2023

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***Scientific Interests***

- Biochemistry: Structure and Function of Proteins.
- Protein polymorphism and macromolecular interactions.
- Protein production and crystallization.
- Studies of proteins associated with pharmaceutical importance and virus proteins important for drug development.
- X-ray crystallographic methods and structural determination of materials focusing on biomacromolecules.
- Method development for structural biology.
- Synchrotron radiation, data collection – analytical methods and instrumentation for the structural characterization of biomacromolecules (X-ray single crystal/ powder diffraction).

# [CURRICULUM VITAE]

## Table of Contents

## Personal Information

Family name, First name: Margiolaki, Irene, Nationality: Greek

## Education

**2004 (20/02/ 2004)** DPhil, School of Chemistry, Physics and Environmental Science, University of Sussex, Brighton, UK, Supervisor: Prof. Kosmas Prassides
**1999** BSc, Department of Physics, University of Crete, Heraklion, Crete, Greece

## Current Positions

**2023–present** Professor, Section of Genetics, Cell & Developmental Biology/Department of Biology/University of Patras/ Patras/ Greece

## Previous Positions

**2023–today** Professor, Section of Genetics, Cell & Developmental Biology/Department of Biology/University of Patras/ Patras/ Greece

**2019–2023** Associate Professor, Section of Genetics, Cell & Developmental Biology/Department of Biology/University of Patras/ Patras/ Greece

**2015–2019** Assistant Professor, Section of Genetics, Cell & Developmental Biology/Department of Biology/University of Patras/ Patras/ Greece
**2010–2015** Lecturer, Section of Genetics, Cell & Developmental Biology/ Department of Biology/University of Patras/ Patras/ Greece
**2006–2010** Instrument Scientist, ID31 Beamline, European Synchrotron Radiation Facility (ESRF), Grenoble, France.
**2003–2006** Post Doctoral Fellow, ID31 Beamline, European ESRF, Grenoble, France.
**1998-1999** Research Trainee (undergraduate student), IESL/FORTH, Heraklion, Crete, Greece

Related article & Web link

## Brief CV

Irene Margiolaki is currently employed as a Professor at the Department of Biology of the University of Patras (UPAT, Patras, Greece). She graduated in Physics in 1999 (University of Crete, Heraklion, Greece). Her D.Phil. thesis on "Structural, Magnetic and Dynamic properties of fullerene-based materials" was completed in 2004 at the Department of Physics, Chemistry and Environmental Sciences, of the University of Sussex, UK (official date of graduation: 20 February 2004). During the period, 2003-2010, she has been employed, initially as a post doctorate fellow and later as an instrument scientist, by the European Synchrotron Radiation Facility (ESRF), in Grenoble, France. An important part of her research at the ID31 High resolution powder diffraction beamline of the ESRF (2003-2010) and future research activities is the development of innovative powder diffraction methods for the structural characterisation of biological macromolecules, when data-quality single crystals for X-ray crystallography cannot be obtained. Since 2010, she leads her 15 member research team. In 2013 she inaugurated a Biochemistry, Structural Biology and X-ray crystallography laboratory at the Department of Biology equipped with 2 modern diffractometers for single crystal and powder diffraction measurements. In 2015, she created a laboratory for protein expression, purification and crystallisation at the same Department. Her work to date has been recognised by internationally distinguished organisations.

## Awards, Fellowships, Committees & Boards

**2003** "*Blue John Crystal*" award from the biological structures group of the British Crystallographic

Association (BCA) (data shown on the cover). Related interview on page 16 of the ESRF Newsletter is available from here.
**2006** European Powder Diffraction Conference (EPDIC 10) young scientist award. To date, she is the only female researcher among all recipients since 1994. Related ESRF-Press release.
**2010** UNESCO- L'OREAL Co-sponsored International Fellowship for Young Women in Life Sciences.
Dr. Margiolaki is the only Greek woman who has received this international fellowship.
**2012** Academic and Research Excellence in Higher Education: Promotion and Support, Hellenic Ministry of Education.
**2014-2015** *Scientific Excellence* research fellowship, "*Aristeia II*", awarded by the Hellenic Ministry of Education, for the development & application of innovative methods in structural biology.
**2015** Presentation of research results on the cover and article (page 18) of the recent volume of the ESRF newsletter.
**2016** Presentation of research results in PANalytical X'Press article 2/2016.
**Committees & Boards:** Dr. Margiolaki is the youngest member of the following committees:
**2009 - present:** Elected member of the European Powder Diffraction (EPDIC) Committee;
**2013 - present:** Elected member of the Hellenic Crystallographic Association Committee (HECRA).
**2015 - 2021:** Appointed member of the Board of Directors: Patras Science Park (PSP).
**2019-present:** Director of the Section of Genetics, Cell Biology and Development, Department of Biology, University of Patras, Patras, Greece.
**2020-present:** Appointed, by the International Union of Crystallography (IUCr) executive committee, Co-editor of Acta Crystallographica section A: Foundations and Advances.
**2021** Press release of the Paul Scherrer Institute (PSI- Switzerland) on our recent publication and cover of the May 2021 issue of Acta Cryst. A (International Union of Crystallography journals).
**2022** Interview for the ESRFNews, December 2022.

**Research Experience**
Irene Margiolaki's research focuses on:
- Biochemistry: Structure and Function of Proteins.
- Protein Polymorphism and macromolecular interactions.
- Protein production and crystallization.
- Studies of proteins associated with pharmaceutical importance and virus proteins important for drug development.
- X-ray Crystallographic methods and structural determination of materials focusing on biomacromolecules.
- Method development for structural biology.
- Synchrotron radiation, data collection – analytical methods and instrumentation for the structural characterization of biomacromolecules (X-ray single crystal/ powder diffraction).

More details related to her research are provided below.

**(a)** Structural characterization of proteins associated with pharmaceutical importance [A.1: 1, 32, B.1: 1-4, C: 1-2] [A.1: 1, 32, B.1: 1-4, C: 1-2]. The long-term aim is the relation between their structure and function and the development of new (drug design) or improvement existing pharmaceuticals (drug delivery). Along this axis, she collaborates with a broad scientific network from Academic Institutes (University of Manchester, University of Hamburg, EPFL, AFMB) and the *R&D* departments of 3 major pharmaceutical companies: Sanofi Aventis (France) [A.1: 8], Novo Nordisk (Denmark) [A1: 10, 12-14, 15, 18, 23-24, 27, 30, 31] and more recently CBL (Greece) [A.1: 21, 29]. Since 2002, she collaborates with the research team of Prof. Bruno Canard (Research Director, AFMB, CNRS) in Marseille, France [A.1: 13, 17, 19, 26; B.1: 3]. Regarding the structure- function relation, we focus on the study of protein-protein and protein-ligand interactions via the synergistic use of diffraction methods with: (a) Nuclear Magnetic Resonance [A.1: 13, 30], Small angle X-ray Scattering, Differential Scanning Fluorimetry-DSF, Isothermal Titration Calorimetry-ITC and Molecular Dynamics [A.1: 26, 31].

**(b)** Method development for structural biochemistry. Since 2003, significant part of her research at ESRF and later at UPAT is dedicated on the development and application of methods for the structural characterization of proteins from microcrystalline samples using the X-ray Powder Diffraction (XRPD) technique [all related papers are provided in Sections A.1 ; B.1; C]. Today she continues her work combining the XRPD technique with other uprising methods: Precession Electron Diffraction Method (PED), Automated Diffraction Tomography (ADT), Serial Synchrotron X-ray crystallography (SSX). The main aim is the combinatorial use of the 3 techniques for structurally characterizing nano-crystalline proteins [articles:1, 2, 3]. Her contribution to both the development of instruments and analytical algorithms as well as their application on pharmaceutically interesting proteins has been internationally recognised, with 6 international/national awards & fellowships, 7 invited review articles & 2 book chapters (monographs), several press releases & ESRF Scientific Highlights, more than 100 invited lectures at conferences and 15 EU & industrial grants; some of these elements are listed below. To date, there are many structures in the *Protein Data Bank* (PDB) derived from these methods and 35 related articles/ 2 book chapters produced by our team; for most of them IM is corresponding author.

**(c)** Development of modern laboratory XRPD systems for collecting high resolution data from protein polycrystalline samples. The main advantage of this approach is that a major bottleneck associated with difficulties in the production of good quality protein crystals can be overcome. She has worked on this project since 2003 as Instrument Scientist at ESRF and since 2010 at UPAT. She collaborates with international companies producing scientific instruments including: PANalytical (*X-ray powder diffraction instruments*), BRUKER (*X-ray single crystal diffraction instruments*) & NanoMEGAS (*electron diffraction instruments*).

**(d)** Method development for biochemistry and the characterization of structural and dynamical characteristics of complex materials. A great part of her published work described in Sections A2; B2, is related to this axis of research. Especially her collaboration with the research team of Prof. Gerard Ferey (Université de Versailles - UVSQ) on the synthesis and structural characterization of the new family of materials, *metal organic framework materials* (*MOF's*), has attracted high scientific interest worldwide. Their work since 2004 has produced 15 papers with high number of citations [A.2: 40, 44, 46, 51, 57, 59, 63, 64, 65, 69, 70, 74, 77, 79, 85]. Especially the article in **Science** has been selected as one of the most cited papers in 2007 (Sciencewatch) with **4,013** citations to date [**46**].

## *Experimental Techniques*

- **Protein production:** protein expression in bacteria and purification via liquid chromatography.
- **Crystallography – Structural Analysis:** Protein Crystallization, method development for structural biology, user of most synchrotrons around the world, X-ray powder and single crystal diffraction, structure solution and refinement methods.
- **Electron diffraction:** using the methods *Precession Electron Diffraction Method, PED & Automated Diffraction Tomography, ADT*. Ερμηνεία των δεδομένων με χρήση κρυσταλλογραφικών μεθόδων.
- **Neutron diffraction:** user since 1999 of nuclear reactors (ILL, France) and Neutron Spallation Sources (ISIS, UK). Ερμηνεία των δεδομένων με χρήση κρυσταλλογραφικών μεθόδων.
- **Other experimental techniques that she has obtained basic knowledge include:** Small angle X-ray scattering, Optical microscopy, Inelastic neutron scattering, Positive muon spin relaxation.

# Development of Infrastructures at UPAT (2010- present)

**2012:** Establishment of a *wet lab* for protein production and crystallization at the Department of Biology (UPAT). The lab (100 $m^2$) can accommodate up to 15 people (4 fully equipped benches): cold room, fume-hood, Leica DM2500 Microscope, biochemistry equipment such as incubators, orbital shakers (Thermo Scientific), a liquid chromatography system (ActaSTART FPLC), a sonicator, bench-top centrifuges, classic gel electrophoresis system for analysis of protein samples and UV-Vis light absorption spectrometers, Oryx Nano protein crystallization robot (Douglas Instruments).

**2013:** Establishment of a Biochemistry, Structural Biology and X-ray Crystallography lab (200 $m^2$) at the department of biology (UPAT). Two X-ray diffractometers were installed in 2013: a single crystal diffractometer (BRUKER, Kappa-CCD) equipped with an Oxford nitrogen Cryostream (400 series) for sample cooling down to 80K and a modern powder diffractometer, specially modified for protein powder diffraction measurements (PANalytical, X'Pert PRO) with focusing optics, robotic sample changer for thin films and a PIXcel (MEDIPIX) ultra-fast detector. Both instruments are routinely used for measurements on single crystals of small organics/inorganics and powder samples of mainly biological macromolecules, respectively. The instruments are supported by an EATON UPS (80KVA) system installed in the lab. The lab is visited routinely by users coming from national and international institutes. In 2023, an Anton Paar MHC-trans chamber was installed in the X'Pert PRO diffractometer for in situ XRPD measurements of compounds upon controlled humidity- temperature variation. The latter is unique at an international level for measurements of microcrystalline proteins and was one of the main goals of an H.F.R.I. grant.

**2013:** The long term collaboration of NanoMEGAS with Irene Margiolaki, led to the installation of scientific equipment at the Inter-departmental Electron Microscopy & Microanalysis lab located at the basement of the department of Biology. The equipment and software provided are used for electron diffraction experiments using the uprising methods: *Precession Electron Diffraction Method, PED & Automated Diffraction Tomography, ADT.* Specifically, the system *«Spinning Star»* was installed on the Transmission Electron Microscope ((TEM/HRTEM) JEM-2100) and is available for measurements to the whole scientific community.

# Teaching Experience

## *Supervision of students and postdoctoral fellows*

**2010–present** 3 Post-docs/5 PhD candidates (5 completed)/13 Master Students (10 completed and 3 currently ongoing)/37 Undergraduate Research trainees (1 year research project each, 30 completed and 7 currently ongoing), Section of Genetics, Cell & Developmental Biology/ Department of Biology/ University of Patras/ Patras/Greece. Selected theses are available.

## *Teaching Activities*

**2011–present** Lecturer (2010-2015), Assistant Professor (2015- 2019), Associate Professor (2019- 2023) and Professor (2023-today) – "*Biochemistry I: Theory & Lab work*", "Biochemistry II" (Undergraduate courses), University of Patras/Department of Biology/Greece

**2011–present** Lecturer (2010-2015), Assistant Professor (2015- 2019), Associate Professor (2019- 2023) and Professor (2023-today) – "Introduction to Structural Biology - X-ray Crystallography" (course in the frame of the postgraduate program "Biological Technology"), University of Patras/Department of Biology/Greece

**2011–present** Lecturer (2010-2015), Assistant Professor (2015- 2019) & Associate Professor (2019- 2023) and Professor (2023-today) – "Structural Biology: Methods for Protein Crystallization & Crystallography" (course in the frame of the postgraduate program "Informatics in Life Sciences"), University of Patras/Faculty of Medicine/Greece

**2012-present** Lecturer (2010-2015), Assistant Professor (2015- 2019), Associate Professor (2019- 2023) and Professor (2023-today) – "Structural Biology: Methods for Protein Crystallization & Crystallography" (course in the frame of the postgraduate program "Biomedical Sciences"), University of Patras/Faculty of Medicine/

# Other Scientific Activities

## *Reviewer for International Scientific Journals*

Journal of Physics: Condensed Matter, Journal of Synchrotron Radiation, Zeitschrift für Kristallographie,

Acta Crystallographica D (Biological Crystallography), Acta Crystallographica B, European Physical Journal B, Solid State Sciences, Journal of Physics and Chemistry of Solids, IUCrJ, Journal of Applied Crystallography, Molecular Biotechnology, Biomolecules, Journal of Molecular Sciences, Crystals, Molecules.

## *Selected Institutional Responsibilities (UPAT)*

**2016-2017** Representative of the Biology Department for the EU mobility program, Erasmus+.
**2012-present** Committee member of the Lab of Electron Microscopy & Microanalysis.
**2014-present** University committee member for "Advancing Research Infrastructures" (School of Natural Sciences).
**2019-2022** Director of Section of Genetics, Cell Biology and Development, Department of Biology, University of Patras.

## *Participation in Scientific Societies (selected)*

**2012-present** Member, FP7 Network for access to large scale facilities "*BiostructX*"
**2008-present** Member of the "IUCr: *World Directory of Crystallographers*".
**2005-present** Member of the French Crystallographic Association
**2020-present** Appointed, by the International Union of Crystallography (IUCr) executive committee, Co-editor of Acta Crystallographica section A: Foundations and Advances.

# Publications

## A.1 Publications related to Biochemistry-Structural Biology and X-ray Powder Diffraction Method Development for the Structural Characterization of Microcrystalline Proteins.

**1.** "Synchrotron X-ray powder diffraction study of Turkey egg-white Lysozyme", Acta Cryst. D61, 423-432 (2005) & ESRF Scientific Highlights, p. 30-31 (2004), I. Margiolaki*, J. P. Wright*, A. N. Fitch, G. C. Fox & R. B. Von Dreele (article available online). Cover of the British Crystallographic Association News (2004).

**2.** "High Throughput Phase Diagram Mapping via Powder Diffraction: A case-study of HEWL versus pH.", Acta Cryst. D 61, 1612-1625 (2005), S. Basso, A. N. Fitch, G. C. Fox, I. Margiolaki* & J. P. Wright* (article available online).

**3.** "Successful protein cryocooling for powder diffraction.", J. Appl. Cryst. 40, 121 (2007), M. Jenner, J. P. Wright*, I. Margiolaki and A. N. Fitch (article available online)

**4.** "Powder diffraction studies for proteins: An overview of data collection approaches", **Invited Review Article associated with the EPDIC Young Scientist Award 2006, (Related ESRF article).** Z. Kristallogr. Suppl. 26, 1-13 (2007), I. Margiolaki*, J. P. Wright, A. N. Fitch, G. C. Fox, A. Labrador, R. B. Von Dreele, K. Miura, F. Gozzo, M. Schiltz, C. Besnard, F. Camus, P. Pattison, D. Beckers, T. Degen (article available online).

**5.** "Second SH3 domain of ponsin solved from powder diffraction.", J. Am. Chem. Soc. 129, 11865 (2007) & ESRF Press release. I. Margiolaki*, J. P. Wright, M. Wilmanns, A. N. Fitch & N. Pinotsis* (article available online).

**6.** "Molecular envelopes derived from X-ray diffraction on polycrystalline protein powders.", J. Appl. Cryst. 41, 329-339 (2008) & ESRF Scientific Highlights, p. 61-62 (2006), J. P. Wright, C. Besnard, I. Margiolaki, S. Basso, F. Camus, A. N. Fitch, G. Fox, P. Pattison, M. Schiltz (article available online).

**7.** "Powder Crystallography on Macromolecules", Acta Cryst. A64, 169-180 (2008). I. Margiolaki* & J. P. Wright*, **Invited Review Article for Special Issue of International Union of Crystallography (IUCr)[3]**

**8.** "Polymorphism of microcrystalline Urate Oxidase from Aspergillus flavus", Acta Cryst. D 66, 539-548

(2010), I. Collings, Y. Watier, M. Giffard, S. Dagogo, R. Kahn, F. Bonnete, J. P. Wright, A. N. Fitch, I. Margiolaki*[4] (article available online). ESRF press release.

**9.** "Features of the Secondary Structure of the Protein Molecule from Powder Diffraction data", Acta Cryst. D 66, 756-761 (2010)- Cover article, S. Basso, C. Besnard, J. P. Wright, I. Margiolaki, A. N. Fitch, P. Pattison, M. Sciltz (article available online).

**10.** "Structural studies of human insulin co-crystallized with phenol or resorcinol via powder diffraction.", Acta Cryst. D68, 1632-1641 (2012), F. Karavassili, A. E. Giannopoulou, E. Kotsiliti, L. Knight, M. Norrman, G. Schluckebier, L. Drube, A. N. Fitch, J. P. Wright & I. Margiolaki* (article available online).

**11.** "X-ray resonant powder diffraction", Eur. Phys. J. Special Topics 208, 275–289 (2012) – Invited Review article, H. Palancher, S. Bos, J.F. Berar, I. Margiolaki & J. L. Hodeau.

**12.** "High-resolution powder X-ray data reveal the T6 hexameric form of bovine insulin.", Acta Cryst. D69, 978-990 (2013), I. Margiolaki*, A. E. Giannopoulou, J. P. Wright, L. Knight, M. Norrman, G. Schluckebier, A. N. Fitch & R. B. Von Dreele (article available online).

**13.** "NMR study of non-structural proteins—part I: 1H, 13C, 15N backbone and side-chain resonance assignment of macro domainfrom Mayaro virus (MAYV)" Biomolecular NMR Assignments 9, 1, 191–195 (2015), E. Melekis, A. C. Tsika, J. Lichière, C. T. Chasapis, I. Margiolaki, N. Papageorgiou, B. Coutard, D. Bentrop, G. A. Spyroulias (article available online).

**14.** "Novel crystalline phase and first-order phase transitions of human insulin complexed with two distinct phenol derivatives", Acta Cryst. D71, 819-828 (2015), A. Valmas, K. Magiouf, S. Fili, M. Norrman, G. Schluckebier, D. Beckers, T. Degen, J. P. Wright, A. Fitch, F. Gozzo, A. E. Giannopoulou, F. Karavassili & I. Margiolaki* (article available online).

**15.** "Human insulin polymorphism upon ligand binding and pH variation: the case of 4-ethylresorcinol", IUCrJ. 4, 2:534-44 (2015) – open access, S. Fili, A. Valmas, M. Norrman, G. Schluckebier, D. Beckers, T. Degen, J. P. Wright, A. Fitch, F. Gozzo, A. E. Giannopoulou, F. Karavassili & I. Margiolaki*.

**16.** "Macromolecular Powder Diffraction: Ready for Genuine Biological Problems", Protein & Peptide Letters, 23 (3):232-41 (2016) - **Invited review article**, F. Karavassili & I. Margiolaki*.

**17.** "Coxsackievirus B3 protease 3C: expression, purification, crystallization and preliminary structural insights", Acta Cryst. F72, 877-884 (2016), S. Fili, A. Valmas, M. Christopoulou, M. Spiliopoulou, N. Nikolopoulos, J. Lichiere, S. Logotheti, F. Karavassili, E. Rosmaraki, A. Fitch, J. Wright, D. Beckers, T. Degen, G. Nenert, R. Hilgenfeld, N. Papageorgiou, B. Canard, B. Coutard & I. Margiolaki* (article available online).

**18.** "In Quest for Improved Drugs against Diabetes: The Added Value of X-ray Powder Diffraction Methods" (**Invited review article for Biomolecules: Special Issue "Protein Crystallography**"), Biomolecules 2017, 7 (3), 63 (OPEN ACCESS), F. Karavassili, A. Valmas, S. Fili, C. Georgiou & I. Margiolaki*.

**19.** "Dengue Virus 3 NS5 methyltransferase domain: expression, purification, crystallization and first structural data from microcrystalline specimens.", Zeitschrift für Kristallographie – Crystalline Materials 2017, 233 (5), 309-316 (Available online), A. Valmas , S. Fili, N. Nikolopoulos, M. Spiliopoulou, M. Christopoulou, F. Karavassili, C. Kosinas, K. Bastalias, E. Rosmaraki, J. Lichiére, A. Fitch, D. Beckers, T. Degen, N. Papageorgiou , B. Canard, B. Coutard & I. Margiolaki*.

**20.** "In situ detection of a novel lysozyme monoclinic crystal form upon controlled relative humidity variation." Journal of Applied Crystallography 2018, 51, 1-13 (article available online), S. Trampari, A. Valmas, S. Logotheti, S. Saslis, S. Fili, M. Spiliopoulou, D. Beckers, T. Degen, G. Nenert, A. Fitch, M. Calamiotou, F. Karavassili and I. Margiolaki*.

**21.** "Revisiting the structure of a synthetic Somatostatin analogue for peptide drug design." Acta Cryst. B75, 611-620 (2019): Structural Science, Crystal Engineering and Materials (article available online) S. Fili, A.

Valmas, M. Spiliopoulou, P. Kontou, A. Fitch, D. Beckers, T. Degen, Kl. Barlos*, K. Barlos, F. Karavassili and I. Margiolaki*.

**22.** "Unit Cell Response of Tetragonal Hen-Egg White Lysozyme upon Controlled Relative Humidity Variation." Journal of Applied Crystallography 52, 816-822 (2019) (article available online), S. Logotheti, A. Valmas, S. Trampari, S. Fili, S. Saslis, M. Spiliopoulou, D. Beckers, T. Degen, G. Nenert , A. Fitch, F. Karavassili and I. Margiolaki*.

**23.** "Applications of X-ray Powder Diffraction in Protein Crystallography and Drug Screening ." Crystals 10, 54 (2020) (**Invited review article for Crystals Special Issue "Crystallization under special and physical environments"**), M. Spiliopoulou, A. Valmas, D. P. Triandafillidis, C. Kosinas, A. Fitch, F. Karavassili and I. Margiolaki* (article available online).

**24.** "Exploring the complex map of insulin polymorphism: A novel crystalline form in the presence of m-Cresol.." Acta Cryst. D76, 4, 375-384 (2020), F. Karavassili, A. Valmas, M. Dimarogona, A. E. Giannopoulou, S. Fili, M. Norrman, G. Schluckebier, D. Beckers, A. N. Fitch and I. Margiolaki* (article available online).

**25.** "Rapid screening of in cellulo grown protein crystals via a small-angle X-ray scattering/X-ray powder diffraction synergistic approach." Journal of Applied Crystallography 53, 1169-1180 (2020) & **Cover article**, J. M. Lahey-Rudolph, R. Schonherr, C. Michael Jeffries, C. E. Blanchet, J. Boger, A. S. Ferreira Ramos, W. M. Riekehr, D. P. Triandafillidis, A. Valmas, I. Margiolaki, D. Svergun and L. Redecke* (article available online) & Scientific Commentary by T. Bergfors & S. Mayumdar.

**26.** "Brothers in Arms: Structure, Assembly and Function of Arenaviridae Nucleoprotein." Viruses 12, 772 (2020), N. Papageorgiou, M. Spiliopoulou, T. Van Nguyen, A. Vaitsopoulou, E. Yekwa Laban, K. Alvarez, I. Margiolaki, B. Canard and F. Ferron* (article available onlne).

**27.** "Insulin polymorphism induced by two polyphenols: New crystal forms and advances in macromolecular powder diffraction." Acta Cryst. D76, 1065-1079 (2020), D. Triandafillidis, N. Parthenios, M. Spiliopoulou, A. Valmas, F. Gozzo, M. Reinle-Schmitt, D. Beckers, T. Degens, M. Pop, A. N. Fitch, J. Wollenhaupt, M. S. Weiss, F. Karavassili and I. Margiolaki* (article available online).

**28.** "Rietveld refinement for macromolecular powder diffraction." Crystal Growth and Design 20, 12, 8101–8123 (2020), Invited review article for the Virtual Special Issue entitled “The Rietveld Refinement Method – Half of a Century Anniversary.” M. Spiliopoulou, D. Triandafillidis, A. Valmas, C. Kosinas, A. N. Fitch, R. B. Von Dreele and I. Margiolaki* (article available online).

**29.** "New perspectives in macromolecular powder diffraction using single photon counting strip detectors: High resolution structure of the pharmaceutical peptide, Octreotide." Acta Cryst. A77, 186-195 (2021) & **Cover article**, M. Spiliopoulou, F. Karavassili, D. Triandafillidis, A. Valmas, C. Kosinas, K. Barlos, K. K. Barlos, M. Morin , M. L. Reinle-Schmitt, F. Gozzo* and I. Margiolaki* (article available online) & **Scientific Highlights of the Paul Scherrer Institute** (PSI- Switzerland).

**30.** "High throughput macromolecular polymorph screening via NMR and X-ray powder diffraction synergistic approach: The case of human insulin co-crystallized with resorcinol derivatives." J. Appl. Cryst. 54, 963-975 (2021)., M. Spiliopoulou, A. Valmas, D. Triandafillidis, S. Fili, M. Christopoulou, A. J. Filopoulou, A. Piskopou, P. Papadea, A. N. Fitch, D. Beckers, T. Degen, F. Gozzo, M. Morin, M. L. Reinle-Schmitt, F. Karavassili, E. Rosmaraki, C. T. Chasapis and I. Margiolaki* (article available online).

**31.** "The T2 structure of polycrystalline cubic human insulin." Acta Cryst. D (in press)., D. P. Triandafillidis, F. Karavassili, M. Spiliopoulou, A. Valmas, M. Athanasiadou, G. Nikolaras, S. Fili, P.i Kontou, M. W. Bowler, C. T. Chasapis, R. B. Von Dreele, A. N. Fitch and . Margiolaki*.

**32.** "Methods on LDL particle isolation, characterization and component fractionation for the development of novel specific oxidized LDL status markers for atherosclerotic disease risk assessment." Frontiers in Medicine, Section - Translational Medicine (published online 5/1/2023), doi: 10.3389/fmed.2022.1078492., P. Papadea, M. Skipitari, E. Kalaitzopoulou, A. Varemmenou, M. Spiliopoulou, M. Papasotiriou, E. Papachristou, D. Goumenos, A. Onoufriou, E. Rosmaraki, I. I. Margiolaki, C. D. Georgiou (open access).

## A.2 Publications related to Method Development: Applications to Biochemistry and the Characterization of Structural and Dynamical Characteristics of Complex Materials.

**33.** Macromolecules, 34, 5295-5305 (2001), H. Retsos, I. Margiolaki, A. Messaritaki, S. H. Anastasiadis (article available online).

**34.** Physica B, 318, 372-377 (2002). I. Margiolaki, S. Margadona, K. Prassides, I. Tsilika, K. P. Meletov, G. A. Kourouklis, T. J. S. Dennis, H. Shinohara (article available online).

**35.** Phys. Rev. B, 65, 184514-1:5 (2002), M. Pissas, G. Papavassiliou, M. Karayanni, M. Fardis, I. Maurin, I. Margiolaki, K. Prassides (article available online).

**36.** Journal of American Chemical Society, 124, 11288-11289, (2002). I.Margiolaki, S. Margadonna, K. Prassides, T. Hansen, K. Ishii and H. Suematsu. ILL-Grenoble Highlights, (article available online).

**37.** *Physic*a B, 326, 572-576 (2003), J. Arvanitidis, K. Papagelis, T. Takenobu, I. Margiolaki, K. Brigatti, K. Prassides, Y. Iwasa and A. Lappas (article available online).

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**87.** Symmetry, *14*, 2355 (2022), Special Issue "Electron Diffraction and Structural Imaging II", P. P. Das, S. Plana-Ruiz, A. Galanis, A. Stewart, F.i Karavassili, S. Nicolopulos, . Margiolaki, M. Calamiotou, H. Putz, G. Iezzi (article available online).

## *B. Peer reviewed Conference Proceedings*

### B.1 Biochemistry-Structural Biology and X-ray Powder Diffraction Method Development for the Structural Characterization of Microcrystalline Proteins.

**1.** "Exploiting X-ray induced anisotropic lattice changes to improve intensity extraction in protein powder diffraction: application to heavy atom detection.", Z. Kristallogr.

Suppl. 26, 39-44 (2007), C. Besnard, F. Camus, M. Fleurant, A. Dahlström, J. P. Wright, I. Margiolaki, P. Pattison, M. Schiltz (article available online).

**2.** "Likelihood Methods With Protein Powder Diffraction Data.", Z. Kristallogr. Suppl. 26, 27-32 (2007), J. P. Wright, A. Markvardsen and I. Margiolaki (article available online).

**3.** **"**Preliminary insights into the non structural protein 3 macro domain of the Mayaro virus by powder diffraction.", Z. Kristallogr. 225, 576–580 (2010), N. Papageorgiou, J. P. Wright , A. N. Fitch, Y. Watiers, L. Saunders, B. Coutard , V. Lantez, E. A. Gould, B. Canard, I. Margiolaki* (article available online).

**4.** "Time-dependent analysis of K2PtBr6 binding to lysozyme studied by protein powder and single crystal X-ray analysis.", Z. Kristallogr. 225, 570–575 (2010), J R Helliwell, A M T Bell, P Bryant , S Fisher, J Habash , M Helliwell, I Margiolaki , K Surasak , Y Watier, J Wright & S Yalamanchilli (article available online).

### B.2 Method Development: Applications to Biochemistry and the Characterization of Structural and Dynamical Characteristics of Complex Materials.

**5.** High Pressure Research, 22, 63-67, (2002), S. Assimopoulos, K. P. Meletov, G. A. Kourouklis, I. Margiolaki, S. Margadonna, K. Prassides, T. J. S. Dennis and H. Shinohara (article available online).

**6.** Acta Physica Polonica A , 117, 2, 323-327 (2010), W. Paszkowicz, P. Piszora, W. Lasocha, I. Margiolaki, M. Brunelli, A. Fitch (article available online).

### C. Book Chapters related to Biochemistry-Structural Biology and X-ray Powder Diffraction Method Development for the Structural Characterization of Microcrystalline Proteins.

**1.** *"Macromolecular Powder Diffraction",* Book Chapter for the International Tables of Crystallography- Volume H: Powder Diffraction, chapter 7.1, 718-736, 2019, (available online), I. Margiolaki

**2.** "Proteins and Powders: An Overview", I. Margiolaki In: *Uniting Electron Crystallography and Powder Diffraction*, Eds. U. Kolb, K. Shankland, L. Meshi, A. Avilov & W. David. (2012). Springer Netherlands, 137-147.

## Bibliometric Analysis.

93 publications; 2 invited book chapters, 11 structural models in PDB, 1 in *Science* (Ferey et al., 2005); 1 in *Nature Comm.* (Georgiou *et al.*, 2015); 38 as first/last author; 25 as corresponding author; 7 invited review articles; 8,552 citations (8,242 without self-citations) & H-index: 27 (source: Isis web of Knowledge).

## Invited presentations to internationally established conferences and schools

### *Selected Invited Presentations to International Conferences:*

**2005** XX International Union of Crystallography (IUCr) Meeting- Florence, Italy

Title: “Powder Diffraction- A complementary tool in Macromolecular Research”
**2005** European Molecular Biology Laboratory (EMBL- Hamburg)
Title: “High Resolution Powder Diffraction: A useful tool for structural biology”
**2006** Pharmaceutical Powder X-ray Diffraction Symposium 5- New Jersey, USA
Title: “Synchrotron Powder Diffraction: applications in macromolecular crystallography”
**2006** Annual Meeting of the crystallographic society of Japan- Tokyo (Japan)
Title: “Complementary techniques in structural biology”
**2006** European Powder Diffraction Conference (EPDIC 10)- Geneva, Switzerland
Plenary lecture: “Synchrotron X-ray powder diffraction as it begins to make an impact in structural biology” & “***EPDIC young scientist award***”
**2007** 1st Meeting of the Italian and Spanish Crystallographic Associations (MISCA), Italy
Title: “Biocrystallography via powder diffraction; an emerging method in structural biology”
**2009** MX-Frontiers at the One Micron Scale, NSLS2, US
Title: "Complementary methods for structural biology"
**2010** 13th International Conference on the Crystallisation of Biological Macromolecules (ICCBM13)- Dublin, Ireland
Title:"Protein Powder Diffraction: Stories of Success and Dreams for the Future”

The year **2014** was announced as the **International Year of Crystallography** (IYCr). During this year, the PI participated as invited speaker at the following international conferences in the frame of IYCr. **(a)** IYCr- Opening Ceremony & Annual Meeting of the French Crystallographic Assdociation, Unesco, Paris, France. Title: “Macromolecular Powder Diffraction”. **(b)** *One day Symposium on Recent Applications of X-ray Crystallography*, Collegio Nacional, Mexico City, Mexico**.** Title: "Macromolecular Powder Diffraction: Current status & Future prospects". **(c)** Invited Seminar at UNAM, Mexico city, Mexico. Title: “Protein Poly-crystallography: Why, What & How”

**2015** Invited Seminar Series, ANSTO, Sydney, Australia.
Title: " "The Power of Powder: Protein-based drug screening"
**2017** First International Mexican Meeting on Diffraction and the VII Meeting of Synchrotron Light Users, Merida, Mexico. Title: “Macromolecular Powder Diffraction: Ready for Genuine Biological Problems.”
**2017** Invited Seminar Series, University of Puebla, Mexico. Title: “SMALLER crystals, FASTER experiments, BRIGHTER beams: Uprising methods for Drug Screening & Innovation.”
**2018** 3rd Joint AIC-SILS conference, Rome, Italy, Title: “Uprising methodologies for structural biology.”
**2018** Energy Materials Nanotechnology (EMN) Greece Meeting, Heraklion, Crete, Title: “In Quest for Improved Drugs against Diabetes: The Added Value of X-ray Powder Diffraction (XRPD) Methods.”
**2018** Working group on Biology regarding the construction of the new synchrotron source PETRA IV, Hamburg, Germany.
**2019** FEBS, Biomolecules in Action II, Title: “Hybrid methods in protein poly-crystallography”, Hamburg, Germany.
**2020** XXIV International School of Pure and Applied Biophysics, Title: “X-ray Powder Diffraction on Biological Macromolecules”, Venice, Italy.
**2021** ESRF User Meeting, Plenary lecture, Grenoble, France.
**2022** Invited Seminar Series, University of Milan, Italy. Title: “The role of structural biology in biological sciences: case studies of microcrystalline proteins characterised via X-ray powder diffraction methods.”
**2022** FEBS, Biomolecules in Action III, Title: “Macromolecular Powder Diffraction: Ready for Genuine Biological Problems", Hamburg, Germany.
**2022** SASBDB, Workshop on the the database of small-angle scattering data and models for biology and soft matter, EMBL Hamburg, Germany.

**2022** 10 Years celebration of Excelsus Structural Solutions**,** Title: "The Protein Powder Diffraction Challenge", Park Innovaare, Villigen, Switzerland.

## *Organisation of International Conferences& Workshops*

**2007** Workshop Organiser, Title: "Development and future directions of powder diffraction in protein crystallography", ESRF, Grenoble, France.

**2008** XXI- International Union of Crystallography (IUCr) meeting - Osaka, Japan

- Invited Keynote Lecturer on the use of powder diffraction in macromolecular research
- In the organising committee and lecturer for the Satellite Meeting:

"Powder Diffraction on Proteins- Current Status and Future Prospect"

- Invited Speaker for the Satellite Meeting:

"Future of Female Crystallographers"

**2008** 11th European Powder Diffraction Conference (EPDIC 11) - Warsaw, Poland
Session Organiser: "Powder Diffraction on Proteins"

**2010** 12th European Powder Diffraction Conference (EPDIC 12) – Darmstadt, Germany.
Session Organiser together with Fabia Gozzo (SLS) for session: "Biomaterials, supramolecular chemistry, pharmaceuticals"

**2011** XXII- International Union of Crystallography (IUCr) Congress – Madrid, Spain
Session Organiser together with Joel Sussman (Israel) for session: "Challenges of low-resolution crystallography".

**2012** 13th European Powder Diffraction Conference (EPDIC 12) – Grenoble, France
Session Organiser together with Jonathan Wright (ESRF) for session: "Molecular and Biomolecular Materials"

**2012** International Workshop on Electron Crystallography, Patras, Greece.

**2013** International Workshop on Fundamentals of Crystallography, Patras, Greece.

**2013** NMR Basics and Applications in Life Sciences, Patras, Greece.

**2013** International Workshop on Powder and Electron Crystallography, Patras, Greece.

**2013** Emerging Analytical Techniques in Protein Characterization, Patras, Greece.

**2013** 2nd Research Coordination Meeting (RCM) on Utilization of Accelerator – Based Real – Time Methods in Investigation of Materials with High Technological Importance (International Atomic Energy Agency, IAEA), Patras, Greece.

**2014** Current Trends in Structural Biology & 7th International Conference of the Hellenic Crystallographic Association, FORTH, Crete, Greece.

**2016** 15th European Powder Diffraction Conference (EPDIC 15), Bari, Italy. Session co-organiser together with C. Tedesco (Italy) for session: "Biological and molecular materials"

**2018** 16th European Powder Diffraction Conference (EPDIC 16) – Edinburgh, UK. Session co-organiser together with Fabia Gozzo (Excelsus) for session: " Pharmaceutical and biological materials"

**2018** 9th International Conference of the Hellenic Crystallographic Association (HeCrA9), UPAT, Patras, Greece.

**2022** 17th European Powder Diffraction Conference (EPDIC17) – Sibenik, Croatia. Session co-organiser together with Fabia Gozzo (Excelsus) for session: "Pharmaceutical and biological materials"

**2022 ESRF Information Day: The use of synchrotron radiation in science** – UPAT, Patras, Greece. The info day, co-organised by the European Synchrotron Radiation Facility (ESRF), the University of Patras and the Greek Synchrotron Users Network (GrSUN), took place at the Conference and Cultural Center of the University of Patras in Greece. This action is in the frame of the panhellenic effort for Greece to participate in the ESRF as an associate country. The youtube links for the distinct Sessions are listed below.

**Session 1:** ESRF Overview
**Session 2:** Biomedical imaging & Cultural heritage
**Session 3:** Life Sciences
**Session 4:** Energy – Catalysis – Environment
**Session 5:** Nanoscale matter & Quantum Materials & Session 6: Industrial Research & Activities

**2022 1st Greek Summer School on Synchrotron Radiation: Properties and Applications,** Aristotle University of Thessaloniki, Greece.
**2022 72$^{d}$ Panhellenic conference of the Hellenic Society of Biochemistry and Molecular Biology**, UPAT, Patras, Greece.

## *Invited Presentations to International Conferences available online*:

1. Protein Powder Diffraction at ESRF, Pharmaceutical Powder X-ray Diffraction Symposium (PPXRD-8), Scotland, 2009.
2. Proteins and Powders - An Overview, International Union of Crystallography (Erice School 2011, Italy).
3. Macromolecular Powder Diffraction, "International Year of Crystallography – IYCr2014" & "Annee Internationale de la Cristallographie en France – AICr2014" UNESCO, Paris, France, 2014.
4. The Power of Powder: Protein based Drug Screening, Pharmaceutical Powder X-ray Diffraction Symposium (PPXRD-13), Germany, 2015.
5. InnovCrete Seminar, IMBB, Heraklion, Crete, Greece, 2016.
6. Screening of protein-based pharmaceuticals, free webinar, PANalytical & UPAT, 2016.
7. 40 Years Anniversary Colloguium series at the Department of Physics, University of Crete, March 2018 "SMALLER crystals, FASTER experiments, BRIGHTER beams: Drug screening and innovation via X-ray powder diffraction".
9. The Power of Powder Humidity induced phase transitions of HEWLysozyme, Collaborative project between Malvern PANalytical and UPAT, 2016.
10. Women in Science, discussion organized by BiTUP (Bioscientific Team University of Patras) 2020 (Greek language).
10. Macromolecular Powder Diffraction: Ready for Genuine Biological Problems, Plenary lecture, European Synchrotron Radiation Facility (ESRF) user meeting 2021.
11. Biotrends: Structural Biology and Bioinformatics, BiTUP (Bioscientific Team University of Patras) 2021 (Greek language).