

Supplementary materials for:

**Deregulation of the purine pathway in pre-transplant liver biopsies
associates with graft function and survival after transplantation**

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Table S1. Misclassification table for the test dataset based on the training dataset model.

True classes	Calculated classes		
	DBD	DCD	Accuracy
DBD	5	0	100%
DCD	1	6	85.71%
Total		12	91.67%
Fisher's prob.			0.0076

Table S2. Annotation of markers based on molecular weight, retention time and collision induced dissociation fragmentation of 5 metabolites.

Identified as	m/z	Retention time (min)	Observed ion	QC RSD (%)
Adenine monophosphate	348.08	17.3	[M+H] ⁺	12.80
Adenosine	268.10	14.2	[M+H] ⁺	5.88
Adenine	136.06	17.1	[M+H] ⁺	7.16
Hypoxanthine	137.05	9.75	[M+H] ⁺	6.07
Urate	169.04	11.8	[M+H] ⁺	21.33

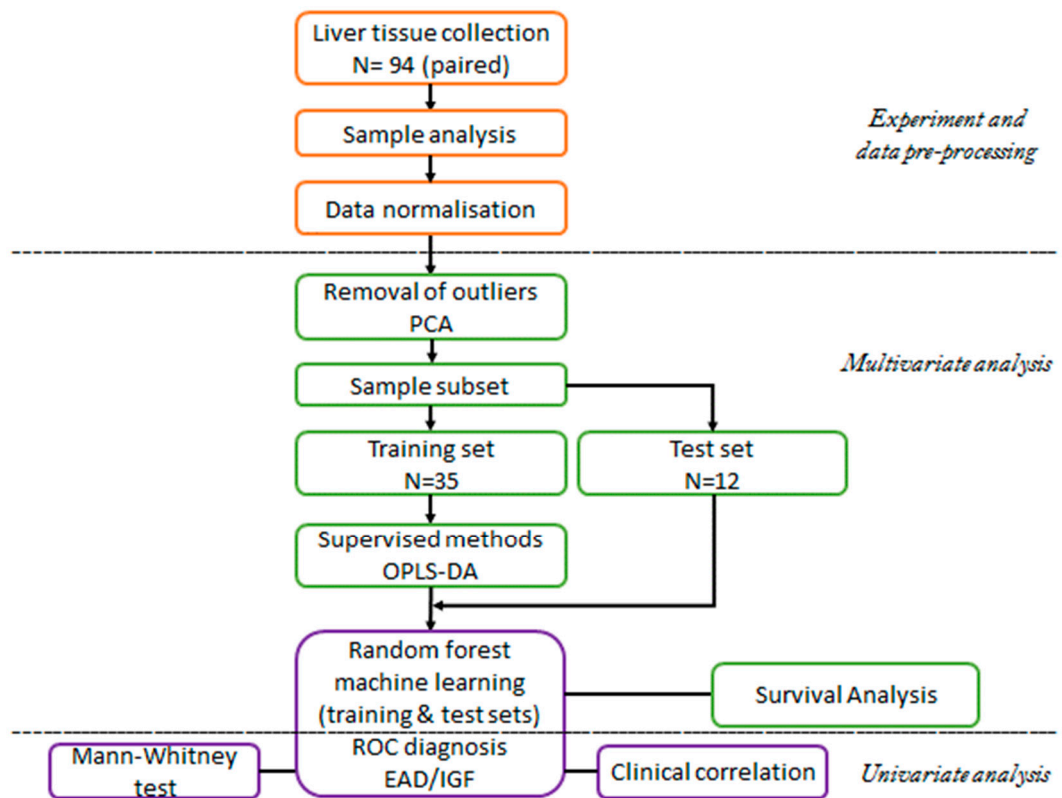


Figure S1. Study workflow.

PCA, principle component analysis; OPLS-DA, orthogonal projections to latent structures-discriminant analysis; EAD; early allograft dysfunction; IGF, immediate graft function; ROC, receiver operating characteristic.

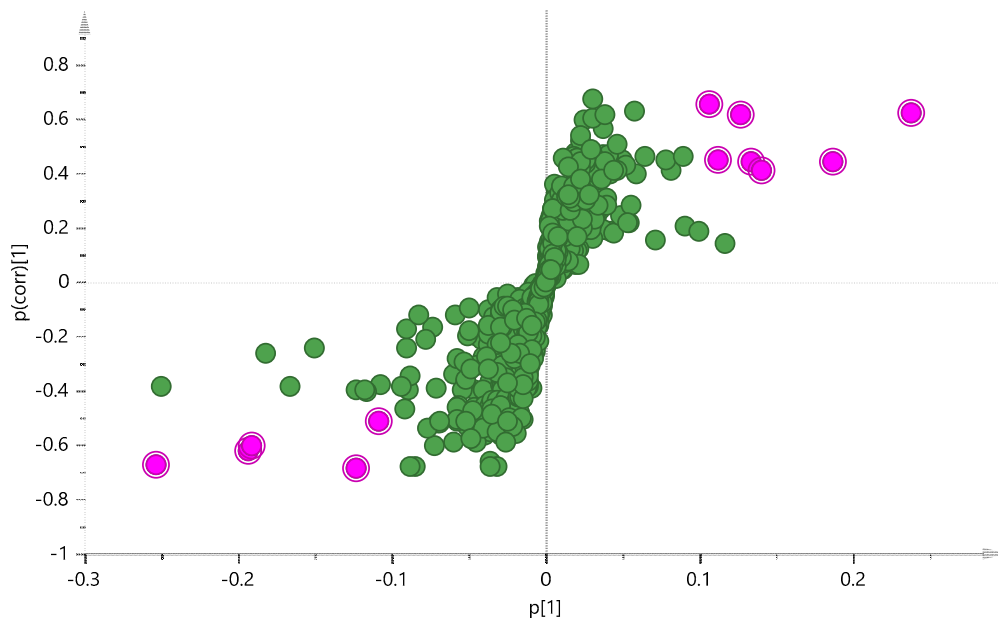


Figure S2. Metabolic feature selection from the S-plot.

All the dots represent detected features, and the pink dots were selected for annotation.

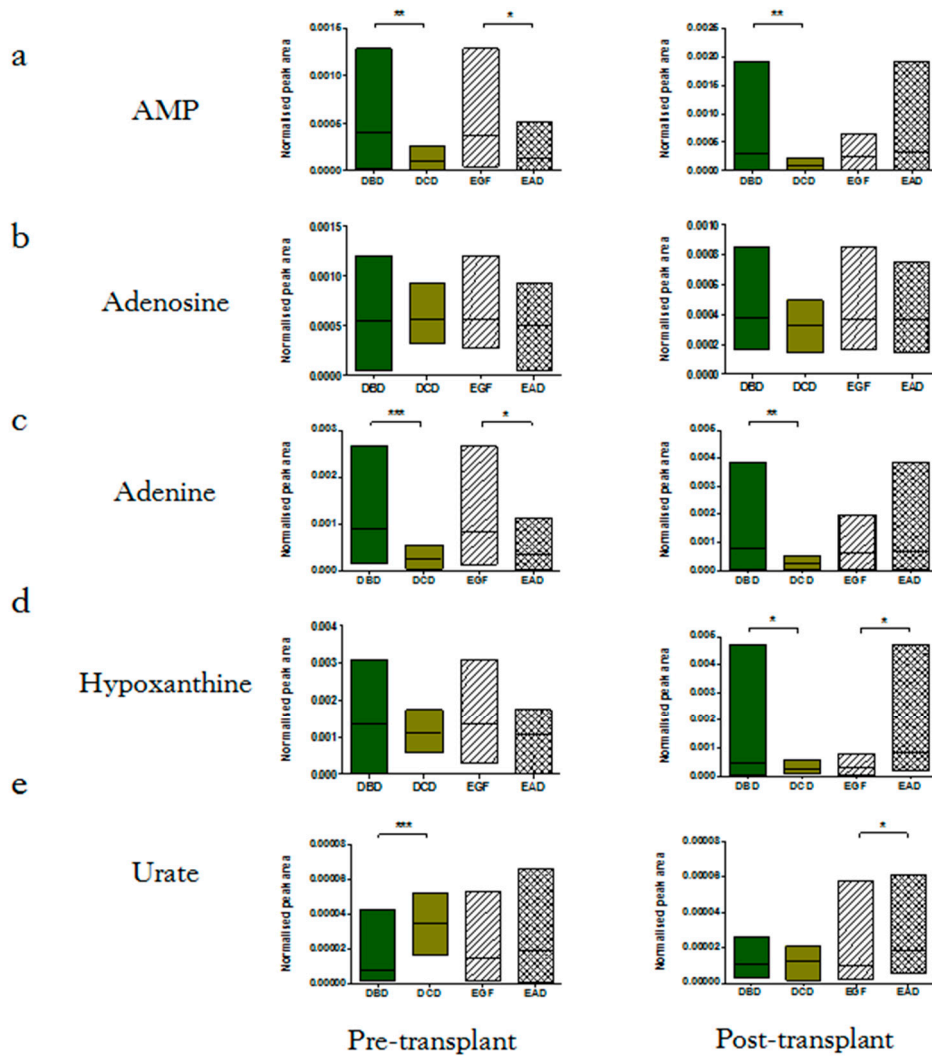


Figure S3. Box plots of 5 metabolites in four groups at both transplant stages. (A) AMP, (B) Adenosine, (C) Adenine, (D) Hypoxanthine and (E) Urate.

AMP, adenosine monophosphate; DBD, donation after brain death; DCD, donation after circulatory death; EGF, early graft function; EAD, early allograft dysfunction. Results represented as low-mean-high, p-value was derived from Mann-Whitney test, followed by Benjamini-Hochberg FDR correction (* $q < 0.05$, ** $q < 0.01$, *** $q < 0.001$).

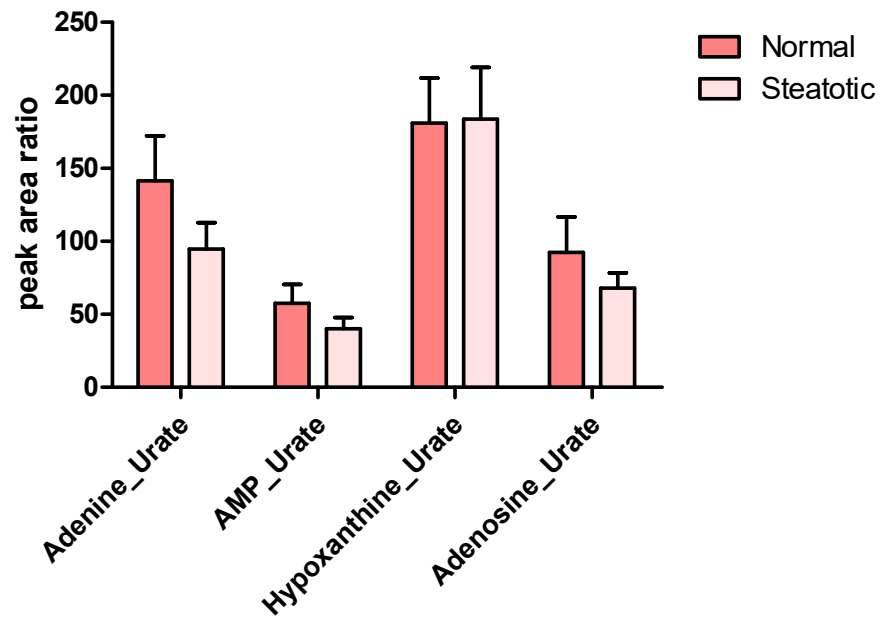


Figure S4. Bar plots of 4 purine ratios in normal (no steatotic, n=21) and steatotic (mild and moderate steatotic, n=26) groups.

AMP, adenosine monophosphate. Results represented as mean with SEM.