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ProbingtheinteractionofCytochromesP450 with new derivatives of 1,3,4-oxadiazole-2-thione using molecular dynamic and docking

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Biography

Reihaneh Sabbaghzadeh is a Laboratory Expert and Faculty of sciences in Department of biology, Hakim Sabzevari, University ,Sabzevar, Iran.

Her recent publications are Various aspects of in vivo drug analysis by QM / MM simulation methods and Evaluation of regional medicinal plants antioxidant activity.

Abstarct

Heterocycles containing more than two hetero atoms are important group of compounds that have many applications in produce organic compounds. Identification evaluation of new 1,3,4-oxadiazole derivatives is the subject of this paper that are obtained from furan and replaced of two CH groups in the ring by nitrogen atoms.In vacuum the system was simulated using molecular dynamic and Langevin dynamics with the HyperChem 7.0 program. The potential energy (kcal/mol) was calculated and temperature was kept at 298,310 and 313 K. The geometry of compounds were optimized using molecular mechanics employing force field designed by Kollman for the simulation of peptides.These studies were demonstrated the chemical interaction between the 5-(((4,5-diphenyl-4H-1,2,4-triazol-3-yl)thio) methyl)-1,3,4-oxadiazole-2-thiol and 2-(5-(((5-mercapto-1,3,4-oxadiazol-2-yl)methyl)thio)-4-phenyl-4H-1,2,4-triazol-3-yl)phenol compounds and shown the potential energy and temperature have a minimum deviation throughout the simulations. Also indicates a stable trajectory of 5-(((4,5-diphenyl-4H-1,2,4-triazol-3-yl)thio) methyl)-1,3,4-oxadiazole-2-thiol compound and the ligating ARG105 residue of active site Cytochromes P450.

Publications

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