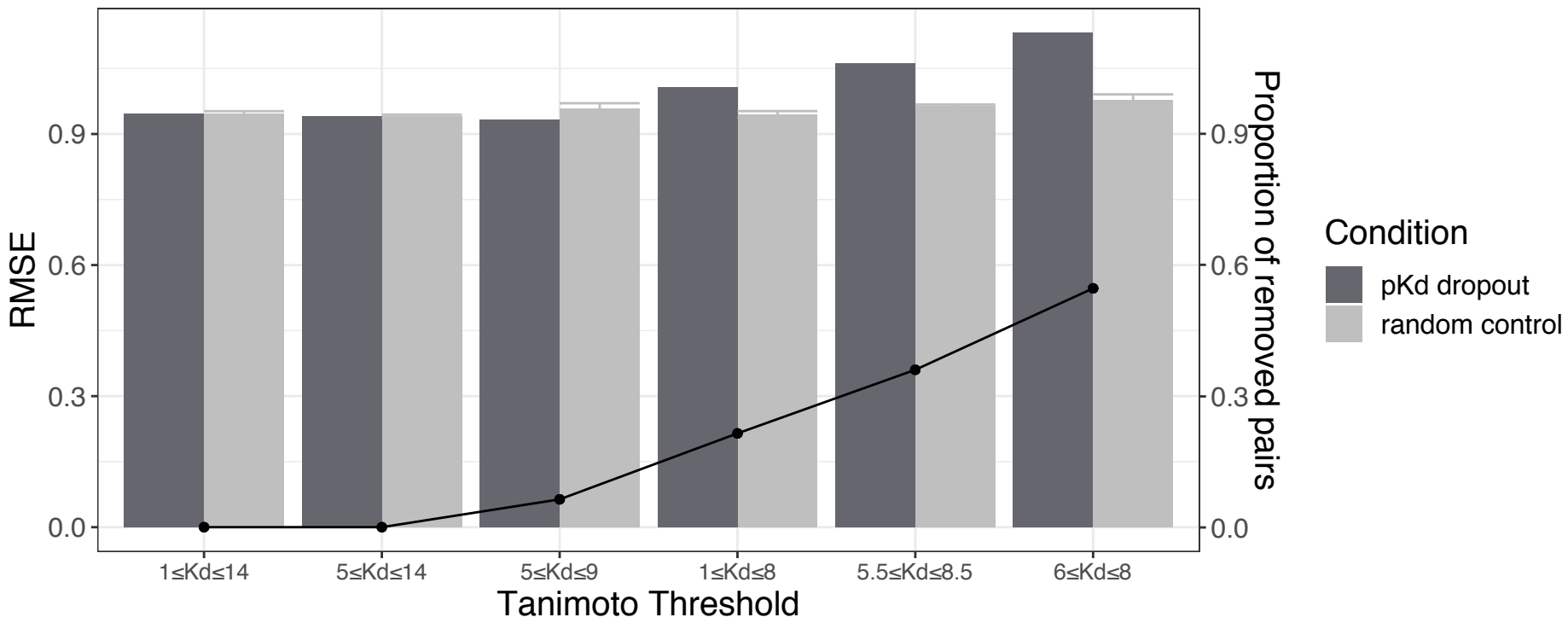
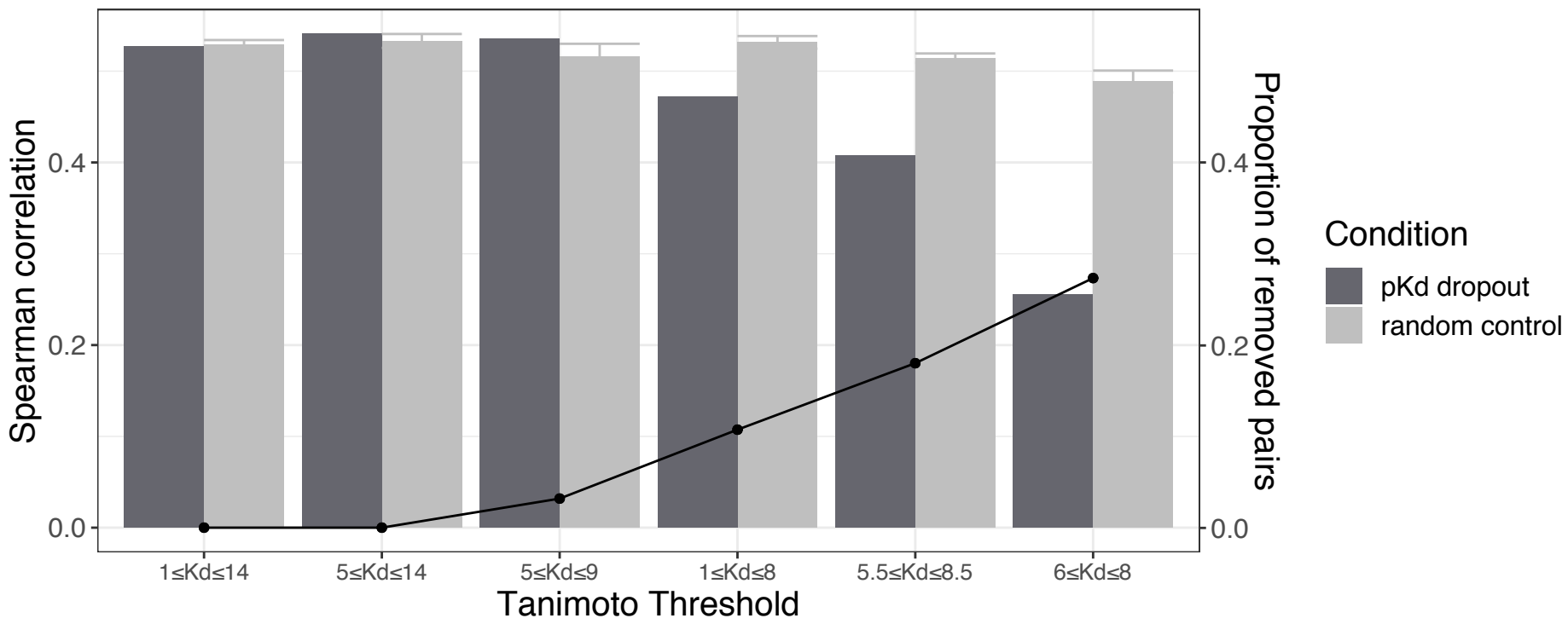
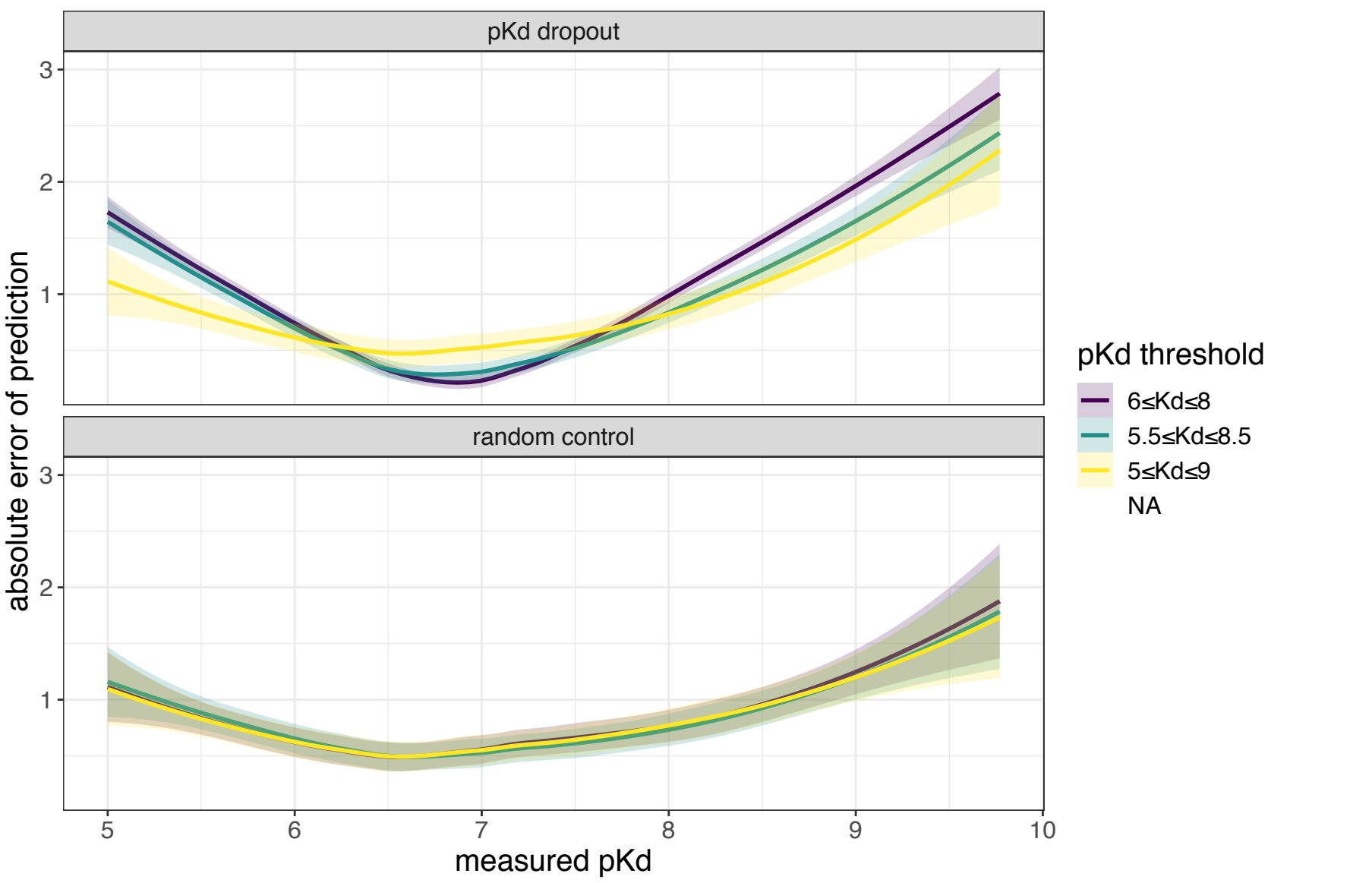
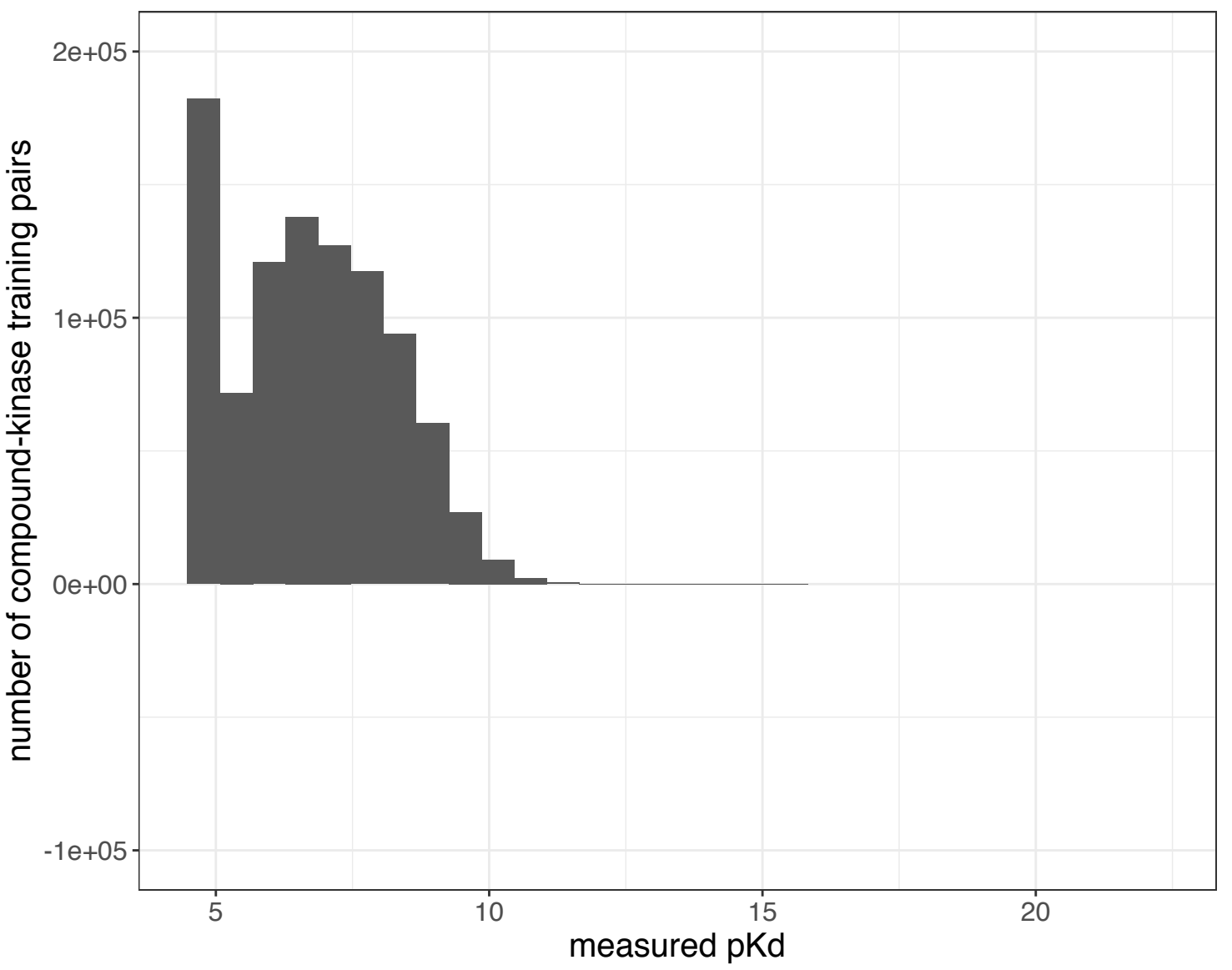

RMSE
Proportion of removed pairs
0.0
0.3
0.6
0.9
1≤Kd≤14
5≤Kd≤14
5≤Kd≤9
1≤Kd≤8
5.5≤Kd≤8.5
6≤Kd≤8
Tanimoto Threshold
Condition
pKd dropout
random control


Spearman correlation
Proportion of removed pairs
0.0
0.2
0.4
1≤Kd≤14
5≤Kd≤14
5≤Kd≤9
1≤Kd≤8
5.5≤Kd≤8.5
6≤Kd≤8
Tanimoto Threshold
Condition
pKd dropout
random control


pKd dropout
random control
absolute error of prediction
1
2
3
5
6
7
8
9
10
measured pKd
pKd threshold
6≤Kd≤8
5.5≤Kd≤8.5
5≤Kd≤9
NA


number of compound-kinase training pairs
2e+05
1e+05
0e+00
-1e+05
5
10
15
20
measured pKd