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Network based side-effects prediction system

Kamal Rawal[3], Jaisri Jagannadham[1], Stuti Agrawal[1,2] and Hitesh Kumar Jaiswal[1]
[1]Department of Biotechnology, Jaypee Institute of Information Technology, India
[2]Department of Biological Sciences, Carnegie Mellon University, USA
[3]Mediplex Obesity Clinics, India

Obesity is a global epidemic affecting over 1.5 billion people and one of the risk factor for several diseases such as type 2 diabetes mellitus. We have constructed a comprehensive map of the molecules reported to be implicated in obesity. A new semi-automated text mining system was developed to complement deep curation strategy to screen over 80,863 abstracts. Our map shows bow-tie architecture with 804 nodes and 971 edges classified into 510 proteins, 115 genes, 62 complexes, 23 RNA molecules, 83 simple molecules, 3 phenotype, and 3 drugs. This network fits into power law distribution and shows scale free nature with distinct topological properties. We classify this network into 5 modules and identify new links between newly found genes such as fat mass and obesity associated with well studied examples such as insulin and leptin. Comparison of network with randomized maps reveals interesting aspects about molecular patho-physiology of obesity. We attempt to perturb this network using molecule docking approach using FDA approved drugs such as orlistat, rimnobant, sibutramine etc. We find that these drugs bind strongly to several of their targets as well as off targets in the obesity network. Several of side-effects reported by these drugs such as abdominal pain, nausea, vomiting and loose motions can be explained and predicted using our strategy of network based docking. Our results help in identifying potential drug targets and also serve as a model to test off-targets for existing drugs.

Biography

Kamal Rawal is an interdisciplinary clinical scientist with interests in genomics and systems biology. He integrates advances in sciences in the medical practice. He has published several papers in prestigious international journals and has been invited to deliver talks in international and national conferences. He was a research fellow of Department of Biotechnology (DBT) and Indian Council of Medical Research. He has been awarded grants from Genetic Information Research Institute California, USA; Council for Scientific and Industrial Research and Department of Science and Technology (DST). His medical and research group is actively working in the area of systems biology of obesity and its induced disorders. Previously Consultant and In expert Panel with-Jamia Milia Islamia University; Nehru Homeopathic Medical College and Hospitals Delhi University, NIIT Ltd, Baidynath Ltd, Silico Bioinformatics Ltd, Tekk Source Ltd, Amity University and Rai University.

kamal.rawal@gmail.com