Georgios Leonis

List of Publications by Year
in descending order

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33	574	623734	610901
papers	citations	14	24
		h-index	g-index

33	33	33	1003
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Losartan Interactions with 2-Hydroxypropyl-Î²-CD. Molecules, 2022, 27, 2421.	3.8	4
2	Application of Neutralization and Technique for the Preparation of the BeneficialÂin Drug 2-Hydroxypropyl-Î²-Cyclodextrin with. Methods in Molecular Biology, 2021, 2207, 1-11.	0.9	2
3	Applications of NMR in Drug:Cyclodextrin. Methods in Molecular Biology, 2021, 2207, 313-325.	0.9	0
4	Molecular Protocols for the Study of Cyclodextrin Drug Systems. Methods in Molecular Biology, 2021, 2207, 109-125.	0.9	0
5	Discovery of a stable tripeptide targeting the N-domain of CRF1 receptor. Amino Acids, 2020, 52, 1337-1351.	2.7	0
6	Antihypertensive activity and molecular interactions of irbesartan in complex with 2â€hydroxypropylâ€Î²â€cyclodextrin. Chemical Biology and Drug Design, 2020, 96, 668-683.	3.2	6
7	Hostâ€“Guest Interactions between Candesartan and Its Prodrug Candesartan Cilexetil in Complex with 2-Hydroxypropyl-Î²-cyclodextrin: On the Biological Potency for Angiotensin II Antagonism. Molecular Pharmaceutics, 2019, 16, 1255-1271.	4.6	17
8	Vinblastine. Advances in Biomembranes and Lipid Self-Assembly, 2019, 29, 127-157.	0.6	2
9	Diabetic skin and UV light: Protection by antioxidants. European Journal of Pharmaceutical Sciences, 2019, 127, 1-8.	4.0	14
10	Topical Treatment of Skin Injury Inflicted in Mice by X-Ray Irradiation. Skin Pharmacology and Physiology, 2018, 31, 175-183.	2.5	10
11	Consensus Predictive Model for Human K562 Cell Growth Inhibition through Enalos Cloud Platform. ChemMedChem, 2018, 13, 555-563.	3.2	2
12	In Silico Discovery of Plant-Origin Natural Product Inhibitors of Tumor Necrosis Factor (TNF) and Receptor Activator of NF-ÎºB Ligand (RANKL). Frontiers in Pharmacology, 2018, 9, 800.	3.5	17
13	Current Status and Future Prospects of Smallâ€“molecule Proteinâ€“protein Interaction (PPI) Inhibitors of Tumor Necrosis Factor (TNF) and Receptor Activator of NF-ÎºB Ligand (RANKL). Current Topics in Medicinal Chemistry, 2018, 18, 661-673.	2.1	13
14	Computational investigation of fullerene-DNA interactions: Implications of fullereneâ€™s size and functionalization on DNA structure and binding energetics. Journal of Molecular Graphics and Modelling, 2017, 74, 177-192.	2.4	6
15	Compilation of Data and Modelling of Nanoparticle Interactions and Toxicity in the NanoPUZZLES Project. Advances in Experimental Medicine and Biology, 2017, 947, 303-324.	1.6	8
16	Strategy for Identification of Nanomaterialsâ€™ Critical Properties Linked to Biological Impacts: Interlinking of Experimental and Computational Approaches. Challenges and Advances in Computational Chemistry and Physics, 2017, , 385-424.	0.6	5
17	Cheminformatics-aided discovery of small-molecule Protein-Protein Interaction (PPI) dual inhibitors of Tumor Necrosis Factor (TNF) and Receptor Activator of NF-ÎºB Ligand (RANKL). PLoS Computational Biology, 2017, 13, e1005372.	3.2	49
18	Discovery of HIV Typeâ€…1 Aspartic Protease Hit Compounds through Combined Computational Approaches. ChemMedChem, 2016, 11, 1646-1652.	3.2	3

#	Article	IF	Citations
19	Development of a potent 2-oxoamide inhibitor of secreted phospholipase A2 guided by molecular docking calculations and molecular dynamics simulations. Bioorganic and Medicinal Chemistry, 2016, 24, 1683-1695.	3.0	23
20	Biological and computational evaluation of resveratrol inhibitors against Alzheimerâ€™s disease. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 67-77.	5.2	32
21	Investigation of the Interactions of Silibinin with 2-Hydroxypropyl-Î²-cyclodextrin through Biophysical Techniques and Computational Methods. Molecular Pharmaceutics, 2015, 12, 954-965.	4.6	55
22	A Comprehensive Computational Study of the Interaction between Human Serum Albumin and Fullerenes. Journal of Physical Chemistry B, 2015, 119, 14971-14985.	2.6	22
23	Elucidation of the binding mechanism of renin using a wide array of computational techniques and biological assays. Journal of Molecular Graphics and Modelling, 2015, 62, 138-149.	2.4	3
24	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
25	Systematic Molecular Dynamics, MMâ€“PBSA, and Ab Initio Approaches to the Saquinavir Resistance Mechanism in HIV-1 PR Due to 11 Double and Multiple Mutations. Journal of Physical Chemistry B, 2014, 118, 9538-9552.	2.6	14
26	Elucidation of Conformational States, Dynamics, and Mechanism of Binding in Human Îº-Opioid Receptor Complexes. Journal of Chemical Information and Modeling, 2014, 54, 2294-2308.	5.4	25
27	A Contribution to the Drug Resistance Mechanism of Darunavir, Amprenavir, Indinavir, and Saquinavir Complexes with HIV-1 Protease Due to Flap Mutation I50V: A Systematic MMâ€“PBSA and Thermodynamic Integration Study. Journal of Chemical Information and Modeling, 2013, 53, 2141-2153.	5.4	68
28	A Comparative Molecular Dynamics, MMâ€“PBSA and Thermodynamic Integration Study of Saquinavir Complexes with Wild-Type HIV-1 PR and L10I, G48V, L63P, A71V, G73S, V82A and I84V Single Mutants. Journal of Chemical Theory and Computation, 2013, 9, 1754-1764.	5.3	47
29	Dual Inhibitors for Aspartic Proteases HIV-1 PR and Renin: Advancements in AIDSâ€“Hypertensionâ€“Diabetes Linkage via Molecular Dynamics, Inhibition Assays, and Binding Free Energy Calculations. Journal of Medicinal Chemistry, 2012, 55, 5784-5796.	6.4	37
30	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
31	Computational Studies of Darunavir into HIV-1 Protease and DMPC Bilayer: Necessary Conditions for Effective Binding and the Role of the Flaps. Journal of Chemical Information and Modeling, 2012, 52, 1542-1558.	5.4	29
32	Binding of novel fullerene inhibitors to HIV-1 protease: insight through molecular dynamics and molecular mechanics Poissonâ€“Boltzmann surface area calculations. Journal of Computer-Aided Molecular Design, 2011, 25, 959-976.	2.9	45
33	Conformational Properties and Energetic Analysis of Aliskiren in Solution and Receptor Site. Molecular Informatics, 2011, 30, 973-985.	2.5	12