

Georgios Leonis

List of Publications by Year in descending order

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33
papers

574
citations

623734

14
h-index

610901

24
g-index

33
all docs

33
docs citations

33
times ranked

1003
citing authors

#	ARTICLE	IF	CITATIONS
1	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. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 2141-2153.	5.4	68
2	Investigation of the Interactions of Silibinin with 2-Hydroxypropyl-Î²-cyclodextrin through Biophysical Techniques and Computational Methods. <i>Molecular Pharmaceutics</i> , 2015, 12, 954-965.	4.6	55
3	Cheminformatics-aided discovery of small-molecule Protein-Protein Interaction (PPI) dual inhibitors of Tumor Necrosis Factor (TNF) and Receptor Activator of NF-Î²B Ligand (RANKL). <i>PLoS Computational Biology</i> , 2017, 13, e1005372.	3.2	49
4	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. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1754-1764.	5.3	47
5	Binding of novel fullerene inhibitors to HIV-1 protease: insight through molecular dynamics and molecular mechanics Poissonâ€‘Boltzmann surface area calculations. <i>Journal of Computer-Aided Molecular Design</i> , 2011, 25, 959-976.	2.9	45
6	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. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 5784-5796.	6.4	37
7	Biological and computational evaluation of resveratrol inhibitors against Alzheimerâ€™s disease. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2016, 31, 67-77.	5.2	32
8	Computational Studies of Darunavir into HIV-1 Protease and DMPC Bilayer: Necessary Conditions for Effective Binding and the Role of the Flaps. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 1542-1558.	5.4	29
9	Elucidation of Conformational States, Dynamics, and Mechanism of Binding in Human Î²-Opioid Receptor Complexes. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 2294-2308.	5.4	25
10	Development of a potent 2-oxoamide inhibitor of secreted phospholipase A2 guided by molecular docking calculations and molecular dynamics simulations. <i>Bioorganic and Medicinal Chemistry</i> , 2016, 24, 1683-1695.	3.0	23
11	A Comprehensive Computational Study of the Interaction between Human Serum Albumin and Fullerenes. <i>Journal of Physical Chemistry B</i> , 2015, 119, 14971-14985.	2.6	22
12	In Silico Discovery of Plant-Origin Natural Product Inhibitors of Tumor Necrosis Factor (TNF) and Receptor Activator of NF-Î²B Ligand (RANKL). <i>Frontiers in Pharmacology</i> , 2018, 9, 800.	3.5	17
13	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. <i>Molecular Pharmaceutics</i> , 2019, 16, 1255-1271.	4.6	17
14	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. <i>Journal of Physical Chemistry B</i> , 2014, 118, 9538-9552.	2.6	14
15	Diabetic skin and UV light: Protection by antioxidants. <i>European Journal of Pharmaceutical Sciences</i> , 2019, 127, 1-8.	4.0	14
16	Current Status and Future Prospects of Smallâ€‘molecule Proteinâ€‘protein Interaction (PPI) Inhibitors of Tumor Necrosis Factor (TNF) and Receptor Activator of NF-Î²B Ligand (RANKL). <i>Current Topics in Medicinal Chemistry</i> , 2018, 18, 661-673.	2.1	13
17	Conformational Properties and Energetic Analysis of Aliskiren in Solution and Receptor Site. <i>Molecular Informatics</i> , 2011, 30, 973-985.	2.5	12
18	Topical Treatment of Skin Injury Inflicted in Mice by X-Ray Irradiation. <i>Skin Pharmacology and Physiology</i> , 2018, 31, 175-183.	2.5	10

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19	Compilation of Data and Modelling of Nanoparticle Interactions and Toxicity in the NanoPUZZLES Project. <i>Advances in Experimental Medicine and Biology</i> , 2017, 947, 303-324.	1.6	8
20	Computational investigation of fullerene-DNA interactions: Implications of fullerene's size and functionalization on DNA structure and binding energetics. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 74, 177-192.	2.4	6
21	Antihypertensive activity and molecular interactions of irbesartan in complex with 2-hydroxypropyl- β -cyclodextrin. <i>Chemical Biology and Drug Design</i> , 2020, 96, 668-683.	3.2	6
22	Strategy for Identification of Nanomaterials' Critical Properties Linked to Biological Impacts: Interlinking of Experimental and Computational Approaches. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2017, , 385-424.	0.6	5
23	Losartan Interactions with 2-Hydroxypropyl- β -CD. <i>Molecules</i> , 2022, 27, 2421.	3.8	4
24	Elucidation of the binding mechanism of renin using a wide array of computational techniques and biological assays. <i>Journal of Molecular Graphics and Modelling</i> , 2015, 62, 138-149.	2.4	3
25	Stability and binding effects of silver(I) complexes at lipoxygenase-1. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2015, 30, 539-549.	5.2	3
26	Discovery of HIV Type-1 Aspartic Protease Hit Compounds through Combined Computational Approaches. <i>ChemMedChem</i> , 2016, 11, 1646-1652.	3.2	3
27	Consensus Predictive Model for Human K562 Cell Growth Inhibition through Enalos Cloud Platform. <i>ChemMedChem</i> , 2018, 13, 555-563.	3.2	2
28	Vinblastine. <i>Advances in Biomembranes and Lipid Self-Assembly</i> , 2019, 29, 127-157.	0.6	2
29	Application of Neutralization and Technique for the Preparation of the Beneficial Drug 2-Hydroxypropyl- β -Cyclodextrin with. <i>Methods in Molecular Biology</i> , 2021, 2207, 1-11.	0.9	2
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. <i>Bioorganic and Medicinal Chemistry</i> , 2012, 20, 6276-6284.	3.0	1
31	Discovery of a stable tripeptide targeting the N-domain of CRF1 receptor. <i>Amino Acids</i> , 2020, 52, 1337-1351.	2.7	0
32	Applications of NMR in Drug:Cyclodextrin. <i>Methods in Molecular Biology</i> , 2021, 2207, 313-325.	0.9	0
33	Molecular Protocols for the Study of Cyclodextrin Drug Systems. <i>Methods in Molecular Biology</i> , 2021, 2207, 109-125.	0.9	0