## **Gerd Folkers**

## List of Publications by Year in descending order

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81351 108046 6,294 131 37 76 citations h-index g-index papers 168 168 168 8203 docs citations times ranked citing authors all docs

#	Article	IF	CITATIONS
1	Guest Editorial: Critical Thinking in Education and Research—Why and How?. Angewandte Chemie - International Edition, 2018, 57, 16574-16575.	7.2	4
2	Gastâ€Editorial: Kritisches Denken in Lehre und Forschung – warum und wie?. Angewandte Chemie, 2018, 130, 16812-16813.	1.6	2
3	Innovation Programs Lead to Innovation. , 2017, , 51-53.		O
4	A Continuum of Reproducible Research in Drug Development. , 2016, , 315-323.		0
5	Salivary Alpha-Amylase Correlates with Subjective Heat Pain Perception. Pain Medicine, 2016, 17, pnv085.	0.9	11
6	Quality of Animal Experiments in Anti-Angiogenic Cancer Drug Development – A Systematic Review. PLoS ONE, 2015, 10, e0137235.	1.1	13
7	How much reproducibility do we need in human and veterinary pathology?. Experimental and Toxicologic Pathology, 2015, 67, 77-80.	2.1	1
8	Temporal Processing in Bistable Perception of the Necker Cube. Perception, 2015, 44, 157-168.	0.5	16
9	Help-Seeking in People with Exceptional Experiences: Results from a General Population Sample. Frontiers in Public Health, 2014, 2, 51.	1.3	14
10	Thermodynamics of the interaction between oxytocin and its myometrial receptor in sheep: A stepwise binding mechanism. Biochemical Pharmacology, 2014, 91, 119-127.	2.0	4
11	Combinatorial chemistry by ant colony optimization. Future Medicinal Chemistry, 2014, 6, 267-280.	1.1	16
12	Naloxone modulates visual judgments of similarity but not dissimilarity. Cognitive, Affective and Behavioral Neuroscience, 2013, 13, 567-574.	1.0	2
13	Exhaustive Proteome Mining for Functional MHC-I Ligands. ACS Chemical Biology, 2013, 8, 1876-1881.	1.6	12
14	Scrutinizing MHC-I Binding Peptides and Their Limits of Variation. PLoS Computational Biology, 2013, 9, e1003088.	1.5	33
15	A New Tool for Real-Time Pain Assessment in Experimental and Clinical Environments. PLoS ONE, 2012, 7, e51014.	1.1	3
16	Placebo-mediated, Naloxone-sensitive suggestibility of short-term memory performance. Neurobiology of Learning and Memory, 2011, 95, 326-334.	1.0	16
17	Pleasure-Related Analgesia Activates Opioid-Insensitive Circuits. Journal of Neuroscience, 2011, 31, 4148-4153.	1.7	20
18	Prefrontal cortex modulates placebo analgesia. Pain, 2010, 148, 368-374.	2.0	268

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19	Wearable monitoring of stage fright in professional musicians. , 2010, , .		1
20	The crystal structure of PfFabZ, the unique $\hat{l}^2$ -hydroxyacyl-ACP dehydratase involved in fatty acid biosynthesis of Plasmodium falciparum. Protein Science, 2009, 14, 1570-1580.	3.1	54
21	Heat pain threshold and tolerance show no left–right perceptual differences at complementary sites of the human forearm. Neuroscience Letters, 2008, 440, 309-313.	1.0	14
22	Characterization of two splice variants of human organic anion transporting polypeptide 3A1 isolated from human brain. American Journal of Physiology - Cell Physiology, 2007, 292, C795-C806.	2.1	142
23	Changes in self-perceived role identity modulate pain perception. Pain, 2007, 131, 191-201.	2.0	14
24	Drug Design and Emotion. AIP Conference Proceedings, 2007, , .	0.3	0
25	Development and validation of a capillary electrophoresis method for the characterization of herpes simplex virus type 1 (HSV-1) thymidine kinase substrates and inhibitors. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2007, 846, 281-290.	1.2	23
26	High-level expression and purification of human thymidine kinase 1: Quaternary structure, stability, and kinetics. Protein Expression and Purification, 2006, 47, 506-515.	0.6	24
27	Imaging in Biomedical Research: Mini-Symposium of the Division for Medicinal Chemistry (DMC) of the Swiss Chemical Society (SCS), at the Department of Chemistry, University of Basel, May 18, 2006. Chimia, 2006, 60, 805-814.	0.3	0
28	The Crystal Structure of Aspergillus fumigatus Cyclophilin Reveals 3D Domain Swapping of a Central Element. Structure, 2006, 14, 185-195.	1.6	27
29	Random Chemistry as a New Tool for the Generation of Small-Compound Libraries. Archiv Der Pharmazie, 2006, 339, 489-497.	2.1	1
30	N-Glycan structures and N-glycosylation sites of mouse soluble intercellular adhesion molecule-1 revealed by MALDI-TOF and FTICR mass spectrometry. Glycobiology, 2006, 16, 1033-1044.	1.3	33
31	Recombinant Expression and Biochemical Characterization of the Unique Elongating $\hat{l}^2$ -Ketoacyl-Acyl Carrier Protein Synthase Involved in Fatty Acid Biosynthesis of Plasmodium falciparum Using Natural and Artificial Substrates. Journal of Biological Chemistry, 2006, 281, 9538-9546.	1.6	26
32	Application of QSAR analysis to organic anion transporting polypeptide 1a5 (Oatp1a5) substrates. Bioorganic and Medicinal Chemistry, 2005, 13, 463-471.	1.4	28
33	Incidence of drug-induced liver injury in medical inpatients. European Journal of Clinical Pharmacology, 2005, 61, 135-143.	0.8	176
34	Maternal dietary alpine butter intake affects human milk: Fatty acids and conjugated linoleic acid isomers. Lipids, 2005, 40, 581-587.	0.7	17
35	Density-functional Theory Applications in Computational Medicinal Chemistry. Methods and Principles in Medicinal Chemistry, 2005, , 41-71.	0.3	0
36	Patupilone Acts as Radiosensitizing Agent in Multidrug-Resistant Cancer Cells In vitro and In vivo. Clinical Cancer Research, 2005, $11$ , $1588-1596$ .	3.2	42

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37	Binding Mode Prediction of Cytochrome P450 and Thymidine Kinase Proteinâ^Ligand Complexes by Consideration of Water and Rescoring in Automated Docking. Journal of Medicinal Chemistry, 2005, 48, 2308-2318.	2.9	121
38	Strongly Altered Receptor Binding Properties in PP and NPY Chimeras Are Accompanied by Changes in Structure and Membrane Binding,. Biochemistry, 2005, 44, 9255-9264.	1.2	27
39	Structure of a type II thymidine kinase with bound dTTP. FEBS Letters, 2005, 579, 1376-1382.	1.3	48
40	Random Chemistry as a New Tool for the Generation of Small Compound Libraries:  Development of a New Acetylcholinesterase Inhibitor. Journal of Medicinal Chemistry, 2005, 48, 7496-7499.	2.9	7
41	Sialylated Complex-type N-Glycans Enhance the Signaling Activity of Soluble Intercellular Adhesion Molecule-1 in Mouse Astrocytes. Journal of Biological Chemistry, 2004, 279, 35201-35209.	1.6	36
42	Calpain-1 Regulates Bax and Subsequent Smac-dependent Caspase-3 Activation in Neutrophil Apoptosis. Journal of Biological Chemistry, 2004, 279, 5947-5957.	1.6	141
43	Synthesis, 18Fâ€Radiolabelling and Biological Evaluations of Câ€6 Alkylated Pyrimidine Nucleoside Analogues. Nucleosides, Nucleotides and Nucleic Acids, 2004, 23, 1707-1721.	0.4	25
44	A Molecular Dynamics Study of Reovirus Attachment Protein $\ddot{l}f1$ Reveals Conformational Changes in $\ddot{l}f1$ Structure. Biophysical Journal, 2004, 86, 3423-3431.	0.2	10
45	Thermodynamics of Protein–Ligand Interactions: History, Presence, and Future Aspects. Journal of Receptor and Signal Transduction Research, 2004, 24, 1-52.	1.3	308
46	Increased radiation toxicity by enhanced apoptotic clearance of HL-60 cells in the presence of the pentapeptide thymopentin, which selectively binds to apoptotic cells. Mutation Research - Genetic Toxicology and Environmental Mutagenesis, 2004, 558, 19-26.	0.9	9
47	Pharmaceutical Chemistry at the ETH Zürich. Chimia, 2004, 58, 707-710.	0.3	O
48	Molecular structures and ab initio molecular orbital calculations of the optically active derivatives of 1-aminocyclopropane-1-carboxylic acid. Journal of Molecular Structure, 2003, 655, 229-241.	1.8	3
49	Homology modelling and docking studies on Varicella Zoster Virus Thymidine kinase. European Journal of Medicinal Chemistry, 2003, 38, 413-419.	2.6	11
50	Synthesis and Biological Evaluation of Iodinated and Fluorinated 9-(2-Hydroxypropyl) and 9-(2-Hydroxyethoxy)methyl Purine Nucleoside Analogues. Journal of Medicinal Chemistry, 2003, 46, 5763-5772.	2.9	21
51	Synthesis and Biological Evaluation of 5-Substituted Derivatives of the Potent Antiherpes Agent (north)-Methanocarbathymine. Journal of Medicinal Chemistry, 2003, 46, 5045-5054.	2.9	53
52	Tautomerism in Computerâ€Aided Drug Design. Journal of Receptor and Signal Transduction Research, 2003, 23, 361-371.	1.3	110
53	Protonation States of Methionine Aminopeptidase and Their Relevance for Inhibitor Binding and Catalytic Activity. Journal of Biological Chemistry, 2003, 278, 47862-47867.	1.6	13
54	Pharmasquare (Pharma2). Chimia, 2003, 57, 116-120.	0.3	1

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55	Vireal Lab – From Instruction to Construction. Chimia, 2003, 57, 121-127.	0.3	0
56	pnn ag: Pharma Nation Network AG – CME online. Chimia, 2003, 57, 345-348.	0.3	0
57	Comparison of the Crystal Structures of the Human Manganese Superoxide Dismutase and the Homologous Aspergillus fumigatus Allergen at 2-Ã Resolution. Journal of Immunology, 2002, 168, 1267-1272.	0.4	70
58	Immunological and Structural Analysis of IgE-Mediated Cross-Reactivity between Manganese Superoxide Dismutases. International Archives of Allergy and Immunology, 2002, 128, 292-303.	0.9	62
59	Methodology and Problems of Proteinâ€Ligand Docking: Case Study of Dihydroorotate Dehydrogenase, Thymidine Kinase, and Phosphodiesterase 4. Journal of Receptor and Signal Transduction Research, 2002, 22, 141-154.	1.3	25
60	Probing the Cysteine-34 Position of Endogenous Serum Albumin with Thiol-Binding Doxorubicin Derivatives. Improved Efficacy of an Acid-Sensitive Doxorubicin Derivative with Specific Albumin-Binding Properties Compared to That of the Parent Compound. Journal of Medicinal Chemistry, 2002, 45, 5523-5533.	2.9	251
61	Bovine Pancreatic Polypeptide (bPP) Undergoes Significant Changes in Conformation and Dynamics upon Binding to DPC Micelles. Journal of Molecular Biology, 2002, 322, 1117-1133.	2.0	44
62	Synthesis, Kinetics, and Molecular Docking of Novel 9-(2-Hydroxypropyl)purine Nucleoside Analogs as Ligands of Herpesviral Thymidine Kinases. Helvetica Chimica Acta, 2002, 85, 3237-3250.	1.0	18
63	The production of macrophage inflammatory protein-2 induced by soluble intercellular adhesion molecule-1 in mouse astrocytes is mediated by src tyrosine kinases and p42/44 mitogen-activated protein kinase. Journal of Neurochemistry, 2002, 80, 824-834.	2.1	44
64	Folding and self-assembly of herpes simplex virus type 1 thymidine kinase. Journal of Molecular Biology, 2001, 313, 657-670.	2.0	12
65	A rationally designed oligopeptide shows significant conformational changes upon binding to sulphate ions. Biosensors and Bioelectronics, 2001, 16, 783-789.	5.3	8
66	Three-dimensional model of the cyclin-dependent kinase 1 (CDK1): Ab initio active site parameters for molecular dynamics studies of CDKS. Proteins: Structure, Function and Bioinformatics, 2001, 45, 478-485.	1.5	27
67	A Spectrophotometric Assay for Quantitative Determination of kcat of Herpes Simplex Virus Type 1 Thymidine Kinase Substrates. Analytical Biochemistry, 2001, 295, 82-87.	1.1	33
68	Cell fingerprinting: An approach to classifying cells according to mass profiles of digests of protein extracts. Proteomics, 2001, 1, 683-690.	1.3	17
69	Computational Methods Facilitate the Assignment of Protein Functions. Angewandte Chemie - International Edition, 2001, 40, 4175-4177.	7.2	4
70	NMR-restrained docking of a peptidic inhibitor to the N-terminal domain of the phosphoenolpyruvate:sugar phosphotransferase enzyme I. Journal of Computer-Aided Molecular Design, 2001, 15, 103-115.	1.3	7
71	The effect of substrate binding on the conformation and structural stability of Herpes simplex virus type 1 thymidine kinase. Protein Science, 2001, 10, 63-73.	3.1	31
72	Use of fluorescence polarization to monitor MHC–peptide interactions in solution. Journal of Immunological Methods, 2001, 255, 57-66.	0.6	32

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73	l̂ <sup>2</sup> -Amino Acid Scan of a Class I Major Histocompatibility Complex-restricted Alloreactive T-cell Epitope. Journal of Biological Chemistry, 2001, 276, 24525-24530.	1.6	40
74	Mutation of Cys-67 Alters the Thermodynamic Stability of the Human Leukocyte Antigen HLA-B*2705. Journal of Biological Chemistry, 2001, 276, 18472-18477.	1.6	15
<b>7</b> 5	The Rational of Catalytic Activity of Herpes Simplex Virus Thymidine Kinase. Journal of Biological Chemistry, 2001, 276, 21692-21697.	1.6	27
76	An analysis of the helix-to-strand transition between peptides with identical sequence. Proteins: Structure, Function and Bioinformatics, 2000, 41, 248-256.	1.5	36
77	Nucleoside binding site ofHerpes simplex type 1 thymidine kinase analyzed by X-ray crystallography. Proteins: Structure, Function and Bioinformatics, 2000, 41, 545-553.	1.5	60
78	Compulsory Order of Substrate Binding to Herpes Simplex Virus Type 1 Thymidine Kinase. Journal of Biological Chemistry, 2000, 275, 16139-16145.	1.6	34
79	Highly Purified Recombinant Varicella Zoster Virus Thymidine Kinase Is a Homodimer. Protein Expression and Purification, 2000, 18, 338-345.	0.6	11
80	Protein-Based Virtual Screening of Chemical Databases. 1. Evaluation of Different Docking/Scoring Combinations. Journal of Medicinal Chemistry, 2000, 43, 4759-4767.	2.9	724
81	Kinetics and Crystal Structure of the Wild-Type and the Engineered Y101F Mutant ofHerpes simplexVirus Type 1 Thymidine Kinase Interacting with (North)-methanocarba-thymidineâ€,‡. Biochemistry, 2000, 39, 9597-9603.	1.2	49
82	Thermodynamic Stability of HLA-B*2705Â-Peptide Complexes. Journal of Biological Chemistry, 2000, 275, 27055-27061.	1.6	23
83	Interaction of the Recombinant Herpes Simplex Virus Type 1 Thymidine Kinase with Thymidine and Aciclovir: A Kinetic Study. Nucleosides & Nucleotides, 1999, 18, 311-330.	0.5	12
84	Substrate Diversity of Herpes Simplex Virus Thymidine Kinase. Journal of Biological Chemistry, 1999, 274, 31967-31973.	1.6	74
85	Directed evolution of thymidine kinase for AZT phosphorylation using DNA family shuffling. Nature Biotechnology, 1999, 17, 259-264.	9.4	126
86	Temperature-Dependent NMR and CD Spectra of $\hat{l}^2$ -Peptides: On the Thermal Stability of $\hat{l}^2$ -Peptide Helices - Is the Folding Process of $\hat{l}^2$ -Peptides Non-cooperative?. Helvetica Chimica Acta, 1999, 82, 1-11.	1.0	59
87	Quantitative Structure-Activity Relationships of Phenyltropanes as Inhibitors of Three Monoamine Transporters: Classical and CoMFA studies. QSAR and Combinatorial Science, 1999, 18, 342-353.	1.4	20
88	Nonapeptide Analogues Containing (R)-3-Hydroxybutanoate and β-Homoalanine Oligomers:  Synthesis and Binding Affinity to a Class I Major Histocompatibility Complex Protein. Journal of Medicinal Chemistry, 1999, 42, 2318-2331.	2.9	30
89	Dimethyl Phosphate:  Stereoelectronic versus Environmental Effects. Journal of Physical Chemistry B, 1999, 103, 6121-6126.	1.2	44
90	Structure-Based Design of Nonnatural Ligands for the HLA-B27 Protein. Journal of Receptor and Signal Transduction Research, 1999, 19, 645-657.	1.3	11

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91	Shapes of membrane permeability–lipophilicity curves: Extension of theoretical models with an aqueous pore pathway. European Journal of Pharmaceutical Sciences, 1998, 6, 321-329.	1.9	51
92	Drug resistance of herpes simplex virus type 1. Structural considerations at the molecular level of the thymidine kinase. FEBS Journal, 1998, 255, 472-481.	0.2	43
93	Binding of rationally designed non-natural peptides to the human leukocyte antigen HLA-B*2705. , 1998, 4, 378-388.		11
94	PrGen: Pseudoreceptor Modeling Using Receptor-mediated Ligand Alignment and Pharmacophore Equilibration. QSAR and Combinatorial Science, 1998, 17, 122-130.	1.4	18
95	A fast and inexpensive method for N-terminal fluorescein-labeling of peptides. Bioorganic and Medicinal Chemistry Letters, 1998, 8, 597-600.	1.0	87
96	Estimation of permeability by passive diffusion through Caco-2 cell monolayers using the drugs' lipophilicity and molecular weight. European Journal of Pharmaceutical Sciences, 1998, 6, 313-319.	1.9	297
97	Substituting Nonpeptidic Spacers for the T Cell Receptor-binding Part of Class I Major Histocompatibility Complex-binding Peptides. Journal of Biological Chemistry, 1998, 273, 19072-19079.	1.6	23
98	Estimation of Blood-Brain Barrier Crossing of Drugs Using Molecular Size and Shape, and H-Bonding Descriptors. Journal of Drug Targeting, 1998, 6, 151-165.	2.1	517
99	Integrated Homology Modelling and X-Ray Study of Herpes Simplex Virus I Thymidine Kinase. , 1998, , 271-283.		4
100	Integrated Homology Modelling and X-Ray Study of Herpes Simplex Virus I Thymidine Kinase: A Case Study. Journal of Receptor and Signal Transduction Research, 1997, 17, 475-494.	1.3	7
101	Comparison of passive drug transport through Caco-2 cells and artificial membranes. International Journal of Pharmaceutics, 1997, 147, 61-70.	2.6	59
102	Oligonucleotide-directed mutagenesis and subsequent expression of the corresponding recombinant proteins without changing the bacterial vector system. Pharmaceutica Acta Helvetiae, 1997, 72, 139-143.	1.2	4
103	Structure-activity relationships of cannabinoids: a joint CoMFA and pseudoreceptor modelling study. Journal of Computer-Aided Molecular Design, 1997, 11, 278-292.	1.3	21
104	Fine specificity of antigen binding to two class I major histocompatibility proteins (B*2705 and B*2703) differing in a single amino acid residue. Journal of Computer-Aided Molecular Design, 1997, 11, 463-478.	1.3	25
105	A new approach to secondary structure evaluation: Secondary structure prediction of porcine adenylate kinase and yeast guanylate kinase by CD spectroscopy of overlapping synthetic peptide segments. Biopolymers, 1997, 41, 213-231.	1.2	12
106	The structures of thymidine kinase from <i>Herpes simplex</i> virus type 1 in complex with substrates and a substrate analogue. Protein Science, 1997, 6, 2097-2106.	3.1	114
107	A New Method for Quantitative Determination of Tritium-Labeled Nucleoside Kinase Products Adsorbed on DEAE-Cellulose. Biochemical and Biophysical Research Communications, 1996, 225, 263-267.	1.0	22
108	Evaluation of the Secondary Structure of Vaccinia-Virus Thymidine Kinase by Circular-Dichroism Spectroscopy of Overlapping Synthetic Peptides. FEBS Journal, 1996, 241, 126-132.	0.2	2

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109	Review of theoretical passive drug absorption models: Historical background, recent developments and limitations. Pharmaceutica Acta Helvetiae, 1996, 71, 309-327.	1.2	156
110	A transferred NOE study of a tricyclic analog of acyclovir bound to thymidine kinase. Journal of Biomolecular NMR, 1996, 8, 261-272.	1.6	8
111	Estimation of Caco-2 Cell Permeability using Calculated Molecular Descriptors. QSAR and Combinatorial Science, 1996, 15, 480-490.	1.4	165
112	A pseudoreceptor modelling study of the varicella-zoster virus and human thymidine kinase binding sites. Journal of Computer-Aided Molecular Design, 1995, 9, 473-478.	1.3	2
113	Secondary structure prediction of adenylate kinase by circular dichroism spectroscopy of synthetic peptides. Pharmaceutica Acta Helvetiae, 1995, 70, 33-41.	1.2	6
114	Fatalism or efficiency?. Pharmaceutica Acta Helvetiae, 1995, 70, 1.	1.2	0
115	Serendipity!. Pharmaceutica Acta Helvetiae, 1995, 70, 93.	1.2	0
116	Snails and shells teach us. Pharmaceutica Acta Helvetiae, 1995, 70, 267-268.	1.2	0
117	MD simulations in Pseudo-Particle Fluids: Applications to active-site Protein Complexes. QSAR and Combinatorial Science, 1995, 14, 229-241.	1.4	2
118	The three-dimensional structure of thymidine kinase from Herpes simplex virus type 1. FEBS Letters, 1995, 368, 289-292.	1.3	83
119	Lock and key. Pharmaceutica Acta Helvetiae, 1995, 69, 175-176.	1.2	12
120	Immunogenetic profiles correlate with pro-MMP expression in rheumatoid arthritis. Acta Orthopaedica, 1995, 66, 154-155.	1.4	0
121	Nucleotide-binding properties of adenylate kinase from Escherichia coli: A molecular dynamics study in aqueous and vacuum environments. Journal of Computer-Aided Molecular Design, 1994, 8, 367-388.	1.3	20
122	Recommendations for CoMFA Studies and 3D QSAR Publications. QSAR and Combinatorial Science, 1994, 13, 1-3.	1.4	28
123	Molecular Dynamics Simulation of MHC-Peptide Complexes as a Tool for Predicting Potential T Cell Epitopes. Biochemistry, 1994, 33, 11476-11485.	1.2	98
124	Siteâ€Directed Mutagenesis Clarifies the Substrate Position within the Threeâ€Dimensional Model of the Active Site of Herpes Simplex Virus Typeâ€1 Thymidine Kinase. FEBS Journal, 1994, 226, 219-226.	0.2	2
125	Site-Directed Mutagenesis Clarifies the Substrate Position within the Three-Dimensional Model of the Active Site of Herpes Simplex Virus Type-1 Thymidine Kinase. FEBS Journal, 1994, 226, 219-226.	0.2	4
126	Site-directed mutagenesis in the active site of the herpes simplex virus type 1 thymidine kinase gene. Virus Genes, 1993, 7, 205-209.	0.7	8

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127	Molecular modeling of an antigenic complex between a viral peptide and a class I major histocompatibility glycoprotein. Proteins: Structure, Function and Bioinformatics, 1992, 13, 70-85.	1.5	38
128	Molecular dynamics study of a complex between the human histocompatibility antigen HLA-A2 and the IMP58-66 nonapeptide from influenza virus matrix protein. FEBS Journal, 1992, 208, 101-113.	0.2	44
129	Conformational and epitope mapping of herpes-simplex-virus type-1 thymidine kinase using synthetic peptide segments. FEBS Journal, 1991, 200, 519-528.	0.2	23
130	Computer-aided active-site-directed modeling of the Herpes Simplex Virus 1 and human thymidine kinase. Journal of Computer-Aided Molecular Design, 1991, 5, 385-404.	1.3	26
131	Hydrogen Bond Strength Estimation by Means of the HYBOT Program Package. , 0, , 367-378.		25