Curriculum Vitae

Demetres D. Leonidas

Department of Biochemistry and Biotechnology
University of Thessaly

Larissa, November 2019

PERSONAL DATA

Name: Demetres D. Leonidas

Address: Department of Biochemistry and Biotechnology, University of Thessaly, Biopolis, 41500, Larissa, Greece. Tel. +30 2410 565278, Fax. +30 2410 565290, email: ddleonidas@bio.uth.gr

Date and Place of Birth: 25 November 1964, Athens, Greece

Nationality: Hellenic

EDUCATION

1992: Ph.D. Thessis, 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 CAREER

20/12/2016-today	**Professor of Biochemisry**, Department of Biochemistry and Biotechnology, University of Thessaly
1/10/2009-19/12/2016	**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**, Insitute of Biology and Biotechnology, National Hellenic Research Foundation.
7/1999 – 4/2000	**Reasearcher**, Inistute of Biology, N.C.R. S "Demokritos"
10/1993 – 6/1999	**Reasearcher,** Department of Biology and Biochemistry, University of Bath, U.K.

RESEARCH INTERESTS

Structural Biochemistry and X-ray crystallography of proteins of pharmaceutical interest with particular emphasis on proteins involved in glycogen metabolism and diabetes type 2, angiogenesis and tumor development, metaloproteases and matrix restructuring and structure-based drug design.

SCIENTIFIC ACTIVITIES

Member of the Board (2003-2012, 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, Research Foundation Flanders Belgium, Hellenic Foundation for Research and Innovation.

Reviewer for: Journal of the American Chemical Society, The FEBS Journal, International Journal of Biological Macromolecules, Acta Crystallographica Section F, Biorganic and Medicinal Chemistry, Protein & Peptide Letters, PROTEINS: Structure, Function, and Bioinformatics, Acta Crystallographica Section D, Amino Acids, African Journal of Biotechnology, Biochimie, Biophysical Chemistry, Chemical Biology & Drug Design, Chemistry and Physics of Lipids, Diabetes Metabolic Syndrome and Obesity Targets and Therapy, European Journal of Medicinal Chemistry, European Journal of Pharmaceutical Sciences, Expert Opinion On Therapeutic Patents, Food and Chemical Toxicology, Glycobiology, Molecules, International Journal of Biological Macromolecules, ISRN Structural Biology, Biorganic and Medicinal Chemistry Letters, Current Drug Discovery Technologies, etc

SCIENTIFIC PUBLICATIONS

Number of Publications	**106**
Number of citations (excluding self)	**2438**
***h* index**	**31**

1. *The architecture of hydrogen and sulfur σ-hole interactions explain differences in the inhibitory potency of C-β-D-glucopyranosyl thiazoles, imidazoles and an N-β-D glucopyranosyl tetrazole for human liver glycogen phosphorylase and offer new insights to structure-based design.* Kyriakis, E. Karra, A.G., Papaioannou, O., Solovou, T., Skamnaki, V.T., Liggri, P.G.V., Zographos, S.E., Szennyes, E., Bokor, E., Kun, S., Psarra A.-M. G, Somsák, L., Leonidas, D.D. **(2019) Bioorg. Med. Chem.** In press.
2. *Glucopyranosylidene-spiro-imidazolinones, a New Ring System: Synthesis and Evaluation as Glycogen Phosphorylase Inhibitors by Enzyme Kinetics and X-ray Crystallography.* Szabó, K.E., Kyriakis, E., Psarra, A.G., Karra, A.G., Sipos, Á., Docsa, T., Stravodimos, G.A.,

Katsidou, E., Skamnaki, V.T., Liggri, P.G.V., Zographos, S.E., Mándi, A., Király, S.B., Kurtán, T., Leonidas, D.D., Somsák. L. **(2019) J Med Chem. 11**, 6116-6136.

3. *High Consistency of Structure-Based Design and X-Ray Crystallography: Design, Synthesis, Kinetic Evaluation and Crystallographic Binding Mode Determination of Biphenyl-N-acyl-β-d-Glucopyranosylamines as Glycogen Phosphorylase Inhibitors.* Fischer, T., Koulas, S.M., Tsagkarakou, A.S., Kyriakis, E., Stravodimos, G.A., Skamnaki, V.T., Liggri, P.G.V., Zographos, S.E., Riedl, R., Leonidas. D.D. (**2019) Molecules 3,** 24(7)
4. *Potential interference of aluminum chlorohydrate with estrogen receptor signaling in breast cancer cells.* Gorgogietas, V.A., Tsialtas, I., Sotiriou, N., Laschou, V.C., Karra, A.G., Leonidas, D.D., Chrousos, G.P., Protopapa, E., Psarra, A.G. **(2018) J Mol Biochem. 7**, 1-13.
5. *Probing the β-pocket of the active site of human liver glycogen phosphorylase with 3-(C-β-D-glucopyranosyl)-5-(4-substituted-phenyl)-1, 2, 4-triazole inhibitors.* Kyriakis, E., Solovou, T.G.A., Kun, S., Czifrák, K., Szőcs, B., Juhász, L., Bokor, É., Stravodimos, G.A., Kantsadi, A.L., Chatzileontiadou, D.S.M., Skamnaki, V.T., Somsák, L., Leonidas, D.D. **(2018) Bioorg Chem. 77**, 485-493.
6. *A multidisciplinary study of 3-(β-d-glucopyranosyl)-5-substituted-1,2,4-triazole derivatives as glycogen phosphorylase inhibitors: Computation, synthesis, crystallography and kinetics reveal new potent inhibitors.* Kun, S., Begum, J., Kyriakis, E., Stamati, E.C.V., Barkas, T.A., Szennyes, E., Bokor, É., Szabó, K.E., Stravodimos, G.A., Sipos, Á., Docsa, T., Gergely, P., Moffatt, C., Patraskaki, M.S., Kokolaki, M.C., Gkerdi, A., Skamnaki, V.T., Leonidas, D.D., Somsák, L., Hayes, J.M. **(2018) Eur. J. Med. Chem. 147**, 266-278.
7. *Evidence for novel action at the cell binding site of human Angiogenin revealed by heteronuclear NMR spectroscopy, in silico and in vivo studies*. Chatzileontiadou, D.S.M., Tsika, A.C., Diamantopoulou, Z., Delbé, J., Badet, J., Courty, J., Skamnaki, V.T., Parmenopoulou, V., Komiotis, D., Hayes, J.M., Spyroulias, G.A., and Leonidas, D.D. **(2018) ChemMedChem 13**, 259-269.
8. *Affinity crystallography reveals the bioactive compounds of industrial juicing byproducts of Punica granatum for glycogen phosphorylase.* Stravodimos, G.A., Kantsadi, A.L., Apostolou, A., Kyriakis, E., Kafaski-Kanelli, V.N., Solovou, T.G.A., Gatzona, P., Liggri, P.C., Theofanous, S., Gorgogietas, V.A., Kissa, A., Psachoula, C., Chatzileontiadou, D.S.M., Lemonakis, A., Psarra, A.G., Skamnaki, V.T., Haroutounian, S., Leonidas, D.D. (**2018**) **Curr Drug Discov Technol. 15**, 41-53.
9. *Nanomolar Inhibitors of Glycogen Phosphorylase Based on β-d-Glucosaminyl Heterocycles: A Combined Synthetic, Enzyme Kinetic, and Protein Crystallography Study.* Bokor, É., Kyriakis, E., Solovou, T.G.A., Koppány, C., Kantsadi, A.L., Szabó, K.E., Szakács, A., Stravodimos, G.A., Docsa, T., Skamnaki, V.T., Zographos, S.E., Gergely, P., Leonidas, D.D., Somsák, L. (**2017**) **J Med Chem. 60**, 9251-9262.
10. *Proteomic Analysis of Human Angiogenin Interactions Reveals Cytoplasmic PCNA as a Putative Binding Partner* Chatzileontiadou, D.S.M., Samiotaki, M., Alexopoulou, A.N., Cotsiki, M., Panayotou, G., Stamatiadi, M., Balatsos, N.A.A., Leonidas, D.D., Kontou, M. (**2017**) **J Proteome Res. 16**, 3606-3622
11. *Oxidation of human serum albumin exhibits inter-individual variability after an ultra-marathon mountain race.* Spanidis, Y., Priftis, A., Stagos, D., Stravodimos, G.A., Leonidas, D.D., Spandidos, D.A., Tsatsakis, A.M., Kouretas, D. (**2017**) **Exp Ther Med. 13,** 2382-2390
12. *van der Waals interactions govern C-β-d-glucopyranosyl triazoles' nM inhibitory potency in human liver glycogen phosphorylase.* Kantsadi, A.L., Stravodimos, G.A., Kyriakis, E., Chatzileontiadou, D.S.M., Solovou, T.G.A., Kun, S., Bokor, É., Somsák, L., Leonidas, D.D. (**2017**) **J Struct Biol. 199**, 57-67
13. *Phytogenic Polyphenols as Glycogen Phosphorylase Inhibitors: The Potential of Triterpenes and Flavonoids for Glycaemic Control in Type 2 Diabetes.* Stravodimos, G.A., Chetter, B.A.,

Kyriakis, E., Kantsadi, A.L., Chatzileontiadou, D.S., Skamnaki, V.T., Kato, A., Hayes, J.M., Leonidas, D.D. (**2017**) **Curr Med Chem. 24,** 384-403

14. *NMR study of Met-1 human Angiogenin: (1)H, (13)C, (15)N backbone and side-chain resonance assignment.* Tsika, A.C., Chatzileontiadou, D.S., Leonidas, D.D., Spyroulias, G.A. (**2016**) **Biomol NMR Assign. 10,** 379-383
15. *Synthetic, enzyme kinetic, and protein crystallographic studies of C-β-d-glucopyranosyl pyrroles and imidazoles reveal and explain low nanomolar inhibition of human liver glycogen phosphorylase.* Kantsadi, A.L., Bokor, É., Kun, S., Stravodimos, G.A., Chatzileontiadou, D.S.M., Leonidas, D.D., Juhász-Tóth, É., Szakács, A., Batta, G., Docsa, T., Gergely, P., Somsák, L. (**2016**) **Eur J Med Chem. 123**, 737-774
16. *The ammonium sulfate inhibition of human angiogenin.*Chatzileontiadou, D.S., Tsirkone, V.G., Dossi, K., Kassouni, A.G., Liggri, P.G., Kantsadi, A.L., Stravodimos, G.A., Balatsos, N.A., Skamnaki, V.T., Leonidas, D.D. (**2016**) **FEBS Lett. 590**, 3005-3018.
17. *AtHESPERIN: A Novel Regulator of Circadian Rhythms with Poly(A)-degrading Activity in Plants.* Delis, C., Krokida, A., Tomatsidou, A., Tsikou, D., Beta, R.A., Tsioumpekou, M., Moustaka, J., Stravodimos, G., Leonidas, D.D., Balatsos, N.A., Papadopoulou, K.K. (**2016) RNA Biol. 13,** 68-82
18. *Triazole double-headed ribonucleosides as inhibitors of eosinophil derived neurotoxin.* Chatzileontiadou, D.S., Parmenopoulou, V., Manta, S., Kantsadi, A.L., Kylindri, P., Griniezaki, M., Kontopoulou, F., Telopoulou, A., Prokova, H., Panagopoulos, D., Boix, E., Balatsos, N.A., Komiotis, D., Leonidas D.D. **(2015) Bioorg Chem. 63**, 152-165.
19. *An evaluation of indirubin analogues as phosphorylase kinase inhibitors.* Begum, J., Skamnaki, V.T., Moffatt, C., Bischler, N., Sarrou, J., Skaltsounis, A.L., Leonidas, D.D., Oikonomakos, N.G., Hayes, J.M. **(2015) J Mol Graph Model. 61**, 231-242.
20. *Glycogen Phosphorylase as a Target for Type 2 Diabetes: Synthetic, Biochemical, Structural and Computational Evaluation of Novel N-acyl-N′-(β-D-glucopyranosyl) Urea Inhibitors.* Kantsadi, A,L,, Parmenopoulou, V., Bakalov, D.N., Snelgrove, L., Stravodimos, G.A., Chatzileontiadou, D.S., Manta, S., Panagiotopoulou, A., Hayes, J.M., Komiotis, D., Leonidas, D.D. **(2015) Curr Top Med Chem.15** (23), 2373-2389.
21. *Molecular Cloning, Carbohydrate Specificity and the Crystal Structure of Two Sclerotium rolfsii Lectin Variants.* Peppa, V.I., Venkat, H., Kantsadi, A.L., Inamdar, S.R., Bhat, G.G., Eligar, S., Shivanand, A., Chachadi, V.B., Satisha, G.J., Swamy, B.M., Skamnaki, V.T., Zographos, S.E., Leonidas, D.D. **(2015) Molecules 20** (6), 10848-10865.
22. *Natural flavonoids as antidiabetic agents. The binding of gallic and ellagic acids to glycogen phosphorylase b.* Kyriakis, E., Stravodimos, G.A., Kantsadi, A.L., Chatzileontiadou, D.S., Skamnaki, V.T., Leonidas, D.D. (**2015) FEBS Lett. 589** (15), 1787-1794.
23. *Non-contact Current Transfer Induces the Formation and Improves the X-ray Diffraction Quality of Protein Crystals.* Boltsis, I., Lagoumintzis, G., Chatzileontiadou, D.S.M., Giastas, P., Tzartos, S.J., Leonidas, D.D., Poulas, K. (**2014) Cryst. Growth & Design 14** (9) 4347-4354.
24. *Structure based inhibitor design targeting glycogen phosphorylase b. Virtual screening, synthesis, biochemical and biological assessment of novel N-acyl-beta-D-glucopyranosylamines.* Parmenopoulou, V., Kantsadi, A.L., Tsirkone, V.G., Chatzileontiadou, D.S.M., Manta, S., Zographos, S.E., Molfeta, C., Archontis, G., Agius, L., Hayes, J.M., Leonidas, D.D., and Komiotis, D. **(2014) Bioorg. & Med. Chem. 22** (17), 4810-4825.
25. *Glucopyranosylidene-spiro-iminothiazolidinone, a new bicyclic ring system: Synthesis, derivatization, and evaluation for inhibition of glycogen phosphorylase by enzyme kinetic and crystallographic methods.* Czifrak, K., Pahi, A., Deak, S., Kiss-Szikszai, A., Kover, K.E., Docsa, T., Gergerly. P., Alexacou, K.M., Papakonstantinou, M., Leonidas, D.D., Zographos, S.E., Chrysina, E.D., Somsak, L. **(2014) Bioorg. & Med. Chem. 22** (15), 4028-404

26. *Natural products and their derivatives as inhibitors of glycogen phosphorylase: potential treatment for type 2 diabetes.* Hayes, J.M., Kantsadi, A.L., Leonidas, D.D. **(2014) Phytochem. Rev. 13** (2), 471-498
27. *Biochemical and biological assessment of the inhibitory potency of extracts from vinification byproducts of Vitis vinifera extracts against glycogen phosphorylase.* Kantsadi, A.L., Apostolou, A., Theofanous, S., Stravodimos, G.A., Kyriakis, E., Gorgogietas, V.A., Chatzileontiadou, D.S.M., Pegiou, K., Skamnaki, V.T., Stagos, D., Kouretas, D., Psarra, A.-M. G., Haroutounian, S.A., Leonidas, D.D. **(2014) Food Chem. Toxicol. 67**, 35-43
28. *Structural analysis of the Rhizoctonia solani agglutinin reveals a domain-swapping dimeric assembly.*Skamnaki, V.T., Peumans, W.J., Kantsadi, A.L., Cubeta, M.A., Plas, K., Pakala, S., Zographos, S.E., Smagghe, G., Nierman, W.C., Van Damme, E.J., Leonidas, D.D. (**2013**) **FEBS J. 280,** 1750-1763.
29. *Sourcing the affinity of flavonoids for the glycogen phosphorylase inhibitor site via crystallography, kinetics and QM/MM-PBSA binding studies: Comparison of chrysin and flavopiridol.*Tsitsanou, K.E., Hayes, J.M., Keramioti, M., Mamais, M., Oikonomakos, N.G., Kato, A., Leonidas, D.D., Zographos, S.E. (**2013**) **Food Chem Toxicol.61**, 14-27.
30. *Glycogen metabolism enzymes as molecular targets for drug development* Skamnaki, V. T., Kantsadi, A. L., Chatzileontiadou, D. S. M., Stravodimos, G. & Leonidas, D. D. **(2013)** in **Glycogen Structure, Functions in the body and role in disease** (Weiss, P. L. & Faulkner, B. D., eds) pp. 109-135, Nova Science Publishers, Inc., New York.
31. *Studies on the essential intramolecular interaction between the A1 and A2 domains of von Willebrand factor.* Karoulia, Z., Papadopoulos, G., Nomikos, M., Thanassoulas, A., Choli-Papadopoulou, T., Nounessis, G., Kontou, M., Stathopoulos, C., and Leonidas, D.D**. (2013). Prot. & Pept. Lett**. 20, 231-240.
32. *Triazole pyrimidine nucleosides as inhibitors of Ribonuclease A. Synthesis, biochemical, and structural evaluation.* Parmenopoulou, V., Chatzileontiadou, D.S.M., Manta, S., Bougiatioti, S., Maragozidis, P., Gkaragkouni,D.-N., Kaffesaki, E., Kantsadi, A.L., Skamnaki, V.T., Zographos, S.E., Zoumpoulakis, P., Balatsos, N.A.A., Komiotis, D., and Leonidas, D.D. (**2012**). **Bioorg Med Chem. 20,** 7184-7193
33. *The binding of C5-alkynyl and alkylfurano[2,3-d]pyrimidine glucopyranonucleosides to glycogen phosphorylase b. Synthesis, biochemical and biological assessment.* Kantsadi, A.L., Manta, S., Psarra, A.-M.G., Dimopoulou, A., Kiritsis, C., Parmenopoulou, V., Skamnaki, V.T., Zoumpoulakis, P., Zographos, S.E., Leonidas, D.D., and Komiotis D. **(2012) Eur. J. Med. Chem. 54,** 740-749**.**
34. *The σ-hole phenomenon of halogen atoms form the structural basis of the strong inhibitory potency of C-5 halogen substituted glucopyranosyl nucleosides towards glycogen phosphorylase b.* Kantsadi, A.L., Hayes, J.M., Manta, S., Skamnaki, V.T., Kiritsis, C., Psarra, A.-M.G., Koutsogiannis, Z., Dimopoulou, A., Theofanous, S., Nikoleousakos, N., Zoumpoulakis, P., Kontou, M., Papadopoulos, G., Zographos, S.E., Komiotis, D., and Leonidas, D.D. **(2012). ChemMedChem 7**, 722-732.
35. *3′-axial CH2OH substitution on glucopyranose does not increase glycogen phosphorylase inhibitory potency.* QM/MM-PBSA calculations suggest why. Manta, S., Xipnitou, A., Kiritsis, A., Kantsadi, A.L., Hayes, J.M., Skamnaki, V.T., Lamprakis, C., Kontou, M., Zoumpoulakis, P., Zographos, S.E., Leonidas, D.D., and Komiotis, D. **(2012). Chem. Biol. & Drug Des. 79**, 663-673.
36. *N-(4-Substituted-benzoyl)-N'-(β-d-glucopyranosyl)ureas as inhibitors of glycogen phosphorylase: Synthesis and evaluation by kinetic, crystallographic, and molecular modelling methods.*Nagy V, Felföldi N, Kónya B, Praly JP, Docsa T, Gergely P, Chrysina ED, Tiraidis C, Kosmopoulou MN, Alexacou KM, Konstantakaki M, Leonidas DD, Zographos SE, Oikonomakos NG, Kozmon S, Tvaroška I, Somsák L. **(2012).Bioorg Med Chem. 20**, 1801-1816.

37. *Anopheles gambiae odorant binding protein crystal complex with the synthetic repellent DEET: implications for structure-based design of novel mosquito repellents.* Tsitsanou K. E., Thireou, T., Drakou, C.E., Koussis, K. Keramioti, M.V., Leonidas, D.D., Eliopoulos, E., Iatrou, K., and Zographos, S.E. **(2012). Cell Mol Life Sci. 69**, 283-297.
38. *hCINAP is an atypical mammalian nuclear adenylate kinase with an ATPase motif: structural and functional studies.* Drakou CE, Malekkou A, Hayes JM, Lederer CW, Leonidas DD, Oikonomakos NG, Lamond AI, Santama N, Zographos SE. **(2012) Proteins Structure-Function and Bioinformatics 80**, 206-220.
39. *Halogen-substituted (C-β-D-glucopyranosyl)-hydroquinone regioisomers: Synthesis, enzymatic evaluation and their binding to glycogen phosphorylase.* Alexacou, K.M., Zhang Y.Z., Praly, J.-P., Zographos, S.E., Chrysina, E.D., Oikonomakos, N.G., and Leonidas, D.D. **(2011) Biorg. Med. Chem. 19**, 5125-5136.
40. *The binding of β-D-glucopyranosyl-thiosemicarbazone derivatives to glycogen phosphorylase: A new class of inhibitors.* Alexacou K.-M., Tenchiu-Deleanu A.C., Chrysina, E.D., Charavgi M.D., Kostas, I.D., Zographos S.E., Oikonomakos, N.G., and Leonidas, D.D. **(2010) Biorg. Med. Chem. 18**, 7911-7922.
41. *Computation as a tool for glycogen phosphorylase inhibitor design*. Hayes, J.M., and Leonidas, D.D. **(2010) Mini Rev. Med. Chem. 10**, 1156-1174.
42. *The binding of beta-D-glucopyranosyl-thiosemicarbazone derivatives to glycogen phosphorylase: A new class of inhibitors.* Alexacou, K.-M., Tenchiu-Deleanu, A.C., Chrysina, E.D., Charavgi, M.-D., Kostas, I.D., Zographos, S.E., Oikonomakos, N.G. Leonidas, D.D. **(2010) Biorg. Med. Chem. 18**, 7911-7922.
43. *1-(3-Deoxy-3-fluoro-beta-d-glucopyranosyl) pyrimidine derivatives as inhibitors of glycogen phosphorylase b: Kinetic, crystallographic and modelling studies.* Tsirkone, V.G., Tsoukala, E., Lamprakis, C., Manta, S., Hayes, J.M., Skamnaki, V.T., Drakou, C., Zographos, S.E., Komiotis, D., Leonidas, D.D. **(2010) Biorg. Med. Chem. 18**, 3413-3425.
44. *Glucose-based spiro-isoxazolines: a new family of potent glycogen phosphorylase inhibitors.* Benltifa M, Hayes JM, Vidal S, Gueyrard D, Goekjian PG, Praly JP, Kizilis G, Tiraidis C, Alexacou KM, Chrysina ED, Zographos SE, Leonidas DD, Archontis G, Oikonomakos NG. **(2009) Biorg. Med. Chem. 17**, 7368-7380.
45. *Mapping the ribonucleolytic active site of bovine seminal ribonuclease. The binding of pyrimidinyl phosphonucleotide inhibitors*. K Dossi, V.G. Tsirkone, J.M. Hayes, J. Matoušek, P. Poučková, J. Souček, M. Zadinova, S.E. Zographos, and D.D. Leonidas (**2009**) **Eur. J. Med. Chem. 44**, 4496-4508.
46. *Inhibitor design to Ribonuclease A: The binding of two 5′phosphate uridine analogues* V.G. Tsirkone, K. Dossi, C. Drakou, S.E. Zographos, M. Kontou and D.D. Leonidas (**2009**) **Acta Crystallogr. F65**, 671-677.
47. *Influence of Naturally-occurring 5'-Pyrophosphate-linked Substituents on the Binding of Adenylic Inhibitors to Ribonuclease A: an X-Ray Crystallographic Study.* Holloway, D.E., Chavali, G.B., Leonidas, D.D., Baker, M.D., and Acharya, K.R. (**2009**). **Biopolymers 91**, 995-1008.
48. *Amide-1,2,3-triazole bioisosterism: the glycogen phosphorylase case*. E. D Chrysina, É. Bokor, K.-M. Alexacou, M.-D. Charavgi, G.N. Oikonomakos, S.E. Zographos, D.D. Leonidas, N.G. Oikonomakos, and L. Somsák **(2009) Tetrahedron Asymm. 20, 733-740**.
49. *Morpholino, piperidino, and pyrrolidino derivatives of pyrimidines as inhibitors of Ribonuclease A: synthesis, kinetic and crystallographic evaluation.* A. Samanta, D. D.

Leonidas, S. Dasgupta, T. Pathak, S.E. Zographos, and N.G. Oikonomakos **(2009). J. Med. Chem. 52**, 932-942**.**

50. *Naturally Occurring Pentacyclic Triterpenes as Inhibitors of Glycogen Phosphorylase: Synthesis, Structure-Activity Relationships and X-ray Crystallographic Studies.* X. Wen, H. Sun, J. Liu, K. Cheng, P. Zhang, L. Zhang, J. Hao, L. Zhang, P. Ni, S.E. Zographos, D.D. Leonidas, K.-M. Alexacou, T. Gimisis, J. M. Hayes, and N.G. Oikonomakos **(2008) J. Med. Chem. 51,** 3540-3554
51. *Pentacyclic triterpenes, inhibitors of glycogen phosphorylase, as potential drugs for type 2 diabetes: X-ray crystallographic studies.* Zographos, S.E., Leonidas, D.D., Alexacou, K.M., Gimisis, T., Hayes, J.M., Oikonomakos, N.G, Wen, X., Sun, H., Liu, J., Cheng, K., Zhang, P., Zhang, L., Hao, J., Zhang, L., and Ni, P. **(2008). Planta Medica 74**, 1146-1147.
52. *Crystallographic and computational studies on N-(β-D-glucopyranosyl)-4-phenyl-1,2,3-triazoleacetamide, an inhibitor of glycogen phosphorylase: comparison with α-D-glucose, N-acetyl-β-D-glucopyranosylamine and N-benzoyl-N′-β-D-glucopyranosyl urea binding.* K.-M. Alexacou, J.M. Hayes, C. Tiraidis, S.E. Zographos, D.D. Leonidas, E.D. Chrysina, G. Archontis, N.G. Oikonomakos, J.V. Paul, B. Varghese, and D. Loganathan **(2008). Proteins, Structure, Function, and Bioinformatics 71,** 301-317.
53. *X-ray sequence ambiguities of Sclerotium rolfsii lectin resolved by mass spectrometry*. G. J. Sathisha, Y. K. Subrahmanya Prakash, V. B. Chachadi, N. N. Nagaraja, S. R. Inamdar, D. D. Leonidas, H. S. Savithri, and B. M. Swamy **(2008) Amino Acids 5**, 309-320
54. *New inhibitors of Glycogen Phosphorylase as potential Antidiabetic Agents.* Somsak, L., Czifrak, K., Toth, M., Bokor, E., Chrysina, E.D., Alexacou, K.-M., Hayes, J.M., Tiraidis, C., Lazoura, E., Leonidas, D.D., Zographos, S.E., and Oikonomakos, N.G. **(2008). Curr. Med. Chem. 15**, 2933-2983.
55. *FR25900, a potential anti-hyperglycemic drug, binds at the allosteric site of glycogen phosphorylase.* C. Tiraidis, K.-M. Alexacou, S.E. Zographos, D.D. Leonidas, T. Gimisis, and N.G. Oikonomakos **(2007). Protein Sci. 16**, 1773-1782.
56. *Structural basis of the carbohydrate recognition of the Sclerotium rolfsii lectin.* D.D. Leonidas, B.M. Swamy, G.N. Hatzopoulos, S.J. Gonchigar, S.R. Inamdar, S.E. Zographos, and N.G. Oikonomakos **(2007)**. **J. Mol. Biol. 368**, 1145-1161.
57. *In the Search of Glycogen Phosphorylase Inhibitors: Synthesis of C-D-Glycopyranosyl-Hydroquinones and -Benzoquinones. Inhibition of and binding to glycogen phosphorylase in the crystal.* L. He, Y.Z. Zang, M. Tanoh, G.-R. Chen, J.-P. Praly, E.D. Chrysina, M.N. Kosmopoulou, D.D. Leonidas, and N.G. Oikonomakos **(2007). Eur. J. Org. Chem.** 596-606.
58. *Recognition of Ribonuclease A by 3 '-5'-Pyrophosphate-linked Dinucleotide Inhibitors: a Molecular Dynamics/Continuum Electrostatics Analysis.* S. Polydoridis, D.D. Leonidas, N.G. Oikonomakos, and G. Archontis. **(2007). Biophys. J. 92**, 1659-1672.
59. *Bioactivity of glycogen phosphorylase inhibitors that bind to the purine nucleoside site*. L.J. Hampson, C. Arden, L. Agius, M. Ganotidis, M.N. Kosmopoulou, C. Tiraidis, Y. Elemes, C. Sakarellos, D.D. Leonidas, and N.G. Oikonomakos, (**2006**). **Bioorg. Med. Chem.** 14, 7835-7845.
60. *Iminosugars as potential inhibitors of glycogenolysis: structural insights into the molecular basis of glycogen phosphorylase inhibition*. N.G. Oikonomakos, C. Tiraidis, D.D. Leonidas, S.E. Zographos, M. Kristiansen, C.U. Jessen, L. Nørskov-Lauritsen, and L. Agius **(2006). J. Med. Chem**. **49**, 5697-5701.

61. *The binding of a 3'-N-Alkylamino-3'-deoxy-ara-uridine to Ribonuclease A in the crystal*. D.D. Leonidas, S. Dasgupta**,** T.K. Maiti, D. Soumya, T. Pathak, S.E. Zographos, and N.G. Oikonomakos **(2006). Bioorg. Med. Chem**. **14**, 6055-6064.
62. *Crystallographic studies on N-azidoacetyl-beta-D-glucopyranosylamine, an inhibitor of glycogen phosphorylase: comparison with N-acetyl-beta-D-glucopyranosylamine.* E.I. Petsalakis, E.D. Chrysina, C. Tiraidis, T. Hadjiloi, D.D. Leonidas, N.G. Oikonomakos, U. Aich, B. Varghese, and D. Loganatha**n (2006). Bioorg. Med. Chem. 14,** 5316-5324.
63. *Binding of oxalyl derivatives of β-D-glucopyranosylamine to muscle glycogen phosphorylase b* T. Hadjiloi, C. Tiraidis, E.D. Chrysina, D.D. Leonidas, N.G. Oikonomakos, P. Tsipos, and T. Gimisis **(2006). Bioorg. Med. Chem**.**14**, 3872-3882.
64. *Crystallographic studies on two bioisosteric analogues, N-acetyl-β-D-glucopyranosylamine and N-trifluoracetyl-β-D-glucopyranosylamine, potent inhibitors of muscle glycogen phosphorylase.* E., Anagnostou, M.N. Kosmopoulou, E.D. Chrysina, D.D. Leonidas, T. Hadjiloi, C. Tiraidis, Z. Györgydeák, L. Somsák, T. Docsa, P. Gergely, and N.G. Oikonomakos **(2006) Biorg. Med. Chem. 14,** 181-189. **Cover Story**
65. *Crystallographic studies on acyl ureas, a new class of glycogen phosphorylase inhibitors, as potential antidiabetic drugs.* N.G. Oikonomakos, M.N. Kosmopoulou, E.D. Chrysina, D.D. Leonidas, I.D. Kostas, K.U. Wendt, T. Klabunde, E. Defossa, **(2005) Protein Sci.** 14, 1760-1771.
66. *Indirubin-3'-aminooxy-acetate inhibits glycogen phosphorylase by binding at the inhibitor and the allosteric site. Broad specificities of the two sites.* M.N. Kosmopoulou, D.D. Leonidas, E.D. Chrysina, G. Eisenbrand, and N.G. Oikonomakos **(2005) Lett. Drug Des. Discov. 2**, 377-390. **Cover Story**
67. *The binding of IMP to ribonuclease A*. G.N. Hatzopoulos, D.D. Leonidas, R. Kardakaris, J. Kobe, and N.G. Oikonomakos. **(2005) FEBS J 272**, 3988-4001.
68. *Kinetic and crystallographic studies on 2-((-D-glucopyranosyl)-5-methyl-1,3,4-oxadiazole,-benothiazole, and -benzimidazole, inhibitors of muscle glycogen phosphorylase b. Evidence for a new binding site.* E.D. Chrysina, M.N. Kosmopoulou, C. Tiraidis, R. Kardakaris, N. Bischler, D.D. Leonidas, Z. Hadady, L. Somsak, T. Docsa, P. Gergely, and N.G. Oikonomakos. **(2005) Protein Sci. 14,** 873-888.
69. *Binding of beta-D-glucopyranosyl bismethoxyphosphoramidate to glycogen phosphorylase b: Kinetic and crystallographic studies*. E.D. Chrysina, M.N. Kosmopoulou, R. Kardakaris, N. Bischler, D.D. Leonidas, T. Kannan, D. Loganathan, and N.G. Oikonomakos **(2005) Bioorg. Med. Chem. 13**, 765-772.
70. *Binding of the potential antitumour agent indirubin-5-sulphonate at the inhibitor site of rabbit muscle glycogen phosphorylase b.* M.N. Kosmopoulou, D.D. Leonidas, E.D. Chrysina, N. Bischler, G. Eisenbrand, C.E. Sakarellos, R. Pauptit, and N.G. Oikonomakos. **(2004) Eur. J. Biochem. 271,** 2280-2290.
71. *High resolution crystal structures of Ribonuclease A complexed with adenylic and uridylic nucleotide inhibitors. Implications for structure-based design of ribonucleolytic inhibitors.* D.D. Leonidas, G.B. Chavali, N.G. Oikonomakos, E.D. Chrysina, M.N. Kosmopoulou, M. Vlassi, C. Frankling, and K.R. Acharya **(2003) Protein Sci. 12**, 2559-2574. **Cover Story**
72. *Crystallographic studies on α- and β-D-glucopyranosyl formamide analogues, inhibitors of glycogen phosphorylase.* E.D. Chrysina, N.G. Oikonomakos, S.E. Zographos, M.N.

Kosmopoulou, N. Bischler, D.D. Leonidas, L. Kovács, T. Docsa, P. Gergely, and L. Somsák **(2003) Biocatal. & Biotransfor. 21**, 233-242.

73. *The binding of β- and γ-cyclodextrins to glycogen phosphorylase b: kinetic and crystallographic studies.* N. Pinotsis, D.D. Leonidas, E.D. Chrysina, N.G. Oikonomakos, and I.M. Mavridis **(2003) Protein Sci. 11**, 1914-1924. **Cover Story**
74. *Crystallization and preliminary X-ray crystallographic analysis of Sclerotium rolfsii lectin.* D.D. Leonidas, B.M. Swamy, A.G. Bhat, S.R. Inamdar, M.N. Kosmopoulou, E.D. Chrysina, and N.G. Oikonomakos **(2003 Acta Cryst. D59**, 363-365.
75. *Crystal structure of rabbit muscle glycogen phosphorylase a in complex with a potential hypoglycaemic drug at 2.0 Å resolution.* N.G. Oikonomakos, E.D. Chrysina, M.N. Kosmopoulou, and D.D. Leonidas **(2003) Biochim. Biophys. Acta 1647**, 325-332.
76. *Guest-host crosstalk in angiogenin/RNase A chimeric protein.* D.E. Holloway, R. Shapiro, M.C. Hares, D.D. Leonidas and K.R. Acharya **(2002) Biochemistry 41,** 10482-10489.
77. *Charcot-Leyden Crystal protein (galectin-10) is not a dual-function galectin with lysophospholipase activity, but binds a lysophospholipase inhibitor in a novel structural function.* S.J. Ackerman, L. Liu, M.A. Kwatia, M.P. Savage, D.D. Leonidas, G.J. Swaminathan, and K.R. Acharya **(2002) J. Biol. Chem. 277,** 14859-14868.
78. *The binding of N-acetyl- and N-benzoyl-N' -beta-D-glucopyranosyl urea to glycogen phosphorylase b: Kinetic and crystallographic studies*. N.G. Oikonomakos, M. Kosmopoulou, S.E. Zographos, D.D. Leonidas, E.D. Chrysina, L. Somsak, V. Nagy, J.-P. Praly, T. Docsa, B. Toth, and P. Gergely **(2002) Eur. J. Biochem. 269**, 1684-1696. **Cover Story**
79. *Crystallographic Studies on the Role of the C-terminal Segment of Human Angiogenin in Defining Enzymatic Potency.* D.D. Leonidas, R. Shapiro, G.V. Subbarao, A. Russo and K.R. Acharya **(2002) Biochemistry 41**, 2552-2562.
80. *Cleavage of 3', 5'-pyrophosphate-linked dinucleotides by Ribonuclease A and Angiogenin.* A.M. Jardine, D.D. Leonidas, J.L. Jenkins, C. Park, R.T. Raines, K.R. Acharya and R. Shapiro **(2001). Biochemistry 40**, 10262-10272.
81. *Binding of phosphate and pyrophosphate ions at the active site of human angiogenin as revealed by X-ray crystallography.* D.D. Leonidas, G.B. Chavali, A.M. Jardine, S. Li, R. Shapiro, and K.R. Acharya, **(2001). Protein Sci. 10**, 1669-1676.
82. *Crystal structure of the Eosinophil Major Basic Protein at 1.8 Å: An atypical lectin with a paradigm shift in specificity.* G.J. Swaminathan, A.J. Weaver, D.A. Loegering, J.L. Checkel, D.D. Leonidas, G.J. Gleich & K.R. Acharya **(2001). J. Biol. Chem. 276**, 26197-26203.
83. *Mapping the ribonucleolytic active site of eosinophil-derived neurotoxin (EDN): High resolution crystal structures of EDN complexes with adenylic nucleotide inhibitors.* D.D. Leonidas, E. Boix, R. Prill, M. Suzuki, R. Turton, K. Minson, G.J. Swaminathan, R.J. Youle, and K.R. Acharya **(2001). J. Biol. Chem. 276**, 15009-15017.
84. *Crystallization and preliminary investigations on a telomeric repeat sequence $C_4A_2C_4A_2$.* G. Savitha, D. Leonidas, K.R. Acharya and M.A. Viswamitra **(2001). Acta Cryst. D57**, 873-875.
85. *The crystal structure of human placenta growth factor-1 (PlGF-1), an angiogenic protein at 2.0 Å resolution.* S. Iyer, D.D. Leonidas, G.J. Swaminathan, D. Maglione, M. Battisti, M. Tucci, M.G. Persico, and K.R. Acharya**, (2001). J. Biol. Chem. 276,** 12153-12161.
86. *The crystal structure of the Fab fragment of a rat monoclonal antibody against the main immunogenic region of the human muscle acetylcholine receptor.* M. Kontou, D.D. Leonidas,

E.H. Vatzaki, P. Tsantili, A. Mamalaki, N.G. Oikonomakos, K. R. Acharya, and S.J. Tzartos **(2000). Eur. J. Biochem. 267**, 2389-2397.

87. *Crystal structure of eosinophil cationic protein at 2.4 Å resolution*. E. Boix, D.D. Leonidas, Z. Nikolovski, M.V. Nogues, C.M. Cuchillo and K.R. Acharya, **(1999). Biochemistry 38**, 16794-16801.
88. *Selective recognition of mannose by human eosinophil Charcot-Leyden crystal protein (Galectin-10): A crystallographic study at 1.8 Å resolution*. G.J. Swaminathan, D.D. Leonidas, M.P. Savage, S.J. Ackerman and K.R. Acharya, **(1999). Biochemistry 38**, 13837-13843.
89. *Towards rational design of Ribonuclease inhibitors: High resolution crystal structure of a Ribonuclease A complex with a potent 3', 5' pyrophosphate-linked dinucleotide inhibitor.* D.D. Leonidas, R. Shapiro, L.I. Irons, N. Russo and K.R. Acharya, **(1999). Biochemistry 38**, 10287-10297.
90. *Refined crystal structures of native human Angiogenin and two active site mutants: Implications for the unique functional properties of an enzyme involved in neovascularization during tumor growth.* D.D. Leonidas, R. Shapiro, S.C. Allen, G.V. Subbarao, K. Veluraja, and K.R. Acharya, **(1999). J. Mol. Biol. 283**, 1209-1233.
91. *Crystal structure of a hybrid between Ribonuclease A and Bovine Seminal Ribonuclease: The Basic surface, at 2.0 Å resolution*. E. H.Vatzaki, S.C. Allen, D.D. Leonidas, K. Trautwein-Frirz, J. Stackhouse, S.A. Benner, and K.R. Acharya, **(1999). Eur. J. Biochem. 260,** 176-182.
92. *Structural basis for the recognition of carbohydrates by human Galectin-7.* D.D. Leonidas, E.H. Vatzaki, H. Vorum, J.E. Celis, P. Madsen, and K.R. Acharya, **(1998). Biochemistry 37**, 13930-13940.
93. *The structure of glycogen phosphorylase b with an alkyl-dicarboxylic acid compound, novel and potent inhibitor.* S.E. Zographos, N.G. Oikonomakos, K.E. Tsitsanou, D.D. Leonidas, E.D. Chrysina, V.T. Skamnaki, H. Bischoff, S. Goldmann, M. Schramm, K.A. Watson, and L.N. Johnson, **(1997). Structure 5**, 1413-1425.
94. *Crystal structures of Ribonuclease complexes with 5' diphosphoadenosine 3'-phosphate and 5' diphosphoadenosine 2'-phosphate at 1.7 Å resolution.* D.D. Leonidas, R. Shapiro, L.I. Irons, N. Russo, and K.R. Acharya, **(1997). Biochemistry 36**, 5584-5588.
95. *The refined crystal structure of Toxic shock Syndrome Toxin-1 at 2.07 Å resolution*. A.C. Papageorgiou, R.D. Brehm, D.D. Leonidas, H.S. Tranter, and K.R. Acharya, **(1996). J. Mol. Biol. 260,** 553-569.
96. *Crystal structure of human Charcot-Leyden crystal protein, an eosinophil lysophospholipase, identifies it as a new member of the carbohydrate binding family of galectins.* D.D. Leonidas, B.L. Elbert, Z. Zhou, H. Leffler, S.J. Ackerman, and K.R. Acharya, **(1995). Structure 3,** 1379-1393. **Cover Story**
97. *Sulphate-activated phosphorylase b: the pH-dependence of catalytic activity*. S.E. Zographos, N.G. Oikonomakos, H.B.F. Dixon, W.G. Griffin, L.N. Johnson, and D.D. Leonidas, **(1995). Biochem. J. 310**, 565-570.
98. *The design of potential antidiabetic drugs - experimental investigation of a number of (-D-glucose analog inhibitors of glycogen phosphorylase.* N.G. Oikonomakos, M. Kontou, S.E. Zographos, H.S. Tsitoura, L.N. Johnson, K.A. Watson, E.P. Mitchell, G.W.J. Fleet, J.C. Son, C.J.F. Bitchard, D.D. Leonidas, and K.R. Acharya, **(1994). Eur. J. Drug Metab. Pharmacokinet. 19**, 185-192.

99. *Design of inhibitors of glycogen phosphorylase: A study of α αnd β glucoheptonamides and 1-thio-α-D-glucose compounds.* K.A. Watson, E.P. Mitchell, L.N. Johnson, J.C. Son, C.J.F. Bitchard, M.G. Orchard, G.W.J. Fleet, N.G. Oikonomakos, D.D. Leonidas, M. Kontou, and A.C. Papageorgiou, **(1994). Biochemistry 33**, 5745-5758.

100. *Kinetic Properties of tetrameric glycogen phosphorylase b in solution and in the crystalline state.* D.D. Leonidas, N.G. Oikonomakos, A.C. Papageorgiou, and T.G. Sotiroudis, **(1992). Protein Sci. 1**, 1123-1132.

101. *Control of phosphorylase b by a modified cofactor : Crystallographic studies on R-state Glycogen Phosphorylase reconstituted with Pyridoxal 5'-diphosphate.* D.D. Leonidas, N.G. Oikonomakos, A.C. Papageorgiou, K.R. Acharya, D. Barford, and L.N. Johnson, **(1992). Protein Sci. 1,** 1112-1122.

102. *Glucose analogue inhibitors of glycogen phosphorylase : the design of potential drugs for diabetes.* J.L. Martin, K. Velouraja, L.N. Johnson, G.W.J. Fleet, N.G. Ramsden, I. Bruce, N.G. Oikonomakos, A.C. Papageorgiou, D.D. Leonidas, and H.S. Tsitoura, **(1991). Biochemistry 30**, 10101-10116.

103. *Sulphate activates phosphorylase b by binding to the Ser (P) site.* D.D. Leonidas, N.G. Oikonomakos, and A.C. Papageorgiou, **(1991). Biochim. Biophys. Acta 1076**, 305-307.

104. *The binding of D-gluconhydroximo-1,5-lactone to glycogen phosphorylase: Kinetic, ultracentrifugation, and crystallographic studies.* A.C. Papageorgiou, N.G. Oikonomakos, D.D. Leonidas, D. Barford, J.L. Martin, K.R. Acharya, L.N. Johnson, B. Bernet, D. Beer, and A. Vasella, **(1991). Biochem. J. 274**, 329-338.

105. *The ammonium sulfate activation of phosphorylase b.* D.D. Leonidas, N.G. Oikonomakos, A.C. Papageorgiou, A. Xenakis, C.T. Cazianis, and F. Bem, **(1990). Febs Lett. 261**, 23-27.

106. *Inhibition of rabbit muscle glycogen phosphorylase by D-Gluconhydroximo-1,5 lactone-N-phenylurethane.* A.C. Papageorgiou, N.G. Oikonomakos, and D.D. Leonidas, **(1989). Arch. Biochem. Biophys. 272**, 376-385.