Demetres Leonidas

[Google Scholar Profile]

Personal Data

Name & Surname: Demetres D. Leonidas

Address: Department of Biochemistry & Biotechnology, University of Thessaly, Biopolis, Larissa 41500, Greece, Tel. +302410 565278, email: ddleonidas@bio.uth.gr

Date and Place of Birth: 25 November 1964, Athens

Nationality: Greek

Education

1992: Ph.D., Department of Biology, National and Kapodistrian University of Athens, Greece (Performed at the Institute of Biological Research & Biotechnology, National Hellenic Research Foundation). Title: "*Allosteric and catalytic mechanism of glycogen phosphorylase: kinetic and crystallographic studies on the R (active) conformation of the enzyme*"

1987: B.Sc. in Chemistry, Department of Chemistry, Aristotelian University of Thessaloniki, Greece.

Professional Experience

Since 20/12/2016	**Professor of Biochemistry**, Department of Biochemistry and Biotechnology, University of Thessaly
10/2009-19/12/2016	**Associate Professor of Biochemistry**, Department of Biochemistry and Biotechnology, University of Thessaly
3/2007-9/2009	**Senior Researcher**, Institute of Organic and Pharmaceutical Chemistry, National Hellenic Research Foundation.
7/2003 – 2/2007	**Researcher**, Institute of Organic and Pharmaceutical Chemistry, National Hellenic Research Foundation.
5/2000 – 6/2003	**Junior Researcher**, Institute of Biological Research and Biotechnology, National Hellenic Research Foundation.
7/1999 – 4/2000	**Researcher**, Institute of Biology, NCSR "Demokritos".
10/1993 – 9/1995	**Researcher**, Department of Biology and Biochemistry, University of Bath, U.K.
10/1995 – 6/1996	**Researcher,** Division of Infectious Diseases, Department of Medicine, Harvard Medical School, U.S.A.
7/1996 – 6/1999	**Researcher,** Department of Biology and Biochemistry, University of Bath, U.K.

Scholarships - Awards

1995 Beth Israel Hospital and Harvard Medical School Research Fellow in Medicine, Division of Infectious Diseases, Department of Medicine, Boston, U.S.A.

1992 1st Prize for PhD Thesis, "Leonidas Zervas" Foundation

1992 (3μήνες) EMBO Predoctoral Fellowship for work in the Laboratory of Molecular Biophysics, University of Oxford, U.K

1992 (3μήνες) Royal Society U.K., Predoctoral Fellowship for work in the Laboratory of Molecular Biophysics, University of Oxford, U.K.

1988 - 1992 PhD Fellowship, National Hellenic Research Foundation.

Research Specialization

- Biochemistry, Enzymology, Protein Chemistry
- Allosterism, Structure Function relationship
- Structural Biochemistry
- X-ray crystallography of biomolecules
- Structure guided drug design

Administration Experience

2024 – today: President of The Regional Council for Research and Innovation of Thessaly

2009 – today: Member of the General Assembly of the Department of Biochemistry and Biotechnology, University of Thessaly

2012 - 2016: Elected Chair of the Department of Biochemistry and Biotechnology, University of Thessaly (Rector's Acts 3122/5-4-2013 and 10338/10-7-2014

2012–today: Member of the Academic Development and Planning Committee of The Department of Biochemistry and Biotechnology, University of Thessaly 2012 - 2014: Member of the Senate of the University of Thessaly.

2012 - 2016: Member of the Deanery of the School of Health Sciences, University of Thessaly.

2015 - today: Director of the Structural and Functional Biochemistry Laboratory

2015 - today: Director of the Inter-Institutional Postgraduate Program "Bioentrepreneurship"

2015: Member of the Thematic Groups of Priorities 1 (Agro-Dietary Complex) and 8 (Horizontal Activities of Institutional Strengthening of the Regional Planning System) of the Strategic Smart Specialization of the Region of Thessaly (Regional Governor's Act 315/15-12-2015).

Academic Teaching

1. Lecturing

1.1. Undergraduate courses of the 1st semester "Basic Principles of Biochemistry", 2nd semester "Biochemistry of proteins and nucleic acids" and the optional courses "Structural Biochemistry" and "From science to business-Innovation and entrepreneurship in biotechnology" at the Department of Biochemistry and Biotechnology.

1.2. Postgraduate course "Biochemistry of nutrition" at the postgraduate program «Biotechnology – Quality assessment in nutrition and the environment" of the Department of Biochemistry and Biotechnology

1.3. Postgraduate course "Methods of Biomolecular Analysis" at the postgraduate program «Advanced Experimental & Computational Biosciences" of the Department of Biochemistry and Biotechnology

1.4. Postgraduate course Basic and advanced methods for the analysis of biomolecules" at the postgraduate program «Biotechnology «Molecular Biology and Genetics Applications" of the Department of Biochemistry and Biotechnology.

1.5. Postgraduate course "Drugs and Health" at the postgraduate program «Bioentrepreneurship" of the Department of Biochemistry and Biotechnology.

2. PhD Theses Supervision

2.1. Anastasia Tsagkarakou (2023) Structural basis of carbohydrate recognition by human galectins, Department of Biochemistry & Biotechnology, University of Thessaly.

2.2. Symeon Koulas (2023) Structural and functional studies on alpha-glucan phosphorylases, Department of Biochemistry & Biotechnology, University of Thessaly.

2.3. Aikaterini Karageorgou (2023). Study of new autoantibodies as biomarkers of autoimmune neurological diseases, Department of Biochemistry & Biotechnology, University of Thessaly.

2.4. Olga Papaioannou (2022). The function of human angiogenin in angiogenesis, Department of Biochemistry & Biotechnology, University of Thessaly.

2.5. Theodora Solovou (2022). Biochemical studies on *Lotus japonicus* gsk3β-like kinase ljsk1, Department of Biochemistry & Biotechnology, University of Thessaly.

2.6. Efthimios Kyriakis (2020) Biochemical Studies on glycogen metabolism, Department of Biochemistry & Biotechnology, University of Thessaly. Currently in Faculty of Medicine Department of Anesthesiology, The University of British Columbia, Vancouver Canada

2.7. George Stravodimos (2018) Biochemical studies of glycogen metabolism enzymes, Department of Biochemistry & Biotechnology, University of Thessaly.

2.8. Demetra Chatzileontiadou (2016) Biochemical studies on human angiogenin. Department of Biochemistry & Biotechnology, University of Thessaly. Currently Adjunct research associate, Monash University, La Trobe Institute for Molecular Science, La Trobe University, Victoria, Australia

2.9. Anastasia Kantsadi (2015) Glycogen phosphorylase as molecular target for the design of new anti-hypergycaemic drugs. Department of Biochemistry & Biotechnology, University of Thessaly. Currently at Department of Biochemistry, University of Oxford, Oxford, U.K.

2.10. Zoi Karoulia (2011) Structural and functional studies of the von willebrand factor and its role in the individual reactions of haemostasis. Department of Biochemistry & Biotechnology, University of Thessaly. Currently at Department of Oncological Sciences and Department of Dermatology, The Tisch Cancer Institute, Icahn School of Medicine at Mount Sinai, New York, USA.

2.11. Kyriaki Melinda Alexacou (2010) Kinetic and X-ray crystallographic studies of glycogen phosphorylase. On the way to structure based drug design for diabetes type 2. Free University of Berlin, Germany

3. Member of Advisory Committee of completed PhD Theses (6 other in progress)

3.1. Theochari Ioanna (2020) Development of nanodispersions as carriers for bioactive compounds and their biological applications Department of Biochemistry & Biotechnology, University of Thessaly.

3.2. Moros Georgios (2020) Finding biomarkers related to Intrauterine Growth Restriction with metabolomics. Department of Biochemistry & Biotechnology, University of Thessaly.

3.3. Michou Myrsini (2020) Development of optimized bacterial strains for recombinant production of prokaryotic and eukaryotic integral membrane proteins. Department of Biochemistry & Biotechnology, University of Thessaly.

3.4. Gorgogietas Vyronas (2018) Role of steroid hormone receptors in the regulation of cellular pathophysiology. Department of Biochemistry & Biotechnology, University of Thessaly.

3.5. Parmenopoulou Vanessa (2016). Synthesis of novel pyranozylamide and furanosylnucleoside inhibitors of glycogen phosphorylase and ribonucleases as potential antidiabetic and antitumor agents. Department of Biochemistry & Biotechnology, University of Thessaly.

4. Member of the Examination Committee of PhD Theses abroad

4.1. Rachel T. Mathomes (2022), Combined in silico docking, enzyme kinetics, X-ray crystallography and glioblastoma cellular studies of baicalein acting as a glycogen phosphorylase inhibitor. School of Pharmacy & Biomedical Sciences, University of Central Lancashire, Preston, United Kingdom

4.2. Guillem Prats Ejarque (2020), Exploring the pharmacological properties of human antimicrobial ribonucleases. Department of Biochemistry and Molecular Biology, Autonomous University of Barcelona, Barcelona, Spain.

4.3. Vandna Sharma (2018), Studies on fibrillation of human γD-crystallin and its inhibition by using small molecules and nanoparticles. Department of Chemistry, National Institute of Technology Hamirpur, Himachal Pradesh, India

4.4. Priyanka Chauhan (2018), Shiff βases and φlavonoids as ınhibitors of ηuman γD-crystallin αggregation and their interactions with human α-crystallin: an approach to impede ψataract. Chemistry Department, NIT, Hamirpur (HP), India.

4.5. Javier Arranz Trullın (2016), Unveiling the multifaceted antimicrobial mechanism of action of human host defence RNases. Department of Biochemistry and Molecular Biology, Autonomous University of Barcelona, Barcelona, Spain.

4.6. Vassiliki Tsirkoni (2016), Tansportin-SR2, de nucleaire import factor van HIV-1 integrase. KU Leuven, Biomedical Sciences Group, Faculty of Pharmaceutical Sciences, Belgium.

5. Supervision of 38 MSc Theses

6. Supervision of 52 Diploma Projects

Editor

1. Principals of Biophysical Chemistry, K.E. van Holde, W.C. Johnson, P.S. Ho. Chapters 7 (Macromolecule Scattering) and 16 (Single molecule Methods). Embrio Publications, 2010.
2. Basic Elements of Enzymology N.C. Price & L. Stevens. Greek version, Parisianou press 2015
3. Biochemistry, R.S. Ochs. Greek version, Parisianou press 2015
4. Laboratory guide for Structural and Functional analysis of biomolecules, University of Thessaly press, 2010
5. Laboratory guide for Metabolism, University of Thessaly press, 2014
6. Biochemistry Basic Principles, Tymoczko J., Berg J., Stryer L. Chapter 30 (Aminoacid metabolism and the urea cycle) Broken Hills Publications 2018.
7. Lehninger's Basic Principals of Biochemistry, Chapter 15 (Metabolic regulation) Broken Hills Publications 2018.
8. Bioprocess Engineering Principles, P. M. Doran, Broken Hills Publications 2019.

Research Projects

My current research activities are mainly focused in understanding the action of, (1) ribonucleases of the pancreatic ribonuclease A family, (2) enzymes involved in glycogen metabolism and (3) lectins involved in carbohydrate and cell-cell interaction.

Specific projects are:

Ribonucleases in pathological conditions

The project includes kinetic, biochemical, biological and crystallographic experiments as well as modeling studies using molecular dynamics and electrostatic analysis to determine the factors that determine the molecular recognition of ribonuclease inhibitors, pancreatic ribonuclease A (RNase A), human angiogenin (hAng), eosinophil derived neurotoxin (EDN), eosinophilic cationic protein (ECP), and bovine seminal ribonuclease (BS-RNase). The analysis of the factors that govern small molecule binding to ribonucleases, at the molecular level, offers the means to control their enzymatic activity and lead to the development of new specific pharmaceutical agents with anti-angiogenic, anti-inflammatory and tumor suppressant potential. To date, we have studied the binding of approximately 50 inhibitors to RNase A (an inhibitor complex shown in Figure 1), hAng, BS-RNase and EDN with significant bioactivity, *in vitro* and *in vivo*.

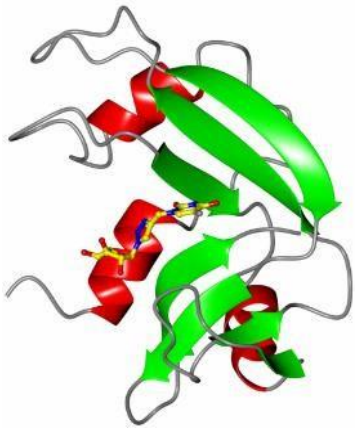

Figure 11

Active collaborations:

- Prof. G. Spyroulias, Department of Pharmacy, University of Patras, Greece.
- Prof. E. Boix, Dept. of Biochemistry and Molecular Biology, Autonomous University of Barcelona, Barcelona, Spain.

Discovery of glycogen metabolism enzyme inhbitors for the development of novel antihyperglycaemic agents.

The project focuses on the discovery of new compounds for the treatment of type 2 diabetes. Type 2 diabetes mainly affects adults and is characterized by inability to regulate glucose levels and insulin resistance. It is the most common form of diabetes and affects 90-95% of cases. The project's objectives are to understand the molecular basis for the recognition of small organic molecules by the enzymes involved in glycogen metabolism. The macromolecular targets studied are hepatic glycogen phosphorylase (GP, EC 2.4.1.1), phosphorylase kinase (PhK, EC 2.7.1.38) and glycogen degradation enzyme (GDE, EC 2.4.1.25). These targets play a central regulatory role in the metabolic pathways of glycogenolysis.

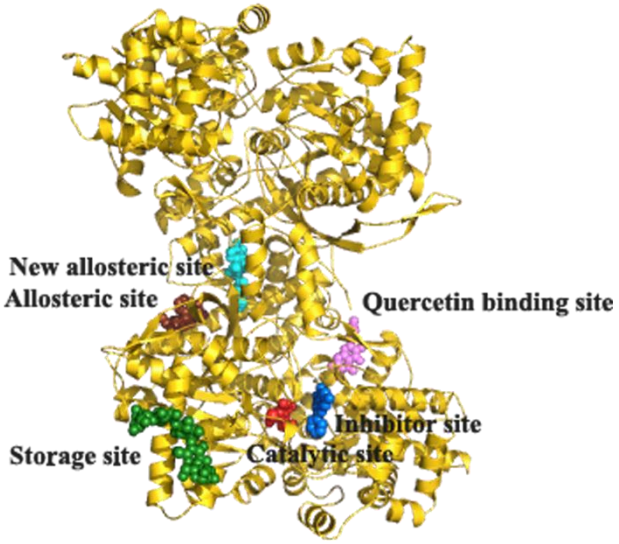

Figure 2

GP is considered an enzyme with a central role in the catabolism of glycogen and is responsible for the production of glucose in the blood (glycogenolysis).

The enzyme catalyzes the first stage of intracellular degradation of glycogen to glucose 1-phosphate (Glc-1-P). Detailed analysis of the factors that determine the binding of micromolecular compounds (inhibitors) to the GP at the molecular level, provides the possibility of controlling its enzymatic activity or the unwanted degradation of glycogen, in type 2 diabetes, where hyperglycemia is a serious medical problem. We have studied by kinetic, spectroscopic, ultracentrifugal and crystallographic methods the binding of more than 300 compounds to glycogen phosphorylase. Several of these compounds have significant antihyperglycemic activity both *in vivo* in hepatocytes and diabetic mice. In addition, our studies led to the discovery of a new allosteric center in the enzyme, the quercetin binding center (Figure 2). PhK also plays an important role in glycogen

metabolism and is a target for the development of antidiabetic drugs. PhK catalyzes the phosphorylation of a single serine (Ser14) of GPb, converting it to active form (GPa) (via allosteric transition). It is the first protein kinase to be discovered and the only known kinase that activates GPb. The enzyme, one of the most complex protein kinases, has a molecular weight of 1.3 kDa and a hexahedron stoichiometry. Four different subunits form tetramers of formula (αβγδ)4. Although its structure has been determined by electron microscopy (EM), the localization of the various subunits in the structure has not been achieved. The aim of the research project is to elucidate its structure with EM techniques and to understand the mechanism of regulation of PhK action by subunits α and β. Attempts are also made to determine the structure of subunits α and β both individually and their complex by X-ray crystallography or molecular modeling methods. Finally, the research work focuses on the determination of the three-dimensional structure of the γ-PhK catalytic subunit in complexes with commercially available kinase inhibitors, such as stavosporine, but also with compounds obtained by computational screening of libraries of imidazole and indole derivatives. Glycogen degradation enzyme (GDE) is a dual-function enzyme. It has a transfer function (oligo-1,4 → 1,4-glucotransferase, EC 2.4.1.25) and glucosidase (amyl-1,6-glucosidase, EC 3.2.1.33). Both enzymes are located in a peptide chain and each of the activities has its own separate catalytic center. GDE is a key enzyme in carbohydrate metabolism in mammals and yeast. GDE together with GP ensures the complete degradation of glycogen and the production of glucose and glucose 1-phosphate. Genetic deficiency of the enzyme in humans causes type III glycogen storage disease (GSD-III or Cori disease) which is characterized by hepatomegaly, hypoglycemia, variable myopathy and cardiomyopathy. GDE inhibitors provide the ability to control its enzymatic activity and the undesired degradation of glycogen in type 2 diabetes mellitus. In the research project we examine the action of various inhibitors by kinetic and crystallographic methods in GDE. To date we have tested 10 GP inhibitors in GDE and the first results show that some inhibitors show significant bioactivity in both enzymes (GP and GDE).

Active Collaborations:

- Dr J.M. Hayes, School of Physical Sciences & Computing, University of Central Lancashire, U.K.
- Prof. László Somsák, Dept. of Organic Chemistry, University of Debrecen.
- Prof. R. Riedl, Institute for Chemistry and Biological Chemistry, Zurich University of Applied Sciences, Zurich, Switzerland.
- Dr S.E. Zographos, Institute of Chemical Biology, National Hellenic Research Foundation.

Molecular recognition of carbohydrates by lectins and human galectins

The aim of this project is to investigate the structure - function relationship and specialization of lectins and galectins. Lectins are proteins found in almost all prokaryotic and eukaryotic organisms and bind sugars, which are either free or bound to the cell surface, with excellent selectivity. Cell surface glycosylation patterns are characteristic of the cancer phenotype and several lectins have a high selectivity for binding to glycosides in neoplastic over healthy tissues. Of particular interest are lectins that are highly specific for saccharides that specifically express cancer cells such as the TF antigen (Galß1GalNAc-□-), as they have the potential to be used as cancer markers to detect tumors at an early stage. As part of the research project, biochemical studies of lectins SRL, ACL, AFL, AML and RSA are carried out, while the structures of SRL and RSA have also been determined (Figure 3).

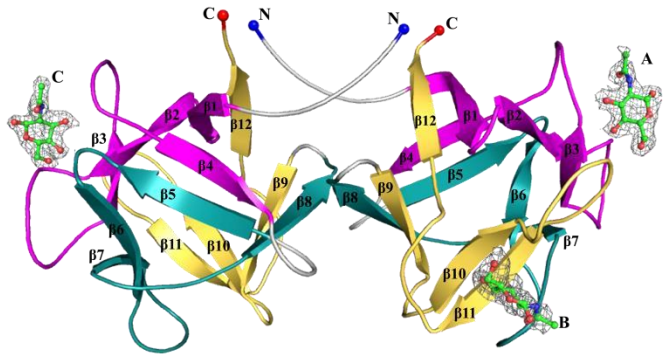

Figure 3

Galectins are a family of proteins that bind β-galactosides. Despite their high homology each galectin exhibits a different affinity for saccharides. In the last decade, a wide range of studies have highlighted the role of human galectins in many biological and pathological processes making them the drug targets for a variety of diseases. The development of competitors specific for each galectin through comparative structural analysis and elucidation of the relationship between the structure and action of the binding of each inhibitor to different human galectins (1, 3, 4, 7, 8, 9 and 10) is a major goal of this project. The structures of Galectin-7 and Galectin-10 were also determined. In the framework of this project I participate in the Consortium for Functional Glycomics (CFG), which is funded by The National Institute of General Medical Sciences (NIGMS) U.S.A.

Active Collaborations:

- Prof. H. Leffler, Department of Laboratory Medicine, Section MIG, Lund University, Lund, Sweden.
- Prof. U.J. Nilson, Department of Chemistry, Lund University, Lund, Sweden.

Research Grants (2020 – today)

1. Program:	**Strengthening of National Research Infrastructures**
Funding	Hellenic Ministry of Development
Title:	Synthetic Biology: From omics technologies to genomic engineering (OMIC-ENGINE)
Position:	Leader of the Thessaly hub
Duration:	2017 – 2020
Budget:	1,870,000 € for the Thessaly hub
2. Program:	**Proprietary Research**
Funding	Unichem Laboratories Ltd
Title:	Structure determination of protein-carbohydrate complex
Position:	Coordinator
Duration:	2018
Budget:	10,000 €
3. Program:	Operational Programme «Human Resources Development, Education and Lifelong Learning 2014-2020"
Funding:	Hellenic Ministry of Development
Title:	GLYDESIGN – Structure guided design of glycogenolysis modulators for the development of new therapeutic agents
Position:	Coordinator
Duration:	2020-2021
Budget:	45.545 €
4. Program:	**Strengthening of National Research Infrastructures**
Funding	Hellenic Ministry of Development
Title:	INSPIRED-THESSALY - The National Research Infrastructures on Integrated Structural Biology, Drug Screening Efforts and Drug Target Functional Characterization.
Position:	Coordinator
Duration.:	2018-2021
Budget:	140.000 €
5. Program:	**Research Projects to support Postdoctoral Researchers 2nd call**
Funding:	Hellenic Foundation for Research and Innovation (HFRI)
Title:	Odorant Degrading Enzymes as molecular targets for controlling the olive fruit fly's behavior (ODEsOFF) Postdoctoral Researcher C. Drakou
Position:	Supervisor
Duration.:	2020-2023

Budget:	170.000 €
6. Program:	**Research Projects to support Postdoctoral Researchers 3rd call**
Funding:	Hellenic Foundation for Research and Innovation (HFRI)
Title:	Development of new generation antimalarial drugs to protect the infection of human erythrocytes (DeMaND) Postdoctoral Researcher A. Kantsadi
Position:	Supervisor
Duration:	2022-2024
Budget:	120.000 €
7. Program:	**HU-RIZON international research excellence cooperation programme**
Funding:	National Hungarian Research, Development and Innovation Office
Title:	New galectin inhibitor scaffolds - design, synthesis and investigation by biochemical and biophysical methods
Position:	Partner
Duration:	2025-2028
Budget:	100.000 €

Other Scientific Activities

Member of the Board (2003-2012, 2014-2016) and Vice-President (2014-2016) of the Hellenic Crystallographic Association

Member of the Association of Greek Chemists, Hellenic Society of Biochemistry and Molecular Biology, British Association of Crystallography.

Program Evaluator: The Medical Research Council, U.K., Hellenic Ministry of Development, General Secretariat of Research and Technology, National State Scholarship Foundation, ., i-Next EU (Access to large research infrastructures), FWO Research Foundation – Flanders, Belgium (2019 – today, member of the Medical and Pharmaceutical Sciences committee).

Reviewer for: Acta Crystallographica Section D, Acta Crystallographica Section F, Advances in Pharmacological Sciences, African Journal of Biotechnology, Amino Acids, Austin Journal of Pharmacology and Therapeutics, Biochimie, Bioorganic and Medicinal Chemistry, Bioorganic and Medicinal Chemistry Letters, Biophysical Chemistry, Chemical Biology & Drug Design, Chemistry and Physics of Lipids, ChemMedChem, Diabetes Metabolic Syndrome and Obesity Targets and Therapy, European Journal of Medicinal Chemistry, European Journal of Pharmaceutical Sciences, Expert Opinion On Therapeutic Patents, FEBS Letters, Food and Chemical Toxicology, Glycobiology, International Journal of Biological Macromolecules, International Journal of Bioorganic Chemistry & Molecular Biology, International Journal of Molecular Sciences, ISRN Structural Biology, Journal of the American Chemical Society, Journal of Molecular Biology, Journal of Functional Food, Journal of Molecular Graphics and Modelling, Medicinal Chemistry Communications, Medicinal Research Reviews, Mini-Reviews in Medicinal Chemistry, Molecules, Nature Communications, Nutrients, Proceedings of the National Academy of Sciences (USA),Protein & Peptide Letters, PROTEINS: Structure, Function, and Bioinformatics, Studies

in Natural Products Chemistry (Bioactive Natural Products), The FEBS Journal, The Scientific World Journal, World Journal of Microbiology, etc.

Registered user of Synchrotron radiation at EMBL-DESY (Hamburg, Germany), Elletra (Trieste, Italy), European Synchrotron Radiation Facility (ESRF, Grenoble, France), Diamond Light Source (Oxford, U.K).

Vice-President of Scientific and Organizing Committee of the 69th Panhellenic Conference of the Hellenic Society of Biochemistry and Molecular Biology, 23-25 November, 2018

Associated Editor: International Journal of Bioorganic Chemistry & Molecular Biology (IJBCMB), Frontiers in Chemistry.

Publications

Number of publication	126
Number of citations (Scopus/ Google Scholar)	3953/4793
h index (Scopus/ Google Scholar)	35/38
Number of depositions in the Protein Data Bank (PDB)	241
https://orcid.org/0000-0002-3874-2523	
Google Scholar	

1. *Expression, purification, and biophysical analysis of a part of the C-terminal domain of human hypoxia inducible factor-2α (HIF-2α).* Diseri, K., Stravodimos, G., Argyriou, A., Spyroulias, G.A., Leonidas, D.D. Liakos, P. **(2024)**, **Biochem. Biophys. Res. Commun. 739**, 150965.
2. *Kinetic and Structural Studies of the Plastidial Solanum tuberosum Phosphorylase.* Koulas, S.M., Kyriakis, E., Tsagkarakou, A.S., Leonidas, D.D. **(2024) ACS Omega, 9,** 41841-41854.
3. *Evidence for the Quercetin Binding Site of Glycogen Phosphorylase as a Target for Liver-Isoform-Selective Inhibitors against Glioblastoma: Investigation of Flavanols Epigallocatechin Gallate and Epigallocatechin.* Alexopoulos, S., McGawley, M., Mathews, R., Papakostopoulou, S., Koulas, S., Leonidas, D.D., Zwain, T., Hayes, J.M., Skamnaki, V. **(2024) J. Agric. Food. Chem., 72**, 24070-24081.
4. *Silver ciprofloxacin (CIPAG): a multitargeted metallodrug in the development of breast cancer therapy.* Banti, C.N., Kalousi, F.D., Psarra, A.G., Moushi, E.E., Leonidas, D.D., Hadjikakou, S.K. (**2024) J. Biol. Inorg. Chem., 29**, 177-186.
5. *Biochemical and Structural Studies of LjSK1, a Lotus japonicus GSK3beta/SHAGGY-like Kinase, Reveal Its Functional Role.* Solovou, T.G.A., Stravodimos, G., Papadopoulos, G.E.,

Skamnaki, V.T., Papadopoulou, K.K., Leonidas, D.D. **(2024) J. Agric. Food. Chem.**, **72**, 3763-3772.

6. *The structure of AgamOBP5 in complex with the natural insect repellents Carvacrol and Thymol: Crystallographic, fluorescence and thermodynamic binding studies.* Liggri, P.G.V., Tsitsanou, K.E., Stamati, E.C.V., Saitta, F., Drakou, C.E., Leonidas, D.D., Fessas, D., Zographos, S.E. (**2023**) **Int. J. Biol. Macromol., 237**, 124009
7. *Structural and Biochemical Characterization of the Human Angiogenin-Proliferating Cell Nuclear Antigen Interaction.* Papaioannou, O. S. E., A. C. Tsika, M. Rovoli, Papadopoulos, G. E., Kontopidis, G., Spyroulias, G.A., Leonidas, D.D. (**2023) Biochemistry 62**, 1706-1715.
8. *Multidisciplinary docking, kinetics, and X-ray crystallography studies of baicalein acting as a glycogen phosphorylase inhibitor and determination of its' potential against glioblastoma in cellular models.* Mathomes, R. T., Koulas, S. M., Tsialtas, I., Stravodimos, G., Welsby, P. J., Psarra, A. G., Stasik, I., Leonidas, D.D. Hayes, J.M. (**2023**) **Chem. Biol. Interact. 382**, 110568.
9. *Strong Binding of C-Glycosylic1,2-Thiodisaccharides to Galectin-3 horizontal line Enthalpy-Driven Affinity Enhancement by Water-Mediated Hydrogen Bonds.* Lazar, L., Tsagkarakou, A.S., Stravodimos, G., Kontopidis,G., Leffler, H., Nilsson, U.J., Somsak, L., Leonidas, D.D. (**2023**) **J. Med. Chem. 66**, 12420-12431.
10. *The druggability of the ATP binding site of glycogen phosphorylase kinase probed by coumarin analogues.* Alexopoulos, S., Gkouskou, A., Stravodimos, G., Tsagkarakou, A. S., Tsialtas, I., Katounis, D., Psarra, A.-M. G., Leonidas, D., Brahmachari, G., Hayes, J. M. and Skamnaki, V. **(2022) Current Research in Chemical Biology 2**, 100022.
11. *Biochemical and in silico identification of the active site and the catalytic mechanism of the circadian deadenylase HESPERIN.* Beta R.A.A., Kyritsis, A., Douka, V., Papanastasi, E., Rizouli, M., Leonidas, D.D., Vlachakis, D., Balatsos, N.A.A. **(2022) FEBS Open Bio** 12(5), 1036–1049.
12. *Structure activity relationship of the binding of p-coumaroyl glucose to glycogen phosphorylase and its effect on hepatic cell metabolic pathways.* Tsagkarakou, A.S., Chasapi, S.A. Koulas, S.M., Tsialtas, I. Kyriakis, E., Drakou, C.E., Kun, S., Somsak, L., Spyroulias, G.A., Psarra, A.-M. G, and Leonidas, D.D. **(2021) Eur. J. Med. Chem. Rep. 3**, 100011.
13. *Glycogen phosphorylase revisited: Extending the resolution of the R- And T-state structures of the free enzyme and in complex with allosteric activators.* Leonidas, D.D., Zographos, S.E.,

Tsitsanou, K.E., Skamnaki, V.T, Stravodimos, G., Kyriakis, E. (**2021) Acta Crystallogr. F, 77,** 303-311.

14. *Anti-apoptotic and antioxidant activities of the mitochondrial estrogen receptor beta in n2a neuroblastoma cells.* Tsialtas, I., Georgantopoulos, A., Karipidou, M.E., Kalousi, F.D., Karra, A.G., Leonidas, D.D., Psarra, A.-M.G. **(2021) Int. J. Mol. Sci. 22**(14), 7620.
15. *Mutagenesis of a Lotus japonicus GSK3β/Shaggy-like kinase reveals functionally conserved regulatory residues.* Solovou, T.G.A., Garagounis, C., Kyriakis, E., Papadopoulou, K.K., Leonidas, D.D. **(2021) Phytochemistry 186,** 112707.
16. *Nicotinic cholinergic system and COVID-19: In silico evaluation of nicotinic acetylcholine receptor agonists as potential therapeutic interventions.* Alexandris, N., Lagoumintzis, G., Chasapis, C.T., Leonidas, D.D., Papadopoulos, G.E., Tzartos, S.J., Tsatsakis, A., Eliopoulos, E., Poulas, K., Farsalinos, K. **(2021) Toxicology Reports 8**, 73-83.
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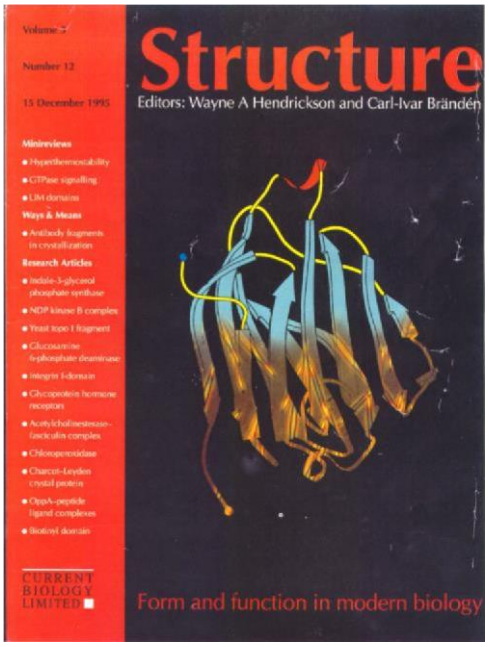

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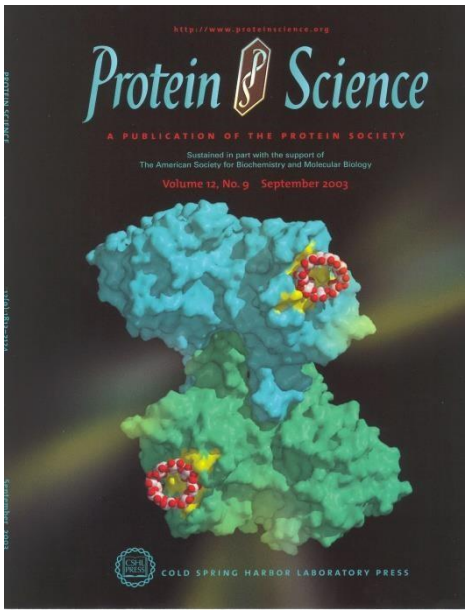

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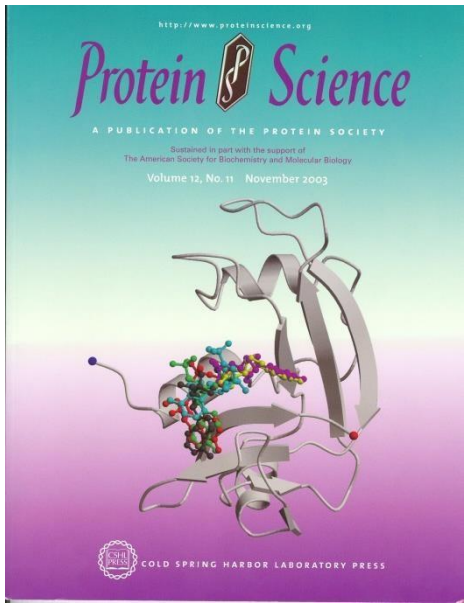

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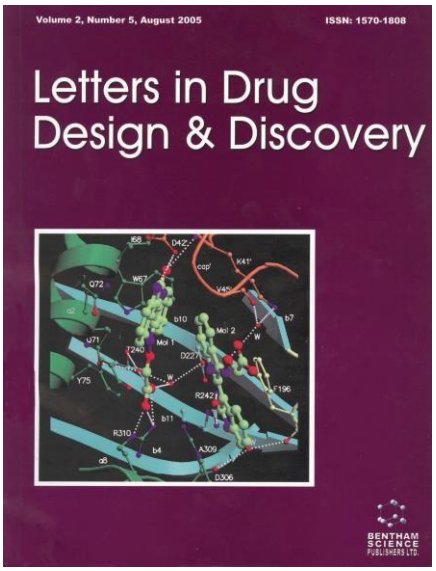

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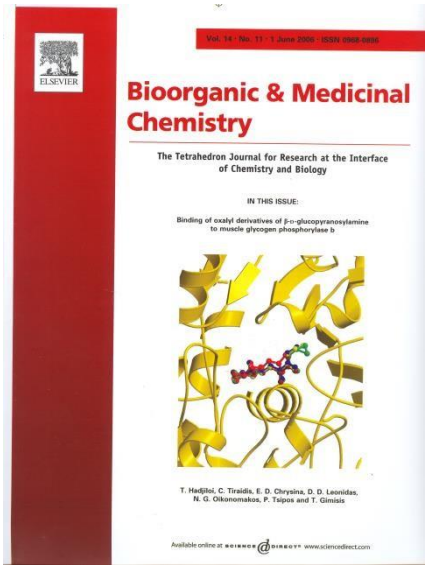

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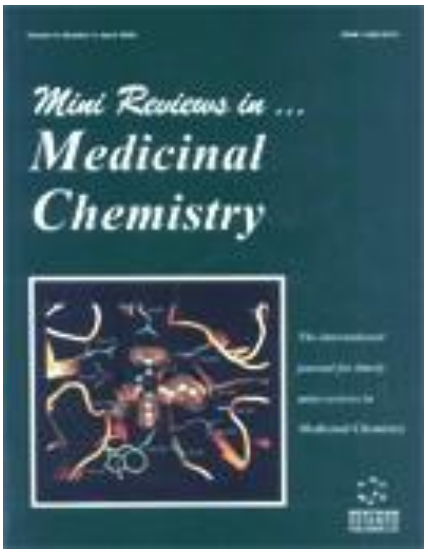

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