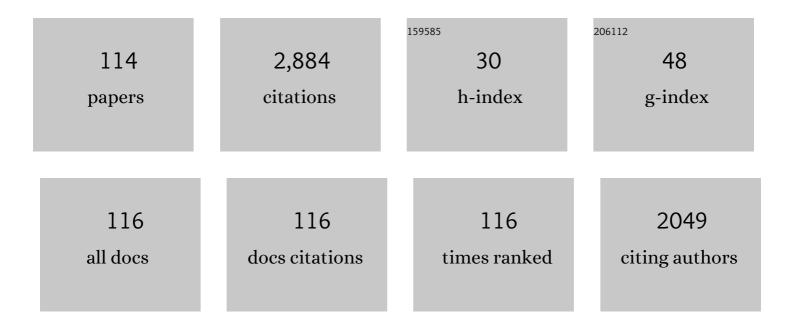
## Vytas Svedas

List of Publications by Year in descending order

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VIVTAS SVEDAS

#	Article	IF	CITATIONS
1	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
2	Guidelines for reporting of biocatalytic reactions. Trends in Biotechnology, 2010, 28, 171-180.	9.3	144
3	Biocatalytic approach to enantiomerically pure β-amino acids. Tetrahedron: Asymmetry, 1995, 6, 1601-1610.	1.8	94
4	Substrate specificity of penicillin amidase from E. coli. Biochimica Et Biophysica Acta - Biomembranes, 1980, 616, 283-289.	2.6	90
5	Biomimetic Transamination of α-Alkyl β-Keto Carboxylic Esters. Chemoenzymatic Approach to the Stereochemically Defined α-Alkyl β-Fluoroalkyl β-Amino Acids. Journal of Organic Chemistry, 1998, 63, 1878-1884.	3.2	80
6	Enzymatic synthesis of $\hat{1}^2$ -lactam antibiotics: A thermodynamic background. Enzyme and Microbial Technology, 1980, 2, 138-144.	3.2	78
7	Chemo-enzymatic approach to the synthesis of each of the four isomers of α-alkyl-β-fluoroalkyl-substituted β-amino acids. Tetrahedron: Asymmetry, 1994, 5, 1225-1228.	1.8	77
8	Biocatalytic resolution of $\hat{I}^2$ -fluoroalkyl- $\hat{I}^2$ -amino acids. Tetrahedron: Asymmetry, 1994, 5, 1119-1126.	1.8	74
9	Robust enzyme design: Bioinformatic tools for improved protein stability. Biotechnology Journal, 2015, 10, 344-355.	3.5	65
10	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
11	Kinetic study of penicillin acylase from Alcaligenes faecalis. FEBS Letters, 1997, 417, 414-418.	2.8	62
12	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
13	Penicillin acylase-catalyzed resolution of amines in aqueous organic solvents. Tetrahedron: Asymmetry, 2000, 11, 4593-4600.	1.8	59
14	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.	1.8	58
15	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
16	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
17	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
18	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

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19	Highly efficient and enantioselective enzymatic acylation of amines in aqueous medium. Tetrahedron: Asymmetry, 2001, 12, 1645-1650.	1.8	49
20	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
21	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
22	Preparation and properties of penicillin amidase immobilized in polyelectrolyte complexes. Biochimica Et Biophysica Acta - Biomembranes, 1981, 660, 359-365.	2.6	47
23	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
24	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
25	Penicillin acylase-catalyzed ampicillin synthesis using a pH gradient: A new approach to optimization. Biotechnology and Bioengineering, 2002, 78, 589-593.	3.3	40
26	Kinetics of the enzymatic synthesis of benzylpenicillin. Enzyme and Microbial Technology, 1980, 2, 313-317.	3.2	35
27	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
28	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
29	Saturation mutagenesis reveals the importance of residues αR145 and αF146 of penicillin acylase in the synthesis of β-lactam antibiotics. Journal of Biotechnology, 2008, 133, 18-26.	3.8	34
30	Zebra: a web server for bioinformatic analysis of diverse protein families. Journal of Biomolecular Structure and Dynamics, 2014, 32, 1752-1758.	3.5	34
31	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 <i>Aeromonas jandaei</i> . FEBS Open Bio, 2018, 8, 1013-1028.	2.3	33
32	Soluble-insoluble immobilized enzymes. Biotechnology and Bioengineering, 1982, 24, 237-240.	3.3	31
33	Mustguseal: a server for multiple structure-guided sequence alignment of protein families. Bioinformatics, 2018, 34, 1583-1585.	4.1	31
34	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
35	A kinetic study of hog kidney aminoacylase. BBA - Proteins and Proteomics, 1982, 701, 389-394.	2.1	29
36	A green, fully enzymatic procedure for amine resolution, using a lipase and a penicillin G acylase. Green Chemistry, 2008, 10, 415.	9.0	28

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37	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
38	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
39	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
40	Application of aminoacylase I to the enantioselective resolution of α-amino acid esters and amides. Tetrahedron: Asymmetry, 2004, 15, 1933-1936.	1.8	25
41	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
42	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. ACS Catalysis, 2014, 4, 2521-2529.	11.2	24
43	Resolution of (RS)-phenylglycinonitrile by penicillin acylase-catalyzed acylation in aqueous medium. Tetrahedron: Asymmetry, 2003, 14, 2613-2617.	1.8	23
44	An â€~easy-on, easy-off' protecting group for the enzymatic resolution of (±)-1-phenylethylamine in an aqueous medium. Tetrahedron: Asymmetry, 2004, 15, 2901-2906.	1.8	22
45	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
46	Continuous Spectrophotometric Assay of Human Lysosomal Cathepsin A/Protective Protein in Normal and Galactosialidosis Cells. Analytical Biochemistry, 1995, 230, 303-307.	2.4	20
47	Molecular Mechanisms of PARP-1 Inhibitor 7-Methylguanine. International Journal of Molecular Sciences, 2020, 21, 2159.	4.1	20
48	Penicillin Acylase-Catalyzed Solid-State Ampicillin Synthesis. Advanced Synthesis and Catalysis, 2002, 344, 894-898.	4.3	19
49	Chiral high-performance liquid chromatography analysis of α-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.	3.7	19
50	Yosshi: a web-server for disulfide engineering by bioinformatic analysis of diverse protein families. Nucleic Acids Research, 2019, 47, W308-W314.	14.5	18
51	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
52	Molecular modeling of formate dehydrogenase: the formation of the Michaelis complex. Journal of Biomolecular Structure and Dynamics, 2012, 30, 170-179.	3.5	17
53	Neuraminidase A from <i>Streptococcus pneumoniae</i> has a modular organization of catalytic and lectin domains separated by a flexible linker. FEBS Journal, 2018, 285, 2428-2445.	4.7	17
54	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

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55	Prospects of Using Biocatalysis for the Synthesis and Modification of Polymers. Molecules, 2021, 26, 2750.	3.8	16
56	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
57	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.	1.1	15
58	Aliphatic Amidase from Rhodococcus rhodochrous M8 Is Related to the Nitrilase/Cyanide Hydratase Family. Biochemistry (Moscow), 2005, 70, 1280-1287.	1.5	15
59	Structural insights into the broad substrate specificity of carboxypeptidase T from <i>ThermoactinomycesÂvulgaris</i> . FEBS Journal, 2015, 282, 1214-1224.	4.7	15
60	Comparative Modeling of Substrate Binding in the S1†Subsite of Serine Carboxypeptidases from Yeast, Wheat, and Humanâ€. Biochemistry, 1996, 35, 14899-14909.	2.5	14
61	Hydrophobicity of $\hat{I}^2$ -lactam antibiotics. Journal of Chromatography A, 1991, 585, 3-34.	3.7	13
62	pH stability of penicillin acylase from Escherichia coli. Biochemistry (Moscow), 2004, 69, 1386-1390.	1.5	13
63	Molecular modeling of different substrateâ€binding modes and their role in penicillin acylase catalysis. FEBS Journal, 2013, 280, 115-126.	4.7	13
64	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
65	Human p38α 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
66	Inhibitory Effect of New Semisynthetic Usnic Acid Derivatives on Human Tyrosyl-DNA Phosphodiesterase 1. Planta Medica, 2019, 85, 103-111.	1.3	13
67	Thermodynamic and kinetic stability of penicillin acylase from Escherichia coli. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2008, 1784, 736-746.	2.3	12
68	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
69	2,5-Diketopiperazines: A New Class of Poly(ADP-ribose)polymerase Inhibitors. Biochemistry (Moscow), 2018, 83, 152-158.	1.5	12
70	Inhibition of Poly(ADP-Ribose) Polymerase by Nucleic Acid Metabolite 7-Methylguanine. Acta Naturae, 2016, 8, 108-115.	1.7	12
71	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
72	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

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73	Quantum chemical studies of the catalytic mechanism of N-terminal nucleophile hydrolase. Biochemistry (Moscow), 2007, 72, 495-500.	1.5	11
74	Bioinformatic Analysis of the Nicotinamide Binding Site in Poly(ADP-Ribose) Polymerase Family Proteins. Cancers, 2021, 13, 1201.	3.7	11
75	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
76	Increased nucleophile reactivity of amino acid β-naphthylamides in α-chymotrypsin-catalyzed peptide synthesis. BBA - Proteins and Proteomics, 1990, 1041, 71-78.	2.1	10
77	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
78	Study of nucleophile binding in the penicillin acylase active center. Kinetic analysis. Biochemistry (Moscow), 2003, 68, 334-338.	1.5	9
79	EasyAmber: A comprehensive toolbox to automate the molecular dynamics simulation of proteins. Journal of Bioinformatics and Computational Biology, 2020, 18, 2040011.	0.8	9
80	Force field parametrization for 6-aminopenicillanic acid. Computational and Theoretical Chemistry, 2003, 631, 117-125.	1.5	8
81	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
82	Molecular modeling studies of substrate binding by penicillin acylase. Biochemistry (Moscow), 2008, 73, 56-64.	1.5	7
83	Biologically active cyclic polypeptides with fragments of β-amino acid derivatives isolated from marine organisms (review). Chemistry of Heterocyclic Compounds, 2011, 47, 395-417.	1.2	7
84	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.	3.5	7
85	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
86	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
87	Comparative Bioinformatic Analysis of Active Site Structures in Evolutionarily Remote Homologues of α,β-Hydrolase Superfamily Enzymes. Acta Naturae, 2011, 3, 93-98.	1.7	6
88	Bifunctional Inhibitors of Influenza Virus Neuraminidase: Molecular Design of a Sulfonamide Linker. International Journal of Molecular Sciences, 2021, 22, 13112.	4.1	6
89	The methyl ester of α-aminophenylacetic acid: pH-dependence and phosphate catalysis of hydrolysis. Journal of the Chemical Society Perkin Transactions II, 1986, , 1537-1540.	0.9	5
90	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

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91	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
92	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
93	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
94	Preparative Biocatalytic Synthesis of α-Ketoglutaramate. International Journal of Molecular Sciences, 2021, 22, 12748.	4.1	5
95	Soft Tissue Sarcoma Study: Association of Genetic Alterations in the Apoptosis Pathways with Chemoresistance to Doxorubicin. Cancers, 2022, 14, 1796.	3.7	5
96	BESSICC, a COSMOâ€RS based tool for in silico solvent screening of biocatalyzed reactions. Biotechnology and Bioengineering, 2012, 109, 1864-1868.	3.3	4
97	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
98	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.	2.5	4
99	Mutation of Residue βF71 of Escherichia coli Penicillin Acylase Results in Enhanced Enantioselectivity and Improved Catalytic Properties. Acta Naturae, 2009, 1, 94-98.	1.7	4
100	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
101	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
102	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
103	A new method for spectrophotometric assay of activity of cross-linked penicillin acylase aggregates. Biochemistry (Moscow), 2006, 71, 315-319.	1.5	3
104	Cloning of penicillin acylase from Escherichia coli: Catalytic properties of recombinant enzymes. Moscow University Chemistry Bulletin, 2008, 63, 103-107.	0.6	3
105	Crystal structures of carboxypeptidase T complexes with transition-state analogs. Journal of Biomolecular Structure and Dynamics, 2018, 36, 3958-3966.	3.5	3
106	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
107	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
108	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

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109	The βD484N 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
110	Professor Dr Roger A. Sheldon—65 years on. Green Chemistry, 2008, 10, 270.	9.0	0
111	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	Ο
112	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
113	Identification of New Structural Fragments for the Design of Lactate Dehydrogenase A Inhibitors. Acta Naturae, 2016, 8, 118-122.	1.7	0
114	High-Performance Hybrid Computing for Bioinformatic Analysis of Protein Superfamilies. Communications in Computer and Information Science, 2019, , 249-264.	0.5	0