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Molecular dynamics simulations and ADME studies of benzopyran class of selective COX-2 inhibitors for inflammatory activity

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In the present work, 3D-QSAR model was derived by partial least squares method for the prediction of anti-inflammatory activity of benzopyran class of compounds against the COX-2 (cyclooxygenase-2). Partial least squares showed high correlation significant model with (R2training=0.866) and predictability (Q2training=0.66) and indicated that physiochemical descriptors namely, steric, electrostatic, hydrophobic and hydrogen bond acceptor field indicators, correlate well with activity, whereas the potential field contributions indicate that the steric and hydrophobic features of the molecules play an important role in governing their biological activity. A molecular docking interaction pattern analysis reveals the importance of Tyr-361 and Ser-516 of the COX-2 active site for X-ray crystal structures and this class of molecules. Thus the molecular modeling based approaches provided an improved understanding in the interaction between benzopyran class and COX-2 inhibition. These findings may be of immense importance in the anti-inflammatory drug development of an inexpensive and benzopyran class of compounds.

Recent Publications

- Yadav DK, Kumar S, Saloni, Singh H, Kim MH, Sharma P Misra S, Khan F (2017) Molecular docking, QSAR and ADMET studies of withanolide analogs against breast cancer. Drug Design, Development and Therapy 11:1859-1870.
- Yadav DK, Rai R, Kumar N, Singh S, Misra S, Sharma P, Shaw P, Pérez-Sánchez H, Mancera RL, Choi EH, Kim MH, Pratap R (2016) New arylated benzo[h]quinolines induce anti-cancer activity by oxidative stress-mediated DNA damage. Scientific reports 6:38128.
- Yadav DK, Dhawan S, Chauhan A, Qidwai T, Sharma P, Bhakuni RS, Dhawan OP, Khan F (2014) QSAR and docking based semi-synthesis and *in vivo* evaluation of artemisinin derivatives for antimalarial activity. Current Drug Target 15(8):753-61.
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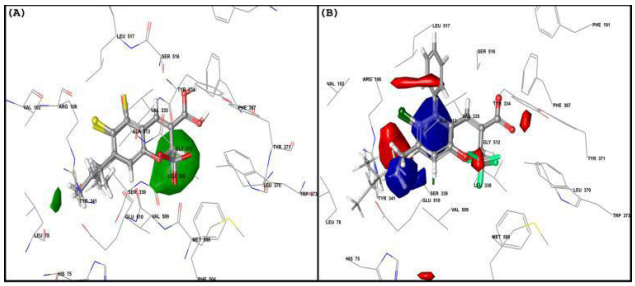
- Yadav DK, Kalani K, Singh AK, Khan F, Srivastava SK, Pant AB (2014) Design, synthesis and *in vitro* evaluation of 18β-glycyrrhetinic Acid derivatives for anticancer activity against human breast cancer cell line MCF-7. Curr Med Chem 21(9):1160-70



Contour maps in protein binding pocket for Gaussian-based 3D-QSAR model. (A) Steric favored regions are shown in green and disfavored regions are shown in yellow. B) Electrostatic favorable electropositive regions are shown in blue and favorable electronegative regions are shown in red

Biography

Saloni received her Post-graduation in Applied Chemistry from Amity University, Noida, UP, India in 2016. During her Post-graduation, she completed her summer training at the 'Centre for Aromatic Plants', Uttarakhand, India where she got brief knowledge of the different medicinal properties of various aromatic plants and also learned to use few instruments in the lab. She also worked as the Research Trainee in the Dept. of Chemistry, University of Delhi, India. She is presently working as a PhD student in College of Pharmacy, Gachon University, Incheon city, Korea. She has published two research articles in reputed international journals with high impact factor. She is continuing her research in Computer-Aided Drug Design Dynamics Simulation of Biological Networks and Plasma Medicine, etc.

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