

Table S3. Study 1: Misclassification rate of PLS with 1 to 10 latent components to classify Study 1 samples based on leave-one-out cross validation, R_2 , Q_2 and percent of variance explained for 1 to 10 latent components.

Number of Latent Components	1	2	3	4	5	6	7	8	9	10
(A) Adjusted for sex and age										
Misclassification Rate	47.4%	36.8%	47.4%	47.4%	52.6%	50.0%	52.6%	52.6%	52.6%	52.6%
Sensitivity	55.6%	66.7%	55.6%	55.6%	55.6%	55.6%	50.0%	55.6%	50.0%	50.0%
Specificity	50.0%	60.0%	50.0%	50.0%	40.0%	45.0%	45.0%	40.0%	45.0%	45.0%
R_2	64.6%	88.7%	93.8%	97.9%	99.4%	99.8%	99.9%	100.0	100.0	100.0
Q_2	-0.213	-0.188	-0.358	-0.295	-0.264	-0.268	-0.253	-0.245	-0.239	-0.236
% of Variance explained by components	5.46%	9.75%	19.6%	23.8%	27.9%	31.9%	35.2%	39.6%	44.2%	47.3%
(B) Not Adjusted for sex and age										
Misclassification Rate	57.9%	42.1%	42.1%	39.5%	42.1%	39.5%	39.5%	39.5%	42.1%	42.1%
Sensitivity	33.3%	50.0%	50.0%	44.4%	50.0%	50.0%	50.0%	50.0%	50.0%	50.0%
Specificity	50.0%	65.0%	65.0%	75.0%	65.0%	70.0%	70.0%	70.0%	65.0%	65.0%
R_2	0.702	0.867	0.956	0.986	0.995	0.999	1.00	1.00	1.00	1.00
Q_2	-0.288	-0.143	-0.096	-0.077	-0.089	-0.087	-0.095	-0.099	-0.102	-0.102
% of Variance explained by components	5.14%	13.9%	20.7%	25.3%	29.5%	32.7%	36.5%	40.4%	44.5%	47.8%

Table S4. Misclassification rate of PLS with 1 to 10 latent components to classify Study 2 samples based on leave-one-out cross validation, R_2 , Q_2 and percent of variance explained for 1 to 10 latent components.

Number of Latent Components	1	2	3	4	5	6	7	8	9	10
(A) Metabolite intensities were adjusted for sex or age										
Misclassification Rate	40.9%	31.8%	40.9%	45.4%	50.0%	54.5%	54.5%	54.5%	54.5%	54.5%
Sensitivity	54.5%	63.6%	54.5%	54.5%	54.5%	54.5%	54.5%	54.5%	54.5%	54.5%
Specificity	63.6%	72.7%	63.6%	54.5%	45.5%	36.3%	36.3%	36.3%	36.3%	36.3%
R_2	87.5%	95.9%	98.4%	99.7%	100.0%	100.0%	100.0%	100.0%	100.0%	100.0%
Q_2	0.250	0.604	0.581	0.583	0.585	0.586	0.586	0.587	0.587	0.587
% X Variance	7.93%	19.5%	45.1%	49.3%	53.3%	57.5%	61.5%	65.0%	68.4%	71.5%
(B) Metabolite intensities were not adjusted for sex or age										
Misclassification Rate	57.9%	42.1%	42.1%	39.5%	42.1%	39.5%	39.5%	39.5%	42.1%	42.1%
Sensitivity	33.3%	50.0%	50.0%	44.4%	50.0%	50.0%	50.0%	50.0%	50.0%	50.0%
Specificity	50.0%	65.0%	65.0%	75.0%	65.0%	70.0%	70.0%	70.0%	65.0%	65.0%
R_2	0.702	0.867	0.956	0.986	0.995	0.999	1.00	1.00	1.00	1.00
Q_2	-0.288	-0.143	-0.096	-0.077	-0.089	-0.087	-0.095	-0.099	-0.102	-0.102
% X Variance	5.14%	13.9%	20.7%	25.3%	29.5%	32.7%	36.5%	40.4%	44.5%	47.8%