Eleni Vrontaki

List of Publications by Year
in descending order

17	168	1163117 8	1125743 13
papers	citations	h-index	g-index

19	19	19	328
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Searching for anthranilic acid-based thumb pocket 2 HCV NS5B polymerase inhibitors through a combination of molecular docking, 3D-QSAR and virtual screening. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 38-52.	5.2	30
2	Discovery of Novel Adenosine Receptor Antagonists through a Combined Structure- and Ligand-Based Approach Followed by Molecular Dynamics Investigation of Ligand Binding Mode. Journal of Chemical Information and Modeling, 2018, 58, 794-815.	5.4	22
3	Exploiting ChEMBL database to identify indole analogs as HCV replication inhibitors. Methods, 2015, 71, 4-13.	3.8	20
4	Pharmacological characterisation of novel adenosine A3 receptor antagonists. Scientific Reports, 2020, 10, 20781.	3.3	16
5	Insights to the Binding of a Selective Adenosine A₃ Receptor Antagonist Using Molecular Dynamic Simulations, MM-PBSA and MM-GBSA Free Energy Calculations, and Mutagenesis. Journal of Chemical Information and Modeling, 2019, 59, 5183-5197.	5.4	15
6	Synthetic Analogues of Aminoadamantane as Influenza Viral Inhibitorsâ€"In Vitro, In Silico and QSAR Studies. Molecules, 2020, 25, 3989.	3.8	10
7	Development of a Predictive Pharmacophore Model and a 3D-QSAR Study for an in silico Screening of New Potent Bcr-Abl Kinase Inhibitors. Mini-Reviews in Medicinal Chemistry, 2017, 17, 188-204.	2.4	10
8	Searching for Novel Janus Kinase-2 Inhibitors Using a Combination of Pharmacophore Modeling, 3D-QSAR Studies and Virtual Screening. Mini-Reviews in Medicinal Chemistry, 2017, 17, 268-294.	2.4	9
9	Structural Characterization of Agonist Binding to an A₃ Adenosine Receptor through Biomolecular Simulations and Mutagenesis Experiments. Journal of Medicinal Chemistry, 2019, 62, 8831-8846.	6.4	8
10	Integrating computational methods to predict mutagenicity of aromatic azo compounds. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2017, 35, 239-257.	2.9	7
11	Pharmacophore Generation and 3D-QSAR Model Development Using PHASE. Methods in Molecular Biology, 2018, 1824, 387-401.	0.9	5
12	Drug Delivery Systems Based on Modified Polysaccharides: Synthesis and. Methods in Molecular Biology, 2021, 2207, 151-161.	0.9	4
13	Stability and binding effects of silver(I) complexes at lipoxygenase-1. Journal of Enzyme Inhibition and Medicinal Chemistry, 2015, 30, 539-549.	5.2	3
14	Conformational analysis of two novel cytotoxic C2-substituted pyrrolo[2,3-f]quinolines in aqueous media, organic solvents, membrane bilayers and at the putative active site. Bioorganic and Medicinal Chemistry, 2012, 20, 6276-6284.	3.0	1
15	Quantitative Nanostructure-Activity Relationship Models for the Risk Assessment of NanoMaterials. , 2017, , 1314-1338.		1
16	Quantitative Nanostructure-Activity Relationship Models for the Risk Assessment of NanoMaterials. Advances in Chemical and Materials Engineering Book Series, 2015, , 535-559.	0.3	0
17	Quantitative Nanostructure-Activity Relationship Models for the Risk Assessment of NanoMaterials. , 2017, , 20-44.		0