Features for level k1 versus other

correlation(feature,t1)

1.0
0.5
0.0
-0.5
-1.0

k1

other

relative covariance(feature,t1)

-1.0   -0.5   0.0   0.5   1.0

Scores (OPLS−DA)

other
k1

to1

40000
20000
0
-20000
-40000

R12S94
R12S31
R12S228
R12S92
R12S32
R12S227
R12S139
R12S162
R12S117
R12S18
R12S145
R1xS1

−20000 −10000   0   10000 20000

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

Model overview

0.35
0.30
0.25
0.20
0.15
0.10
0.05
0.00

R2Y   Q2Y

p1   o1

k1 versus other

Features influencing orthogonal projection for k1 versus other

correlation(feature,to1)

1.0
0.5
0.0
-0.5
-1.0

-1.0   -0.5   0.0   0.5   1.0

relative covariance(feature,to1)

Features for level k2 versus other

correlation(feature,t1)

k2

other

relative covariance(feature,t1)

Scores (OPLS−DA)

other

k2

to1

R12S94

R12S31

R12S1

R12S32

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

R2X   R2Y   Q2Y   RMSEE pre ort
0.564 0.634 0.569   **t1 (20%)**   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)

to1

other

k4

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
R12S107   R12S209
R12S84   R12S266
R12S86   R12S211   R12S156
R12S14   R12S154
R12S28   R12S218   R12S110
R12S87   R12S196
R12S180   R12S142
R12S332   R12S212   R12S221
R12S205   R12S167   R12S138
R12S210
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

correlation(feature,t1)

k1   k3

relative covariance(feature,t1)

Scores (OPLS–DA)

k3
k1

to1

R2X	R2Y	Q2Y		RMSEE	pre	ort
0.401	0.721	0.607	**t1 (23%)**	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)

relative covariance(feature,t1)

k1 k4

Scores (OPLS−DA)

to1

k4
k1

R12S94
R12S31
R12S32
R12S92
R12S228
R12S162
R12S133
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

Scores (OPLS−DA)

R2X	R2Y	Q2Y		RMSEE	pre	ort
0.524	0.9	0.874	**t1 (38%)**	0.159	1	1

Model overview

k2 versus k3

Features influencing orthogonal projection for k2 versus k3

Features for level k3 versus k4

correlation(feature,t1)

k3

k4

relative covariance(feature,t1)

Scores (OPLS−DA)

k4

k3

to1

R12S94

R12S31

R12S32

R12S99

R12S228

R12S162

R12S139

R12S227

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

Model overview

R2Y

Q2Y

p1

o1

k3 versus k4

Features influencing orthogonal projection for k3 versus k4

correlation(feature,to1)

relative covariance(feature,to1)