Stefano Artin Serapian

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7239619/publications.pdf

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28	622	567281	610901
papers	citations	15 h-index	24 g-index

39	39	39	1174
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Protein Allostery and Ligand Design: Computational Design Meets Experiments to Discover Novel Chemical Probes. Journal of Molecular Biology, 2022, 434, 167468.	4.2	10
2	Path to Actinorhodin: Regio- and Stereoselective Ketone Reduction by a Type II Polyketide Ketoreductase Revealed in Atomistic Detail. Jacs Au, 2022, 2, 972-984.	7.9	1
3	New perspectives in cancer drug development: computational advances with an eye to design. RSC Medicinal Chemistry, 2021, 12, 1491-1502.	3.9	6
4	Exploiting Folding and Degradation Machineries To Target Undruggable Proteins: What Can a Computational Approach Tell Us?. ChemMedChem, 2021, 16, 1593-1599.	3.2	4
5	Bow to the enemy: How flexibility of host protein receptors can favor SARS-CoV-2. Biophysical Journal, 2021, 120, 977-979.	0.5	1
6	Atomistic Simulations of the Mechanisms of the Poorly Catalytic Mitochondrial Chaperone Trap1: Insights into the Effects of Structural Asymmetry on Reactivity. ACS Catalysis, 2021, 11, 8605-8620.	11.2	6
7	The molecular chaperone TRAP1 in cancer: From the basics of biology to pharmacological targeting. Seminars in Cancer Biology, 2021, 76, 45-53.	9.6	18
8	Targeting the mitochondrial chaperone TRAP1: strategies and therapeutic perspectives. Trends in Pharmacological Sciences, 2021, 42, 566-576.	8.7	19
9	The tumor suppressor folliculin inhibits lactate dehydrogenase A and regulates the Warburg effect. Nature Structural and Molecular Biology, 2021, 28, 662-670.	8.2	19
10	SARS-CoV-2 Spike Protein Mutations and Escape from Antibodies: A Computational Model of Epitope Loss in Variants of Concern. Journal of Chemical Information and Modeling, 2021, 61, 4687-4700.	5.4	26
11	Designing Molecular Spanners to Throw in the Protein Networks. Chemistry - A European Journal, 2020, 26, 4656-4670.	3.3	28
12	Dynamically Shaping Chaperones. Allosteric Modulators of HSP90 Family as Regulatory Tools of Cell Metabolism in Neoplastic Progression. Frontiers in Oncology, 2020, 10, 1177.	2.8	28
13	The Answer Lies in the Energy: How Simple Atomistic Molecular Dynamics Simulations May Hold the Key to Epitope Prediction on the Fully Glycosylated SARS-CoV-2 Spike Protein. Journal of Physical Chemistry Letters, 2020, 11, 8084-8093.	4.6	39
14	Chemical Perturbation of Oncogenic Protein Folding: from the Prediction of Locally Unstable Structures to the Design of Disruptors of Hsp90â€“Client Interactions. Chemistry - A European Journal, 2020, 26, 9459-9465.	3.3	39
15	Frontispiece: Designing Molecular Spanners to Throw in the Protein Networks. Chemistry - A European Journal, 2020, 26, .	3.3	2
16	Impact of Mutations on NPAC Structural Dynamics: Mechanistic Insights from MD Simulations. Journal of Chemical Information and Modeling, 2019, 59, 3927-3937.	5.4	27
17	Unpicking the Cause of Stereoselectivity in Actinorhodin Ketoreductase Variants with Atomistic Simulations. ACS Catalysis, 2019, 9, 2381-2394.	11.2	28
18	Photochromism and Dualâ€Color Fluorescence in a Polyoxometalateâ€“Benzospiropyran Molecular Switch. Angewandte Chemie - International Edition, 2017, 56, 4872-4876.	13.8	64

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19	Photochromism and Dualâ€Color Fluorescence in a Polyoxometalateâ€“Benzospiropyran Molecular Switch. Angewandte Chemie, 2017, 129, 4950-4954.	2.0	10
20	Electronic and relativistic contributions to ion-pairing in polyoxometalate model systems. Physical Chemistry Chemical Physics, 2017, 19, 8715-8725.	2.8	23
21	Hierarchical Self-Assembly of Polyoxometalate-Based Hybrids Driven by Metal Coordination and Electrostatic Interactions: From Discrete Supramolecular Species to Dense Monodisperse Nanoparticles. Journal of the American Chemical Society, 2016, 138, 5093-5099.	13.7	94
22	Simulating the Favorable Aggregation of Monolacunary Keggin Anions. Journal of Physical Chemistry B, 2016, 120, 12959-12971.	2.6	11
23	Molecular Basis for the Recognition of Higher Fullerenes into Ureidopyrimidinoneâ€“Cyclotriveratrylene Selfâ€Assembled Capsules. Chemistry - A European Journal, 2016, 22, 13496-13505.	3.3	18
24	Molecular Motion and Conformational Interconversion of IrIÂ·COD Included in Rebekâ€™s Self-Folding Octaamide Cavitand. Journal of the American Chemical Society, 2016, 138, 2273-2279.	13.7	11
25	Ring-Closing Metathesis and Nanoparticle Formation Based on Diallyldithiocarbamate Complexes of Gold(I): Synthetic, Structural, and Computational Studies. Inorganic Chemistry, 2014, 53, 2404-2416.	4.0	35
26	The shape of Au8: gold leaf or gold nugget?. Nanoscale, 2013, 5, 6445.	5.6	41
27	Assessing the preferred solution conformation of an interacting senseâ€“antisense (complementary) peptide pair. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 496-502.	2.2	4
28	The statistical significance of selected senseâ€“antisense peptide interactions. Journal of Computational Chemistry, 2012, 33, 1440-1447.	3.3	5