WALTER F. DE AZEVEDO JR.

Professor

PROFILE

My scientific interests are interdisciplinary, with three main emphases: computational structural biology, artificial intelligence, and complex systems. In my studies, I developed several free software programs to explore the concept of Scoring Function Space.
As a result of my research, I published over 200 scientific works about protein structures, computer models, and simulations of proteins. These publications have generated over 12,000 citations on Google Scholar (h-index of 64) and more than 10,000 citations and an h-index of 58 in Scopus.

CONTACT

SITE: https://github.com/azevedolab/

EMAILS: walter@azevedolab.net
prof.walter.filgueira@gmail.com

ADDRESS: Federal University of Alfenas. Rua Gabriel Monteiro da Silva, 700. Alfenas-MG. Brazil. 37130-001

SKILLS

- Machine-learning developer
- Programming in Python
- Leadership of international teams of researchers
- Editorial experience
- Teaching undergraduate and graduate coarses
- Supervising PhD and Master students
- Interdiscplinary research (Computing, Biology, Chemistry, and Physics)

OBJECTIVES

My goal is to establish an international group focused on interdisciplinary research projects. This joint-research group will work on machine-learning models to address drug development. It will integrate interdisciplinary and international researchers. To reach this goal, I will establish a team of researchers with extensive experience in collaborative networks to impact science and education. My experience in supervising international teams is well-documented in recent publications where I am the corresponding author of these papers (e.g., de Azevedo et al., 2024, de Azevedo et al., 2026). My current group of collaborators has participation of researchers from nine countries (Argentina, Brazil, France, Italy, Mexico, Portugal, Russia, Turkey, and the USA). This group will work as a seed to further integrate my future colleagues on research projects focused on modeling complex systems using machine learning techniques. I also aim to invite PhD students to participate in my research projects. I have experience linking my teaching to research projects where students participate in activities that generate publishable results (e.g., de Azevedo et al., 2021). I advocate an educational approach called education through science. My editorial experience includes multiple scientific journals (e.g., Current Medicinal Chemistry, Molecular Diversity, and Methods of Molecular Biology). For all these journals, I frequently lead issues dedicated to my research goals (e.g., Current Medicinal Chemistry: Volume 32, Issue 28, 2025 Published on: 29 May, 2025). I will work on new volumes on topics of common interest with my future colleagues and students. In summary, my previous experience in research (ranked among the most influential researchers), editing (e.g., Editor-in-Chief for Current Drug Therapy), and teaching will be an interesting addition to any international university or scientific journal pursuing interdisciplinary projects that impact science. Furthermore, I will bring my enthusiasm and scientific experience to contribute to research, teaching, and cultural exchange.

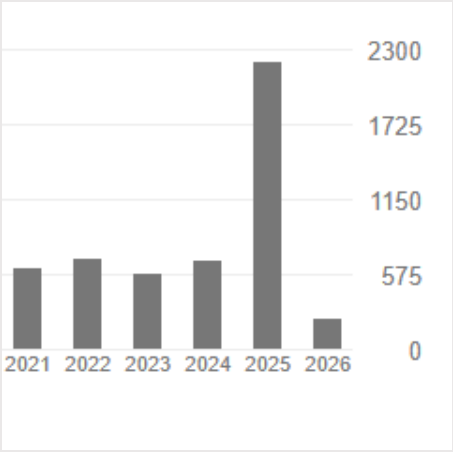
PERSONAL INFORMATION

Nane: Walter Filgueira de Azevedo Junior

Date of Birth: January 10, 1963

Local of Birth: Rio de Janeiro, RJ. Brazil

RESEARCH HIGHLIGHTS



Times cited and publications over time (Google Scholar: 2021-2026) (May 12, 2026)
Data Source: https://scholar.google.com.br/citations?hl=en-BR&user=HWwJXJUAAAAJ

EDUCATION

São Paulo State University
2004 Habilitation (Livre Docência) in Physics

State University of São Paulo (University of California, Berkeley)
1992-1997 Doctor of Science (Ph.D.) in Applied Physics. Split PhD program.

State University of São Paulo
1991-1992 Master of Science (M.Sc.) in Applied Physics

State University of São Paulo
1986-1990 Bachelor in Physics (BSc)

WORKING EXPERIENCE

Bharath Institute of Higher Education and Research Bharath University (India) (September 2025-) (Honorary Professor)
Leading international and interdiciplinary research and editorial projects. Supervise PhD students.

Federal University of Alfenas (Brazil) (May 2023-) (Professor)
Teaching undergraduate and graduate courses. Leading international and interdiciplinary research and editorial projects. Supervise Master and PhD students.

Pontifical Catholic University of Rio Grande do Sul (Brazil) (August 2005-January 2023) (Professor)
Coordinate courses. Teaching undergraduate and graduate courses. Leading international and interdiciplinary research and editorial projects. Supervise Master and PhD students.

São Paulo State University (Brazil) (May 1998-July 2005) (Professor)
Coordinate courses. Teaching undergraduate and graduate courses. Leading international and interdiciplinary research and editorial projects. Supervise Master and PhD students.

University of California, Berkeley (USA) (October 1993-July 1996) (Visiting Researcher)
Participate in structural biological research projects.

CITATION METRICS

Scopus
Documents by author: 226 Total citations: 10,236 H-index: 58
Link: https://www.scopus.com/authid/detail.uri?authorId=7006435557

Web of Science
Documents by author: 241 Total citations: 8,465 H-index: 50
Link: https://www.webofscience.com/wos/author/record/581112

Google Scholar (Curated by the Author)
Documents by author: 257 Total citations: 12,715 H-index: 64
Link: https://scholar.google.com/citations?user=HWwJXJUAAAAJ

Researcher Gate
Documents by author: 248 Total citations: 11,020 H-index: 60
Link: https://www.researchgate.net/profile/Walter-De-Azevedo-Jr

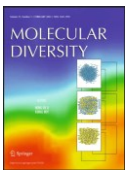
Updated on May 12, 2026.

RESEARCH HIGHLIGHTS

Current Drug Therapy
Since March 2026, I have been the Editor-in-Chief of Current Drug Therapy (Editorial Board)
Image Source: https://www.benthamscience.com/images/bentham/CDTH_0.gif

EDITORIAL EXPERIENCE

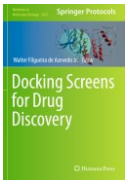
Current Drug Therapy
ISSN: 1574-8855 (Print) 2212-3903 (Online)
Editor-in-Chief
Link: https://www.benthamscience.com/journal/14/editorial-board



Molecular Diversity Electronic
ISSN: 1381-1991 (Print) 1573-501X (Online)
Member of the Editorial Board
Link: https://link.springer.com/journal/11030/editorial-board

Current Drug Targets
ISSN: 1873-5592 (Online) 1389-4501 (Print)
Section Editor (Section: Bioinformatics and Biophysics)
Link: https://www.benthamscience.com/journal/13/editorial-board

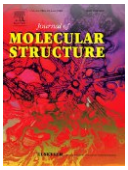
Current Medicinal Chemistry
ISSN: 0929-8673 (Print) 1875-533X (Online)
Section Editor (Bioinformatics in Drug Design and Discovery)
Link: https://www.benthamscience.com/journal/25/editorial-board



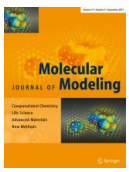
Methods of Molecular Biology-Docking Screens for Drug Discovery
ISBN: 978-1-4939-9751-0 978-1-4939-9752-7 (Online)
Editor for Springer Nature
Link: https://www.springer.com/gp/book/9781493997510

PeerJ
ISSN: 2167-8359
Member of the Editorial Board
Link: https://peerj.com/Walter/

Organic & Medicinal Chemistry International Journal
ISSN: 2474-7610
Honorable Editor
Link: https://juniperpublishers.com/omcij/editorialboard.php

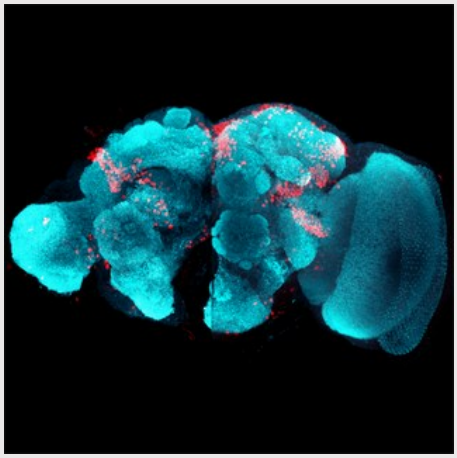


Journal of Molecular Structure
ISSN: 0022-2860 (Print) 1872-8014 (Online)
Member of the Editorial Board (2023-26) and Guest Editor
Link: https://www.sciencedirect.com/special-issue/329534/quantum-chemical-methods-in-molecular-structure-and-reactivity-for-applications-in-quantum-biology



Journal of Molecular Modeling
ISSN: 1610-2940 (Print) 0948-5023 (Online)
Guest Editor
Link: https://link.springer.com/collections/gdgeagaecd

RESEARCH HIGHLIGHTS



PLOS Biology
Due to the impact of my work, I have been ranked among the most influential researchers in the world (Fields: Biophysics, Biochemistry & Molecular Biology, and Biomedical Research) according to a database created by Journal Plos Biology (https://journals.plos.org/plosbiology/article?id=10.1371/journal.pbio.3000918)
Image Source: https://journals.plos.org/plosbiology/article/figure/image?size=inline&id=10.1371/image.pbio.v18.i10.g001

HONORS AND AWARDS

2025
Most influential researchers in the world according to a database created by Journal Plos Biology. Link: https://elsevier.digitalcommonsdata.com/datasets/btchxktzyw/8

2024
Most influential researchers in the world according to a database created by Journal Plos Biology. Link: https://elsevier.digitalcommonsdata.com/datasets/btchxktzyw/7

2023
Most influential researchers in the world according to a database created by Journal Plos Biology. Link: https://elsevier.digitalcommonsdata.com/datasets/btchxktzyw/6

2022
Most influential researchers in the world according to a database created by Journal Plos Biology. Link: https://elsevier.digitalcommonsdata.com/datasets/btchxktzyw/4

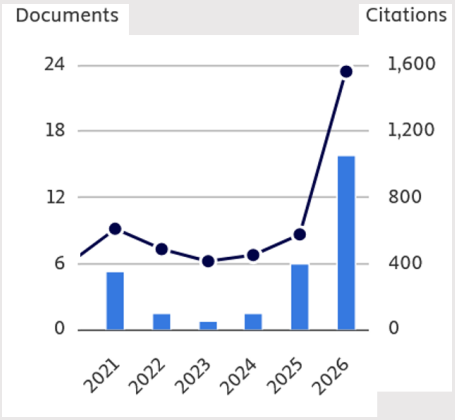
2022
Keynote lecturer: Harnessing Machine Learning for Drug Discovery., XXVIII Symposium on Bioinformatics and Computer-Aided Drug Discovery

2021
Most influential researchers in the world according to a database created by Journal Plos Biology. Link: https://elsevier.digitalcommonsdata.com/datasets/btchxktzyw/3

2020
Most influential researchers in the world according to a database created by Journal Plos Biology. Link: https://doi.org/10.1371/journal.pbio.300091, Journal of PLOS Biology.
See news: https://www.pucrs.br/en/blog/research-database-includes-7-pucrs-professors-among-most-influential-in-the-world/

2019
Most influential researchers in the world according to a database created by Journal Plos Biology. Link: https://elsevier.digitalcommonsdata.com/datasets/btchxktzyw/1

RESEARCH HIGHLIGHTS



Times cited and publications over time (Scopus: 2021-2026) (May 12, 2026)
Data Source: https://www.scopus.com/authid/detail.uri?authorId=7006435557

RECENT RESEARCH GRANT

2023-2027
Funding agency: CNPq (Conselho Nacional de Desenvolvimento Científico e Tecnológico-Brazil). R$ 120.000,00 (one-hundred and twenty thousand reais). Process Number: 306298/2022-8
Title: Development of Scoring Functions to Predict Protein-Ligand Binding Affinity

Abstract
In this project, we study protein-ligand binding affinity using computational approaches. We employed a workflow to integrate advanced machine learning techniques and docking simulations. This workflow combines protein-ligand binding affinity data from the BindingDB and crystal structures of proteins available at the Protein Data Bank. These two databases are the sources for training sets for machine learning models used to predict binding affinity based on the crystallographic atomic coordinates of protein-ligand complexes. It is also possible to use docked poses to create machine learning models to predict binding affinity. Our approach explores the concept of scoring function space, allowing the development of a machine learning model targeted to the protein of interest. An international team of researchers with experience in using computational tools to address biological systems participated in this project.

International Team
Damla Dere (Scopus ID: 58396726400) (Turkey)
Enrique González-Vergara (Scopus ID: 6603132110)(Mexico)
Marcos Ariel Villarreal (Scopus ID: 56011459000)(Argentine)
Nelson José Freitas da Silveira (Scopus ID: 6602182638)(Brazil)
Marco Tutone (Scopus ID: 23494181200)(Italy)
Martina Veit-Acosta (Scopus ID: 57210831489)(USA)
Olga Tarasova (Scopus ID: 55914745500)(Russia)
Rodrigo Quiroga (Scopus ID: 26432219400)(Argentine)
Rui Fausto (Scopus ID: 7004333128)(Portugal)
Sema Nur Pehlivan (Scopus ID: 60136674400) (Turkey)
Stéphaine Baud (Scopus ID: 55556463100)(France)
Vladimir Poroikov (Scopus ID: 7004294720)(Russia)

RESEARCH ID, SCOPUS, ORCID, AND RELATED METRICS

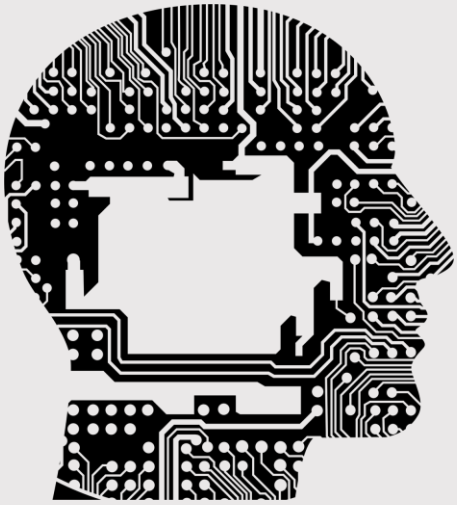
WEB OF SCIENCE RESEARCHER ID: N-5585-2018
Link: https://www.webofscience.com/wos/author/record/581112

SCOPUS ID: 7006435557
Link: https://www.scopus.com/authid/detail.uri?authorId=7006435557

ORCID: 0000-0001-8640-357X
Link: http://orcid.org/0000-0001-8640-357X

RESEARCH GATE
Link: https://www.researchgate.net/profile/Walter-De-Azevedo-Jr

RESEARCH HIGHLIGHTS



Machine-learning models to address protein-ligand interactions (GitHub)
My research focuses on machine-learning models to address complex biological systems.
Image Source: https://pixabay.com/vectors/cranium-head-human-male-man-2099120/

TEACHING EXPERIENCE

Undergraduate Courses
Biophysics
Molecular Biophysics
Bioinformatics
General Physics
Quantum Physics
Computational Physics
Mathematical Methods for Physicists
Biochemistry

Graduate Courses
Bioinformatics
Drug Discovery (taught in English)
Machine Learning (taught in English)
Structural Biology (taught in English)
Crystallography
Docking Screens for Drug Discovery (taught in English) (Course based on my book)

SCIENTIFIC IMPACT

My research is interdisciplinary, with three main emphases: computational structural biology, artificial intelligence, and complex systems. In my studies, I developed several free software programs to explore the concept of Scoring Function Space (Heck et al., 2017). As a result of my research, I published over 200 publications focused on protein structures, computer models of complex systems, and simulations of protein systems. These publications have generated over 12,000 citations on Google Scholar (h-index of 64) and more than 10,000 citations and an h-index of 58 in Scopus.

Due to the impact of my work, I have been ranked among the most influential researchers in the world (Fields: Biophysics, Biochemistry & Molecular Biology, and Biomedical Research) according to a database created by Journal Plos Biology (see news here). The application of the same set of metrics acknowledged the influence of my work from 2021 to 2025 (Baas et al., 2021; Ioannidis, 2022; Ioannidis, 2023; Ioannidis, 2024; Ioannidis, 2025). Not bad for a poor dreamer who was a shoe seller in São Paulo and had the opportunity to study at the University of São Paulo with a scholarship for food and housing. I was 23 when I initiated my undergraduate studies and was the first in my family to have access to higher education.

Regarding scientific impact (Peterson, 2005), for a physicist, a value for the h-index of 45 or higher could mean membership in the National Academy of Sciences of the USA. So far, there have been no invitations. No hard feelings because I am in good company. Carl Sagan was never allowed into the National Academy of Sciences. According to Google Scholar, his work accumulates more than 1,000 citations per year (search performed in November 2024). Indeed, his current citation rate exceeds that of many members of the National Academy of Sciences.

RESEARCH HIGHLIGHTS

Launch of Shuttle Discovery on STS-95 Mission (News)
In 1998, we sent proteins to crystallize in a microgravity environment during the Space Shuttle Discovery flight.
Image Source: https://www.nasa.gov/wp-content/uploads/2023/03/98pc1450.jpg
Link to video with news about crystallization of proteins in microgravity (Portuguese): https://www.youtube.com/watch?v=N9IFiQNY8mE

SHORT BIOGRAPHY

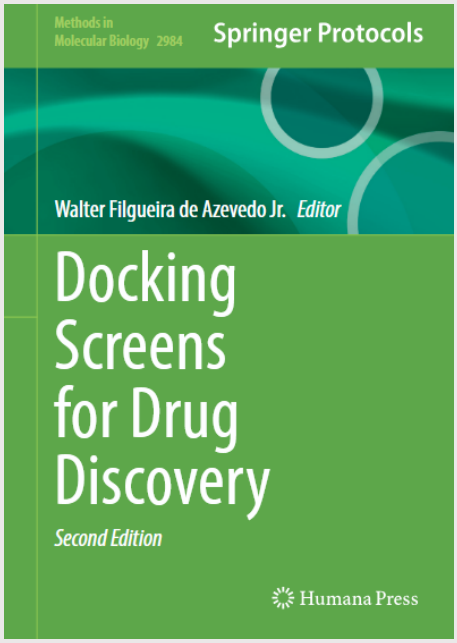
Dr. Walter F. de Azevedo, Jr. earned a BSc in Physics (1990), an MSc in Applied Physics (1992), and a DSc in Applied Physics (1997) from the University of São Paulo (Brazil). Dr Azevedo worked under the supervision of Prof. Yvonne Primerano Mascarenhas (University of São Paulo) and Prof. Sung-Hou Kim (University of California, Berkeley) on a split Doctoral program with a fellowship from the Brazilian Research Council (CNPq). During the first two years of his stay at Berkeley, he was under a CNPq fellowship (1993-95). Due to his performance during these first years, Prof. S.-H. Kim hired him as a Visiting Researcher for the Department of Chemistry at the University of California, Berkeley (1995-96). The work developed at Berkeley resulted in his thesis about the structure of CDK2 (PDB code: 2A4L) (https://www.rcsb.org/structure/2A4L) (Azevedo et al., 1996)(https://doi.org/10.1073/pnas.93.7.2735); (Azevedo et al., 1997)(https://doi.org/10.1111/j.1432-1033.1997.0518a.x). Dr Azevedo is the first author of both papers, and these publications have more than 1,000 citations on the Web of Science (https://www.webofscience.com/wos/author/record/581112).

During 1997-1998, he had a postdoc position at São Paulo State University (Unesp) with a Fapesp fellowship (https://bv.fapesp.br/pt/bolsas/75932/determinacao-de-estruturas-de-proteinas-por-tecnicas-de-difracao-de-raios-x/). He holds a habilitation degree in Physics (livre-docência) from São Paulo State University (Unesp)(2004). In 1998, Dr. Azevedo participated in a research project with NASA. This project focused on protein crystallization in a microgravity environment onboard the Space Shuttle Discovery (STS-95). Brazilian TV networks covered this research (https://www.youtube.com/watch?v=N9IFiQNY8mE). In 2019, he published the book Docking Screens for Drug Discovery. This book sold more than 63,000 copies (March 2026) with over 2 million dollars in sales (https://link.springer.com/book/10.1007/978-1-4939-9752-7). The second edition was published in October 2025 (https://doi.org/10.1007/978-1-0716-4949-7).

In 2020, the Journal Plos Biology ranked Dr. Azevedo among the most influential researchers in the world (https://journals.plos.org/plosbiology/article?id=10.1371/journal.pbio.3000918). The application of the same set of metrics recognized the influence of my work from 2021 to 2025 (Baas et al., 2021; Ioannidis, 2022, 2023, 2024, and 2025).

Since March 2026, he has been the Editor in Chief for the Current Drug Therapy (https://www.benthamscience.com/journal/14/editorial-board). Dr. Azevedo works as an editor of several journals. Among them, he is the frontiers section editor (Bioinformatics/Biophysics) for the Current Drug Targets (https://benthamscience.com/journals/current-drug-targets/editorial-board/#top), section editor for the Current Medicinal Chemistry (https://benthamscience.com/journals/current-medicinal-chemistry/editorial-board/#top), member of the editorial board of Molecular Diversity (https://www.springer.com/journal/11030/editors), and editor of Docking Screens for Drug Discovery (Methods of Molecular Biology)-Springer Nature. He is a reviewer for over 60 high-impact journals, including Nature Communications and Briefings in Bioinformatics.

RESEARCH HIGHLIGHTS



Publication of Docking Screens for Drug Discovery (doi: 10.1007/978-1-0716-4949-7) (12 October 2025) (de Azevedo et al., 2024)
This new edition concentrates on the development of computational models to predict binding affinity based on the atomic coordinates of protein-ligand complexes. All codes are Python snippets based on the program SAnDReS 2.0.
Image Source: https://media.springernature.com/w316/springer-static/cover/book/978-1-0716-4949-7.jpg?as=webp

PUBLICATIONS (2026-1995)

Dos Santos Bezerra WA, da Rocha CQ, da Silva Vaz Junior I, Ullah S, de Azevedo Junior WF, Soares AMDS. In vitro and in silico evaluation of plant compounds as inhibitors of glutathione S-transferase from Rhipicephalus microplus and R. decoloratus. Mol Biochem Parasitol. 2026;266:111735. doi: 10.1016/j.molbiopara.2026.111735.

de Azevedo WF Jr. Tree-Based Methods to Predict Enzyme Inhibition. Methods Mol Biol. 2026;2984:295-311. doi: 10.1007/978-1-0716-4949-7_20. PMID: 41075100.

de Azevedo WF Jr. Neural Networks to Calculate CDK2 Inhibition. Methods Mol Biol. 2026;2984:277-293. doi: 10.1007/978-1-0716-4949-7_19. PMID: 41075099.

de Azevedo WF Jr. Molegro Data Modeller to Estimate CDK6 Inhibition. Methods Mol Biol. 2026;2984:259-275. doi: 10.1007/978-1-0716-4949-7_18. PMID: 41075098.

de Azevedo WF Jr. CDK7 as a Target for Docking Screens. Methods Mol Biol. 2026;2984:243-258. doi: 10.1007/978-1-0716-4949-7_17. PMID: 41075097.

de Azevedo WF Jr. Targeting CDK9 with Molegro Virtual Docker. Methods Mol Biol. 2026;2984:227-242. doi: 10.1007/978-1-0716-4949-7_16. PMID: 41075096.

de Azevedo WF Jr. Machine Learning to Predict CDK4 Inhibition. Methods Mol Biol. 2026;2984:211-225. doi: 10.1007/978-1-0716-4949-7_15. PMID: 41075095.

da Silva AD, Russo S, González-Vergara E, de Azevedo WF Jr. Differential Evolution for Docking Simulations. Methods Mol Biol. 2026;2984:197-210. doi: 10.1007/978-1-0716-4949-7_14. PMID: 41075094.

da Silva AD, de Azevedo WF Jr. AlphaFold for Docking Screens. Methods Mol Biol. 2026;2984:183-196. doi: 10.1007/978-1-0716-4949-7_13. PMID: 41075093.

da Silva AD, de Azevedo WF Jr. Neural Networks with Molegro Data Modeller. Methods Mol Biol. 2026;2984:167-181. doi: 10.1007/978-1-0716-4949-7_12. PMID: 41075092.

da Silva AD, da Silveira NJF, Oliveira PR, de Azevedo WF Jr. Molegro Data Modeller for Machine Learning. Methods Mol Biol. 2026;2984:153-166. doi: 10.1007/978-1-0716-4949-7_11. PMID: 41075091.

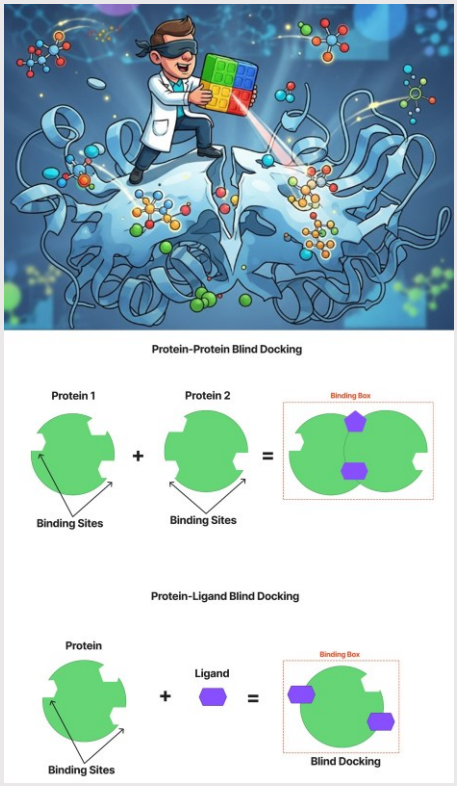
Oliveira JMV, da Silva AD, Soares AMDS, de Azevedo WF Jr. Molegro Virtual Docker for Docking Screens. Methods Mol Biol. 2026;2984:139-152. doi: 10.1007/978-1-0716-4949-7_10. PMID: 41075090.

Dere D, Pehlivan SN, da Silva AD, de Azevedo WF Jr. Hands-On Docking with Molegro Virtual Docker. Methods Mol Biol. 2026;2984:125-138. doi: 10.1007/978-1-0716-4949-7_9. PMID: 41075089.

da Silva AD, de Azevedo WF Jr. Extremely Randomized Trees to Determine Binding Affinity. Methods Mol Biol. 2026;2984:111-123. doi: 10.1007/978-1-0716-4949-7_8. PMID: 41075088.

da Silva AD, de Azevedo WF Jr. Calculating Enzyme Inhibition with Random Forests. Methods Mol Biol. 2026;2984:97-110. doi: 10.1007/978-1-0716-4949-7_7. PMID: 41075087.

RESEARCH HIGHLIGHTS



Docking in the Dark (Roomi et al., 2025)
This review focuses on blind docking simulations.
Image Source: https://pub.mdpi-res.com/pharmaceuticals/pharmaceuticals-18-01777/article_deploy/html/images/pharmaceuticals-18-01777-ag.png?1763977668

PUBLICATIONS (CONTINUATION)

da Silva AD, de Azevedo WF Jr. Decision Tree for Prediction of Binding Affinity. Methods Mol Biol. 2026;2984:81-95. doi: 10.1007/978-1-0716-4949-7_6. PMID: 41075086.

da Silva AD, de Azevedo WF Jr. Gradient Descent to Predict Enzyme Inhibition. Methods Mol Biol. 2026;2984:65-79. doi: 10.1007/978-1-0716-4949-7_5. PMID: 41075085.

da Silva AD, de Azevedo WF Jr. Elastic Net Regression to Predict CDK2 Inhibition. Methods Mol Biol. 2026;2984:51-64. doi: 10.1007/978-1-0716-4949-7_4. PMID: 41075084.

da Silva AD, de Azevedo WF Jr. Elastic Net Regression to Predict CDK2 Inhibition. Methods Mol Biol. 2026;2984:51-64. doi: 10.1007/978-1-0716-4949-7_4. PMID: 41075084.

Pehlivan SN, da Silva AD, de Azevedo WF Jr. Combining MVD and Ridge Method to Predict CDK2 Inhibition. Methods Mol Biol. 2026;2984:35-49. doi: 10.1007/978-1-0716-4949-7_3. PMID: 41075083.

da Silva AD, Baud S, de Azevedo WF Jr. Exploring the Scoring Function Space with Lasso Regression. Methods Mol Biol. 2026;2984:19-34. doi: 10.1007/978-1-0716-4949-7_2. PMID: 41075082.

de Azevedo WF Jr, editor. Docking screens for drug discovery. 2nd ed. New York, NY: Springer; 2025. doi: 10.1007/978-1-0716-4949-7.

Roomi MS, Culletta G, Longo L, Filgueira de Azevedo W Jr, Perricone U, Tutone M. Docking in the Dark: Insights into Protein-Protein and Protein-Ligand Blind Docking. Pharmaceuticals (Basel). 2025;18(12):1777. doi: 10.3390/ph18121777. PMID: 41471265.

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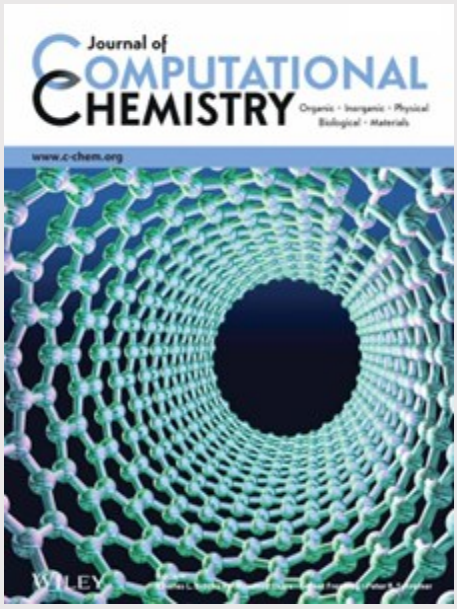

SAnDReS 2.0.0 (de Azevedo Jr et al., 2024)
This program brings together the most advanced tools for protein-ligand docking simulation and machine-learning modeling.
Code available at https://github.com/azevedolab/sandres
Image Source: https://onlinelibrary.wiley.com/cms/asset/a820fc27-aee3-4d6e-abda-076bcabe3248/jcc.v45.27.cover.gif

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Cover of the Journal of Computational Chemistry showing the mass-spring model employed by the program Taba (da Silva et al., 2022) The basic idea behind the Taba is that the determinant structural features responsible for ligand-binding affinity are already somehow imprinted in the three-dimensional structures of protein-ligand complexes.
Image Source: https://onlinelibrary.wiley.com/cms/asset/d431cd58-6058-4c32-8b80-2334ce90cb9a/jcc.v41.1.cover.gif

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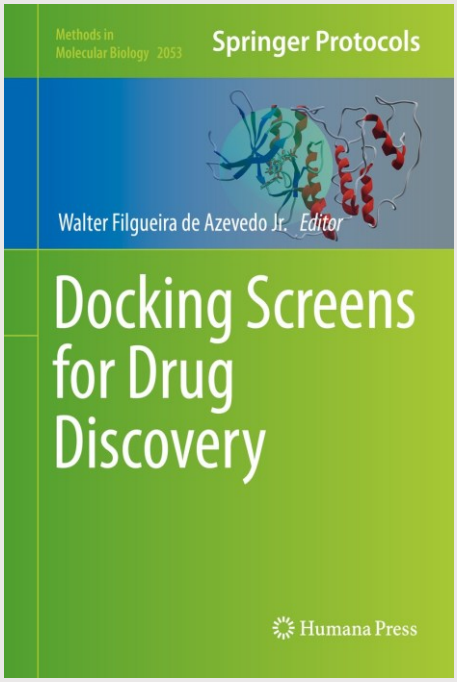

Publication of Docking Screens for Drug Discovery (26 August 2019) (de Azevedo et al., 2019)
This book focuses on recent developments in docking simulations for target proteins with chapters on specific techniques or applications for docking simulations, including the major docking programs
Image Source: https://media.springernature.com/w316/springer-static/cover/book/978-1-4939-9752-7.jpg?as=webp

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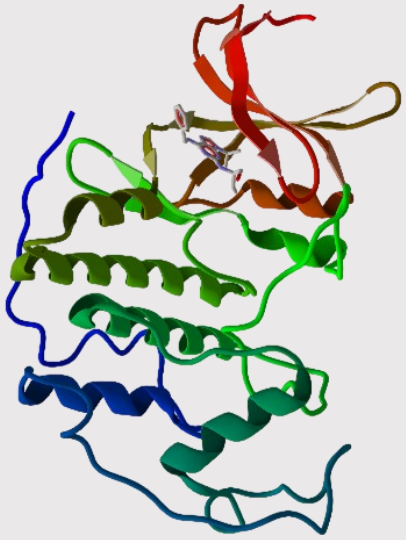
RESEARCH HIGHLIGHTS



Structure of CDK2 in complex with an inhibitor (de Azevedo, 2016)
Cyclin-dependent kinases (CDKs) comprise an important protein family for development of drugs, mostly aimed for use in treatment of cancer but there is also potential for development of drugs for neurodegenerative diseases and diabetes. Since the early 1990s, structural studies have been carried out on CDKs, in order to determine the structural basis for inhibition of this protein target.

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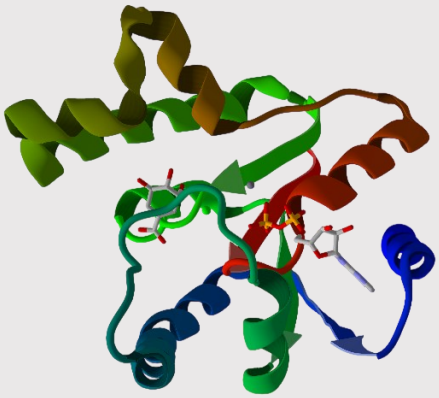

Structure of Shikimate Kinase used fo docking simulations (Vianna & de Azevedo, 2012)
Among targets identified in Mycobacterium tuberculosis genome, enzymes of the shikimate pathway deserve special attention, since they are essential to the survival of the microorganism and absent in mammals. The object of our study is shikimate kinase (SK), the fifth enzyme of this pathway.
Data Source: https://www.rcsb.org/structure/1WE2

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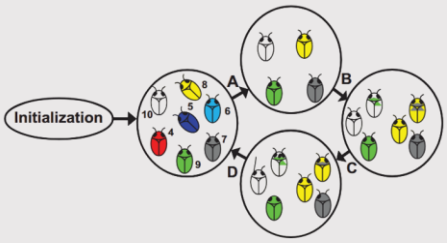

Evolutionary process of a bio-inspired algorithm (Heberlé and de Azevedo, 2011)
Initially a population with different individuals is generated (initialization). Selection (A) is then carried out, and the individuals
with the highest scores are chosen. In the next step, recombination (B) is performed followed by a step in which mutation (C) takes place. Finally, the fitness function is calculated for these new individuals (D).
Nature as a source of inspiration has been shown to have a great beneficial impact on the development of new computational methodologies. In this scenario, analyses of the interactions between a protein target and a ligand can be simulated by biologically inspired algorithms (BIAs). These algorithms mimic biological systems to create new paradigms for computation, such as neural networks, evolutionary computing, and swarm intelligence.
Source: https://www.eurekaselect.com/article/18551

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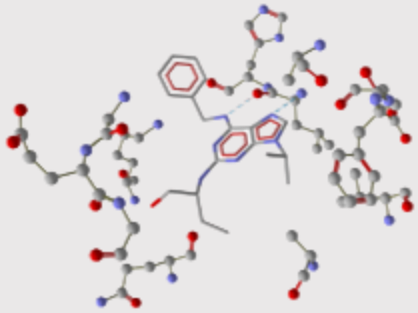
RESEARCH HIGHLIGHTS



Analysis of protein-drug interactions (de Azevedo, 2008)
One of the most interesting and important challenges in the so-called "Post- genomic Era" is the understanding of protein networks. Until the 1980s, most of our knowledge about drugs, drug mechanisms and drug receptors could fit in a few encyclopedic books and a couple dozen schematic figures. However, with the recent explosion in biological and chemical knowledge, this is no longer the case. The development of drug-binding databases plays an important role in the understanding of protein-drug interaction and is reviewed in this volume.

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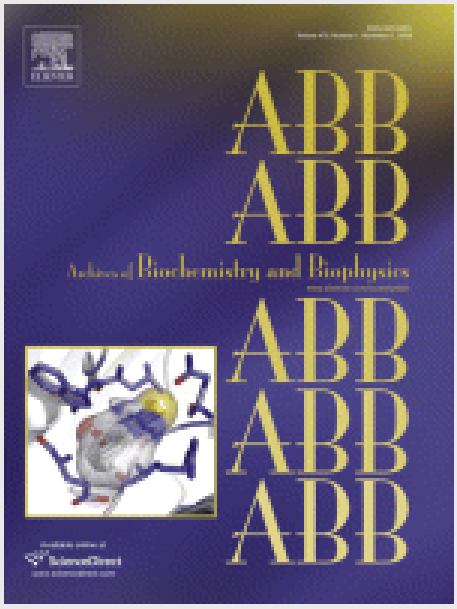

Structural studies of human purine nucleoside phosphorylase (Cover) (Timmers et al., 2008)
Human purine nucleoside phosphorylase (HsPNP) is a target for inhibitor development aiming at T-cell immune response modulation. In this work, we report the development of a new set of empirical scoring functions and its application to evaluate binding affinities and docking results. To test these new functions, we solved the structure of HsPNP and 2-mercapto-4(3H)-quinazolinone (HsPNP:MQU) binary complex at 2.7A resolution using synchrotron radiation, and used these functions to predict ligand position obtained in docking simulations.
Image Source: https://ars.els-cdn.com/content/image/1-s2.0-S0003986108X00207-cov200h.gif

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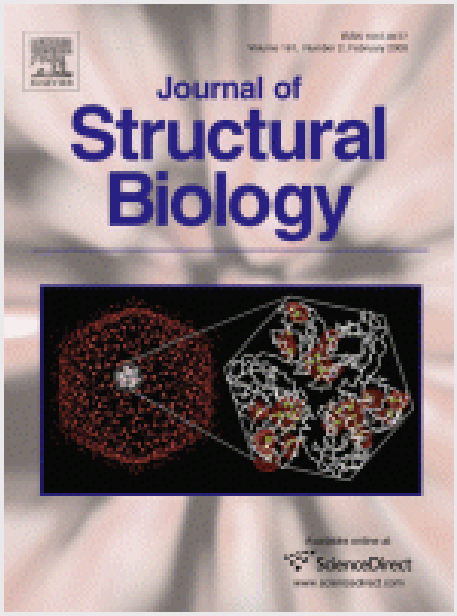
RESEARCH HIGHLIGHTS



Identification of a new quaternary association for legume lectins (Moreno et al., 2008)
The crystal structure of Lotus tetragonolobus lectin (LTA) at 2.0 Å resolution reveals a different legume lectin tetramer. Its structure consists of a homotetramer composed of two back-to-back GS4-like dimers arranged in a new mode, resulting in a novel tetramer.
Image Source: https://ars.els-cdn.com/content/image/1-s2.0-S1047847708X0156X-cov200h.gif

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RESEARCH HIGHLIGHTS

Crystallographic studies on the binding of isonicotinyl-NAD adduct to wild-type and isoniazid resistant 2-trans-enoyl-ACP (CoA) reductase (Dias et al., 2007)
To understand the mechanism of resistance to INH, we have solved the structure of two InhA mutants (I21V and S94A), identified in INH-resistant clinical isolates, and compare them to INH-sensitive WT InhA structure in complex with the INH-NAD adduct.
Image Source: https://ars.els-cdn.com/content/image/1-s2.0-S1047847707X01515-cov200h.gif

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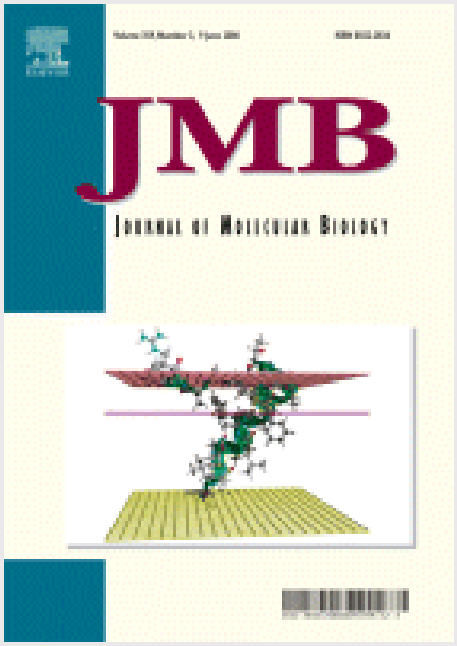

Crystallographic and pre-steady-state kinetics studies on binding of NADH to wild-type and isoniazid-resistant enoyl-ACP(CoA) reductase (Oliveira et al., 2006)
Here, in trying to identify structural changes between wild-type and INH-resistant InhA enzymes, we have solved the crystal structures of wild-type and of S94A, I47T and I21V InhA proteins in complex with NADH to resolutions of, respectively, 2.3A, 2.2A, 2.0 A, and 1.9A.
Image Source: https://ars.els-cdn.com/content/image/1-s2.0-S0022283606X2003X-cov200h.gif

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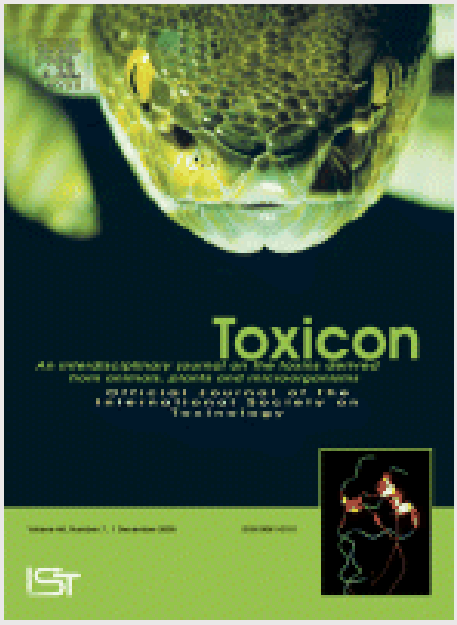

NMR structure of crotaimine (Fadel et al., 2005)
Crotamine is one of four major components of the venom of the South American rattlesnake Crotalus durissus terrificus. Similar to its counterparts in the family of the myotoxins, it induces myonecrosis of skeletal muscle cells. This paper describes a new NMR structure determination of crotamine in aqueous solution at pH 5.8 and 20 degrees C, using standard homonuclear 1H NMR spectroscopy at 900MHz and the automated structure calculation software ATNOS/CANDID/DYANA. The automatic NOESY spectral analysis included the identification of a most likely combination of the six cysteines into three disulfide bonds, i.e. Cys4-Cys36, Cys11-Cys30 and Cys18-Cys37; thereby a generally applicable new computational protocol is introduced to determine unknown disulfide bond connectivities in globular proteins.
Image Source: https://ars.els-cdn.com/content/image/1-s2.0-S0041010105X0383X-cov200h.gif

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RESEARCH HIGHLIGHTS

Parmodel (Uchôa et al., 2004)
Parmodel is a web server for automated comparative modeling and evaluation of protein structures. The aim of this tool is to help inexperienced users to perform modeling, assessment, visualization, and optimization of protein models as well as crystallographers to evaluate structures solved experimentally. It is subdivided in four modules: Parmodel Modeling, Parmodel Assessment, Parmodel Visualization, and Parmodel Optimization. The main module is the Parmodel Modeling that allows the building of several models for a same protein in a reduced time, through the distribution of modeling processes on a Beowulf cluster. Parmodel automates and integrates the main softwares used in comparative modeling as MODELLER, Whatcheck, Procheck, Raster3D, Molscript, and Gromacs.
Image Source: https://ars.els-cdn.com/content/image/X0006291X.jpg

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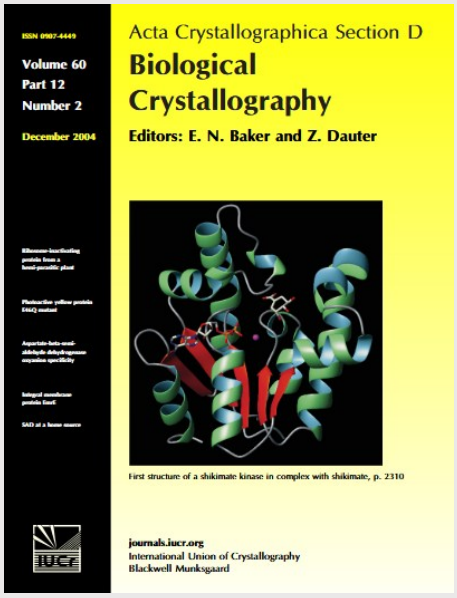
RESEARCH HIGHLIGHTS



Structure of Shikikmate Kinase (Cover) (Pereira et al., 2004)
Crystal structure of shikimate kinase from Mycobacterium tuberculosis (MtSK) complexed with MgADP and shikimic acid (shikimate) has been determined at 2.3 Å resolution, clearly revealing the amino-acid residues involved in shikimate binding. This is the first three-dimensional structure of SK complexed with shikimate. The LID domain (residues 112-124) and shikimate binding domain (SB) (residues 33-61) are responsible for large conformational changes during catalysis.
Image Source: https://journals.iucr.org/d/issues/2004/12/02/graphics/coverill.gif

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RESEARCH HIGHLIGHTS

Docking and small angle X-ray scattering studies of purine nucleoside phosphorylase (Filgueira de Azevedo W Jr et al., 2003)

Docking simulations have been used to assess protein complexes with some success. Small angle X-ray scattering (SAXS) is a well-established technique to investigate protein spatial configuration. This work describes the integration of geometric docking with SAXS to investigate the quaternary structure of recombinant human purine nucleoside phosphorylase. Image Source: https://ars.els-cdn.com/content/image/X0006291X.jpg

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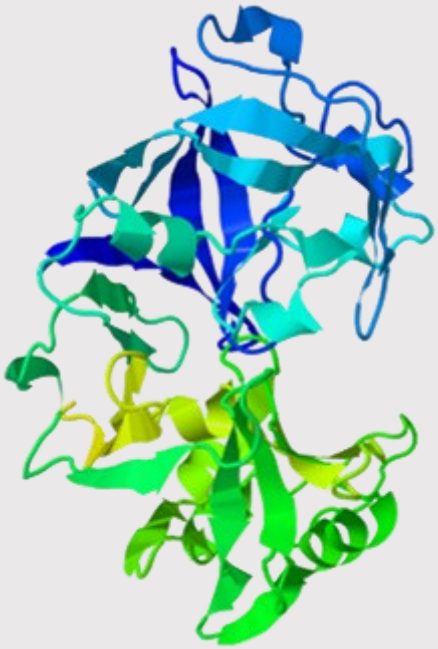

Structure of human uropepsin at 2.45 A resolution (Canduri et al., 2001)
The molecular structure of human uropepsin, an aspartic proteinase from the urine produced in the form of pepsinogen A in the gastric mucosa, has been determined by molecular replacement using human pepsin as the search model.
Data Source: https://www.rcsb.org/structure/1FLH

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Fonseca JC, Honda RT, Delatorre P, Fadel V, Bonilla-Rodriguez GO, de Azevedo WF Jr. Crystallization, preliminary X-ray analysis and molecular-replacement solution of haemoglobin-II from the fish matrinxã (Brycon cephalus). Acta Crystallogr D Biol Crystallogr. 2003;59(Pt 4):752-754. doi: 10.1107/s0907444903003408. PMID: 12657802.

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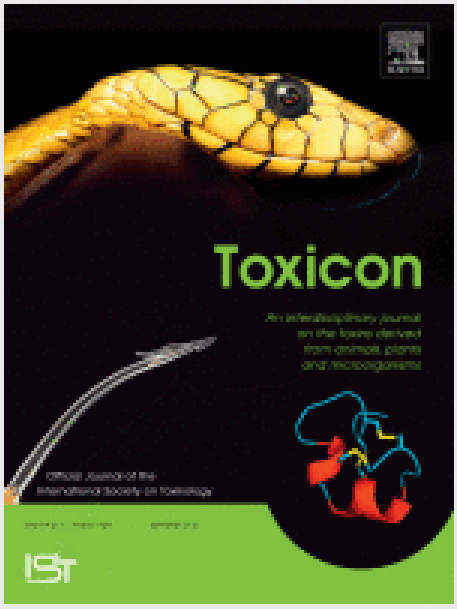

Structure of phospholipase A2 (de Azevedo et al., 1999)
Lys49-Phospholipase A2 (Lys49-PLA2) homologues damage membranes by a Ca^{2+}-independent mechanism which does not involve catalytic activity. We have solved the structure of myotoxin-I, a Lys49-PLA2 homologue isolated from the venom of Bothrops nummifer (jumping viper) at 2.4 Å resolution using molecular replacement techniques.
Image Source: https://ars.els-cdn.com/content/image/1-s2.0-S0041010126X20025-cov150h.gif

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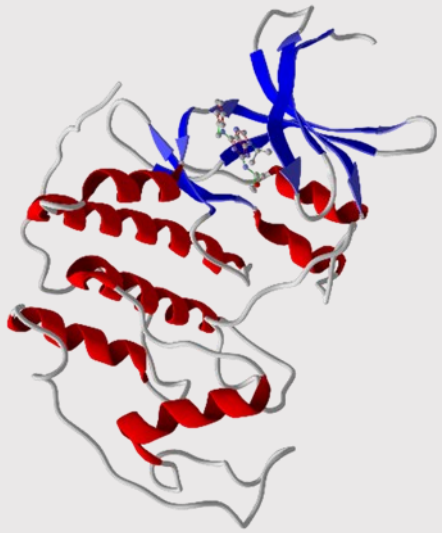
RESEARCH HIGHLIGHTS



Crystal structure of human cdk2 complexed with roscovitine (de Azevedo et al., 1997)
The structure cdk2-roscovitine reveals that the (R)-stereoisomer of roscovitine is bound to cdk2. The (R)isomer is about twice as potent in inhibiting cdc2/cyclin B than the (S)-isomer. Results from structure/activity studies and from analysis of the cdk2/roscovitine complex crystal structure should allow the design of even more potent cdk inhibitors.
Data Source: https://www.rcsb.org/structure/2A4L

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