Vsevolod Katritch

List of Publications by Citations

124 papers	19,074 citations	62 h-index	136 g-index
136 ext. papers	21,476 ext. citations	19.1 avg, IF	6.44 L-index

#	Paper	IF	Citations
124	Structures of the CXCR4 chemokine GPCR with small-molecule and cyclic peptide antagonists. *Science*, **2010**, 330, 1066-71	33.3	1432
123	Structure of the human dopamine D3 receptor in complex with a D2/D3 selective antagonist. *Science*, **2010**, 330, 1091-5	33.3	938
122	Structure-function of the G protein-coupled receptor superfamily. *Annual Review of Pharmacology and Toxicology*, **2013**, 53, 531-56	17.9	758
121	Structural basis for allosteric regulation of GPCRs by sodium ions. *Science*, **2012**, 337, 232-6	33.3	714
120	Structure of an agonist-bound human A2A adenosine receptor. *Science*, **2011**, 332, 322-7	33.3	706
119	Structure of the human □opioid receptor in complex with JDTic. *Nature*, **2012**, 485, 327-32	50.4	695
118	Structure of the human histamine H1 receptor complex with doxepin. *Nature*, **2011**, 475, 65-70	50.4	630
117	Crystal structure of rhodopsin bound to arrestin by femtosecond X-ray laser. *Nature*, **2015**, 523, 561-7	50.4	572
116	Biased signaling pathways in □2-adrenergic receptor characterized by 19F-NMR. *Science*, **2012**, 335, 1106-10	33.3	523
115	Structural features for functional selectivity at serotonin receptors. *Science*, **2013**, 340, 615-9	33.3	492
114	Lipidic cubic phase injector facilitates membrane protein serial femtosecond crystallography. *Nature Communications*, **2014**, 5, 3309	17.4	416
113	Structure of a class C GPCR metabotropic glutamate receptor 1 bound to an allosteric modulator. *Science*, **2014**, 344, 58-64	33.3	406
112	Structure of the nociceptin/orphanin FQ receptor in complex with a peptide mimetic. *Nature*, **2012**, 485, 395-9	50.4	383
111	Structure of the human smoothened receptor bound to an antitumour agent. *Nature*, **2013**, 497, 338-43	50.4	375
110	Structural basis for molecular recognition at serotonin receptors. *Science*, **2013**, 340, 610-4	33.3	370
109	Serial femtosecond crystallography of G protein-coupled receptors. *Science*, **2013**, 342, 1521-4	33.3	367
108	Molecular control of □opioid receptor signalling. *Nature*, **2014**, 506, 191-6	50.4	355

107	Diversity and modularity of G protein-coupled receptor structures. *Trends in Pharmacological Sciences*, **2012**, 33, 17-27	13.2	348
106	Allosteric sodium in class A GPCR signaling. *Trends in Biochemical Sciences*, **2014**, 39, 233-44	10.3	314
105	Structure of the human glucagon class B G-protein-coupled receptor. *Nature*, **2013**, 499, 444-9	50.4	312
104	Conserved binding mode of human beta2 adrenergic receptor inverse agonists and antagonist revealed by X-ray crystallography. *Journal of the American Chemical Society*, **2010**, 132, 11443-5	16.4	297
103	Structure of the human P2Y12 receptor in complex with an antithrombotic drug. *Nature*, **2014**, 509, 115-8	50.4	272
102	Fusion partner toolchest for the stabilization and crystallization of G protein-coupled receptors. *Structure*, **2012**, 20, 967-76	5.2	272
101	Structure of the Angiotensin receptor revealed by serial femtosecond crystallography. *Cell*, **2015**, 161, 833-44	56.2	262
100	Generic GPCR residue numbers - aligning topology maps while minding the gaps. *Trends in Pharmacological Sciences*, **2015**, 36, 22-31	13.2	259
99	Status of GPCR modeling and docking as reflected by community-wide GPCR Dock 2010 assessment. *Structure*, **2011**, 19, 1108-26	5.2	243
98	Two disparate ligand-binding sites in the human P2Y1 receptor. *Nature*, **2015**, 520, 317-21	50.4	239
97	Community-wide assessment of GPCR structure modelling and ligand docking: GPCR Dock 2008. *Nature Reviews Drug Discovery*, **2009**, 8, 455-63	64.1	236
96	Agonist-bound structure of the human P2Y12 receptor. *Nature*, **2014**, 509, 119-22	50.4	222
95	Geometry and physics of knots. *Nature*, **1996**, 384, 142-145	50.4	218
94	Structure-based discovery of novel chemotypes for adenosine A(2A) receptor antagonists. *Journal of Medicinal Chemistry*, **2010**, 53, 1799-809	8.3	211
93	The GPCR Network: a large-scale collaboration to determine human GPCR structure and function. *Nature Reviews Drug Discovery*, **2013**, 12, 25-34	64.1	207
92	Structure of the Nanobody-Stabilized Active State of the Kappa Opioid Receptor. *Cell*, **2018**, 172, 55-67.e15	56.2	205
91	Determination of DNA persistence length by cryo-electron microscopy. Separation of the static and dynamic contributions to the apparent persistence length of DNA. *Journal of Molecular Biology*, **1995**, 254, 579-94	6.5	189
90	Structural basis for Smoothened receptor modulation and chemoresistance to anticancer drugs. *Nature Communications*, **2014**, 5, 4355	17.4	175

89	Crystal Structure of the Human Cannabinoid Receptor CB2. *Cell*, **2019**, 176, 459-467.e13	56.2	175
88	Crystal structure-based virtual screening for fragment-like ligands of the human histamine H(1) receptor. *Journal of Medicinal Chemistry*, **2011**, 54, 8195-206	8.3	171
87	Electrophoretic mobility of DNA knots. *Nature*, **1996**, 384, 122	50.4	152
86	Advances in GPCR modeling evaluated by the GPCR Dock 2013 assessment: meeting new challenges. *Structure*, **2014**, 22, 1120-1139	5.2	136
85	Structural basis for bifunctional peptide recognition at human δ-opioid receptor. *Nature Structural and Molecular Biology*, **2015**, 22, 265-8	17.6	133
84	Genetically encoded chemical probes in cells reveal the binding path of urocortin-I to CRF class B GPCR. *Cell*, **2013**, 155, 1258-69	56.2	131
83	Structural basis for selectivity and diversity in angiotensin II receptors. *Nature*, **2017**, 544, 327-332	50.4	128
82	5-HT Receptor Structures Reveal the Structural Basis of GPCR Polypharmacology. *Cell*, **2018**, 172, 719-736.e14	36.2	123
81	Structural Basis for Ligand Recognition and Functional Selectivity at Angiotensin Receptor. *Journal of Biological Chemistry*, **2015**, 290, 29127-39	5.4	111
80	Ligand-dependent perturbation of the conformational ensemble for the GPCR β adrenergic receptor revealed by HDX. *Structure*, **2011**, 19, 1424-32	5.2	111
79	GPCR 3D homology models for ligand screening: lessons learned from blind predictions of adenosine A2a receptor complex. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 197-211	4.2	111
78	Tightness of random knotting. *Physical Review E*, **2000**, 61, 5545-9	2.4	108
77	Sedimentation and electrophoretic migration of DNA knots and catenanes. *Journal of Molecular Biology*, **1998**, 278, 1-3	6.5	106
76	Analysis of full and partial agonists binding to beta2-adrenergic receptor suggests a role of transmembrane helix V in agonist-specific conformational changes. *Journal of Molecular Recognition*, **2009**, 22, 307-18	2.6	100
75	Structural basis of ligand recognition at the human MT melatonin receptor. *Nature*, **2019**, 569, 284-288	50.4	98
74	The role of a sodium ion binding site in the allosteric modulation of the A(2A) adenosine G protein-coupled receptor. *Structure*, **2013**, 21, 2175-85	5.2	98
73	High resolution structure of the ba3 cytochrome c oxidase from Thermus thermophilus in a lipidic environment. *PLoS ONE*, **2011**, 6, e22348	3.7	94
72	Native phasing of x-ray free-electron laser data for a G protein-coupled receptor. *Science Advances*, **2016**, 2, e1600292	14.3	85

71	Pulling chromatin fibers: computer simulations of direct physical micromanipulations. *Journal of Molecular Biology*, **2000**, 295, 29-40	6.5	78
70	XFEL structures of the human MT melatonin receptor reveal the basis of subtype selectivity. *Nature* , **2019**, 569, 289-292	50.4	77
69	Structural Connection between Activation Microswitch and Allosteric Sodium Site in GPCR Signaling. *Structure*, **2018**, 26, 259-269.e5	5.2	77
68	Ligand binding and subtype selectivity of the human A(2A) adenosine receptor: identification and characterization of essential amino acid residues. *Journal of Biological Chemistry*, **2010**, 285, 13032-44	5.4	77
67	Nucleotides Acting at P2Y Receptors: Connecting Structure and Function. *Molecular Pharmacology*, **2015**, 88, 220-30	4.3	74
66	Structure based prediction of subtype-selectivity for adenosine receptor antagonists. *Neuropharmacology*, **2011**, 60, 108-15	5.5	71
65	Properties of ideal composite knots. *Nature*, **1997**, 388, 148-51	50.4	71
64	Structure-based ligand discovery targeting orthosteric and allosteric pockets of dopamine receptors. *Molecular Pharmacology*, **2013**, 84, 794-807	4.3	69
63	Single-molecule view of basal activity and activation mechanisms of the G protein-coupled receptor A2AR. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 14254-9	11.5	65
62	Synthesis of Photoswitchable Tetrahydrocannabinol Derivatives Enables Optical Control of Cannabinoid Receptor 1 Signaling. *Journal of the American Chemical Society*, **2017**, 139, 18206-18212	16.4	61
61	Sodium ion binding pocket mutations and adenosine A2A receptor function. *Molecular Pharmacology*, **2015**, 87, 305-13	4.3	60
60	An autism spectrum disorder-related de novo mutation hotspot discovered in the GEF1 domain of Trio. *Nature Communications*, **2017**, 8, 601	17.4	60
59	Identifying conformational changes of the beta(2) adrenoceptor that enable accurate prediction of ligand/receptor interactions and screening for GPCR modulators. *Journal of Computer-Aided Molecular Design*, **2009**, 23, 273-88	4.2	57
58	Optimization of adenosine 5′-carboxamide derivatives as adenosine receptor agonists using structure-based ligand design and fragment screening. *Journal of Medicinal Chemistry*, **2012**, 55, 4297-308	8.3	55
57	Aminoglycoside binding in the major groove of duplex RNA: the thermodynamic and electrostatic forces that govern recognition. *Journal of Molecular Biology*, **2000**, 298, 95-110	6.5	55
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55	The Importance of Ligand-Receptor Conformational Pairs in Stabilization: Spotlight on the N/OFQ G Protein-Coupled Receptor. *Structure*, **2015**, 23, 2291-2299	5.2	53
54	GPCR agonist binding revealed by modeling and crystallography. *Trends in Pharmacological Sciences* , **2011**, 32, 637-43	13.2	52

53	Crystal structure of the Frizzled 4 receptor in a ligand-free state. *Nature*, **2018**, 560, 666-670	50.4	51
52	Harnessing Ion-Binding Sites for GPCR Pharmacology. *Pharmacological Reviews*, **2019**, 71, 571-595	22.5	49
51	Structural basis of the activation of a metabotropic GABA receptor. *Nature*, **2020**, 584, 298-303	50.4	49
50	Chemotype-selective modes of action of κ-opioid receptor agonists. *Journal of Biological Chemistry*, **2013**, 288, 34470-83	5.4	45
49	Structural insights into the extracellular recognition of the human serotonin 2B receptor by an antibody. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 8223-8228	11.5	43
48	Structure-based mechanism of cysteinyl leukotriene receptor inhibition by antiasthmatic drugs. *Science Advances*, **2019**, 5, eaax2518	14.3	41
47	Computational design of thermostabilizing point mutations for G protein-coupled receptors. *ELife*, **2018**, 7,	8.9	40
46	Geometry and physics of catenanes applied to the study of DNA replication. *Biophysical Journal*, **1998**, 74, 2815-22	2.9	39
45	In vitro expression and analysis of the 826 human G protein-coupled receptors. *Protein and Cell*, **2016**, 7, 325-37	7.2	38
44	Elucidating the active δ-opioid receptor crystal structure with peptide and small-molecule agonists. *Science Advances*, **2019**, 5, eaax9115	14.3	38
43	In meso crystal structure and docking simulations suggest an alternative proteoglycan binding site in the OpcA outer membrane adhesin. *Proteins: Structure, Function and Bioinformatics*, **2008**, 71, 24-34	4.2	37
42	Evaluation of molecular modeling of agonist binding in light of the crystallographic structure of an agonist-bound A2A adenosine receptor. *Journal of Medicinal Chemistry*, **2012**, 55, 538-52	8.3	36
41	Discovery of small molecule inhibitors of ubiquitin-like poxvirus proteinase I7L using homology modeling and covalent docking approaches. *Journal of Computer-Aided Molecular Design*, **2007**, 21, 549-58	4.2	36
40	Structure-Based Discovery of New Antagonist and Biased Agonist Chemotypes for the Kappa Opioid Receptor. *Journal of Medicinal Chemistry*, **2017**, 60, 3070-3081	8.3	35
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38	Ligand-guided receptor optimization. *Methods in Molecular Biology*, **2012**, 857, 189-205	1.4	34
37	The effect of intrinsic curvature on conformational properties of circular DNA. *Biophysical Journal*, **1997**, 72, 1070-9	2.9	32
36	Structural basis of ligand selectivity and disease mutations in cysteinyl leukotriene receptors. *Nature Communications*, **2019**, 10, 5573	17.4	31

35	Exploring a 2-naphthoic acid template for the structure-based design of P2Y14 receptor antagonist molecular probes. *ACS Chemical Biology*, **2014**, 9, 2833-42	4.9	30
34	Opposite effect of counterions on the persistence length of nicked and non-nicked DNA. *Journal of Molecular Biology*, **1997**, 266, 711-21	6.5	28
33	Structural insight into the activation of a class B G-protein-coupled receptor by peptide hormones in live human cells. *ELife*, **2017**, 6,	8.9	25
32	Extrinsic Tryptophans as NMR Probes of Allosteric Coupling in Membrane Proteins: Application to the A Adenosine Receptor. *Journal of the American Chemical Society*, **2018**, 140, 8228-8235	16.4	24
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30	Crystal structure of misoprostol bound to the labor inducer prostaglandin E receptor. *Nature Chemical Biology*, **2019**, 15, 11-17	11.7	23
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28	O-GlcNAc Engineering of GPCR Peptide-Agonists Improves Their Stability and in Vivo Activity. *Journal of the American Chemical Society*, **2019**, 141, 14210-14219	16.4	19
27	Structure-based discovery of potent and selective melatonin receptor agonists. *ELife*, **2020**, 9,	8.9	19
26	Biased Signaling of the G-Protein-Coupled Receptor βAR Is Governed by Conformational Exchange Kinetics. *Structure*, **2020**, 28, 371-377.e3	5.2	18
25	IDEAL KNOTS AND THEIR RELATION TO THE PHYSICS OF REAL KNOTS. *Series on Knots and Everything*, **1998**, 1-19	2	17
24	Controlling opioid receptor functional selectivity by targeting distinct subpockets of the orthosteric site. *ELife*, **2021**, 10,	8.9	16
23	An Intellectual Disability-Related Missense Mutation in Rac1 Prevents LTP Induction. *Frontiers in Molecular Neuroscience*, **2018**, 11, 223	6.1	15
22	Synthon-based ligand discovery in virtual libraries of over 11 billion compounds.. *Nature*, **2021**,	50.4	15
21	Design, synthesis, pharmacological characterization of a fluorescent agonist of the P2Y receptor. *Bioorganic and Medicinal Chemistry Letters*, **2015**, 25, 4733-4739	2.9	14
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19	Single Amino Acid Variation Underlies Species-Specific Sensitivity to Amphibian Skin-Derived Opioid-like Peptides. *Chemistry and Biology*, **2015**, 22, 764-75		11
18	SimiCon: a web tool for protein-ligand model comparison through calculation of equivalent atomic contacts. *Bioinformatics*, **2010**, 26, 2784-5	7.2	11

17	Influence of nucleosome structure on the three-dimensional folding of idealized minichromosomes. *Structure*, **1999**, 7, 1009-22	5.2	11
16	Optical Control of Cannabinoid Receptor 2-Mediated Ca Release Enabled by Synthesis of Photoswitchable Probes. *Journal of the American Chemical Society*, **2021**, 143, 736-743	16.4	10
15	Novel Dual-Target Opioid Receptor and Dopamine D Receptor Ligands as Potential Nonaddictive Pharmacotherapeutics for Pain Management. *Journal of Medicinal Chemistry*, **2021**, 64, 7778-7808	8.3	8
14	Activation Stoichiometry and Pore Architecture of TRPA1 Probed with Channel Concatemers. *Scientific Reports*, **2018**, 8, 17104	4.9	8
13	Computational design for thermostabilization of GPCRs. *Current Opinion in Structural Biology*, **2019**, 55, 25-33	8.1	7
12	Exploring Pairwise Chemical Crosslinking To Study Peptide-Receptor Interactions. *ChemBioChem*, **2019**, 20, 683-692	3.8	5
11	Breaking the Enigma Code of Angiotensin II Type 2 Receptor Signaling. *Structure*, **2020**, 28, 390-392	5.2	4
10	Structural insights on ligand recognition at the human leukotriene B4 receptor 1. *Nature Communications*, **2021**, 12, 2971	17.4	4
9	Ligand-Dependent Effects of Methionine-8 Oxidation in Parathyroid Hormone Peptide Analogues. *Endocrinology*, **2021**, 162,	4.8	3
8	Structure-Based Virtual Screening of Ultra-Large Library Yields Potent Antagonists for a Lipid GPCR. *Biomolecules*, **2020**, 10,	5.9	3
7	Structure and Modeling of GPCRs: Implications for Drug Discovery **2010**, 385-433		2
6	Schizophrenia-associated SAP97 mutations increase glutamatergic synapse strength in the dentate gyrus and impair contextual episodic memory in rats.. *Nature Communications*, **2022**, 13, 798	17.4	1
5	Chiral Cyclic Aliphatic Linkers as Building Blocks for Selective Dopamine D or D Receptor Agonists. *Journal of Medicinal Chemistry*, **2021**, 64, 16088-16105	8.3	1
4	Novel Class of Psychedelic Iboga Alkaloids Disrupts Opioid Addiction States		1
3	Structural Characterization of KOR Inactive and Active States for 3D Pharmacology and Drug Discovery. *Handbook of Experimental Pharmacology*, **2022**, 271, 41-64	3.2	1
2	Expression and purification of an engineered human endothelin receptor B in a monomeric form. *Doklady Biochemistry and Biophysics*, **2016**, 467, 157-61	0.8	
1	Biased Signaling Pathways in -Adrenergic Receptor Characterized by 19F-NMR **2021**, 179-183		