

S4 Table.

LV	R ² Y(cum)(%)	Q ² Y(cum)(%)
t1	28.54	25.25
t2	51.20	44.25
t3	74.28	62.19
t4	78.24	63.68
t5	81.83	65.62
t6	87.21	71.55
t7	88.52	72.64
t8	90.09	74.16
t9	91.09	74.88
t10	92.29	69.09

R²Y(cum): cumulative explained variation of the class response (Y) explained by each latent variables (LV) in %, Q²Y(cum): cumulative predicted variation (cross-validated) in %.