

Identification of Diosmin and Flavin Adenine Dinucleotide as Repurposing Treatments for Monkeypox Virus: A Computational Study

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Abbreviations:

CS-E: chondroitin sulfate-E

MPXV: monkeypox virus

RMSD: Root mean square deviation

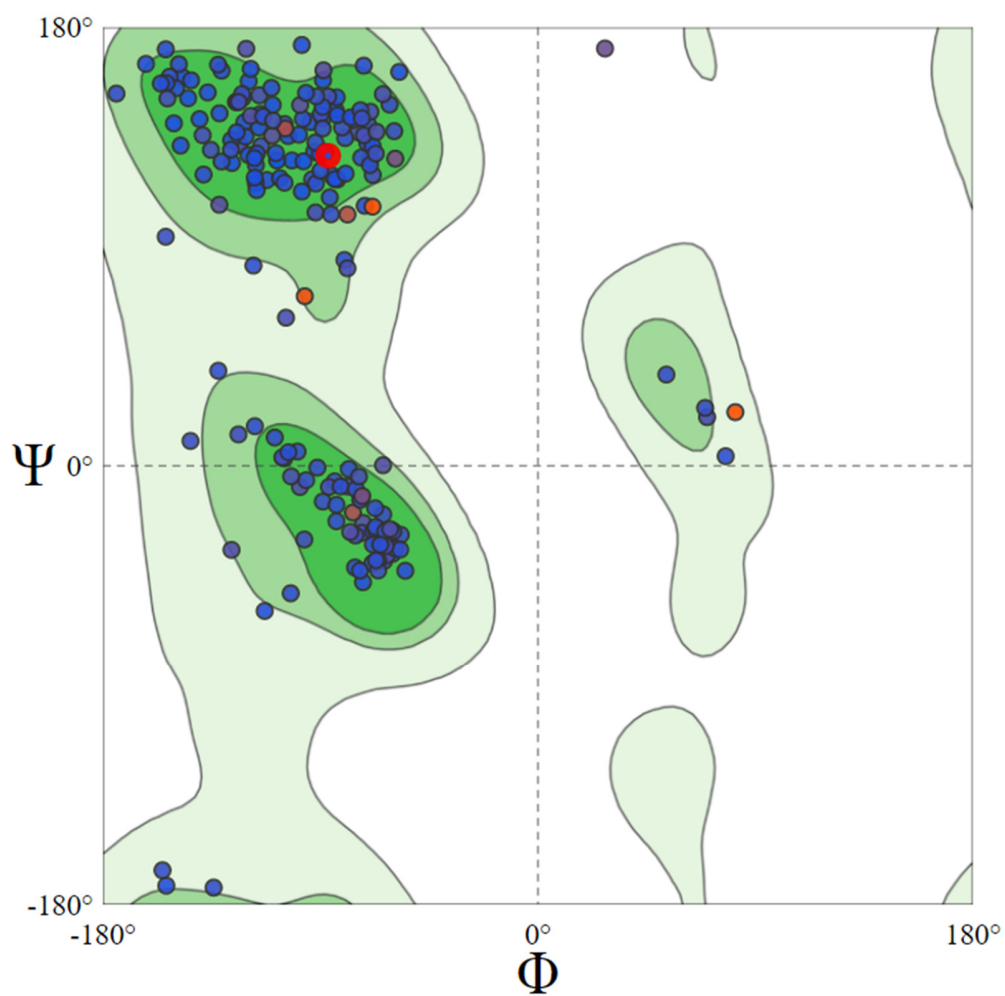
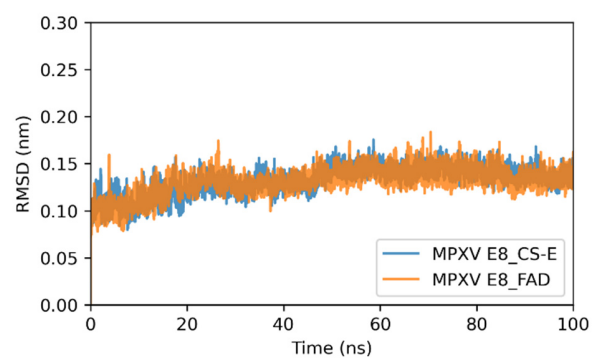
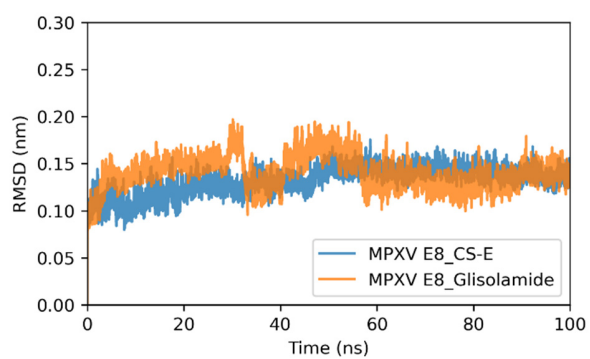
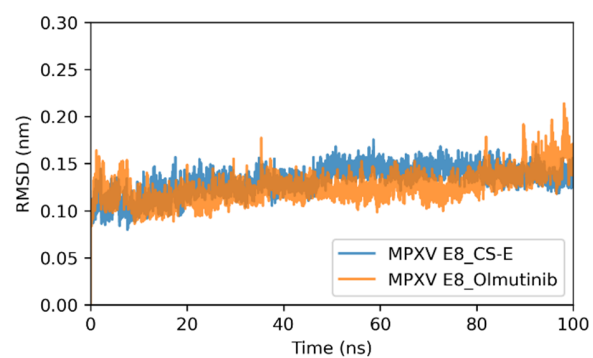
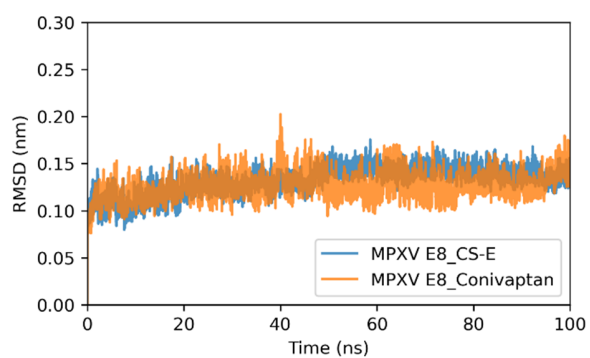
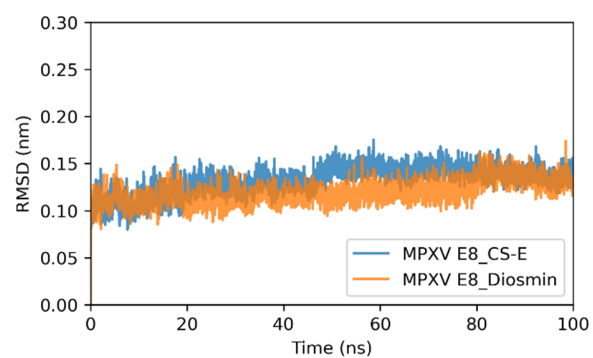
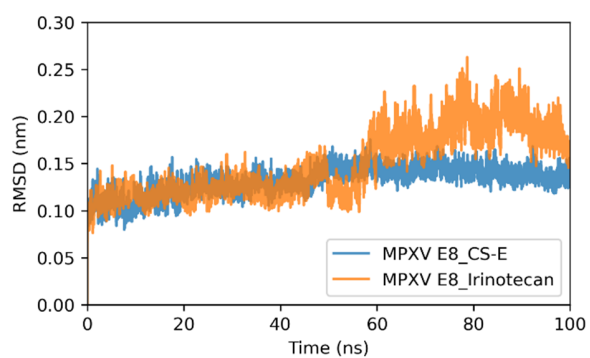
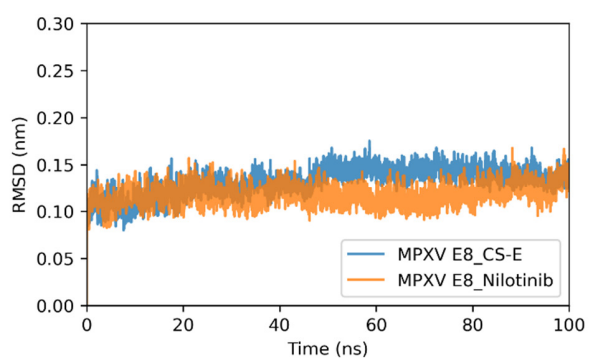
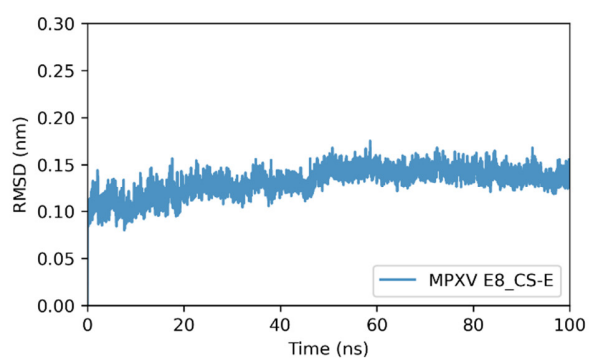


Figure S1. Ramachandran plot of the MPXV E8 protein first domain (residue 1–235)



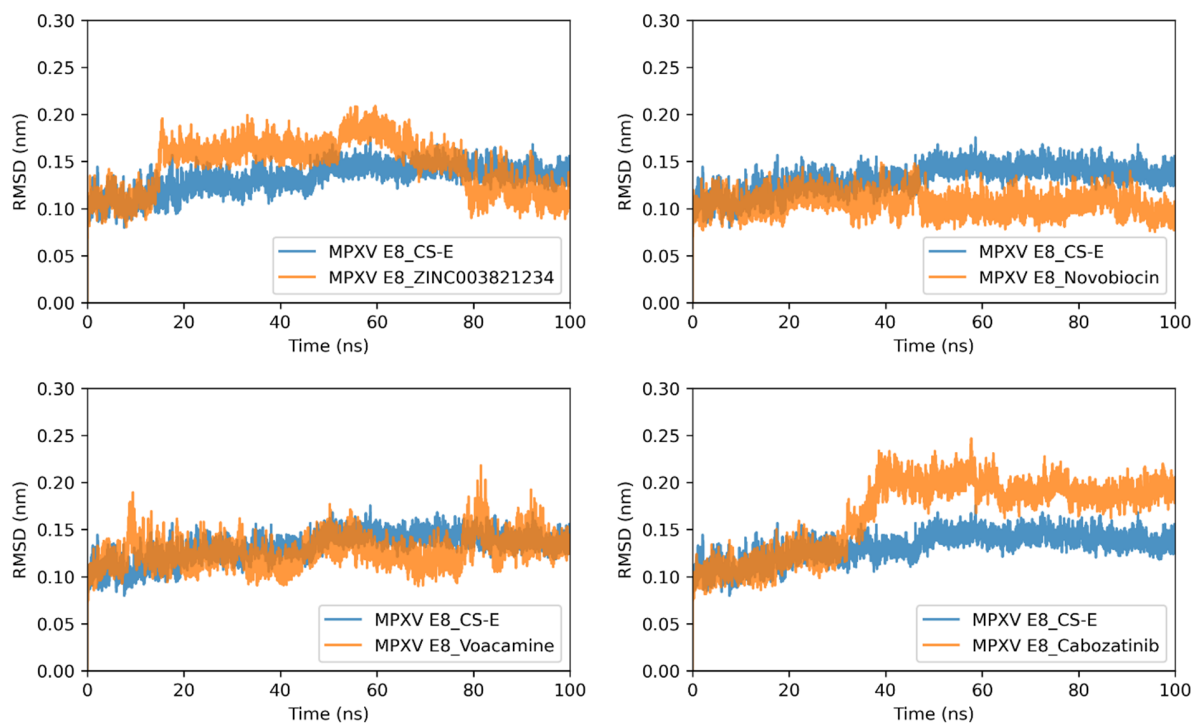
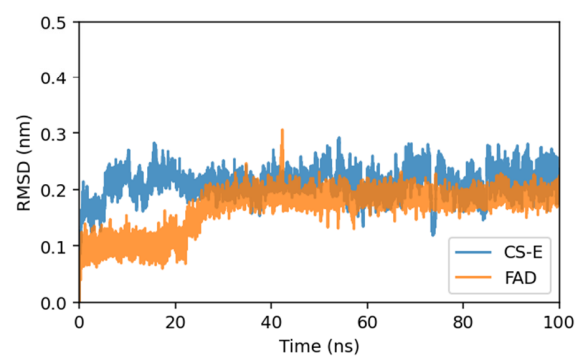
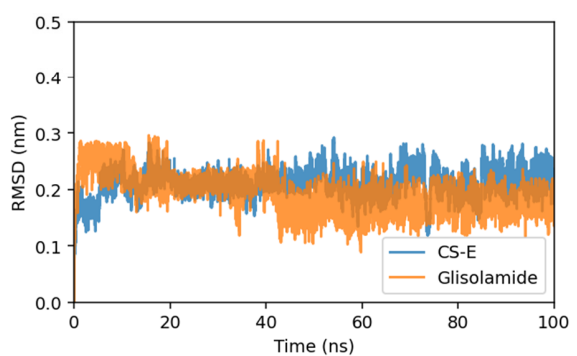
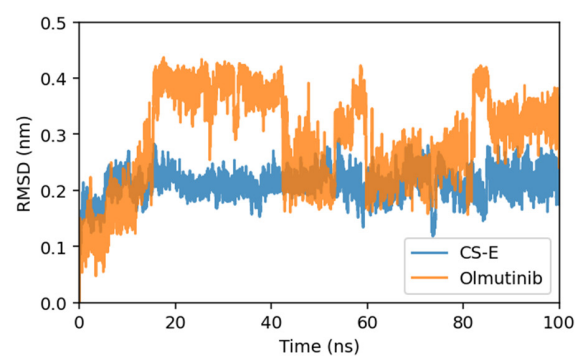
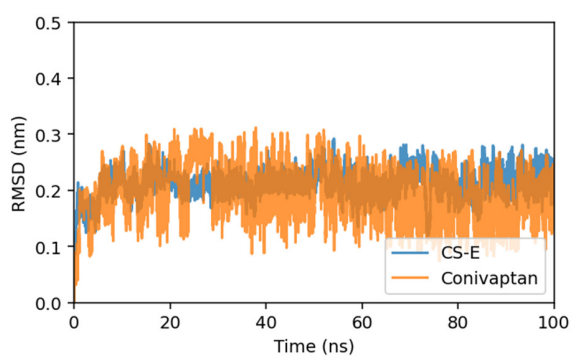
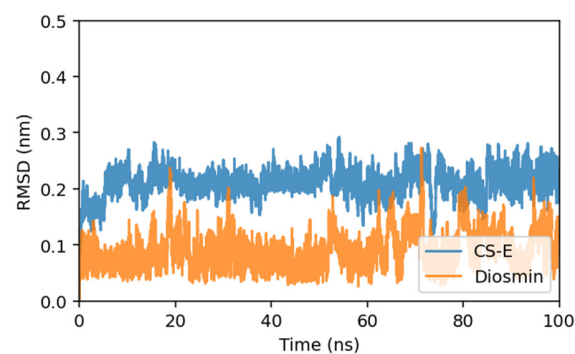
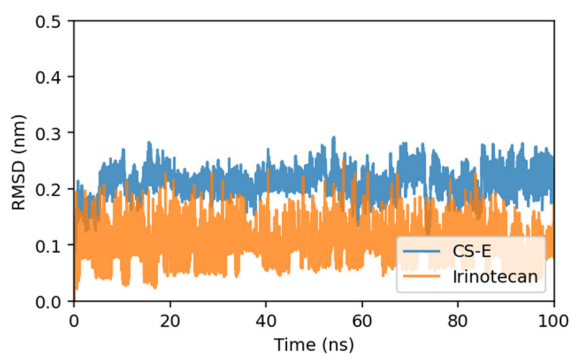
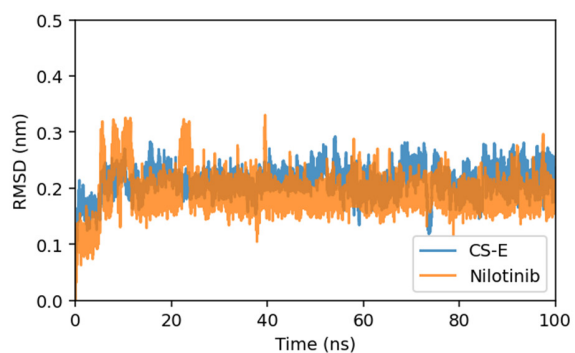
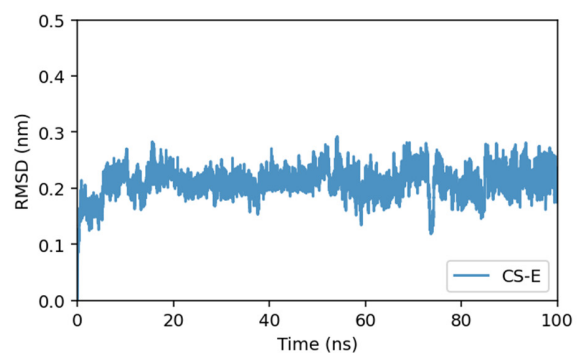


Figure S2. Protein RMSD plot (carbon backbone) of 11 complexes of the MPXV E8 protein with the top 11 small-molecule drugs during the 100 nanoseconds molecular dynamics simulations



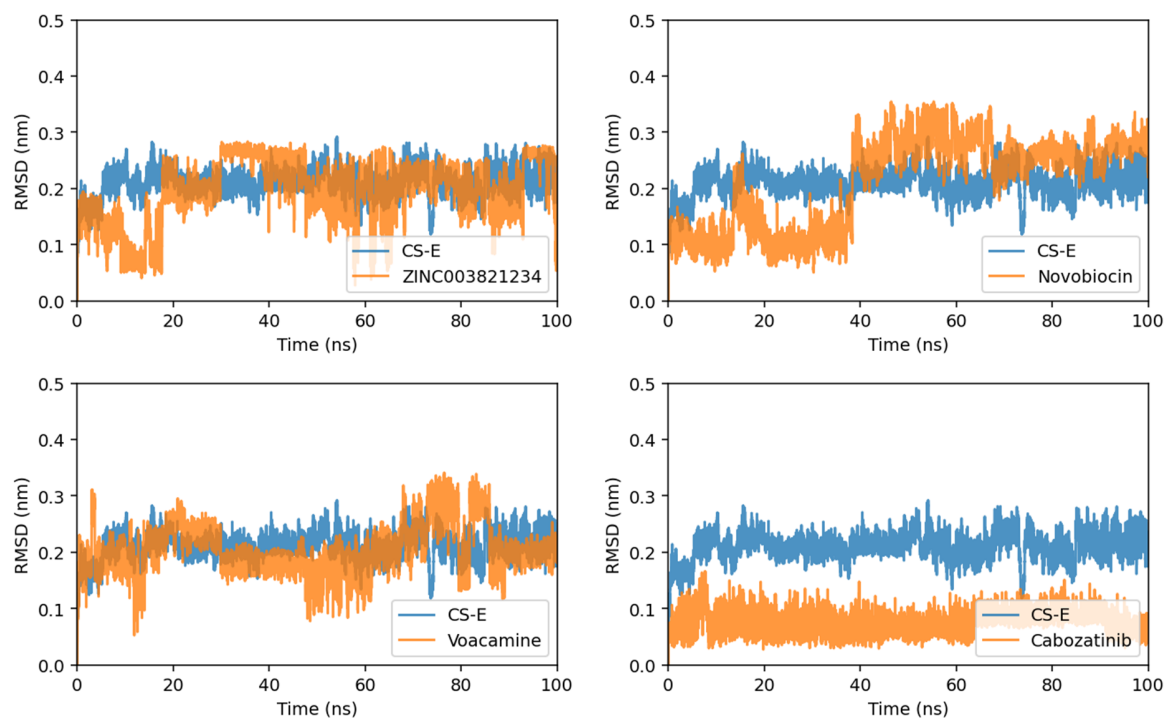


Figure S3. RMSD plot of ligand heavy atoms in 11 complexes with the MPXV E8 protein during the 100 nanoseconds molecular dynamics simulations