Andrea R Beccari

List of Publications by Year in Descending Order

20 papers	474 citations	12 h-index	21 g-index
29 ext. papers	765 ext. citations	7.9 avg, IF	3.79 L-index

#	Paper	IF	Citations
20	Natural Compounds Inhibit SARS-CoV-2 nsp13 Unwinding and ATPase Enzyme Activities.. *ACS Pharmacology and Translational Science*, **2022**, 5, 226-239	5.9	5
19	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,	11.5	3
18	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	5.9	15
17	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	5.9	31
16	X-ray screening identifies active site and allosteric inhibitors of SARS-CoV-2 main protease. *Science*, **2021**, 372, 642-646	33.3	95
15	"Molecular Anatomy": a new multi-dimensional hierarchical scaffold analysis tool. *Journal of Cheminformatics*, **2021**, 13, 54	8.6	2
14	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,	4.8	5
13	Binding Mode Exploration of B1 Receptor Antagonistsaby the Use of Molecular Dynamics and Docking Simulation-How Different Target Engagement Can Determine Different Biological Effects. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	2
12	Targeting SARS-CoV-2 Proteases and Polymerase for COVID-19 Treatment: State of the Art and Future Opportunities. *Journal of Medicinal Chemistry*, **2020**,	8.3	57
11	Computational Studies of SARS-CoV-2 3CLpro: Insights from MD Simulations. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	29
10	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,	6.3	17
9	SARS-CoV-2 Entry Inhibitors: Small Molecules and Peptides Targeting Virus or Host Cells. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	35
8	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,	6.3	9
7	ADPredict: ADP-ribosylation site prediction based on physicochemical and structural descriptors. *Bioinformatics*, **2018**, 34, 2566-2574	7.2	10
6	PARP1-produced poly-ADP-ribose causes the PARP12 translocation to stress granules and impairment of Golgi complex functions. *Scientific Reports*, **2017**, 7, 14035	4.9	49
5	Novel selective, potent naphthyl TRPM8 antagonists identified through a combined ligand- and structure-based virtual screening approach. *Scientific Reports*, **2017**, 7, 10999	4.9	14
4	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, 16937-42	11.5	44

3	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, 1503-17	6.1	18
2	LiGen: a high performance workflow for chemistry driven de novo design. *Journal of Chemical Information and Modeling*, **2013**, 53, 1518-27	6.1	29
1	Identification of inhibitors of SARS-CoV-2 3CL-Pro enzymatic activity using a small molecule in-vitro repurposing screen		1