<https://link.springer.com/article/10.1007%2FBF03256811>

https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3285382/

W. Scott Spangler

<https://researcher.watson.ibm.com/researcher/view_person_pubs.php?person=us-spangles&t=1>

Stephen Wong, Ph.D.

<https://www.houstonmethodist.org/faculty/stephen_wong/>

<https://www.bcm.edu/people/view/stephen-wong-ph-d/b265f2dd-ffed-11e2-be68-080027880ca6>

Scott J. Weir, Pharm.D., Ph.D.

<http://www.kumc.edu/school-of-medicine/pharmacology-toxicology-and-therapeutics/faculty/tenured-and-tenure-track-faculty/scott-weir-pharmd-phd.html>

Tudor Oprea

<https://scholar.google.com/citations?hl=en&user=2O0vLx8AAAAJ&view_op=list_works&sortby=pubdate>

<https://vivo.health.unm.edu/display/n7948>

https://stc.unm.edu/tudor-i-oprea-m-d-ph-d/

\*\*\* https://www.ncbi.nlm.nih.gov/myncbi/tudor.oprea.1/cv/47761/

Description

Computer-assisted drug repurposing. Historical background: Since 1999, most HTS campaigns start by screening the Prestwick library (880 out of patent drugs and natural products) or an equivalent library. This increased availability of drug-target interactions information leads many scientists to believe that these newly-found activities can easily be translated into the clinic. Central finding: After screening up to 1,789 drugs in-house at UNM, an academic setting, and after developing DrugCentral (a database that uses controlled vocabularies for on- and off-label indications, contra-indications, as well as extensive drug-target annotations), Oprea concluded that efficacy and safety are the two most important elements for successful drug repurposing. Influence of the finding: Several academic drug repurposing efforts are now incorporating safety and efficacy in their drug repurposing strategy. Specific role: Oprea introduced drug repurposing in his academic setting by purchasing the first copy of the Prestwick chemical library at UNM, which was later enhanced to nearly 1,800 drugs that are computationally annotated with respect to drug-target interactions, clinical use and formulations (DrugCentral). Oprea served as advisor on nine drug repurposing efforts, of which Raltegravir (NCT01275183) and Ketorolac (NCT01670799) are in phase I clinical trials; Nortriptyline was recently granted a US Patent for treatment of melanoma (8,835,506), whereas R-ketorolac recently got notice of approval from USPTO.

1. Oprea TI, Nielsen SK, Ursu O, Yang JJ, Taboureau O, Mathias SL, Kouskoumvekaki L, Sklar LA, Bologa CG. Associating Drugs, Targets and Clinical Outcomes into an Integrated Network Affords a New Platform for Computer-Aided Drug Repurposing. Mol Inform. 2011 Mar 14;30(2-3):100-111. PubMed PMID: 22287994; NIHMSID: NIHMS347774; PubMed Central PMCID: PMC3266123.
2. Oprea TI, Overington JP. Computational and Practical Aspects of Drug Repositioning. Assay Drug Dev Technol. 2015 Jul-Aug;13(6):299-306. PubMed PMID: 26241209; PubMed Central PMCID: PMC4533090.

Assignment: Describe the research of a leader in your field

Student name: Youcheng ZHANG

Course: BB2899 Project in Molecular Life Science

Principal investigator: Tudor I. Oprea, M.D., Ph.D. Professor and Chief, Translational Informatics Division, UNM School

Website: <https://vivo.health.unm.edu/display/n7948>

Research description:

Professor Oprea lab focuses on translational data science, lead & probe identification, drug informatics and drug repurposing with knowledge and data mining in drug discovery. His central finding is developing DrugCentral database that contains indications as well as drug-target annotations, which brings the influence that several academic drug repurposing efforts incorporated safety and efficacy in their repositioning strategy. Other previous researches also provides understanding biomarker drugability profiling, molecular drug targets mapping and drugs-targets-clinical outcomes network integrations as new approaches for Computer-Aided Drug Repurposing.