Takatsugu Hirokawa

List of Publications by Year
in descending order

100	3,844	218677	133252
papers	citations	26 h-index	59 g-index

105	105	105	7998
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Ubiquitin is phosphorylated by PINK1 to activate parkin. Nature, 2014, 510, 162-166.	27.8	1,185
2	Structural Basis for a Broad But Selective Ligand Spectrum of a Mouse Olfactory Receptor: Mapping the Odorant-Binding Site. Journal of Neuroscience, 2005, 25, 1806-1815.	3.6	278
3	Aryl hydrocarbon receptor suppresses intestinal carcinogenesis in Apc ^{Min /+} mice with natural ligands. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 13481-13486.	7.1	238
4	Alterations of structure and hydrolase activity of parkinsonism-associated human ubiquitin carboxyl-terminal hydrolase L1 variants. Biochemical and Biophysical Research Communications, 2003, 304, 176-183.	2.1	151
5	Analysis of multiple compoundâ€“protein interactions reveals novel bioactive molecules. Molecular Systems Biology, 2011, 7, 472.	7.2	134
6	Potential anti-COVID-19 agents, cepharanthine and nelfinavir, and their usage for combination treatment. IScience, 2021, 24, 102367.	4.1	126
7	Ligand binding to human prostaglandin E receptor EP4 at the lipid-bilayer interface. Nature Chemical Biology, 2019, 15, 18-26.	8.0	85
8	Temperature-Sensitive Substrate and Product Binding Underlie Temperature-Compensated Phosphorylation in the Clock. Molecular Cell, 2017, 67, 783-798.e20.	9.7	79
9	Engineering PQQ glucose dehydrogenase with improved substrate specificity. New Biotechnology, 2004, 21, 81-89.	2.7	61
10	Molecular Mechanisms for Sweet-suppressing Effect of Gymnemic Acids. Journal of Biological Chemistry, 2014, 289, 25711-25720.	3.4	56
11	Proportion of membrane proteins in proteomes of 15 single-cell organisms analyzed by the SOSUI prediction system. Biophysical Chemistry, 1999, 82, 165-171.	2.8	55
12	Crystal Structures of Human Orexin 2 Receptor Bound to the Subtype-Selective Antagonist EMPA. Structure, 2018, 26, 7-19.e5.	3.3	55
13	Generation of KS-58 as the first K-Ras(G12D)-inhibitory peptide presenting anti-cancer activity in vivo. Scientific Reports, 2020, 10, 21671.	3.3	54
14	Site-specific Interaction Mapping of Phosphorylated Ubiquitin to Uncover Parkin Activation. Journal of Biological Chemistry, 2015, 290, 25199-25211.	3.4	50
15	Porin Associates with Tom22 to Regulate the Mitochondrial Protein Gate Assembly. Molecular Cell, 2019, 73, 1044-1055.e8.	9.7	47
16	A small-molecule compound inhibits a collagen-specific molecular chaperone and could represent a potential remedy for fibrosis. Journal of Biological Chemistry, 2017, 292, 20076-20085.	3.4	45
17	Discovery of indenopyrazoles as EGFR and VEGFR-2 tyrosine kinase inhibitors by in silico high-throughput screening. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 285-288.	2.2	41
18	Investigation of the Bioactive Conformation of Histamine H₃ Receptor Antagonists by the Cyclopropylic Strain-Based Conformational Restriction Strategy. Journal of Medicinal Chemistry, 2010, 53, 3585-3593.	6.4	40

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19	RCAI-56, a carbocyclic analogue of KRN7000: its synthesis and potent activity for natural killer (NK) T cells to preferentially produce interferon-Î³. Tetrahedron Letters, 2007, 48, 3343-3347.	1.4	39
20	Correlation Analyses on Binding Affinity of Sialic Acid Analogues and Anti-Influenza Drugs with Human Neuraminidase Using ab Initio MO Calculations on Their Complex Structures â€“ LERE-QSAR Analysis (IV). Journal of Chemical Information and Modeling, 2011, 51, 2706-2716.	5.4	35
21	Current Challenges and Opportunities in Designing Proteinâ€“Protein Interaction Targeted Drugs . Advances and Applications in Bioinformatics and Chemistry, 2020, Volume 13, 11-25.	2.6	34
22	Identification of potential inhibitors based on compound proposal contest: Tyrosine-protein kinase Yes as a target. Scientific Reports, 2015, 5, 17209.	3.3	33
23	JBIR-22, An Inhibitor for Proteinâ^'Protein Interaction of the Homodimer of Proteasome Assembly Factor 3. Journal of Natural Products, 2010, 73, 628-631.	3.0	31
24	The Effect of Conformational Flexibility on Binding Free Energy Estimation between Kinases and Their Inhibitors. Journal of Chemical Information and Modeling, 2016, 56, 2445-2456.	5.4	29
25	Design and Synthesis of a Berberine Dimer: A Fluorescent Ligand with High Affinity towards Gâ€Quadruplexes. Chemistry - A European Journal, 2015, 21, 14519-14528.	3.3	28
26	An iterative compound screening contest method for identifying target protein inhibitors using the tyrosine-protein kinase Yes. Scientific Reports, 2017, 7, 12038.	3.3	28
27	RCAI-37, 56, 59, 60, 92, 101, and 102, cyclitol and carbasugar analogs of KRN7000: Their synthesis and bioactivity for mouse lymphocytes to produce Th1-biased cytokines. Bioorganic and Medicinal Chemistry, 2009, 17, 6360-6373.	3.0	27
28	Trichostatin Analogues JBIR-109, JBIR-110, and JBIR-111 from the Marine Sponge-Derived Streptomyces sp. RM72. Journal of Natural Products, 2012, 75, 285-289.	3.0	27
29	Interaction of dopamine and acetylcholine with an amphiphilic resorcinarene receptor in aqueous micelle system. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 1367-1370.	2.2	26
30	Synthesis of Skeletal Analogues of Saxitoxin Derivatives and Evaluation of Their Inhibitory Activity on Sodium Ion Channels Na_V1.4 and Na_V1.5. Chemistry - A European Journal, 2011, 17, 12144-12152.	3.3	26
31	A Continuum theory for the prediction of lateral and rotational positioning of Î±-helices in membrane proteins: Bacteriorhodopsin. Proteins: Structure, Function and Bioinformatics, 1995, 22, 363-377.	2.6	25
32	Protease-resistant modified human Î²-hexosaminidase B ameliorates symptoms in GM2 gangliosidosis model. Journal of Clinical Investigation, 2016, 126, 1691-1703.	8.2	25
33	A unique amino acid substitution, T126I, in human genotype C of hepatitis B virus S gene and its possible influence on antigenic structural change. Gene, 2006, 383, 43-51.	2.2	24
34	Investigation of the Noncovalent Binding Mode of Covalent Proteasome Inhibitors around the Transition State by Combined Use of Cyclopropylic Strain-Based Conformational Restriction and Computational Modeling. Journal of Medicinal Chemistry, 2013, 56, 5829-5842.	6.4	24
35	Detailed Analysis of the Binding Mode of Vanilloids to Transient Receptor Potential Vanilloid Type I (TRPV1) by a Mutational and Computational Study. PLoS ONE, 2016, 11, e0162543.	2.5	24
36	Thymine at â€”5 Is Crucial for cpc Promoter Activity of Synechocystis sp. Strain PCC 6714. Journal of Bacteriology, 2003, 185, 6477-6480.	2.2	22

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37	Structure and dynamics of RNA polymerase II elongation complex. Biochemical and Biophysical Research Communications, 2006, 343, 90-98.	2.1	22
38	Discovery of Chemical Compound Groups with Common Structures by a Network Analysis Approach (Affinity Prediction Method). Journal of Chemical Information and Modeling, 2011, 51, 61-68.	5.4	21
39	Synthesis of saxitoxin derivatives bearing guanidine and urea groups at C13 and evaluation of their inhibitory activity on voltage-gated sodium channels. Organic and Biomolecular Chemistry, 2013, 11, 6642.	2.8	20
40	Evaluating cepharanthine analogues as natural drugs against SARSâ€CoVâ€2. FEBS Open Bio, 2022, 12, 285-294.	2.3	20
41	Stratifin Inhibits SCFFBW7 Formation and Blocks Ubiquitination of Oncoproteins during the Course of Lung Adenocarcinogenesis. Clinical Cancer Research, 2019, 25, 2809-2820.	7.0	19
42	Development of G-quadruplex ligands for selective induction of a parallel-type topology. Organic and Biomolecular Chemistry, 2018, 16, 7375-7382.	2.8	18
43	Structural insights into the differences among lactisole derivatives in inhibitory mechanisms against the human sweet taste receptor. PLoS ONE, 2019, 14, e0213552.	2.5	18
44	Design and Synthesis of Cyclic ADPâ€4â€Thioribose as a Stable Equivalent of Cyclic ADPâ€Ribose, a Calcium Ionâ€Mobilizing Second Messenger. Angewandte Chemie - International Edition, 2013, 52, 6633-6637.	13.8	17
45	Probing the Hydrophobic Binding Pocket of G-Protein-Coupled Lysophosphatidylserine Receptor GPR34/LPS₁ by Docking-Aided Structureâ€“Activity Analysis. Journal of Medicinal Chemistry, 2017, 60, 6384-6399.	6.4	17
46	Synthesis and Telomeric G-Quadruplex-Stabilizing Ability of Macrocyclic Hexaoxazoles Bearing Three Side Chains. Molecules, 2019, 24, 263.	3.8	16
47	Design and synthesis of unsymmetric macrocyclic hexaoxazole compounds with an ability to induce distinct G-quadruplex topologies in telomeric DNA. Organic and Biomolecular Chemistry, 2016, 14, 5109-5116.	2.8	15
48	A prospective compound screening contest identified broader inhibitors for Sirtuin 1. Scientific Reports, 2019, 9, 19585.	3.3	15
49	Molecular action of larvicidal flavonoids on ecdysteroidogenic glutathione S-transferase Noppera-bo in Aedes aegypti. BMC Biology, 2022, 20, 43.	3.8	15
50	Cyclopropane-based stereochemical diversity-oriented conformational restriction strategy: Histamine H₃and/or H₄receptor ligands with the 2,3-methanobutane backbone. Organic and Biomolecular Chemistry, 2012, 10, 736-745.	2.8	14
51	An integrated approach to unravel a crucial structural property required for the function of the insect steroidogenic Halloween protein Noppera-bo. Journal of Biological Chemistry, 2020, 295, 7154-7167.	3.4	14
52	Total synthesis and characterization of thielocin B1 as a proteinâ€“protein interaction inhibitor of PAC3 homodimer. Chemical Science, 2014, 5, 1860-1868.	7.4	13
53	Design and synthesis of 2-phenyl-1,4-dioxa-spiro[4.5]deca-6,9-dien-8-ones as potential anticancer agents starting from cytotoxic spiromamakone A. European Journal of Medicinal Chemistry, 2013, 66, 180-184.	5.5	12
54	Mode of substrate recognition by the Josephin domain of ataxinâ€3, which has an endoâ€type deubiquitinase activity. FEBS Letters, 2014, 588, 4422-4430.	2.8	12

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55	Synthesis of C12â€Keto Saxitoxin Derivatives with Unusual Inhibitory Activity Against Voltageâ€Gated Sodium Channels. Chemistry - A European Journal, 2020, 26, 2025-2033.	3.3	12
56	Relationship between Human Evolution and Neurally Mediated Syncope Disclosed by the Polymorphic Sites of the Adrenergic Receptor Gene Î±2B-AR. PLoS ONE, 2015, 10, e0120788.	2.5	12
57	The transcriptional corepressor CtBP2 serves as a metabolite sensor orchestrating hepatic glucose and lipid homeostasis. Nature Communications, 2021, 12, 6315.	12.8	12
58	Structure Activity Relationships of Quinoxalin-2-one Derivatives as Platelet-Derived Growth Factor-.BETA. Receptor (PDGF.BETA. R) Inhibitors, Derived from Molecular Modeling. Chemical and Pharmaceutical Bulletin, 2008, 56, 682-687.	1.3	11
59	Extended Template-Based Modeling and Evaluation Method Using Consensus of Binding Mode of GPCRs for Virtual Screening. Journal of Chemical Information and Modeling, 2014, 54, 3153-3161.	5.4	11
60	Discovery of Novel Indazole Derivatives as Orally Available Î²₃-Adrenergic Receptor Agonists Lacking Off-Target-Based Cardiovascular Side Effects. Journal of Medicinal Chemistry, 2017, 60, 3252-3265.	6.4	11
61	Analysis by metadynamics simulation of binding pathway of influenza virus M2 channel blockers. Microbiology and Immunology, 2018, 62, 34-43.	1.4	11
62	Exploring the Odorant Binding Site of a G-Protein-Coupled Olfactory Receptor. Current Computer-Aided Drug Design, 2008, 4, 123-131.	1.2	10
63	Unnatural Tripeptides as Potent Positive Allosteric Modulators of T1R2/T1R3. ACS Medicinal Chemistry Letters, 2019, 10, 800-805.	2.8	10
64	EFCAB2 is a novel calcium-binding protein in mouse testis and sperm. PLoS ONE, 2019, 14, e0214687.	2.5	10
65	Molecular Dynamics Simulation and Experimental Verification of the Interaction between Cyclin T1 and HIV-1 Tat Proteins. PLoS ONE, 2015, 10, e0119451.	2.5	10
66	Ibuprofen, a Nonsteroidal Anti-Inflammatory Drug, is a Potent Inhibitor of the Human Sweet Taste Receptor. Chemical Senses, 2020, 45, 667-673.	2.0	9
67	2-Carba-lysophosphatidic acid is a novel Î²-lysophosphatidic acid analogue with high potential for lysophosphatidic acid receptor activation and autotaxin inhibition. Scientific Reports, 2021, 11, 17360.	3.3	9
68	Synthesis of vitamin D3 derivatives with nitrogen-linked substituents at A-ring C-2 and evaluation of their vitamin D receptor-mediated transcriptional activity. Organic and Biomolecular Chemistry, 2012, 10, 7826.	2.8	8
69	Non-steroidal inhibitors of <i>Drosophila melanogaster</i> steroidogenic glutathione <i>S</i>-transferase Noppera-bo. Journal of Pesticide Sciences, 2021, 46, 75-87.	1.4	8
70	Differences in Intestinal Hydrolytic Activities between Cynomolgus Monkeys and Humans: Evaluation of Substrate Specificities Using Recombinant Carboxylesterase 2 Isozymes. Molecular Pharmaceutics, 2016, 13, 3176-3186.	4.6	7
71	Linear consecutive hexaoxazoles as G4 ligands inducing chair-type anti-parallel topology of a telomeric G-quadruplex. RSC Advances, 2020, 10, 43319-43323.	3.6	7
72	Discrimination of Golgi Type II Membrane Proteins Based on Their Hydropathy Profiles and the Amino Acid Propensities of Their Transmembrane Regions. Bioscience, Biotechnology and Biochemistry, 2011, 75, 82-88.	1.3	6

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73	Tertiary Structure Prediction of RNAâ€“RNA Complexes Using a Secondary Structure and Fragment-Based Method. Journal of Chemical Information and Modeling, 2014, 54, 672-682.	5.4	6
74	Re-Docking Scheme for Generating Near-Native Protein Complexes by Assembling Residue Interaction Fingerprints. PLoS ONE, 2013, 8, e69365.	2.5	6
75	Tailored Synthesis of 162â€Residue Sâ€Monoglycosylated GM2â€Activator Protein (GM2AP) Analogues that Allows Facile Access to a Protein Library. ChemBioChem, 2016, 17, 1986-1992.	2.6	5
76	MD simulation of the Tat/Cyclin T1/CDK9 complex revealing the hidden catalytic cavity within the CDK9 molecule upon Tat binding. PLoS ONE, 2017, 12, e0171727.	2.5	5
77	Computer-Aided Modeling of Pentachlorophenol 4-Monooxygenase and Site-Directed Mutagenesis of Its Active Site. Chemical and Pharmaceutical Bulletin, 2003, 51, 1293-1298.	1.3	4
78	Novel pH-dependent regulation of human cytosolic sialidase 2 (NEU2) activities by siastatin B and structural prediction of NEU2/siastatin B complex. Biochemistry and Biophysics Reports, 2015, 4, 234-242.	1.3	4
79	Funiculosin variants and phosphorylated derivatives promote innate immune responses via the Toll-like receptor 4/myeloid differentiation factor-2 complex. Journal of Biological Chemistry, 2017, 292, 15378-15394.	3.4	4
80	Synthesis and biological evaluation of thielocin B1 analogues as protein-protein interaction inhibitors of PAC3 homodimer. Bioorganic and Medicinal Chemistry, 2018, 26, 6023-6034.	3.0	4
81	Vinylnaphthalene-bearing hexaoxazole as a fluorescence turn-on type G-quadruplex ligand. Organic and Biomolecular Chemistry, 2021, 19, 8035-8040.	2.8	4
82	Chemosynthetic ethanolamine plasmalogen stimulates gonadotropin secretion from bovine gonadotrophs by acting as a potential GPR61 agonist. Animal Reproduction Science, 2022, 241, 106992.	1.5	4
83	Design, Synthesis, and Chemical and Biological Properties of Cyclic ADP-4-Thioribose as a Stable Equivalent of Cyclic ADP-Ribose. Messenger (Los Angeles, Calif: Print), 2014, 3, 35-51.	0.3	3
84	Combined replacement effects of human modified Î²-hexosaminidase B and GM2 activator protein on GM2 gangliosidoses fibroblasts. Biochemistry and Biophysics Reports, 2016, 7, 157-163.	1.3	3
85	JBIR-155, a Specific Class D Î²-Lactamase Inhibitor of Microbial Origin. Organic Letters, 2021, 23, 4415-4419.	4.6	3
86	Structural Insights into the Interaction of Filovirus Glycoproteins with the Endosomal Receptor Niemann-Pick C1: A Computational Study. Viruses, 2021, 13, 913.	3.3	3
87	Identification of Glycosyltransferases Focusing on Golgi Transmembrane Region. Trends in Glycoscience and Glycotechnology, 2007, 19, 41-47.	0.1	3
88	Hemeâ€dependent recognition of 5â€aminolevulinate synthase by the human mitochondrial molecular chaperone ClpX. FEBS Letters, 2021, 595, 3019.	2.8	3
89	Unfolding is the driving force for mitochondrial import and degradation of the Parkinson's disease-related protein DJ-1. Journal of Cell Science, 2021, 134, .	2.0	3
90	Site-Directed Chemical Mutations on Abzymes: Large Rate Accelerations in the Catalysis by Exchanging the Functionalized Small Nonprotein Components. ACS Chemical Biology, 2016, 11, 2803-2811.	3.4	2

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91	MDContactCom: a tool to identify differences of protein molecular dynamics from two MD simulation trajectories in terms of interresidue contacts. Bioinformatics, 2021, 38, 273-274.	4.1	2
92	Modeling of Human Neuraminidase-1 and Its Validation by LERE-Correlation Analysis. Chem-Bio Informatics Journal, 2013, 13, 30-44.	0.3	2
93	Ligandâ€“Phospholipid Conjugation: A Versatile Strategy for Developing Long-Acting Ligands That Bind to Membrane Proteins by Restricting the Subcellular Localization of the Ligand. Journal of Medicinal Chemistry, 2018, 61, 4020-4029.	6.4	1
94	Protein druggability assessment for natural products using in silico simulation: A case study with estrogen receptor and the flavonoid genistein. Gene, 2021, 791, 145726.	2.2	1
95	Synthesis and Biological Evaluation of NMDI14 Derivatives as Anti-Mesothelioma Agents. Heterocycles, 2020, 100, 253.	0.7	1
96	Contributory presentations/posters. Journal of Biosciences, 1999, 24, 33-198.	1.1	0
97	2P-284 Protein-protein docking with protein flexibility from bioinformatic approach(Invited Talk for) Tj ETQq1 1 0.784314 rgBT /Overl	0.1	0
98	Computational analysis of ligand recognition mechanisms by prostaglandin E2 (subtype 2) and D2 receptors. Theoretical Chemistry Accounts, 2011, 130, 1131-1143.	1.4	0
99	Structural insights from an in silico molecular docking simulation of complement component 3a receptor 1 with an antagonist. Journal of Molecular Graphics and Modelling, 2021, 106, 107914.	2.4	0
100	Inverse Mixed-Solvent Molecular Dynamics for Visualization of the Residue Interaction Profile of Molecular Probes. International Journal of Molecular Sciences, 2022, 23, 4749.	4.1	0