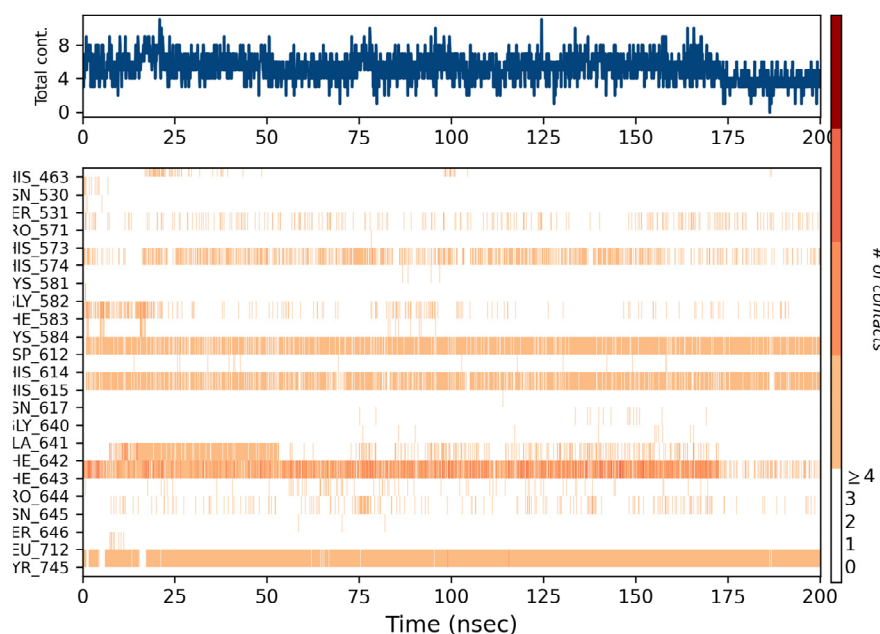
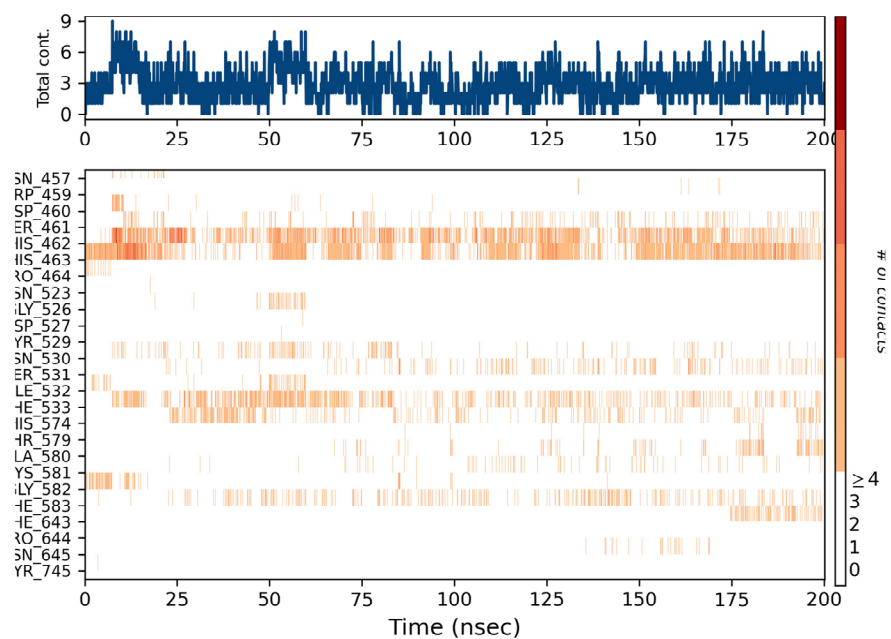


Supplementary Materials

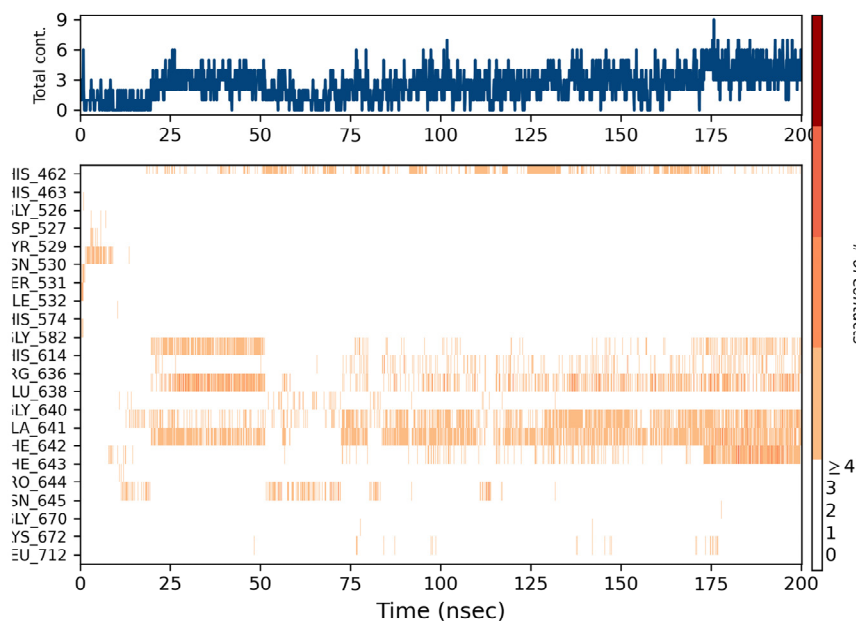
Identification of Novel Natural Dual HDAC and Hsp90 Inhibitors for Metastatic TNBC Using e-Pharmacophore Modeling, Molecular Docking, and Molecular Dynamics Studies



A

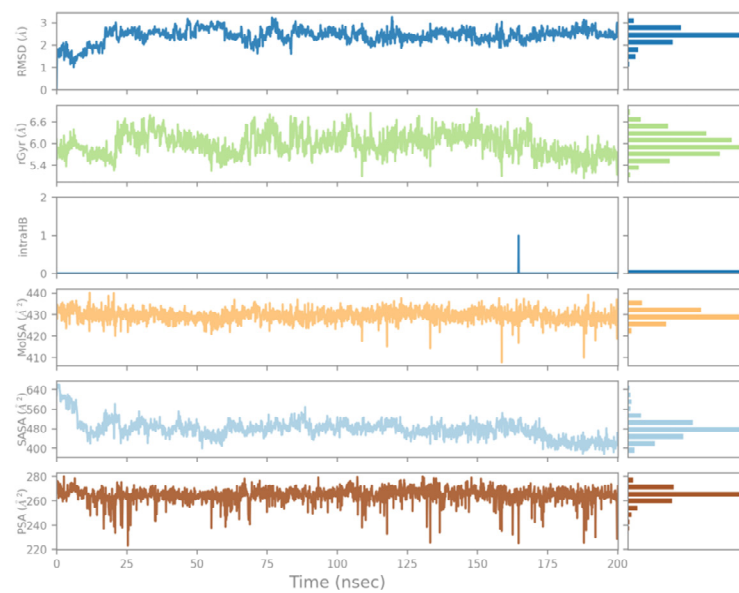


B



C

Figure S1. A timeline representation of the interactions and contacts (H-bonds, Hydrophobic, Ionic, Water bridges) of the top three compounds complexed with HDAC6 (PDB ID: 6PYE) during 200 ns molecular dynamics simulation using Desmond software. (A) compound A, (B) compound B, and (C) compound C.

**A****B**

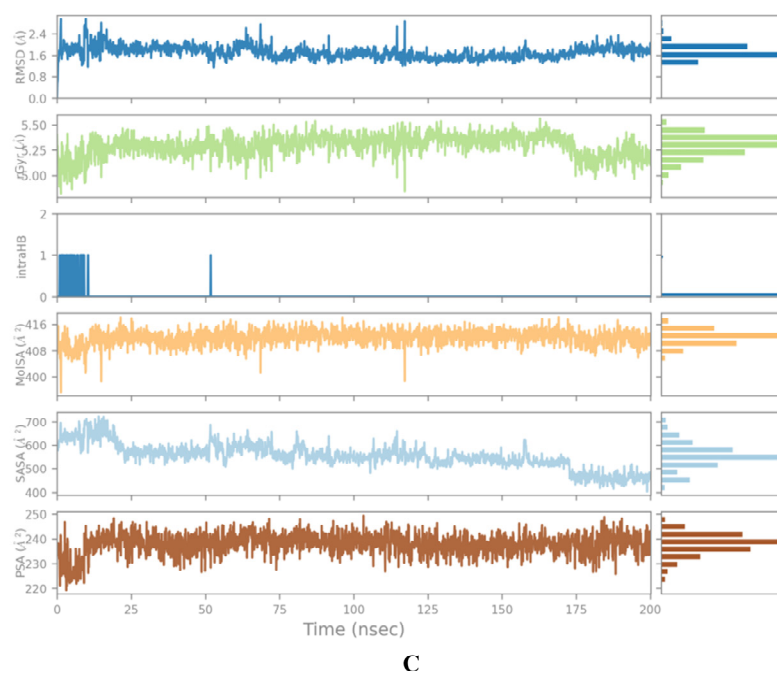
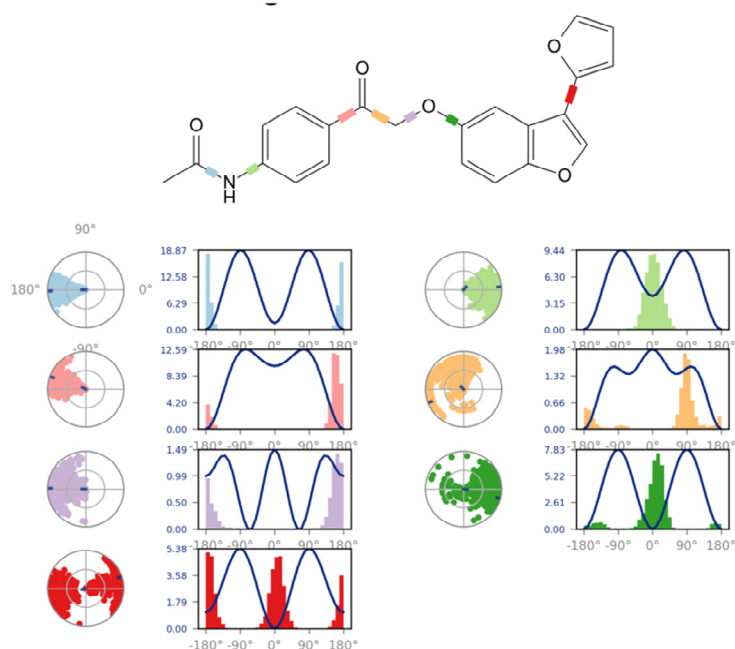


Figure S2. Ligand properties of the top three compounds complexed with HDAC6 (PDB ID: 6PYE) during 200 ns molecular dynamics simulation using Desmond software. (A) compound A, (B) compound B, and (C) compound C.



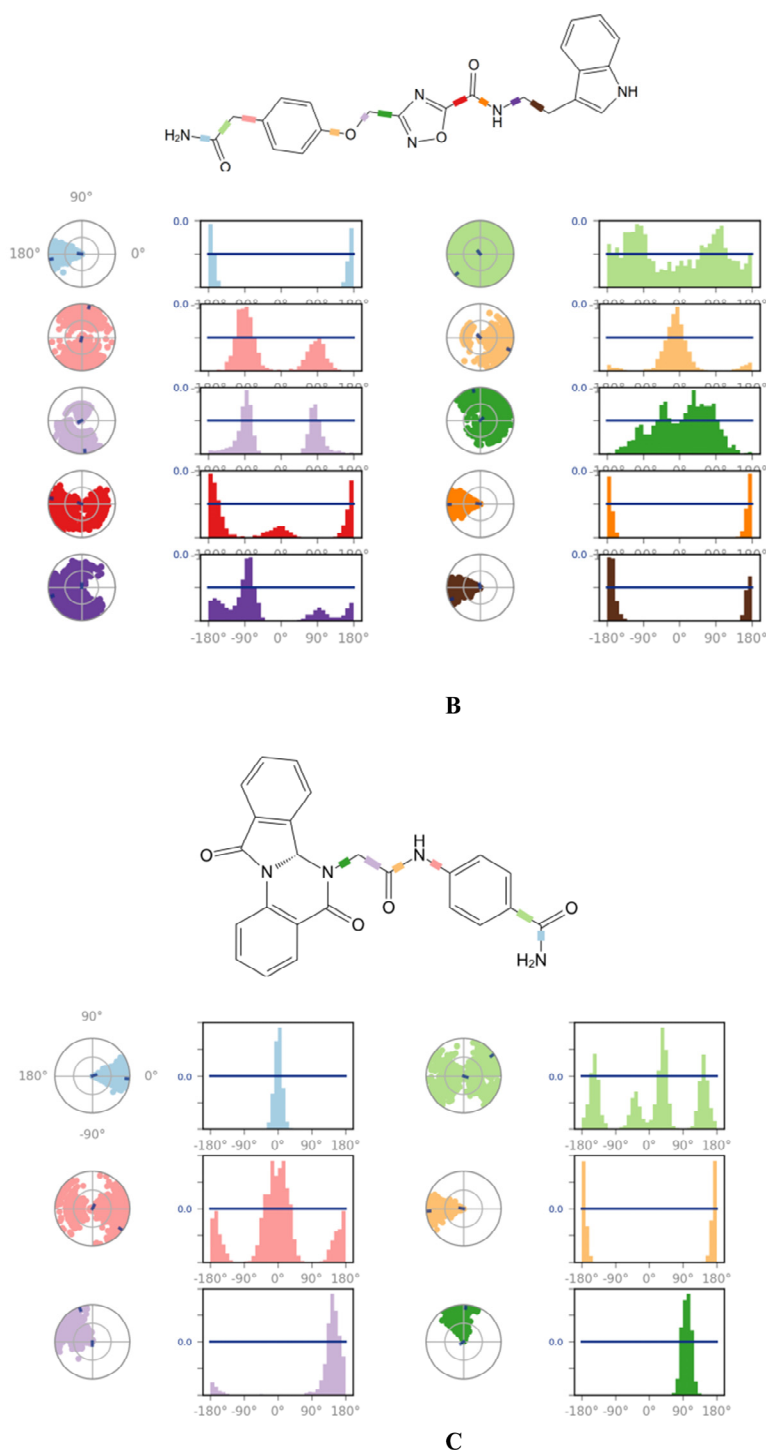


Figure S3. Ligand torsion Profile of the top three compounds complexed with HDAC6 (PDB ID: 6PYE) during 200 ns molecular dynamics simulation using Desmond software. The top panel shows the 2d schematic of a ligand with color-coded rotatable bonds. Each rotatable bond torsion is accompanied by a dial plot and bar plots of the same color. (A) compound A, (B) compound B, and (C) compound C.