Andrea R Beccari

List of Publications by Year
in descending order

23	1,061	623188	610482
papers	citations	14 h-index	24 g-index

29	29	29	1871
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	X-ray screening identifies active site and allosteric inhibitors of SARS-CoV-2 main protease. Science, 2021, 372, 642-646.	6.0	240
2	Targeting SARS-CoV-2 Proteases and Polymerase for COVID-19 Treatment: State of the Art and Future Opportunities. Journal of Medicinal Chemistry, 2022, 65, 2716-2746.	2.9	149
3	Identification of Inhibitors of SARS-CoV-2 3CL-Pro Enzymatic Activity Using a Small Molecule in Vitro Repurposing Screen. ACS Pharmacology and Translational Science, 2021, 4, 1096-1110.	2.5	101
4	PARP1-produced poly-ADP-ribose causes the PARP12 translocation to stress granules and impairment of Golgi complex functions. Scientific Reports, 2017, 7, 14035.	1.6	76
5	SARS-CoV-2 Entry Inhibitors: Small Molecules and Peptides Targeting Virus or Host Cells. International Journal of Molecular Sciences, 2020, 21, 5707.	1.8	58
6	Targeting the minor pocket of C5aR for the rational design of an oral allosteric inhibitor for inflammatory and neuropathic pain relief. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 16937-16942.	3.3	56
7	Computational Studies of SARS-CoV-2 3CLpro: Insights from MD Simulations. International Journal of Molecular Sciences, 2020, 21, 5346.	1.8	48
8	LiGen: A High Performance Workflow for Chemistry Driven de Novo Design. Journal of Chemical Information and Modeling, 2013, 53, 1518-1527.	2.5	45
9	A Blueprint for High Affinity SARS-CoV-2 Mpro Inhibitors from Activity-Based Compound Library Screening Guided by Analysis of Protein Dynamics. ACS Pharmacology and Translational Science, 2021, 4, 1079-1095.	2.5	44
10	Natural Compounds Inhibit SARS-CoV-2 nsp13 Unwinding and ATPase Enzyme Activities. ACS Pharmacology and Translational Science, 2022, 5, 226-239.	2.5	43
11	A Comprehensive Mapping of the Druggable Cavities within the SARS-CoV-2 Therapeutically Relevant Proteins by Combining Pocket and Docking Searches as Implemented in Pockets 2.0. International Journal of Molecular Sciences, 2020, 21, 5152.	1.8	34
12	Use of Experimental Design To Optimize Docking Performance: The Case of LiGenDock, the Docking Module of Ligen, a New De Novo Design Program. Journal of Chemical Information and Modeling, 2013, 53, 1503-1517.	2.5	28
13	Novel selective, potent naphthyl TRPM8 antagonists identified through a combined ligand- and structure-based virtual screening approach. Scientific Reports, 2017, 7, 10999.	1.6	23
14	ADPredict: ADP-ribosylation site prediction based on physicochemical and structural descriptors. Bioinformatics, 2018, 34, 2566-2574.	1.8	17
15	Cytopathic SARS-CoV-2 screening on VERO-E6 cells in a large-scale repurposing effort. Scientific Data, 2022, 9, .	2.4	17
16	PKD-dependent PARP12-catalyzed mono-ADP-ribosylation of Golgin-97 is required for E-cadherin transport from Golgi to plasma membrane. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	16
17	Combining Molecular Dynamics and Docking Simulations to Develop Targeted Protocols for Performing Optimized Virtual Screening Campaigns on the hTRPM8 Channel. International Journal of Molecular Sciences, 2020, 21, 2265.	1.8	15
18	Combining Different Docking Engines and Consensus Strategies to Design and Validate Optimized Virtual Screening Protocols for the SARS-CoV-2 3CL Protease. Molecules, 2021, 26, 797.	1.7	14

#	Article	IF	Citations
19	â€œMolecular Anatomyâ€: a new multi-dimensional hierarchical scaffold analysis tool. Journal of Cheminformatics, 2021, 13, 54.	2.8	12
20	Altered Local Interactions and Long-Range Communications in UK Variant (B.1.1.7) Spike Glycoprotein. International Journal of Molecular Sciences, 2021, 22, 5464.	1.8	9
21	Characterization of raloxifene as a potential pharmacological agent against SARS-CoV-2 and its variants. Cell Death and Disease, 2022, 13, .	2.7	9
22	Binding Mode Exploration of B1 Receptor Antagonistsâ€™ by the Use of Molecular Dynamics and Docking Simulationâ€”How Different Target Engagement Can Determine Different Biological Effects. International Journal of Molecular Sciences, 2020, 21, 7677.	1.8	2
23	Extensive Sampling of Molecular Dynamics Simulations to Identify Reliable Protein Structures for Optimized Virtual Screening Studies: The Case of the hTRPM8 Channel. International Journal of Molecular Sciences, 2022, 23, 7558.	1.8	1