Table S1 : A collection of successful drug repositioning examples

Drug name	Origin indication	New indication	Mining Approaches	Ref
Atomoxetine	Parkinson's disease	ADHD	Network Approach	[1,8]
Allopurinol	Tumor lysis syndrome	Gout	Experiment	[1]
Amphetamine	Stimulant	Hyperkinesis in children (attention deficit hyperactivity disorder, ADHD)	Semantic Approach	[1,9]
Apomorphine	Parkinson's disease	Erectile dysfunction	Experiment	[3]
Aspirin	Analgesic, antipyretic	Colorectal cancer	Experiment	[3]
Budesonide	Asthma	Colitis,Ulcerative	Computational Approach	[4,10]
Bupropion	Depression	Smoking cessation	Experiment	[1, 2]
Celecoxib	Osteoarthritis and adult rheumatoid arthritis	Familial adenomatous polyposis, colon,colorectal,lung and breast cancer	Computational Approach	[4,11]
Chlorpromazine	Antiemetic/antihistamine	Non-sedating tranquillizer	Experiment	[4]
Crizotinib	Clinical trials for anaplastic large-cell lymphoma	NSCLC	Experiment	[5]
Cymbalta	Depression	Diabetic peripheral neuropathy	Experiment	[1]
Dapoxetine	Analgesia and depression	Premature ejaculation	Experiment	[1]
Doxepin	Antidepressant	Insomnia antipruritic	Experiment	[2]
Drospirenone	Oral contraceptive	Hypertension	Experiment	[6]
Duloxetine	Depression	Stress urinary incontinence, fibromyalgia, chronic, musculoskeletal pain	Computational Approach	[2,12]
Duloxetine	Diabetic Neuropathies	Shoulder pain, back pain, osteoa-rthritis, knee	Experiment	[4]
Eflornithine	Anti-infective	Reduction of unwanted facial hair in women	Experiment	[4,13]
Etanercept	Rheumatoid arthritis	Asthma	Network Approach	[6,14]

Everolimus	Immunosuppressant	Pancreatic neuroendocrine tumors	Text-mining Approach	[5,15]
Finasteride	Benign prostatic hyperplasia	Hair loss	Experiment	[1, 4]
Fludrocortisone	Cerebral salt wasting syndrome	Hypertension	Experiment	[6]
Fluoxetine	Depression	Premenstrual dysphoric disorder	Network Propagation	[1,16]
Furosemide	Edema associated with congestive heart failure	Bartter syndrome	Experiment	[6]
Galantamine	Polio, paralysis and anaesthesia	Alzheimer's disease	Network Approach	[4,17]
Gemcitabine	Antiviral	Anticancer agent	Experiment	[3]
Hydroxychloroquine	Antiparasitic	Anti-arthritic systemic lupus erythematosus	Experiment	[2]
Imatinib	BCR-ABL	GIST	Experiment	[5]
Imidapril	Hypertension	Cancer cachexia	Experiment	[2]
Infliximab	Crohn's disease	Different arthritis forms; Alzheimer's disease	Experiment	[2]
Leflunomide	Rheumatoid arthritis	Prostate cancer	Network Approach	[3,18]
Lidocaine	Local anaesthesia	Oral corticosteroid dependentas- thma, arrhythmia	Experiment	[1]
Lumigan	Glaucoma	Hypotrichosis simplex	Experiment	[1]
Mecamylamine	Moderately severe to severe essential hypertension and uncomplicated cases of malignant hypertension	ADHD	Experiment	[4]
Metformin	Diabetes mellitus	Breast, adenocarcinoma, prostate, colorectal cancer	Experiment	[3]
Methotrexate	Acute leukemia	Osteosarcoma, breast cancer, Hodgkin lymphoma	Network Approach	[1]
Methotrexate	Cancer	Rheumatoid arthritis	Experiment	[3]
Mifepristone	Pregnancy termination	Psychotic major depression,Cushing's	Experiment	[1]

		syndrome		
Milnacipran	Depression	Fibromyalgia	Experiment	[1]
Miltefosine	Breast cancer	Visceral and cutaneous leishmaniosis	Experiment	[2]
Minocycline	Acne	Ovarian cancer, glioma	Experiment	[3]
Monoxide	Hypertension	Hair loss	Experiment	[1]
Mycophenolate mofetil	Transplanted organ rejection	Renal symptoms of systemic lupus erythematosus	Experiment	[2]
Naltrexone	Opioid addiction	Alcohol withdrawal	Experiment	[2]
Nelfinavir	AIDS	In clinical trials for multiple cancer	Network Approach	[5,16]
Nitroxoline	Antibiotic	Bladder, breast cancer	Experiment	[3]
Noscapine	Antitussive,antimalarial,analgesic	Multiple cancer types	Experiment	[3]
Paclitaxel	Cancer	Restenosis	Network Approach	[1,19]
Pegvisomant	Acromegaly	Hypercholesterolemia	Experiment	[6]
Perindopril	Hypertension	Alzheimer's disease	Experiment	[6]
Phentolamine	Hypertension	Impaired night vision,dental anesthesia reversal agent	Network Approach	[1,20]
Pioglitazone	Type 2 diabetes mellitus	Nonalcoholic steatohepatitis	Network Approach	[7,21]
Raloxifene	Breast and prostate cancer	Osteoporosis	Experiment	[2]
Rapamycin	Immunosuppressant	Colorectal cancer, lymphoma, leukemia	Computational Approach	[3,22]
Requip	Parkinson's disease	Restless legs	Experiment	[1]
Retinoic acid	Acne	Acute promyelocytic leukemia	Experiment	[2]
Ropinerole	Hypertension	Parkinson's, restless legs syndrome	Experiment	[4]
Sibutramine	Depression	Obesity	Experiment	[1, 2]
Sildenafil citrate	Hypertension, angina	Erectile dysfunction (approved)	Experiment	[1, 2]
Statins	Myocardial infarction	cancer, leukemia	Network Approach	[3,16]
Sunitinib	GIST, renal cell carcinoma	Pancreatic tumors/Gastrointestinal Tumor	Network Approach	[5,23]

Tadalafil	Inflammation and cardiovascular disease	Male erectile dysfunction	Experiment	[4]
Tadalafil	Impotence	Hypertension,pulmonary,prostatic hyperplasia,prostate cancer	Network Approach	[4,24]
Thalidomide	Sedation, nausea and insomnia	Cutaneous manifestations of moderate to severe erythema nodosum leprosum in leprosy and multiple myeloma	Experiment	[4]
Thalidomide	Morning sickness	Leprosy,multiple myeloma	Network Approach	[1,25]
Thalidomide	Anti-emetic	Erythema nodosum leprosum	Experiment	[2]
Thiocolchicoside	Muscle relaxant	Leukemia, multiple myeloma	Network Approach	[3]
Tofisopam	Anxiety-related conditions	Irritable bowel syndrome	Experiment	[4]
Topiramate	Epilepsy	Migraine,bulimia	Experiment	[1]
Trastuzumab	HER2-positive breast cancer	HER2-positive metastatic gastric cancer	Network Approach	[5]
Valproic acid	Antiepileptic	Leukemia, solid tumors	Experiment	[3]
Vesnarinone	Cardioprotective	Oral cancer, leukemia, lymphoma	Experiment	[3]
Wortmannin	Antifungal	Leukemia	Experiment	[3]
Zidovudine	Cancer	HIV/AIDS	Experiment	[1]
Zoledronic acid	Anti-bone resorption	Multiple myeloma, prostate cancer, breast cancer	Experiment	[3]

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Table S2: A collection of successful drug reposition resources

	Database	*Link*	*Description*	*Ref*
1	Adverse Reaction Database (Canada)	http://www.hc-sc.gc.ca	A database contains information about suspected adverse reactions (also known as side effects) to health products.	[1]
2	ArrayExpress	http://www.ebi.ac.uk/arrayexpress/	A public database contains high throughput functional genomics data,	[2]
3	BindingDB	http://www.bindingdb.org/bind/index.jsp	A public, web-accessible database includes measured binding affinities.	[3]
4	BioCarta	http://www.biocarta.com	A database contains biological pathways.	[4]
5	BioGRID	http://thebiogrid.org/	A database contains biological interaction data.	[5]
6	Cancer Cell Line Encyclopedia(CCLE)	http://www.broadinstitute.org/ccle	A database contains a large panel of human cancer cell lines.	[6]
7	CellMiner	http://discover.nci.nih.gov/cellminer/	A database is designed for querying molecular information on NCI-60.	[7]
8	ChemBank	http://chembank.broad.harvard.edu	A web-based informatics environment includes freely available data derived from small molecules and small-molecule screens.	[8]
9	ChEMBL	https://www.ebi.ac.uk/chembl/	An open database contains binding, functional and ADMET information for a large number of drug-like bioactive compounds.	[9]
10	ChemDB	http://www.chemdb.com	A public database include small molecules data on the Web.	[10]
11	ChemFrog	http://www.chemfrog.com	A chemical search engine provides a sourcing platform for chemical buyers and sellers worldwide.	[4]

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12	Chemicalize (ChemAxon)	http://www.chemicalize.org	A powerful online platform is designed for chemical calculations, search, and text processing.	[11]
13	ChemSpider	http://www.chemspider.com	A free chemical structure database provides fast access to over 34 million structures, properties and associated information.	[12]
14	Clinicaltrial.gov	http://clinicaltrials.gov	A registry and results database provides publicly and privately supported clinical studies of human participants conducted around the world.	[4]
15	Collaborative Drug Discovery Vault	https://www.collaborativedrug.com	A hosted biological and chemical database contains chemical structures and biological study data.	[13]
16	DailyMed (US FDA)	http://dailymed.nlm.nih.gov/dailymed/about.cfm	A web site provides latest electronic drug label information approved by the FDA.	[14]
17	Database for Annotation Visualization and Integrated Discovery (DAVID)	http://david.abcc.ncifcrf.gov	A web-accessible program integrates functional genomic annotations with intuitive graphical summaries	[15]
18	Database of Interacting Proteins (DIP)	http://dip.doe-mbi.ucla.edu/dip/Main.cgi	A database includes experimentally determined protein–protein interactions.	[16]
19	DbSNP	http://www.ncbi.nlm.nih.gov/projects/SNP/	A free public archive contains genetic variation within and across different species	[17]
20	DistilBio	http://distilbio.com	A platform is designed for knowledge discovery and exploration.	[4]
21	Drug Drug Combination Database(DCDB)	http://www.cls.zju.edu.cn/dcdb	An available database collects and organizes information on drug combinations.	[18]

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22	Drug versus Disease (DvD)	www.ebi.ac.uk/saezrodriguez/dvd	An R package is designed to 'match' drug and disease profiles.	[19]
23	Drugbank	http://www.drugbank.ca/	A unique bioinformatics and cheminformatics resource combines detailed drug data with comprehensive drug target information.	[20]
24	DrugMap Central (DMC)	http://r2d2drug.org/index.html	An on-line query and visualization tool is designed to facilitate drug repositioning studies.	[21]
25	Drugs@FDA Database	http://www.fda.gov/Drugs/InformationOnDrugs/	A database collects FDA approved drug data.	[22]
26	FAERS (US FDA)	http://www.fda.gov/Drugs/	A database contains information on adverse event and medication error reports submitted to FDA.	[4]
27	FDALABEL (US FDA)	http://www.fda.gov/ScienceResearch/ BioinformaticsTools/	A tool is designed to search of drug labeling.	[4]
28	Gene Expression Atlas	http://www.ebi.ac.uk/gxa	An open science resource gives users a powerful way to find information about gene and protein expression.	[23]
29	Gene Expression Omnibus (GEO)	http://www.ncbi.nlm.nih.gov/geo	A database repository contains high throughput gene expression data and hybridization arrays, chips, microarrays.	[24]
30	Gene Set Enrichment Analysis(GSEA)	http://www.broadinstitute.org/gsea	A computational method defined set of genes shows statistically significant, concordant differences between two biological states	[25]
31	Gene Signature Database(GeneSigDB)	http://compbio.dfci.harvard.edu/genesigdb	A searchable database includes fully traceable, standardized, annotated gene signatures	[26]
32	GeneCards Databases	http://www.genecards.org/	A searchable, integrated, database of human genes provides concise genomic related information, on all known and predicted human genes	[27]

	Continue			
33	Genome Array Express	http://www.ebi.ac.uk/arrayexpress	A database accepts data generated by sequencing or array-based technologies and currently contains data from almost a million assays, from over 30 000 experiments.	[28]
34	GPCR-Ligand Database (GLIDA)	http://pharminfo.pharm.kyoto-u.ac.jp/services/glida/	A database is developed for the field of GPCRs-related drug discovery	[29]
35	Human Metabolome Database (HMDB)	http://www.hmdb.ca	A freely available electronic database contains detailed information about small molecule metabolites	[30]
36	Human Protein Reference Database (HPRD)	http://www.hprd.org/	A database contains manually curated scientific information pertaining to the biology of most human proteins	[31]
37	IntAct	http://www.ebi.ac.uk/intact/	A database provides protein interactions data	[32]
38	International Cancer Genome Consortium	https://icgc.org	A research project obtain a comprehensive description of genomic, transcriptomic and epigenomic changes in 50 different tumor types and/or subtypes	[33]
39	Iowa Drug Information Service (IDIS)	http://itsnt14.its.uiowa.edu	A database provides access to the serial literature of medicine and pharmacy	[34]
40	iScienceSearch	http://cwmglobalsearch.com/gs/Default.aspx	An Internet search engine is designed for searching chemical data.	[4]
41	Johns Hopkins University HTS Core	http://www.molecularinteraction.org/HIT%20center.htm	An integrated robotics database contains chemical data.	[4]

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42	Kansas University HTS Lab Services	http://www.hts.ku.edu	A free service provide researchers with the ability to run high-throughput chemical, siRNA, and high-content screens (HCS)	[4]
43	Kyoto Encyclopedia of Genes and Genomes (KEGG)	http://www.genome.jp/kegg	A database resource is developed for understanding high-level functions and the biological system	[35]
44	Library of Integrated Network based Cellular Signatures(LINCS)	http://www.lincsproject.org	A database contain details about the assays, cell types, and perturbagens.	[35]
45	MATADOR (manually annotated)	http://matador.embl.de	A resource includes protein-chemical interactions	[36]
46	MIPS (mammalian protein-protein interaction database)	http://mips.helmholtz-muenchen.de/proj/ppi/	A new resource contains high-quality experimental protein interaction data in mammals	[37]
47	Molecular Signature Database(MsigDB)	http://www.broadinstitute.org/gsea/msigdb	A collection contains annotated gene sets for use with GSEA software.	[38]
48	NCI Pathway Interaction Database (NCI-PID)	http://pid.nci.nih.gov/	A database includes pathway data and interactions.	[39]
49	NCGC Database	http://www.genome.gov/12512295	A comprehensive resource of clinically approved drugs enabling repurposing and chemical genomics	[40]
50	NIMH Psychoactive Drug Screening Program(PDSP)	http://pdsp.cwru.edu/	A service provides screening of novel psychoactive compounds for pharmacological and functional activity at cloned human or rodent CNS receptors, channels, and transporters	[4]
51	OCA	http://oca.weizmann.ac.il/oca-bin/ocamain	A browser-database is developed for protein structure/function	[41]
52	Oncomine	https://www.oncomine.org	A cancer microarray database and web-based data-mining platform aimed at facilitating discovery from genome-wide expression analyses.	[42]

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53	Online Mendelian Inheritance in Man (OMIM)	http://www.omim.org	A continuously updated catalog of human genes and genetic disorders and traits, with particular focus on the molecular relationship between genetic variation and phenotypic expression	[43]
54	OPM(membrane proteins)	http://opm.phar.umich.edu	A database provides spatial arrangements of membrane proteins with respect to the hydrocarbon core of the lipid bilayer	[44]
55	PathwayCommons	http://www.pathwaycommons.org/about/	A collection includes publicly available pathway information from multiple organisms	[45]
56	Princeton University MicroArray database (PUMAdb)	http://puma.princeton.edu	A database stores raw and normalized data from microarray experiments	[46]
57	Protein Data Bank (PDB)	http://www.rcsb.org/pdb/home/home.do	A crystallographic database is designed for the three-dimensional structural data of large biological molecules	[47]
58	Proteopedia	http://proteopedia.org	A database includes 3D encyclopedia of proteins and other molecules	[48]
59	Psychoactive Drug Screening Program Ki (PDSP Ki)	http://pdsp.med.unc.edu/pdsp.php	A unique resource in the public domain provides information on the abilities of drugs to interact with an expanding number of molecular targets.	[49]
60	PubChem	https://pubchem.ncbi.nlm.nih.gov/	A database includes chemical molecules and their activities against biological assays	[50]
61	Reactome	http://www.reactome.org	A free, open-source, curated and peer database includes pathway database	[51]
62	Rockefeller University HTS Core Facility	http://www.rockefeller.edu/	A source includes bioassays and drug data	[4]

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63	Sequence Read Archive (SRA)	http://www.ncbi.nlm.nih.gov/Traces/sra/	A database makes biological sequence data available to the research community to enhance reproducibility and allow for new discoveries by comparing data sets.	[52]
64	Side Effect Resource (SIDER)	http://sideeffects.embl.de	A resource contains information on marketed medicines and their recorded adverse drug reactions	[53]
65	Stanford Microarray Database	http://smd.princeton.edu	A database stores raw and normalized data from microarray experiments, and provides web interfaces for researchers to retrieve, analyze and visualize their data	[54]
66	STITCH (Chemical-Protein Interactions)	http://stitch.embl.de/	A resource integrates disparate data sources for 430 000 chemicals into a single, easy-to-use way	[55]
67	STRING	http://string-db.org/	A biological database and web resource is known of predicting protein–protein interactions	[56]
68	Structured Product Labeling (SPL)	http://www.fda.gov/	A document markup standard is approved by Health Level Seven	[4]
69	SuperTarget	http://bioinf-apache.charite.de/supertarget_v2/	A database is developed in the first place to collect informations about drug-target relations.	[36]
70	SWEETLEAD	https://simtk.org/home/sweetlead	A highly-curated in silico database lcontains chemical structures representing approved drugs, chemical isolates from traditional medicinal herbs, and regulated chemicals	[57]
71	The Cancer Genome Atlas (TCGA)	http://cancergenome.nih.gov	A public funded project aims to catalogue and discover major cancer-causing genomic alterations to create a comprehensive “atlas” of cancer genomic profiles.	[58]

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72	The Connectivity Map (CMap)	http://www.broadinstitute.org/cmap	A database includes genome-wide transcriptional expression data from cultured human cells treated with bioactive small molecules	[59]
73	The NCGC Pharmaceutical Collection (NPC)	http://tripod.nih.gov/npc/	A comprehensive, publically-accessible collection of approved and investigational drugs for high-throughput screening	[40]
74	Pharmacogenomics Knowledge Base (PharmGKB)	http://www.pharmgkb.org	A comprehensive resource curates knowledge about the impact of genetic variation on drug response for clinicians and researchers.	[60]
75	Therapeutic Target Database (TTD)	http://bidd.nus.edu.sg/group/cjttd/	A database provides information about the known and explored therapeutic protein and nucleic acid targets, the targeted disease, pathway information and the corresponding drugs directed at each of these targets.	[61]
76	TOPSAN	http://www.topsan.org	A web-based collaboration platform is developed for exploring and annotating structures determined by structural genomics efforts	[62]

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