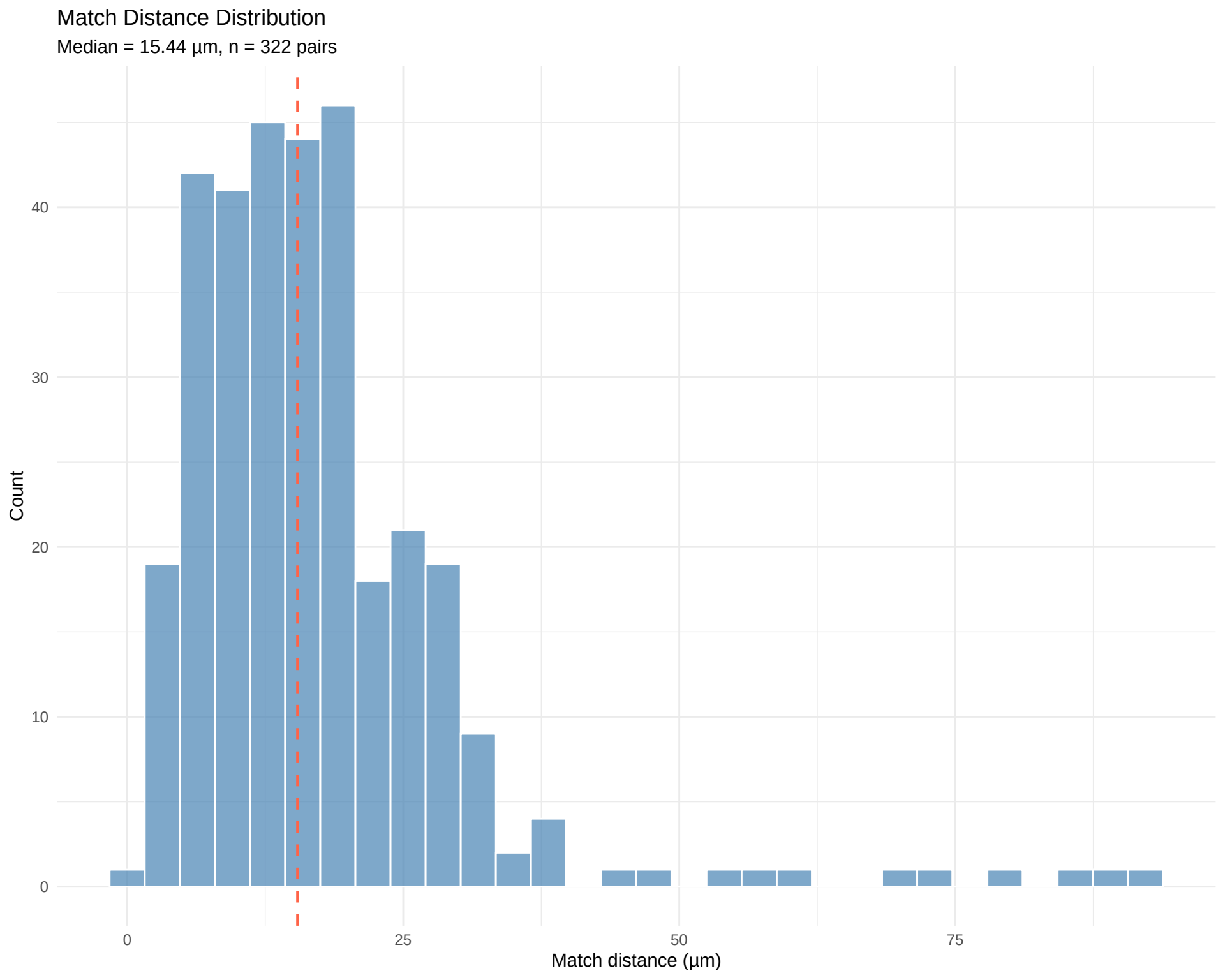
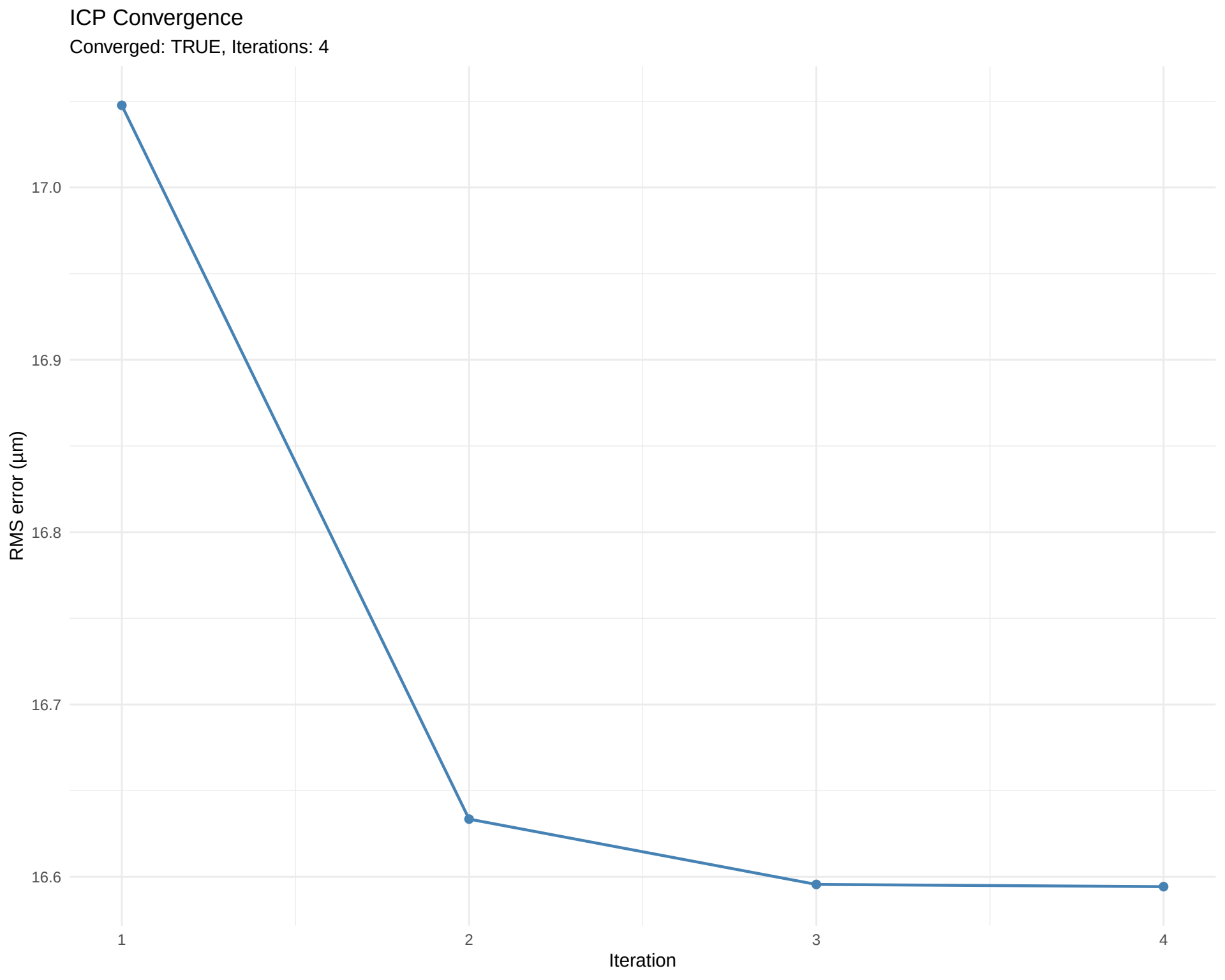
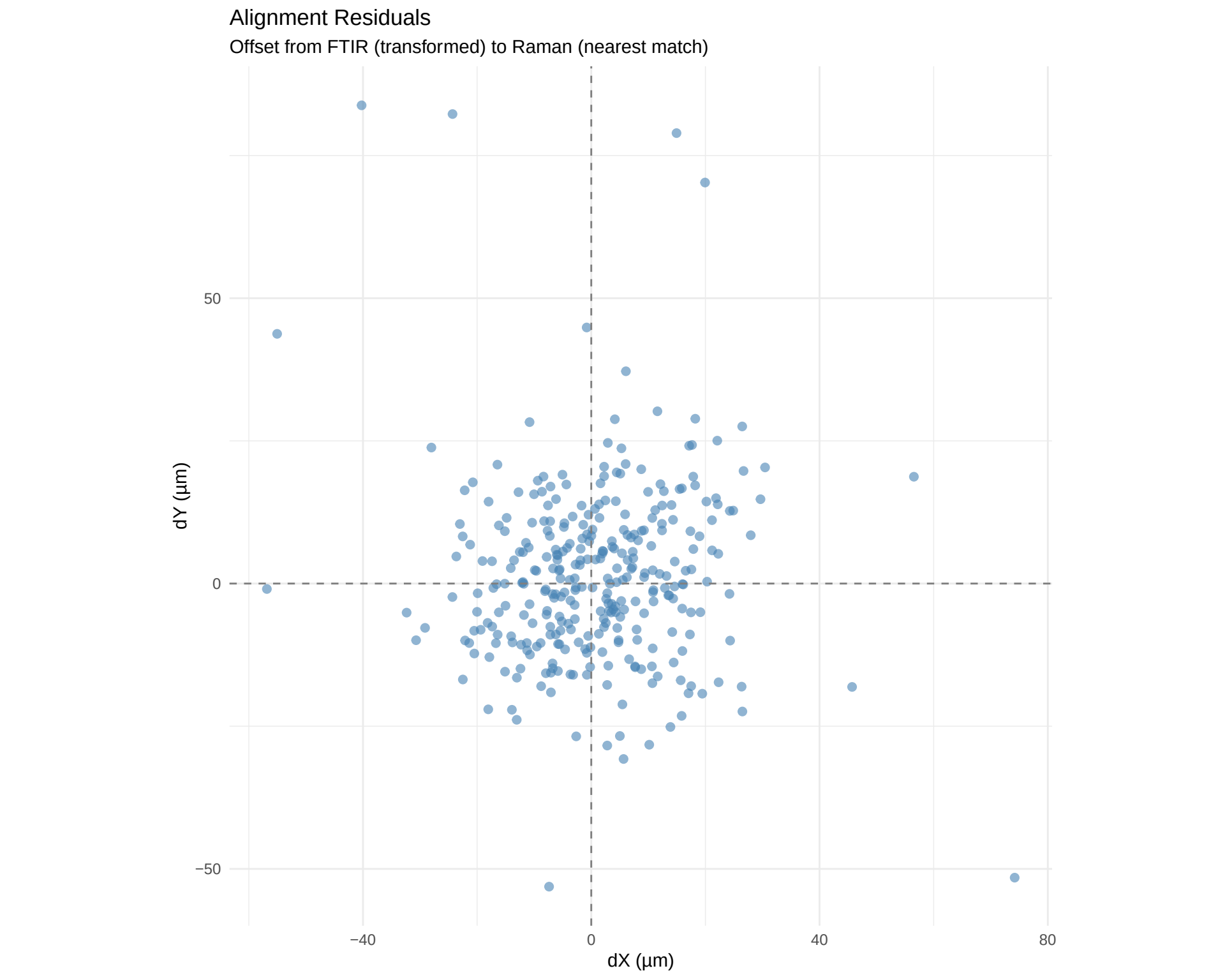
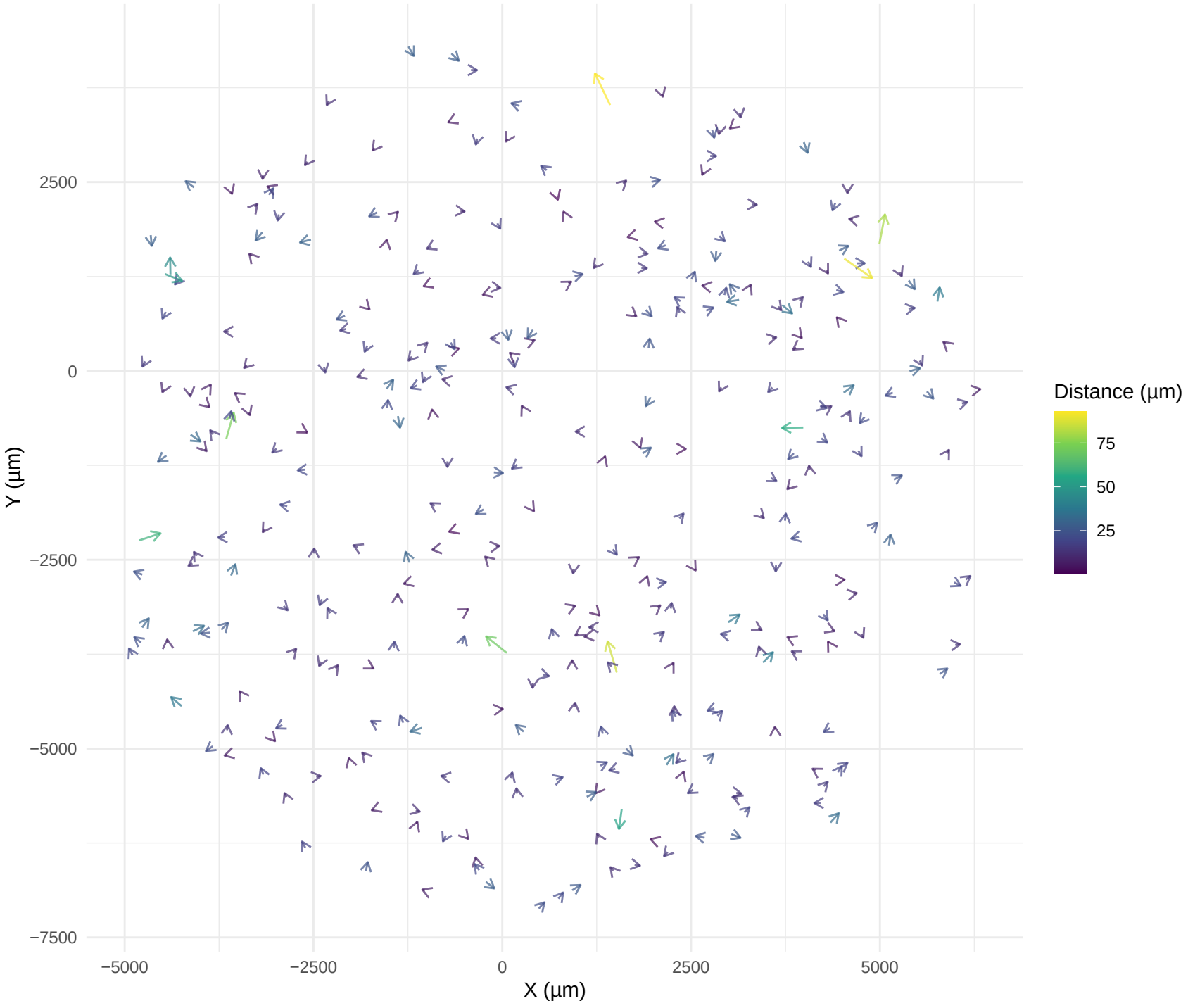
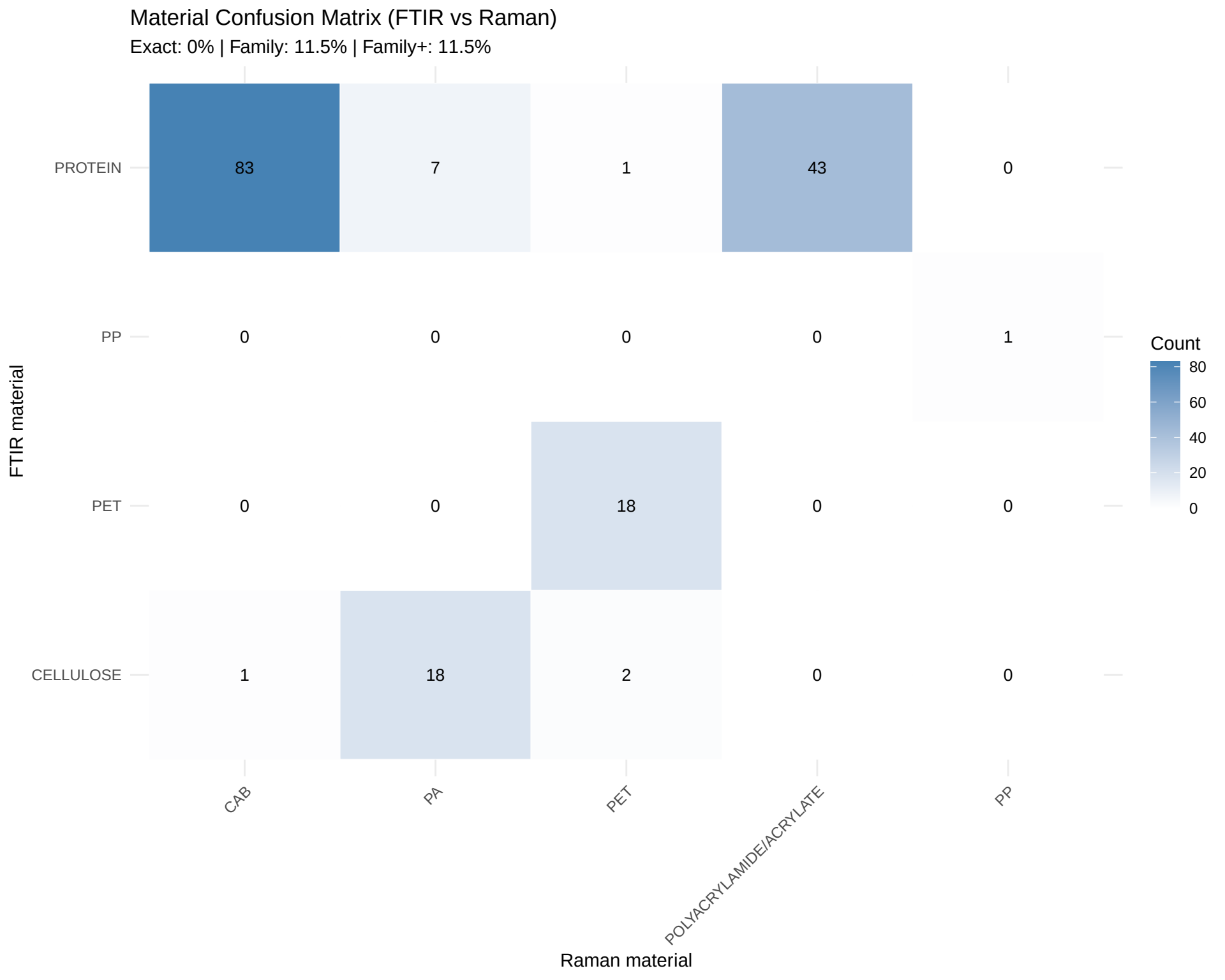
FTIR...Raman Particle Overlay (aligned coordinates)
Red triangles = FTIR, Blue circles = Raman, Lines = matched pairs
5000
2500
0
−2500
−5000
−7500
Y (µm, normalized)
−6000
−3000
0
3000
6000
X (µm, normalized)

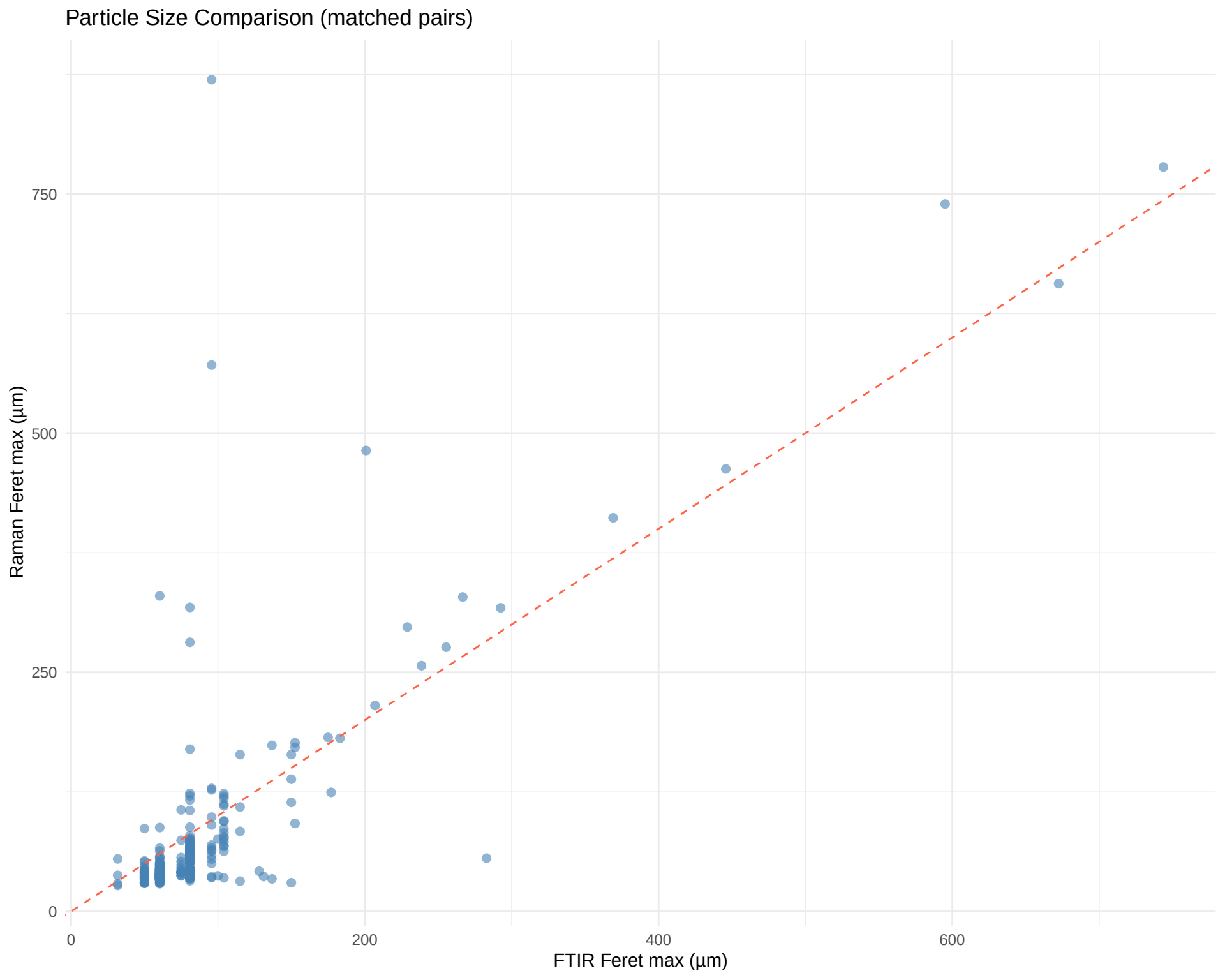

Match Distance Distribution
Median = 15.44 µm, n = 322 pairs
Count
0
10
20
30
40
0
25
50
75
Match distance (µm)

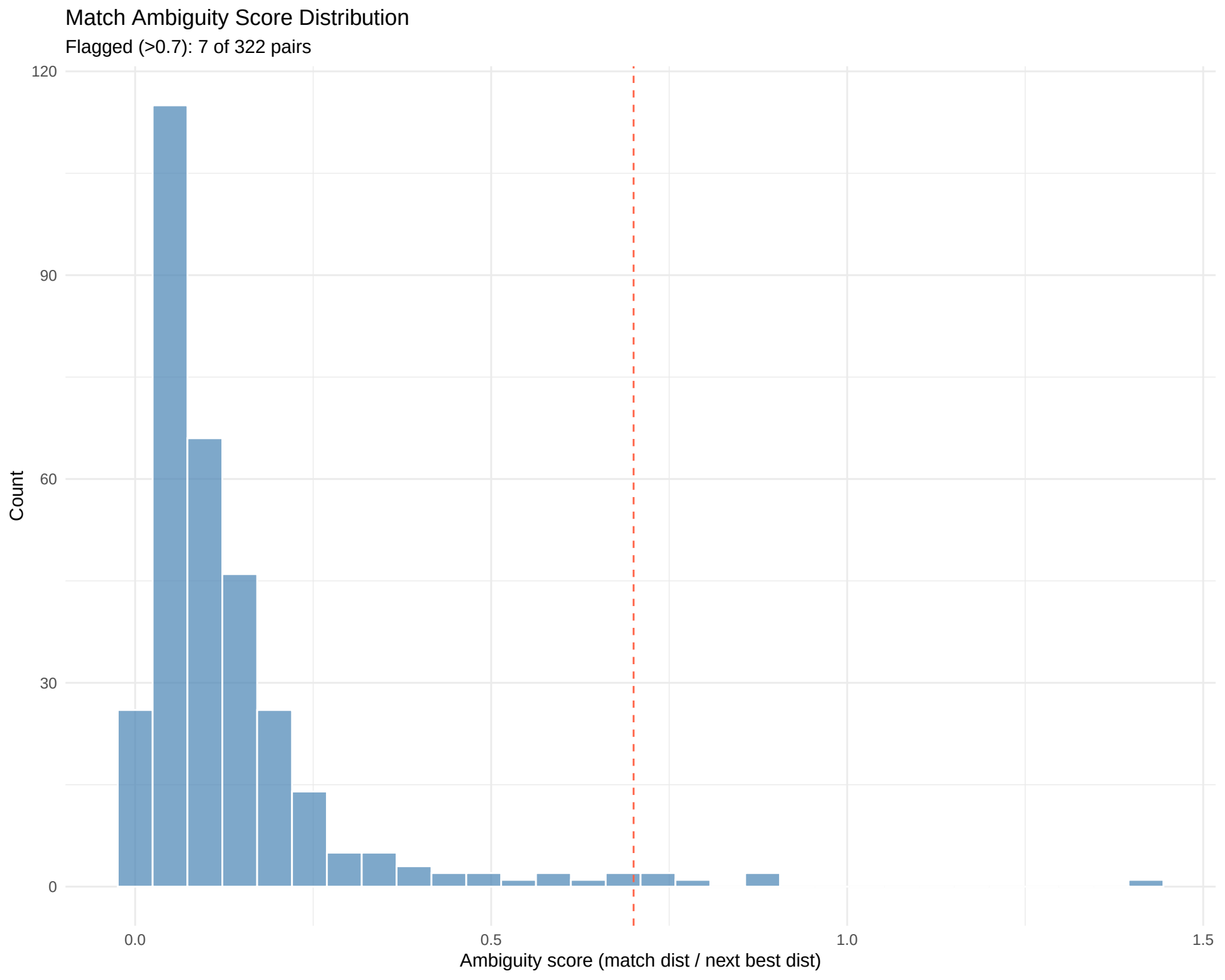

ICP Convergence
Converged: TRUE, Iterations: 4
RMS error (µm)
17.0
16.9
16.8
16.7
16.6
1
2
3
4
Iteration

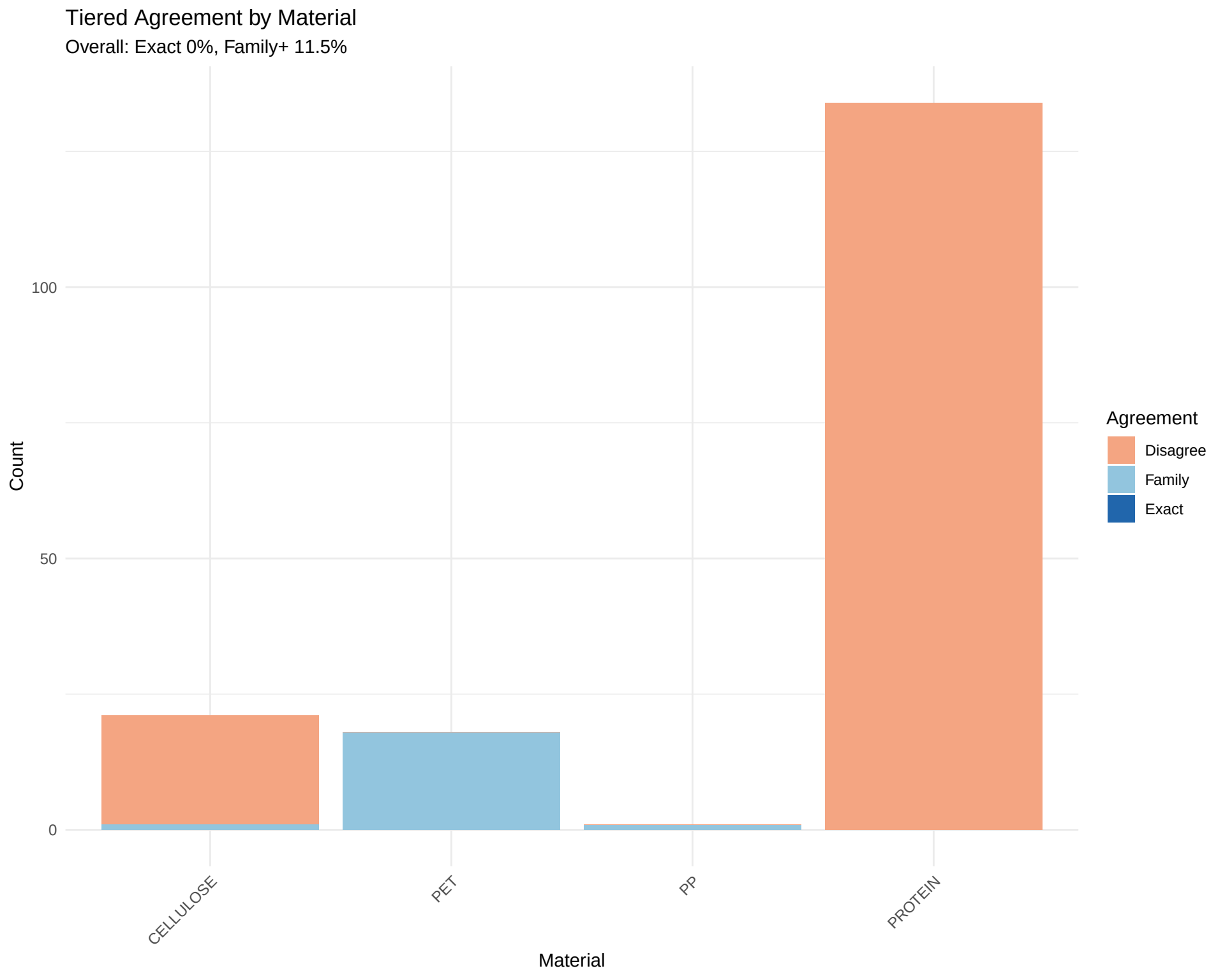

Alignment Residuals
Offset from FTIR (transformed) to Raman (nearest match)
50
0
−50
dY (µm)
−40
0
40
80
dX (µm)

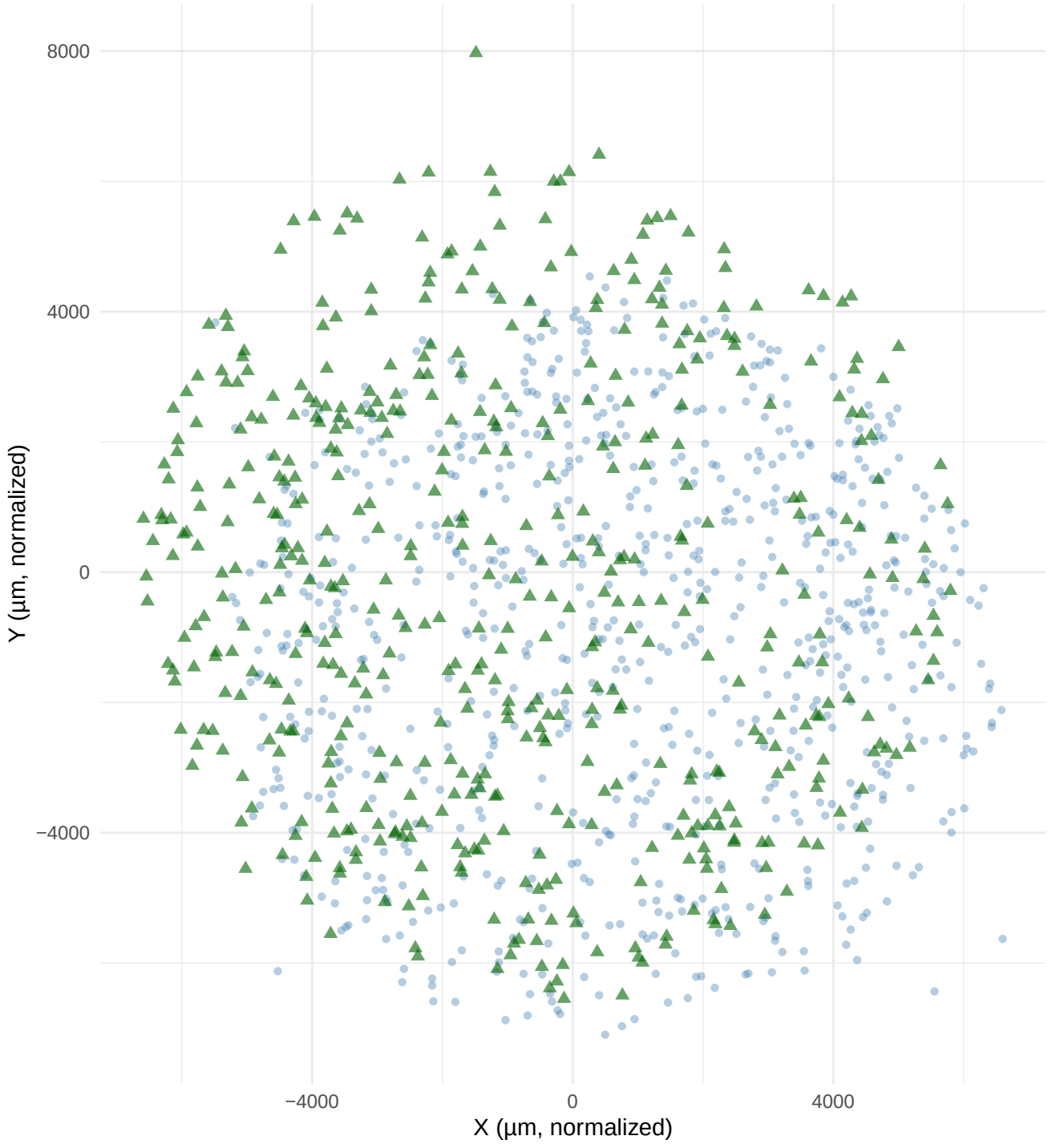

Residual Vector Field
Arrows magnified 5x | Systematic patterns indicate local distortion
2500
0
−2500
−5000
−7500
Y (µm)
−5000
−2500
0
2500
5000
X (µm)
Distance (µm)
75
50
25

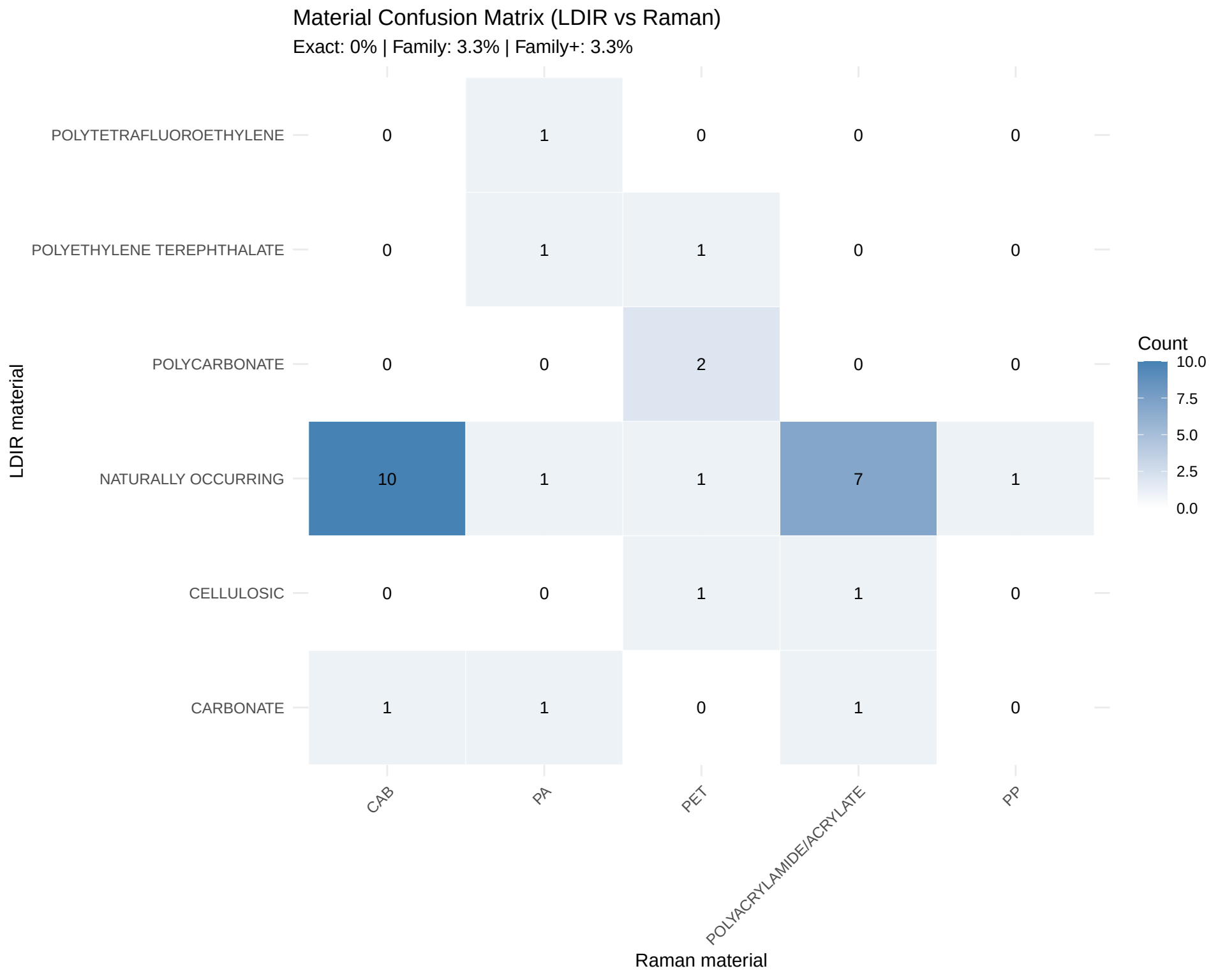

Material Confusion Matrix (FTIR vs Raman)
Exact: 0% | Family: 11.5% | Family+: 11.5%
FTIR material
PROTEIN
PP
PET
CELLULOSE
83
7
1
43
0
0
0
0
0
1
0
0
18
0
0
1
18
2
0
0
CAB
PA
PET
POLYACRYLAMIDE/ACRYLATE
PP
Raman material
Count
80
60
40
20
0


Particle Size Comparison (matched pairs)
Raman Feret max (µm)
FTIR Feret max (µm)
0
250
500
750
0
200
400
600


Match Ambiguity Score Distribution
Flagged (>0.7): 7 of 322 pairs
120
90
60
30
0
Count
0.0
0.5
1.0
1.5
Ambiguity score (match dist / next best dist)


Tiered Agreement by Material
Overall: Exact 0%, Family+ 11.5%
Count
100
50
0
CELLULOSE
PET
PP
PROTEIN
Material
Agreement
Disagree
Family
Exact


LDIR...Raman Particle Overlay (aligned coordinates)
Green triangles = LDIR, Blue circles = Raman
8000
4000
0
−4000
Y (µm, normalized)
−4000
0
4000
X (µm, normalized)


Material Confusion Matrix (LDIR vs Raman)
Exact: 0% | Family: 3.3% | Family+: 3.3%
LDIR material
POLYTETRAFLUOROETHYLENE
POLYETHYLENE TEREPHTHALATE
POLYCARBONATE
NATURALLY OCCURRING
CELLULOSIC
CARBONATE
0 1 0 0 0
0 1 1 0 0
0 0 2 0 0
10 1 1 7 1
0 0 1 1 0
1 1 0 1 0
CAB
PA
PET
POLYACRYLAMIDE/ACRYLATE
PP
Raman material
Count
10.0
7.5
5.0
2.5
0.0