pR2Y = 0.05, pQ2 = 0.05

Similarity($\mathbf{y}$, $\mathbf{y_{perm}}$)

Q2Y

R2Y

Observation diagnostics

Orthogonal distance (OD)

Score distance (SD)

Scores (PLS−DA)

pre
8
6
4
2
10

t2 (11%)

t1 (15%)

R2X	R2Y	Q2Y		RMSEE	pre
0.262	0.234	0		0.341	2

pR2Y = 0.25, pQ2 = 0.2

Similarity($\mathbf{y}$, $\mathbf{y_{perm}}$)

Q2Y
R2Y

Observation diagnostics

Orthogonal distance (OD)

Score distance (SD)

Scores (OPLS−DA)

to1

R2X	R2Y	Q2Y		RMSEE	pre	ort
0.219	0.597	−0.182	**t1 (9%)**	0.332	1	1

Scores (OPLS–DA)

R2X	R2Y	Q2Y	**t1 (9%)**	RMSEE	pre	ort
0.219	0.597	−0.182		0.332	1	1