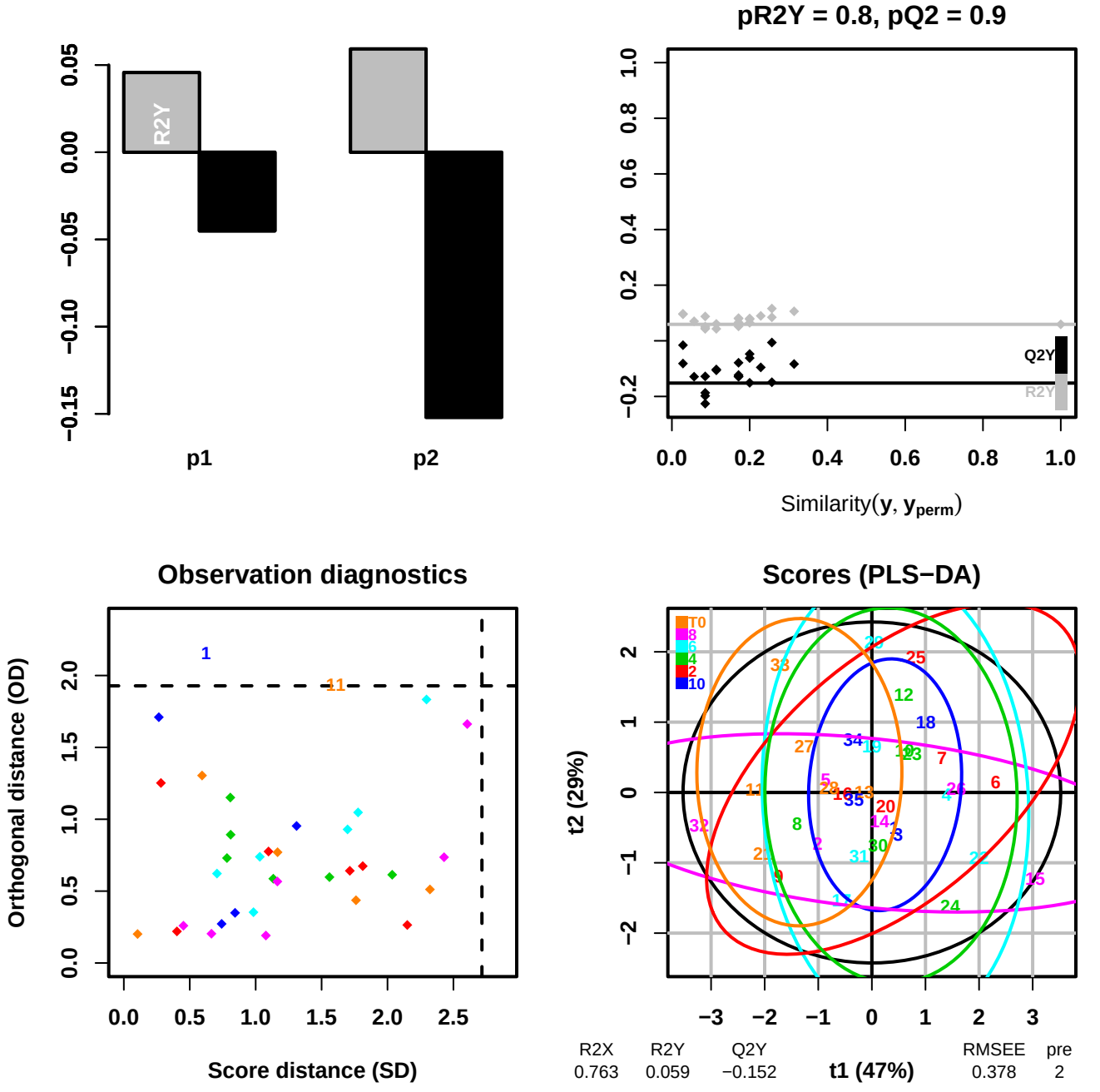
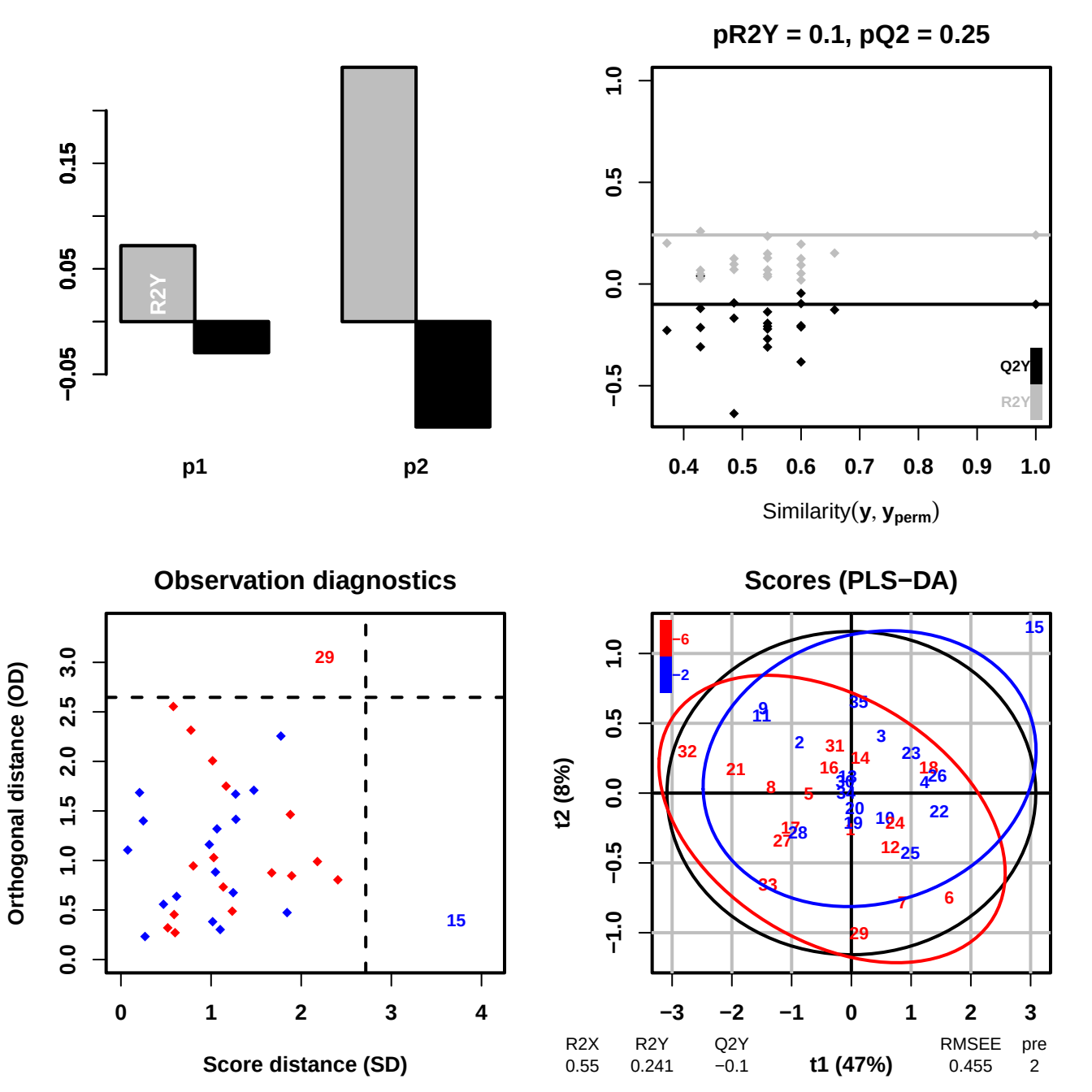
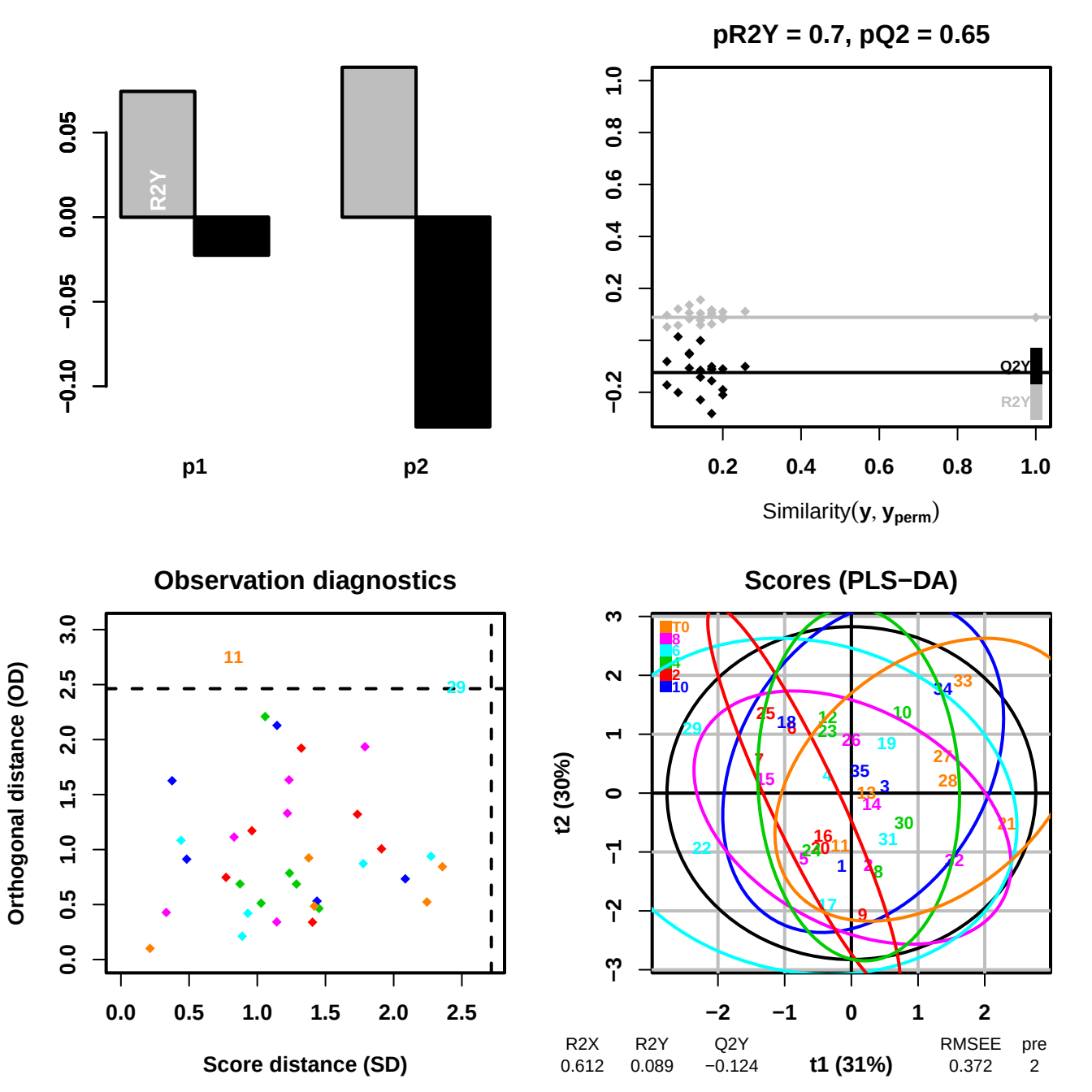
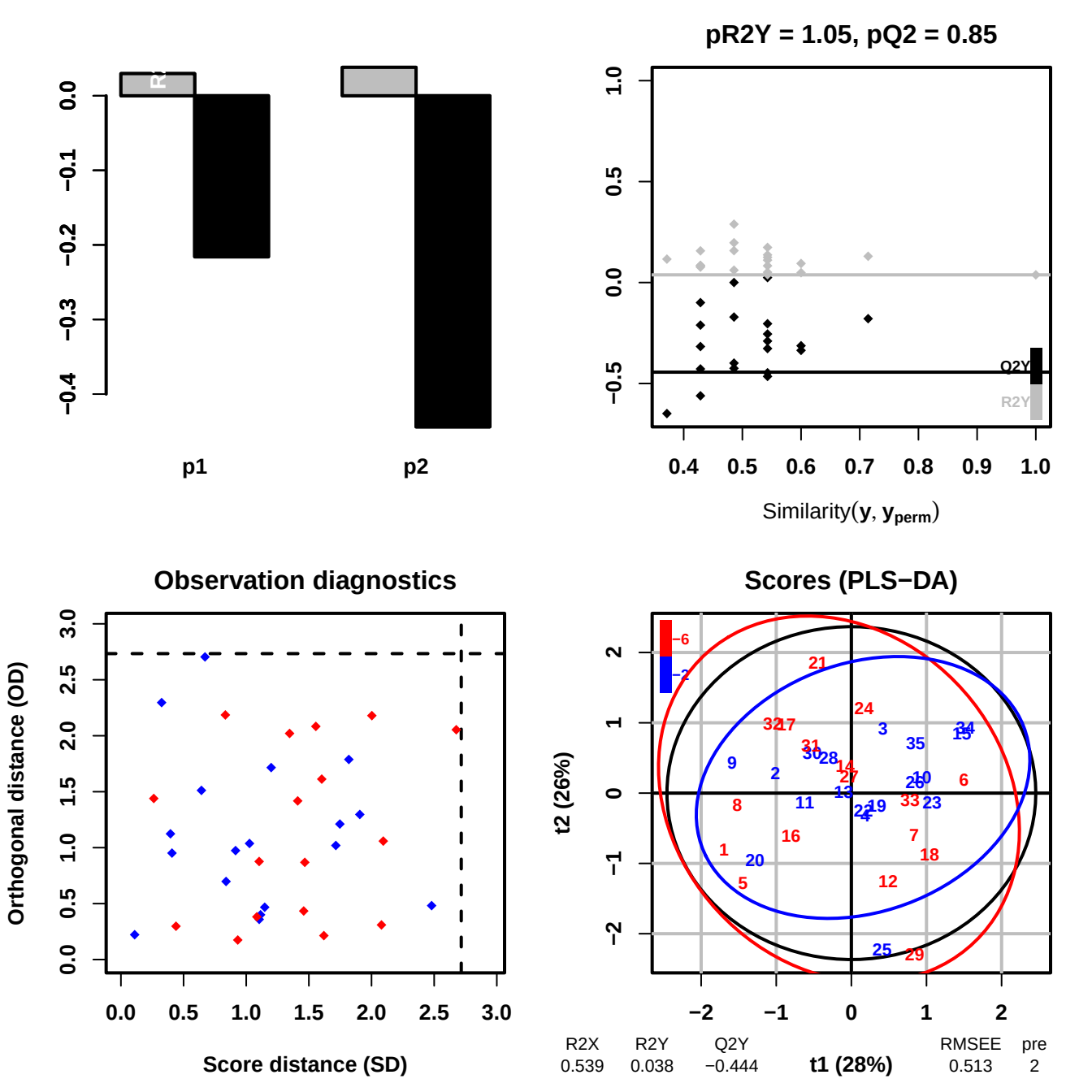
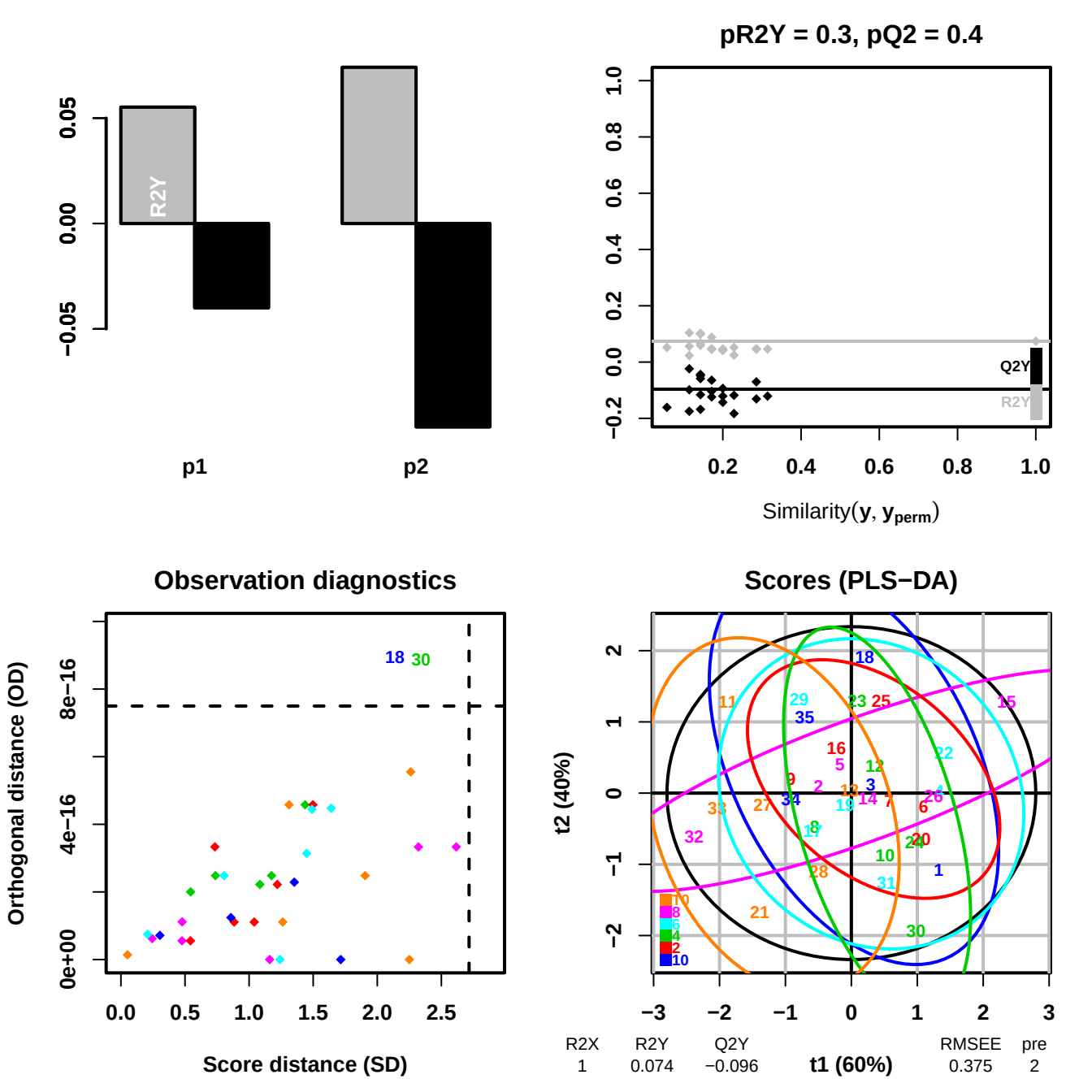
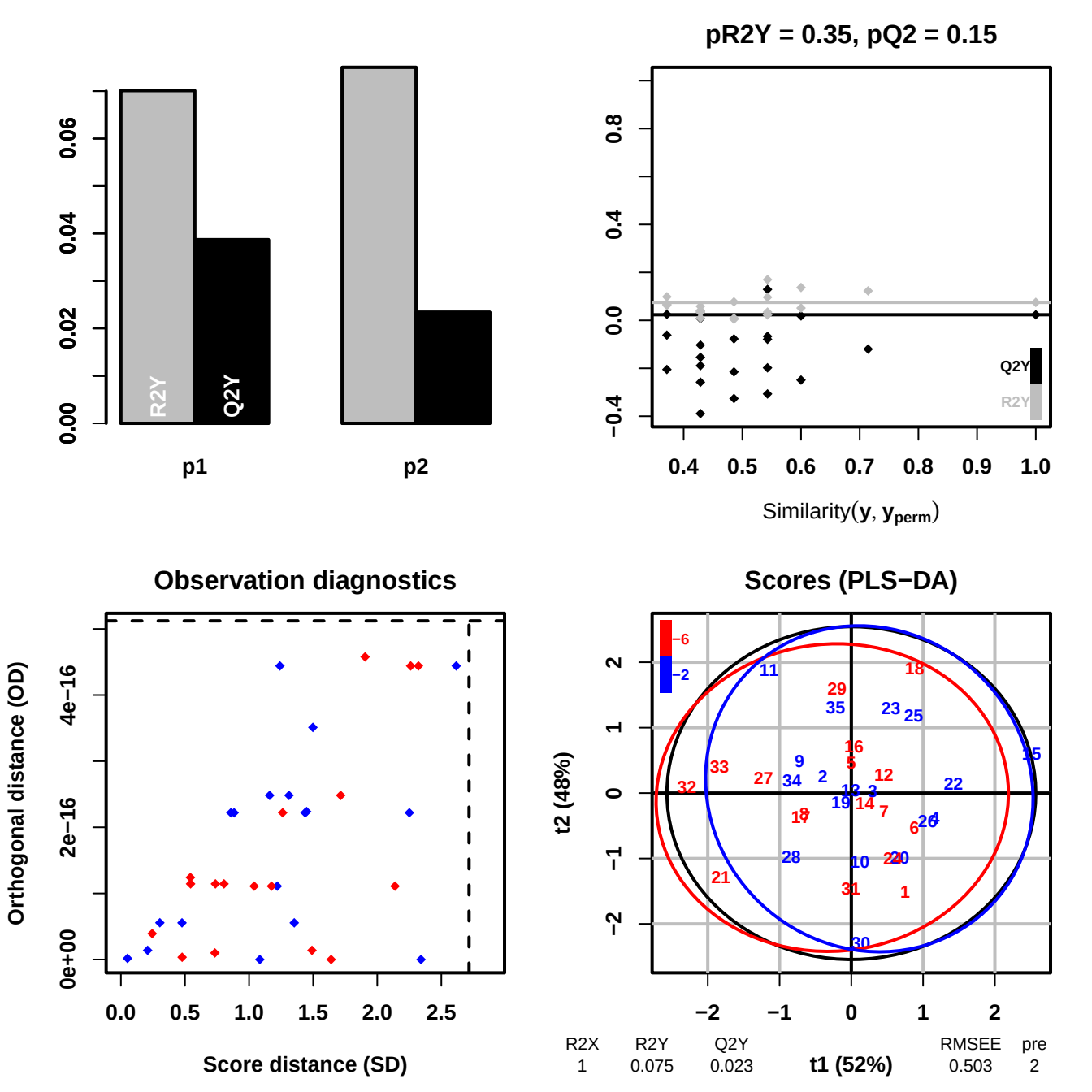

R2Y
p1
p2
pR2Y = 0.8, pQ2 = 0.9
Q2Y
R2Y
Similarity(y, y_perm)
Observation diagnostics
Orthogonal distance (OD)
Score distance (SD)
Scores (PLS−DA)
t2 (29%)
t1 (47%)
T0
8
6
4
2
10
R2X
0.763
R2Y
0.059
Q2Y
−0.152
RMSEE
0.378
pre
2


R2Y
0.15
0.05
−0.05
p1
p2
pR2Y = 0.1, pQ2 = 0.25
1.0
0.5
0.0
−0.5
Q2Y
R2Y
0.4
0.5
0.6
0.7
0.8
0.9
1.0
Similarity(y, y_perm)
Observation diagnostics
Orthogonal distance (OD)
Score distance (SD)
Scores (PLS−DA)
t2 (8%)
t1 (47%)
R2X
0.55
R2Y
0.241
Q2Y
−0.1
RMSEE
0.455
pre
2


R2Y
0.05
0.00
−0.05
−0.10
p1
p2
pR2Y = 0.7, pQ2 = 0.65
1.0
0.8
0.6
0.4
0.2
−0.2
Q2Y
R2Y
0.2
0.4
0.6
0.8
1.0
Similarity(y, y_perm)
Observation diagnostics
Orthogonal distance (OD)
Score distance (SD)
Scores (PLS−DA)
t2 (30%)
t1 (31%)
T0
8
6
4
2
10
R2X 0.612
R2Y 0.089
Q2Y −0.124
RMSEE 0.372
pre 2


R2
0.0
−0.1
−0.2
−0.3
−0.4
p1
p2
pR2Y = 1.05, pQ2 = 0.85
1.0
0.5
0.0
−0.5
Q2Y
R2Y
0.4
0.5
0.6
0.7
0.8
0.9
1.0
Similarity(y, y_perm)
Observation diagnostics
Orthogonal distance (OD)
Score distance (SD)
Scores (PLS−DA)
t2 (26%)
t1 (28%)
−6
−2
R2X
0.539
R2Y
0.038
Q2Y
−0.444
RMSEE
0.513
pre
2


R2Y
0.05
0.00
−0.05
p1
p2
pR2Y = 0.3, pQ2 = 0.4
Q2Y
R2Y
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
0.2
0.4
0.6
0.8
1.0
Similarity(y, y_perm)
Observation diagnostics
Orthogonal distance (OD)
8e−16
4e−16
0e+00
0.0
0.5
1.0
1.5
2.0
2.5
Score distance (SD)
Scores (PLS−DA)
t2 (40%)
t1 (60%)
−3
−2
−1
0
1
2
3
R2X
1
R2Y
0.074
Q2Y
−0.096
RMSEE
0.375
pre
2


pR2Y = 0.35, pQ2 = 0.15
R2Y
Q2Y
p1
p2
Similarity(y, y_perm)
Observation diagnostics
Orthogonal distance (OD)
Score distance (SD)
Scores (PLS−DA)
t2 (48%)
t1 (52%)
R2X 1
R2Y 0.075
Q2Y 0.023
RMSEE 0.503
pre 2