Curr Synthetic Sys Biol 2015, 3:3
http://dx.doi.org/10.4172/2332-0737.C1.003



## N-QCCA-Novel fragment-based QSAR modeling and combinatorial design of pyrazole derived CRK3 inhibitors as potent anti-leishmanials

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The CRK3 cyclin-dependent kinase of *Leishmania* plays an important role in regulating the cellcycleprogression at the G2-M phase checkpoint transition, proliferation and viability inside thehost macrophage. In this study, a novel fragment based QSAR model has been developed using22 pyrazole derived compounds exhibiting inhibitory activity against Leishmanial CRK3. Unlikeother QSAR methods, this fragment based method gives flexibility to study the relationship between molecular fragments of interest and their contribution for the variation in the biologicalresponse by evaluating cross-term fragment descriptors. Based on the fragment-based QSARmodel, a combinatorial library was generated and top two compounds were reported afterpredicting their activity. The QSAR model showed satisfactory statistical parameters for the dataset (r2=0.8752, q2=0.6690, F-ratio=30.37 and pred-r2=0.8632) with four descriptorsdescribing the nature of substituent groups and the environment of the substitution site. Evaluation of the model implied that electron-rich substitution at R1 position improves theinhibitory activity while decline in inhibitory activity was observed in presence of nitrogen at R2 position. The analysis carried out in this study provides a substantial basis for consideration ofthe designed pyrazole-based leads as potent anti-leishmanial drugs.

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## Randomness and preserved patterns in cancer network

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Breast cancer has been reported to account for the maximum cases among all female cancers till date. Complexity as well as variations at every stage of the cancer renders designing drug targets very difficult. The ample availability of data in functional genomic and proteomic information and the development of high-throughput data-collection techniques have resulted from basic gene-based traditional molecular biology to a systems approach of network biology. In this approach, biological processes are considered as complex networks of interactions between numerous components of the cell rather than as independent interactions involving only a few molecules. We analyze the breast cancer network and its normal counterpart at the proteomic level. The spectral analysis reflects that robustness of the overall system is decreased in the disease but the interactions of the important proteins involved in promoting the disease are preserved and might be one of the reasons behind making those pathways involved with the important proteins highly resistant to various treatments. Detection of important proteins involved in breast cancer using random matrix theory platform provides a time efficient and cost effective approach for those diseases, which lack in-depth information about important genes. The analysis provides a benchmark for designing drugs, which can target a sub graph instead of individual proteins.

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