Adriaan P Ijzerman

List of Publications by Year
in descending order

290 papers	15,542 citations	20759 60 h-index	24915 109 g-index
300 all docs	300 docs citations	300 times ranked	14842 citing authors

#	Article	IF	Citations
1	MPP+-Induced Changes in Cellular Impedance as a Measure for Organic Cation Transporter (SLC22A1-3) Activity and Inhibition. International Journal of Molecular Sciences, 2022, 23, 1203.	1.8	2
2	International Union of Basic and Clinical Pharmacology. CXII: Adenosine Receptors: A Further Update. Pharmacological Reviews, 2022, 74, 340-372.	7.1	67
3	Oncological drug discovery: AI meets structure-based computational research. Drug Discovery Today, 2022, 27, 1661-1670.	3.2	9
4	Kinetic profiling and functional characterization of 8-phenylxanthine derivatives as A2B adenosine receptor antagonists. Biochemical Pharmacology, 2022, 200, 115027.	2.0	3
5	Impedance-Based Phenotypic Readout of Transporter Function: A Case for Glutamate Transporters. Frontiers in Pharmacology, 2022, 13, .	1.6	2
6	Cancerâ€related somatic mutations alter adenosine A ₁ receptor pharmacologyâ€”A focus on mutations in the loops and Câ€terminus. FASEB Journal, 2022, 36, .	0.2	3
7	Cancer-Related Somatic Mutations in Transmembrane Helices Alter Adenosine A1 Receptor Pharmacology. Molecules, 2022, 27, 3742.	1.7	1
8	Targeting the Kv11.1 (hERG) channel with allosteric modulators. Synthesis and biological evaluation of three novel series of LUF7346 derivatives. European Journal of Medicinal Chemistry, 2021, 212, 113033.	2.6	6
9	Molecular probes for the human adenosine receptors. Purinergic Signalling, 2021, 17, 85-108.	1.1	11
10	Medicinal chemistry of P2 and adenosine receptors: Common scaffolds adapted for multiple targets. Biochemical Pharmacology, 2021, 187, 114311.	2.0	29
11	A study of the dopamine transporter using the TRACT assay, a novel in vitro tool for solute carrier drug discovery. Scientific Reports, 2021, 11, 1312.	1.6	8
12	Design and Characterization of an Intracellular Covalent Ligand for CC Chemokine Receptor 2. Journal of Medicinal Chemistry, 2021, 64, 2608-2621.	2.9	13
13	Rollover Cyclometalation vs Nitrogen Coordination in Tetrapyridyl Anticancer Gold(III) Complexes: Effect on Protein Interaction and Toxicity. Jacs Au, 2021, 1, 380-395.	3.6	14
14	Crystal Structure and Subsequent Ligand Design of a Nonriboside Partial Agonist Bound to the Adenosine A_{2A} Receptor. Journal of Medicinal Chemistry, 2021, 64, 3827-3842.	2.9	29
15	G protein-coupled receptors expressed and studied in yeast. The adenosine receptor as a prime example. Biochemical Pharmacology, 2021, 187, 114370.	2.0	5
16	Label-free high-throughput screening assay for the identification of norepinephrine transporter (NET/SLC6A2) inhibitors. Scientific Reports, 2021, 11, 12290.	1.6	4
17	Adenosine receptors in GtoPdb v.2021.2. IUPHAR/BPS Guide To Pharmacology CITE, 2021, 2021, .	0.2	5
18	Identification of V6.51L as a selectivity hotspot in stereoselective A2B adenosine receptor antagonist recognition. Scientific Reports, 2021, 11, 14171.	1.6	11

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19	An Overview of Cell-Based Assay Platforms for the Solute Carrier Family of Transporters. Frontiers in Pharmacology, 2021, 12, 722889.	1.6	31
20	Gonadotrophin-releasing hormone receptors in GtoPdb v.2021.3. IUPHAR/BPS Guide To Pharmacology CITE, 2021, 2021, .	0.2	0
21	THE CONCISE GUIDE TO PHARMACOLOGY 2021/22: G proteinâ€coupled receptors. British Journal of Pharmacology, 2021, 178, S27-S156.	2.7	337
22	Computational Approaches for De Novo Drug Design: Past, Present, and Future. Methods in Molecular Biology, 2021, 2190, 139-165.	0.4	26
23	Deciphering conformational selectivity in the A2A adenosine G protein-coupled receptor by free energy simulations. PLoS Computational Biology, 2021, 17, e1009152.	1.5	5
24	DrugEx v2: de novo design of drug molecules by Pareto-based multi-objective reinforcement learning in polypharmacology. Journal of Cheminformatics, 2021, 13, 85.	2.8	30
25	Allosteric modulation of G proteinâ€coupled receptors by amiloride and its derivatives. Perspectives for drug discovery?. Medicinal Research Reviews, 2020, 40, 683-708.	5.0	21
26	Affinity, binding kinetics and functional characterization of draflazine analogues for human equilibrative nucleoside transporter 1 (SLC29A1). Biochemical Pharmacology, 2020, 172, 113747.	2.0	16
27	Annotation of Allosteric Compounds to Enhance Bioactivity Modeling for Class A GPCRs. Journal of Chemical Information and Modeling, 2020, 60, 4664-4672.	2.5	2
28	Successive Statistical and Structure-Based Modeling to Identify Chemically Novel Kinase Inhibitors. Journal of Chemical Information and Modeling, 2020, 60, 4283-4295.	2.5	4
29	Quantitative prediction of selectivity between the A1 and A2A adenosine receptors. Journal of Cheminformatics, 2020, 12, 33.	2.8	10
30	Design and pharmacological profile of a novel covalent partial agonist for the adenosine A1 receptor. Biochemical Pharmacology, 2020, 180, 114144.	2.0	10
31	Characterization of cancer-related somatic mutations in the adenosine A2B receptor. European Journal of Pharmacology, 2020, 880, 173126.	1.7	15
32	LUF7244 plus Dofetilide Rescues Aberrant Kv11.1 Trafficking and Produces Functional IKv11.1. Molecular Pharmacology, 2020, 97, 355-364.	1.0	10
33	Novel natural and synthetic inhibitors of solute carriers SGLT1 and SGLT2. Pharmacology Research and Perspectives, 2019, 7, e00504.	1.1	8
34	LUF7244, an allosteric modulator/activator of K_v11.1 channels, counteracts dofetilideâ€induced torsades de pointes arrhythmia in the chronic atrioventricular block dog model. British Journal of Pharmacology, 2019, 176, 3871-3885.	2.7	16
35	THE CONCISE GUIDE TO PHARMACOLOGY 2019/20: G proteinâ€coupled receptors. British Journal of Pharmacology, 2019, 176, S21-S141.	2.7	519
36	Label-free detection of transporter activity via GPCR signalling in living cells: A case for SLC29A1, the equilibrative nucleoside transporter 1. Scientific Reports, 2019, 9, 13802.	1.6	16

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37	Squalene-Adenosine Nanoparticles: Ligands of Adenosine Receptors or Adenosine Prodrug?. Journal of Pharmacology and Experimental Therapeutics, 2019, 369, 144-151.	1.3	15
38	An exploration strategy improves the diversity of de novo ligands using deep reinforcement learning: a case for the adenosine A2A receptor. Journal of Cheminformatics, 2019, 11, 35.	2.8	58
39	Drugâ€"Target Association Kinetics in Drug Discovery. Trends in Biochemical Sciences, 2019, 44, 861-871.	3.7	42
40	Long residence time adenosine A1 receptor agonists produce sustained wash-resistant antilipolytic effect in rat adipocytes. Biochemical Pharmacology, 2019, 164, 45-52.	2.0	17
41	Development of Covalent Ligands for G Protein-Coupled Receptors: A Case for the Human Adenosine A₃ Receptor. Journal of Medicinal Chemistry, 2019, 62, 3539-3552.	2.9	31
42	A live cell NanoBRET binding assay allows the study of ligand-binding kinetics to the adenosine A3 receptor. Purinergic Signalling, 2019, 15, 139-153.	1.1	35
43	TLR-Induced IL-12 and CCL2 Production by Myeloid Cells Is Dependent on Adenosine A3 Receptorâ€"Mediated Signaling. Journal of Immunology, 2019, 202, 2421-2430.	0.4	7
44	Identification of novel small molecule inhibitors for solute carrier SGLT1 using proteochemometric modeling. Journal of Cheminformatics, 2019, 11, 15.	2.8	17
45	Advances and Challenges in Computational Target Prediction. Journal of Chemical Information and Modeling, 2019, 59, 1728-1742.	2.5	76
46	Proteochemometricsâ€¯â€"â€¯recent developments in bioactivity and selectivity modeling. Drug Discovery Today: Technologies, 2019, 32-33, 89-98.	4.0	25
47	Lymphoblast-derived hiPS cell lines generated from four individuals of a family of genetically unrelated parents and their female monozygotic twins. Stem Cell Research, 2019, 41, 101654.	0.3	1
48	Synthesis and Pharmacological Evaluation of Triazolopyrimidinone Derivatives as Noncompetitive, Intracellular Antagonists for CC Chemokine Receptors 2 and 5. Journal of Medicinal Chemistry, 2019, 62, 11035-11053.	2.9	11
49	Application of portfolio optimization to drug discovery. Information Sciences, 2019, 475, 29-43.	4.0	9
50	Covalent Allosteric Probe for the Metabotropic Glutamate ReceptorÂ2: Design, Synthesis, and Pharmacological Characterization. Journal of Medicinal Chemistry, 2019, 62, 223-233.	2.9	17
51	Adenosine receptors (version 2019.4) in the IUPHAR/BPS Guide to Pharmacology Database. IUPHAR/BPS Guide To Pharmacology CITE, 2019, 2019, .	0.2	3
52	Gonadotrophin-releasing hormone receptors (version 2019.4) in the IUPHAR/BPS Guide to Pharmacology Database. IUPHAR/BPS Guide To Pharmacology CITE, 2019, 2019, .	0.2	0
53	Hydroxycarboxylic acid receptors (version 2019.4) in the IUPHAR/BPS Guide to Pharmacology Database. IUPHAR/BPS Guide To Pharmacology CITE, 2019, 2019, .	0.2	1
54	Data-driven approaches used for compound library design, hit triage and bioactivity modeling in high-throughput screening. Briefings in Bioinformatics, 2018, 19, bbw105.	3.2	17

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55	A twoâ€state model for the kinetics of competitive radioligand binding. British Journal of Pharmacology, 2018, 175, 1719-1730.	2.7	14
56	Intracellular Receptor Modulation: Novel Approach to Target GPCRs. Trends in Pharmacological Sciences, 2018, 39, 547-559.	4.0	43
57	Selective Photoaffinity Probe That Enables Assessment of Cannabinoid CB₂ Receptor Expression and Ligand Engagement in Human Cells. Journal of the American Chemical Society, 2018, 140, 6067-6075.	6.6	68
58	A binding kinetics study of human adenosine A3 receptor agonists. Biochemical Pharmacology, 2018, 153, 248-259.	2.0	11
59	Constitutive activity of the metabotropic glutamate receptor 2 explored with a whole-cell label-free biosensor. Biochemical Pharmacology, 2018, 152, 201-210.	2.0	16
60	Species differences and mechanism of action of A3 adenosine receptor allosteric modulators. Purinergic Signalling, 2018, 14, 59-71.	1.1	17
61	Molecular Basis of Ligand Dissociation from G Protein-Coupled Receptors and Predicting Residence Time. Methods in Molecular Biology, 2018, 1705, 197-206.	0.4	3
62	Kinetics of human cannabinoid 1 (CB1) receptor antagonists: Structure-kinetics relationships (SKR) and implications for insurmountable antagonism. Biochemical Pharmacology, 2018, 151, 166-179.	2.0	9
63	Pyrrolone Derivatives as Intracellular Allosteric Modulators for Chemokine Receptors: Selective and Dual-Targeting Inhibitors of CC Chemokine Receptors 1 and 2. Journal of Medicinal Chemistry, 2018, 61, 9146-9161.	2.9	21
64	An Affinity-Based Probe for the Human Adenosine A_{2A} Receptor. Journal of Medicinal Chemistry, 2018, 61, 7892-7901.	2.9	39
65	Impact of allosteric modulation: Exploring the binding kinetics of glutamate and other orthosteric ligands of the metabotropic glutamate receptor 2. Biochemical Pharmacology, 2018, 155, 356-365.	2.0	6
66	Kinetic Aspects of the Interaction between Ligand and G Protein-Coupled Receptor: The Case of the Adenosine Receptors. Chemical Reviews, 2017, 117, 38-66.	23.0	51
67	Kinetics for Drug Discovery: an industry-driven effort to target drug residence time. Drug Discovery Today, 2017, 22, 896-911.	3.2	165
68	A novel CCR2 antagonist inhibits atherogenesis in apoE deficient mice by achieving high receptor occupancy. Scientific Reports, 2017, 7, 52.	1.6	50
69	Phenotypic screening of cannabinoid receptor 2 ligands shows different sensitivity to genotype. Biochemical Pharmacology, 2017, 130, 60-70.	2.0	4
70	A covalent antagonist for the human adenosine A2A receptor. Purinergic Signalling, 2017, 13, 191-201.	1.1	22
71	Structure-Activity Relationships of the Sustained Effects of Adenosine A2A Receptor Agonists Driven by Slow Dissociation Kinetics. Molecular Pharmacology, 2017, 91, 25-38.	1.0	18
72	From receptor binding kinetics to signal transduction; a missing link in predicting in vivo drug-action. Scientific Reports, 2017, 7, 14169.	1.6	7

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73	A New Class of Fluorinated A_{2A} Adenosine Receptor Agonist with Application to Lastâ€Step Enzymatic [¹⁸F]Fluorination for PET Imaging. ChemBioChem, 2017, 18, 2156-2164.	1.3	12
74	A Novel Selective Inverse Agonist of the CB₂ Receptor as a Radiolabeled Tool Compound for Kinetic Binding Studies. Molecular Pharmacology, 2017, 92, 389-400.	1.0	17
75	Label-free technology and patient cells: from early drug development to precision medicine. Drug Discovery Today, 2017, 22, 1808-1815.	3.2	28
76	Beyond the hype: deep neural networks outperform established methods using a ChEMBL bioactivity benchmark set. Journal of Cheminformatics, 2017, 9, 45.	2.8	219
77	Structureâ€“Affinity Relationships and Structureâ€“Kinetics Relationships of Pyrido[2,1-f]purine-2,4-dione Derivatives as Human Adenosine A₃ Receptor Antagonists. Journal of Medicinal Chemistry, 2017, 60, 7555-7568.	2.9	26
78	Reduced hepatitis B and D viral entry using clinically applied drugs as novel inhibitors of the bile acid transporter NTCP. Scientific Reports, 2017, 7, 15307.	1.6	72
79	Structureâ€“Affinity Relationships and Structureâ€“Kinetic Relationships of 1,2-Diarylimidazol-4-carboxamide Derivatives as Human Cannabinoid 1 Receptor Antagonists. Journal of Medicinal Chemistry, 2017, 60, 9545-9564.	2.9	6
80	Discovery and Kinetic Profiling of 7-Aryl-1,2,4-triazolo[4,3-a]pyridines: Positive Allosteric Modulators of the Metabotropic Glutamate Receptor 2. Journal of Medicinal Chemistry, 2017, 60, 6704-6720.	2.9	35
81	Synthesis and evaluation of N-substituted 2-amino-4,5-diarylpyrimidines as selective adenosine A1 receptor antagonists. European Journal of Medicinal Chemistry, 2017, 125, 586-602.	2.6	9
82	Small molecule absorption by PDMS in the context of drug response bioassays. Biochemical and Biophysical Research Communications, 2017, 482, 323-328.	1.0	312
83	Molecular mechanism of positive allosteric modulation of the metabotropic glutamate receptor 2 by JNJâ€46281222. British Journal of Pharmacology, 2016, 173, 588-600.	2.7	39
84	A new <scp>hERG</scp> allosteric modulator rescues genetic and drugâ€induced longâ€<scp>QT</scp> syndrome phenotypes in cardiomyocytes from isogenic pairs of patient induced pluripotent stem cells. EMBO Molecular Medicine, 2016, 8, 1065-1081.	3.3	77
85	Structure of CC chemokine receptor 2 with orthosteric and allosteric antagonists. Nature, 2016, 540, 458-461.	13.7	220
86	Equilibrium and kinetic selectivity profiling on the human adenosine receptors. Biochemical Pharmacology, 2016, 105, 34-41.	2.0	18
87	Allosteric Modulation of K _v 11.1 (hERG) Channels Protects Against Drug-Induced Ventricular Arrhythmias. Circulation: Arrhythmia and Electrophysiology, 2016, 9, e003439.	2.1	24
88	5â€²-Substituted Amiloride Derivatives as Allosteric Modulators Binding in the Sodium Ion Pocket of the Adenosine A_{2A} Receptor. Journal of Medicinal Chemistry, 2016, 59, 4769-4777.	2.9	30
89	Getting personal: Endogenous adenosine receptor signaling in lymphoblastoid cell lines. Biochemical Pharmacology, 2016, 115, 114-122.	2.0	5
90	Data-Driven Derivation of an â€œInformer Compound Setâ€• for Improved Selection of Active Compounds in High-Throughput Screening. Journal of Chemical Information and Modeling, 2016, 56, 1622-1630.	2.5	14

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91	Characterization of 12 GnRH peptide agonists â€“ a kinetic perspective. British Journal of Pharmacology, 2016, 173, 128-141.	2.7	29
92	Predicting Binding Affinities for GPCR Ligands Using Free-Energy Perturbation. ACS Omega, 2016, 1, 293-304.	1.6	108
93	The Added Value of Assessing Ligandâ€“Receptor Binding Kinetics in Drug Discovery. ACS Medicinal Chemistry Letters, 2016, 7, 819-821.	1.3	27
94	Kinetic binding and activation profiles of endogenous tachykinins targeting the NK1 receptor. Biochemical Pharmacology, 2016, 118, 88-95.	2.0	14
95	Interacting with GPCRs: Using Interaction Fingerprints for Virtual Screening. Journal of Chemical Information and Modeling, 2016, 56, 2053-2060.	2.5	12
96	In search of novel ligands using a structure-based approach: a case study on the adenosine A2A receptor. Journal of Computer-Aided Molecular Design, 2016, 30, 863-874.	1.3	20
97	Kinetic Profile of Neuropeptideâ€“Receptor Interactions. Trends in Neurosciences, 2016, 39, 830-839.	4.2	8
98	Controlling the Dissociation of Ligands from the Adenosine A_{2A} Receptor through Modulation of Salt Bridge Strength. Journal of Medicinal Chemistry, 2016, 59, 6470-6479.	2.9	151
99	Getting from A to Bâ€”exploring the activation motifs of the class B adhesion G proteinâ€coupled receptor subfamily G member 4/GPR112. FASEB Journal, 2016, 30, 1836-1848.	0.2	17
100	Analysis of Iterative Screening with Stepwise Compound Selection Based on Novartis In-house HTS Data. ACS Chemical Biology, 2016, 11, 1255-1264.	1.6	42
101	Scintillation proximity assay (SPA) as a new approach to determine a ligandâ€™s kinetic profile. A case in point for the adenosine A1 receptor. Purinergic Signalling, 2016, 12, 115-126.	1.1	38
102	On the Relation between HERG Channel Block in Cell Line and Action Potential Prolongation in Human iPSC Cardiomyocytes. Biophysical Journal, 2016, 110, 527a.	0.2	0
103	Persistent GnRH receptor activation in pituitary Î±T3-1 cells analyzed with a label-free technology. Biosensors and Bioelectronics, 2016, 79, 721-727.	5.3	9
104	Human G protein-coupled receptor studies in Saccharomyces cerevisiae. Biochemical Pharmacology, 2016, 114, 103-115.	2.0	22
105	Molecular Basis of Ligand Dissociation from the Adenosine A_{2A} Receptor. Molecular Pharmacology, 2016, 89, 485-491.	1.0	72
106	The role of the C-terminus of the human hydroxycarboxylic acid receptors 2 and 3 in G protein activation using Gî±-engineered yeast cells. European Journal of Pharmacology, 2016, 770, 70-77.	1.7	5
107	Mass spectrometry-based ligand binding assays on adenosine A1 and A2A receptors. Purinergic Signalling, 2015, 11, 581-594.	1.1	20
108	Evaluation of (4â€Arylpiperidinâ€1â€yl)cyclopentanecarboxamides As Highâ€Affinity and Longâ€Residenceâ€Time Antagonists for the CCR2 Receptor. ChemMedChem, 2015, 10, 1249-1258.	1.6	7

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109	The Role of Target Binding Kinetics in Drug Discovery. ChemMedChem, 2015, 10, 1793-1796.	1.6	37
110	Indanesâ€"Properties, Preparation, and Presence in Ligands for G Protein Coupled Receptors. Medicinal Research Reviews, 2015, 35, 1097-1126.	5.0	36
111	Affinity and kinetics study of anthranilic acids as HCA2 receptor agonists. Bioorganic and Medicinal Chemistry, 2015, 23, 4013-4025.	1.4	5
112	When structureâ€"affinity relationships meet structureâ€"kinetics relationships: 3-((Inden-1-yl)amino)-1-isopropyl-cyclopentane-1-carboxamides as CCR2 antagonists. European Journal of Medicinal Chemistry, 2015, 93, 121-134.	2.6	23
113	<scp>K_v11.1</scp> (<scp>hERG</scp>)â€induced cardiotoxicity: a molecular insight from a binding kinetics study of prototypical <scp>K_v11.1</scp> (<scp>hERG</scp>) inhibitors. British Journal of Pharmacology, 2015, 172, 940-955.	2.7	32
114	Structure-kinetics relationships of Capadenoson derivatives as adenosine A 1 receptor agonists. European Journal of Medicinal Chemistry, 2015, 101, 681-691.	2.6	28
115	Whole-cell biosensor for label-free detection of GPCR-mediated drug responses in personal cell lines. Biosensors and Bioelectronics, 2015, 74, 233-242.	5.3	34
116	Structureâ€"Affinity Relationships (SARs) and Structureâ€"Kinetics Relationships (SKRs) of K_v11.1 Blockers. Journal of Medicinal Chemistry, 2015, 58, 5916-5929.	2.9	22
117	Synthesis and biological evaluation of a new series of 2-amino-3-aroyl thiophene derivatives as agonist allosteric modulators of the A 1 adenosine receptor. A position-dependent effect study. European Journal of Medicinal Chemistry, 2015, 101, 185-204.	2.6	13
118	Sodium Ion Binding Pocket Mutations and Adenosine A_{2A}Receptor Function. Molecular Pharmacology, 2015, 87, 305-313.	1.0	79
119	Scanning mutagenesis in a yeast system delineates the role of the NPxxY(x) 5,6 F motif and helix 8 of the adenosine A 2B receptor in G protein coupling. Biochemical Pharmacology, 2015, 95, 290-300.	2.0	18
120	Proteochemometric modelling coupled to in silico target prediction: an integrated approach for the simultaneous prediction of polypharmacology and binding affinity/potency of small molecules. Journal of Cheminformatics, 2015, 7, 15.	2.8	29
121	Synthesis and biological evaluation of negative allosteric modulators of the Kv11.1(hERG) channel. European Journal of Medicinal Chemistry, 2015, 106, 50-59.	2.6	16
122	Polypharmacology modelling using proteochemometrics (PCM): recent methodological developments, applications to target families, and future prospects. MedChemComm, 2015, 6, 24-50.	3.5	109
123	A3Adenosine Receptor Allosteric Modulator Induces an Anti-Inflammatory Effect:In VivoStudies and Molecular Mechanism of Action. Mediators of Inflammation, 2014, 2014, 1-8.	1.4	27
124	Caffeine increases light responsiveness of the mouse circadian pacemaker. European Journal of Neuroscience, 2014, 40, 3504-3511.	1.2	54
125	Molecular mechanism of allosteric modulation at <scp>GPCRs</scp>: insight from a binding kinetics study at the human <scp>A</scp>₁ adenosine receptor. British Journal of Pharmacology, 2014, 171, 5295-5312.	2.7	20
126	Discovery and Mapping of an Intracellular Antagonist Binding Site at the Chemokine Receptor CCR2. Molecular Pharmacology, 2014, 86, 358-368.	1.0	35

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127	Allosteric modulators of the hERG K+ channel. Toxicology and Applied Pharmacology, 2014, 274, 78-86.	1.3	23
128	A yeast screening method to decipher the interaction between the adenosine A2B receptor and the C-terminus of different G protein Î±-subunits. Purinergic Signalling, 2014, 10, 441-453.	1.1	16
129	Bias in chemokine receptor signalling. Trends in Immunology, 2014, 35, 243-252.	2.9	75
130	Drugâ€Target Residence Timeâ€"A Case for G Proteinâ€Coupled Receptors. Medicinal Research Reviews, 2014, 34, 856-892.	5.0	145
131	How Diverse Are Diversity Assessment Methods? A Comparative Analysis and Benchmarking of Molecular Descriptor Space. Journal of Chemical Information and Modeling, 2014, 54, 230-242.	2.5	62
132	Design and synthesis of novel small molecule CCR2 antagonists: Evaluation of 4-aminopiperidine derivatives. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 5377-5380.	1.0	8
133	Selecting an Optimal Number of Binding Site Waters To Improve Virtual Screening Enrichments Against the Adenosine A_{2A} Receptor. Journal of Chemical Information and Modeling, 2014, 54, 1737-1746.	2.5	49
134	Binding Kinetics of ZM241385 Derivatives at the Human Adenosine A_{2A} Receptor. ChemMedChem, 2014, 9, 752-761.	1.6	45
135	Synthesis and Biological Evaluation of Novel Allosteric Enhancers of the A₁ Adenosine Receptor Based on 2-Amino-3-(4â€²-Chlorobenzoyl)-4-Substituted-5-Arylethynyl Thiophene. Journal of Medicinal Chemistry, 2014, 57, 7673-7686.	2.9	26
136	Domains for activation and inactivation in G protein-coupled receptors â€“ A mutational analysis of constitutive activity of the adenosine A2B receptor. Biochemical Pharmacology, 2014, 92, 348-357.	2.0	9
137	Agonists for the Adenosine A₁ Receptor with Tunable Residence Time. A Case for Nonribose 4-Amino-6-aryl-5-cyano-2-thiopyrimidines. Journal of Medicinal Chemistry, 2014, 57, 3213-3222.	2.9	47
138	Insights into Molecular Basis of hERG Inhibition by Studying a Library of Dofetilide Derivatives. Biophysical Journal, 2014, 106, 138a.	0.2	0
139	The Role of a Sodium Ion Binding Site in the Allosteric Modulation of the A2A Adenosine G Protein-Coupled Receptor. Structure, 2013, 21, 2175-2185.	1.6	118
140	Removal of Human Ether-Ã-go-go Related Gene (hERG) K⁺ Channel Affinity through Rigidity: A Case of Clofilium Analogues. Journal of Medicinal Chemistry, 2013, 56, 9427-9440.	2.9	30
141	Benchmarking of protein descriptor sets in proteochemometric modeling (part 2): modeling performance of 13 amino acid descriptor sets. Journal of Cheminformatics, 2013, 5, 42.	2.8	73
142	Benchmarking of protein descriptor sets in proteochemometric modeling (part 1): comparative study of 13 amino acid descriptor sets. Journal of Cheminformatics, 2013, 5, 41.	2.8	82
143	Complementarity between in Silico and Biophysical Screening Approaches in Fragment-Based Lead Discovery against the A2A Adenosine Receptor. Journal of Chemical Information and Modeling, 2013, 53, 2701-2714.	2.5	65
144	Structureâ€"Kinetic Relationshipsâ€"An Overlooked Parameter in Hit-to-Lead Optimization: A Case of Cyclopentylamines as Chemokine Receptor 2 Antagonists. Journal of Medicinal Chemistry, 2013, 56, 7706-7714.	2.9	60

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145	Structure-Based Identification of OATP1B1/3 Inhibitors. Molecular Pharmacology, 2013, 83, 1257-1267.	1.0	110
146	Functional selectivity of adenosine A1 receptor ligands?. Purinergic Signalling, 2013, 9, 91-100.	1.1	21
147	Strategies To Reduce hERG K⁺ Channel Blockade. Exploring Heteroaromaticity and Rigidity in Novel Pyridine Analogues of Dofetilide. Journal of Medicinal Chemistry, 2013, 56, 2828-2840.	2.9	35
148	Significantly Improved HIV Inhibitor Efficacy Prediction Employing Proteochemometric Models Generated From Antivirogram Data. PLoS Computational Biology, 2013, 9, e1002899.	1.5	42
149	Multiple Binding Sites for Small-Molecule Antagonists at the CC Chemokine Receptor 2. Molecular Pharmacology, 2013, 84, 551-561.	1.0	48
150	Dual-Point Competition Association Assay: A Fast and High-Throughput Kinetic Screening Method for Assessing Ligand-Receptor Binding Kinetics. Journal of Biomolecular Screening, 2013, 18, 309-320.	2.6	65
151	5â€²-AMP impacts lymphocyte recirculation through activation of A2Breceptors. Journal of Leukocyte Biology, 2013, 94, 89-98.	1.5	4
152	Adenosine A_{2B}Receptor Agonism Inhibits Neointimal Lesion Development After Arterial Injury in Apolipoprotein Eâ€“Deficient Mice. Arteriosclerosis, Thrombosis, and Vascular Biology, 2012, 32, 2197-2205.	1.1	20
153	Protection from Myocardial Ischemia/Reperfusion Injury by a Positive Allosteric Modulator of the A₃ Adenosine Receptor. Journal of Pharmacology and Experimental Therapeutics, 2012, 340, 210-217.	1.3	29
154	A Novel Nonribose Agonist, LUF5834, Engages Residues That Are Distinct from Those of Adenosine-Like Ligands to Activate the Adenosine A_{2a} Receptor. Molecular Pharmacology, 2012, 81, 475-487.	1.0	39
155	Effects of pyrazole partial agonists on HCA₂â€mediated flushing and VLDLâ€triglyceride levels in mice. British Journal of Pharmacology, 2012, 167, 818-825.	2.7	5
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