applied sciences

MDPI

Communication

Supplementary material: Experimental and Simulation Identification of Xanthohumol as an Inhibitor and Substrate of ABCB1

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Table S1: Residue Interactions with DOX and XN Ligands

DOX complex	XN complex
ILE 340[1]	PHE 336[1]
PHE 983[1]	PHE 983[1]
ASN 839[1]	ALA 980[1]
GLN 990[1]	PHE 728[1]
TYR 307[1]	ASN 842
GLN 725[1]	TYR 953
PHE 343[1]	PHE 732

[1]Interactions that occur more than 30.0% of the simulation time in the selected trajectory

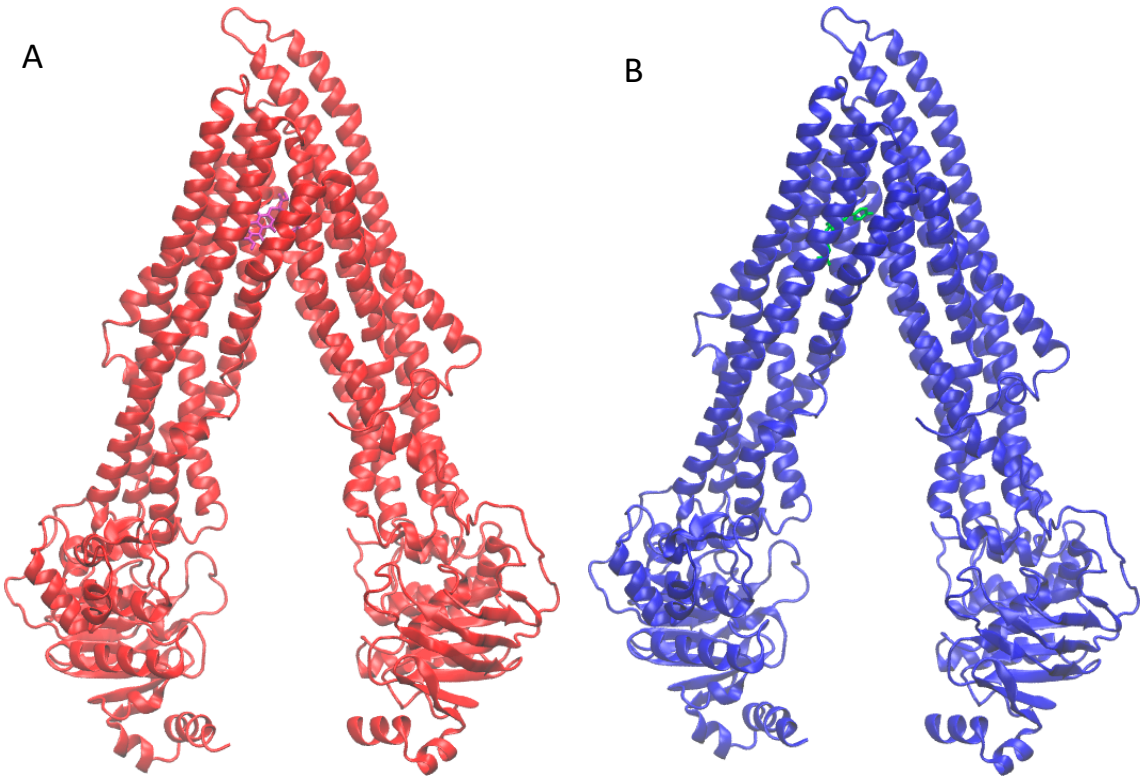
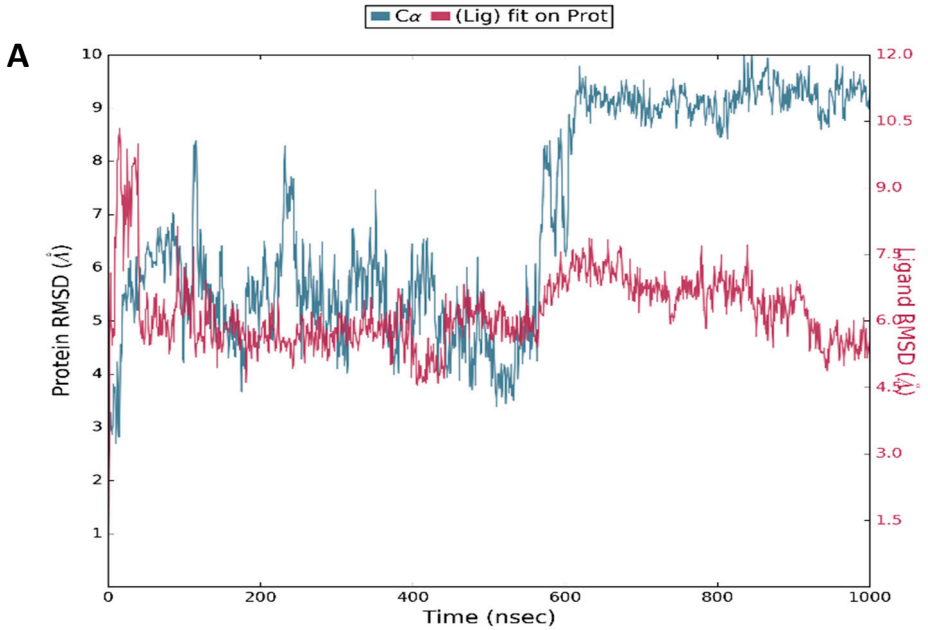


Figure S1. Complexes from IFD docking. Closed, original crystal structure (PDB ID: 4Q9I). (A) DOX docked. (B) XN docked.



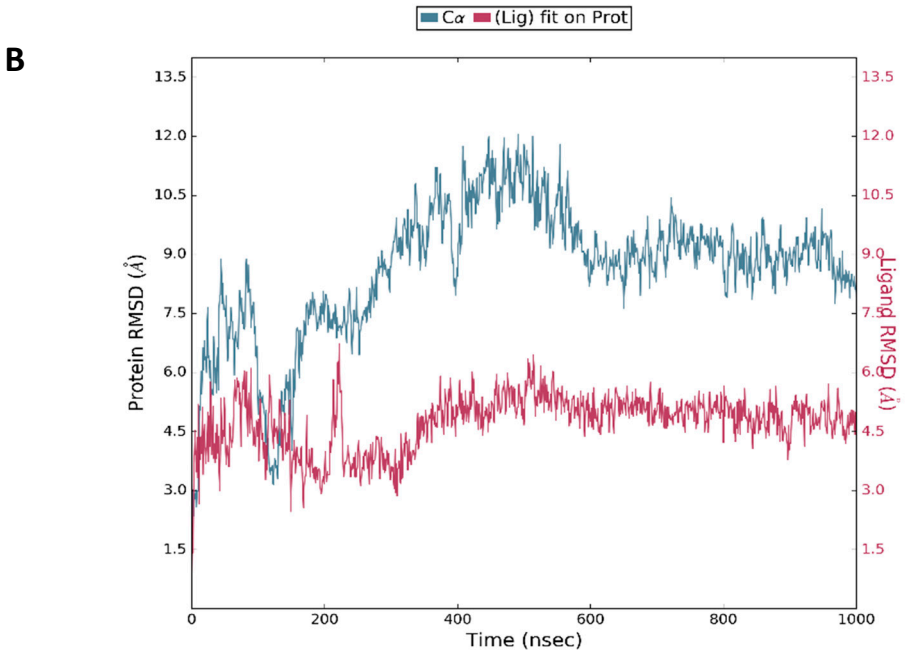
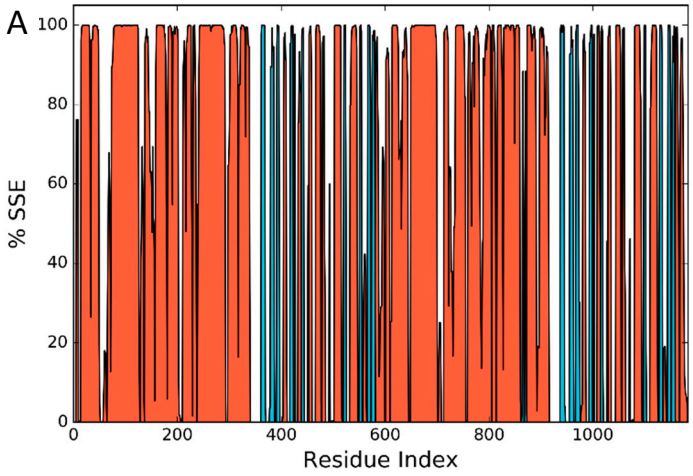


Figure S2. Protein/Ligand Root Mean Square Deviation (RMSD) Comparison. RMSD measures the average change in displacement of a selection of atoms for a particular frame with respect to a reference frame. All protein frames are first aligned on the reference frame backbone (i.e. the initial frame), and then RMSD is calculated based on the atom selection. (A) DOX complex. (B) XN complex.



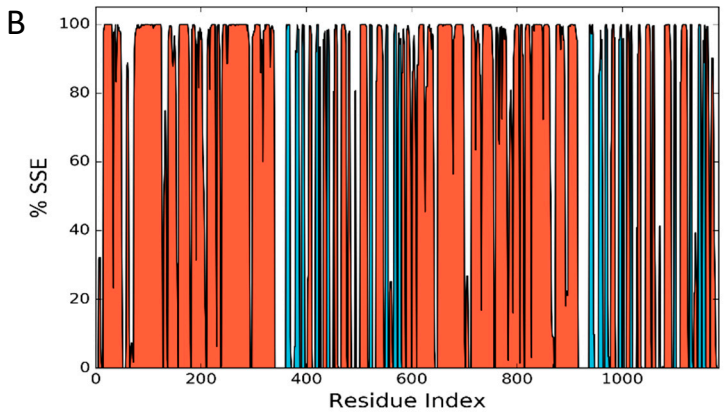


Figure S3. Protein Secondary Structure. Protein secondary structure elements (SSE) are monitored throughout simulation. This plot reports the SSE distribution by residue index throughout the protein structure. (A) DOX complex. (B) XN complex. Purple: alpha-helices Blue: beta-strands White: Coils.

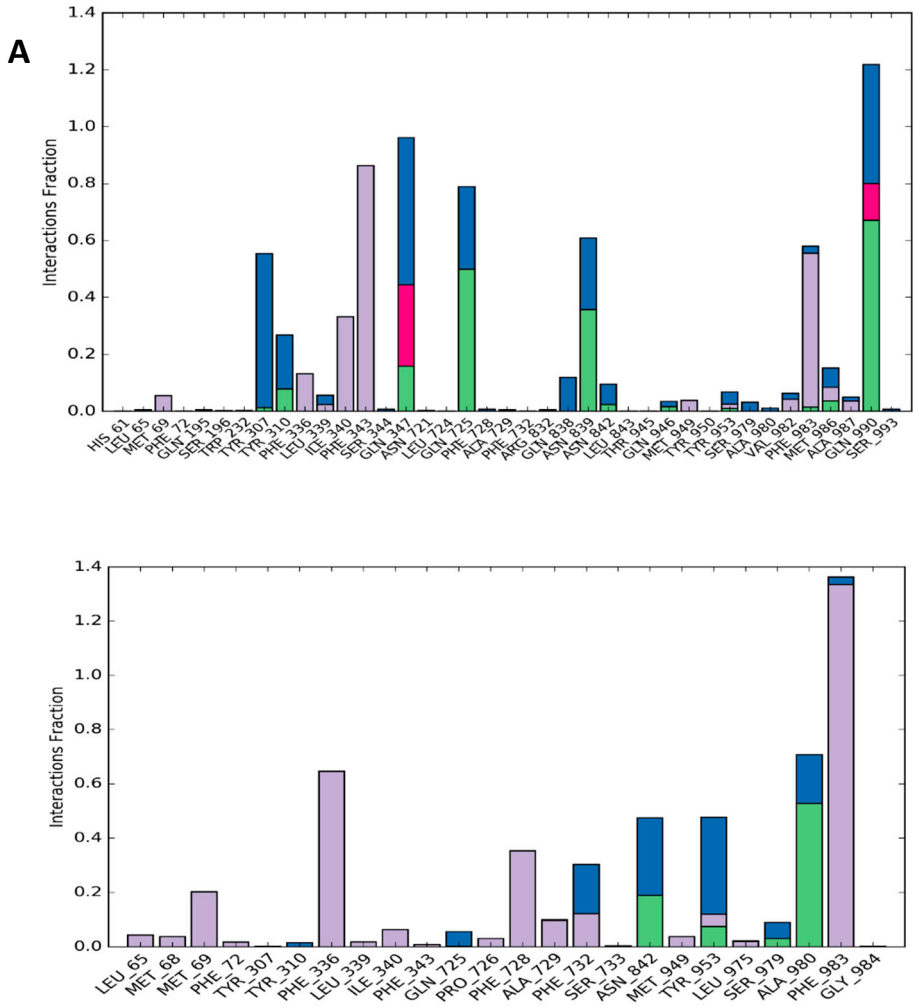


Figure S4. Protein-Ligand Contacts. (**A**) DOX complex. (**B**) XN complex.

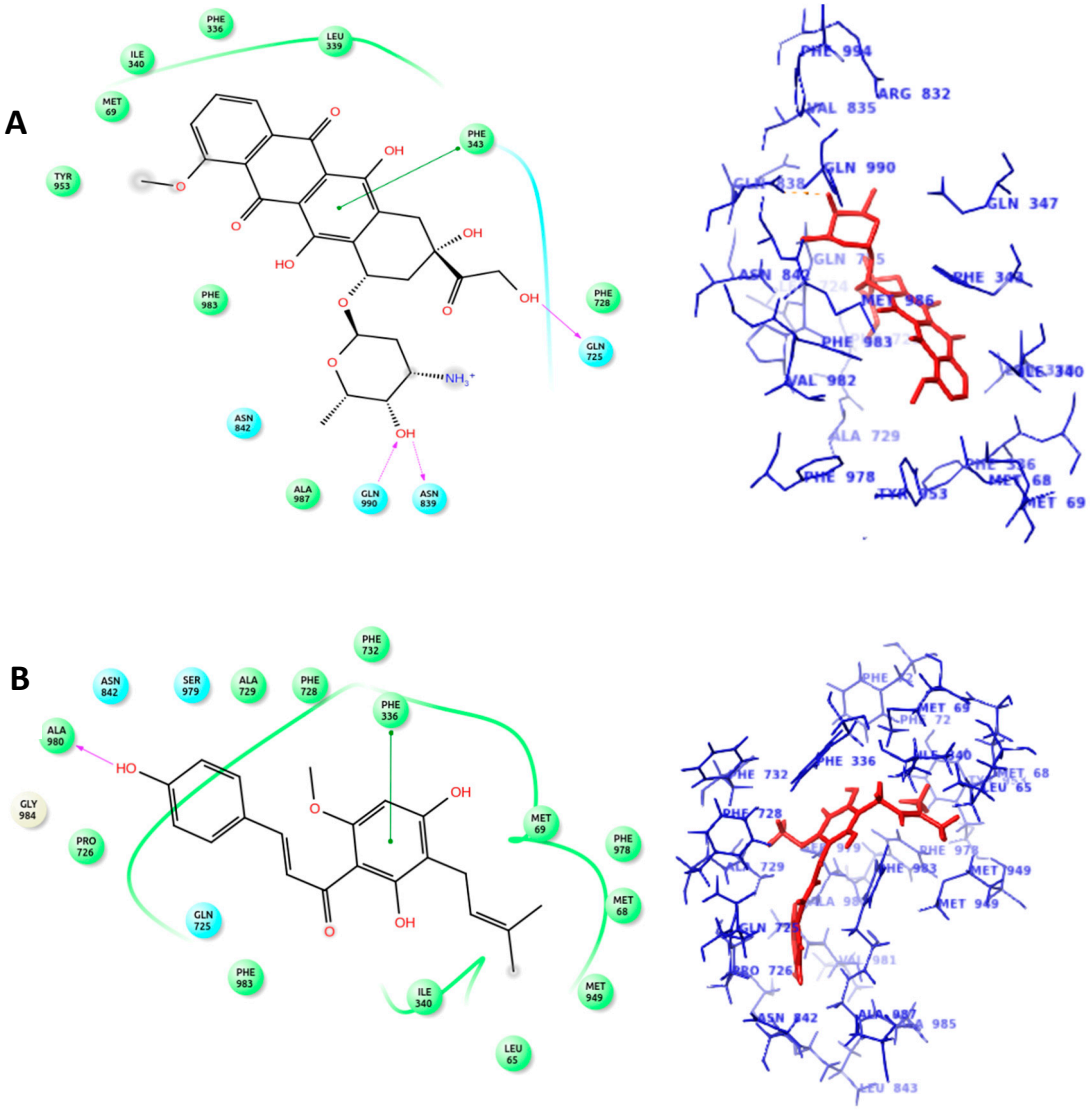
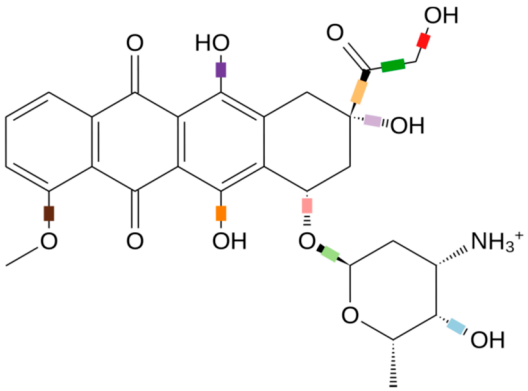
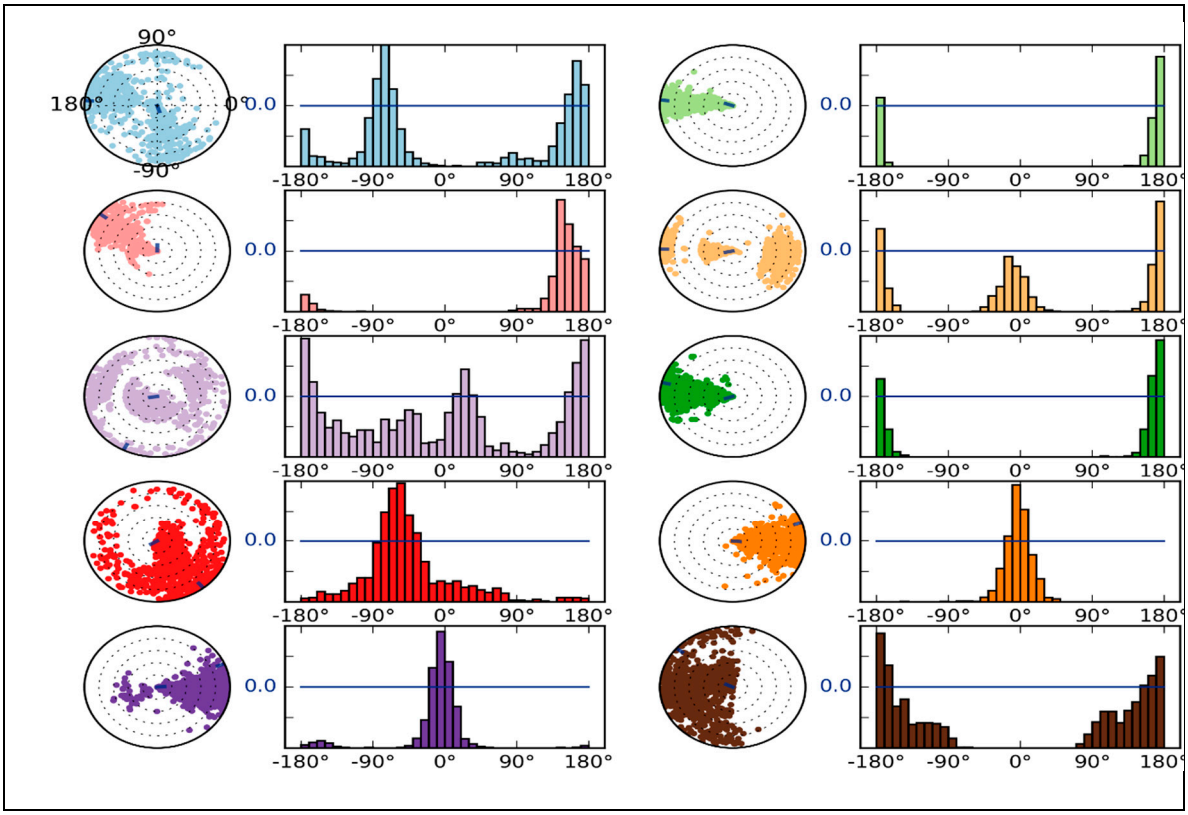


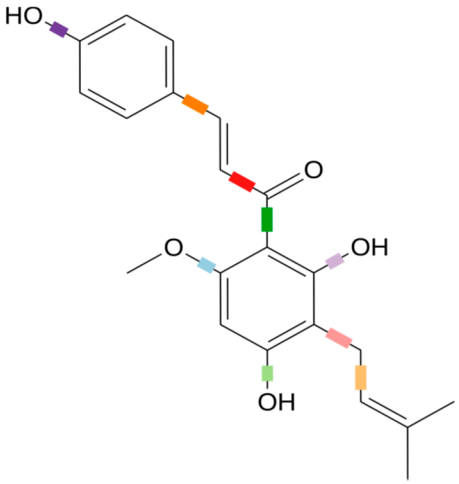
Figure S5. Protein Interactions Diagrams. (A) Shows the 2D interaction diagram and the 3D interaction diagram from the last snapshot structure for the DOX complex. (B) Shows the 2D interaction diagram and the 3D interaction diagram from the last snap shot structure for the XN complex.

A





B



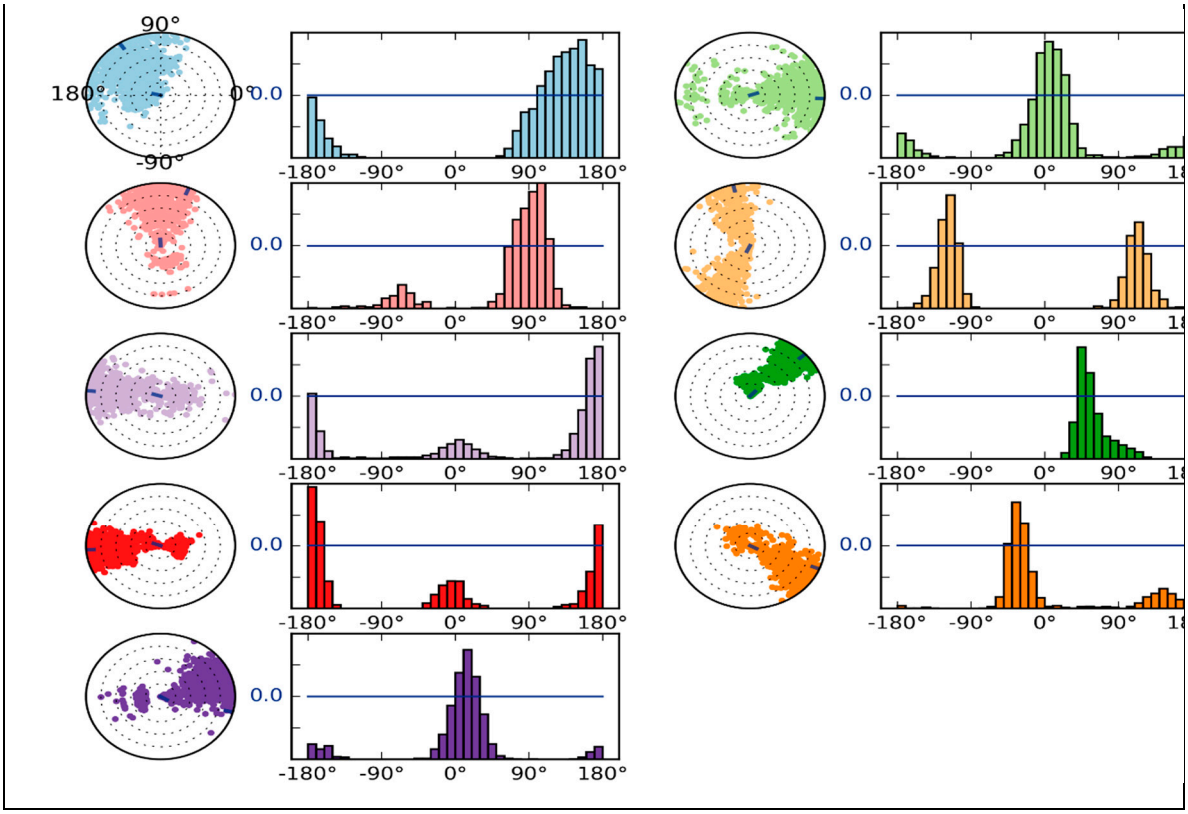


Figure S6. Ligand Torsion Profile. The ligand torsions plot summarizes the conformational evolution of every rotatable bond in the ligand throughout the simulation trajectory. (A) DOX. (B) XN.