

Figure S1. Dynamic cross-correlation analysis (DCCM) results. **A** TrkA-co-crystal ligand complex B) TrkA-Entrectinib complex, **C** TrkA-PHUB000399 complex and **D** TrkA-NPACT01417 complex.

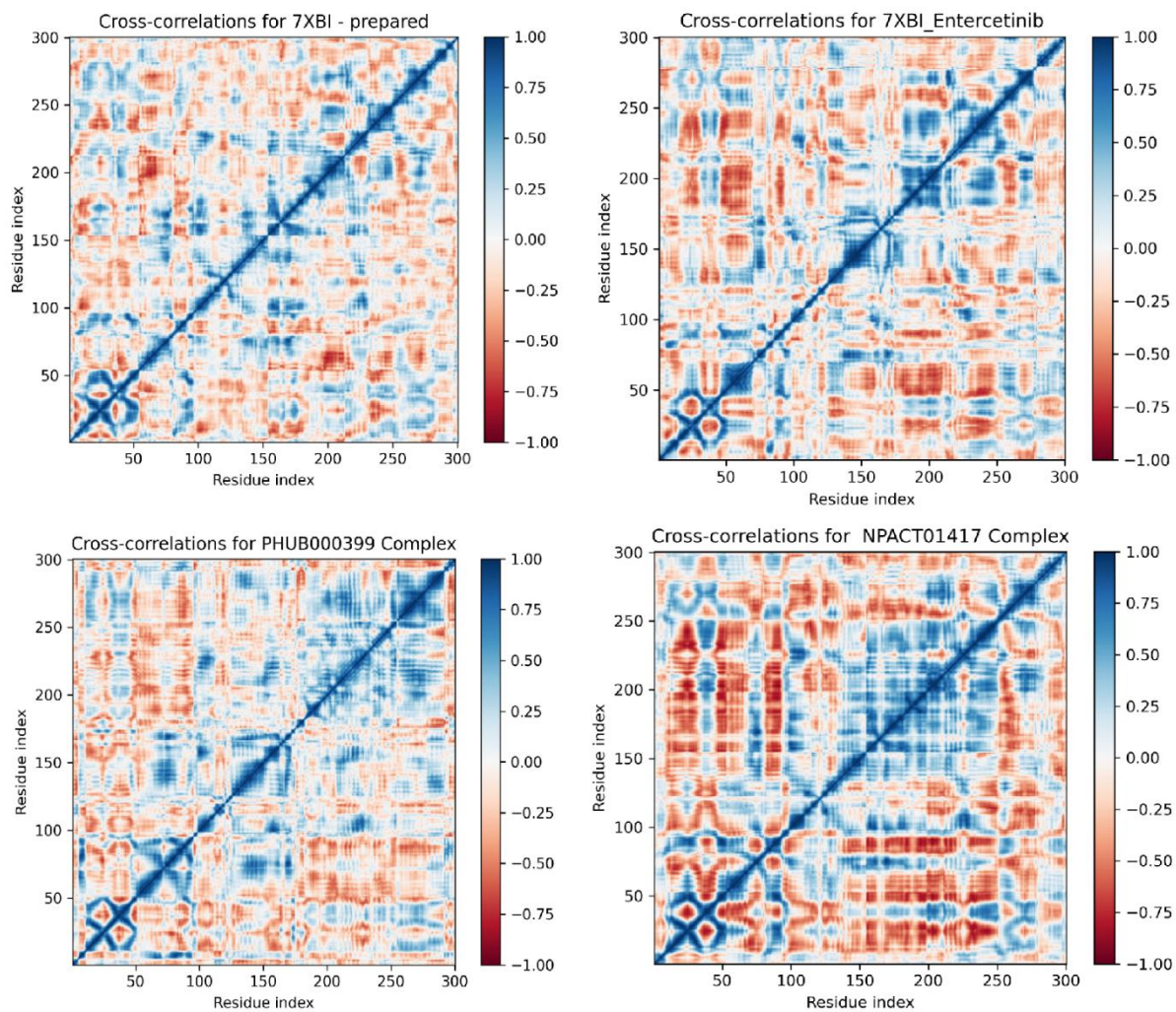


Figure S2. PCA analysis results. **A** TrkA-co-crystal ligand (Control) complex, **B** TrkA-Entrectinib complex, **C** TrkA-PHUB000399 complex and **D**) TrkA-NPACT01417 complex.

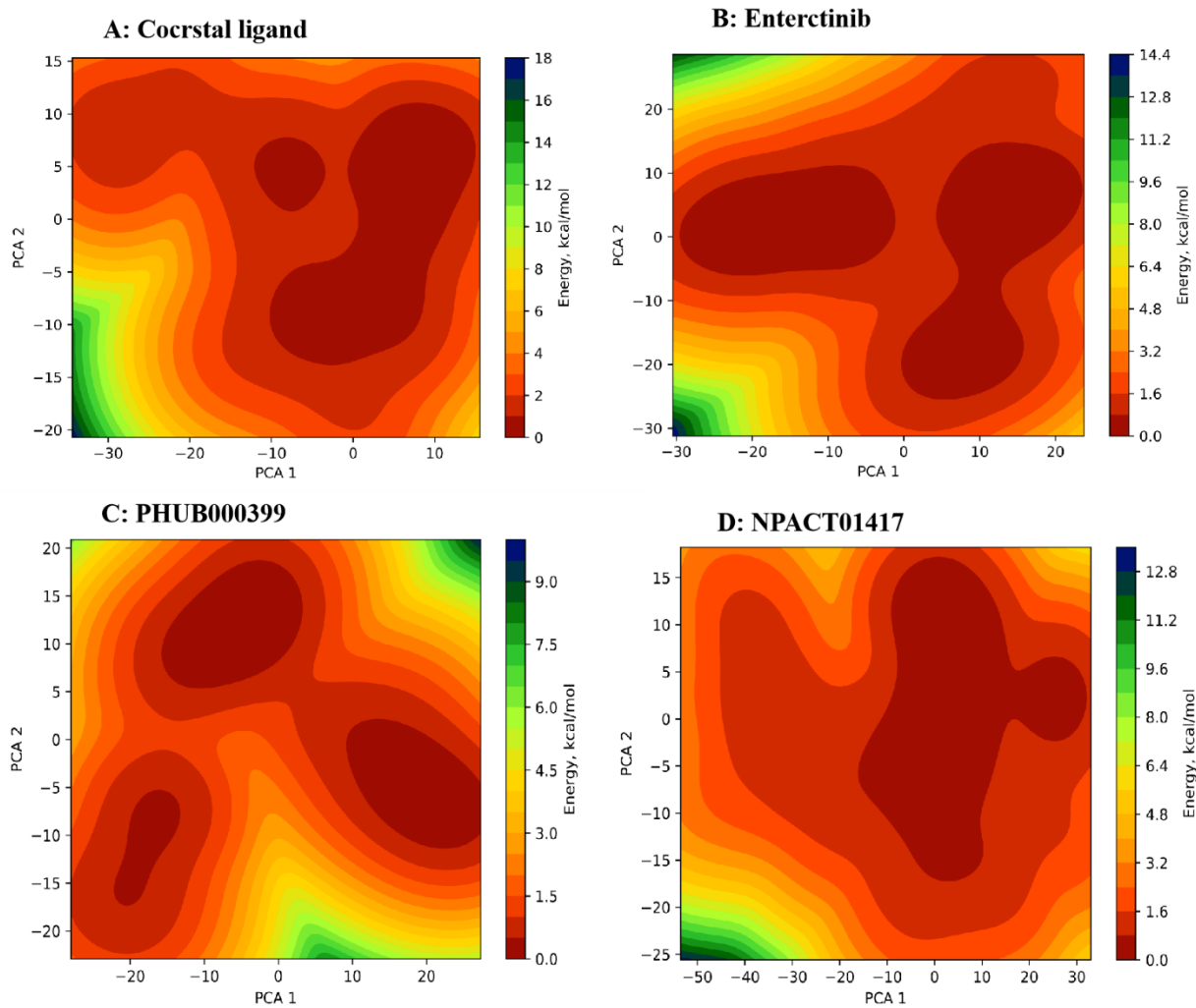
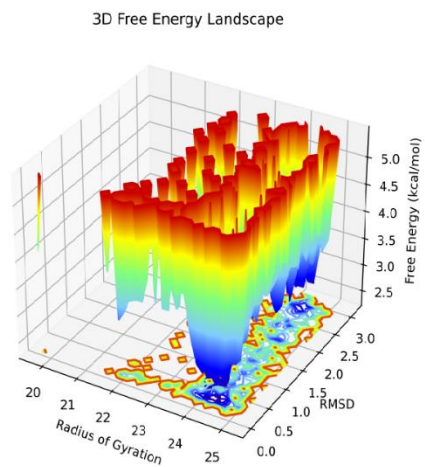
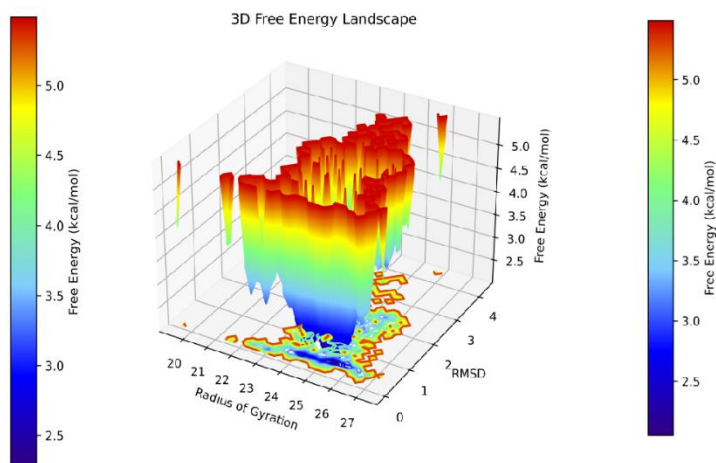


Figure S3. FEL analysis results. **A** TrkA-co-crystal ligand complex, **B** TrkA-Entrectinib complex, **C** TrkA-PHUB000399 complex and **D** TrkA-NPACT01417 complex.

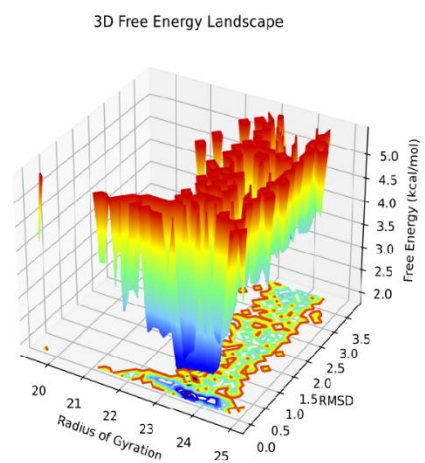
A: Cocrystal ligand



B: Entrectinib



C: PHUB000399



D: NPACT01417

