

Spyros E. Zographos

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Scopus Author ID: [6603926262](#)

WoS ResearcherID: [H-9058-2013](#)

CV (Last updated May, 2022)



Spyros E. Zographos is principal investigator of the Structural Biology and Chemistry Group at the Institute of Biology, Medicinal Chemistry and Biotechnology (IBMCB). He is a chemist with vast experience in molecular biology, biochemistry and structural biology. He earned his Bachelor's (1992) and Ph.D. degree from the Department of Chemistry at the University of Athens, Greece, in 1992 and 2000, respectively. He served as a visiting lecturer in the Department of Chemistry at the University of Cyprus (UCY) (2000-2001) and afterwards as a Marie Curie postdoctoral research fellow in the Department of Biological Sciences, UCY (2001-2004). He was awarded a Marie Curie reintegration grant and in 2004 joined IBMCB as a postdoctoral research fellow. He became an Assistant researcher in 2006, a senior researcher in 2010 and Research Director in 2018.

His scientific achievements are presented in 62 peer-reviewed articles (WoS: h-index: 27, Times Cited: total 2,531, without self-citations: 2,421. Google Scholar: i10-index: 54, Times Cited: total 2,968), 3 reviews, 4 chapters in books, 70 oral /poster presentations in conferences and 24 short communications. He has deposited as audit author 113 protein structures at the Protein Data Bank.

Dr. Spyros Zographos has significant teaching experience. As a visiting lecturer at the Chemistry Department of University of Cyprus, he taught Medicinal Chemistry, Biochemistry, X-ray Protein Crystallography to undergraduate students and also Enzymology-Structural Biology as part of a postgraduate course. He also taught Enzymology at the MSc Program in Food Science and Technology of the Technological Educational Institute of Athens. Currently he is teaching Enzymology at the joint MSc program "Bioentrepreneurship" (University of Thessaly - NHRF) and Structural Biology at the joint MSc program "Biotechnology" (National and Kapodistrian university of Athens – NHRF). He is supervising /has supervised 8 Post-doctoral researchers, 4 PhD and 16 MSc Theses, 9 final year research projects and 3 Internships.

His research activities have been supported by 10 EU grants (2 as coordinator), 12 national grants from GSRT, NSRF-EPAnEK, Hellenic Foundation for Research and

Innovation (H.F.R.I.), State Scholarships Foundation (IKY) (4 as coordinator) and 3 research grants from Cyprus RPF (1 as coordinator) as well as by 2 collaborative projects with Sanofi-Aventis Pharma and Pfizer Inc., USA. He has received 33 EU travel/access grants for X-ray crystallographic data collection (more than 500 shifts) and HT-protein expression at EU large scale facilities/laboratories.

He was elected Board member (2010-2014) and President (2014-2020) of the Hellenic Crystallographic Association (HeCrA). Currently, he serves as elected member of the Scientific Council of ICB (ΕΣΙ) and Deputy Director and member of the Coordination Committee of the MSc program "Bioentrepreneurship".

Research interests

The general theme that underlies the work of Dr. Zographos' research team is the functional and structural studies of proteins of pharmaceutical and biotechnological interest. His team utilizes recombinant DNA technology, protein expression and advanced protein purification techniques in conjunction with biochemical binding assays, enzyme kinetics and X-ray protein crystallography to gain a deep understanding of the structure/function relationship and regulation of protein targets of interest. This information can guide both computational and synthetic chemists to the rational design, synthesis and discovery of novel therapeutic agents and other products of biotechnological interest.

His current research interest include pharmacological and biotechnological targets involved in: Type 2 diabetes mellitus (glycogen phosphorylase and glucokinase), Cancer (human Coilin Interacting Nuclear ATPase; hCINAP and BRAF(V600E), Inflammation (Ligand Binding Domain of Glycocorticoid Receptor; GR-LBD), Aging (human Proteasome) Melanogenesis and enzymatic browning in foods and beverages (Tyrosinase) and Chemoreception in insects (mosquito and oriental fruit fly Odorant Binding Proteins; OBPs and mosquito Odorant Receptor co-receptor ORco).

Over the past decade, structure-assisted inhibitor design studies, have led to the discovery of more than 100 inhibitors of **glycogen phosphorylase (GP)** enzyme (target for type 2 diabetes mellitus), including new synthetic inhibitor classes and natural products such as flavonoids and terpenes.

Since 2010, Dr. Zographos' research focuses on biochemical, molecular, functional and structural characterization of Mosquito and Pest insects **Odorant Binding Proteins (OBPs)**, as molecular targets for the structure-based discovery of novel host-seeking disruptors, repellents or attractants. Since 2020, the research in insect olfaction was expanded to the mosquito **7-transmembrane Odorant Receptor coreceptor (ORco)**. The goal of this direction is the application of OBP- and ORco-structure-based approaches for the discovery of multiple new and effective agents to be employed in the effort to reduce the spread of insect-transmitted infectious diseases as well as control insects of agricultural importance.

Education and qualifications

2000: PhD in Chemistry, National and Kapodistrian University of Athens

1996: X-ray protein crystallography trainee, University of Oxford, U.K.

1994: X-ray protein crystallography trainee, University of Oxford, U.K.

1993: X-ray protein crystallography trainee, University of Oxford, U.K.

1992: BSc in Chemistry, National and Kapodistrian University of Athens

Fellowships

2005-2007: Marie Curie Reintegration Fellowship by the European Union (24 months)
2001-2004: Marie Curie Postdoctoral Fellowship by the European Union (36 months)
1992-1997: Doctoral studentship from the National Hellenic Research Foundation (48 months)

Appointments

Jul 2018 - present: Research Director, ICB, NHRF
Mar 2010-Jul 2018: Senior Researcher, IBMCB, NHRF
Mar 2006-Feb 2009: Research Assistant, IOPC, NHRF
Sep 2004-Feb 2006: Marie Curie Postdoctoral Fellow, IOPC, NHRF
Aug 2001-Aug 2004: Marie Curie Postdoctoral Fellow, Dept. of Biol. Sciences, UCY
Sep 2000-Jun 2001: Visiting Lecturer, Dept. of Chemistry, UCY
Feb 2000-Aug 2000: Postdoctoral Fellow, IBRB, NHRF
Jan 1998-Dec 2000: Second Lieutenant, Supply and Transp. Corps, Hellenic Army

Committee membership

2014-present: Member of the Scientific Advisory Board of Institute of Biology, Medicinal Chemistry and Biotechnology, NHRF.
2014-present: Deputy Director & Member of the Coordination committee of MSc program "Bioentrepreneurship"
2014-2020: President of the Hellenic Crystallographic Association
2010-2014: Elected board member (treasurer) of the Hellenic Crystallographic Association
2008-present: Permanent board member of the "Nikos Oikonomakos award" for structural biology
2001-2002: Biology panel member (question selection committee) of the 2001 and 2002 pancyprian examinations for the admission of graduate secondary students to the Universities of Cyprus and Greece.
2001: Final year projects qualifying examination committee, Dept. of Chemistry, UCY
2008-present: Co-organizer for 21 conferences/workshops (7 as president of the organizing committee)

Professional activities

- Member of the Hellenic Crystallographic Association
- Member of the Hellenic Society of Biochemistry and Molecular Biology
- Member of the American Society of Molecular Biology and Biochemistry
- Member of the Greek Chemists' Association
- Member of the Hellenic Marie Curie fellows Association

Registered user (*since 1992*) of the synchrotron radiation sources: SRS (Daresbury, UK), Elletra (Trieste, Italy), EMBL-DESY (Hamburg, Germany) and MAX-Lab (Lund, Sweden), Diamond Light source (Oxford, UK)

Publications in refereed journals

1. Fytrou A, Papachristos, DP, Milonas, PG, Giatropoulos, A, **Zographos, SE**, and Michaelakis, A. (2022) Behavioural response of *Culex pipiens* biotype *molestus* to oviposition pheromone. *Journal of Insect Physiology* [Epub 2022 Mar 18] → [Journal](#) | [PubMed](#)

*JIF*²⁰²¹: **2.354**

2. Leonidas DD*, **Zographos SE***, Tsitsanou KE, Skamnaki VT, Stravodimos G, Kyriakis E (2021) Glycogen phosphorylase revisited: extending the resolution of the R- and T-state structures of the free enzyme and in complex with allosteric activators. *Acta Crystallogr F* 77, 303-311 → [Journal](#) | [PubMed](#)

*JIF*²⁰²¹: **1.056**

PDBs: [3E3L](#), [3E3N](#), [3E3O](#), [7P7D](#)

3. Kyriakis E, Karra AG, Papaioannou O, Solovou T, Skamnaki VT, Liggri PGV, **Zographos SE**, Szennyes E, Bokor E, Kun S, Psarra AG, Somsak L, Leonidas DD (2020) The architecture of hydrogen and sulfur sigma-hole interactions explain differences in the inhibitory potency of C-beta-d-glucopyranosyl thiazoles, imidazoles and an N-beta-d glucopyranosyl tetrazole for human liver glycogen phosphorylase and offer new insights to structure-based design. *Bioorg Med Chem.* 28, 115196 → [Journal](#) | [PubMed](#)

*JIF*²⁰²⁰: **3.409**

PDBs: [6S4H](#), [6S4K](#), [6S4O](#), [6S4P](#), [6S4R](#), [6S51](#), [6S52](#)

4. Szabo, KE, Kyriakis, E, Psarra, AG, Karra, AG, Sipos, A, Docsa, T, Stravodimos, GA, Katsidou, E, Skamnaki, VT, Liggri, PGV, **Zographos, SE**, Mandi, A, Kiraly, SB, Kurtan, T, Leonidas, DD, and Somsak, L (2019) Glucopyranosylidene-spiro-imidazolinones, a New Ring System: Synthesis and Evaluation as Glycogen Phosphorylase Inhibitors by Enzyme Kinetics and X-ray Crystallography. *J Med Chem.* 62, 6116-6136 → [Journal](#) | [PubMed](#)

*JIF*²⁰¹⁹: **6.336**

PDBs: [6QA6](#), [6QA7](#), [6QA8](#)

5. Fischer T, Koulas SM, Tsagkarakou AS, Kyriakis E, Stravodimos GA, Skamnaki VT, Liggri PGV, **Zographos SE**, Riedl R, Leonidas DD (2019) 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. *Molecules* 24, 1322+ → [Journal](#) | [PubMed](#)

*JIF*²⁰¹⁹: **3.309**

PDBs: [6ROH](#), [6ROI](#)

6. Thireou T, Kythreoti G, Tsitsanou KE, Koussis K, Drakou CE, Kinnersley J, Krober T, Guerin PM, Zhou, J-J, Iatrou K, Eliopoulos E, **Zographos SE*** (2018). Identification of novel bioinspired synthetic mosquito repellents by combined ligand-based screening and OBP-structure-based molecular docking. *Insect Biochem Mol Biol.* 98, 48–61 → [Journal](#) | [PubMed](#)

*JIF*²⁰¹⁸: **3.737**

7. Bokor E, Kyriakis E, Solovou TG, Koppány C, Kantsadi AL, Szabo KE, Szakacs A, Stravodimos GA, Docsa T, Skamnaki VT, **Zographos SE**, Gergely P, Leonidas DD, Somsak L (2017) Nanomolar inhibitors of glycogen phosphorylase based on beta-D-glucosaminyl heterocycles: a combined synthetic, enzyme kinetic and protein crystallography study. *J Med Chem.* 60, 9251–9262 → [Journal](#) | [PubMed](#)

*JIF*²⁰¹⁷: **6.590**

PDBs: [5050](#), [5052](#), [5054](#), [5056](#)

8. Drakou CE, Tsitsanou KE, Potamitis C, Fessas D, Zervou M, **Zographos SE*** (2017) The crystal structure of the AgamOBP1*Icaridin complex reveals alternative binding modes and stereo-selective repellent recognition. *Cell Mol Life Sci.* 74, 319–338 → [Journal](#) | [PubMed](#)

*JIF*²⁰¹⁷: **6.998**

PDBs: [5EL2](#)

9. Peppas VI, Venkat H, Kantsadi AL, Inamdar SR, Bhat GG, Eligar S, Shivanand A, Chachadi VB, Satisha GJ, Swamy BM, Skamnaki VT, **Zographos SE**, Leonidas DD (2015) Molecular Cloning, Carbohydrate Specificity and the Crystal Structure of Two Sclerotium rolfsii Lectin Variants. *Molecules* 20, 10848-65 → [Journal](#) | [PubMed](#)

*JIF*²⁰¹⁵: **2.465**

PDBs: [4YLD](#), [4Z2F](#), [4Z2Q](#), [4Z2S](#)

10. Parmenopoulou V, Kantsadi AL, Tsirkone VG, Chatzileontiadou DS, Manta S, **Zographos SE**, Molfeta C, Archontis G, Agius L, Hayes JM, Leonidas DD, Komiotis D. (2014) "Structure based inhibitor design targeting glycogen phosphorylase b. Virtual screening, synthesis, biochemical and biological assessment of novel N-acyl-β-d-glucopyranosylamines" *Bioorg Med Chem.* 22, 4810-25 → [Journal](#) | [PubMed](#)

*JIF*²⁰¹⁴: **2.793**

PDBs: [4MHO](#), [4MHS](#), [4MIC](#), [4MI3](#), [4MI6](#) & [4MI9](#)

11. Czifrák K, Páhi A, Deák S, Kiss-Szicszai A, Kövér KE, Docsa T, Gergely P, Alexacou KM, Papakonstantinou M, Leonidas DD, **Zographos SE**, Chrysiná ED, Somsák L. (2014) "Glucopyranosylidene-spiro-iminothiazolidinone, a new bicyclic ring system: synthesis, derivatization, and evaluation for inhibition of glycogen phosphorylase by enzyme kinetic and crystallographic methods" *Bioorg Med Chem.* 22, 4028-41 → [Journal](#) | [PubMed](#)

*JIF*²⁰¹⁴: **2.793**

PDBs: [4CTM](#), [4CTN](#) & [4CTO](#)

12. Tsitsanou KE, Drakou CE, Thireou T, Gruber AV, Kythreoti G, Azem A, Fessas D, Eliopoulos E, Iatrou K, **Zographos SE*** (2013) "The crystal and solution studies of the "Plus-C" odorant binding protein 48 from *Anopheles gambiae*: Control of binding specificity through 3D domain-swapping" *J Biol Chem* **288**, 33427-38 → [Journal](#) | [PubMed](#)

*JIF*²⁰¹³: **4.600**

PDBs: [4IJ7](#) & [4KYN](#)

13. Skamnaki VT, Peumans WJ, Kantsadi AL, Cubeta MA, Plas K, Pakala S, **Zographos SE**, Smaghe G, Nierman WC, Van Damme EJ, Leonidas DD. (2013) "Structural analysis of the *Rhizoctonia solani* agglutinin reveals a domain swapping dimeric assembly" *FEBS J.* **280**, 1750-1763 → [Journal](#) | [PubMed](#)

*JIF*²⁰¹³: **3.986**

PDBs: [4G9M](#) & [4G9N](#)

14. Tsitsanou KE, Hayes JM, Keramioti M, Mamais M, Oikonomakos NG, Kato A, Leonidas DD, **Zographos SE*** (2013) "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." *Food Chem Toxicol* **61**, 14-27 → [Journal](#) | [PubMed](#)

*JIF*²⁰¹³: **2.610**

PDBs: [3EBO](#) & [3EBP](#)

15. Parmenopoulou V, Chatzileontiadou DS, Manta S, Bougiatioti S, Maragozidis P, Gkaragkouni DN, Kaffesaki E, Kantsadi AL, Skamnaki VT, **Zographos SE**, Zounpoulakis P, Balatsos NA, Komiotis D, Leonidas DD (2012) "Triazole pyrimidine nucleosides as inhibitors of Ribonuclease A. Synthesis, biochemical, and structural evaluation." *Bioorg Med Chem.* **20**, 7184-7193. → [Journal](#) | [PubMed](#)

*JIF*²⁰¹²: **2.903**

PDBs: [4G90](#), [4G8V](#) & [4G8Y](#)

16. A.L. Kantsadi, S. Manta, A.-M.G. Psarra, A. Dimopoulou, C. Kiritsis, V. Parmenopoulou, V.T. Skamnaki, P. Zoumpoulakis, **S.E. Zographos**, D.D. Leonidas, and D. Komiotis (2012) "The binding of C5-alkynyl and alkylfurano[2,3-d]pyrimidine glucopyranonucleosides to glycogen phosphorylase b. Synthesis, biochemical and biological assessment." *European Journal of Medicinal Chemistry* **54**, 740-749. → [Journal](#) | [PubMed](#)

*JIF*²⁰¹²: **3.499**

PDBs: [4EJ2](#), [4EKE](#), [4EL5](#), [4EKY](#) & [4ELO](#)

17. 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) "N-(4-Substituted-benzoyl)-N'-(β-d-glucopyranosyl)ureas as inhibitors of glycogen phosphorylase: Synthesis and evaluation by kinetic, crystallographic, and molecular modelling methods" *Bioorg Med Chem.* **20**, 1801-1816. → [Journal](#) | [PubMed](#)

*JIF*²⁰¹²: **2.903**

PDBs: [2QNB](#), [2QLM](#), [2QLN](#), [2QN3](#), [2QN7](#), [2QN8](#) & [2QN9](#)

18. Manta S, Xipnitou A, Kiritsis C, Kantsadi AL, Hayes JM, Skamnaki VT, Lamprakis C, Kontou M, Zoumpoulakis P, **Zographos SE**, Leonidas DD, Komiotis D. (2012) "3'-axial CH₂ OH substitution on glucopyranose does not increase glycogen phosphorylase inhibitory potency. QM/MM-PBSA calculations suggest why." *Chem Biol Drug Des.* 79, 663-673. → [Journal](#) | [PubMed](#)

*JIF*²⁰¹²: 2.469

PDBs: [3SYM](#) & [3SYR](#)

19. Kantsadi AL, Hayes JM, Manta S, Skamnaki VT, Kiritsis C, Psarra AM, Koutsogiannis Z, Dimopoulou A, Theofanous S, Nikoleousakos N, Zoumpoulakis P, Kontou M, Papadopoulos G, **Zographos SE**, Komiotis D, Leonidas DD. (2012) "The σ -hole phenomenon of halogen atoms forms the structural basis of the strong inhibitory potency of C5 halogen substituted glucopyranosyl nucleosides towards glycogen phosphorylase b" *ChemMedChem.* 7, 722-732. → [Journal](#) | [PubMed](#)

*JIF*²⁰¹²: 2.835

PDBs: [3T3D](#), [3T3E](#), [3T3G](#), [3T3H](#) & [3T3I](#)

20. Christina E. Drakou, Anna Malekkou, Joseph M. Hayes, Carsten W. Lederer, Demetres D. Leonidas, Nikos G. Oikonomakos, Angus I. Lamond, Niovi Santama, and **Zographos SE*** (2012) "hCINAP is an atypical mammalian nuclear adenylate kinase with an ATPase motif: Structural and functional studies" *Proteins* 80, 206-220. → [Journal](#) | [PubMed](#)

*JIF*²⁰¹²: 3.337

PDBs: [3I1J](#), [3I1K](#), [3I1L](#) & [3I1M](#)

21. Tsitsanou KE, Thireou T, Drakou CE, Koussis K, Keramioti MV, Leonidas DD, Eliopoulos E, Iatrou K, **Zographos SE*** (2012) "Anopheles gambiae odorant binding protein crystal complex with the synthetic repellent DEET: implications for structure-based design of novel mosquito repellents" *Cellular Molecular Life Sci.* 69, 283-297. → [Journal](#) | [PubMed](#)

*JIF*²⁰¹²: 5.615

PDB: [3N7H](#)

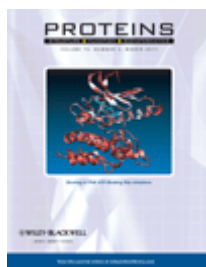
22. Alexacou KM, Zhang YZ, Praly JP, **Zographos SE**, Chrysina ED, Oikonomakos NG, Leonidas DD (2011) "Halogen-substituted (C- β -d-glucopyranosyl)-hydroquinone regioisomers: Synthesis, enzymatic evaluation and their binding to glycogen phosphorylase" *Bioorgan Med Chem* 19, 5125-5136. → [Journal](#) | [PubMed](#)

*JIF*²⁰¹¹: 2.921.

PDBs: [3NP7](#), [3NP9](#), [3NPA](#) & [3SOJ](#)

23. J.M. Hayes, V.T. Skamnaki, G. Archontis, C. Lamprakis, J. Sarrou, N. Bischler, A-L. Skaltsounis, **S.E. Zographos**, N.G. Oikonomakos (2011) "Kinetics, in silico docking, molecular dynamics and MM-GBSA binding studies on prototype indirubins, KT5720 and staurosporine as phosphorylase kinase ATP-binding site inhibitors: The role of water molecules examined" *Proteins* 79, 703-719. → [Journal](#) | [PubMed](#)

Cover Story



*JIF*²⁰¹¹: **3.392**

24. V.G. Tsirkone, E. Tsoukala, C. Lamprakis, S. Manta, J.M. Hayes, V.T. Skamnaki, C. Drakou, **S.E. Zographos**, D. Komiotis, D.D. Leonidas (2010) "1-(3-Deoxy-3-fluoro-beta-D-glucopyranosyl) pyrimidine derivatives as inhibitors of glycogen phosphorylase b: Kinetic, crystallographic and modelling studies" *Bioorgan Med Chem* **18**, 3413-3425. → [Journal](#) | [PubMed](#)

*JIF*²⁰¹⁰: **2.978**.

PDBs: [3L79](#), [3L7A](#), [3L7B](#), [3L7C](#) & [3L7D](#)

25. K.M. Alexacou, A.C. Tenchiu Deleanu, E.D. Chrysina, M.D. Charavgi, I.D. Kostas, **S.E. Zographos**, N.G. Oikonomakos, D.D. Leonidas (2010) "The binding of β -D-glucopyranosyl-thiosemicarbazone derivatives to glycogen phosphorylase: A new class of inhibitors" *Bioorgan Med Chem* **18**, 7911-7922. → [Journal](#) | [PubMed](#)

*JIF*²⁰¹⁰: **2.978**.

PDBs: [3MQF](#), [3MTA](#), [3MTZ](#), [3MS7](#), [3MTB](#), [3MT8](#), [3MS4](#), [3MSC](#), [3MT9](#), [3NC4](#), [3MRV](#), [3MTD](#), [3MRX](#), [3MS2](#) & [3MRT](#)

26. Dossi K, Tsirkone VG, Hayes JM, Matousek J, Pouckova P, Soucek J, Zadinova M, **Zographos SE**, & Leonidas DD (2009) "Mapping the ribonucleolytic active site of bovine seminal ribonuclease. The binding of pyrimidinyl phosphonucleotide inhibitors" *Eur J Med Chem* **44**, 4496-4508. → [Journal](#) | [PubMed](#)

*JIF*²⁰⁰⁹: **3.269**

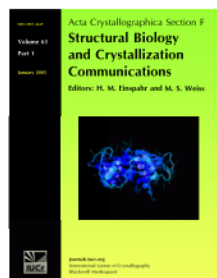
PDBs: [3DJO](#), [3DJP](#), [3DJQ](#), [3DJV](#) & [3DJX](#)

27. Benlifa M, Hayes JM, Vidal S, Gueyrard D, Goekjian PG, Praly J-P, Kizilis G, Tiraidis C, Alexacou K-M, Chrysina ED, **Zographos SE**, Leonidas DD, Archontis G & Oikonomakos NG (2009) "Glucose-based Spiro-isoxazolines: A New Family of Potent Glycogen Phosphorylase Inhibitors" *Bioorgan Med Chem* **17**, 7368-7380. → [Journal](#) | [PubMed](#)

*JIF*²⁰⁰⁹: **2.822**

PDBs: [2QRG](#), [2QRH](#), [2QRM](#), [2QRP](#) & [2QRQ](#)

28. Tsirkone VG, Dossi K, Drakou C, **Zographos SE**, Kontou M & Leonidas DD (2009) "Inhibitor design for ribonuclease A: the binding of two 5'-phosphate uridine analogues" *Acta Crystallogr F* **65**, 671-677. → [Journal](#) | [PubMed](#)
Cover Story



*JIF*²⁰⁰⁹: **0.551**

PDBs: [3DXG](#) & [3DXH](#)

29. Chrysina ED, Bokor E, Alexacou KM, Charavgi MD, Oikonomakos GN, **Zographos SE**, Leonidas DD, Oikonomakos NG & Laszlo S (2009) "Amide-1,2,3-triazole bioisosterism: the glycogen phosphorylase case" *Tetrahedron-Asymmetry* **20**, 733-740. → [Journal](#)

*JIF*²⁰⁰⁹: **2.625**

PDBs: [3G2H](#), [3G2L](#), [3G2K](#), [3G2I](#), [3G2N](#) & [3G2J](#)

30. Samanta A, Leonidas DD, Dasgupta S, Pathak T, **Zographos SE** & Oikonomakos NG (2009) "Morpholino, Piperidino, and Pyrrolidino Derivatives of Pyrimidine Nucleosides as Inhibitors of Ribonuclease A: Synthesis, Biochemical, and Crystallographic Evaluation" *J Med Chem* **52**, 932-942. → [Journal](#) | [PubMed](#)

*JIF*²⁰⁰⁹: **4.802**

PDBs: [3D6Q](#), [3D6P](#), [3D6Q](#), [3D7B](#), [3D8Y](#) & [3D8Z](#)

31. Wen XA, Sun HB, Liu J, Cheng KG, Zhang P, Zhang LY, Hao J, Ni PZ, **Zographos SE**, Leonidas DD, Alexacou KM, Gimisis T, Hayes JM & Oikonomakos NG (2008) "Naturally occurring pentacyclic triterpenes as inhibitors of glycogen phosphorylase: Synthesis, structure-activity relationships, and X-ray crystallographic studies" *J Med Chem* **51**, 3540-3554. → [Journal](#) | [PubMed](#)

*JIF*²⁰⁰⁸: **4.898**

PDBs: [2QN1](#) & [2QN2](#)

32. Alexacou KM, Hayes JM, Tiraidis C, **Zographos SE**, Leonidas DD, Chrysina ED, Archontis G, Oikonomakos NG, Paul JV, Varghese B & Loganathan D (2008) "Crystallographic and computational studies on 4-phenyl-N-(beta-D-glucopyranosyl)-1H-1,2,3-triazole-1-acetamide, an inhibitor of glycogen phosphorylase: Comparison with alpha-D-glucose, N-acetyl-beta-D-glucopyranosylamine and N-benzoyl-N'-beta-D-glucopyranosyl urea binding" *Proteins* **71**, 1307-1323. → [Journal](#) | [PubMed](#)

*JIF*²⁰⁰⁸: **3.419**

PDBs: [2PYD](#) & [2PYI](#)

33. Tiraidis C, Alexacou KM, **Zographos SE**, Leonidas DD, Gimisis T & Oikonomakos NG (2007) "FR258900, a potential anti-hyperglycemic drug, binds at the allosteric site of glycogen phosphorylase" *Protein Sci* **16**, 1773-1782. → [Journal](#) | [PubMed](#)

*JIF*²⁰⁰⁷: **3.135**

PDB: [2OFF](#)

34. Pantelidou M, **Zographos SE**, Lederer CW, Kyriakides T, Pfaffl MW & Santama N (2007) "Differential expression of molecular motors in the motor cortex of sporadic ALS" *Neurobiol Dis* **26**, 577-589. → [Journal](#) | [PubMed](#)

*JIF*²⁰⁰⁷: **4.377**

NCBI GeneBank: [AM177178](#), [AM177179](#), [AM177180](#), [AM180763](#), [AM180764](#),
[AM180765](#) & [AM231689](#)

NCBI dbSNP: [ss52050753](#), [ss52085996](#), [ss65640445](#)

35. Leonidas DD, Swamy BM, Hatzopoulos GN, Gonchigar SJ, Chachadi VB, Inamdar SR, **Zographos SE** & Oikonomakos NG (2007) "Structural basis for the carbohydrate recognition of the *Sclerotium rolfsii* lectin" *J Mol Biol* **368**, 1145-1161. → [Journal](#) | [PubMed](#)

*JIF*²⁰⁰⁷: **4.472**

PDBs: [20FC](#), [20FD](#) & [20FE](#)

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PDBs: [2G9Q](#), [2G9V](#), [2G9R](#) & [2G9U](#)

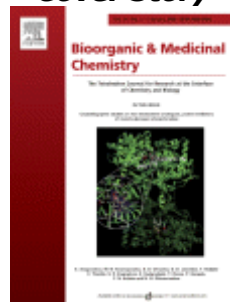
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PDBs: [2G8Q](#) & [2G8R](#)

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PDBs: [1WW2](#) & [1WW3](#)

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PDB: [1H5U](#)

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PDBs: [1K06](#), [1K08](#) & [1KTI](#)

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Interviews

- Interview "Research on the development of plant repellents from the Greek flora" on the morning show of Ms. K. Houzouri, at the **radio station of the Church of Greece, 98.5 FM 30/62020**. → [Listen the interview \(in Greek\)](#)
- Newspaper article entitled "A daisy that can cut the wings of a...tiger" about research of QFytoTera consortium on insect repellents. **In newspaper "Kathimerini", Sunday edition, published on 28/6/2020, No. sheet 30.455, p.32** (Editor Ms. Ioanna Fotiadi). → [Digital edition \(in Greek\)](#)
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Research Funding

Running funded projects

➤ As coordinator and/or Scientific Responsible

- "3D-ORco: Advanced Research on the 3D structure of Mosquito Odorant Receptor coreceptor". Hellenic Foundation for Research and Innovation (H.F.R.I.) under the "1st Call for H.F.R.I. Research Projects to support Faculty members and Researchers and the procurement of high-cost research equipment" (Project Number: HFRI-FM17-637) in collaboration with NCSR-Demokritos, Hellenic Pasteur Institute, University of Helsinki, Finland and University of Dublin, Ireland (28/2/2020-31/8/2023). **Budget: 180.000 €**.

- **"QFytoTera:** Nanoemulsions of plant oils with moisturizing and insect repellent properties" under the Operational Programme "Research, Entrepreneurship and Innovation" EPAnEK-NSRF 2014-2020 (MIS 5030853) for collaborative R&D projects between academic institutions and the private sector (in collaboration with Qualia Pharma Ltd., Benaki Phytopathological Institute and the University of Patras). **(9/7/2018-8/7/2022). Budget: 630,005.37 €**

➤ *As partner*

- **"INSPIRED:** The National Research Infrastructures on Integrated Structural Biology, Drug Screening Efforts and Drug target functional characterization" National Research Infrastructures NSRF (ΕΠΑνΕΚ) 2014-2020. Coordinator Dr. E. Chrysina **(3/9/2018-30/9/2022). Budget for SBC1: 76,000€ (Upgrade of Crystallization Infrastructure).** Role: **Partner/member of the steering committee**
- **"OMIC-ENGINE** Synthetic Biology: from omics technologies to genomic engineering" National Research Infrastructures NSRF (ΕΠΑνΕΚ) 2014-2020. Coordinator Prof. K. Mathiopoulos, University of Thessaly (Scientist in charge for ICB/NHRF Dr. G. Skretas), **(1/1/2018-30/6/2022) Budget for SBC1: 500€ (travels).** Role: **Partner**

Completed funded projects

➤ *As coordinator and/or Scientific Responsible for ICB*

- **"IKYMOS:** Mosquito Odorant Binding Proteins as molecular targets for the discovery of new effective repellents/attractants. "State Scholarships Foundation (IKY) Doctorate Scholarship 2016-2019 to Ms. P. Liggri" NSRF (ΕΣΠΑ) 2014-2020 **(8/12/2016-7/12/2019). Scholarship: 29.408,4 €.**
Role: Supervisor
- **"PREVENT:** Molecular, functional and structural analysis of Mosquito OBPs for Prevention of Vector-Borne Infectious Diseases" General Secretariat for Research and Technology, Research grant ESPA R&D project of bilateral cooperation Greece-Turkey 2013-2014 in collaboration with Ass. Prof. M. Senay Sengul, Department of Molecular Biology and Genetics, Gaziosmanpasa University, Tokat, Turkey **(20/12/2013-31/12/2015).** Coordinator Dr. S. E. Zographos, IBMCB/NHRF. **Budget: 30,000 €**
Role : Coordinator/ Scientific Responsible
- **"ENAROMaTIC:** European Network for Advanced Research on Olfaction for Malaria Transmitting Insect Control." FP7-HEALTH-2007-2.3.2-9 (GA-222927), **(1/12/2008-30/11/2012);** Coordinator Dr. K. Iatrou, NCR Demokritos. **Budget for SBC1: 280,000 €**
Role : Scientist in charge for ICB /WP5 leader
- **"EUROSTRUCT:** European consolidation and promotion of research capacity in the area of structure based drug discovery". FP7-REGPOT-2008-1, (GA-230146), **(1/2/2009-31/1/2012);** Coordinator Dr. S. E. Zographos, IBMCB/NHRF. **Budget: 970,300 €.**
Role: Coordinator.
<http://www.eie.gr/nhrf/institutes/iopc/eu-projects/eurostruct/index-en.html>
- **"Protein complexes of CINAP:** composite molecular targets for the understanding of human disease". Cyprus Research Promotion Foundation, Thematic Research Grant YGEIA,

GA-0506/05 (2007-2009). Coordinator Prof. N. Santama, University of Cyprus. **Budget for PI: 16,879 €**

Role : Scientist in charge for ICB

- **"Structure-function relationship of TAF9 proteins"** Human Resources and Mobility activity, Marie Curie European Reintegration Grant, MERGE-CT-2004-006358, (2004-2005). **Budget: 40,000 €.**
Role : Coordinator
- **"Structure/function relationships of recombinant human TAFs9 proteins"** Greek General Secretariat for Research and Technology, Research Grant ENTER 2001, GA-01ER 115 (2004-2006). Coordinator Dr. N. Oikonomakos, NHRF. **Budget: 65,588 €.**
Role : Reintegrated Researcher/ Scientist in charge for ICB

➤ *As partner*

- **"STHENOS-β:** Targeted therapeutic approaches against degenerative diseases, with emphasis on cancer and aging: Optimization of targeted bioactive compounds" Ministry of Education, Lifelong Learning, and Religious Affairs, "Development Proposals of Research Institutions - KRIPIS", NSRF 2014-2020. O.P. "Competitiveness & Entrepreneurship" and Regions in Transition" (1/1/2017-30/06/2021); Coordinator Dr. A. Pintzas (IBM CB Director), IBM CB/ NHRF. **Budget for SBC1: 46,800€ (Personnel and consumables).**
Role: Partner/WP1 leader
- **"INSTRUCT-Ultra:** Releasing the full potential of Instruct (Integrating infrastructures for Structural Biology) to expand and consolidate infrastructure services for integrated structural life science research". H2020-INFRADEV-2016-1 (GA-731005) (01/01/2017-31/12/2020). Coordinator D. Stuart, University of Oxford (Scientist in charge for IBM CB/NHRF Dr. E. Chrysina), **Budget for SBC1: 750€ (travels).** **Role: Partner/Member of the general assembly.**
- **"IKYMOS-Pos:** A combined methodology for the discovery of compounds with insect repellency properties" IKY Fellowships of Excellence for Postgraduate Studies in Greece-Siemens Program to Dr. E. Kritsi. (16/04/2017- 31/08/2017) Scientific Responsible: P.Zoumpoulakis. **Budget: 13,500 €**
Role : Partner
- **'STHENOS:** Targeted therapeutic approaches against degenerative diseases, with emphasis on cancer and aging" Ministry of Education, Lifelong Learning, and Religious Affairs, "Development Proposals of Research Institutions - KRIPIS", NSRF 2007-2013. O.P. "Competitiveness & Entrepreneurship" and Regions in Transition" (1/1/2013-31/12/2015); Coordinator Dr. A. Pintzas (IBM CB Director), IBM CB/ NHRF. **Budget for SBC1: 120,000 €**
Role : Partner
- **"ARCADE:** Advancement of Research Capability for the Development of New Functional Compounds" FP7-REGPOT-2009-1, (GA-245866), (01/12/2009-30/5/2013); Coordinator Dr. B. Steele, IBM CB/NHRF. **Budget for SBC1: 205,000 €**
Role : Partner

- **“Crystallisation, co-crystallisation, and crystallographic studies with human pancreatic glucokinase, a molecular target for types 2 diabetes therapy”** by Aventis Pharma Deutschland GmbH, a company of the sanofi-aventis group, Frankfurt, Germany (2005-2006). Coordinator Dr. N. Oikonomakos, NHRF **Budget: 10,000 €**.
Role : Principal Investigator.
- **“Structure/function relationships of new human protein CIP1 with molecular pathogenesis of neurodegenerative disorders”**. Cyprus Research Promotion Foundation, Research Grant PENEK 2004-2005, ENISX 0603/03 (2004-2006). Coordinator Prof. N. Santama, University of Cyprus. **Budget Total/for PI: 60,000/3,595 €**. Role: **Scientist in charge from 1.06.2004 to 31.8.200. From 01.09.2004 PI moved back to Greece and continued the project as Principal Investigator at NHRF.**
- **“Inhibitors of glycogen phosphorylase and phosphorylase kinase as potential antidiabetic drugs”** Greek General Secretariat for Research and Technology, Research grant ENTER 2004, GA-04ER 70 (2006-2008). Coordinator Dr. N. Oikonomakos (**passed away on 31.08.2008**), NHRF. **Budget: 78,000 €** (Business Partner **Pfizer Inc**, Pfizer Global Research & Development, Groton Laboratories, USA; Contribution **8,000 €**) Role: **Principal Investigator. Coordinator from 1.09.2008 to 31.10.2008.**
- **“DRUGDESI: Drug design at the molecular level using approximate and exact computational methods”** Marie Curie Host Fellowships for the Transfer of Knowledge, MTKD-CT-2006-042776 (2007-2011). Coordinator Dr. N. Oikonomakos, (Dr. E. Chrysina since 1.09.2008), NHRF. **Budget: 186,396.40 €**.
Role: Collaborator (Structural and kinetic studies).
- **“EURODESY: A European Research Training Site for the Design and Synthesis of Novel Neuroprotective and Hypoglycaemic Agents through a Multi-disciplinary approach”** Marie Curie Early Stage Training (EST), MEST-CT-020575 (2006-2010). Coordinator Dr. N. Oikonomakos (Dr. D. Leonidas and Dr. I. Kostas since 1.09.2008), NHRF. **Budget: 984,182 €**.
Role: Collaborator (Structural and kinetic studies of glycogen phosphorylase, co-organizer/tutor of the workshop entitled “Workshop on Structure Based Drug Discovery” in the frame of EURODESY, NHRF, 2-6 June 2008).
- **“EURORES: European Researchers’ Night in Greece”** FP7-PEOPLE-NIGHT-2008, CN-22, (2008). Coordinator Dr. N. Oikonomakos, NHRF. **Budget: 50,000 €**.
Role: Member of the implementation team.
- **“A Training, Implementation and Discrimination (TID) centre** (Heraklion TID-Centre) of the EU project «BIOXHIT»”. BIOXHIT stands for Biocrystallography (X) on a Highly Integrated Technology Platform for European Structural Genomics and is funded under the FP6 of the EC (LSHG-CT-2003-503420) (2006-2008). Coordinator for Heraklion TID-Centre: Dr. K. Petratos, Institute of Molecular Biology and Biotechnology, Crete. **Budget: 60,000 €**.
Role: Collaborator (co-organizer of the international workshop entitled “From Crystals to Structures: Crystallization, Diffraction Data Collection, Processing and Phasing” 23-25 June 2008, IMBB-FORTH, Crete, Greece).
- **“Discovery of small-molecule inhibitors of glycogen phosphorylase, as potential hypoglycaemic agents, guided by structure-based drug design and in silico virtual ligand screening”** Greek General Secretariat for Research and Technology (EPAN) Research Grant for Scientific and Technological cooperation between Greece and USA, Prof.

Alexander D. MacKerell, Jr., Computer-Aided Drug Design Center, School of Pharmacy, Univ. of Maryland, Baltimore, MD, USA (USA 046) (**2004-2006**). Coordinator Dr. N. Oikonomakos, NHRF. **Budget: 60,000 €.**

Role: Collaborator (Structural and kinetic studies of glycogen phosphorylase).

- **"Kinesin Molecular Motors and Neurodegenerative Diseases: The case of ALS (Amyotrophic Lateral Sclerosis)"**, TELETHON Foundation (Cyprus), Research Grant (**2004-2005**). Coordinator Prof. N. Santama, University of Cyprus. **Budget: 60,000 €.**
Role: Post doctoral fellow (2 months).
- **"Structure-based design of new potential hypoglycaemic drugs"** General Secretariat for Research and Technology, Research grant EPAN R&D project of bilateral cooperation Greece-Hungary in collaboration with Prof. László Somsák, Department of Organic Chemistry, University of Debrecen, Hungary (**2003-2005**). Coordinator Dr. N. Oikonomakos, NHRF. **Budget: 11,740 €.**
Role: Collaborator (Structural and kinetic studies of glycogen phosphorylase).
- **"Cellular functions of kinesin like proteins and their role in human diseases"**, FP5-Improving Human Research Potential, Marie Curie Research Training Networks, GA IHP-RTN-99-1 (**2000-2004**). A collaborative research programme with 6 participating laboratories. Coordinator for University of Cyprus Prof. N. Santama. **Budget: 260,000 €.** **Role: Post doctoral fellow** (36 months).
- **"Structure-function relationship of allosteric proteins of muscle cells: molecular recognition and rational design of potential drugs"**. PENED-1999 (**1999-2000**), Ministry of Development, General Secretariat of Research and Technology (EPET II). Coordinator Dr. N. Oikonomakos, NHRF
Role: Post doctoral fellow
- **"Crystallographic studies of glycogen phosphorylase-inhibitor complexes of pharmacological importance"**, Access to modern instrumentation for X-ray crystallography". Institute of Molecular Biotechnology, Centre for Design and Structure in Biology (CDSB), Jena, Germany, (**1999-2000**). Coordinator Dr. N. Oikonomakos, NHRF.
Role : Post doctoral fellow

Access to European Large Infrastructures

- **"OBP structure-based discovery of novel marine-, plant-derived and bio-inspired compounds with mosquito repellent activity"** Project ID: 13686 (**2020**). iNEXT-DISCOVERY: Structural biology research infrastructures for translational research and discovery; H2020 project #871037, **Budget:** Expenses for shipment of samples. **Role : Principal Investigator**
- **"OBP-based reverse chemical ecology for the discovery of novel host-seeking disruptors of insects"** Project IDs: 2660 (**2017**), 6690 (**2018**). iNEXT: Access for translational research to European NMR, EM and X-rays infrastructures; H2020 project #653706. **Budget:** Travel, accommodation and shipment expenses.
Role : Principal Investigator
- **"Design of novel inhibitors of the oncogenic BRAFV600E protein kinase"** Project ID: 6668 (**2018**). iNEXT: Access for translational research to European NMR, EM and X-rays

infrastructures; H2020 project #653706. **Budget:** Travel, accommodation and shipment expenses.

Role : Principal Investigator

- **"Greek network of protein crystallographers 2018, 2020, 2021, 2022"**. Block Allocation Group (BAG) application for Access to EMBL synchrotron radiation facilities **2018-2022**; Project IDs: MX-619, MX-726, MX-840, MX-868. Coordinator: Dr E. Stratikos/Dr. P. Giastas.
Role: Principal Investigator
- **"Greek network of protein crystallographers 2016"**. Block Allocation Group (BAG) application for Access to EMBL synchrotron radiation facilities **2016-2017**; Project ID: MX-345, MX-372.
Role : Coordinator/Principal Investigator
- **"Greek network of protein crystallographers 2014"**. Block Allocation Group (BAG) application for Access to ALBA, Spain synchrotron radiation facilities **2015**; Project ID: **2014060919**. Coordinator: Dr S.E. Zographos.
Role : Coordinator/Principal Investigator
- **"Greek network of protein crystallographers 2014"**. Block Allocation Group (BAG) application for Access to EU synchrotron radiation facilities in the frame of FP7 project "BioStruct-X" (GA-283570), **2014-2015**; Coordinator: Dr G. Kontopidis. **Budget:** Travel and accommodation expenses.
Role : Principal Investigator
- **"Greek network of protein crystallographers 2013"**. Block Allocation Group (BAG) application for long-term Access to Max-lab, Sweden synchrotron radiation facilities **August 2013-July 2015**; Project ID: **20130015**. Coordinator: Dr S.E. Zographos.
Role : Coordinator/Principal Investigator
- **"Greek network of protein crystallographers 2013"**. Block Allocation Group (BAG) application for Access to ALBA, Spain synchrotron radiation facilities **2014**; Project ID: **2013100608**. Coordinator: Dr S.E. Zographos.
Role : Coordinator/Principal Investigator
- **"Greek network of protein crystallographers 2013"**. Block Allocation Group (BAG) Access to EU synchrotron radiation facilities in the frame of FP7 project "BioStruct-X" (GA-283570), **2013-2014**; Coordinator: Dr G. Kontopidis. **Budget:** Travel and accommodation expenses.
Role : Principal Investigator
- **"Advanced research for Mosquito Repellents"**, (Project No: PC-215; **2012**). Access to Structural Proteomics Facility OPPF, Rutherford Appleton Laboratory, Harwell Research Complex, Oxford, UK under the FP7 Capacities Specific Programme Research Infrastructures, "P-CUBE" (Infrastructure for Protein Production Platforms), (GA-227764). **Budget:** Travel, accommodation and subsistent expenses for a two (2) week visit.
Role : Principal Investigator
- **"Structural Studies using synchrotron Radiation of The Hellenic Structural Biology Network" (2011)**. Block Allocation Group (BAG) application for long-term Access to Max-

lab, Sweden synchrotron radiation facilities **July 2011-June 2013**; Project ID: **20110270**.
Coordinator: Dr D.D. Leonidas.

Role : Principal Investigator

- **"Instruct-Ellas, National consortium"**. Block Allocation Group (BAG) application for Access to EU synchrotron radiation facilities in the frame of FP7 project "BioStruct-X" (GA-283570), **(2011-2012)**. Coordinator: Dr E. Chrysina. **Budget:** Travel and accommodation expenses.
Role : Principal Investigator
- **"X-ray data collection at EU Synchrotron Radiation Sources"**. Access to EU synchrotron radiation facilities in the frame of FP6 Research Infrastructure Actions "Structuring the European Research Area", "ELISA" (European Light Sources Activities) **Budget:** Travel and accommodation expenses for visits to: **Synchrotron Radiation Source CCLRC Daresbury Laboratory, UK**, Project No: 44229, **(2005)**; 46131 **(2006)**; 48049 **(2007)**; 50114 **(2007)**, **MAX-lab, Lund, Sweden** Project No: PX-151-2007 **(2007)**; SAXS-149, **(2007)**; PX-178, **(2008)**; PX-184, **(2009-2010)**; Project No PX-123, **(2011-2012)**, **EMBL Hamburg Outstation, Germany** Project No: PX-03-16 **(2003)**; PX-05-181, **(2005)**; SAXS-07-12/SAXS-07-13, **(2007)**; SAXS-09-142/PX-09-29/PX-09-30 **(2009)**; PX-10-57/PX-10-58/PX-10-60/PX-10-61 **(2010)**; PX-10-80/PX-10-81, **(2011)**; MX-3, **(2012)**. **Role : Coordinator/Principal Investigator**