

List of scientific publications citing TTD (Aug 12th, 2017)

1. Yang, S. (2007). "Gene amplifications at chromosome 7 of the human gastric cancer genome." *International Journal of Molecular Medicine* 20(2): 225-231.
2. Chen, X. (2013). "Target network analysis of adiponectin, a multifaceted adipokine." *Journal of Cellular Biochemistry* 114(5): 1145-1152.
3. Mayburd, A. L., et al. (2008). "Successful anti-cancer drug targets able to pass FDA review demonstrate the identifiable signature distinct from the signatures of random genes and initially proposed targets." *Bioinformatics* 24(3): 389-395.
4. Porollo, A., et al. (2012). "Analysis of Current Antifungal Agents and Their Targets within the *Pneumocystis carinii* Genome." *Current Drug Targets* 13(12): 1575-1585.
5. Omar, M. A., et al. (2016). "Evaluation of in vitro inhibitory effect of, enoxacin on *Babesia* and *Theileria* parasites." *Experimental Parasitology* 161: 62-67.
6. Legehar, A., et al. (2016). "IDAAPM: integrated database of ADMET and adverse effects of predictive modeling based on FDA approved drug data." *Journal of Cheminformatics* 8.
7. Mora, A. and I. M. Donaldson (2012). "Effects of protein interaction data integration, representation and reliability on the use of network properties for drug target prediction." *Bmc Bioinformatics* 13.
8. Song, Y. and P. Buchwald (2015). "TNF Superfamily Protein-Protein Interactions: Feasibility of Small-Molecule Modulation." *Current Drug Targets* 16(4): 393-408.
9. Tang, J. and T. Aittokallio (2014). "Network Pharmacology Strategies Toward Multi-Target Anticancer Therapies: From Computational Models to Experimental Design Principles." *Current Pharmaceutical Design* 20(1): 23-36.
10. Tian, Z. and Y. Dong (2015). "A network pharmacology study of Sendeng-4, a Mongolian medicine." *Chinese Journal of Natural Medicines* 13(2): 108-118.
11. Kell, D. B., et al. (2013). "The promiscuous binding of pharmaceutical drugs and their transporter-mediated uptake into cells: what we (need to) know and how we can do so." *Drug Discovery Today* 18(5-6): 218-239.
12. Bull, S. C. and A. J. Doig (2015). "Properties of Protein Drug Target Classes." *Plos One* 10(3).
13. Lederer, C. W., et al. (2007). "Pathways and genes differentially expressed in the motor cortex of patients with sporadic amyotrophic lateral sclerosis." *Bmc Genomics* 8.
14. Southan, C., et al. (2011). "Analysis of in vitro bioactivity data extracted from drug discovery literature and patents: Ranking 1654 human protein targets by assayed compounds and molecular scaffolds." *Journal of Cheminformatics* 3.
15. Southan, C., et al. (2013). "Comparing the Chemical Structure and Protein Content of ChEMBL, DrugBank, Human Metabolome Database and the Therapeutic Target Database." *Molecular Informatics* 32(11-12): 881-897.

List of scientific publications citing TTD (Aug 12th, 2017)

16. Wishart, D. S. (2007). "Discovering drug targets through the web." *Comparative Biochemistry and Physiology D-Genomics & Proteomics* 2(1): 9-17.
17. Wishart, D. S. (2012). "Chapter 3: Small Molecules and Disease." *Plos Computational Biology* 8(12).
18. Wishart, D. S., et al. (2006). "DrugBank: a comprehensive resource for in silico drug discovery and exploration." *Nucleic Acids Research* 34: D668-D672.
19. Wishart, D. S., et al. (2008). "DrugBank: a knowledgebase for drugs, drug actions and drug targets." *Nucleic Acids Research* 36: D901-D906.
20. Jadamba, E. and M. Shin (2016). "A Systematic Framework for Drug Repositioning from Integrated Omics and Drug Phenotype Profiles Using Pathway-Drug Network." *Biomed Research International*.
21. Han, L., et al. (2006). "Recent progresses in the application of machine learning approach for predicting protein functional class independent of sequence similarity." *Proteomics* 6(14): 4023-4037.
22. Gao, Z., et al. (2008). "PDTD: a web-accessible protein database for drug target identification." *Bmc Bioinformatics* 9.
23. Lee, S., et al. (2009). "Building a drug-target network and its applications." *Expert Opinion on Drug Discovery* 4(11): 1177-1189.
24. Zhu, F., et al. (2009). "What Are Next Generation Innovative Therapeutic Targets? Clues from Genetic, Structural, Physicochemical, and Systems Profiles of Successful Targets." *Journal of Pharmacology and Experimental Therapeutics* 330(1): 304-315.
25. Gao, N., et al. (2010). "DIGAP - a Database of Improved Gene Annotation for Phytopathogens." *Bmc Genomics* 11.
26. Zhu, F., et al. (2010). "Update of TTD: Therapeutic Target Database." *Nucleic Acids Research* 38: D787-D791.
27. Zhu, F., et al. (2011). "Clustered patterns of species origins of nature-derived drugs and clues for future bioprospecting." *Proceedings of the National Academy of Sciences of the United States of America* 108(31): 12943-12948.
28. Yan, G., et al. (2011). "Genome sequencing and comparison of two nonhuman primate animal models, the cynomolgus and Chinese rhesus macaques." *Nature Biotechnology* 29(11): 1019-U1089.
29. Liu, X., et al. (2011). "The Therapeutic Target Database: an Internet resource for the primary targets of approved, clinical trial and experimental drugs." *Expert Opinion on Therapeutic Targets* 15(8): 903-912.
30. Sun, J., et al. (2012). "DTome: a web-based tool for drug-target interactome construction." *Bmc Bioinformatics* 13.
31. Tao, W., et al. (2012). "Mechanism of Sini Decoction on Coronary Heart Disease in Molecular Level." *Proceedings of the 2nd International Conference on Computer and Information Applications (Iccia 2012)*: 596-599.
32. Zou, J., et al. (2012). "Neighbor communities in drug combination networks characterize synergistic effect." *Molecular Biosystems* 8(12): 3185-3196.

List of scientific publications citing TTD (Aug 12th, 2017)

33. Zhu, F., et al. (2012). "Therapeutic target database update 2012: a resource for facilitating target-oriented drug discovery." *Nucleic Acids Research* 40(D1): D1128-D1136.
34. Qin, C., et al. (2012). "What Does It Take to Synergistically Combine Sub-Potent Natural Products into Drug-Level Potent Combinations?" *Plos One* 7(11).
35. Xie, L., et al. (2012). Novel Computational Approaches to Polypharmacology as a Means to Define Responses to Individual Drugs. *Annual Review of Pharmacology and Toxicology*, Vol 52. P. A. Insel, S. G. Amara and T. F. Blaschke. 52: 361-+.
36. Liu, X., et al. (2013). "Predicting Targeted Polypharmacology for Drug Repositioning and Multi-Target Drug Discovery." *Current Medicinal Chemistry* 20(13): 1646-1661.
37. Tao, W., et al. (2013). Computational Simulation on the Material Basis of Sini Decoction in Treating Coronary Heart Disease. *Advances in Mechatronics and Control Engineering*, Pts 1-3. Y. H. Kim and P. Yarlagadda. 278-280: 535-538.
38. Liu, Y., et al. (2014). "DCDB 2.0: a major update of the drug combination database." *Database-the Journal of Biological Databases and Curation*.
39. Gao, L., et al. (2014). "Discovery of the neuroprotective effects of alvespimycin by computational prioritization of potential anti-parkinson agents." *Febs Journal* 281(4): 1110-1122.
40. Liu, X., et al. (2014). "In Silico target fishing: addressing a "Big Data" problem by ligand-based similarity rankings with data fusion." *Journal of Cheminformatics* 6.
41. Sun, J., et al. (2014). "Network-Assisted Prediction of Potential Drugs for Addiction." *Biomed Research International*.
42. Luo, F., et al. (2014). "Systems pharmacology strategies for anticancer drug discovery based on natural products." *Molecular Biosystems* 10(7): 1912-1917.
43. Qin, C., et al. (2014). "Therapeutic target database update 2014: a resource for targeted therapeutics." *Nucleic Acids Research* 42(D1): D1118-D1123.
44. Guo, Q., et al. (2015). "A Systems Biology Perspective on the Molecular Mechanisms Underlying the Therapeutic Effects of Buyang Huanwu Decoction on Ischemic Stroke." *Rejuvenation Research* 18(4): 313-325.
45. Tao, L., et al. (2015). "Clustered Distribution of Natural Product Leads of Drugs in the Chemical Space as Influenced by the Privileged Target-Sites." *Scientific Reports* 5.
46. Tao, L., et al. (2015). "Co-targeting cancer drug escape pathways confers clinical advantage for multi-target anticancer drugs." *Pharmacological Research* 102: 123-131.
47. Tao, C., et al. (2015). "Colorectal cancer drug target prediction using ontology-based inference and network analysis." *Database-the Journal of Biological Databases and Curation*.

List of scientific publications citing TTD (Aug 12th, 2017)

48. Sun, Y., et al. (2015). "Combining genomic and network characteristics for extended capability in predicting synergistic drugs for cancer." *Nature Communications* 6.
49. Yoo, M., et al. (2015). "DSigDB: drug signatures database for gene set analysis." *Bioinformatics* 31(18): 3069-3071.
50. Lei, Q., et al. (2015). "In silico target fishing and pharmacological profiling for the isoquinoline alkaloids of *Macleaya cordata* (Bo Luo Hui)." *Chinese Medicine* 10.
51. Lin, L., et al. (2015). "SLC transporters as therapeutic targets: emerging opportunities." *Nature Reviews Drug Discovery* 14(8): 543-560.
52. Hur, J., et al. (2015). "Systems Pharmacological Analysis of Drugs Inducing Stevens - Johnson Syndrome and Toxic Epidermal Necrolysis." *Chemical Research in Toxicology* 28(5): 927-934.
53. Qin, C., et al. (2015). "The Assessment of the Readiness of Molecular Biomarker-Based Mobile Health Technologies for Healthcare Applications." *Scientific Reports* 5.
54. Wei, S., et al. (2016). "A network pharmacology approach to discover active compounds and action mechanisms of San-Cao Granule for treatment of liver fibrosis." *Drug Design Development and Therapy* 10: 733-743.
55. Liu, H., et al. (2016). "A Network Pharmacology Approach to Explore the Pharmacological Mechanism of Xiaoyao Powder on Anovulatory Infertility." *Evidence-Based Complementary and Alternative Medicine*.
56. Liu, Z., et al. (2016). "BATMAN-TCM: a Bioinformatics Analysis Tool for Molecular mechanism of Traditional Chinese Medicine." *Scientific Reports* 6.
57. Lee, H., et al. (2016). "Drug Repositioning for Cancer Therapy Based on Large-Scale Drug-Induced Transcriptional Signatures." *Plos One* 11(3).
58. Lin, Y., et al. (2016). "Effect of Glycyrrhiza on the Diuretic Function of *Euphorbia kansui*: An Ascites Mouse Model." *Evidence-Based Complementary and Alternative Medicine*.
59. Xue, W., et al. (2016). "Identification of the inhibitory mechanism of FDA approved selective serotonin reuptake inhibitors: an insight from molecular dynamics simulation study." *Physical Chemistry Chemical Physics* 18(4): 3260-3271.
60. Tan, Y., et al. (2016). "Improving drug safety: From adverse drug reaction knowledge discovery to clinical implementation." *Methods* 110: 14-25.
61. Wei, H., et al. (2016). "Pharmaceutical applications of affinity-ultrafiltration mass spectrometry: Recent advances and future prospects." *Journal of Pharmaceutical and Biomedical Analysis* 131: 444-453.
62. Sun, J., et al. (2016). "To Unveil the Molecular Mechanisms of Qi and Blood through Systems Biology-Based Investigation into Si-Jun-Zi-Tang and Si-Wu-Tang formulae." *Scientific Reports* 6.
63. Liu, R., et al. (2016). "Using Chemical-Induced Gene Expression in Cultured Human Cells to Predict Chemical Toxicity." *Chemical Research in Toxicology* 29(11): 1883-1893.

List of scientific publications citing TTD (Aug 12th, 2017)

64. Lee, A., et al. (2016). "Using reverse docking for target identification and its applications for drug discovery." *Expert Opinion on Drug Discovery* 11(7): 707-715.
65. Kim, P., et al. (2016). "Y ccmGDB: a database for cancer cell metabolism genes." *Nucleic Acids Research* 44(D1): D959-D968.
66. Han, Y., et al. (2017). "Microarray analysis of copy-number variations and gene expression profiles in prostate cancer." *Medicine* 96(28).
67. Mao, Y., et al. (2017). "Network pharmacology-based and clinically relevant prediction of the active ingredients and potential targets of Chinese herbs in metastatic breast cancer patients." *Oncotarget* 8(16): 27007-27021.
68. Han, K., et al. (2017). "Synergistic drug combinations for cancer identified in a CRISPR screen for pairwise genetic interactions." *Nature Biotechnology* 35(5): 463-+.
69. Jasmine, F., et al. (2012). "A Genome-Wide Study of Cytogenetic Changes in Colorectal Cancer Using SNP Microarrays: Opportunities for Future Personalized Treatment." *Plos One* 7(2).
70. Doss, C. G. P., et al. (2014). Computational Approaches and Resources in Single Amino Acid Substitutions Analysis Toward Clinical Research. *Advances in Protein Chemistry and Structural Biology*, Vol 94. R. Donev. 94: 365-423.
71. Nair, D. G., et al. (2015). "Interactions of some commonly used drugs with human alpha-thrombin." *Journal of Biomolecular Structure & Dynamics* 33(5): 1008-1015.
72. Loetsch, J. and A. Ultsch (2016). "A machine-learned computational functional genomics-based approach to drug classification." *European Journal of Clinical Pharmacology* 72(12): 1449-1461.
73. George, J. J. and V. Umrana (2011). "In silico identification of putative drug targets in *Klebsiella pneumoniae* MGH78578." *Indian Journal of Biotechnology* 10(4): 432-439.
74. George, J. J. and V. V. Umrana (2012). "Subtractive Genomics Approach to Identify Putative Drug Targets and Identification of Drug-like Molecules for Beta Subunit of DNA Polymerase III in *Streptococcus* Species." *Applied Biochemistry and Biotechnology* 167(5): 1377-1395.
75. Roix, J. J., et al. (2014). "Systematic Repurposing Screening in Xenograft Models Identifies Approved Drugs with Novel Anti-Cancer Activity." *Plos One* 9(8).
76. Chan, W. K. B., et al. (2015). "GLASS: a comprehensive database for experimentally validated GPCR-ligand associations." *Bioinformatics* 31(18): 3035-3042.
77. Wong, V. K.-W., et al. (2016). "Advanced research technology for discovery of new effective compounds from Chinese herbal medicine and their molecular targets." *Pharmacological Research* 111: 546-555.
78. Perlman, L., et al. (2011). "Combining Drug and Gene Similarity Measures for Drug-Target Elucidation." *Journal of Computational Biology* 18(2): 133-145.

List of scientific publications citing TTD (Aug 12th, 2017)

79. Ghemtio, L., et al. (2016). "Predictive Modeling of Ocular Pharmacokinetics and Adverse Effects." *Current Pharmaceutical Design* 22(46): 6928-6934.
80. Imamura, M., et al. (2016). "Genome-wide association studies in the Japanese population identify seven novel loci for type 2 diabetes." *Nature Communications* 7.
81. Neelapu, N. R. R. and T. Pavani (2013). "Identification of Novel Drug Targets in HpB38, HpP12, HpG27, Hpshi470, HpSJM180 Strains of *Helicobacter pylori* : An In Silico Approach for Therapeutic Intervention." *Current Drug Targets* 14(5): 601-611.
82. Chan, J. N. Y., et al. (2010). "Recent advances and method development for drug target identification." *Trends in Pharmacological Sciences* 31(2): 82-88.
83. Faherty, N., et al. (2016). "Negative autoregulation of BMP dependent transcription by SIN3B splicing reveals a role for RBM39." *Scientific Reports* 6.
84. Hacariz, O. and G. P. Sayers (2016). "The omic approach to parasitic trematode research-a review of techniques and developments within the past 5 years." *Parasitology Research* 115(7): 2523-2543.
85. Kharkar, P. S., et al. (2014). "Reverse docking: a powerful tool for drug repositioning and drug rescue." *Future Medicinal Chemistry* 6(3): 333-342.
86. Tang, Z. Q., et al. (2007). "Derivation of stable microarray cancer-differentiating signatures using consensus scoring of multiple random sampling and gene-ranking consistency evaluation." *Cancer Research* 67(20): 9996-10003.
87. Guimera, R., et al. (2007). "A network-based method for target selection in metabolic networks." *Bioinformatics* 23(13): 1616-1622.
88. Akhondi, S. A., et al. (2015). "Ambiguity of non-systematic chemical identifiers within and between small-molecule databases." *Journal of Cheminformatics* 7.
89. Akhondi, S. A., et al. (2016). "Chemical entity recognition in patents by combining dictionary-based and statistical approaches." *Database-the Journal of Biological Databases and Curation*.
90. Azam, S. S. and A. Shamim (2014). "An insight into the exploration of druggable genome of *Streptococcus gordonii* for the identification of novel therapeutic candidates." *Genomics* 104(3): 203-214.
91. Pezzino, S., et al. (2011). "Systems Biology of Apoptosis and Survival: Implications for Drug Development." *Current Pharmaceutical Design* 17(3): 190-203.
92. Hall, A. S., et al. (2013). "An Overview of Computational Life Science Databases & Exchange Formats of Relevance to Chemical Biology Research." *Combinatorial Chemistry & High Throughput Screening* 16(3): 189-198.
93. Bundela, S., et al. (2014). "Potential Therapeutic Targets for Oral Cancer: ADM, TP53, EGFR, LYN, CTLA4, SKIL, CTGF, CD70." *Plos One* 9(7).

List of scientific publications citing TTD (Aug 12th, 2017)

94. Bundela, S., et al. (2015). "Potential Compounds for Oral Cancer Treatment: Resveratrol, Nimbolide, Lovastatin, Bortezomib, Vorinostat, Berberine, Pterostilbene, Deguelin, Andrographolide, and Colchicine." *Plos One* 10(11).
95. Wong, H. S.-C., et al. (2016). "Characterization of cytokinome landscape for clinical responses in human cancers." *Oncolmmunology* 5(11).
96. Wong, H. S.-C., et al. (2016). "Integrative bioinformatic analyses of an oncogenomic profile reveal the biology of endometrial cancer and guide drug discovery." *Oncotarget* 7(5): 5909-5923.
97. Ou-Yang, S.-s., et al. (2012). "Computational drug discovery." *Acta Pharmacologica Sinica* 33(9): 1131-1140.
98. Brettin, T., et al. (2015). "RASTtk: A modular and extensible implementation of the RAST algorithm for building custom annotation pipelines and annotating batches of genomes." *Scientific Reports* 5.
99. Chen, Y. Z. and C. Y. Ung (2002). "Computer automated prediction of potential therapeutic and toxicity protein targets of bioactive compounds from Chinese medicinal plants." *American Journal of Chinese Medicine* 30(1): 139-154.
100. Prabahar, A. and J. Natarajan (2017). "MicroRNA mediated network motifs in autoimmune diseases and its crosstalk between genes, functions and pathways." *Journal of Immunological Methods* 440: 19-26.
101. Kamburov, A., et al. (2013). "The ConsensusPathDB interaction database: 2013 update." *Nucleic Acids Research* 41(D1): D793-D800.
102. Moskalev, A., et al. (2015). "Geroprotectors.org: a new, structured and curated database of current therapeutic interventions in aging and age-related disease." *Aging-Us* 7(9): 616-628.
103. Verbanac, D., et al. (2005). "Combined in silico and in vitro approach to drug screening." *Croatica Chemica Acta* 78(2): 133-139.
104. Widmeier, E., et al. (2017). "A small molecule screening to detect potential therapeutic targets in human podocytes." *American Journal of Physiology-Renal Physiology* 312(1): F157-F171.
105. Chen, X., et al. (2003). "Can an in silico drug-target search method be used to probe potential mechanisms of medicinal plant ingredients?" *Natural Product Reports* 20(4): 432-444.
106. Wang, L., et al. (2006). "Reconstruction and in silico analysis of the MAPK signaling pathways in the human blood fluke, *Schistosoma japonicum*." *Febs Letters* 580(15): 3677-3686.
107. Knox, C., et al. (2007). Biospider: A web server for automating metabolome annotations.
108. Kuhn, M., et al. (2008). "Large-scale prediction of drug-target relationships." *Febs Letters* 582(8): 1283-1290.
109. Yang, L., et al. (2009). "Harvesting Candidate Genes Responsible for Serious Adverse Drug Reactions from a Chemical-Protein Interactome." *Plos Computational Biology* 5(7).
110. Zhou, X., et al. (2010). "Computational identification of bioactive natural products by structure activity relationship." *Journal of Molecular Graphics & Modelling* 29(1): 38-45.

List of scientific publications citing TTD (Aug 12th, 2017)

111. Tang, Z., et al. (2010). "Identification of N-Glycan Serum Markers Associated with Hepatocellular Carcinoma from Mass Spectrometry Data." *Journal of Proteome Research* 9(1): 104-112.
112. Yang, L., et al. (2010). "Identifying Unexpected Therapeutic Targets via Chemical-Protein Interactome." *Plos One* 5(3): A71-A81.
113. Tian, Y., et al. (2010). "Mapping Tissue-Specific Expression of Extracellular Proteins Using Systematic Glycoproteomic Analysis of Different Mouse Tissues." *Journal of Proteome Research* 9(11): 5837-5847.
114. Zhao, J., et al. (2010). "Molecular networks for the study of TCM Pharmacology." *Briefings in Bioinformatics* 11(4): 417-430.
115. Knox, C., et al. (2011). "DrugBank 3.0: a comprehensive resource for 'Omics' research on drugs." *Nucleic Acids Research* 39: D1035-D1041.
116. Yang, L., et al. (2011). "Exploring Off-Targets and Off-Systems for Adverse Drug Reactions via Chemical-Protein Interactome - Clozapine-Induced Agranulocytosis as a Case Study." *Plos Computational Biology* 7(3).
117. Liao, C., et al. (2011). "Software and resources for computational medicinal chemistry." *Future Medicinal Chemistry* 3(8): 1057-1085.
118. Kuhn, M., et al. (2012). "STITCH 3: zooming in on protein-chemical interactions." *Nucleic Acids Research* 40(D1): D876-D880.
119. Zhou, T., et al. (2013). "Bioinformatics for spermatogenesis: annotation of male reproduction based on proteomics." *Asian Journal of Andrology* 15(5): 594-602.
120. Tian, S., et al. (2013). "Modeling Compound-Target Interaction Network of Traditional Chinese Medicines for Type II Diabetes Mellitus: Insight for Polypharmacology and Drug Design." *Journal of Chemical Information and Modeling* 53(7): 1787-1803.
121. Yang, M., et al. (2013). "Navigating Traditional Chinese Medicine Network Pharmacology and Computational Tools." *Evidence-Based Complementary and Alternative Medicine*.
122. Chen, L., et al. (2013). "Prediction of Effective Drug Combinations by Chemical Interaction, Protein Interaction and Target Enrichment of KEGG Pathways." *Biomed Research International*.
123. Wang, X., et al. (2013). "Systems pharmacology uncovers Janus functions of botanical drugs: activation of host defense system and inhibition of influenza virus replication." *Integrative Biology* 5(2): 351-371.
124. Tang, J., et al. (2013). "Target Inhibition Networks: Predicting Selective Combinations of Druggable Targets to Block Cancer Survival Pathways." *Plos Computational Biology* 9(9).
125. Jeon, J., et al. (2014). "A systematic approach to identify novel cancer drug targets using machine learning, inhibitor design and high-throughput screening." *Genome Medicine* 6.

List of scientific publications citing TTD (Aug 12th, 2017)

126. Quan, Y., et al. (2014). "Dissecting Traditional Chinese Medicines by Omics and Bioinformatics." *Natural Product Communications* 9(9): 1391-1396.
127. Tang, J., et al. (2014). "Making Sense of Large-Scale Kinase Inhibitor Bioactivity Data Sets: A Comparative and Integrative Analysis." *Journal of Chemical Information and Modeling* 54(3): 735-743.
128. Wang, L., et al. (2014). "Potential synergistic effects of Chinese herbal prescription FTZ components detected in blood towards hepatic lipid-modulating targets." *Complementary Therapies in Medicine* 22(5): 887-893.
129. Zhao, M., et al. (2014). "Predicting Protein-Ligand Interactions Based on Chemical Preference Features with its Application to New D-Amino Acid Oxidase Inhibitor Discovery." *Current Pharmaceutical Design* 20(32): 5202-5211.
130. Kuhn, M., et al. (2014). "STITCH 4: integration of protein-chemical interactions with user data." *Nucleic Acids Research* 42(D1): D401-D407.
131. Fang, H., et al. (2015). "Analysis of Cynandione A's Anti-Ischemic Stroke Effects from Pathways and Protein-Protein Interactome." *Plos One* 10(5).
132. Wang, C., et al. (2015). "Construction of a genome-scale metabolic network of the plant pathogen *Pectobacterium carotovorum* provides new strategies for bactericide discovery." *Febs Letters* 589(3): 285-294.
133. Chen, C., et al. (2015). "Creation of a free, Internet-accessible database: the Multiple Target Ligand Database." *Journal of Cheminformatics* 7.
134. Fang, J., et al. (2015). "Discovery of Multitarget-Directed Ligands against Alzheimer's Disease through Systematic Prediction of Chemical Protein Interactions." *Journal of Chemical Information and Modeling* 55(1): 149-164.
135. Isik, Z., et al. (2015). "Drug target prioritization by perturbed gene expression and network information." *Scientific Reports* 5.
136. Amar, D., et al. (2015). "Integrated analysis of numerous heterogeneous gene expression profiles for detecting robust disease-specific biomarkers and proposing drug targets." *Nucleic Acids Research* 43(16): 7779-7789.
137. Kang, X., et al. (2015). "Personalized targeted therapy for esophageal squamous cell carcinoma." *World Journal of Gastroenterology* 21(25): 7648-7658.
138. Paik, H., et al. (2015). "Repurpose terbutaline sulfate for amyotrophic lateral sclerosis using electronic medical records." *Scientific Reports* 5.
139. Chen, X., et al. (2015). "Systematic Analysis of the Associations between Adverse Drug Reactions and Pathways." *Biomed Research International*.
140. Wang, Y., et al. (2015). "Systems Pharmacology Dissecting Holistic Medicine for Treatment of Complex Diseases: An Example Using Cardiocerebrovascular Diseases Treated by TCM." *Evidence-Based Complementary and Alternative Medicine*.

List of scientific publications citing TTD (Aug 12th, 2017)

141. Tang, H., et al. (2016). "A Network Pharmacology Approach to Uncover the Pharmacological Mechanism of XuanHuSuo Powder on Osteoarthritis." *Evidence-Based Complementary and Alternative Medicine*.
142. Dong, J., et al. (2016). "BioTriangle: a web-accessible platform for generating various molecular representations for chemicals, proteins, DNAs/RNAs and their interactions." *Journal of Cheminformatics* 8.
143. Wang, H., et al. (2016). "Current situation and future usage of anticancer drug databases." *Apoptosis* 21(7): 778-794.
144. Chen, X., et al. (2016). "Drug-target interaction prediction: databases, web servers and computational models." *Briefings in Bioinformatics* 17(4): 696-712.
145. Chen, X., et al. (2016). "Large-scale identification of adverse drug reaction-related proteins through a random walk model." *Scientific Reports* 6.
146. Guan, M., et al. (2016). "Pd-Catalyzed sequential beta-C(sp³)-H arylation and intramolecular amination of delta-C(sp²)-H bonds for synthesis of quinolinones via an N,O-bidentate directing group." *Chemical Communications* 52(43): 7043-7046.
147. Wang, C., et al. (2016). "PDID: database of molecular-level putative protein-drug interactions in the structural human proteome." *Bioinformatics* 32(4): 579-586.
148. Zhou, J., et al. (2016). "Progress in the Rational Design for Polypharmacology Drug." *Current Pharmaceutical Design* 22(21): 3182-3189.
149. Wang, L., et al. (2016). "Synthesis and biological evaluation of Oblongifolin C derivatives as c-Met inhibitors." *Bioorganic & Medicinal Chemistry* 24(18): 4120-4128.
150. Zhou, W., et al. (2016). "Systems pharmacology exploration of botanic drug pairs reveals the mechanism for treating different diseases." *Scientific Reports* 6.
151. Zhou, W., et al. (2016). "The antipsychotic drug pimozide inhibits cell growth in prostate cancer through suppression of STAT3 activation." *International Journal of Oncology* 48(1): 322-328.
152. Yang, H., et al. (2016). "Therapeutic target database update 2016: enriched resource for bench to clinical drug target and targeted pathway information." *Nucleic Acids Research* 44(D1): D1069-D1074.
153. Wang, B., et al. (2016). System Prediction of Drug-Drug Interactions Through the Integration of Drug Phenotypic, Therapeutic, Structural, and Genomic Similarities. *Intelligent Computing Theories and Application, Ictic 2016, Pt I*. D. S. Huang, V. Bevilacqua and P. Premaratne. 9771: 377-385.
154. Fang, J., et al. (2017). "AlzhCPI: A knowledge base for predicting chemical-protein interactions towards Alzheimer's disease." *Plos One* 12(5).
155. Mock, A., et al. (2017). "CVE: an R package for interactive variant prioritisation in precision oncology." *Bmc Medical Genomics* 10.

List of scientific publications citing TTD (Aug 12th, 2017)

156. Wang, P., et al. (2017). "Differentiating Physicochemical Properties between Addictive and Nonaddictive ADHD Drugs Revealed by Molecular Dynamics Simulation Studies." *Acs Chemical Neuroscience* 8(6): 1416-1428.
157. Park, S., et al. (2017). "Network mirroring for drug repositioning." *Bmc Medical Informatics and Decision Making* 17.
158. Wang, X., et al. (2017). "Treatment of rheumatoid arthritis with combination of methotrexate and Tripterygium wilfordii: A meta-analysis." *Life Sciences* 171: 45-50.
159. Musshoff, F., et al. (2010). "Pharmacogenetics and forensic toxicology." *Forensic Science International* 203(1-3): 53-62.
160. Cochrane, G. R. and M. Y. Galperin (2010). "The 2010 Nucleic Acids Research Database Issue and online Database Collection: a community of data resources." *Nucleic Acids Research* 38: D1-D4.
161. Heinrich, J. C., et al. (2016). "New HSP27 inhibitors efficiently suppress drug resistance development in cancer cells." *Oncotarget* 7(42): 68156-68169.
162. Griffith, M., et al. (2013). "DGIdb: mining the druggable genome." *Nature Methods* 10(12): 1209-+.
163. Tarasova, O. A., et al. (2015). "QSAR Modeling Using Large-Scale Databases: Case Study for HIV-1 Reverse Transcriptase Inhibitors." *Journal of Chemical Information and Modeling* 55(7): 1388-1399.
164. Csermely, P., et al. (2013). "Structure and dynamics of molecular networks: A novel paradigm of drug discovery A comprehensive review." *Pharmacology & Therapeutics* 138(3): 333-408.
165. Winquist, R. J., et al. (2014). "The fall and rise of pharmacology - (Re-)defining the discipline?" *Biochemical Pharmacology* 87(1): 4-24.
166. Nagaraju, R., et al. (2012). "Design and Evaluation of Fast Dissolving Films Containing Nizatidine." *Indian Journal of Pharmaceutical Education and Research* 46(4): 318-322.
167. Kunimoto, R., et al. (2017). "Application of a New Scaffold Concept for Computational Target Deconvolution of Chemical Cancer Cell Line Screens." *Acs Omega* 2(4): 1463-1468.
168. Corsello, S. M., et al. (2017). "The Drug Repurposing Hub: a next-generation drug library and information resource." *Nature Medicine* 23(4): 405-+.
169. Guenther, S., et al. (2008). "SuperTarget and Matador: resources for exploring drug-target relationships." *Nucleic Acids Research* 36: D919-D922.
170. Blondeau, S., et al. (2010). "Reverse Pharmacognosy: Another Way to Harness the Generosity of Nature." *Current Pharmaceutical Design* 16(15): 1682-1696.
171. Mocellin, S., et al. (2010). "Targeted Therapy Database (TTD): A Model to Match Patient's Molecular Profile with Current Knowledge on Cancer Biology." *Plos One* 5(8).

List of scientific publications citing TTD (Aug 12th, 2017)

172. Paratore, S., et al. (2012). "Identification of Pharmacological Targets in Amyotrophic Lateral Sclerosis Through Genomic Analysis of Deregulated Genes and Pathways." *Current Genomics* 13(4): 321-333.
173. Porcelli, S., et al. (2016). "Possible biomarkers modulating haloperidol efficacy and/or tolerability." *Pharmacogenomics* 17(5): 507-529.
174. Chandran, U., et al. (2015). "Network Pharmacology of Ayurveda Formulation Triphala with Special Reference to Anti-Cancer Property." *Combinatorial Chemistry & High Throughput Screening* 18(9): 846-854.
175. Grolmusz, V. I. (2015). "Identifying diabetes-related important protein targets with few interacting partners with the PageRank algorithm." *Royal Society Open Science* 2(4).
176. Reisdorf, W. C., et al. (2017). "Harnessing public domain data to discover and validate therapeutic targets." *Expert Opinion on Drug Discovery* 12(7): 687-693.
177. Wang, Y.-C., et al. (2010). "Computationally Probing Drug-Protein Interactions Via Support Vector Machine." *Letters in Drug Design & Discovery* 7(5): 370-378.
178. Zhao, X.-M., et al. (2011). "Prediction of Drug Combinations by Integrating Molecular and Pharmacological Data." *Plos Computational Biology* 7(12).
179. Gonzalez-Medina, M., et al. (2016). "Cheminformatic expedition of the chemical space of fungal products." *Future Medicinal Chemistry* 8(12): 1399-1412.
180. Gonzalez-Medina, M., et al. (2016). "Consensus Diversity Plots: a global diversity analysis of chemical libraries." *Journal of Cheminformatics* 8.
181. Yang, H.-T., et al. (2017). "Literature-based discovery of new candidates for drug repurposing." *Briefings in Bioinformatics* 18(3): 488-497.
182. Chen, X.-W., et al. (2012). "Interaction of Herbal Compounds with Biological Targets: A Case Study with Berberine." *Scientific World Journal*.
183. Wang, Z.-Y., et al. (2013). "Metabolite Concentration as a Criterion for Antibacterial Discovery." *Current Computer-Aided Drug Design* 9(3): 412-416.
184. Wang, J.-Y., et al. (2017). "Identifying prognostic signature in ovarian cancer using DirGenerank." *Oncotarget* 8(28): 46398-46413.
185. Okada, Y. (2014). "From the era of genome analysis to the era of genomic drug discovery: a pioneering example of rheumatoid arthritis." *Clinical Genetics* 86(5): 432-440.
186. Tendi, E. A., et al. (2010). "Drug Target Identification for Neuronal Apoptosis Through a Genome Scale Screening." *Current Medicinal Chemistry* 17(26): 2906-2920.
187. Bispo, N. A., et al. (2013). "A Systematic In Silico Search for Target Similarity Identifies Several Approved Drugs with Potential Activity against the Plasmodium falciparum Apicoplast." *Plos One* 8(3).

List of scientific publications citing TTD (Aug 12th, 2017)

188. Silva, L. A., et al. (2015). "In Silico Search of Energy Metabolism Inhibitors for Alternative Leishmaniasis Treatments." *Biomed Research International*.
189. Dahab, A. A., et al. (2016). "Pharmacokinetic variations in cancer patients with liver dysfunction: applications and challenges of pharmacometabolomics." *Cancer Chemotherapy and Pharmacology* 78(3): 465-489.
190. Sneha, P. and C. G. P. Doss (2016). "Gliptins in managing diabetes - Reviewing computational strategy." *Life Sciences* 166: 108-120.
191. Sneha, P. and C. G. P. Doss (2016). *Molecular Dynamics: New Frontier in Personalized Medicine. Advances in Protein Chemistry and Structural Biology, Vol 102: Personalized Medicine*. R. Donev. 102: 181-224.
192. Poret, A. and J.-P. Boissel (2014). "An in silico target identification using Boolean network attractors: Avoiding pathological phenotypes." *Comptes Rendus Biologies* 337(12): 661-678.
193. Egner, U. and R. C. Hillig (2008). "A structural biology view of target drugability." *Expert Opinion on Drug Discovery* 3(4): 391-401.
194. Li, Y. Y. and S. J. M. Jones (2012). "Drug repositioning for personalized medicine." *Genome Medicine* 4.
195. Cheng, F. and Z. Zhao (2014). "Machine learning-based prediction of drug-drug interactions by integrating drug phenotypic, therapeutic, chemical, and genomic properties." *Journal of the American Medical Informatics Association* 21(E2): E278-E286.
196. Engin, H. B., et al. (2012). "A Strategy Based on Protein-Protein Interface Motifs May Help in Identifying Drug Off-Targets." *Journal of Chemical Information and Modeling* 52(8): 2273-2286.
197. Engin, H. B., et al. (2014). "Network-Based Strategies Can Help Mono-and Poly-pharmacology Drug Discovery: A Systems Biology View." *Current Pharmaceutical Design* 20(8): 1201-1207.
198. Boran, A. D. W. and R. Iyengar (2010). "Systems approaches to polypharmacology and drug discovery." *Current Opinion in Drug Discovery & Development* 13(3): 297-309.
199. Myler, P. J. (2008). Searching the Tritryp genomes for drug targets. *Drug Targets in Kinetoplastid Parasites*. H. K. Majumder. 625: 133-140.
200. Haupt, V. J. and M. Schroeder (2011). "Old friends in new guise: repositioning of known drugs with structural bioinformatics." *Briefings in Bioinformatics* 12(4): 312-326.
201. Lopes, T. J. S., et al. (2015). "Identifying problematic drugs based on the characteristics of their targets." *Frontiers in Pharmacology* 6.
202. Zheng, C. J., et al. (2004). "Drug ADME-associated protein database as a resource for facilitating pharmacogenomics research." *Drug Development Research* 62(2): 134-142.
203. Zheng, C. J., et al. (2004). "TRMP: a database of therapeutically relevant multiple pathways." *Bioinformatics* 20(14): 2236-2241.

List of scientific publications citing TTD (Aug 12th, 2017)

204. Zheng, C. J., et al. (2006). "Therapeutic targets: Progress of their exploration and investigation of their characteristics." *Pharmacological Reviews* 58(2): 259-279.
205. Zheng, C. J., et al. (2007). "PharmGED: Pharmacogenetic effect database." *Nucleic Acids Research* 35: D794-D799.
206. Haupt, V. J., et al. (2013). "Drug Promiscuity in PDB: Protein Binding Site Similarity Is Key." *Plos One* 8(6).
207. Neves, B. J., et al. (2015). "In Silico Repositioning-Chemogenomics Strategy Identifies New Drugs with Potential Activity against Multiple Life Stages of *Schistosoma mansoni*." *Plos Neglected Tropical Diseases* 9(1).
208. Yadav, M. K., et al. (2014). "A Knowledge-Based Approach for Identification of Drugs Against Vivapain-2 Protein of *Plasmodium vivax* Through Pharmacophore-Based Virtual Screening with Comparative Modelling." *Applied Biochemistry and Biotechnology* 173(8): 2174-2188.
209. Lahti, J. L., et al. (2012). "Bioinformatics and variability in drug response: a protein structural perspective." *Journal of the Royal Society Interface* 9(72): 1409-1437.
210. Padhy, B. M. and Y. K. Gupta (2011). "Drug repositioning: Re-investigating existing drugs for new therapeutic indications." *Journal of Postgraduate Medicine* 57(2): 153-160.
211. Islam, M. M. and Z. Mohamed (2015). "Computational and Pharmacological Target of Neurovascular Unit for Drug Design and Delivery." *Biomed Research International*.
212. Labbe, C. M., et al. (2013). "iPPI-DB: a manually curated and interactive database of small non-peptide inhibitors of protein-protein interactions." *Drug Discovery Today* 18(19-20): 958-968.
213. Njogu, P. M., et al. (2016). "Computer-Aided Drug Discovery Approaches against the Tropical Infectious Diseases Malaria, Tuberculosis, Trypanosomiasis, and Leishmaniasis." *Acs Infectious Diseases* 2(1): 8-31.
214. Jiang, Z. R. and Y. H. Zhou (2005). "Using bioinformatics for drug target identification from the genome." *American Journal of Pharmacogenomics* 5(6): 387-396.
215. Brown, A. S. and C. J. Patel (2017). "MeSHDD: Literature-based drug-drug similarity for drug repositioning." *Journal of the American Medical Informatics Association* 24(3): 614-618.
216. Zhang, J. W., et al. (2004). "Development of KiBank, a database supporting structure-based drug design." *Computational Biology and Chemistry* 28(5-6): 401-407.
217. Ho, R. J. Y., et al. (2015). "Systems Approach to targeted and long-acting HIV/AIDS therapy." *Drug Delivery and Translational Research* 5(6): 531-539.
218. Ji, Z. L., et al. (2006). "Increasing the odds of drug hit identification by screening against receptor homologs?" *Letters in Drug Design & Discovery* 3(3): 200-204.
219. Zheng, C., et al. (2006). "Progress and problems in the exploration of therapeutic targets." *Drug Discovery Today* 11(9-10): 412-420.

List of scientific publications citing TTD (Aug 12th, 2017)

220. Scior, T., et al. (2007). "Large compound databases for structure-activity relationships studies in drug discovery." *Mini-Reviews in Medicinal Chemistry* 7(8): 851-860.
221. Klipp, E., et al. (2010). "Biochemical network-based drug-target prediction." *Current Opinion in Biotechnology* 21(4): 511-516.
222. Bahar, I., et al. (2010). "Normal Mode Analysis of Biomolecular Structures: Functional Mechanisms of Membrane Proteins." *Chemical Reviews* 110(3): 1463-1497.
223. Ahmed, J., et al. (2011). "CancerResource: a comprehensive database of cancer-relevant proteins and compound interactions supported by experimental knowledge." *Nucleic Acids Research* 39: D960-D967.
224. Cheng, T., et al. (2011). "Identifying Compound-Target Associations by Combining Bioactivity Profile Similarity Search and Public Databases Mining." *Journal of Chemical Information and Modeling* 51(9): 2440-2448.
225. Huang, H., et al. (2012). "C(2)Maps: a network pharmacology database with comprehensive disease-gene-drug connectivity relationships." *Bmc Genomics* 13.
226. Cheng, F., et al. (2012). "Prediction of Chemical-Protein Interactions Network with Weighted Network-Based Inference Method." *Plos One* 7(7).
227. Scior, T., et al. (2012). "Recognizing Pitfalls in Virtual Screening: A Critical Review." *Journal of Chemical Information and Modeling* 52(4): 867-881.
228. Wu, C.-C., et al. (2012). "TARGETgene: A Tool for Identification of Potential Therapeutic Targets in Cancer." *Plos One* 7(8).
229. Ma, X. H., et al. (2012). "Virtual Screening Methods as Tools for Drug Lead Discovery from Large Chemical Libraries." *Current Medicinal Chemistry* 19(32): 5562-5571.
230. Li, G.-B., et al. (2013). "A combined molecular docking-based and pharmacophore-based target prediction strategy with a probabilistic fusion method for target ranking." *Journal of Molecular Graphics & Modelling* 44: 278-285.
231. Zhang, Y., et al. (2013). "A Systems Biology-Based Investigation into the Pharmacological Mechanisms of Wu Tou Tang Acting on Rheumatoid Arthritis by Integrating Network Analysis." *Evidence-Based Complementary and Alternative Medicine*.
232. Cheng, F., et al. (2013). "Adverse Drug Events: Database Construction and in Silico Prediction." *Journal of Chemical Information and Modeling* 53(4): 744-752.
233. Kumar, R., et al. (2013). "CancerDR: Cancer Drug Resistance Database." *Scientific Reports* 3.
234. Zheng, M., et al. (2013). "Computational methods for drug design and discovery: focus on China." *Trends in Pharmacological Sciences* 34(10): 549-559.
235. Cheng, F., et al. (2013). "Prediction of Polypharmacological Profiles of Drugs by the Integration of Chemical, Side Effect, and Therapeutic Space." *Journal of Chemical Information and Modeling* 53(4): 753-762.

List of scientific publications citing TTD (Aug 12th, 2017)

236. Zhang, Y., et al. (2014). "A systems biology-based investigation into the therapeutic effects of Gansui Banxia Tang on reversing the imbalanced network of hepatocellular carcinoma." *Scientific Reports* 4.
237. Huang, Z., et al. (2014). "ASD v2.0: updated content and novel features focusing on allosteric regulation." *Nucleic Acids Research* 42(D1): D510-D516.
238. Okada, Y., et al. (2014). "Genetics of rheumatoid arthritis contributes to biology and drug discovery." *Nature* 506(7488): 376-+.
239. Xiong, M., et al. (2014). "Identification of transcription factors for drug-associated gene modules and biomedical implications." *Bioinformatics* 30(3): 305-309.
240. Kumar, P., et al. (2014). "Information Gateway for Integrated Pharmacogenomics Data-IGIPD." 2014 IEEE International Conference on Big Data (Big Data).
241. Zhang, X., et al. (2014). "Network pharmacology study on the mechanism of traditional Chinese medicine for upper respiratory tract infection." *Molecular Biosystems* 10(10): 2517-2525.
242. Kumar, A., et al. (2014). "PfalDB: An Integrated Drug Target and Chemical Database for *Plasmodium falciparum*." *Current Drug Targets* 15(12): 1089-1093.
243. Jiang, Y., et al. (2014). "Predicting putative adverse drug reaction related proteins based on network topological properties." *Analytical Methods* 6(8): 2692-2698.
244. Cheng, F., et al. (2014). "Quantitative network mapping of the human kinome interactome reveals new clues for rational kinase inhibitor discovery and individualized cancer therapy." *Oncotarget* 5(11): 3697-3710.
245. Zhang, J., et al. (2014). "Systems Pharmacology Dissection of Multi-Scale Mechanisms of Action for Herbal Medicines in Stroke Treatment and Prevention." *Plos One* 9(8).
246. Huang, C., et al. (2014). "Systems pharmacology in drug discovery and therapeutic insight for herbal medicines." *Briefings in Bioinformatics* 15(5): 710-733.
247. Zhang, C., et al. (2015). "Biomarker-based drug safety assessment in the age of systems pharmacology: from foundational to regulatory science." *Biomarkers in Medicine* 9(11): 1241-1252.
248. Zhang, C., et al. (2015). "CFam: a chemical families database based on iterative selection of functional seeds and seed-directed compound clustering." *Nucleic Acids Research* 43(D1): D558-D565.
249. Huang, H., et al. (2015). "DMAP: a connectivity map database to enable identification of novel drug repositioning candidates." *Bmc Bioinformatics* 16.
250. Gupta, A., et al. (2015). "Integrative analysis of ocular complications in atherosclerosis unveils pathway convergence and crosstalk." *Journal of Receptors and Signal Transduction* 35(2): 149-164.
251. Iwata, H., et al. (2015). "Large-Scale Prediction of Beneficial Drug Combinations Using Drug Efficacy and Target Profiles." *Journal of Chemical Information and Modeling* 55(12): 2705-2716.

List of scientific publications citing TTD (Aug 12th, 2017)

252. Zhang, J., et al. (2015). "Systems Pharmacology Dissection of the Anti-Inflammatory Mechanism for the Medicinal Herb Folium Eriobotryae." *International Journal of Molecular Sciences* 16(2): 2913-2941.
253. Zhang, Y., et al. (2015). "Uncovering pharmacological mechanisms of Wu-tou decoction acting on rheumatoid arthritis through systems approaches: drug-target prediction, network analysis and experimental validation." *Scientific Reports* 5.
254. Cheng, F., et al. (2016). "A network-based drug repositioning infrastructure for precision cancer medicine through targeting significantly mutated genes in the human cancer genomes." *Journal of the American Medical Informatics Association* 23(4): 681-691.
255. Zhang, M., et al. (2016). "Drug Repositioning for Alzheimer's Disease Based on Systematic 'omics' Data Mining." *Plos One* 11(12).
256. Zheng, G., et al. (2016). "Exploring the Inhibitory Mechanism of Approved Selective Norepinephrine Reuptake Inhibitors and Reboxetine Enantiomers by Molecular Dynamics Study." *Scientific Reports* 6.
257. Huang, G., et al. (2016). "Large-Scale Prediction of Drug Targets Based on Local and Global Consistency of Chemical-Chemical Networks." *Combinatorial Chemistry & High Throughput Screening* 19(2): 121-128.
258. Zhang, B., et al. (2016). "New strategy for drug discovery by large-scale association analysis of molecular networks of different species." *Scientific Reports* 6.
259. Okada, Y., et al. (2016). "Significant impact of miRNA-target gene networks on genetics of human complex traits." *Scientific Reports* 6.
260. Li, Y. H., et al. (2016). "SVM-Prot 2016: A Web-Server for Machine Learning Prediction of Protein Functional Families from Sequence Irrespective of Similarity." *Plos One* 11(8).
261. Cheng, F., et al. (2016). "Systems Biology-Based Investigation of Cellular Antiviral Drug Targets Identified by Gene-Trap Insertional Mutagenesis." *Plos Computational Biology* 12(9).
262. Zhang, W., et al. (2016). "Systems Pharmacology Dissection of the Integrated Treatment for Cardiovascular and Gastrointestinal Disorders by Traditional Chinese Medicine." *Scientific Reports* 6.
263. Kumar, A., et al. (2016). "Target identification in *Fusobacterium nucleatum* by subtractive genomics approach and enrichment analysis of host-pathogen protein-protein interactions." *Bmc Microbiology* 16.
264. Li, Y. H., et al. (2016). "The Human Kinome Targeted by FDA Approved Multi-Target Drugs and Combination Products: A Comparative Study from the Drug-Target Interaction Network Perspective." *Plos One* 11(11).
265. Xiang, Z., et al. (2016). "The study on serum and urine of renal interstitial fibrosis rats induced by unilateral ureteral obstruction based on metabonomics and network analysis methods." *Analytical and Bioanalytical Chemistry* 408(10): 2607-2619.
266. Zheng, C., et al. (2016). "Understanding the diverse functions of Huatan Tongluo Fang on rheumatoid arthritis from a pharmacological perspective." *Experimental and Therapeutic Medicine* 12(1): 87-94.

List of scientific publications citing TTD (Aug 12th, 2017)

267. Iwata, M., et al. (2017). "Elucidating the modes of action for bioactive compounds in a cell-specific manner by large-scale chemically-induced transcriptomics." *Scientific Reports* 7.
268. Mirza, N., et al. (2017). "Identifying new antiepileptic drugs through genomics-based drug repurposing." *Human Molecular Genetics* 26(3): 527-537.
269. Cheng, F., et al. (2017). "Individualized network-based drug repositioning infrastructure for precision oncology in the panomics era." *Briefings in Bioinformatics* 18(4): 682-697.
270. Liang, X., et al. (2017). "LRSSL: predict and interpret drug-disease associations based on data integration using sparse subspace learning." *Bioinformatics* 33(8): 1187-1196.
271. Mayer, B., et al. (2017). "Predictive Biomarkers for Linking Disease Pathology and Drug Effect." *Current Pharmaceutical Design* 23(1): 29-54.
272. Finan, C., et al. (2017). "The druggable genome and support for target identification and validation in drug development." *Science Translational Medicine* 9(383).
273. Huang, L.-C., et al. (2015). "A weighted and integrated drug-target interactome: drug repurposing for schizophrenia as a use case." *Bmc Systems Biology* 9.
274. Zhang, X.-D., et al. (2016). "The exploration of network motifs as potential drug targets from post-translational regulatory networks." *Scientific Reports* 6.
275. Chung, F.-H., et al. (2014). "Functional Module Connectivity Map (FMCM): A Framework for Searching Repurposed Drug Compounds for Systems Treatment of Cancer and an Application to Colorectal Adenocarcinoma." *Plos One* 9(1).
276. Chung, F.-H., et al. (2015). "Gene-Set Local Hierarchical Clustering (GSLHC)-A Gene Set-Based Approach for Characterizing Bioactive Compounds in Terms of Biological Functional Groups." *Plos One* 10(10).
277. Zheng, C.-S., et al. (2013). "Network pharmacology-based prediction of the multi-target capabilities of the compounds in Taohong Siwu decoction, and their application in osteoarthritis." *Experimental and Therapeutic Medicine* 6(1): 125-132.
278. Zheng, C.-S., et al. (2014). "In silico search for multi- target therapies for osteoarthritis based on 10 common Huoxue Huayu herbs and potential applications to other diseases." *Molecular Medicine Reports* 9(3): 857-862.
279. Zheng, C.-S., et al. (2014). "Understanding the polypharmacological anticancer effects of Xiao Chai Hu Tang via a computational pharmacological model." *Experimental and Therapeutic Medicine* 7(6): 1777-1783.
280. Lavecchia, A. and C. Cerchia (2016). "In silico methods to address polypharmacology: current status, applications and future perspectives." *Drug Discovery Today* 21(2): 288-298.
281. Boumehira, A. Z., et al. (2016). "Recent progress on the development of antibiotics from the genus *Micromonospora*." *Biotechnology and Bioprocess Engineering* 21(2): 199-223.

List of scientific publications citing TTD (Aug 12th, 2017)

282. Cichonska, A., et al. (2015). "Identification of drug candidates and repurposing opportunities through compound-target interaction networks." *Expert Opinion on Drug Discovery* 10(12): 1333-1345.
283. Martorana, A., et al. (2016). "The Repurposing of Old Drugs or Unsuccessful Lead Compounds by in Silico Approaches: New Advances and Perspectives." *Current Topics in Medicinal Chemistry* 16(19): 2088-2106.
284. Jamali, A. A., et al. (2016). "DrugMiner: comparative analysis of machine learning algorithms for prediction of potential druggable proteins." *Drug Discovery Today* 21(5): 718-724.
285. Pawson, A. J., et al. (2014). "The IUPHAR/BPS Guide to PHARMACOLOGY: an expert-driven knowledgebase of drug targets and their ligands." *Nucleic Acids Research* 42(D1): D1098-D1106.
286. Bansal, A. K. (2008). "Role of bioinformatics in the development of new antibacterial therapy." *Expert Review of Anti-Infective Therapy* 6(1): 51-65.
287. Wattam, A. R., et al. (2017). "Improvements to PATRIC, the all-bacterial Bioinformatics Database and Analysis Resource Center." *Nucleic Acids Research* 45(D1): D535-D542.
288. Merino, A., et al. (2010). "Drug profiling: knowing where it hits." *Drug Discovery Today* 15(17-18): 749-756.
289. Kim, J.-A., et al. (2016). "Comprehensive functional analysis of the tousel-like kinase 2 frequently amplified in aggressive luminal breast cancers." *Nature Communications* 7.
290. Lauria, A., et al. (2016). "Drugs Polypharmacology by In Silico Methods: New Opportunities in Drug Discovery." *Current Pharmaceutical Design* 22(21): 3073-3081.
291. Shanmugham, B. and A. Pan (2013). "Identification and Characterization of Potential Therapeutic Candidates in Emerging Human Pathogen Mycobacterium abscessus: A Novel Hierarchical In Silico Approach." *Plos One* 8(3).
292. Duardo-Sanchez, A., et al. (2015). "MI-NODES Multiscale Models of Metabolic Reactions, Brain Connectome, Ecological, Epidemic, World Trade, and Legal-Social Networks." *Current Bioinformatics* 10(5): 692-713.
293. Jin, G. and S. T. C. Wong (2014). "Toward better drug repositioning: prioritizing and integrating existing methods into efficient pipelines." *Drug Discovery Today* 19(5): 637-644.
294. Koutsoukas, A., et al. (2011). "From in silico target prediction to multi-target drug design: Current databases, methods and applications." *Journal of Proteomics* 74(12): 2554-2574.
295. Pan, J.-B., et al. (2014). "High-throughput identification of off-targets for the mechanistic study of severe adverse drug reactions induced by analgesics." *Toxicology and Applied Pharmacology* 274(1): 24-34.
296. Ligeti, B., et al. (2015). "A Network-Based Target Overlap Score for Characterizing Drug Combinations: High Correlation with Cancer Clinical Trial Results." *Plos One* 10(6).
297. Ligeti, B., et al. (2017). "Propagation on Molecular Interaction Networks: Prediction of Effective Drug Combinations and Biomarkers in Cancer Treatment." *Current Pharmaceutical Design* 23(1): 5-28.

List of scientific publications citing TTD (Aug 12th, 2017)

298. Gohlke, B.-O., et al. (2016). "CancerResource-updated database of cancer-relevant proteins, mutations and interacting drugs." *Nucleic Acids Research* 44(D1): D932-D937.
299. Hao, D. C. and P. G. Xiao (2014). "Network Pharmacology: A Rosetta Stone for Traditional Chinese Medicine." *Drug Development Research* 75(5): 299-312.
300. Greene, C. S. and B. F. Voight (2016). "Pathway and network-based strategies to translate genetic discoveries into effective therapies." *Human Molecular Genetics* 25(R2): R94-R98.
301. Greene, C. S., et al. (2015). "Understanding multicellular function and disease with human tissue-specific networks." *Nature Genetics* 47(6): 569-576.
302. Senger, C., et al. (2012). "Mining and evaluation of molecular relationships in literature." *Bioinformatics* 28(5): 709-714.
303. Lin, C.-C., et al. (2015). "Regulation rewiring analysis reveals mutual regulation between STAT1 and miR-155-5p in tumor immunosurveillance in seven major cancers." *Scientific Reports* 5.
304. Peragovics, A., et al. (2016). "Modeling Polypharmacological Profiles by Affinity Fingerprinting." *Current Pharmaceutical Design* 22(46): 6885-6894.
305. Barlow, D. J., et al. (2012). "In-silico studies in Chinese herbal medicines' research: Evaluation of in-silico methodologies and phytochemical data sources, and a review of research to date." *Journal of Ethnopharmacology* 140(3): 526-534.
306. Rhodes, D. R., et al. (2004). "ONCOMINE: A cancer microarray database and integrated data-mining platform." *Neoplasia* 6(1): 1-6.
307. Borckholder, C., et al. (2013). A generic, service-based data integration framework applied to linking drugs & clinical trials. 4th International Conference on Computational Systems-Biology and Bioinformatics. S. B. Cho, J. H. Chan and K. B. Hwang. 23: 24-35.
308. Danishuddin, M. and A. U. Khan (2015). "Structure based virtual screening to discover putative drug candidates: Necessary considerations and successful case studies." *Methods* 71: 135-145.
309. Ilardi, E. A., et al. (2013). "An In-Pharm-ative Educational Poster Anthology Highlighting the Therapeutic Agents That Chronicle Our Medicinal History." *Journal of Chemical Education* 90(10): 1403-1405.
310. Fadhal, E., et al. (2014). "Modelling human protein interaction networks as metric spaces has potential in disease research and drug target discovery." *Bmc Systems Biology* 8.
311. Soysal, E., et al. (2017). "CATTLE (CAnCER treatment treasury with linked evidence): An integrated knowledge base for personalized oncology research and practice." *Cpt-Pharmacometrics & Systems Pharmacology* 6(3): 188-196.
312. Villoutreix, B. O., et al. (2007). "Free resources to assist structure-based virtual ligand screening experiments." *Current Protein & Peptide Science* 8(4): 381-411.

List of scientific publications citing TTD (Aug 12th, 2017)

313. Goonesekere, N. C. W., et al. (2014). "A Meta Analysis of Pancreatic Microarray Datasets Yields New Targets as Cancer Genes and Biomarkers." *Plos One* 9(4).
314. Garcia-Serna, R., et al. (2015). "Large-Scale Predictive Drug Safety: From Structural Alerts to Biological Mechanisms." *Chemical Research in Toxicology* 28(10): 1875-1887.
315. Li, H., et al. (2006). "TarFisDock: a web server for identifying drug targets with docking approach." *Nucleic Acids Research* 34: W219-W224.
316. Xu, H., et al. (2007). "Learning the drug target-likeness of a protein." *Proteomics* 7(23): 4255-4263.
317. Ye, H., et al. (2011). "HIT: linking herbal active ingredients to targets." *Nucleic Acids Research* 39: D1055-D1059.
318. Li, X., et al. (2012). "A System-Level Investigation into the Mechanisms of Chinese Traditional Medicine: Compound Danshen Formula for Cardiovascular Disease Treatment." *Plos One* 7(9).
319. Yu, H., et al. (2012). "A Systematic Prediction of Multiple Drug-Target Interactions from Chemical, Genomic, and Pharmacological Data." *Plos One* 7(5).
320. Gu, J., et al. (2013). "CVDHD: a cardiovascular disease herbal database for drug discovery and network pharmacology." *Journal of Cheminformatics* 5.
321. Fu, C., et al. (2013). "DrugMap Central: an on-line query and visualization tool to facilitate drug repositioning studies." *Bioinformatics* 29(14): 1834-1836.
322. Ge, H., et al. (2013). "Molecular Dynamics-Based Virtual Screening: Accelerating the Drug Discovery Process by High-Performance Computing." *Journal of Chemical Information and Modeling* 53(10): 2757-2764.
323. Gu, J., et al. (2013). "Use of Natural Products as Chemical Library for Drug Discovery and Network Pharmacology." *Plos One* 8(4).
324. Xu, H., et al. (2014). "A Systems Biology-Based Approach to Uncovering the Molecular Mechanisms Underlying the Effects of Dragon's Blood Tablet in Colitis, Involving the Integration of Chemical Analysis, ADME Prediction, and Network Pharmacology." *Plos One* 9(7).
325. Li, B., et al. (2014). "Elucidating Polypharmacological Mechanisms of Polyphenols by Gene Module Profile Analysis." *International Journal of Molecular Sciences* 15(7): 11245-11254.
326. Li, P., et al. (2014). "Insights from systems pharmacology into cardiovascular drug discovery and therapy." *Bmc Systems Biology* 8.
327. Li, Y., et al. (2014). "Investigation into the mechanism of *Eucommia ulmoides* Oliv. based on a systems pharmacology approach." *Journal of Ethnopharmacology* 151(1): 452-460.
328. Li, P., et al. (2014). "Systems pharmacology strategies for drug discovery and combination with applications to cardiovascular diseases." *Journal of Ethnopharmacology* 151(1): 93-107.

List of scientific publications citing TTD (Aug 12th, 2017)

329. Fu, P., et al. (2014). "Target network differences between western drugs and Chinese herbal ingredients in treating cardiovascular disease." *Bmc Bioinformatics* 15.
330. Ru, J., et al. (2014). "TCMSP: a database of systems pharmacology for drug discovery from herbal medicines." *Journal of Cheminformatics* 6.
331. Li, P., et al. (2015). "An Effective Method to Identify Shared Pathways and Common Factors among Neurodegenerative Diseases." *Plos One* 10(11).
332. Fu, Y., et al. (2015). "Exploring the relationship between hub proteins and drug targets based on GO and intrinsic disorder." *Computational Biology and Chemistry* 56: 41-48.
333. Li, W., et al. (2015). "Identifying Prognostic Features by Bottom-Up Approach and Correlating to Drug Repositioning." *Plos One* 10(3).
334. Li, P., et al. (2015). "Large-scale exploration and analysis of drug combinations." *Bioinformatics* 31(12): 2007-2016.
335. Li, Y., et al. (2015). "Systems pharmacology to decipher the combinational anti-migraine effects of Tianshu formula." *Journal of Ethnopharmacology* 174: 45-56.
336. Li, X., et al. (2016). "Biomolecular Network-Based Synergistic Drug Combination Discovery." *Biomed Research International*.
337. Xu, J., et al. (2016). "Comparison of FDA Approved Kinase Targets to Clinical Trial Ones: Insights from Their System Profiles and Drug-Target Interaction Networks." *Biomed Research International*.
338. Ye, H., et al. (2016). "Drug Repositioning Through Network Pharmacology." *Current Topics in Medicinal Chemistry* 16(30): 3646-3656.
339. Xu, H., et al. (2016). "Identification of key active constituents of Buchang Naoxintong capsules with therapeutic effects against ischemic stroke by using an integrative pharmacology-based approach." *Molecular Biosystems* 12(1): 233-245.
340. Yi, F., et al. (2016). "In silico profiling for secondary metabolites from *Lepidium meyenii* (maca) by the pharmacophore and ligand-shape-based joint approach." *Chinese Medicine* 11.
341. Li, B., et al. (2016). "Performance Evaluation and Online Realization of Data-driven Normalization Methods Used in LC/MS based Untargeted Metabolomics Analysis." *Scientific Reports* 6.
342. Xu, X., et al. (2016). "SM-TF: A Structural Database of Small Molecule-Transcription Factor Complexes." *Journal of Computational Chemistry* 37(17): 1559-1564.
343. Xu, Q., et al. (2017). "ADMETNet: The knowledge base of pharmacokinetics and toxicology network." *Journal of Genetics and Genomics* 44(5): 273-276.
344. Ma, W., et al. (2017). "An analysis of human microbe-disease associations." *Briefings in Bioinformatics* 18(1): 85-97.

List of scientific publications citing TTD (Aug 12th, 2017)

345. Wu, H., et al. (2017). "DrugSig: A resource for computational drug repositioning utilizing gene expression signatures." *Plos One* 12(5).
346. Yu, L., et al. (2017). "Identification of MYST3 as a novel epigenetic activator of ER alpha frequently amplified in breast cancer." *Oncogene* 36(20): 2910-2918.
347. Li, B., et al. (2017). "NOREVA: normalization and evaluation of MS-based metabolomics data." *Nucleic Acids Research* 45(W1): W162-W170.
348. Xu, T., et al. (2017). "Systematically characterize the absorbed effective substances of Wutou Decoction and their metabolic pathways in rat plasma using UHPLC-Q-TOF-MS combined with a target network pharmacological analysis." *Journal of Pharmaceutical and Biomedical Analysis* 141: 95-107.
349. Bezhentsev, V. M., et al. (2017). "WEB RESOURCES FOR DISCOVERY AND DEVELOPMENT OF NEW MEDICINES." *Pharmaceutical Chemistry Journal* 51(2): 91-99.
350. de Chasse, B., et al. (2014). "Virus-host interactomics: new insights and opportunities for antiviral drug discovery." *Genome Medicine* 6.
351. Lin, S.-F., et al. (2008). A tool for finding possible explanation for adverse drug reactions through drug and drug target interactions. *Bmei 2008: Proceedings of the International Conference on Biomedical Engineering and Informatics, Vol 1*: 580-+.
352. Lin, S.-F., et al. (2010). "Analysis of adverse drug reactions using drug and drug target interactions and graph-based methods." *Artificial Intelligence in Medicine* 48(2-3): 161-166.
353. Vitali, F., et al. (2016). "A Network-Based Data Integration Approach to Support Drug Repurposing and Multi-Target Therapies in Triple Negative Breast Cancer." *Plos One* 11(9).
354. Schomburg, K. T., et al. (2014). "Facing the Challenges of Structure-Based Target Prediction by Inverse Virtual Screening." *Journal of Chemical Information and Modeling* 54(6): 1676-1686.
355. Dac-Trung, N., et al. (2017). "Pharos: Collating protein information to shed light on the druggable genome." *Nucleic Acids Research* 45(D1): D995-D1002.
356. Nicola, G., et al. (2012). "Public Domain Databases for Medicinal Chemistry." *Journal of Medicinal Chemistry* 55(16): 6987-7002.
357. Manyam, G., et al. (2012). "Relax with CouchDB - Into the non-relational DBMS era of bioinformatics." *Genomics* 100(1): 1-7.
358. Shende, G., et al. (2017). "PBIT: Pipeline Builder for Identification of drug Targets for infectious diseases." *Bioinformatics* 33(6): 929-931.
359. Roider, H. G., et al. (2014). "Drug2Gene: an exhaustive resource to explore effectively the drug-target relation network." *Bmc Bioinformatics* 15.

List of scientific publications citing TTD (Aug 12th, 2017)

360. Lee, J.-H., et al. (2012). "CDA: Combinatorial Drug Discovery Using Transcriptional Response Modules." *Plos One* 7(8).
361. Lee, J.-H., et al. (2015). "PharmDB-K: Integrated Bio-Pharmacological Network Database for Traditional Korean Medicine." *Plos One* 10(11).
362. Hindumathi, V., et al. (2014). "The prediction of candidate genes for cervix related cancer through gene ontology and graph theoretical approach." *Molecular Biosystems* 10(6): 1450-1460.
363. Daminelli, S., et al. (2012). "Drug repositioning through incomplete bi-cliques in an integrated drug-target-disease network." *Integrative Biology* 4(7): 778-788.
364. Yamanishi, Y., et al. (2014). "DINIES: drug-target interaction network inference engine based on supervised analysis." *Nucleic Acids Research* 42(W1): W39-W45.
365. Subramaniam, S., et al. (2011). "Bioinformatics and Systems Biology of the Lipidome." *Chemical Reviews* 111(10): 6452-6490.
366. Toro-Dominguez, D., et al. (2017). "Support for phosphoinositol 3 kinase and mTOR inhibitors as treatment for lupus using in-silico drug-repurposing analysis." *Arthritis Research & Therapy* 19.
367. Nickel, J., et al. (2014). "SuperPred: update on drug classification and target prediction." *Nucleic Acids Research* 42(W1): W26-W31.
368. Yue, S.-J., et al. (2017). "Herb pair Danggui-Honghua: mechanisms underlying blood stasis syndrome by system pharmacology approach." *Scientific Reports* 7.
369. Kuchta, K., et al. (2012). "DNAtraffic-a new database for systems biology of DNA dynamics during the cell life." *Nucleic Acids Research* 40(D1): D1235-D1240.
370. Jensen, K., et al. (2014). "Integrated Text Mining and Chemoinformatics Analysis Associates Diet to Health Benefit at Molecular Level." *Plos Computational Biology* 10(1).
371. Jensen, K., et al. (2015). "Developing a Molecular Roadmap of Drug-Food Interactions." *Plos Computational Biology* 11(2).
372. Jensen, K., et al. (2015). "NutriChem: a systems chemical biology resource to explore the medicinal value of plant-based foods." *Nucleic Acids Research* 43(D1): D940-D945.
373. Papanikolaou, N., et al. (2016). "DrugQuest - a text mining workflow for drug association discovery." *Bmc Bioinformatics* 17.
374. Carazzolle, M. F., et al. (2014). "IIS - Integrated Interactome System: A Web-Based Platform for the Annotation, Analysis and Visualization of Protein-Metabolite-Gene-Drug Interactions by Integrating a Variety of Data Sources and Tools." *Plos One* 9(6).
375. Pavlopoulou, A., et al. (2015). "Human cancer databases." *Oncology Reports* 33(1): 3-18.

List of scientific publications citing TTD (Aug 12th, 2017)

376. Rashmi, M. and D. Swati (2015). "In silico drug re-purposing against African sleeping sickness using GlcNAc-PI de-N-acetylase as an experimental target." *Computational Biology and Chemistry* 59: 87-94.
377. Bredel, M. and E. Jacoby (2004). "Chemogenomics: An emerging strategy for rapid target and drug discovery." *Nature Reviews Genetics* 5(4): 262-275.
378. Grover, M. P., et al. (2014). "Identification of novel therapeutics for complex diseases from genome-wide association data." *Bmc Medical Genomics* 7.
379. Grover, M. P., et al. (2015). "Novel therapeutics for coronary artery disease from genome-wide association study data." *Bmc Medical Genomics* 8.
380. Sovizi, M. R. and S. G. Hosseini (2013). "Studies on the thermal behavior and decomposition kinetic of drugs cetirizine and simvastatin." *Journal of Thermal Analysis and Calorimetry* 111(3): 2143-2148.
381. Kibble, M., et al. (2015). "Network pharmacology applications to map the unexplored target space and therapeutic potential of natural products." *Natural Product Reports* 32(8): 1249-1266.
382. Teruel, M., et al. (2017). "Omics studies: their use in diagnosis and reclassification of SLE and other systemic autoimmune diseases." *Rheumatology* 56: 78-87.
383. Venkatraman, V., et al. (2016). "Computer-aided molecular design of imidazole-based absorbents for CO₂ capture." *International Journal of Greenhouse Gas Control* 49: 55-63.
384. Montero-Melendez, T. (2015). "ACTH: The forgotten therapy." *Seminars in Immunology* 27(3): 216-226.
385. Andersson, C. R., et al. (2011). "Quantitative Chemogenomics: Machine-Learning Models of Protein-Ligand Interaction." *Current Topics in Medicinal Chemistry* 11(15): 1978-1993.
386. Quoc Tuan, D., et al. (2015). "How to Valorize Biodiversity? Let's Go Hashing, Extracting, Filtering, Mining, Fishing." *Planta Medica* 81(6): 436-449.
387. Van Allen, E. M., et al. (2013). "Clinical Analysis and Interpretation of Cancer Genome Data." *Journal of Clinical Oncology* 31(15): 1825-1833.
388. Rasmussen, H. B. and C. M. Dahmcke (2012). "Genome-wide identification of structural variants in genes encoding drug targets: possible implications for individualized drug therapy." *Pharmacogenetics and Genomics* 22(7): 471-483.
389. Henriksen, K., et al. (2011). "Serological biochemical markers of surrogate efficacy and safety as a novel approach to drug repositioning." *Drug Discovery Today* 16(21-22): 967-975.
390. Kowalsman, N. and M. Y. Niv (2014). *GPCR & Company: Databases and Servers for GPCRs and Interacting Partners. G Protein-Coupled Receptors - Modeling and Simulation. M. Filizola. 796: 185-204.*
391. Damodaran, S., et al. (2015). "Cancer Driver Log (CanDL) Catalog of Potentially Actionable Cancer Mutations." *Journal of Molecular Diagnostics* 17(5): 554-559.

List of scientific publications citing TTD (Aug 12th, 2017)

392. Sugaya, N. and T. Furuya (2011). "Dr. PIAS: an integrative system for assessing the druggability of protein-protein interactions." *Bmc Bioinformatics* 12.
393. Sugaya, N., et al. (2012). "Dr. PIAS 2.0: an update of a database of predicted druggable protein-protein interactions." *Database-the Journal of Biological Databases and Curation*.
394. Hecker, N., et al. (2012). "SuperTarget goes quantitative: update on drug-target interactions." *Nucleic Acids Research* 40(D1): D1113-D1117.
395. Ma, H. and H. Zhao (2012). "iFad: an integrative factor analysis model for drug-pathway association inference." *Bioinformatics* 28(14): 1911-1918.
396. Li, Q. and L. Lai (2007). "Prediction of potential drug targets based on simple sequence properties." *Bmc Bioinformatics* 8.
397. Sadok Menna-Barreto, R. F., et al. (2014). "Proteomic and Bioinformatic Analysis of *Trypanosoma cruzi* Chemotherapy and Potential Drug Targets: New Pieces for an Old Puzzle." *Current Drug Targets* 15(3): 255-271.
398. Chirivino, E., et al. (2007). "Tuning sensitivity in paramagnetic NMR detection of ligand-DNA interactions." *Chemmedchem* 2(8): 1153-1156.
399. Sperandio, O., et al. (2006). "Receptor-based computational screening of compound databases: The main docking-scoring engines." *Current Protein & Peptide Science* 7(5): 369-393.
400. Sharma, O. P. and M. S. Kumar (2016). "Essential proteins and possible therapeutic targets of *Wolbachia* endosymbiont and development of FiloBase-a comprehensive drug target database for Lymphatic filariasis." *Scientific Reports* 6.
401. dos Santos, E. C., et al. (2012). "PREDICTING NEW HUMAN DRUG TARGETS BY USING FEATURE SELECTION TECHNIQUES." *Bioinformatics: Proceedings of the International Conference on Bioinformatics Models, Methods and Algorithms*: 137-142.
402. dos Santos, E. C., et al. (2013). "A Semantic-based Similarity of Human Drug Target Proteins." *Bioinformatics 2013: Proceedings of the International Conference on Bioinformatics Models, Methods and Algorithms*: 300-303.
403. Imming, P. (2010). "Molecular Targets of Natural Drug Substances: Idiosyncrasies and Preferences." *Planta Medica* 76(16): 1794-1801.
404. Ambure, P. and K. Roy (2017). "CADD Modeling of Multi-Target Drugs Against Alzheimer's Disease." *Current Drug Targets* 18(5): 522-533.
405. Kumari, P., et al. (2015). "Identification of human drug targets using machine-learning algorithms." *Computers in Biology and Medicine* 56: 175-181.
406. Wei, W.-Q., et al. (2013). "Development and evaluation of an ensemble resource linking medications to their indications." *Journal of the American Medical Informatics Association* 20(5): 954-961.

List of scientific publications citing TTD (Aug 12th, 2017)

407. Marhoefer, R. J., et al. (2011). "Drug discovery and the use of computational approaches for infectious diseases." *Future Medicinal Chemistry* 3(8): 1011-1025.
408. Abubucker, S., et al. (2011). "HelmCoP: An Online Resource for Helminth Functional Genomics and Drug and Vaccine Targets Prioritization." *Plos One* 6(7).
409. Gacche, R. N. and R. J. Meshram (2013). "Targeting tumor micro-environment for design and development of novel anti-angiogenic agents arresting tumor growth." *Progress in Biophysics & Molecular Biology* 113(2): 333-354.
410. Atreya, R. V., et al. (2013). "Exploring drug-target interaction networks of illicit drugs." *Bmc Genomics* 14.
411. Danger, R., et al. (2010). "A comparison of machine learning techniques for detection of drug target articles." *Journal of Biomedical Informatics* 43(6): 902-913.
412. Sawada, R., et al. (2015). "Target-Based Drug Repositioning Using Large-Scale Chemical-Protein Interactome Data." *Journal of Chemical Information and Modeling* 55(12): 2717-2730.
413. Santos, R., et al. (2017). "A comprehensive map of molecular drug targets." *Nature Reviews Drug Discovery* 16(1): 19-34.
414. Nongonierma, A. B. and R. J. FitzGerald (2016). "Strategies for the discovery, identification and validation of milk protein-derived bioactive peptides." *Trends in Food Science & Technology* 50: 26-43.
415. Magarinos, M. P., et al. (2012). "TDR Targets: a chemogenomics resource for neglected diseases." *Nucleic Acids Research* 40(D1): D1118-D1127.
416. Madagi, S. B. and U. Balekundri (2013). Identification of Anti-prostate Cancer Targets for Resveratrol: an Inverse Screening Approach. *World Congress on Engineering and Computer Science, Wcecs 2013, Vol II. S. I. Ao, C. Douglas, W. S. Grundfest and J. Burgstone. Ao: 610-612.*
417. Cao, D.-S., et al. (2012). "Large-scale prediction of drug-target interactions using protein sequences and drug topological structures." *Analytica Chimica Acta* 752: 1-10.
418. Cao, D.-S., et al. (2013). "PyDPI: Freely Available Python Package for Chemoinformatics, Bioinformatics, and Chemogenomics Studies." *Journal of Chemical Information and Modeling* 53(11): 3086-3096.
419. Medina, S., et al. (2013). "The effects of the intake of plant foods on the human metabolome." *Trac-Trends in Analytical Chemistry* 52: 88-99.
420. Deghou, S., et al. (2016). "CART-a chemical annotation retrieval toolkit." *Bioinformatics* 32(18): 2869-2871.
421. Jaeger, S., et al. (2017). "Quantification of Pathway Cross-talk Reveals Novel Synergistic Drug Combinations for Breast Cancer." *Cancer Research* 77(2): 459-469.
422. Prachayasittikul, V., et al. (2015). "Computer-Aided Drug Design of Bioactive Natural Products." *Current Topics in Medicinal Chemistry* 15(18): 1780-1800.

List of scientific publications citing TTD (Aug 12th, 2017)

423. Umland, T. C., et al. (2012). "In Vivo-Validated Essential Genes Identified in *Acinetobacter baumannii* by Using Human Ascites Overlap Poorly with Essential Genes Detected on Laboratory Media." *Mbio* 3(4).
424. Ehrman, T. M., et al. (2007). "Phytochemical informatics of traditional Chinese medicine and therapeutic relevance." *Journal of Chemical Information and Modeling* 47(6): 2316-2334.
425. Ehrman, T. M., et al. (2010). "Phytochemical Informatics and Virtual Screening of Herbs Used in Chinese Medicine." *Current Pharmaceutical Design* 16(15): 1785-1798.
426. Santra, T., et al. (2014). "Navigating the Multilayered Organization of Eukaryotic Signaling: A New Trend in Data Integration." *Plos Computational Biology* 10(2).
427. Siramshetty, V. B., et al. (2016). "WITHDRAWN-a resource for withdrawn and discontinued drugs." *Nucleic Acids Research* 44(D1): D1080-D1086.
428. Muramatsu, M. and Y. Arisue (2011). "New Drug Approvals over Three Decades from 1980 to 2009 in Japan -Their Therapeutic Targets and Biochemical Properties." *Yakugaku Zasshi-Journal of the Pharmaceutical Society of Japan* 131(4): 603-619.
429. Muramatsu, M. and Y. Arisue (2012). "Characteristics of Reactions of Target Enzymes of Drugs Containing New Active Ingredients (NAIs) and Changes of the NAIs Approvals over Three Decades from 1980 to 2009 in Japan." *Yakugaku Zasshi-Journal of the Pharmaceutical Society of Japan* 132(6): 733-752.
430. Sharma, V. and I. N. Sarkar (2013). "Leveraging concept-based approaches to identify potential phyto-therapies." *Journal of Biomedical Informatics* 46(4): 602-614.
431. Brandt, W., et al. (2010). "Chemoinformatic Analysis of Biologically Active Macrocycles." *Current Topics in Medicinal Chemistry* 10(14): 1361-1379.
432. Koscielny, G., et al. (2017). "Open Targets: a platform for therapeutic target identification and validation." *Nucleic Acids Research* 45(D1): D985-D994.
433. Han, L. Y., et al. (2007). "Support vector machines approach for predicting druggable proteins: recent progress in its exploration and investigation of its usefulness." *Drug Discovery Today* 12(7-8): 304-313.
434. Chatr-aryamontri, A., et al. (2017). "The BioGRID interaction database: 2017 update." *Nucleic Acids Research* 45(D1): D369-D379.
435. Karthikeyan, M., et al. (2015). "ChemScreener: A Distributed Computing Tool for Scaffold based Virtual Screening." *Combinatorial Chemistry & High Throughput Screening* 18(6): 544-561.
436. Karthikeyan, M., et al. (2015). "MegaMiner: A Tool for Lead Identification Through Text Mining Using Chemoinformatics Tools and Cloud Computing Environment." *Combinatorial Chemistry & High Throughput Screening* 18(6): 591-603.
437. Szklarczyk, D., et al. (2016). "STITCH 5: augmenting protein-chemical interaction networks with tissue and affinity data." *Nucleic Acids Research* 44(D1): D380-D384.
-

List of scientific publications citing TTD (Aug 12th, 2017)

438. Fernandez-de Gortari, E. and J. L. Medina-Franco (2015). "Epigenetic relevant chemical space: a chemoinformatic characterization of inhibitors of DNA methyltransferases." *Rsc Advances* 5(106): 87465-87476.