

METAXIA I. VLASSI

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Education:

1984: BSc in Physics, University of Patras (Physics Dept.), Greece

1985-1989: Post-graduate Student, University of Patras, Greece/ Université Catholique de Louvain-la-Neuve, Belgium (doctoral research in chemical and theoretical crystallography)

1989: PhD in Chemistry (x-ray crystallography), University of Patras (Chem Dept), Greece

Positions held:

2008-today: Researcher A', Institute of Biosciences & Applications (IB-A, former Institute of Biology), National Center for Scientific Research (NCSR) "Demokritos", Athens, Greece. Head of the Protein Structure & Molecular Modeling group

1999-2007: Researcher B', Institute of Biology (IB) NCSR "Demokritos", Athens, Greece

1995-1999: Researcher C', IB, NCSR "Demokritos", Athens, Greece

1994-1995: Research associate, Institute of Molecular Biology & Biotechnology, Division of Macromolecular Structures, Heraklion, Crete, Greece.

1989-1993: Postdoctoral Fellow in the field of Protein Crystallography, Institute of Molecular Biology & Biotechnology and Univ. of Crete, Heraklion, Crete, Greece.

1993: Short term post-doctoral fellow in the field of Protein Crystallography, EMBL/DESY Hamburg, Germany

Research interests:

- Protein structure
- Sequence-structure relationships
- Dynamics of protein structure
- Molecular dynamics simulations
- Conformational preferences of amino-acid repeats
- Protein-protein interactions
- Kinases
- Intrinsically disordered proteins

Expertise/Research activities:

M. Vlassi has long experience (since her postdoctoral research) in protein structural biology using both experimental methods (such as X-ray crystallography and circular dichroism) and currently, *in silico* approaches, such as homology-modelling and molecular dynamics (MD) simulations. Her research activities focus on the elucidation of sequence-structure relationships of proteins aiming at understanding the atomic details of their function under physiological and/or pathological conditions with emphasis on amino-acid repeats mediating protein interactions and on proteins mainly linked to diseases. For example, she has studied experimentally the structure and stability of hydrophobic amino-acid repeats, such as heptad- and TPR-repeats (Vlassi et al 1994; Vlassi et al 1998; Vlassi et al 1999; Gounalaki et al 2000; ...Vlassi et al 2006; Palaiomylitou et

al 2008) and has employed mainly MD simulations to predict the folding of highly disordered amino-acid repeats serving as protein-protein interaction modules, such as arginine-serine repeats (both in isolation and in complex with Srpk1 and Akt kinases), short repeats identified in the inhibitory domain of the mineralocorticoid receptor and polyglutamine-stretches (Sellis et al 2012; Vlasi et al 2013; Voukkalis et al 2016; Tartas et al 2017). A parallel interest is on MD simulations and development of related tools. For example, MV and her group developed the software, Gromita (Sellis et al 2009), a GUI to Gromacs for molecular dynamics simulations of proteins in solution (<http://bio.demokritos.gr/gromita>). Her current activities focus on *in silico* studies of proteins mainly linked to diseases, with emphasis on kinases. For example, her recent work using comparative analyses of MD simulations of the Tyk2 kinase and a variant linked to protection against autoimmune diseases, shed light on the structural/functional consequences of the corresponding *TYK2* gene polymorphism and contributed to understanding the atomic details of the related protection mechanism against such diseases (Lesgidou et al, 2018).

Other activities related to Structural Molecular Biology

- Active role (PI from IB) in establishing (1998) the “*Centre for Crystallographic Studies of Macromolecules*” (CCM), an infrastructure of NCSR “D” comprising an x-ray system and a circular dichroism (CD) spectropolarimeter that was financed by a grant from the General Secretariat for Research & Technology (GSRT) in the framework of EPETII/*Infrastructure of Research Centers* program (approved Nov. 1996) and served a network of academic institutions nationwide, including three Institutes inside NCSR “Demokritos” (the former: Biology, Physical Chemistry and Radioisotopes & Radiodiagnostic Products). The CCM equipment is currently part of the *INSPIRED* research infrastructure of NCSR “D” (see below).
- Organizer of the **1st Hellenic workshop on “Crystallographic Data Collection and Processing”** (IB, NCSR “Demokritos”, 1999). The workshop took place at the CCM and was supported by a GSRT grant in the framework of the EPETII/*Career opportunities for Greek speaking scientists* program (coordinator: M. Vlasi), and was attended by students and scientists from various Greek universities and research institutions.
- Member (2000-2002) of the Structural Molecular Biology (SMB) sub-committee of the **SESAME (Synchrotron-light source for Experimental Science and Applications in the Middle East) project** aiming to prepare and design related to structural biology SESAME beamlines.
- Presentation on current status of SMB related research activities in Greece in the Inaugural Meeting of the SMB Science Sub-committee of SESAME in the framework of the **1st Workshop on Structural Molecular Biology at SESAME** 6-7 April, 2000, Athens, Greece (see SRN Vol 13, No 4, pp 25-27)
- Presentation (December 2000), as member of the SESAME SMB sub-committee, on the current status of SMB related research activities in Greece and in charge (in collaboration with Pierre Rizkallah) for the **preparation of a proposal for an SMB Institute at SESAME** in the framework of the **2nd Workshop on Structural Molecular Biology at SESAME**, 6-7 December, 2000, Nicosia, Cyprus
- **Founding member** (2001) and member of the 1st administrative board (2001-2003) of the **Hellenic Crystallographic Association (HeCra)**.
- Co-organizer of the **International workshop on Bioinformatics and Structural Modeling**, Sabanci University, Istanbul, Turkey, September 2001 (see errata, Synchrotron Radiation

News, 15:1, 22-22, doi:10.1080/08940880208602928) of SRN, 14:6, 24-25)

- Co-organizer and responsible for the preparation of practical exercises of the **1st Hellenic workshop on Bioinformatics**, University of Athens (May 2002)
- Co-organizer of the **1st Congress of HeCra**, Agricultural University of Athens (May 2002)
- Member (2002-2007) of the **Scientific Advisory Committee** of the International Research Center, **SESAME** (see above) that is established in Jordan.
- Participation as member of the SESAME SAC in the: **1st** (20-21 December 2002, CCLRC Daresbury Laboratory, UK), **2nd** (15-16 April, 2004 at UNESCO, Paris, France), **3rd** (5-6 May 2005 at UNESCO, Paris, France) and **4th** (November 2006, Cairo, Egypt) **Joint Meetings of the SESAME Beamlines & Science Committees**.
- Presentation of research activities related to Bioinformatics & Computational Biology at NCSR “Demokritos” in the Joint Meeting of the Hellenic Society of Computational Biology & Bioinformatics (HSCBB) – the GSRT – Coordinators of the European **ELIXIR project**, 30-31 March, 2009, Athens, Greece.
- Member (PI of NCSR “D”) of the national network **BE/OPT-XFEL: Network to Optimize use of the European X-FEL by the Greek Research Community** financed by a GSRT grant in the framework of National Research Infrastructures roadmap (2009-2011)
- **Organizer** of the **International workshop: “XFEL Radiation & its Applications”** at NCSR “Demokritos” (18-19 June 2010) aiming at adequately preparing the Greek scientific community for research opportunities created by the European X-FEL facility. The workshop was organized in the framework of the **BE/OPT-XFEL program** (see above). The speakers (13) were invited scientists, experts in X-Ray Free Electron Lasers (XFELs), including members of the European X-FEL scientific advisory board and users of similar infrastructures (CFEL/Germany, SLAC/Stanford/USA, Spring-8 Center/Japan). The presentations covered basic principles of XFEL operations and scientific applications in a wide range of fields that were inaccessible prior to XFEL.
- Contribution to a **survey** (2019) of the **status of Computational Biology in Greece and Cyprus** in collaboration with other Scientists from the two counties (see: Chasapi et al 2019, PLoS Comput Biol 15(12): e1007532).
- Member of the **Scientific Committee** of the **10th International Conference of HeCra** (2021).
- In charge of the **Circular Dichroism (CD) lab**, which is a service unit of IB_A (since 2013). The CD lab is equipped with the **CD spectropolarimeter of CCM** (see above) and continues to serve research groups from NCSR “D” and other academic institutions nationwide, as well as the private sector. The CD lab is also part of the **INSPIRED** research infrastructure (see below) of NCSR “D”.
- Member of the **INSTRUCT-GR** network (linked to the European **INSTRUCT: An Integrated Structural Biology Infrastructure for Europe**) and in charge of the *in silico* structural studies platform of the NCSR “D” node of the related National research infrastructure: **INSPIRED-RIS** which is financed by GSRT in the framework of NSRF 2014-2020/Action: Reinforcement of the Research and Innovation Infrastructure (MIS:5002550) (*approved in 2018, ongoing*)

Other Scientific Activities

- Ad-hoc reviewer of international scientific journals (Cancers, Cells, ACS Omega, J. of Information & Modelling, Acta Crystallographica D, Nucleic Acid Research, Neurochemical Research, Theoretical Chemistry Accounts)

Educational activities/Teaching

- Supervisor/co-supervisor of more than 20 students and young researchers, including 5 postdocs, 5 PhD students (*1 in progress*) and 4 Master's students, as well as undergraduate- and intramural PhD rotation-students.

University Postgraduate (Masters) programs:

- (2019-**today**): Lectures in the framework of the course: "*Computational Analysis of Biomolecular Structure*" of the **postgraduate (Masters) program: "Bioinformatics - Computational Biology"** of the National & Kapodistrian University of Athens (Dept. of Biology).
- (2018-**today**): Lectures in the framework of the course: "*Advanced Biochemistry*" of the **postgraduate (Masters) program: "Applied Biochemistry: Clinical Chemistry, Biotechnology, Pharmaceutical Products evaluation"** co-organized by IB_A of NCSR "Demokritos" and the University of Patras (Dept of Chemistry).
- (2003-**today**): Lectures in the framework of the course "*Current Biochemical & Biophysical Approaches*" of the **postgraduate (Masters) program: "Clinical Biochemistry – Molecular Diagnosis"** of the National & Kapodistrian University of Athens (Depts. of Biology-Chemistry).
- (2003-2010): Lectures in the framework of the course: "*Introduction to Research Methodology*" of the **postgraduate (Masters) program: "Molecular Medicine"** of the Medical School, University of Athens.

Other courses/workshops/practical courses:

- (2012): Lecture entitled: "*Prediction of protein structure using molecular dynamics simulations*" to students of the University of Texas at Arlington (UTA) in the framework of the **Study abroad program** co-organized by UTA and NCSR "D", May 28-30, 2012.
- (2002): Tutor (lectures & **preparation of practical exercises**) of the **1st Hellenic workshop on Bioinformatics**, May 2002, University of Athens, Athens, Greece
- (2001): Tutor (lectures and **preparation of practical exercises**) of the **1st Workshop in Bioinformatics & Structural Modeling**, 3-9 Sept 2001, Istanbul, Turkey.
- (May 2000): Instructor in the framework of the "**Intensive Course on Plant Biotechnology and Applications 1999-2000**", Mediterranean Agronomic Institute of Chania (MAICH), May 2000, Crete
- (1996) Instructor (invited speaker/lectures and preparation of practical exercises) of the practical course "**Computer Applications in Structural Biology and Sequence Analysis**" organized at the University of Crete, Dept. of Biology, 2-6 Sept 1996, Heraklion-Crete, Greece (sponsored by ICSU/COBIOTECH)
- (1991) Tutor of the 2nd practical course: "**Protein Design**" organized under the support of Directorate-General for Science, Research and Development of the EU, at the IMBB Institute, Heraklion-Crete, Greece (Sept. 1991).

- (1990) Tutor in the framework of the European practical course: "*Protein Design*" organized with the support of the Doctorate-General for Science, Research & Development of the EU (Bridge Program) at the IMBB Institute, Heraklion-Crete, Greece (Sept.-Oct. 1990).

IB-A Postgraduate courses

- (1998-2007): Lectures in the framework of the course "*Structural & Computational Biology*" of the **postgraduate program of the IB-A** (former IB), NCSR "D".

NCSR "D" Summer Schools

- Presentations in the framework of NCSR "D" Summer Schools (1998,1999, 2001,2002,2005)

Other activities (Administrative)

- (2021) Member of the ad-hoc **advisory committee for the recruitment of a Researcher** (one position) at the Institute of Chemical Biology of the National Hellenic Research Foundation, Athens, Greece
- (2021) Member of the evaluation committee **for the recruitment of external research associates** in the framework of a HORIZON 2020/Marie Curie grant of the Institute of Informatics & Telecommunications of NCSR "D" (**2 evaluations**)
- (2019) Member of one ad-hoc **evaluation committee for Researcher promotion** (BRFAA, Athens, Greece)
- (2018) Member of one ad-hoc **evaluation committee for Researcher promotion** (INRASTES, NCSR "D")
- (2017) Member of one ad-hoc **evaluation committee for Researcher promotion (IB-A, NCSR "D")**
- (2012) Member of one ad-hoc **evaluation committee of the University of Thessaly** (School of Health Sciences, Dept. of Biochemistry & Biotechnology) **for the appointment of an Associate Professor** in the field of Biophysics with emphasis on structure/function studies of proteins
- (2012) Member of the ad-hoc **evaluation committee of IB-A/NCSR "D" for the appointment** of an Associate Research Scientist in the field of the "Design, Synthesis and Evaluation of Chemicals with Biological and Pharmaceutical Activity"
- (2000-2008, 2010-2012) Member and (2002-2004) President of the **Scientific Advisory Board the Institute of Biology** (IB; currently:IB-A) of NCSR "Demokritos"
- (Nov 2010-2011) **Deputy Director** of the IB/NCSR "D"
- (2008) Member and (2010- 2013) deputy member of the **Research Committee of NCSR "D"**
- (2003): Member of **ad hoc evaluation committees of grant applications** in the framework of **bilateral** research programs (GSRT, Greece).
- (2001-2003): Member of the **education (postgraduate-level) committee** of IB/NCSR "D"
- (1996) Responsible Scientist for the establishment of the computer local area network of IB
- (1998-2002) Responsible Scientist for the design and maintenance of the Institute's web site

LIST of PUBLICATIONS
(in peer-reviewed International journals)

Aubry, A., **Vlassi, M.**, Marraud, M. (1986). Backbone side chain interactions in peptides. VI. Crystal structures of four t-BuCO-Pro-X-NHMe dipeptides with X=His, His⁺, PF₆⁻, His(τ-Me) and His(π-Me). *Int. Journal Peptide Protein Research*, 28, 637-648. [doi:10.1111/j.1399-3011.1986.tb03302.x](https://doi.org/10.1111/j.1399-3011.1986.tb03302.x)

Vlassi, M., Germain, G., Matsoukas, J., Psachoulia, C., Voliotis, S., Leban, I (1987). Structures of Two N-Boc Amino-Acid Phenacyl Esters. *Acta Crystallogr*, C43, 2173-2175. [doi:10.1107/S0108270187088565](https://doi.org/10.1107/S0108270187088565)

Arrieta, J.M., Badia, D., Dominquez, E., Lete, E., de Mariquorta, E.M., Germain, G., **Vlassi, M.**, Debaerdemaeker, T. (1988). The X-Ray Structure of N-(2,2-Dimethoxyethyl)-3-(3,4-dimethoxyphenyl)-6,7,8-trimethoxy-1-methyl-1,2,3,4-tetrahydroisoquinoline. *J. Chem. Res.*, 70-71.

Arrieta, J.M., Badia, D., Dominquez, E., Lete, E., Igartua, A., Germain, G., **Vlassi, M.**, Debaerdemaeker, T. (1988). Trans-3-(3,4-Dimethoxyphenyl)-6,7,8-trimethoxy-1-methyl-1,2,3,4-tetrahydroisoquinoline-Methanol(1/1). *Acta Crystallogr*, C44, 1931-1933. [doi:10.1107/S0108270188007292](https://doi.org/10.1107/S0108270188007292)

Gili, P., Zarza, P.M., Nunez, P., Medina, A., Diaz, M.C., Martin, M.G., Arrieta, J.M., **Vlassi, M.**, Germain, G., Vermeire, M., Dupont L. (1989). Synthesis, spectroscopic and magnetic studies of Cobalt(II), Nickel(II) and Copper(II) complexes with 3'-and 5'-methoxysalicylaldehyde-3-ethylene-1H-indole. X-Ray structure of Bis(1H-indole-3-ethylene-5Ymethoxysalicylaldehyde)Copper(II). *J. Coord. Chem.*, 20, 273-287. [doi:10.1080/00958978909408169](https://doi.org/10.1080/00958978909408169)

Vlassi, M., Germain, G., Cervello, J., Marquet, J., Morano-Manas, M., Piniella, J.F (1989). Trans-Bis(methyl 3,5-dioxohexanoato) dipyridinenickel (II). *Z. Kristallogr*, 189, 263-268. [doi:10.1524/zkri.1989.189.3-4.263](https://doi.org/10.1524/zkri.1989.189.3-4.263)

Vlassi, M., Germain, G., Barlos, K., Mamos, P., Refaat, L.S. (1990). Crystal structure of Na-tritylleucyl-(1-benzotriazolyl ester). *Z. Kristallogr*, 192, 59-66.

Stavropoulos, G., Papaioannou, D., Karagiannis, C., **Vlassi, M.**, Nastopoulos, V.(1990). Structure of cis-4-hydroxy-N-triphenylmethyl-L-proline methyl ester. *Acta Crystallogr*, C46, 1461-1464. [doi:10.1107/S0108270189012084](https://doi.org/10.1107/S0108270189012084)

Arrieta, J.M., Dominquez, E., Lete, E., Villa, M.J., Germain, G., **Vlassi, M.** (1990). 5-(2-bromo-4,5-dimethoxyphenyl)-4-(2-hydroxy-3,4-dimethoxyphenyl) pyrimidine. *Acta Crystallogr*, C46, 660-663. [doi:10.1107/S0108270189008656](https://doi.org/10.1107/S0108270189008656)

Mederos, A., Gili, P., Dominquez, S., Benitez, A., Palacios, M.S., Henandez, M., Martin, P., Rodriguez, M.L., Ruiz, C., Lahoz, F.J., Oro, L., Brito, F., Arrieta, J.M., **Vlassi, M.**, Germain, G (1990). Dimer Species in Aqueous Solutions of m-phenylenediamine-N,N,N',N'-tetra-acetic acid(m-H4pdta) with Copper(II) and pyridine-2,6-diamine-N,N,N',N'-tetra-acetic acid(2,6-H4pydta) with Nickel(II). X-Ray structures of Na₄(Cu₂(m-pdta)₂)18H₂O, Na₄(Co₂(m-pdta)₂)10H₂O and Na₄(Ni₂(m-pdta)₂)8H₂O. *Dalton Trans*, 1, 1477-1491. [doi:10.1039/dt9900001477](https://doi.org/10.1039/dt9900001477)

- Arrieta, J.M., Dominquez, E. Lete, E., Villa, M.J., Germain, G., **Vlassi, M.**, Prewo, R., Bieri, J.H (1991). N-2-(2-bromo-4,5-Dimethoxyphenyl)-1-(2,3,4-Trimethoxyphenyl) Ethylformamide. *Acta Crystallogr*, C47, 2115-2118. [doi:10.1107/S0108270191003141](https://doi.org/10.1107/S0108270191003141)
- Arrieta, J.M., Germain, G., **Vlassi, M.**, Craciunescu, D.G., Iglesias, E.P., Debaerdemaeker, T. (1992). Bis[2 - (2-hydroxyethyl) piperazinium] hexachloroosmate (IV) Dichloride. *Acta Crystallogr*, C48, 1305-1307. [doi:10.1107/S0108270191014117](https://doi.org/10.1107/S0108270191014117)
- Vlassi, M.**, Brueckner, H., Kokkinidis, M. (1992). The crystal structure of the conformationally constrained peptide Z-(Aib)6-Obut. *Z. Kristallogr*, 202, 89-98. [doi:10.1524/zkri.1992.202.1-2.89](https://doi.org/10.1524/zkri.1992.202.1-2.89)
- Arrieta, J.M., Arnaiz, A.R., Santiago, C., Lorente, L., Zunica, F.J., Madariaga, G., Germain, G., **Vlassi, M.** (1993). Structure of hexakis(3-methylpyridinium) decavanadate bis(3-methylpyridinium perchlorate). *Acta Crystallogr*, C49, 1417-1421. [doi:10.1107/S0108270193001362](https://doi.org/10.1107/S0108270193001362)
- Kokkinidis, M., **Vlassi, M.**, Papanikolaou, Y., Kotsifaki, D., Kingswell, A., Tsernoglou, D., Hinz H.J. (1993). Correlation between protein stability and crystal properties of designed ROP variants. *Proteins*, 16, 214-216. [doi:10.1002/prot.340160208](https://doi.org/10.1002/prot.340160208)
- Vlassi, M.**, Brueckner, H., Kokkinidis, M. (1993). A peptide with built-in conformational constraints: The crystal structure of Z-(Aib)7-Obut. *Acta Crystallogr*, B49, 560-564. [doi:10.1107/S0108768192007171](https://doi.org/10.1107/S0108768192007171)
- Athanasiadis, A., **Vlassi, M.**, Kotsifaki, D., Tucker, P.A., Wilson, K.S., Kokkinidis, M. (1994). Crystal structure of PVUII endonuclease reveals extensive structural homologies to EcoRV. *Nature Struct Biol*, 1 (No 7), 469-475. [doi:10.1038/nsb0794-469](https://doi.org/10.1038/nsb0794-469) (Note: An editorial referring to this work was published in Nature, see: Riddihough G.(1994) *Nature* 370 (6484): 78-78)
- Vlassi, M.**, Steif, C., Weber, P., Tsernoglou, D., Wilson, K.S., Hinz, H-J., Kokkinidis, M. (1994). Restored heptad pattern continuity does not alter the folding of a 4- α -helical bundle. *Nature Struct Biol*, 1 (No 10), 706-716. [doi:10.1038/nsb1094-706](https://doi.org/10.1038/nsb1094-706)
- Vlassi, M.**, Dauter, Z., Wilson, K.S., Kokkinidis, M. (1998). Structural parameters for proteins derived from the atomic-resolution (1.09Å) structure of a designed variant of the *ColE1* ROP protein. *Acta Crystallogr*, D54, 1245-1260. [doi:10.1107/S0907444998002492](https://doi.org/10.1107/S0907444998002492)
- Lassalle, M.W., Hinz, H-J., Wenzel, H., **Vlassi, M.**, Kokkinidis, M., Cesareni, G. (1998). Dimer-to-tetramer transformation: loop excision dramatically alters structure and stability of the ROP 4- α -helix bundle protein. *J Mol Biol* 279, 987-1000. [doi:10.1006/jmbi.1998.1776](https://doi.org/10.1006/jmbi.1998.1776)
- Vlassi, M.**, Cesareni, G., Kokkinidis, M. (1999) A correlation between the loss of hydrophobic core packing interactions and protein stability. *J Mol Biol* 285, 817-27. [doi:10.1006/jmbi.1998.2342](https://doi.org/10.1006/jmbi.1998.2342)
- Zhou, B., Nelson, T.R., Kashtan, C., Gleason, B., Michael, A.F., **Vlassi, M.**, Charonis, A.S (2000). Identification of two alternatively spliced forms of Human Tubulointestinal Nephritis Antigen (TIN-ag). *J Am Soc Nephrol* 11(4):658-68. [doi:10.1681/asn.v114658](https://doi.org/10.1681/asn.v114658)
- Gounalaki, N., Tzamarias, D., **Vlassi M*** (2000). Identification of residues in the TPR domain of Ssn6 responsible for interaction with the Tup1 protein. *FEBS Lett* 473(1):37-41. [doi:10.1016/S0014-5793\(00\)01480-0](https://doi.org/10.1016/S0014-5793(00)01480-0) (Note: This work was used as cover illustration) (*Corresponding author)
- Mounaji, K., **Vlassi M.**, Erraiss, N-E., Wegnez, M., Serrano, A., Soukri, A (2003). In vitro effect of metal ions on the activity of two amphibian glyceraldehyde-3-phosphate dehydrogenases: Potential metal binding sites. *Comp Biochem Phys B*, 135(2), 241-254. [doi:10.1016/S1096-](https://doi.org/10.1016/S1096-)

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Pyrpassopoulos, S, Ladopoulou, A., **Vlassi, M.**, Papanikolaou, Y., Vorgias, C.E., Yannoukakos, D., Nounesis, G (2005). Thermal denaturation of the BRCT tandem repeat region of human tumour suppressor gene product BRCA1. *Biophys Chem* 114, 1-12. doi:10.1002/prot.21003

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Pyrpassopoulos, S, **Vlassi, M.**, Tsortos, A., Papanikolaou, Y., Petratos, K., Vorgias, CE, Nounesis G. (2006) Equilibrium heat-induced denaturation of chitinase 40 from *Streptomyces thermoviolaceus*. *Proteins* 64(2):513-23. doi:10.1002/prot.21003

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Selected Presentations at National Conferences

Sellis, D., Giannakouros, T., **Vlassi, M*** (2012) Molecular dynamics simulations of arginine/serine repeats: Implications for their role in molecular recognition. **6th International Conference of the Hellenic Crystallographic Association**, 28-29 September, 2012, Univ. of Athens, Athens, Greece

Zarkadas, C., D. Sellis, **M. Vlassi** (2014) GROMITA-4.6: A Graphical User Interface to facilitate molecular simulations with GROMACS GPU-CPU versions 4.6.x. **Current Trends in Structural Biology & 7th International Conference of the Hellenic Crystallographic Association**, September 19-21, 2014, FORTH, Crete, Greece

C. Zarkadas, **M. Vlassi** (2014) Molecular dynamics simulations of the human apolipoprotein E3. **9th Conference of the Hellenic Society for Computational Biology & Bioinformatics (HSCBB14)** – Agricultural University of Athens, Athens, Greece, 10-12 October 2014

Zarkadas, C., **M. Vlassi** (2015) GROMITA-5.0: An up-to-date and easy to install version of the GROMITA GUI for GROMACS Molecular Dynamics package versions 5.0.x. **66th Congress of the Hellenic Society of Biochemistry and Molecular Biology (HSBMB)**, 11-13 December, 2015, Eugenides Foundation, Athens, Greece

Zarkadas, C., **M. Vlassi*** (2016). Free energy calculations of the binding of RS-repeat containing peptides to AKT kinase based on molecular dynamics simulations: a comparative study. **Joint Conference of the Hellenic Crystallographic Association and the Hellenic Society for Computational Biology & Bioinformatics (HECRA-HSCBB16)**, October 7-9, 2016, Agricultural University of Athens, Athens, Greece (*Oral presentation)

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Lesgidou, N., **M Vlassi (2021)** Using large-scale molecular dynamics simulations to elucidate sequence-structure-function relationships of a tyrosine kinase. **10th International Conference of the Hellenic Crystallographic Association (HeCrA)**, NCSR "Demokritos", Athens, Greece, 15-17 October 2021. Book of abstracts (Proceedings of the 10th International Conference of HeCrA), Pg 89-90. <https://drive.google.com/file/d/11y0ruC7NPmy2Kw6B4y1ZibiWIpgQjw36/view>

Selected funding programs (competitive grants)

- GSRT-EPETII/*Infrustrure of Research Centers "Centre for Crystallographic Studies of Macromolecules"* (M. Vlassi; PI IB-NCSR "D"), Nov 1996.
- EU/BIOTECHNOLOGY, Area 6 "*Structural Biology*", (contract: BIO-CT98-0086) (10/1998-10/2000) "The European Bio-Crystallogenesis Initiative" (Coordinator: R. Hilgenfeld, IMB, Jena, Germany/M.Vlassi: sub-contractor).
- EU/BIOTECHNOLOGY, Area 6 "*Structural Biology*", (contract: BIO-CT98-0328) (10/1998-10/2000) "Restriction Endonucleases And Methyltransferases" (M.Vlassi: sub-contractor)
- GSRT-EPETII/*Career opportunities for Greek speaking scientists* (1/1/2000-30/4/2001) "Structure and function of proteins" (Coordinator: M. Vlassi)
- NCSR "D"/*DHMOEREVNA'99* (1/4/1999-31/3/2001) "Structural Studies on the Ssn6-Tup1 transcriptional co-repressor" (Coordinator: M. Vlassi).
- GSRT/*PENED99* (1/1/2000-31/8/2001). "Structural and functional analysis of the Ssn6(Cyc8) transcriptional regulator" (Coordinator: M. Vlassi)
- GSRT/*PRAXE Phase A'* (30/12/2003-30/6/2005) "Structure-based design of compounds against pathologic bacteria" (Coordinator: M. Vlassi)
- GSRT/ *05Non-EU-356* (1/9/2006-31/3/2008) "Structural and Functional Characterization of Deflated: a new target for rational anti-cancer drug design" (Coordinator: M. Vlassi)
- NCSR "D"/*Dhmoerevna-06*: "Development of computational tools for molecular dynamics simulations of proteins in water solutions" (Coordinator: M. Vlassi)
- GSRT: *BE/OPT-XFEL* (20/1/2010 – 31/3/2011) "BE/OPT-XFEL Network to Optimize use of the European X-FEL by the Greek Research Community" (M.Vlassi, PI NCSR "D")
- ESF&NSRF2007-2013/*THALIS-UoI* (1/1/2012-30/11/2015) «THALIS-UoI: The new Biology of Intrinsically Disordered Proteins: A targeted, multidisciplinary analysis of IDP structure, function and properties in real time and true cellular conditions» (MIE 379440) (M. Vlassi: PI NCSR "D").
- ESF&NSRF2007-2013/*THALIS-UoC* (22/6/2012-30/11/2015) "THALIS-UoC: Mitochondrial dysfunction in neurodegenerative diseases" (MIE 377226) (M. Vlassi: PI NCSR "D").

- NSRF2014-2020/**INSPIRED-RIS** (3/9/2018-30/9/2022) "INPSIRED-The National Research Infrastructures on Integrated Structural Biology, Drug Screening Efforts and Drug Target Functional Characterization" (MIS:5002550).

Computing time grants:

- **ARIS @ GRNET/ 6th Call for Production Projects Accessing the supercomputer system ARIS** (6/12/2018-6/12/2019) (Coordinator: Metaxia Vlassi). Granted computing resources: 900.000,0 core hours
- **ARIS @ GRNET/ 8th Call for Production Projects Accessing the supercomputer system ARIS** (10/12/2019-10/12/2020) (Coordinator: Metaxia Vlassi). Granted computing resources: 1.500.000,0 core hours
- **ARIS @ GRNET/ 10th Call for Production Projects Accessing the supercomputer system ARIS** (10/3/2021-10/3/2022) (Coordinator: Metaxia Vlassi). Granted computing resources: 1.900.000,0 core hours
- **ARIS @ GRNET/ 12th Call for Production Projects Accessing the supercomputer system ARIS** (10/3/2022-10/3/2023) (Coordinator: Metaxia Vlassi). Granted computing resources: 1.400.000,0 core hours