

Vsevolod Katritch

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Schizophrenia-associated SAP97 mutations increase glutamatergic synapse strength in the dentate gyrus and impair contextual episodic memory in rats.. <i>Nature Communications</i> , 2022 , 13, 798	17.4	1
123	Structural Characterization of KOR Inactive and Active States for 3D Pharmacology and Drug Discovery. <i>Handbook of Experimental Pharmacology</i> , 2022 , 271, 41-64	3.2	1
122	Synthon-based ligand discovery in virtual libraries of over 11 billion compounds.. <i>Nature</i> , 2021 ,	50.4	15
121	Ligand-Dependent Effects of Methionine-8 Oxidation in Parathyroid Hormone Peptide Analogues. <i>Endocrinology</i> , 2021 , 162,	4.8	3
120	Chiral Cyclic Aliphatic Linkers as Building Blocks for Selective Dopamine D or D Receptor Agonists. <i>Journal of Medicinal Chemistry</i> , 2021 , 64, 16088-16105	8.3	1
119	Structural insights on ligand recognition at the human leukotriene B4 receptor 1. <i>Nature Communications</i> , 2021 , 12, 2971	17.4	4
118	Novel Dual-Target μ Opioid Receptor and Dopamine D Receptor Ligands as Potential Nonaddictive Pharmacotherapeutics for Pain Management. <i>Journal of Medicinal Chemistry</i> , 2021 , 64, 7778-7808	8.3	8
117	Optical Control of Cannabinoid Receptor 2-Mediated Ca Release Enabled by Synthesis of Photoswitchable Probes. <i>Journal of the American Chemical Society</i> , 2021 , 143, 736-743	16.4	10
116	Controlling opioid receptor functional selectivity by targeting distinct subpockets of the orthosteric site. <i>ELife</i> , 2021 , 10,	8.9	16
115	Biased Signaling Pathways in β -Adrenergic Receptor Characterized by 19F-NMR 2021 , 179-183		
114	Structural basis of the activation of a metabotropic GABA receptor. <i>Nature</i> , 2020 , 584, 298-303	50.4	49
113	Biased Signaling of the G-Protein-Coupled Receptor μ AR Is Governed by Conformational Exchange Kinetics. <i>Structure</i> , 2020 , 28, 371-377.e3	5.2	18
112	Breaking the Enigma Code of Angiotensin II Type 2 Receptor Signaling. <i>Structure</i> , 2020 , 28, 390-392	5.2	4
111	Structure-based discovery of potent and selective melatonin receptor agonists. <i>ELife</i> , 2020 , 9,	8.9	19
110	Structure-Based Virtual Screening of Ultra-Large Library Yields Potent Antagonists for a Lipid GPCR. <i>Biomolecules</i> , 2020 , 10,	5.9	3
109	Harnessing Ion-Binding Sites for GPCR Pharmacology. <i>Pharmacological Reviews</i> , 2019 , 71, 571-595	22.5	49
108	Structural basis of ligand recognition at the human MT melatonin receptor. <i>Nature</i> , 2019 , 569, 284-288	50.4	98

107	XFEL structures of the human MT melatonin receptor reveal the basis of subtype selectivity. <i>Nature</i> , 2019 , 569, 289-292	50.4	77
106	Computational design for thermostabilization of GPCRs. <i>Current Opinion in Structural Biology</i> , 2019 , 55, 25-33	8.1	7
105	O-GlcNAc Engineering of GPCR Peptide-Agonists Improves Their Stability and in Vivo Activity. <i>Journal of the American Chemical Society</i> , 2019 , 141, 14210-14219	16.4	19
104	Structure-based mechanism of cysteinyl leukotriene receptor inhibition by antiasthmatic drugs. <i>Science Advances</i> , 2019 , 5, eaax2518	14.3	41
103	Elucidating the active μ -opioid receptor crystal structure with peptide and small-molecule agonists. <i>Science Advances</i> , 2019 , 5, eaax9115	14.3	38
102	Structural basis of ligand selectivity and disease mutations in cysteinyl leukotriene receptors. <i>Nature Communications</i> , 2019 , 10, 5573	17.4	31
101	Exploring Pairwise Chemical Crosslinking To Study Peptide-Receptor Interactions. <i>ChemBioChem</i> , 2019 , 20, 683-692	3.8	5
100	Crystal Structure of the Human Cannabinoid Receptor CB2. <i>Cell</i> , 2019 , 176, 459-467.e13	56.2	175
99	Crystal structure of misoprostol bound to the labor inducer prostaglandin E receptor. <i>Nature Chemical Biology</i> , 2019 , 15, 11-17	11.7	23
98	A Thieno[2,3- d]pyrimidine Scaffold Is a Novel Negative Allosteric Modulator of the Dopamine D Receptor. <i>Journal of Medicinal Chemistry</i> , 2019 , 62, 174-206	8.3	12
97	5-HT Receptor Structures Reveal the Structural Basis of GPCR Polypharmacology. <i>Cell</i> , 2018 , 172, 719-730.e14	36.1	123
96	Structural Connection between Activation Microswitch and Allosteric Sodium Site in GPCR Signaling. <i>Structure</i> , 2018 , 26, 259-269.e5	5.2	77
95	Intracellular Transfer of Na in an Active-State G-Protein-Coupled Receptor. <i>Structure</i> , 2018 , 26, 171-180.e2	5.2	54
94	Structure of the Nanobody-Stabilized Active State of the Kappa Opioid Receptor. <i>Cell</i> , 2018 , 172, 55-67.e15	36.1	205
93	An Intellectual Disability-Related Missense Mutation in Rac1 Prevents LTP Induction. <i>Frontiers in Molecular Neuroscience</i> , 2018 , 11, 223	6.1	15
92	Crystal structure of the Frizzled 4 receptor in a ligand-free state. <i>Nature</i> , 2018 , 560, 666-670	50.4	51
91	Extrinsic Tryptophans as NMR Probes of Allosteric Coupling in Membrane Proteins: Application to the A Adenosine Receptor. <i>Journal of the American Chemical Society</i> , 2018 , 140, 8228-8235	16.4	24
90	Activation Stoichiometry and Pore Architecture of TRPA1 Probed with Channel Concatemers. <i>Scientific Reports</i> , 2018 , 8, 17104	4.9	8

89	Computational design of thermostabilizing point mutations for G protein-coupled receptors. <i>ELife</i> , 2018 , 7,	8.9	40
88	Structure-Based Discovery of New Antagonist and Biased Agonist Chemotypes for the Kappa Opioid Receptor. <i>Journal of Medicinal Chemistry</i> , 2017 , 60, 3070-3081	8.3	35
87	Structural basis for selectivity and diversity in angiotensin II receptors. <i>Nature</i> , 2017 , 544, 327-332	50.4	128
86	An autism spectrum disorder-related de novo mutation hotspot discovered in the GEF1 domain of Trio. <i>Nature Communications</i> , 2017 , 8, 601	17.4	60
85	Structural insights into the extracellular recognition of the human serotonin 2B receptor by an antibody. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, 8223-8228	11.5	43
84	Dynamic Strategic Bond Analysis Yields a Ten-Step Synthesis of 20-nor-Salvinorin A, a Potent μ OR Agonist. <i>ACS Central Science</i> , 2017 , 3, 1329-1336	16.8	23
83	Synthesis of Photoswitchable Δ^9 Tetrahydrocannabinol Derivatives Enables Optical Control of Cannabinoid Receptor 1 Signaling. <i>Journal of the American Chemical Society</i> , 2017 , 139, 18206-18212	16.4	61
82	Structural insight into the activation of a class B G-protein-coupled receptor by peptide hormones in live human cells. <i>ELife</i> , 2017 , 6,	8.9	25
81	Native phasing of x-ray free-electron laser data for a G protein-coupled receptor. <i>Science Advances</i> , 2016 , 2, e1600292	14.3	85
80	Expression and purification of an engineered human endothelin receptor B in a monomeric form. <i>Doklady Biochemistry and Biophysics</i> , 2016 , 467, 157-61	0.8	
79	In vitro expression and analysis of the 826 human G protein-coupled receptors. <i>Protein and Cell</i> , 2016 , 7, 325-37	7.2	38
78	Single Amino Acid Variation Underlies Species-Specific Sensitivity to Amphibian Skin-Derived Opioid-like Peptides. <i>Chemistry and Biology</i> , 2015 , 22, 764-75		11
77	Crystal structure of rhodopsin bound to arrestin by femtosecond X-ray laser. <i>Nature</i> , 2015 , 523, 561-7	50.4	572
76	Modeling ligand recognition at the P2Y12 receptor in light of X-ray structural information. <i>Journal of Computer-Aided Molecular Design</i> , 2015 , 29, 737-56	4.2	34
75	Structure of the Angiotensin receptor revealed by serial femtosecond crystallography. <i>Cell</i> , 2015 , 161, 833-44	56.2	262
74	Sodium ion binding pocket mutations and adenosine A2A receptor function. <i>Molecular Pharmacology</i> , 2015 , 87, 305-13	4.3	60
73	Two disparate ligand-binding sites in the human P2Y1 receptor. <i>Nature</i> , 2015 , 520, 317-21	50.4	239
72	Nucleotides Acting at P2Y Receptors: Connecting Structure and Function. <i>Molecular Pharmacology</i> , 2015 , 88, 220-30	4.3	74

71	The Importance of Ligand-Receptor Conformational Pairs in Stabilization: Spotlight on the N/OFQ G Protein-Coupled Receptor. <i>Structure</i> , 2015 , 23, 2291-2299	5.2	53
70	Single-molecule view of basal activity and activation mechanisms of the G protein-coupled receptor μ AR. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015 , 112, 14254-9	11.5	65
69	Design, synthesis, pharmacological characterization of a fluorescent agonist of the P2Y ₁₂ receptor. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2015 , 25, 4733-4739	2.9	14
68	Structural Basis for Ligand Recognition and Functional Selectivity at Angiotensin Receptor. <i>Journal of Biological Chemistry</i> , 2015 , 290, 29127-39	5.4	111
67	Generic GPCR residue numbers - aligning topology maps while minding the gaps. <i>Trends in Pharmacological Sciences</i> , 2015 , 36, 22-31	13.2	259
66	Structural basis for bifunctional peptide recognition at human μ opioid receptor. <i>Nature Structural and Molecular Biology</i> , 2015 , 22, 265-8	17.6	133
65	Structure of a class C GPCR metabotropic glutamate receptor 1 bound to an allosteric modulator. <i>Science</i> , 2014 , 344, 58-64	33.3	406
64	Lipidic cubic phase injector facilitates membrane protein serial femtosecond crystallography. <i>Nature Communications</i> , 2014 , 5, 3309	17.4	416
63	Structure of the human P2Y ₁₂ receptor in complex with an antithrombotic drug. <i>Nature</i> , 2014 , 509, 115-8	50.4	272
62	Allosteric sodium in class A GPCR signaling. <i>Trends in Biochemical Sciences</i> , 2014 , 39, 233-44	10.3	314
61	Molecular control of μ opioid receptor signalling. <i>Nature</i> , 2014 , 506, 191-6	50.4	355
60	Structural basis for Smoothed receptor modulation and chemoresistance to anticancer drugs. <i>Nature Communications</i> , 2014 , 5, 4355	17.4	175
59	Advances in GPCR modeling evaluated by the GPCR Dock 2013 assessment: meeting new challenges. <i>Structure</i> , 2014 , 22, 1120-1139	5.2	136
58	Agonist-bound structure of the human P2Y ₁₂ receptor. <i>Nature</i> , 2014 , 509, 119-22	50.4	222
57	Exploring a 2-naphthoic acid template for the structure-based design of P2Y ₁₄ receptor antagonist molecular probes. <i>ACS Chemical Biology</i> , 2014 , 9, 2833-42	4.9	30
56	Structure of the human glucagon class B G-protein-coupled receptor. <i>Nature</i> , 2013 , 499, 444-9	50.4	312
55	The role of a sodium ion binding site in the allosteric modulation of the A(2A) adenosine G protein-coupled receptor. <i>Structure</i> , 2013 , 21, 2175-85	5.2	98
54	Chemotype-selective modes of action of μ opioid receptor agonists. <i>Journal of Biological Chemistry</i> , 2013 , 288, 34470-83	5.4	45

53	Structure-based ligand discovery targeting orthosteric and allosteric pockets of dopamine receptors. <i>Molecular Pharmacology</i> , 2013 , 84, 794-807	4.3	69
52	Genetically encoded chemical probes in cells reveal the binding path of urocortin-I to CRF class B GPCR. <i>Cell</i> , 2013 , 155, 1258-69	56.2	131
51	Serial femtosecond crystallography of G protein-coupled receptors. <i>Science</i> , 2013 , 342, 1521-4	33.3	367
50	The GPCR Network: a large-scale collaboration to determine human GPCR structure and function. <i>Nature Reviews Drug Discovery</i> , 2013 , 12, 25-34	64.1	207
49	Structure-function of the G protein-coupled receptor superfamily. <i>Annual Review of Pharmacology and Toxicology</i> , 2013 , 53, 531-56	17.9	758
48	Structural features for functional selectivity at serotonin receptors. <i>Science</i> , 2013 , 340, 615-9	33.3	492
47	Structural basis for molecular recognition at serotonin receptors. <i>Science</i> , 2013 , 340, 610-4	33.3	370
46	Structure of the human smoothened receptor bound to an antitumour agent. <i>Nature</i> , 2013 , 497, 338-43	50.4	375
45	Fusion partner toolchest for the stabilization and crystallization of G protein-coupled receptors. <i>Structure</i> , 2012 , 20, 967-76	5.2	272
44	Structural basis for allosteric regulation of GPCRs by sodium ions. <i>Science</i> , 2012 , 337, 232-6	33.3	714
43	Diversity and modularity of G protein-coupled receptor structures. <i>Trends in Pharmacological Sciences</i> , 2012 , 33, 17-27	13.2	348
42	Biased signaling pathways in α -adrenergic receptor characterized by 19F-NMR. <i>Science</i> , 2012 , 335, 1106-10	39.3	523
41	Structure of the nociceptin/orphanin FQ receptor in complex with a peptide mimetic. <i>Nature</i> , 2012 , 485, 395-9	50.4	383
40	Structure of the human μ -opioid receptor in complex with JDTic. <i>Nature</i> , 2012 , 485, 327-32	50.4	695
39	Optimization of adenosine 5'-carboxamide derivatives as adenosine receptor agonists using structure-based ligand design and fragment screening. <i>Journal of Medicinal Chemistry</i> , 2012 , 55, 4297-308	8.3	55
38	Evaluation of molecular modeling of agonist binding in light of the crystallographic structure of an agonist-bound A _{2A} adenosine receptor. <i>Journal of Medicinal Chemistry</i> , 2012 , 55, 538-52	8.3	36
37	Ligand-guided receptor optimization. <i>Methods in Molecular Biology</i> , 2012 , 857, 189-205	1.4	34
36	Crystal structure-based virtual screening for fragment-like ligands of the human histamine H(1) receptor. <i>Journal of Medicinal Chemistry</i> , 2011 , 54, 8195-206	8.3	171

35	GPCR agonist binding revealed by modeling and crystallography. <i>Trends in Pharmacological Sciences</i> , 2011 , 32, 637-43	13.2	52
34	Structure based prediction of subtype-selectivity for adenosine receptor antagonists. <i>Neuropharmacology</i> , 2011 , 60, 108-15	5.5	71
33	Structure of an agonist-bound human A2A adenosine receptor. <i>Science</i> , 2011 , 332, 322-7	33.3	706
32	High resolution structure of the ba3 cytochrome c oxidase from <i>Thermus thermophilus</i> in a lipidic environment. <i>PLoS ONE</i> , 2011 , 6, e22348	3.7	94
31	Status of GPCR modeling and docking as reflected by community-wide GPCR Dock 2010 assessment. <i>Structure</i> , 2011 , 19, 1108-26	5.2	243
30	Ligand-dependent perturbation of the conformational ensemble for the GPCR β adrenergic receptor revealed by HDX. <i>Structure</i> , 2011 , 19, 1424-32	5.2	111
29	Structure of the human histamine H1 receptor complex with doxepin. <i>Nature</i> , 2011 , 475, 65-70	50.4	630
28	Ligand binding and subtype selectivity of the human A(2A) adenosine receptor: identification and characterization of essential amino acid residues. <i>Journal of Biological Chemistry</i> , 2010 , 285, 13032-44	5.4	77
27	SimiCon: a web tool for protein-ligand model comparison through calculation of equivalent atomic contacts. <i>Bioinformatics</i> , 2010 , 26, 2784-5	7.2	11
26	Structure of the human dopamine D3 receptor in complex with a D2/D3 selective antagonist. <i>Science</i> , 2010 , 330, 1091-5	33.3	938
25	Structures of the CXCR4 chemokine GPCR with small-molecule and cyclic peptide antagonists. <i>Science</i> , 2010 , 330, 1066-71	33.3	1432
24	Conserved binding mode of human beta2 adrenergic receptor inverse agonists and antagonist revealed by X-ray crystallography. <i>Journal of the American Chemical Society</i> , 2010 , 132, 11443-5	16.4	297
23	Structure and Modeling of GPCRs: Implications for Drug Discovery 2010 , 385-433		2
22	Structure-based discovery of novel chemotypes for adenosine A(2A) receptor antagonists. <i>Journal of Medicinal Chemistry</i> , 2010 , 53, 1799-809	8.3	211
21	GPCR 3D homology models for ligand screening: lessons learned from blind predictions of adenosine A2a receptor complex. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010 , 78, 197-211	4.2	111
20	Analysis of full and partial agonists binding to beta2-adrenergic receptor suggests a role of transmembrane helix V in agonist-specific conformational changes. <i>Journal of Molecular Recognition</i> , 2009 , 22, 307-18	2.6	100
19	Identifying conformational changes of the beta(2) adrenoceptor that enable accurate prediction of ligand/receptor interactions and screening for GPCR modulators. <i>Journal of Computer-Aided Molecular Design</i> , 2009 , 23, 273-88	4.2	57
18	Community-wide assessment of GPCR structure modelling and ligand docking: GPCR Dock 2008. <i>Nature Reviews Drug Discovery</i> , 2009 , 8, 455-63	64.1	236

17	In meso crystal structure and docking simulations suggest an alternative proteoglycan binding site in the OpcA outer membrane adhesin. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008 , 71, 24-34	4.2	37
16	Discovery of small molecule inhibitors of ubiquitin-like poxvirus proteinase I7L using homology modeling and covalent docking approaches. <i>Journal of Computer-Aided Molecular Design</i> , 2007 , 21, 549-582	4.2	36
15	ICFF: a new method to incorporate implicit flexibility into an internal coordinate force field. <i>Journal of Computational Chemistry</i> , 2003 , 24, 254-65	3.5	22
14	Tightness of random knotting. <i>Physical Review E</i> , 2000 , 61, 5545-9	2.4	108
13	Pulling chromatin fibers: computer simulations of direct physical micromanipulations. <i>Journal of Molecular Biology</i> , 2000 , 295, 29-40	6.5	78
12	Aminoglycoside binding in the major groove of duplex RNA: the thermodynamic and electrostatic forces that govern recognition. <i>Journal of Molecular Biology</i> , 2000 , 298, 95-110	6.5	55
11	Influence of nucleosome structure on the three-dimensional folding of idealized minichromosomes. <i>Structure</i> , 1999 , 7, 1009-22	5.2	11
10	Sedimentation and electrophoretic migration of DNA knots and catenanes. <i>Journal of Molecular Biology</i> , 1998 , 278, 1-3	6.5	106
9	Geometry and physics of catenanes applied to the study of DNA replication. <i>Biophysical Journal</i> , 1998 , 74, 2815-22	2.9	39
8	IDEAL KNOTS AND THEIR RELATION TO THE PHYSICS OF REAL KNOTS. <i>Series on Knots and Everything</i> , 1998 , 1-19	2	17
7	The effect of intrinsic curvature on conformational properties of circular DNA. <i>Biophysical Journal</i> , 1997 , 72, 1070-9	2.9	32
6	Opposite effect of counterions on the persistence length of nicked and non-nicked DNA. <i>Journal of Molecular Biology</i> , 1997 , 266, 711-21	6.5	28
5	Properties of ideal composite knots. <i>Nature</i> , 1997 , 388, 148-51	50.4	71
4	Electrophoretic mobility of DNA knots. <i>Nature</i> , 1996 , 384, 122	50.4	152
3	Geometry and physics of knots. <i>Nature</i> , 1996 , 384, 142-145	50.4	218
2	Determination of DNA persistence length by cryo-electron microscopy. Separation of the static and dynamic contributions to the apparent persistence length of DNA. <i>Journal of Molecular Biology</i> , 1995 , 254, 579-94	6.5	189
1	Novel Class of Psychedelic Iboga Alkaloids Disrupts Opioid Addiction States		1