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Computational predictions of intracellular thiazovivin interactions as one of the best hESCs apoptosis inhibitors

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Background and Aims: Unlike mouse embryonic stem cells (mESCs), human embryonic stem cells (hESCs) are vulnerable to apoptosis upon dissociation. Considering that apoptosis (which is caused by Rock dependent hyperactivation of actomyosin) can efficiently be suppressed by Rock(Rho dependent kinase) inhibitor, here we compared five common Rock inhibitors to select the most efficient one for preserving the maintenance of dissociated hESCs .
Methods: At first , a computational work carried out using PDB(Protein Data Bank) and Chemspider database to obtain structures of Rock and our candidate inhibitors. Then the number of hydrophobic cavities and their size were determined by CASTp database. After that, 3DLigand server was used to choose suitable cavity, considering its active site. Finally inhibitors binding affinity were compared by the use of Molegro virtual docker software.
Results: Among five selected Rock inhibitors including Thiazovivin, GSK429286A, Fasudil Hcl and Y-27632, Thiazovivin indicated the most efficient binding to the Rock(ΔG=-120 kcal/mol).
Conclusions: Despite common notion about Y-27632 as the best Rock inhibitor, Thiazovivin has much more efficient docking to the Rock and is the best inhibitor among our candidate inhibitors. Thus its efficacy should be checked in an in vivo experiment whether it is a potential ability to maintain the dissociated hESCs.

Keywords: Thizovivin;Y-27632; Rock; hESC.apoptosis