

# Yasushi Okuno

## List of Publications by Year in descending order

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Version: 2024-02-01

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	Brigatinib combined with anti-EGFR antibody overcomes osimertinib resistance in EGFR-mutated non-small-cell lung cancer. <i>Nature Communications</i> , 2017, 8, 14768.	12.8	306
2	Two Novel ALK Mutations Mediate Acquired Resistance to the Next-Generation ALK Inhibitor Alectinib. <i>Clinical Cancer Research</i> , 2014, 20, 5686-5696.	7.0	261
3	Analysis of multiple compound-protein interactions reveals novel bioactive molecules. <i>Molecular Systems Biology</i> , 2011, 7, 472.	7.2	134
4	Exome Sequencing Landscape Analysis in Ovarian Clear Cell Carcinoma Shed Light on Key Chromosomal Regions and Mutation Gene Networks. <i>American Journal of Pathology</i> , 2017, 187, 2246-2258.	3.8	104
5	Prediction of ALK mutations mediating ALK-TKIs resistance and drug re-purposing to overcome the resistance. <i>EBioMedicine</i> , 2019, 41, 105-119.	6.1	93
6	Landscape and function of multiple mutations within individual oncogenes. <i>Nature</i> , 2020, 582, 95-99.	27.8	79
7	A secondary RET mutation in the activation loop conferring resistance to vandetanib. <i>Nature Communications</i> , 2018, 9, 625.	12.8	75
8	Classification of glomerular pathological findings using deep learning and nephrologist-AI collective intelligence approach. <i>International Journal of Medical Informatics</i> , 2020, 141, 104231.	3.3	59
9	CGBVS-DNN: Prediction of Compound-protein Interactions Based on Deep Learning. <i>Molecular Informatics</i> , 2017, 36, 1600045.	2.5	58
10	Combination of host immune metabolic biomarkers for the PD-1 blockade cancer immunotherapy. <i>JCI Insight</i> , 2020, 5, .	5.0	58
11	Tivantinib (ARQ 197) Exhibits Antitumor Activity by Directly Interacting with Tubulin and Overcomes ABC Transporter-Mediated Drug Resistance. <i>Molecular Cancer Therapeutics</i> , 2014, 13, 2978-2990.	4.1	57
12	Clinical sequencing using a next-generation sequencing-based multiplex gene assay in patients with advanced solid tumors. <i>Cancer Science</i> , 2017, 108, 1440-1446.	3.9	57
13	Extraction of protein dynamics information from cryo-EM maps using deep learning. <i>Nature Machine Intelligence</i> , 2021, 3, 153-160.	16.0	57
14	kGCN: a graph-based deep learning framework for chemical structures. <i>Journal of Cheminformatics</i> , 2020, 12, 32.	6.1	55
15	Association between homologous recombination repair gene mutations and response to oxaliplatin in pancreatic cancer. <i>Oncotarget</i> , 2018, 9, 19817-19825.	1.8	54
16	Gilteritinib overcomes lorlatinib resistance in ALK-rearranged cancer. <i>Nature Communications</i> , 2021, 12, 1261.	12.8	52
17	Prediction and Interpretable Visualization of Retrosynthetic Reactions Using Graph Convolutional Networks. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 5026-5033.	5.4	48
18	Prediction of blood pressure variability using deep neural networks. <i>International Journal of Medical Informatics</i> , 2020, 136, 104067.	3.3	46

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19	Accurate Prediction of Complex Structure and Affinity for a Flexible Protein Receptor and Its Inhibitor. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2389-2399.	5.3	43
20	Molecular dynamics simulation-guided drug sensitivity prediction for lung cancer with rare EGFR mutations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 10025-10030.	7.1	41
21	Repertoires of G protein-coupled receptors for Ciona-specific neuropeptides. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 7847-7856.	7.1	39
22	Establishment of the culture model system that reflects the process of terminal differentiation of connective tissue-type mast cells. <i>FEBS Letters</i> , 2008, 582, 1444-1450.	2.8	38
23	Antipsychotics-Associated Serious Adverse Events in Children: An Analysis of the FAERS Database. <i>International Journal of Medical Sciences</i> , 2015, 12, 135-140.	2.5	34
24	Metagenomic analysis of bacterial species in tongue microbiome of current and never smokers. <i>Npj Biofilms and Microbiomes</i> , 2020, 6, 11.	6.4	32
25	Machine learning accelerates MD-based binding pose prediction between ligands and proteins. <i>Bioinformatics</i> , 2018, 34, 770-778.	4.1	31
26	Calculation of absolute binding free energies between the hERG channel and structurally diverse drugs. <i>Scientific Reports</i> , 2019, 9, 16586.	3.3	30
27	The Effect of Conformational Flexibility on Binding Free Energy Estimation between Kinases and Their Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 2445-2456.	5.4	29
28	Fibronectin type III domain-containing protein 5 interacts with APP and decreases amyloid $\beta$ production in Alzheimer's disease. <i>Molecular Brain</i> , 2018, 11, 61.	2.6	29
29	Metagenomic profiling of gut microbiome in early chronic kidney disease. <i>Nephrology Dialysis Transplantation</i> , 2021, 36, 1675-1684.	0.7	29
30	Novel inhibitor candidates of TRPV2 prevent damage of dystrophic myocytes and ameliorate against dilated cardiomyopathy in a hamster model. <i>Oncotarget</i> , 2018, 9, 14042-14057.	1.8	28
31	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). <i>Environmental Health and Preventive Medicine</i> , 2017, 22, 51.	3.4	27
32	Combination treatment with highly bioavailable curcumin and NQO1 inhibitor exhibits potent antitumor effects on esophageal squamous cell carcinoma. <i>Journal of Gastroenterology</i> , 2019, 54, 687-698.	5.1	27
33	The possibility of clinical sequencing in the management of cancer. <i>Japanese Journal of Clinical Oncology</i> , 2016, 46, 399-406.	1.3	26
34	Efficient construction method for phase diagrams using uncertainty sampling. <i>Physical Review Materials</i> , 2019, 3, .	2.4	26
35	Exploring ligand binding pathways on proteins using hypersound-accelerated molecular dynamics. <i>Nature Communications</i> , 2021, 12, 2793.	12.8	24
36	Adjuvant chemotherapy improves survival of patients with high-risk upper urinary tract urothelial carcinoma: a propensity score-matched analysis. <i>BMC Urology</i> , 2017, 17, 110.	1.4	22

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37	Dynamic Docking of a Medium-Sized Molecule to Its Receptor by Multicanonical MD Simulations. <i>Journal of Physical Chemistry B</i> , 2019, 123, 2479-2490.	2.6	22
38	A deep learning system to diagnose the malignant potential of urothelial carcinoma cells in cytology specimens. <i>Cancer Cytopathology</i> , 2021, 129, 984-995.	2.4	22
39	Exhaustive search of the configurational space of heat shock protein 90 with its inhibitor by multicanonical molecular dynamics based dynamic docking. <i>Journal of Computational Chemistry</i> , 2020, 41, 1606-1615.	3.3	20
40	Future possibilities for artificial intelligence in the practical management of hypertension. <i>Hypertension Research</i> , 2020, 43, 1327-1337.	2.7	19
41	CompRet: a comprehensive recommendation framework for chemical synthesis planning with algorithmic enumeration. <i>Journal of Cheminformatics</i> , 2020, 12, 52.	6.1	19
42	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. <i>PLoS ONE</i> , 2017, 12, e0183291.	2.5	19
43	<i>&lt;i&gt;CBNplot&lt;/i&gt;</i> : Bayesian network plots for enrichment analysis. <i>Bioinformatics</i> , 2022, 38, 2959-2960.	4.1	19
44	The relationship between cigarette smoking and the tongue microbiome in an East Asian population. <i>Journal of Oral Microbiology</i> , 2020, 12, 1742527.	2.7	18
45	Stabilization Mechanism for a Nonfibrillar Amyloid $\beta^2$ Oligomer Based on Formation of a Hydrophobic Core Determined by Dissipative Particle Dynamics. <i>ACS Chemical Neuroscience</i> , 2020, 11, 385-394.	3.5	15
46	Evaluation of Kidney Histological Images Using Unsupervised Deep Learning. <i>Kidney International Reports</i> , 2021, 6, 2445-2454.	0.8	15
47	AI-Driven Synthetic Route Design Incorporated with Retrosynthesis Knowledge. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 1357-1367.	5.4	15
48	Core Binding Site of a Thioflavin-T-Derived Imaging Probe on Amyloid $\beta^2$ Fibrils Predicted by Computational Methods. <i>ACS Chemical Neuroscience</i> , 2018, 9, 957-966.	3.5	14
49	eSkip-Finder: a machine learning-based web application and database to identify the optimal sequences of antisense oligonucleotides for exon skipping. <i>Nucleic Acids Research</i> , 2021, 49, W193-W198.	14.5	13
50	<i>&lt;i&gt;De novo&lt;/i&gt;</i> Drug Design â€œ Ye olde Scoring Problem Revisited. <i>Molecular Informatics</i> , 2017, 36, 1681031.	2.5	12
51	Prediction and visualization of acute kidney injury in intensive care unit using one-dimensional convolutional neural networks based on routinely collected data. <i>Computer Methods and Programs in Biomedicine</i> , 2021, 206, 106129.	4.7	12
52	Hydrophobic interactions at subsite S1 <sup>â€²</sup> of human dipeptidyl peptidase IV contribute significantly to the inhibitory effect of tripeptides. <i>Heliyon</i> , 2020, 6, e04227.	3.2	11
53	Microsecond-timescale MD simulation of EGFR minor mutation predicts the structural flexibility of EGFR kinase core that reflects EGFR inhibitor sensitivity. <i>Npj Precision Oncology</i> , 2021, 5, 32.	5.4	11
54	Accurate Binding Configuration Prediction of a G-Protein-Coupled Receptor to Its Antagonist Using Multicanonical Molecular Dynamics-Based Dynamic Docking. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5161-5171.	5.4	10

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55	Protein–ligand binding affinity prediction of cyclin–dependent kinase–2 inhibitors by dynamically averaged fragment molecular orbital–based interaction energy. <i>Journal of Computational Chemistry</i> , 2022, 43, 1362-1371.	3.3	10
56	Constructing a Foundational Platform Driven by Japan’s K Supercomputer for Next-Generation Drug Design. <i>Molecular Informatics</i> , 2014, 33, 732-741.	2.5	9
57	Improving the Accuracy of Protein–Ligand Binding Mode Prediction Using a Molecular Dynamics–Based Pocket Generation Approach. <i>Journal of Computational Chemistry</i> , 2018, 39, 2679-2689.	3.3	9
58	Suppression of IgE-Independent Degranulation of Murine Connective Tissue-Type Mast Cells by Dexamethasone. <i>Cells</i> , 2019, 8, 112.	4.1	9
59	System-Based Differential Gene Network Analysis for Characterizing a Sample-Specific Subnetwork. <i>Biomolecules</i> , 2020, 10, 306.	4.0	9
60	Structural modification of indomethacin toward selective inhibition of COX-2 with a significant increase in van der Waals contributions. <i>Bioorganic and Medicinal Chemistry</i> , 2019, 27, 1789-1794.	3.0	8
61	An <i>in silico</i> Approach for Integrating Phenotypic and Target–based Approaches in Drug Discovery. <i>Molecular Informatics</i> , 2020, 39, e1900096.	2.5	8
62	Efficient Search for Energetically Favorable Molecular Conformations against Metastable States via Gray-Box Optimization. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5419-5427.	5.3	8
63	Structure-based design and discovery of novel anti-tissue factor antibodies with cooperative double-point mutations, using interaction analysis. <i>Scientific Reports</i> , 2020, 10, 17590.	3.3	7
64	Improvement in predicting drug sensitivity changes associated with protein mutations using a molecular dynamics based alchemical mutation method. <i>Scientific Reports</i> , 2020, 10, 2161.	3.3	7
65	Novel Resistance Mechanisms Including L1196Q, P1094H, and R1248_D1249 Insertion in Three Patients With NSCLC After ALK Tyrosine Kinase Inhibitor Treatment. <i>Journal of Thoracic Oncology</i> , 2021, 16, 477-482.	1.1	7
66	MGeND: an integrated database for Japanese clinical and genomic information. <i>Human Genome Variation</i> , 2019, 6, 53.	0.7	6
67	Identification of a new class of non-electrophilic TRPA1 agonists by a structure-based virtual screening approach. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2020, 30, 127142.	2.2	6
68	Health improvement framework for actionable treatment planning using a surrogate Bayesian model. <i>Nature Communications</i> , 2021, 12, 3088.	12.8	6
69	Novel cancer subtyping method based on patient-specific gene regulatory network. <i>Scientific Reports</i> , 2021, 11, 23653.	3.3	6
70	Lipocalin-type prostaglandin D synthase regulates light-induced phase advance of the central circadian rhythm in mice. <i>Communications Biology</i> , 2020, 3, 557.	4.4	5
71	Impact of BRCAness on the efficacy of oxaliplatin-based chemotherapy in patients with unresectable pancreatic cancer.. <i>Journal of Clinical Oncology</i> , 2017, 35, 250-250.	1.6	5
72	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. <i>Ultrasound in Medicine and Biology</i> , 2017, 43, 1703-1715.	1.5	4

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73	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
74	E487K-Induced Disorder in Functionally Relevant Dynamics of Mitochondrial Aldehyde Dehydrogenase 2. Biophysical Journal, 2020, 119, 628-637.	0.5	4
75	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
76	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
77	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
78	Dynamic changes in gene-to-gene regulatory networks in response to SARS-CoV-2 infection. Scientific Reports, 2021, 11, 11241.	3.3	3
79	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
80	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
81	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
82	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
83	A Platform for Comprehensive Genomic Profiling in Human Cancers and Pharmacogenomics Therapy Selection. Methods in Molecular Biology, 2018, 1825, 413-424.	0.9	0
84	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
85	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
86	Overview of Life Intelligence Consortium "LINC". Proceedings for Annual Meeting of the Japanese Pharmacological Society, 2020, 93, 2-CS-1.	0.0	0