

Mattia Sturlese

List of Publications by Year in descending order

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papers

1,252
citations

430442

18
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433756

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74
docs citations

74
times ranked

1818
citing authors

#	ARTICLE	IF	CITATIONS
1	Deciphering the Complexity of Ligand-Protein Recognition Pathways Using Supervised Molecular Dynamics (SuMD) Simulations. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 687-705.	2.5	88
2	Molecular architecture and the structural basis for anion interaction in prestin and SLC26 transporters. <i>Nature Communications</i> , 2014, 5, 3622.	5.8	74
3	MMsINC: a large-scale chemoinformatics database. <i>Nucleic Acids Research</i> , 2009, 37, D284-D290.	6.5	71
4	Exploring Protein-Peptide Recognition Pathways Using a Supervised Molecular Dynamics Approach. <i>Structure</i> , 2017, 25, 655-662.e2.	1.6	67
5	Dopamine-derived Quinones Affect the Structure of the Redox Sensor DJ-1 through Modifications at Cys-106 and Cys-53. <i>Journal of Biological Chemistry</i> , 2012, 287, 18738-18749.	1.6	61
6	Supervised Molecular Dynamics (SuMD) Insights into the mechanism of action of SARS-CoV-2 main protease inhibitor PF-07321332. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2021, 36, 1645-1649.	2.5	60
7	SAR and QSAR study on 2-aminothiazole derivatives, modulators of transcriptional repression in Huntington's disease. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 5695-5703.	1.4	49
8	Targeting the coronavirus SARS-CoV-2: computational insights into the mechanism of action of the protease inhibitors lopinavir, ritonavir and nelfinavir. <i>Scientific Reports</i> , 2020, 10, 20927.	1.6	44
9	DockBench: An Integrated Informatic Platform Bridging the Gap between the Robust Validation of Docking Protocols and Virtual Screening Simulations. <i>Molecules</i> , 2015, 20, 9977-9993.	1.7	40
10	Iron-Sulfur Cluster Binding by Mitochondrial Monothiol Glutaredoxin-1 of <i>Trypanosoma brucei</i> : Molecular Basis of Iron-Sulfur Cluster Coordination and Relevance for Parasite Infectivity. <i>Antioxidants and Redox Signaling</i> , 2013, 19, 665-682.	2.5	37
11	Identification of a Novel Mcl-1 Protein Binding Motif. <i>Journal of Biological Chemistry</i> , 2011, 286, 39829-39835.	1.6	34
12	AquaMMapS: An Alternative Tool to Monitor the Role of Water Molecules During Protein-Ligand Association. <i>ChemMedChem</i> , 2018, 13, 522-531.	1.6	29
13	The rise of molecular simulations in fragment-based drug design (FBDD): an overview. <i>Drug Discovery Today</i> , 2020, 25, 1693-1701.	3.2	29
14	Polyamine-Based Thiols in Trypanosomatids: Evolution, Protein Structural Adaptations, and Biological Functions. <i>Antioxidants and Redox Signaling</i> , 2018, 28, 463-486.	2.5	27
15	Novel coumarin-pyridazine hybrids as selective MAO-B inhibitors for the Parkinson's disease therapy. <i>Bioorganic Chemistry</i> , 2020, 104, 104203.	2.0	27
16	Combining self- and cross-docking as benchmark tools: the performance of DockBench in the D3R Grand Challenge 2. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 251-264.	1.3	26
17	Synthesis, biological evaluation and molecular modeling studies of phthalazin-1(2H)-one derivatives as novel cholinesterase inhibitors. <i>RSC Advances</i> , 2016, 6, 46170-46185.	1.7	22
18	Computationally driven discovery of SARS-CoV-2 M ^{pro} inhibitors: from design to experimental validation. <i>Chemical Science</i> , 2022, 13, 3674-3687.	3.7	21

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19	Side Chain Cyclization Based on Serine Residues: Synthesis, Structure, and Activity of a Novel Cyclic Analogue of the Parathyroid Hormone Fragment 1-11. <i>Journal of Medicinal Chemistry</i> , 2010, 53, 8072-8079.	2.9	20
20	Supervised Molecular Dynamics (SuMD) Approaches in Drug Design. <i>Methods in Molecular Biology</i> , 2018, 1824, 287-298.	0.4	18
21	Deciphering the Molecular Recognition Mechanism of Multidrug Resistance Staphylococcus aureus NorA Efflux Pump Using a Supervised Molecular Dynamics Approach. <i>International Journal of Molecular Sciences</i> , 2019, 20, 4041.	1.8	18
22	Re-Exploring the Ability of Common Docking Programs to Correctly Reproduce the Binding Modes of Non-Covalent Inhibitors of SARS-CoV-2 Protease Mpro. <i>Pharmaceuticals</i> , 2022, 15, 180.	1.7	18
23	A Deep-Learning Approach toward Rational Molecular Docking Protocol Selection. <i>Molecules</i> , 2020, 25, 2487.	1.7	17
24	Targeting Protein Kinase CK1 β with Riluzole: Could It Be One of the Possible Missing Bricks to Interpret Its Effect in the Treatment of ALS from a Molecular Point of View?. <i>ChemMedChem</i> , 2018, 13, 2601-2605.	1.6	16
25	Exploring the RNA-Recognition Mechanism Using Supervised Molecular Dynamics (SuMD) Simulations: Toward a Rational Design for Ribonucleic-Targeting Molecules?. <i>Frontiers in Chemistry</i> , 2020, 8, 107.	1.8	16
26	A Computational Workflow for the Identification of Novel Fragments Acting as Inhibitors of the Activity of Protein Kinase CK1 β . <i>International Journal of Molecular Sciences</i> , 2021, 22, 9741.	1.8	15
27	From the Wuhan-Hu-1 strain to the XD and XE variants: is targeting the SARS-CoV-2 spike protein still a pharmaceutically relevant option against COVID-19?. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2022, 37, 1704-1714.	2.5	15
28	NMR-Assisted Molecular Docking Methodologies. <i>Molecular Informatics</i> , 2015, 34, 513-525.	1.4	14
29	The role of 5-arylalkylamino- and 5-piperazino- moieties on the 7-aminopyrazolo[4,3-d]pyrimidine core in affecting adenosine A ₁ and A _{2A} receptor affinity and selectivity profiles. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2017, 32, 248-263.	2.5	14
30	Can We Still Trust Docking Results? An Extension of the Applicability of DockBench on PDBbind Database. <i>International Journal of Molecular Sciences</i> , 2019, 20, 3558.	1.8	14
31	Revisiting the Allosteric Regulation of Sodium Cation on the Binding of Adenosine at the Human A _{2A} Adenosine Receptor: Insights from Supervised Molecular Dynamics (SuMD) Simulations. <i>Molecules</i> , 2019, 24, 2752.	1.7	14
32	DockBench as docking selector tool: the lesson learned from D3R Grand Challenge 2015. <i>Journal of Computer-Aided Molecular Design</i> , 2016, 30, 773-789.	1.3	13
33	Synthesis, structure-activity relationships and biological evaluation of 7-phenyl-pyrroloquinolinone 3-amide derivatives as potent antimetabolic agents. <i>European Journal of Medicinal Chemistry</i> , 2017, 127, 643-660.	2.6	13
34	A new inactive conformation of SARS-CoV-2 main protease. <i>Acta Crystallographica Section D: Structural Biology</i> , 2022, 78, 363-378.	1.1	13
35	Inspecting the Mechanism of Fragment Hits Binding on SARS-CoV-2 M ^{pro} by Using Supervised Molecular Dynamics (SuMD) Simulations. <i>ChemMedChem</i> , 2021, 16, 2075-2081.	1.6	12
36	Implementing a Scoring Function Based on Interaction Fingerprint for Autogrow4: Protein Kinase CK1 β as a Case Study. <i>Frontiers in Molecular Biosciences</i> , 0, 9, .	1.6	11

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37	Evaluating the effects of fluorine on biological properties and metabolic stability of some antitubulin 3-substituted 7-phenyl-pyrroloquinolinones. <i>European Journal of Medicinal Chemistry</i> , 2019, 178, 297-314.	2.6	10
38	HT-SuMD: making molecular dynamics simulations suitable for fragment-based screening. A comparative study with NMR. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2021, 36, 1-14.	2.5	10
39	Ribose and Non-Ribose A2A Adenosine Receptor Agonists: Do They Share the Same Receptor Recognition Mechanism?. <i>Biomedicines</i> , 2022, 10, 515.	1.4	10
40	Sulfonamido-derivatives of unsubstituted carbazoles as BACE1 inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2017, 27, 4812-4816.	1.0	9
41	Scaffold Repurposing of in-House Chemical Library toward the Identification of New Casein Kinase 1 γ Inhibitors. <i>ACS Medicinal Chemistry Letters</i> , 2020, 11, 1168-1174.	1.3	9
42	Synthesis and structural studies of new analogues of PTH(1-11) containing C β -tetra-substituted amino acids in position 8. <i>Amino Acids</i> , 2010, 39, 1369-1379.	1.2	8
43	Targeting tubulin polymerization by novel 7-aryl-pyrroloquinolinones: Synthesis, biological activity and SARs. <i>European Journal of Medicinal Chemistry</i> , 2018, 143, 244-258.	2.6	8
44	Binding mode of AIF(370-394) peptide to CypA: insights from NMR, label-free and molecular docking studies. <i>Biochemical Journal</i> , 2018, 475, 2377-2393.	1.7	8
45	Sodium or Not Sodium: Should Its Presence Affect the Accuracy of Pose Prediction in Docking GPCR Antagonists?. <i>Pharmaceuticals</i> , 2022, 15, 346.	1.7	8
46	FRET-Protease-Coupled Peptidyl-Prolyl cis-trans Isomerase Assay. <i>Journal of Biomolecular Screening</i> , 2016, 21, 701-712.	2.6	7
47	Design, conformational studies and analysis of structure-function relationships of PTH (1-11) analogues: the essential role of Val in position 2. <i>Amino Acids</i> , 2012, 43, 207-218.	1.2	6
48	The Influence of the 1-(3-Trifluoromethyl-Benzyl)-1H-Pyrazole-4-yl Moiety on the Adenosine Receptors Affinity Profile of Pyrazolo[4,3-e][1,2,4]Triazolo[1,5-c]Pyrimidine Derivatives. <i>PLoS ONE</i> , 2015, 10, e0143504.	1.1	6
49	The Multifaceted Role of GPCRs in Amyotrophic Lateral Sclerosis: A New Therapeutic Perspective?. <i>International Journal of Molecular Sciences</i> , 2022, 23, 4504.	1.8	6
50	¹ H, ¹³ C and ¹⁵ N resonance assignment of the mature form of monothiol glutaredoxin 1 from the pathogen <i>Trypanosoma brucei</i> . <i>Biomolecular NMR Assignments</i> , 2015, 9, 143-146.	0.4	5
51	¹ H, ¹³ C and ¹⁵ N resonance assignment of the cytosolic dithiol glutaredoxin 1 from the pathogen <i>Trypanosoma brucei</i> . <i>Biomolecular NMR Assignments</i> , 2016, 10, 85-88.	0.4	5
52	Synthesis and preliminary structure-activity relationship study of 2-aryl-2H-pyrazolo[4,3-c]quinolin-3-ones as potential checkpoint kinase 1 (Chk1) inhibitors. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2018, 33, 171-183.	2.5	5
53	Coupling Supervised Molecular Dynamics (SuMD) with Entropy Estimations To Shine Light on the Stability of Multiple Binding Sites. <i>ACS Medicinal Chemistry Letters</i> , 2019, 10, 444-449.	1.3	5
54	Design, synthesis, structural analysis and biochemical studies of stapled AIF(370-394) analogues as ligand of CypA. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2020, 1864, 129717.	1.1	5

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55	New Insights into Key Determinants for Adenosine 1 Receptor Antagonists Selectivity Using Supervised Molecular Dynamics Simulations. <i>Biomolecules</i> , 2020, 10, 732.	1.8	5
56	Shedding Light on the Molecular Recognition of Sub-Kilodalton Macrocyclic Peptides on Thrombin by Supervised Molecular Dynamics. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 707661.	1.6	5
57	Pyridazinones containing dithiocarbamoyl moieties as a new class of selective MAO-B inhibitors. <i>Bioorganic Chemistry</i> , 2021, 115, 105203.	2.0	5
58	In Silico 3D Modeling of Binding Activities. <i>Methods in Molecular Biology</i> , 2016, 1425, 23-35.	0.4	4
59	The lineage-specific, intrinsically disordered N-terminal extension of monothiol glutaredoxin 1 from trypanosomes contains a regulatory region. <i>Scientific Reports</i> , 2018, 8, 13716.	1.6	4
60	Targeting G Protein-Coupled Receptors with Magnetic Carbon Nanotubes: The Case of the A ₃ Adenosine Receptor. <i>ChemMedChem</i> , 2020, 15, 1909-1920.	1.6	4
61	Comparing Fragment Binding Poses Prediction Using HSP90 as a Key Study: When Bound Water Makes the Difference. <i>Molecules</i> , 2020, 25, 4651.	1.7	4
62	Bat coronaviruses related to SARS-CoV-2: what about their 3CL proteases (MPro)? <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2022, 37, 1077-1082.	2.5	4
63	New Trends in Inspecting GPCR-Ligand Recognition Process: the Contribution of the Molecular Modeling Section (MMS) at the University of Padova. <i>Molecular Informatics</i> , 2016, 35, 440-448.	1.4	3
64	Comparative Molecular Dynamics Investigation of the Electromotile Hearing Protein Prestin. <i>International Journal of Molecular Sciences</i> , 2021, 22, 8318.	1.8	2
65	A molecular dynamics strategy for CS \pm peptides disulfide-assisted model refinement. <i>Journal of Biomolecular Structure and Dynamics</i> , 2017, 35, 2736-2744.	2.0	1
66	A Structural Model for Prestin and Related SLC26 Anion Transporters. <i>Biophysical Journal</i> , 2013, 104, 112a.	0.2	0
67	Abstract 8: Identification of a non-canonical BH3 peptide that binds the BH3 pocket of Mcl-1. , 2011, , .		0