

Stefano Artin Serapian

List of Publications by Year in descending order

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Version: 2024-02-01

28
papers

622
citations

567281

15
h-index

610901

24
g-index

39
all docs

39
docs citations

39
times ranked

1174
citing authors

#	ARTICLE	IF	CITATIONS
1	Hierarchical Self-Assembly of Polyoxometalate-Based Hybrids Driven by Metal Coordination and Electrostatic Interactions: From Discrete Supramolecular Species to Dense Monodisperse Nanoparticles. <i>Journal of the American Chemical Society</i> , 2016, 138, 5093-5099.	13.7	94
2	Photochromism and Dual-Color Fluorescence in a Polyoxometalate-Benzospiropyran Molecular Switch. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 4872-4876.	13.8	64
3	The shape of Au ₈ : gold leaf or gold nugget?. <i>Nanoscale</i> , 2013, 5, 6445.	5.6	41
4	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. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 8084-8093.	4.6	39
5	Chemical Perturbation of Oncogenic Protein Folding: from the Prediction of Locally Unstable Structures to the Design of Disruptors of Hsp90-Client Interactions. <i>Chemistry - A European Journal</i> , 2020, 26, 9459-9465.	3.3	39
6	Ring-Closing Metathesis and Nanoparticle Formation Based on Diallyldithiocarbamate Complexes of Gold(I): Synthetic, Structural, and Computational Studies. <i>Inorganic Chemistry</i> , 2014, 53, 2404-2416.	4.0	35
7	Unpicking the Cause of Stereoselectivity in Actinorhodin Ketoreductase Variants with Atomistic Simulations. <i>ACS Catalysis</i> , 2019, 9, 2381-2394.	11.2	28
8	Designing Molecular Spanners to Throw in the Protein Networks. <i>Chemistry - A European Journal</i> , 2020, 26, 4656-4670.	3.3	28
9	Dynamically Shaping Chaperones. Allosteric Modulators of HSP90 Family as Regulatory Tools of Cell Metabolism in Neoplastic Progression. <i>Frontiers in Oncology</i> , 2020, 10, 1177.	2.8	28
10	Impact of Mutations on NPAC Structural Dynamics: Mechanistic Insights from MD Simulations. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3927-3937.	5.4	27
11	SARS-CoV-2 Spike Protein Mutations and Escape from Antibodies: A Computational Model of Epitope Loss in Variants of Concern. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4687-4700.	5.4	26
12	Electronic and relativistic contributions to ion-pairing in polyoxometalate model systems. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 8715-8725.	2.8	23
13	Targeting the mitochondrial chaperone TRAP1: strategies and therapeutic perspectives. <i>Trends in Pharmacological Sciences</i> , 2021, 42, 566-576.	8.7	19
14	The tumor suppressor folliculin inhibits lactate dehydrogenase A and regulates the Warburg effect. <i>Nature Structural and Molecular Biology</i> , 2021, 28, 662-670.	8.2	19
15	Molecular Basis for the Recognition of Higher Fullerenes into Ureidopyrimidinone-Cyclotrimeratrylene Self-Assembled Capsules. <i>Chemistry - A European Journal</i> , 2016, 22, 13496-13505.	3.3	18
16	The molecular chaperone TRAP1 in cancer: From the basics of biology to pharmacological targeting. <i>Seminars in Cancer Biology</i> , 2021, 76, 45-53.	9.6	18
17	Simulating the Favorable Aggregation of Monolacunary Keggin Anions. <i>Journal of Physical Chemistry B</i> , 2016, 120, 12959-12971.	2.6	11
18	Molecular Motion and Conformational Interconversion of Ir-COD Included in Rebeck's Self-Folding Octaamide Cavitand. <i>Journal of the American Chemical Society</i> , 2016, 138, 2273-2279.	13.7	11

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19	Photochromism and Dual-Color Fluorescence in a Polyoxometalate-Benzospiropyran Molecular Switch. <i>Angewandte Chemie</i> , 2017, 129, 4950-4954.	2.0	10
20	Protein Allostery and Ligand Design: Computational Design Meets Experiments to Discover Novel Chemical Probes. <i>Journal of Molecular Biology</i> , 2022, 434, 167468.	4.2	10
21	New perspectives in cancer drug development: computational advances with an eye to design. <i>RSC Medicinal Chemistry</i> , 2021, 12, 1491-1502.	3.9	6
22	Atomistic Simulations of the Mechanisms of the Poorly Catalytic Mitochondrial Chaperone Trap1: Insights into the Effects of Structural Asymmetry on Reactivity. <i>ACS Catalysis</i> , 2021, 11, 8605-8620.	11.2	6
23	The statistical significance of selected sense-antisense peptide interactions. <i>Journal of Computational Chemistry</i> , 2012, 33, 1440-1447.	3.3	5
24	Assessing the preferred solution conformation of an interacting sense-antisense (complementary) peptide pair. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2013, 23, 496-502.	2.2	4
25	Exploiting Folding and Degradation Machineries To Target Undruggable Proteins: What Can a Computational Approach Tell Us?. <i>ChemMedChem</i> , 2021, 16, 1593-1599.	3.2	4
26	Frontispiece: Designing Molecular Spanners to Throw in the Protein Networks. <i>Chemistry - A European Journal</i> , 2020, 26, .	3.3	2
27	Bow to the enemy: How flexibility of host protein receptors can favor SARS-CoV-2. <i>Biophysical Journal</i> , 2021, 120, 977-979.	0.5	1
28	Path to Actinorhodin: Regio- and Stereoselective Ketone Reduction by a Type II Polyketide Ketoreductase Revealed in Atomistic Detail. <i>Jacs Au</i> , 2022, 2, 972-984.	7.9	1