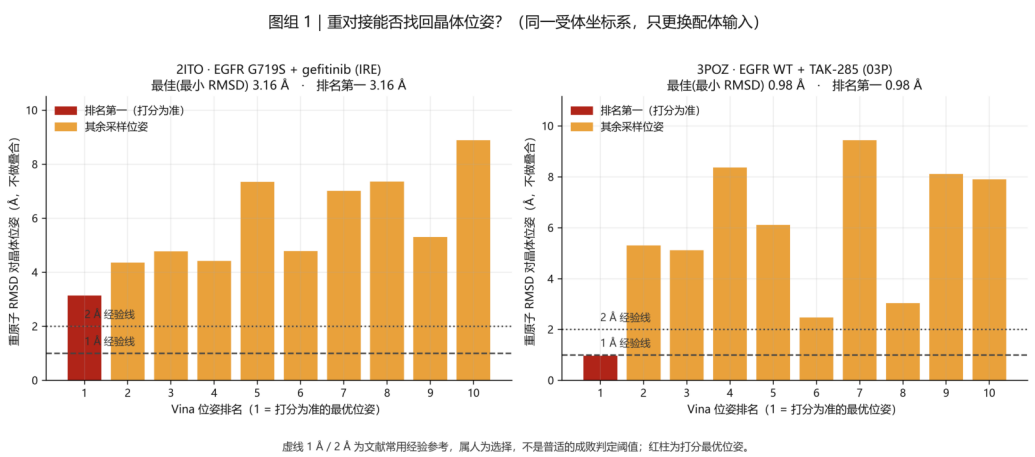
□□□□□□□□□□□□□□□□□□□□□□

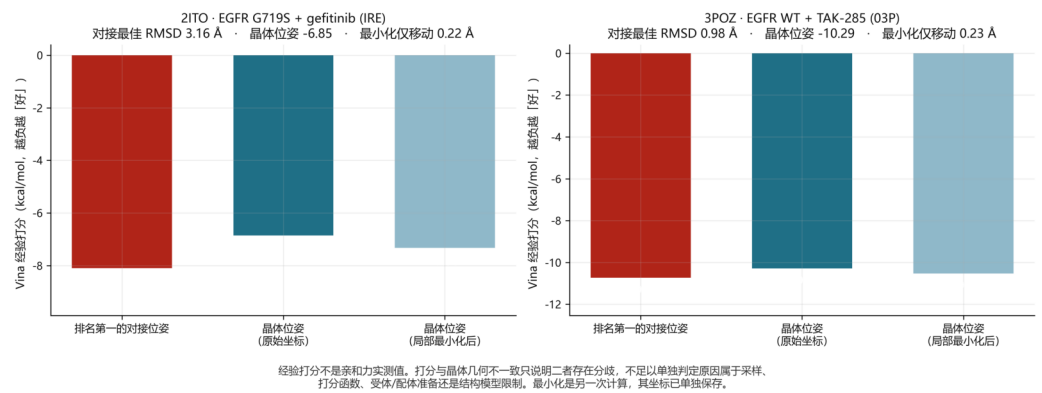
□□□□□□□□□□□□□□□□□□□□□□□□□□Vina seed 42 / exhaustiveness 8 / 10 poses□

A □□□□□□□□□□□□□□



□□□□□□□□□□□□□□□□□□□□□□ RMSD□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□ 1/2 Å □□□□□□□□□□□□□□□□□□

B □□□□ vs □□□□



□□□□□□□□□□□□□□□□□□□□□□ RMSD□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□□ 1/2 Å □□□□□□□□□□□□□□□□□□

□□□ 0.22 Å□□□ 2ITO □□□□□□□□□□□□□□□□□□□□