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	An Effort To Understand the Molecular Basis of Hypertension through the Study of Conformational Analysis of Losartan and Sarmesin Using a Combination of Nuclear Magnetic Resonance Spectroscopy and Theoretical Calculations. Journal of Medicinal Chemistry, 1999, 42, 1714-1722.	6.4	115
2	Synthesis, pH-Dependent Structural Characterization, and Solution Behavior of Aqueous Aluminum and Gallium Citrate Complexes. Inorganic Chemistry, 2001, 40, 1734-1744.	4.0	106
3	Functional Components of Carob Fruit: Linking the Chemical and Biological Space. International Journal of Molecular Sciences, 2016, 17, 1875.	4.1	101
4	Computational design of novel fullerene analogues as potential HIV-1 PR inhibitors: Analysis of the binding interactions between fullerene inhibitors and HIV-1 PR residues using 3D QSAR, molecular docking and molecular dynamics simulations. Bioorganic and Medicinal Chemistry, 2008, 16, 9957-9974.	3.0	93
5	Strategies in the Rational Drug Design. Current Medicinal Chemistry, 2011, 18, 2517-2530.	2.4	92
6	Comparison of classical and ultrasound-assisted isolation procedures of cellulose from kenaf (Hibiscus cannabinus L.) and eucalyptus (Eucalyptus rodustrus Sm.). Ultrasonics Sonochemistry, 2002, 9, 19-23.	8.2	91
7	A New Dinuclear Ti(IV)â^'Peroxoâ^'Citrate Complex from Aqueous Solutions. Synthetic, Structural, and Spectroscopic Studies in Relevance to Aqueous Titanium(IV)â^'Peroxoâ^'Citrate Speciation. Inorganic Chemistry, 2003, 42, 4632-4639.	4.0	85
8	Role of the NH2-terminal domain of angiotensin II (ANG II) and [Sar1]angiotensin II on conformation and activity. NMR evidence for aromatic ring clustering and peptide backbone folding compared with [des-1,2,3]angiotensin II.. Journal of Biological Chemistry, 1994, 269, 5303-5312.	3.4	78
9	Synthesis and Spectroscopic and Structural Studies of a New Cadmium(II)â^'Citrate Aqueous Complex. Potential Relevance to Cadmium(II)â^'Citrate Speciation and Links to Cadmium Toxicity. Inorganic Chemistry, 2003, 42, 2531-2537.	4.0	75
10	Effects of non-steroid anti-inflammatory drugs in membrane bilayers. Chemistry and Physics of Lipids, 2004, 132, 157-169.	3.2	74
11	¹H NMR-Based Protocol for the Detection of Adulterations of Refined Olive Oil with Refined Hazelnut Oil. Journal of Agricultural and Food Chemistry, 2009, 57, 11550-11556.	5.2	74
12	Hematocrit-lowering Effect Following Inactivation of Renin-Angiotensin System with Angiotensin Converting Enzyme Inhibitors and Angiotensin Receptor Blockers. Current Topics in Medicinal Chemistry, 2004, 4, 483-486.	2.1	72
13	Antagonistic Effects of Human Cyclic MBP87-99 Altered Peptide Ligands in Experimental Allergic Encephalomyelitis and Human T-Cell Proliferation. Journal of Medicinal Chemistry, 2002, 45, 275-283.	6.4	70
14	Structural, compositional and acidic characteristics of nanosized amorphous or partially crystalline ZSM-5 zeolite-based materials. Microporous and Mesoporous Materials, 2004, 75, 89-100.	4.4	70
15	Design And Synthesis of a Novel Potent Myelin Basic Protein Epitope 87â^'99 Cyclic Analogue:Â Enhanced Stability and Biological Properties of Mimics Render Them a Potentially New Class of Immunomodulatorsâ€. Journal of Medicinal Chemistry, 2005, 48, 1470-1480.	6.4	62
16	3D QSAR CoMFA/CoMSIA, molecular docking and molecular dynamics studies of fullerene-based HIV-1 PR inhibitors. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 6283-6289.	2.2	60
17	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
18	Development of accurate binding affinity predictions of novel renin inhibitors through molecular docking studies. Journal of Molecular Graphics and Modelling, 2010, 29, 425-435.	2.4	56

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19	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
20	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
21	Role of the NH2-terminal domain of angiotensin II (ANG II) and [Sar1]angiotensin II on conformation and activity. NMR evidence for aromatic ring clustering and peptide backbone folding compared with [des-1,2,3]angiotensin II. Journal of Biological Chemistry, 1994, 269, 5303-12.	3.4	54
22	Losartanâ€™s molecular basis of interaction with membranes and AT1 receptor. Chemistry and Physics of Lipids, 2003, 125, 13-25.	3.2	52
23	In Silico Drug Screening Approach for the Design of Magic Bullets: A Successful Example with Anti-HIV Fullerene Derivatized Amino Acids. Journal of Chemical Information and Modeling, 2009, 49, 1139-1143.	5.4	52
24	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
25	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
26	Design and Synthesis of a Potent Cyclic Analogue of the Myelin Basic Protein Epitope MBP72-85:â€‰ Importance of the Ala81 Carboxyl Group and of a Cyclic Conformation for Induction of Experimental Allergic Encephalomyelitis. Journal of Medicinal Chemistry, 1999, 42, 1170-1177.	6.4	48
27	Interactions of the AT1 antagonist valsartan with dipalmitoyl-phosphatidylcholine bilayers. Biochimica Et Biophysica Acta - Biomembranes, 2011, 1808, 1753-1763.	2.6	48
28	Mapping the interactions and bioactivity of quercetinâ¿¿(2-hydroxypropyl)-Î²-cyclodextrin complex. International Journal of Pharmaceutics, 2016, 511, 303-311.	5.2	48
29	The Application of 3D-QSAR Studies for Novel Cannabinoid Ligands Substituted at the C1â€˜ Position of the Alkyl Side Chain on the Structural Requirements for Binding to Cannabinoid Receptors CB1 and CB2. Journal of Medicinal Chemistry, 2007, 50, 2875-2885.	6.4	47
30	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
31	The design and synthesis of a potent angiotensin II cyclic analogue confirms the ring cluster receptor conformation of the hormone angiotensin II. Bioorganic and Medicinal Chemistry, 2000, 8, 1-10.	3.0	45
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	A novel analytical method to detect adulteration of virgin olive oil by other oils. JAOCS, Journal of the American Oil Chemists' Society, 2000, 77, 405-411.	1.9	44
34	Application of 3D QSAR CoMFA/CoMSIA and in silico docking studies on novel renin inhibitors against cardiovascular diseases. European Journal of Medicinal Chemistry, 2009, 44, 3703-3711.	5.5	44
35	Antileishmanial Ring-Substituted Ether Phospholipids. Journal of Medicinal Chemistry, 2003, 46, 755-767.	6.4	42
36	Study of the topography of cannabinoids in model membranes using X-ray diffraction. Biochimica Et Biophysica Acta - Biomembranes, 1990, 1024, 336-344.	2.6	41

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37	Amphipathic interactions of cannabinoids with membranes. A comparison between Î”8-THC and its O-methyl analog using differential scanning calorimetry, X-ray diffraction and solid state 2H-NMR. Biochimica Et Biophysica Acta - Biomembranes, 1992, 1103, 25-36.	2.6	41
38	Losartan's affinity to fluid bilayers modulates lipidâ€“cholesterol interactions. Physical Chemistry Chemical Physics, 2012, 14, 4780.	2.8	40
39	The use of high-resolution solid-state NMR spectroscopy and differential scanning calorimetry to study interactions of anaesthetic steroids with membrane. Biochimica Et Biophysica Acta - Biomembranes, 1997, 1328, 65-73.	2.6	39
40	Authenticity of the Traditional Cypriot Spirit â€œZivaniaâ€•on the Basis of Metal Content Using a Combination of Coupled Plasma Spectroscopy and Statistical Analysis. Journal of Agricultural and Food Chemistry, 2003, 51, 6233-6239.	5.2	39
41	Antihypertensive Drug Valsartan in Solution and at the AT₁ Receptor: Conformational Analysis, Dynamic NMR Spectroscopy, in Silico Docking, and Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2009, 49, 726-739.	5.4	39
42	Treatment of experimental allergic encephalomyelitis (EAE) by a rationally designed cyclic analogue of myelin basic protein (MBP) epitope 72â€“85. Bioorganic and Medicinal Chemistry Letters, 2000, 10, 2713-2717.	2.2	37
43	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
44	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
45	Effects of the anesthetic steroid alphaxalone and its inactive Î”16-analog on the thermotropic properties of membrane bilayers. A model for membrane perturbation. Biochimica Et Biophysica Acta - Biomembranes, 1995, 1239, 257-264.	2.6	36
46	Mononuclear Titanium(IV)â€“Citrate Complexes from Aqueous Solutions:â€‰ pH-Specific Synthesis and Structural and Spectroscopic Studies in Relevance to Aqueous Titanium(IV)â€“Citrate Speciation. Inorganic Chemistry, 2005, 44, 2596-2605.	4.0	36
47	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
48	Synthesis and Contractile Activities of Cyclic Thrombin Receptor-Derived Peptide Analogues with a Phe-Leu-Leu-Arg Motif:Â Importance of the Phe/Arg Relative Conformation and the Primary Amino Group for Activityâ€‡. Journal of Medicinal Chemistry, 1996, 39, 3585-3591.	6.4	35
49	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
50	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
51	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
52	Authenticity of the Traditional Cypriot Spirit â€œZivaniaâ€•on the Basis of1H NMR Spectroscopy Diagnostic Parameters and Statistical Analysis. Journal of Agricultural and Food Chemistry, 2005, 53, 5293-5303.	5.2	34
53	Molecular Docking and 3D-QSAR CoMFA Studies on Indole Inhibitors of GIIA Secreted Phospholipase A₂. Journal of Chemical Information and Modeling, 2010, 50, 1589-1601.	5.4	34
54	Ether Phospholipid-AZT Conjugates Possessing Anti-HIV and Antitumor Cell Activity. Synthesis, Conformational Analysis, and Study of Their Thermal Effects on Membrane Bilayers. Journal of Medicinal Chemistry, 2001, 44, 1702-1709.	6.4	33

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55	Differences in Backbone Structure between Angiotensin II Agonists and Type I Antagonists. Journal of Medicinal Chemistry, 1995, 38, 4660-4669.	6.4	32
56	Synthesis of 2-(2-adamantyl)piperidines and structure anti-influenza virus a activity relationship study using a combination of NMR spectroscopy and molecular modeling. Bioorganic and Medicinal Chemistry Letters, 1999, 9, 3465-3470.	2.2	32
57	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
58	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
59	13C NMR analysis of the triacylglycerol composition of Greek virgin olive oils. Magnetic Resonance in Chemistry, 1997, 35, S3-S7.	1.9	31
60	Biological activity of myricetin and its derivatives against human leukemic cell lines in vitro. Pharmacological Research, 2000, 42, 475-478.	7.1	31
61	A comparative study of the effects of cholesterol and sclareol, a bioactive labdane type diterpene, on phospholipid bilayers. Chemistry and Physics of Lipids, 2005, 133, 125-134.	3.2	31
62	A computational study on cannabinoid receptors and potent bioactive cannabinoid ligands: homology modeling, docking, de novo drug design and molecular dynamics analysis. Molecular Diversity, 2010, 14, 257-276.	3.9	31
63	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
64	Synthesis and study of a cyclic angiotensin II antagonist analogue reveals the role of Ï€*â€“Ï€* interactions in the C-terminal aromatic residue for agonist activity and its structure resemblance with AT1 non-peptide antagonists. Bioorganic and Medicinal Chemistry, 2001, 9, 1639-1647.	3.0	30
65	A molecular basis explanation of the dynamic and thermal effects of vinblastine sulfate upon dipalmitoylphosphatidylcholine bilayer membranes. Biochimica Et Biophysica Acta - Biomembranes, 2002, 1567, 49-55.	2.6	30
66	The modulation of thermal properties of vinblastine by cholesterol in membrane bilayers. Biochimica Et Biophysica Acta - Biomembranes, 2004, 1661, 1-8.	2.6	30
67	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
68	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
69	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
70	Conformation and Bioactivity. Design and Discovery of Novel Antihypertensive Drugs. Current Topics in Medicinal Chemistry, 2004, 4, 385-401.	2.1	30
71	Combined 3D QSAR and molecular docking studies to reveal novel cannabinoid ligands with optimum binding activity. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 6754-6763.	2.2	29
72	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

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73	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
74	Structural Requirements for Binding of Myelin Basic Protein (MBP) Peptides to MHC II: Effects on Immune Regulation. Current Medicinal Chemistry, 2005, 12, 1521-1535.	2.4	27
75	pH-Specific Aqueous Synthetic Chemistry in the Binary Cadmium(II)â^'Citrate System. Gaining Insight into Cadmium(II)â^'Citrate Speciation with Relevance to Cadmium Toxicity. Inorganic Chemistry, 2005, 44, 4818-4828.	4.0	27
76	Novel 17Î²-Substituted Conformationally Constrained Neurosteroids that Modulate GABAAReceptors. Journal of Medicinal Chemistry, 2005, 48, 5203-5214.	6.4	27
77	Design and synthesis of novel antihypertensive drugs. Bioorganic and Medicinal Chemistry Letters, 2003, 13, 1737-1740.	2.2	26
78	Molecular dynamics at the receptor level of immunodominant myelin basic protein epitope 87â€“99 implicated in multiple sclerosis and its antagonists altered peptide ligands: Triggering of immune response. Journal of Molecular Graphics and Modelling, 2007, 26, 471-481.	2.4	26
79	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
80	pHEMA@AGMNA-1: A novel material for the development of antibacterial contact lens. Materials Science and Engineering C, 2020, 111, 110770.	7.3	26
81	Thermodynamic origin ofcis/trans isomers of a proline-containing Î²-turn model dipeptide in aqueous solution: A combined variable temperature1H-NMR, two-dimensional1H,1H gradient enhanced nuclear overhauser effect spectroscopy (NOESY), one-dimensional steady-state intermolecular13C,1H NOE, and molecular dynamics study. Biopolymers, 2000, 53, 72-83.	2.4	25
82	AT1 antagonists: a patent review (2008 â€“ 2012). Expert Opinion on Therapeutic Patents, 2013, 23, 1483-1494.	5.0	25
83	Studies on the thermotropic effects of cannabinoids on phosphatidylcholine bilayers using differential scanning calorimetry and small angle X-ray diffraction. Biochimica Et Biophysica Acta - Biomembranes, 1996, 1281, 235-244.	2.6	24
84	Differential membrane fluidization by active and inactive cannabinoid analogues. Biochimica Et Biophysica Acta - Biomembranes, 2001, 1512, 183-190.	2.6	24
85	Design of new secreted phospholipase A2 inhibitors based on docking calculations by modifying the pharmacophore segments of the FPL67047XX inhibitor. Journal of Computer-Aided Molecular Design, 2010, 24, 107-115.	2.9	24
86	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
87	Effects of cannabinoids in membrane bilayers containing cholesterol. Biochimica Et Biophysica Acta - Biomembranes, 1999, 1420, 252-265.	2.6	23
88	Comparison of Proposed Putative Active Conformations of Myelin Basic Protein Epitope 87â^'99 Linear Altered Peptide Ligands by Spectroscopic and Modelling Studies:Â The Role of Positions 91 and 96 in T-Cell Receptor Activation. Journal of Medicinal Chemistry, 2006, 49, 6683-6691.	6.4	23
89	Delving into the complex picture of Ti(IV)â€“citrate speciation in aqueous media: Synthetic, structural, and electrochemical considerations in mononuclear Ti(IV) complexes containing variably deprotonated citrate ligands. Inorganica Chimica Acta, 2008, 361, 2210-2224.	2.4	23
90	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

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91	The Application of Rational Design on Phospholipase A2 Inhibitors. Current Medicinal Chemistry, 2011, 18, 2566-2582.	2.4	23
92	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
93	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
94	Calixarenes in Lipase Biocatalysis and Cancer Therapy. Current Organic Chemistry, 2016, 20, 1043-1057.	1.6	23
95	Structure elucidation and conformational properties of eprosartan a non peptide Angiotensin II AT1 antagonist. Journal of Pharmaceutical and Biomedical Analysis, 2002, 28, 125-135.	2.8	22
96	Interactions at the bilayer interface and receptor site induced by the novel synthetic pyrrolidinone analog MMK3. Biochimica Et Biophysica Acta - Biomembranes, 2010, 1798, 422-432.	2.6	22
97	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
98	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
99	Efforts to Understand the Molecular Basis of Hypertension Through Drug:Membrane Interactions. Current Topics in Medicinal Chemistry, 2004, 4, 445-459.	2.1	22
100	Small angle X-ray diffraction studies on the topography of cannabinoids in synaptic plasma membranes. Pharmacology Biochemistry and Behavior, 1991, 40, 547-552.	2.9	21
101	The role of the anticancer drug vinorelbine in lipid bilayers using differential scanning calorimetry and molecular modeling. Chemistry and Physics of Lipids, 2006, 144, 85-95.	3.2	21
102	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
103	Studies of the conformational properties of the cannabimimetic aminoalkylindole pravadoline using NMR and molecular modeling. European Journal of Medicinal Chemistry, 1995, 30, 227-234.	5.5	20
104	Synthesis, binding studies and in vivo biological evaluation of novel non-peptide antihypertensive analogues. Bioorganic and Medicinal Chemistry, 2006, 14, 4353-4360.	3.0	20
105	3D-Quantitative structureâ€“activity relationships of synthetic antileishmanial ring-substituted ether phospholipids. Bioorganic and Medicinal Chemistry, 2007, 15, 1252-1265.	3.0	20
106	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
107	Partial interdigitation of lipid bilayers. International Journal of Quantum Chemistry, 2011, 111, 1172-1183.	2.0	20
108	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

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109	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
110	Exploiting ChEMBL database to identify indole analogs as HCV replication inhibitors. Methods, 2015, 71, 4-13.	3.8	20
111	Pharmaceutical compositions for antihypertensive treatments: a patent review. Expert Opinion on Therapeutic Patents, 2015, 25, 1305-17.	5.0	20
112	Small angle X-ray diffraction and differential scanning calorimetric studies on O-methyl-(â^')-Î”8-tetrahydrocannabinol and its 5â€² iodinated derivative in membrane bilayers. Biochimica Et Biophysica Acta - Biomembranes, 1995, 1237, 183-188.	2.6	19
113	A combined use of 13C-cross polarization/magic angle spinning, 13C-magic angle spinning and 31P-nuclear magnetic resonance spectroscopy with differential scanning calorimetry to study cannabinoid-membrane interactions. Chemistry and Physics of Lipids, 1998, 92, 37-52.	3.2	19
114	Design, Synthesis, and Modeling of Novel Cyclic Thrombin Receptor-Derived Peptide Analogues of the Ser42-Phe-Leu-Leu-Arg46Motif Sequence with Fixed Conformations of Pharmacophoric Groups:Â Importance of a Phe/Arg/NH2Cluster for Receptor Activation and Implications in the Design of Nonpeptide Thrombin Receptor Mimeticsâ€. Journal of Medicinal Chemistry, 2001, 44, 328-339.	6.4	19
115	Design, synthesis and biological evaluation of cyclic angiotensin II analogues with 3,5 side-Chain bridges. Bioorganic and Medicinal Chemistry Letters, 2002, 12, 2627-2633.	2.2	19
116	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
117	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
118	Molecular Dynamics Simulations of Angiotensin II in Aqueous and Dimethyl Sulfoxide Environments. Journal of Physical Chemistry B, 2005, 109, 17743-17751.	2.6	18
119	Biocompatible PEO-b-PCL Nanosized Micelles as Drug Carriers: Structure and Drugâ€“Polymer Interactions. Nanomaterials, 2020, 10, 1872.	4.1	18
120	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
121	Topography of tetrahydrocannabinol in model membranes using neutron diffraction. Biochimica Et Biophysica Acta - Biomembranes, 1993, 1151, 51-58.	2.6	17
122	Topography of alphaxalone and Î”16-alphaxalone in membrane bilayers containing cholesterol. Biochimica Et Biophysica Acta - Biomembranes, 1994, 1194, 69-74.	2.6	17
123	A combined NMR and molecular dynamics simulation study to determine the conformational properties of agonists and antagonists against experimental autoimmune encephalomyelitis. Bioorganic and Medicinal Chemistry, 2008, 16, 2171-2182.	3.0	17
124	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
125	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
126	A putative bioactive conformation for the altered peptide ligand of myelin basic protein and inhibitor of experimental autoimmune encephalomyelitis [Arg91, Ala96] MBP87â€“99. Journal of Molecular Graphics and Modelling, 2006, 25, 17-29.	2.4	16

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127	An efficient synthesis of a rationally designed 1,5 disubstituted imidazole AT1 Angiotensin II receptor antagonist: reorientation of imidazole pharmacophore groups in losartan reserves high receptor affinity and confirms docking studies. Journal of Computer-Aided Molecular Design, 2010, 24, 749-758.	2.9	16
128	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
129	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
130	Enhancement of glioblastoma multiforme therapy through a novel Quercetin-Losartan hybrid. Free Radical Biology and Medicine, 2020, 160, 391-402.	2.9	16
131	Structure elucidation, conformational analysis and thermal effects on membrane bilayers of an antimicrobial myricetin ether derivative. Journal of Heterocyclic Chemistry, 2001, 38, 703-710.	2.6	15
132	Block copolymers with crystalline/amorphous, crystalline/polyelectrolyte and amorphous/polyelectrolyte blocks. Macromolecular Chemistry and Physics, 2002, 203, 1317-1327.	2.2	15
133	Structure elucidation and conformational study of V8. Journal of Pharmaceutical and Biomedical Analysis, 2006, 40, 1097-1104.	2.8	15
134	Development of a CP 31P NMR Broadline Simulation Methodology for Studying the Interactions of Antihypertensive AT1 Antagonist Losartan with Phospholipid Bilayers. Biophysical Journal, 2009, 96, 2227-2236.	0.5	15
135	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
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