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Interactomics: Computational analysis of novel drug opportunities

We have developed a Computational Analysis of Novel Drug Opportunities (CANDO) platform that analyses compound-proteome interaction signatures to determine drug behavior, in contrast to traditional single target approaches. The platform uses similarity of interaction signatures across all proteins as indicative of similar functional behavior and non similar signatures (or regions of signatures) as indicative of off- and anti-target (side) effects, in effect inferring homology of compound/drug behavior at a proteomic level. We have created a matrix of predicted interactions between 3,733 human ingestible compounds (including FDA approved drugs and supplements)×48,278 proteins using our hierarchical chem and bio-informatic fragment-based docking with dynamics protocol (from over one billion predicted interactions total). We applied our compound-proteome signature comparison and ranking approach to 2030 indications with one approved compound and yielded benchmarking accuracies of 12-25% for 1439 indications with more than approved compound. We are prospectively validating "high value" predictions in vitro, in vivo, and by clinical studies for more than forty indications, including dental caries, dengue, tuberculosis, ovarian cancer, cholangiocarinomas, among many others. 57/1162 predictions over eleven studies show comparable or better activity to existing therapies, or micromolar inhibition at the cellular level, and serve as novel repurposeable therapies. Our approach is applicable to any compound beyond those approved by the FDA, and also include can readily consider mutations in protein structures to enable personalization based on genotype, foreshadowing a new era of faster, safer, better and cheaper drug discovery.

Biography

Ram Samudrala is Professor and Chief of the Division of Bioinformatics at SUNY Buffalo researching multiscale modelling of atomic, molecular, cellular, and physiological systems with more than 110 publications. He was on the University of Washington faculty from 2001-2014 after completing his Postdoctoral work with Michael Levitt (2013 Nobel in Chemistry), Stanford University from 1997-2000 and PhD thesis with John Moult, CARB from 1993-1997. His honours include a Searle Scholar Award (2002). He got MIT Technology Review TR100 selection (2003), Science in Medicine Lecture (2004), a NSF CAREER Award (2005), Alberta Heritage Foundation Visiting Scientist Award (2008), and a NIH Director's Pioneer Award (2010).

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