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List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/7903870/publications.pdf

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25 papers	1,459 citations	471509 17 h-index	580821 25 g-index
26 all docs	26 docs citations	26 times ranked	2047 citing authors

#	Article	IF	Citations
1	Computationally driven discovery of SARS-CoV-2 M^{pro}inhibitors: from design to experimental validation. Chemical Science, 2022, 13, 3674-3687.	7.4	21
2	From Target to Drug: Generative Modeling for the Multimodal Structure-Based Ligand Design. Molecular Pharmaceutics, 2019, 16, 4282-4291.	4.6	81
3	Defining and Exploiting Hypersensitivity Hotspots to Facilitate Abscisic Acid Agonist Optimization. ACS Chemical Biology, 2019, 14, 332-336.	3.4	19
4	Insecticidal spider toxins are high affinity positive allosteric modulators of the nicotinic acetylcholine receptor. FEBS Letters, 2019, 593, 1336-1350.	2.8	23
5	Shape-Based Generative Modeling for de Novo Drug Design. Journal of Chemical Information and Modeling, 2019, 59, 1205-1214.	5.4	145
6	Supervised Molecular Dynamics (SuMD) Approaches in Drug Design. Methods in Molecular Biology, 2018, 1824, 287-298.	0.9	18
7	New Trends in Inspecting GPCRâ€ligand Recognition Process: the Contribution of the Molecular Modeling Section (MMS) at the University of Padova. Molecular Informatics, 2016, 35, 440-448.	2.5	3
8	Deciphering the Complexity of Ligandâ€"Protein Recognition Pathways Using Supervised Molecular Dynamics (SuMD) Simulations. Journal of Chemical Information and Modeling, 2016, 56, 687-705.	5.4	88
9	Modeling ligand recognition at the P2Y12 receptor in light of X-ray structural information. Journal of Computer-Aided Molecular Design, 2015, 29, 737-756.	2.9	42
10	Exploring the recognition pathway at the human A_{2A} adenosine receptor of the endogenous agonist adenosine using supervised molecular dynamics simulations. MedChemComm, 2015, 6, 1081-1085.	3.4	36
11	Advances in Computational Techniques to Study GPCRâ€"Ligand Recognition. Trends in Pharmacological Sciences, 2015, 36, 878-890.	8.7	40
12	The xylanase inhibitor <scp>TAXIâ€II</scp> counteracts the necrotic activity of a <scp>F</scp>usarium graminearum xylanase inâ€‰vitro and in durum wheat transgenic plants. Molecular Plant Pathology, 2015, 16, 583-592.	4.2	22
13	Carboxylation-dependent conformational changes of human osteocalcin. Frontiers in Bioscience - Landmark, 2014, 19, 1105.	3.0	12
14	Bridging Molecular Docking to Membrane Molecular Dynamics To Investigate GPCRâ€"Ligand Recognition: The Human A_{2A} Adenosine Receptor as a Key Study. Journal of Chemical Information and Modeling, 2014, 54, 169-183.	5.4	59
15	Advances in GPCR Modeling Evaluated by the GPCR Dock 2013 Assessment: Meeting New Challenges. Structure, 2014, 22, 1120-1139.	3.3	149
16	Perturbation of Fluid Dynamics Properties of Water Molecules during G Protein-Coupled Receptorâ€"Ligand Recognition: The Human A_{2A} Adenosine Receptor as a Key Study. Journal of Chemical Information and Modeling, 2014, 54, 2846-2855.	5.4	24
17	Supervised Molecular Dynamics (SuMD) as a Helpful Tool To Depict GPCRâ€"Ligand Recognition Pathway in a Nanosecond Time Scale. Journal of Chemical Information and Modeling, 2014, 54, 372-376.	5.4	135
18	The mitochondrial calcium uniporter is a multimer that can include a dominant-negative pore-forming subunit. EMBO Journal, 2013, 32, 2362-2376.	7.8	408

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19	MMsDusty: an Alternative InChIâ€Based Tool to Minimize Chemical Redundancy. Molecular Informatics, 2013, 32, 681-684.	2.5	2
20	Implementing the â€œBest Template Searchingâ€•tool into Adenosiland platform. In Silico Pharmacology, 2013, 1, 25.	3.3	10
21	New insight into adenosine receptors selectivity derived from a novel series of [5-substituted-4-phenyl-1,3-thiazol-2-yl] benzamides and furamides. European Journal of Medicinal Chemistry, 2013, 63, 924-934.	5.5	30
22	Adenosiland: Walking through adenosine receptors landscape. European Journal of Medicinal Chemistry, 2012, 58, 248-257.	5.5	29
23	Exploring the Directionality of 5-Substitutions in a New Series of 5-Alkylaminopyrazolo[4,3-e]1,2,4-triazolo[1,5-c]pyrimidine as a Strategy To Design Novel Human A₃ Adenosine Receptor Antagonists.. Journal of Medicinal Chemistry, 2012, 55, 9654-9668.	6.4	17
24	3-Hydroxy-1H-quinazoline-2,4-dione derivatives as new antagonists at ionotropic glutamate receptors: Molecular modeling and pharmacological studies. European Journal of Medicinal Chemistry, 2012, 54, 470-482.	5.5	31
25	Molecular modelling studies on Arylthioindoles as potent inhibitors of tubulin polymerization. European Journal of Medicinal Chemistry, 2011, 46, 3519-3525.	5.5	15