

Ivaylo Ivanov

<https://orcid.org/0000-0002-5306-1005>

Websites & Social Links

Ivaylo Ivanov's Web Page at Georgia State University (<https://chemistry.gsu.edu/profile/ivaylo-ivanov/>)
Ivaylo Ivanov's Research Group Website (<https://ivanov-group.org>)
Ivaylo Ivanov's Google Scholar Profile (<https://scholar.google.com/citations?user=0y-asqwAAAAJ&hl=en>)
Ivaylo Ivanov's Linked-in Profile (<https://www.linkedin.com/in/ivaylo-ivanov-75a57471>)
Ivaylo Ivanov's ResearchGate Profile (<https://www.researchgate.net/profile/Ivaylo-Ivanov-4>)
Ivaylo Ivanov's Dimensions Profile (<https://app.dimensions.ai/details/entities/publication/author/ur.01321432365.41>)
NIH MyNCBI Bibliography (<https://www.ncbi.nlm.nih.gov/myncbi/ivaylo.ivanov.2/bibliography/public/>)

Country

United States

Keywords

Computational biology and biophysics, Molecular modeling and simulations, Biological assemblies and mechanisms, genome maintenance, gene expression, gene regulation

Other IDs

ResearcherID: A-7613-2013 (<http://www.researcherid.com/rid/A-7613-2013>)
Loop profile: 126638 (http://loop.frontiersin.org/people/126638/overview?referrer=orcid_profile)

Email

iiivanov@gsu.edu

Biography

Ivaylo Ivanov completed his Ph.D. at the University of Pennsylvania and his postdoctoral training at the University of California, San Diego. He is a Professor of Chemistry at Georgia State University in Atlanta, GA. Research in the Ivanov group focuses on the molecular machines and intricate mechanisms of genome maintenance, gene expression and gene regulation. Computational modeling has emerged as a powerful tool for understanding these complex systems, significant for human health. His group develops and applies hybrid methods to integrate data from biophysical techniques that can probe flexible macromolecular assemblies – cryo-electron microscopy, single-molecule spectroscopy and small angle X-ray scattering. The group also has extensive expertise in enhanced sampling, path optimization and free energy methods. Novel computational analyses and data from biochemistry, genetics and genomics are being leveraged to understand how disease mutations interfere with the structure and dynamics of key gene expression assemblies. In turn, such analysis reveals the complex interplay between genetic impairment and disease phenotypes. Recently, the research team has elucidated key pathway selection mechanisms in the DNA damage response, unveiled the molecular architecture of transcription initiation complexes, and contributed to understanding the etiology of genetic disorders associated with cancer, aging, and developmental defects.

Employment (3)

Georgia State University: Atlanta, GA, US

2020 to present | Professor (Department of Chemistry)

Employment

Source:Ivaylo Ivanov

Georgia State University: Atlanta, Georgia, US

2015 to 2020 | Associate Professor (Chemistry)

Employment

Source:Ivaylo Ivanov

Georgia State University: Atlanta, Georgia, US

2009 to 2015 | Assistant Professor (Chemistry)

Employment

Source:Ivaylo Ivanov

Education and qualifications (4)

University of California San Diego: La Jolla, CA, US

2005 to 2009 | Postdoctoral Scholar (Department of Chemistry & Biochemistry)

Qualification

Source: Iwaylo Ivanov

University of Pennsylvania: Philadelphia, PA, US

1999 to 2004 | Ph.D. (Department of Chemistry)

Education

Source: Iwaylo Ivanov

Carnegie Mellon University: Pittsburgh, PA, US

1997 to 1999 | M.S. (Department of Chemistry)

Education

Source: Iwaylo Ivanov

Sofia University Saint Kliment Ohridski: Sofia, BG

1992 to 1996 | B.S. (Department of Chemistry)

Education

Source: Iwaylo Ivanov

Invited positions and distinctions (7)

U.S. Department of Energy Office of Science: Washington, District of Columbia, US

I Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Award (2019–2026)

Distinction

Source: Iwaylo Ivanov

Georgia State University: Atlanta, Georgia, US

2018 | Cleon C. Arrington Research Initiation Award

Distinction

Source: Iwaylo Ivanov

U.S. Department of Energy Office of Science: Washington, District of Columbia, US

2013 | ASCR Leadership Computing Challenge Award

Distinction

Source: Iwaylo Ivanov

U.S. National Science Foundation: Alexandria, Virginia, US

2012 | NSF CAREER Award (2012–2018)

Distinction

Source: Iwaylo Ivanov

Georgia State University: Atlanta, Georgia, US

2012 | Dean's Early Career Award (College of Arts & Sciences)

Distinction

Source: Iwaylo Ivanov

U.S. Department of Energy Office of Science: Washington, District of Columbia, US

2011 | NERSC Initiative for Scientific Exploration (NISE) Award

Distinction

Source: Iwaylo Ivanov

Burroughs Wellcome Fund: Durham, North Carolina, US

2005 | Burroughs Wellcome Fund (La Jolla Interfaces in Science) Postdoctoral Fellowship (2005–2007)

Distinction

Source: Iwaylo Ivanov

Membership and service (7)

National Institutes of Health: Bethesda, Maryland, US

I Ad hoc reviewer of NIH grants (MSFA and MSFC study sections) (Center for Scientific Review)
Service

Source:Ivaylo Ivanov

U.S. National Science Foundation: Alexandria, Virginia, US

2017 to present I NSF ACCESS Resource Allocation Committee
Service

Source:Ivaylo Ivanov

European Science Foundation: Strasbourg, Grand Est, FR

2017 to present I European Science Foundation (ESF) College of Expert Reviewers
Service

Source:Ivaylo Ivanov

Frontiers in Physics (ISSN 2296-424X):

2016 to present I Reviewing Editor
Service

ISSN: 2296-4240

Source:Ivaylo Ivanov

Frontiers in Molecular Biosciences (ISSN: 2296-889X):

2016 to present I Reviewing Editor
Service

ISSN: 2296-8890

Source:Ivaylo Ivanov

National Science Foundation: Alexandria, Virginia, US

2013 to present I Ad hoc reviewer of NSF/NSF-CAREER grants
Service

Source:Ivaylo Ivanov

American Society for Biochemistry and Molecular Biology: Rockville, Maryland, US

2022 to 2023 I Organizer, ASBMB 2023 meeting in Seattle, WA
Service

Source:Ivaylo Ivanov

Funding (6)

Integrative Modeling of Biomolecular Machinery in Nucleotide Excision Repair

National Institutes of Health (Md., Md.)
2022-03 to 2027-01Grant
GRANT_NUMBER: R01ES032786
URL: <https://reporter.nih.gov/search/bnTfDF9LgkmzwnSU6D6NOA/project-details/10362051> (<https://reporter.nih.gov/search/bnTfDF9LgkmzwnSU6D6NOA/project-details/10362051>)
Source:Ivaylo Ivanov

Advanced Computational Modeling of Molecular Machines in Gene Regulation and DNA Repair

National Institute of General Medical Sciences (Bethesda)
2021-03-01 to 2026-02-28Grant
GRANT_NUMBER: R35GM139382
URL: <https://app.dimensions.ai/details/grant/grant.9615541> (<https://app.dimensions.ai/details/grant/grant.9615541>)
Source:Ivaylo IvanovviaDimensionsWizard

Advanced Computational Modeling of Molecular Machines in Gene Regulation and DNA Repair

National Institute of General Medical Sciences (Md., Md.)
2021-03 to 2026-02Grant
GRANT_NUMBER: 1R35GM139382
Source:Ivaylo Ivanov

Advanced Computational Modeling of Pathways for Epigenetic Regulation and Genome Maintenance

National Science Foundation (VA, VA)
2020-08 to 2024-07Grant
GRANT_NUMBER: 2027902
Source:Ivaylo Ivanov

Integrative modeling of PCNA assemblies engaged in genome duplication and repair

National Institute of General Medical Sciences (Bethesda)

2015-09-01 to 2020-08-31Grant

GRANT_NUMBER: 1R01GM110387-01A1

GRANT_NUMBER: 1R01GM110387-01A1

Source:Ivaylo IvanovviaDimensionsWizard

CAREER: Modeling Assemblies and Interactions at the Replication Fork: Sliding Clamps and Clamp Loaders

National Science Foundation (Arlington)

2012-05-01 to 2017-04-30Grant

GRANT_NUMBER: 1149521

GRANT_NUMBER: 1149521

Source:Ivaylo IvanovviaDimensionsWizard

Research resources (1 of 1)

Control of intestinal t cell homeostasis by commenal bacteria

Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support (Alexandria, Virginia, US)

2024-11-15 to 2025-11-14

URL: <https://www.xras.org/public/requests/173722-ACCESS-BIO240332>

Source:ACCESS

Works (79 of 79)

Translocation mechanism of xeroderma pigmentosum group D protein on single-stranded DNA and genetic disease

etiology

Nature Communications

2025-11-28 | journal-article

DOI: 10.1038/s41467-025-66834-1

PMID: 41315283

Source:Ivaylo Ivanov

Engineering a cell-based orthogonal ubiquitin transfer cascade for profiling the substrates of RBR E3 Parkin

iScience

2025-07 | journal-article

DOI: 10.1016/j.isci.2025.112913

PMID: 40687836

PMC: PMC12271601

Source:Ivaylo Ivanov

The interaction of XPG with TFIIH through p62 and XPD is required for the completion of nucleotide excision repair

2025-05-23 | preprint

DOI: 10.1101/2025.05.20.655039

PMC: PMC12139914

PMID: 40475541

Source:Ivaylo Ivanov

Molecular model of TFIIH recruitment to the transcription-coupled repair machinery

Nature Communications

2025-03-08 | journal-article

DOI: 10.1038/s41467-025-57593-0

PMC: PMC11890784

PMID: 40057514

Source:Ivaylo Ivanov

Oligomerization of protein arginine methyltransferase 1 and its functional impact on substrate arginine methylation

Journal of Biological Chemistry

2024-12 | journal-article

DOI: 10.1016/j.jbc.2024.107947

PMC: PMC11681865

PMID: 39491649

Source:Ivaylo Ivanov

Molecular architecture and functional dynamics of the pre-incision complex in nucleotide excision repair

Nature Communications

2024-10-01 | journal-article

DOI: 10.1038/s41467-024-52860-y

PMC: PMC11445577

PMID: 39353945

Source:lvaylo Ivanov

ASCC1 structures and bioinformatics reveal a novel helix-clasp-helix RNA-binding motif linked to a two-histidine phosphodiesterase

Journal of Biological Chemistry

2024-06 | journal-article

DOI: 10.1016/j.jbc.2024.107368

PMC: PMC11214414

PMID: 38750793

Source:lvaylo Ivanov

Dynamic conformational switching underlies TFIIH function in transcription and DNA repair and impacts genetic diseases

Nature Communications

2023-05-13 | journal-article

DOI: 10.1038/s41467-023-38416-6

PMC: PMC10183003

PMID: 37179334

Source:lvaylo Ivanov

A scanning-to-incision switch in TFIIH-XPG induced by DNA damage licenses nucleotide excision repair

Nucleic Acids Research

2023-02-22 | journal-article

DOI: 10.1093/nar/gkac1095

PMC: PMC9943652

PMID: 36477609

Source:lvaylo Ivanov

Universally Accessible Structural Data on Macromolecular Conformation, Assembly, and Dynamics by Small Angle X-Ray Scattering for DNA Repair Insights.

Methods in molecular biology (Clifton, N.J.)

2022-01-01 | journal-article

PMID: 35290631

PMC: PMC9020468

DOI: 10.1007/978-1-0716-2063-2_4

Source:lvaylo Ivanov

Decoding Cancer Variants of Unknown Significance for Helicase-Nuclease-RPA Complexes Orchestrating DNA Repair During Transcription and Replication.

Frontiers in molecular biosciences

2021-12-14 | journal-article

PMID: 34966786

PMC: PMC8710748

DOI: 10.3389/fmolb.2021.791792

Source:lvaylo Ivanov

Mechanism of Rad26-assisted rescue of stalled RNA polymerase II in transcription-coupled repair

Nature Communications

2021-12-01 | journal-article

DOI: 10.1038/s41467-021-27295-4

PMC: PMC8636621

PMID: 34853308

Source:lvaylo Ivanov

Subsets of adjacent nodes (SOAN): a fast method for computing suboptimal paths in protein dynamic networks

Molecular Physics

2021-10-18 | journal-article

DOI: 10.1080/00268976.2021.1893847

Source:lvaylo Ivanov

Pharmacophore-based screening of diamidine small molecule inhibitors for protein arginine methyltransferases

RSC Medicinal Chemistry

2021 | journal-article

DOI: 10.1039/d0md00259c

PMC: PMC8130551

PMID: 34046601

Source:lvaylo Ivanov

Envisioning how the prototypic molecular machine TFIIH functions in transcription initiation and DNA repair

DNA Repair

2020-12 | journal-article

DOI: 10.1016/j.dnarep.2020.102972

PMC: PMC7669588

PMID: 33007515

Source:lvaylo Ivanov

Polymerization and editing modes of a high-fidelity DNA polymerase are linked by a well-defined path

Nature Communications

2020-10-23 | journal-article

DOI: 10.1038/s41467-020-19165-2

PMC: PMC7584608

PMID: 33097731

Source:lvaylo Ivanov

Structural mechanism of helicase loading onto replication origin DNA by ORC-Cdc6

Proceedings of the National Academy of Sciences

2020-07-28 | journal-article

DOI: 10.1073/pnas.2006231117

PMC: PMC7395460

PMID: 32669428

Source:lvaylo Ivanov

Human XPG nuclease structure, assembly, and activities with insights for neurodegeneration and cancer from pathogenic mutations.

Proceedings of the National Academy of Sciences of the United States of America

2020-06-10 | journal-article

PMID: 32522879

PMC: PMC7321962

DOI: 10.1073/pnas.1921311117

Source:lvaylo Ivanov

Simulation-based methods for model building and refinement in cryoelectron microscopy

Journal of Chemical Information and Modeling

2020-05-26 | journal-article

DOI: 10.1021/acs.jcim.0c00087

PMC: PMC7284120

PMID: 32202798

Source:lvaylo Ivanov

Small angle X-ray scattering-assisted protein structure prediction in CASP13 and emergence of solution structure differences.

Proteins

2019-10-16 | journal-article

PMID: 31589784

PMC: PMC6851496

DOI: 10.1002/prot.25827

Source:lvaylo Ivanov

Recognition of a key anchor residue by a conserved hydrophobic pocket ensures subunit interface integrity in DNA clamps

Journal of Molecular Biology

2019-06 | journal-article

DOI: 10.1016/j.jmb.2019.04.035

PMC: PMC6527350

PMID: 31051173

Source:lvaylo Ivanov

Transcription preinitiation complex structure and dynamics provide insight into genetic diseases

Nature Structural & Molecular Biology

2019-06 | journal-article

DOI: 10.1038/s41594-019-0220-3

PMC: PMC6642811

PMID: 31110295

Source:lvaylo Ivanov

Small molecule binders recognize DNA microstructural variations via an induced fit mechanism

Physical Chemistry Chemical Physics

2019 | journal-article

DOI: 10.1039/c8cp05537h

PMC: PMC6497476

PMID: 30629058

Source:lvaylo Ivanov

Structural visualization of RNA polymerase III transcription machineries

Cell Discovery

2018-07-31 | journal-article

DOI: 10.1038/s41421-018-0044-z

PMC: PMC6066478

PMID: 30083386

Source:lvaylo Ivanov

Uncovering universal rules governing the selectivity of the archetypal DNA glycosylase TDG

Proceedings of the National Academy of Sciences

2018-06-05 | journal-article

DOI: 10.1073/pnas.1803323115

PMC: PMC6003370

PMID: 29784784

Source:lvaylo Ivanov

Dissection of DNA double-strand-break repair using novel single-molecule forceps.

Nature structural & molecular biology

2018-05-21 | journal-article

PMID: 29786079

PMC: PMC5990469

DOI: 10.1038/s41594-018-0065-1

Source:lvaylo Ivanov

Natural product Micheliolide (MCL) irreversibly activates pyruvate kinase M2 and suppresses leukemia

Journal of Medicinal Chemistry

2018-05-10 | journal-article

DOI: 10.1021/acs.jmedchem.8b00241

PMC: PMC5949721

PMID: 29641204

Source:lvaylo Ivanov

Small angle X-ray scattering and cross-linking for data assisted protein structure prediction in CASP 12 with prospects for improved accuracy.

Proteins

2018-02-07 | journal-article

PMID: 29314274

PMC: PMC6003418

DOI: 10.1002/prot.25452

Source:lvaylo Ivanov

Phosphate steering by Flap Endonuclease 1 promotes 5'-flap specificity and incision to prevent genome instability.

Nature communications

2017-06-27 | journal-article

PMID: 28653660

PMC: PMC5490271

DOI: 10.1038/ncomms15855

Source:lvaylo Ivanov

Structural mechanism of ATP-independent transcription initiation by RNA polymerase I

eLife

2017-06-17 | journal-article

DOI: 10.7554/elife.27414

PMC: PMC5489313

PMID: 28623663

Source:lvaylo Ivanov

Single-molecule FRET unveils induced-fit mechanism for substrate selectivity in flap endonuclease 1

eLife

2017-02-23 | journal-article

DOI: 10.7554/elife.21884

PMC: PMC5358979

PMID: 28230529

Source:lvaylo Ivanov

DNA microstructure influences selective binding of small molecules designed to target mixed-site DNA sequences

Nucleic Acids Research

2017-02-17 | journal-article

DOI: 10.1093/nar/gkw1232

PMC: PMC5388402

PMID: 28180310

Source:lvaylo Ivanov

Discovery of decamidine as a new and potent PRMT1 inhibitor

MedChemComm

2017 | journal-article

DOI: 10.1039/c6md00573j

PMC: PMC5477784

PMID: 28649316

Source:lvaylo Ivanov

Secondary interaction interfaces with PCNA control conformational switching of DNA polymerase PolB from polymerization to editing

The Journal of Physical Chemistry B

2016-08-25 | journal-article

DOI: 10.1021/acs.jpcb.6b02082

PMC: PMC5001886

PMID: 27109703

Source:lvaylo Ivanov

Discovery of selective inhibitors of tyrosyl-DNA phosphodiesterase 2 by targeting the enzyme DNA-binding cleft

Bioorganic & Medicinal Chemistry Letters

2016-07 | journal-article

DOI: 10.1016/j.bmcl.2016.05.065

PMC: PMC4939481

PMID: 27262595

Source:lvaylo Ivanov

Rational design of a protein that binds integrin $\alpha v\beta 3$ outside the ligand binding site

Nature Communications

2016-05-31 | journal-article

DOI: 10.1038/ncomms11675

PMC: PMC4895024

PMID: 27241473

Source:lvaylo Ivanov

Near-atomic resolution visualization of human transcription promoter opening

Nature

2016-05-19 | journal-article

DOI: 10.1038/nature17970

PMC: PMC4940141

PMID: 27193682

Source:lvaylo Ivanov

Distal substitutions drive divergent DNA specificity among paralogous transcription factors through subdivision of conformational space

Proceedings of the National Academy of Sciences

2016-01-12 | journal-article

DOI: 10.1073/pnas.1518960113

PMC: PMC4720311

PMID: 26715749

Source:lvaylo Ivanov

Unexpected allosteric network contributes to LRR-1 co-regulator selectivity

Journal of Biological Chemistry

2016-01 | journal-article

DOI: 10.1074/jbc.m115.662874

PMC: PMC4714224

PMID: 26553876

Source:lvaylo Ivanov

Functional dynamics in replication protein A DNA binding and protein recruitment domains

Structure

2015-06 | journal-article

DOI: 10.1016/j.str.2015.04.008

PMC: PMC4456234

PMID: 26004442

Source:lvaylo Ivanov

Structurally distinct ubiquitin- and SUMO-modified PCNA: Implications for their distinct roles in the DNA damage response.

Structure (London, England : 1993)

2015-03-12 | journal-article

PMID: 25773143

PMC: PMC4394044

DOI: 10.1016/j.str.2015.02.008

Source:lvaylo Ivanov

Integrative modeling of macromolecular assemblies from low to near-atomic resolution

Computational and Structural Biotechnology Journal

2015 | journal-article

DOI: 10.1016/j.csbj.2015.08.005

PMC: PMC4588362

PMID: 26557958

Source:lvaylo Ivanov

Alkylpurine glycosylase D employs DNA sculpting as a strategy to extrude and excise damaged bases

PLoS Computational Biology

2014-07-03 | journal-article

DOI: 10.1371/journal.pcbi.1003704

PMC: PMC4081403

PMID: 24992034

Source:lvaylo Ivanov

Diamidine compounds for selective inhibition of protein arginine methyltransferase 1

Journal of Medicinal Chemistry

2014-03-27 | journal-article

DOI: 10.1021/jm401884z

PMC: PMC3983339

PMID: 24564570

Source:lvaylo Ivanov

Opening pathways of the DNA clamps proliferating cell nuclear antigen and Rad9-Rad1-Hus1

Nucleic Acids Research

2013-12-01 | journal-article

DOI: 10.1093/nar/gkt810

PMC: PMC3905852

PMID: 24038358

Source:lvaylo Ivanov

Probing DNA clamps with single-molecule force spectroscopy

Nucleic Acids Research

2013-09 | journal-article

DOI: 10.1093/nar/gkt487

PMC: PMC3763527

PMID: 23783571

Source:lvaylo Ivanov

Conserved structural chemistry for incision activity in structurally non-homologous apurinic/apyrimidinic endonuclease APE1 and endonuclease IV DNA repair enzymes

Journal of Biological Chemistry

2013-03 | journal-article

DOI: 10.1074/jbc.m112.422774

PMC: PMC3605660

PMID: 23355472

Source:lvaylo Ivanov

A new structural framework for integrating replication protein A into DNA processing machinery

Nucleic Acids Research

2013-02 | journal-article

DOI: 10.1093/nar/gks1332

PMC: PMC3575853

PMID: 23303776

Source:lvaylo Ivanov

Enzyme cofactors: Double-edged sword for catalysis

Nature Chemistry

2013-01 | journal-article

DOI: 10.1038/nchem.1529

PMID: 23247167

Source:lvaylo Ivanov

Repair complexes of FEN1 endonuclease, DNA, and Rad9-Hus1-Rad1 are distinguished from their PCNA counterparts by functionally important stability

Proceedings of the National Academy of Sciences

2012-05-29 | journal-article

DOI: 10.1073/pnas.1121116109

PMC: PMC3365210

PMID: 22586102

Source: Ivaylo Ivanov

Molecular dynamics

Methods in Molecular Biology

2012 | book-chapter

DOI: 10.1007/978-1-62703-050-2_11

PMID: 23007433

Source: Ivaylo Ivanov

Solution X-ray scattering combined with computational modeling reveals multiple conformations of covalently bound ubiquitin on PCNA

Proceedings of the National Academy of Sciences

2011-10-25 | journal-article

DOI: 10.1073/pnas.1110480108

PMC: PMC3203759

PMID: 22006297

Source: Ivaylo Ivanov

Histone H4 acetylation differentially modulates arginine methylation by an in cis mechanism

Journal of Biological Chemistry

2011-06 | journal-article

DOI: 10.1074/jbc.m110.207258

PMC: PMC3121530

PMID: 21502321

Source: Ivaylo Ivanov

New insights into the GABA(a) receptor structure and orthosteric ligand binding: Receptor modeling guided by experimental data

Proteins: Structure, Function, and Bioinformatics

2011-05 | journal-article

DOI: 10.1002/prot.22975

PMC: PMC3076690

PMID: 21365676

Source: Ivaylo Ivanov

Ion selectivity mechanism in a bacterial pentameric ligand-gated ion channel

Biophysical Journal

2011-01 | journal-article

DOI: 10.1016/j.bpj.2010.11.077

PMC: PMC3021669

PMID: 21244835

Source: Ivaylo Ivanov

Recognition of the ring-opened state of proliferating cell nuclear antigen by replication factor C promotes eukaryotic clamp-loading

Journal of the American Chemical Society

2010-06-02 | journal-article

DOI: 10.1021/ja100365x

PMC: PMC2876781

PMID: 20455582

Source: Ivaylo Ivanov

Molecular dynamics simulations of ELIC — a prokaryotic homologue of the nicotinic acetylcholine receptor

Biophysical Journal

2009-06 | journal-article

DOI: 10.1016/j.bpj.2009.03.018

PMC: PMC2711484

PMID: 19486673

Source:lvaylo Ivanov

Characterizing loop dynamics and ligand recognition in human- and avian-type influenza neuraminidases via Generalized Born molecular dynamics and end-point free energy calculations

Journal of the American Chemical Society

2009-04-08 | journal-article

DOI: 10.1021/ja8085643

PMC: PMC2665887

PMID: 19296611

Source:lvaylo Ivanov

Dynamics of the acetylcholinesterase tetramer

Biophysical Journal

2008-02 | journal-article

DOI: 10.1529/biophysj.107.117879

PMC: PMC2212707

PMID: 17921202

Source:lvaylo Ivanov

Synthetic mimics of antimicrobial peptides

Peptide Science

2008-01 | journal-article

DOI: 10.1002/bip.20970

PMID: 18314892

Source:lvaylo Ivanov

Nanosecond-timescale conformational dynamics of the human $\alpha 7$ nicotinic acetylcholine receptor

Biophysical Journal

2007-10 | journal-article

DOI: 10.1529/biophysj.107.109843

PMC: PMC1989720

PMID: 17573436

Source:lvaylo Ivanov

Barriers to ion translocation in cationic and anionic receptors from the Cys-loop family

Journal of the American Chemical Society

2007-07-01 | journal-article

DOI: 10.1021/ja070778l

PMID: 17552523

Source:lvaylo Ivanov

Unraveling the three-metal-ion catalytic mechanism of the DNA repair enzyme endonuclease IV

Proceedings of the National Academy of Sciences

2007-01-30 | journal-article

DOI: 10.1073/pnas.0603468104

PMC: PMC1780068

PMID: 17242363

Source:lvaylo Ivanov

Proliferating cell nuclear antigen loaded onto double-stranded DNA: dynamics, minor groove interactions and functional implications

Nucleic Acids Research

2006-11 | journal-article

DOI: 10.1093/nar/gkl744

PMC: PMC1635319

PMID: 17071716

Source:lvaylo Ivanov

Ab initio calculations of intramolecular parameters for a class of arylamide polymers

Journal of Computational Chemistry

2006-04-30 | journal-article

DOI: 10.1002/jcc.20382

PMID: 16634095

Source:lvaylo Ivanov

Controlling the shape and flexibility of arylamides: A combined ab initio, ab initio molecular dynamics, and classical molecular dynamics study

The Journal of Physical Chemistry B

2006-03-01 | journal-article

DOI: 10.1021/jp054306

PMID: 16494407

Source:lvaylo Ivanov

Relative pKa values from first-principles molecular dynamics: The case of histidine deprotonation

The Journal of Physical Chemistry B

2006-03-01 | journal-article

DOI: 10.1021/jp056750i

PMID: 16553455

Source:lvaylo Ivanov

Characterization of nonbiological antimicrobial polymers in aqueous solution and at water–lipid interfaces from all-atom molecular dynamics

Journal of the American Chemical Society

2006-02-01 | journal-article

DOI: 10.1021/ja0564665

PMID: 16464062

Source:lvaylo Ivanov

The design and evaluation of heparin-binding foldamers

Angewandte Chemie International Edition

2005-10-21 | journal-article

DOI: 10.1002/anie.200501279

PMID: 16094685

Source:lvaylo Ivanov

Dynamical flexibility and proton transfer in the arginase active site probed by ab initio molecular dynamics

Journal of the American Chemical Society

2005-03-01 | journal-article

DOI: 10.1021/ja043693i

PMID: 15771538

Source:lvaylo Ivanov

Terascale ab initio molecular dynamics simulations of proton transfer and dissociation processes in chemical and biological systems.

2004-12 | dissertation-thesis

ISBN: 978-0-496-12390-2

Source:lvaylo Ivanov

Transmembrane peptide-induced lipid sorting and mechanism of L-to-inverted phase transition using coarse-grain molecular dynamics

Biophysical Journal

2004-10 | journal-article

DOI: 10.1529/biophysj.104.040311

PMC: PMC1304638

PMID: 15454415

Source:lvaylo Ivanov

First principles computational study of the active site of arginase

Proteins: Structure, Function, and Bioinformatics

2004-01 | journal-article

DOI: 10.1002/prot.10572

PMID: 14705018

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Hydrogen bonding in water

Physical Review Letters

2003-11-20 | journal-article

DOI: 10.1103/physrevlett.91.215503

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Solution characterization of monodisperse atactic polystyrenes by static and dynamic light scattering

International Journal of Polymer Analysis and Characterization

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DOI: 10.1080/10236660304875

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Deprotonation of a histidine residue in aqueous solution using constrained ab initio molecular dynamics

Journal of the American Chemical Society

2002-11-01 | journal-article

DOI: 10.1021/ja027972m

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Solvation structure and mobility mechanism of OH⁻: A Car-Parrinello molecular dynamics investigation of alkaline solutions

The Journal of Physical Chemistry B

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DOI: 10.1021/jp026504w

Source:lvaylo Ivanov

First-principles study of aqueous hydroxide solutions

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2002-07-01 | journal-article

DOI: 10.1021/ja020350g

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Comparison of the INDO band structures of polyacetylene, polythiophene, polyfuran, and polypyrrole

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2001-01 | journal-article

DOI: 10.1016/s0379-6779(00)00526-9

Source:lvaylo Ivanov

Peer review (14)

- review activity for **Accounts of chemical research**. (1)
- review activity for **ACS catalysis**. (1)
- review activity for **Chemical reviews**. (1)
- review activity for **eLife** (2)
- review activity for **Journal of chemical information and modeling**. (8)
- review activity for **Journal of chemical theory and computation** : (3)
- review activity for **Journal of medicinal chemistry**. (1)
- review activity for **Journal of the American Chemical Society**. (4)
- review activity for **Nature** (1)
- review activity for **Nature communications** (2)
- review activity for **Nature structural & molecular biology**. (1)
- review activity for **Nucleic acids research**. (20)
- review activity for **Proceedings of the National Academy of Sciences of the United States of America**. (1)
- review activity for **The journal of physical chemistry letters**. (3)

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