Visvaldas Kairys

List of Publications by Year
in descending order

58 papers	2,135 citations	331642 21 h-index	233409 45 g-index
60 all docs	60 docs citations	60 times ranked	2733 citing authors

#	Article	IF	Citations
1	Polyester Dendrimers Based on Bis-MPA for Doxorubicin Delivery. Biomacromolecules, 2022, 23, 20-33.	5.4	5
2	Beta and Gamma Amino Acid-Substituted Benzenesulfonamides as Inhibitors of Human Carbonic Anhydrases. Pharmaceuticals, 2022, 15, 477.	3.8	5
3	Enhanced nucleosome assembly at CpG sites containing an extended 5-methylcytosine analogue. Nucleic Acids Research, 2022, 50, 6549-6561.	14.5	5
4	Structure and mechanism of secondary sulfonamide binding to carbonic anhydrases. European Biophysics Journal, 2021, 50, 993-1011.	2.2	5
5	Biphenyl substituted lysine derivatives as recognition elements for the matrix metalloproteinases MMP-2 and MMP-9. Bioorganic Chemistry, 2021, 115, 105155.	4.1	7
6	Templateâ€based modeling of diverse protein interactions in CAPRI rounds 38â€45. Proteins: Structure, Function and Bioinformatics, 2020, 88, 939-947.	2.6	3
7	Isoform-Selective Enzyme Inhibitors by Exploring Pocket Size According to the Lock-and-Key Principle. Biophysical Journal, 2020, 119, 1513-1524.	0.5	6
8	The hydrolysis of indoxyl acetate: A versatile reaction to assay carbonic anhydrase activity by high-throughput screening. Enzyme and Microbial Technology, 2020, 139, 109584.	3.2	3
9	Recent Developments in Medicinal Chemistry of Allosteric Activators of Human Glucokinase for Type 2 Diabetes Mellitus Therapeutics. Current Pharmaceutical Design, 2020, 26, 2510-2552.	1.9	19
10	Mycobacterium tuberculosis Î²-Carbonic Anhydrases: Novel Targets for Developing Antituberculosis Drugs. International Journal of Molecular Sciences, 2019, 20, 5153.	4.1	28
11	Engineered Carbonic Anhydrase VI-Mimic Enzyme Switched the Structure and Affinities of Inhibitors. Scientific Reports, 2019, 9, 12710.	3.3	5
12	In Silico Modeling of Inhibitor Binding to Carbonic Anhydrases. , 2019, , 215-232.		0
13	Binding affinity in drug design: experimental and computational techniques. Expert Opinion on Drug Discovery, 2019, 14, 755-768.	5.0	75
14	Benzimidazole design, synthesis, and docking to build selective carbonic anhydrase VA inhibitors. Bioorganic and Medicinal Chemistry, 2018, 26, 675-687.	3.0	11
15	Molecular basis for potentiation of Cx36 gap junction channel conductance by n-alcohols and general anesthetics. Bioscience Reports, 2018, 38, .	2.4	6
16	Genome scale metabolic models as tools for drug design and personalized medicine. PLoS ONE, 2018, 13, e0190636.	2.5	35
17	Acetylcholine molecular arrays enable quantum information processing. Chemical Physics Letters, 2017, 684, 39-43.	2.6	0
18	Fluorinated benzenesulfonamide anticancer inhibitors of carbonic anhydrase IX exhibit lower toxic effects on zebrafish embryonic development than ethoxzolamide. Drug and Chemical Toxicology, 2017, 40, 309-319.	2.3	13

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19	Predicting Isoform-specific Binding Selectivities of Benzensulfonamides Using QSAR and 3D-QSAR. Current Computer-Aided Drug Design, 2017, 13, 75-83.	1.2	2
20	Spintronic characteristics of self-assembled neurotransmitter acetylcholine molecular complexes enable quantum information processing in neural networks and brain. Chemical Physics Letters, 2016, 660, 189-198.	2.6	2
21	COD::CIF::Parser: an error-correcting CIF parser for the Perl language. Journal of Applied Crystallography, 2016, 49, 292-301.	4.5	139
22	Synthesis and antiproliferative activity of Î±-branched Î±,Î²-unsaturated ketones in human hematological and solid cancer cell lines. European Journal of Medicinal Chemistry, 2015, 98, 30-48.	5.5	6
23	CLEA-Based Immobilization of Methylotropic Yeast Alcohol Oxidase: Influence on Storage Stability and Reaction Efficiency. Organic Process Research and Development, 2015, 19, 2025-2033.	2.7	7
24	Comparison of performance of docking, LIE, metadynamics and QSAR in predicting binding affinity of benzenesulfonamides. Current Computer-Aided Drug Design, 2015, 11, 237-244.	1.2	2
25	Saccharin Sulfonamides as Inhibitors of Carbonic Anhydrases I, II, VII, XII, and XIII. BioMed Research International, 2014, 2014, 1-9.	1.9	9
26	Monoclonal antibodies raised against 167â€"180 aa sequence of human carbonic anhydrase XII inhibit its enzymatic activity. Journal of Enzyme Inhibition and Medicinal Chemistry, 2014, 29, 804-810.	5.2	15
27	Conformational Analysis of Processivity Clamps in Solution Demonstrates that Tertiary Structure Does Not Correlate with Protein Dynamics. Structure, 2014, 22, 572-581.	3.3	30
28	Discovery and Characterization of Novel Selective Inhibitors of Carbonic Anhydrase IX. Journal of Medicinal Chemistry, 2014, 57, 9435-9446.	6.4	72
29	Intrinsic Thermodynamics and Structure Correlation of Benzenesulfonamides with a Pyrimidine Moiety Binding to Carbonic Anhydrases I, II, VII, XII, and XIII. PLoS ONE, 2014, 9, e114106.	2.5	19
30	Structural and functional analysis of rare missense mutations in human chorionic gonadotrophin Î²-subunit. Molecular Human Reproduction, 2012, 18, 379-390.	2.8	21
31	Insight into the role of N,N-dimethylaminoethyl methacrylate (DMAEMA) conjugation onto poly(ethylenimine): cell viability and gene transfection studies. Journal of Materials Science: Materials in Medicine, 2012, 23, 2967-2980.	3.6	21
32	Interaction of antimicrobial peptides, BP100 and pepR, with model membrane systems as explored by brownian dynamics simulations on a coarseâ€grained model. Biopolymers, 2012, 98, 294-312.	2.4	7
33	Enantioseparation and chiral recognition mechanism of new chiral derivatives of xanthones on macrocyclic antibiotic stationary phases. Journal of Chromatography A, 2012, 1241, 60-68.	3.7	48
34	Design of [(2-pyrimidinylthio)acetyl]benzenesulfonamides as inhibitors of human carbonic anhydrases. European Journal of Medicinal Chemistry, 2012, 51, 259-270.	5.5	33
35	Evaluating the Substrate-Envelope Hypothesis: Structural Analysis of Novel HIV-1 Protease Inhibitors Designed To Be Robust against Drug Resistance. Journal of Virology, 2010, 84, 5368-5378.	3.4	104
36	Study on the cyclization of 6-arylethynylpyrimidine-5-carbaldehydes with tert-butylamine: microwave versus thermal preparation of pyrido[4,3-d]pyrimidines. Tetrahedron, 2009, 65, 5752-5759.	1.9	17

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37	Quantitative Structureâ€“Activity Relationship Models with Receptorâ€Dependent Descriptors for Predicting Peroxisome Proliferatorâ€Activated Receptor Activities of Thiazolidinedione and Oxazolidinedione Derivatives. Chemical Biology and Drug Design, 2009, 73, 428-441.	3.2	4
38	Toward the Design of Mutationâ€Resistant Enzyme Inhibitors: Further Evaluation of the Substrate Envelope Hypothesis. Chemical Biology and Drug Design, 2009, 74, 234-245.	3.2	20
39	HIV-1 Protease Inhibitors from Inverse Design in the Substrate Envelope Exhibit Subnanomolar Binding to Drug-Resistant Variants. Journal of the American Chemical Society, 2008, 130, 6099-6113.	13.7	105
40	SitCon: Binding site residue conservation visualization and protein sequence-to-function tool. International Journal of Quantum Chemistry, 2007, 107, 2100-2110.	2.0	0
41	Evaluation of the substrate envelope hypothesis for inhibitors of HIV-1 protease. Proteins: Structure, Function and Bioinformatics, 2007, 68, 561-567.	2.6	48
42	Design of Mutation-resistant HIV Protease Inhibitors with the Substrate Envelope Hypothesis. Chemical Biology and Drug Design, 2007, 69, 298-313.	3.2	51
43	Screening Drug-Like Compounds by Docking to Homology Models:Â A Systematic Study. Journal of Chemical Information and Modeling, 2006, 46, 365-379.	5.4	82
44	Using Protein Homology Models for Structure-Based Studies: Approaches to Model Refinement. Scientific World Journal, The, 2006, 6, 1542-1554.	2.1	15
45	Structural model for an AxxxGâ€mediated dimer of surfactantâ€associated protein C. FEBS Journal, 2004, 271, 2086-2092.	0.2	28
46	Comparing Ligand Interactions with Multiple Receptors via Serial Docking. Journal of Chemical Information and Computer Sciences, 2004, 44, 1961-1970.	2.8	29
47	Solution Structure and Functional Ligand Screening of HI0719, a Highly Conserved Protein from Bacteria to Humans in the YjgF/YER057c/UK114 Familyâ€,â€¡. Biochemistry, 2003, 42, 80-89.	2.5	58
48	Enhanced docking with the mining minima optimizer: Acceleration and side-chain flexibility. Journal of Computational Chemistry, 2002, 23, 1656-1670.	3.3	51
49	The Effective Fragment Potential Method:Â A QM-Based MM Approach to Modeling Environmental Effects in Chemistry. Journal of Physical Chemistry A, 2001, 105, 293-307.	2.5	570
50	Accurate Intraprotein Electrostatics Derived from First Principles:Â An Effective Fragment Potential Method Study of the Proton Affinities of Lysine 55 and Tyrosine 20 in Turkey Ovomucoid Third Domain. Journal of Physical Chemistry A, 2001, 105, 3829-3837.	2.5	45
51	QM/MM Boundaries Across Covalent Bonds:Â A Frozen Localized Molecular Orbital-Based Approach for the Effective Fragment Potential Method. Journal of Physical Chemistry A, 2000, 104, 6656-6665.	2.5	136
52	Evaluation of the charge penetration energy between non-orthogonal molecular orbitals using the Spherical Gaussian Overlap approximation. Chemical Physics Letters, 1999, 315, 140-144.	2.6	61
53	Computation of adsorbate vibrational frequencies: methyl, methylidyne and methoxy adsorbed on the Al(111) surface. Computational and Theoretical Chemistry, 1999, 464, 153-162.	1.5	6
54	A quantum chemical cluster study of hydrated halide adsorption on the cathodic Al(111) surface. Surface Science, 1999, 440, 169-186.	1.9	9

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55	Electric field effects on the geometry and vibrations of charged molecules: the hydroxide ion case. Chemical Physics Letters, 1998, 288, 423-428.	2.6	4
56	Geometry Optimization of Charged Molecules in an External Electric Field Applied to F-Â·H2O and I-Â·H2O. Journal of Physical Chemistry A, 1998, 102, 1365-1370.	2.5	7
57	A theoretical investigation of adsorbate-induced surface relaxation effects using cluster models: Al on Si(111). Surface Science, 1997, 380, 283-292.	1.9	9
58	The mechanism of electroreduction of silver cyanide complexes in aqueous electrolytesâ€"II. Interpretation of SERS data. Electrochimica Acta, 1997, 42, 1345-1350.	5.2	12