Thomas Mavromoustakos

List of Publications by Year
in descending order

281	5,757	81900 39	155660 55
papers	citations	h-index	g-index

290	290	290	5785
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Molecular investigation of artificial and natural sweeteners as potential anti-inflammatory agents. Journal of Biomolecular Structure and Dynamics, 2022, 40, 12608-12620.	3.5	7
2	Development of a DHA-Losartan hybrid as a potent inhibitor of multiple pathway-induced platelet aggregation. Journal of Biomolecular Structure and Dynamics, 2022, 40, 13889-13900.	3.5	0
3	Insights into molecular mechanism of action of citrus flavonoids hesperidin and naringin on lipid bilayers using spectroscopic, calorimetric, microscopic and theoretical studies. Journal of Molecular Liquids, 2022, 347, 118411.	4.9	15
4	Losartan Interactions with 2-Hydroxypropyl-Î²-CD. Molecules, 2022, 27, 2421.	3.8	4
5	Discovery of a new generation of angiotensin receptor blocking drugs: Receptor mechanisms and in silico binding to enzymes relevant to SARS-CoV-2. Computational and Structural Biotechnology Journal, 2022, 20, 2091-2111.	4.1	18
6	Biophysical Evaluation and In Vitro Controlled Release of Two Isomeric Adamantane Phenylalkylamines with Antiproliferative/Anticancer and Analgesic Activity. Molecules, 2022, 27, 7.	3.8	0
7	Conformational Properties of New Thiosemicarbazone and Thiocarbohydrazone Derivatives and Their Possible Targets. Molecules, 2022, 27, 2537.	3.8	8
8	Effects of cholesterol on the GPCR AT1 receptor and its interplay with AT1 antagonists. , 2022, , 147-168.		0
9	Understanding the Driving Forces That Trigger Mutations in SARS-CoV-2: Mutational Energetics and the Role of Arginine Blockers in COVID-19 Therapy. Viruses, 2022, 14, 1029.	3.3	17
10	Conformational Properties and Putative Bioactive Targets for Novel Thiosemicarbazone Derivatives. Molecules, 2022, 27, 4548.	3.8	2
11	Charting the structural and thermodynamic determinants in phenolic acid natural product â€“ cyclodextrin encapsulations. Journal of Biomolecular Structure and Dynamics, 2021, 39, 2642-2658.	3.5	9
12	Structureâ€“function analysis of naturally occurring apolipoprotein A-I L144R, A164S and L178P mutants provides insight on their role on HDL levels and cardiovascular risk. Cellular and Molecular Life Sciences, 2021, 78, 1523-1544.	5.4	8
13	Interplay of cholesterol, membrane bilayers and the AT1R: A cholesterol consensus motif on AT1R is revealed. Computational and Structural Biotechnology Journal, 2021, 19, 110-120.	4.1	7
14	Ligandâ€“Receptor Interactions and Drug Design. Methods in Molecular Biology, 2021, 2266, 89-104.	0.9	6
15	Hydrogels containing water soluble conjugates of silver(<scp>i</scp>) ions with amino acids, metabolites or natural products for non infectious contact lenses. Dalton Transactions, 2021, 50, 13712-13727.	3.3	4
16	Silver Nanoparticles from Oregano Leavesâ€™ Extracts as Antimicrobial Components for Non-Infected Hydrogel Contact Lenses. International Journal of Molecular Sciences, 2021, 22, 3539.	4.1	14
17	Organotin derivatives of cholic acid induce apoptosis into breast cancer cells and interfere with mitochondrion; Synthesis, characterization and biological evaluation. Steroids, 2021, 167, 108798.	1.8	13
18	Nano-Assemblies from Amphiphilic PnBA-b-POEGA Copolymers as Drug Nanocarriers. Polymers, 2021, 13, 1164.	4.5	11

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19	Anti-Ageing Potential of S. euboea Heldr. Phenolics. Molecules, 2021, 26, 3151.	3.8	9
20	Advancing the Therapeutic Efficacy of Bioactive Molecules by Delivery Vehicle Platforms. Current Medicinal Chemistry, 2021, 28, 2697-2706.	2.4	6
21	Rational Design and Synthesis of AT1R Antagonists. Molecules, 2021, 26, 2927.	3.8	6
22	An Overview on Target-Based Drug Design against Kinetoplastid Protozoan Infections: Human African Trypanosomiasis, Chagas Disease and Leishmaniases. Molecules, 2021, 26, 4629.	3.8	50
23	Poly(2-oxazoline)-Based Amphiphilic Gradient Copolymers as Nanocarriers for Losartan: Insights into Drugâ€“Polymer Interactions. Macromol, 2021, 1, 177-200.	4.4	7
24	Dissolution and sorption mechanisms at the aluminosilicate and carbonate mineral-AMD (Acid Mine) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	3.0	9
25	Silver Nanoparticles Using Eucalyptus or Willow Extracts (AgNPs) as Contact Lens Hydrogel Components to Reduce the Risk of Microbial Infection. Molecules, 2021, 26, 5022.	3.8	7
26	From Angiotensin II to Cyclic Peptides and Angiotensin Receptor Blockers (ARBs): Perspectives of ARBs in COVID-19 Therapy. Molecules, 2021, 26, 618.	3.8	15
27	Unveiling the Thermodynamic Aspects of Drug-Cyclodextrin Interactions Through Isothermal Titration Calorimetry. Methods in Molecular Biology, 2021, 2207, 187-198.	0.9	3
28	A Differential Scanning Calorimetry (DSC) Experimental Protocol for Evaluating the Modified Thermotropic Behavior of Liposomes with Incorporated Guest Molecules. Methods in Molecular Biology, 2021, 2207, 299-312.	0.9	6
29	Study of Candesartan Cilexetil: 2-Hydroxypropyl-Î²-Cyclodextrin : A Computational Approach Using Steered Simulations. Methods in Molecular Biology, 2021, 2207, 45-70.	0.9	1
30	Drug Incorporation in the Drug Delivery of. Methods in Molecular Biology, 2021, 2207, 99-108.	0.9	1
31	On the Rational Drug Design for Hypertension through NMR Spectroscopy. Molecules, 2021, 26, 12.	3.8	3
32	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
33	Drug Delivery Systems Based on Modified Polysaccharides: Synthesis and. Methods in Molecular Biology, 2021, 2207, 151-161.	0.9	4
34	Differential Scanning Calorimetry (DSC) on Sartan/Cyclodextrin Delivery Formulations. Methods in Molecular Biology, 2021, 2207, 163-174.	0.9	2
35	Association of the Thermodynamics with the Functionality of Thermoresponsive Chimeric Nanosystems. Methods in Molecular Biology, 2021, 2207, 221-233.	0.9	1
36	2D NMR: A Valuable Tool to Confirm the in Drug Systems. Methods in Molecular Biology, 2021, 2207, 235-246.	0.9	2

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37	Applications of NMR in Drug:Cyclodextrin. Methods in Molecular Biology, 2021, 2207, 313-325.	0.9	0
38	Molecular Protocols for the Study of Cyclodextrin Drug Systems. Methods in Molecular Biology, 2021, 2207, 109-125.	0.9	0
39	Novel Approaches in the Immunotherapy of Multiple Sclerosis: Cyclization of Myelin Epitope Peptides and Conjugation with Mannan. Brain Sciences, 2021, 11, 1583.	2.3	5
40	Structure assignment, conformational properties and discovery of potential targets of the Ugi cinnamic adduct NGI25. Journal of Biomolecular Structure and Dynamics, 2021, , 1-14.	3.5	3
41	The boundary lipid around DMPC-spanning influenza A M2 transmembrane domain channels: Its structure and potential for drug accommodation. Biochimica Et Biophysica Acta - Biomembranes, 2020, 1862, 183156.	2.6	4
42	Exploring the role of the membrane bilayer in the recognition of candesartan by its GPCR AT1 receptor. Biochimica Et Biophysica Acta - Biomembranes, 2020, 1862, 183142.	2.6	15
43	Cheminformatics and virtual screening studies of COMT inhibitors as potential Parkinsonâ€™s disease therapeutics. Expert Opinion on Drug Discovery, 2020, 15, 53-62.	5.0	8
44	Discovery of a stable tripeptide targeting the N-domain of CRF1 receptor. Amino Acids, 2020, 52, 1337-1351.	2.7	0
45	Enhancement of glioblastoma multiforme therapy through a novel Quercetin-Losartan hybrid. Free Radical Biology and Medicine, 2020, 160, 391-402.	2.9	16
46	Preparation and Biophysical Characterization of Quercetin Inclusion Complexes with Î²-Cyclodextrin Derivatives to be Formulated as Possible Nose-to-Brain Quercetin Delivery Systems. Molecular Pharmaceutics, 2020, 17, 4241-4255.	4.6	35
47	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
48	Biocompatible PEO-b-PCL Nanosized Micelles as Drug Carriers: Structure and Drugâ€“Polymer Interactions. Nanomaterials, 2020, 10, 1872.	4.1	18
49	Synthetic Analogues of Aminoadamantane as Influenza Viral Inhibitorsâ€”In Vitro, In Silico and QSAR Studies. Molecules, 2020, 25, 3989.	3.8	10
50	Unveiling the interaction profile of rosmarinic acid and its bioactive substructures with serum albumin. Journal of Enzyme Inhibition and Medicinal Chemistry, 2020, 35, 786-804.	5.2	15
51	A Journey to the Conformational Analysis of T-Cell Epitope Peptides Involved in Multiple Sclerosis. Brain Sciences, 2020, 10, 356.	2.3	4
52	pHEMA@AGMNA-1: A novel material for the development of antibacterial contact lens. Materials Science and Engineering C, 2020, 111, 110770.	7.3	26
53	Synthesis, biology, computational studies and in vitro controlled release of new isoniazid-based adamantane derivatives. Future Medicinal Chemistry, 2019, 11, 2779-2802.	2.3	4
54	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

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55	Effects of Cholesterol on GPCR Function: Insights from Computational and Experimental Studies. Advances in Experimental Medicine and Biology, 2019, 1135, 89-103.	1.6	32
56	Drug-Membrane Interactions in the Renin Angiotensin System. Series in Bioengineering, 2019, , 339-364.	0.6	1
57	Inclusion of Quercetin in Gold Nanoparticles Decorated with Supramolecular Hosts Amplifies Its Tumor Targeting Properties. ACS Applied Bio Materials, 2019, 2, 2715-2725.	4.6	30
58	Vinblastine. Advances in Biomembranes and Lipid Self-Assembly, 2019, 29, 127-157.	0.6	2
59	An Efficient Disinfectant, Composite Material {SLS@[Zn3(CitH)2]} as Ingredient for Development of Sterilized and Non Infectious Contact Lens. Antibiotics, 2019, 8, 213.	3.7	9
60	The dynamic properties of angiotensin II type 1 receptor inverse agonists in solution and in the receptor site. Arabian Journal of Chemistry, 2019, 12, 5062-5078.	4.9	19
61	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
62	Discovery of selective dengue virus inhibitors using combination of molecular fingerprint-based virtual screening protocols, structure-based pharmacophore model development, molecular dynamics simulations and in vitro studies. Journal of Molecular Graphics and Modelling, 2018, 79, 88-102.	2.4	23
63	Comparison of the thermal behavior and conformational changes in partially and fully hydrated dipalmitoylphosphatidylcholine systems. Journal of Thermal Analysis and Calorimetry, 2018, 131, 887-898.	3.6	6
64	Comparative Perturbation Effects Exerted by the Influenza A M2 WT Protein Inhibitors Amantadine and the Spiro[pyrrolidine-2,2â€²-adamantane] Variant AK13 to Membrane Bilayers Studied Using Biophysical Experiments and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2018, 122, 9877-9895.	2.6	11
65	Small Peptides Able to Suppress Prostaglandin E2 Generation in Renal Mesangial Cells. Molecules, 2018, 23, 158.	3.8	7
66	Molecular Dynamics Simulations on the Bioactive Molecule of hIAPP22â€“29 (NFGAILSS) and Rational Drug Design. Methods in Molecular Biology, 2018, 1824, 1-16.	0.9	0
67	Designing Natural Product Hybrids Bearing Triple Antiplatelet Profile and Evaluating Their Human Plasma Stability. Methods in Molecular Biology, 2018, 1824, 371-385.	0.9	4
68	Three Regioselectively Acylated Flavonoid Aglycone Derivatives in Equimolar Yield at One Blow. ChemistrySelect, 2018, 3, 5207-5211.	1.5	2
69	Exploring the oxidation and iron binding profile of a cyclodextrin encapsulated quercetin complex unveiled a controlled complex dissociation through a chemical stimulus. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 1913-1924.	2.4	28
70	Current Status and Future Prospects of Smallâ€“molecule Proteinâ€“protein Interaction (PPI) Inhibitors of Tumor Necrosis Factor (TNF) and Receptor Activator of NF-Î¹B Ligand (RANKL). Current Topics in Medicinal Chemistry, 2018, 18, 661-673.	2.1	13
71	Exploring the interactions of irbesartan and irbesartanâ€“2-hydroxypropyl-Î²-cyclodextrin complex with model membranes. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 1089-1098.	2.6	26
72	Molecular requirements involving the human platelet protease-activated receptor-4 mechanism of activation by peptide analogues of its tethered-ligand. Platelets, 2017, 28, 812-821.	2.3	13

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73	In vitro Controlled Release from Solid Pharmaceutical Formulations of two new Adamantane Aminoethers with Antitubercular Activity (I).. Drug Research, 2017, 67, 447-450.	1.7	8
74	Crystal structure analysis, covalent docking, and molecular dynamics calculations reveal a conformational switch in PhaZ7 PHB depolymerase. Proteins: Structure, Function and Bioinformatics, 2017, 85, 1351-1361.	2.6	7
75	Unveiling and tackling guanidinium peptide coupling reagent side reactions towards the development of peptide-drug conjugates. RSC Advances, 2017, 7, 50519-50526.	3.6	21
76	Rational design and structureâ€“activity relationship studies of quercetinâ€“amino acid hybrids targeting the anti-apoptotic protein Bcl-xL. Organic and Biomolecular Chemistry, 2017, 15, 7956-7976.	2.8	24
77	In vitro Controlled Release of two new Tuberculocidal Adamantane Aminoethers from Solid Pharmaceutical Formulations (II). Drug Research, 2017, 67, 653-660.	1.7	7
78	Publisher Note. Journal of Molecular Graphics and Modelling, 2017, 77, 338.	2.4	2
79	A combined NMR and molecular dynamics simulation study to determine the conformational properties of rat/mouse 35-55 myelin oligodendrocyte glycoprotein epitope implicated in the induction of experimental autoimmune encephalomyelitis. Journal of Biomolecular Structure and Dynamics, 2017, 35, 1559-1567.	3.5	3
80	The use of J-coupling as a sole criterion to assign the total absolute stereochemistry of new pyrrolidinone class synthetic analogs, derived from S -pyroglutamic acid. Journal of Molecular Structure, 2017, 1129, 195-199.	3.6	0
81	Copolymerization of Norbornene and Norbornadiene Using a cis-Selective Bimetallic W-Based Catalytic System. Polymers, 2017, 9, 141.	4.5	10
82	Family B G Protein-coupled Receptors and their Ligands: From Structure to Function. Current Medicinal Chemistry, 2017, 24, 3323-3355.	2.4	11
83	Cheminformatics-aided discovery of small-molecule Protein-Protein Interaction (PPI) dual inhibitors of Tumor Necrosis Factor (TNF) and Receptor Activator of NF-Î¹B Ligand (RANKL). PLoS Computational Biology, 2017, 13, e1005372.	3.2	49
84	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
85	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
86	Quantitative Nanostructure-Activity Relationship Models for the Risk Assessment of NanoMaterials. , 2017, , 1314-1338.		1
87	Functional Components of Carob Fruit: Linking the Chemical and Biological Space. International Journal of Molecular Sciences, 2016, 17, 1875.	4.1	101
88	Mapping the interactions and bioactivity of quercetinâ¿¿(2-hydroxypropyl)-Î²-cyclodextrin complex. International Journal of Pharmaceutics, 2016, 511, 303-311.	5.2	48
89	New hydrazones of 5-nitro-2-furaldehyde with adamantanealkanohydrazides: synthesis and in vitro trypanocidal activity. MedChemComm, 2016, 7, 1229-1236.	3.4	12
90	Deconvoluting the Dual Antiplatelet Activity of a Plant Extract. Journal of Agricultural and Food Chemistry, 2016, 64, 4511-4521.	5.2	13

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91	Antiplatelet effect of the main triterpenoids of an olive leaf extract. Atherosclerosis, 2016, 252, e98.	0.8	1
92	Exploring new scaffolds for angiotensin II receptor antagonism. Bioorganic and Medicinal Chemistry, 2016, 24, 4444-4451.	3.0	7
93	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
94	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
95	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
96	Computer Aided Drug Design Approaches for Identification of Novel Autotaxin (ATX) Inhibitors. Current Medicinal Chemistry, 2016, 23, 1708-1724.	2.4	3
97	Calixarenes in Lipase Biocatalysis and Cancer Therapy. Current Organic Chemistry, 2016, 20, 1043-1057.	1.6	23
98	Leveraging NMR and X-ray Data of the Free Ligands to Build Better Drugs Targeting Angiotensin II Type 1 G-Protein Coupled Receptor. Current Medicinal Chemistry, 2015, 23, 36-59.	2.4	20
99	Rational Drug Design and Synthesis of Molecules Targeting the Angiotensin II Type 1 and Type 2 Receptors. Molecules, 2015, 20, 3868-3897.	3.8	36
100	Comparative study of interactions of aliskiren and AT 1 receptor antagonists with lipid bilayers. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 984-994.	2.6	10
101	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
102	Branched-chain sugar nucleosides: stereocontrolled synthesis and bioevaluation of novel 3â€²-C-trifluoromethyl and 3â€²-C-methyl pyranonucleosides. Carbohydrate Research, 2015, 407, 170-178.	2.3	2
103	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
104	Exploiting ChEMBL database to identify indole analogs as HCV replication inhibitors. Methods, 2015, 71, 4-13.	3.8	20
105	A novel synthetic luteinizing hormone-releasing hormone (LHRH) analogue coupled with modified Î²-cyclodextrin: Insight into its intramolecular interactions. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 159-168.	2.4	8
106	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
107	Pharmaceutical compositions for antihypertensive treatments: a patent review. Expert Opinion on Therapeutic Patents, 2015, 25, 1305-17.	5.0	20
108	Rational Drug Design Paradigms: The Odyssey for Designing Better Drugs. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 238-256.	1.1	8

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109	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
110	Structural-Functional Analysis of the Third Transmembrane Domain of the Corticotropin-releasing Factor Type 1 Receptor. Journal of Biological Chemistry, 2014, 289, 18966-18977.	3.4	16
111	Insights into the molecular basis of action of the AT1 antagonist losartan using a combined NMR spectroscopy and computational approach. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 1031-1046.	2.6	35
112	Monounsaturated Fatty Acid Ether Oligomers Formed during Heating of Virgin Olive Oil Show Agglutination Activity against Human Red Blood Cells. Journal of Agricultural and Food Chemistry, 2014, 62, 867-874.	5.2	9
113	32nd Cyprus-Noordwijkerhout-Camerino Symposium: Trends in Drug Research 2014. ChemMedChem, 2014, 9, n/a-n/a.	3.2	0
114	The application of solid-state NMR spectroscopy to study candesartan cilexetil (TCV-116) membrane interactions. Comparative study with the AT1R antagonist drug olmesartan. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 2439-2450.	2.6	16
115	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
116	Distinctive Spectral and Microscopic Features for Characterizing the Three-Dimensional Local Aluminosilicate Structure of Perlites. Journal of Physical Chemistry C, 2014, 118, 26649-26658.	3.1	13
117	An Efficient Synthetic Method and Theoretical Calculations of Olmesartan Methyl Ether: Study of Biological Function of AT1 Antagonism. Combinatorial Chemistry and High Throughput Screening, 2014, 17, 652-662.	1.1	4
118	Interactions of the potent synthetic AT1 antagonist analog BV6 with membrane bilayers and mesoporous silicate matrices. Biochimica Et Biophysica Acta - Biomembranes, 2013, 1828, 1846-1855.	2.6	6
119	AT1 antagonists: a patent review (2008 â€“ 2012). Expert Opinion on Therapeutic Patents, 2013, 23, 1483-1494.	5.0	25
120	Molecular insights into the AT1 antagonism based on biophysical and in silico studies of telmisartan. Medicinal Chemistry Research, 2013, 22, 4842-4857.	2.4	8
121	Rational design, efficient syntheses and biological evaluation of N , N â€²-symmetrically bis-substituted butylimidazole analogs as a new class of potent Angiotensin II receptor blockers. European Journal of Medicinal Chemistry, 2013, 62, 352-370.	5.5	28
122	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
123	Synthesis of New Optically Active 2-Pyrrolidinones. Molecules, 2013, 18, 50-73.	3.8	7
124	Facile and Efficient Syntheses of a Series of N-Benzyl and N-Biphenylmethyl Substituted Imidazole Derivatives Based on (E)-Urocanic acid, as Angiotensin II AT1 Receptor Blockers. Molecules, 2013, 18, 7510-7532.	3.8	7
125	Molecular Modeling on Pyrimidine-Urea Inhibitors of TNF-Î± Production: An Integrated Approach Using a Combination of Molecular Docking, Classification Techniques, and 3D-QSAR CoMSIA. Journal of Chemical Information and Modeling, 2012, 52, 711-723.	5.4	57
126	Comparative Binding Effects of Aspirin and Anti-Inflammatory Cu Complex in the Active Site of LOX-1. Journal of Chemical Information and Modeling, 2012, 52, 3293-3301.	5.4	10

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127	Chapter 8. Theoretical Studies of Interactions in Nanomaterials and Biological Systems. RSC Nanoscience and Nanotechnology, 2012, , 148-186.	0.2	0
128	Losartan's affinity to fluid bilayers modulates lipidâ€“cholesterol interactions. Physical Chemistry Chemical Physics, 2012, 14, 4780.	2.8	40
129	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
130	Comparative study of the AT1 receptor prodrug antagonist candesartan cilexetil with other sartans on the interactions with membrane bilayers. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 3107-3120.	2.6	19
131	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
132	The discovery of new potent non-peptide Angiotensin II AT1 receptor blockers: A concise synthesis, molecular docking studies and biological evaluation ofÂN-substituted 5-butylimidazole derivatives. European Journal of Medicinal Chemistry, 2012, 55, 358-374.	5.5	31
133	Binding Conformation of 2-Oxoamide Inhibitors to Group IVA Cytosolic Phospholipase A₂ Determined by Molecular Docking Combined with Molecular Dynamics. Journal of Chemical Information and Modeling, 2012, 52, 243-254.	5.4	20
134	Copper(I)/(II) or silver(I) ions towards 2-mercaptopyrimidine: An exploration of a chemical variability with possible biological implication. Inorganica Chimica Acta, 2012, 382, 146-157.	2.4	30
135	An effort to discover the preferred conformation of the potent AMG3 cannabinoid analog when reaching the active sites of the cannabinoid receptors. European Journal of Medicinal Chemistry, 2012, 47, 44-51.	5.5	4
136	Comparative Biophysical Studies of Sartan Class Drug Molecules Losartan and Candesartan (CV-11974) with Membrane Bilayers. Journal of Physical Chemistry B, 2011, 115, 6180-6192.	2.6	37
137	Interactions of the AT1 antagonist valsartan with dipalmitoyl-phosphatidylcholine bilayers. Biochimica Et Biophysica Acta - Biomembranes, 2011, 1808, 1753-1763.	2.6	48
138	Thermal, dynamic and structural properties of drug AT1 antagonist olmesartan in lipid bilayers. Biochimica Et Biophysica Acta - Biomembranes, 2011, 1808, 2995-3006.	2.6	23
139	Editorial [Hot Topic:Methodologies and Applied Strategies in the Rational Drug Design (Guest Editor:) Tj ETQq1 1 0.784314 rgBT /Ove	2.4	2
140	Synthesis, structural characterization and biological studies of novel mixed ligand Ag(I) complexes with triphenylphosphine and aspirin or salicylic acid. Inorganica Chimica Acta, 2011, 375, 114-121.	2.4	55
141	Conformational analysis of the Îœ[Ì¡83â€“99 (Phe91) and Îœ[Ì¡83â€“99 (Tyr91) peptide analogues and study of their interactions with the HLA-DR2 and human TCR receptors by using Molecular Dynamics. Journal of Computer-Aided Molecular Design, 2011, 25, 837-853.	2.9	5
142	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
143	Comparison of thermal effects of stilbenoid analogs in lipid bilayers using differential scanning calorimetry and molecular dynamics: correlation of thermal effects and topographical position with antioxidant activity. European Biophysics Journal, 2011, 40, 865-875.	2.2	20
144	Partial interdigitation of lipid bilayers. International Journal of Quantum Chemistry, 2011, 111, 1172-1183.	2.0	20

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145	Docking and Molecular Dynamics Calculations of Pyrrolidinone Analog MMK16 Bound to COX and LOX Enzymes. Molecular Informatics, 2011, 30, 473-486.	2.5	9
146	Conformational Properties and Energetic Analysis of Aliskiren in Solution and Receptor Site. Molecular Informatics, 2011, 30, 973-985.	2.5	12
147	Inhibition of secreted phospholipases A2 by 2-oxoamides based on Î±-amino acids: Synthesis, in vitro evaluation and molecular docking calculations. Bioorganic and Medicinal Chemistry, 2011, 19, 735-743.	3.0	35
148	Synthesis, in silico docking experiments of new 2-pyrrolidinone derivatives and study of their anti-inflammatory activity. Bioorganic and Medicinal Chemistry, 2011, 19, 2888-2902.	3.0	22
149	The Application of Rational Design on Phospholipase A2 Inhibitors. Current Medicinal Chemistry, 2011, 18, 2566-2582.	2.4	23
150	Strategies in the Rational Drug Design. Current Medicinal Chemistry, 2011, 18, 2517-2530.	2.4	92
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