

# Vytas Svedas

## List of Publications by Citations

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108  
papers

2,406  
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29  
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116  
ext. papers

2,579  
ext. citations

4.2  
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4.78  
L-index

#	Paper	IF	Citations
108	The interaction of amino acids with ophthaldialdehyde: a kinetic study and spectrophotometric assay of the reaction product. <i>Analytical Biochemistry</i> , <b>1980</b> , 101, 188-95	3.1	130
107	Guidelines for reporting of biocatalytic reactions. <i>Trends in Biotechnology</i> , <b>2010</b> , 28, 171-80	15.1	126
106	Biocatalytic approach to enantiomerically pure $\alpha$ -amino acids. <i>Tetrahedron: Asymmetry</i> , <b>1995</b> , 6, 1601-1610		88
105	Biomimetic Transamination of $\beta$ -Alkyl $\beta$ -Keto Carboxylic Esters. Chemoenzymatic Approach to the Stereochemically Defined $\beta$ -Alkyl $\beta$ -Fluoroalkyl $\beta$ -Amino Acids. <i>Journal of Organic Chemistry</i> , <b>1998</b> , 63, 1878-1884	4.2	75
104	Substrate specificity of penicillin amidase from <i>E. coli</i> . <i>Biochimica Et Biophysica Acta - Biomembranes</i> , <b>1980</b> , 616, 283-9	3.8	75
103	Chemo-enzymatic approach to the synthesis of each of the four isomers of $\beta$ -alkyl- $\beta$ -fluoroalkyl-substituted $\beta$ -amino acids. <i>Tetrahedron: Asymmetry</i> , <b>1994</b> , 5, 1225-1228		74
102	Enzymatic synthesis of $\beta$ -lactam antibiotics: A thermodynamic background. <i>Enzyme and Microbial Technology</i> , <b>1980</b> , 2, 138-144	3.8	72
101	Biocatalytic resolution of $\beta$ -fluoroalkyl- $\beta$ -amino acids. <i>Tetrahedron: Asymmetry</i> , <b>1994</b> , 5, 1119-1126		69
100	Quantitative characterization of the nucleophile reactivity in penicillin acylase-catalyzed acyl transfer reactions. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , <b>2002</b> , 1599, 134-40	4	53
99	Penicillin acylase-catalyzed resolution of amines in aqueous organic solvents. <i>Tetrahedron: Asymmetry</i> , <b>2000</b> , 11, 4593-4600		53
98	Kinetic study of penicillin acylase from <i>Alcaligenes faecalis</i> . <i>FEBS Letters</i> , <b>1997</b> , 417, 414-8	3.8	51
97	Highly efficient synthesis of ampicillin in an "aqueous solution-precipitate" system: repetitive addition of substrates in a semicontinuous process. <i>Biotechnology and Bioengineering</i> , <b>2001</b> , 73, 426-30	4.9	51
96	Robust enzyme design: bioinformatic tools for improved protein stability. <i>Biotechnology Journal</i> , <b>2015</b> , 10, 344-55	5.6	49
95	Tyrosyl-DNA Phosphodiesterase 1 Inhibitors: Usnic Acid Enamines Enhance the Cytotoxic Effect of Camptothecin. <i>Journal of Natural Products</i> , <b>2016</b> , 79, 2961-2967	4.9	48
94	Penicillin acylase-catalyzed synthesis of beta-lactam antibiotics in highly condensed aqueous systems: beneficial impact of kinetic substrate supersaturation. <i>Biotechnology and Bioengineering</i> , <b>2004</b> , 85, 323-9	4.9	48
93	Penicillin acylase-catalyzed synthesis of ampicillin in aqueous solution-precipitate systems. High substrate concentration and supersaturation effect. <i>Journal of Molecular Catalysis B: Enzymatic</i> , <b>2000</b> , 10, 509-515		48
92	Preparation of optically active 1-aminoalkylphosphonic acids by stereoselective enzymatic hydrolysis of racemic N-acylated 1-aminoalkylphosphonic acids. <i>Tetrahedron</i> , <b>1991</b> , 47, 3989-3998	2.4	46

91	Highly efficient and enantioselective enzymatic acylation of amines in aqueous medium. <i>Tetrahedron: Asymmetry</i> , <b>2001</b> , 12, 1645-1650		43
90	Computational design of a pH stable enzyme: understanding molecular mechanism of penicillin acylase's adaptation to alkaline conditions. <i>PLoS ONE</i> , <b>2014</b> , 9, e100643	3.7	42
89	Bioinformatic analysis of $\beta$ / $\gamma$ -hydrolase fold enzymes reveals subfamily-specific positions responsible for discrimination of amidase and lipase activities. <i>Protein Engineering, Design and Selection</i> , <b>2012</b> , 25, 689-97	1.9	41
88	Quantitative characteristic of the catalytic properties and microstructure of cross-linked enzyme aggregates of penicillin acylase. <i>Journal of Molecular Catalysis B: Enzymatic</i> , <b>2009</b> , 56, 202-207		39
87	Active site titration as a tool for the evaluation of immobilization procedures of penicillin acylase. <i>Biotechnology and Bioengineering</i> , <b>2002</b> , 79, 224-8	4.9	39
86	Penicillin acylase-catalyzed protection and deprotection of amino groups as a promising approach in enzymatic peptide synthesis. <i>FEBS Letters</i> , <b>1991</b> , 287, 31-3	3.8	38
85	Penicillin acylase-catalyzed ampicillin synthesis using a pH gradient: a new approach to optimization. <i>Biotechnology and Bioengineering</i> , <b>2002</b> , 78, 589-93	4.9	36
84	Preparation and properties of penicillin amidase immobilized in polyelectrolyte complexes. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , <b>1981</b> , 660, 359-65	3.8	35
83	Enzymatic preparation of both L- and D-enantiomers of phosphonic and phosphonous analogues of alanine using penicillin acylase. <i>Tetrahedron: Asymmetry</i> , <b>1993</b> , 4, 1965-1968		33
82	Penicillin acylase-catalyzed peptide synthesis: a chemo-enzymatic route to stereoisomers of 3,6-diphenylpiperazine-2,5-dione. <i>Tetrahedron: Asymmetry</i> , <b>2000</b> , 11, 1077-1083		31
81	Zebra: a web server for bioinformatic analysis of diverse protein families. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2014</b> , 32, 1752-8	3.6	29
80	Kinetics of the enzymatic synthesis of benzylpenicillin. <i>Enzyme and Microbial Technology</i> , <b>1980</b> , 2, 313-317	3.8	29
79	Bioinformatic analysis of protein families for identification of variable amino acid residues responsible for functional diversity. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2014</b> , 32, 75-87	3.6	26
78	Saturation mutagenesis reveals the importance of residues alphaR145 and alphaF146 of penicillin acylase in the synthesis of beta-lactam antibiotics. <i>Journal of Biotechnology</i> , <b>2008</b> , 133, 18-26	3.7	25
77	Acyl group transfer by proteases forming an acylenzyme intermediate: kinetic model analysis (including hydrolysis of acylenzyme- nucleophile complex). <i>Journal of Theoretical Biology</i> , <b>1989</b> , 140, 193-204	2.3	25
76	A green, fully enzymatic procedure for amine resolution, using a lipase and a penicillin G acylase. <i>Green Chemistry</i> , <b>2008</b> , 10, 415	10	24
75	Mustguseal: a server for multiple structure-guided sequence alignment of protein families. <i>Bioinformatics</i> , <b>2018</b> , 34, 1583-1585	7.2	23
74	A kinetic study of hog kidney aminoacylase. <i>BBA - Proteins and Proteomics</i> , <b>1982</b> , 701, 389-94		23

73	pocketZebra: a web-server for automated selection and classification of subfamily-specific binding sites by bioinformatic analysis of diverse protein families. <i>Nucleic Acids Research</i> , <b>2014</b> , 42, W344-9	20.1	22
72	Kinetics of ampicillin synthesis catalyzed by penicillin acylase from <i>E. coli</i> in homogeneous and heterogeneous systems. Quantitative characterization of nucleophile reactivity and mathematical modeling of the process. <i>Biochemistry (Moscow)</i> , <b>2000</b> , 65, 1367-75	2.9	22
71	Application of aminoacylase I to the enantioselective resolution of $\beta$ -amino acid esters and amides. <i>Tetrahedron: Asymmetry</i> , <b>2004</b> , 15, 1933-1936		21
70	Penicillin acylase-catalyzed peptide synthesis in aqueous medium: a chemo-enzymatic route to stereoisomerically pure diketopiperazines. <i>Tetrahedron: Asymmetry</i> , <b>2003</b> , 14, 3123-3128		21
69	Resolution of (RS)-phenylglycinonitrile by penicillin acylase-catalyzed acylation in aqueous medium. <i>Tetrahedron: Asymmetry</i> , <b>2003</b> , 14, 2613-2617		21
68	Soluble-insoluble immobilized enzymes. <i>Biotechnology and Bioengineering</i> , <b>1982</b> , 24, 237-40	4.9	21
67	Catalytic Cycle of Penicillin Acylase from <i>Escherichia coli</i> : QM/MM Modeling of Chemical Transformations in the Enzyme Active Site upon Penicillin G Hydrolysis. <i>ACS Catalysis</i> , <b>2014</b> , 4, 2521-2529	13.1	19
66	An Easy-on, easy-off protecting group for the enzymatic resolution of ( $\beta$ )-1-phenylethylamine in an aqueous medium. <i>Tetrahedron: Asymmetry</i> , <b>2004</b> , 15, 2901-2906		19
65	Bioinformatic analysis of the fold type I PLP-dependent enzymes reveals determinants of reaction specificity in l-threonine aldolase from. <i>FEBS Open Bio</i> , <b>2018</b> , 8, 1013-1028	2.7	18
64	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. <i>Journal of Chromatography A</i> , <b>2005</b> , 1095, 89-93	4.5	18
63	Continuous spectrophotometric assay of human lysosomal cathepsin A/protective protein in normal and galactosialidosis cells. <i>Analytical Biochemistry</i> , <b>1995</b> , 230, 303-7	3.1	18
62	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. <i>Journal of Chromatography A</i> , <b>2007</b> , 1175, 89-95	4.5	16
61	Penicillin Acylase-Catalyzed Solid-State Ampicillin Synthesis. <i>Advanced Synthesis and Catalysis</i> , <b>2002</b> , 344, 894-898	5.6	15
60	Neuraminidase A from <i>Streptococcus pneumoniae</i> has a modular organization of catalytic and lectin domains separated by a flexible linker. <i>FEBS Journal</i> , <b>2018</b> , 285, 2428-2445	5.7	14
59	Yosshi: a web-server for disulfide engineering by bioinformatic analysis of diverse protein families. <i>Nucleic Acids Research</i> , <b>2019</b> , 47, W308-W314	20.1	13
58	Aliphatic amidase from <i>Rhodococcus rhodochrous</i> M8 is related to the nitrilase/cyanide hydratase family. <i>Biochemistry (Moscow)</i> , <b>2005</b> , 70, 1280-7	2.9	13
57	Enzymatic hydrolysis of $\beta$ -lactam antibiotics at low pH in a two-phase "aqueous solution - water-immiscible organic solvent" system. <i>Canadian Journal of Chemistry</i> , <b>2002</b> , 80, 699-707	0.9	13
56	Structural insights into the broad substrate specificity of carboxypeptidase T from <i>Thermoactinomyces vulgaris</i> . <i>FEBS Journal</i> , <b>2015</b> , 282, 1214-24	5.7	12

55	Molecular Mechanisms of PARP-1 Inhibitor 7-Methylguanine. <i>International Journal of Molecular Sciences</i> , <b>2020</b> , 21,	6.3	12
54	The visualCMAT: A web-server to select and interpret correlated mutations/co-evolving residues in protein families. <i>Journal of Bioinformatics and Computational Biology</i> , <b>2018</b> , 16, 1840005	1	12
53	Molecular modeling of formate dehydrogenase: the formation of the Michaelis complex. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2012</b> , 30, 170-9	3.6	12
52	Thermodynamic and kinetic stability of penicillin acylase from <i>Escherichia coli</i> . <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , <b>2008</b> , 1784, 736-46	4	12
51	pH Stability of penicillin acylase from <i>Escherichia coli</i> . <i>Biochemistry (Moscow)</i> , <b>2004</b> , 69, 1386-90	2.9	12
50	Comparative modeling of substrate binding in the S1' subsite of serine carboxypeptidases from yeast, wheat, and human. <i>Biochemistry</i> , <b>1996</b> , 35, 14899-909	3.2	12
49	Zebra2: advanced and easy-to-use web-server for bioinformatic analysis of subfamily-specific and conserved positions in diverse protein superfamilies. <i>Nucleic Acids Research</i> , <b>2020</b> , 48, W65-W71	20.1	12
48	Molecular modeling of different substrate-binding modes and their role in penicillin acylase catalysis. <i>FEBS Journal</i> , <b>2013</b> , 280, 115-26	5.7	11
47	Novel inhibitors of glyceraldehyde-3-phosphate dehydrogenase: covalent modification of NAD-binding site by aromatic thiols. <i>Biochemistry (Moscow)</i> , <b>2010</b> , 75, 1444-9	2.9	11
46	Hydrophobicity of beta-lactam antibiotics. Explanation and prediction of their behaviour in various partitioning solvent systems and reversed-phase chromatography. <i>Journal of Chromatography A</i> , <b>1991</b> , 585, 3-34	4.5	11
45	Human p38 $\beta$ mitogen-activated protein kinase in the Asp168-Phe169-Gly170-in (DFG-in) state can bind allosteric inhibitor Doramapimod. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2019</b> , 37, 2049-2060	3.6	10
44	Increased nucleophile reactivity of amino acid beta-naphthylamides in alpha-chymotrypsin-catalyzed peptide synthesis. <i>BBA - Proteins and Proteomics</i> , <b>1990</b> , 1041, 71-8		10
43	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. <i>FEBS Letters</i> , <b>1975</b> , 49, 325-8	3.8	10
42	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. <i>FEBS Journal</i> , <b>1973</b> , 38, 529-36		10
41	Parallel workflow manager for non-parallel bioinformatic applications to solve large-scale biological problems on a supercomputer. <i>Journal of Bioinformatics and Computational Biology</i> , <b>2016</b> , 14, 1641008	1	10
40	Inhibitory Effect of New Semisynthetic Usnic Acid Derivatives on Human Tyrosyl-DNA Phosphodiesterase 1. <i>Planta Medica</i> , <b>2019</b> , 85, 103-111	3.1	9
39	Influence of the immunization against heterologous alcohol dehydrogenase on liver alcohol dehydrogenase isozymes and alcohol abuse of rats. <i>FEBS Journal</i> , <b>1993</b> , 212, 757-61		9
38	2,5-Diketopiperazines: A New Class of Poly(ADP-ribose)polymerase Inhibitors. <i>Biochemistry (Moscow)</i> , <b>2018</b> , 83, 152-158	2.9	8

37	Quantum chemical studies of the catalytic mechanism of N-terminal nucleophile hydrolase. <i>Biochemistry (Moscow)</i> , <b>2007</b> , 72, 495-500	2.9	8
36	Study of nucleophile binding in the penicillin acylase active center. Kinetic analysis. <i>Biochemistry (Moscow)</i> , <b>2003</b> , 68, 334-8	2.9	8
35	Force field parametrization for 6-aminopenicillanic acid. <i>Computational and Theoretical Chemistry</i> , <b>2003</b> , 631, 117-125		8
34	Prospects of Using Biocatalysis for the Synthesis and Modification of Polymers. <i>Molecules</i> , <b>2021</b> , 26,	4.8	8
33	Structure of the carboxypeptidase B complex with N-sulfamoyl-L-phenylalanine - a transition state analog of non-specific substrate. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2018</b> , 36, 956-965	3.6	7
32	Inhibition of Poly(ADP-Ribose) Polymerase by Nucleic Acid Metabolite 7-Methylguanine. <i>Acta Naturae</i> , <b>2016</b> , 8, 108-115	2.1	7
31	Bioinformatic Analysis of the Nicotinamide Binding Site in Poly(ADP-Ribose) Polymerase Family Proteins. <i>Cancers</i> , <b>2021</b> , 13,	6.6	7
30	EasyAmber: A comprehensive toolbox to automate the molecular dynamics simulation of proteins. <i>Journal of Bioinformatics and Computational Biology</i> , <b>2020</b> , 18, 2040011	1	6
29	Molecular modeling studies of substrate binding by penicillin acylase. <i>Biochemistry (Moscow)</i> , <b>2008</b> , 73, 56-64	2.9	6
28	Bioinformatic analysis of subfamily-specific regions in 3D-structures of homologs to study functional diversity and conformational plasticity in protein superfamilies. <i>Computational and Structural Biotechnology Journal</i> , <b>2021</b> , 19, 1302-1311	6.8	6
27	Biologically active cyclic polypeptides with fragments of $\alpha$ -amino acid derivatives isolated from marine organisms (review). <i>Chemistry of Heterocyclic Compounds</i> , <b>2011</b> , 47, 395-417	1.4	5
26	Totally enzymatic synthesis of peptides. Penicillin acylase-catalyzed protection and deprotection of amino groups as important building blocks of this strategy. <i>Annals of the New York Academy of Sciences</i> , <b>1998</b> , 864, 524-7	6.5	5
25	Modeling of the Full-Size 3D Structure of Human Chaperone Hsp70 and Study of Its Interdomain Interactions. <i>Acta Naturae</i> , <b>2010</b> , 2, 66-71	2.1	5
24	BESSICC, a COSMO-RS based tool for in silico solvent screening of biocatalyzed reactions. <i>Biotechnology and Bioengineering</i> , <b>2012</b> , 109, 1864-8	4.9	4
23	The methyl ester of $\beta$ -aminophenylacetic acid: pH-dependence and phosphate catalysis of hydrolysis. <i>Journal of the Chemical Society Perkin Transactions II</i> , <b>1986</b> , 1537-1540		4
22	Penicillin Acylase-Catalyzed Effective and Stereoselective Acylation of 1-phenylethylamine in Aqueous Medium using Non-Activated Acyl Donor. <i>Acta Naturae</i> , <b>2010</b> , 2, 94-96	2.1	4
21	Comparative Bioinformatic Analysis of Active Site Structures in Evolutionarily Remote Homologues of $\beta$ , $\beta$ -Hydrolase Superfamily Enzymes. <i>Acta Naturae</i> , <b>2011</b> , 3, 93-98	2.1	4
20	Building a Full-Atom Model of L,D-transpeptidase 2 from <i>Mycobacterium tuberculosis</i> for Screening New Inhibitors. <i>Acta Naturae</i> , <b>2017</b> , 9, 44-51	2.1	4

19	The nature of the ligand's side chain interacting with the S1'-subsite of metalloprotease T (from <i>Thermoactinomyces vulgaris</i> ) determines the geometry of the tetrahedral transition complex. <i>PLoS ONE</i> , <b>2019</b> , 14, e0226636	3.7	4
18	Mustguseal and Sister Web-Methods: A Practical Guide to Bioinformatic Analysis of Protein Superfamilies. <i>Methods in Molecular Biology</i> , <b>2021</b> , 2231, 179-200	1.4	4
17	Thermodynamics of phenylacetamides synthesis: Linear free energy relationship with the pK of amine. <i>Journal of Molecular Catalysis B: Enzymatic</i> , <b>2012</b> , 74, 48-53		3
16	Investigation of formate transport through the substrate channel of formate dehydrogenase by steered molecular dynamics simulations. <i>Biochemistry (Moscow)</i> , <b>2011</b> , 76, 172-4	2.9	3
15	A new method for spectrophotometric assay of activity of cross-linked penicillin acylase aggregates. <i>Biochemistry (Moscow)</i> , <b>2006</b> , 71, 315-9	2.9	3
14	Use of high acyl donor concentrations leads to penicillin acylase inactivation in the course of peptide synthesis. <i>Journal of Molecular Catalysis B: Enzymatic</i> , <b>2004</b> , 31, 63-65		3
13	Bioinformatic Analysis, Molecular Modeling of Role of Lys65 Residue in Catalytic Triad of D-aminopeptidase from <i>Ochrobactrum anthropi</i> . <i>Acta Naturae</i> , <b>2010</b> , 2, 66-70	2.1	3
12	Catalytic and lectin domains in neuraminidase A from <i>Streptococcus pneumoniae</i> are capable of an intermolecular assembly: Implications for biofilm formation. <i>FEBS Journal</i> , <b>2021</b> , 288, 3217-3230	5.7	3
11	Crystal structures of carboxypeptidase T complexes with transition-state analogs. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2018</b> , 36, 3958-3966	3.6	3
10	Cloning of penicillin acylase from <i>Escherichia coli</i> : Catalytic properties of recombinant enzymes. <i>Moscow University Chemistry Bulletin</i> , <b>2008</b> , 63, 103-107	0.5	2
9	Mutation of Residue E71 of <i>Escherichia coli</i> Penicillin Acylase Results in Enhanced Enantioselectivity and Improved Catalytic Properties. <i>Acta Naturae</i> , <b>2009</b> , 1, 94-98	2.1	2
8	Molecular Modeling of the Binding of the Allosteric Inhibitor Optactin at a New Binding Site in Neuraminidase A from <i>Streptococcus pneumoniae</i> . <i>Moscow University Chemistry Bulletin</i> , <b>2018</b> , 73, 205-211	0.5	2
7	Study of the Conformational Variety of the Oligosaccharide Substrates of Neuraminidases from Pathogens using Molecular Modeling. <i>Moscow University Chemistry Bulletin</i> , <b>2018</b> , 73, 39-45	0.5	2
6	The D484N mutant of penicillin acylase from <i>Escherichia coli</i> is more resistant to inactivation by substrates and can effectively perform peptide synthesis in aqueous medium. <i>Journal of Molecular Catalysis B: Enzymatic</i> , <b>2015</b> , 112, 66-68		1
5	Co-designing HPC-systems by computing capabilities and management flexibility to accommodate bioinformatic workflows at different complexity levels. <i>Journal of Supercomputing</i> , 1	2.5	1
4	Bifunctional Inhibitors of Influenza Virus Neuraminidase: Molecular Design of a Sulfonamide Linker. <i>International Journal of Molecular Sciences</i> , <b>2021</b> , 22,	6.3	1
3	Probing the Substrate Specificity and Intersubunit Interactions of <i>Brevundimonas Diminuta</i> Glutaryl Acylase with Site-Directed Mutagenesis. <i>American Journal of Biochemistry and Biotechnology</i> , <b>2014</b> , 10, 169-179	0.4	
2	Synthesis of Schiff bases from 3-amino-3-arylpropionic acid esters in aqueous medium. <i>Russian Journal of Organic Chemistry</i> , <b>2012</b> , 48, 860-863	0.7	

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