Carmine Talarico

List of Publications by Year in Descending Order

21 papers	259 citations	10 h-index	15 g-index
28 ext. papers	406 ext. citations	6.1 avg, IF	3.09 L-index

#	Paper	IF	Citations
21	Natural Compounds Inhibit SARS-CoV-2 nsp13 Unwinding and ATPase Enzyme Activities.. *ACS Pharmacology and Translational Science*, **2022**, 5, 226-239	5.9	5
20	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
19	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
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,	4.8	5
17	Repurposing the estrogen receptor modulator raloxifene to treat SARS-CoV-2 infection. *Cell Death and Differentiation*, **2021**,	12.7	6
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,	6.3	2
15	Molecular modelling of epitopes recognized by neoplastic B lymphocytes in Chronic Lymphocytic Leukemia. *European Journal of Medicinal Chemistry*, **2020**, 185, 111838	6.8	12
14	Computational Studies of SARS-CoV-2 3CLpro: Insights from MD Simulations. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	29
13	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
12	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
11	Computer-based techniques for lead identification and optimization I: Basics. *Physical Sciences Reviews*, **2019**, 4,	1.4	10
10	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	6.8	23
9	Real-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	19.7	6
8	Pathway involving the N155H mutation in HIV-1 integrase leads to dolutegravir resistance. *Journal of Antimicrobial Chemotherapy*, **2018**, 73, 1158-1166	5.1	8
7	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	4.3	13
6	The Mu.Ta.Lig. Chemotheca: A Community-Populated Molecular Database for Multi-Target Ligands Identification and Compound-Repurposing. *Frontiers in Chemistry*, **2018**, 6, 130	5	6
5	Structural Modeling of New Polymorphism Clusters of HCV Polymerase Isolated from Direct-Acting Antiviral Naïve Patients: Focus on Dasabuvir and Setrobuvir Binding Affinity. *ChemistrySelect*, **2018**, 3, 6009-6017	1.8	5

List of Publications

4	Molecular recognition of a carboxy pyridostatin toward G-quadruplex structures: Why does it prefer RNA?. *Chemical Biology and Drug Design*, **2017**, 90, 919-925	2.9	18
3	Identification of G-quadruplex DNA/RNA binders: Structure-based virtual screening and biophysical characterization. *Biochimica Et Biophysica Acta - General Subjects*, **2017**, 1861, 1329-1340	4	25
2	A Comparative Docking Strategy to Identify Polyphenolic Derivatives as Promising Antineoplastic Binders of G-quadruplex DNA c-myc and bcl-2 Sequences. *Molecular Informatics*, **2016**, 35, 391-402	3.8	12
1	Identification of inhibitors of SARS-CoV-2 3CL-Pro enzymatic activity using a small molecule in-vitro repurposing screen		1