Yasushi Okuno

List of Publications by Year
in descending order

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86 papers	2,649 citations	201674 27 h-index	214800 47 g-index
92 all docs	92 docs citations	92 times ranked	4215 citing authors

#	Article	IF	Citations
1	Integrated approach to functional analysis of an ERBB2 variant of unknown significance detected by a cancer gene panel test. Cellular Oncology (Dordrecht), 2022, 45, 121.	4.4	1
2	CBNplot: Bayesian network plots for enrichment analysis. Bioinformatics, 2022, 38, 2959-2960.	4.1	19
3	AI-Driven Synthetic Route Design Incorporated with Retrosynthesis Knowledge. Journal of Chemical Information and Modeling, 2022, 62, 1357-1367.	5.4	15
4	Proteinâ€“ligand binding affinity prediction of cyclinâ€dependent kinaseâ€2 inhibitors by dynamically averaged fragment molecular orbitalâ€based interaction energy. Journal of Computational Chemistry, 2022, 43, 1362-1371.	3.3	10
5	Using incomplete Cholesky factorization to increase the time step in molecular dynamics simulations. Journal of Computational and Applied Mathematics, 2022, 415, 114519.	2.0	1
6	Single-Image Super-Resolution Improvement of X-ray Single-Particle Diffraction Images Using a Convolutional Neural Network. Journal of Chemical Information and Modeling, 2022, 62, 3352-3364.	5.4	1
7	Metagenomic profiling of gut microbiome in early chronic kidney disease. Nephrology Dialysis Transplantation, 2021, 36, 1675-1684.	0.7	29
8	Novel Resistance Mechanisms Including L1196Q, P1094H, and R1248_D1249 Insertion in Three Patients With NSCLC After ALK Tyrosine Kinase Inhibitor Treatment. Journal of Thoracic Oncology, 2021, 16, 477-482.	1.1	7
9	Topical application of toll-like receptor 3 inhibitors ameliorates chronic allergic skin inflammation in mice. Journal of Dermatological Science, 2021, 101, 141-144.	1.9	3
10	Discovery of natural TRPA1 activators through pharmacophore-based virtual screening and a biological assay. Bioorganic and Medicinal Chemistry Letters, 2021, 31, 127639.	2.2	3
11	Extraction of protein dynamics information from cryo-EM maps using deep learning. Nature Machine Intelligence, 2021, 3, 153-160.	16.0	57
12	Gilteritinib overcomes lorlatinib resistance in ALK-rearranged cancer. Nature Communications, 2021, 12, 1261.	12.8	52
13	Microsecond-timescale MD simulation of EGFR minor mutation predicts the structural flexibility of EGFR kinase core that reflects EGFR inhibitor sensitivity. Npj Precision Oncology, 2021, 5, 32.	5.4	11
14	Exploring ligand binding pathways on proteins using hypersound-accelerated molecular dynamics. Nature Communications, 2021, 12, 2793.	12.8	24
15	A deep learning system to diagnose the malignant potential of urothelial carcinoma cells in cytology specimens. Cancer Cytopathology, 2021, 129, 984-995.	2.4	22
16	Health improvement framework for actionable treatment planning using a surrogate Bayesian model. Nature Communications, 2021, 12, 3088.	12.8	6
17	Dynamic changes in gene-to-gene regulatory networks in response to SARS-CoV-2 infection. Scientific Reports, 2021, 11, 11241.	3.3	3
18	eSkip-Finder: a machine learning-based web application and database to identify the optimal sequences of antisense oligonucleotides for exon skipping. Nucleic Acids Research, 2021, 49, W193-W198.	14.5	13

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19	Efficient Search for Energetically Favorable Molecular Conformations against Metastable States via Gray-Box Optimization. Journal of Chemical Theory and Computation, 2021, 17, 5419-5427.	5.3	8
20	Prediction and visualization of acute kidney injury in intensive care unit using one-dimensional convolutional neural networks based on routinely collected data. Computer Methods and Programs in Biomedicine, 2021, 206, 106129.	4.7	12
21	Oncogenic mutations Q61L and Q61H confer active form-like structural features to the inactive state (state 1) conformation of H-Ras protein. Biochemical and Biophysical Research Communications, 2021, 565, 85-90.	2.1	3
22	Evaluation of Kidney Histological Images Using Unsupervised Deep Learning. Kidney International Reports, 2021, 6, 2445-2454.	0.8	15
23	Accurate Binding Configuration Prediction of a G-Protein-Coupled Receptor to Its Antagonist Using Multicanonical Molecular Dynamics-Based Dynamic Docking. Journal of Chemical Information and Modeling, 2021, 61, 5161-5171.	5.4	10
24	Novel cancer subtyping method based on patient-specific gene regulatory network. Scientific Reports, 2021, 11, 23653.	3.3	6
25	An in silico Approach for Integrating Phenotypic and Targetâ€based Approaches in Drug Discovery. Molecular Informatics, 2020, 39, e1900096.	2.5	8
26	Stabilization Mechanism for a Nonfibrillar Amyloid Î² Oligomer Based on Formation of a Hydrophobic Core Determined by Dissipative Particle Dynamics. ACS Chemical Neuroscience, 2020, 11, 385-394.	3.5	15
27	Classification of glomerular pathological findings using deep learning and nephrologistâ€“AI collective intelligence approach. International Journal of Medical Informatics, 2020, 141, 104231.	3.3	59
28	Future possibilities for artificial intelligence in the practical management of hypertension. Hypertension Research, 2020, 43, 1327-1337.	2.7	19
29	E487K-Induced Disorder in Functionally Relevant Dynamics of Mitochondrial Aldehyde Dehydrogenase 2. Biophysical Journal, 2020, 119, 628-637.	0.5	4
30	Structure-based design and discovery of novel anti-tissue factor antibodies with cooperative double-point mutations, using interaction analysis. Scientific Reports, 2020, 10, 17590.	3.3	7
31	Lipocalin-type prostaglandin D synthase regulates light-induced phase advance of the central circadian rhythm in mice. Communications Biology, 2020, 3, 557.	4.4	5
32	CompRet: a comprehensive recommendation framework for chemical synthesis planning with algorithmic enumeration. Journal of Cheminformatics, 2020, 12, 52.	6.1	19
33	The relationship between cigarette smoking and the tongue microbiome in an East Asian population. Journal of Oral Microbiology, 2020, 12, 1742527.	2.7	18
34	kGCN: a graph-based deep learning framework for chemical structures. Journal of Cheminformatics, 2020, 12, 32.	6.1	55
35	Coarse-Grained Diffraction Template Matching Model to Retrieve Multiconformational Models for Biomolecule Structures from Noisy Diffraction Patterns. Journal of Chemical Information and Modeling, 2020, 60, 2803-2818.	5.4	3
36	Landscape and function of multiple mutations within individual oncogenes. Nature, 2020, 582, 95-99.	27.8	79

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37	Metagenomic analysis of bacterial species in tongue microbiome of current and never smokers. Npj Biofilms and Microbiomes, 2020, 6, 11.	6.4	32
38	Hydrophobic interactions at subsite S1â€² of human dipeptidyl peptidase IV contribute significantly to the inhibitory effect of tripeptides. Heliyon, 2020, 6, e04227.	3.2	11
39	Improvement in predicting drug sensitivity changes associated with protein mutations using a molecular dynamics based alchemical mutation method. Scientific Reports, 2020, 10, 2161.	3.3	7
40	System-Based Differential Gene Network Analysis for Characterizing a Sample-Specific Subnetwork. Biomolecules, 2020, 10, 306.	4.0	9
41	Prediction of blood pressure variability using deep neural networks. International Journal of Medical Informatics, 2020, 136, 104067.	3.3	46
42	Identification of a new class of non-electrophilic TRPA1 agonists by a structure-based virtual screening approach. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 127142.	2.2	6
43	Exhaustive search of the configurational space of heatâ€shock protein 90 with its inhibitor by multicanonical molecular dynamics based dynamic docking. Journal of Computational Chemistry, 2020, 41, 1606-1615.	3.3	20
44	Combination of host immune metabolic biomarkers for the PD-1 blockade cancer immunotherapy. JCI Insight, 2020, 5, .	5.0	58
45	Overview of Life Intelligence Consortium â€œLINCâ€• Proceedings for Annual Meeting of the Japanese Pharmacological Society, 2020, 93, 2-CS-1.	0.0	0
46	Prediction of ALK mutations mediating ALK-TKIs resistance and drug re-purposing to overcome the resistance. EBioMedicine, 2019, 41, 105-119.	6.1	93
47	Molecular dynamics simulation-guided drug sensitivity prediction for lung cancer with rare EGFR mutations. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 10025-10030.	7.1	41
48	Structural modification of indomethacin toward selective inhibition of COX-2 with a significant increase in van der Waals contributions. Bioorganic and Medicinal Chemistry, 2019, 27, 1789-1794.	3.0	8
49	Repertoires of G protein-coupled receptors for Ciona -specific neuropeptides. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 7847-7856.	7.1	39
50	Suppression of IgE-Independent Degranulation of Murine Connective Tissue-Type Mast Cells by Dexamethasone. Cells, 2019, 8, 112.	4.1	9
51	Combination treatment with highly bioavailable curcumin and NQO1 inhibitor exhibits potent antitumor effects on esophageal squamous cell carcinoma. Journal of Gastroenterology, 2019, 54, 687-698.	5.1	27
52	Dynamic Docking of a Medium-Sized Molecule to Its Receptor by Multicanonical MD Simulations. Journal of Physical Chemistry B, 2019, 123, 2479-2490.	2.6	22
53	Calculation of absolute binding free energies between the hERG channel and structurally diverse drugs. Scientific Reports, 2019, 9, 16586.	3.3	30
54	MGeND: an integrated database for Japanese clinical and genomic information. Human Genome Variation, 2019, 6, 53.	0.7	6

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55	Prediction and Interpretable Visualization of Retrosynthetic Reactions Using Graph Convolutional Networks. Journal of Chemical Information and Modeling, 2019, 59, 5026-5033.	5.4	48
56	Efficient construction method for phase diagrams using uncertainty sampling. Physical Review Materials, 2019, 3, .	2.4	26
57	A secondary RET mutation in the activation loop conferring resistance to vandetanib. Nature Communications, 2018, 9, 625.	12.8	75
58	Core Binding Site of a Thioflavin-T-Derived Imaging Probe on Amyloid Î² Fibrils Predicted by Computational Methods. ACS Chemical Neuroscience, 2018, 9, 957-966.	3.5	14
59	Machine learning accelerates MD-based binding pose prediction between ligands and proteins. Bioinformatics, 2018, 34, 770-778.	4.1	31
60	Improving the Accuracy of Proteinâ€Ligand Binding Mode Prediction Using a Molecular Dynamicsâ€Based Pocket Generation Approach. Journal of Computational Chemistry, 2018, 39, 2679-2689.	3.3	9
61	Novel inhibitor candidates of TRPV2 prevent damage of dystrophic myocytes and ameliorate against dilated cardiomyopathy in a hamster model. Oncotarget, 2018, 9, 14042-14057.	1.8	28
62	Fibronectin type III domain-containing protein 5 interacts with APP and decreases amyloid Î² production in Alzheimerâ€™s disease. Molecular Brain, 2018, 11, 61.	2.6	29
63	A Platform for Comprehensive Genomic Profiling in Human Cancers and Pharmacogenomics Therapy Selection. Methods in Molecular Biology, 2018, 1825, 413-424.	0.9	0
64	Association between homologous recombination repair gene mutations and response to oxaliplatin in pancreatic cancer. Oncotarget, 2018, 9, 19817-19825.	1.8	54
65	Suppression of IgE-independent degranulation of murine mast cells by dexamethasone. Proceedings for Annual Meeting of the Japanese Pharmacological Society, 2018, WCP2018, PO3-4-14.	0.0	0
66	Clinical characterization and in silico drug sensitivity prediction model of rare EGFR mutations in non-small cell lung cancer.. Journal of Clinical Oncology, 2018, 36, e21221-e21221.	1.6	0
67	De novo Drug Design â€“ Ye olde Scoring Problem Revisited. Molecular Informatics, 2017, 36, 1681031.	2.5	12
68	Accurate Prediction of Complex Structure and Affinity for a Flexible Protein Receptor and Its Inhibitor. Journal of Chemical Theory and Computation, 2017, 13, 2389-2399.	5.3	43
69	Relationships Between Quantitative Pulse-Echo Ultrasound Parameters from the Superficial Zone of the Human Articular Cartilage and Changes in Surface Roughness, Collagen Content or Collagen Orientation Caused by Early Degeneration. Ultrasound in Medicine and Biology, 2017, 43, 1703-1715.	1.5	4
70	Clinical sequencing using a nextâ€generation sequencingâ€based multiplex gene assay in patients with advanced solid tumors. Cancer Science, 2017, 108, 1440-1446.	3.9	57
71	Brigatinib combined with anti-EGFR antibody overcomes osimertinib resistance in EGFR-mutated non-small-cell lung cancer. Nature Communications, 2017, 8, 14768.	12.8	306
72	Exome Sequencing Landscape Analysis in Ovarian Clear Cell Carcinoma Shed Light on Key Chromosomal Regions and Mutation Gene Networks. American Journal of Pathology, 2017, 187, 2246-2258.	3.8	104

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73	Analysis of the evidence-practice gap to facilitate proper medical care for the elderly: investigation, using databases, of utilization measures for National Database of Health Insurance Claims and Specific Health Checkups of Japan (NDB). Environmental Health and Preventive Medicine, 2017, 22, 51.	3.4	27
74	Association between UGT1A1*28*28 genotype and lung cancer in the Japanese population. International Journal of Clinical Oncology, 2017, 22, 269-273.	2.2	4
75	CGBVSâ€DNN: Prediction of Compoundâ€protein Interactions Based on Deep Learning. Molecular Informatics, 2017, 36, 1600045.	2.5	58
76	Adjuvant chemotherapy improves survival of patients with high-risk upper urinary tract urothelial carcinoma: a propensity score-matched analysis. BMC Urology, 2017, 17, 110.	1.4	22
77	Impact of BRCAness on the efficacy of oxaliplatin-based chemotherapy in patients with unresectable pancreatic cancer.. Journal of Clinical Oncology, 2017, 35, 250-250.	1.6	5
78	Development and validation of a set of six adaptable prognosis prediction (SAP) models based on time-series real-world big data analysis for patients with cancer receiving chemotherapy: A multicenter case crossover study. PLoS ONE, 2017, 12, e0183291.	2.5	19
79	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
80	The possibility of clinical sequencing in the management of cancer. Japanese Journal of Clinical Oncology, 2016, 46, 399-406.	1.3	26
81	Antipsychotics-Associated Serious Adverse Events in Children: An Analysis of the FAERS Database. International Journal of Medical Sciences, 2015, 12, 135-140.	2.5	34
82	Constructing a Foundational Platform Driven by Japanâ€™s K Supercomputer for Next-Generation Drug Design. Molecular Informatics, 2014, 33, 732-741.	2.5	9
83	Two Novel ALK Mutations Mediate Acquired Resistance to the Next-Generation ALK Inhibitor Alectinib. Clinical Cancer Research, 2014, 20, 5686-5696.	7.0	261
84	Tivantinib (ARQ 197) Exhibits Antitumor Activity by Directly Interacting with Tubulin and Overcomes ABC Transporterâ€“Mediated Drug Resistance. Molecular Cancer Therapeutics, 2014, 13, 2978-2990.	4.1	57
85	Analysis of multiple compoundâ€“protein interactions reveals novel bioactive molecules. Molecular Systems Biology, 2011, 7, 472.	7.2	134
86	Establishment of the culture model system that reflects the process of terminal differentiation of connective tissueâ€type mast cells. FEBS Letters, 2008, 582, 1444-1450.	2.8	38