

Julio Caballero

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/7267820/publications.pdf>

Version: 2024-02-01

154
papers

4,088
citations

109137

35
h-index

161609

54
g-index

160
all docs

160
docs citations

160
times ranked

4826
citing authors

#	ARTICLE	IF	CITATIONS
1	Is It Reliable to Take the Molecular Docking Top Scoring Position as the Best Solution without Considering Available Structural Data?. <i>Molecules</i> , 2018, 23, 1038.	1.7	267
2	Is It Reliable to Use Common Molecular Docking Methods for Comparing the Binding Affinities of Enantiomer Pairs for Their Protein Target?. <i>International Journal of Molecular Sciences</i> , 2016, 17, 525.	1.8	114
3	Immobilization of Adamantane-Modified Cytochrome c Electrode Surfaces through Supramolecular Interactions. <i>Langmuir</i> , 2002, 18, 5051-5054.	1.6	88
4	Quantitative structure–activity relationship to predict differential inhibition of aldose reductase by flavonoid compounds. <i>Bioorganic and Medicinal Chemistry</i> , 2005, 13, 3269-3277.	1.4	87
5	LigRMSD: a web server for automatic structure matching and RMSD calculations among identical and similar compounds in protein-ligand docking. <i>Bioinformatics</i> , 2020, 36, 2912-2914.	1.8	84
6	Genetic algorithm optimization in drug design QSAR: Bayesian-regularized genetic neural networks (BRGNN) and genetic algorithm-optimized support vectors machines (GA-SVM). <i>Molecular Diversity</i> , 2011, 15, 269-289.	2.1	81
7	QSAR for non-nucleoside inhibitors of HIV-1 reverse transcriptase. <i>Bioorganic and Medicinal Chemistry</i> , 2006, 14, 5876-5889.	1.4	80
8	Minimizing the Risk of Reporting False Aromaticity and Antiaromaticity in Inorganic Heterocycles Following Magnetic Criteria. <i>Inorganic Chemistry</i> , 2014, 53, 3579-3585.	1.9	80
9	Chlorogenic Acid Inhibits Human Platelet Activation and Thrombus Formation. <i>PLoS ONE</i> , 2014, 9, e90699.	1.1	78
10	Linear and nonlinear modeling of antifungal activity of some heterocyclic ring derivatives using multiple linear regression and Bayesian-regularized neural networks. <i>Journal of Molecular Modeling</i> , 2006, 12, 168-181.	0.8	73
11	Artificial Neural Networks from MATLAB; in <i>Medicinal Chemistry. Bayesian-Regularized Genetic Neural Networks (BRGNN): Application to the Prediction of the Antagonistic Activity Against Human Platelet Thrombin Receptor (PAR-1)</i> . <i>Current Topics in Medicinal Chemistry</i> , 2008, 8, 1580-1605.	1.0	72
12	Study of the Differential Activity of Thrombin Inhibitors Using Docking, QSAR, Molecular Dynamics, and MM-GBSA. <i>PLoS ONE</i> , 2015, 10, e0142774.	1.1	70
13	Linear and nonlinear QSAR study of N-hydroxy-2-[(phenylsulfonyl)amino]acetamide derivatives as matrix metalloproteinase inhibitors. <i>Bioorganic and Medicinal Chemistry</i> , 2006, 14, 4137-4150.	1.4	63
14	Inhibition of Platelet Activation and Thrombus Formation by Adenosine and Inosine: Studies on Their Relative Contribution and Molecular Modeling. <i>PLoS ONE</i> , 2014, 9, e112741.	1.1	63
15	Rosmarinic acid prevents fibrillization and diminishes vibrational modes associated to β sheet in tau protein linked to Alzheimer's disease. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2017, 32, 945-953.	2.5	63
16	Modeling of farnesyltransferase inhibition by some thiol and non-thiol peptidomimetic inhibitors using genetic neural networks and RDF approaches. <i>Bioorganic and Medicinal Chemistry</i> , 2006, 14, 200-213.	1.4	62
17	3D-QSAR (CoMFA and CoMSIA) and pharmacophore (GALAHAD) studies on the differential inhibition of aldose reductase by flavonoid compounds. <i>Journal of Molecular Graphics and Modelling</i> , 2010, 29, 363-371.	1.3	61
18	Modeling of activity of cyclic urea HIV-1 protease inhibitors using regularized-artificial neural networks. <i>Bioorganic and Medicinal Chemistry</i> , 2006, 14, 280-294.	1.4	60

#	ARTICLE	IF	CITATIONS
19	Rationalizing the stability and interactions of 2,4-diamino-5-(4-chlorophenyl)-6-ethylpyrimidin-1-ium 2-hydroxy-3,5-dinitrobenzoate salt. <i>Journal of Molecular Structure</i> , 2019, 1193, 185-194.	1.8	60
20	Study of Interaction Energies between the PAMAM Dendrimer and Nonsteroidal Anti-Inflammatory Drug Using a Distributed Computational Strategy and Experimental Analysis by ESI-MS/MS. <i>Journal of Physical Chemistry B</i> , 2012, 116, 2031-2039.	1.2	59
21	Performance of the MM/GBSA scoring using a binding site hydrogen bond network-based frame selection: the protein kinase case. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 14047-14058.	1.3	58
22	Amino Acid Sequence Autocorrelation Vectors and Ensembles of Bayesian-Regularized Genetic Neural Networks for Prediction of Conformational Stability of Human Lysozyme Mutants. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 1255-1268.	2.5	57
23	Insights into the Structural Basis of N2 and O6 Substituted Guanine Derivatives as Cyclin-Dependent Kinase 2 (CDK2) Inhibitors: Prediction of the Binding Modes and Potency of the inhibitors by Docking and ONIOM Calculations. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 886-899.	2.5	57
24	Modeling of Cyclin-Dependent Kinase Inhibition by 1H-Pyrazolo[3,4-d]Pyrimidine Derivatives Using Artificial Neural Network Ensembles. <i>Journal of Chemical Information and Modeling</i> , 2005, 45, 1884-1895.	2.5	54
25	Proteometric study of ghrelin receptor function variations upon mutations using amino acid sequence autocorrelation vectors and genetic algorithm-based least square support vector machines. <i>Journal of Molecular Graphics and Modelling</i> , 2007, 26, 166-178.	1.3	53
26	Protective mechanisms of adenosine 5â€²-monophosphate in platelet activation and thrombus formation. <i>Thrombosis and Haemostasis</i> , 2014, 111, 491-507.	1.8	52
27	Secondary Metabolites in <i>Ramalina terebrata</i> Detected by UHPLC/ESI/MS/MS and Identification of Parietin as Tau Protein Inhibitor. <i>International Journal of Molecular Sciences</i> , 2016, 17, 1303.	1.8	50
28	Amino acid sequence autocorrelation vectors and bayesian-regularized genetic neural networks for modeling protein conformational stability: Gene V protein mutants. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 67, 834-852.	1.5	46
29	Identification of a potent and selective Î²1 receptor agonist potentiating NGF-induced neurite outgrowth in PC12 cells. <i>Bioorganic and Medicinal Chemistry</i> , 2011, 19, 6210-6224.	1.4	45
30	Study of differences in the VEGFR2 inhibitory activities between semaxanib and SU5205 using 3D-QSAR, docking, and molecular dynamics simulations. <i>Journal of Molecular Graphics and Modelling</i> , 2012, 32, 39-48.	1.3	44
31	QSAR analysis for heterocyclic antifungals. <i>Bioorganic and Medicinal Chemistry</i> , 2007, 15, 2680-2689.	1.4	42
32	Supramolecular assembly of Î²-cyclodextrin-modified gold nanoparticles and Cu, Zn-superoxide dismutase on catalase. <i>Journal of Molecular Catalysis B: Enzymatic</i> , 2005, 35, 79-85.	1.8	41
33	QSAR modeling of matrix metalloproteinase inhibition by N-hydroxy-Î±-phenylsulfonylacetamide derivatives. <i>Bioorganic and Medicinal Chemistry</i> , 2007, 15, 6298-6310.	1.4	40
34	A Novel Class of Selective Acetylcholinesterase Inhibitors: Synthesis and Evaluation of (E)-2-(Benzo[d]thiazol-2-yl)-3-heteroarylacrylonitriles. <i>Molecules</i> , 2012, 17, 12072-12085.	1.7	40
35	Quantitative Structureâ€“Activity Relationship of Rubiscolin Analogues as Î³ Opioid Peptides Using Comparative Molecular Field Analysis (CoMFA) and Comparative Molecular Similarity Indices Analysis (CoMSIA). <i>Journal of Agricultural and Food Chemistry</i> , 2007, 55, 8101-8104.	2.4	36
36	Bayesian-regularized genetic neural networks applied to the modeling of non-peptide antagonists for the human luteinizing hormone-releasing hormone receptor. <i>Journal of Molecular Graphics and Modelling</i> , 2006, 25, 410-422.	1.3	35

#	ARTICLE	IF	CITATIONS
37	Considerations for Docking of Selective Angiotensin-Converting Enzyme Inhibitors. <i>Molecules</i> , 2020, 25, 295.	1.7	35
38	1,3-Dipolar cycloaddition of nitrile imines with $\hat{1},\hat{1}^2$ -unsaturated lactones, thiolactones and lactams: synthesis of ring-fused pyrazoles. <i>Tetrahedron</i> , 2012, 68, 3319-3328.	1.0	34
39	Design, synthesis and cellular dynamics studies in membranes of a new coumarin-based "turn-off" fluorescent probe selective for Fe ²⁺ . <i>European Journal of Medicinal Chemistry</i> , 2013, 67, 60-63.	2.6	34
40	Modeling of the Inhibition Constant (K _i) of Some Cruzain Ketone-Based Inhibitors Using 2D Spatial Autocorrelation Vectors and Data-Diverse Ensembles of Bayesian-Regularized Genetic Neural Networks. <i>QSAR and Combinatorial Science</i> , 2007, 26, 27-40.	1.5	33
41	Computational Study on the Interaction of N1 Substituted Pyrazole Derivatives with B-Raf Kinase: An Unusual Water Wire Hydrogen-Bond Network and Novel Interactions at the Entrance of the Active Site. <i>Journal of Chemical Information and Modeling</i> , 2010, 50, 1101-1112.	2.5	33
42	Structural requirements of pyrido[2,3-d]pyrimidin-7-one as CDK4/D inhibitors: 2D autocorrelation, CoMFA and CoMSIA analyses. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 6103-6115.	1.4	32
43	Quality Threshold Clustering of Molecular Dynamics: A Word of Caution. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 467-472.	2.5	31
44	Docking and Quantitative Structure-Activity Relationship Studies for the Bisphenylbenzimidazole Family of Non-Nucleoside Inhibitors of HIV-1 Reverse Transcriptase. <i>Chemical Biology and Drug Design</i> , 2008, 72, 360-369.	1.5	30
45	Study of the Interaction between Progesterone and $\hat{1}^2$ -Cyclodextrin by Electrochemical Techniques and Steered Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2008, 112, 10194-10201.	1.2	30
46	Direct and Auger Electron-Induced, Single- and Double-Strand Breaks on Plasmid DNA Caused by ^{99m} Tc-Labeled Pyrene Derivatives and the Effect of Bonding Distance. <i>PLoS ONE</i> , 2016, 11, e0161973.	1.1	30
47	2D Autocorrelation modeling of the activity of trihalobenzocycloheptapyridine analogues as farnesyl protein transferase inhibitors. <i>Molecular Simulation</i> , 2005, 31, 575-584.	0.9	29
48	2D Autocorrelation modeling of the negative inotropic activity of calcium entry blockers using Bayesian-regularized genetic neural networks. <i>Bioorganic and Medicinal Chemistry</i> , 2006, 14, 3330-3340.	1.4	29
49	2D Autocorrelation, CoMFA, and CoMSIA modeling of protein tyrosine kinases™ inhibition by substituted pyrido[2,3-d]pyrimidine derivatives. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 810-821.	1.4	29
50	The latest automated docking technologies for novel drug discovery. <i>Expert Opinion on Drug Discovery</i> , 2021, 16, 625-645.	2.5	29
51	2D Autocorrelation Modelling of the Inhibitory Activity of Cytokinin-Derived Cyclin-Dependent Kinase Inhibitors. <i>Bulletin of Mathematical Biology</i> , 2006, 68, 735-751.	0.9	28
52	Insights into the Interactions between Maleimide Derivates and GSK3 ² Combining Molecular Docking and QSAR. <i>PLoS ONE</i> , 2014, 9, e102212.	1.1	28
53	Docking and quantitative structure-activity relationship studies for 3-fluoro-4-(pyrrolo[2,1-f][1,2,4]triazin-4-yloxy)aniline, 3-fluoro-4-(1H-pyrrolo[2,3-b]pyridin-4-yloxy)aniline, and 4-(4-amino-2-fluorophenoxy)-2-pyridinylamine derivatives as c-Met kinase inhibitors. <i>Journal of Computer-Aided Molecular Design</i> , 2011, 25, 349-369.	1.3	27
54	Synthesis, in silico, in vitro, and in vivo investigation of 5-[¹¹ C]methoxy-substituted sunitinib, a tyrosine kinase inhibitor of VEGFR-2. <i>European Journal of Medicinal Chemistry</i> , 2012, 58, 272-280.	2.6	27

#	ARTICLE	IF	CITATIONS
55	Association of nicotinic acid with a poly(amidoamine) dendrimer studied by molecular dynamics simulations. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 39, 71-78.	1.3	27
56	Flavonoids as CDK1 Inhibitors: Insights in Their Binding Orientations and Structure-Activity Relationship. <i>PLoS ONE</i> , 2016, 11, e0161111.	1.1	27
57	The receptor-like pseudokinase MRH1 interacts with the voltage-gated potassium channel AKT2. <i>Scientific Reports</i> , 2017, 7, 44611.	1.6	25
58	Modeling of acetylcholinesterase inhibition by tacrine analogues using Bayesian-regularized Genetic Neural Networks and ensemble averaging. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2006, 21, 647-661.	2.5	23
59	Docking and quantitative structure-activity relationship of oxadiazole derivatives as inhibitors of GSK3 β . <i>Molecular Diversity</i> , 2014, 18, 149-159.	2.1	23
60	Improved Anti-Inflammatory and Pharmacokinetic Properties for Superoxide Dismutase by Chemical Glycosidation with Carboxymethylchitin. <i>Macromolecular Bioscience</i> , 2005, 5, 118-123.	2.1	22
61	Ensembles of Bayesian-regularized Genetic Neural Networks for Modeling of Acetylcholinesterase Inhibition by Huprines. <i>Chemical Biology and Drug Design</i> , 2006, 68, 201-212.	1.5	22
62	Computational Study of the Interactions between Guanine Derivatives and Cyclin-Dependent Kinase 2 (CDK2) by CoMFA and QM/MM. <i>Journal of Chemical Information and Modeling</i> , 2010, 50, 110-122.	2.5	22
63	Insights into the structure of urea-like compounds as inhibitors of the juvenile hormone epoxide hydrolase (JHEH) of the tobacco hornworm <i>Manduca sexta</i> : Analysis of the binding modes and structure-activity relationships of the inhibitors by docking and CoMFA calculations. <i>Chemosphere</i> , 2011, 82, 1604-1613.	4.2	22
64	Computational study of the binding orientation and affinity of PPAR β agonists: inclusion of ligand-induced fit by cross-docking. <i>RSC Advances</i> , 2016, 6, 64756-64768.	1.7	22
65	Computational Studies of Snake Venom Toxins. <i>Toxins</i> , 2018, 10, 8.	1.5	22
66	Molecular dynamics simulations and CD spectroscopy reveal hydration-induced unfolding of the intrinsically disordered LEA proteins COR15A and COR15B from <i>Arabidopsis thaliana</i> . <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 25806-25816.	1.3	21
67	Folding and Lipid Composition Determine Membrane Interaction of the Disordered Protein COR15A. <i>Biophysical Journal</i> , 2018, 115, 968-980.	0.2	21
68	Omega hydroxylated JA-Ile is an endogenous bioactive jasmonate that signals through the canonical jasmonate signaling pathway. <i>Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids</i> , 2019, 1864, 158520.	1.2	21
69	Classification of conformational stability of protein mutants from 3D pseudo-folding graph representation of protein sequences using support vector machines. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 70, 167-175.	1.5	20
70	Molecular Dynamics of Protein Kinase-Inhibitor Complexes: A Valid Structural Information. <i>Current Pharmaceutical Design</i> , 2012, 18, 2946-2963.	0.9	20
71	The pH sensor of the plant K ⁺ -uptake channel KAT1 is built from a sensory cloud rather than from single key amino acids. <i>Biochemical Journal</i> , 2012, 442, 57-63.	1.7	20
72	Structural and Affinity Determinants in the Interaction between Alcohol Acyltransferase from <i>F. x ananassa</i> and Several Alcohol Substrates: A Computational Study. <i>PLoS ONE</i> , 2016, 11, e0153057.	1.1	20

#	ARTICLE	IF	CITATIONS
73	Adenosine A _{2A} receptor agonists with potent antiplatelet activity. <i>Platelets</i> , 2018, 29, 292-300.	1.1	20
74	BitClust: Fast Geometrical Clustering of Long Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 444-448.	2.5	20
75	Protein radial distribution function (P-RDF) and Bayesian-Regularized Genetic Neural Networks for modeling protein conformational stability: Chymotrypsin inhibitor 2 mutants. <i>Journal of Molecular Graphics and Modelling</i> , 2007, 26, 748-759.	1.3	19
76	Docking and quantitative structure-activity relationship studies for sulfonyl hydrazides as inhibitors of cytosolic human branched-chain amino acid aminotransferase. <i>Molecular Diversity</i> , 2009, 13, 493-500.	2.1	19
77	Effects of β -cyclodextrin-dextran polymer on stability properties of trypsin. <i>Biotechnology and Bioengineering</i> , 2003, 83, 743-747.	1.7	18
78	Investigation of the Differences in Activity between Hydroxycycloalkyl N1 Substituted Pyrazole Derivatives As Inhibitors of B-Raf Kinase by Using Docking, Molecular Dynamics, QM/MM, and Fragment-Based <i>De Novo</i> Design: Study of Binding Mode of Diastereomer Compounds. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 2920-2931.	2.5	18
79	Binding Studies and Quantitative Structure-Activity Relationship of 3-Amino-1H-Indazoles as Inhibitors of GSK3 β . <i>Chemical Biology and Drug Design</i> , 2011, 78, 631-641.	1.5	18
80	A coumarinyldoxime as a specific sensor for Cu ²⁺ and its biological application. <i>Tetrahedron Letters</i> , 2014, 55, 873-876.	0.7	18
81	Mycobacterium tuberculosis serine/threonine protein kinases: structural information for the design of their specific ATP-competitive inhibitors. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 1315-1336.	1.3	18
82	Estimation of 2D autocorrelation descriptors and 2D Monte Carlo descriptors as a tool to build up predictive models for acetylcholinesterase (AChE) inhibitory activity. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2019, 184, 14-21.	1.8	18
83	QSAR models for predicting the activity of non-peptide luteinizing hormone-releasing hormone (LHRH) antagonists derived from erythromycin A using quantum chemical properties. <i>Journal of Molecular Modeling</i> , 2007, 13, 465-476.	0.8	17
84	Ultrasound-assisted phase-transfer catalysis method in an aqueous medium to promote the Knoevenagel reaction: Advantages over the conventional and microwave-assisted solvent-free/catalyst-free method. <i>Ultrasonics Sonochemistry</i> , 2014, 21, 1666-1674.	3.8	17
85	Analyzing torquoselectivity in electrocyclic ring opening reactions of trans-3,4-dimethylcyclobutene and 3-formylcyclobutene through electronic structure principles. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 23104-23111.	1.3	17
86	K2P channels in plants and animals. <i>Pflügers Archiv European Journal of Physiology</i> , 2015, 467, 1091-1104.	1.3	17
87	Study of the Affinity between the Protein Kinase PKA and Peptide Substrates Derived from Kemptide Using Molecular Dynamics Simulations and MM/GBSA. <i>PLoS ONE</i> , 2014, 9, e109639.	1.1	17
88	A computational ONIOM model for the description of the H-bond interactions between NU2058 analogues and CDK2 active site. <i>Chemical Physics Letters</i> , 2009, 479, 149-155.	1.2	16
89	1-Benzyl-2,3,4-Tetrahydro- β -Carboline as Channel Blocker of N-Methyl-D-Aspartate Receptors. <i>Chemical Biology and Drug Design</i> , 2012, 79, 594-599.	1.5	16
90	Discovery of Novel TASK-3 Channel Blockers Using a Pharmacophore-Based Virtual Screening. <i>International Journal of Molecular Sciences</i> , 2019, 20, 4014.	1.8	16

#	ARTICLE	IF	CITATIONS
91	Genetic neural network modeling of the selective inhibition of the intermediate-conductance Ca ²⁺ -activated K ⁺ channel by some triarylmethanes using topological charge indexes descriptors. <i>Journal of Computer-Aided Molecular Design</i> , 2005, 19, 771-789.	1.3	15
92	Studying the phosphoryl transfer mechanism of the <i>E. coli</i> phosphofructokinase-2: from X-ray structure to quantum mechanics/molecular mechanics simulations. <i>Chemical Science</i> , 2019, 10, 2882-2892.	3.7	15
93	Docking, Interaction Fingerprint, and Three-Dimensional Quantitative Structure-Activity Relationship (3D-QSAR) of Sigma1 Receptor Ligands, Analogs of the Neuroprotective Agent RC-33. <i>Frontiers in Chemistry</i> , 2019, 7, 496.	1.8	14
94	In silico Comparison of Antimycobacterial Natural Products with Known Antituberculosis Drugs. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 649-660.	2.5	13
95	Understanding the comparative molecular field analysis (CoMFA) in terms of molecular quantum similarity and DFT-based reactivity descriptors. <i>Journal of Molecular Modeling</i> , 2015, 21, 156.	0.8	13
96	Synthesis of the Indolo[2,3-a]quinolizidine Ring through the Addition of 2-Siloxyfurans to Imines and Intrinsic Reaction Coordinate Calculations. <i>Synthesis</i> , 2012, 44, 144-150.	1.2	12
97	The Dynamic Nonprime Binding of Sampatrilat to the C-Domain of Angiotensin-Converting Enzyme. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 2486-2494.	2.5	12
98	Synthesis and in silico analysis of the quantitative structure-activity relationship of heteroaryl acrylonitriles as AChE inhibitors. <i>Journal of the Taiwan Institute of Chemical Engineers</i> , 2016, 59, 45-60.	2.7	12
99	In-Silico Design, Synthesis and Evaluation of a Nanostructured Hydrogel as a Dimethoate Removal Agent. <i>Nanomaterials</i> , 2018, 8, 23.	1.9	12
100	1,3-Dipolar Cycloaddition of Nitrile Imines with Cyclic Unsaturated Ketones: A Regiochemical Route to Ring-Fused Pyrazoles. <i>European Journal of Organic Chemistry</i> , 2011, 2011, 4806-4813.	1.2	11
101	Structural Requirements of N-alpha-Mercaptoacetyl Dipeptide (NAMdP) Inhibitors of <i>Pseudomonas Aeruginosa</i> Virulence Factor LasB: 3D-QSAR, Molecular Docking, and Interaction Fingerprint Studies. <i>International Journal of Molecular Sciences</i> , 2019, 20, 6133.	1.8	11
102	Development of indazolylpyrimidine derivatives as high-affine EphB4 receptor ligands and potential PET radiotracers. <i>Bioorganic and Medicinal Chemistry</i> , 2015, 23, 6025-6035.	1.4	10
103	A study of the cis-trans isomerization preference of N-alkylated peptides containing phosphorus in the side chain and backbone. <i>New Journal of Chemistry</i> , 2019, 43, 12804-12813.	1.4	10
104	New Insights into the Opening of the Occluded Ligand-Binding Pocket of Sigma1 Receptor: Binding of a Novel Bivalent RC-33 Derivative. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 756-765.	2.5	10
105	Coarse-Grained Parameters for Divalent Cations within the SIRAH Force Field. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3935-3943.	2.5	10
106	Study of the interactions between Edaglitazone and Ciglitazone with PPAR ^γ and their antiplatelet profile. <i>Life Sciences</i> , 2017, 186, 59-65.	2.0	9
107	On the Nature of the Enzyme-Substrate Complex and the Reaction Mechanism in Human Arginase I. A Combined Molecular Dynamics and QM/MM Study. <i>ACS Catalysis</i> , 2020, 10, 8321-8333.	5.5	9
108	Improved Pharmacological Properties for Superoxide Dismutase Modified with Carboxymethylcellulose. <i>Journal of Bioactive and Compatible Polymers</i> , 2005, 20, 557-570.	0.8	8

#	ARTICLE	IF	CITATIONS
109	Analyses of Synthetic <i>N</i> -Acyl Dopamine Derivatives Revealing Different Structural Requirements for Their Anti-inflammatory and Transient-Receptor-Potential-Channel-of-the-Vanilloid-Receptor-Subfamily-Subtype-1 (TRPV1)-Activating Properties. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 3126-3137.	2.9	8
110	Mechanistic insights into the phosphoryl transfer reaction in cyclin-dependent kinase 2: A QM/MM study. <i>PLoS ONE</i> , 2019, 14, e0215793.	1.1	8
111	Continental and Antarctic Lichens: isolation, identification and molecular modeling of the depside tenuiorin from the Antarctic lichen <i>Umbilicaria antarctica</i> as tau protein inhibitor. <i>Natural Product Research</i> , 2020, 34, 646-650.	1.0	8
112	Analysis of protegrin structure-activity relationships: the structural characteristics important for antimicrobial activity using smoothed amino acid sequence descriptors. <i>Molecular Simulation</i> , 2007, 33, 689-702.	0.9	7
113	Quantitative Structure-Activity Relationship Modeling of Growth Hormone Secretagogues Agonist Activity of some Tetrahydroisoquinoline 1-Carboxamides. <i>Chemical Biology and Drug Design</i> , 2007, 69, 48-55.	1.5	7
114	Inclusion complexes containing poly(ϵ -caprolactone)diol and cyclodextrins. Experimental and theoretical studies. <i>Polymer</i> , 2009, 50, 2926-2932.	1.8	7
115	Quantitative Structure-Activity Relationship of Organosulphur Compounds as Soybean 15-Lipoxygenase Inhibitors Using CoMFA and CoMSIA. <i>Chemical Biology and Drug Design</i> , 2010, 76, 511-517.	1.5	7
116	Identification of <i>Mycobacterium tuberculosis</i> CtpF as a target for designing new antituberculous compounds. <i>Bioorganic and Medicinal Chemistry</i> , 2020, 28, 115256.	1.4	7
117	Improved pharmacological properties for superoxide dismutase modified with mannan. <i>Biotechnology and Applied Biochemistry</i> , 2006, 44, 159.	1.4	6
118	Docking and quantitative structure-activity relationship studies for imidazo[1,2-a]pyrazines as inhibitors of checkpoint kinase-1. <i>Medicinal Chemistry Research</i> , 2012, 21, 1912-1920.	1.1	6
119	New insights into steric and electronic effects in a series of phosphine ligands from the perspective of local quantum similarity using the Fukui function. <i>Journal of Molecular Modeling</i> , 2015, 21, 45.	0.8	6
120	Study of the affinity between the protein kinase PKA and homoarginine-containing peptides derived from kemptide: Free energy perturbation (FEP) calculations. <i>Journal of Computational Chemistry</i> , 2018, 39, 986-992.	1.5	6
121	Insights into the Structural Requirements of 2(S)-Amino-6-Borono-hexanoic Acid Derivatives as Arginase I Inhibitors: 3D-QSAR, Docking, and Interaction Fingerprint Studies. <i>International Journal of Molecular Sciences</i> , 2018, 19, 2956.	1.8	6
122	Chalcone derivatives as non-canonical ligands of TRPV1. <i>International Journal of Biochemistry and Cell Biology</i> , 2019, 112, 18-23.	1.2	6
123	Dammarane triterpenes targeting \pm -synuclein: biological activity and evaluation of binding sites by molecular docking. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2021, 36, 154-162.	2.5	6
124	Computational Modeling to Explain Why 5,5-Diarylpentadienamides are TRPV1 Antagonists. <i>Molecules</i> , 2021, 26, 1765.	1.7	6
125	Bitopic Sigma 1 Receptor Modulators to Shed Light on Molecular Mechanisms Underpinning Ligand Binding and Receptor Oligomerization. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 14997-15016.	2.9	6
126	A CoMSIA study on the adenosine kinase inhibition of pyrrolo[2,3-d]pyrimidine nucleoside analogues. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 5103-5108.	1.4	5

#	ARTICLE	IF	CITATIONS
127	Proteometric Modeling of the Inhibition Complexes of Matrix Metalloproteinases with α -Hydroxy- β -(Phenylsulfonyl)Amino]Acetamide Derivatives Using Topological Autocorrelation Interaction Matrix and Model Ensemble Averaging. <i>Chemical Biology and Drug Design</i> , 2008, 72, 65-78.	1.5	5
128	Synthesis of coumarin derivatives as fluorescent probes for membrane and cell dynamics studies. <i>European Journal of Medicinal Chemistry</i> , 2014, 76, 79-86.	2.6	5
129	Optimal graph-based and Simplified Molecular Input Line Entry System-based descriptors for quantitative structure-activity relationship analysis of arylalkylaminoalcohols, arylalkenylamines, and arylalkylamines as 1 receptor ligands. <i>Journal of Chemometrics</i> , 2015, 29, 13-20.	0.7	5
130	Radiofluorinated ^{18}F -Octanoyl Dopamine (^{18}F -NOD) as a Tool To Study Tissue Distribution and Elimination of NOD in Vitro and in Vivo. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 9855-9865.	2.9	5
131	Docking and quantitative structure-activity relationship of bi-cyclic heteroaromatic pyridazinone and pyrazolone derivatives as phosphodiesterase 3A (PDE3A) inhibitors. <i>PLoS ONE</i> , 2017, 12, e0189213.	1.1	5
132	PSIQUE: Protein Secondary Structure Identification on the Basis of Quaternions and Electronic Structure Calculations. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 1789-1800.	2.5	5
133	Classification of conformational stability of protein mutants from 2D graph representation of protein sequences using support vector machines. <i>Molecular Simulation</i> , 2007, 33, 889-896.	0.9	4
134	Comparative modeling of the conformational stability of chymotrypsin inhibitor 2 protein mutants using amino acid sequence autocorrelation (AASA) and amino acid 3D autocorrelation (AA3DA) vectors and ensembles of Bayesian-regularized genetic neural networks. <i>Molecular Simulation</i> , 2007, 33, 1045-1056.	0.9	4
135	Modeling of the Inhibition of the Intermediate-Conductance Ca^{2+} -Activated K^{+} Channel (IKCa1) by Some Triarylmethanes Using Quantum Chemical Properties Derived From Ab Initio Calculations. <i>QSAR and Combinatorial Science</i> , 2008, 27, 866-875.	1.5	4
136	Models of the pharmacophoric pattern and affinity trend of methyl 2-(aminomethyl)-1-phenylcyclopropane-1-carboxylate derivatives as 1 ligands. <i>Molecular Simulation</i> , 2012, 38, 227-235.	0.9	4
137	HQSAR and molecular docking studies of furanyl derivatives as adenosine A2A receptor antagonists. <i>Medicinal Chemistry Research</i> , 2016, 25, 1316-1328.	1.1	4
138	BitQT: a graph-based approach to the quality threshold clustering of molecular dynamics. <i>Bioinformatics</i> , 2021, 38, 73-79.	1.8	4
139	RCDPeaks: memory-efficient density peaks clustering of long molecular dynamics. <i>Bioinformatics</i> , 2022, 38, 1863-1869.	1.8	4
140	Proteometric modelling of protein conformational stability using amino acid sequence autocorrelation vectors and genetic algorithm-optimised support vector machines. <i>Molecular Simulation</i> , 2008, 34, 857-872.	0.9	3
141	Transforming Non-Selective Angiotensin-Converting Enzyme Inhibitors in C- and N-domain Selective Inhibitors by Using Computational Tools. <i>Mini-Reviews in Medicinal Chemistry</i> , 2020, 20, 1436-1446.	1.1	3
142	SAR and QSAR Modeling of Juvenile Hormone Mimics. , 2013, , 159-188.		2
143	Molecular Modeling of Tau Proline-Directed Protein Kinase (PDPK) Inhibitors. <i>Neuromethods</i> , 2018, , 305-345.	0.2	2
144	Energetic differences between non-domain-swapped and domain-swapped chain connectivities in the K2P potassium channel TRAAK. <i>RSC Advances</i> , 2018, 8, 26610-26618.	1.7	2

#	ARTICLE	IF	CITATIONS
145	3D-QSAR Modeling of Non-peptide Antagonists for the Human Luteinizing Hormone-releasing Hormone Receptor. <i>Medicinal Chemistry</i> , 2013, 9, 560-570.	0.7	2
146	Graphical Representations of Protein Sequences for Alignment-Free Comparative and Predictive Studies. Recognition of Protease Inhibition Pattern from H-Depleted Molecular Graph Representation of Protease Sequences. <i>Current Bioinformatics</i> , 2010, 5, 241-252.	0.7	2
147	Easy Identification of Residues Involved on Structural Differences Between Nonphosphorylated and Phosphorylated CDK2/Cyclin A Complexes Using Two-Dimensional Networks. <i>Molecular Informatics</i> , 2014, 33, 151-162.	1.4	1
148	Genetic Algorithm Optimization of Bayesian-Regularized Artificial Neural Networks in Drug Design. , 2016, , 83-102.		1
149	Predicting the stability of human lysozyme mutants using the tree-based classifier TTOSOM. <i>Chemometrics and Intelligent Laboratory Systems</i> , 2017, 162, 65-72.	1.8	1
150	Synthesis of diN-Substituted Glycyl-Phenylalanine Derivatives by Using Ugi Four Component Reaction and Their Potential as Acetylcholinesterase Inhibitors. <i>Molecules</i> , 2019, 24, 189.	1.7	1
151	Multi-scale simulation reveals that an amino acid substitution increases photosensitizing reaction inputs in Rhodopsins. <i>Journal of Computational Chemistry</i> , 2020, 41, 2278-2295.	1.5	1
152	Editorial [Hot Topic: Protein Kinase Inhibitors: Current Strategies and Future Prospects (Executive) Tj ETQq0 0 0 rgBT/Overlock 10 Tf 50	0.9	0
153	Kristallografie - New Crystal Structures, 2016, 231, 171-173.	0.1	0
154	Free energy theoretical calculations of PKA-Kemptide complex formation, and effect of mutation of Kemptide arginines to homoarginines. , 0, , .		0