Latin American Journal of Pharmacy
(formerly *Acta Farmacéutica Bonaerense)*
Lat. Am. J. Pharm. **29** (3): 362-8 (2010)

Original Article

Received: August 16, 2009
Accepted: October 3, 2009

2 D QSAR and Docking of Novel N-substitutedAryl Amine Derivatives as Potential Inhibitors of Lumazine Synthase

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SUMMARY. Fungi play a predominant role in microbial infections with serious health risk to immuno-compromised individuals, including AIDS, cancer, diabetics, newborns and elderly patients. Fungi specific riboflavin metabolism involves lumazine synthase catalyzed synthesis of 6,7-dimethyl-8-D-ribityl lumazine which is converted to riboflavin by a riboflavin synthase. Therefore lumazine synthase has been targeted for design of newer antifungal agents. 32 novel N-substituted aryl amine derivatives have been designed, synthesized, characterized and screened as antifungals. Molecular modelling and docking studies with fungal lumazine synthase using the 32 inhibitors have elucidated unique binding areas within the active site of the enzyme. Amongst the selected 2-D QSAR descriptors, chiV3Cluster and Most +ve Potential show positive correlation with antifungal activity while XX Polarizability, XY Polarizability, Heat of Formation and Quadruple 3 show negative correlation with antifungal activity.

KEY WORDS: 2 D QSAR, Docking, Lumazine synthase.

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ISSN 0326-2383