Gianni De Fabritiis

List of Publications by Year
in descending order

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73 papers	5,629 citations	117453 34 h-index	85405 71 g-index
77 all docs	77 docs citations	77 times ranked	6735 citing authors

#	Article	IF	Citations
1	Structure based virtual screening: Fast and slow. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1544.	6.2	25
2	PlayMolecule Glimpse: Understanding Proteinâ€“Ligand Property Predictions with Interpretable Neural Networks. Journal of Chemical Information and Modeling, 2022, 62, 225-231.	2.5	11
3	TorchMD: A Deep Learning Framework for Molecular Simulations. Journal of Chemical Theory and Computation, 2021, 17, 2355-2363.	2.3	101
4	The Role of Hydrophobic Nodes in the Dynamics of Class A Î²-Lactamases. Frontiers in Microbiology, 2021, 12, 720991.	1.5	6
5	Machine learning for protein folding and dynamics. Current Opinion in Structural Biology, 2020, 60, 77-84.	2.6	116
6	GPCRmd uncovers the dynamics of the 3D-GPCRome. Nature Methods, 2020, 17, 777-787.	9.0	90
7	Coarse graining molecular dynamics with graph neural networks. Journal of Chemical Physics, 2020, 153, 194101.	1.2	103
8	Small Molecule Modulation of Intrinsically Disordered Proteins Using Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2020, 60, 5003-5010.	2.5	9
9	Characterization of partially ordered states in the intrinsically disordered N-terminal domain of p53 using millisecond molecular dynamics simulations. Scientific Reports, 2020, 10, 12402.	1.6	12
10	SkeleDock: A Web Application for Scaffold Docking in PlayMolecule. Journal of Chemical Information and Modeling, 2020, 60, 2673-2677.	2.5	9
11	AdaptiveBandit: A Multi-armed Bandit Framework for Adaptive Sampling in Molecular Simulations. Journal of Chemical Theory and Computation, 2020, 16, 4685-4693.	2.3	21
12	PlayMolecule CrypticScout: Predicting Protein Cryptic Sites Using Mixed-Solvent Molecular Simulations. Journal of Chemical Information and Modeling, 2020, 60, 2314-2324.	2.5	15
13	Generative Models for Molecular Design. Journal of Chemical Information and Modeling, 2020, 60, 5635-5636.	2.5	9
14	LigVoxel: inpainting binding pockets using 3D-convolutional neural networks. Bioinformatics, 2019, 35, 243-250.	1.8	48
15	From Target to Drug: Generative Modeling for the Multimodal Structure-Based Ligand Design. Molecular Pharmaceutics, 2019, 16, 4282-4291.	2.3	81
16	A Scalable Molecular Force Field Parameterization Method Based on Density Functional Theory and Quantum-Level Machine Learning. Journal of Chemical Information and Modeling, 2019, 59, 3485-3493.	2.5	52
17	Reconstruction of apo A2A receptor activation pathways reveal ligand-competent intermediates and state-dependent cholesterol hotspots. Scientific Reports, 2019, 9, 14199.	1.6	24
18	The Aminotriazole Antagonist Cmpdâ€1 Stabilises a Distinct Inactive State of the Adenosine 2A Receptor. Angewandte Chemie, 2019, 131, 9499-9503.	1.6	1

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19	The Aminotriazole Antagonist Cmpdâ€1 Stabilises a Distinct Inactive State of the Adenosine 2A Receptor. Angewandte Chemie - International Edition, 2019, 58, 9399-9403.	7.2	3
20	Machine Learning of Coarse-Grained Molecular Dynamics Force Fields. ACS Central Science, 2019, 5, 755-767.	5.3	306
21	Shape-Based Generative Modeling for de Novo Drug Design. Journal of Chemical Information and Modeling, 2019, 59, 1205-1214.	2.5	145
22	DeltaDelta neural networks for lead optimization of small molecule potency. Chemical Science, 2019, 10, 10911-10918.	3.7	48
23	PathwayMap: Molecular Pathway Association with Self-Normalizing Neural Networks. Journal of Chemical Information and Modeling, 2019, 59, 1172-1181.	2.5	20
24	PlayMolecule BindScope: large scale CNN-based virtual screening on the web. Bioinformatics, 2019, 35, 1237-1238.	1.8	42
25	Simulations meet machine learning in structural biology. Current Opinion in Structural Biology, 2018, 49, 139-144.	2.6	40
26	Molecular-Simulation-Driven Fragment Screening for the Discovery of New CXCL12 Inhibitors. Journal of Chemical Information and Modeling, 2018, 58, 683-691.	2.5	20
27	Dopamine D3 receptor antagonist reveals a cryptic pocket in aminergic GPCRs. Scientific Reports, 2018, 8, 897.	1.6	39
28	K_{DEEP}: Proteinâ€“Ligand Absolute Binding Affinity Prediction via 3D-Convolutional Neural Networks. Journal of Chemical Information and Modeling, 2018, 58, 287-296.	2.5	586
29	Regulation of Androgen Receptor Activity by Transient Interactions of Its Transactivation Domain with General Transcription Regulators. Structure, 2018, 26, 145-152.e3.	1.6	45
30	PlayMolecule ProteinPrepare: A Web Application for Protein Preparation for Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2017, 57, 1511-1516.	2.5	179
31	Dynamic and Kinetic Elements of Âμ-Opioid Receptor Functional Selectivity. Scientific Reports, 2017, 7, 11255.	1.6	44
32	High-Throughput Automated Preparation and Simulation of Membrane Proteins with HTMD. Journal of Chemical Theory and Computation, 2017, 13, 4003-4011.	2.3	27
33	Complete proteinâ€“protein association kinetics in atomic detail revealed by molecular dynamics simulations and Markov modelling. Nature Chemistry, 2017, 9, 1005-1011.	6.6	304
34	Drug Discovery and Molecular Dynamics: Methods, Applications and Perspective Beyond the Second Timescale. Current Topics in Medicinal Chemistry, 2017, 17, 2617-2625.	1.0	33
35	Binding Kinetics in Drug Discovery. Molecular Informatics, 2016, 35, 216-226.	1.4	40
36	The pathway of ligand entry from the membrane bilayer to a lipid G protein-coupled receptor. Scientific Reports, 2016, 6, 22639.	1.6	77

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37	Multibody cofactor and substrate molecular recognition in the myo-inositol monophosphatase enzyme. Scientific Reports, 2016, 6, 30275.	1.6	17
38	Emergence of Multiple EGFR Extracellular Mutations during Cetuximab Treatment in Colorectal Cancer. Clinical Cancer Research, 2015, 21, 2157-2166.	3.2	227
39	High throughput molecular dynamics for drug discovery. In Silico Pharmacology, 2015, 3, 3.	1.8	12
40	Detection of New Biased Agonists for the Serotonin 5-HT_{2A} Receptor: Modeling and Experimental Validation. Molecular Pharmacology, 2015, 87, 740-746.	1.0	29
41	Progress in studying intrinsically disordered proteins with atomistic simulations. Progress in Biophysics and Molecular Biology, 2015, 119, 47-52.	1.4	30
42	Spontaneous Inward Opening of the Dopamine Transporter Is Triggered by PIP₂-Regulated Dynamics of the N-Terminus. ACS Chemical Neuroscience, 2015, 6, 1825-1837.	1.7	95
43	Insights from Fragment Hit Binding Assays by Molecular Simulations. Journal of Chemical Information and Modeling, 2015, 55, 2200-2205.	2.5	25
44	Kinetic modulation of a disordered protein domain by phosphorylation. Nature Communications, 2014, 5, 5272.	5.8	60
45	Membrane lipids are key modulators of the endocannabinoid-hydrolase FAAH. Biochemical Journal, 2014, 457, 463-472.	1.7	42
46	Understanding Molecular Recognition by Kinetic Network Models Constructed from Molecular Dynamics Simulations. Advances in Experimental Medicine and Biology, 2014, 797, 107-114.	0.8	3
47	Rapid Conformational Fluctuations of Disordered HIV-1 Fusion Peptide in Solution. Journal of Chemical Theory and Computation, 2013, 9, 2870-2874.	2.3	8
48	Computational Modeling of an Epidermal Growth Factor Receptor Single-Mutation Resistance to Cetuximab in Colorectal Cancer Treatment. Journal of Chemical Information and Modeling, 2013, 53, 3123-3126.	2.5	6
49	Identification of slow molecular order parameters for Markov model construction. Journal of Chemical Physics, 2013, 139, 015102.	1.2	777
50	Kinetic characterization of the critical step in HIV-1 protease maturation. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 20449-20454.	3.3	92
51	Thumbs Down for HIV: Domain Level Rearrangements Do Occur in the NNRTI-Bound HIV-1 Reverse Transcriptase. Journal of the American Chemical Society, 2012, 134, 12885-12888.	6.6	22
52	High-throughput molecular dynamics: the powerful new tool for drug discovery. Drug Discovery Today, 2012, 17, 1059-1062.	3.2	76
53	A survey of computational molecular science using graphics processing units. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2012, 2, 734-742.	6.2	33
54	Membrane-Sensitive Conformational States of Helix 8 in the Metabotropic Glu2 Receptor, a Class C GPCR. PLoS ONE, 2012, 7, e42023.	1.1	31

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55	Optimized Potential of Mean Force Calculations for Standard Binding Free Energies. Journal of Chemical Theory and Computation, 2011, 7, 1765-1772.	2.3	37
56	Capturing the Initial Autocatalytic Maturation Mechanism of HIV-1 protease at Atomic Resolution. Biophysical Journal, 2011, 100, 228a.	0.2	0
57	A High-Throughput Steered Molecular Dynamics Study on the Free Energy Profile of Ion Permeation through Gramicidin A. Journal of Chemical Theory and Computation, 2011, 7, 1943-1950.	2.3	35
58	Complete reconstruction of an enzyme-inhibitor binding process by molecular dynamics simulations. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 10184-10189.	3.3	601
59	Distributed computing as a virtual supercomputer: Tools to run and manage large-scale BOINC simulations. Computer Physics Communications, 2010, 181, 1402-1409.	3.0	4
60	Explicit solvent dynamics and energetics of HIVâ€1 protease flap opening and closing. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2873-2885.	1.5	61
61	Induced Effects of Sodium Ions on Dopaminergic G-Protein Coupled Receptors. PLoS Computational Biology, 2010, 6, e1000884.	1.5	93
62	Amyloid-dependent triosephosphate isomerase nitrotyrosination induces glycation and tau fibrillation. Brain, 2009, 132, 1335-1345.	3.7	93
63	Insights from the energetics of water binding at the domainâ€ligand interface of the Src SH2 domain. Proteins: Structure, Function and Bioinformatics, 2008, 72, 1290-1297.	1.5	10
64	Energetics of K⁺ permeability through Gramicidin A by forwardâ€reverse steered molecular dynamics. Proteins: Structure, Function and Bioinformatics, 2008, 73, 185-194.	1.5	26
65	A COUPLED MOLECULAR-CONTINUUM HYBRID MODEL FOR THE SIMULATION OF MACROMOLECULAR DYNAMICS. International Journal of Modern Physics C, 2007, 18, 520-527.	0.8	3
66	Embedding molecular dynamics within fluctuating hydrodynamics in multiscale simulations of liquids. Physical Review E, 2007, 76, 036709.	0.8	53
67	Integrative Biology â€" the challenges of developing a collaborative research environment for heart and cancer modelling. Future Generation Computer Systems, 2007, 23, 457-465.	4.9	11
68	Energy controlled insertion of polar molecules in dense fluids. Journal of Chemical Physics, 2004, 121, 12139.	1.2	34
69	Multiscale dissipative particle dynamics. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2002, 360, 317-331.	1.6	12
70	Mesoscopic dynamics of Voronoi fluid particles. Journal of Physics A, 2002, 35, 1605-1625.	1.6	31
71	Foundations of dissipative particle dynamics. Physical Review E, 2000, 62, 2140-2157.	0.8	133
72	PERFORMANCE EVALUATION OF A FD-TD PARALLEL CODE FOR MICROWAVE OVENS DESIGN. , 2000, , .		0

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73	Discrete random walk models for symmetric LÃ©vyâ€“Feller diffusion processes. Physica A: Statistical Mechanics and Its Applications, 1999, 269, 79-89.	1.2	61