Mattia Sturlese

List of Publications by Year
in descending order

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67 papers	1,252 citations	430442 18 h-index	433756 31 g-index
74 all docs	74 docs citations	74 times ranked	1818 citing authors

#	Article	IF	Citations
1	Re-Exploring the Ability of Common Docking Programs to Correctly Reproduce the Binding Modes of Non-Covalent Inhibitors of SARS-CoV-2 Protease Mpro. Pharmaceuticals, 2022, 15, 180.	1.7	18
2	Computationally driven discovery of SARS-CoV-2 M^{pro}inhibitors: from design to experimental validation. Chemical Science, 2022, 13, 3674-3687.	3.7	21
3	A new inactive conformation of SARS-CoV-2 main protease. Acta Crystallographica Section D: Structural Biology, 2022, 78, 363-378.	1.1	13
4	Ribose and Non-Ribose A2A Adenosine Receptor Agonists: Do They Share the Same Receptor Recognition Mechanism?. Biomedicines, 2022, 10, 515.	1.4	10
5	Sodium or Not Sodium: Should Its Presence Affect the Accuracy of Pose Prediction in Docking GPCR Antagonists?. Pharmaceuticals, 2022, 15, 346.	1.7	8
6	The Multifaceted Role of GPCRs in Amyotrophic Lateral Sclerosis: A New Therapeutic Perspective?. International Journal of Molecular Sciences, 2022, 23, 4504.	1.8	6
7	Bat coronaviruses related to SARS-CoV-2: what about their 3CL proteases (MPro)?. Journal of Enzyme Inhibition and Medicinal Chemistry, 2022, 37, 1077-1082.	2.5	4
8	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?. Journal of Enzyme Inhibition and Medicinal Chemistry, 2022, 37, 1704-1714.	2.5	15
9	HT-SuMD: making molecular dynamics simulations suitable for fragment-based screening. A comparative study with NMR. Journal of Enzyme Inhibition and Medicinal Chemistry, 2021, 36, 1-14.	2.5	10
10	Supervised Molecular Dynamics (SuMD) Insights into the mechanism of action of SARS-CoV-2 main protease inhibitor PF-07321332. Journal of Enzyme Inhibition and Medicinal Chemistry, 2021, 36, 1645-1649.	2.5	60
11	Inspecting the Mechanism of Fragment Hits Binding on SARSâ€CoVâ€2 M^{pro} by Using Supervised Molecular Dynamics (SuMD) Simulations. ChemMedChem, 2021, 16, 2075-2081.	1.6	12
12	Comparative Molecular Dynamics Investigation of the Electromotile Hearing Protein Prestin. International Journal of Molecular Sciences, 2021, 22, 8318.	1.8	2
13	Shedding Light on the Molecular Recognition of Sub-Kilodalton Macrocyclic Peptides on Thrombin by Supervised Molecular Dynamics. Frontiers in Molecular Biosciences, 2021, 8, 707661.	1.6	5
14	A Computational Workflow for the Identification of Novel Fragments Acting as Inhibitors of the Activity of Protein Kinase CK1Î´. International Journal of Molecular Sciences, 2021, 22, 9741.	1.8	15
15	Pyridazinones containing dithiocarbamoyl moieties as a new class of selective MAO-B inhibitors. Bioorganic Chemistry, 2021, 115, 105203.	2.0	5
16	Design, synthesis, structural analysis and biochemical studies of stapled AIF(370-394) analogues as ligand of CypA. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129717.	1.1	5
17	Targeting G Proteinâ€Coupled Receptors with Magnetic Carbon Nanotubes: The Case of the A 3 Adenosine Receptor. ChemMedChem, 2020, 15, 1909-1920.	1.6	4
18	Novel coumarin-pyridazine hybrids as selective MAO-B inhibitors for the Parkinsonâ€™s disease therapy. Bioorganic Chemistry, 2020, 104, 104203.	2.0	27

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19	Targeting the coronavirus SARS-CoV-2: computational insights into the mechanism of action of the protease inhibitors lopinavir, ritonavir and nelfinavir. Scientific Reports, 2020, 10, 20927.	1.6	44
20	Comparing Fragment Binding Poses Prediction Using HSP90 as a Key Study: When Bound Water Makes the Difference. Molecules, 2020, 25, 4651.	1.7	4
21	New Insights into Key Determinants for Adenosine 1 Receptor Antagonists Selectivity Using Supervised Molecular Dynamics Simulations. Biomolecules, 2020, 10, 732.	1.8	5
22	A Deep-Learning Approach toward Rational Molecular Docking Protocol Selection. Molecules, 2020, 25, 2487.	1.7	17
23	Exploring the RNA-Recognition Mechanism Using Supervised Molecular Dynamics (SuMD) Simulations: Toward a Rational Design for Ribonucleic-Targeting Molecules?. Frontiers in Chemistry, 2020, 8, 107.	1.8	16
24	The rise of molecular simulations in fragment-based drug design (FBDD): an overview. Drug Discovery Today, 2020, 25, 1693-1701.	3.2	29
25	Scaffold Repurposing of in-House Chemical Library toward the Identification of New Casein Kinase 1 Î´ Inhibitors. ACS Medicinal Chemistry Letters, 2020, 11, 1168-1174.	1.3	9
26	Deciphering the Molecular Recognition Mechanism of Multidrug Resistance Staphylococcus aureus NorA Efflux Pump Using a Supervised Molecular Dynamics Approach. International Journal of Molecular Sciences, 2019, 20, 4041.	1.8	18
27	Can We Still Trust Docking Results? An Extension of the Applicability of DockBench on PDBbind Database. International Journal of Molecular Sciences, 2019, 20, 3558.	1.8	14
28	Revisiting the Allosteric Regulation of Sodium Cation on the Binding of Adenosine at the Human A2A Adenosine Receptor: Insights from Supervised Molecular Dynamics (SuMD) Simulations. Molecules, 2019, 24, 2752.	1.7	14
29	Evaluating the effects of fluorine on biological properties and metabolic stability of some antitubulin 3-substituted 7-phenyl-pyrroloquinolinones. European Journal of Medicinal Chemistry, 2019, 178, 297-314.	2.6	10
30	Coupling Supervised Molecular Dynamics (SuMD) with Entropy Estimations To Shine Light on the Stability of Multiple Binding Sites. ACS Medicinal Chemistry Letters, 2019, 10, 444-449.	1.3	5
31	Polyamine-Based Thiols in Trypanosomatids: Evolution, Protein Structural Adaptations, and Biological Functions. Antioxidants and Redox Signaling, 2018, 28, 463-486.	2.5	27
32	Combining self- and cross-docking as benchmark tools: the performance of DockBench in the D3R Grand Challenge 2. Journal of Computer-Aided Molecular Design, 2018, 32, 251-264.	1.3	26
33	AquaMMapS: An Alternative Tool to Monitor the Role of Water Molecules During Proteinâ€“Ligand Association. ChemMedChem, 2018, 13, 522-531.	1.6	29
34	Targeting tubulin polymerization by novel 7-aryl-pyrroloquinolinones: Synthesis, biological activity and SARs. European Journal of Medicinal Chemistry, 2018, 143, 244-258.	2.6	8
35	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. Journal of Enzyme Inhibition and Medicinal Chemistry, 2018, 33, 171-183.	2.5	5
36	The lineage-specific, intrinsically disordered N-terminal extension of monothiol glutaredoxin 1 from trypanosomes contains a regulatory region. Scientific Reports, 2018, 8, 13716.	1.6	4

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37	Targeting Protein Kinase CK1Î´ 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?. ChemMedChem, 2018, 13, 2601-2605.	1.6	16
38	Supervised Molecular Dynamics (SuMD) Approaches in Drug Design. Methods in Molecular Biology, 2018, 1824, 287-298.	0.4	18
39	Binding mode of AIF(370â€“394) peptide to CypA: insights from NMR, label-free and molecular docking studies. Biochemical Journal, 2018, 475, 2377-2393.	1.7	8
40	The role of 5-arylalkylamino- and 5-piperazino- moieties on the 7-aminopyrazolo[4,3-d]pyrimidine core in affecting adenosine A₁ and A_{2A} receptor affinity and selectivity profiles. Journal of Enzyme Inhibition and Medicinal Chemistry, 2017, 32, 248-263.	2.5	14
41	Exploring Protein-Peptide Recognition Pathways Using a Supervised Molecular Dynamics Approach. Structure, 2017, 25, 655-662.e2.	1.6	67
42	Sulfonamido-derivatives of unsubstituted carbazoles as BACE1 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 4812-4816.	1.0	9
43	Synthesis, structure-activity relationships and biological evaluation ofÂ7-phenyl-pyrroloquinolinone 3-amide derivatives as potent antimitotic agents. European Journal of Medicinal Chemistry, 2017, 127, 643-660.	2.6	13
44	A molecular dynamics strategy for CSÎ±Î² peptides disulfide-assisted model refinement. Journal of Biomolecular Structure and Dynamics, 2017, 35, 2736-2744.	2.0	1
45	Synthesis, biological evaluation and molecular modeling studies of phthalazin-1(2H)-one derivatives as novel cholinesterase inhibitors. RSC Advances, 2016, 6, 46170-46185.	1.7	22
46	In Silico 3D Modeling of Binding Activities. Methods in Molecular Biology, 2016, 1425, 23-35.	0.4	4
47	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.	1.4	3
48	DockBench as docking selector tool: the lesson learned from D3R Grand Challenge 2015. Journal of Computer-Aided Molecular Design, 2016, 30, 773-789.	1.3	13
49	FRET-Protease-Coupled Peptidyl-Prolyl cis-trans Isomerase Assay. Journal of Biomolecular Screening, 2016, 21, 701-712.	2.6	7
50	Deciphering the Complexity of Ligandâ€“Protein Recognition Pathways Using Supervised Molecular Dynamics (SuMD) Simulations. Journal of Chemical Information and Modeling, 2016, 56, 687-705.	2.5	88
51	1H, 13C and 15N resonance assignment of the cytosolic dithiol glutaredoxin 1 from the pathogen Trypanosoma brucei. Biomolecular NMR Assignments, 2016, 10, 85-88.	0.4	5
52	NMRâ€Assisted Molecular Docking Methodologies. Molecular Informatics, 2015, 34, 513-525.	1.4	14
53	DockBench: An Integrated Informatic Platform Bridging the Gap between the Robust Validation of Docking Protocols and Virtual Screening Simulations. Molecules, 2015, 20, 9977-9993.	1.7	40
54	1H, 13C and 15N resonance assignment of the mature form of monothiol glutaredoxin 1 from the pathogen Trypanosoma brucei. Biomolecular NMR Assignments, 2015, 9, 143-146.	0.4	5

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55	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. PLoS ONE, 2015, 10, e0143504.	1.1	6
56	Molecular architecture and the structural basis for anion interaction in prestin and SLC26 transporters. Nature Communications, 2014, 5, 3622.	5.8	74
57	Ironâ€“Sulfur Cluster Binding by Mitochondrial Monothiol Glutaredoxin-1 ofTrypanosoma brucei: Molecular Basis of Ironâ€“Sulfur Cluster Coordination and Relevance for Parasite Infectivity. Antioxidants and Redox Signaling, 2013, 19, 665-682.	2.5	37
58	A Structural Model for Prestin and Related SLC26 Anion Transporters. Biophysical Journal, 2013, 104, 112a.	0.2	0
59	Dopamine-derived Quinones Affect the Structure of the Redox Sensor DJ-1 through Modifications at Cys-106 and Cys-53. Journal of Biological Chemistry, 2012, 287, 18738-18749.	1.6	61
60	Design, conformational studies and analysis of structureâ€“function relationships of PTH (1â€“11) analogues: the essential role of Val in position 2. Amino Acids, 2012, 43, 207-218.	1.2	6
61	Identification of a Novel Mcl-1 Protein Binding Motif. Journal of Biological Chemistry, 2011, 286, 39829-39835.	1.6	34
62	Abstract 8: Identification of a non-canonical BH3 peptide that binds the BH3 pocket of Mcl-1. , 2011, , .		0
63	Synthesis and structural studies of new analogues of PTH(1â€“11) containing CÎ±-tetra-substituted amino acids in position 8. Amino Acids, 2010, 39, 1369-1379.	1.2	8
64	Side Chain Cyclization Based on Serine Residues: Synthesis, Structure, and Activity of a Novel Cyclic Analogue of the Parathyroid Hormone Fragment 1â¯11â€. Journal of Medicinal Chemistry, 2010, 53, 8072-8079.	2.9	20
65	MMsINC: a large-scale chemoinformatics database. Nucleic Acids Research, 2009, 37, D284-D290.	6.5	71
66	SAR and QSAR study on 2-aminothiazole derivatives, modulators of transcriptional repression in Huntingtonâ€™s disease. Bioorganic and Medicinal Chemistry, 2008, 16, 5695-5703.	1.4	49
67	Implementing a Scoring Function Based on Interaction Fingerprint for Autogrow4: Protein Kinase CK1Î´ as a Case Study. Frontiers in Molecular Biosciences, 0, 9, .	1.6	11