Amiram Goldblum, Pharm Anal Acta 2016, 7:1 (Suppl)
http://dx.doi.org/10.4172/2153-2435.C1.026

OMICS International
conferenceseries.com

8th International Conference and Exhibition on
Pharmaceutics & Novel Drug Delivery Systems
March 07-09, 2016 Madrid, Spain

Amiram Goldblum
The Hebrew University of Jerusalem, Israel

Current Problems in Drug Discovery and some *in silico* Solutions

Main concepts in drug discovery and design will be examined using protein structures from X-rays for docking and discovering drugs, the single disease single target concept as well as associated issues of selectivity and side effects. Targeting two or more proteins in order to produce single multi-targeted molecules may prove to be a better avenue to effective drugs. Many disease conditions like cancers, bacterial and viral infections, hypertension, neurological disorders and diabetes are currently treated by "drug cocktails" or by single targeted drugs. Those and others have more than a single biochemical pathway or several targets in a pathway leading to disease, therefore multi-targeted single drugs could be more effective than current treatments. Attempts to block proteins to prevent harmful enzyme reactions or protein-protein interactions are failing due to the involvement of these proteins in reactions with other substrates or partners. Therefore the concept of "substrate selective inhibition" (SSI), the tailoring of an inhibitor to block a single or a few and to avoid other substrates has been developed earlier but may be advanced by using computations. I will present an algorithm called "Iterative Stochastic Elimination" that can supply ideas for novel and diverse molecules that are predicted and proven to have multi-targeting abilities and will suggest approaches to the SSI problem.

Biography

Amiram Goldblum is the Head of the Molecular Modeling at the Hebrew University of Jerusalem. He has completed his PhD in Organic Reaction Mechanisms, Jerusalem and Postdoctoral studies of Quantum Biochemistry in Paris and QSAR and QM reaction mechanisms in California. He has developed semi-empirical MNDO/H for dealing with H-bonding in large molecular systems and moved to algorithmic development for dealing with extremely complex problems, for which he received an Award of the COMP division of ACS in 2000.

amiramg@ekmd.huji.ac.il

Notes: