Kei Terayama

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/9055037/publications.pdf

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22	460	758635 12	752256 20
papers	citations	h-index	g-index

22	22	22	482
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	De novo creation of a naked eyeâ€“detectable fluorescent molecule based on quantum chemical computation and machine learning. Science Advances, 2022, 8, eabj3906.	4.7	14
2	Enhanced Conformational Sampling with an Adaptive Coarse-Grained Elastic Network Model Using Short-Time All-Atom Molecular Dynamics. Journal of Chemical Theory and Computation, 2022, 18, 2062-2074.	2.3	11
3	AI-Driven Synthetic Route Design Incorporated with Retrosynthesis Knowledge. Journal of Chemical Information and Modeling, 2022, 62, 1357-1367.	2.5	15
4	Integrating Incompatible Assay Data Sets with Deep Preference Learning. ACS Medicinal Chemistry Letters, 2022, 13, 70-75.	1.3	2
5	Black-Box Optimization for Automated Discovery. Accounts of Chemical Research, 2021, 54, 1334-1346.	7.6	57
6	Extraction of protein dynamics information from cryo-EM maps using deep learning. Nature Machine Intelligence, 2021, 3, 153-160.	8.3	57
7	Discovery of polymer electret material via de novo molecule generation and functional group enrichment analysis. Applied Physics Letters, 2021, 118, .	1.5	12
8	Efficient Search for Energetically Favorable Molecular Conformations against Metastable States via Gray-Box Optimization. Journal of Chemical Theory and Computation, 2021, 17, 5419-5427.	2.3	8
9	Structure-Based de Novo Molecular Generator Combined with Artificial Intelligence and Docking Simulations. Journal of Chemical Information and Modeling, 2021, 61, 3304-3313.	2.5	41
10	Looking represents choosing in toddlers: Exploring the equivalence between multimodal measures in forcedâ€choice tasks. Infancy, 2021, 26, 148-167.	0.9	3
11	CompRet: a comprehensive recommendation framework for chemical synthesis planning with algorithmic enumeration. Journal of Cheminformatics, 2020, 12, 52.	2.8	19
12	Computer Vision-Based Approach for Quantifying Occupational Therapistsâ€™ Qualitative Evaluations of Postural Control. Occupational Therapy International, 2020, 2020, 1-9.	0.3	2
13	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.	2.5	3
14	Pushing property limits in materials discoveryviaboundless objective-free exploration. Chemical Science, 2020, 11, 5959-5968.	3.7	20
15	Exploring Successful Parameter Region for Coarse-Grained Simulation of Biomolecules by Bayesian Optimization and Active Learning. Biomolecules, 2020, 10, 482.	1.8	5
16	Experimental Establishment of Phase Diagrams Guided by Uncertainty Sampling: An Application to the Deposition of Znâ€“Snâ€“P Films by Molecular Beam Epitaxy. , 2020, 2, 571-575.		13
17	Enhancing Biomolecular Sampling with Reinforcement Learning: A Tree Search Molecular Dynamics Simulation Method. ACS Omega, 2019, 4, 13853-13862.	1.6	25
18	Prediction and Interpretable Visualization of Retrosynthetic Reactions Using Graph Convolutional Networks. Journal of Chemical Information and Modeling, 2019, 59, 5026-5033.	2.5	48

#	Article	IF	Citations
19	Deep-learning-based quality filtering of mechanically exfoliated 2D crystals. Npj Computational Materials, 2019, 5, .	3.5	46
20	evERdock BAI: Machine-learning-guided selection of protein-protein complex structure. Journal of Chemical Physics, 2019, 151, 215104.	1.2	8
21	Machine learning accelerates MD-based binding pose prediction between ligands and proteins. Bioinformatics, 2018, 34, 770-778.	1.8	31
22	Fine-grained optimization method for crystal structure prediction. Npj Computational Materials, 2018, 4, .	3.5	20