

Doc. RNDr Jiří Vondrášek CSc - Publikace pro jmenovací řízení

1. **vědecké monografie** (jejich význam a závažnost posoudí příslušná hodnotící, event. habilitační komise a konkrétně se k nim v předkládaném Stanovisku hodnotící, resp. habilitační komise vyjádří)

N/A

2. **kapitoly v monografiích,**

Boris Fackovec and Jiri Vondrasek (2011). Decomposition of Intramolecular Interactions Between Amino-Acids in Globular Proteins - A Consequence for Structural Classes of Proteins and Methods of Their Classification, Systems and Computational Biology - Molecular and Cellular Experimental Systems, Editor: Prof. Ning-Sun Yang (Ed.), ISBN: 978-953-307-280-7, InTech publishing
Available from: <http://www.intechopen.com/books/systems-andcomputational-biology-molecular-and-cellular-experimental-systems/decomposition-of-intramolecularinteractions-between-amino-acids-in-globular-proteins-a-consequence->

3. **původní práce a práce v recenzovaných sbornících** – národních/mezinárodních

Celkový počet prací k 31.1.2021: **120**

Record 1

Title: Intrinsically disordered protein domain of human ameloblastin in synthetic fusion with calmodulin increases calmodulin stability and modulates its function

Authors: Monika Zouharova , Jiri Vymetal , Lucie Bednarova , Ondrej Vanek , Petr Herman , Veronika Vetyskova , Klara Postulkova , Petter S Lingstaadas , Jiri Vondrasek , Kristyna Bousova

Source: *International Journal of Biological Macromolecules*; Volume 168, 2021 Jan 31, pages :1-12.

doi: 10.1016/j.ijbiomac.2020.11.216. Epub 2020 Dec 5.

PMID: 33290768

IF: 5.162

Record 2

Title: GigaSOM.jl: High-performance clustering and visualization of huge cytometry datasets

Author(s): Miroslav Kratochvíl, Oliver Hunewald, Laurent Heirendt, Vasco Verissimo, Jiří Vondrášek, Venkata P Satagopam, Reinhard Schneider, Christophe Trefois, Markus Ollert

Source: *GigaScience*, Volume 9, Issue 11, November 2020, g127, **Published:** 18 November 2020

DOI: <https://doi.org/10.1093/gigascience/giaa127>

PMID: 33205814 **PMCID:** PMC7672468

IF: 5.999

Record 3

Title: Characterization of AMBN I and II Isoforms and Study of Their Ca²⁺-Binding Properties

Author(s): Vetyskova, V (Vetyskova, Veronika); Zouharova, M (Zouharova, Monika); Bednarova, L (Bednarova, Lucie); Vanek, O (Vanek, Ondrej); Sazelova, P (Sazelova, Petra); Kasicka, V (Kasicka, Vaclav); Vymetal, J (Vymetal, Jiri); Srp, J (Srp, Jaroslav);

Rumlova, M (Rumlova, Michaela); Charnavets, T (Charnavets, Tatsiana); Postulkova, K (Postulkova, Klara); Reseland, JE (Reseland, Janne E.); Bousova, K (Bousova, Kristyna); Vondrasek, J (Vondrasek, Jiri)
Source: INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES Volume: 21 Issue: 23 Article Number: 9293 DOI: 10.3390/ijms21239293 Published: DEC 2020
Accession Number: WOS:000597881700001
PubMed ID: 33291486
eISSN: 1422-0067
IF: 4.556

Record 4

Title: Mapping of CaM, S100A1 and PIP2-Binding Epitopes in the Intracellular N- and C-Termini of TRPM4
Author(s): Bousova, K (Bousova, Kristyna); Barvik, I (Barvik, Ivan); Herman, P (Herman, Petr); Hofbauerova, K (Hofbauerova, Katerina); Monincova, L (Monincova, Lenka); Majer, P (Majer, Pavel); Zouharova, M (Zouharova, Monika); Vetyskova, V (Vetyskova, Veronika); Postulkova, K (Postulkova, Klara); Vondrasek, J (Vondrasek, Jiri)
Source: INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES Volume: 21 Issue: 12 Article Number: 4323 DOI: 10.3390/ijms21124323 Published: JUN 2020
Accession Number: WOS:000549496800001
PubMed ID: 32560560
eISSN: 1422-0067
IF: 4.556

Record 5

Title: Hydrophobic Amino Acids as Universal Elements of Protein-Induced DNA Structure Deformation
Author(s): Faltejskova, K (Faltejskova, Katerina); Jakubec, D (Jakubec, David); Vondrasek, J (Vondrasek, Jiri)
Source: INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES Volume: 21 Issue: 11 Article Number: 3986 DOI: 10.3390/ijms21113986 Published: JUN 2020
Accession Number: WOS:000543400300248
PubMed ID: 32498246
eISSN: 1422-0067
IF: 4.556

Record 6

Title: ShinySOM: graphical SOM-based analysis of single-cell cytometry data
Author(s): Kratochvil, M (Kratochvil, Miroslav); Bednarek, D (Bednarek, David); Sieger, T (Sieger, Tomas); Fiser, K (Fiser, Karel); Vondrasek, J (Vondrasek, Jiri)
Source: BIOINFORMATICS Volume: 36 Issue: 10 Pages: 3288-3289 DOI: 10.1093/bioinformatics/btaa091 Published: MAY 15 2020
Accession Number: WOS:000537447900056
PubMed ID: 32049322
ISSN: 1367-4803
eISSN: 1460-2059
IF: 5.61

Record 7

Title: Efficient Estimation of Absolute Binding Free Energy for a Homeodomain-DNA Complex from Nonequilibrium Pulling Simulations
Author(s): Jakubec, D (Jakubec, David); Vondrasek, J (Vondrasek, Jiri)
Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION Volume: 16 Issue: 4 Pages: 2034-2041 DOI: 10.1021/acs.jctc.0c00006 Published: APR 14 2020
Accession Number: WOS:000526313000004
PubMed ID: 32208691
ISSN: 1549-9618
eISSN: 1549-9626
IF: 5.011

Record 8

Title: Interoperable chemical structure search service (vol 11, 45, 2019)
Author(s): Kratochvil, M (Kratochvil, Miroslav); Vondrasek, J (Vondrasek, Jiri); Galgonek, J (Galgonek, Jakub)
Source: JOURNAL OF CHEMINFORMATICS Volume: 12 Issue: 1 Article Number: 13 DOI: 10.1186/s13321-020-0418-8
Published: FEB 13 2020

Accession Number: WOS:000514894400001
PubMed ID: 33431019
ISSN: 1758-2946
IF: 5.362

Record 9

Title: TRPM6 N-Terminal CaM- and S100A1-Binding Domains
Author(s): Zouharova, M (Zouharova, Monika); Herman, P (Herman, Petr); Hofbauerova, K (Hofbauerova, Katerina); Vondrasek, J (Vondrasek, Jiri); Bousova, K (Bousova, Kristyna)
Source: INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES Volume: 20 Issue: 18 Article Number: 4430 DOI: 10.3390/ijms20184430 Published: SEP 2 2019
Accession Number: WOS:000489100500109
PubMed ID: 31505788
eISSN: 1422-0067
IF: 4.556

Record 10

Title: The bio.tools registry of software tools and data resources for the life sciences
Author(s): Ison, J (Ison, Jon); Ienasescu, H (Ienasescu, Hans); Chmura, P (Chmura, Piotr); Rydza, E (Rydza, Emil); Menager, H (Menager, Herve); Kalas, M (Kalas, Matus); Schwammle, V (Schwammle, Veit); Gruning, B (Gruening, Bjoern); Beard, N (Beard, Niall); Lopez, R (Lopez, Rodrigo); Duvaud, S (Duvaud, Severine); Stockinger, H (Stockinger, Heinz); Persson, B (Persson, Bengt); Varekova, RS (Varekova, Radka Svobodova); Racek, T (Racek, Tomas); Vondrasek, J (Vondrasek, Jiri); Peterson, H (Peterson, Hedi); Salumets, A (Salumets, Ahto); Jonassen, I (Jonassen, Inge); Hooft, R (Hooft, Rob); Nyronen, T (Nyronen, Tommi); Valencia, A (Valencia, Alfonso); Capella, S (Capella, Salvador); Gelpi, J (Gelpi, Josep); Zambelli, F (Zambelli, Federico); Savakis, B (Savakis, Babis); Leskosek, B (Leskosek, Brane); Rapacki, K (Rapacki, Kristoffer); Blanchet, C (Blanchet, Christophe); Jimenez, R (Jimenez, Rafael); Oliveira, A (Oliveira, Arlindo); Vriend, G (Vriend, Gert); Collin, O (Collin, Olivier); van Helden, J (van Helden, Jacques); Longreen, P (Longreen, Peter); Brunak, S (Brunak, Soren)
Source: GENOME BIOLOGY Volume: 20 Issue: 1 Article Number: 164 DOI: 10.1186/s13059-019-1772-6 Published: AUG 12 2019
Accession Number: WOS:000480534400002
PubMed ID: 31405382
ISSN: 1474-760X
IF: 10.806

Record 11

Title: Sequence Versus Composition: What Prescribes IDP Biophysical Properties?
Author(s): Vymetal, J (Vymetal, Jiri); Vondrasek, J (Vondrasek, Jiri); Hlouchova, K (Hlouchova, Klara)
Source: ENTROPY Volume: 21 Issue: 7 Article Number: 654 DOI: 10.3390/e21070654 Published: JUL 2019
Accession Number: WOS:000478585200086
PubMed ID: 33267368
eISSN: 1099-4300
IF: 2.494

Record 12

Title: Interoperable chemical structure search service
Author(s): Kratochvil, M (Kratochvil, Miroslav); Vondrasek, J (Vondrasek, Jiri); Galgonek, J (Galgonek, Jakub)
Source: JOURNAL OF CHEMINFORMATICS Volume: 11 Article Number: 45 DOI: 10.1186/s13321-019-0367-2 Published: JUN 28 2019
Accession Number: WOS:000473238100001
PubMed ID: 31254167
ISSN: 1758-2946
IF: 5.326

Record 13

Title: Can All-Atom Molecular Dynamics Simulations Quantitatively Describe Homeodomain-DNA Binding Equilibria?
Author(s): Jakubec, D (Jakubec, David); Vondrasek, J (Vondrasek, Jiri)
Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION Volume: 15 Issue: 4 Pages: 2635-2648 DOI: 10.1021/acs.jctc.8b01144 Published: APR 2019
Accession Number: WOS:000464475500043
PubMed ID: 30807142
ISSN: 1549-9618

eISSN: 1549-9626

IF: 5.011

Record 14

Title: Toward Ab Initio Protein Folding: Inherent Secondary Structure Propensity of Short Peptides from the Bioinformatics and Quantum-Chemical Perspective

Author(s): Culka, M (Culka, Martin); Galgonek, J (Galgonek, Jakub); Vymetal, J (Vymetal, Jiri); Vondrasek, J (Vondrasek, Jiri); Rulisek, L (Rulisek, Lubomir)

Source: JOURNAL OF PHYSICAL CHEMISTRY B Volume: 123 Issue: 6 Pages: 1215-1227 DOI: 10.1021/acs.jpcb.8b09245

Published: FEB 14 2019

Accession Number: WOS:000459223800001

PubMed ID: 30645123

ISSN: 1520-6106

eISSN: 1520-5207

IF: 2.857

Record 15

Title: 3DPatch: fast 3D structure visualization with residue conservation

Author(s): Jakubec, D (Jakubec, David); Vondrasek, J (Vondrasek, Jiri); Finn, RD (Finn, Robert D.)

Source: BIOINFORMATICS Volume: 35 Issue: 2 Pages: 332-334 DOI: 10.1093/bioinformatics/bty464 Published: JAN 15 2019

Accession Number: WOS:000459314900019

PubMed ID: 29931189

ISSN: 1367-4803

eISSN: 1460-2059

IF: 5.61

Record 16

Title: Exquisite ligand stereoselectivity of a Drosophila juvenile hormone receptor contrasts with its broad agonist repertoire

Author(s): Bittova, L (Bittova, Lenka); Jedlicka, P (Jedlicka, Pavel); Dracinsky, M (Dracinsky, Martin); Kirubakaran, P (Kirubakaran, Palani); Vondrasek, J (Vondrasek, Jiri); Hanus, R (Hanus, Robert); Jindra, M (Jindra, Marek)

Source: JOURNAL OF BIOLOGICAL CHEMISTRY Volume: 294 Issue: 2 Pages: 410-423 DOI: 10.1074/jbc.RA118.005992

Published: JAN 11 2019

Accession Number: WOS:000456263600003

PubMed ID: 30455350

ISSN: 0021-9258

eISSN: 1083-351X

IF: 4.238

Record 17

Title: AMBER and CHARMM Force Fields Inconsistently Portray the Microscopic Details of Phosphorylation

Author(s): Vymetal, J (Vymetal, Jiri); Juraskova, V (Juraskova, Veronika); Vondrasek, J (Vondrasek, Jiri)

Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION Volume: 15 Issue: 1 Pages: 665-679 DOI: 10.1021/acs.jctc.8b00715 Published: JAN 2019

Accession Number: WOS:000455558200058

PubMed ID: 30468703

ISSN: 1549-9618

eISSN: 1549-9626

IF: 5.011

Record 18

Title: An ameloblastin C-terminus variant is present in human adipose tissue

Author(s): Stakkestad, O (Stakkestad, Oystein); Heyward, C (Heyward, Catherine); Lyngstadaas, SP (Lyngstadaas, Stale Petter); Medin, T (Medin, Tirill); Vondrasek, J (Vondrasek, Jiri); Lian, AM (Lian, Aina-Mari); Pezeshki, G (Pezeshki, Gita); Reseland, JE (Reseland, Janne Elin)

Source: HELIYON Volume: 4 Issue: 12 Article Number: e01075 DOI: 10.1016/j.heliyon.2018.e01075 Published: DEC 2018

Accession Number: WOS:000454725700029

PubMed ID: 30603708

ISSN: 2405-8440

IF: N/A

Record 19

Title: Widespread evolutionary crosstalk among protein domains in the context of multi- domain proteins

Author(s): Jakubec, D (Jakubec, David); Kratochvil, M (Kratochvil, Miroslav); Vymetal, J (Vymetal, Jiri); Vondrasek, J (Vondrasek, Jiri)

Source: PLOS ONE Volume: 13 Issue: 8 Article Number: e0203085 DOI: 10.1371/journal.pone.0203085 Published: AUG 31 2018

Accession Number: WOS:000443374400020

PubMed ID: 30169546

ISSN: 1932-6203

IF: 2.74

Record 20

Title: Sachem: a chemical cartridge for high-performance substructure search

Author(s): Kratochvil, M (Kratochvil, Miroslav); Vondrasek, J (Vondrasek, Jiri); Galgonek, J (Galgonek, Jakub)

Source: JOURNAL OF CHEMINFORMATICS Volume: 10 Article Number: 27 DOI: 10.1186/s13321-018-0282-y Published: MAY 23 2018

Accession Number: WOS:000433128300001

PubMed ID: 29797000

ISSN: 1758-2946

IF: 5.326

Record 21

Title: Substituents at the C3 ' and C3 ' N positions are critical for taxanes to overcome acquired resistance of cancer cells to paclitaxel

Author(s): Jelinek, M (Jelinek, Michael); Balusikova, K (Balusikova, Kamila); Daniel, P (Daniel, Petr); Nemcova-Furstova, V (Nemcova-Furstova, Vlasta); Kirubakaran, P (Kirubakaran, Palani); Jacek, M (Jacek, Martin); Wei, LF (Wei, Longfei); Wang, X (Wang, Xin); Vondrasek, J (Vondrasek, Jiri); Ojima, I (Ojima, Iwao); Kovar, J (Kovar, Jan)

Source: TOXICOLOGY AND APPLIED PHARMACOLOGY Volume: 347 Pages: 79-91 DOI: 10.1016/j.taap.2018.04.002

Published: MAY 15 2018

Accession Number: WOS:000431165000009

PubMed ID: 29625142

ISSN: 0041-008X

eISSN: 1096-0333

IF: 3.347

Record 22

Title: SmSP2: A serine protease secreted by the blood fluke pathogen *Schistosoma mansoni* with anti-hemostatic properties

Author(s): Leontovyc, A (Leontovyc, Adrian); Ulrychova, L (Ulrychova, Lenka); O'Donoghue, AJ (O'Donoghue, Anthony J.); Vondrasek, J (Vondrasek, Jiri); Maresova, L (Maresova, Lucie); Hubalek, M (Hubalek, Martin); Fajtova, P (Fajtova, Pavla); Chanova, M (Chanova, Marta); Jiang, ZZ (Jiang, Zhenze); Craik, CS (Craik, Charles S.); Caffrey, CR (Caffrey, Conor R.); Mares, M (Mares, Michael); Dvorak, J (Dvorak, Jan); Horn, M (Horn, Martin)

Source: PLOS NEGLECTED TROPICAL DISEASES Volume: 12 Issue: 4 Article Number: e0006446 DOI:

10.1371/journal.pntd.0006446 Published: APR 2018

Accession Number: WOS:000433487700071

PubMed ID: 29677188

ISSN: 1935-2735

IF: 3.885

Record 23

Title: Shared CaM- and S100A1-binding epitopes in the distal TRPM4 N terminus

Author(s): Bousova, K (Bousova, Kristyna); Herman, P (Herman, Petr); Vecer, J (Vecer, Jaroslav); Bednarova, L (Bednarova, Lucie); Monincova, L (Monincova, Lenka); Majer, P (Majer, Pavel); Vyklicky, L (Vyklicky, Ladislav); Vondrasek, J (Vondrasek, Jiri); Teisinger, J (Teisinger, Jan)

Source: FEBS JOURNAL Volume: 285 Issue: 3 Pages: 599-613 DOI: 10.1111/febs.14362 Published: FEB 2018

Accession Number: WOS:000424168600012

PubMed ID: 29240297

ISSN: 1742-464X
eISSN: 1742-4658
IF: 4.392

Record 24

Title: Novel Structural Mechanism of Allosteric Regulation of Aspartic Peptidases via an Evolutionarily Conserved Exosite
Author(s): Hanova, I (Hanova, Iva); Brynda, J (Brynda, Jiri); Houstecka, R (Houstecka, Radka); Alam, N (Alam, Nawsad); Sojka, D (Sojka, Daniel); Kopacek, P (Kopacek, Petr); Maresova, L (Maresova, Lucie); Vondrasek, J (Vondrasek, Jiri); Horn, M (Horn, Martin); SchuelerFurman, O (SchuelerFurman, Ora); Mares, M (Mares, Michael)
Source: CELL CHEMICAL BIOLOGY Volume: 25 Issue: 3 Pages: 318+
DOI: 10.1016/j.chembiol.2018.01.001 Published: MAR 15 2018
Accession Number: WOS:000427600400012
PubMed ID: 29396291
ISSN: 24519448
IF: 7.739

Record 25

Title: The identification of new substrates of human DHRS7 by molecular modeling and in vitro testing
Author(s): Zemanova, L (Zemanova, Lucie); Kirubakaran, P (Kirubakaran, Palani); Pato, IH (Pato, Ignacio Hernando); Stambergova, H (Stambergova, Hana); Vondrasek, J (Vondrasek, Jiri)
Source: INTERNATIONAL JOURNAL OF BIOLOGICAL MACROMOLECULES Volume: 105 Pages: 171182
DOI: 10.1016/j.ijbiomac.2017.07.012 Part: 1 Published: DEC 2017
Accession Number: WOS:000414882900019
PubMed ID: 28687384
ISSN: 01418130
eISSN: 18790003
IF: 5.162

Record 26

Title: Random protein sequences can form defined secondary structures and are well tolerated in vivo
Author(s): Tretyachenko, V (Tretyachenko, Vyacheslav); Vymetal, J (Vymetal, Jiri); Bednarova, L (Bednarova, Lucie); Kopecky, V (Kopecky, Vladimir, Jr.); Hofbauerova, K (Hofbauerova, Katerina); Jindrova, H (Jindrova, Helena); Hubalek, M (Hubalek, Martin); Soucek, R (Soucek, Radko); Konvalinka, J (Konvalinka, Jan); Vondrasek, J (Vondrasek, Jiri); Hlouchova, K (Hlouchova, Klara)
Source: SCIENTIFIC REPORTS Volume: 7 Article Number: 15449 DOI: 10.1038/s41598017156358
Published: NOV 13 2017
Accession Number: WOS:000415023200010
PubMed ID: 29133927
ISSN: 20452322
IF: 3.998

Record 27

Title: Phosphorylation Modulates Ameloblastin Selfassembly and Ca²⁺ Binding
Author(s): Stakkestad, O (Stakkestad, Oystein); Lyngstadaas, SP (Lyngstadaas, Stale P.); Thiede, B (Thiede, Bernd); Vondrasek, J (Vondrasek, Jiri); Skalhogg, BS (Skalhogg, Bjorn S.); Reseland, JE (Reseland, Janne E.)
Source: FRONTIERS IN PHYSIOLOGY Volume: 8 Article Number: 531 DOI: 10.3389/fphys.2017.00531 Published: JUL 27 2017
Accession Number: WOS:000406530400001
PubMed ID: 28798693
ISSN: 1664042X
IF:3.367

Record 28

Title: Amino Acid Interaction (INTAA) web server
Author(s): Galgonek, J (Galgonek, Jakub); Vymetal, J (Vymetal, Jiri); Jakubec, D (Jakubec, David); Vondrasek, J (Vondrasek, Jiri)
Source: NUCLEIC ACIDS RESEARCH Volume: 45 Issue: W1 Pages: W388W392
DOI: 10.1093/nar/gkx352 Published: JUL 3 2017
Accession Number: WOS:000404427000058

PubMed ID: 28472475

ISSN: 03051048

eISSN: 13624962

IF:11.502

Record 29

Title: Ameloblastin Peptides Modulates the Osteogenic Capacity of Human Mesenchymal Stem Cells

Author(s): Stakkestad, O (Stakkestad, Oystein); Lyngstadaas, SP (Lyngstadaas, Stale P.); Vondrasek, J (Vondrasek, Jiri);

Gordeladze, JO (Gordeladze, Jan O.); Reseland, JE (Reseland, Janne Elin)

Source: FRONTIERS IN PHYSIOLOGY Volume: 8 Article Number: 58 DOI: 10.3389/fphys.2017.00058 Published: FEB 7 2017

Accession Number: WOS:000393307100002

PubMed ID: 28223942

ISSN: 1664042X

IF:3.367

Record 30

Title: Noncovalent Interactions in Specific Recognition Motifs of Protein-DNA Complexes

Author(s): Stasyuk, OA (Stasyuk, Olga A.); Jakubec, D (Jakubec, David); Vondrasek, J (Vondrasek, Jiri); Hobza, P (Hobza, Pavel)

Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION Volume: 13 Issue: 2 Pages: 877885

DOI: 10.1021/acs.jctc.6b00775 Published:

FEB 2017

Accession Number: WOS:000394924000044

PubMed ID: 27992205

ISSN: 15499618

eISSN: 15499626

IF:5.011

Record 31

Title: Artificial proteins as allosteric modulators of PDZ3 and SH3 in two domain constructs: A computational characterization of novel chimeric proteins

Author(s): Kirubakaran, P (Kirubakaran, Palani); Pfeiferova, L (Pfeiferova, Lucie); Bousova, K (Bousova, Kristyna); Bednarova, L (Bednarova, Lucie); Obsilova, V (Obsilova, Veronika); Vondrasek, J (Vondrasek, Jiri)

Source: PROTEINS STRUCTURE FUNCTION AND BIOINFORMATICS Volume: 84 Issue: 10 Pages: 13581374

DOI: 10.1002/prot.25082 Published: OCT 2016

Accession Number: WOS:000383678800003

PubMed ID: 27273513

ISSN: 08873585

eISSN: 10970134

IF:2.828

Record 32

Title: The characterization of a novel S100A1 binding site in the N terminus of TRPM1

Author(s): Jirku, M (Jirku, Michaela); Lansky, Z (Lansky, Zdenek); Bednarova, L (Bednarova, Lucie); Sulc, M (Sulc, Miroslav);

Monincova, L (Monincova, Lenka); Majer, P (Majer, Pavel); Vyklicky, L (Vyklicky, Ladislav); Vondrasek, J (Vondrasek, Jiri);

Teisinger, J (Teisinger, Jan); Bousova, K (Bousova, Kristyna)

Source: INTERNATIONAL JOURNAL OF BIOCHEMISTRY & CELL BIOLOGY Volume: 78 Pages: 186193

DOI: 10.1016/j.biocel.2016.07.014 Published: SEP 2016

Accession Number: WOS:000383297300020

PubMed ID: 27435061

ISSN: 13572725

eISSN: 18785875

IF:3.673

Record 33

Title: Sequence Specific Recognition of DNA by Proteins: Binding Motifs Discovered Using a Novel Statistical/Computational Analysis

Author(s): Jakubec, D (Jakubec, David); Laskowski, RA (Laskowski, Roman A.); Vondrasek, J (Vondrasek, Jiri)

Source: PLOS ONE Volume: 11 Issue: 7 Article Number: e0158704

DOI: 10.1371/journal.pone.0158704 Published: JUL 6 2016

Accession Number: WOS:000379809400077

PubMed ID: 27384774

ISSN: 19326203

IF:2.74

Record 34

Title: Advanced SPARQL querying in small molecule databases

Author(s): Galgonek, J (Galgonek, Jakub); Hurt, T (Hurt, Tomas); Michlikova, V (Michlikova, Vendula); Onderka, P (Onderka, Petr); Schwarz, J (Schwarz, Jan); Vondrasek, J (Vondrasek, Jiri)

Source: JOURNAL OF CHEMINFORMATICS Volume: 8 Article Number: 31

DOI: 10.1186/s1332101601444

Published: JUN 6 2016

Accession Number: WOS:000377064900001

PubMed ID: 27275187

ISSN: 17582946

IF:5.326

Record 35

Title: Regioselective Palmitoylation of 9(2,3Dihydroxypropyl) adenine Catalyzed by a Glycopolymerenzyme Conjugate

Author(s): Brabcova, J (Brabcova, Jana); Blazek, J (Blazek, Jiri); Krecmerova, M (Krecmerova, Marcela); Vondrasek, J (Vondrasek, Jiri); Palomo, JM (Palomo, Jose M.); Zarevucka, M (Zarevucka, Marie)

Source: MOLECULES Volume: 21 Issue: 5 Article Number: 648 DOI: 10.3390/molecules21050648 Published: MAY 2016

Accession Number: WOS:000380241600111

PubMed ID: 27196879

ISSN: 14203049

IF:3.267

Record 36

Title: Conformational States of Amino Acids in Proteins and Peptides by Means of Computational Chemistry Methods

Author(s): Vondrasek, J (Vondrasek, Jiri); Vymetal, J (Vymetal, Jiri)

Source: CHEMISCHE LISTE Volume: 110 Issue: 5 Pages: 385393

Published: MAY 2016

Accession Number: WOS:000376591500010

ISSN: 00092770

eISSN: 12137103

IF:0.39

Record 37

Title: Effect of TFE on the Helical Content of AK17 and HAL1 Peptides: Theoretical Insights into the Mechanism of Helix Stabilization

Author(s): Vymetal, J (Vymetal, Jiri); Bednarova, L (Bednarova, Lucie); Vondrasek, J (Vondrasek, Jiri)

Source: JOURNAL OF PHYSICAL CHEMISTRY B Volume: 120 Issue: 6 Pages: 10481059

DOI: 10.1021/acs.jpcc.5b11228 Published: FEB 18 2016

Accession Number: WOS:000370678500002

PubMed ID: 26786280

ISSN: 15206106

IF:2.857

Record 38

Title: Computational methods for the description of pharmacologically relevant platinum complexes molecular structure and bond dissociation

Author(s): Kokoschka, M (Kokoschka, Malte); Galgonek, J (Galgonek, Jakub); Vondrasek, J (Vondrasek, Jiri); Hobza, P (Hobza, Pavel)

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS Volume: 18 Issue: 5 Pages: 40514062

DOI: 10.1039/c5cp03391h Published: FEB 7 2016

Accession Number: WOS:000369508100080

PubMed ID: 26777459

ISSN: 14639076

eISSN: 14639084

IF: 3.43

Record 39

Title: Insights into Unfolded Proteins from the Intrinsic phi/psi Propensities of the AAXAA HostGuest Series

Author(s): Towse, CL (Towse, ClareLouise); Vymetal, J (Vymetal, Jiri); Vondrasek, J (Vondrasek, Jiri); Daggett, V (Daggett, Valerie)

Source: BIOPHYSICAL JOURNAL Volume: 110 Issue: 2 Pages: 348361

DOI: 10.1016/j.bpj.2015.12.008 Published: JAN 19 2016

Accession Number: WOS:000368354700009

PubMed ID: 26789758

ISSN: 00063495

eISSN: 15420086

IF: 3.854

Record 40

Title: Characterization of the part of Nterminal PIP2 binding site of the TRPM1 channel

Author(s): Jirku, M (Jirku, Michaela); Bumba, L (Bumba, Ladislav); Bednarova, L (Bednarova, Lucie); Kubala, M (Kubala, Martin); Sulc, M (Sulc, Miroslav); Franek, M (Franek, Miloslav); Vyklicky, L (Vyklicky, Ladislav); Vondrasek, J (Vondrasek, Jiri); Teisinger, J (Teisinger, Jan); Bousova, K (Bousova, Kristyna)

Source: BIOPHYSICAL CHEMISTRY Volume: 207 Pages: 135142

DOI: 10.1016/j.bpc.2015.10.005 Published: DEC 2015

Accession Number: WOS:000366442800016

PubMed ID: 26544986

ISSN: 03014622

eISSN: 18734200

IF: 1.995

Record 41

Title: PIP2 and PIP3 interact with Nterminus region of TRPM4 channel

Author(s): Bousova, K (Bousova, Kristyna); Jirku, M (Jirku, Michaela); Sumba, L (Sumba, Ladislav); Bednarova, L (Bednarova, Lucie); Sulc, M (Sulc, Miroslav); Franek, M (Franek, Miloslav); Vyklicky, L (Vyklicky, Ladislav); Vondrasek, J (Vondrasek, Jiri); Teisinger, J (Teisinger, Jan)

Source: BIOPHYSICAL CHEMISTRY Volume: 205 Pages: 2432

DOI: 10.1016/j.bpc.2015.06.004 Published: OCT 2015

Accession Number: WOS:000358806500004

PubMed ID: 26071843

ISSN: 03014622

eISSN: 18734200

IF: 1.995

Record 42

Title: Representative Amino Acid Side Chain Interactions in ProteinDNA Complexes: A Comparison of Highly Accurate Correlated Ab Initio Quantum Mechanical Calculations and Efficient Approaches for Applications to Large Systems

Author(s): Hostas, J (Hostas, Jiri); Jakubec, D (Jakubec, David); Laskowski, RA (Laskowski, Roman A.); Gnanasekaran, R (Gnanasekaran, Ramachandran); Rezac, J (Rezac, Jan); Vondrasek, J (Vondrasek, Jiri); Hobza, P (Hobza, Pavel)

Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION Volume: 11 Issue: 9 Pages: 40864092

DOI: 10.1021/acs.jctc.5b00398 Published: SEP 2015

Accession Number: WOS:000361087600013

PubMed ID: 26575904

ISSN: 15499618

eISSN: 15499626

IF: 5.011

Record 43

Title: Prolyl Oligopeptidase from the Blood Fluke Schistosoma mansoni: From Functional Analysis to Antischistosomal Inhibitors

Author(s): Fajtova, P (Fajtova, Pavla); Stefanic, S (Stefanic, Sasa); Hradilek, M (Hradilek, Martin); Dvorak, J (Dvorak, Jan); Vondrasek, J (Vondrasek, Jiri); Jilkova, A (Jilkova, Adela); Ulrychova, L (Ulrychova, Lenka); McKerrow, JH (McKerrow, James H.); Caffrey, CR (Caffrey, Conor R.); Mares, M (Mares, Michael); Horn, M (Horn, Martin)

Source: PLOS NEGLECTED TROPICAL DISEASES Volume: 9 Issue: 6 Article Number: e0003827 DOI:

10.1371/journal.pntd.0003827 Published: JUN 2015

Accession Number: WOS:000357398100031

PubMed ID: 26039195

ISSN: 19352735

IF: 3.885

Record 44

Title: Large Scale Quantitative Assessment of Binding Preferences in Protein Nucleic Acid Complexes

Author(s): Jakubec, D (Jakubec, David); Hostas, J (Hostas, Jiri); Laskowski, RA (Laskowski, Roman A.); Hobza, P (Hobza, Pavel); Vondrasek, J (Vondrasek, Jiri)

Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION Volume: 11 Issue: 4 Pages: 19391948

DOI: 10.1021/ct501168n Published: APR 2015

Accession Number: WOS:000353176500058

PubMed ID: 26894243

ISSN: 15499618

eISSN: 15499626

IF: 5.011

Record 45

Title: Activation Route of the Schistosoma mansoni Cathepsin B1 Drug Target: Structural Map with a Glycosaminoglycan Switch

Author(s): Jilkova, A (Jilkova, Adela); Horn, M (Horn, Martin); Rezacova, P (Rezacova, Pavlina); Maresova, L (Maresova, Lucie); Fajtova, P (Fajtova, Pavla); Brynda, J (Brynda, Jiri); Vondrasek, J (Vondrasek, Jiri); McKerrow, JH (McKerrow, James H.); Caffrey, CR (Caffrey, Conor R.); Mares, M (Mares, Michael)

Source: STRUCTURE Volume: 22 Issue: 12 Pages: 17861798

DOI: 10.1016/j.str.2014.09.015 Published: DEC 2 2014

Accession Number: WOS:000345898700012

PubMed ID: 25456815

ISSN: 09692126

eISSN: 18784186

IF:4.862

Record 46

Title: Retro operation on the Trp cage miniprotein sequence produces an unstructured molecule capable of folding similar to the original only upon 2,2,2trifluoroethanol addition

Author(s): Vymetal, J (Vymetal, Jiri); Bathula, SR (Bathula, Sreenivas Reddy); Cerny, J (Cerny, Jiri); Chaloupkova, R (Chaloupkova, Radka); Zidek, L (Zidek, Lukas); Sklenar, V (Sklenar, Vladimir); Vondrasek, J (Vondrasek, Jiri)

Source: PROTEIN ENGINEERING DESIGN & SELECTION Volume: 27 Issue: 12 Pages: 463472

DOI: 10.1093/protein/gzu046 Published: DEC 2014

Accession Number: WOS:000345837300001

PubMed ID: 25344682

ISSN: 17410126

eISSN: 17410134

IF: 1.774

Record 47

Title: Parametrization of 2,2,2Trifluoroethanol Based on the Generalized Amber Force Field Provides Realistic Agreement between Experimental and Calculated Properties of Pure Liquid as Well as Water Mixed Solutions

Author(s): Vymetal, J (Vymetal, Jiri); Vondrasek, J (Vondrasek, Jiri)

Source: JOURNAL OF PHYSICAL CHEMISTRY B Volume: 118 Issue: 35 Pages: 1039010404

DOI: 10.1021/jp505861b Published: SEP 4 2014

Accession Number: WOS:000341337500008

PubMed ID: 25110944

ISSN: 15206106

IF: 2.857

Record 48

Title: On InChI and evaluating the quality of cross reference links

Author(s): Galgonek, J (Galgonek, Jakub); Vondrasek, J (Vondrasek, Jiri)

Source: JOURNAL OF CHEMINFORMATICS Volume: 6 Article Number: 15 DOI: 10.1186/17582946615

Published: APR 17 2014

Accession Number: WOS:000335606300001

PubMed ID: 24742140

ISSN: 17582946

IF: 5.326

Record 49

Title: Trypsin and Chymotrypsin Like Serine Proteases in Schistosoma mansoni ' The Undiscovered Country'

Author(s): Horn, M (Horn, Martin); Fajtova, P (Fajtova, Pavla); Arreola, LR (Arreola, Liliana Rojo); Ulrychova, L (Ulrychova, Lenka); BartosovaSojkova, P (Bartosova Sojkova, Pavla); Franta, Z (Franta, Zdenek); Protasio, AV (Protasio, Anna V.);

Opavsky, D (Opavsky, David); Vondrasek, J (Vondrasek, Jiri); McKerrow, JH (McKerrow, James H.); Mares, M (Mares, Michael); Caffrey, CR (Caffrey, Conor R.); Dvorak, J (Dvorak, Jan)
Source: PLOS NEGLECTED TROPICAL DISEASES Volume: 8 Issue: 3 Article Number: e2766 DOI: 10.1371/journal.pntd.0002766 Published: MAR 2014
Accession Number: WOS:000337348800041
PubMed ID: 24676141
ISSN: 19352735
IF:3.885

Record 50

Title: Highly selective purification of three lipases from *Geotrichum candidum* 4013 and their characterization and biotechnological applications
Author(s): Brabcova, J (Brabcova, Jana); Demianova, Z (Demianova, Zuzana); Vondrasek, J (Vondrasek, Jiri); Jagr, M (Jagr, Michal); Zarevucka, M (Zarevucka, Marie); Palomo, JM (Palomo, Jose M.)
Source: JOURNAL OF MOLECULAR CATALYSIS B ENZYMATIC
Volume: 98 Pages: 6272
DOI: 10.1016/j.molcatb.2013.09.012 Published: DEC 30 2013
Accession Number: WOS:000328237400010
ISSN: 13811177
eISSN: 18733158
IF:2.269

Record 51

Title: A systematic method for analysing the protein hydration structure of T4 lysozyme
Author(s): Kysilka, J (Kysilka, J.); Vondrasek, J (Vondrasek, J.)
Source: JOURNAL OF MOLECULAR RECOGNITION Volume: 26 Issue: 10 Pages: 479487
DOI: 10.1002/jmr.2290 Published: OCT 2013
Accession Number: WOS:000323674900006
PubMed ID: 23996490
ISSN: 09523499
eISSN: 10991352
IF:2.214

Record 52

Title: Intrinsically Disordered Enamel Matrix Protein Ameloblastin Forms Ribbonlike Supramolecular Structures via an N-terminal Segment Encoded by Exon 5
Author(s): Wald, T (Wald, Tomas); Osickova, A (Osickova, Adriana); Sulc, M (Sulc, Miroslav); Benada, O (Benada, Oldrich); Semeradtova, A (Semeradtova, Alena); Rezabkova, L (Rezabkova, Lenka); Veverka, V (Veverka, Vaclav); Bednarova, L (Bednarova, Lucie); Maly, J (Maly, Jan); Macek, P (Macek, Pavel); Sebo, P (Sebo, Peter); Slaby, I (Slaby, Ivan); Vondrasek, J (Vondrasek, Jiri); Osicka, R (Osicka, Radim)
Source: JOURNAL OF BIOLOGICAL CHEMISTRY Volume: 288 Issue: 31 Pages: 2233322345
DOI: 10.1074/jbc.M113.456012 Published: AUG 2 2013
Accession Number: WOS:000330596300015
PubMed ID: 23782691
ISSN: 00219258
eISSN: 1083351X
IF:4.238

Record 53

Title: Increasing Affinity of Interferon gamma Receptor 1 to Interferon gamma by Computer Aided Design
Author(s): Mikulecky, P (Mikulecky, Pavel); Cerny, J (Cerny, Jiri); Biedermannova, L (Biedermannova, Lada); Petrokova, H (Petrokova, Hana); Kuchar, M (Kuchar, Milan); Vondrasek, J (Vondrasek, Jiri); Maly, P (Maly, Petr); Sebo, P (Sebo, Peter); Schneider, B (Schneider, Bohdan)
Source: BIOMED RESEARCH INTERNATIONAL Article Number: 752514 DOI: 10.1155/2013/752514 Published: 2013
Accession Number: WOS:000325638500001
PubMed ID: 24199198
ISSN: 23146133
eISSN: 23146141
IF:2.276

Record 54

Title: Critical Assessment of Current Force Fields. Short Peptide Test Case

Author(s): Vymetal, J (Vymetal, Jiri); Vondrasek, J (Vondrasek, Jiri)
Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION Volume: 9 Issue: 1 Pages: 441451
DOI: 10.1021/ct300794a Published: JAN 2013
Accession Number: WOS:000313378700047
PubMed ID: 26589046
ISSN: 15499618
IF: 5.011

Record 55

Title: Towards a better understanding of the specificity of protein-protein interaction
Author(s): Kysilka, J (Kysilka, Jiri); Vondrasek, J (Vondrasek, Jiri)
Source: JOURNAL OF MOLECULAR RECOGNITION Volume: 25 Issue: 11 Special Issue: SI Pages: 604615
DOI: 10.1002/jmr.2219 Published: NOV 2012
Accession Number: WOS:000310555100011
PubMed ID: 23108620
ISSN: 09523499
IF: 2.214

Record 56

Title: Optimal Definition of Inter Residual Contact in Globular Proteins Based on Pairwise Interaction Energy Calculations, Its Robustness, and Applications
Author(s): Fackovec, B (Fackovec, Boris); Vondrasek, J (Vondrasek, Jiri)
Source: JOURNAL OF PHYSICAL CHEMISTRY B Volume: 116 Issue: 42 Pages: 1265112660
DOI: 10.1021/jp303088n Published: OCT 25 2012
Accession Number: WOS:000310120900002
PubMed ID: 22988914
ISSN: 15206106
IF: 2.857

Record 57

Title: Effect of Enamel Matrix Derivative and of Proline Rich Synthetic Peptides on the Differentiation of Human Mesenchymal Stem Cells Toward the Osteogenic Lineage
Author(s): Ramis, JM (Maria Ramis, Joana); Rubert, M (Rubert, Marina); Vondrasek, J (Vondrasek, Jiri); Gaya, A (Gaya, Antoni); Lyngstadaas, SP (Lyngstadaas, Staale Petter); Monjo, M (Monjo, Marta)
Source: TISSUE ENGINEERING PART A Volume: 18 Issue: 1112
Pages: 12531263
DOI: 10.1089/ten.tea.2011.0404 Published: JUN 2012
Accession Number: WOS:000304779400015
PubMed ID: 22429009
ISSN: 19373341
IF: 3.508

Record 58

Title: Novel high affinity binders of human interferon gamma derived from albumin binding domain of protein G
Author(s): Ahmad, JN (Ahmad, Jawid N.); Li, JJ (Li, Jingjing); Biedermannova, L (Biedermannova, Lada); Kuchar, M (Kuchar, Milan); Sipova, H (Sipova, Hana); Semeradtova, A (Semeradtova, Alena); Cerny, J (Cerny, Jiri); Petrokova, H (Petrokova, Hana); Mikulecky, P (Mikulecky, Pavel); Polinek, J (Polinek, Jiri); Stanek, O (Stanek, Ondrej); Vondrasek, J (Vondrasek, Jiri); Homola, J (Homola, Jiri); Maly, J (Maly, Jan); Osicka, R (Osicka, Radim); Sebo, P (Sebo, Peter); Maly, P (Maly, Petr)
Source: PROTEINS STRUCTURE FUNCTION AND BIOINFORMATICS Volume: 80 Issue: 3 Pages: 774789
DOI: 10.1002/prot.23234 Published: MAR 2012
Accession Number: WOS:000300053500026
PubMed ID: 22113774
ISSN: 08873585
eISSN: 10970134
IF: 2.828

Record 59

Title: Synthetic Peptides Analogue to Enamel Proteins Promote Osteogenic Differentiation of MC3T3E1 and Mesenchymal Stem Cells
Author(s): Rubert, M (Rubert, Marina); Ramis, JM (Ramis, Joana Maria); Vondrasek, J (Vondrasek, Jiri); Gaya, A (Gaya, Antoni); Lyngstadaas, SP (Lyngstadaas, Staale Petter); Monjo, M (Monjo, Marta)
Source: JOURNAL OF BIOMATERIALS AND TISSUE ENGINEERING Volume: 1 Issue: 2 Pages: 198209
DOI: 10.1166/jbt.2011.1018 Published: DEC

2011

Accession Number: WOS:000312570600009

ISSN: 21579083

IF: 0.511

Record 60

Title: Biophysical characterization of recombinant human ameloblastin

Authors: Wald, T ; Bednarova, L ; Osicka, R ; Pacht, P ; Sulc, M ; Lyngstadaas, SP ; Slaby, I; Vondrasek, J.:

Source: EUROPEAN JOURNAL OF ORAL SCIENCES, Volume: 119, Special Issue:

DOI: 10.1111/j.1600-0722.2011.00913.x

Published: DEC 2011

IF: 2.22

Record 61

Title: Like Charge Guanidinium Pairing from Molecular Dynamics and Ab Initio Calculations

Author(s): Vazdar, M (Vazdar, Mario); Vymetal, J (Vymetal, Jiri); Heyda, J (Heyda, Jan); Vondrasek, J (Vondrasek, Jiri); Jungwirth, P (Jungwirth, Pavel)

Source: JOURNAL OF PHYSICAL CHEMISTRY A Volume: 115 Issue: 41 Pages: 1119311201

DOI: 10.1021/jp203519p Published: OCT 20 2011

Accession Number: WOS:000295700600009

PubMed ID: 21721561

ISSN: 10895639

IF: 2.6

Record 62

Title: Gyration and InertiaTensor Based Collective Coordinates for Metadynamics. Application on the Conformational Behavior of Polyalanine Peptides and Trp Cage Folding,

Author(s): Vymetal, J (Vymetal, Jiri); Vondrasek, J (Vondrasek, Jiri)

Source: JOURNAL OF PHYSICAL CHEMISTRY A Volume: 115 Issue: 41 Pages: 1145511465

DOI: 10.1021/jp2065612 Published: OCT 20 2011

Accession Number: WOS:000295700600037

PubMed ID: 21961799

ISSN: 10895639

IF: 2.6

Record 63

Title: Urea and Guanidinium Induced Denaturation of a Trp Cage Miniprotein

Author(s): Heyda, J (Heyda, Jan); Kozisek, M (Kozisek, Milan); Bednarova, L (Bednarova, Lucie); Thompson, G (Thompson, Gary); Konvalinka, J (Konvalinka, Jan); Vondrasek, J (Vondrasek, Jiri); Jungwirth, P (Jungwirth, Pavel)

Source: JOURNAL OF PHYSICAL CHEMISTRY B Volume: 115 Issue: 28 Pages: 89108924

DOI: 10.1021/jp200790h Published: JUL 21 2011

Accession Number: WOS:000292893200012

PubMed ID: 21634379

ISSN: 15206106

IF: 2.857

Record 64

Title: Hypertrophic cardiomyopathy: from mutation to functional analysis of defective protein

Author(s): Capek, P (Capek, Pavel); Vondrasek, J (Vondrasek, Jiri); Skvor, J (Skvor, Jiri); Brdicka, R (Brdicka, Radim)

Source: CROATIAN MEDICAL JOURNAL Volume: 52 Issue: 3 Pages: 384391

DOI: 10.3325/cmj.2011.52.384 Published: JUN 2011

Accession Number: WOS:000292873600016

PubMed ID: 21674835

ISSN: 03539504

IF: 1.247

Record 65

Title: Mapping the Pro Peptide of the Schistosoma mansoni Cathepsin B1 Drug Target: Modulation of Inhibition by Heparin and Design of Mimetic Inhibitors

Author(s): Horn, M (Horn, Martin); Jilkova, A (Jilkova, Adela); Vondrasek, J (Vondrasek, Jiri); Maresova, L (Maresova, Lucie); Caffrey, CR (Caffrey, Conor R.); Mares, M (Mares, Michael)

Source: ACS CHEMICAL BIOLOGY Volume: 6 Issue: 6 Pages: 609617

DOI: 10.1021/cb100411v Published: JUN 2011
Accession Number: WOS:000291896400011
PubMed ID: 21375333
ISSN: 15548929
IF: 4.434

Record 66

Title: The DFLCCSD(T0) correction of the phi/psi force field dihedral parameters significantly influences the free energy profile of the alanine dipeptide
Author(s): Vymetal, J (Vymetal, Jiri); Vondrasek, J (Vondrasek, Jiri)
Source: CHEMICAL PHYSICS LETTERS Volume: 503 Issue: 46
Pages: 301304
DOI: 10.1016/j.cplett.2011.01.030 Published: FEB 17 2011
Accession Number: WOS:000287187800024
ISSN: 00092614
IF:2.029

Record 67

Title: HOW TO FRAGMENT A POLYPEPTIDE? AN ab initio COMPUTATIONAL STUDY OF PAIR INTERACTIONS BETWEEN AMINO ACIDS AND LIGAND AMINO ACIDS IN PROTEINS
Author(s): Klusak, V (Klusak, Vojtech); Dobes, P (Dobes, Petr); Cerny, J (Cerny, Jiri); Vondrasek, J (Vondrasek, Jiri)
Source: COLLECTION OF CZECHOSLOVAK CHEMICAL COMMUNICATIONS Volume: 76 Issue: 5 Pages: 605618
DOI: 10.1135/cccc2011033 Published: 2011
Accession Number: WOS:000290280100016
ISSN: 00100765
IF: 1.137

Record 68

Title: Energy Matrix of Structurally Important SideChain/SideChain Interactions in Proteins
Author(s): Berka, K (Berka, Karel); Laskowski, RA (Laskowski, Roman A.); Hobza, P (Hobza, Pavel); Vondrasek, J (Vondrasek, Jiri)
Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION Volume: 6 Issue: 7 Pages: 21912203
DOI: 10.1021/ct100007y Published: JUL 2010
Accession Number: WOS:000279751500026
PubMed ID: 26615945
ISSN: 15499618
eISSN: 15499626
IF: 5.011

Record 69

Title: Metadynamics As a Tool for Mapping the Conformational and Free Energy Space of Peptides The Alanine Dipeptide Case Study
Author(s): Vymetal, J (Vymetal, Jiri); Vondrasek, J (Vondrasek, Jiri)
Source: JOURNAL OF PHYSICAL CHEMISTRY B Volume: 114 Issue: 16 Pages: 56325642
DOI: 10.1021/jp100950w Published: APR 29 2010
Accession Number: WOS:000276889100050
PubMed ID: 20361773
ISSN: 15206106
IF: 2.857

Record 70

Title: Rigid Duplex alpha Cyclodextrin Reversibly Connected With Disulfide Bonds. Synthesis and Inclusion Complexes (vol 74, pg 1082, 2009)
Author(s): Kumprecht, L (Kumprecht, Lukas); Budesinsky, M (Budesinsky, Milos); Vondrasek, J (Vondrasek, Jiri); Vymetal, J (Vymetal, Jiri); Cerny, J (Cerny, Jiri); Cisarova, I (Cisarova, Ivana); Brynda, J (Brynda, Jiri); Herzig, V (Herzig, Vladimir); Koutnik, P (Koutnik, Petr); Zavada, J (Zavada, Jiri); Kraus, T (Kraus, Tomas)
Source: JOURNAL OF ORGANIC CHEMISTRY Volume: 74 Issue: 21 Pages: 84968496
DOI: 10.1021/jo9020612 Published: NOV 6 2009
Accession Number: WOS:000271113400073
ISSN: 00223263
IF: 4.335

Record 71

Title: The Molecular Origin of LikeCharge Arginine-Arginine Pairing in Water

Author(s): Vondrasek, J (Vondrasek, Jiri); Mason, PE (Mason, Philip E.); Heyda, J (Heyda, Jan); Collins, KD (Collins, Kim D.); Jungwirth, P (Jungwirth, Pavel)

Source: JOURNAL OF PHYSICAL CHEMISTRY B Volume: 113 Issue: 27 Pages: 90419045

DOI: 10.1021/jp902377q Published: JUL 9 2009

Accession Number: WOS:000267651600001

PubMed ID: 19354258

ISSN: 15206106

IF: 2.857

Record 72

Title: Structure and Stability of the Water-Graphite Complexes

Author(s): Rubes, M (Rubes, Miroslav); Nachtigall, P (Nachtigall, Petr); Vondrasek, J (Vondrasek, Jiri); Bludsky, O (Bludsky, Ota)

Source: JOURNAL OF PHYSICAL CHEMISTRY C Volume: 113 Issue: 19 Pages: 84128419

DOI: 10.1021/jp901410m Published: MAY 14 2009

Accession Number: WOS:000265895500063

ISSN: 19327447

IF: 4.189

Record 73

Title: Loss of Dispersion Energy Changes the Stability and Folding/Unfolding Equilibrium of the Trp Cage Protein

Author(s): Cerny, J (Cerny, Jiri); Vondrasek, J (Vondrasek, Jiri); Hobza, P (Hobza, Pavel)

Source: JOURNAL OF PHYSICAL CHEMISTRY B Volume: 113 Issue: 16 Pages: 56575660

DOI: 10.1021/jp9004746 Published: APR 23 2009

Accession Number: WOS:000265269100038

PubMed ID: 19444987

ISSN: 15206106

IF: 2.857

Record 74

Title: Representative Amino Acid Side Chain Interactions in Proteins. A Comparison of Highly Accurate Correlated ab Initio Quantum Chemical and Empirical Potential Procedures

Author(s): Berka, K (Berka, Karel); Laskowski, R (Laskowski, Roman); Riley, KE (Riley, Kevin E.); Hobza, P (Hobza, Pavel); Vondrasek, J (Vondrasek, Jiri)

Source: JOURNAL OF CHEMICAL THEORY AND COMPUTATION Volume: 5 Issue: 4 Pages: 982992

DOI: 10.1021/ct800508v Published: APR 2009

Accession Number: WOS:000265268800037

PubMed ID: 26609607

ISSN: 15499618

IF: 5.011

Record 75

Title: Ions at aqueous interfaces: From water surface to hydrated proteins

Author(s): Heyda, J (Heyda, Jan); Vacha, R (Vacha, Robert); Vondrasek, J (Vondrasek, Jiri); Jungwirth, P (Jungwirth, Pavel)

Source: ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY Meeting Abstract: 94COLL

Volume: 237 Published: MAR 22 2009

Accession Number: WOS:000207857803016

ISSN: 00657727

IF: N/A

Record 76

Title: Analysis of Energy Stabilization inside the Hydrophobic Core of Rubredoxin

Author(s): Berka, K (Berka, Karel); Hobza, P (Hobza, Pavel); Vondrasek, J (Vondrasek, Jiri)

Source: CHEMPHYSCHEM Volume: 10 Issue: 3 Pages: 543548

DOI: 10.1002/cphc.200800401 Published: FEB 23 2009

Accession Number: WOS:000264229900014

PubMed ID: 19170065

ISSN: 14394235

IF: 3.144

Record 77

Title: Rigid Duplex alpha Cyclodextrin Reversibly Connected With Disulfide Bonds. Synthesis and Inclusion Complexes
Author(s): Kumprecht, L (Kumprecht, Lukas); Budesinsky, M (Budesinsky, Milos); Vondrasek, J (Vondrasek, Jiri); Vymetal, J (Vymetal, Jiri); Cerny, J (Cerny, Jiri); Cisarova, I (Cisarova, Ivana); Brynda, J (Brynda, Jiri); Herzig, V (Herzig, Vladimir); Koutnik, P (Koutnik, Petr); Zavada, J (Zavada, Jiri); Kraus, T (Kraus, Tomas)
Source: JOURNAL OF ORGANIC CHEMISTRY Volume: 74 Issue: 3 Pages: 10821092
DOI: 10.1021/jo802139s Published: FEB 6 2009
Accession Number: WOS:000263004300015
PubMed ID: 19113826
ISSN: 00223263
IF:4.335

Record 78

Title: Ion specific effects of sodium and potassium on the catalytic activity of HIV1 protease
Author(s): Heyda, J (Heyda, Jan); Pokorna, J (Pokorna, Jana); Vrbka, L (Vrbka, Lubos); Vacha, R (Vacha, Robert); JagodaCwiklik, B (JagodaCwiklik, Barbara); Konvalinka, J (Konvalinka, Jan); Jungwirth, P (Jungwirth, Pavel); Vondrasek, J (Vondrasek, Jiri)
Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS Volume: 11 Issue: 35 Pages: 75997604
DOI: 10.1039/b905462f Published: 2009
Accession Number: WOS:000269400500010
PubMed ID: 19950498
ISSN: 14639076
IF: 3.43

Record 79

Title: MedusaScore: An accurate force field based scoring function for virtual drug screening
Author(s): Yin, S (Yin, Shuangye); Biedermannova, L (Biedermannova, Lada); Vondrasek, J (Vondrasek, Jiri); Dokholyan, NV (Dokholyan, Nikolay V.)
Source: JOURNAL OF CHEMICAL INFORMATION AND MODELING Volume: 48 Issue: 8 Pages: 16561662
DOI: 10.1021/ci8001167 Published: AUG 2008
Accession Number: WOS:000258697400010
PubMed ID: 18672869
ISSN: 15499596
eISSN: 1549960X
IF: 4.549

Record 80

Title: Identifying stabilizing key residues in proteins using interresidue interaction energy matrix
Author(s): BendovaBiedermannova, L (BendovaBiedermannova, Lada); Hobza, P (Hobza, Pavel); Vondrasek, J (Vondrasek, Jiri)
Source: PROTEINS STRUCTURE FUNCTION AND BIOINFORMATICS Volume: 72 Issue: 1 Pages: 402413
DOI: 10.1002/prot.21938 Published: JUL 2008
Accession Number: WOS:000256609800035
PubMed ID: 18214960
ISSN: 08873585
IF:2.828

Record 81

Title: Bioinformatic analysis and molecular modelling of human ameloblastin suggest a twodomain intrinsically unstructured calcium binding protein
Author(s): Vymetal, J (Vymetal, Jiri); Slaby, I (Slaby, Ivan); Spahr, A (Spahr, Axel); Vondrasek, J (Vondrasek, Jiri); Lyngstadaas, SP (Lyngstadaas, S. Petter)
Source: EUROPEAN JOURNAL OF ORAL SCIENCES Volume: 116 Issue: 2 Pages: 124134
DOI: 10.1111/j.16000722.2008.00526.
Accession Number: WOS:000254126200005
PubMed ID: 18353005
ISSN: 09098836
IF:2.22

Record 82

Title: Quasiplanarity of the peptide bond
Author(s): Chalupsky, J (Chalupsky, Jakub); Vondrasek, J (Vondrasek, Jiri); Spirko, V (Spirko, Vladimir)
Source: JOURNAL OF PHYSICAL CHEMISTRY A Volume: 112 Issue: 4 Pages: 693699

DOI: 10.1021/jp0750699 Published: JAN 31 2008

Accession Number: WOS:000252618700015

PubMed ID: 18177024

ISSN: 10895639

IF:2.6

Record 83

Title: THE STABILIZATION ENERGY OF THE GLULYS SALT BRIDGE IN THE PROTEIN/WATER ENVIRONMENT: CORRELATED QUANTUM

CHEMICAL ab initio, DFT AND EMPIRICAL POTENTIAL STUDIES

Author(s): Rezac, J (Rezac, Jan); Berka, K (Berka, Karel); Horinek, D (Horinek, Dominik); Hobza, P (Hobza, Pavel); Vondrasek, J (Vondrasek, Jiri)

Source: COLLECTION OF CZECHOSLOVAK CHEMICAL COMMUNICATIONS Volume: 73 Issue: 67

Pages: 921936

DOI: 10.1135/cccc20080921 Published: 2008

Accession Number: WOS:000260536700014

ISSN: 00100765

IF:1.137

Record 84

Title: QUANTUM CHEMICAL BENCHMARK ENERGY AND GEOMETRY DATABASE FOR MOLECULAR CLUSTERS AND COMPLEX MOLECULAR SYSTEMS (www.begdb.com): A USERS MANUAL AND EXAMPLES

Author(s): Rezac, J (Rezac, Jan); Jurecka, P (Jurecka, Petr); Riley, KE (Riley, Kevin E.); Cerny, J (Cerny, Jiri); Valdes, H (Valdes, Haydee); Pluhackova, K (Pluhackova, Kristyna); Berka, K (Berka, Karel); Rezac, T (Rezac, Tomas); Pitonak, M (Pitonak, Michal); Vondrasek, J (Vondrasek, Jiri); Hobza, P (Hobza, Pavel)

Source: COLLECTION OF CZECHOSLOVAK CHEMICAL COMMUNICATIONS Volume: 73 Issue: 10 Pages: 12611270

DOI: 10.1135/cccc20081261 Published: 2008

Accession Number: WOS:000263121400003

ISSN: 00100765

IF:1.137

Record 85

Title: Another role of proline: stabilization interactions in proteins and protein complexes concerning proline and tryptophane

Author(s): Biedermannova, L (Biedermannova, Lada); Riley, KE (Riley, Kevin E.); Berka, K (Berka, Karel); Hobza, P (Hobza, Pavel); Vondrasek, J (Vondrasek, Jiri)

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS Volume: 10 Issue: 42 Pages: 63506359

DOI: 10.1039/b805087b Published: 2008

Accession Number: WOS:000260485600002

PubMed ID: 18972023

ISSN: 14639076

IF: 3.43

Record 86

Title: Model of peptide bond aromatic ring interaction: Correlated ab initio quantum chemical study

Author(s): Bendova, L (Bendova, Lada); Jurecka, P (Jurecka, Petr); Hobza, P (Hobza, Pavel); Vondrasek, J (Vondrasek, Jiri)

Source: JOURNAL OF PHYSICAL CHEMISTRY B Volume: 111 Issue: 33 Pages: 99759979

DOI: 10.1021/jp072859+ Published: AUG 23 2007

Accession Number: WOS:000248759000037

PubMed ID: 17672495

ISSN: 15206106

IF: 2.857

Record 87

Title: Dispersion interactions govern the strong thermal stability of a protein

Author(s): Vondrasek, J (Vondrasek, Jiri); Kubar, T (Kubar, Tomas); Jenney, FE (Jenney, Francis E., Jr.); Adams, MWW (Adams, Michael W. W.); Kozisek, M (Kozisek, Milan); Cerny, J (Cerny, Jiri); Sklenar, V (Sklenar, Vladimir); Hobza, P (Hobza, Pavel)

Source: CHEMISTRY A EUROPEAN JOURNAL Volume: 13 Issue: 32 Pages: 90229027

DOI: 10.1002/chem.200700428 Published: 2007

Accession Number: WOS:000250913900012

PubMed ID: 17696186

ISSN: 09476539

IF: 4.857

Record 88

Title: Performance of the DFTD method, paired with the PCM implicit solvation model, for the computation of interaction energies of solvated complexes of biological interest

Author(s): Riley, KE (Riley, Kevin E.); Vondrasek, J (Vondrasek, Jiri); Hobza, P (Hobza, Pavel)

Source: PHYSICAL CHEMISTRY CHEMICAL PHYSICS Volume: 9 Issue: 41 Pages: 55555560

DOI: 10.1039/b708089a Published: 2007

Accession Number: WOS:000250366900005

PubMed ID: 17957311

ISSN: 14639076

eISSN: 14639084

IF: 3.43

Record 89

Title: Cathepsin D propeptide: Mechanism and regulation of its interaction with the catalytic core

Author(s): Masa, M (Masa, Martin); Maresova, L (Maresova, Lucie); Vondrasek, J (Vondrasek, Jiri); Horn, M (Horn, Martin); Jezek, J (Jezek, Jan); Mares, M (Mares, Michael)

Source: BIOCHEMISTRY Volume: 45 Issue: 51 Pages: 1547415482

Article Number: PII S00062960(06)01498X

DOI: 10.1021/bi0614986 Published: DEC 26 2006

Accession Number: WOS:000242935600035

PubMed ID: 17176069

ISSN: 00062960

IF:2.865

Record 90

Title: Quantification and rationalization of the higher affinity of sodium over potassium to protein surfaces

Author(s): Vrbka, L (Vrbka, Lubos); Vondrasek, J (Vondrasek, Jiri); JagodaCwiklik, B (JagodaCwiklik, Barbara); Vacha, R (Vacha, Robert); Jungwirth, P (Jungwirth, Pavel)

Source: PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA Volume: 103 Issue: 42 Pages: 1544015444

DOI: 10.1073/pnas.0606959103 Published: OCT 17 2006

Accession Number: WOS:000241476200031

PubMed ID: 17032760

ISSN: 00278424

IF:9.412

Record 91

Title: Thermodynamic penalty arising from burial of a ligand polar group within a hydrophobic pocket of a protein receptor

Author(s): Barratt, E (Barratt, Elizabeth); Bronowska, A (Bronowska, Agnieszka); Vondrasek, J (Vondrasek, Jiri); Cerny, J (Cerny, Jiri); Bingham, R (Bingham, Richard); Phillips, S (Phillips, Simon); Homans, SW (Homans, Steve W.)

Source: JOURNAL OF MOLECULAR BIOLOGY Volume: 362 Issue: 5 Pages: 9941003

DOI: 10.1016/j.jmb.2006.07.067 Published: OCT 6 2006

Accession Number: WOS:000241324800011

PubMed ID: 16935302

ISSN: 00222836

IF: 4.76

Record 92

Title: Chemical compound navigator: A web based chemBLAST, chemical taxonomy based search engine for browsing compounds

Author(s): Prasanna, MD (Prasanna, MD); Vondrasek, J (Vondrasek, J); Wlodawer, A (Wlodawer, A); Rodriguez, H (Rodriguez, H); Bhat, TN (Bhat, TN)

Source: PROTEINS STRUCTURE FUNCTION AND BIOINFORMATICS Volume: 63 Issue: 4 Pages: 907917

DOI: 10.1002/prot.20914 Published: JUN 1 2006

Accession Number: WOS:000237863100017

PubMed ID: 16508960

ISSN: 08873585

IF:2.828

Record 93

Title: Propeptide interaction with cathepsin D: Mechanism and regulation

Author(s): Masa, M (Masa, M.); Maresova, L (Maresova, L.); Vondrasek, J (Vondrasek, J.); Horn, M (Horn, M.); Jezek, J (Jezek, J.); Mares, M (Mares, M.)

Source: JOURNAL OF PEPTIDE SCIENCE Volume: 12 Pages: 155155

Supplement: S Published: 2006

Accession Number: WOS:000239905600284

ISSN: 10752617

IF:1.877

Record 94

Title: Structure and IR spectrum of phenylalanylglycylglycine tripeptide in the gasphase: IR/UV experiments, ab initio quantum chemical calculations, and molecular dynamic Simulations

Author(s): Reha, D (Reha, D); Valdes, H (Valdes, H); Vondrasek, J (Vondrasek, J); Hobza, P (Hobza, P); AbuRiziq, A (AbuRiziq, A); Crews, B (Crews, B); de Vries, MS (de Vries, MS)

Source: CHEMISTRY A EUROPEAN JOURNAL Volume: 11 Issue: 23 Pages: 68036817

DOI: 10.1002/chem.200500465 Published: NOV 18 2005

Accession Number: WOS:000233508800002

PubMed ID: 16092140

ISSN: 09476539

IF: 4.857

Record 95

Title: Application of InChI to curate, index, and query 3D structures

Author(s): Prasanna, MD (Prasanna, MD); Vondrasek, J (Vondrasek, J); Wlodawer, A (Wlodawer, A); Bhat, TN (Bhat, TN)

Source: PROTEINS STRUCTURE FUNCTION AND BIOINFORMATICS Volume: 60 Issue: 1 Pages: 14

DOI: 10.1002/prot.20469 Published: JUL 1 2005

Accession Number: WOS:000229454200001

PubMed ID: 15861385

ISSN: 08873585

IF:2.828

Record 96

Title: 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)

Author(s): Vondrasek, J (Vondrasek, J); Bendova, L (Bendova, L); Klusak, V (Klusak, V); Hobza, P (Hobza, P)

Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY Volume: 127 Issue: 22 Pages: 82328232

DOI: 10.1021/ja0599081 Published: JUN 8 2005

Accession Number: WOS:000229619500063

ISSN: 00027863

IF: 14.612

Record 97

Title: 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

Author(s): Caffrey, CR (Caffrey, CR); Placha, L (Placha, L); Barinka, C (Barinka, C); Hradilek, M (Hradilek, M); Dostal, J (Dostal, J); Sajid, M (Sajid, M); McKerrow, JH (McKerrow, JH); Majer, P (Majer, P); Konvalinka, J (Konvalinka, J); Vondrasek, J (Vondrasek, J)

Source: BIOLOGICAL CHEMISTRY Volume: 386 Issue: 4 Pages: 339349

DOI: 10.1515/BC.2005.041 Published: APR 2005

Accession Number: WOS:000228817700005

PubMed ID: 15899696

ISSN: 14316730

IF:3.27

Record 98

Title: Unexpectedly strong energy stabilization inside the hydrophobic core of small protein rubredoxin mediated by aromatic residues: Correlated ab initio quantum chemical calculations

Author(s): Vondrasek, J (Vondrasek, J); Bendova, L (Bendova, L); Klusak, V (Klusak, V); Hobza, P (Hobza, P)

Source: JOURNAL OF THE AMERICAN CHEMICAL SOCIETY Volume: 127 Issue: 8 Pages: 26152619

DOI: 10.1021/ja044607h Published: MAR 2 2005
Accession Number: WOS:000227308100046
PubMed ID: 15725017
ISSN: 00027863
IF:14.612

Record 99

Title: Molecular dynamics study of the effect of the gamma abu insert on the conformational behavior of the glycopeptide endrimers based on the oligolysine scaffold in N,N 'dimethylformamide
Author(s): Veprek, P (Veprek, P); Jezek, J (Jezek, J); Trnka, T (Trnka, T); Vondrasek, J (Vondrasek, J)
Source: JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS Volume: 22 Issue: 1 Pages: 7990
Published: AUG 2004
Accession Number: WOS:000222865400009
PubMed ID: 15214808
ISSN: 07391102
IF: 3.31

Record 100

Title: MOLECULAR DYNAMICS STUDY OF THE EFFECT OF GABU INSERT ON THE CONFORMATIONAL BEHAVIOR OF THE MULTIPLE ANTIGEN GLYCOPEPTIDES DURING THE SOLIDPHASE SYNTHESIS
Author(s): Veprek, P (Veprek, P.); Vondrasek, J (Vondrasek, J.); Trnka, T (Trnka, T.); Jezek, J (Jezek, J.)
Source: JOURNAL OF PEPTIDE SCIENCE Volume: 10 Pages: 233233
Published: 2004
Accession Number: WOS:000207131001324
ISSN: 10752617
IF: 1.877

Record 101

Title: Sexual attraction in the silkworm moth: Nature of binding of bombykol in pheromone binding protein An ab initio study
Author(s): Klusak, V (Klusak, V); Havlas, Z (Havlas, Z); Rulisek, L (Rulisek, L); Vondrasek, J (Vondrasek, J); Svatos, A (Svatos, A)
Source: CHEMISTRY & BIOLOGY Volume: 10 Issue: 4 Pages: 331340
DOI: 10.1016/S10745521(03)000747
Published: APR 2003
Accession Number: WOS:000183647300005
PubMed ID: 12725861
ISSN: 10745521
IF: 5.915

Record 102

Title: Unusual binding mode of an HIV1 protease inhibitor explains its potency against multidrug resistant virus strains
Author(s): Weber, J (Weber, J); Mesters, JR (Mesters, JR); Lepsik, M (Lepsik, M); Prejdova, J (Prejdova, J); Svec, M (Svec, M); Sponarova, J (Sponarova, J); Mlcochova, P (Mlcochova, P); Skalicka, K (Skalicka, K); Strisovsky, K (Strisovsky, K); Uhlíkova, T (Uhlíkova, T); Soucek, M (Soucek, M); Machala, L (Machala, L); Stankova, M (Stankova, M); Vondrasek, J (Vondrasek, J); Klimkait, T (Klimkait, T); Kraeusslich, HG (Kraeusslich, HG); Hilgenfeld, R (Hilgenfeld, R); Konvalinka, J (Konvalinka, J)
Source: JOURNAL OF MOLECULAR BIOLOGY Volume: 324 Issue: 4 Pages: 739754
DOI: 10.1016/S00222836(02)011397
Published: DEC 6 2002
Accession Number: WOS:000179825300014
PubMed ID: 12460574
ISSN: 00222836
IF: 4.76

Record 103

Title: HIVdb: A database of the structures of human immunodeficiency virus protease
Author(s): Vondrasek, J (Vondrasek, J); Wlodawer, A (Wlodawer, A)
Source: PROTEINS STRUCTURE FUNCTION AND GENETICS Volume: 49 Issue: 4 Pages: 429431
DOI: 10.1002/prot.10246 Published: DEC 1 2002
Accession Number: WOS:000179475800001
PubMed ID: 12402352
ISSN: 08873585
IF:2.828

Record 104

Title: Freethiol Cys331 exposed during activation process is critical for native tetramer structure of cathepsin C (dipeptidyl peptidase I)

Author(s): Horn, M (Horn, M); Baudys, M (Baudys, M); Voburka, Z (Voburka, Z); Kluh, I (Kluh, I); Vondrasek, J (Vondrasek, J); Mares, M (Mares, M)

Source: PROTEIN SCIENCE Volume: 11 Issue: 4 Pages: 933943

DOI: 10.1110/ps.2910102 Published: APR 2002

Accession Number: WOS:000174594200019

PubMed ID: 11910036

ISSN: 09618368

IF: 3.876

Record 105

Title: Magnesium and biological activity of oxytocin analogues modified on aromatic ring of amino acid in position 2

Author(s): Slaninova, J (Slaninova, J); Maletinska, L (Maletinska, L); Vondrasek, J (Vondrasek, J); Prochazka, Z (Prochazka, Z)

Source: JOURNAL OF PEPTIDE SCIENCE Volume: 7 Issue: 8 Pages: 413424

DOI: 10.1002/psc.334 Published: AUG 2001

Accession Number: WOS:000171014000003

PubMed ID: 11548057

ISSN: 10752617

IF: 1.877

Record 106

Title: A picomolar inhibitor of resistant strains of human immunodeficiency virus protease identified by a combinatorial approach

Author(s): Rinnova, M (Rinnova, M); Hradilek, M (Hradilek, M); Barinka, C (Barinka, C); Weber, J (Weber, J); Soucek, M (Soucek, M); Vondrasek, J (Vondrasek, J); Klimkait, T (Klimkait, T); Konvalinka, J (Konvalinka, J)

Source: ARCHIVES OF BIOCHEMISTRY AND BIOPHYSICS Volume: 382 Issue: 1 Pages: 2230

DOI: 10.1006/abbi.2000.2017 Published: OCT 1 2000

Accession Number: WOS:000089687400004

PubMed ID: 11051093

ISSN: 00039861

IF: 3.391

Record 107

Title: Protein folding: State of the problem at the end of millenium

Author(s): Svec, M (Svec, M); Vondrasek, J (Vondrasek, J)

Source: CHEMICAL LISTY Volume: 94 Issue: 8 Pages: 494500

Published: 2000

Accession Number: WOS:000088956500003

ISSN: 00092770

IF:0.39

Record 108

Title: Solid phase synthesis of glycopeptide dendrimers with Tn antigenic structure and their biological activities. Part I

Author(s): Jezek, J (Jezek, J); Velek, J (Velek, J); Veprek, P (Veprek, P); Velkova, V (Velkova, V); Trnka, T (Trnka, T); Pecka, J (Pecka, J); Ledvina, M (Ledvina, M); Vondrasek, J (Vondrasek, J); Pisacka, M (Pisacka, M)

Source: JOURNAL OF PEPTIDE SCIENCE Volume: 5 Issue: 1 Pages: 4655

Published: JAN 1999

Accession Number: WOS:000079363500006

ISSN: 10752617

IF:1.877

Record 109

Title: Coordination geometries of selected transition metal ions (Co²⁺, Ni²⁺, Cu²⁺, Zn²⁺, Cd²⁺, and Hg²⁺) in metalloproteins

Author(s): Rulisek, L (Rulisek, L); Vondrasek, J (Vondrasek, J)

Source: JOURNAL OF INORGANIC BIOCHEMISTRY Volume: 71 Issue: 34

Pages: 115127

DOI: 10.1016/S01620134(98)100429

Published: SEP 1998

Accession Number: WOS:000077038800002

PubMed ID: 9833317

ISSN: 01620134

IF:3.212

Record 110

Title: Inhibitors of HIV1 protease: A major success of structure assisted drug design

Author(s): Wlodawer, A (Wlodawer, A); Vondrasek, J (Vondrasek, J)

Source: ANNUAL REVIEW OF BIOPHYSICS AND BIOMOLECULAR STRUCTURE Volume: 27 Pages: 249284

DOI: 10.1146/annurev.biophys.27.1.249 Published: 1998

Accession Number: WOS:000074324000011

PubMed ID: 9646869

ISSN: 10568700

IF:18.955

Record 111

Title: Configurations of diastereomeric hydroxyethylene isosteres strongly affect biological activities of a series of specific inhibitors of human immunodeficiency virus proteinase

Author(s): Konvalinka, J (Konvalinka, J); Litera, J (Litera, J); Weber, J (Weber, J); Vondrasek, J (Vondrasek, J); Hradilek, M (Hradilek, M); Soucek, M (Soucek, M); Pichova, I (Pichova, I); Majer, P (Majer, P); Strop, P (Strop, P); Sedlacek, J (Sedlacek, J); Heuser, AM (Heuser, AM); Kottler, H (Kottler, H); Krausslich, HG (Krausslich, HG)

Source: EUROPEAN JOURNAL OF BIOCHEMISTRY Volume: 250 Issue: 2 Pages: 559566

DOI: 10.1111/j.14321033.1997.0559a.x

Published: DEC 1 1997

Accession Number: WOS:A1997YK84000043

PubMed ID: 9428710

ISSN: 00142956

IF:3.579

Record 112

Title: Performance of empirical potentials (AMBER, CFF95, CVFF, CHARMM, OPLS, POLTEV), semiempirical quantum chemical methods (AM1, MNDO/M, PM3), and ab initio Hartree-Fock method for interaction of DNA bases: Comparison with nonempirical beyond Hartree-Fock results

Author(s): Hobza, P (Hobza, P); Kabelac, M (Kabelac, M); Sponer, J (Sponer, J); Mejzlik, P (Mejzlik, P); Vondrasek, J (Vondrasek, J)

Source: JOURNAL OF COMPUTATIONAL CHEMISTRY Volume: 18 Issue: 9 Pages: 11361150

DOI: 10.1002/(SICI)1096987X(19970715)18:9<1136::AIDJCC3>3.0.CO;2S

Published: JUL 15 1997

Accession Number: WOS:A1997XG19500003

ISSN: 01928651

IF: 2.976

Record 113

Title: Potency comparison of peptidomimetic inhibitors against HIV1 and HIV2 proteinases: Design of equipotent lead compounds

Author(s): Weber, J (Weber, J); Majer, P (Majer, P); Litera, J (Litera, J); Urban, J (Urban, J); Soucek, M (Soucek, M); Vondrasek, J (Vondrasek, J); Konvalinka, J (Konvalinka, J); Novek, P (Novek, P); Sedlacek, J (Sedlacek, J); Strop, P (Strop, P); Krausslich, HG (Krausslich, HG); Pichova, I (Pichova, I)

Source: ARCHIVES OF BIOCHEMISTRY AND BIOPHYSICS Volume: 341 Issue: 1 Pages: 6269

DOI: 10.1006/abbi.1997.9945 Published: MAY 1 1997

Accession Number: WOS:A1997WX13400008

PubMed ID: 9143353

ISSN: 00039861

IF:3.391

Record 114

Title: Database of HIV proteinase structures

Author(s): Vondrasek, J (Vondrasek, J); Wlodawer, A (Wlodawer, A)

Source: TRENDS IN BIOCHEMICAL SCIENCES Volume: 22 Issue: 5 Pages: 183183

DOI: 10.1016/S09680004(97)010244

Published: MAY 1997

Accession Number: WOS:A1997WZ50400015

PubMed ID: 9175479

ISSN: 09680004

IF:14.732

Record 115

Title: Data base of three dimensional structures of HIV proteinases

Author(s): Vondrasek, J (Vondrasek, J); vanBuskirk, CP (vanBuskirk, CP); Wlodawer, A (Wlodawer, A)

Source: NATURE STRUCTURAL BIOLOGY Volume: 4 Issue: 1 Pages: 88

DOI: 10.1038/nsb01978

Published: JAN 1997

Accession Number: WOS:A1997WA81000004

PubMed ID: 8989313

ISSN: 10728368

IF:11.579

Record 116

Title: A new approach for screening of cadmium binding by synthetic peptides

Author(s): Kotrba, P (Kotrba, P); Doleckova, L (Doleckova, L); Pavlik, M (Pavlik, M); Vondrasek, J (Vondrasek, J); Ruml, T (Ruml, T)

Source: CHEMICKE LISTY Volume: 90 Issue: 9 Pages: 709709

Published: SEP 1996

Accession Number: WOS:A1996VG96800153

ISSN: 00092770

IF:0.39

Record 117

Title: Ability of empirical potentials (AMBER, CHARMM, CVFF, OPLS, Poltev) and semiempirical quantum chemical methods (AM1, MNDO/M, PM3) to describe H bonding in DNA base pairs; Comparison with ab initio results

Author(s): Hobza, P (Hobza, P); Hubalek, F (Hubalek, F); Kabelac, M (Kabelac, M); Mejzlik, P (Mejzlik, P); Sponer, J (Sponer, J); Vondrasek, J (Vondrasek, J)

Source: CHEMICAL PHYSICS LETTERS Volume: 257 Issue: 12

Pages: 3135

DOI: 10.1016/00092614(96)005374

Published: JUL 19 1996

Accession Number: WOS:A1996UY12200005

ISSN: 00092614

IF: 2.029

Record 118

Title: A modular approach to HIV1 proteinase inhibitor design

Author(s): Uhlikova, T (Uhlikova, T); Konvalinka, J (Konvalinka, J); Pichova, I (Pichova, I); Soucek, M (Soucek, M); Krausslich, HG (Krausslich, HG); Vondrasek, J (Vondrasek, J)

Source: BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS Volume: 222 Issue: 1 Pages: 3843

DOI: 10.1006/bbrc.1996.0694 Published: MAY 6 1996

Accession Number: WOS:A1996UJ62500007

PubMed ID: 8630071

ISSN: 0006291X

IF:2.985

Record 119

Title: New database

Author(s): Vondrasek, J (Vondrasek, J); Wlodawer, A (Wlodawer, A)

Source: SCIENCE Volume: 272 Issue: 5260 Pages: 337338

Published: APR 19 1996

Accession Number: WOS:A1996UG25200009

PubMed ID: 8602518

ISSN: 00368075

IF: 41.846

Record 120

Title: AN EMPIRICAL POTENTIAL STUDY OF THE INTERACTION OF LYSINELANINELANINE TRIPEPTIDE WITH 4 MODELS OF B-DNA WITH DIFFERENT COMPOSITIONS

Author(s): VONDRASEK, J (VONDRASEK, J); SPONAR, J (SPONAR, J); HOBZA, P (HOBZA, P)

Source: JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS Volume: 11 Issue: 4 Pages: 869880

DOI: 10.1080/07391102.1994.10508038 Published: FEB 1994

Accession Number: WOS:A1994MZ78400012
PubMed ID: 8204220
ISSN: 07391102
IF:3.31

4. **učebnice a učební texty,**

Jiří Vondrášek (2006), Molekulární modelování, Molekulární biologie a genetika XII, editor: J.Jonák jr and J.Jonák, Ústav molekulární genetiky AV ČR, ISBN: 80-902588-5-9

5. **různé závažné práce** (např. recenze v odborných časopisech, dobrozdání, expertizy, encyklopedie, slovníky, příručky, překlady atd.)

- cca 20 recenzí pro ACS journals – Journal of Physical Chemistry B, Journal of Chemical Theory and Computations, Journal of Chemical Modelling, cca 15 recenzí pro International Journal of Molecular Sciences, cca 20 recenzí pro Biophysics, Proteins: Structure Function and Bioinformatics, Nucleic Acid Research atd..
- oponent více jak 20 disertačních prací, 10 diplomových prací

6. **přednášky typu "invited speaker"**

1 How to build up Biological Data infrastructure in conditions of central Europe; Polish Bioinformatic Society, Bioinformatics in Toruń 2017, June 22-24, 2017

2 From direct to indirect readout. DNA/Protein recognition by means of computational analysis
Vienna, 19/05/2016 , Host: Bojan Zagrovic, *Location: Lecture Hall A, VBC 5*, Organizer: VBC seminars, Seminar Series "Modern Concepts in Structural Biology"

3 From direct to indirect readout, DNA/Protein recognition by means of bioinformatics and computational analysis; CIISB Kick-off Meeting; 5–7/12/2016 Hotel Kurdějov

4 Keynote lecture by ELIXIR Czech Republic – Good practices in the Node, ELIXIR-SI LAUNCH & 11TH CFGBC SYMPOSIUM: "DATA FOR LIFE" , CANKARJEV DOM & FACULTY OF MEDICINE, UNIVERSITY OF LJUBLJANA, LJUBLJANA, SEPTEMBER 20 – SEPTEMBER 21, 2016

5 Large-Scale Quantitative Assessment of Binding Preferences in Protein–Nucleic Acid Complexes, [BC]2 Basel Computational Biology Conference, June 7-10, 2015

6 Intrinsically Disordered Proteins in Biomineralization - the case of Ameloblastin, MATERIALS FOR TISSUE ENGINEERING - HAFJELL, NORWAY, 2013, 6th Annual meeting of the Scandinavian Society for ScandiniBiomaterials (ScSB), Hafjell, Norway, 13th-15th of March 2013

7 Protein-Protein interactions via stabilization energy between side chains of amino acids at the interaction interface, Affinity 2011, 16. - 19. Juni 2011 Tavira, Portugal

8 Computational Chemistry as a tool for structural Biology, National Center for Biomolecular Research NCBR Seminar – CA050 and CC060 FACULTY OF SCIENCE, MASARYK UNIVERSITY Spring semestr 2009/2010

9 Hydrophobic (dispersion) interactions contribute to stability of small protein rubredoxin more than H-bonded and ion-neutral electrostatic interactions; Czech-Japan Theoretical Chemistry Symposium, Sep. 14 - 16, 2005, Prague

7. přehledy a souborné referáty

N/A

8. patenty národní a zahraniční, objevy

N/A

9. disertační, rigorózní práce, habilitační práce (u profesorských řízení)

Disertační práce:

INHIBITORY HIV-1 PROTEINASY. MOLEKULÁRNÍ MODELOVÁNÍ A TEORETICKÉ VÝPOČTY, Akademie věd české republiky, školitel: prof. Ing. Pavel Hobza DRSc, Praha 1995

Habilitační práce:

INTRAMOLECULAR STABILIZATION OF PROTEINS BY MEANS OF COMPUTATIONAL METHODS
INTRAMOLEKULÁRNÍ STABILIZACE PROTEINU PODHLEDEM VÝPOČETNÍCH METOD, Přírodovědecká fakulta Univerzity Karlovy, Praha 2018

10. abstrakta ze sjezdů a sympozií

Novel calmodulin and S100A1 binding site in distal TRPM4 N-terminus; Vargova, M.; Frtus, A.; Vyklicky, L.; Teisinger, J.; Vondrasek, J.; Bousova, K. ;FEBS JOURNAL,SEP 2017,2017, 284, 42nd Congress of the Federation-of-European-Biochemical-Societies (FEBS) on From Molecules to Cells and Back SEP 10-14, 2017

Is the structure and function of fusion proteins dependent on order of their domains? Bousova, K.; Bednarova, L.; Teisinger, J.; Vondrasek, J.; FEBS JOURNAL, SEP 2017, 2017,284, 42nd Congress of the Federation-of-European-Biochemical-Societies (FEBS) on From Molecules to Cells and Back SEP 10-14, 2017

Novel structural mechanism of allosteric regulation of aspartic peptidases via evolutionary conserved exosite; Hanova, I.; Brynda, J.; Hobizalova, R.; Alam, N.; Sojka, D.; Kopacek, P.; Maresova, L.; Vondrasek, J.; Horn, M.; Schueler-Furman, O.; Mares, M., FEBS JOURNAL, SEP 2017, 2017, 284, 42nd Congress of the Federation-of-European-Biochemical-Societies (FEBS) on From Molecules to Cells and Back SEP 10-14, 2017

Mapping Allostery in the Two Domain Constructs of PDZ3 and SH3 with Artificial Domains; Palani, Kirubakaran; Pfeiferova, Lucie; Vondrasek, Jiri, BIOPHYSICAL JOURNAL, FEB 16 2016, 2016, 110, DOI10.1016/j.bpj.2015.11.347, 60th Annual Meeting of the Biophysical-Society, FEB 27-MAR 02, 2016

DHRS7 enzyme - important player in human health and diseases?; Zemanova, Lucie; Stambergova, Hana; Lundova, Tereza; Andrys, Rudolf; Vondrasek, Jiri; Wsol, Vladimir; PROTEIN SCIENCE, OCT 2015, 2015, 29th Annual Symposium of the Protein-Society, JUL 22-25, 2015

Biophysical characterization of recombinant human ameloblastin; Wald, Tomas; Bednarova, Lucie; Osicka, Radim; Pacht, Petr; Sulc, Miroslav; Lyngstadaas, Stale Petter; Slaby, Ivan; Vondrasek, Jiri; EUROPEAN JOURNAL OF ORAL SCIENCES, DEC 2011, 2011, DOI: 10.1111/j.1600-0722.2011.00913.x, 8th International Symposium on Development, Properties and Pathology of Tooth Enamel, JUN 12-18, 2011

Molecular dynamics study of the conformational behavior of branched glycopeptides during the solid-phase synthesis - The effect of insert and terminal groups; Veprek, Pavel; Trnka, Tomas; Jezek, Jan; Vondrasek, Jiri; Flegel, M; Fridkin, M; Gilon, C; Slaninova, J; Peptides 2004, Proceedings: BRIDGES BETWEEN DISCIPLINES, 3rd International Peptide Symposium/28th European Peptide Symposium, SEP 05-10, 2004

11. **účasť na řešení grantů**, (název a číslo grantu, VZ nebo VC, poskytovatel, roky realizace)

Poskytovatel: MŠMT

Reg. Č. a nezkrácený název projektu: LH11020 - Systematické mapování konformačního prostoru krátkých peptidů pomocí výpočetních metod - cesta k porozumění struktury proteinů a jejich sbalování

Celková výše podpory:1650

Doba řešení: 2011-03-15 - 2015-04-15

Pracovní úvazek:10

Název instituce která podporu přijímá: Ústav organické chemie a biochemie AV ČR

Role: řešitel

Poskytovatel: GAČR

Reg. Č. a nezkrácený název projektu: P302/10/0427 - Ameloblastin - protein indukující růst tvrdých tkání

Celková výše podpory: 3700

Doba řešení: 2010-01-01 - 2012-12-31

Pracovní úvazek:20

Název instituce která podporu přijímá: Biotechnologický ústav AV ČR

Role: řešitel

Poskytovatel: GAČR

Reg. Č. a nezkrácený název projektu: P106/12/G015 - Vývoj nových nanoporézních adsorbentů a katalyzátorů

Celková výše podpory: 9728

Doba řešení: 2012-01-01 - 2018-12-31

Pracovní úvazek: 5

Název instituce která podporu přijímá: Ústav fyzikální chemie J. Heyrovského AV ČR, v.v.i.

Role: člen týmu

Poskytovatel: GAČR

Reg. Č. a nezkrácený název projektu: P208/10/0725 - Intermolecular Interactions in Molecular Solids and Proteins

Celková výše podpory: 2678

Doba řešení: 2010-01-01 - 2013-12-31

Pracovní úvazek 10

Název instituce která podporu přijímá: Ústav organické chemie a biochemie AV ČR, v.v.i.

Role: člen týmu

Poskytovatel: GAČR

Reg. Č. a nezkrácený název projektu: P305/10/2184 - Vztahy mezi strukturou a funkcí v proteinových interakcích

Celková výše podpory: 8276

Doba řešení: 2010-01-01 - 2014-12-31

Pracovní úvazek:5

Název instituce která podporu přijímá: Biotechnologický ústav AV ČR

Role: člen týmu

Poskytovatel: MŠMT

Reg. Č. a nezkrácený název projektu: LM 2015047 Česká národní infrastruktura pro biologická data

Celková výše podpory: 22 662

Doba řešení: 2016-01-01 - 2019-12-31

Pracovní úvazek: 50

Název instituce která podporu přijímá: Ústav organické chemie a biochemie AV ČR, v.v.i.

Role: řešitel

Poskytovatel: European Comission

Reg. Č. a nezkrácený název projektu: 676559 ELIXIR-EXCELERATE: Fast-track ELIXIR implementation and drive early user exploitation across the life-sciences.

Celková výše podpory: 40896

Doba řešení: 2015-09-01 - 2019-8-31

Pracovní úvazek: 20

Název instituce která podporu přijímá: Ústav organické chemie a biochemie AV ČR, v.v.i.

Role: řešitel

Poskytovatel: MŠMT

Reg. Č. a nezkrácený název projektu: LM 2015047 Česká národní infrastruktura pro biologická data, hlavní řešitel

Celková výše podpory: 1650

Doba řešení: 2019-01-01 - 2022-31-12

Pracovní úvazek: 20

Název instituce která podporu přijímá: Ústav organické chemie a biochemie AV ČR

Role: řešitel

Poskytovatel: European Comission

Reg. Č. a nezkrácený název projektu: 871075 ELIXIR-Converge, Connect and align ELIXIR Nodes to deliver sustainable FAIR life-science data management services

Celková výše podpory: 40896

Doba řešení: 2020-01-03 - 2022-28-02

Pracovní úvazek: 20

Název instituce která podporu přijímá: Ústav organické chemie a biochemie AV ČR, v.v.i.

Role: řešitel

Poskytovatel: GAČR

Reg. Č. a nezkrácený název projektu: 19-03488S Ovladání na dálku: Allostेरická kontrola selektivity PDZ3 domény ze ZO-1 Proteinu v chimérických fúzních proteinech

Celková výše podpory: 11 200

Doba řešení: 2019-01-01 - 2021-12-31

Pracovní úvazek: 20

Název instituce která podporu přijímá: Ústav organické chemie a biochemie AV ČR

Role: řešitel

12. **ostatní publikace** (populární články, recenze atd.).

Radka Štorchová, Petr Divina, Jan Pačes, Jiří Vondrášek , Biologie in silico - Ekologie genů z pohledu bioinformatiky , 13. 10. 2005 | Vesmír 84, 582, 2005/10