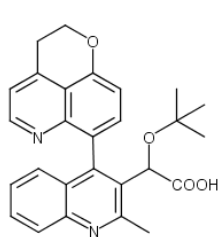


Biophysical Journal, Volume 119

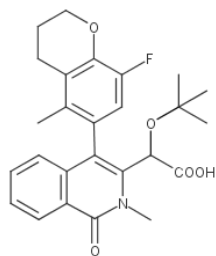
Supplemental Information

Exploring the Free-Energy Landscape and Thermodynamics of Protein-Protein Association

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BI-224436
 $EC_{50} = 15 \text{ nM}$



GSK1264
 $IC_{50} = 38 \text{ nM}$

Figure S1. Structures of ALLINIs BI-224436 and GSK1264.

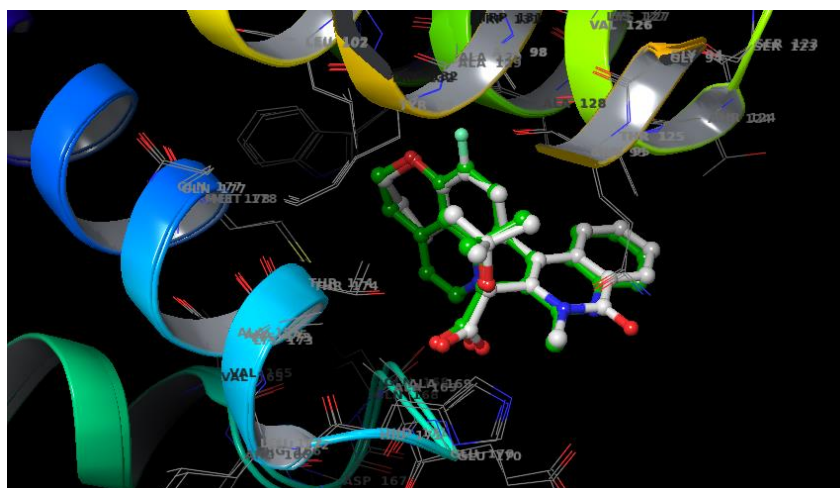


Figure S2. Overlay of GSK1264 and BI-224436 in the HIV-1 IN dimer, obtained by superimposing the protein residues in the PDB 4ojr (containing GSK1264) and the protein residues in the PDB 6nuj (containing BI224436). The carbon atoms in GSK1264 are colored white, while the carbon atoms in BI224436 are green.