

Supplementary Materials: Renal Cell Carcinoma: A Study through NMR-Based Metabolomics Combined with Transcriptomics

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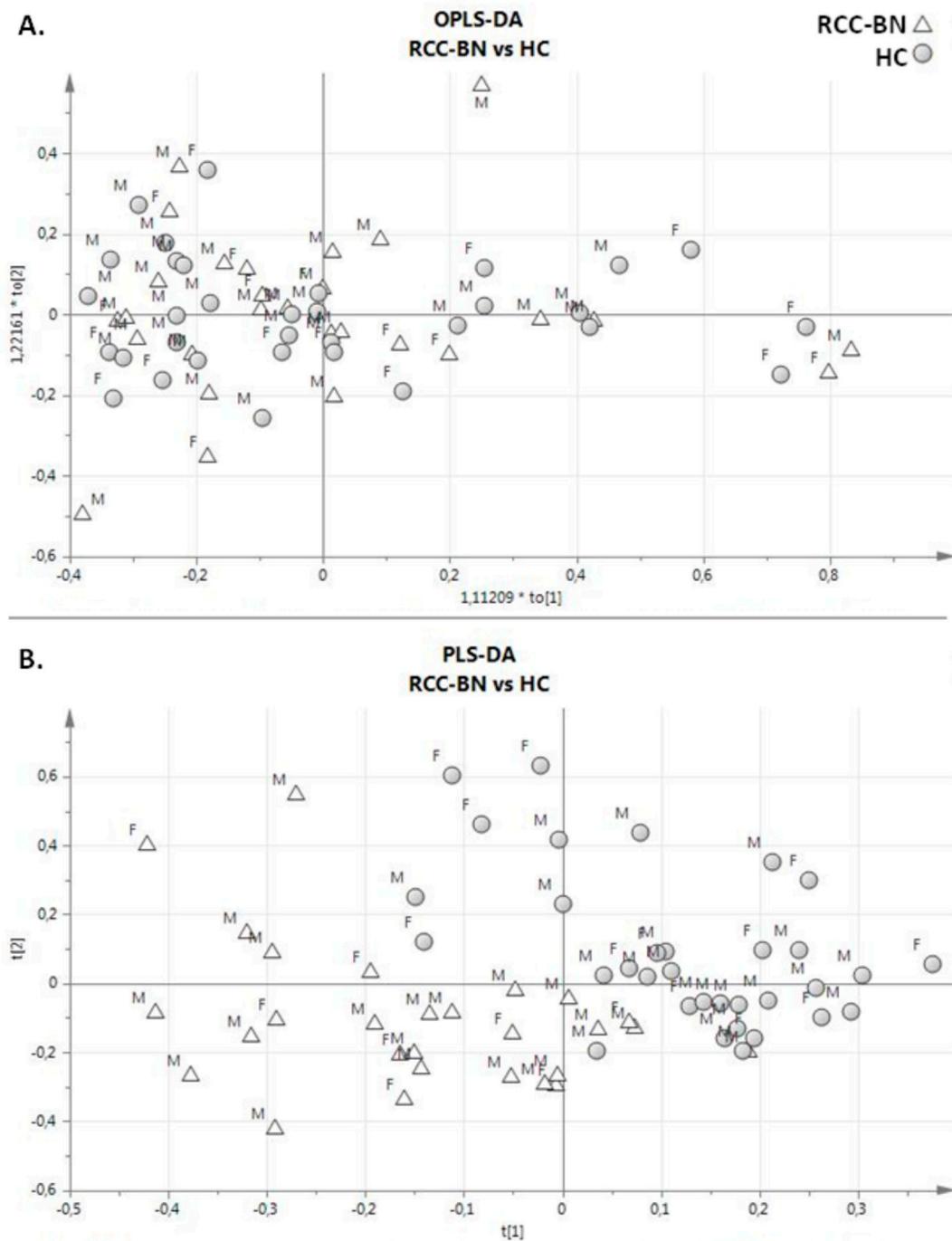


Figure S1. Cont.

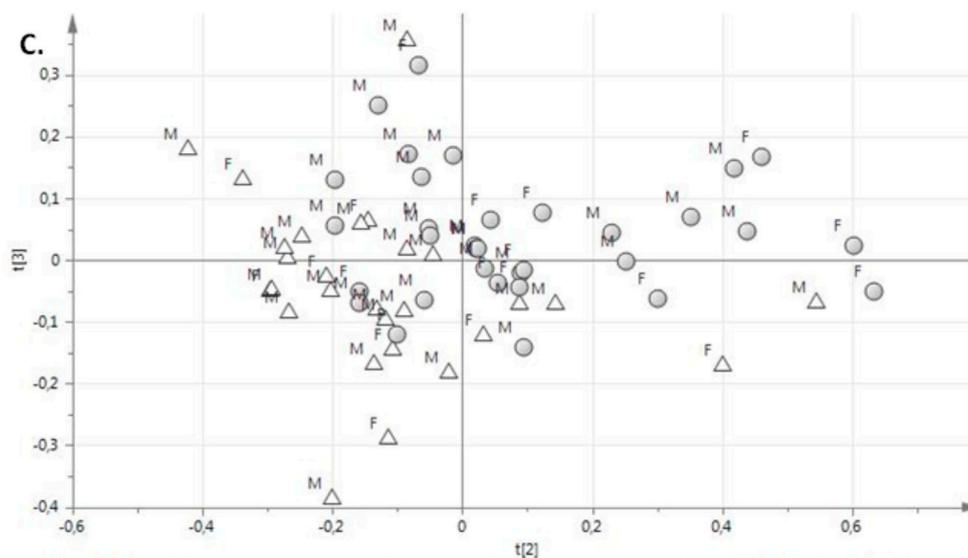


Figure S1. Score plot of OPLS-DA model for RCC-BN *vs.* HC, showing the first (to1) and the second (to2) orthogonal components (A). Score plots of PLS-DA model for RCC-BN *vs.* HC, showing the first (t1) *vs.* the second (t2) components (B) and the second (t2) *vs.* the third (t3) components (C). Samples are labeled with F for females and M for males. There is no grouping according to gender neither along orthogonal components in OPLS-DA (to1 *vs.* to2) nor along minor components in PLS-DA (t2 *vs.* t3).

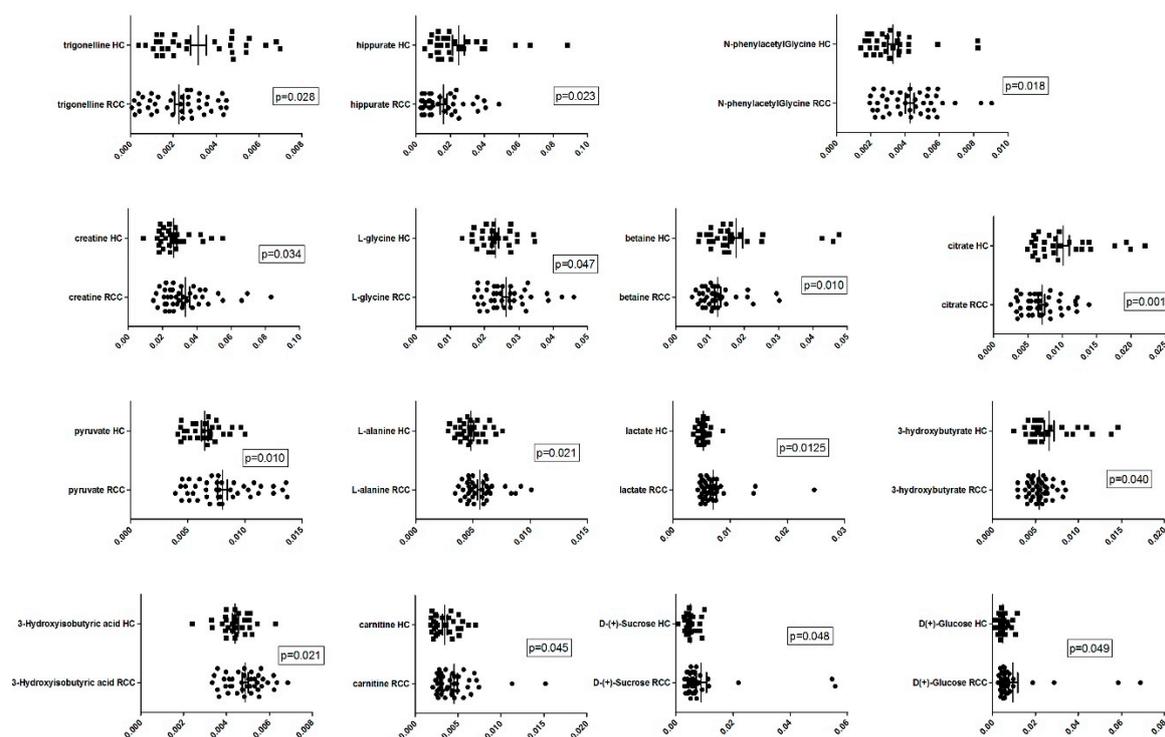


Figure S2. Quantitative differences and the *p*-value *t*-test for each metabolite calculated on the basis of the intensity of the corresponding signals in the different samples.

Table S1. Parameters describing the models (OPLS-DA and PLS-DA) built using only the spectral data of male subjects.

ccRCC-BN vs. HC Only Males							
OPLS-DA Model				PLS-DA Model			
Component	R ² X(cum)	R ² (cum)	Q ² (cum)	Component	R ² X(cum)	R ² Y(cum)	Q ² (cum)
Model	0.367	0.662	0.426	1	0.226	0.421	0.27
Predictive	0.112	0.662	0.426	2	0.367	0.662	0.452
P1	0.112	0.662	0.426				
Orthogonal in X	0.254	0					
O1	0.254	0					
Specificity	0.8			Specificity	0.8		
Sensitivity	0.905			Sensitivity	0.905		
Accuracy	0.855			Accuracy	0.855		
Cohen's K in cross-validation	0.706			Cohen's K in cross-validation	0.706		