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A study on quantitative structure-activity relationship and molecular docking of Hsp90 inhibitors based on 3, 4-isoxazolediamide scaffold

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In the present study, 3, 4-isoxazolediamide derivatives were proposed as Hsp90 inhibitors for anti-cancer therapy. Genetic algorithm of partial least square (GA-PLS) methods as ligand-based methods was performed to build models to predict the inhibitory activity of Hsp90. The validation of models was performed by leave-one out (LOO) cross-validation method and Y-randomization test to check their predictability. The created GA-PLS model indicated the importance of size, shape, symmetry, and branching in a molecule in inhibitory activities of Hsp90. Applicability domain of the models was determined to screen new compounds. Also, molecular docking studies as a structure-based method were conducted to study the mode of interaction of 3, 4-isoxazolediamide derivatives with Hsp90. The Hsp90 binding site was verified according to the previous studies. The two main residues at the bottom of pocket were Asp93 and Thr184. The docking study indicated that two hydroxyl groups in the resorcinol ring were very important in interacting with Asp93 and the orientation of these groups was related to substitution of different R1 groups.

Biography

Maryam Abbasi is PhD candidate at Department of Medicinal Chemistry in Isfahan University of Medical Sciences. Her thesis is about prediction of new Hsp90 inhibitors by pharmacophore modeling and virtual screening, synthesis and biological test of predicted ligands.

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