Vytas Svedas

List of Publications by Year
in descending order

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114 papers	2,884 citations	159585 30 h-index	206112 48 g-index
116 all docs	116 docs citations	116 times ranked	2049 citing authors

#	Article	IF	Citations
1	Soft Tissue Sarcoma Study: Association of Genetic Alterations in the Apoptosis Pathways with Chemoresistance to Doxorubicin. Cancers, 2022, 14, 1796.	3.7	5
2	The role of Tyr102 residue in the functioning of bacterial NAD+-dependent formate dehydrogenase of Pseudomonas sp. 101. Biochemical and Biophysical Research Communications, 2022, 616, 134-139.	2.1	4
3	Mustguseal and Sister Web-Methods: A Practical Guide to Bioinformatic Analysis of Protein Superfamilies. Methods in Molecular Biology, 2021, 2231, 179-200.	0.9	6
4	Catalytic and lectin domains in neuraminidase A from Streptococcus pneumoniae are capable of an intermolecular assembly: Implications for biofilm formation. FEBS Journal, 2021, 288, 3217-3230.	4.7	7
5	Bioinformatic Analysis of the Nicotinamide Binding Site in Poly(ADP-Ribose) Polymerase Family Proteins. Cancers, 2021, 13, 1201.	3.7	11
6	Design, Synthesis, and Molecular Docking Study of New Tyrosyl-DNA Phosphodiesterase 1 (TDP1) Inhibitors Combining Resin Acids and Adamantane Moieties. Pharmaceuticals, 2021, 14, 422.	3.8	10
7	Prospects of Using Biocatalysis for the Synthesis and Modification of Polymers. Molecules, 2021, 26, 2750.	3.8	16
8	Bioinformatic analysis of subfamily-specific regions in 3D-structures of homologs to study functional diversity and conformational plasticity in protein superfamilies. Computational and Structural Biotechnology Journal, 2021, 19, 1302-1311.	4.1	11
9	Preparative Biocatalytic Synthesis of Î±-Ketoglutaramate. International Journal of Molecular Sciences, 2021, 22, 12748.	4.1	5
10	Bifunctional Inhibitors of Influenza Virus Neuraminidase: Molecular Design of a Sulfonamide Linker. International Journal of Molecular Sciences, 2021, 22, 13112.	4.1	6
11	Molecular Mechanisms of PARP-1 Inhibitor 7-Methylguanine. International Journal of Molecular Sciences, 2020, 21, 2159.	4.1	20
12	EasyAmber: A comprehensive toolbox to automate the molecular dynamics simulation of proteins. Journal of Bioinformatics and Computational Biology, 2020, 18, 2040011.	0.8	9
13	Zebra2: advanced and easy-to-use web-server for bioinformatic analysis of subfamily-specific and conserved positions in diverse protein superfamilies. Nucleic Acids Research, 2020, 48, W65-W71.	14.5	18
14	Human p38Î± mitogen-activated protein kinase in the Asp168-Phe169-Gly170-in (DFG-in) state can bind allosteric inhibitor Doramapimod. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2049-2060.	3.5	13
15	Inhibitory Effect of New Semisynthetic Usnic Acid Derivatives on Human Tyrosyl-DNA Phosphodiesterase 1. Planta Medica, 2019, 85, 103-111.	1.3	13
16	Yosshi: a web-server for disulfide engineering by bioinformatic analysis of diverse protein families. Nucleic Acids Research, 2019, 47, W308-W314.	14.5	18
17	The nature of the ligandâ€™s side chain interacting with the S1'-subsite of metallocarboxypeptidase T (from Thermoactinomyces vulgaris) determines the geometry of the tetrahedral transition complex. PLoS ONE, 2019, 14, e0226636.	2.5	4
18	High-Performance Hybrid Computing for Bioinformatic Analysis of Protein Superfamilies. Communications in Computer and Information Science, 2019, , 249-264.	0.5	0

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19	2,5-Diketopiperazines: A New Class of Poly(ADP-ribose)polymerase Inhibitors. Biochemistry (Moscow), 2018, 83, 152-158.	1.5	12
20	The visualCMAT: A web-server to select and interpret correlated mutations/co-evolving residues in protein families. Journal of Bioinformatics and Computational Biology, 2018, 16, 1840005.	0.8	16
21	Mustguseal: a server for multiple structure-guided sequence alignment of protein families. Bioinformatics, 2018, 34, 1583-1585.	4.1	31
22	Neuraminidase A from Streptococcus pneumoniae has a modular organization of catalytic and lectin domains separated by a flexible linker. FEBS Journal, 2018, 285, 2428-2445.	4.7	17
23	Structure of the carboxypeptidase B complex with N-sulfamoyl-L-phenylalanine â€“ a transition state analog of non-specific substrate. Journal of Biomolecular Structure and Dynamics, 2018, 36, 956-965.	3.5	7
24	Crystal structures of carboxypeptidase T complexes with transition-state analogs. Journal of Biomolecular Structure and Dynamics, 2018, 36, 3958-3966.	3.5	3
25	Molecular Modeling of the Binding of the Allosteric Inhibitor Optactin at a New Binding Site in Neuraminidase A from Streptococcus pneumoniae. Moscow University Chemistry Bulletin, 2018, 73, 205-211.	0.6	2
26	Study of the Conformational Variety of the Oligosaccharide Substrates of Neuraminidases from Pathogens using Molecular Modeling. Moscow University Chemistry Bulletin, 2018, 73, 39-45.	0.6	2
27	Bioinformatic analysis of the fold type I <scp>PLP</scp>â€dependent enzymes reveals determinants of reaction specificity in <scp>l</scp>â€threonine aldolase from Aeromonas jandaei. FEBS Open Bio, 2018, 8, 1013-1028.	2.3	33
28	Building a Full-Atom Model of L,Dtranspeptidase 2 from Mycobacterium tuberculosis for Screening New Inhibitors. Acta Naturae, 2017, 9, 44-51.	1.7	5
29	Parallel workflow manager for non-parallel bioinformatic applications to solve large-scale biological problems on a supercomputer. Journal of Bioinformatics and Computational Biology, 2016, 14, 1641008.	0.8	13
30	Tyrosyl-DNA Phosphodiesterase 1 Inhibitors: Usnic Acid Enamines Enhance the Cytotoxic Effect of Camptothecin. Journal of Natural Products, 2016, 79, 2961-2967.	3.0	65
31	Inhibition of Poly(ADP-Ribose) Polymerase by Nucleic Acid Metabolite 7-Methylguanine. Acta Naturae, 2016, 8, 108-115.	1.7	12
32	Identification of New Structural Fragments for the Design of Lactate Dehydrogenase A Inhibitors. Acta Naturae, 2016, 8, 118-122.	1.7	0
33	Robust enzyme design: Bioinformatic tools for improved protein stability. Biotechnology Journal, 2015, 10, 344-355.	3.5	65
34	The Î²D484N mutant of penicillin acylase from Escherichia coli is more resistant to inactivation by substrates and can effectively perform peptide synthesis in aqueous medium. Journal of Molecular Catalysis B: Enzymatic, 2015, 112, 66-68.	1.8	1
35	Structural insights into the broad substrate specificity of carboxypeptidase T from ThermoactinomycesÂvulgaris. FEBS Journal, 2015, 282, 1214-1224.	4.7	15
36	Computational Design of a pH Stable Enzyme: Understanding Molecular Mechanism of Penicillin Acylase's Adaptation to Alkaline Conditions. PLoS ONE, 2014, 9, e100643.	2.5	54

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37	Probing the Substrate Specificity and Intersubunit Interactions of <i>Brevundimonas Diminuta</i> Glutaryl Acylase with Site-Directed Mutagenesis. American Journal of Biochemistry and Biotechnology, 2014, 10, 169-179.	0.4	0
38	Bioinformatic analysis of protein families for identification of variable amino acid residues responsible for functional diversity. Journal of Biomolecular Structure and Dynamics, 2014, 32, 75-87.	3.5	30
39	Zebra: a web server for bioinformatic analysis of diverse protein families. Journal of Biomolecular Structure and Dynamics, 2014, 32, 1752-1758.	3.5	34
40	Catalytic Cycle of Penicillin Acylase from Escherichia coli: QM/MM Modeling of Chemical Transformations in the Enzyme Active Site upon Penicillin G Hydrolysis. ACS Catalysis, 2014, 4, 2521-2529.	11.2	24
41	pocketZebra: a web-server for automated selection and classification of subfamily-specific binding sites by bioinformatic analysis of diverse protein families. Nucleic Acids Research, 2014, 42, W344-W349.	14.5	28
42	Molecular modeling of different substrateâ€binding modes and their role in penicillin acylase catalysis. FEBS Journal, 2013, 280, 115-126.	4.7	13
43	Bioinformatic analysis of alpha/beta-hydrolase fold enzymes reveals subfamily-specific positions responsible for discrimination of amidase and lipase activities. Protein Engineering, Design and Selection, 2012, 25, 689-697.	2.1	48
44	Synthesis of Schiff bases from 3-amino-3-arylpropionic acid esters in aqueous medium. Russian Journal of Organic Chemistry, 2012, 48, 860-863.	0.8	0
45	Molecular modeling of formate dehydrogenase: the formation of the Michaelis complex. Journal of Biomolecular Structure and Dynamics, 2012, 30, 170-179.	3.5	17
46	BESSICC, a COSMOâ€RS based tool for in silico solvent screening of biocatalyzed reactions. Biotechnology and Bioengineering, 2012, 109, 1864-1868.	3.3	4
47	Thermodynamics of phenylacetamides synthesis: Linear free energy relationship with the pK of amine. Journal of Molecular Catalysis B: Enzymatic, 2012, 74, 48-53.	1.8	4
48	Investigation of formate transport through the substrate channel of formate dehydrogenase by steered molecular dynamics simulations. Biochemistry (Moscow), 2011, 76, 172-174.	1.5	5
49	Biologically active cyclic polypeptides with fragments of Î²-amino acid derivatives isolated from marine organisms (review). Chemistry of Heterocyclic Compounds, 2011, 47, 395-417.	1.2	7
50	Comparative Bioinformatic Analysis of Active Site Structures in Evolutionarily Remote Homologues of Î±,Î²-Hydrolase Superfamily Enzymes. Acta Naturae, 2011, 3, 93-98.	1.7	6
51	Guidelines for reporting of biocatalytic reactions. Trends in Biotechnology, 2010, 28, 171-180.	9.3	144
52	Novel inhibitors of glyceraldehyde-3-phosphate dehydrogenase: Covalent modification of NAD-binding site by aromatic thiols. Biochemistry (Moscow), 2010, 75, 1444-1449.	1.5	12
53	Penicillin Acylase-Catalyzed Effective and Stereoselective Acylation of 1-phenylethylamine in Aqueous Medium using Non-Activated Acyl Donor. Acta Naturae, 2010, 2, 94-96.	1.7	4
54	Bioinformatic Analysis, Molecular Modeling of Role of Lys65 Residue in Catalytic Triad of D-aminopeptidase from Ochrobactrum anthropi. Acta Naturae, 2010, 2, 66-70.	1.7	5

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55	Modeling of the Full-Size 3D Structure of Human Chaperone Hsp70 and Study of Its Interdomain Interactions. Acta Naturae, 2010, 2, 66-71.	1.7	5
56	Quantitative characteristic of the catalytic properties and microstructure of cross-linked enzyme aggregates of penicillin acylase. Journal of Molecular Catalysis B: Enzymatic, 2009, 56, 202-207.	1.8	45
57	Mutation of Residue Î²F71 of Escherichia coli Penicillin Acylase Results in Enhanced Enantioselectivity and Improved Catalytic Properties. Acta Naturae, 2009, 1, 94-98.	1.7	4
58	Thermodynamic and kinetic stability of penicillin acylase from Escherichia coli. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2008, 1784, 736-746.	2.3	12
59	Cloning of penicillin acylase from Escherichia coli: Catalytic properties of recombinant enzymes. Moscow University Chemistry Bulletin, 2008, 63, 103-107.	0.6	3
60	Molecular modeling studies of substrate binding by penicillin acylase. Biochemistry (Moscow), 2008, 73, 56-64.	1.5	7
61	A green, fully enzymatic procedure for amine resolution, using a lipase and a penicillin G acylase. Green Chemistry, 2008, 10, 415.	9.0	28
62	Saturation mutagenesis reveals the importance of residues Î±R145 and Î±F146 of penicillin acylase in the synthesis of Î²-lactam antibiotics. Journal of Biotechnology, 2008, 133, 18-26.	3.8	34
63	Professor Dr Roger A. Sheldonâ€"65 years on. Green Chemistry, 2008, 10, 270.	9.0	0
64	Chiral high-performance liquid chromatography analysis of Î±-amino acid mixtures using a novel SH reagentâ€"N-R-mandelyl-l-cysteine and traditional enantiomeric thiols for precolumn derivatization. Journal of Chromatography A, 2007, 1175, 89-95.	3.7	19
65	Quantum chemical studies of the catalytic mechanism of N-terminal nucleophile hydrolase. Biochemistry (Moscow), 2007, 72, 495-500.	1.5	11
66	A new method for spectrophotometric assay of activity of cross-linked penicillin acylase aggregates. Biochemistry (Moscow), 2006, 71, 315-319.	1.5	3
67	Efficient enantiomeric analysis of primary amines and amino alcohols by high-performance liquid chromatography with precolumn derivatization using novel chiral SH-reagent N-(R)-mandelyl-(S)-cysteine. Journal of Chromatography A, 2005, 1095, 89-93.	3.7	21
68	Aliphatic Amidase from Rhodococcus rhodochrous M8 Is Related to the Nitrilase/Cyanide Hydratase Family. Biochemistry (Moscow), 2005, 70, 1280-1287.	1.5	15
69	Use of high acyl donor concentrations leads to penicillin acylase inactivation in the course of peptide synthesis. Journal of Molecular Catalysis B: Enzymatic, 2004, 31, 63-65.	1.8	3
70	An â€˜easy-on, easy-offâ€™ protecting group for the enzymatic resolution of (Â±)-1-phenylethylamine in an aqueous medium. Tetrahedron: Asymmetry, 2004, 15, 2901-2906.	1.8	22
71	pH stability of penicillin acylase from Escherichia coli. Biochemistry (Moscow), 2004, 69, 1386-1390.	1.5	13
72	Penicillin acylase-catalyzed synthesis of ?-lactam antibiotics in highly condensed aqueous systems: Beneficial impact of kinetic substrate supersaturation. Biotechnology and Bioengineering, 2004, 85, 323-329.	3.3	54

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73	Application of aminoacylase I to the enantioselective resolution of Î±-amino acid esters and amides. Tetrahedron: Asymmetry, 2004, 15, 1933-1936.	1.8	25
74	Study of nucleophile binding in the penicillin acylase active center. Kinetic analysis. Biochemistry (Moscow), 2003, 68, 334-338.	1.5	9
75	Penicillin acylase-catalyzed peptide synthesis in aqueous medium: a chemo-enzymatic route to stereoisomerically pure diketopiperazines. Tetrahedron: Asymmetry, 2003, 14, 3123-3128.	1.8	24
76	Force field parametrization for 6-aminopenicillanic acid. Computational and Theoretical Chemistry, 2003, 631, 117-125.	1.5	8
77	Resolution of (RS)-phenylglycinonitrile by penicillin acylase-catalyzed acylation in aqueous medium. Tetrahedron: Asymmetry, 2003, 14, 2613-2617.	1.8	23
78	Enzymatic hydrolysis of Î²-lactam antibiotics at low pH in a two-phase "aqueous solution - water-immiscible organic solvent" system. Canadian Journal of Chemistry, 2002, 80, 699-707.	1.1	15
79	Penicillin Acylase-Catalyzed Solid-State Ampicillin Synthesis. Advanced Synthesis and Catalysis, 2002, 344, 894-898.	4.3	19
80	Penicillin acylase-catalyzed ampicillin synthesis using a pH gradient: A new approach to optimization. Biotechnology and Bioengineering, 2002, 78, 589-593.	3.3	40
81	Active site titration as a tool for the evaluation of immobilization procedures of penicillin acylase. Biotechnology and Bioengineering, 2002, 79, 224-228.	3.3	48
82	Quantitative characterization of the nucleophile reactivity in penicillin acylase-catalyzed acyl transfer reactions. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2002, 1599, 134-140.	2.3	60
83	Highly efficient and enantioselective enzymatic acylation of amines in aqueous medium. Tetrahedron: Asymmetry, 2001, 12, 1645-1650.	1.8	49
84	Highly efficient synthesis of ampicillin in an ?aqueous solution-precipitate? system: Repetitive addition of substrates in a semicontinuous process. Biotechnology and Bioengineering, 2001, 73, 426-430.	3.3	56
85	Penicillin acylase-catalyzed peptide synthesis: a chemo-enzymatic route to stereoisomers of 3,6-diphenylpiperazine-2,5-dione. Tetrahedron: Asymmetry, 2000, 11, 1077-1083.	1.8	34
86	Penicillin acylase-catalyzed resolution of amines in aqueous organic solvents. Tetrahedron: Asymmetry, 2000, 11, 4593-4600.	1.8	59
87	Penicillin acylase-catalyzed synthesis of ampicillin in â€œaqueous solutionâ€“precipitateâ€•systems. High substrate concentration and supersaturation effect. Journal of Molecular Catalysis B: Enzymatic, 2000, 10, 509-515.	1.8	58
88	Kinetics of ampicillin synthesis catalyzed by penicillin acylase from E. coli in homogeneous and heterogeneous systems. Quantitative characterization of nucleophile reactivity and mathematical modeling of the process. , 2000, 65, 1367-1375.		26
89	Totally Enzymatic Synthesis of Peptides: Penicillin Acylase-Catalyzed Protection and Deprotection of Amino Groups as Important Building Blocks of This Strategy. Annals of the New York Academy of Sciences, 1998, 864, 524-527.	3.8	7
90	Biomimetic Transamination of Î±-Alkyl Î²-Keto Carboxylic Esters. Chemoenzymatic Approach to the Stereochemically Defined Î±-Alkyl Î²-Fluoroalkyl Î²-Amino Acids. Journal of Organic Chemistry, 1998, 63, 1878-1884.	3.2	80

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91	Kinetic study of penicillin acylase from Alcaligenes faecalis. FEBS Letters, 1997, 417, 414-418.	2.8	62
92	Comparative Modeling of Substrate Binding in the S1â€˜ Subsite of Serine Carboxypeptidases from Yeast, Wheat, and Humanâ€. Biochemistry, 1996, 35, 14899-14909.	2.5	14
93	Continuous Spectrophotometric Assay of Human Lysosomal Cathepsin A/Protective Protein in Normal and Galactosialidosis Cells. Analytical Biochemistry, 1995, 230, 303-307.	2.4	20
94	Biocatalytic approach to enantiomerically pure Î²-amino acids. Tetrahedron: Asymmetry, 1995, 6, 1601-1610.	1.8	94
95	Biocatalytic resolution of Î²-fluoroalkyl-Î²-amino acids. Tetrahedron: Asymmetry, 1994, 5, 1119-1126.	1.8	74
96	Chemo-enzymatic approach to the synthesis of each of the four isomers of Î±-alkyl-Î²-fluoroalkyl-substituted Î²-amino acids. Tetrahedron: Asymmetry, 1994, 5, 1225-1228.	1.8	77
97	Enzymatic preparation of both L- and D-enantiomers of phosphonic and phosphonous analogues of alanine using penicillin acylase. Tetrahedron: Asymmetry, 1993, 4, 1965-1968.	1.8	35
98	Influence of the immunization against heterologous alcohol dehydrogenase on liver alcohol dehydrogenase isozymes and alcohol abuse of rats. FEBS Journal, 1993, 212, 757-761.	0.2	11
99	Penicillin acylase-catalyzed protection and deprotection of amino groups as a promising approach in enzymatic peptide synthesis. FEBS Letters, 1991, 287, 31-33.	2.8	46
100	Hydrophobicity of Î²-lactam antibiotics. Journal of Chromatography A, 1991, 585, 3-34.	3.7	13
101	Preparation of optically active 1-aminoalkylphosphonic acids by stereoselective enzymatic hydrolysis of racemic N-acylated 1-aminoalkylphosphonic acids. Tetrahedron, 1991, 47, 3989-3998.	1.9	49
102	Increased nucleophile reactivity of amino acid Î²-naphthylamides in Î±-chymotrypsin-catalyzed peptide synthesis. BBA - Proteins and Proteomics, 1990, 1041, 71-78.	2.1	10
103	Acyl group transfer by proteases forming an acylenzyme intermediate: Kinetic model analysis (including hydrolysis of acylenzyme-nucleophile complex). Journal of Theoretical Biology, 1989, 140, 193-204.	1.7	25
104	The methyl ester of Î±-aminophenylacetic acid: pH-dependence and phosphate catalysis of hydrolysis. Journal of the Chemical Society Perkin Transactions II, 1986, , 1537-1540.	0.9	5
105	A kinetic study of hog kidney aminoacylase. BBA - Proteins and Proteomics, 1982, 701, 389-394.	2.1	29
106	Soluble-insoluble immobilized enzymes. Biotechnology and Bioengineering, 1982, 24, 237-240.	3.3	31
107	Preparation and properties of penicillin amidase immobilized in polyelectrolyte complexes. Biochimica Et Biophysica Acta - Biomembranes, 1981, 660, 359-365.	2.6	47
108	The interaction of amino acids with o-phthaldialdehyde: A kinetic study and spectrophotometric assay of the reaction product. Analytical Biochemistry, 1980, 101, 188-195.	2.4	146

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109	Enzymatic synthesis of Î²-lactam antibiotics: A thermodynamic background. Enzyme and Microbial Technology, 1980, 2, 138-144.	3.2	78
110	Kinetics of the enzymatic synthesis of benzylpenicillin. Enzyme and Microbial Technology, 1980, 2, 313-317.	3.2	35
111	Substrate specificity of penicillin amidase from E. coli. Biochimica Et Biophysica Acta - Biomembranes, 1980, 616, 283-289.	2.6	90
112	The effect of ultrasound as a new method of studying conformational transitions in enzyme active sites. FEBS Letters, 1975, 49, 325-328.	2.8	15
113	The Mechanism of the alpha-Chymotrypsin and Trypsin-Catalyzed Hydrolysis of Amides. Evidence for the Participation of the Active Serine in the amidase Activity of Trypsin. FEBS Journal, 1973, 38, 529-536.	0.2	11
114	Co-designing HPC-systems by computing capabilities and management flexibility to accommodate bioinformatic workflows at different complexity levels. Journal of Supercomputing, 0, , 1.	3.6	2