Vytas Svedas

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

108 papers	2,406 citations	29 h-index	44 g-index
116 ext. papers	2,579 ext. citations	4.2 avg, IF	4.78 L-index

#	Paper	IF	Citations
108	Bioinformatic Analysis of the Nicotinamide Binding Site in Poly(ADP-Ribose) Polymerase Family Proteins. *Cancers*, **2021**, 13,	6.6	7
107	Prospects of Using Biocatalysis for the Synthesis and Modification of Polymers. *Molecules*, **2021**, 26,	4.8	8
106	Mustguseal and Sister Web-Methods: A Practical Guide to Bioinformatic Analysis of Protein Superfamilies. *Methods in Molecular Biology*, **2021**, 2231, 179-200	1.4	4
105	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	5.7	3
104	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	6.8	6
103	Bifunctional Inhibitors of Influenza Virus Neuraminidase: Molecular Design of a Sulfonamide Linker. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	1
102	Molecular Mechanisms of PARP-1 Inhibitor 7-Methylguanine. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	12
101	EasyAmber: A comprehensive toolbox to automate the molecular dynamics simulation of proteins. *Journal of Bioinformatics and Computational Biology*, **2020**, 18, 2040011	1	6
100	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	20.1	12
99	Yosshi: a web-server for disulfide engineering by bioinformatic analysis of diverse protein families. *Nucleic Acids Research*, **2019**, 47, W308-W314	20.1	13
98	Human p38□ 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	3.6	10
97	Inhibitory Effect of New Semisynthetic Usnic Acid Derivatives on Human Tyrosyl-DNA Phosphodiesterase 1. *Planta Medica*, **2019**, 85, 103-111	3.1	9
96	High-Performance Hybrid Computing for Bioinformatic Analysis of Protein Superfamilies. *Communications in Computer and Information Science*, **2019**, 249-264	0.3	
95	The nature of the ligand'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	3.7	4
94	2,5-Diketopiperazines: A New Class of Poly(ADP-ribose)polymerase Inhibitors. *Biochemistry (Moscow)*, **2018**, 83, 152-158	2.9	8
93	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	1	12
92	Mustguseal: a server for multiple structure-guided sequence alignment of protein families. *Bioinformatics*, **2018**, 34, 1583-1585	7.2	23

91	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	5.7	14
90	Structure of the carboxypeptidase B complex with N-sulfamoyl-L-phenylalanine - a transition state analog of non-specific substrate. *Journal of Biomolecular Structure and Dynamics*, **2018**, 36, 956-965	3.6	7
89	Bioinformatic analysis of the fold type I PLP-dependent enzymes reveals determinants of reaction specificity in l-threonine aldolase from. *FEBS Open Bio*, **2018**, 8, 1013-1028	2.7	18
88	Crystal structures of carboxypeptidase T complexes with transition-state analogs. *Journal of Biomolecular Structure and Dynamics*, **2018**, 36, 3958-3966	3.6	3
87	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	0.5	2
86	Study of the Conformational Variety of the Oligosaccharide Substrates of Neuraminidases from Pathogens using Molecular Modeling. *Moscow University Chemistry Bulletin*, **2018**, 73, 39-45	0.5	2
85	Building a Full-Atom Model of L,Dtranspeptidase 2 from Mycobacterium tuberculosis for Screening New Inhibitors. *Acta Naturae*, **2017**, 9, 44-51	2.1	4
84	Tyrosyl-DNA Phosphodiesterase 1 Inhibitors: Usnic Acid Enamines Enhance the Cytotoxic Effect of Camptothecin. *Journal of Natural Products*, **2016**, 79, 2961-2967	4.9	48
83	Inhibition of Poly(ADP-Ribose) Polymerase by Nucleic Acid Metabolite 7-Methylguanine. *Acta Naturae*, **2016**, 8, 108-115	2.1	7
82	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	1	10
81	Structural insights into the broad substrate specificity of carboxypeptidase T from Thermoactinomyces vulgaris. *FEBS Journal*, **2015**, 282, 1214-24	5.7	12
80	Robust enzyme design: bioinformatic tools for improved protein stability. *Biotechnology Journal*, **2015**, 10, 344-55	5.6	49
79	The D484N 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
78	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	13.1	19
77	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, W344-9	20.1	22
76	Computational design of a pH stable enzyme: understanding molecular mechanism of penicillin acylase's adaptation to alkaline conditions. *PLoS ONE*, **2014**, 9, e100643	3.7	42
75	Probing the Substrate Specificity and Intersubunit Interactions of Brevundimonas Diminuta Glutaryl Acylase with Site-Directed Mutagenesis. *American Journal of Biochemistry and Biotechnology*, **2014**, 10, 169-179	0.4	
74	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	3.6	26

73	Zebra: a web server for bioinformatic analysis of diverse protein families. *Journal of Biomolecular Structure and Dynamics*, **2014**, 32, 1752-8	3.6	29
72	Molecular modeling of different substrate-binding modes and their role in penicillin acylase catalysis. *FEBS Journal*, **2013**, 280, 115-26	5.7	11
71	Thermodynamics of phenylacetamides synthesis: Linear free energy relationship with the pK of amine. *Journal of Molecular Catalysis B: Enzymatic*, **2012**, 74, 48-53		3
70	Synthesis of Schiff bases from 3-amino-3-arylpropionic acid esters in aqueous medium. *Russian Journal of Organic Chemistry*, **2012**, 48, 860-863	0.7	
69	Molecular modeling of formate dehydrogenase: the formation of the Michaelis complex. *Journal of Biomolecular Structure and Dynamics*, **2012**, 30, 170-9	3.6	12
68	BESSICC, a COSMO-RS based tool for in silico solvent screening of biocatalyzed reactions. *Biotechnology and Bioengineering*, **2012**, 109, 1864-8	4.9	4
67	Bioinformatic analysis of □/□hydrolase fold enzymes reveals subfamily-specific positions responsible for discrimination of amidase and lipase activities. *Protein Engineering, Design and Selection*, **2012**, 25, 689-97	1.9	41
66	Investigation of formate transport through the substrate channel of formate dehydrogenase by steered molecular dynamics simulations. *Biochemistry (Moscow)*, **2011**, 76, 172-4	2.9	3
65	Biologically active cyclic polypeptides with fragments of □amino acid derivatives isolated from marine organisms (review). *Chemistry of Heterocyclic Compounds*, **2011**, 47, 395-417	1.4	5
64	Comparative Bioinformatic Analysis of Active Site Structures in Evolutionarily Remote Homologues of □,□Hydrolase Superfamily Enzymes. *Acta Naturae*, **2011**, 3, 93-98	2.1	4
63	Novel inhibitors of glyceraldehyde-3-phosphate dehydrogenase: covalent modification of NAD-binding site by aromatic thiols. *Biochemistry (Moscow)*, **2010**, 75, 1444-9	2.9	11
62	Guidelines for reporting of biocatalytic reactions. *Trends in Biotechnology*, **2010**, 28, 171-80	15.1	126
61	Penicillin Acylase-Catalyzed Effective and Stereoselective Acylation of 1-phenylethylamine in Aqueous Medium using Non-Activated Acyl Donor. *Acta Naturae*, **2010**, 2, 94-96	2.1	4
60	Bioinformatic Analysis, Molecular Modeling of Role of Lys65 Residue in Catalytic Triad of D-aminopeptidase from Ochrobactrum anthropi. *Acta Naturae*, **2010**, 2, 66-70	2.1	3
59	Modeling of the Full-Size 3D Structure of Human Chaperone Hsp70 and Study of Its Interdomain Interactions. *Acta Naturae*, **2010**, 2, 66-71	2.1	5
58	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		39
57	Mutation of Residue □71 of Escherichia coli Penicillin Acylase Results in Enhanced Enantioselectivity and Improved Catalytic Properties. *Acta Naturae*, **2009**, 1, 94-98	2.1	2
56	Molecular modeling studies of substrate binding by penicillin acylase. *Biochemistry (Moscow)*, **2008**, 73, 56-64	2.9	6

55	A green, fully enzymatic procedure for amine resolution, using a lipase and a penicillin G acylase. *Green Chemistry*, **2008**, 10, 415	10	24
54	Saturation mutagenesis reveals the importance of residues alphaR145 and alphaF146 of penicillin acylase in the synthesis of beta-lactam antibiotics. *Journal of Biotechnology*, **2008**, 133, 18-26	3.7	25
53	Thermodynamic and kinetic stability of penicillin acylase from Escherichia coli. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2008**, 1784, 736-46	4	12
52	Cloning of penicillin acylase from Escherichia coli: Catalytic properties of recombinant enzymes. *Moscow University Chemistry Bulletin*, **2008**, 63, 103-107	0.5	2
51	Chiral high-performance liquid chromatography analysis of alpha-amino acid mixtures using a novel SH reagent--N-R-mandelyl-L-cysteine and traditional enantiomeric thiols for precolumn derivatization. *Journal of Chromatography A*, **2007**, 1175, 89-95	4.5	16
50	Quantum chemical studies of the catalytic mechanism of N-terminal nucleophile hydrolase. *Biochemistry (Moscow)*, **2007**, 72, 495-500	2.9	8
49	A new method for spectrophotometric assay of activity of cross-linked penicillin acylase aggregates. *Biochemistry (Moscow)*, **2006**, 71, 315-9	2.9	3
48	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	4.5	18
47	Aliphatic amidase from Rhodococcus rhodochrous M8 is related to the nitrilase/cyanide hydratase family. *Biochemistry (Moscow)*, **2005**, 70, 1280-7	2.9	13
46	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		3
45	An easy-on, easy-off protecting group for the enzymatic resolution of (±)-1-phenylethylamine in an aqueous medium. *Tetrahedron: Asymmetry*, **2004**, 15, 2901-2906		19
44	pH Stability of penicillin acylase from Escherichia coli. *Biochemistry (Moscow)*, **2004**, 69, 1386-90	2.9	12
43	Penicillin acylase-catalyzed synthesis of beta-lactam antibiotics in highly condensed aqueous systems: beneficial impact of kinetic substrate supersaturation. *Biotechnology and Bioengineering*, **2004**, 85, 323-9	4.9	48
42	Application of aminoacylase I to the enantioselective resolution of α-amino acid esters and amides. *Tetrahedron: Asymmetry*, **2004**, 15, 1933-1936		21
41	Study of nucleophile binding in the penicillin acylase active center. Kinetic analysis. *Biochemistry (Moscow)*, **2003**, 68, 334-8	2.9	8
40	Penicillin acylase-catalyzed peptide synthesis in aqueous medium: a chemo-enzymatic route to stereoisomerically pure diketopiperazines. *Tetrahedron: Asymmetry*, **2003**, 14, 3123-3128		21
39	Force field parametrization for 6-aminopenicillanic acid. *Computational and Theoretical Chemistry*, **2003**, 631, 117-125		8
38	Resolution of (RS)-phenylglycinonitrile by penicillin acylase-catalyzed acylation in aqueous medium. *Tetrahedron: Asymmetry*, **2003**, 14, 2613-2617		21

37	Penicillin Acylase-Catalyzed Solid-State Ampicillin Synthesis. *Advanced Synthesis and Catalysis*, **2002**, 344, 894-898	5.6	15
36	Penicillin acylase-catalyzed ampicillin synthesis using a pH gradient: a new approach to optimization. *Biotechnology and Bioengineering*, **2002**, 78, 589-93	4.9	36
35	Active site titration as a tool for the evaluation of immobilization procedures of penicillin acylase. *Biotechnology and Bioengineering*, **2002**, 79, 224-8	4.9	39
34	Quantitative characterization of the nucleophile reactivity in penicillin acylase-catalyzed acyl transfer reactions. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2002**, 1599, 134-40	4	53
33	Enzymatic hydrolysis of β-lactam antibiotics at low pH in a two-phase "aqueous solution - water-immiscible organic solvent" system. *Canadian Journal of Chemistry*, **2002**, 80, 699-707	0.9	13
32	Highly efficient and enantioselective enzymatic acylation of amines in aqueous medium. *Tetrahedron: Asymmetry*, **2001**, 12, 1645-1650		43
31	Highly efficient synthesis of ampicillin in an "aqueous solution-precipitate" system: repetitive addition of substrates in a semicontinuous process. *Biotechnology and Bioengineering*, **2001**, 73, 426-30	4.9	51
30	Penicillin acylase-catalyzed peptide synthesis: a chemo-enzymatic route to stereoisomers of 3,6-diphenylpiperazine-2,5-dione. *Tetrahedron: Asymmetry*, **2000**, 11, 1077-1083		31
29	Penicillin acylase-catalyzed resolution of amines in aqueous organic solvents. *Tetrahedron: Asymmetry*, **2000**, 11, 4593-4600		53
28	Penicillin acylase-catalyzed synthesis of ampicillin in "aqueous solution–precipitate" systems. High substrate concentration and supersaturation effect. *Journal of Molecular Catalysis B: Enzymatic*, **2000**, 10, 509-515		48
27	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. *Biochemistry (Moscow)*, **2000**, 65, 1367-75	2.9	22
26	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, 524-7	6.5	5
25	Biomimetic Transamination of α-Alkyl β-Keto Carboxylic Esters. Chemoenzymatic Approach to the Stereochemically Defined β-Alkyl β-Fluoroalkyl β-Amino Acids. *Journal of Organic Chemistry*, **1998**, 63, 1878-1884	4.2	75
24	Kinetic study of penicillin acylase from Alcaligenes faecalis. *FEBS Letters*, **1997**, 417, 414-8	3.8	51
23	Comparative modeling of substrate binding in the S1' subsite of serine carboxypeptidases from yeast, wheat, and human. *Biochemistry*, **1996**, 35, 14899-909	3.2	12
22	Biocatalytic approach to enantiomerically pure β-amino acids. *Tetrahedron: Asymmetry*, **1995**, 6, 1601-1610		88
21	Continuous spectrophotometric assay of human lysosomal cathepsin A/protective protein in normal and galactosialidosis cells. *Analytical Biochemistry*, **1995**, 230, 303-7	3.1	18
20	Biocatalytic resolution of β-Fluoroalkyl-β-amino acids. *Tetrahedron: Asymmetry*, **1994**, 5, 1119-1126		69

19	Chemo-enzymatic approach to the synthesis of each of the four isomers of □-alkyl-□fluoroalkyl-substituted □amino acids. *Tetrahedron: Asymmetry*, **1994**, 5, 1225-1228		74
18	Enzymatic preparation of both L- and D-enantiomers of phosphonic and phosphonous analogues of alanine using penicillin acylase. *Tetrahedron: Asymmetry*, **1993**, 4, 1965-1968		33
17	Influence of the immunization against heterologous alcohol dehydrogenase on liver alcohol dehydrogenase isozymes and alcohol abuse of rats. *FEBS Journal*, **1993**, 212, 757-61		9
16	Hydrophobicity of beta-lactam antibiotics. Explanation and prediction of their behaviour in various partitioning solvent systems and reversed-phase chromatography. *Journal of Chromatography A*, **1991**, 585, 3-34	4.5	11
15	Preparation of optically active 1-aminoalkylphosphonic acids by stereoselective enzymatic hydrolysis of racemic N-acylated 1-aminoalkylphosphonic acids. *Tetrahedron*, **1991**, 47, 3989-3998	2.4	46
14	Penicillin acylase-catalyzed protection and deprotection of amino groups as a promising approach in enzymatic peptide synthesis. *FEBS Letters*, **1991**, 287, 31-3	3.8	38
13	Increased nucleophile reactivity of amino acid beta-naphthylamides in alpha-chymotrypsin-catalyzed peptide synthesis. *BBA - Proteins and Proteomics*, **1990**, 1041, 71-8		10
12	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	2.3	25
11	The methyl ester of □-aminophenylacetic acid: pH-dependence and phosphate catalysis of hydrolysis. *Journal of the Chemical Society Perkin Transactions II*, **1986**, 1537-1540		4
10	A kinetic study of hog kidney aminoacylase. *BBA - Proteins and Proteomics*, **1982**, 701, 389-94		23
9	Soluble-insoluble immobilized enzymes. *Biotechnology and Bioengineering*, **1982**, 24, 237-40	4.9	21
8	Preparation and properties of penicillin amidase immobilized in polyelectrolyte complexes. *Biochimica Et Biophysica Acta - Biomembranes*, **1981**, 660, 359-65	3.8	35
7	The interaction of amino acids with ophthaldialdehyde: a kinetic study and spectrophotometric assay of the reaction product. *Analytical Biochemistry*, **1980**, 101, 188-95	3.1	130
6	Enzymatic synthesis of □lactam antibiotics: A thermodynamic background. *Enzyme and Microbial Technology*, **1980**, 2, 138-144	3.8	72
5	Kinetics of the enzymatic synthesis of benzylpenicillin. *Enzyme and Microbial Technology*, **1980**, 2, 313-317	3.8	29
4	Substrate specificity of penicillin amidase from E. coli. *Biochimica Et Biophysica Acta - Biomembranes* , **1980**, 616, 283-9	3.8	75
3	The effect of ultrasound as a new method of studying conformational transitions in enzyme active sites. pH- and temperature-induced conformational transitions in the active centre of penicillin amidase. *FEBS Letters*, **1975**, 49, 325-8	3.8	10
2	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, 529-36		10

1	Co-designing HPC-systems by computing capabilities and management flexibility to accommodate bioinformatic workflows at different complexity levels. *Journal of Supercomputing*,1	2.5	1