



Massimo Domenico Sammito

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Summary of CV

This section describes briefly a summary of your career in science, academic and research; the main scientific and technological achievements and goals in your line of research in the medium -and long- term. It also includes other important aspects or peculiarities.

My previous training and research experience have been designed from a purpose to integrate theoretical, computing and practical skills essential in the solution of biomedical problems resulting in pharmaceutical development.

After a three-year degree with highest marks in Computer Science (2009) at the University of Catania, Italy. I chose to join the two-year International Master in Bioinformatics for Health Sciences at the University of Bologna in Italy and at the University Pompeu Fabra in Barcelona obtaining both Master qualifications with highest marks. Beyond learning theoretical and practical fundamentals, I discovered upcoming research topics in this field. Being attracted by the link between structure and function as well as by the emergent in silico methods and the prediction of protein structures from primary sequences, I focused on structural and computational biology. Simultaneously, I was set to develop expertise in experimental research. On these grounds, I applied and was accepted for a Ph.D position in Prof. Usón's research group the leading group in Spain for applied computing methods in crystallography. During my Ph.D, I developed scientific software ARCIMBOLDO, BORGES and SHREDDER, methods to solve difficult macromolecular structures and study the complexity of local fold in proteins. I applied these methods to the study of a viral immunomodulator. The original idea of combining small local unspecific folds for phasing macromolecular structure received a very positive resonance, evidenced in a publication in Nature Methods in 2013, highlighted by the Nature Publishing Group as one of 50 milestones in structural biology. I have been talking in several European Crystallography Meeting. My active participation in more than 6 international conferences, 5 schools and 8 meetings allowed me to improve my scientific training and oral communication skills. I lectured bioinformatics at the Biotechnology Master at the University of Barcelona and crystallographic methods at international courses. After my thesis in June 2015, for which I received an award from the Faculty of Pharmacy, I joined a post-doctoral position at Prof. George M. Sheldrick's Structural Chemistry group, University Göttingen. I worked on the integration of SHELX programs in the European Collaborative Computing Project for crystallography CCP4. I obtained a grant to share my time between Göttingen and Cambridge University, spending one year at CIMR group of Prof. Randy Read with the aim of integrating ARCIMBOLDO into CCP4 and continue developing new methods exploiting distributed computing and supercomputing facilities. In 2018 I have been awarded with an individual fellowship European Marie Curie grant to work with Prof. Randy Read where I am developing the new framework for automatic molecular replacement PhaserVoyager. In 2019 I have been invited to talk at the CCP4 Study Weekend where I presented my new software ALEPH. This is a bioinformatics tool to analyse, interpret and process protein structure model with the aim of generating fragment libraries for molecular replacement. I have been part of two publications related to the CASP13 task force where we establish new statistical metrics to evaluate and compare results.

My aim is to progress developing new algorithms for biology and health sciences, applying my knowledge computer science to experimental methods for structural biology to understand processes relating structure and disease.



General quality indicators of scientific research

This section describes briefly the main quality indicators of scientific production (periods of research activity, experience in supervising doctoral theses, total citations, articles in journals of the first quartile, H index...). It also includes other important aspects or peculiarities.

All Since 2015
Citations 404 385
h-index 12 12
i10-index 13 13



Massimo Domenico Sammito

Surname(s): **Sammito**
Name: **Massimo Domenico**
ORCID: **0000-0002-8346-9247**
ResearcherID: **I-2546-2015**

Current professional situation

Employing entity: University of Cambridge **Type of entity:** University
Department: Cambridge Institute for Medical Research
Professional category: Marie Curie Fellow Post Doctoral Researcher
Start date: 01/06/2018
Type of contract: Grant-assisted student (pre or post-doctoral, others) **Dedication regime:** Full time

Previous positions and activities

	Employing entity	Professional category	Start date
1	Consejo Superior de Investigaciones Científicas	Post doctoral researcher	01/01/2017
2	Institute of Inorganic Chemistry	Post doctoral researcher	15/10/2015
3	Consejo Superior de Investigaciones Científicas	Post doctoral researcher	22/06/2015
4	Consejo Superior de Investigaciones Científicas	Pre doctoral researcher	14/02/2011

- 1** **Employing entity:** Consejo Superior de Investigaciones Científicas **Type of entity:** State agency
Department: Structural Biology, Instituto de Biología Molecular de Barcelona
City employing entity: Barcelona, Catalonia, Spain
Professional category: Post doctoral researcher
Start-End date: 01/01/2017 - 31/05/2018 **Duration:** 1 year - 5 months
Type of contract: Temporary employment contract
Performed tasks: Developing of machine learning approaches to analyse and learn from deposited protein structures, with the aim to reveal emergent features in protein folding, functional studies and structural properties
Applicability in teaching and/or research: Teaching to Master and Ph.D students.
- 2** **Employing entity:** Institute of Inorganic Chemistry **Type of entity:** University
City employing entity: Goettingen, Hannover, Germany
Professional category: Post doctoral researcher
Start-End date: 15/10/2015 - 31/12/2016



Primary (UNESCO code): 120317 - Informatics; 120323 - Programming languages; 120601 - Algorithm construction

Secondary (UNESCO code): 120300 - Computer Sciences; 230418 - Polypeptides and proteins; 240401 - Biostatistics

Tertiary (UNESCO code): 239000 - Pharmaceutical Chemistry

Performed tasks: Research in Structural Biology and Bioinformatics: development of computational methods and their application to Biomedical and Biotechnological projects. -Design and development of distributed computing software for Structural Biology and Bioinformatics. -Determination of protein structures involved in Immunodeficiency through crystallographic experiments. -Developing ab initio phasing methods. -Programming web servers for scientific software and graphical user interfaces. -Training undergraduate, graduate and Ph.D students in Bioinformatics and Crystallography.

3 **Employing entity:** Consejo Superior de Investigaciones Científicas **Type of entity:** State agency

Department: Structural Biology, Instituto de Biología Molecular de Barcelona

City employing entity: Barcelona, Catalonia, Spain

Professional category: Post doctoral researcher

Start-End date: 22/06/2015 - 15/10/2015

Duration: 3 months - 15 days

Type of contract: Temporary employment contract

4 **Employing entity:** Consejo Superior de Investigaciones Científicas **Type of entity:** State agency

Department: Structural Biology, Instituto de Biología Molecular de Barcelona

City employing entity: Barcelona, Catalonia, Spain

Professional category: Pre doctoral researcher

Start-End date: 14/02/2011 - 21/06/2015

Duration: 4 years - 4 months - 6 days

Type of contract: Temporary employment contract



Education

University education

1st and 2nd cycle studies and pre-Bologna degrees

- 1** **University degree:** Higher degree
Name of qualification: Computer Science
City degree awarding entity: Catania, Sicilia, Italy
Degree awarding entity: Università degli Studi di Catania **Type of entity:** University
Date of qualification: 12/11/2009
Average mark: Excellent
Prize: Archimede
Standardised degree: Yes **Date of homologation:** 20/01/2015
Foreign qualification: Laurea in Informatica
- 2** **University degree:** Higher degree
Name of qualification: Master in Bioinformatics for Health Sciences
City degree awarding entity: Barcelona, Catalonia, Spain
Degree awarding entity: Universidad Pompeu Fabra **Type of entity:** University
Date of qualification: 05/05/2012
Average mark: Excellent
- 3** **University degree:** Higher degree
Name of qualification: Master in Bioinformatics
City degree awarding entity: Bologna, Emilia-Romagna, Italy
Degree awarding entity: Alma Mater Studiorum - Università di Bologna **Type of entity:** University
Date of qualification: 22/07/2011
Average mark: Excellent
Standardised degree: Yes **Date of homologation:** 21/03/2012
Foreign qualification: Laurea Magistrale in Bioinformatica

Doctorates

Doctorate programme: Biothecnology
Degree awarding entity: Universitat de Barcelona **Type of entity:** University
City degree awarding entity: Barcelona, Catalonia, Spain
Date of degree: 22/06/2015
European doctorate: No
Thesis title: Enforcing secondary and tertiary structure for crystallographic phasing. Developing ARCIMBOLDO and BORGES.
Thesis director: Isabel Usón Finkenzeller
Obtained qualification: Sobresaliente Cum Laude
Recognition of quality: Yes



Special doctorate award: Yes

Specialised, lifelong, technical, professional and refresher training (other than formal academic and healthcare studies)

- 1** **Type of training:** Course
Training title: Cryo 3D Electron Microscopy
City awarding entity: Erice, Sicilia, Italy
Awarding entity: Ettore Majorana Centre **Type of entity:** Foundation
End date: 2019 **Duration in hours:** 60 hours
- 2** **Type of training:** Course
Training title: Análisis avanzado de Big Data. analytics con R software
City awarding entity: Barcelona, Catalonia, Spain
Awarding entity: Consejo Superior de Investigaciones Científicas **Type of entity:** State agency
End date: 2017 **Duration in hours:** 80 hours
- 3** **Type of training:** Course
Training title: Protein-Ligand Complexes: Understanding Biological Chemistry
City awarding entity: Nottingham University, East Anglia, United Kingdom
Awarding entity: Nottingham University and CCP4 **Type of entity:** Associations and Groups
End date: 2016 **Duration in hours:** 25 hours
- 4** **Type of training:** Practical work
Training title: Advanced Computing School for Crystallography
City awarding entity: Lossburg-Wittendorf, Germany
Awarding entity: ECACOMSIG9
Training manager: Harry Powell
End date: 2016 **Duration in hours:** 20 hours
- 5** **Type of training:** Course
Training title: Advanced Software Development for Crystallographers
City awarding entity: Rovinj, Croatia
Awarding entity: the European Crystallographic Association's Computing Special Interest Group **Type of entity:** Associations and Groups
End date: 2015 **Duration in hours:** 16 hours
- 6** **Type of training:** Course
Training title: Campus Gutemberg
City awarding entity: Barcelona, Catalonia, Spain
Awarding entity: Universidad Pompeu Fabra **Type of entity:** University
End date: 2014 **Duration in hours:** 10 hours
- 7** **Type of training:** Course
Training title: Introducción a la estadística aplicada
City awarding entity: Barcelona, Catalonia, Spain
Awarding entity: Consejo Superior de Investigaciones Científicas **Type of entity:** State agency
End date: 2014 **Duration in hours:** 20 hours



- 8** **Type of training:** Course
Training title: MCS2014. Macromolecular Crystallography School
City awarding entity: Madrid, Community of Madrid, Spain
Awarding entity: Institute of Physical-Chemistry "Rocasolano" - CSIC
End date: 2014
Type of entity: Public Research Body
Duration in hours: 30 hours
- 9** **Type of training:** Course
Training title: Transporters and other Molecular Machines
City awarding entity: Barcelona, Catalonia, Spain
Awarding entity: Institute for Research in Biomedicine
End date: 2014
Type of entity: R&D Centre
Duration in hours: 18 hours
- 10** **Training title:** Gestión Eficaz del Tiempo CSIC
Awarding entity: Consejo Superior de Investigaciones Científicas
End date: 2014
Type of entity: State agency
Duration in hours: 20 hours
- 11** **Training title:** Ingles técnico
Awarding entity: Consejo Superior de Investigaciones Científicas
End date: 2014
Type of entity: State agency
Duration in hours: 20 hours
- 12** **Type of training:** Course
Training title: Introduction to Software Development for Crystallographers
City awarding entity: Warwick, West Midlands, United Kingdom
Awarding entity: the European Crystallographic Association's Computing Special Interest Group
End date: 2013
Type of entity: Associations and Groups
Duration in hours: 12 hours
- 13** **Type of training:** Course
Training title: BioCrys2012: Fundamental of Modern Methods of BioCrystallography
City awarding entity: Oeiras, Lisboa, Portugal
Awarding entity: Instituto de Tecnologia Química e Biológica and FEBS
End date: 2012
Type of entity: University Department
Duration in hours: 36 hours
- 14** **Type of training:** Course
Training title: Present and Future Methods for Biomolecular Crystallography
City awarding entity: Erice, Sicilia, Italy
Awarding entity: Ettore Majorana Centre
End date: 2012
Type of entity: Foundation
Duration in hours: 60 hours
- 15** **Type of training:** Course
Training title: Computational Methods for System Biology
City awarding entity: Bologna, Emilia-Romagna, Italy
Awarding entity: Alma Mater Studiorum - Università di Bologna
End date: 2010
Type of entity: University
Duration in hours: 30 hours



Language skills

Language	Listening skills	Reading skills	Spoken interaction	Speaking skills	Writing skills
French	A2	A2	A2	A2	A2
Catalan	B1	A1	B1	B1	B1
Spanish	C2	C2	C2	C2	C1
English	C2	C2	C2	C2	C1
Italian	C2	C2	C2	C2	C2

Teaching experience

General teaching experience

- 1 Name of the course:** Bioinformatics
University degree: Master Molecular Biotechnology. Genomics, Proteomics, Bioinformatics
Start date: 17/10/2017 **End date:** 24/10/2017
End date: 2017
Entity: Universitat de Barcelona **Type of entity:** University
Faculty, institute or centre: Facultat de Farmacia
- 2 Name of the course:** Bioinformatics
University degree: Master Molecular Biotechnology. Genomics, Proteomics, Bioinformatics
Start date: 17/10/2016 **End date:** 24/10/2016
End date: 2016
Entity: Universitat de Barcelona **Type of entity:** University
Faculty, institute or centre: Facultat de Farmacia
- 3 Name of the course:** Bioinformatics
University degree: Master Molecular Biotechnology. Genomics, Proteomics, Bioinformatics
Start date: 18/10/2015 **End date:** 24/10/2015
End date: 2015
Entity: Universitat de Barcelona **Type of entity:** University
Faculty, institute or centre: Facultat de Farmacia
- 4 Name of the course:** Bioinformatics
University degree: Master Molecular Biotechnology. Genomics, Proteomics, Bioinformatics
Start date: 09/10/2014 **End date:** 15/10/2014
End date: 2014
Entity: Universitat de Barcelona **Type of entity:** University
Faculty, institute or centre: Facultat de Farmacia



Experience supervising doctoral thesis and/or final year projects

Project title: Retrieval of fold properties for structure interpretation with BORGES_MATRIX

Type of project: End of course project

Student: Ana Medina

Date of reading: 21/07/2017

Teaching experience in courses and seminars for university teacher training

- 1** **Type of event:** School
Name of the event: BCA School in Crystallography
Organising entity: British Crystallographic Association
Hours of teaching: 2
Teaching date: 30/08/2018
- 2** **Type of event:** Workshop
Name of the event: Advanced Computing School
City organizing entity: Lossburg-Wittendorf, Germany
Organising entity: ECACOMSIG9-ECA **Type of entity:** Associations and Groups
Hours of teaching: 4
Teaching date: 08/2016
Type of participation: Participatory - invited/keynote talk
- 3** **Name of the event:** SHELX Workshops at the ACA Meeting
City organizing entity: Denver, United States of America
Organising entity: American Crystallographic Association
Hours of teaching: 1
Teaching date: 07/2016
- 4** **Type of event:** Workshop
Name of the event: CCP4 Crystallography School
City organizing entity: Okinawa, Japan
Organising entity: Okinawa Institute of Science and Technology and CCP4 **Type of entity:** University Research Institute
Hours of teaching: 60 **Teaching language:** English
Teaching date: 11/2015
- 5** **Type of event:** Workshop
Name of the event: Software Fayre at ECM29
City organizing entity: Rovinj, Croatia
Organising entity: European Crystallographic Association **Type of entity:** Associations and Groups
Hours of teaching: 1 **Teaching language:** English
Teaching date: 08/2015
- 6** **Type of event:** Workshop
Name of the event: Software Fayre at ECM28
City organizing entity: Warwick, West Midlands, United Kingdom



Organising entity: European Crystallographic Association

Type of entity: Associations and Groups

Hours of teaching: 1

Teaching language: English

Teaching date: 08/2013

Scientific and technological experience

Scientific or technological activities

R&D projects funded through competitive calls of public or private entities

- 1** **Name of the project:** VW-Stiftung Niedersachsenprofessur
Entity where project took place: Georg-August-Universität Göttingen
City of entity: Göttingen, Braunschweig, Germany
Name principal investigator (PI, Co-PI....): George Sheldrick
N° of researchers: 1
Start-End date: 2012 - 2016
Type of entity: University
- 2** **Name of the project:** Desarrollo de métodos cristalográficos(IV) y su aplicación a aspectos del metabolismo del azufre
Entity where project took place: Instituto de Biología Molecular de Barcelona
City of entity: Barcelona, Catalonia, Spain
Name principal investigator (PI, Co-PI....): Isabel Usón Finkenzeller
Funding entity or bodies: Ministerio de Economía y Competitividad Tipo de entidad: Agencia Estatal
Type of entity: State agency
Start-End date: 01/01/2013 - 31/12/2015
- 3** **Name of the project:** ARCIMBOLDO CLOUD: Cloud computing con ARCIMBOLDO para una solución de estructuras cristalográficas por supercomputación en la FCSCCL
Entity where project took place: Insituto de Biología Molecular de Barcelona
City of entity: Barcelona, Catalonia, Spain
Name principal investigator (PI, Co-PI....): Isabel Usón Finkenzeller
Funding entity or bodies: Centro para el Desarrollo Tecnológico Industrial Tipo de entidad: Entidad Empresarial Ciudad entidad financiadora: Madrid
Type of entity: State agency
Start-End date: 01/01/2010 - 31/12/2012
- 4** **Name of the project:** Ayuda a Grupos de Investigación consolidados de Cataluña (2009SGR 1036)
Entity where project took place: Instituto de Biología Molecular de Barcelona
City of entity: Barcelona, Catalonia, Spain
Name principal investigator (PI, Co-PI....): Isabel Usón Finkenzeller
Start-End date: 01/01/2009 - 31/12/2012
Type of entity: State agency



- 5 Name of the project:** Desarrollo de métodos cristalográficos(III) y su aplicación a aspectos del metabolismo del azufre
- Entity where project took place:** Instituto de Biología Molecular de Barcelona
- Type of entity:** State agency
- City of entity:** Barcelona, Catalonia, Spain
- Start-End date:** 01/01/2009 - 31/12/2012

R&D non-competitive contracts, agreements or projects with public or private entities

Name of the project: ARCIMBOLDO phasing software joins CCP4 7.0 release

Degree of contribution: Researcher

Name principal investigator (PI, Co-PI...): Massimo Domenico Sammito; Claudia Millán Nebot

Nº of researchers: 2

Funding entity or bodies: THE SCIENCE AND TECHNOLOGY FACILITIES COUNCIL (STFC)

Type of entity: State agency

City funding entity: Cambridge, East Anglia, United Kingdom

Start date: 01/09/2015

Duration: 11 months

Total amount: 26.211,28 €

Scientific and technological activities

Scientific production

Publications, scientific and technical documents

- 1** Ana Medina; Josep Triviño; Rafael J. Borges; Claudia Millán; Isabel Usón; Massimo D. Sammito. ALEPH: a network-oriented approach for the generation of fragment-based libraries and for structure interpretation}. Acta Crystallographica Section D. 76 - 3, pp. 193 - 208. 03/2020. Available on-line at: <<https://doi.org/10.1107/S2059798320001679>>.
- Type of production:** Scientific paper
- Format:** Journal
- Corresponding author:** Yes
- 2** Rafael Junqueira Borges; Kathrin Meindl; Josep Triviño; Massimo Sammito; Ana Medina; Claudia Millán; Martin Alcorlo; Juan A. Hermoso; Marcos Roberto de Mattos Fontes; Isabel Usón. SEQUENCE SLIDER: expanding polyalanine fragments for phasing with multiple side-chain hypotheses}. Acta Crystallographica Section D. 76 - 3, pp. 221 - 237. 03/2020. Available on-line at: <<https://doi.org/10.1107/S2059798320000339>>.
- Type of production:** Scientific paper
- Format:** Journal
- 3** Kaushik S. Hatti; Airlie J. McCoy; Robert D. Oeffner; Massimo D. Sammito; Randy J. Read. Factors influencing estimates of coordinate error for molecular replacement. Acta Crystallographica Section D. 76 - 1, pp. 19 - 27. 01/2020. Available on-line at: <<https://doi.org/10.1107/S2059798319015730>>.
- Type of production:** Scientific paper
- Format:** Journal
- 4** Dorothee Liebschner; Pavel V. Afonine; Matthew L. Baker; Gabor Bunkóczi; Vincent B. Chen; Tristan I. Croll; Bradley Hintze; Li-Wei Hung; Swati Jain; Airlie J. McCoy; Nigel W. Moriarty; Robert D. Oeffner; Billy K. Poon; Michael G. Prisant; Randy J. Read; Jane S. Richardson; David C. Richardson; Massimo D. Sammito; Oleg V.



Sobolev; Duncan H. Stockwell; Thomas C. Terwilliger; Alexandre G. Urzhumtsev; Lizbeth L. Videau; Christopher J. Williams; Paul D. Adams. Macromolecular structure determination using X-rays, neutrons and electrons: recent developments in Phenix. *Acta Crystallographica Section D*. 75 - 10, pp. 861 - 877. 10/2019. Available on-line at: <<https://doi.org/10.1107/S2059798319011471>>.

Type of production: Scientific paper

Format: Journal

- 5 Randy J. Read; Massimo D. Sammito; Andriy Kryshtafovych; Tristan I. Croll. Evaluation of model refinement in CASP13. *Proteins: Structure, Function, and Bioinformatics*. 87 - 12, pp. 1249 - 1262. 2019. Available on-line at: <<https://onlinelibrary.wiley.com/doi/abs/10.1002/prot.25794>>.

Type of production: Scientific paper

Format: Journal

- 6 Tristan I. Croll; Massimo D. Sammito; Andriy Kryshtafovych; Randy J. Read. Evaluation of template-based modeling in CASP13. *Proteins: Structure, Function, and Bioinformatics*. 87 - 12, pp. 1113 - 1127. 2019. Available on-line at: <<https://onlinelibrary.wiley.com/doi/abs/10.1002/prot.25800>>.

Type of production: Scientific paper

Format: Journal

- 7 Iracema Caballero; Massimo Sammito; Claudia Millán; Andrey Lebedev; Nicolas Soler; Isabel Usón. ARCIMBOLDO on coiled coils. *Acta Crystallographica D*. 74 - 3, pp. 194 - 204. 01/03/2018.

Type of production: Scientific paper

Format: Journal

- 8 Sofiya Fedosyuk; Gustavo Arruda Bezerra; Katharina Radakovics; Terry K. Smith; Massimo Sammito; Nina Bobik; Adam Round; Lynn F. Ten Eyck; Kristina Djinovi? Carugo; Isabel Usón; Tim Skern. Vaccinia Virus Immunomodulator A46: A Lipid and Protein-Binding Scaffold for Sequestering Host TIR-Domain Proteins. *PLoS Pathogens*. 12 - 12, pp. 1 - 24. 14/12/2016.

Type of production: Scientific paper

Format: Journal

- 9 Massimo Sammito; Claudia Millán; Dawid Frieske; Eloy Rodríguez-Freire; Rafael Junqueira-Borges; Isabel Usón. ARCIMBOLDO_LITE: single workstation implementation and use. *Acta Crystallographica D*. 71 - 9, pp. 1921 - 1930. 01/09/2015.

Type of production: Scientific paper

Format: Journal

- 10 Claudia Millán; Massimo Sammito; Irene García-Ferrer; Theodoros Goulas; George M. Sheldrick; Isabel Usón. Combining phase information in reciprocal space for ARCIMBOLDO. *Acta Crystallographica D*. 71 - 9, pp. 1931 - 1945. 01/09/2015.

Type of production: Scientific paper

Format: Journal

- 11 Guillaume A Schoch; Massimo Sammito; Claudia Millán; Isabel Usón; Markus G Rudolph. Structure of a 13-fold superhelix (almost) determined from first principles. *IUCrJ*. 2 - Pt 2, pp. 177 - 264. 01/03/2015. ISSN 2052-2525

Type of production: Scientific paper

Format: Journal

- 12 Claudia Millán; Massimo Sammito; Isabel Usón. Macromolecular ab initio phasing enforcing secondary and tertiary structure. *IUCrJ*. 2 - Pt 1, pp. 95 - 200. 01/01/2015. ISSN 2052-2525

Type of production: Scientific paper

Format: Journal

- 13 Massimo Sammito; Kathrin Meindl; Iñaki M de Ilarduya; Claudia Millán; Cecilia Artola Recolons; Juan A Hermoso; Isabel Usón. Structure solution with ARCIMBOLDO using fragments derived from distant homology models. *The FEBS journal*. 281 - 18, pp. 4029 - 4074. 01/09/2014. ISSN 1742-4658

Type of production: Scientific paper

Format: Journal

- 14 Kevin Pröpper; Kathrin Meindl; Massimo Sammito; Birger Dittrich; George M Sheldrick; Ehmke Pohl; Isabel Usón. Structure solution of DNA-binding proteins and complexes with ARCIMBOLDO libraries. *Acta crystallographica. Section D, Biological crystallography*. 70 - Pt 6, pp. 1743 - 1800. 30/05/2014. ISSN 1399-0047

Type of production: Scientific paper

Format: Journal

- 15** Massimo Sammito; Claudia Millán; Dayté D Rodríguez; Iñaki M de Ilarduya; Kathrin Meindl; Ivan De Marino; Giovanna Petrillo; Rubén M Buey; José M de Pereda; Kornelius Zeth; George M Sheldrick; Isabel Usón. Exploiting tertiary structure through local folds for crystallographic phasing. *Nature methods*. 10 - 11, pp. 1099 - 1200. 01/11/2013. ISSN 1548-7105
Type of production: Scientific paper **Format:** Journal
- 16** Dayté Rodríguez; Massimo Sammito; Kathrin Meindl; Iñaki M de Ilarduya; Marianus Potratz; George M Sheldrick; Isabel Usón. Practical structure solution with ARCIMBOLDO. *Acta crystallographica. Section D, Biological crystallography*. 68 - Pt 4, pp. 336 - 379. 16/03/2012. ISSN 1399-0047
Type of production: Scientific paper **Format:** Journal
- 17** Massimo Sammito; Claudia Millán. *Bioinformática para la cristalografía. MoleQla*. 8, 21/12/2012.
Type of production: Popular science article **Format:** Journal
- 18** Isabel Usón; Claudia Millán; Massimo Sammito; Kathrin Meindl; Iñaki Martínez de Ilarduya; Ivan De Marino; Dayté Rodríguez. Phasing Through Location of Small Fragments and Density Modification with ARCIMBOLDO. *Advancing Methods for Biomolecular Crystallography*. pp. 123 - 132. Springer, 01/01/2013.
Type of production: Book chapter **Format:** Book

Works submitted to national or international conferences

- 1** **Title of the work:** How to map a protein structure into a network graph to understand protein folding.
Name of the conference: PyData 2017
City of event: Barcelona, Spain
Date of event: 19/05/2017
End date: 21/05/2017
Organising entity: NumFocus and Python
Massimo Sammito.
- 2** **Title of the work:** Using BORGES_MATRIX for X-ray ab initio phasing and structure interpretation
Name of the conference: Understanding biology through structure
City of event: Santa Fe, United States of America
Date of event: 13/05/2017
End date: 17/05/2017
Organising entity: Los Alamos National Laboratory and the New Mexico Consortium
Massimo Sammito; Claudia Millán; Ana Medina; Iracema Caballero; Nicolas Soler; Isabel Usón.
- 3** **Title of the work:** ARCIMBOLDO_SHREDDER's contribution to MR: phasing with fragments from distant homologs
Name of the conference: 30th European Crystallographic Meeting
City of event: Basel, Switzerland
Date of event: 28/08/2016
End date: 01/09/2016
Organising entity: European Crystallographic Association
Claudia Millán; Massimo Sammito; Andrey Nascimiento; Isabel Usón.
- 4** **Title of the work:** BORGES_MATRIX: a tool to generate models for ab initio phasing and for structure interpretation
Name of the conference: 30th European Crystallographic Meeting



City of event: Basel, Switzerland

Date of event: 28/08/2016

End date: 01/09/2016

Organising entity: European Crystallographic Association

Massimo Sammito; Claudia Millán; Rafael Borges; George Sheldrick; Isabel Usón.

5 Title of the work: Solving protein structures without a model or experimental phases.

Name of the conference: 66th Annual Meeting of ACA

City of event: Denver, United States of America

Date of event: 22/07/2016

End date: 26/07/2016

Organising entity: American Crystallographic Association

Massimo Sammito; Claudia Millán; Rafael Borges; Andrey Nascimiento; George Sheldrick; Isabel Usón.

6 Title of the work: Molecular replacement with small fragments: ARCIMBLDO and PHASER

Name of the conference: Diffraction Methods in Structural Biology: Gordon Conferences

City of event: Lewiston, United States of America

Date of event: 17/07/2016

End date: 22/07/2016

Organising entity: Gordon Conference

Isabel Usón; Airlie McCoy; Claudia Millán; Massimo Sammito; Andrey Nascimiento; Robert Oeffner; Randy Read.

7 Title of the work: BORGES libraries: from phasing to structural bioinformatics

Name of the conference: The 29th European Crystallographic Meeting

Type of participation: 'Participatory - poster

Corresponding author: No

City of event: Rovinj, Croatia

Date of event: 23/08/2015

End date: 28/08/2015

Organising entity: European Crystallographic Association

Massimo Sammito; Claudia Millán; Rafael Junqueira Borges; Lynn Ten Eyck; Isabel Usón.

8 Title of the work: SEQUENCE SLIDER: a multi sequence evaluator and its application in venomics

Name of the conference: The 29th European Crystallographic Meeting

Type of participation: Participatory - oral communication

Corresponding author: No

City of event: Rovinj, Croatia

Date of event: 23/08/2015

End date: 28/08/2015

Organising entity: European Crystallographic Association

Rafael Junqueira Borges; Massimo Sammito; Claudia Millán; Marcos Fontes; Isabel Usón.

9 Title of the work: Use of clustering algorithms to combine partial solutions in reciprocal space

Name of the conference: The 29th European Crystallographic Meeting

Type of participation: Participatory - oral communication

Corresponding author: No

City of event: Rovinj, Croatia

Date of event: 23/08/2015

End date: 28/08/2015

Organising entity: European Crystallographic Association

Claudia Millán; Massimo Sammito; Rafael Junqueira Borges; Isabel Usón.

- 10** **Title of the work:** Phasing your XALOC data with ARCIMBOLDO
Name of the conference: VII Congress of the Spanish Synchrotron User Association (AUSE) and the II ALBA User's Meeting
Type of participation: Participatory - oral communication
Corresponding author: No
City of event: Barcelona, Catalonia, Spain
Date of event: 16/06/2015
End date: 19/06/2015
Organising entity: ALBA Synchrotron
Rafael Junqueira Borges; Massimo Sammito; Claudia Millán; Jordi Juanhuix; Isabel Usón.
- 11** **Title of the work:** Structure of a thirteen-fold superhelix (almost) determined from first principles
Name of the conference: The Biophysical Society Annual Meeting
Type of participation: 'Participatory - poster
Corresponding author: No
City of event: Baltimore, United States of America
Date of event: 07/02/2015
End date: 11/02/2015
Organising entity: Biophysical Society
Guillaume Schoch; Massimo Sammito; Claudia Millán; Isabel Usón; Markus Rudolph.
- 12** **Title of the work:** Exploiting tertiary folds as fragment libraries for phasing
Name of the conference: BAC2014 (Biotech annual Congress 2014)
Type of participation: Participatory - oral communication
City of event: Barcelona, Catalonia, Spain
Date of event: 09/07/2014
End date: 11/07/2014
Organising entity: FEBiotec
- 13** **Title of the work:** BORGES-ARCIMBOLDO exploiting tertiary folds as fragments libraries for phasing
Name of the conference: ECM28 (28th European Crystallography Meeting)
Type of participation: Participatory - oral communication
Corresponding author: No
City of event: Warwick, West Midlands, United Kingdom
Date of event: 26/08/2013
End date: 29/08/2013
Organising entity: European Crystallographic Association
Type of entity: Associations and Groups
Massimo Sammito; Claudia Millán; Kathrin Meindl; Iñaki Martínez de Ilarduya; Isabel Usón.
- 14** **Title of the work:** Reciprocal space clustering of BORGES-ARCIMBOLDO partial solutions: Practical cases
Name of the conference: ECM28 (28th European Crystallography Meeting)
Type of participation: 'Participatory - poster
Corresponding author: No
City of event: Warwick, West Midlands, United Kingdom
Date of event: 25/08/2013
End date: 29/08/2013
Organising entity: European Crystallographic Association
Type of entity: Associations and Groups



Claudia Millán; Massimo Sammito; Kathrin Meindl; Iñaki Martínez de Ilarduya; Isabel Usón.

- 15** **Title of the work:** DNA - Protein Complex Structure Prediction
Name of the conference: The 27th Meeting of the European Crystallographic Association
Type of participation: 'Participatory - poster
Corresponding author: No
City of event: Bergen, Norway
Date of event: 06/08/2012
End date: 11/08/2012
Organising entity: European Crystallographic Association
K. Propper; K. Meindl; D.D Rodríguez; M. Sammito; B. Dittrich; G.M. Sheldrick; E. Pohl; I. Usón.
- 16** **Title of the work:** ARCIMBOLDO structure solution with customized and clustered fragment libraries from Borges
Name of the conference: International School of Crystallography 45th Course Present and Future Methods for Biomolecular Crystallography
Type of participation: 'Participatory - poster
Corresponding author: Yes
City of event: Erice, Sicilia, Italy
Date of event: 31/05/2012
End date: 10/06/2012
Organising entity: Ettore Majorana Foundation and **Type of entity:** R&D Centre
Center for Scientific Culture
Massimo Sammito; Claudia Millán; Dayté D. Rodríguez; Kathrin Meindl; Iñaki Martínez de Ilarduya; George M. Sheldrick; Isabel Usón.
- 17** **Title of the work:** Clustering fragments for ARCIMBOLDO phasing
Name of the conference: International School of Crystallography 45th Course Present and Future Methods for Biomolecular Crystallography
Type of participation: 'Participatory - poster
Corresponding author: No
City of event: Erice, Sicilia, Italy
Date of event: 31/05/2012
End date: 10/06/2012
Organising entity: Ettore Majorana Foundation and **Type of entity:** R&D Centre
Center for Scientific Culture
Claudia Millán; Massimo Sammito; Dayté D. Rodríguez; Kathrin Meindl; Iñaki M. de Ilarduya; George M. Sheldrick; Isabel Usón.
- 18** **Title of the work:** Clustering for ARCIMBOLDO
Name of the conference: ZCAM-Daresbury Laboratory collaborative tutorial: Computational methods for macromolecular phasing and refinement
Type of participation: 'Participatory - poster
Corresponding author: No
City of event: Zaragoza, Aragon, Spain
Date of event: 11/03/2012
End date: 17/03/2012
Organising entity: Nodos CECAM de Zaragoza y Daresbury
Claudia Millán; Massimo Sammito; Dayté Dayana Rodríguez; Kathrin Meindl; Iñaki Martínez de Ilarduya; George M. Sheldrick; Isabel Usón.



- 19** **Title of the work:** ARCIMBOLDO goes super: ab Initio phasing on the supercomputer Calendula FCSC
Name of the conference: XXII Congress and General Assembly of International Union of Crystallography
Type of participation: 'Participatory - poster
Corresponding author: No
City of event: Madrid, Community of Madrid, Spain
Date of event: 22/08/2011
End date: 29/08/2011
Organising entity: International Union of Crystallography
I. Usón.; D.D. Rodríguez; M. Sammito; K. Meindl; I. M. de Ilarduya.
- 20** **Title of the work:** BORGES a tool to generate customised, secondary structure libraries for phasing
Name of the conference: XXII Congress and General Assembly of International Union of Crystallography
Type of participation: 'Participatory - poster
Corresponding author: Yes
City of event: Madrid, Community of Madrid, Spain
Date of event: 22/08/2011
End date: 29/08/2011
Organising entity: International Union of Crystallography
M. Sammito; D.D. Rodríguez; K. Meindl; I. M. de Ilarduya; I. Usón.
- 21** **Title of the work:** New features in ARCIMBOLDO: a tutorial
Name of the conference: XXII Congress and General Assembly of International Union of Crystallography
Type of participation: 'Participatory - poster
Corresponding author: Yes
City of event: Madrid, Community of Madrid, Spain
Date of event: 22/08/2011
End date: 29/08/2011
Organising entity: International Union of Crystallography
D.D. Rodríguez; M. Sammito; I. M. de Ilarduya; K. Meindl; I. Usón.

Other achievements

Stays in public or private R&D centres

- 1** **Entity:** Cambridge University **Type of entity:** University
Faculty, institute or centre: The Cambridge Institute for Medical Research (CIMR)
City of entity: Cambridge, East Anglia, United Kingdom
Start-End date: 01/09/2015 - 31/07/2016 **Duration:** 11 months
Goals of the stay: Guest
Provable tasks: Research stay at CIMR, hosted by Prof. Read's group, 11 month, developing structural and bioinformatic computing methods and algorithms for Biomedicine. Integrating ARCIMBOLDO, BORGES and SHREDDER in the Collaborative Computing Project dedicated to Crystallography community (CCP4) and PHASER.
- 2** **Entity:** Georg-August-Universität Göttingen
City of entity: Göttingen, Germany
Start-End date: 30/06/2015 - 28/07/2015
Goals of the stay: Guest



Provable tasks: Research stay hosted by Prof. Sheldrick's group at the University of Göttingen of one month, working on methods and software development of SHELXE and its integration in ARCIMBOLDO pipeline to phase difficult macromolecular structures.

3 Entity: Georg-August-Universität Göttingen

City of entity: Göttingen, Germany

Start-End date: 03/07/2014 - 31/08/2014

Goals of the stay: Guest

Provable tasks: Research stay hosted by Prof. Sheldrick's group at the University of Göttingen of one month, working on methods and software development of SHELXE and its integration in ARCIMBOLDO pipeline to phase difficult macromolecular structures.

4 Entity: Medical Research Council

Type of entity: State agency

City of entity: Cambridge, United Kingdom

Start-End date: 05/2014 - 05/2014

Goals of the stay: Guest

Provable tasks: Meeting between CCP4 and ARCIMBOLDO software developers

Obtained grants and scholarships

1 Name of the grant: MSCA-ST-IF: Marie Curie Individual Fellowship

Aims: Post-doctoral

Awarding entity: European Commission

Conferral date: 01/06/2018

Duration: 2 years

End date: 31/05/2020

Entity where activity was carried out: MRC-CIMR

2 Name of the grant: Grant for attending "Advanced Software Development for Crystallographers"

City awarding entity:

Aims: Pre-doctoral

Awarding entity: the European Crystallographic Association's Computing Special Interest Group

Type of entity: Associations and Groups

Amount of the grant: 125 €

Conferral date: 12/08/2015

Duration: 3 days

Entity where activity was carried out: 29th European Crystallographic Meeting in Rovinj

3 Name of the grant: Georg-August-Universität Göttingen grant for project "Exploiting tertiary folds as fragment libraries for phasing"

City awarding entity:

Aims: Pre-doctoral

Awarding entity: Georg-August-Universität Göttingen

Type of entity: University

Amount of the grant: 1.365 €

Conferral date: 30/07/2015

Duration: 2 months

Entity where activity was carried out: Georg-August-Universität Göttingen

4 Name of the grant: Travel grant for attending the 29th European Crystallographic Meeting

City awarding entity:

Aims: Pre-doctoral

Awarding entity: the European Crystallographic Association

Type of entity: Associations and Groups



Amount of the grant: 220 €

Conferral date: 09/06/2015

Duration: 8 days

Entity where activity was carried out: 29th European Crystallographic Meeting in Rovinj

- 5 Name of the grant:** Georg-August-Universität Göttingen grant for project "Exploiting tertiary folds as fragment libraries for phasing"

City awarding entity:

Aims: Pre-doctoral

Awarding entity: Georg-August-Universität Göttingen

Type of entity: University

Amount of the grant: 1.365 €

Conferral date: 30/07/2014

Duration: 2 months

Entity where activity was carried out: Georg-August-Universität Göttingen

- 6 Name of the grant:** Grant for attending "An introduction to Software Development for Crystallographers"

City awarding entity:

Aims: Pre-doctoral

Awarding entity: the European Crystallographic Association's Computing Special Interest Group

Type of entity: Associations and Groups

Amount of the grant: 130,88 €

Conferral date: 24/07/2013

Duration: 3 days

Entity where activity was carried out: 28th European Crystallographic Meeting in Warwick

- 7 Name of the grant:** Travel grant for attending the 28th European Crystallographic Meeting

City awarding entity:

Aims: Pre-doctoral

Awarding entity: the European Crystallographic Association

Type of entity: Associations and Groups

Amount of the grant: 327,2 €

Conferral date: 11/06/2013

Duration: 8 days

Entity where activity was carried out: 28th European Crystallographic Meeting in Warwick

- 8 Name of the grant:** 45th International School of Crystallography

City awarding entity:

Aims: Pre-doctoral

Awarding entity: «Ettore Majorana» Foundation and International Centre for Scientific Culture

Type of entity: Foundation

Amount of the grant: 800 €

Conferral date: 23/01/2012

Duration: 10 days

Entity where activity was carried out: Erice NATO Advanced Study Institute

Scientific societies and professional associations

- 1 Name of the society:** European Crystallographic Association (ECA)

Affiliation entity: International Union of Crystallography (IUCr)

Start date: 10/07/2015

- 2 Name of the society:** Associació de Biotecnòlegs de Catalunya (Asbtec)

Affiliation entity: Federación Española de Biotecnólogos (FEBiotec)

Type of entity: Associations and Groups



Start date: 01/06/2014

Prizes, mentions and distinctions

- 1** **Description:** Best Ph.D thesis 2015
Awarding entity: Faculty of Pharmacy. University of Barcelona
City awarding entity: Barcelona, Catalonia, Spain
Conferral date: 19/04/2018
- 2** **Description:** Best Poster at ACA 2016
Awarding entity: Taylor and Francis Group
City awarding entity: Denver, United States of America
Conferral date: 2016