Carmine Talarico

List of Publications by Year in descending order

23 papers	558 citations	623188 14 h-index	642321 23 g-index
28 all docs	28 docs citations	28 times ranked	994 citing authors

#	Article	IF	Citations
1	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
2	Computational Studies of SARS-CoV-2 3CLpro: Insights from MD Simulations. International Journal of Molecular Sciences, 2020, 21, 5346.	1.8	48
3	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
4	Natural Compounds Inhibit SARS-CoV-2 nsp13 Unwinding and ATPase Enzyme Activities. ACS Pharmacology and Translational Science, 2022, 5, 226-239.	2.5	43
5	Repurposing the estrogen receptor modulator raloxifene to treat SARS-CoV-2 infection. Cell Death and Differentiation, 2022, 29, 156-166.	5.0	38
6	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
7	Identification of G-quadruplex DNA/RNA binders: Structure-based virtual screening and biophysical characterization. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 1329-1340.	1.1	33
8	Novel natural non-nucleoside inhibitors of HIV-1 reverse transcriptase identified by shape- and structure-based virtual screening techniques. European Journal of Medicinal Chemistry, 2019, 161, 1-10.	2.6	31
9	Molecular recognition of a carboxy pyridostatin toward Gâ€quadruplex structures: Why does it prefer <scp>RNA</scp>?. Chemical Biology and Drug Design, 2017, 90, 919-925.	1.5	25
10	In Silico Identification of Piperidinyl-amine Derivatives as Novel Dual Binders of Oncogene c-myc/c-Kit G-quadruplexes. ACS Medicinal Chemistry Letters, 2018, 9, 848-853.	1.3	19
11	Molecular modelling of epitopes recognized by neoplastic B lymphocytes in Chronic Lymphocytic Leukemia. European Journal of Medicinal Chemistry, 2020, 185, 111838.	2.6	17
12	Computer-based techniques for lead identification and optimization I: Basics. Physical Sciences Reviews, 2019, 4, .	0.8	16
13	A Comparative Docking Strategy to Identify Polyphenolic Derivatives as Promising Antineoplastic Binders of Gâ€quadruplex DNA câ€myc and bclâ€2 Sequences. Molecular Informatics, 2016, 35, 391-402.	1.4	15
14	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
15	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
16	Pathway involving the N155H mutation in HIV-1 integrase leads to dolutegravir resistance. Journal of Antimicrobial Chemotherapy, 2018, 73, 1158-1166.	1.3	13
17	The Mu.Ta.Lig. Chemotheca: A Community-Populated Molecular Database for Multi-Target Ligands Identification and Compound-Repurposing. Frontiers in Chemistry, 2018, 6, 130.	1.8	13
18	Realâ€life 3D therapy failure: Analysis of NS5A 93H RAS plus 108 K polymorphism in complex with ombitasvir by molecular modeling. Journal of Medical Virology, 2018, 90, 1257-1263.	2.5	9

#	Article	IF	Citations
19	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
20	Characterization of raloxifene as a potential pharmacological agent against SARS-CoV-2 and its variants. Cell Death and Disease, 2022, 13, .	2.7	9
21	Structural Modeling of New Polymorphism Clusters of HCV Polymerase Isolated from Directâ€Acting Antiviral NaÃ¯ve Patients: Focus on Dasabuvir and Setrobuvir Binding Affinity. ChemistrySelect, 2018, 3, 6009-6017.	0.7	7
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