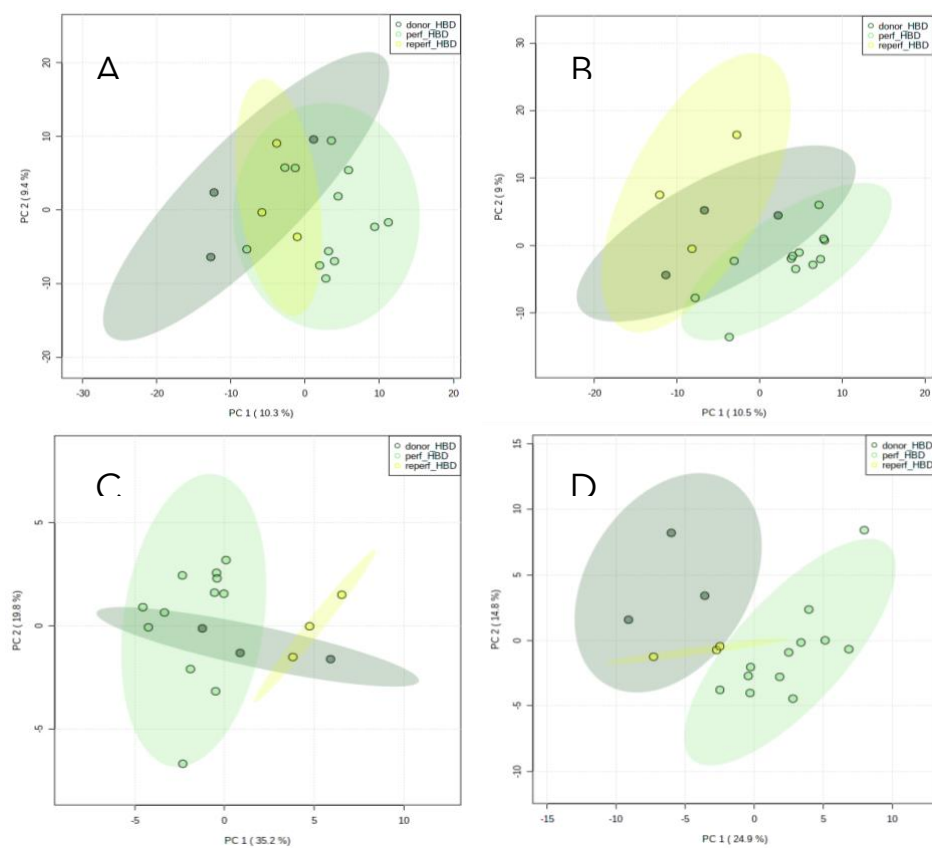
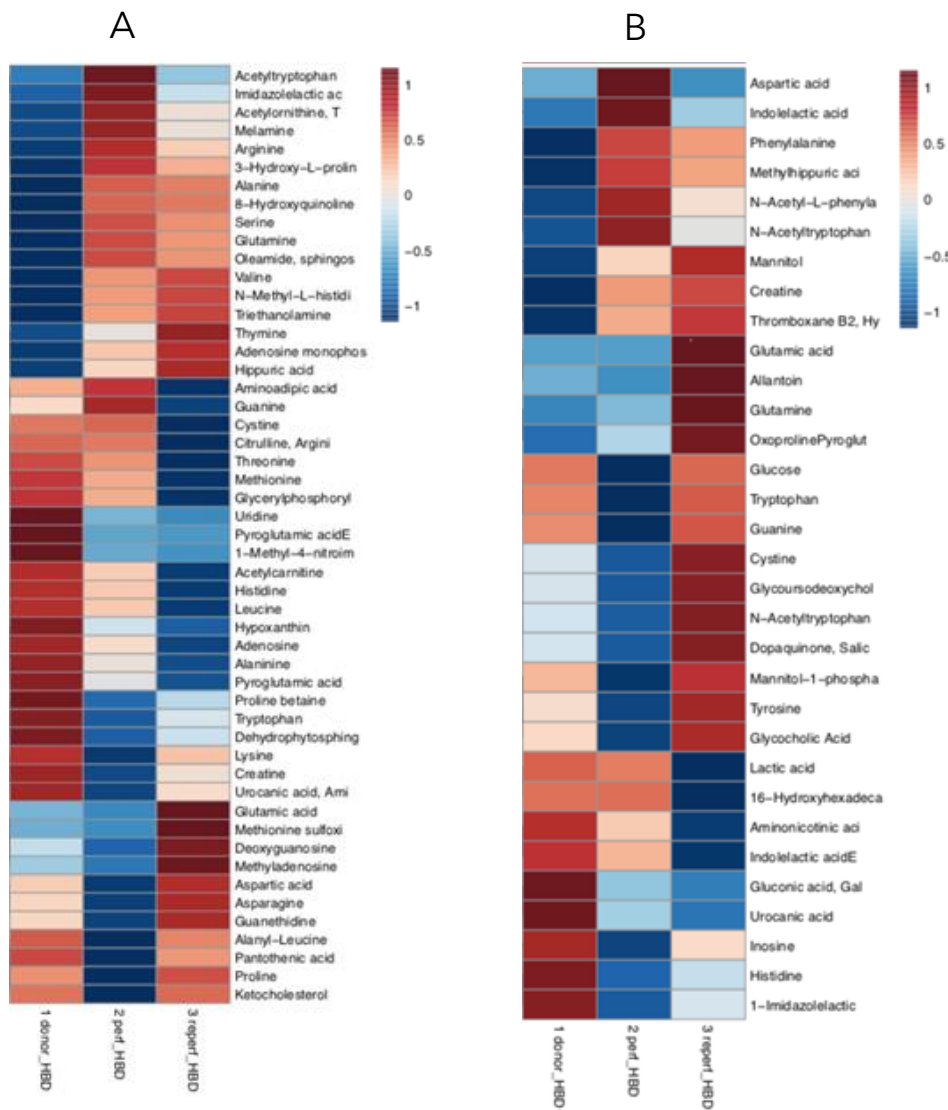
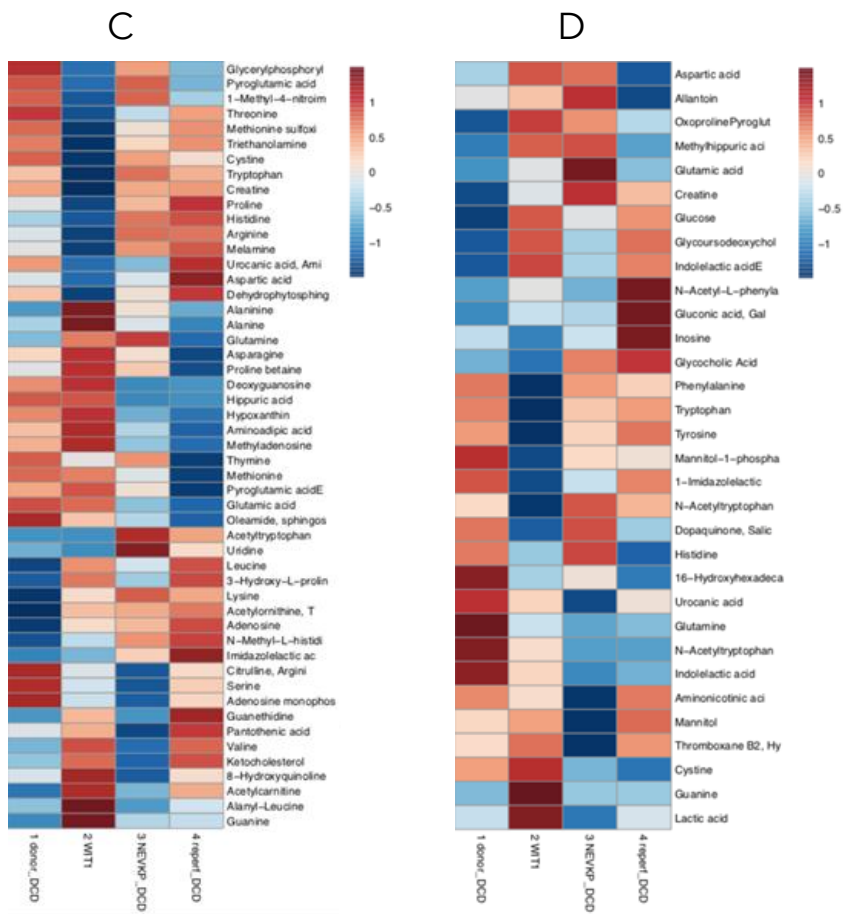


Fig. S4 Principal Component Analysis score plots of HBD metabolomic and lipidomic data. A – metabolomics, RP, positive ionization mode; B – metabolomics, RP, negative ionization mode; C – lipidomics, HILIC, positive ionization mode; D – lipidomics, RP, positive ionization mode





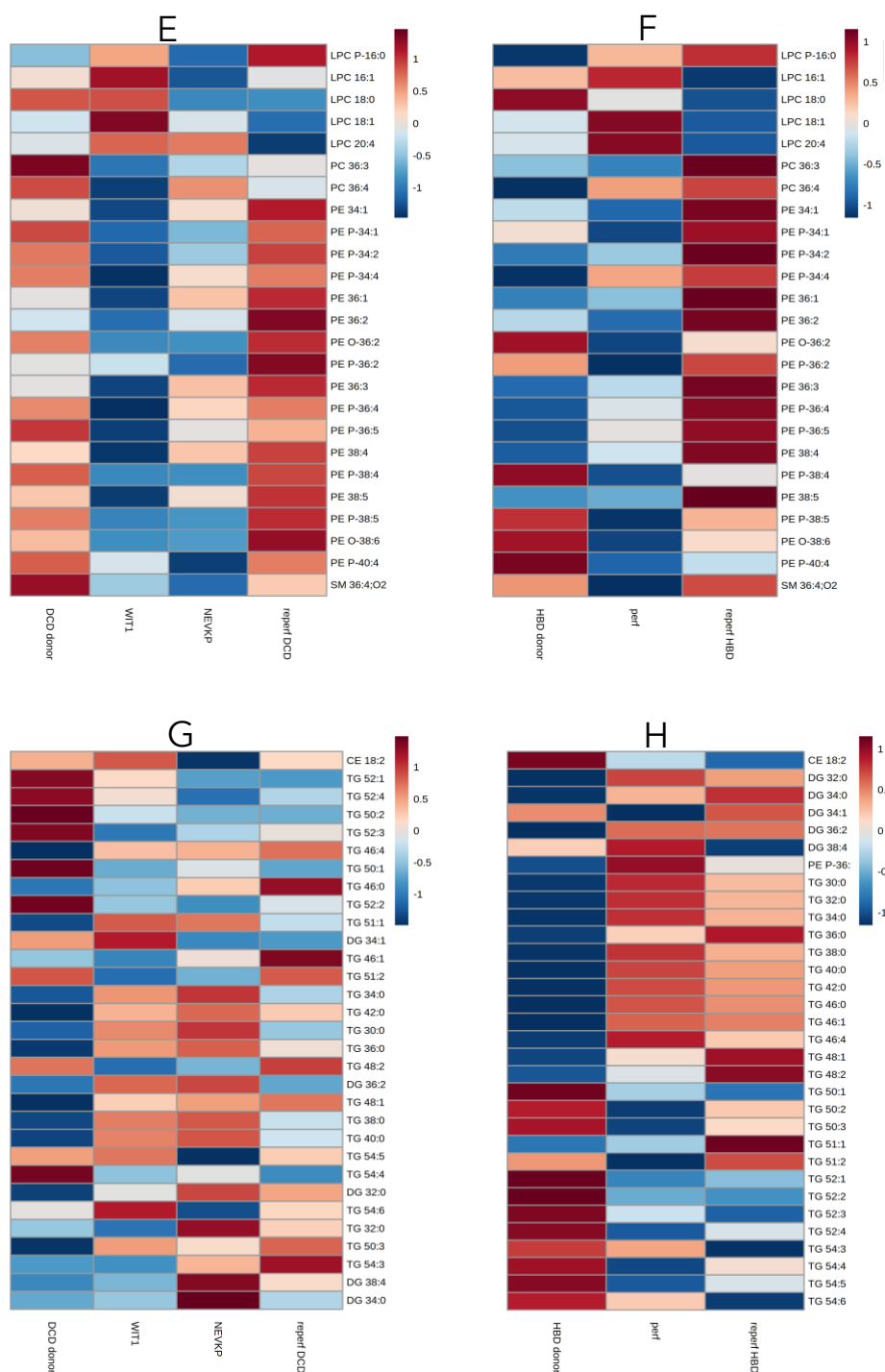


Fig. S5 Heat-maps showing overall trends in identified metabolites levels during autotransplantation procedure. A- HBD donor, metabolomics, RP, positive ionization mode; B- HBD donor, metabolomics, RP, negative ionization mode; C- DCD donor, metabolomics, RP, positive ionization mode; D- DCD donor, metabolomics, RP, negative ionization mode; E- DCD donor, lipidomics, HILIC; F- HBD donor, lipidomics, HILIC; G- DCD donor, lipidomic RP; H- HBD donor, lipidomic, RP