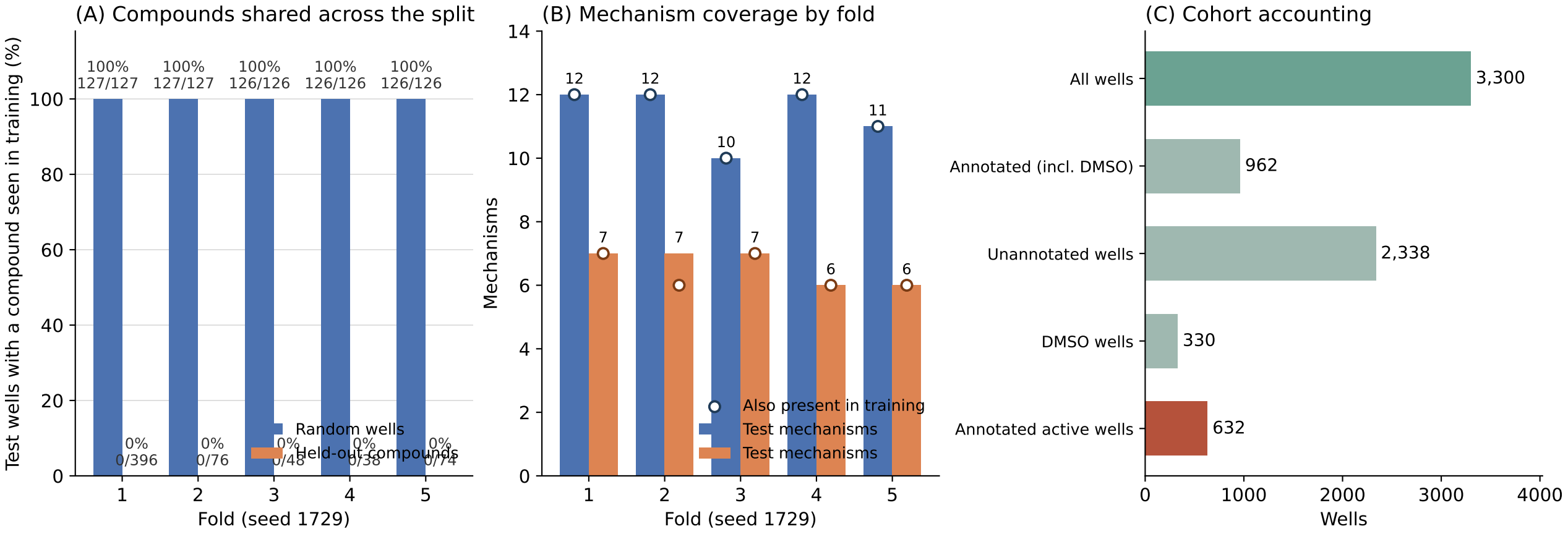

(A) Compounds shared across the split
Test wells with a compound seen in training (%)
100%
127/127
100%
127/127
100%
126/126
100%
126/126
100%
126/126
0%
0/396
0%
0/76
0%
0/48
0%
0/38
0%
0/74
Random wells
Held-out compounds
Fold (seed 1729)
(B) Mechanism coverage by fold
Mechanisms
12
12
10
12
11
7
7
7
6
6
Also present in training
Test mechanisms
Test mechanisms
Fold (seed 1729)
(C) Cohort accounting
All wells
3,300
Annotated (incl. DMSO)
962
Unannotated wells
2,338
DMSO wells
330
Annotated active wells
632
Wells