Mattia Sturlese

List of Publications by Year
in descending order

67 papers	**1,252** citations	430874 **18** h-index	434195 **31** g-index
74 all docs	**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. Journal of Chemical Information and Modeling, 2016, 56, 687-705.	5.4	88
2	Molecular architecture and the structural basis for anion interaction in prestin and SLC26 transporters. Nature Communications, 2014, 5, 3622.	12.8	74
3	MMsINC: a large-scale chemoinformatics database. Nucleic Acids Research, 2009, 37, D284-D290.	14.5	71
4	Exploring Protein-Peptide Recognition Pathways Using a Supervised Molecular Dynamics Approach. Structure, 2017, 25, 655-662.e2.	3.3	67
5	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.	3.4	61
6	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.	5.2	60
7	SAR and QSAR study on 2-aminothiazole derivatives, modulators of transcriptional repression in Huntington's disease. Bioorganic and Medicinal Chemistry, 2008, 16, 5695-5703.	3.0	49
8	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.	3.3	44
9	DockBench: An Integrated Informatic Platform Bridging the Gap between the Robust Validation of Docking Protocols and Virtual Screening Simulations. Molecules, 2015, 20, 9977-9993.	3.8	40
10	Iron–Sulfur Cluster Binding by Mitochondrial Monothiol Glutaredoxin-1 of *Trypanosoma brucei*: Molecular Basis of Iron–Sulfur Cluster Coordination and Relevance for Parasite Infectivity. Antioxidants and Redox Signaling, 2013, 19, 665-682.	5.4	37
11	Identification of a Novel Mcl-1 Protein Binding Motif. Journal of Biological Chemistry, 2011, 286, 39829-39835.	3.4	34
12	AquaMMapS: An Alternative Tool to Monitor the Role of Water Molecules During Protein–Ligand Association. ChemMedChem, 2018, 13, 522-531.	3.2	29
13	The rise of molecular simulations in fragment-based drug design (FBDD): an overview. Drug Discovery Today, 2020, 25, 1693-1701.	6.4	29
14	Polyamine-Based Thiols in Trypanosomatids: Evolution, Protein Structural Adaptations, and Biological Functions. Antioxidants and Redox Signaling, 2018, 28, 463-486.	5.4	27
15	Novel coumarin-pyridazine hybrids as selective MAO-B inhibitors for the Parkinson's disease therapy. Bioorganic Chemistry, 2020, 104, 104203.	4.1	27
16	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.	2.9	26
17	Synthesis, biological evaluation and molecular modeling studies of phthalazin-1(2H)-one derivatives as novel cholinesterase inhibitors. RSC Advances, 2016, 6, 46170-46185.	3.6	22
18	Computationally driven discovery of SARS-CoV-2 M^{pro} inhibitors: from design to experimental validation. Chemical Science, 2022, 13, 3674-3687.	7.4	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 1â´'11â€. Journal of Medicinal Chemistry, 2010, 53, 8072-8079.	6.4	20
20	Supervised Molecular Dynamics (SuMD) Approaches in Drug Design. Methods in Molecular Biology, 2018, 1824, 287-298.	0.9	18
21	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.	4.1	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. Pharmaceuticals, 2022, 15, 180.	3.8	18
23	A Deep-Learning Approach toward Rational Molecular Docking Protocol Selection. Molecules, 2020, 25, 2487.	3.8	17
24	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.	3.2	16
25	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.	3.6	16
26	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.	4.1	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?. Journal of Enzyme Inhibition and Medicinal Chemistry, 2022, 37, 1704-1714.	5.2	15
28	NMRâ€Assisted Molecular Docking Methodologies. Molecular Informatics, 2015, 34, 513-525.	2.5	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. Journal of Enzyme Inhibition and Medicinal Chemistry, 2017, 32, 248-263.	5.2	14
30	Can We Still Trust Docking Results? An Extension of the Applicability of DockBench on PDBbind Database. International Journal of Molecular Sciences, 2019, 20, 3558.	4.1	14
31	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.	3.8	14
32	DockBench as docking selector tool: the lesson learned from D3R Grand Challenge 2015. Journal of Computer-Aided Molecular Design, 2016, 30, 773-789.	2.9	13
33	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.	5.5	13
34	A new inactive conformation of SARS-CoV-2 main protease. Acta Crystallographica Section D: Structural Biology, 2022, 78, 363-378.	2.3	13
35	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.	3.2	12
36	Implementing a Scoring Function Based on Interaction Fingerprint for Autogrow4: Protein Kinase CK1Î´ as a Case Study. Frontiers in Molecular Biosciences, 0, 9, .	3.5	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. European Journal of Medicinal Chemistry, 2019, 178, 297-314.	5.5	10
38	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.	5.2	10
39	Ribose and Non-Ribose A2A Adenosine Receptor Agonists: Do They Share the Same Receptor Recognition Mechanism?. Biomedicines, 2022, 10, 515.	3.2	10
40	Sulfonamido-derivatives of unsubstituted carbazoles as BACE1 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 4812-4816.	2.2	9
41	Scaffold Repurposing of in-House Chemical Library toward the Identification of New Casein Kinase 1 δ Inhibitors. ACS Medicinal Chemistry Letters, 2020, 11, 1168-1174.	2.8	9
42	Synthesis and structural studies of new analogues of PTH(1–11) containing Cα-tetra-substituted amino acids in position 8. Amino Acids, 2010, 39, 1369-1379.	2.7	8
43	Targeting tubulin polymerization by novel 7-aryl-pyrroloquinolinones: Synthesis, biological activity and SARs. European Journal of Medicinal Chemistry, 2018, 143, 244-258.	5.5	8
44	Binding mode of AIF(370–394) peptide to CypA: insights from NMR, label-free and molecular docking studies. Biochemical Journal, 2018, 475, 2377-2393.	3.7	8
45	Sodium or Not Sodium: Should Its Presence Affect the Accuracy of Pose Prediction in Docking GPCR Antagonists?. Pharmaceuticals, 2022, 15, 346.	3.8	8
46	FRET-Protease-Coupled Peptidyl-Prolyl cis-trans Isomerase Assay. Journal of Biomolecular Screening, 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. Amino Acids, 2012, 43, 207-218.	2.7	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. PLoS ONE, 2015, 10, e0143504.	2.5	6
49	The Multifaceted Role of GPCRs in Amyotrophic Lateral Sclerosis: A New Therapeutic Perspective?. International Journal of Molecular Sciences, 2022, 23, 4504.	4.1	6
50	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.	0.8	5
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.	0.8	5
52	Synthesis and preliminary structure-activity relationship study of 2-aryl-2*H*-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.	5.2	5
53	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.	2.8	5
54	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.	2.4	5

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55	New Insights into Key Determinants for Adenosine 1 Receptor Antagonists Selectivity Using Supervised Molecular Dynamics Simulations. Biomolecules, 2020, 10, 732.	4.0	5
56	Shedding Light on the Molecular Recognition of Sub-Kilodalton Macrocyclic Peptides on Thrombin by Supervised Molecular Dynamics. Frontiers in Molecular Biosciences, 2021, 8, 707661.	3.5	5
57	Pyridazinones containing dithiocarbamoyl moieties as a new class of selective MAO-B inhibitors. Bioorganic Chemistry, 2021, 115, 105203.	4.1	5
58	In Silico 3D Modeling of Binding Activities. Methods in Molecular Biology, 2016, 1425, 23-35.	0.9	4
59	The lineage-specific, intrinsically disordered N-terminal extension of monothiol glutaredoxin 1 from trypanosomes contains a regulatory region. Scientific Reports, 2018, 8, 13716.	3.3	4
60	Targeting G Protein–Coupled Receptors with Magnetic Carbon Nanotubes: The Case of the A 3 Adenosine Receptor. ChemMedChem, 2020, 15, 1909-1920.	3.2	4
61	Comparing Fragment Binding Poses Prediction Using HSP90 as a Key Study: When Bound Water Makes the Difference. Molecules, 2020, 25, 4651.	3.8	4
62	Bat coronaviruses related to SARS-CoV-2: what about their 3CL proteases (MPro)?. Journal of Enzyme Inhibition and Medicinal Chemistry, 2022, 37, 1077-1082.	5.2	4
63	New Trends in Inspecting GPCR–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
64	Comparative Molecular Dynamics Investigation of the Electromotile Hearing Protein Prestin. International Journal of Molecular Sciences, 2021, 22, 8318.	4.1	2
65	A molecular dynamics strategy for CSÎ±Î² peptides disulfide-assisted model refinement. Journal of Biomolecular Structure and Dynamics, 2017, 35, 2736-2744.	3.5	1
66	A Structural Model for Prestin and Related SLC26 Anion Transporters. Biophysical Journal, 2013, 104, 112a.	0.5	0
67	Abstract 8: Identification of a non-canonical BH3 peptide that binds the BH3 pocket of Mcl-1. , 2011, , .		0