Features for level k1 versus other

Scores (OPLS–DA)

R2X	R2Y	Q2Y		RMSEE	pre	ort
0.547	0.547	0.45	**t1 (18%)**	0.229	1	1

Model overview

k1 versus other

Features influencing orthogonal projection for k1 versus other

Features for level k2 versus other

k2

other

correlation(feature,t1)

relative covariance(feature,t1)

Scores (OPLS−DA)

other

k2

to1

t1 (21%)

R2X	R2Y	Q2Y		RMSEE	pre	ort
0.375	0.831	0.76		0.196	1	1

Model overview

R2Y

Q2Y

p1

o1

k2 versus other

Features influencing orthogonal projection for k2 versus other

correlation(feature,to1)

relative covariance(feature,to1)

Features for level k3 versus other

correlation(feature,t1)

relative covariance(feature,t1)

k3

other

Scores (OPLS−DA)

other

k3

to1

t1 (20%)

R2X	R2Y	Q2Y		RMSEE	pre	ort
0.564	0.634	0.569		0.307	1	1

Model overview

R2Y

Q2Y

p1

o1

k3 versus other

Features influencing orthogonal projection for k3 versus other

correlation(feature,to1)

relative covariance(feature,to1)

Features for level k4 versus other

correlation(feature,t1)

k4

other

relative covariance(feature,t1)

Scores (OPLS−DA)

other

k4

R12S228

R12S92   R12S227

R12S31   R12S139

R12S32

R12S94

to1

R2X	R2Y	Q2Y		RMSEE	pre	ort
0.584	0.915	0.892	**t1 (39%)**	0.083	1	1

Model overview

R2Y Q2Y

p1   o1

k4 versus other

Features influencing orthogonal projection for k4 versus other

correlation(feature,to1)

relative covariance(feature,to1)

Features for level k1 versus k2

correlation(feature,t1)

k1

k2

relative covariance(feature,t1)

Scores (OPLS−DA)

k2

k1

to1

R12S117

R12S135 R12S161
R12S145
R12S209
R12S107 R12S166
R12S84 R12S156
R12S86 R12S211 R12S154
R12S14
R12S28 R12S218 R12S110
R12S87
R12S180 R12S196
R12S332 R12S212 R12S167
R12S205 R12S189
R12S224
R12S133
R12S217
R12S183
R12S1
R12S15

R2X	R2Y	Q2Y		RMSEE	pre	ort
0.572	0.879	0.805	**t1 (44%)**	0.163	1	1

Model overview

R2Y Q2Y

p1   o1

k1 versus k2

Features influencing orthogonal projection for k1 versus k2

correlation(feature,to1)

relative covariance(feature,to1)

Features for level k1 versus k3

k1

k3

correlation(feature,t1)

relative covariance(feature,t1)

Scores (OPLS–DA)

k3

k1

to1

t1 (23%)

R2X	R2Y	Q2Y		RMSEE	pre	ort
0.401	0.721	0.607		0.224	1	1

Model overview

R2Y Q2Y

p1

o1

k1 versus k3

Features influencing orthogonal projection for k1 versus k3

correlation(feature,to1)

relative covariance(feature,to1)

Features for level k1 versus k4

correlation(feature,t1)

k1

k4

relative covariance(feature,t1)

Scores (OPLS−DA)

k4

k1

to1

R12S94

R12S31

R12S32

R12S92

R12S228

R12S162
R12S138
R12S227

R2X	R2Y	Q2Y		RMSEE	pre	ort
0.747	0.97	0.941	**t1 (61%)**	0.092	1	1

Model overview

R2Y Q2Y

p1

o1

k1 versus k4

Features influencing orthogonal projection for k1 versus k4

correlation(feature,to1)

relative covariance(feature,to1)

Features for level k2 versus k3

correlation(feature,t1)

k2

k3

relative covariance(feature,t1)

Scores (OPLS−DA)

k3

k2

to1

t1 (38%)

R2X	R2Y	Q2Y		RMSEE	pre	ort
0.524	0.9	0.874		0.159	1	1

Model overview

R2Y Q2Y

p1

o1

k2 versus k3

Features influencing orthogonal projection for k2 versus k3

correlation(feature,to1)

relative covariance(feature,to1)

Features for level k2 versus k4

correlation(feature,t1)

relative covariance(feature,t1)

k2

k4

Scores (OPLS−DA)

to1

k4

k2

R12S94

R12S115

R12S31

R12S32

R12S92

R12S188 R12S139

R12S228

R12S227

R2X	R2Y	Q2Y		RMSEE	pre	ort
0.669	0.943	0.926	**t1 (56%)**	0.102	1	1

Model overview

R2Y

Q2Y

p1

o1

k2 versus k4

Features influencing orthogonal projection for k2 versus k4

correlation(feature,to1)

relative covariance(feature,to1)

Features for level k3 versus k4

Scores (OPLS−DA)

R2X	R2Y	Q2Y		RMSEE	pre	ort
0.68	0.968	0.95	**t1 (56%)**	0.067	1	1

Model overview

k3 versus k4

Features influencing orthogonal projection for k3 versus k4