

The Effect of Amino Substituents on the Interactions of Quinazolone Derivatives with *c*-KIT G-Quadruplex: Insight from Molecular Dynamics Simulation Study to Rational Design of Ligands

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Supplementary Information

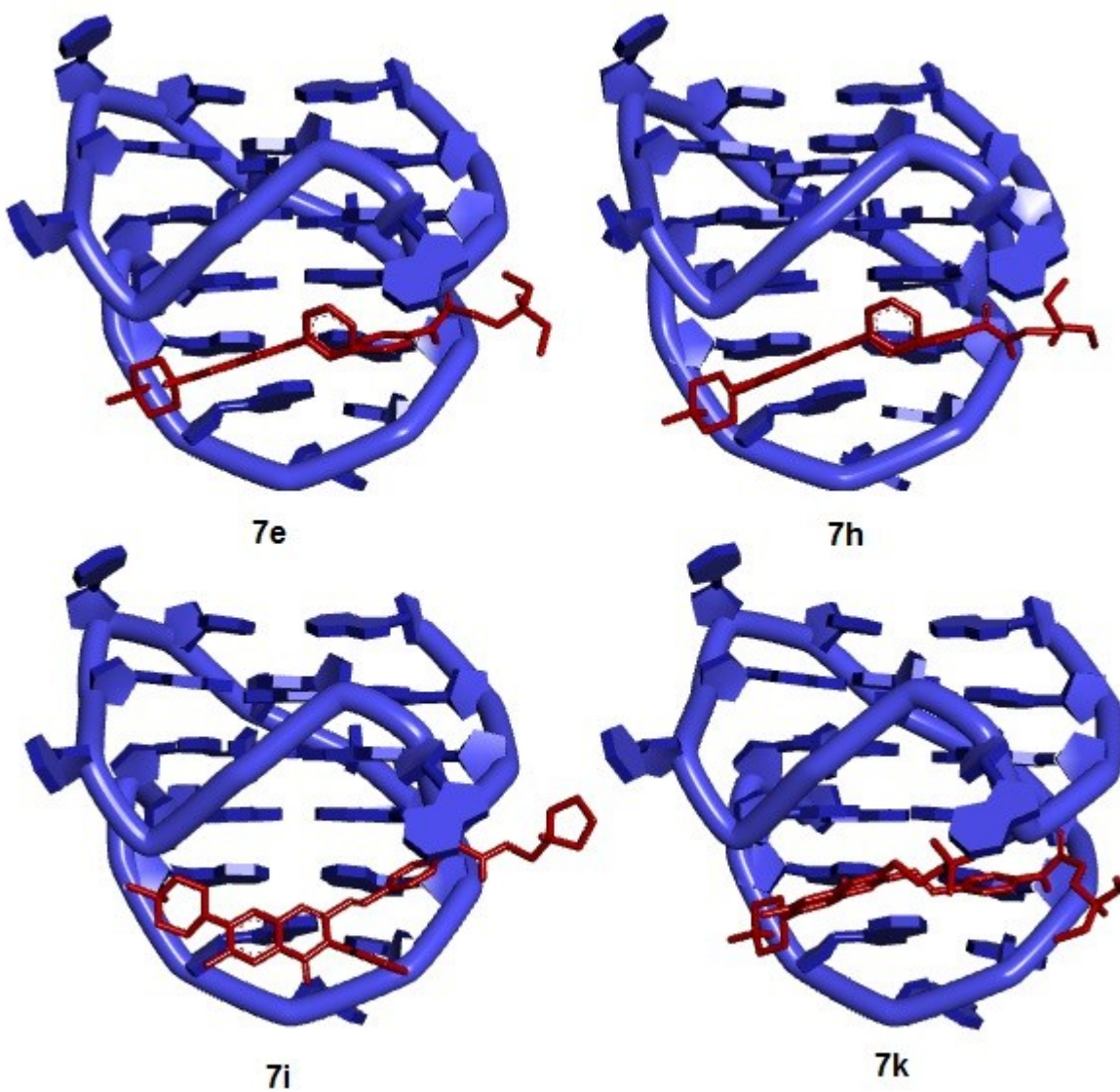


Fig. S1. Structures of ligands and *c-KIT* G-quadruplex after molecular docking are shown in red and blue, respectively.

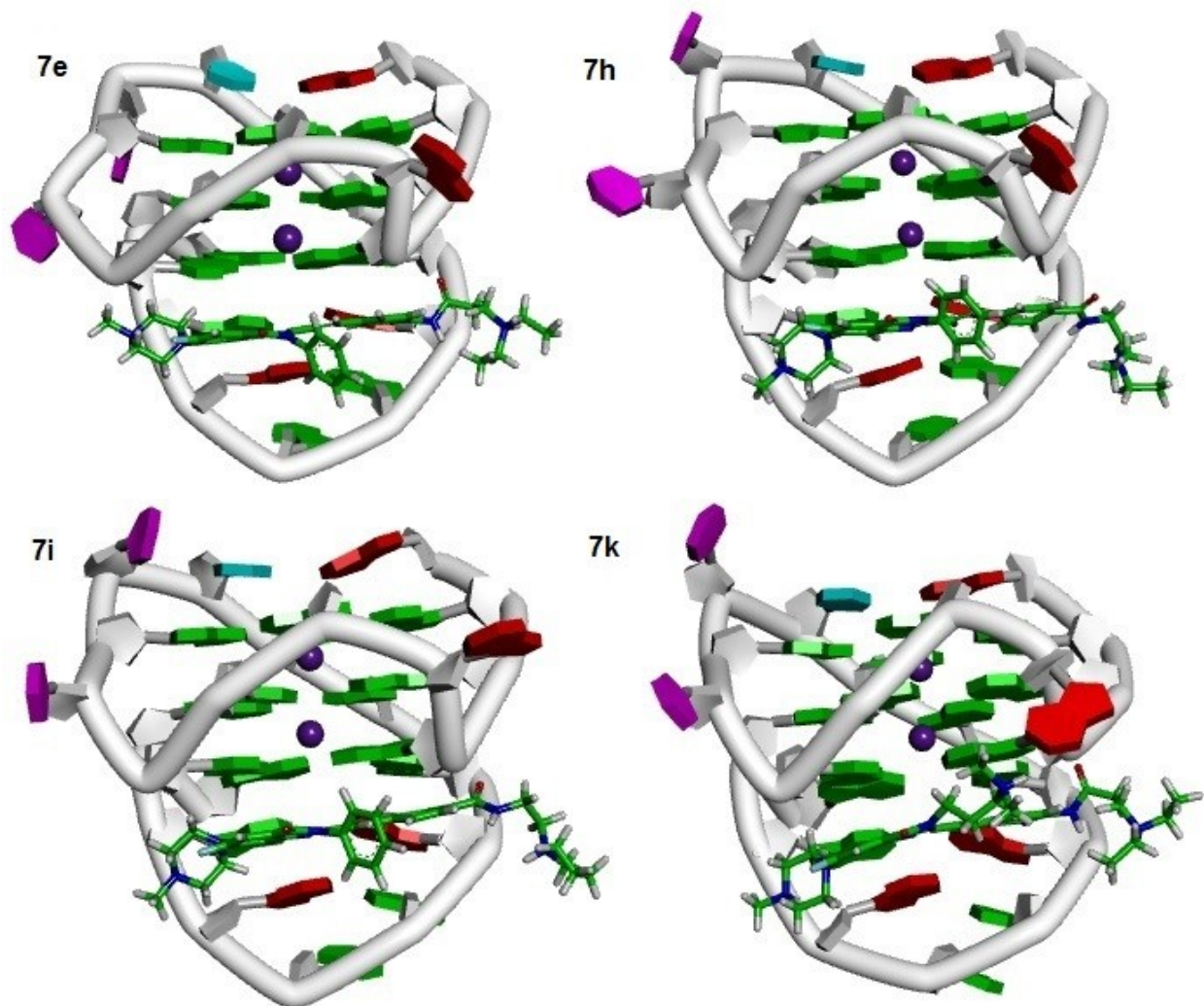


Fig. S2. Final MD structures of the G-quadruplex-ligand complexes after 50 ns simulations. The K^+ ions in the middle of G-quartets are shown as purple spheres.

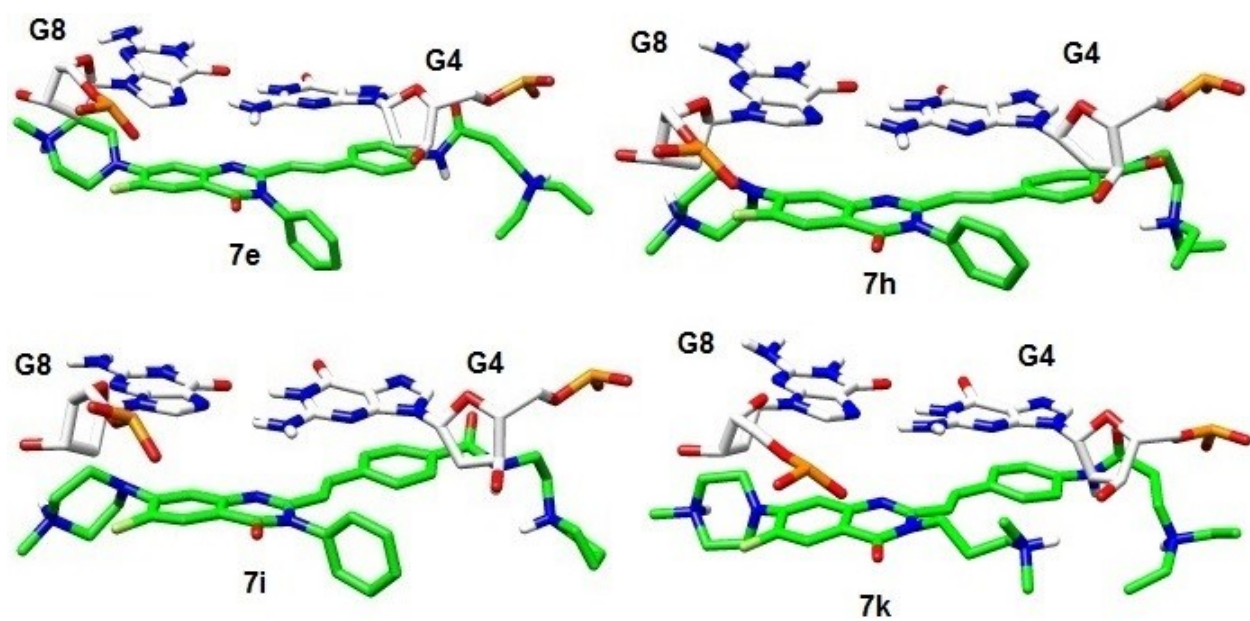


Fig. S3. Stacking interactions between ligands and *c-KIT* G-quadruplex.