

S3 Table.

N. dataset	R ² X(cum)(%)	R ² Y(cum)(%)	Q ² Y(cum)(%)	LV
1	71.31	73.39	55.90	3
2	70.24	74.55	53.15	3
3	69.27	72.66	61.85	3
4	69.35	72.49	59.91	3
5	73.60	73.81	59.29	3
6	72.40	74.25	55.29	3
7	69.78	73.81	62.20	3
8	71.51	73.03	62.48	3
9	74.55	73.92	61.40	3
10	70.87	72.92	50.83	3
11	64.16	62.87	55.53	2
12	72.08	72.98	63.40	3
13	70.64	74.26	56.85	3
14	70.89	74.34	58.23	3
15	71.45	73.76	61.40	3
16	62.76	61.72	53.31	2
17	70.71	72.53	55.30	3
18	68.62	74.28	62.19	3
19	69.41	74.14	58.70	3
20	70.90	74.46	58.23	3
21	69.55	74.02	54.89	3
22	65.23	62.23	55.92	2
23	70.07	71.02	62.23	3
24	69.63	73.95	56.86	3
25	69.45	74.86	64.47	3
26	68.52	71.75	59.43	3
27	69.92	74.64	59.25	3
28	70.47	73.33	58.48	3
29	69.07	75.83	60.18	3
30	70.06	73.08	56.47	3
31	71.67	72.34	60.09	3
32	71.01	72.77	59.69	3
33	68.50	71.40	56.80	3
34	69.60	74.82	64.57	3
35	72.02	74.16	63.22	3
36	70.36	71.52	61.09	3
37	68.76	75.54	61.72	3
38	70.86	73.45	58.62	3
39	67.62	72.89	61.23	3
40	70.12	71.89	55.37	3
41	63.50	63.84	61.26	2
42	73.99	74.04	55.87	3
43	72.94	73.52	59.48	3
44	69.97	75.14	64.40	3
45	68.83	72.68	59.67	3
46	71.33	74.68	59.77	3
47	71.16	72.19	59.05	3
48	68.88	74.49	58.81	3
49	70.57	74.31	47.62	3
50	71.29	70.71	58.49	3

R²X, R²Y: fraction of the variance of descriptor matrix (X) and class response (Y) explained by each latent variables (LV) in %, Q²Y: fraction of the variance predicted (cross-validated) in %; R²X(cum), R²Y(cum): cumulative explained variation and Q²Y(cum) predicted variation in %.