

Irina Kufareva

List of Publications by Year in descending order

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102
papers

7,705
citations

76196

40
h-index

54797

84
g-index

116
all docs

116
docs citations

116
times ranked

11325
citing authors

#	ARTICLE	IF	CITATIONS
1	Sirtuin 2 Inhibitors Rescue α -Synuclein-Mediated Toxicity in Models of Parkinson's Disease. <i>Science</i> , 2007, 317, 516-519.	6.0	995
2	Structure of the CCR5 Chemokine Receptor-HIV Entry Inhibitor Maraviroc Complex. <i>Science</i> , 2013, 341, 1387-1390.	6.0	606
3	Crystal Structure of the Human Cannabinoid Receptor CB1. <i>Cell</i> , 2016, 167, 750-762.e14.	13.5	468
4	The emerging mutational landscape of G proteins and G-protein-coupled receptors in cancer. <i>Nature Reviews Cancer</i> , 2013, 13, 412-424.	12.8	462
5	Methods of Protein Structure Comparison. <i>Methods in Molecular Biology</i> , 2011, 857, 231-257.	0.4	378
6	Crystal structure of the chemokine receptor CXCR4 in complex with a viral chemokine. <i>Science</i> , 2015, 347, 1117-1122.	6.0	325
7	Status of GPCR Modeling and Docking as Reflected by Community-wide GPCR Dock 2010 Assessment. <i>Structure</i> , 2011, 19, 1108-1126.	1.6	269
8	Structure-Based Discovery of Novel Chemotypes for Adenosine A _{2A} Receptor Antagonists. <i>Journal of Medicinal Chemistry</i> , 2010, 53, 1799-1809.	2.9	231
9	Structure of CC chemokine receptor 2 with orthosteric and allosteric antagonists. <i>Nature</i> , 2016, 540, 458-461.	13.7	220
10	Four-Dimensional Docking: A Fast and Accurate Account of Discrete Receptor Flexibility in Ligand Docking. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 397-406.	2.9	172
11	Type-II Kinase Inhibitor Docking, Screening, and Profiling Using Modified Structures of Active Kinase States. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 7921-7932.	2.9	162
12	Chemokine and chemokine receptor structure and interactions: implications for therapeutic strategies. <i>Immunology and Cell Biology</i> , 2015, 93, 372-383.	1.0	162
13	3-Hydroxyanthranilic acid inhibits PDK1 activation and suppresses experimental asthma by inducing T cell apoptosis. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 18619-18624.	3.3	161
14	Pocketome: an encyclopedia of small-molecule binding sites in 4D. <i>Nucleic Acids Research</i> , 2012, 40, D535-D540.	6.5	149
15	Advances in GPCR Modeling Evaluated by the GPCR Dock 2013 Assessment: Meeting New Challenges. <i>Structure</i> , 2014, 22, 1120-1139.	1.6	149
16	Structure of CC Chemokine Receptor 5 with a Potent Chemokine Antagonist Reveals Mechanisms of Chemokine Recognition and Molecular Mimicry by HIV. <i>Immunity</i> , 2017, 46, 1005-1017.e5.	6.6	148
17	Viral Infection Controlled by a Calcium-Dependent Lipid-Binding Module in ALIX. <i>Developmental Cell</i> , 2013, 25, 364-373.	3.1	107
18	PIER: Protein interface recognition for structural proteomics. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 67, 400-417.	1.5	104

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19	Signal transmission through the CXC chemokine receptor 4 (CXCR4) transmembrane helices. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 9928-9933.	3.3	96
20	Towards a structural understanding of allosteric drugs at the human calcium-sensing receptor. Cell Research, 2016, 26, 574-592.	5.7	85
21	Structural basis of ligand interaction with atypical chemokine receptor 3. Nature Communications, 2017, 8, 14135.	5.8	83
22	Structure based prediction of subtype-selectivity for adenosine receptor antagonists. Neuropharmacology, 2011, 60, 108-115.	2.0	81
23	What Do Structures Tell Us About Chemokine Receptor Function and Antagonism?. Annual Review of Biophysics, 2017, 46, 175-198.	4.5	81
24	Tyrosine Phosphorylation of the G12-Interacting Protein GIV Promotes Activation of Phosphoinositide 3-Kinase During Cell Migration. Science Signaling, 2011, 4, ra64.	1.6	78
25	A new method for ligand docking to flexible receptors by dual alanine scanning and refinement (SCARE). Journal of Computer-Aided Molecular Design, 2008, 22, 311-325.	1.3	74
26	Stoichiometry and geometry of the CXC chemokine receptor 4 complex with CXC ligand 12: Molecular modeling and experimental validation. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E5363-72.	3.3	70
27	Identifying ligands at orphan GPCRs: current status using structure-based approaches. British Journal of Pharmacology, 2016, 173, 2934-2951.	2.7	70
28	Inactivating mutations in GNA13 and RHOA in Burkitt's lymphoma and diffuse large B-cell lymphoma: a tumor suppressor function for the G12/RhoA axis in B cells. Oncogene, 2016, 35, 3771-3780.	2.6	66
29	Pivotal role of P450-P450 interactions in CYP3A4 allostery: the case of 1-naphthoflavone. Biochemical Journal, 2013, 453, 219-230.	1.7	60
30	Improved docking, screening and selectivity prediction for small molecule nuclear receptor modulators using conformational ensembles. Journal of Computer-Aided Molecular Design, 2010, 24, 459-471.	1.3	59
31	TLR4 signaling and macrophage inflammatory responses are dampened by GIV/Girdin. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 26895-26906.	3.3	57
32	Molecular Mechanisms Deployed by Virally Encoded G Protein-Coupled Receptors in Human Diseases. Annual Review of Pharmacology and Toxicology, 2013, 53, 331-354.	4.2	55
33	The Flexible Pocketome Engine for Structural Chemogenomics. Methods in Molecular Biology, 2009, 575, 249-279.	0.4	55
34	Structural basis for activation of trimeric Gi proteins by multiple growth factor receptors via GIV/Girdin. Molecular Biology of the Cell, 2014, 25, 3654-3671.	0.9	54
35	Sulfopeptide Probes of the CXCR4/CXCL12 Interface Reveal Oligomer-Specific Contacts and Chemokine Allostery. ACS Chemical Biology, 2013, 8, 1955-1963.	1.6	51
36	<i>In Silico</i> Analysis of the Conservation of Human Toxicity and Endocrine Disruption Targets in Aquatic Species. Environmental Science & Technology, 2014, 48, 1964-1972.	4.6	51

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37	Normalization of cholesterol metabolism in spinal microglia alleviates neuropathic pain. <i>Journal of Experimental Medicine</i> , 2021, 218, .	4.2	51
38	The Angiotensin Receptor Blocker Losartan Suppresses Growth of Pulmonary Metastases via AT1R-Independent Inhibition of CCR2 Signaling and Monocyte Recruitment. <i>Journal of Immunology</i> , 2019, 202, 3087-3102.	0.4	48
39	Optimization of High Throughput Virtual Screening by Combining Shape-Matching and Docking Methods. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 489-497.	2.5	46
40	Discovery of novel membrane binding structures and functions. <i>Biochemistry and Cell Biology</i> , 2014, 92, 555-563.	0.9	46
41	Activation of G β γ at the Golgi by GIV/Girdin Imposes Finiteness in Arf1 Signaling. <i>Developmental Cell</i> , 2015, 33, 189-203.	3.1	46
42	Structural basis for GPCR-independent activation of heterotrimeric Gi proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 16394-16403.	3.3	43
43	Compound Activity Prediction Using Models of Binding Pockets or Ligand Properties in 3D. <i>Current Topics in Medicinal Chemistry</i> , 2012, 12, 1869-1882.	1.0	42
44	Membrane and Protein Interactions of the Pleckstrin Homology Domain Superfamily. <i>Membranes</i> , 2015, 5, 646-663.	1.4	42
45	AMP-activated protein kinase fortifies epithelial tight junctions during energetic stress via its effector GIV/Girdin. <i>ELife</i> , 2016, 5, .	2.8	41
46	The GAPs, GEFs, GDIs and now, GEMs: New kids on the heterotrimeric G protein signaling block. <i>Cell Cycle</i> , 2017, 16, 607-612.	1.3	40
47	Dual Targeting of the Chemokine Receptors CXCR4 and ACKR3 with Novel Engineered Chemokines. <i>Journal of Biological Chemistry</i> , 2015, 290, 22385-22397.	1.6	37
48	Lapatinib-Binding Protein Kinases in the African Trypanosome: Identification of Cellular Targets for Kinase-Directed Chemical Scaffolds. <i>PLoS ONE</i> , 2013, 8, e56150.	1.1	36
49	In Silico Identification and Pharmacological Evaluation of Novel Endocrine Disrupting Chemicals That Act via the Ligand-Binding Domain of the Estrogen Receptor β . <i>Toxicological Sciences</i> , 2014, 141, 188-197.	1.4	36
50	A Tyrosine Switch on NEDD4-2 E3 Ligase Transmits GPCR Inflammatory Signaling. <i>Cell Reports</i> , 2018, 24, 3312-3323.e5.	2.9	36
51	Chemokines and their receptors: insights from molecular modeling and crystallography. <i>Current Opinion in Pharmacology</i> , 2016, 30, 27-37.	1.7	35
52	Structure-Based Predictions of Activity Cliffs. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 1062-1076.	2.5	34
53	Identification of Novel Serotonin Transporter Compounds by Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 933-943.	2.5	32
54	Molecular mechanism of serotonin transporter inhibition elucidated by a new flexible docking protocol. <i>European Journal of Medicinal Chemistry</i> , 2012, 47, 24-37.	2.6	26

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55	Convergence of Wnt, growth factor, and heterotrimeric G protein signals on the guanine nucleotide exchange factor Daple. <i>Science Signaling</i> , 2018, 11, .	1.6	26
56	Novel cGMP Efflux Inhibitors Identified by Virtual Ligand Screening (VLS) and Confirmed by Experimental Studies. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 3049-3057.	2.9	25
57	2-Aminothiazole Derivatives as Selective Allosteric Modulators of the Protein Kinase CK2. 1. Identification of an Allosteric Binding Site. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 1803-1816.	2.9	25
58	Functional anatomy of the full-length CXCR4-CXCL12 complex systematically dissected by quantitative model-guided mutagenesis. <i>Science Signaling</i> , 2020, 13, .	1.6	24
59	Crosslinking-guided geometry of a complete CXC receptor-chemokine complex and the basis of chemokine subfamily selectivity. <i>PLoS Biology</i> , 2020, 18, e3000656.	2.6	24
60	A General Method for Site Specific Fluorescent Labeling of Recombinant Chemokines. <i>PLoS ONE</i> , 2014, 9, e81454.	1.1	21
61	Identification of Global and Ligand-Specific Calcium Sensing Receptor Activation Mechanisms. <i>Molecular Pharmacology</i> , 2018, 93, 619-630.	1.0	20
62	CCR2-Mediated Uptake of Constitutively Produced CCL2: A Mechanism for Regulating Chemokine Levels in the Blood. <i>Journal of Immunology</i> , 2019, 203, 3157-3165.	0.4	19
63	Receptor tyrosine kinases activate heterotrimeric G proteins via phosphorylation within the interdomain cleft of G β γ . <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 28763-28774.	3.3	19
64	Discovery of holoenzyme-disrupting chemicals as substrate-selective CK2 inhibitors. <i>Scientific Reports</i> , 2019, 9, 15893.	1.6	18
65	2-Aminothiazole Derivatives as Selective Allosteric Modulators of the Protein Kinase CK2. 2. Structure-Based Optimization and Investigation of Effects Specific to the Allosteric Mode of Action. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 1817-1836.	2.9	17
66	Disulfide Trapping for Modeling and Structure Determination of Receptor. <i>Methods in Enzymology</i> , 2016, 570, 389-420.	0.4	15
67	A Novel Approach to Quantify G-Protein-Coupled Receptor Dimerization Equilibrium Using Bioluminescence Resonance Energy Transfer. <i>Methods in Molecular Biology</i> , 2013, 1013, 93-127.	0.4	15
68	Quantum mechanics approaches to drug research in the era of structural chemogenomics. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1669-1675.	1.0	14
69	Homology modeling and ligand docking of Mitogen-activated protein kinase-activated protein kinase 5 (MK5). <i>Theoretical Biology and Medical Modelling</i> , 2013, 10, 56.	2.1	13
70	A Structural Snapshot of CYP2B4 in Complex with Paroxetine Provides Insights into Ligand Binding and Clusters of Conformational States. <i>Journal of Pharmacology and Experimental Therapeutics</i> , 2013, 346, 113-120.	1.3	13
71	PeptiSite: A structural database of peptide binding sites in 4D. <i>Biochemical and Biophysical Research Communications</i> , 2014, 445, 717-723.	1.0	13
72	Dual Action Calcium-Sensing Receptor Modulator Unmasks Novel Mode-Switching Mechanism. <i>ACS Pharmacology and Translational Science</i> , 2018, 1, 96-109.	2.5	13

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73	Design and Characterization of an Intracellular Covalent Ligand for CC Chemokine Receptor 2. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 2608-2621.	2.9	13
74	Negative allosteric modulators of the human calcium-sensing receptor bind to overlapping and distinct sites within the 7-transmembrane domain. <i>British Journal of Pharmacology</i> , 2020, 177, 1917-1930.	2.7	12
75	Experiment-Guided Molecular Modeling of Protein-Protein Complexes Involving GPCRs. <i>Methods in Molecular Biology</i> , 2015, 1335, 295-311.	0.4	11
76	Synthesis, Antidepressant Evaluation and Docking Studies of Long-Chain Alkylnitroquipazines as Serotonin Transporter Inhibitors. <i>Chemical Biology and Drug Design</i> , 2013, 81, 695-706.	1.5	10
77	Differential activity and selectivity of N-terminal modified CXCL12 chemokines at the CXCR4 and ACKR3 receptors. <i>Journal of Leukocyte Biology</i> , 2020, 107, 1123-1135.	1.5	9
78	Tyrosine-Based Signals Regulate the Assembly of Daple-PARD3 Complex at Cell-Cell Junctions. <i>IScience</i> , 2020, 23, 100859.	1.9	9
79	A long isoform of GIV/Girdin contains a PDZ-binding module that regulates localization and G-protein binding. <i>Journal of Biological Chemistry</i> , 2021, 296, 100493.	1.6	8
80	Orphan receptor GPR37L1 remains unliganded. <i>Nature Chemical Biology</i> , 2021, 17, 383-386.	3.9	6
81	Synthesis, in-vitro binding studies and docking of long-chain arylpiperazine nitroquipazine analogues, as potential serotonin transporter inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2012, 49, 200-210.	2.6	5
82	Strategies for Network GWAS Evaluated Using Classroom Crowd Science. <i>Cell Systems</i> , 2019, 8, 275-280.	2.9	5
83	Docking, Screening and Selectivity Prediction for Small-molecule Nuclear Receptor Modulators. <i>RSC Drug Discovery Series</i> , 2012, , 84-109.	0.2	4
84	Nilotinib, an approved leukemia drug, inhibits smoothened signaling in Hedgehog-dependent medulloblastoma. <i>PLoS ONE</i> , 2019, 14, e0214901.	1.1	4
85	Predicting Molecular Interactions in Structural Proteomics. , 2009, , 185-209.		3
86	Tackling the complexities of orphan GPCR ligand discovery with rationally assisted approaches. , 2020, , 295-334.		2
87	Druggable exosites of the human kino-pocketome. <i>Journal of Computer-Aided Molecular Design</i> , 2020, 34, 219-230.	1.3	2
88	Role of 3D Structures in Understanding, Predicting, and Designing Molecular Interactions in the Chemokine Receptor Family. <i>Topics in Medicinal Chemistry</i> , 2014, , 41-85.	0.4	1
89	Equivalence Checking of Arithmetic Circuits. , 2004, , 77-123.		0
90	Investigating Chemokine Receptor CCR2 Dynamics and Druggability by Ensemble Based Approaches. <i>Biophysical Journal</i> , 2018, 114, 399a.	0.2	0

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91	Dynamic Structural Modeling Revealed That Nilotinib Inhibits Smoothed Signaling. Neurosurgery, 2019, 66, .	0.6	0
92	Abstract 4202: Deciphering the effects of GNA13 mutations in B-cell lymphomas. , 2014, , .		0
93	Abstract 2059: Novel roles for GNA13 and RHOA as tumor suppressor genes. , 2015, , .		0
94	Abstract A168: Towards an understanding of the structural basis of CXCR7 ligand binding and signaling. , 2016, , .		0
95	â€œArrestin ARRDC3 is a Multifunctional Adaptor That Regulates G Proteinâ€Coupled Receptor Signaling and Breast Cancer Invasion. FASEB Journal, 2020, 34, 1-1.	0.2	0
96	Tyrosineâ€based Signals Converge on Daple&[bull]PARD3 Complex to Fineâ€tune Polarized Planar Cell Migration. FASEB Journal, 2020, 34, 1-1.	0.2	0
97	Title is missing!. , 2020, 18, e3000656.		0
98	Title is missing!. , 2020, 18, e3000656.		0
99	Title is missing!. , 2020, 18, e3000656.		0
100	Title is missing!. , 2020, 18, e3000656.		0
101	Title is missing!. , 2020, 18, e3000656.		0
102	Title is missing!. , 2020, 18, e3000656.		0