

Halogen Bonding in Haspin-Halogenated Tubercidin Complexes: Molecular Dynamics and Quantum Chemical Calculations

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Supporting Information

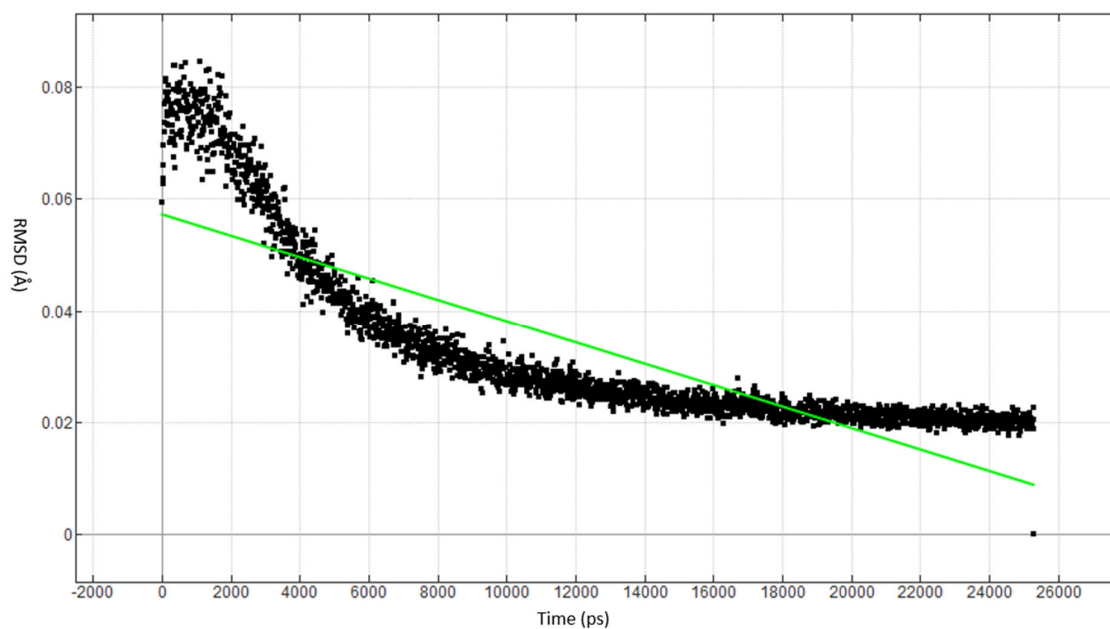


Figure S1. Root mean square deviation (RMSD) plot of complex between 5-iTU and Haspin.

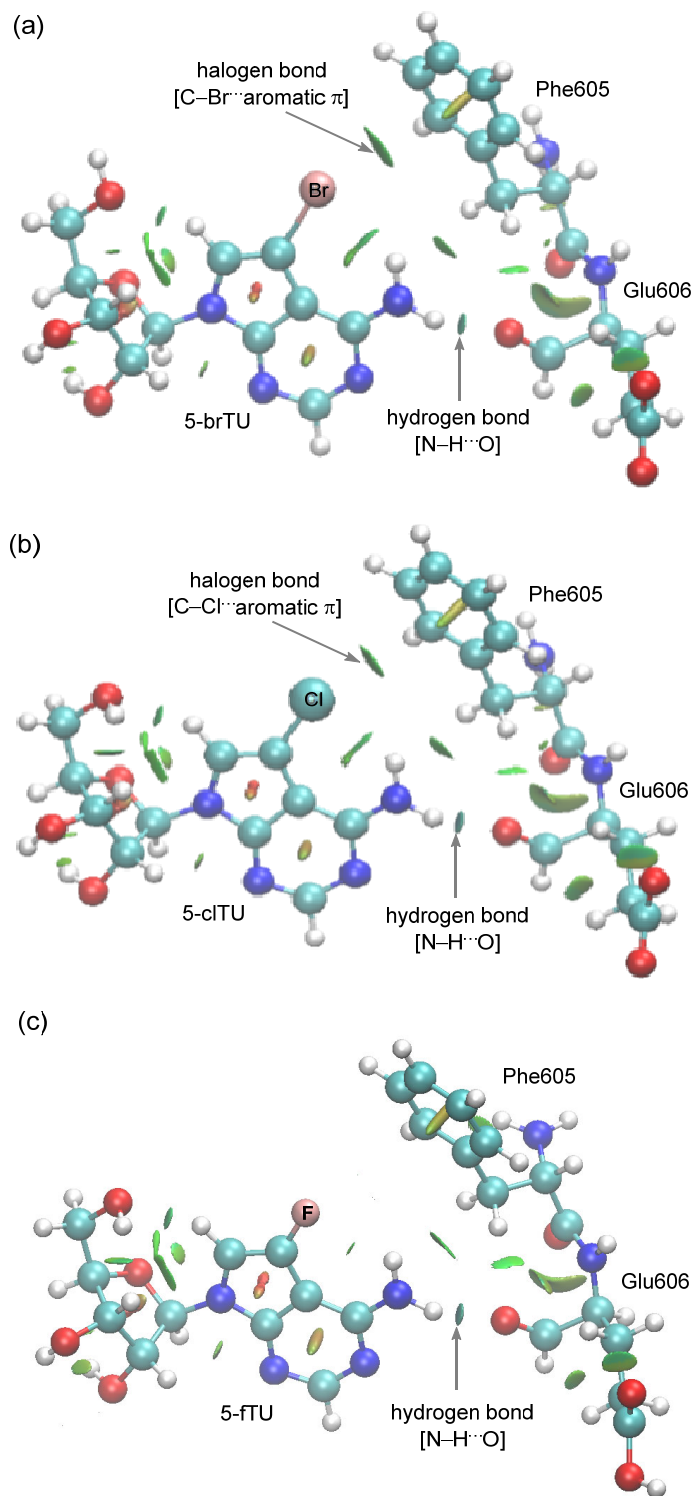


Figure S2. NCI isosurface between the tubercidin ligand 5-XTU and Haspin key residues (Phe605-Glu606): (a) 5-brTU, (b) 5-clTU, and (c) 5-ftU.