

Citation report for 125 results from Web of Science Core Collection between 1... and 2... Go

You searched for: AUTHOR: (vondrasek j) ...More

This report reflects citations to source items indexed within Web of Science Core Collection. Perform a Cited Reference Search to include citations to items not indexed within Web of Science Core Collection.

Export Data: Save to Excel ...

Total Publications

125 Analyze



h-Index

28

Average citations per item  
27.66

Sum of Times Cited

3,458

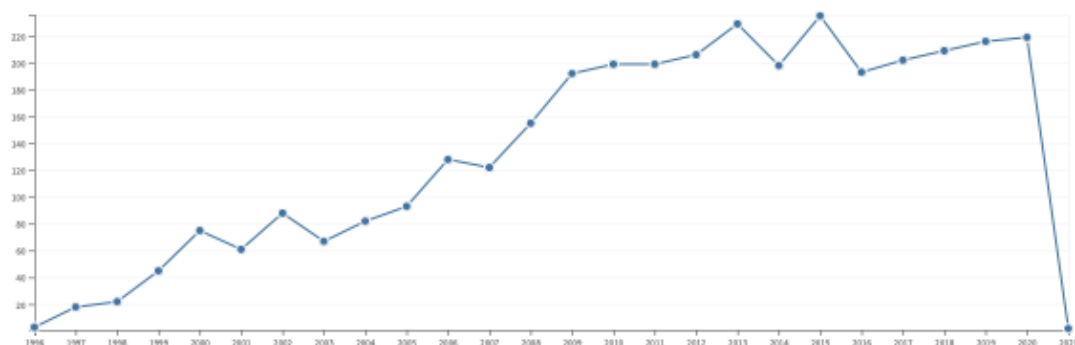
Without self citations  
3,301

Citing articles

3,054 Analyze

Without self citations  
2,981 Analyze

Sum of Times Cited per Year



Sort by: Times Cited 17 Date More

1 of 13

How are these totals calculated?

Use the checkboxes to remove individual items from this Citation Report

or restrict to items published between 1... and 2... Go

- ☐ 1. **Inhibitors of HIV-1 protease: A major success of structure-assisted drug design**  
By: Wlodawer, A; Vondrasek, J  
ANNUAL REVIEW OF BIOPHYSICS AND BIOMOLECULAR STRUCTURE Volume: 27 Pages: 249-284  
Published: 1998

2017	2018	2019	2020	2021	Total	Average Citations per Year
202	209	216	219	2	3458	133.00
14	18	13	17	0	531	22.13



- ☐ 11. **Representative Amino Acid Side Chain Interactions in Proteins. A Comparison of Highly Accurate Correlated ab Initio Quantum Chemical and Empirical Potential Procedures**  
By: Berka, Karel; Laskowski, Roman; Riley, Kevin E.; et al.  
JOURNAL OF CHEMICAL THEORY AND COMPUTATION Volume: 5 Issue: 4 Pages: 982-992 Published: APR 2009
- ☐ 12. **Another role of proline: stabilization interactions in proteins and protein complexes concerning proline and tryptophane**  
By: Biedermannova, Lada; Riley, Kevin E.; Berka, Karel; et al.  
PHYSICAL CHEMISTRY CHEMICAL PHYSICS Volume: 10 Issue: 42 Pages: 6350-6359 Published: 2008
- ☐ 13. **Performance of the DFT-D method, paired with the PCM implicit solvation model, for the computation of interaction energies of solvated complexes of biological interest**  
By: Riley, Kevin E.; Vondrasek, Jiri; Hobza, Pavel  
PHYSICAL CHEMISTRY CHEMICAL PHYSICS Volume: 9 Issue: 41 Pages: 5555-5560 Published: 2007
- ☐ 14. **Urea and Guanidinium Induced Denaturation of a Trp-Cage Mini-protein**  
By: Heyda, Jan; Kozisek, Milan; Bednarova, Lucie; et al.  
JOURNAL OF PHYSICAL CHEMISTRY B Volume: 115 Issue: 28 Pages: 8910-8924 Published: JUL 21 2011
- ☐ 15. **HIVdb: A database of the structures of human immunodeficiency virus protease**  
By: Vondrasek, J; Wlodawer, A  
PROTEINS-STRUCTURE FUNCTION AND GENETICS Volume: 49 Issue: 4 Pages: 429-431 Published: DEC 1 2002
- ☐ 16. **Unusual binding mode of an HIV-1 protease inhibitor explains its potency against multi-drug-resistant virus strains**  
By: Weber, J; Mesters, JR; Lepsik, M; et al.  
JOURNAL OF MOLECULAR BIOLOGY Volume: 324 Issue: 4 Pages: 739-754 Published: DEC 6 2002
- ☐ 17. **Metadynamics As a Tool for Mapping the Conformational and Free-Energy Space of Peptides - The Alanine Dipeptide Case Study**  
By: Vymetal, Jiri; Vondrasek, Jiri  
JOURNAL OF PHYSICAL CHEMISTRY B Volume: 114 Issue: 16 Pages: 5632-5642 Published: APR 29 2010
- ☐ 18. **Data base of three-dimensional structures of HIV proteinases**  
By: Vondrasek, J; vanBuskirk, CP; Wlodawer, A  
NATURE STRUCTURAL BIOLOGY Volume: 4 Issue: 1 Pages: 8-8 Published: JAN 1997
- ☐ 19. **Like-Charge Guanidinium Pairing from Molecular Dynamics and Ab Initio Calculations**  
By: Vazdar, Mario; Vymetal, Jiri; Heyda, Jan; et al.  
JOURNAL OF PHYSICAL CHEMISTRY A Volume: 115 Issue: 41 Pages: 11193-11201 Published: OCT 20 2011
- ☐ 20. **Ability of empirical potentials (AMBER, CHARMM, CVFF, OPLS, Poltev) and semi-empirical quantum chemical methods (AM1, MNDO/M, PM3) to describe H-bonding in DNA base pairs; Comparison with ab initio results**  
By: Hobza, P; Hubalek, F; Kabelac, M; et al.  
CHEMICAL PHYSICS LETTERS Volume: 257 Issue: 1-2 Pages: 31-35 Published: JUL 19 1996

5	1	4	0	0	68	5.23
9	3	4	6	0	57	4.07
3	2	1	1	0	55	3.67
6	9	3	4	0	52	4.73
1	0	0	0	0	51	2.55
1	0	0	0	0	46	2.30
4	3	4	3	0	44	3.67
0	0	1	0	0	44	1.76
5	3	5	6	1	43	3.91
0	0	0	1	0	39	1.50

☐ Select Page | |

<input type="checkbox"/>	21. Ion specific effects of sodium and potassium on the catalytic activity of HIV-1 protease By: Heyda, Jan; Pokorna, Jana; Vrbka, Lubos; et al. PHYSICAL CHEMISTRY CHEMICAL PHYSICS Volume: 11 Issue: 35 Pages: 7599-7604 Published: 2009	4	2	9	1	0	36	2.77
<input type="checkbox"/>	22. Sexual attraction in the silkworm moth: Nature of binding of bombykol in pheromone binding protein - An ab initio study By: Klusak, V; Havlas, Z; Rullsek, L; et al. CHEMISTRY & BIOLOGY Volume: 10 Issue: 4 Pages: 331-340 Published: APR 2003	1	2	0	0	0	35	1.84
<input type="checkbox"/>	23. Configurations of diastereomeric hydroxyethylene isosteres strongly affect biological activities of a series of specific inhibitors of human-immunodeficiency-virus protease By: Konvalinka, J; Litera, J; Weber, J; et al. EUROPEAN JOURNAL OF BIOCHEMISTRY Volume: 250 Issue: 2 Pages: 559-566 Published: DEC 1 1997	0	0	0	0	0	34	1.36
<input type="checkbox"/>	24. Thermodynamic penalty arising from burial of a ligand polar group within a hydrophobic pocket of a protein receptor By: Barratt, Elizabeth; Bronowska, Agnieszka; Vondrasek, Jiri; et al. JOURNAL OF MOLECULAR BIOLOGY Volume: 362 Issue: 5 Pages: 994-1003 Published: OCT 6 2006	1	2	3	3	0	33	2.06
<input type="checkbox"/>	25. <a href="#">Rigid Duplex alpha-Cyclodextrin Reversibly Connected With Disulfide Bonds. Synthesis and Inclusion Complexes</a> ✖ By: Kumprecht, Lukas; Budesinsky, Milos; Vondrasek, Jiri; et al. JOURNAL OF ORGANIC CHEMISTRY Volume: 74 Issue: 3 Pages: 1082-1092 Published: FEB 6 2009	2	1	1	2	0	32	2.46
<input type="checkbox"/>	26. Evolution by any other name: Antibiotic resistance and avoidance of the E-word By: Antonovics, Janis; Abbate, Jessica L.; Baker, Christi Howell; et al. PLOS BIOLOGY Volume: 5 Issue: 2 Pages: 137-140 Article Number: e30 Published: FEB 2007	4	2	1	3	0	32	2.13
<input type="checkbox"/>	27. Model of peptide bond-aromatic ring interaction: Correlated ab initio quantum chemical study By: Bendova, Lada; Jurecka, Petr; Hobza, Pavel; et al. JOURNAL OF PHYSICAL CHEMISTRY B Volume: 111 Issue: 33 Pages: 9975-9979 Published: AUG 23 2007	1	2	0	0	0	31	2.07
<input type="checkbox"/>	28. Cathepsin D propeptide: Mechanism and regulation of its interaction with the catalytic core By: Masa, Martin; Maresova, Lucie; Vondrasek, Jiri; et al. BIOCHEMISTRY Volume: 45 Issue: 51 Pages: 15474-15482 Article Number: PII S0006-2960(06)01498-X Published: DEC 26 2006	1	3	1	1	0	30	1.88
<input type="checkbox"/>	29. Gyration- and Inertia-Tensor-Based Collective Coordinates for Metadynamics. Application on the Conformational Behavior of Polyalanine Peptides and Trp-Cage Folding By: Vymetal, Jiri; Vondrasek, Jiri JOURNAL OF PHYSICAL CHEMISTRY A Volume: 115 Issue: 41 Pages: 11455-11465 Published: OCT 20 2011	3	4	6	2	0	28	2.55
<input type="checkbox"/>	30. Bioinformatic analysis and molecular modelling of human ameloblastin suggest a two-domain intrinsically unstructured calcium-binding protein By: Vymetal, Jiri; Slaby, Ivan; Spahr, Axel; et al. EUROPEAN JOURNAL OF ORAL SCIENCES Volume: 116 Issue: 2 Pages: 124-134 Published: APR 2008	3	1	1	1	0	28	2.00

☐ Select Page | | Save to Excel ... ▾

<input type="checkbox"/>	31. <b>Identifying stabilizing key residues in proteins using interresidue interaction energy matrix</b> By: Bendova-Biedermannova, Lada; Hobza, Pavel; Vondrasek, Jiri PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS Volume: 72 Issue: 1 Pages: 402-413 Published: JUL 2008	1	1	2	2	0	25	1.79
<input type="checkbox"/>	32. <b>Critical Assessment of Current Force Fields. Short Peptide Test Case</b> By: Vymetal, Jiri; Vondrasek, Jiri JOURNAL OF CHEMICAL THEORY AND COMPUTATION Volume: 9 Issue: 1 Pages: 441-451 Published: JAN 2013	1	2	2	1	0	24	2.67
<input type="checkbox"/>	33. <b>Novel high-affinity binders of human interferon gamma derived from albumin-binding domain of protein G</b> By: Ahmad, Jawid N.; Li, Jingjing; Biedermannova, Lada; et al. PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS Volume: 80 Issue: 3 Pages: 774-789 Published: MAR 2013	3	4	5	1	1	24	2.40
<input type="checkbox"/>	34. <b>Solid phase synthesis of glycopeptide dendrimers with Tn antigenic structure and their biological activities. Part I</b> By: Jezek, J; Velek, J; Veprek, P; et al. JOURNAL OF PEPTIDE SCIENCE Volume: 5 Issue: 1 Pages: 46-55 Published: JAN 1999	0	0	0	0	0	24	1.04
<input type="checkbox"/>	35. <b>Dispersion Interactions govern the strong thermal stability of a protein</b> By: Vondrasek, Jiri; Kubar, Tomas; Jenney, Francis E., Jr.; et al. CHEMISTRY-A EUROPEAN JOURNAL Volume: 13 Issue: 32 Pages: 9022-9027 Published: 2007	3	2	2	0	0	23	1.53
<input type="checkbox"/>	36. <b>Intrinsically Disordered Enamel Matrix Protein Ameloblastin Forms Ribbon-like Supramolecular Structures via an N-terminal Segment Encoded by Exon 5</b> By: Wald, Tomas; Osickova, Adriana; Sulc, Miroslav; et al. JOURNAL OF BIOLOGICAL CHEMISTRY Volume: 288 Issue: 31 Pages: 22333-22345 Published: AUG 2 2013	5	1	1	5	0	22	2.44
<input type="checkbox"/>	37. <b>Energy Matrix of Structurally Important Side-Chain/Side-Chain Interactions in Proteins</b> By: Berka, Karel; Laskowski, Roman A.; Hobza, Pavel; et al. JOURNAL OF CHEMICAL THEORY AND COMPUTATION Volume: 6 Issue: 7 Pages: 2191-2203 Published: JUL 2010	1	2	1	0	0	22	1.83
<input type="checkbox"/>	38. <b>Loss of Dispersion Energy Changes the Stability and Folding/Unfolding Equilibrium of the Trp-Cage Protein</b> By: Cerny, Jiri; Vondrasek, Jiri; Hobza, Pavel JOURNAL OF PHYSICAL CHEMISTRY B Volume: 113 Issue: 16 Pages: 5657-5660 Published: APR 23 2009	1	0	0	1	0	20	1.54
<input type="checkbox"/>	39. <b>Prolyl Oligopeptidase from the Blood Fluke Schistosoma mansoni: From Functional Analysis to Anti-schistosomal Inhibitors</b> By: Fajtova, Pavla; Stefanic, Sasa; Hradilek, Martin; et al. PLOS NEGLECTED TROPICAL DISEASES Volume: 9 Issue: 6 Article Number: e0003827 Published: JUN 2015	2	9	1	3	0	19	2.71
<input type="checkbox"/>	40. <b>Mapping the Pro-Peptide of the Schistosoma mansoni Cathepsin B1 Drug Target: Modulation of Inhibition by Heparin and Design of Mimetic Inhibitors</b> By: Horn, Martin; Jilkova, Adela; Vondrasek, Jiri; et al. ACS CHEMICAL BIOLOGY Volume: 6 Issue: 6 Pages: 609-617 Published: JUN 2011	0	7	0	2	0	19	1.73

☐ Select Page

<input type="checkbox"/>	41. <b>Application of InChI to curate, index, and query 3-D structures</b> By: Prasanna, MD; Vondrasek, J; Wlodawer, A; et al. PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS Volume: 60 Issue: 1 Pages: 1-4 Published: JUL 1 2005	0	0	0	0	0	19	1.12
<input type="checkbox"/>	42. <b>Highly selective purification of three lipases from Geotrichum candidum 4013 and their characterization and biotechnological applications</b> By: Brabcova, Jana; Demianova, Zuzana; Vondrasek, Jiri; et al. JOURNAL OF MOLECULAR CATALYSIS B-ENZYMATIC Volume: 98 Pages: 62-72 Published: DEC 30 2013	1	4	3	2	0	18	2.00
<input type="checkbox"/>	43. <b>Potency comparison of peptidomimetic inhibitors against HIV-1 and HIV-2 proteinases: Design of equipotent lead compounds</b> By: Weber, J; Majer, P; Litera, J; et al. ARCHIVES OF BIOCHEMISTRY AND BIOPHYSICS Volume: 341 Issue: 1 Pages: 62-69 Published: MAY 1 1997	0	0	0	0	0	18	0.72
<input type="checkbox"/>	44. <b>PIP2 and PIP3 interact with N-terminus region of TRPM4 channel</b> By: Bousova, Kristyna; Jirku, Michaela; Sumba, Ladislav; et al. BIOPHYSICAL CHEMISTRY Volume: 205 Pages: 24-32 Published: OCT 2015	2	5	2	3	0	17	2.43
<input type="checkbox"/>	45. <b>Trypsin- and Chymotrypsin-Like Serine Proteases in Schistosoma mansoni - 'The Undiscovered Country'</b> By: Horn, Martin; Fajtova, Pavla; Arreola, Lilliana Rojo; et al. PLOS NEGLECTED TROPICAL DISEASES Volume: 8 Issue: 3 Article Number: e2766 Published: MAR 2014	2	4	1	3	0	17	2.13
<input type="checkbox"/>	46. <b>Effect of Enamel Matrix Derivative and of Proline-Rich Synthetic Peptides on the Differentiation of Human Mesenchymal Stem Cells Toward the Osteogenic Lineage</b> By: Maria Ramis, Joana; Rubert, Marina; Vondrasek, Jiri; et al. TISSUE ENGINEERING PART A Volume: 18 Issue: 11-12 Pages: 1253-1263 Published: JUN 2012	1	0	2	4	0	17	1.70
<input type="checkbox"/>	47. <b>Activation Route of the Schistosoma mansoni Cathepsin B1 Drug Target: Structural Map with a Glycosaminoglycan Switch</b> By: Jilkova, Adela; Horn, Martin; Rezacova, Pavlina; et al. STRUCTURE Volume: 22 Issue: 12 Pages: 1786-1798 Published: DEC 2 2014	1	7	1	3	0	16	2.00
<input type="checkbox"/>	48. <b>Quasiplanarity of the peptide bond</b> By: Chalupsky, Jakub; Vondrasek, Jiri; Spirko, Vladimir JOURNAL OF PHYSICAL CHEMISTRY A Volume: 112 Issue: 4 Pages: 693-699 Published: JAN 31 2008	1	0	0	0	0	16	1.14
<input type="checkbox"/>	49. <b>Chemical compound navigator: A web-based chem-BLAST, chemical taxonomy-based search engine for browsing compounds</b> By: Prasanna, M. D.; Vondrasek, Jiri; Wlodawer, Alexander; et al. PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS Volume: 63 Issue: 4 Pages: 907-917 Published: JUN 1 2006	0	0	0	0	0	16	1.00
<input type="checkbox"/>	50. <b>A picomolar inhibitor of resistant strains of human immunodeficiency virus protease identified by a combinatorial approach</b> By: Rinnova, M; Hradlilek, M; Barinka, C; et al. ARCHIVES OF BIOCHEMISTRY AND BIOPHYSICS Volume: 382 Issue: 1 Pages: 22-30 Published: OCT 1 2000	0	0	0	0	0	16	0.73

☐ Select Page

Sort by: **Times Cited** Date More 

5 of 13



<input type="checkbox"/>	51. <b>Random protein sequences can form defined secondary structures and are well-tolerated in vivo</b> By: Tretiyachenko, Vyacheslav; Vymetal, Jiri; Bednarova, Lucie; et al. SCIENTIFIC REPORTS Volume: 7 Article Number: 15449 Published: NOV 13 2017	0	4	5	6	0	15	3.00
<input type="checkbox"/>	52. <b>Effect of TFE on the Helical Content of AK17 and HAL-1 Peptides: Theoretical Insights Into the Mechanism of Helix Stabilization</b> By: Vymetal, Jiri; Bednarova, Lucie; Vondrasek, Jiri JOURNAL OF PHYSICAL CHEMISTRY B Volume: 120 Issue: 6 Pages: 1048-1059 Published: FEB 18 2016	0	3	3	7	0	15	2.50
<input type="checkbox"/>	53. <b>Representative Amino Acid Side-Chain Interactions in Protein-DNA Complexes: A Comparison of Highly Accurate Correlated Ab Initio Quantum Mechanical Calculations and Efficient Approaches for Applications to Large Systems</b> By: Hostas, Jiri; Jakubec, David; Laskowski, Roman A.; et al. JOURNAL OF CHEMICAL THEORY AND COMPUTATION Volume: 11 Issue: 9 Pages: 4086-4092 Published: SEP 2015	5	3	0	2	0	14	2.00
<input type="checkbox"/>	54. <b>Biophysical characterization of recombinant human ameloblastin</b> By: Wald, Tomas; Bednarova, Lucie; Osicka, Radim; et al. Conference: 8th International Symposium on Development, Properties and Pathology of Tooth Enamel Location: N Utica, IL Date: JUN 12-18, 2011 EUROPEAN JOURNAL OF ORAL SCIENCES Volume: 119 Special Issue: SI Supplement: 1 Pages: 261-269 Published: DEC 2011	3	1	1	2	0	14	1.27
<input type="checkbox"/>	55. <b>A modular approach to HIV-1 protease inhibitor design</b> By: Uhlíkova, T; Konvalinka, J; Pichova, I; et al. BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS Volume: 222 Issue: 1 Pages: 38-43 Published: MAY 6 1996	0	0	0	1	0	14	0.54
<input type="checkbox"/>	56. <b>Exquisite ligand stereoselectivity of a Drosophila juvenile hormone receptor contrasts with its broad agonist repertoire</b> By: Bittova, Lenka; Jedlicka, Pavel; Dracinsky, Martin; et al. JOURNAL OF BIOLOGICAL CHEMISTRY Volume: 294 Issue: 2 Pages: 410-423 Published: JAN 11 2019	0	0	5	8	0	13	4.33
<input type="checkbox"/>	57. <b>Parametrization of 2,2,2-Trifluoroethanol Based on the Generalized Amber Force Field Provides Realistic Agreement between Experimental and Calculated Properties of Pure Liquid as Well as Water-Mixed Solutions</b> By: Vymetal, Jiri; Vondrasek, Jiri JOURNAL OF PHYSICAL CHEMISTRY B Volume: 118 Issue: 35 Pages: 10390-10404 Published: SEP 4 2014	1	4	2	0	0	12	1.50
<input type="checkbox"/>	58. <b>Homology modeling and SAR analysis of Schistosoma japonicum cathepsin D (SjCD). with statin inhibitors identify a unique active site steric barrier with potential for the design of specific inhibitors</b> By: Caffrey, CR; Placha, L; Barinka, C; et al. BIOLOGICAL CHEMISTRY Volume: 386 Issue: 4 Pages: 339-349 Published: APR 2005	0	1	0	0	0	12	0.71
<input type="checkbox"/>	59. <b>Free-thiol Cys331 exposed during activation process is critical for native tetramer structure of cathepsin C (dipeptidyl peptidase I)</b> By: Horn, M; Baudys, M; Voburka, Z; et al. PROTEIN SCIENCE Volume: 11 Issue: 4 Pages: 933-943 Published: APR 2002	0	0	3	0	0	12	0.60
<input type="checkbox"/>	60. <b>Synthetic Peptides Analogue to Enamel Proteins Promote Osteogenic Differentiation of MC3T3-E1 and Mesenchymal Stem Cells</b> By: Rubert, Marina; Ramis, Joana Maria; Vondrasek, Jiri; et al. JOURNAL OF BIOMATERIALS AND TISSUE ENGINEERING Volume: 1 Issue: 2 Pages: 198-209 Published: DEC 2011	1	0	2	2	0	11	1.00

☐ Select Page | | Save to Excel ...

Sort by: Times Cited Date More

◀ 6 of 13 ▶

<input type="checkbox"/>	61. <b>SmSP2: A serine protease secreted by the blood fluke pathogen <i>Schistosoma mansoni</i> with anti-hemostatic properties</b> By: Leontovyc, Adrian; Ulrychova, Lenka; O'Donoghue, Anthony J.; et al. PLOS NEGLECTED TROPICAL DISEASES Volume: 12 Issue: 4 Article Number: e0006446 Published: APR 2018	0	2	0	8	0	10	2.50
<input type="checkbox"/>	62. <b>Noncovalent Interactions in Specific Recognition Motifs of Protein-DNA Complexes</b> By: Stasyuk, Olga A.; Jakubec, David; Vondrasek, Jiri; et al. JOURNAL OF CHEMICAL THEORY AND COMPUTATION Volume: 13 Issue: 2 Pages: 877-885 Published: FEB 2017	1	1	4	4	0	10	2.00
<input type="checkbox"/>	63. <b>Amino Acid Interaction (INTAA) web server</b> By: Galgonek, Jakub; Vymetal, Jiri; Jakubec, David; et al. NUCLEIC ACIDS RESEARCH Volume: 45 Issue: W1 Pages: W388-W392 Published: JUL 3 2017	0	1	5	3	0	9	1.80
<input type="checkbox"/>	64. <b>Insights into Unfolded Proteins from the Intrinsic phi/psi Propensities of the AAXAA Host-Guest Series</b> By: Towse, Clare-Louise; Vymetal, Jiri; Vondrasek, Jiri; et al. BIOPHYSICAL JOURNAL Volume: 110 Issue: 2 Pages: 348-361 Published: JAN 19 2016	3	1	1	1	0	8	1.33
<input type="checkbox"/>	65. <b>Database of HIV protease structures</b> By: Vondrasek, J.; Wlodawer, A TRENDS IN BIOCHEMICAL SCIENCES Volume: 22 Issue: 5 Pages: 183-183 Published: MAY 1997	0	0	0	0	0	8	0.32
<input type="checkbox"/>	66. <b>Characterization of the part of N-terminal PIP2 binding site of the TRPM1 channel</b> By: Jirku, Michaela; Bumba, Ladislav; Bednarova, Lucie; et al. BIOPHYSICAL CHEMISTRY Volume: 207 Pages: 135-142 Published: DEC 2015	1	3	1	1	0	7	1.00
<input type="checkbox"/>	67. <b>Large-Scale Quantitative Assessment of Binding Preferences in Protein-Nucleic Acid Complexes</b> By: Jakubec, David; Hostas, Jiri; Laskowski, Roman A.; et al. JOURNAL OF CHEMICAL THEORY AND COMPUTATION Volume: 11 Issue: 4 Pages: 1939-1948 Published: APR 2015	4	1	0	0	0	7	1.00
<input type="checkbox"/>	68. <b>The DF-LCCSD(T0) correction of the phi/psi force field dihedral parameters significantly influences the free energy profile of the alanine dipeptide</b> By: Vymetal, Jiri; Vondrasek, Jiri CHEMICAL PHYSICS LETTERS Volume: 503 Issue: 4-6 Pages: 301-304 Published: FEB 17 2011	0	0	0	2	0	7	0.64
<input type="checkbox"/>	69. <b>Magnesium and biological activity of oxytocin analogues modified on aromatic ring of amino acid in position 2</b> By: Slaninova, J; Maletinska, L; Vondrasek, J; et al. JOURNAL OF PEPTIDE SCIENCE Volume: 7 Issue: 8 Pages: 413-424 Published: AUG 2001	0	0	2	0	0	7	0.33
<input type="checkbox"/>	70. <b>Novel Structural Mechanism of Allosteric Regulation of Aspartic Peptidases via an Evolutionarily Conserved Exosite</b> By: Hanova, Iva; Brynda, Jiri; Houstecka, Radka; et al. CELL CHEMICAL BIOLOGY Volume: 25 Issue: 3 Pages: 318 -+ Published: MAR 15 2018	0	2	1	3	0	6	1.50

☐ Select Page



<input type="checkbox"/>	71. Unexpectedly strong energy stabilization inside the hydrophobic core of small protein rubredoxin mediated by aromatic residues: Correlated ab initio quantum chemical calculations (vol 127, pg 2615, 2005) By: Vondrasek, J; Bendova, L; Klusak, V; et al. JOURNAL OF THE AMERICAN CHEMICAL SOCIETY Volume: 127 Issue: 22 Pages: 8232-8232 Published: JUN 8 2005	0	0	0	0	0	6	0.35
<input type="checkbox"/>	72. Molecular dynamics study of the effect of the gamma-abu Insert on the conformational behavior of the glycopeptide dendrimers based on the oligolysine scaffold in N,N'-dimethylformamide By: Veprek, P; Jezek, J; Trnka, T; et al. JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS Volume: 22 Issue: 1 Pages: 79-90 Published: AUG 2004	0	0	0	0	0	6	0.33
<input type="checkbox"/>	73. New database By: Vondrasek, J; Wlodawer, A SCIENCE Volume: 272 Issue: 5260 Pages: 337-338 Published: APR 19 1996	0	0	0	0	0	6	0.23
<input type="checkbox"/>	74. Sachem: a chemical cartridge for high-performance substructure search By: Kratochvil, Miroslav; Vondrasek, Jiri; Galgonek, Jakub JOURNAL OF CHEMINFORMATICS Volume: 10 Article Number: 27 Published: MAY 23 2018	0	0	5	0	0	5	1.25
<input type="checkbox"/>	75. Shared CaM- and S100A1-binding epitopes in the distal TRPM4 N terminus By: Bousova, Kristyna; Herman, Petr; Vecer, Jaroslav; et al. FEBS JOURNAL Volume: 285 Issue: 3 Pages: 599-613 Published: FEB 2018	0	1	1	3	0	5	1.25
<input type="checkbox"/>	76. Ameloblastin Peptides Modulates the Osteogenic Capacity of Human Mesenchymal Stem Cells By: Stakkestad, Oystein; Lyngstadaas, Stale P.; Vondrasek, Jiri; et al. FRONTIERS IN PHYSIOLOGY Volume: 8 Article Number: 58 Published: FEB 7 2017	1	1	0	3	0	5	1.00
<input type="checkbox"/>	77. Sequence-Specific Recognition of DNA by Proteins: Binding Motifs Discovered Using a Novel Statistical/Computational Analysis By: Jakubec, David; Laskowski, Roman A.; Vondrasek, Jiri PLOS ONE Volume: 11 Issue: 7 Article Number: e0158704 Published: JUL 6 2016	2	1	2	0	0	5	0.83
<input type="checkbox"/>	78. On InChI and evaluating the quality of cross-reference links By: Galgonek, Jakub; Vondrasek, Jiri JOURNAL OF CHEMINFORMATICS Volume: 6 Article Number: 15 Published: APR 17 2014	0	0	0	0	0	5	0.63
<input type="checkbox"/>	79. A systematic method for analysing the protein hydration structure of T4 lysozyme By: Kyslik, J.; Vondrasek, J. JOURNAL OF MOLECULAR RECOGNITION Volume: 26 Issue: 10 Pages: 479-487 Published: OCT 2013	0	0	1	0	0	5	0.56
<input type="checkbox"/>	80. Increasing Affinity of Interferon-gamma Receptor 1 to Interferon-gamma by Computer-Aided Design By: Mikulecky, Pavel; Cerny, Jiri; Biedermannova, Lada; et al. BIOMED RESEARCH INTERNATIONAL Volume: 2013 Article Number: 752514 Published: 2013	0	2	1	0	0	5	0.56

☐ Select Page | |

Sort by: **Times Cited** Date More

8 of 13

<input type="checkbox"/>	81. <b>Towards a better understanding of the specificity of protein-protein interaction</b> By: Kyslikova, Jiri; Vondrasek, Jiri JOURNAL OF MOLECULAR RECOGNITION Volume: 25 Issue: 11 Special Issue: SI Pages: 604-615 Published: NOV 2012	1	1	0	0	0	5	0.50
<input type="checkbox"/>	82. <b>AMBER and CHARMM Force Fields Inconsistently Portray the Microscopic Details of Phosphorylation</b> By: Vymetal, Jiri; Juraskova, Veronika; Vondrasek, Jiri JOURNAL OF CHEMICAL THEORY AND COMPUTATION Volume: 15 Issue: 1 Pages: 665-679 Published: JAN 2019	0	0	2	2	0	4	1.33
<input type="checkbox"/>	83. <b>Phosphorylation Modulates Ameloblastin Self-assembly and Ca2+ Binding</b> By: Stakkestad, Oystein; Lyngstadaas, Stale P.; Thiede, Bernd; et al. FRONTIERS IN PHYSIOLOGY Volume: 8 Article Number: 531 Published: JUL 27 2017	0	1	1	2	0	4	0.80
<input type="checkbox"/>	84. <b>The characterization of a novel S100A1 binding site in the N-terminus of TRPM1</b> By: Jirku, Michaela; Lansky, Zdenek; Bednarova, Lucie; et al. INTERNATIONAL JOURNAL OF BIOCHEMISTRY & CELL BIOLOGY Volume: 78 Pages: 186-193 Published: SEP 2016	0	1	1	2	0	4	0.67
<input type="checkbox"/>	85. <b>Optimal Definition of Inter-Residual Contact in Globular Proteins Based on Pairwise Interaction Energy Calculations, Its Robustness, and Applications</b> By: Fackovec, Boris; Vondrasek, Jiri JOURNAL OF PHYSICAL CHEMISTRY B Volume: 116 Issue: 42 Pages: 12651-12660 Published: OCT 25 2012	1	0	3	0	0	4	0.40
<input type="checkbox"/>	86. <b>Analysis of Energy Stabilization Inside the Hydrophobic Core of Rubredoxin</b> By: Berka, Karel; Hobza, Pavel; Vondrasek, Jiri CHEMPHYSCHEM Volume: 10 Issue: 3 Pages: 543-548 Published: FEB 23 2009	0	0	0	0	0	4	0.31
<input type="checkbox"/>	87. <b>Can All-Atom Molecular Dynamics Simulations Quantitatively Describe Homeodomain-DNA Binding Equilibria?</b> By: Jakubec, David; Vondrasek, Jiri JOURNAL OF CHEMICAL THEORY AND COMPUTATION Volume: 15 Issue: 4 Pages: 2635-2648 Published: APR 2019	0	0	0	3	0	3	1.00
<input type="checkbox"/>	88. <b>Toward Ab Initio Protein Folding: Inherent Secondary Structure Propensity of Short Peptides from the Bioinformatics and Quantum-Chemical Perspective</b> By: Culik, Martin; Galgonek, Jakub; Vymetal, Jiri; et al. JOURNAL OF PHYSICAL CHEMISTRY B Volume: 123 Issue: 6 Pages: 1215-1227 Published: FEB 14 2019	0	0	1	2	0	3	1.00
<input type="checkbox"/>	89. <b>Substituents at the C3' and C3' N positions are critical for taxanes to overcome acquired resistance of cancer cells to paclitaxel</b> By: Jelinek, Michael; Balusikova, Kamila; Daniel, Petr; et al. TOXICOLOGY AND APPLIED PHARMACOLOGY Volume: 347 Pages: 79-91 Published: MAY 15 2018	0	0	1	2	0	3	0.75
<input type="checkbox"/>	90. <b>Computational methods for the description of pharmacologically relevant platinum complexes - molecular structure and bond dissociation</b> By: Kokoschka, Malte; Galgonek, Jakub; Vondrasek, Jiri; et al. PHYSICAL CHEMISTRY CHEMICAL PHYSICS Volume: 18 Issue: 5 Pages: 4051-4062 Published: FEB 7 2016	0	0	2	0	0	3	0.50

☐ Select Page

<input type="checkbox"/>	91. <b>Retro operation on the Trp-cage miniprotein sequence produces an unstructured molecule capable of folding similar to the original only upon 2,2,2-trifluoroethanol addition</b> By: Vymetal, Jiri; Bathula, Sreenivas Reddy; Cerny, Jiri; et al. PROTEIN ENGINEERING DESIGN & SELECTION Volume: 27 Issue: 12 Pages: 463-472 Published: DEC 2014	0	0	2	0	0	3	0.38
<input type="checkbox"/>	92. <b>Interoperable chemical structure search service</b> By: Kratochvil, Miroslav; Vondrasek, Jiri; Galgonek, Jakub JOURNAL OF CHEMINFORMATICS Volume: 11 Article Number: 45 Published: JUN 28 2019	0	0	0	2	0	2	0.67
<input type="checkbox"/>	93. <b>Regioselective Palmitoylation of 9-(2,3-Dihydroxy-propyl)adenine Catalyzed by a Glycopolymer-enzyme Conjugate</b> By: Brabcova, Jana; Blazek, Jiri; Krecmerova, Marcela; et al. MOLECULES Volume: 21 Issue: 5 Article Number: 648 Published: MAY 2016	1	0	0	1	0	2	0.33
<input type="checkbox"/>	94. <b>Hypertrophic cardiomyopathy: from mutation to functional analysis of defective protein</b> By: Capek, Pavel; Vondrasek, Jiri; Sikvor, Jiri; et al. CROATIAN MEDICAL JOURNAL Volume: 52 Issue: 3 Pages: 384-391 Published: JUN 2011	0	0	0	1	0	2	0.18
<input type="checkbox"/>	95. <b>THE STABILIZATION ENERGY OF THE GLU-LYS SALT BRIDGE IN THE PROTEIN/WATER ENVIRONMENT: CORRELATED QUANTUM CHEMICAL ab Initio, DFT AND EMPIRICAL POTENTIAL STUDIES</b> By: Rezac, Jan; Berka, Karel; Horinek, Dominik; et al. COLLECTION OF CZECHOSLOVAK CHEMICAL COMMUNICATIONS Volume: 73 Issue: 6-7 Pages: 921-936 Published: 2008	0	0	0	0	0	2	0.14
<input type="checkbox"/>	96. <b>Efficient Estimation of Absolute Binding Free Energy for a Homeodomain-DNA Complex from Nonequilibrium Pulling Simulations</b> By: Jakubec, David; Vondrasek, Jiri JOURNAL OF CHEMICAL THEORY AND COMPUTATION Volume: 16 Issue: 4 Pages: 2034-2041 Published: APR 14 2020	0	0	0	1	0	1	0.50
<input type="checkbox"/>	97. <b>TRPM6 N-Terminal CaM- and S100A1-Binding Domains</b> By: Zouharova, Monika; Herman, Petr; Hofbauerova, Katerina; et al. INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES Volume: 20 Issue: 18 Article Number: 4430 Published: SEP 2 2019	0	0	0	1	0	1	0.33
<input type="checkbox"/>	98. <b>The bio.tools registry of software tools and data resources for the life sciences</b> By: Ison, Jon; Ienasescu, Hans; Chmura, Piotr; et al. GENOME BIOLOGY Volume: 20 Issue: 1 Article Number: 164 Published: AUG 12 2019	0	0	1	0	0	1	0.33
<input type="checkbox"/>	99. <b>An ameloblastin C-terminus variant is present in human adipose tissue</b> By: Stakkestad, Oystein; Heyward, Catherine; Lyngstadaas, Stale Petter; et al. HELIXON Volume: 4 Issue: 12 Article Number: e01075 Published: DEC 2018	0	0	0	1	0	1	0.25
<input type="checkbox"/>	100. <b>Artificial proteins as allosteric modulators of PDZ3 and SH3 in two-domain constructs: A computational characterization of novel chimeric proteins</b> By: Kirubakaran, Palani; Pfeifferova, Lucie; Bousova, Kristyna; et al. PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS Volume: 84 Issue: 10 Pages: 1358-1374 Published: OCT 2016	0	1	0	0	0	1	0.17

☐ Select Page | |

<input type="checkbox"/>	101. <b>Advanced SPARQL querying in small molecule databases</b> By: Galgonek, Jakub; Hurt, Tomas; Michlikova, Vendula; et al. JOURNAL OF CHEMINFORMATICS Volume: 8 Article Number: 31 Published: JUN 6 2016	0	0	1	0	0	1	0.17
<input type="checkbox"/>	102. <b>AN EMPIRICAL POTENTIAL STUDY OF THE INTERACTION OF L-LYSINE-L-ALANINE-L-ALANINE TRIPEPTIDE WITH 4 MODELS OF B-DNA WITH DIFFERENT COMPOSITIONS</b> By: VONDRASEK, J; SPONAR, J; HOBZA, P JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS Volume: 11 Issue: 4 Pages: 869-880 Published: FEB 1994	0	0	0	0	0	1	0.04
<input type="checkbox"/>	103. <b>Characterization of AMBN I and II Isoforms and Study of Their Ca<sup>2+</sup>-Binding Properties</b> By: Vetyiskova, Veronika; Zouharova, Monika; Bednarova, Lucie; et al. INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES Volume: 21 Issue: 23 Article Number: 9293 Published: DEC 2020	0	0	0	0	0	0	0.00
<input type="checkbox"/>	104. <b>Mapping of CaM, S100A1 and PIP2-Binding Epitopes in the Intracellular N- and C-Termini of TRPM4</b> By: Bousova, Kristyna; Barvik, Ivan; Herman, Petr; et al. INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES Volume: 21 Issue: 12 Article Number: 4323 Published: JUN 2020	0	0	0	0	0	0	0.00
<input type="checkbox"/>	105. <b>Hydrophobic Amino Acids as Universal Elements of Protein-Induced DNA Structure Deformation</b> By: Faltejskova, Katerina; Jakubec, David; Vondrasek, Jiri INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES Volume: 21 Issue: 11 Article Number: 3986 Published: JUN 2020	0	0	0	0	0	0	0.00
<input type="checkbox"/>	106. <b>ShinySOM: graphical SOM-based analysis of single-cell cytometry data</b> By: Kratochvil, Miroslav; Bednarek, David; Sieger, Tomas; et al. BIOINFORMATICS Volume: 36 Issue: 10 Pages: 3288-3289 Published: MAY 15 2020	0	0	0	0	0	0	0.00
<input type="checkbox"/>	107. <b>Interoperable chemical structure search service (vol 11, 45, 2019)</b> By: Kratochvil, Miroslav; Vondrasek, Jiri; Galgonek, Jakub JOURNAL OF CHEMINFORMATICS Volume: 12 Issue: 1 Article Number: 13 Published: FEB 13 2020	0	0	0	0	0	0	0.00
<input type="checkbox"/>	108. <b>Sequence Versus Composition: What Prescribes IDP Biophysical Properties?</b> By: Vymetal, Jiri; Vondrasek, Jiri; Hlouchova, Klara ENTROPY Volume: 21 Issue: 7 Article Number: 654 Published: JUL 2019	0	0	0	0	0	0	0.00
<input type="checkbox"/>	109. <b>3DPatch: fast 3D structure visualization with residue conservation</b> By: Jakubec, David; Vondrasek, Jiri; Finn, Robert D. BIOINFORMATICS Volume: 35 Issue: 2 Pages: 332-334 Published: JAN 15 2019	0	0	0	0	0	0	0.00
<input type="checkbox"/>	110. <b>Widespread evolutionary crosstalk among protein domains in the context of multi-domain proteins</b> By: Jakubec, David; Kratochvil, Miroslav; Vymetal, Jiri; et al. PLOS ONE Volume: 13 Issue: 8 Article Number: e0203085 Published: AUG 31 2018	0	0	0	0	0	0	0.00

☐ Select Page | | Save to Excel ...

<input type="checkbox"/>	111. <b>The identification of new substrates of human DHR57 by molecular modeling and in vitro testing</b> By: Zemanova, Lucie; Kirubakaran, Palani; Pato, Ignacio Hernando; et al. INTERNATIONAL JOURNAL OF BIOLOGICAL MACROMOLECULES Volume: 105 Pages: 171-182 Part: 1 Published: DEC 2017	0	0	0	0	0	0	0.00
<input type="checkbox"/>	112. <b>Novel calmodulin and S100A1 binding site in distal TRPM4 N-terminus</b> By: Vargova, M.; Frtus, A.; Vyklicky, L.; et al. Conference: 42nd Congress of the Federation-of-European-Biochemical-Societies (FEBS) on From Molecules to Cells and Back Location: Jerusalem, ISRAEL Date: SEP 10-14, 2017 Sponsor(s): Federat European Biochem Soc FEBS JOURNAL Volume: 284 Special Issue: SI Supplement: 1 Pages: 157-157 Meeting Abstract: P.2.1-023 Published: SEP 2017	0	0	0	0	0	0	0.00
<input type="checkbox"/>	113. <b>Is the structure and function of fusion proteins dependent on order of their domains?</b> By: Bousova, K.; Bednarova, L.; Telsinger, J.; et al. Conference: 42nd Congress of the Federation-of-European-Biochemical-Societies (FEBS) on From Molecules to Cells and Back Location: Jerusalem, ISRAEL Date: SEP 10-14, 2017 Sponsor(s): Federat European Biochem Soc FEBS JOURNAL Volume: 284 Special Issue: SI Supplement: 1 Pages: 215-215 Meeting Abstract: P.3.1.B014 Published: SEP 2017	0	0	0	0	0	0	0.00
<input type="checkbox"/>	114. <b>Novel structural mechanism of allosteric regulation of aspartic peptidases via evolutionary conserved exosite</b> By: Hanova, I.; Brynda, J.; Hobizalova, R.; et al. Conference: 42nd Congress of the Federation-of-European-Biochemical-Societies (FEBS) on From Molecules to Cells and Back Location: Jerusalem, ISRAEL Date: SEP 10-14, 2017 Sponsor(s): Federat European Biochem Soc FEBS JOURNAL Volume: 284 Special Issue: SI Supplement: 1 Pages: 300-301 Meeting Abstract: P.4.3.A011 Published: SEP 2017	0	0	0	0	0	0	0.00
<input type="checkbox"/>	115. <b>Conformational States of Amino Acids in Proteins and Peptides by Means of Computational Chemistry Methods</b> By: Vondrasek, Jiri; Vymetal, Jiri CHEMICKÉ LISTY Volume: 110 Issue: 5 Pages: 385-393 Published: MAY 2016	0	0	0	0	0	0	0.00
<input type="checkbox"/>	116. <b>Mapping Allostery in the Two Domain Constructs of PDZ3 and SH3 with Artificial Domains</b> By: Palani, Kirubakaran; Pfeiferova, Lucie; Vondrasek, Jiri Conference: 60th Annual Meeting of the Biophysical-Society Location: Los Angeles, CA Date: FEB 27-MAR 02, 2016 Sponsor(s): Biophys Soc BIOPHYSICAL JOURNAL Volume: 110 Issue: 3 Supplement: 1 Pages: 52 A-52A Meeting Abstract: 274-Pos Published: FEB 16 2016	0	0	0	0	0	0	0.00
<input type="checkbox"/>	117. <b>DHR57 enzyme - Important player in human health and diseases?</b> By: Zemanova, Lucie; Stambergova, Hana; Lundova, Tereza; et al. Conference: 29th Annual Symposium of the Protein-Society Location: Barcelona, SPAIN Date: JUL 22-25, 2015 Sponsor(s): Prot Soc PROTEIN SCIENCE Volume: 24 Special Issue: SI Supplement: 1 Pages: 111-112 Meeting Abstract: PE-017 Published: OCT 2015	0	0	0	0	0	0	0.00
<input type="checkbox"/>	118. <b>HOW TO FRAGMENT A POLYPEPTIDE? AN ab Initio COMPUTATIONAL STUDY OF PAIR INTERACTIONS BETWEEN AMINO ACIDS AND LIGAND-AMINO ACIDS IN PROTEINS</b> By: Klusak, Vojtech; Dobes, Petr; Cerny, Jiri; et al. COLLECTION OF CZECHOSLOVAK CHEMICAL COMMUNICATIONS Volume: 76 Issue: 5 Pages: 605-618 Published: 2011	0	0	0	0	0	0	0.00
<input type="checkbox"/>	119. <b>Rigid Duplex alpha-Cyclodextrin Reversibly Connected With Disulfide Bonds. Synthesis and Inclusion Complexes (vol 74, pg 1082, 2009)</b> By: Kumprecht, Lukas; Budesinsky, Milos; Vondrasek, Jiri; et al. JOURNAL OF ORGANIC CHEMISTRY Volume: 74 Issue: 21 Pages: 8496-8496 Published: NOV 6 2009	0	0	0	0	0	0	0.00
<input type="checkbox"/>	120. <b>Ions at aqueous interfaces: From water surface to hydrated proteins</b> By: Heyda, Jan; Vacha, Robert; Vondrasek, Jiri; et al. ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY Volume: 237 Meeting Abstract: 94 - COLL Published: MAR 22 2009	0	0	0	0	0	0	0.00

<input type="checkbox"/>	121. <b>Propeptide interaction with cathepsin D: Mechanism and regulation</b> By: Masa, M.; Maresova, L.; Vondrasek, J.; et al. JOURNAL OF PEPTIDE SCIENCE Volume: 12 Supplement: 5 Pages: 155-155 Published: 2006	0	0	0	0	0	0	0.00
<input type="checkbox"/>	122. <b>Molecular dynamics study of the conformational behavior of branched glycopeptides during the solid-phase synthesis - The effect of insert and terminal groups</b> By: Veprek, Pavel; Trnka, Tomas; Jezek, Jan; et al. Conference: 3rd International Peptide Symposium/28th European Peptide Symposium Location: Prague, CZECH REPUBLIC Date: SEP 05-10, 2004 Peptides 2004, Proceedings: BRIDGES BETWEEN DISCIPLINES Pages: 774-775 Published: 2005	0	0	0	0	0	0	0.00
<input type="checkbox"/>	123. <b>MOLECULAR DYNAMICS STUDY OF THE EFFECT OF GABU INSERT ON THE CONFORMATIONAL BEHAVIOR OF THE MULTIPLE ANTIGEN GLYCOPEPTIDES DURING THE SOLID-PHASE SYNTHESIS</b> By: Veprek, P.; Vondrasek, J.; Trnka, T.; et al. JOURNAL OF PEPTIDE SCIENCE Volume: 10 Pages: 233-233 Published: 2004	0	0	0	0	0	0	0.00
<input type="checkbox"/>	124. <b>Protein folding: State of the problem at the end of millenium</b> By: Svec, M; Vondrasek, J CHEMICKE LISTY Volume: 94 Issue: 8 Pages: 494-500 Published: 2000	0	0	0	0	0	0	0.00
<input type="checkbox"/>	125. <b>A new approach for screening of cadmlum binding by synthetic peptides</b> By: Kotrba, P; Doleckova, L; Pavlik, M; et al. CHEMICKE LISTY Volume: 90 Issue: 9 Pages: 709-709 Published: SEP 1996	0	0	0	0	0	0	0.00