Assessment of New Anti-HER2 Ligands Using Combined Docking, QM/MM Scoring and MD Simulation

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Abstract:

In the development of new anti-cancer drugs to tackle the problem of resistance to current chemotherapeutic agents, a new series of anti-HER2 (human epidermal growth factor receptors 2) agents has been synthesized and investigated using different computational methods. Although non-selective, the most active inhibitor in the new series shows higher activity toward HER2 than EGFR. The induced fit docking protocol (IFD) is performed to find possible binding poses of the new inhibitors in the active site of the HER2 receptor. Molecular dynamic simulations of the inhibitor/protein complexes for the two most active compounds from the new series are carried out. Simulations stability is checked using different stability parameters. Different scoring functions are employed.

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