

Spyros E. Zographos

Senior Researcher

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Short CV (May 2016)



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 and a senior researcher in 2010. Spyros Zographos has deposited 145 protein structures at the Protein Data Bank, 30% of which were released in the last 3 years. His scientific achievements are presented in 55 peer-reviewed articles (h-index: 24, i10-index: 39, Times Cited: total 1,751; excluding self cited 1,538), 3 reviews, 4 chapters in books, 47 oral /poster presentations in conferences and 23 short communications.

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 is teaching Enzymology at the MSc Program in Food Science and Technology of the Technological Educational Institute of Athens and the joint MSc program in "Bioentrepreneurship" of University of Thessaly and NHRF. Furthermore, he has been co-organizer and/or tutor for 9 workshops and 2 international scientific symposiums on structure-based drug design. He is supervising /has supervised 2 PhD Thesis, 7 MSc and 7 final year research projects and 2 Internships.

His research activities have been supported by 10 EU (2 as coordinator), 7 national (3 as coordinator) and 3 Cypriot research grants (1 as coordinator) as well as by 2 collaborative projects with Sanofi-Aventis Pharma and Pfizer Inc., USA. He has received 11 EU travel grants for X-ray crystallographic data collection (more than 500 shifts) and HT-protein expression at EU large scale facilities/laboratories.

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), Inflammation (Ligand Binding Domain of Glycocorticoid Receptor; GR-LBD), Ciliopathies (Nucleotide binding proteins NUBP1 and NUBP2), Melanogenesis and enzymatic browning in foods and beverages (Tyrosinase) and Chemoreception in insects (mosquito and oriental fruit fly Odorant Binding Proteins; OBPs).

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 2009, Dr. Zographos' research focuses on Mosquito Odorant Binding Proteins (OBPs) as molecular targets for the structure-based discovery of novel host-seeking disruptors. His research team has developed and successfully validated a Ligand- & Structure-based Discovery Protocol which has led to the identification of promising novel repellents/attractants. The discovery of multiple disruptors of host seeking behavior of female mosquitoes will provide multiple new and effective tools to be employed in the effort to reduce the vector-borne diseases transmission.

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

1992-1997: Doctoral studentship from the National Hellenic Research Foundation (48 months)

2001-2004: Marie Curie Postdoctoral Fellowship by the European Union (36 months)

2005-2007: Marie Curie Reintegration Fellowship by the European Union (24 months)

Appointments

Mar 2010-present: 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: President of the Hellenic Crystallographic Association

2014-present: Member of the Scientific Advisory Board of Institute of Biology, Medicinal Chemistry and Biotechnology, NHRF.

2014-present: Member of the Coordination committee of MSc program "Bioentrepreneurship"

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

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), Elettra (Trieste, Italy), EMBL-DESY (Hamburg, Germany) and MAX-Lab (Lund, Sweden)

Publications in refereed journals

1. 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*²⁰¹⁵: **5.694**

PDBs: [5EL2](#)

2. 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](#)

3. 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](#)

4. Czifrák K, Páhi A, Deák S, Kiss-Szikszai A, Kövér KE, Dócsa 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](#)

5. 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: [4IJZ](#) & [4KYN](#)

6. Skamnaki VT, Peumans WJ, Kantsadi AL, Cubeta MA, Plas K, Pakala S, **Zographos SE**, Smagghe 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](#)

7. 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](#)

8. Parmenopoulou V, Chatzileontiadiou 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](#)

9. 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](#)

10. Nagy V, Felföldi N, Kónya B, Praly JP, Docsa T, Gergely P, Chrysin 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](#)

11. 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](#)

12. 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](#)

13. 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](#)

14. 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](#)

15. 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](#)

16. 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](#)

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*JIF*²⁰¹¹: **3.392**

17. 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](#)

18. 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](#)

19. 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](#)

20. Bentifa 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](#) & [2QRO](#)

21. 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](#)

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*JIF*²⁰⁰⁹: **0.551**

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

22. 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](#)

23. 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: [3D6O](#), [3D6P](#), [3D6Q](#), [3D7B](#), [3D8Y](#) & [3D8Z](#)

24. 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](#)

25. 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](#)

26. 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](#)

27. 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](#)

28. 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](#)

29. Oikonomakos NG, Tiraidis C, Leonidas DD, **Zographos SE**, Kristiansen M, Jessen CU, Norskov-Lauritsen L & Agius L (2006) "Iminosugars as potential inhibitors of glycogenolysis: Structural insights into the molecular basis of glycogen phosphorylase inhibition" *J Med Chem* 49, 5687-5701. → [Journal](#) | [PubMed](#)

*JIF*²⁰⁰⁶: 5.115

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

30. Leonidas DD, Maiti TK, Samanta A, Dasgupta S, Pathak T, **Zographos SE** & Oikonomakos NG (2006) "The binding of 3'-N-piperidine-4-carboxyl-3'-deoxy-ara-uridine to ribonuclease A in the crystal" *Bioorgan Med Chem* 14, 6055-6064. → [Journal](#) | [PubMed](#)

*JIF*²⁰⁰⁶: 2.624

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

31. Anagnostou E, Kosmopoulou MN, Chrysina ED, Leonidas DD, Hadjiloi T, Tiraidis C, **Zographos SE**, Gyorgydeak Z, Somsak L, Docsa T, Gergely P, Kollis FN & Oikonomakos NG (2006) "Crystallographic studies on two bioisosteric analogues, N-acetyl-beta-D-glucopyranosylamine and N-trifluoroacetyl-beta-D-glucopyranosylamine, potent inhibitors of muscle glycogen phosphorylase" *Bioorgan Med Chem* 14, 181-189. → [Journal](#) | [PubMed](#)

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*JIF*²⁰⁰⁶: 2.624

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

32. Watson KA, Chrysina ED, Tsitsanou KE, **Zographos SE**, Archontis G, Fleet GWJ & Oikonomakos NG (2005) "Kinetic and crystallographic studies of glucopyranose spirohydantoin and glucopyranosylamine analogs inhibitors of glycogen phosphorylase" *Proteins* 61, 966-983. → [Journal](#) | [PubMed](#)

*JIF*²⁰⁰⁵: 4.684

PDBs: [1FS4](#), [1FTQ](#), [1FTW](#), [1FTY](#), [1FU4](#), [1FU7](#) & [1FU8](#)

33. Archontis G, Watson KA, Xie Q, Andreou G, Chrysina ED, **Zographos SE**, Oikonomakos NG & Karplus M (2005) "Glycogen phosphorylase inhibitors: A free energy perturbation analysis of glucopyranose spirohydantoin analogues" *Proteins* **61**, 984-998. → [Journal](#) | [PubMed](#)

*JIF*²⁰⁰⁵: **4.684**

34. Santama N, Ogg SC, Malekku A, **Zographos SE**, Weis K & Lamond AI (2005) "Characterization of hCINAP, a novel coilin-interacting protein encoded by a transcript from the transcription factor TAFII(32) locus" *J Biol Chem* **280**, 36429-36441. → [Journal](#) | [PubMed](#)

*JIF*²⁰⁰⁵: **5.854**

NCBI GeneBank: [AJ878880](#) & [AJ878881](#)

35. Chrysina ED, Oikonomakos NG, **Zographos SE**, Kosmopoulou MN, Bischler N, Leonidas DD, Kovacs L, Docsa T, Gergely P & Somsak L (2003) "Crystallographic studies on alpha- and beta-D-glucopyranosyl formamide analogues, inhibitors of glycogen phosphorylase" *Biocatal Biotransfor* **21**, 233-242. → [Journal](#)

*JIF*²⁰⁰³: **1.085**

PDBs: [1P4G](#), [1P4H](#) & [1P4J](#)

36. Oikonomakos NG, **Zographos SE**, Skamnaki VT & Archontis G (2002) "The 1.76 angstrom resolution crystal structure of glycogen phosphorylase B complexed with glucose, and CP320626, a potential antidiabetic drug" *Bioorgan Med Chem* **10**, 1313-1319. → [Journal](#) | [PubMed](#)

*JIF*²⁰⁰²: **2.043**

PDB: [1H5U](#)

37. Oikonomakos NG, Kosmopoulou M, **Zographos SE**, Leonidas DD, Chrysina ED, Somsak U, Nagy V, Praly JP, Docsa T, Toth A & Gergely P (2002) "Binding of N-acetyl-N '-beta-D-glucopyranosyl urea and N-benzoyl-N '-beta-D-glucopyranosyl urea to glycogen phosphorylase b-Kinetic and crystallographic studies" *Eur J Biochem* **269**, 1684-1696. → [Journal](#) | [PubMed](#)

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*JIF*²⁰⁰²: **2.999**

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

38. Oikonomakos NG, Schnier JB, **Zographos SE**, Skamnaki VT, Tsitsanou KE & Johnson LN (2000) "Flavopiridol inhibits glycogen phosphorylase by binding at the inhibitor site" *J Biol Chem* **275**, 34566-34573. → [Journal](#) | [PubMed](#)

*JIF*²⁰⁰⁰: **7.368**

PDBs: [1C8K](#), [1E1Y](#) & [1GFZ](#)

39. Oikonomakos NG, Tsitsanou KE, **Zographos SE**, Skamnaki VT, Goldmann S & Bischoff H (1999). Allosteric inhibition of glycogen phosphorylase a by the potential antidiabetic drug 3-isopropyl 4-(2-chlorophenyl)-1,4-dihydro-1-ethyl-2-methyl-pyridine-3,5,6-tricarboxylate. *Protein Science* **8**, 1930-1945. → [Journal](#) | [PubMed](#)

*JIF*¹⁹⁹⁹: **4.457**

PDBs: [2GPA](#) & [3AMV](#)

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Cover Story



*JIF*¹⁹⁹⁹: **4.457**

PDBs: [1B4D](#) & [1BX3](#)

41. Heightman TD, Vasella A, Tsitsanou KE, **Zographos SE**, Skamnaki VT & Oikonomakos NG (1998). Cooperative interactions of the catalytic nucleophile and the catalytic acid in the inhibition of beta-glycosidases. Calculations and their validation by comparative kinetic and structural studies of the inhibition of glycogen phosphorylase b. *Helvetica Chimica Acta* **81**, 853-864. → [Journal](#)

*JIF*¹⁹⁹⁸: **2.463**

PDB: [1AXR](#)

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*JIF*¹⁹⁹⁷: **2.499**

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*JIF*¹⁹⁹⁷: **7.633**

PDB: [2AMV](#)

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*JIF*¹⁹⁹⁷: **2.646**

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*JIF*¹⁹⁹⁷: **2.646**

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*JIF*¹⁹⁹⁶: **4.867**

PDBs: [2SKC](#), [2SKD](#) & [2SKE](#)

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*JIF*¹⁹⁹⁶: **2.232**

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*JIF*¹⁹⁹⁶: **2.382**

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*JIF*¹⁹⁹⁵: **5.346**

PDB: [2PRI](#).

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*JIF*¹⁹⁹⁵: **4.806**

PDB: [2PRJ](#)

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*JIF*¹⁹⁹⁵: **2.257**

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*JIF*¹⁹⁹⁵: **4.159**

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*JIF*¹⁹⁹⁵: **4.029**

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*JIF*¹⁹⁹⁵: **2.257**

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*JIF*¹⁹⁹⁴: **0.489**

Reviews/Chapters in books

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2. Somsak L, Czifrak K, Toth M, Bokor E, Chrysina ED, Alexacou KM, Hayes JM, Tiraidis C, Lazoura E, Leonidas DD, **Zographos SE** & Oikonomakos NG (2008). New inhibitors of glycogen phosphorylase as potential antidiabetic agents (**Review**). *Current Medicinal Chemistry* **15**, 2933-2983. → [Journal](#) | [PubMed](#)

*JIF*²⁰⁰⁸: **4.823**

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4. N.G. Oikonomakos, M. N. Kosmopoulou, D. D. Leonidas, E. D. Chrysina, C. Tiraidis, N. Bischler, K. E. Tsitsanou, **S. E. Zographos**, I. D. Kostas, and G. Eisenbrand (2006). Indirubin and indigo analogues as potential inhibitors of glycogenolysis: structural basis of glycogen phosphorylase inhibition. In *Indirubin, the red shade of indigo* (Meijer L., Guyard N., Skaltsounis L. & Eisenbrand G., eds) Editions "Life in Progress", Station Biologique, Roscoff, Chapter 18, pp. 177-189. ISBN: 2-9518029-0-0. → [Publisher](#)

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2. Katerina E. Tsitsanou, Christina E. Drakou, Demetres D. Leonidas, Spyros E. Zographos (2012) Mosquito Odorant Binding Protein 1 as a target for the structure-based discovery of novel host-seeking disruptors. *MAX-lab Activity Report 2012* → [Report Online](#)
3. Katerina E. Tsitsanou, Christina E. Drakou, Maria Keramioti and **Spyros E. Zographos** (2010). Crystal structure of odorant binding protein 4 from *Anopheles gambiae* complexed with *N*-Phenyl-1-naphthylamine. *MAX-lab Activity Report 2010*, pp. 382-383. → [Report Online](#)
4. V.T. Skamnaki, A. Katsandi, S. Manta, E. Tsoukala, **S.E. Zographos**, M. Kontou, P. Zoumpoulakis, D. Komiotis and D.D. Leonidas (2010). The binding of 1-(β -D-glucopyranosyl) pyrimidine derivatives to Glycogen phosphorylase b. *MAX-lab Activity Report 2010*, pp. 374-375. → [Report Online](#)
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7. **Spyros E. Zographos**, Christina E. Drakou, Anna Malekkou, Niovi Santama, Joseph M. Hayes, Demetres D. Leonidas, Angus I. Lamond, A. Sifaka-kapadai and Nikos G. Oikonomakos (2008). Crystal Structure of the nuclear factor hCINAP in complex with ADP refined to 1.8 Å resolution: Insights into the function of hCINAP. *MAX-lab Activity Report 2008*, pp. 412-413. → [Report Online](#)

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9. Tiraidis, C., Alexacou, K.-M., **Zographos, S.E.**, Leonidas, D.D., Gimisis, T., Oikonomakos, N.G.(2007). FR258900, a potential anti-hyperglycaemic drug, isolated from Fungus No. 138354, binds at the allosteric site of glycogen phosphorylase. **EMBL, Hamburg Outstation, Annual Report 2007, Part II**, pp. 135-136. → [Report Online](#)
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11. K. Dossi, D.D. Leonidas, J. Soucek, J. Matoucek, P. Poucková, **S.E. Zographos**, and N.G. Oikonomakos (2007). Structure assisted inhibitor design on bovine seminal ribonuclease: The binding of uridilyl nucleotide inhibitor. **EMBL, Hamburg Outstation, Annual Report 2007, Part II**, pp. 219-220. → [Report Online](#)
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14. Leonidas, D.D., Maiti, T.K., Samanta, A., Dasgupta, S., Pathak, T., **Zographos, S.E.**, Oikonomakos, N.G (2006). The binding of 3'-N-piperidine-4-carboxyl-3'-deoxy-ara uridine to Ribonuclease A in the crystal. **EMBL, Hamburg Outstation, Annual Report 2006, Part II**, pp. 227-228. → [Report Online](#)
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21. Watson, K.A., Gregoriou, M., Garman, E.F., Mitchell, E.P., Johnson, L.N., Bichard, C.J.F., Krulle, T.M., Taylor, H., Fleet, G.W.J., **Zographos, S.E.**, Kontou, M., Koutra, D.D. & Oikonomakos, N.G. (1996). X-ray structural studies of Escherichia coli maltodextrin phosphorylase (ECMP) and high resolution X-ray binding studies of glucose analogue inhibitors of glycogen phosphorylase (GP): Glucose analogue inhibitor studies. *SYNCHROTRON RADIATION DEPARTMENT, Daresbury Laboratory 1995-96, Scientific Reports Volume II*, pp. 733-734.
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Interviews

- **Dr. Spyros E. Zographos** (EUROSTRUCT coordinator) (2012) "The new centre for structural Biology: The Structural Biology and Chemistry Group (SBCG) of the National Hellenic Research Foundation have overseen a project, EUROSTRUCT, which has dramatically transformed their capabilities by creating a centre of excellence in structural biology in Greece" in *Projects magazine, (Insight Publishers Ltd., UK, ed.)*. **27**, 54-55. → [Digital edition](#) | [Individual link](#)
- Dr. Kostas Iatrou (ENAROMaTIC coordinator) and **Dr. Spyros E. Zographos** (ENAROMaTIC partner) (2011) "Greek plants in the fight against malaria" in *Pathfinder Eco-Science* → [View video \(in Greek\)](#)

Research Funding (2002-2015)

Running funded projects

- **"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. Liggrí" NSRF (ΕΣΠΑ) 2014-2020 (**8/12/2016-7/12/2019**). **Scholarship: 29.408,4 €**. Role: **Supervisor**
- **"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). Coordinator D. Stuart, University of Oxford (Scientist in charge for IBMCB/NHRF Dr. E. Chrysina), **Budget Total/for SBCG/NHRF 3,950,000/100,000 €**. Role: **Participant/Member of the general assembly/ Principal Investigator**. (**01/01/2017-31/12/2020**)

Upcoming funded projects

- **"INSPIRED:** The National Research Infrastructures on Integrated Structural Biology, Drug Screening Efforts and Drug target functional characterization" NSRF (ΕΠΑνΕΚ) 2014-2020. Coordinator Dr. V. Gregoriou, president of NHRF. **Budget Total/for IBMCB/NHRF 4,000,000/268,875 €**. Role: **Principal Investigator/member of the steering committee**.
- **"OMIC-ENGINE** Synthetic Biology: from omics technologies to genomic engineering" NSRF (ΕΠΑνΕΚ) 2014-2020. Coordinator Prof. K. Mathiopoulos, University of Thessaly (Scientist in charge for IBMCB/NHRF Dr. G. Skretas), **Budget Total/for IBMCB/NHRF 4,000,000/70,000 €**. Role: **Principal Investigator**.

Completed funded projects

- **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/Principal Investigator**
- **"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 (IBMCB Director), IBMCB/ NHRF. **Budget Total/for SBCT: 1,500,000/120,000 €**.
- **"Greek network of protein crystallographers"**. 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**
- **"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, IBMCB/NHRF. **Budget Total/for PI 2,000,000/205,000 €.** Role: **Principal Investigator.**

- **"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 Total/for PI: 2,500,000/280,000 €.** Role: **Principal Investigator** <http://enaromatic.bio.demokritos.gr/>
- **"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/ Principal Investigator.**
<http://www.eie.gr/nhrf/institutes/iopc/eu-projects/eurostruct/index-en.html>
- **"Advanced research for Mosquito Repellents",** (Project No: PC-215; **2012**). Access to Structural Proteomics Facility OPFF, 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**
- **"Instruct-Ellas, National consortium".** 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**
- **"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 Total/for PI: 135,097 /16,879 €.** Role: **Principal Investigator.**
- **"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/Principal Investigator.**
- **"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.**
- **"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).
- **“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) (**2005-2011**). **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**).