

Polypharmacology: Challenges and Opportunities in Dr

Journal of Medicinal Chemistry

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Citation Report

#	ARTICLE	IF	CITATIONS
1	Multitarget Drugs. , 2008, , 449-472.		5
2	How drugs get into cells: tested and testable predictions to help discriminate between transporter-mediated uptake and lipoidal bilayer diffusion. <i>Frontiers in Pharmacology</i> , 2014, 5, 231.	1.6	136
3	An in silico target identification using Boolean network attractors: Avoiding pathological phenotypes. <i>Comptes Rendus - Biologies</i> , 2014, 337, 661-678.	0.1	16
4	Computational studies to predict or explain G protein coupled receptor polypharmacology. <i>Trends in Pharmacological Sciences</i> , 2014, 35, 658-663.	4.0	29
5	<i>N</i> -Methyl- <i>N</i> -((1-methyl-5-(3-(1-(2-methylbenzyl)piperidin-4-yl)propoxy)-1 <i>H</i> -indol-2-yl)methyl)prop-2-yn-1-amine, a New Cholinesterase and Monoamine Oxidase Dual Inhibitor. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 10455-10463.	2.9	56
6	Î²-Lactam Estrogen Receptor Antagonists and a Dual-Targeting Estrogen Receptor/Tubulin Ligand. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 9370-9382.	2.9	45
7	First Selective Dual Inhibitors of Tau Phosphorylation and Beta-Amyloid Aggregation, Two Major Pathogenic Mechanisms in Alzheimer's Disease. <i>ACS Chemical Neuroscience</i> , 2014, 5, 1198-1202.	1.7	27
9	Selective Negative Allosteric Modulation Of Metabotropic Glutamate Receptors – A Structural Perspective of Ligands and Mutants. <i>Scientific Reports</i> , 2015, 5, 13869.	1.6	38
10	Defining the Schistosoma haematobium kinome enables the prediction of essential kinases as anti-schistosome drug targets. <i>Scientific Reports</i> , 2015, 5, 17759.	1.6	37
12	Exploiting Atropisomerism to Increase the Target Selectivity of Kinase Inhibitors. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 11754-11759.	7.2	51
13	Identification of Orthologous Target Pairs with Shared Active Compounds and Comparison of Organism-specific Activity Patterns. <i>Chemical Biology and Drug Design</i> , 2015, 86, 1105-1114.	1.5	2
14	Synthetic biology for pharmaceutical drug discovery. <i>Drug Design, Development and Therapy</i> , 2015, 9, 6285.	2.0	66
15	Editorial (Thematic Issue: Multi-Target Drug Discovery in Medicinal Chemistry: Current Status and) Tj ETQq0 0 0 rgBT ₁ /Overlock 10 Tf 50	1.1	1
16	Repositioning of Thiourea-Containing Drugs as Tyrosinase Inhibitors. <i>International Journal of Molecular Sciences</i> , 2015, 16, 28534-28548.	1.8	28
17	Anticancer Properties of Lamellarins. <i>Marine Drugs</i> , 2015, 13, 1105-1123.	2.2	133
18	Colon-targeted delivery of piceatannol enhances anti-colitic effects of the natural product: potential molecular mechanisms for therapeutic enhancement. <i>Drug Design, Development and Therapy</i> , 2015, 9, 4247.	2.0	7
19	Ligand Discovery for the Alanine-Serine-Cysteine Transporter (ASCT2, SLC1A5) from Homology Modeling and Virtual Screening. <i>PLoS Computational Biology</i> , 2015, 11, e1004477.	1.5	62
20	Modeling-Enabled Characterization of Novel NLRX1 Ligands. <i>PLoS ONE</i> , 2015, 10, e0145420.	1.1	25

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21	Computational polypharmacology comes of age. <i>Frontiers in Pharmacology</i> , 2015, 6, 157.	1.6	61
23	Computer-aided drug discovery. <i>F1000Research</i> , 2015, 4, 630.	0.8	49
24	Discovery of Multitarget Antivirals Acting on Both the Dengue Virus NS5-NS3 Interaction and the Host Src/Fyn Kinases. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 4964-4975.	2.9	52
25	Design, synthesis and characterization of dual inhibitors against new targets FabG4 and HtdX of <i>Mycobacterium tuberculosis</i> . <i>European Journal of Medicinal Chemistry</i> , 2015, 100, 223-234.	2.6	13
26	The design of multitarget ligands for chronic and neuropathic pain. <i>Future Medicinal Chemistry</i> , 2015, 7, 2469-2483.	1.1	37
27	Antitumor effects of a drug combination targeting glycolysis, glutaminolysis and de novo synthesis of fatty acids. <i>Oncology Reports</i> , 2015, 34, 1533-1542.	1.2	25
28	Searching Hidden Truth behind Clinical Trials. <i>Respiratory Investigation</i> , 2015, 53, 1.	0.9	0
29	Semisynthetic Studies on and Biological Evaluation of <i>N</i> -Methylaurotetanine Analogues as Ligands for 5-HT Receptors. <i>Journal of Natural Products</i> , 2015, 78, 722-729.	1.5	12
30	Recent Advances in Cancer Therapeutics. <i>Progress in Medicinal Chemistry</i> , 2015, 54, 1-63.	4.1	32
31	Selective, Nontoxic CB ₂ Cannabinoid <i>o</i> -Quinone with in Vivo Activity against Triple-Negative Breast Cancer. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 2256-2264.	2.9	33
32	Computational Polypharmacology Analysis of the Heat Shock Protein 90 Interactome. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 676-686.	2.5	31
33	Discovery of Novel Multiacting Topoisomerase I/II and Histone Deacetylase Inhibitors. <i>ACS Medicinal Chemistry Letters</i> , 2015, 6, 239-243.	1.3	64
34	Selective Optimization of Side Activities (SOSA) in Drug Discovery. , 2015, , 473-486.		2
35	Acute Toxicity-Supported Chronic Toxicity Prediction: A <i>k</i> -Nearest Neighbor Coupled Read-Across Strategy. <i>International Journal of Molecular Sciences</i> , 2015, 16, 11659-11677.	1.8	23
36	Discovery of a 6-(pyridin-3-yl)benzo[d]thiazole template for optimization of hedgehog and PI3K/AKT/mTOR dual inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2015, 25, 3665-3670.	1.0	17
37	The design, synthesis and biological evaluation of conformationally restricted 4-substituted-2,6-dimethylfuro[2,3-d]pyrimidines as multi-targeted receptor tyrosine kinase and microtubule inhibitors as potential antitumor agents. <i>Bioorganic and Medicinal Chemistry</i> , 2015, 23, 2408-2423.	1.4	32
38	Indole based peptidomimetics as anti-inflammatory and anti-hyperalgesic agents: Dual inhibition of 5-LOX and COX-2 enzymes. <i>European Journal of Medicinal Chemistry</i> , 2015, 97, 104-123.	2.6	49
39	Rational Design of Dual Peptides Targeting Ghrelin and γ ₂ Receptors to Regulate Food Intake and Body Weight. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 4180-4193.	2.9	9

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40	History and Perspectives of A _{2A} Adenosine Receptor Antagonists as Potential Therapeutic Agents. <i>Medicinal Research Reviews</i> , 2015, 35, 790-848.	5.0	88
41	sc-PDB: a 3D-database of ligandable binding sites—10 years on. <i>Nucleic Acids Research</i> , 2015, 43, D399-D404.	6.5	182
42	Chemical genetics and regeneration. <i>Future Medicinal Chemistry</i> , 2015, 7, 2263-2283.	1.1	4
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45	Rationally Designed Small Molecules That Target Both the DNA and RNA Causing Myotonic Dystrophy Type 1. <i>Journal of the American Chemical Society</i> , 2015, 137, 14180-14189.	6.6	106
46	Repurposing Registered Drugs as Antagonists for Protease-Activated Receptor 2. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 2079-2084.	2.5	10
47	Using quantitative systems pharmacology for novel drug discovery. <i>Expert Opinion on Drug Discovery</i> , 2015, 10, 1315-1331.	2.5	18
48	Investigations into the binding of jadomycin DS to human topoisomerase II ^β by WaterLOGSY NMR spectroscopy. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 10324-10327.	1.5	12
49	Large-Scale Predictive Drug Safety: From Structural Alerts to Biological Mechanisms. <i>Chemical Research in Toxicology</i> , 2015, 28, 1875-1887.	1.7	49
50	Multiple binding sites in the nicotinic acetylcholine receptors: An opportunity for polypharmacology. <i>Pharmacological Research</i> , 2015, 101, 9-17.	3.1	20
51	Thermal proteome profiling for unbiased identification of direct and indirect drug targets using multiplexed quantitative mass spectrometry. <i>Nature Protocols</i> , 2015, 10, 1567-1593.	5.5	481
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53	Polypharmacology in Drug Discovery: A Review from Systems Pharmacology Perspective. <i>Current Pharmaceutical Design</i> , 2016, 22, 3171-3181.	0.9	77
54	Structural insights into the polypharmacological activity of quercetin on serine/threonine kinases. <i>Drug Design, Development and Therapy</i> , 2016, Volume 10, 3109-3123.	2.0	19
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57	Drug Design for CNS Diseases: Polypharmacological Profiling of Compounds Using Cheminformatic, 3D-QSAR and Virtual Screening Methodologies. <i>Frontiers in Neuroscience</i> , 2016, 10, 265.	1.4	62

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59	Incorporating Natural Products, Pharmaceutical Drugs, Self-Care and Digital/Mobile Health Technologies into Molecular-Behavioral Combination Therapies for Chronic Diseases. <i>Current Clinical Pharmacology</i> , 2016, 11, 128-145.	0.2	26
60	Systems psychopharmacology: A network approach to developing novel therapies. <i>World Journal of Psychiatry</i> , 2016, 6, 66.	1.3	15
61	Nature-Inspired Multifunctional Ligands: Focusing on Amyloid-Based Molecular Mechanisms of Alzheimer's Disease. <i>ChemMedChem</i> , 2016, 11, 1309-1317.	1.6	31
62	Analyzing Promiscuity at the Level of Active Compounds and Targets. <i>Molecular Informatics</i> , 2016, 35, 583-587.	1.4	8
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64	Polypharmacology in Drug Development: A Minireview of Current Technologies. <i>ChemMedChem</i> , 2016, 11, 1211-1218.	1.6	39
65	Epigenetic polypharmacology: from combination therapy to multitargeted drugs. <i>Clinical Epigenetics</i> , 2016, 8, 105.	1.8	113
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67	Polypharmacology of dopamine receptor ligands. <i>Progress in Neurobiology</i> , 2016, 142, 68-103.	2.8	57
68	<i>C</i>-Glycosylflavones Alleviate Tau Phosphorylation and Amyloid Neurotoxicity through GSK3 β Inhibition. <i>ACS Chemical Neuroscience</i> , 2016, 7, 912-923.	1.7	50
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72	Chemical Biology Approaches for Characterization of Epigenetic Regulators. <i>Methods in Enzymology</i> , 2016, 574, 79-103.	0.4	5
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95	Chemoproteomic Approach to Explore the Target Profile of GPCR ligands: Application to 5-HT _{1A} and 5-HT ₆ Receptors. <i>Chemistry - A European Journal</i> , 2016, 22, 1313-1321.	1.7	15
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101	De Novo Design at the Edge of Chaos. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 4077-4086.	2.9	124
102	Application of Dual Inhibition Concept within Looped Autoregulatory Systems toward Antivirulence Agents against <i>Pseudomonas aeruginosa</i> Infections. <i>ACS Chemical Biology</i> , 2016, 11, 1279-1286.	1.6	61
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113	The use of novel selectivity metrics in kinase research. <i>BMC Bioinformatics</i> , 2017, 18, 17.	1.2	35
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116	Targeting Oxidative Stress in Stroke. <i>Springer Series in Translational Stroke Research</i> , 2017, , 203-250.	0.1	8
117	Discovery of Multitarget Agents Active as Broad-Spectrum Antivirals and Correctors of Cystic Fibrosis Transmembrane Conductance Regulator for Associated Pulmonary Diseases. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 1400-1416.	2.9	17
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126	Polypharmacological <i>in Silico</i> Bioactivity Profiling and Experimental Validation Uncovers Sedative-Hypnotic Effects of Approved and Experimental Drugs in Rat. <i>ACS Chemical Biology</i> , 2017, 12, 1593-1602.	1.6	9
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128	Outlook for the Future. <i>AAPS Advances in the Pharmaceutical Sciences Series</i> , 2017, , 421-447.	0.2	0
129	Systematic Data Mining Reveals Synergistic H3R/MCHR1 Ligands. <i>ACS Medicinal Chemistry Letters</i> , 2017, 8, 648-653.	1.3	7

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144	Network-Based Approach to Identify Potential Targets and Drugs that Promote Neuroprotection and Neurorepair in Acute Ischemic Stroke. <i>Scientific Reports</i> , 2017, 7, 40137.	1.6	38
145	Synthesis and Docking of Novel 3 ^{â€} Indolylpropyl Derivatives as New Polypharmacological Agents Displaying Affinity for 5 ^{â€} HT _{1A} /SERT. <i>Archiv Der Pharmazie</i> , 2017, 350, e1600271.	2.1	9
146	Trends in GPCR drug discovery: new agents, targets and indications. <i>Nature Reviews Drug Discovery</i> , 2017, 16, 829-842.	21.5	1,773
147	Design and Synthesis of Ligand Efficient Dual Inhibitors of Janus Kinase (JAK) and Histone Deacetylase (HDAC) Based on Ruxolitinib and Vorinostat. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 8336-8357.	2.9	82
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151	Structural and Functional View of Polypharmacology. <i>Scientific Reports</i> , 2017, 7, 10102.	1.6	33
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