Irina Kufareva

List of Publications by Year
in descending order

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	A long isoform of GIV/Girdin contains a PDZ-binding module that regulates localization and G-protein binding. Journal of Biological Chemistry, 2021, 296, 100493.	1.6	8
2	Design and Characterization of an Intracellular Covalent Ligand for CC Chemokine Receptor 2. Journal of Medicinal Chemistry, 2021, 64, 2608-2621.	2.9	13
3	Orphan receptor GPR37L1 remains unliganded. Nature Chemical Biology, 2021, 17, 383-386.	3.9	6
4	Normalization of cholesterol metabolism in spinal microglia alleviates neuropathic pain. Journal of Experimental Medicine, 2021, 218, .	4.2	51
5	Tackling the complexities of orphan GPCR ligand discovery with rationally assisted approaches. , 2020, , 295-334.		2
6	Negative allosteric modulators of the human calciumâ€sensing receptor bind to overlapping and distinct sites within the 7â€transmembrane domain. British Journal of Pharmacology, 2020, 177, 1917-1930.	2.7	12
7	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
8	Functional anatomy of the full-length CXCR4-CXCL12 complex systematically dissected by quantitative model-guided mutagenesis. Science Signaling, 2020, 13, .	1.6	24
9	Receptor tyrosine kinases activate heterotrimeric G proteins via phosphorylation within the interdomain cleft of GÎ±i. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 28763-28774.	3.3	19
10	Differential activity and selectivity of N-terminal modified CXCL12 chemokines at the CXCR4 and ACKR3 receptors. Journal of Leukocyte Biology, 2020, 107, 1123-1135.	1.5	9
11	Tyrosine-Based Signals Regulate the Assembly of Dapleâ‹…PARD3 Complex at Cell-Cell Junctions. IScience, 2020, 23, 100859.	1.9	9
12	Druggable exosites of the human kino-pocketome. Journal of Computer-Aided Molecular Design, 2020, 34, 219-230.	1.3	2
13	Crosslinking-guided geometry of a complete CXC receptor-chemokine complex and the basis of chemokine subfamily selectivity. PLoS Biology, 2020, 18, e3000656.	2.6	24
14	aâ€arrestin 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
15	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
16	Title is missing!. , 2020, 18, e3000656.		0
17	Title is missing!. , 2020, 18, e3000656.		0
18	Title is missing!. , 2020, 18, e3000656.		0

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19	Title is missing!. , 2020, 18, e3000656.		0
20	Title is missing!. , 2020, 18, e3000656.		0
21	Title is missing!. , 2020, 18, e3000656.		0
22	Structural basis for GPCR-independent activation of heterotrimeric Gi proteins. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 16394-16403.	3.3	43
23	Dynamic Structural Modeling Revealed That Nilotinib Inhibits Smoothened Signaling. Neurosurgery, 2019, 66, .	0.6	0
24	Discovery of holoenzyme-disrupting chemicals as substrate-selective CK2 inhibitors. Scientific Reports, 2019, 9, 15893.	1.6	18
25	Nilotinib, an approved leukemia drug, inhibits smoothened signaling in Hedgehog-dependent medulloblastoma. PLoS ONE, 2019, 14, e0214901.	1.1	4
26	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. Journal of Medicinal Chemistry, 2019, 62, 1817-1836.	2.9	17
27	2-Aminothiazole Derivatives as Selective Allosteric Modulators of the Protein Kinase CK2. 1. Identification of an Allosteric Binding Site. Journal of Medicinal Chemistry, 2019, 62, 1803-1816.	2.9	25
28	Strategies for Network GWAS Evaluated Using Classroom Crowd Science. Cell Systems, 2019, 8, 275-280.	2.9	5
29	The Angiotensin Receptor Blocker Losartan Suppresses Growth of Pulmonary Metastases via AT1R-Independent Inhibition of CCR2 Signaling and Monocyte Recruitment. Journal of Immunology, 2019, 202, 3087-3102.	0.4	48
30	CCR2-Mediated Uptake of Constitutively Produced CCL2: A Mechanism for Regulating Chemokine Levels in the Blood. Journal of Immunology, 2019, 203, 3157-3165.	0.4	19
31	Convergence of Wnt, growth factor, and heterotrimeric G protein signals on the guanine nucleotide exchange factor Daple. Science Signaling, 2018, 11, .	1.6	26
32	Identification of Global and Ligand-Specific Calcium Sensing Receptor Activation Mechanisms. Molecular Pharmacology, 2018, 93, 619-630.	1.0	20
33	Dual Action Calcium-Sensing Receptor Modulator Unmasks Novel Mode-Switching Mechanism. ACS Pharmacology and Translational Science, 2018, 1, 96-109.	2.5	13
34	Investigating Chemokine Receptor CCR2 Dynamics and Druggability by Ensemble Based Approaches. Biophysical Journal, 2018, 114, 399a.	0.2	0
35	A Tyrosine Switch on NEDD4-2 E3 Ligase Transmits GPCR Inflammatory Signaling. Cell Reports, 2018, 24, 3312-3323.e5.	2.9	36
36	Structural basis of ligand interaction with atypical chemokine receptor 3. Nature Communications, 2017, 8, 14135.	5.8	83

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37	Structure of CC Chemokine Receptor 5 with a Potent Chemokine Antagonist Reveals Mechanisms of Chemokine Recognition and Molecular Mimicry by HIV. Immunity, 2017, 46, 1005-1017.e5.	6.6	148
38	What Do Structures Tell Us About Chemokine Receptor Function and Antagonism?. Annual Review of Biophysics, 2017, 46, 175-198.	4.5	81
39	The GAPs, GEFs, GDIs andâ€¦now, GEMs: New kids on the heterotrimeric G protein signaling block. Cell Cycle, 2017, 16, 607-612.	1.3	40
40	Identifying ligands at orphan GPCRs: current status using structureâ€based approaches. British Journal of Pharmacology, 2016, 173, 2934-2951.	2.7	70
41	Structure of CC chemokine receptor 2 with orthosteric and allosteric antagonists. Nature, 2016, 540, 458-461.	13.7	220
42	Disulfide Trapping for Modeling and Structure Determination of Receptor. Methods in Enzymology, 2016, 570, 389-420.	0.4	15
43	Chemokines and their receptors: insights from molecular modeling and crystallography. Current Opinion in Pharmacology, 2016, 30, 27-37.	1.7	35
44	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
45	Crystal Structure of the Human Cannabinoid Receptor CB1. Cell, 2016, 167, 750-762.e14.	13.5	468
46	Towards a structural understanding of allosteric drugs at the human calcium-sensing receptor. Cell Research, 2016, 26, 574-592.	5.7	85
47	Inactivating mutations in GNA13 and RHOA in Burkittâ€™s lymphoma and diffuse large B-cell lymphoma: a tumor suppressor function for the Gî±13/RhoA axis in B cells. Oncogene, 2016, 35, 3771-3780.	2.6	66
48	AMP-activated protein kinase fortifies epithelial tight junctions during energetic stress via its effector GIV/Girdin. ELife, 2016, 5, .	2.8	41
49	Abstract A168: Towards an understanding of the structural basis of CXCR7 ligand binding and signaling. , 2016, , .		0
50	Membrane and Protein Interactions of the Pleckstrin Homology Domain Superfamily. Membranes, 2015, 5, 646-663.	1.4	42
51	Crystal structure of the chemokine receptor CXCR4 in complex with a viral chemokine. Science, 2015, 347, 1117-1122.	6.0	325
52	Chemokine and chemokine receptor structure and interactions: implications for therapeutic strategies. Immunology and Cell Biology, 2015, 93, 372-383.	1.0	162
53	Structure-Based Predictions of Activity Cliffs. Journal of Chemical Information and Modeling, 2015, 55, 1062-1076.	2.5	34
54	Activation of Gî±i at the Golgi by GIV/Girdin Imposes Finiteness in Arf1 Signaling. Developmental Cell, 2015, 33, 189-203.	3.1	46

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55	Dual Targeting of the Chemokine Receptors CXCR4 and ACKR3 with Novel Engineered Chemokines. Journal of Biological Chemistry, 2015, 290, 22385-22397.	1.6	37
56	Experiment-Guided Molecular Modeling of Proteinâ€“Protein Complexes Involving GPCRs. Methods in Molecular Biology, 2015, 1335, 295-311.	0.4	11
57	Abstract 2059: Novel roles for GNA13 and RHOA as tumor suppressor genes. , 2015, , .		0
58	A General Method for Site Specific Fluorescent Labeling of Recombinant Chemokines. PLoS ONE, 2014, 9, e81454.	1.1	21
59	Discovery of novel membrane binding structures and functions. Biochemistry and Cell Biology, 2014, 92, 555-563.	0.9	46
60	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
61	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
62	PeptiSite: A structural database of peptide binding sites in 4D. Biochemical and Biophysical Research Communications, 2014, 445, 717-723.	1.0	13
63	In Silico Analysis of the Conservation of Human Toxicity and Endocrine Disruption Targets in Aquatic Species. Environmental Science & Technology, 2014, 48, 1964-1972.	4.6	51
64	Role of 3D Structures in Understanding, Predicting, and Designing Molecular Interactions in the Chemokine Receptor Family. Topics in Medicinal Chemistry, 2014, , 41-85.	0.4	1
65	Advances in GPCR Modeling Evaluated by the GPCR Dock 2013 Assessment: Meeting New Challenges. Structure, 2014, 22, 1120-1139.	1.6	149
66	Identification of Novel Serotonin Transporter Compounds by Virtual Screening. Journal of Chemical Information and Modeling, 2014, 54, 933-943.	2.5	32
67	In Silico Identification and Pharmacological Evaluation of Novel Endocrine Disrupting Chemicals That Act via the Ligand-Binding Domain of theÂEstrogen Receptor Î±. Toxicological Sciences, 2014, 141, 188-197.	1.4	36
68	Abstract 4202: Deciphering the effects of GNA13 mutations in B-cell lymphomas. , 2014, , .		0
69	Homology modeling and ligand docking of Mitogen-activated protein kinase-activated protein kinase 5 (MK5). Theoretical Biology and Medical Modelling, 2013, 10, 56.	2.1	13
70	Structure of the CCR5 Chemokine Receptorâ€“HIV Entry Inhibitor Maraviroc Complex. Science, 2013, 341, 1387-1390.	6.0	606
71	Quantum mechanics approaches to drug research in the era of structural chemogenomics. International Journal of Quantum Chemistry, 2013, 113, 1669-1675.	1.0	14
72	Sulfopeptide Probes of the CXCR4/CXCL12 Interface Reveal Oligomer-Specific Contacts and Chemokine Allostery. ACS Chemical Biology, 2013, 8, 1955-1963.	1.6	51

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73	The emerging mutational landscape of G proteins and G-protein-coupled receptors in cancer. Nature Reviews Cancer, 2013, 13, 412-424.	12.8	462
74	Viral Infection Controlled by a Calcium-Dependent Lipid-Binding Module in ALIX. Developmental Cell, 2013, 25, 364-373.	3.1	107
75	Pivotal role of P450â€“P450 interactions in CYP3A4 allostery: the case of Î±-naphthoflavone. Biochemical Journal, 2013, 453, 219-230.	1.7	60
76	Molecular Mechanisms Deployed by Virally Encoded G Proteinâ€“Coupled Receptors in Human Diseases. Annual Review of Pharmacology and Toxicology, 2013, 53, 331-354.	4.2	55
77	A Structural Snapshot of CYP2B4 in Complex with Paroxetine Provides Insights into Ligand Binding and Clusters of Conformational States. Journal of Pharmacology and Experimental Therapeutics, 2013, 346, 113-120.	1.3	13
78	Synthesis, Antidepressant Evaluation and Docking Studies of Longâ€Chain Alkylnitroquipazines as Serotonin Transporter Inhibitors. Chemical Biology and Drug Design, 2013, 81, 695-706.	1.5	10
79	Lapatinib-Binding Protein Kinases in the African Trypanosome: Identification of Cellular Targets for Kinase-Directed Chemical Scaffolds. PLoS ONE, 2013, 8, e56150.	1.1	36
80	A Novel Approach to Quantify G-Protein-Coupled Receptor Dimerization Equilibrium Using Bioluminescence Resonance Energy Transfer. Methods in Molecular Biology, 2013, 1013, 93-127.	0.4	15
81	Pocketome: an encyclopedia of small-molecule binding sites in 4D. Nucleic Acids Research, 2012, 40, D535-D540.	6.5	149
82	Compound Activity Prediction Using Models of Binding Pockets or Ligand Properties in 3D. Current Topics in Medicinal Chemistry, 2012, 12, 1869-1882.	1.0	42
83	Docking, Screening and Selectivity Prediction for Small-molecule Nuclear Receptor Modulators. RSC Drug Discovery Series, 2012, , 84-109.	0.2	4
84	Novel cGMP Efflux Inhibitors Identified by Virtual Ligand Screening (VLS) and Confirmed by Experimental Studies. Journal of Medicinal Chemistry, 2012, 55, 3049-3057.	2.9	25
85	Molecular mechanism of serotonin transporter inhibition elucidated by a new flexible docking protocol. European Journal of Medicinal Chemistry, 2012, 47, 24-37.	2.6	26
86	Synthesis, inÂvitro binding studies and docking of long-chain arylpiperazine nitroquipazine analogues, as potential serotonin transporter inhibitors. European Journal of Medicinal Chemistry, 2012, 49, 200-210.	2.6	5
87	Structure based prediction of subtype-selectivity for adenosine receptor antagonists. Neuropharmacology, 2011, 60, 108-115.	2.0	81
88	Status of GPCR Modeling and Docking as Reflected by Community-wide GPCR Dock 2010 Assessment. Structure, 2011, 19, 1108-1126.	1.6	269
89	Methods of Protein Structure Comparison. Methods in Molecular Biology, 2011, 857, 231-257.	0.4	378
90	Tyrosine Phosphorylation of the GÎ±-Interacting Protein GIV Promotes Activation of Phosphoinositide 3-Kinase During Cell Migration. Science Signaling, 2011, 4, ra64.	1.6	78

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91	Structure-Based Discovery of Novel Chemotypes for Adenosine A_{2A} Receptor Antagonists. Journal of Medicinal Chemistry, 2010, 53, 1799-1809.	2.9	231
92	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
93	Four-Dimensional Docking: A Fast and Accurate Account of Discrete Receptor Flexibility in Ligand Docking. Journal of Medicinal Chemistry, 2009, 52, 397-406.	2.9	172
94	The Flexible Pocketome Engine for Structural Chemogenomics. Methods in Molecular Biology, 2009, 575, 249-279.	0.4	55
95	Predicting Molecular Interactions in Structural Proteomics. , 2009, , 185-209.		3
96	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
97	Type-II Kinase Inhibitor Docking, Screening, and Profiling Using Modified Structures of Active Kinase States. Journal of Medicinal Chemistry, 2008, 51, 7921-7932.	2.9	162
98	Optimization of High Throughput Virtual Screening by Combining Shape-Matching and Docking Methods. Journal of Chemical Information and Modeling, 2008, 48, 489-497.	2.5	46
99	3-Hydroxyanthranilic acid inhibits PDK1 activation and suppresses experimental asthma by inducing T cell apoptosis. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 18619-18624.	3.3	161
100	Sirtuin 2 Inhibitors Rescue Â-Synuclein-Mediated Toxicity in Models of Parkinson's Disease. Science, 2007, 317, 516-519.	6.0	995
101	PIER: Protein interface recognition for structural proteomics. Proteins: Structure, Function and Bioinformatics, 2007, 67, 400-417.	1.5	104
102	Equivalence Checking of Arithmetic Circuits. , 2004, , 77-123.		0