Andrea R Beccari

List of Publications by Year
in descending order

23 papers	1,061 citations	623188 14 h-index	610482 24 g-index
29 all docs	29 docs citations	29 times ranked	1871 citing authors

#	Article	IF	Citations
1	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
2	Natural Compounds Inhibit SARS-CoV-2 nsp13 Unwinding and ATPase Enzyme Activities. ACS Pharmacology and Translational Science, 2022, 5, 226-239.	2.5	43
3	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
4	Characterization of raloxifene as a potential pharmacological agent against SARS-CoV-2 and its variants. Cell Death and Disease, 2022, 13, .	2.7	9
5	Cytopathic SARS-CoV-2 screening on VERO-E6 cells in a large-scale repurposing effort. Scientific Data, 2022, 9, .	2.4	17
6	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
7	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
8	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
9	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
10	X-ray screening identifies active site and allosteric inhibitors of SARS-CoV-2 main protease. Science, 2021, 372, 642-646.	6.0	240
11	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
12	"Molecular Anatomy" a new multi-dimensional hierarchical scaffold analysis tool. Journal of Cheminformatics, 2021, 13, 54.	2.8	12
13	Computational Studies of SARS-CoV-2 3CLpro: Insights from MD Simulations. International Journal of Molecular Sciences, 2020, 21, 5346.	1.8	48
14	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
15	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
16	Binding Mode Exploration of B1 Receptor Antagonists' by the Use of Molecular Dynamics and Docking Simulation—How Different Target Engagement Can Determine Different Biological Effects. International Journal of Molecular Sciences, 2020, 21, 7677.	1.8	2
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	ADPredict: ADP-ribosylation site prediction based on physicochemical and structural descriptors. Bioinformatics, 2018, 34, 2566-2574.	1.8	17

#	Article	IF	Citations
19	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
20	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
21	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
22	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
23	LiGen: A High Performance Workflow for Chemistry Driven de Novo Design. Journal of Chemical Information and Modeling, 2013, 53, 1518-1527.	2.5	45