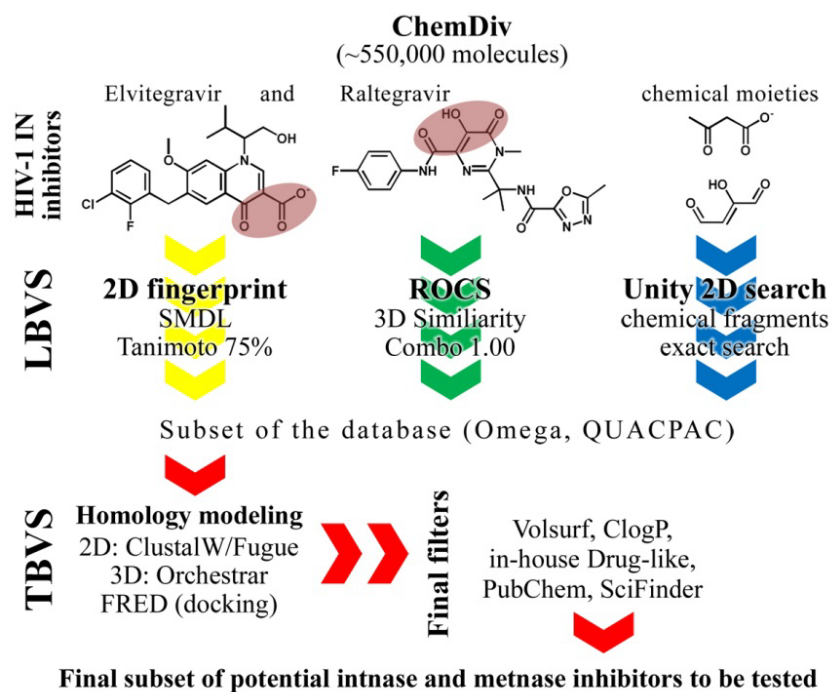


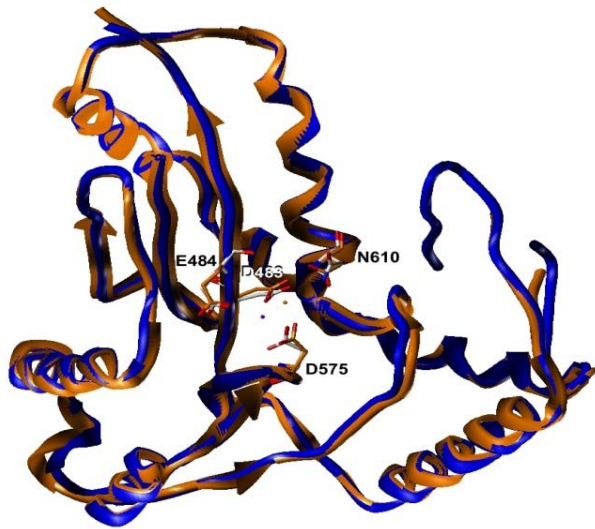
## Supplementary Information

### For Targeting the Transposase Domain of the DNA Repair Component Metnase to Enhance Chemotherapy

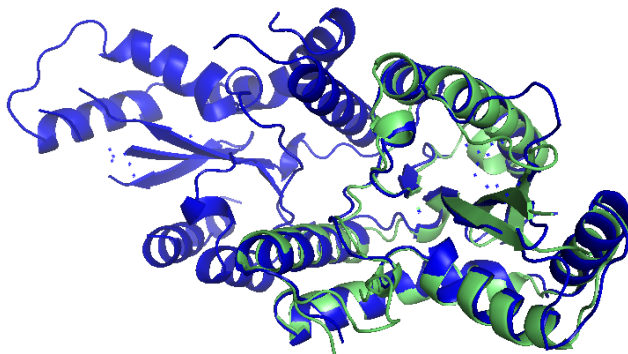
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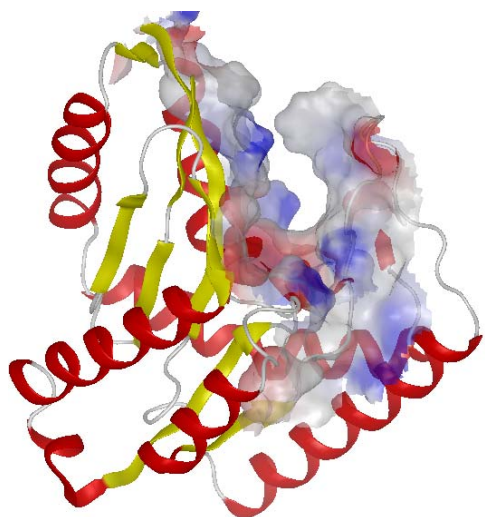
**Figure S1.** The composite approach for *in silico* compound selection.



**Figure S2.** Superposition of the 3D structures of Metnase (model, blue) and MOS-1 active sites (2F7T, orange).



**Figure S3.** Comparison between two metnase structures: monomer from the homology modeling (green) and the dimeric X-rays crystallography structure 3F2K (blue).  
RMSD: C-alpha carbon: 0.89 Å. All atoms: 0.94 Å



**Figure S4.** Electrostatic surface of the metnase Transposase domain. Ribbon representation:  $\alpha$ -helices (red),  $\beta$ -sheet (yellow), loops (gray). Electrostatic surface: red (high electron density), blue (low density region).