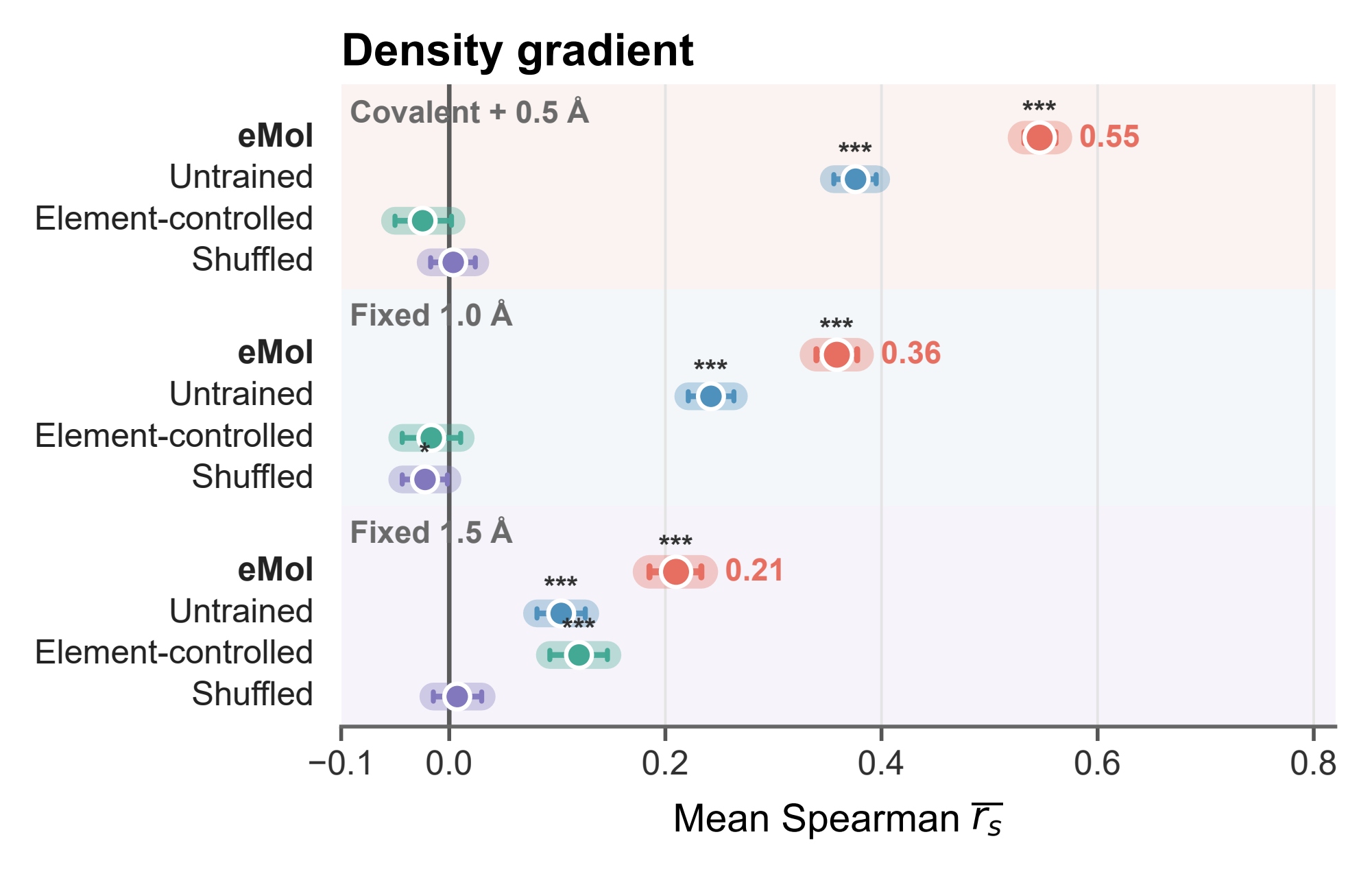

Density gradient
Covalent + 0.5 Å
eMol
Untrained
Element-controlled
Shuffled
***
0.55
***
Fixed 1.0 Å
eMol
Untrained
Element-controlled
Shuffled
***
0.36
***
*
Fixed 1.5 Å
eMol
Untrained
Element-controlled
Shuffled
***
0.21
***
***
−0.1
0.0
0.2
0.4
0.6
0.8
Mean Spearman $\overline{r_s}$