Table S3 Statistical parameters of multivariate PCA models of metabolomic data

Model	N	k	A	R^2X	Q^2	Scaling	Comparison	Figure
M1	34	9151	6	0.919	0.85	Pareto	All samples	3A
M2	11	9151	3	0.876	0.698	Pareto	F0 *vs.* F2 in YNB medium	3B & C
M3	11	9151	2	0.936	0.889	Centre	F0 *vs.* F2 in YNB medium	3B & C
M4	12	9151	3	0.785	0.458	Pareto	F0 *vs.* F2 in YPD medium	S5A & B
M5	12	9151	5	0.98	0.866	Centre	F0 *vs.* F2 in YPD medium	S5A & B
M6	12	9151	4	0.916	0.826	Pareto	F2 in YNB *vs.* YPD medium	S5C & D
M7	12	9151	3	0.986	0.961	Centre	F2 in YNB *vs.* YPD medium	S5C & D
M8	11	9151	3	0.848	0.545	Pareto	F0 in YNB *vs.* YPD medium	S5E & F
M9	11	9151	2	0.838	0.567	Centre	F0 in YNB *vs.* YPD medium	S5E & F

N= number of samples, k= number of x-variables (buckets), A= number of principal components in the model, R^2X=sum of squares of all x-variables explained by the model, Q^2= cumulative cross-validated R^2.