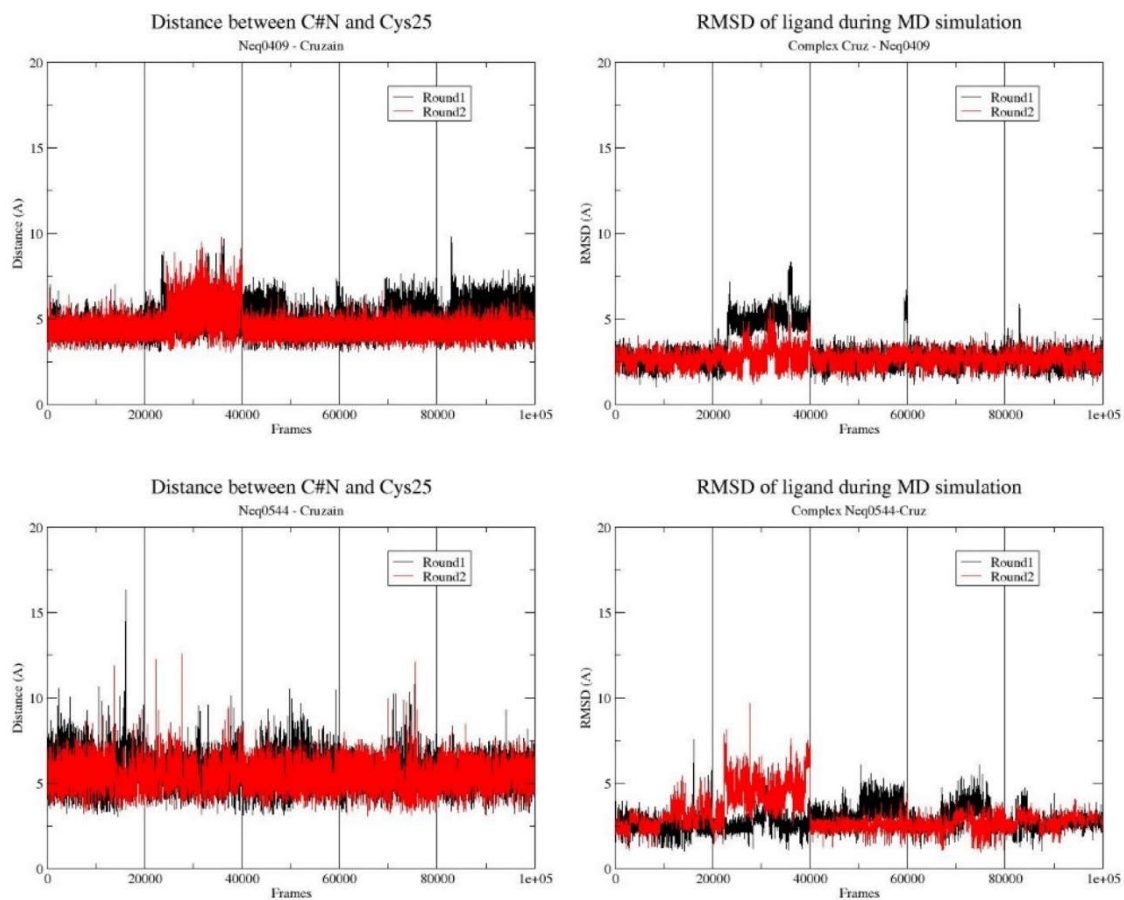
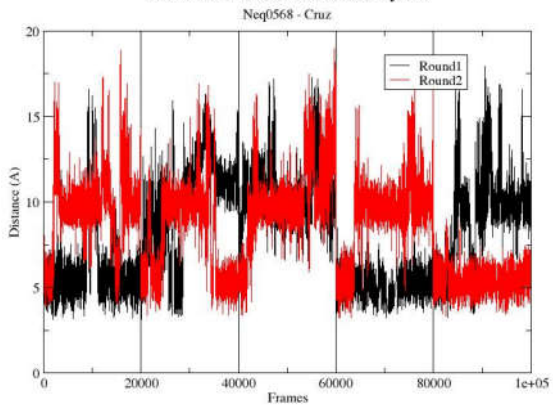


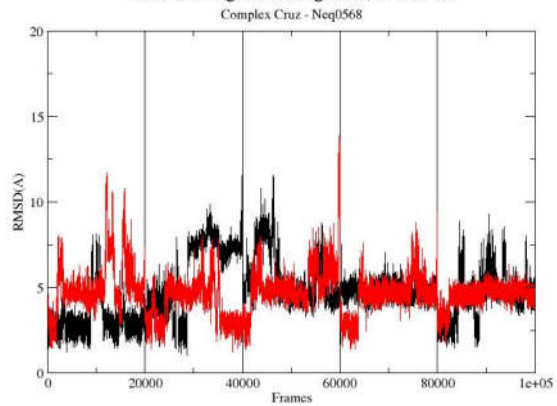
Figure S 6 - Distance (first column) between ligand nitrile and sulfur from Cys25 residue and RMSD of ligand (second column) complexed with cruzain. Black vertical bars delimit the replicates. Black and red lines represent respectively Round 1 and 2 simulations. The rows are respectively Neq0409, Neq0544, Neq0569, Neq0568.



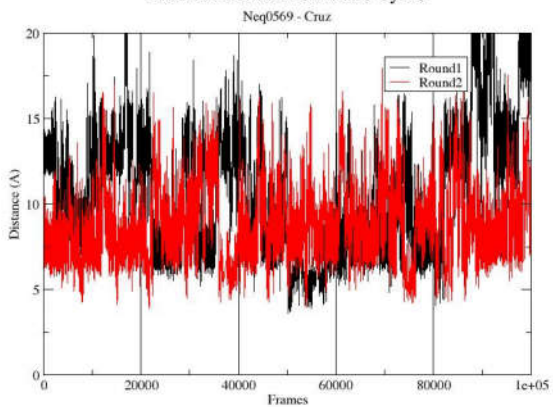
Distance between C#N and Cys25



RMSD of ligand during MD simulation



Distance between C#N and Cys25



RMSD of ligand during MD simulation

