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Present **IBMB-CSIC/PCB**

Since Sept. 03 ICREA Research Professor vinculated to the Spanish Research Council. *Maria de Maeztu* 2014 Excellence Unit Departament of Structural Biology at Instituto de Biología Molecular de Barcelona (IBMB-CSIC). Development of computational methods for macromolecular crystallography and structural characterization of proteins involved in catalysis. Author of the structure solution methods programmed in ARCIMBOLDO (fragment search plus density modification in a supercomputer frame), SUBIX (geometrical phasing of DNA and its complexes), BORGES (local geometry analysis and customized libraries) and SHREDDER (phasing with distant homologs). Developer of SHELX.

Habilitation **University of Göttingen (Germany)**

Jul.01-Aug.03 Lecturer (Privat Dozentin) at the Department of Structural Chemistry.
4 Juli. 01 Habilitation *Venia legendi* in the area „Structural Chemistry”.

Habilitation Thesis: „On *ab initio* structure solution, the IGF-II-binding domain of the MIR-receptor and the catalytic mechanism of sulfatases“.

Apr. 96- Jul. 01 Lecturer (Habilitation) in the group of Prof. G.M. Sheldrick.
Working in methods development in macromolecular crystallography.

Dual-space recycling *ab Initio* and substructure solution.

Structural basis of sulfatase deficiencies and the IGFII-regulación.

Design and execution of the „Environmental Chemistry“ course for Chemistry Students.

In charge of the general chemistry introductory practical course (Grundkurs) for Chemistry Students.

Postdoctoral **University of Göttingen (Germany)**

Feb.94-Apr.96 Postdoctoral Fellowship (Human Capital and Mobility European Union Program: HCM). Project: "New catalysts on the basis of organometallic fluorides" directed by Prof. H. W. Roesky.

Studies

University of Zaragoza (Spain)

July 1992 Doctor Thesis (Tesis Doctoral) "Synthesis and structure of homonuclear platinum (II) compounds and heteropolinuclear platinum (II) compounds with silver, lead, tin, thallium and mercury", Doctor examination with the highest grade ("Apto cum Laude").

Oct. 91-Oct.92 Associate Lecturer in the Inorganic Chemistry Department
In charge of the General Chemistry courses at the Polytechnical School in Huesca.

Jan. 88-Sept.91 Postgraduate Scholarship from the Spanish Ministerio de Educación y Ciencia at "Instituto de Ciencia de Materiales de Aragón, Universidad de Zaragoza-CSIC" (Institute for Science and Technology of Materials).

Working on the project "Organometallic Compounds with metal-to-metal bonds between Platinum (II) and Silver (I), Thallium (I), Tin (II), or Lead (II): Synthesis and structural characterization".

1988 Master Thesis (Tesis de Licenciatura) "Organometallic platinum(II) compounds with pentafluorophenyl groups", with the highest grade (Sobresaliente).

Oct.82-June 87 Degree (Licenciatura) in Sciences with specialization in Inorganic Chemistry with grade A (Sobresaliente).

Publications 183

Patents 1

Lectures, meetings 100 main contributions, organization of CCP4SW 2019, "Integrated, rational molecular replacement" and of a conference on "Methods and applications in the frontier between MX and CryoEM, Barcelona 19-21 September 2017. Co-organization of workshops on computational methods for macromolecular crystallography (2004 and 2006 in Barcelona at IBMB and CESCO, 2007 in York, 2012 in Zaragoza at ZCAM and 2016, 2017, 2018, 2019 in Madrid).

Honours Life member of Clare Hall College, University of Cambridge

Organisatorial Co-authoring and leading the proposal for a second beamline dedicated to macromolecular crystallography at the Synchrotron Alba, now under construction. Member of the construction project board of the XAIRA beamline and external advisor and reviewer of Alba's Structural and Molecular Biology planning for the upgrade to a 4th generation synchrotron source. Member of ESRF proposal-grading panel.

Projects Funded by MICINN, CDTI, AGAUR, CSIC, Royal Society, CCP4-STFC

Ph.D. / MSc

Theses directed 17 / 11

Further experience in structural biophysical and computational methods:
Low temperature X-ray crystallography with laboratory and synchrotron equipment
Computer networks under Linux, UNIX and VMS. Middleware.
FORTRAN, Python.

Work experience **Procter & Gamble** European Technical Center
Temselaan 100, 1853 Strombeek-Bever, Belgium.

Nov.92-Feb.94 Product Research Scientist in Research and Development Department
Responsible for the development of trace analysis methods, to evaluate the performance and guide the development of perfume in laundry and household cleaning products.

Languages Spanish, mother tongue, English and German, excellent, French, good.

Research Group Dra. Iracema Caballero Elisabeth Jiménez
Dr. Roberto Navarro Josep Triviño
Dr. Rafael Borges Maria del Carmen Martín
Marc Hsiao Lee

Attachment I: Publications

- 1.- (NBu₄)[Sn{Pt(μ-Cl)(C₆F₅)₂}₃], an unusual Cluster with Three Pt^{II}→Sn^{II} Bonds".
Angew. Chem. Int. Ed. Engl. **29** (1990)1449.
Rafael Usón*, Juan Forniés, Milagros Tomás and Isabel Usón.
- 2.- Synthesis and molecular structure of (NBu₄)₂{Pb[Pt(C₆F₅)₄]₂}, the first lead(II) compound linearly bonded to two metal atoms".
Inorg. Chem. **31** (1992) 3697.
Rafael Usón*, Juan Forniés, Larry R. Falvello, Miguel A. Usón and Isabel Usón.
- 3.- A highly symmetrical octa-Palladium(I) compound: Crystal Structure of {[Pd(μ-SC₆F₅)(μ-dppm)Pd](μ-SC₆F₅)}₄•2 O(C₂H₅)₂.
Inorg. Chem. **32** (1993) 1066.
Rafael Usón*, Juan Forniés, Larry R. Falvello, Miguel A. Usón, Isabel Usón and Santiago Herrero.
- 4.- Pentafluorophenyl trinuclear Pt₂Hg und hexanuclear Pt₄Hg₂ anionic complexes containing unbridged Pt-Hg bonds and OH bridges.
Inorg. Chim. Acta **212** (1993) 105.
Rafael Usón*, Juan Forniés, Larry R. Falvello, Irene Ara and Isabel Usón.
- 5.- Lösliche organische Derivate von Alumosilicaten mit Al₂Si₂O₄- und Al₄Si₂O₆-Gerüsten.
Angew. Chem. **106** (1994) 2198; *Int. Ed. Engl.* **33** (1994) 2103.
Mavis L. Montero, Isabel Usón and Herbert W. Roesky*.
- 6.- Pentahalophenyl ethylxanthate complexes of platinum (II). Structures of (NBu₄)[Pt(C₆F₅)₂(S₂COEt)] and (NBu₄)₂{Pt₄(C₆F₅)₈[(μ₃-S)SCOEt]₂}. Unprecedented coordination of the xanthate ligands in the tetranuclear complex.
Inorg. Chim. Acta **232** (1995) 35.
Rafael Usón*, Juan Forniés, Larry R. Falvello, Milagros Tomás, Irene Ara and Isabel Usón.
- 7.- Synthesis and structure of metal-containing eight- and twelve-membered M-N-C-O-heterocycles (M= Al, Ga, In).
Main Group Chemistry **1** (1995) 127.
Andreas Klemp, Isabel Usón, Jens-Thomas Ahlemann, Thomas Belgardt, Jens Storre and Herbert W. Roesky*.
- 8.- Lösliche Alumosilicaten mit Grundgerüsten von Mineralien.
Angew. Chem. **107** (1995) 2761; *Int. Ed. Engl.* **34** (1995) 2504.
Mavis L. Montero, Andreas Voigt, Markus Teichert, Isabel Usón and Herbert W. Roesky*.
- 9.- Synthesis and structure of bisphosphaallyl complexes with two-co-ordinate phosphorus.
J. Chem. Soc. Dalton Trans. (1995) 1951.
Uwe Wirringa, Heike Voelker, Herbert W. Roesky*, Yuri Shermolovich, Leonid Markovski, Isabel Usón, Mathias Noltemeyer and Hans-Georg Schmidt.

- 10.-Synthesis and structure of cyclopentadienyl fluoro and chloro complexes of the triad (Ti Zr, Hf) containing acyclic and cyclic siloxane building blocks.
J. Chem. Soc. Dalton Trans. (1995) 2453.
Feng-Quan Liu, Isabel Usón and Herbert W. Roesky*.
- 11.-Syntheses and structure of the first eight-membered fluoro and chloro hafnium siloxane complexes.
Z. Anorg. Allg. Chem. **622** (1996) 819-822.
Feng-Quan Liu, Isabel Usón and Herbert W. Roesky*.
- 12.-Syntheses and properties of cyclopentadienyl-substituted imidotitanium fluorides.
Inorg. Chem. **35** (1996) 741.
Feng-Quan Liu, Axel Herzog, Herbert W. Roesky* and Isabel Usón.
- 13.-Synthesis and characterisation of quinoide bridged dinuclear complexes of titanium and zirconium.
J. Chem. Soc. Dalton Trans. (1996) 913.
Antje Künzel, Maxim Sokolow, Feng-Quan Liu, Herbert W. Roesky*, Mathias Noltemeyer, Hans-Georg Schmidt and Isabel Usón.
- 14.-Syntheses, structure and reactivity of a series of (pentamethylcyclopentadienyl)molibdenum (V) and -tungsten (V) imido complexes.
Inorg. Chem. **35** (1996) 1773.
Katrin Köhler, Herbert W. Roesky*, Axel Herzog, Heinz Gornitzka, Alexander Steiner and Isabel Usón.
- 15.-Facile and rational route for high-yield synthesis of titanasilsesquioxanes from aminosilanetriols
Organometallics **15** (1996) 1610.
Andreas Voigt, Ramaswamy Murugavel, Vadapalli Chandrasekhar, Norbert Winkhofer, Herbert W. Roesky*, Hans-Georg Schmidt and Isabel Usón.
- 16.-Contribution of the intramolecular disulfide bridge to the folding stability of REI_v, the variable domain of a human immunoglobulin kappa-light chain.
Folding & Design **1**(1996) 431.
Christian Frisch, Harald Kolmar, Arno Schmidt, Gerd Kleemann, Astrid Reinhardt, Ehmke Pohl, Isabel Usón, Thomas R. Schneider and Hans-Joachim Fritz*.
- 17.-Über die Reaktion primärer und sekundärer Amine mit LiAlH₄ und Na(AlHET₃).
Angew. Chem. **109** (1997) 644; *Int. Ed. Engl.* **36** (1997) 629.
Mavis L. Montero, Helge Wessel, Herbert W. Roesky*, Markus Teichert and Isabel Usón.
- 18.-Synthesis and characterisation of (4-Fluorophenyl) amino-based amino- and iminometallanes of group 13. Crystal structures of (MeAlNRf)₄, (MeMNRf)_{6.n} THF (M= Al, n=2; M= Ga, n= 7) and (MeIn(THF)NRf)₄. (Rf = 4-C₆H₄F)
Organometallics **16** (1997) 1197-1202.

Christoph Schnitter, Said D. Waezsada, Herbert W. Roesky*, Markus Teichert, Isabel Usón and Emilio Parisini.

- 19.-Aminodimethylalanes ($R^1R^2NAlMe_2$) as useful synthetic precursors of aminoalane difluorides using trimethyltin fluoride; crystal structures of (2,6-i-Pr₂C₆H₃)N(SiMe₃)AlMe₂ and (2,6-i-Pr₂C₆H₃)N(SiMe₃)AlF₂.
Organometallics **16** (1997) 1260-1264.
Said D. Waezsada, Feng-Quan Liu, Eamonn F. Murphy, Herbert W. Roesky*, Markus Teichert, Isabel Usón, Hans-Georg Schmidt, Thomas Albers, Emilio Parisini and Mathias Noltemeyer.
- 20.-Lösliche, molekulare Titanosilicate. Soluble molecular titanosilicates.
Angew. Chem. **109** (1997) 1020; *Int. Ed. Engl.* **36** (1997) 1001.
Andreas Voigt, Ramaswamy Murugavel, Mavis L. Montero, Helge Wessel, Feng-Quan Liu, Herbert W. Roesky*, Isabel Usón, Thomas Albers and Emilio Parisini.
- 21.-Reactions of $\{[Pd(\mu-SC_6F_5)(\mu-dppm)Pd](\mu-SC_6F_5)\}_4 \cdot 2 O(C_2H_5)_2$. Crystal structures of the complexes $[(Ph_3P)Pd(\mu-SC_6F_5)(\mu-dppm)Pd(SC_6F_5)] \cdot 1.4 CH_2Cl_2$ and $[(Ph_3P)Pd(\mu-SC_6F_5)(\mu-dppm)Pd(PPh_3)]SO_3CF_3 \cdot 2 CH_2Cl_2$ and ab Initio MO calculations on the model systems $[(H_3P)Pd(\mu-H_2PCH_2PH_2)(\mu-SH)Pd(PH_3)]^+$ and $[(H_3P)Pd(\mu-H_2PCH_2PH_2)Pd(PH_3)]^{2+}$.
Inorg. Chem. **36** (1997) 1912-1922.
Rafael Usón*, Juan Forniés, Javier Fernández Sanz, Miguel A. Usón, Isabel Usón and Santiago Herrero.
- 22.-Formation of a tantalum siloxane cage complex in the reaction of $(\eta^5-C_5Me_5)TaMe_4$ with a silanetriol.
Inorg. Chem. **36** (1997) 3392-3393.
Alexander I. Gouzyr, Helge Wessel, Craig E. Barnes, Herbert W. Roesky*, Markus Teichert and Isabel Usón.
- 23.-Isostructural molecular amino- and oxo-aminoalumosilicates.
Organometallics **16** (1997) 3243-3245.
Helge Wessel, Carsten Rennekamp, Said D. Waezsada, Herbert W. Roesky*, Mavis L. Montero and Isabel Usón.
- 24.-X-ray crystallography reveals stringent conservation of protein fold after removal of the only disulfide bridge from a stabilized immunoglobulin variable domain. *Folding & Design* **2** (1997) 357-361.
Isabel Usón*, M. Teresa Bes, George M. Sheldrick, Thomas R. Schneider, Thomas Hartsch and Hans-Joachim Fritz.
- 25.-Synthese und Struktur von Aluminium-Fluor-Sauerstoff Clustern.
Angew. Chem. **109** (1997) 2738-2739; *Int. Ed. Engl.* **36** (1997) 2625-2626.
Said D. Waezsada, Feng-Quan Liu, Craig E. Barnes, Herbert W. Roesky*, Mavis L. Montero and Isabel Usón.

- 26.-Bildung adamantanartiger Strukturen durch Reaktion von Titanocenfluoriden mit einem Iminoalan. Formation of adamantane-like structures by reaction of titanocene fluorides with an iminoalane.
Angew. Chem. **110** (1998) 862-864; *Int. Ed. Engl.* **37** (1998) 843-845.
Helge Wessel, Mavis L. Montero, Carsten Rennekamp, Herbert W. Roesky*, Peihua Yu and Isabel Usón.
- 27.-Gallophosphonates containing alkali metal ions - Part 2: Synthesis and structure of gallophosphonates incorporating Na⁺ and K⁺ ions.
Inorg. Chem. **37** (1998) 473-478.
Mrinalli G. Walawalkar, Ramaswamy Murugavel, Herbert W. Roesky*, Isabel Usón and Ralph Krätzner.
- 28.-Formation of [Cp₂Ti(eta²-F)₂AlEt₂]₂ and [Cp(C₅H₄)Ti(eta²-H)AlEt₂]₂ in the reaction of Cp₂TiF₂ with AlEt₃; Structure of [Cp₂Ti(eta²-F)₂AlEt₂]₂.
Inorg. Chem. **37** (1998) 2595-2597.
Peihua Yu, Mavis L. Montero, Craig E. Barnes, Herbert W. Roesky*, and Isabel Usón.
- 29.-Syntheses and Structure of (CH₃Si)₆(NH)₉: A Si-N cage made from methyltrichlorosilane and ammonia.
Angew. Chem. **110** (1998) 1508-1510; *Int. Ed. Engl.* **37** (1998) 1432-1433.
Bodo Räge, Herbert W. Roesky*, Isabel Usón and Peter Müller.
- 30.-Reactions of group 4 metal cyclopentadienyl trifluorides with a trimeric iminoalane.
Organometallics **17** (1998) 1919-1921.
Helge Wessel, Carsten Rennekamp, Herbert W. Roesky*, Mavis L. Montero, Peter Müller and Isabel Usón.
- 31.-New dichlorosilanes, cyclotrisilanes and silacyclopropanes as precursors of intramolecularly coordinated silylenes.
Chem. Eur. J. **4** (1998) 852-863.
Johannes Belzner*, Uwe Dehnert, Heiko Ihmels, Matthias Hübner, Peter Müller and Isabel Usón.
- 32.-The first stereoselective bifunctionalization of 4-quinolones with organometallics and N-halosuccinimides to 2,3-trans-disubstituted tetrahydroquinolones: expected and unexpected results.
Synlett. (1998) 649-651.
Uwe Beifuss*, Gerald Feder, M.Teresa Bes and Isabel Usón.
- 33.-A hexacyclic estrone derivative.
Acta Crystallogr. **C54** (1998) 1341-1343.
M.Teresa Bes, János Wölfling, Isabel Usón, Szilvia Pelikán, Lutz F. Tietze, Eva Frank and Gyula Schneider.
- 34.-Reactions of organotitanoxane fluorides with AlR₃ (R=Me, Et, CH₂Ph) and Me₃SiCl: X-ray crystal structures of [C₅Me₅Ti(mu-O)]₄F[(mu-F)AlMe₃]₃, [C₅Me₅Ti(mu-

- O)]₄F₃[(μ-F)Al(CH₂Ph)₃], [C₅Me₅Ti(μ-O)Et]₄ and (C₅Me₅)₄Ti₄O₅X₂ (X= Cl and F).
- Inorg. Chem.* **37** (1998) 5117-5124.
- Peihua Yu, Thomas Pape, Isabel Usón, Musa A. Said, Herbert W. Roesky*, Mavis L. Montero, Hans-Georg Schmidt and Alojz Demsar.
- 35.-First structurally characterized organometallic chloro oxo-peroxo compounds of molybdenum and tungsten.
- Organometallics* **18** (1999) 106-108.
- Debashis Chakroborty, Manish Bhattacharjee, Rolf Siefken, Herbert W. Roesky*, Ralph Krätzner, Isabel Usón and Hans-Georg Schmidt.
- 36.-The 1.2 Å crystal structure of hirutasin reveals the intrinsic flexibility of a family of highly disulphide bridged inhibitors.
- Structure.* **7** (1999) 55-63;
- Isabel Usón, George M. Sheldrick, Eric de La Fortelle, Gerard Bricogne, Stefania di Marco, John P. Priestle, Markus G. Grütter and Peer R. E. Mittl
- 37.-Synthese und Struktur von {[MeAl(μ₂-F)]₂N(2,6-iPrC₆H₃)}₄ - eine molekulare Al-F-N-Käfigverbindung.
- Angew. Chem.* **111** (1999) 850-852; *Int. Ed. Engl.* **38** (1998) 813-815.
- Helge Wessel, H.S. Park, Peter Müller, Herbert W. Roesky* and Isabel Usón.
- 38.-V-Amylose at atomic resolution: X-Ray structure of a cycloamylose with 26 glucoses.
- Proc. Natl. Acad. Sci. USA*, **96** (1999) 4246-4251.
- Katrin Geßler, Isabel Usón, Takeshi Takaha, Norbert Krauß, Steven M. Smith, Shigetaka Okada, George M. Sheldrick and Wolfram Saenger*.
- 39.-1.7 Å structure of the stabilised REIv mutant T39K. Application of local NCS restraints.
- Acta Crystallogr.* **D55** (1999) 1158-1167.
- Isabel Usón*, Ehmke Pohl, Thomas R. Schneider, Zbigniew Dauter, Arno Schmidt, Hans-Joachim Fritz and George M. Sheldrick.
- 40.-Variation of a theme: crystal structure with four octakis-(2,3,6-tri-O-methyl) -cyclodextrin molecules hydrated differently by a total of 19.3 water.
- J. Am. Chem. Soc.* **121** (1999) 3321-3327;
- Thammárat Aree, Isabel Usón, Burkhard Schulz, Günter Reck, Helga Hoier, George M. Sheldrick and Wolfram Saenger*.
- 41.-Difference in reactivity of cyclopentadienyltitanium fluorides and chlorides using AlR₃ (R=Me, Et): Syntheses and structures of Ti(III)-F(Cl)-Al compounds (eta-C₅Me₅)₂Ti₂(μ-Cl)₆Al₂Me₄, (eta⁵-C₅Me₅)₂Ti₂(μ-F)₈Al₄Me₈ and [(eta⁵-C₅H₄Me)₂Ti(μ-F)₂AlEt₂]₂.
- Organometallics* **18** (1999)1669-1674.
- Peihua Yu, Peter Müller, Musa A. Said, Herbert W. Roesky*, Isabel Usón, Guangcai Bai and Mathias Noltemeyer.

- 42.-Darstellung und strukturelle Untersuchung des $[(\text{Me}_3\text{Sn})_3\text{O}]\text{Cl}$ - mit einem graphitähnlichen Aufbau.
Angew. Chem. **111** (1999) 2069-2071; *Int. Ed. Engl.* **38** (1998) 2050-2052.
Bodo Räge, Peter Müller, Herbert W. Roesky* and Isabel Usón.
- 43.-Advances in direct methods for protein crystallography.
Curr. Opinion in Struc. Biol. **9** (1999) 643-648.
Isabel Usón and George M. Sheldrick*.
- 44.-New approach to dichloroindiumamides.
J. Chem. Soc. Dalton. Trans. **14** (1999) 2265-2266.
Jörg Prust, Peter Müller, Carsten Rennekamp, Herbert W. Roesky* and Isabel Usón.
- 45.-An alternative approach to Al_2O_2 -ring systems by unexpected cleavage of stable Al-F- and Si-O-bonds.
Inorg. Chem. **38** (1999) 5235-5240.
Karsten Rennekamp, Helge Wessel, Herbert W. Roesky*, Peter Müller, Hans-Georg Schmidt, Mathias Noltemeyer, Isabel Usón and Andrew R. Barron.
- 46.-Synthesis, crystal structure and light absorption of vinylogous N,N'-dialkylindigos.
Tetrahedron **55** (1999) 14421-14428.
Lutz Fitjer, Ralf Gerke, Wolfgang Lüttke*, Peter Müller and Isabel Usón.
- 47.-New indigo chromophores containing disulfide donor groups.
Tetrahedron **55** (1999) 14429-14434.
Ralf Gerke, Lutz Fitjer*, Peter Müller, Isabel Usón, Klaus Kowski and Paul Rademacher.
- 48.-Organotitanfluoride als Matrix zum Abfangen von molekularem ZnF_2 und MeZnF .
Angew. Chem. **111** (1999) 3518-3520; *Int. Ed. Engl.* **38** (1999) 3319-3321. Peihua Yu, Peter Müller, Herbert W. Roesky*, Mathias Noltemeyer, Alojz Demsar and Isabel Usón.
- 49.-The dipotassium salt of p-nitrocatechol sulfate.
Acta Crystallogr. **C56** (2000) 152-153.
Rixa von Bülow and Isabel Usón*.
- 50.-Titanium (III) compounds with neta²-pyrazolato ligands.
Eur. J. Inorg. Chem. (2000)13-16.
Nadia Mösch-Zanetti*, Ralph Krätzner, Thomas R. Schneider, Christopher Lehmann and Isabel Usón.
- 51.-Reaction of dimethylaluminumfluoride with primary amines RNH_2 (R= t-Bu, 2,6-i-Pr₂C₆H₃).
J. Fluorine Chem. **102** (2000) 17-20.
Karsten Rennekamp, Andreas Stasch, Peter Müller, Herbert W. Roesky*, Mathias Noltemeyer, Hans-Georg Schmidt and Isabel Usón.
- 52.-Ammonolysis of trichlorosilanes.
Eur. J. Inorg. Chem. (2000) 827-830.

- Karsten Ackerhans, Bodo Räke, Ralph Krätzner, Peter Müller, Herbert W. Roesky* and Isabel Usón.
- 53.-Si-NH-M cage compounds – molecular iminosilicates containing group 13 metals and their functionalized halogen containing derivatives.
Eur. J. Inorg. Chem. (2000) 1861-1868.
Karsten Rennekamp, Peter Müller, Jörg Prust, Helge Wessel, Herbert W. Roesky* and Isabel Usón.
- 54.-The atomic resolution structure of bucanidin, a novel toxin isolated from the Malayan krait, determined by direct methods.
Acta Crystallogr. **D56** (2000) 1401-1407.
Peter Kuhn, Ashley Deacon, Doina-Silviana Comsa, G. Rajaseger, R. Manjunatha Kini, Isabel Usón and Prasana Kolatkar*.
- 55.-Tetrameric indium trichloride, a new modification of a widely used compound.
Acta Crystallogr. **C56** (2000) 1300-1301.
Peter Müller*, Isabel Usón, Jörg Prust and Herbert W. Roesky.
- 56.-Crystal structure of an enzyme substrate complex provides insight to the interaction between human arylsulfatase A and its substrates during catalysis.
J. Mol. Biol. **305** (2001) 269-277.
Rixa von Bülow, Bernhard Schmidt, Thomas Dierks, Kurt von Figura and Isabel Usón*.
- 57.-Intramolecular coupling of two cyclopentadienyl ring systems of zirconium – Unprecedented formation of a dihydride and preparation of the cluster [$\{(Me C_5H_4)Zr\}_5(\eta^5-N)(\eta^3-NH)_4(-NH_2)_4$] in a two phase system.
Organometallics, **19** (2000) 4675-4677.
Guangcai Bai, Peter Müller, Herbert W. Roesky* and Isabel Usón.
- 58.-*Ab Initio* phasing.
In “International tables for crystallography, Volume F. Crystallography of biological macromolecules”. Editors Rossman, M.G. & Arnold, E. Dordrecht: Kluwer Academic Publishers, 2001, 16.1. Pp. 333-351.
George M. Sheldrick, Herbert A. Hauptman, Charles M. Weeks, Russ Miller and Isabel Usón.
- 59.-*Ab Initio* phasing by dual-space direct methods. In “Advances in structure analysis”. Editors: R. Kuzel & J. Hasek: Czech and Slovak Crystallographic Association, 2001. Pp. 37-64.
Charles M. Weeks, George M. Sheldrick, Russ Miller, Isabel Usón and Herbert A. Hauptman.
- 60.-Crystal structure of a Cyclotetraicosaphenylene.
Helv. Chim. Acta. **84** (2001) 778-785.
Peter Müller, Isabel Usón, Volker Hensel, A. Dieter Schlüter and George M. Sheldrick*.
- 61.-Synthesis and structural characterization of functionalized dimeric aluminophosphonates and a monomeric gallophosphonate anion.

- Inorg. Chem.* **40** (2001) 2620-2624.
Debashis Chakraborty, Sabine Horchler, Ralph Krätzner, Saji P. Varkey, Jiri Pinkas, Herbert W. Roesky*, Isabel Usón, Mathias Noltemeyer and Hans-Georg Schmidt.
- 62.-1.3 Å structure of arylsulfatase from *Pseudomonas aeruginosa* establishes the catalytic mechanism of sulfate ester cleavage in the sulfatase family.
Structure **9** (2001) 483-491.
Imke Boltes, Honorata Czapinska, Antje Kahnert, Rixa von Bülow, Thomas Dierks, Bernhard Schmidt, Kurt von Figura, Michael A. Kertesz and Isabel Usón*.
- 63.-Synthesis and Structures of vinamidine MnII, ZnII and CdII iodine derivatives.
Eur. J. Inorg. Chem. (2001) 1613-1616.
Jörg Prust, Kerstin Most, Ilka Müller, Andreas Stasch, Herbert W. Roesky* and Isabel Usón.
- 64.-Halogenodisilanes: Precursors for new disilane derivatives.
Inorg. Chem. **40** (2001) 3766-3773.
Carsten Ackerhans, Peter Böttcher, Peter Müller, Herbert W. Roesky*, Isabel Usón, Hans-Georg Schmidt and Mathias Noltemeyer.
- 65.-X-ray structure of β -cyclodextrin-2,7-dihydroxy-naphtalene • 4.6 H₂O: an unusually distorted macrocycle.
Carbohydr. res. **333** (2001) 251-256.
Maribel Añibarro, Katrin Geßler, Isabel Usón, George M. Sheldrick and Wolfram Saenger*.
- 66.-An orthorhombic crystal form of cyclohexaicosose, CA26-32.59: comparison with the triclinic form.
Carbohydr. res. **336** (2001) 141-153.
Olaf Nimz, Katrin Geßler, Isabel Usón and Wolfram Saenger*.
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149- Identification of the active site residues in ATP-citrate lyase's carboxy-terminal portion

VH Nguyen, N Singh, A Medina, I Usón, ME Fraser *

Protein Science **28**, (2019) 1840-1849 <https://doi.org/10.1002/pro.3708>

- 150- A conserved filamentous assembly underlies the structure of the meiotic chromosome axis
Alan M.V. West, Scott C. Rosenberg, Sarah N. Ur, Madison K. Lehmer, Qiaozhen Ye,
Elife **8** (2019) e40372
Götz Hagemann, Iracema Caballero Muñoz, Isabel Usón, Franz Herzog, Kevin D.
Corbett*
- 151- Supramolecular arrangement of the full-length Zika virus NS5
PLoS pathogens **15** (2019), e1007656 <https://doi.org/10.1371/journal.ppat.1007656>
DS Ferrero, VM Ruiz-Arroyo, N Soler, I Usón, A Guarné, N Verdaguer*
- 152- Ega3 from the fungal pathogen *Aspergillus fumigatus* is an endo- α -1, 4-galactosaminidase
that disrupts microbial biofilms
J. Biol. Chem. **294** (2019) 13833-13849
NC Bamford, F Le Mauff, AS Subramanian, P Yip, C Millán, Y Zhang, C Zacharias, A. Forman,
M. Nitz, J.D.C. Codée, I. Usón, D.C. Sheppard and P.L. Howell*
- 153- SEQUENCE SLIDER: expanding polyalanine fragments for phasing with multiple side-
chain hypotheses
Acta Crystallogr., **D76** (2020) 221-237
RJ Borges*, K Meindl, J Trivino, M Sammito, A Medina, C Millán, M Alcorlo, J.A. Hermoso,
MRM Fontes, Isabel Usón*
- 154- ALEPH: a network-oriented approach for the generation of fragment-based libraries and
for structure interpretation
Acta Crystallogr., **D75** (2020) 193-208
A Medina, J Trivino, RJ Borges, C Millán, I Usón*, MD Sammito*
- 155- ALIXE: a phase-combination tool for fragment-based molecular replacement
Acta Crystallogr., **D75** (2020) 209-220
C Millán*, E Jiménez, A Schuster, K Diederichs, I Usón*
- 156- The Amphibian Antimicrobial Peptide Uperin 3.5 is a Cross- α /Cross- β Chameleon
Functional Amyloid
BioRxiv doi: <https://doi.org/10.1101/2020.05.31.126045>
Nir Salinas, Einav Tayeb-Fligelman, Massimo Sammito, Daniel Bloch, Raz Jelinek, Dror
Noy, Isabel Uson, Meytal Landau

157- Fragment-based determination of a proteinase K structure from MicroED data using ARCIMBOLDO SHREDDER

Acta Crystallogr. **D76** (2020) 703–712

Logan S. Richards, Claudia Millán, Jennifer Miao, Michael W. Martynowycz, Michael R. Sawaya, Tamir Gonen, Rafael J. Borges, Isabel Uson and Jose A. Rodriguez

158- Biophysical characterization of pro-apoptotic BimBH3 peptides reveals an unexpected capacity for self-association

Structure 29 (2021) 114-124.e3, <https://doi.org/10.1016/j.str.2020.09.002>

Tufa E. Assafa, Sukhendu Nandi, Dariusz Śmiłowicz, Laura Galazzo, Markus Teucher, Christina Elsner, Stefanie Pütz, Stephanie Bleicken, Adeline Y. Robin Dana Westphal, Isabel Uson, Raphael Stoll, Peter E. Czabotar, Nils Metzler-Nolte, Enrica Bordignon*

159- Plasmodium falciparum apicomplexan-specific glucosamine-6-phosphate N-acetyltransferase is key for amino sugar metabolism and asexual blood stage development. *Mbio* (2020) e02045-20; DOI: 10.1128/mBio.02045-20

Jordi Chi, Marta Cova, Matilde de las Rivas, Ana Medina, Rafael Borges, Pablo Leivar, Antoni Planas, Isabel Usón, Ramón Hurtado-Guerrero, and Luis Izquierdo*

160- Structure and dsRNA-binding activity of the Birnavirus Drosophila X Virus VP3 protein *J. Virology*, 95 (2021) 4, e02166-20; DOI: 10.1128/JVI.02166-20

Diego Ferrero, Idoia Busnadiego, Damia Garriga, Pablo Guerra, Maria Teresa Martin, Leonor Kremer, Isabel Usón, José Rodriguez, and Nuria Verdaguer.*

161- Detection of translational non-crystallographic symmetry in Patterson functions

Acta Crystallogr. **D77** (2021) 131-141. doi: 10.1107/S2059798320016836

Iracema Caballero, Massimo Sammito, Pavel V. Afonine, Isabel Usón, Randy J. Read and Airlie J. McCoy*

162- Orientational Ambiguity in Septin Coiled Coils and its Structural Basis

J Mol Biol. **433** (2021) 166889. doi:10.1016/j.jmb.2021.166889

Diego A. Leonardo, Italo A. Cavini, Fernanda A. Sala, Deborah C. Mendonça, Patricia S. Kumagai, Edson Crusca Jr, Napoleão F. Valadares, Ivo A. Marques, José Brandão-Neto, Claudia E. Munte, Hans R. Kalbitzer, Nicolas Soler, Isabel Usón, Ingemar André, Ana P. U. Araujo, Humberto D’Muniz Pereira and Richard Charles Garratt

163- Structure of the class XI myosin globular tail reveals evolutionary hallmarks for cargo recognition in plants

Acta Crystallogr. **77** (2021) 522-533. doi:10.1107/S2059798321001583

Valeria R Turowski, Diego M. Ruiz, Andrey FZ Nascimento, Claudia Millán, Massimo D. Sammito, Judith Juanhuix, Aline Sampaio Cremonesi, Isabel Usón, Priscila O Gioseppe and Mario T. Murakami*

164- Insight into the molecular determinants of thermal stability in halohydrin dehalogenase HheD2

FEBS **288** (2021) 4683-4701 doi:10.1111/febs.15777

Julia Wessel, Giovanna Petrillo, Miquel Estevez-Gay, Sandra Bosch, Margarita Seeger, Willem P. Dijkman, Javier Iglesias-Fernández, Aurelio Hidalgo, Isabel Usón, Sílvia Osuna and Anett Schallmeyer*

165- Model Building in SHELXE

bioRxiv 2022.04.28.489939; doi: <https://doi.org/10.1101/2022.04.28.489939>

Isabel Usón* and George Sheldrick

166- Collinolactone, its Biosynthesis, and Semisynthetic Analogues: Effects of Monoastral Phenotype and Protection from Intracellular Oxidative Stress.

Angew Chem Int Ed Engl. **60** (2021) 23212-23216. doi:10.1002/anie.202106802

Julian C Schmid, Kerstin Frey, Matthias Scheiner, Jaime Felipe Guerrero Garzón, Luise Stafforst, Jan-Niklas Fricke, Michaela Schuppe, Hajo Schiewe, Axel Zeeck, Tilmann Weber, Isabel Usón, Ralf Kemkemer, Michael Decker and Stephanie Grond*

167- Integrated, rational molecular replacement

Acta Crystallogr. **D77** (2021) 129-130. doi: 10.1107/S2059798321001339

Isabel Usón, Charles C. Ballard, Ronan M. Keegan and Randy J. Read

168- BthTX-II from Bothrops jararacussu venom has variants with different oligomeric assemblies: An example of snake venom phospholipases A(2) versatility

Rafael J. Borges, Guilherme H. M. Salvador, Henrique B. Campanelli, Daniel C. Pimenta, Mario de Oliveira Neto, Isabel Usón and Marcos R. M. Fontes.

International Journal of Biological Macromolecules. **191** (2021) 255-266

169- SEQUENCE SLIDER: integration of structural and genetic data to characterize isoforms from natural sources

Nucleic Acids Res. **50** (2022) e50. doi: 10.1093/nar/gkac029.

Rafael J. Borges, Guilherme H. M. Salvador, Daniel C. Pimenta, Lucilene D. Dos Santos, Marcos R. M. Fontes and Isabel Usón.

- 170- Exploring generality of experimental conformational changes with AlphaFold predictions
bioRxiv 2022.04.12.488086; doi: <https://doi.org/10.1101/2022.04.12.488086>
Albert Castellví, Ana Medina, Giovanna Petrillo, Theo Sagmeister, Tea Pavkov- Keller, Fernando Govantes, Kay Diederichs, Massimo D. Sammito* and Isabel Usón*. (2022)
- 171- CCP4 Cloud for structure determination and project management in macromolecular crystallography
Acta Crystallogr. **D78** (2022) 1079-1089; <https://doi.org/10.1107/S2059798322007987>
Krissinel, E., Lebedev, A. A., Uski, V., Ballard, C. B., Keegan, R. M., Kovalevskiy, O., Nicholls, R. A., Pannu, N. S., Skubak, P., Berrisford, J., Fando, M., Lohkamp, B., Wojdyr, M., Simpkin, A. J., Thomas, J. M. H., Oliver, C., Vornrhein, C., Chojnowski, G., Basle, A., Purkiss, A., Isupov, M. N., McNicholas, S., Lowe, E., Trivino, J., Cowtan, K., Agirre, J., Rigden, D. J., Uson, I., Lamzin, V., Tews, I., Bricogne, G., Leslie, A. G. W. & Brown, D. G.
- 172- Verification: model-free phasing with enhanced predicted models in ARCIMBOLDO_SHREDDER
Acta Crystallogr. **D78** (2022) 1283-1293
Ana Medina, Elisabet Jiménez, Iracema Caballero, Albert Castellví, Josep Triviño Valls, Martin Alcorlo, Rafael Molina, Juan A. Hermoso, Massimo D. Sammito, Rafael Borges and Isabel Usón*
- 173- SPACA6 ectodomain structure reveals a conserved superfamily of gamete fusion-associated proteins.
Nature Communications biology 5 (2022), 984; <https://doi.org/10.1038/s42003-022-03883-y>
Tyler DR Vance, Patrick Yip, Elisabet Jiménez, Sheng Li, Diana Gawol, James Byrnes, Isabel Usón, Ahmed Ziyat, Jeffrey E Lee
- 174- Response regulator PorX coordinates oligonucleotide signalling and gene expression to control the secretion of virulence factors
Nucleic Acids Res. **50** (2022) e50. doi: 10.1093/nar/gkac1103
Claus Schmitz, Mariusz Madej, Zuzanna Nowakowska, Anna Cuppari, Anna Jacula, Mirosław Ksiazek, Katarzyna Mikruta, Jerzy Wisniewski, Natalia Pudelko-Malik, Anshu Saran, Natalie Zeytuni, Piotr Mlynarz, Richard J Lamont, Isabel Usón, Virginijus Siksnys, Jan Potempa, Maria Solà
- 175- Structural and functional studies of a snake venom phospholipase A₂-like protein complexed to an inhibitor from *Tabernaemontana catharinensis*.
Biochimie, 206 (2023) 105-115. <https://doi.org/10.1016/j.biochi.2022.10.011>

Rafael J Borges, Fábio F Cardoso, Círcia de Carvalho, Ivan de Marino, Paulo S Pereira, Andreimar M Soares, Maeli Dal-Pai-Silva, Isabel Usón, Marcos RM Fontes

176- Making ripples in the comparison of calculated and experimental maps for real-space refinement and assessment by analytic modelling of local resolution

IUCrJ **9** (2022) 718

Isabel Usón

177- Fragment-based ab initio phasing of peptidic nanocrystals by MicroED

ACS Bio. Med. Chem. Au **3** (2023) 201-210 <https://doi.org/10.1021/acsbiomedchemau.2c00082>

Logan Richards, Maria Flores, Claudia Millan, Calina Glynn, Chih-Te Zee, Michael Sawaya, Marcus Gallagher-Jones, Rafael Borges, Isabel Usón*, Jose Rodriguez*

178- The CCP4 suite: integrative software for macromolecular crystallography

Acta Crystallogr. **D79** (2023) 449-461 <https://doi.org/10.1107/S2059798323003595>

Jon Agirre, Mihaela Atanasova, Haroldas Bagdonas, Charles B Ballard, Arnaud Baslé, James Beilsten-Edmands, Rafael J Borges, David G Brown, J Javier Burgos-Mármol, John M Berrisford, Paul S Bond, Iracema Caballero, Lucrezia Catapano, Grzegorz Chojnowski, Atlanta G Cook, Kevin D Cowtan, Tristan I Croll, Judit É Debreczeni, Nicholas E Devenish, Eleanor J Dodson, Tarik R Drevon, Paul Emsley, Gwyndaf Evans, Phil R Evans, Maria Fando, James Foadi, Luis Fuentes-Montero, Elspeth F Garman, Markus Gerstel, Richard J Gildea, Kaushik Hatti, Maarten L Hekkelman, Philipp Heuser, Soon Wen Hoh, Michael A Hough, Huw T Jenkins, Elisabet Jiménez, Robbie P Joosten, Ronan M Keegan, Nicholas Keep, Eugene B Krissinel, Petr Kolenko, Oleg Kovalevskiy, Victor S Lamzin, David M Lawson, Andrey A Lebedev, Andrew GW Leslie, Bernhard Lohkamp, Fei Long, Martin Malý, Airlie J McCoy, Stuart J McNicholas, Ana Medina, Claudia Millán, James W Murray, Garib N Murshudov, Robert A Nicholls, Martin EM Noble, Robert Oeffner, Navraj S Pannu, James M Parkhurst, Nicholas Pearce, Joana Pereira, Anastassis Perrakis, Harold R Powell, Randy J Read, Daniel J Rigden, William Rochira, Massimo Sammito, Filomeno Sánchez Rodríguez, George M Sheldrick, Kathryn L Shelley, Felix Simkovic, Adam J Simpkin, Pavol Skubak, Egor Sobolev, Roberto A Steiner, Kyle Stevenson, Ivo Tews, Jens MH Thomas, Andrea Thorn, Josep Triviño Valls, Ville Uski, Isabel Usón, Alexei Vagin, Sameer Velankar, Melanie Vollmar, Helen Walden, David Waterman, Keith S Wilson, Martyn D Winn, Graeme Winter, Marcin Wojdyr, Keitaro Yamashita.

179- Predicted models and CCP4

Acta Crystallogr. **D79** (2023) 806-819 <https://doi.org/10.1107/S2059798323006289>

Adam J. Simpkin, Iracema Caballero, Stuart J McNicholas, Kyle Stevenson, Elisabet Jiménez, Filomeno Sánchez Rodríguez, Maria Fando, Ville Uski, Charles Ballard, Grzegorz Chojnowski, Andrey Lebedev, Eugene Krissinel, Isabel Usón, Daniel J Rigden and Ronan M Keegan

- 180- XDSGUI: a graphical user interface for XDS, SHELX and ARCIMBOLDO
J. Appl. Cryst. **56** (2023) 1585-1594 <https://doi.org/10.1107/S1600576723007057>
Wolfgang Brehm, Josep Triviño, Juno M. Krahn, Isabel Usón* and Kay Diederichs*
- 181- Structural characterization of PaaX, the main repressor of the phenylacetate degradation pathway in *Escherichia coli* W: A novel fold of transcription regulator proteins.
Int. J. Biol. Macromol. **254** (2024), 127935
<https://doi.org/10.1016/j.ijbiomac.2023.127935>
Víctor M. Hernández-Rocamora, Rafael Molina, Alejandra Alba, César Carrasco-López, Alzoray Rojas-Altuve, Santosh Panjekar, Ana Medina, Isabel Usón, Carlos Alfonso, Beatriz Galán, Germán Rivas, Juan A. Hermoso, Jesús M. Sanz
- 182- *Vibrio cholerae*'s ToxRS bile sensing system
eLife **12** (2023) e88721 <https://doi.org/10.7554/eLife.88721>
Nina Gubensäk, Theo Sagmeister, Christoph Buhllheller, Bruno Di Geronimo, Gabriel E Wagner, Lukas Petrowitsch, Melissa A Gräwert, Markus Rotzinger, Tamara M Ismael Berger, Jan Schäfer, Isabel Usón, Joachim Reidl, Pedro A Sánchez-Murcia, Klaus Zangger, Tea Pavkov-Keller
- 183- SHELXE modes and model building
Acta Crystallogr. **D80** (2024) 4-15 <https://doi.org/10.1107/S2059798323010082>
Isabel Usón* and George M. Sheldrick

Attachment II:Patent

Inventors (in signing order): Isabel Maria Usón, Hugo Jean Demeyere, Frederick Anthony Hartman, Mark Sivik.

Title: **Active substance delivery system**

Application no.: PCT/US94/10748

Priority country: USA

Priority date: 22-09-1994

Year granted: 1995: WO1995008976 A1

Patent holding body: Procter & Gamble

Countries to which it has been extended: worldwide: Designated state(s): KE MW SD SZ AT
BE CH DE DK ES FR GB GR IE IT LU MC NL PT SE BF BJ CF CG CI CM GA GN
ML MR NE SN TD TG

Designated state(s): AM AU BB BG BR BY CA CN CZ EE FI GE HU JP KG KP KR KZ LK
LR LT LV MD MG MN NO NZ PL RO RU SI SK TJ TT UA US UZ VN

Companies exploiting it: Procter & Gamble

Attachment III: Lectures and Communications

- 1.- "Mono- and polynuclear palladium and platinum xanthate complexes".
October 1991; El Escorial, Organometallic Chemistry Group, IX annual meeting.
- 2.- "Pentafluorophenylplatinate complexes acting as Lewis bases towards Sn²⁺ or Pb²⁺".
October 1991; El Escorial, Organometallic Chemistry Group, IX annual meeting.
- 3.- "Analysis of structural results derived from defective data". Abstract PB83, session
"Problem structures, puzzles and solutions"
August 1992; Pittsburgh, ACA annual meeting.
- 4.- "Intensity scaling: a trick to solve a structure with third row metals on special positions".
Abstract M172, session "Problem structures: solutions, tricks and pleas for help"
July 1995; Montreal, ACA annual meeting.
- 5.- "Structure of an immunoglobulin REIv mutant at 1.7 Å resolution". Abstract M122,
July 1995; Montreal, ACA annual meeting.
- 6.- Tutor beim SHELXL Workshop
July 1995; Montreal.
- 7.- Lecture "Methodische Entwicklungen in der Röntgenstrukturanalyse von Proteinen".
29 - 31 October 1995; Reisenburg, Abschlußkolloquium DFG-Schwerpunkt "Protein
Design"
- 8.- Protein Crystallography of REIv mutants. March 1996 Biochemisches Institutkolloquium.
Institut für Molekular Genetik, Universität Göttingen.
- 9.- Tutor at the EMBO practical course on refinement techniques and Map interpretation.
14 - 20 July 1996; EMBL-Heidelberg.
- 10.-Lecture "Kristallstruktur eines disulfid-freien REIv Immunoglobulinfragments".
27 - 29 October 1996; Reisenburg, DFG-Rundgespräch "Protein Design".
- 11.-"Ab Initio solution of an unknown 55 amino-acid protein".
22-Mai-2 June 1997; 25th International School of Crystallography in Erice, Direct methods
and *ab initio* phasing techniques.
- 12.-Tutor at the SHELXL-97 Workshop. Lecture: "SHELXL refinement at medium resolution".
6-12 Juli 1997; Universität Göttingen.
- 13.-"Alkali metal containing gallium alkyls as precursors to secondary building units (SBUs)
of gallophosphate materials". 21-25 July 1997, OMCOS9, Göttingen.
- 14.-Lecturer at the European CCP4 Workshop on refinement techniques. Lectures on
"Refinement with SHELXL-97" and "Anisotropic refinement and disorder". Tutorials on
the use of SHELXL-97.
1 - 6 September 1997; York, England.
- 15.-Invited speaker at the 11th Rhine-Knee Regional Meeting on X-Ray crystallography of
biomacromolecules. "Ab initio structure solution of hirustasin, a 55-amino acid protease
inhibitor".

- 24 - 26 September 1997; Delemont (JU), Switzerland.
- 16.-Lecture: "Röntgenkristallographische Charakterisierung konformations-stabilisierter und disulfidfreier Immunoglobulin Fragmente".
13 January 1998; Tagung "Diversität und Selektion in der biologischen Synthese".
Göttingen.
- 17.-Invited speaker at the 1998 Annual Meeting of the American Crystallographic Association (ACA). "Examples of *ab initio* structure solution". Session 11.07, Computational methods.
18 - 23 July 1998; Airlington (Virginia), USA.
- 18.-Invited speaker at the 18th European Crystallographic Meeting (ECM). "Examples of macromolecular *ab initio* solution with high resolution data" Session E5: *Ab Initio* methods for structure determination.
"Direct methods in supramolecular chemistry" and participation in the panel discussion for the Session C7: Large supramolecular assemblies and inclusion compounds
15 - 20 August 1998; Prague, Czeck Republic.
- 19.-Lecturer at the European CCP4 Workshop on refinement techniques. Lectures on "Refinement with SHELXL-97" and "High Resolution *ab Initio* Structure Solution".
Tutorials on the use of SHELXL-97.
13 - 18 December 1998; York, England.
- 20.-Lecturer at the 5th European Workshop on crystallography of biological macromolecules.
Lecture on "High Resolution *ab Initio* Structure Solution and location of Se atoms". 15 - 20 May 1999; Centro di cultura scientifica A. Volta, Como, Italy.
- 21.-Invited speaker at the XVIIIth International Union of Crystallography Meeting (IUCr).
"Exploiting the Patterson in *ab initio* phasing" Session 12BB: *Ab Initio* and Molecular replacement.
4 - 13 August 1999; Glasgow, UK.
- 22.-Lecturer at the International School of crystallography of biological macromolecules.
Lectures on "High Resolution *ab Initio* Structure Solution and location of Se atoms", "Refinement with SHELXL-97", Tutorials on the use of SHELXL-97. 9 - 15 September 1999; Centro de Investigacion y Desarrollo, (CSIC), Barcelona, Spain.
- 23.-Invited lecture at the Humbolt Universität Berlin. Institut für Biochemie, Institutsklinikum Charité. "*Ab Initio* dual space recycling (sub)structure Solution". 6.June 2000. Berlin.
- 24.-Lecturer at the Satellite meeting "Frontiers in macromolecular crystallography" to the 19th European Crystallographic Meeting (ECM) in Nancy, France. "*Ab Initio* dual space recycling (sub)structure Solution", 1-3 September 2000; Bischenberg, France.
- 25.-Lecture at the 783rd GDCh Sitzung, Ortsverband Göttingen. "*Von der Röntgenstrukturanalyse zur Funktion – Katalysemechanismus von Sulfatasen*". 7. December 2000. Göttingen.

- 26.-Invited lecture at the Technische Universität Berlin, anorganisch-chemisches Kolloquium. "Von der Röntgenstrukturanalyse zur Funktion- *ab initio* Methoden, Substrukturen anomale Streuer und der Katalysemechanismus von Sulfatasen". 23 April 2001. Berlin.
27. Invited plenary lecture at the annual meeting of Dutch and Flemish Protein Crystallographers, NVK Meeting. "*Ab initio* and substructure solution with dual space recycling methods". 8 June 2001. Brussels.
28. Invited lecture at the Humboldt Universität Berlin, Interdisziplinäres Zentrum für Biophysik und Bioinformatik. "*Ab initio* Methoden, Substrukturen anomaler Streuer und der Katalysemechanismus von Sulfatasen". 6 July 2001. Berlin.
29. Invited speaker at the 20th European Crystallographic Meeting (ECM). "Locating halide substructures with dual space recycling methods" Session 1b4: On-line structure determination through *Ab Initio* and MAD phasing. 25 - 31 August 2001; Kraków, Poland.
30. Invited lecture at the Universität Erlangen-Nürnberg, Naturwissenschaftliche Fakultät II. "Kristallographische Methoden und lysosomale Speicherkrankheiten". 7 November 2001. Erlangen.
31. Lecturer at the 7th European Workshop on crystallography of biological macromolecules. Lecture on "Fragment search and high resolution structure solution". 10 - 14 May 2003; Centro di cultura scientifica A. Volta, Como, Italy.
32. Lecturer at the European Max-Inf-SHELX Workshop on macromolecular phasing and refinement. Lectures on "*Ab Initio* phasing". Tutorials on the use of SHELXD for *ab Initio* structure solution. 18 - 24 September 2003; Goettingen, Germany.
33. Organiser and Lecturer at the European Max-Inf- Workshop on macromolecular phasing and refinement. Lectures on "*Ab Initio* phasing". Tutorials on the use of SHELXD for *ab Initio* structure solution and substructure solution. 18 - 23 March 2004; Barcelona, Spain.
34. Lecture at the European BIOXHIT Kickoff meeting, Fragment search for high resolution structure solution 26-28 April 2004, Hamburg, Germany
35. Invited lecture at the University of Bern, Biochemisches Colloquium, "Lost in Translation, Fragment search for high resolution structure solution". 29-November 2004, Bern, Switzerland
36. Organiser and Lecturer at the European CCP4/Max-Inf- Workshop on macromolecular phasing and refinement. Lectures on "*Ab Initio* solution of macromolecular structures and substructure determination". Tutorials on the use of SHELXD for *ab Initio* structure solution and substructure solution. 2 - 7 March 2006; Barcelona, Spain.

37. Lecturer at the European Max-Inf-SHELX Workshop on macromolecular phasing and refinement. Lectures on “*Ab Initio* direct methods“ and “Experiences with problem structures”. Tutorials on the use of SHELXC/D/E for *ab Initio* structure solution. 7 - 14 September 2006; Goettingen, Germany.
38. Invited lecture at the VIth Iberoamerican Congress of Biophysics IACB “Pushing the resolution limits in structure solution with SHELX”. 24-27-September 2006, Madrid, Spain
39. Co-organiser and Lecturer at the European CCP4/Max-Inf- Workshop on macromolecular phasing and refinement. Lectures on “SHELX in action“. Tutorials on the use of SHELXD for *ab Initio* structure solution and substructure solution. April 2007, York (UK)
40. Invited lecture at 26th European Crystallographic Meeting (ECM). “Ab Initio Phasing with ARCIMBOLDO“. August 2010, Darmstadt (Germany).
41. Invited lecture at CCP4 Study weekend. “New structures solved and built with ARCIMBOLDO... and a glimpse of SUBIX “5-7 January 2011, Warwick (U.K.).
42. Invited lecture at Software Fayre of the IUCr XXII Congress and General Assembly. “ARCIMBOLDO“ 23-28 August 2011, Madrid (Spain).
43. Co-organiser and Lecturer at the ZCAM-CCP4 Daresbury Workshop on macromolecular phasing and refinement. Lectures on “ARCIMBOLDO phasing“. Practicals on the use of Arcimboldo for *ab Initio* structure solution and substructure solution. March 2012, Zaragoza (Spain)
44. Invited lecture at International School of Crystallography. 45th Course on Present and Future Methods for Biomolecular Crystallography. “Phasing with Small Fragments“ 31 May-11 June 2012, Erice (Italy).
45. Invited lecture at Software Fayre of the ECM XXVII Congress. “ARCIMBOLDO“ 6-11 August 2012, Bergen (Norway).
46. Invited lecture at LMB-MRC Crystallography course, “Exploiting Tertiary Structure for Ab Initio Phasing: *Borges* and Arcimboldo” 15 May 2013, Cambridge (UK).
47. Invited lecture at EMBO 2013 Practical Course - Exploiting Anomalous Scattering - ESRF - 10 - 14 June 2013, Grenoble (France).
48. Invited lecture at Software Fayre of the ECM XXVIII Congress. “BORGES“ 25-31 August 2013, Warwick (UK). *Also, co-chairing session on Phasing, refinement and automatic model building.*
49. Invited lecture at International workshop MX2014 - IFSC - USP Macromolecular Crystallography School 2014 "From data processing to structure refinement and beyond". “*MR with ARCIMBOLDO*” 11 April 2014, Sao Carlos. Brazil
50. Invited lecture at UNESP “Development of supercomputing crystallographic methods: ARCIMBOLDO“ 10 April 2013, Botucatu (Brazil).
51. Invited lecture at IUCr 23rd Congress and General Assembly satellite SHELX workshop. “ARCIMBOLDO“ 6 August 2014, Montreal (Canada).

52. Invited Keynote lecture at IUCr 23rd Congress and General Assembly. “Ab Initio Phasing enforcing secondary and tertiary structure“ 11 August 2014, Montreal (Canada).
53. Invited lecture at DGK 23rd Annual Conference. “Macromolecular Phasing with ARCIMBOLDO – single workstation implementations and combination of partial solutions in reciprocal space “ 17 March 2015, Göttingen (Germany).
16 - 19 March 2015; Göttingen, Germany.
54. Invited lecture at the Max Perutz Institute of the University of Vienna, “Ab initio macromolecular phasing with ARCIMBOLDO” 30. April 2015, Vienna (Austria).
55. Invited talk at the Incoatec Users Symposium, “Macromolecular phasing with ARCIMBOLDO: Next challenges” 9. Julio 2015, Göttingen (Germany).
56. Invited lecture at Satellite Meeting - IRTG Methods Course on Macromolecular applications of SHELX. “ARCIMBOLDO_LITE“ 19 March 2015, Göttingen (Germany).
57. Invited lecture at the ECM XXIX Congress. “ARCIMBOLDO, an ab initio approach to MR phasing“ in session on “*Advances in phasing, refinement and autobuilding*” 23-28 August 2015, Rovenj (Croatia). Also, co-chairing the microsposium on *New applications of old algorithms in Crystallography* and George M. Sheldrick’s Keynote Lecture on *Structure determination revisited*.
58. Invited lecture at the Institute of Biochemistry, Universidad of Cambridge, “ARCIMBOLDO, an ab initio approach to MR phasing“ 21 October 2015, Cambridge, UK.
59. Lecturer at International workshop at Diamond Light Source Macromolecular Crystallography School 2015 "SHELXE for MR solutions and ARCIMBOLDO". 5 Dec 2015, Harwell, Oxford UK
60. Invited lecture at the Cambridge Institute for Medical Research, University of Cambridge, “Developing the program ARCIMBOLDO for crystallographic structure solution“. 26 January 2016, Cambridge, UK.
61. Invited lecture at BIFI 2016: International Conference on Molecular Recognition "ARCIMBOLDO and BORGES: Supercomputing Methods for Macromolecular Crystallographic Ab Initio Phasing” 1 February 2016, BIFI, Zaragoza. Spain
62. Invited lecture at the Anorganisches Chemisches Kolloquium, Faculty of Chemistry of the University of Göttingen, “Crystallographic phasing enforcing chemical knowledge” 16. February 2016, Göttingen (Germany).
63. Invited lecture at CCP4 developers meeting - 2016 "ARCIMBOLDO". 16 March 2016, Cosener’s House, Oxford. UK
64. Invited lecture at International workshop MX2016 - IFSC - USP Macromolecular Crystallography School 2016 "From data processing to structure refinement and beyond". “EP with SHELX” and “SHELX for MR” 7 April “MR with ARCIMBOLDO” 8 April 2016, Sao Carlos. Brazil

65. Coorganiser and lecturer at International workshop MCS2016 – IFQR-CSIC Macromolecular Crystallography School 2016 "From data processing to structure refinement and beyond". "General overview about SHELX, PHASER and ARCIMBOLDO" 25 May 2016, Madrid. Spain
66. Invited lecture at Gordon Research Conference on Diffraction Methods in Structural Biology. "Local folds and fragments in phasing, autotracing and structure interpretation" 20 July 2016, Bates College, Lewiston (MAINE, USA).
67. Invited lecture at the SickKids Hospital of the University of Toronto, MOLECULAR STRUCTURE & FUNCTION SEMINAR SERIES, "Fragments in structure interpretation: local folds" 3. November 2016, Toronto (Canada).
68. Invited Keynote lecture at International workshop BHT, McMaster University, Hamilton, Canada. "Small fragment search for high resolution phasing in high throughput crystallography" 4 November 2016, Hamilton. Canada
69. Invited lecture at CCP4 Study weekend. "ARCIMBOLDO at low resolution" 9-11 January 2017, Nottingham (U.K.).
70. Invited lecture at the LNLS, Brazilian Synchrotron. "Fragments in structure solution and interpretation" 21 February 2017, Campinas. Brazil
71. Coorganiser and lecturer at International workshop MCS2016 – IFQR-CSIC Macromolecular Crystallography School 2017 "From data processing to structure refinement and beyond". "General overview about SHELX, PHASER and ARCIMBOLDO" 6 May 2017, Madrid. Spain
72. Invited lecture at symposium *Understanding Biology through Structure 2017*, Santa Fe, USA. "Fragments in phasing, autotracing and structure interpretation" 16 May 2017, Santa Fe. USA
73. Organiser on behalf of the SBU-IBMB (CSIC), together with Garib N. Murshudov, LMB-MRC, Cambridge, of the "Conference on methods and applications in the frontier between MX and CryoEM" for 150 participants. 19-21 September 2017, Barcelona. Spain
74. Invited lecture at CCP4 Macromolecular Crystallography School "Structural Biology to enhance high impact research in health and disease" Institut Pasteur de Montevideo, Uruguay November 13-23, 2017. "EP with SHELX" and "SHELX for MR", "MR with ARCIMBOLDO", Montevideo. Uruguay
75. Coorganiser and lecturer at International workshop MCS2018 – IFQR-CSIC Macromolecular Crystallography School 2018 "From data processing to structure refinement and beyond". "General overview about SHELX, PHASER and ARCIMBOLDO" 21 May 2018, Madrid. Spain
76. Invited lecture at the ECM XXXI Congress. "All is fair in phasing: the combined artillery in ARCIMBOLDO" in session on "Combining methods in macromolecular structure determination, including special conditions MX" 22-27 August 2018, Oviedo (Spain). Also, chairing the microsposium on New approaches to structure solution by

Crystallography and CryoEM: Computational features and new algorithms and Randy J. Read's Keynote Lecture on Understanding and using likelihood in structural biology.

77. Organiser of the CCP4 Study weekend, together with R. J. Read (University Cambridge) and R. Keegan (CCP4). "Rational, integrated molecular replacement" 8-10 January 2019, Nottingham (U.K.).
78. Coorganiser and lecturer at International workshop MCS2019 – IFQR-CSIC Macromolecular Crystallography School 2019 "From data processing to structure refinement and beyond". "General overview about SHELX, PHASER and ARCIMBOLDO" April 2019, Madrid. Spain
79. Invited lecture at the ECM XXXII Congress. "Errors and validation: cryoEM maps for microED structures" in session on "Errors and Validation" 18-23 August 2019, Vienna (Austria).
80. Invited lectures at international workshop CCP4/Shanghai Crystallographic Workshop From Data collection to Structure Refinement and Beyond / Shanghai (China), 11 Oct, 2019 - "16 October: Phasing with SHELX ; Phaser ; Tutorial: SHELX; 18 October: SHELX and Phaser for MR; ARCIMBOLDO; Tutorial ARCIMBOLDO"
81. Invited lecture at CCP4 Study weekend. "Model building in SHELXE" 7-9 January 2020, Nottingham (U.K.).
82. Invited lecture at the phasing@home meeting. "Practical density modification and autotracing in SHELXE". 14 June 2020, Virtual meeting with sites in Cambridge, Konstanz, Göttingen and Sao Paulo.
83. Invited lectures at international workshop CCP4/DLS Crystallographic Workshop From Data collection to Structure Refinement and Beyond / Oxford (UK), 11 Dec, 2020 - "16 October: Phasing with SHELX; 18 October: Model building in SHELXE and ArpWarp"
84. Invited lunchtime Byte virtual lecture at CCP4 Study weekend 2021. "Model building in SHELXE" 7-9 January 2021, Nottingham (U.K.).
85. Invited lectures at international workshop CCP4/South Africa Crystallographic Workshop From Data collection to Structure Refinement and Beyond / University of Cape Town (South Africa)/Diamond Light Source (UK), 22 Feb- 5 March, 2021 - "26 February: Experimental phasing: SHELX, Tutorial case study; 26 February: Automated model building"
86. Invited lectures at international workshop CCP4/APS Virtual School in Macromolecular Crystallography: From data collection to structure refinement and beyond. Argonne National Laboratory June 14 - 25, 2021 - "18 June: SHELXE for Molecular Replacement, and ARCIMBOLDO pipelines; 21 June: SHELXC/D/E"

87. Invited lecture at IUCr 25th Congress and General Assembly hybrid satellite Electron Crystallography School - 3D Electron Diffraction/MicroED Uniting Small Molecule and Macromolecular Crystallography. 11-14 August. "Methods for phasing diffraction data – macromolecules" 12 August 2021, Prague (Czech Republic).
88. Invited lecture at virtual "AIC International School of Crystallography AICS2021 Fundamentals of Crystallographic Knowledge" 1-4 September 2021, Italian Crystallographic Association. 4 Sept: Macromolecular crystallographic refinement and phasing
89. Invited lectures at international workshop CCP4/South America Crystallographic Workshop From Data collection to Structure Refinement and Beyond / Montevideo (Uruguay), 20 Sept-1 Oct, 2021 - "27 Sept: Phasing with SHELX; SHELX and ARCIMBOLDO tutorial"
90. Invited lectures at international virtual workshop CCP4/DLS Crystallographic Workshop From Data collection to Structure Refinement and Beyond / Oxford (UK), 29 Nov, 2021 - "3 December: Phasing with SHELX; 8 December: Model building in SHELXE and ArpWarp"
91. Invited lecture at CCP4 Study weekend on Refinement and Validation. "SHELXL "5-8 January 2022, Nottingham (U.K.). Oral contribution on webinar AlphaFold tools in CCP4.
92. Invited lectures at international workshop CCP4/APS Virtual School in Macromolecular Crystallography: From data collection to structure refinement and beyond. Argonne National Laboratory June 13 - 24, 2022 - "17 June: ARCIMBOLDO; 20 June: SHELXC/D/E"
93. Invited lecture at CCP4 developers meeting - 2022 "ARCIMBOLDO and AlphaFold". 4-6 July 2022, Cosener's House, Oxford. UK
94. Invited lecture at Gordon Research Conference on Diffraction Methods in Structural Biology. "The role of predictions in structure determination" 27 July 2022, Bates College, Lewiston (MAINE, USA).
95. Lecture at the ECM XXXIII Congress. "Exploring generality of experimental conformational changes with AF predictions" in session on "MX/Cryo-EM software development" 23-27 August 2022, Versailles (France). Also, chairing the microsposium on "Opportunities from combining structural biology and fold prediction".
96. Keynote lecture at the X AUSE Conference V ALBA Synchrotron User's meeting. "Synchrotron experimental techniques in the post-AlphaFold2 age" 7 September 2022, Cerdanyola del Valles, Barcelona
97. Invited lectures at international workshop CCP4/DLS Crystallographic Workshop From Data collection to Structure Refinement and Beyond / Oxford (UK), 27 Nov, 2022 - 6 December. Hands-on problem solving. Lecture 2 December: "Verification".

98. Invited lecture at CCP4 Study weekend on A new era in structural biology. "Prediction-based tools to plan and interpret experiments with AF ARCIMBOLDO_AIR" 4-6 January 2023, Nottingham (U.K.).
 99. Lecturer at International workshop MCS2023 – IFQR-CSIC Macromolecular Crystallography School 2023 "From data processing to structure refinement and beyond". "General overview about SHELX and ARCIMBOLDO" 9 May 2023, Madrid. Spain
 100. Invited lecture at CCP4 developers meeting - 2023 "ARCIMBOLDO_AIR: predictions and dynamics". 4-6 July 2023, Cosener's House, Abingdon, Oxfordshire. UK
 101. Invited lecture at BIODRUG ERA meeting - 2023 "Predictions and experiments in structure determination: ARCIMBOLDO and VAIRO". 18-19 September 2023, AVALON HOTEL & Conferences. Riga, Latvia.
 102. Invited lectures at international workshop CCP4/DLS Crystallographic Workshop From Data collection to Structure Refinement and Beyond / Oxford (UK), 26 Nov, 2023 - 5 December. Hands-on problem solving. Talk 1 December: "Verification".
 103. Invited lecture at Intitutscolloquium at the Institute of Molecular Biosciences der Karl Franzens University Graz (Austria), 24 Nov, 2023 "Predictions and experiments in structure determination: ARCIMBOLDO and VAIRO".
 104. Invited lecture at XXXI GE3C meeting - 2024 "Predictions and experiments in structure determination: ARCIMBOLDO and VAIRO" en la sesion "Cristalografía de proteínas y más allá. Participación en mesa redonda sobre "Mujeres y Cristalografía" en la sesión inaugural. 16-19 January 2024, ICIQ Tarragona.
 105. Invited lectures at international workshop South-East Asian Crystallographic Overview And Systematic Training January 29 - February 7, 2024 / King Mongkut's University of Technology Thonburi (KMUTT) Bangkok (Thailand). "2 February: Density modification in phasing with SHELX; 4 February: ARCIMBOLDO; VAIRO and SYMPROFOLD (Guiding predictions with experimental knowledge; Tutorial ARCIMBOLDO". Remote participation.
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PARTICIPATION IN PROJECT GRANTS

TITULO DEL PROYECTO: **Conexiones BCB**

ENTIDAD FINANCIADORA: **Agencia Estatal Consejo Superior Investigaciones Científicas (CSIC)**

DURACION DESDE: **2023**

HASTA: **2026**

INVESTIGADOR PRINCIPAL: **Ana Conesa, Pablo Chacón**

TITULO DEL PROYECTO: **Desarrollo de métodos cristalográficos(VII) y su aplicación a catálisis avanzada (PID2021-128751NB-I00)**

ENTIDAD FINANCIADORA: **Ministerio de Ciencia e Innovación**

DURACION DESDE: **2022**

HASTA: **2024**

INVESTIGADOR PRINCIPAL: **Isabel Usón**

TITULO DEL PROYECTO: **Desarrollo de métodos cristalográficos(VI) y su aplicación a catálisis avanzada (PGC2018-101370-B-100)**

ENTIDAD FINANCIADORA: **Ministerio de Ciencia e Innovación**

DURACION DESDE: **2019**

HASTA: **2022**

INVESTIGADOR PRINCIPAL: **Isabel Usón**

TITULO DEL PROYECTO: **ARCIMBOLDO LOW**

ENTIDAD FINANCIADORA: **CCP4-Science and Technology Facilities Council UK**

DURACION DESDE: **2019**

HASTA: **2023**

INVESTIGADOR PRINCIPAL: **Isabel Usón**

TITULO DEL PROYECTO: **Desarrollo de métodos cristalográficos(V) y su aplicación a catálisis avanzada (BIO2015-64216-P)**

ENTIDAD FINANCIADORA: **Ministerio de Economía y Competitividad**

DURACION DESDE: **2016**

HASTA: **2018**

INVESTIGADOR PRINCIPAL: **Isabel Usón**

TITULO DEL PROYECTO: **Salvador de Madariaga**

ENTIDAD FINANCIADORA: **Ministerio de Educación, Culture y Deporte**

DURACION DESDE: **2015**

HASTA: **2016**

INVESTIGADOR PRINCIPAL: **Isabel Usón**

TITULO DEL PROYECTO: **Unidad de Excelencia “Maria de Maeztu” Biología Estructural (MdM-2014-0435)**

ENTIDAD FINANCIADORA: **Ministerio de economía y competitividad (MINECO)**

DURACION DESDE: **2015**

HASTA: **2019**

INVESTIGADOR PRINCIPAL: **Isabel Usón; Coordinadora Nuria Verdaguer Massana**

TITULO DEL PROYECTO: Ayuda a Grupos de Investigación consolidados de Cataluña (2014SGR 997).

ENTIDAD FINANCIADORA: Generalitat de Catalunya

DURACION DESDE: 2014 HASTA: 2019

INVESTIGADOR PRINCIPAL: María Solà

TITULO DEL PROYECTO: Aleph (BIO2013-49604-EXP)

ENTIDAD FINANCIADORA: Ministerio de economía y competitividad (MINECO)

DURACION DESDE: 2014 HASTA: Mayo 2017

INVESTIGADOR PRINCIPAL: Isabel Usón

TITULO DEL PROYECTO: Desarrollo de métodos cristalográficos(IV) y su aplicación a aspectos del metabolismo del azufre (BFU2012-35367)

ENTIDAD FINANCIADORA: Ministerio de Economía y Competitividad

DURACION DESDE: 2012 HASTA: 2014

INVESTIGADOR PRINCIPAL: Isabel Usón

TITULO DEL PROYECTO: Cloud computing con ARCIMBOLDO para una solución de estructuras cristalográficas por supercomputación en la FCSCCL (ARCIMBOLDO-CLOUD)

ENTIDAD FINANCIADORA: Centro para el Desarrollo Tecnológico Industrial (CDTI)

DURACION DESDE: 2010 HASTA: 2012

INVESTIGADOR PRINCIPAL: Isabel Usón por parte del IBMB-CSIC

COORDINADOR: CATON SISTEMAS ALTERNATIVOS,S.L.

TITULO DEL PROYECTO: Desarrollo de métodos cristalográficos(III) y su aplicación a aspectos del metabolismo del azufre (BIO2009-10576)

ENTIDAD FINANCIADORA: Ministerio de Ciencia y Tecnología

DURACION DESDE: 2009 HASTA: 2012

INVESTIGADOR PRINCIPAL: Isabel Usón

TITULO DEL PROYECTO: Ayuda a Grupos de Investigación consolidados de Cataluña (2009SGR 1036).

ENTIDAD FINANCIADORA: Generalitat de Catalunya

DURACION DESDE: 2009 HASTA: 2012

INVESTIGADOR PRINCIPAL: Francesc-Xavier Gomis-Rüth

TITULO DEL PROYECTO: Fragment-based methods for structure solution (RS International collaboration).

ENTIDAD FINANCIADORA: The Royal Society

DURACION DESDE: 2010 HASTA: 2012

INVESTIGADOR PRINCIPAL: Ehmke Pohl/Isabel Usón/ George M. Sheldrick

TITULO DEL PROYECTO: Desarrollo de métodos cristalográficos(II) y su aplicación a aspectos del metabolismo del azufre y transporte (BIO2006-14139)

ENTIDAD FINANCIADORA: Ministerio de Ciencia y Tecnología

DURACION DESDE: 2006 **HASTA:** 2009

INVESTIGADOR PRINCIPAL: Isabel Usón

TITULO DEL PROYECTO: Fragment Search for high resolution structure solution BIOXHIT("Biocrystallography (X) on a highly integrated technology platform for European structural genomics")

ENTIDAD FINANCIADORA: European Union (VI-PM)

DURACION DESDE: 2004 **HASTA:** 2007

INVESTIGADOR PRINCIPAL: Victor Lamzin

TITULO DEL PROYECTO: Desarrollo de métodos cristalográficos y su aplicación a aspectos del metabolismo del azufre (BIO2003-06653)

ENTIDAD FINANCIADORA: Ministerio de Ciencia y Tecnología

DURACION DESDE: 2004 **HASTA:** 2006

INVESTIGADOR PRINCIPAL: Isabel Usón

TITULO DEL PROYECTO: Genómica Estructural: aplicación a proteínas y complejos proteicos relacionados con el cáncer GENES (GEN2003-20642-C09-01).

ENTIDAD FINANCIADORA: Proyecto Integrado de la Acción Estratégica de Genómica y Proteómica. Ministerio de Ciencia y Tecnología.

DURACION DESDE: 2004 **HASTA:** 2007

INVESTIGADOR PRINCIPAL: Miquel Coll

TITULO DEL PROYECTO: Ayuda a Grupos de Investigación consolidados de Cataluña (2005SGR 00280).

ENTIDAD FINANCIADORA: Generalitat de Catalunya

DURACION DESDE: 2005 **HASTA:** 2008

INVESTIGADOR PRINCIPAL: Miquel Coll

TITULO DEL PROYECTO: US20/1 "Análisis cristalográfico de el dominio de enlace del factor de crecimiento análogo a la insulina II del receptor de fosfato de 6-manosa e IGFII así como de dos sulfatasas bacterianas"

ENTIDAD FINANCIADORA: Deutsche Forschungsgemeinschaft (DFG)

DURACION DESDE: Ago 1999 **HASTA:** Jun 2003

INVESTIGADOR PRINCIPAL: Isabel Usón y Bernhard Schmidt

TITULO DEL PROYECTO: "Síntesis y transformación química y biológica de productos naturales y sus análogos" SFB416-B9

ENTIDAD FINANCIADORA: Deutsche Forschungsgemeinschaft (DFG)

DURACION DESDE: Jul 1999 **HASTA:** Dic 2001

INVESTIGADOR PRINCIPAL: Isabel Usón

TITULO DEL PROYECTO: New catalysts on the basis of organometallic fluorides

ENTIDAD FINANCIADORA: Unión Europea

DURACION DESDE: Nov 1993 **HASTA:** Oct 1996

INVESTIGADOR PRINCIPAL: Herwert W Roesky

TITULO DEL PROYECTO: **Crystal structures in the 100-1000 atom range**

ENTIDAD FINANCIADORA: **Unión Europea**

DURACION DESDE: **Dic 1994** *HASTA:* **Nov 1997**

INVESTIGADOR PRINCIPAL: **George M. Sheldrick**

TITULO DEL PROYECTO: **Determination of macromolecular crystal structures.**

Integrated, automated and user-friendly approaches.

ENTIDAD FINANCIADORA: **Union Europea, Red europea formada, entre otros por: Universidad de Göttingen, Universidad York, EMBL-DESY(Hamburgo), Universidad Cambridge, etc.**

DURACION DESDE: **Nov 1993** *HASTA:* **Oct 1996**

INVESTIGADOR PRINCIPAL: **George M. Sheldrick y Keith Wilson**

Ph.D. THESES

Título: Strukturanalyse zum Katalysemechanismus und zur Stabilität der Arylsulfatase A. (Análisis estructural del mecanismo catalítico y de la estabilidad de la arilsulfatasa A).

Doctorando: Rixa von Bülow
Universidad: Göttingen
Facultad / Escuela: Facultad de Ciencias Químicas
Fecha: 1999
Calificación: Magna cum Laude

Título: Probleme der modernen hochauflösender Einkristall-Röntgenstrukturanalyse. (Problemas de la cristalografía moderna a alta resolución).

Doctorando: Peter Müller
Universidad: Göttingen
Facultad / Escuela: Facultad de Ciencias Químicas
Fecha: 2001
Calificación: Magna cum Laude

Título: Strukturelle Untersuchungen an Varianten des Ecballium elaterium Tripsyn Inhibitors-II (EETI-II). (Determinación estructural de variantes del inhibidor de tripsina-II de Ecballium elaterium (EETI-II)).

Doctorando: Ralph Krätzner
Universidad: Göttingen
Facultad / Escuela: Facultad de Ciencias Químicas
Fecha: 2001
Calificación: Magna cum Laude

Título: Crystal structure of Wind, a PDI-related protein required for drosophila melanogaster dorsal-ventral development

Doctorando: Qingjun Ma
Universidad: Göttingen
Facultad / Escuela: Facultad de Ciencias Químicas
Fecha: 2003
Calificación: Magna cum Laude

Título: Strukturuntersuchungen zum Reaktionsmechanismus an der Alkylsulfatase aus *Pseudomonas putida* S-313.

Doctorando: Ilka Müller
Universidad: Göttingen
Facultad / Escuela: Facultad de Ciencias Químicas

Fecha: 2003
Calificación: Summa cum Laude

Título: Crystallographic and modelling studies of intermolecular interactions of biological interest.

Doctorando: Eftichia Alexopoulos
Universidad: Göttingen
Facultad / Escuela: Facultad de Ciencias Químicas
Fecha: 2004
Calificación: Magna cum Laude

Título: Structural Studies on the LysR-type regulator Tsar.

Doctorando: Dominique Monferrer Ventura
Universidad: Universidad de Barcelona
Facultad / Escuela: Facultad de Ciencias Químicas
Fecha: 19- February 2009
Calificación: Cum Laude

Título: ARCIMBOLDO, a supercomputing method for crystallographic *ab initio* protein structure solution below atomic resolution.

Doctorando: Dayté Dayana Rodríguez Martínez
Universidad: Universidad Ramón Llull
Facultad / Escuela: Facultad de Ciencias Químicas
Fecha: 17 December 2013
Calificación: Excelente Cum Laude

Título: Enforcing Secondary and Tertiary structure for crystallographic phasing.

Doctorando: Massimo Domenico Sammito
Universidad: Universidad de Barcelona
Facultad / Escuela: Facultad de Farmacia
Fecha: 22 June 2015
Calificación: Excelente *cum laude*.

* Awarded "Premi Extraordinari de Doctorat del curs acadèmic 2014-15"

Título: Crystallographic methods exploiting modern computing SUBIX, SHREDDER, Middleware and Web interfaces, Tools for crystallographic teaching.

Doctorando: Iñaki Martínez de Ilarduya Muñoz
Universidad: Universidad de Barcelona
Facultad / Escuela: Facultad de Farmacia
Fecha: 23 June 2015

Calificación: Excelente *cum laude*.

Título: Structural studies of PLA₂-like toxins and development of the structural solution method SEQUENCE SLIDER.

Doctorando: Rafael Junqueira Borges

Universidad: Universidad de Barcelona (Spain) and UNESP (Brazil)

Facultad / Escuela: Facultad de Farmacia (Barcelona) and Instituto de Biociencias (Botucatu)

Fecha: 20 February 2017

Calificación: Highest posible grade in the Brazilian system.

Título: Insight into the structure and function of engineered biocatalysts: Serine hydroxymethyltransferase from *Streptococcus thermophilus* and Halohydrine dehalogenase D2 from *Gammaproteobacterium*.

Doctorando: Giovanna Petrillo

Universidad: Universidad de Barcelona

Facultad / Escuela: Facultad de Farmacia

Fecha: 28 June 2017

Calificación: Excelente *cum laude*.

Título: Phase combination and its application to the solution of macromolecular structures: Developing ALIXE and SHREDDER

Doctorando: Claudia Lucía Millán Nebot

Universidad: Universidad de Barcelona

Facultad / Escuela: Facultad de Farmacia

Fecha: 21 Septiembre 2018

Calificación: Excelente *cum laude*.

* Awarded "Premio Extraordinario de Doctorado del curso académico 2018-19"

Título: Development of crystallographic methods for phasing highly modulated macromolecular structures

Doctorando: Iracema Caballero Muñoz

Universidad: Universidad de Barcelona

Facultad / Escuela: Facultad de Farmacia

Fecha: 26 March 2021

Calificación: Excelente *cum laude*

Título: Structural analysis of macromolecular folds and the application to phasing

Doctorando: Ana del Rocío Medina Bernal

Universidad: Universidad de Barcelona

Facultad / Escuela: Facultad de Farmacia

Fecha: 19 November 2021

Calificación: Excelente *cum laude*

Título: Integrating structure prediction and experimental approaches to elucidate the assembly of Surface Layer Proteins in *Lactobacilli*

Doctorando: Theo Sagmeister

Universidad: Karl-Franzens University of Graz (Austria)

Facultad / Escuela: Institute of Molecular Biosciences

Fecha: 23 November 2023

Calificación: Sehr Gut (Highest possible grade)

Master Theses:

- Lorena Gallardo Carbonell “Laying the foundations for a ligand validation method in X-ray protein crystallography”. University of Barcelona, Facultat de Química, Master in Theoretical Chemistry and Computational Modelling, June 2022
- Elisabet Jiménez Mellado, “Combining phase information with ALIXE for fragment-based molecular replacement”. University of Barcelona, Facultat de Farmàcia, Master de Biotecnologia Molecular, July 2019
 - * Awarded "Premio Extraordinario de Máster del curso académico 2018-19"
- Ana Medina, “Retrieval of fold properties for structure interpretation with BORGES_MATRIX”. University of Barcelona, Facultat de Farmàcia, Master de Biotecnologia Molecular, July 2017
- Iracema Caballero Muñoz, “Solution of coiled-coil protein crystal structures with ARCIMBOLDO_LITE and ARCIMBOLDO_BORGES”. University of Barcelona, Facultat de Farmàcia, Master de Biotecnologia Molecular, July 2016
- Ramón Hernández Moratinos, “Extracting libraries of local folds for crystallographic phasing with BORGES_MATRIX and ARCIMBOLDO” University of Barcelona, Facultat de Farmàcia, Master de Biotecnologia Molecular, July 2016
- Eloy Rodríguez Freire, “ARCIMBOLDO_LITE, ARCIMBOLDO_BORGES and BORGES_MATRIX: tests and parameterization”. University of Barcelona, Facultat de Farmàcia, Master de Biotecnologia Molecular, July 2015
- Claudia Millán, “Clustering for ARCIMBOLDO”. U. Menéndez Pidal-CSIC, Master Cristalografía y cristalización, Jul2012
- Daniela Leyton Puig, “Preliminary structural studies and functional characterization of AtzR, a LysR-type transcriptional regulator” University of Barcelona, Facultat de Farmàcia, Master de Biotecnologia Molecular, July 2011

- Massimo Sammito, BORGES: Programming an interactive tool to generate customized, secondary structure fragment databases for protein structure solution with ARCIMBOLDO. U. Bologna, Máster Bioinformática y Biocomputación, Jul 2011
- Iñaki Martínez de Ilarduya Muñoz, “DNAVectors”. U. Pompeu Fabra, Máster Bioinformática y Biocomputación, July 2009
- Dayté Rodríguez Martínez, “Crystallographic ab Initio Phasing below atomic resolution” U. Menéndez Pidal-CSIC, Master Cristalografía y cristalización, July 2009

Degree Theses:

- César González Griñán “Proyecto Borges Plus”. Open University of Catalonia, Degree in Computer Sciences, June 2015