

Curriculum Vitae

Date and place of birth: 6 January 1970, Athens, Greece

Education

Doctor of Philosophy (DPhil) in Chemistry, University of York, UK (1996)

Πτυχίον Βιολογίας (Bachelor in Biology), University of Athens, Greece (1992)

Απολυτήριον (High School degree), Athens College, Greece (1987)

Pre- and postdoctoral training

1996-1997 EMBO long-term post-doctoral fellow, with Titia Sixma at the NKI

1992-1995 Pre-doctoral fellow, with Keith Wilson at the EMBL-Hamburg Unit

Positions held

2019-present Oncode Institute Investigator

2018-present Professor, University of Utrecht

2005-present Principal Investigator NKI

2001-2005 AvL fellow, NKI (Principal Investigator - assistant professor)

1998-2000 Staff Scientist and Team Leader, EMBL-Grenoble Unit

Honours and awards

EMBO Young Investigator, 2001

EMBO long-term fellowship, 1996

Professional societies

Founding and Board member of the Netherlands Biomolecular Modelling Society

"Proteins" NWO study group (Board member 2013-2015)

"Nucleic Acids" and "Crystallography" NWO study groups

International Union of Crystallography (through both the Dutch and Greek societies)

Funding - Current Research Grants

- **KWF** Membrane glycerophosphodiesterases: novel players in cell differentiation and cancer biology (PRINCIPAL INVESTIGATOR, 498 k€)
- **INSTRUCT-Ultra**, EU H2020 Infradev 731005, Releasing the full potential of Instruct for integrated structural life science research (PRINCIPAL INVESTIGATOR, 250 k€)
- **WEST-life**, EU H2020 675858, World-wide E-infrastructure for structural biology (PRINCIPAL INVESTIGATOR, 250 k€)
- **INEXT**, EU 653706 INFRASTRUCTURE FOR NMR, EM AND X-RAY CRYSTALLOGRAPHY FOR TRANSLATIONAL RESEARCH (PRINCIPAL INVESTIGATOR, DEPUTY CO-ORDINATOR, 660 k€)
- **NWO-TOP** 714.014.002. Structural and chemical basis for the biosynthesis and propagation of base J (PRINCIPAL INVESTIGATOR, 695 k€)
- **KWF** Mechanisms of activation of MPS1, a guardian of genomic stability (Co-Investigator, 640 k€)

Overview of Publications and Research Metrics

Hirsch-index: **49** (Scopus) - **55** (Google Scholar)

Nr. peer reviewed original research papers: **105**

Nr. reviews, books, commentaries, etc: **32**

in which as Corresponding author: **41**

Nr. of citations: **12,860** (Scopus)

Nr. of citations: **16,700** (Google Scholar)

Highly cited publications (Google scholar):

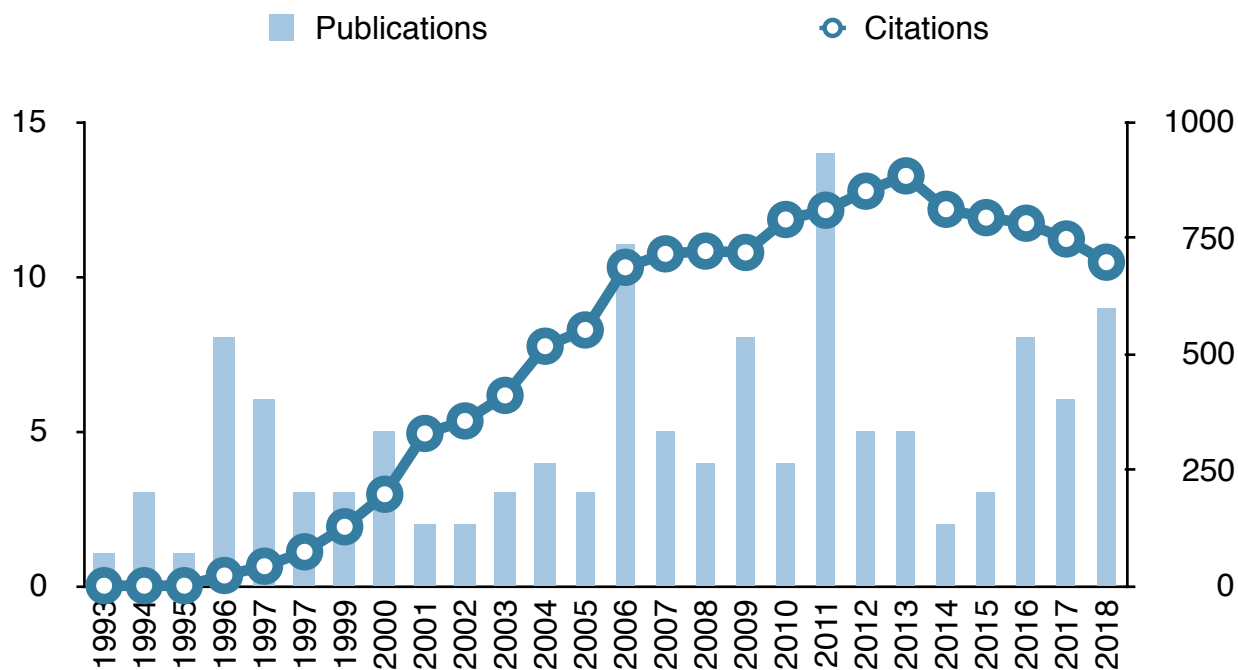
1 publication with 2,930 citations

1 publication with 1,229 citations

6 publications with over 500 citations

11 publications with over 200 citations

18 publications with over 100 citations



Academic Examination Boards

PHD and other higher degree examination boards

- Doctoral Thesis examination board of fifteen PhD candidates in the Netherlands
- Doctoral Thesis examination board in the UK (three students)
- Doctoral Thesis examination board in Denmark (two student)
- "Habilitation" (license to supervise PhD students) for Dr. Carlo Petosa (France)
- "Habilitation" (license to supervise PhD students) for Dr. Montserrat Soler Lozez

Other funding

Current fellowships to lab members

- **NWO VIDI** fellowship to Dr. R. Joosten (career development grant)
- **NWO VENI** fellowship to Dr. Y. Hiruma (personal fellowship)

Previous research grants

- **NWO TOP-GO** L.10.062. Autotaxin, a secreted phosphodiesterase with diverse roles in disease: structural and functional studies (PRINCIPAL INVESTIGATOR, 746 k€)
- **KWF** NKI-2010-4781 Validation of autotaxin, a metastasis-enhancing exo-phosphodiesterase, as theyrapeutic target (Co-Investigator, 640 k€)
- **NWO-Groot** The NKI Protein Facility (Equipment only, 1.4 M€)
- **SPINE-2**, EU FW6 031220, 2006-2010, FROM RECEPTOR TO GENE: STRUCTURES OF MACROMOLECULAR COMPLEXES (Partner, 620 k€).
- **TEACH-SG**, EU FW6, 2006-2010, TRAINING FOR HIGH VOLUME, HIGH VALUE STRUCTURAL GENOMICS METHODOLOGIES (Partner, 50 k€).
- **NIH RO1** DEVELOPMENT OF THE ARP/WARP SOFTWARE PACKAGE, 2006-2010 (900 k\$)
- **3D-Repertoire**, EU FW6 512028, 2005-2009, A MULTIDISCIPLINARY APPROACH FOR STRUCTURES OF PROTEIN COMPLEXES IN A MODEL ORGANISM (Partner, 650 k€).
- **MAX-INF-II** EU Macromolecular Crystallography Infrastructure Network, 2004-2008
- **BIOXHIT**, EU FW6 503420, 2004-2008, BIOCRYSTALLOGRAPHY ON HIGHLY INTEGRATED TECHNOLOGY PLATFORM (Section Coordinator, Partner, 753 k€).
- **KWF** grant NKI 2004-3063, 2004-2008, FUNCTION STRUCTURE STUDY OF POLO-LIKE KINASES (CO-INVESTIGATOR, 600 k€)
- **SPINE**, EU FW6 Pilot 00988, 2002-2005, STRUCTURAL PROTEOMICS IN EUROPE (620 k€)
- **NIH RO1** DEVELOPMENT OF ARP/WARP SOFTWARE PACKAGE, 2002 - 2006 (700 k\$)
- **NWO-OC.01.077** STRUCTURAL AND FUNCTIONAL ANALYSIS OF HUMAN L1/ALU RETROPOSITION, 1/9/2002-30/8/2006 (PRINCIPAL CO-INVESTIGATOR1 PhD student)
- **NWO-OC.01.078** FUNCTION AND STRUCTURE CHARACTERISATION OF THE RLP/RAB7 COMPLEX 1/9/2002-30/8/2006 (PRINCIPAL CO-INVESTIGATOR, 1 PhD student)
- **NWO-OC.01.M.013** PURCHASE OF X-RAY DIFFRACTION EQUIPMENT(with T. Sixma, 250 k€)
- **AUTOSTRUCT** QLRT-1999-30398 (2000-2003, Partner, 105 k€)
- **MAX-INF-II** EU Macromolecular Crystallography Infrastructure Network, 2004-2008

Previous fellowships to lab members

- **Senior SFN fellowship** to Dr. E. von Castelmur
- **NWO Veni** fellowship to Dr. R. Joosten
- **EMBO** fellowship to Dr. E. von Castelmur
- **EMBO** fellowship to Dr. C. Caillat
- **SNF** Swiss Science Foundation post-doctoral fellowship to Dr. E. von Castelmur
- **NWO Veni** fellowship to Dr. S. Cohen
- **NWO Vidi** career development grant to O. Weichenrieder
- **EMBO** fellowship to Dr. V. De Marco
- **Marie Curie** fellowship to Dr. O. Weichenrieder
- **EMBO** fellowship to Dr. O. Weichenrieder

Editorial

► **Editorial and peer review**

- Editorial Board member in Journal of Structural Biology (2011-present)
- Editorial Board member in PROTEINS:Structure, function&Bioinformatics (2008-present)
- Review Editor for Frontiers (Structural Biology)
- F1000 member (Structural Biology)
- Guest Scientific Editor for Emerging Topics In Life Sciences (special issue 2018)
- Guest Scientific Editor for Current Opinion in Structural Biology (special issue 2016)
- Guest Scientific Editor for J. Structural Biology (special issue 2011)
- Guest Scientific Editor for Acta D, Biol. Crystallography (special issue December 2004)
- Referee for research papers in various scientific journals, including Nature, Nature Methods, Nature Protocols, Nature Structural & Molecular Biology, Structure, Acta Cryst.

Activities with industry and commercialisation of research results

- Research Collaboration with Janssen Pharmaceuticals

A research collaboration to improve and customise our software PDB_REDO, for JnJ at Philadelphia, for biologics and small molecule drug discovery. The research agreement is for two years, starting 2016, and involved an amount of 2360,000 US\$.

- ARP/wARP

The ARP/wARP software has been a long term project that has been free for academic users, but licensed for a fee to over 50 companies, with a to-day revenue reaching 2,000,000 Euro.

- X-ray Micro-diffractometer

I co-designed and commissioned the first X-ray micro-diffractometer, between 1998-2000. In the last two decades, the micro-diffractometer has been a success that revolutionised design of many beamlines, having introduced concepts like the on-axis viewing for sample centring. It is commercially exploited by the EMBL through the company MATEL and several units are installed in world synchrotrons.

- Crystallisation Screening

The PACT screen for macromolecular crystallisation has been developed in my laboratory, licensed to Molecular Dimensions Ltd and Qiagen, and is a successful product with both companies.

- Autotaxin

The Autotaxin structure determination project has been a close collaboration with Pfizer, and involved a research grant of 200,000 Euro to fund a PhD position in my lab for this project.

- Human lipase

A human lipase that is a drug target for preventing viral entry, has been a focus for structural studies in my lab; the IP on a new human lipase has been licensed to Haplogen GmbH.

Management

Activities within the Host organisation

- Scientific responsible for the NKI High Performance Computing Cluster (2016 - 2018)
- NKI international Seminar Committee member (2012 -)
- Scientific responsible for the NKI Protein Facility (2010 -)
- Deputy member of the NKI Research Council (2008 - 2015)
- EMBL - ESRF JCSG management committee (1997-1999)

Participation in European Project coordination

- Coordinator of the iNEXT-2 proposal for INFRA Horizon2020 funding.
- Executive Board member for the Instruct ESFRI project (NL representative, 2017-)
- Council member for the Instruct ESFRI project (NL representative, 2011-2017)
- Deputy Coordinator of the iNEXT H2020 project.
- Working Group Coordinator for the INSTRUCT ESFRI project, responsible for coordinating actions for biophysical and crystallisation research infrastructures for Structural Biology in the European level (2006-2010).
- Project Steering Committee member for the 3D-Repertoire project (2005-2009)
- Project Steering Committee member and Section Manager for the BIOXHIT EU project, coordinating the action of five laboratories involved in this section (2004-2008).

Advisory groups

- Member of "site visit" evaluation committee for the Department of Biology, University of Athens, Greece (November 2018)
- Member of "site visit" evaluation committee for the Technical University of Athens, Greece (December 2016)
- Member of the Advisory Board for the EC-REGPOT project InnovCrete (2015-2018)
- Co-chair of the Shanghai Synchrotron Radiation Facility Biology Beamlines (2015)
- Member of the Netherlands "contact committee" to EMBC/EMBL (2014-present)
- Elected European Users representative to the Biostruct-X EC-CSA (2012-2014)
- Member of the Advisory Board for the EC-REGPOT project SEE-DRUG (2012-2015)
- Member of the Review Panel for Diamond beamline BL23 (2011)
- Member of a "site visit" evaluation committee for the Department of Biochemistry , University of Larissa, Greece (February 2011)
- Member of the ESRF synchrotron (France) external consultant panel for Macromolecular Crystallography in the strategic upgrade (2009)
- Member of the DIAMOND synchrotron (UK) working group for macromolecular crystallography beamlines (2001-2005)
- Member of the ALBA synchrotron (Spain) international advisory panel for the macromolecular crystallography beamline (2004)
- Member of advisory committees on two STW projects (Dutch technology projects)

Grant Review

Grant panels, committees and review - International

- Belgian National Research Foundation, FWO (2013-present)
- Vice-chair of the Biostruct-X EC-CSA Project Evaluation Committee (2012-2016)
- Review Board member for NIH grants (2010, 2011)
- Referee for EMBO short and long term fellowships (regularly since 2002)
- Referee and Committee member for grants of the Wellcome Trust (UK, 2006, 2009)
- Referee for research grants of the BBSRC (UK, 2005, 2006, 2008)
- Referee and Committee member for EC FP7 grants
- Referee for beamtime applications at the EMBL/UK-BBSRC BM14 (2001 - 2010)
- Panel member and referee for the National Portuguese Research Foundation; area of Molecular and Structural Biology: 2002, 2004, 2007
- Referee for research grants of the Belgian National Research Foundation

Grant panels, committees and review - National (NWO Netherlands)

- Committee member of the VIDI fellowships panel of NWO-CW (2005, 2006, 2011)
- Committee member of the 'MiddelGroot' grants panel of NWO-CW (2010)
- Committee member of the BAZIS grants panel of NWO-CW (2010)
- Referee for several research grants of the Dutch National Research Organisation (NWO)

Scientific Collaborations

International Collaborations

- Dr. Craig Jamieson, small molecule inhibitors
- Dr. Garib Murshudov, macromolecular refinement
- Prof. Peter Myler, J-base biology
- Prof. Andrew Morris, Autotaxin in cardiovascular disease
- Prof. Mathieu Bollen, Autotaxin family members
- Dr. Victor Lamzin, the ARP/wARP project
- Prof. Julian Blow, DNA replication biochemistry
- Assoc. Prof. Zoe Lygerou and Assoc. Prof. Stavros Taraviras, DNA replication
- Dr. Hideo Nishitani, DNA replication and damage

National Collaborations

- Prof. Ronald Oude-Elfering, Autotaxin function
- Prof. Geert Kops, mitotic kinases
- Prof. Gert Vriend, PDB_REDO
- Dr. Thijn Brummelkamp, host factors for viral entry
- Prof. Piet Borst, J-base biology
- Prof. Rene Medema, mitotic kinases
- Prof. Jacques Neefjes, antigen presentation mechanisms
- Prof. Huib Ovaa, Autotaxin inhibitors

Teaching activities

Organisation of conferences and workshops

- Translating Structural Biology into Biomedical Applications, Grenoble, 2018
- Instruct Biennial Structural Biology meeting, Brno, 2016
- Gordon Conference on "Diffraction Methods in Molecular Biology" 2014 Chair
- Gordon Conference on "Diffraction Methods in Molecular Biology" 2012 Co-chair
- "What is a Macromolecular Complex?", NKI, 1-2 October 2009, NKI, Amsterdam
- Como School on X-ray Crystallography, 21-25 May 2006, Como, Italy
- CCP4 Study Weekend, 4-5 January 2004, Leeds, UK
- Methods for high-throughput structure determination, 1 June 2004, NKI, Amsterdam
- Methods for high-throughput structure determination, 17 May 2002, NKI, Amsterdam

Organisation of Practical courses

- Macromolecular Crystallography, Cold Spring Harbor, US, 2016 - present (annually)
- Master Your Proteins, Amsterdam, 20-23 November 2017, NKI Amsterdam
- HTP crystallisation and information management, 18-20 June 2008, NKI Amsterdam
- Biophysical Characterisation of Macromolecules , 21-23 May 2008, NKI, Amsterdam
- High Throughput Protein crystallisation, 28 February - 3 March 2007, EMBL Hamburg
- High Throughput Protein crystallisation, 13-15 December 2005, NKI, Amsterdam
- EMBO Practical course on "Automated high-throughput macromolecular structure determination", 24-30 May 2004, NKI, Amsterdam
- 1st EMBO YIP PhD course, 29 August - 4 September 2002, EMBL-Heidelberg
- EMBO Practical course on "Automated high-throughput macromolecular structure determination", 8-16 May 2002, EMBL-Heidelberg
- EMBO Practical course on "Automated high-throughput macromolecular structure determination", 20-29 March 2000, EMBL-Grenoble

Invited Tutor in regular Practical Courses

From 1998 – annual	Macromolecular Crystallography, Cold Spring Harbor, US
From 2002 – 2014	Modern Methods in Biocrystallography, IQTB Lisboa, PO
From 2002 – 2005	EMBO YIP PhD course, EMBL–Heidelberg, DE
From 1999 – 2011	Methods for macromolecular crystallography, EMBL-HH, DE

Invited Tutor in Courses and Workshops

19-23 November 2018, Macromolecular complexes, Strasburg, FR
27-29 September 2018, Structural Biology Approaches for drug development, HU
17-21 December 2014, From Genes to Atomic Structures at Trieste, IT
23-29 April 2012, From Genes to Atomic Structures at Trieste, IT
10-16 July 2011, EMBO course on Macromolecular Complexes, Marseille, FR
15-19 September 2008, EMBO Crystallography Course at Soleil, Paris, FR
5-7 June 2008, Biochemistry and Biotechnology course, Heraklion, GR
24-27 May 2008, CCP4 Workshop, APS Chicago, US
2-12 May 2008, Macromolecular Crystallography, CN
9-22 Sept. 2006, Shelx Workshop, Gottingen, DE
6-17 Sept. 2003, Shelx Workshop, Gottingen, DE
22-23 Nov. 2002, High-throughput methods for structural genomics, Argonne N.L., US
8-9 Oct. 2002, X-ray Structure Determination for Structural Genomics, PSF Berlin, DE
13-17 March 2000, New trends in Protein Crystallography, University of Ulu, FI
7-8 Nov. 2000, Crystallographic methods for Structural Genomics, Harima, JP
25 May-4 June 2000, Structural Molecular Biology School, Stanford University, US
15-19 Nov. 1999, High-throughput methods for structural genomics, Argonne, US
14-20 August 1999, IUCr Workshop on Crystallographic Computing, Cambridge, UK
21-22 June, 1999, Automated high-throughput structure determination, Brookhaven, US
11-17 Dec., 1998, Protein structure refinement, University of York, UK

Scientific Meetings and Seminars

Chair in International meetings

- EMBO conference "Towards Novel Therapies", 6-8 March 2017, Groningen, NL
- "New Computational Approaches to Structure Solution and Refinement", International Union of Crystallography (IUCr), 22-30 August 2011, Madrid, ES
- Gordon Conference "Diffraction methods in molecular biology", 11-15 July 2010, Session Chair, USA
- "Experimental Phasing in Structural Biology, Phase Improvement and Refinement.", European Crystallography Meeting (ECM), 29 August - 2 Sept 2010, Darmstadt, DE
- "Computational Methods", American Crystallographic Association (ACA) Annual Meeting, 26-31 July 2004, Chicago, USA
- "Chemistry meets Biology symposium", 5-6 June 2004, Heidelberg, DE
- "Model building and refinement", American Crystallographic Association (ACA) Annual Meeting, 26-31 July 2003, Cincinnati, USA
- "Conference on Structural Genomics", 1-5 November 2000, Yokohama, Co-chairman

Invited Lectures (selected)

- 2018 Protein-protein interactions versus ligand-receptor interactions, Ghent, BE
- 2018 Bioactive Lipids, Athens, GR
- 2017 Protein-Protein Interactions Meeting, Elat, IL
- 2017 Lysophospholipid and Related Mediators - From Bench to Clinic, New Orleans, USA
- 2017 BioTrans17 Meeting, Barcelona, ES
- 2016 Bioactive Lipids, Budapest, HU
- 2016 Greek Crystallographic society meeting, Athens, GR
- 2016 IMBB Seminar Series, Heraklion, GR
- 2016 Max Perutz Institute Seminar Series, Vienna, AU
- 2015 Instruct Biennial meeting, Florence, IT
- 2014 Greek Crystallographic society meeting, Greece
- 2014 Greek Pharmacological society annual meeting, Greece
- 2013 LMB-MRC Cambridge, Seminar Series, J-base binding protein
- 2014 Invited Lecturer, Greek Crystallographic Society, Heraklion, GR
- 2014 Invited Lecturer, Greek Pharmacological Society, Athens, GR
- 2013 Invited lecturer, " The J-base binding protein", LMB-MRC Cambridge,
- 2012 Invited Lecturer, Methods in Macromolecular Crystallography, rice, IT,
- 2011 Invited Lecturer CIMP , "Structure and function of Autotaxin", Vienna, AU,
- 2010 Gent, BE, Guest lecture at University of Gent, BE
- 2010 Invited Lecturer "Medicinal Chemistry of Tropical Diseases", London, UK
- 2010 Invited Lecturer Swedish Structural Biology meeting, Tallberg, SE
- 2010 Invited Lecturer in "Macromolecular Complexes" meeting, Erice, IT
- 2009 Invited Lecturer, University of Dundee, Dundee UK,
- 2008 3rd meeting of the Greek Crystallography Association, Athens, GR
- 2008 Third International Structural Genomics Meeting Oxford UK,
- 2008 Gordon Conference Diffraction methods in molecular biology, UA,
- 2008 Algorithms in crystallography and electron microscopy, NL
- 2007 BCA Spring meeting, Canterbury UK,
- 2006 Greek Biochemistry Association annual meeting, Patra GR,
- 2006 BCA Spring meeting, Lancaster UK,
- 2006 USA, Gordon Conference Diffraction methods in molecular biology
- 2004 London, UK, The SPINE conference
- 2004 USA, Gordon Conference Diffraction Methods in Molecular Biology
- 2004 Meeting on high resolution structures for drug design, Bischoffshausen, FR
- 2003 American Crystallographic Association Annual Meeting, Cincinnati, USA
- 2003 International Symposium on Diffraction Structural Biology, Tsukuba, JA
- 2003 7th European Workshop on Crystallography, Como, IT
- 2002 2nd Conference on Structural Genomics, Berlin, DE
- 2002 Structural Biology applications at PETRA III, Hamburg, DE
- 2002 9th Int.Conference Crystallisation Biological Macromolecules, Jena
- 2001 American Crystallographic Association Meeting, Los Angeles, USA,

- 2001 ESRF user meeting, Grenoble, FR
- 2000 Conference on Structural Genomics, Co-chairman, Yokohama, JA
- 2000 ECM-19: 19th European Crystallographic Meeting, Nancy, FR
- 2000 Methods in Macromolecular Crystallography, Erice, IT
- 1999 American Crystallographic Association Meeting, Buffalo, USA
- 1999 5th European Workshop on Crystallography, Como, IT
- 1999 CCP4 study weekend, 'Data collection and processing', Sheffield, UK
- 1998 American Crystallographic Association Meeting, Washington, USA
- 1998 Gordon Conference Diffraction Methods in Molecular Biology, USA
- 1997 Symposium on the refinement of macromolecules, Porto, PO
- 1997 ECM-17: 17th European Crystallographic Meeting, Lisboa, PO
- 1997 CCP4 study weekend, 'Recent advances in phasing', York, UK
- 1996 Methods and Structures in macromolecular crystallography, Hamburg
- 1996 2nd International Symposium on Chitin Enzymology, Senigalia, IT

Current team members

Dr. Krista Joosten - Post Doc, Methods in macromolecular crystallography (20%)
Dr. Robbie Joosten - Post Doc, Methods in macromolecular crystallography
Dr. Yoshitake Hiruma - Post Doc, Biochemistry and Structural Biology
Dr. Misbha Ud Din Ahmad - Post Doc, Biochemistry and Structural Biology
Mr. Nassos Adamopoulos - PhD Candidate, Biochemistry and Structural Biology
Mr. Bart van Beusekom - PhD Candidate, Methods in macromolecular crystallography
Mr. Fernando Salgado-Polo - PhD Candidate, Biochemistry and Structural Biology
Mr. Maarten Hekkelman - Software Developer, Methods in macromolecular crystallography
Mr. George Damaskos - Software Developer, Methods in macromolecular crystallography
Mrs. Tatjana Heidebrecht - Technician, Biochemistry

Previous team members - NKI

Ms. Foteini Tsakou - Technician (Master student, Denmark)
Ms. Yvetter Stuif-Buitsma - Technician (Laboratory Manager, NKI)
Dr. Wouter Touw - Post Doc (R&D Scientist, DSM)
Dr. Willem Jan Keune - Post Doc (Consultant, FFUND)
Dr. Eleonora von Castelmur - Post Doc, (Assistant Professor, University of Linköping)
Dr. Christophe Caillat - Post Doc, (Post Doc, IBS Grenoble)
Dr. Jens Hausmann - PhD Student, (EMBO fellow, University of Münster)
Dr. Leonie van Zijl - Post Doc (Docent Life Sciences at Hogeschool Utrecht)
Dr. Serge Cohen - Post Doc, (Chargé de recherche, "Ipanema", France)
Dr. Valeria De Marco - Post Doc, (Head of Student Administration, MRC London)
Dr. Eirini Mitisiki - Post- doc, (Application Scientist, Pfizer, Athens)
Dr. Dene Littler - Post Doc, (Post-doc, Melbourne, Australia)
Mr. Evangelos Christodoulou - Technician (Protein expression Facility Manager, MRC London)
Dr. Patrick Celie - Post Doc, (NKI Protein Facility Manager)
Dr. Wijnand Mooij - Post Doc, (Scientific programmer, Dotmatics)
Mr. Diederick de Vries - Database developer, (Software developer, Sogyo)
Mrs. Suzan van Gerwen - Technician, (Research Assistant, MPI Dortmund)
Mrs. Angelina Huseinovic - Technician, (PhD student at Vrije Universiteit Amsterdam)
Mr. Mobien Kassiem - Technician, (Technician, NKI Amsterdam)
Dr. Oliver Weichenrieder – Senior Post Doc, (Group Leader MPG Tübingen, DE)
Mr. Kostas Repanas – PhD Student, (Scientific writer, Singapore)
Dr. Mark Hilge – Post Doc, Biochemistry, (Staff Scientist, Switzerland)
Mr. Marouane Ben Jelloul – Software Engineer (Project Manager, Paris)
Mr. Mattheos Kakaris - Software Engineer (Senior Project Manager, Digitalis, Greece)
Mrs. Cristiane Toaldo – Technician NKI H4 (technician)

Publications List

-Original research publications

105. Hayashi A, Giakoumakis NN, Heidebrecht T, Ishii T, Panagopoulos A, Caillat C, Takahara M, Hibbert RG, Suenaga N, Stadnik-Spiewak M, Takahashi T, Shiomi Y, Taraviras S, von Castelmur E, Lygerou Z, Perrakis A*, Nishitani H. Direct binding of Cdt2 to PCNA is important for targeting the CRL4Cdt2 E3 ligase activity to Cdt1. **Life Sci Alliance**. 2018 Dec 31;1(6):e201800238. doi: 10.26508/lsa.201800238. eCollection 2018 Dec.
104. Roorda JC, Joosten RP, Perrakis A*, Hiruma Y. A crystal structure of the human protein kinase Mps1 reveals an ordered conformation of the activation loop. **Proteins**. 2018 Dec 23. doi: 10.1002/prot.25651. [Epub ahead of print]
102. van Beusekom B, Heidebrecht T, Adamopoulos A, Fish A, Pardon E, Steyaert J, Joosten RP, Perrakis A. Characterization and structure determination of a llama-derived nanobody targeting the J-base binding protein 1 **Acta Crystallogr F Struct Biol Commun**. 2018 Nov 1;74(Pt 11):690-695. doi: 10.1107/S2053230X18010282. Epub 2018 Oct 16.
101. Argenzio E, Klarenbeek J, Kedziora KM, Nahidiazar L, Isogai T, Perrakis A, Jalink K, Moolenaar WH, Innocenti M. Profilin binding couples chloride intracellular channel protein CLIC4 to RhoA-mDia2 signaling and filopodium formation. **J Biol Chem**. 2018 Dec 14;293(50):19161-19176. doi: 10.1074/jbc.RA118.002779. Epub 2018 Oct 31.
100. Sacristan C, Ahmad MUD, Keller J, Fermie J, Groenewold V, Tromer E, Fish A, Melero R, Carazo JM, Klumperman J, Musacchio A, Perrakis A, Kops GJ. Dynamic kinetochore size regulation promotes microtubule capture and chromosome biorientation in mitosis. **Nat Cell Biol**. 2018 Jun 18. doi: 10.1038/s41556-018-0130-3.
99. van Beusekom B, Joosten K, Hekkelman ML, Joosten RP, Perrakis A. Homology-based loop modeling yields more complete crystallographic protein structures. **IUCr** 2018 Aug 8;5(Pt 5):585-594
98. Salgado-Polo F, Fish A, Matsoukas MT, Heidebrecht T, Keune WJ, Perrakis A. Lysophosphatidic acid produced by autotaxin acts as an allosteric modulator of its catalytic efficiency. **J Biol Chem**. 2018 Sep 14;293(37):14312-14327. doi: 10.1074/jbc.RA118.004450. Epub 2018 Jul 19.
97. van Veen M, Mans LA, Matas-Rico E, van Pelt J, Perrakis A, Moolenaar WH, Haramis AG. Glycerophosphodiesterase GDE2/GDPD5 affects pancreas differentiation in zebrafish. **Int J Biochem Cell Biol**. 2018 Jan;94:71-78. doi: 10.1016/j.biocel.2017.11.015. Epub 2017 Dec 22.
96. van Beusekom B, Touw WG, Tatineni M, Somani S, Rajagopal G, Luo J, Gilliland GL, Perrakis A*, Joosten RP. Homology-based hydrogen bond information improves crystallographic structures in the PDB. **Protein Sci**. 2018 Mar;27(3):798-808. doi: 10.1002/pro.3353
95. Nieuwenhuis J, Adamopoulos A, Bleijerveld OB, Mazouzi A, Stickel E, Celie P, Altelaar M, Knipscheer P, Perrakis A, Blomen VA, Brummelkamp TR. Vasohibins encode tubulin detyrosinating activity. **Science**. 2017 Nov 16. pii: eaao5676. doi: 10.1126/science.aao5676.
94. van Veen M, Matas-Rico E, van de Wetering K, Leyton-Puig D, Kedziora KM, De Lorenzi V, Stijf-Bultsma Y, van den Broek B, Jalink K, Sidenius N, Perrakis A, Moolenaar WH. Negative regulation of urokinase receptor activity by a GPI-specific phospholipase C in breast cancer cells. **Elife**. 2017 Aug 29;6. pii: e23649. doi: 10.7554/eLife.23649.
93. Hiruma Y, Koch A, Hazraty N, Tsakou F, Medema RH, Joosten RP, Perrakis A*. Understanding inhibitor resistance in Mps1 kinase through novel biophysical assays and structures. **J Biol Chem**. 2017 Sep 1;292(35):14496-14504. doi: 10.1074/jbc.M117.783555. Epub 2017 Jul 18.
92. Keune W-J, Potjewyd F, Heidebrecht T, Salgado-Polo E, Macdonald, S.J.F., Chelvarajan, L., Abdel Latif, A., Soman, S., Morris, A.J., Watson, A.J.B., Jamieson, C., Perrakis A*. Rational Design of Autotaxin Inhibitors by Structural Evolution of Endogenous Modulators (2017) **Journal of Medicinal Chemistry**, 60 (5), pp. 2006-2017.
91. Miller, L.M., Keune W-J, Castagna, D., Young, L.C., Duffy, E.L., Potjewyd F, Salgado-Polo E, García, P.E., Semaan, D., Pritchard, J.M., Perrakis A, MacDonald, S.J.F., Jamieson, C., Watson, A.J.B. Structure-activity relationships of small molecule autotaxin inhibitors with a discrete binding mode (2017) **Journal of Medicinal Chemistry**, 60 (2), pp. 722-748.

90. Staring, J., von Castelmur, E., Blomen, V.A., van den Hengel, L.G., Brockmann, M., Baggen, J., Thibaut, H.J., Nieuwenhuis, J., Janssen, H., van Kuppeveld, F.J., Perrakis, A., Carette, J.E., Brummelkamp, T.R. PLA2G16 represents a switch between entry and clearance of Picornaviridae (2017) **Nature**, 541 (7637), pp. 412-416.
91. Hiruma, Y., Koch, A., Dharadhar, S., Joosten, R.P., Perrakis, A*. Structural basis of reversine selectivity in inhibiting Mps1 more potently than aurora B kinase (2016) **Proteins: Structure, Function and Bioinformatics**, 84 (12), pp. 1761-1766.
88. Matas-Rico, E., van Veen, M., Leyton-Puig, D., van den Berg, J., Koster, J., Kedziora, K.M., Molenaar, B., Weerts, M.J.A., de Rink, I., Medema, R.H., Giepmans, B.N.G., Perrakis, A., Jalink, K., Versteeg, R., Moolenaar, W.H. Glycerophosphodiesterase GDE2 Promotes Neuroblastoma Differentiation through Glypican Release and Is a Marker of Clinical Outcome (2016) **Cancer Cell**, 30 (4), pp. 548-562.
87. Hausmann, J., Keune, W.-J., Hipgrave Ederveen, A.L., van Zeijl, L., Joosten, R.P., Perrakis, A*. Structural snapshots of the catalytic cycle of the phosphodiesterase Autotaxin (2016) **Journal of Structural Biology**, 195 (2), pp. 199-206.
86. Keune WJ, Hausmann J, Bolier R, Tolenaars D, Kremer A, Heidebrecht T, Joosten RP, Sunkara M, Morris AJ, Matas-Rico E, Moolenaar WH, Oude Elferink RP, Perrakis A*. (2016) Steroid binding to Autotaxin links bile salts and lysophosphatidic acid signalling. **Nature Commun.** Apr 14;7:11248. doi: 10.1038/ncomms11248.
85. Caillat C, Fish A, Pefani DE, Taraviras S, Lygerou Z, Perrakis A*. (2015) The structure of the GemC1 coiled coil and its interaction with the Geminin family of coiled-coil proteins. **Acta Crystallogr D Biol Crystallogr.** 71(Pt 11):2278-86.
84. Hiruma Y, Sacristan C, Pachis ST, Adamopoulos A, Kuijt T, Ubbink M, von Castelmur E, Perrakis A*, Kops GJ. (2015) Competition between MPS1 and microtubules at kinetochores regulates spindle checkpoint signaling. **Science** 348(6240):1264-7.
83. Garstka MA, Fish A, Celie PH, Joosten RP, Janssen GM, Berlin I, Hoppes R, Stadnik M, Janssen L, Ovaa H, van Veelen PA, Perrakis A, Neefjes J. (2015) The first step of peptide selection in antigen presentation by MHC class I molecules. **Proc Natl Acad Sci U S A.** 112(5):1505-10.
82. Joosten RP, Long F, Murshudov GN, and Perrakis A* (2014) "The PDB_REDO Server for Macromolecular Structure Model Optimization.." **IUCrJ** 1 (Pt 4) (June 30): 213-220. doi: 10.1107/S2052252514009324.
81. Caillat C, Pefani DE, Gillespie PJ, Taraviras S, Blow JJ, Lygerou Z, Perrakis A*. (2013) The geminin and idas coiled coils preferentially form a heterodimer that inhibits geminin function in DNA replication licensing. **J Biol Chem.** 2013;288(44):31624-34. Epub 2013/09/26.
80. Nijenhuis W, von Castelmur E, Littler D, De Marco V, Tromer E, Vleugel M, van Osch MH, Snel B, Perrakis A*, Kops GJ. (2013) A TPR domain-containing N-terminal module of MPS1 is required for its kinetochore localization by Aurora B. **J Cell Biol.** 201(2):217-31
79. Houben AJ, van Wijk XM, van Meeteren LA, van Zeijl L, van de Westerloo EM, Hausmann J, Fish A, Perrakis A, van Kuppeveld TH, Moolenaar WH. (2013) The Polybasic Insertion in Autotaxin- α Confers Specific Binding to Heparin and Cell-Surface Heparan Sulfate Proteoglycans. **J Biol Chem.** 4;288:510-9
78. Jansen S, Perrakis A*, Ulens C, Winkler C, Andries M, Joosten RP, Van Acker M, Luyten FP, Moolenaar WH, Bollen M. (2012) Structure of NPP1, an Ectonucleotide Pyrophosphatase/Phosphodiesterase Involved in Tissue Calcification. **Structure.** 20(11):1948-59.
77. Heidebrecht T, Fish A, von Castelmur E, Johnson KA, Zaccai G, Borst P, Perrakis A*. (2012) Binding of the J-binding protein to DNA containing glucosylated hmU (base J) or 5-hmC; evidence for a rapid conformational change upon DNA binding. **J Am Chem Soc.** 134(32): 13357-65.
76. van Luenen HGAM, Farris C, Jan S, Genest PA, Tripathi P, Velds A, Kerkhoven RM, Nieuwland M, Haydock A, Ramasamy G, Vainio S, Heidebrecht T, Perrakis A, van Steensel B., Myler PJ, Borst P. (2012) Glucosylated hydroxymethyluracil (DNA base J) prevents transcriptional read-through in Leishmania. **Cell.** 150:5, 909-921
75. Suijkerbuijk SJ, van Dam TJ, Karagöz GE, von Castelmur E, Hubner NC, Duarte AM, Vleugel M, Perrakis A, Rüdiger SG, Snel B, Kops GJ. (2012) The Vertebrate Mitotic Checkpoint Protein BUBR1 Is an Unusual Pseudokinase. **Dev Cell.** 22(6):1321-9.

74. Joosten RP, Joosten K, Murshudov GN, Perrakis A*. (2012) PDB_REDO: constructive validation, more than just looking for errors. **Acta Crystallogr D Biol Crystallogr.** 69:2293-5
73. Joosten RP, Joosten K, Cohen SX, Vriend G, Perrakis A*. (2011) Automatic rebuilding and optimization of crystallographic structures in the Protein Data Bank. **Bioinformatics.** 2011 Dec 15;27(24):3392-8.
72. Kryshtafovych A, Moutl J, Bartual SG, Bazan JF, Berman H, Casteel DE, Christodoulou E, Everett JK, Hausmann J, Heidebrecht T, Hills T, Hui R, Hunt JF, Seetharaman J, Joachimiak A, Kennedy MA, Kim C, Lingel A, Michalska K, Montelione GT, Otero JM, Perrakis A, Pizarro JC, van Raaij MJ, Ramelot TA, Rousseau F, Tong L, Wernimont AK, Young J, Schwede T. (2011) Target highlights in CASP9: Experimental target structures for the critical assessment of techniques for protein structure prediction. **Proteins.** 79 Suppl 10:6-20
71. Read RJ, Adams PD, Arendall WB III, Brunger AT, Emsley P, Joosten RP, Kleywegt GJ, Krissinel EB, Lütke T, Otwinowski Z, Perrakis A, Richardson JS, Sheffler WH, Smith JL, Tickle IJ, Vriend G and Zwart PH. (2011) A new generation of crystallographic validation tools for the Protein Data Bank. **Structure** 19(10):1395-412.
70. Faesen A, Dirac AMG, Shanmugham A, Ovaa H, Perrakis A and Sixma TK. (2011) Auto-activation of USP7/HAUSP by its C-terminal ubiquitin-like domain (HUBL) is allosterically promoted by GMPS. **Molecular Cell** 44(1):147-59.
69. Albers HM, Hendrickx LJ, van Tol RJ, Hausmann J, Perrakis A, Ovaa H. Structure-Based Design of Novel Boronic Acid-Based Inhibitors of Autotaxin. (2011) **J Med Chem.** 14;54(13): 4619-26.
68. Pefani DE, Dimaki M, Spella M, Karantzelis N, Mitsiki E, Kyrousi C, Symeonidou IE, Perrakis A, Taraviras S, Lygerou Z. Idas, a novel phylogenetically conserved geminin-related protein, binds to geminin and is required for cell cycle progression. (2011) **J Biol Chem.**286(26): 23234-46.
67. Luna-Vargas MP, Christodoulou E, Alfieri A, van Dijk WJ, Stadnik M, Hibbert RG, Sahtoe DD, Clerici M, Marco VD, Littler D, Celie PH, Sixma TK, Perrakis A*. (2011) Enabling high-throughput ligation-independent cloning and protein expression for the family of ubiquitin specific proteases. **J Struct Biol.** 175(2):113-9
66. Heidebrecht T, Christodoulou E, Chalmers MJ, Jan S, Ter Riet B, Grover RK, Joosten RP, Littler D, van Luenen H, Griffin PR, Wentworth P Jr, Borst P, Perrakis A*. (2011) The structural basis for recognition of base J containing DNA by a novel DNA binding domain in JBP1. **Nucleic Acids Res.** 39(13):5715-28
65. Hausmann J, Kamtekar S, Christodoulou E, Day JE, Wu T, Fulkerson Z, Albers HMHG, van Meeteren LA, Houben A, van Zeijl L, Jansen S, Andries M, Hall T, Pegg LE, Benson TE, Kasiem M, Harlos K, Vander Kooi C, Smyth SS, Ovaa H, Bollen M, Morris AJ, Moolenaar WH & Perrakis A* (2011), Structural basis for substrate discrimination and integrin binding by autotaxin. **Nature Structural and Molecular Biology**, 18(2):198-204
64. Busso D, Peleg Y, Heidebrecht T, Romier C, Jacobovitch Y, Dantes A, Salim L, Troesch E, Schuetz A, Heinemann U, Folkers GE, Geerlof A, Wilmanns M, Polewacz A, Quedenau C, Büsow K, Adamson R, Blagova E, Walton J, Cartwright JL, Bird LE, Owens RJ, Berrow NS, Wilson KS, Sussman JL, Perrakis A, Celie PH. (2011) Expression of protein complexes using multiple Escherichia coli protein co-expression systems: A benchmarking study. **J Struct Biol.** 175(2):159-70
63. Monti MC, Cohen SX, Fish A, Winterwerp HH, Barendregt A, Friedhoff P, Perrakis A, Heck AJ, Sixma TK, van den Heuvel RH, Lebbink JH. (2011) Native mass spectrometry provides direct evidence for DNA mismatch-induced regulation of asymmetric nucleotide binding in mismatch repair protein MutS. **Nucleic Acids Res.** 39(18):8052-8064.
62. Hausmann J, Christodoulou E, Kasiem M, De Marco V, van Meeteren L, Moolenaar W, Axford D, Owen R, Evans G, and Perrakis A* (2010). Mammalian cell expression, purification, crystallization and microcrystal data collection of Autotaxin/ENPP2, a secreted mammalian glycoprotein. (2010) **Acta Crystallogr F.** 66(9):1130-5
61. Littler D, Alvarez-Fernández M, Stein A, Hibbert R, Heidebrecht T, Aloy P, Medema R, Perrakis A* (2010) Understanding DNA recognition by FoxM1 through structural studies and functional analysis. **Nucleic Acids Res** 38(13): 4527-38

60. Brooks M, Gewartowski K, Mitsiki E, L  toquart J, Pache RA, Billier Y, Bertero M, Corr  a M, Czarnocki-Cieciura M, Dadlez M, Henriot V, Lazar N, Delbos L, Lebert D, Piwowarski J, Rochaix P, B  ttcher B, Serrano L, S  raphin B, van Tilbeurgh H, Aloy P, Perrakis A*, Dziembowski A. (2010) Systematic bioinformatics and experimental validation of yeast complexes reduces the rate of attrition during structural investigations. **Structure**. 18(9): 1075-82.
59. Littler DR, Brown LJ, Breit SN, Perrakis A, Curmi PM. (2010) Structure of human CLIC3 at 2.0   resolution. **Proteins**. 78(6):1594-600.
58. De Marco V, Gillespie PJ, Li A, Karantzelis N, Christodoulou E, Klompmaker R, van Gerwen S, Fish A, Petoukhov MV, Iliou MS, Lygerou Z, Medema RH, Blow JJ, Svergun DI, Taraviras S, Perrakis A*. (2009) Quaternary structure of the human Cdt1-Geminin complex regulates DNA replication licensing. **Proc Natl Acad Sci U S A**. 106(47):19807-12.
57. Hilge M, Aelen J, Fource A, Perrakis A, Vuister GW. (2009) Ca²⁺ regulation in the Na⁺/Ca²⁺ exchanger features a dual electrostatic switch mechanism. **Proc Natl Acad Sci U S A**. 106(34):14333-8.
56. Rodenko B, Toebes M, Celie PH, Perrakis A, Schumacher TN, Ovaa H. (2009) Class I major histocompatibility complexes loaded by a periodate trigger. **J Am Chem Soc**. 131(34): 12305-135.
55. Celie PH, Toebes M, Rodenko B, Ovaa H, Perrakis A, Schumacher TN. (2009) UV-induced ligand exchange in MHC class I protein crystals. **J Am Chem Soc**. 131(34):12298-304
54. Mooij WT, Mitsiki E, Perrakis A. ProteinCCD: enabling the design of protein truncation constructs for expression and crystallization experiments. **Nucleic Acids Res**.;37(Web Server issue):W402-5.
53. Ulens C, Akdemir A, Jongejan A, van Elk R, Bertrand S, Perrakis A, Leurs R, Smit AB, Sixma TK, Bertrand D, de Esch IJ. (2009) Use of acetylcholine binding protein in the search for novel alpha7 nicotinic receptor ligands. In silico docking, pharmacological screening, and X-ray analysis. **J Med Chem**. ;52(8):2372-83.
52. Mooij WT, Cohen SX, Joosten K, Murshudov GN, Perrakis A. (2009) "Conditional Restraints": Restraining the Free Atoms in ARP/wARP. **Structure**.;17(2):183-9.
51. Repanas K, Fuentes G, Cohen SX, Bonvin AM, Perrakis A. (2009) Insights into the DNA cleavage mechanism of human LINE-1 retrotransposon endonuclease. **Proteins**. 74(4): 917-28
50. Langer G, Cohen SX, Lamzin V, Perrakis A. (2008) Crystallographic Model Building in ARP/wARP 7. **Nature Protocols**. 3(7):1171-9
49. Joosten K, Cohen SX, Emsley P, Mooij W, Lamzin VS, Perrakis A. (2008) A knowledge-driven approach for crystallographic protein model completion. **Acta Crystallogr D Biol Crystallogr**. 64(Pt 4):416-24.
48. van de Weerd BC, Littler DR, Klompmaker R, Huseinovic A, Fish A, Perrakis A, Medema RH. (2008) Polo-box domains confer target specificity to the Polo-like kinase family. **Biochim Biophys Acta**.
47. Kedde M, Strasser MJ, Boldajipour B, Vrielink JA, Slanchev K, le Sage C, Nagel R, Voorhoeve PM, van Duijse J,  rom UA, Lund AH, Perrakis A, Raz E, Agami R. (2008) RNA-binding protein Dnd1 inhibits microRNA access to target mRNA. **Cell**. 131(7):1273-86.
46. Cohen SX, Ben Jelloul M, Long F, Vagin A, Knipscheer P, Lebbink J, Sixma TK, Lamzin VS, Murshudov GN, Perrakis A. (2008) ARP/wARP and molecular replacement: the next generation. **Acta Crystallogr D Biol Crystallogr**. 64:49-60
45. Repanas K, Zingler N, Layer LE, Schumann GG, Perrakis A, Weichenrieder O. (2007) Determinants for DNA target structure selectivity of the human LINE-1 retrotransposon endonuclease. **Nucleic Acids Res**. 35(14):4914-26.
44. Yu Z, Genest PA, Riet BT, Sweeney K, Dipaolo C, Kieft R, Christodoulou E, Perrakis A, Simmons JM, Hausinger RP, van Luenen HG, Rigden DJ, Sabatini R, Borst P. (2007) The protein that binds to DNA base J in trypanosomatids has features of a thymidine hydroxylase. **Nucleic Acids Res**.
43. Evrard GX, Langer GG, Perrakis A, Lamzin VS. (2007) Assessment of automatic ligand building in ARP/wARP. **Acta Crystallogr D Biol Crystallogr**. 63, 108-17.

42. Buchwald G, van der Stoop P, Weichenrieder O, Perrakis A, van Lohuizen M, Sixma TK. (2006) Structure and E3-ligase activity of the Ring-Ring complex of polycomb proteins Bmi1 and Ring1b. **Embo J** 2006;25(11):2465-74.
41. Romier C, Ben Jelloul M, Albeck S, Buchwald G, Busso D, Celie PH, Christodoulou E, De Marco V, van Gerwen S, Knipscheer P, Lebbink JH, Notenboom V, Poterszman A, Rochel N, Cohen SX, Unger T, Sussman JL, Moras D, Sixma TK, Perrakis A. (2006) Co-expression of protein complexes in prokaryotic and eukaryotic hosts: experimental procedures, database tracking and case studies. **Acta Crystallogr D Biol Crystallogr.** 62, 1232-42.
40. Mamely I, van Vugt MA, Smits VA, Semple JI, Lemmens B, Perrakis A, Medema RH, Freire R. (2006) Polo-like Kinase-1 Controls Proteasome-Dependent Degradation of Claspins during Checkpoint Recovery. **Curr Biol.** 16(19), 1950-5.
39. Newman J, Egan D, Walter TS, Meged R, Berry I, Ben Jelloul M, Sussman JL, Stuart DI, Perrakis A. (2005) Towards rationalization of crystallization screening for small- to medium-sized academic laboratories: the PACT/JCSG+ strategy. **Acta Crystallogr D Biol Crystallogr.** 61, 1426-31.
38. Litjens SH, Wilhelmsen K, de Pereda JM, Perrakis A, Sonnenberg A. (2005) Modeling and experimental validation of the binary complex of the plectin actin binding domain and the first pair of FNIII domains of the $\beta 4$ integrin. **J Biol Chem.** 280 (23), 22270-7.
37. van Meeteren LA, Ruurs P, Christodoulou E, Goding JW, Takakusa H, Kikuchi K, Perrakis A, Nagano T, Moolenaar WH. (2005) Inhibition of Autotaxin by Lysophosphatidic Acid and Sphingosine 1-Phosphate. **J Biol Chem.** 280 (22), 21155-21161.
36. Potterton L, McNicholas S, Krissinel E, Gruber J, Cowtan K, Emsley P, Murshudov GN, Cohen S, Perrakis A, Noble M. (2004) Developments in the CCP4 molecular-graphics project. **Acta Crystallogr D Biol Crystallogr.** 60(12), 2288-94
35. Cohen SX, Morris RJ, Fernandez FJ, Ben Jelloul M, Kakaris M, Parthasarathy V, Lamzin VS, Kleywegt GJ, Perrakis A. (2004) Towards complete validated models in the next generation of ARP/wARP. **Acta Crystallogr D Biol Crystallogr.** 60(2), 2222-9
34. Weichenrieder O, Repanas K, Perrakis A. (2004) Crystal structure of the targeting endonuclease of the human LINE-1 retrotransposon. **Structure** 12(6), 975-86.
33. Morris RJ, Zwart PH, Cohen S, Fernandez FJ, Kakaris M, Kirillova O, Vornrhein C, Perrakis A, Lamzin VS. (2004) Breaking good resolutions with ARP/wARP. **J Synchrotron Radiat.** 11,56-9.
32. Natrajan G, Lamers MH, Enzlin JH, Winterwerp HH, Perrakis A, Sixma TK. (2003) Structures of Escherichia coli DNA mismatch repair enzyme MutS in complex with different mismatches: a common recognition mode for diverse substrates. **Nucleic Acids Res.** 31, 4814-21.
31. Xiao B, Spencer J, Clements A, Ali-Khan N, Mittnacht S, Broceno C, Burghammer M, Perrakis A, Marmorstein R, Gamblin SJ. (2003) Crystal structure of the retinoblastoma tumor suppressor protein bound to E2F and the molecular basis of its regulation. **Proc Natl Acad Sci U S A** 5. 2363-8.
30. Ruivenkamp CA, van Wezel T, Zanon C, Stassen AP, Vlcek C, Csikos T, Klous AM, Tripodis N, Perrakis A, Boerrigter L, Groot PC, Lindeman J, Mooi WJ, Meijjer GA, Scholten G, Dauwerse H, Paces V, van Zandwijk N, van Ommen GJ, Demant P. (2002) Ptpn11 is a candidate for the mouse colon-cancer susceptibility locus Scc1 and is frequently deleted in human cancers. **Nature Genet.** 31, 295-300.
29. Morris RJ., Perrakis A, Lamzin VS. (2002) ARP/wARP's model-building algorithms. I. The main chain. **Acta Crystallogr D Biol Crystallogr.** 58, 968-75.
28. Perrakis A*, Harkiolaki M, Wilson KS, Lamzin VS. (2001) ARP/wARP and molecular replacement. **Acta Crystallogr D Biol Crystallogr.** 57, 1445-50.
27. Hilge M, Perrakis A, Abrahams JP, Winterhalter K, Piontek K, Gloor SM. (2001) Structure elucidation of beta-mannanase: from the electron-density map to the DNA sequence. **Acta Crystallogr D Biol Crystallogr.** 57, 37-43.
26. Perrakis A, Lamers, M.H., Enzlin, J.H., Winterwerp, H.H.K., de Wind, N. and Sixma, T.K. - first two authors contributed equally, author order is swapped from printed publication - (2000) The crystal structure of DNA mismatch repair protein MutS binding to a G.T mismatch, **Nature** 407, 711-7.

25. Bracher A., Perrakis A, Dresbach T., Betz H., Weissenhorn W. (2000) The X-ray crystal structure of neuronal Sec1 from squid sheds new light on the role of this protein in exocytosis, **Structure Fold Des.**, **8**, 685-694.
24. Walsh MA, Otwinowski Z, Perrakis A, Anderson PM, Joachimiak A. (2000) Structure of cyanase reveals that a novel dimeric and decameric arrangement of subunits is required for formation of the enzyme active site, **Structure Fold Des.** **8**, 505-514.
23. Perrakis A*, Cypriani F, Castagna JC, Claustre L, Burghammer M, Riek C, and Cusack S. (1999) Protein microcrystals and the design of a microdiffractometer; current experience and plans at EMBL and ESRF/ID13, **Acta Crystallogr D Biol Crystallogr** **55**, 1765-1770.
22. Perrakis A*, Antoniadou-Vyzas E, Tsitsa P, Lamzin VS, Wilson KS and Hamodrakas SJ (1999) Molecular, crystal and solution structure of a β -cyclodextrin complex with ADM-10, a potential antimicrobial drug, **Carbohydrate Research** **317**, 19-28.
21. Perrakis A*, Morris RJ and Lamzin VS (1999) Automated protein model building combined with iterative structure refinement, **Nature Structural Biology** **6**, 458-463.
20. Valegard K, van Scheltiga A, Lloyd MD, Hara T, Ramaswamy S, Perrakis A, Thompson A, Lee HJ, Baldwin JE, Schofield CJ, Hajdu J and Anderssen I. (1998) Structure of a cephalosporin synthase. **Nature** **394**, 805-809.
19. Asselt van E, Perrakis A, Kalk KH, Lamzin VS, and Dijkstra B. (1998) Accelerated X-ray structure elucidation of a 36 kDa muramidase/transglycosylase using wARP. **Acta Crystallographica D54**, 58-73.
18. Perrakis A*, Sixma TK, Wilson KS and Lamzin VS (1997) wARP: improvement and extension of crystallographic phases by weighted averaging of multiple refined dummy atomic models, **Acta Crystallographica D53**, 448-455.
17. Pouderoyen van G, Ketting RF, Perrakis A, Plasterk RHA and Sixma TK (1997) Crystal structure of the specific DNA binding domain of Tc3 transposase of *C.elegans* in complex with transposon DNA, **EMBO journal** **16**, 6044-6054.
16. Tong H, Hateboer G, Perrakis A, Bernards R and Sixma TK (1997) Crystal structure of mammalian Ubc9 provides insight into the variability of the ubiquitin-conjugating system, **Journal of Biological Chemistry** **272**, 21381-21387.
16. Perrakis A, Ouzounis C and Wilson KS (1997) Evolution of immunoglobulin-like modules in chitinases: their structural flexibility and functional implications, **Folding and Design** **2**, 291-294.
14. Perrakis A, Tews I, Terwischa v. Scheltiga A, Wilson KS and Dijkstra B. - *first three authors contributed equally, author order is swapped from printed publication*- (1997) Substrate assisted catalysis unifies two families of chitinolytic enzymes, **Journal American Chemical Society** **119**, 7954-7959.
13. Agianian P, Perrakis A, Kanellopoulos P, Sheldrick B and Hamodrakas SJ (1997) Molecular and crystal structure of 4'-nitrophenyl- α -manopyranoside, **Acta Crystallographica C53**, 543-648.
12. Hamodrakas SJ, Perrakis A and Antoniadou-Vyzas E. (1997) A *de novo* Designed Possible 5-Lipoxygenase Inhibitor: -Acetoxy-*N*-[1-(1-tricyclo[3.3.1.1^{3,7}]dec-1-yl)ethyl]benzeneacetamide **Acta Crystallographica C52**, 677-679
11. Schonbrunn E, Sack S, Eschenburg S, Perrakis A, Krekel F, Amrhein N, and Mandelkow E (1996) Crystal structure of UDP-*N*-acetylglucosamine enolpyruvyltransferase, the target of the antibiotic fosfomycin, **Structure** **4**:10, 1065-1076.
10. Teplyakov A, Sebastiao P, Obmolova G, Perrakis A, Brush GS, Bessman MJ and Wilson KS. (1996) Crystal structure of bacteriophage T4 deoxy-nucleotide kinase with its substrates dGMP and ATP, **EMBO Journal** **15**:14, 3487-3497.
9. Kanellopoulos P, Pavlou K., Perrakis A, Agianian B, Vorgias CE, Mavrommatis C, Soufi M, Tucker P and Hamodrakas SJ (1996) The crystal structure of the complexes of Concanavalin A with 4'-nitrophenyl- β -D-manopyranoside and 4'-nitrophenyl- β -glucopyranoside, **Journal of Structural Biology** **116**, 345-355.
8. Tews I, Perrakis A, Oppenheim A, Dauter Z, Wilson KS and Vorgias CE (1996) A bacterial chitinase: Structure, mechanism and Tay-Sachs disease, **Nature Structural Biology** **3**, 638-648.
7. Hamodrakas S, Perrakis A and Antoniadou-Vyzas A. (1996) A *de novo* designed possible 5-

- lipoxygenase inhibitor, **Acta Crystallographica C52**, 677-679.
6. Perrakis A, Schneider T, Antoniadou-Vyzas E, Dauter Z and Hamodrakas SJ. (1996) Refinement of 2-amino-4-(tricyclo [3.3.1.1.3,7] decyl-1)-6-N-methyl-piperazino-1,3,5-triazine at three different temperatures using Image-Plate data. **Journal of Applied Crystallography** **29**, 261-264.
 5. Perrakis A, Constantinidis C, Athanasiadis A and Hamodrakas SJ (1995) PBM: A software package to create, display and manipulate interactively models of small molecules and proteins on IBM compatible PC's. **CABIOS** **11**, 141-145.
 4. Perrakis A, Tews I, Chet I, Oppenheim A, Dauter Z, Wilson KS and Vorgias CE. (1994) Crystal structure of a bacterial chitinase at 2.3 Å resolution. **Structure** **2**, 12, 1169-1180.
 3. Rypniewski WR, Perrakis A, Vorgias CE and Wilson KS. (1994). Evolutionary divergence and conservation of trypsin. **Protein Engineering** **7**, 57-64.
 2. Piperaki S, Perrakis A and Parissi-Poulou M. (1994) Liquid chromatography retention behaviour and separation of promethazine and isopromethazine on a β-cyclodextrin bonded-phase column. **Journal of Chromatography A** **660**, 339-350.
 1. Perrakis A, Hempel A, Camerman N and Hamodrakas SJ. (1993) Crystal structure of 2-amino-4-(tricyclo[3.3.1.1.3,7]decyl-1-methyl)-6-dimethyl-amino-1,3,5-triazine. **Journal of Crystallographic and Spectroscopic research** **23**, 821-824.

-Reviews

- I. Celie, P.H.N., Parret, A.H.A., Perrakis, A*. Recombinant cloning strategies for protein expression (2016) Current Opinion in Structural Biology, 38, pp. 145-154. Cited 3 times.
- II. Perrakis, A, and W H Moolenaar. (2014). "Autotaxin: Structure-Function and Signaling." **The Journal of Lipid Research** **55** (6) (May 28): 1010-1018. doi:10.1194/jlr.R046391.
- III. Hausmann J, Perrakis A, Moolenaar WH. (2012) Structure-function relationships of autotaxin, a secreted lysophospholipase D. **Adv Biol Regul.** 2012 Sep 28.
- IV. Moolenaar W and Perrakis A, (2011) Insights into Autotaxin: how to produce and present a lipid growth factor. **Nature Reviews in Molecular Cell Biology**, 12(10), 674-9
- V. von Castelmur E and Perrakis A*, (2011) Book Review for "Crystals, x-rays and proteins: comprehensive protein crystallography", by Dennis Sherwood and Jon Cooper, Oxford, Oxford University Press; Crystallography Reviews
- VI. Perrakis A, Romier C. (2008) Assembly of protein complexes by co-expression in prokaryotic and eukaryotic hosts Structural Proteomics. High-Throughput Methods. Series: **Methods Mol Biol**, 426:247-56
- VII. Albeck S, Alzari P, Andreini C, Banci L, Berry IM, Bertini I, Cambillau C, Canard B, Carter L, Cohen SX, Diprose JM, Dym O, Esnouf RM, Felder C, Ferron F, Guillemot F, Hamer R, Ben Jelloul M, Laskowski RA, Laurent T, Longhi S, Lopez R, Luchinat C, Malet H, Mochel T, Morris RJ, Moulinier L, Oinn T, Pajon A, Peleg Y, Perrakis A, Poch O, Prilusky J, Rachedi A, Ripp R, Rosato A, Silman I, Stuart DI, Sussman JL, Thierry JC, Thompson JD, Thornton JM, Unger T, Vaughan B, Vranken W, Watson JD, Whamond G, Henrick K. (2006) SPINE bioinformatics and data-management aspects of high-throughput structural biology. **Acta Crystallogr D Biol Crystallogr** 62(Pt 10):1184-95.
- VIII. Alzari PM, Berglund H, Berrow NS, Blagova E, Busso D, Cambillau C, Campanacci V, Christodoulou E, Eiler S, Fogg MJ, Folkers G, Geerlof A, Hart D, Haouz A, Herman MD, Macieira S, Nordlund P, Perrakis A, Quevillon-Cheruel S, Tarandeu F, van Tilbeurgh H, Unger T, Luna-Vargas MP, Velarde M, Willmanns M, Owens RJ. (2006) Implementation of semi-automated cloning and prokaryotic expression screening: the impact of SPINE. **Acta Crystallogr D Biol Crystallogr** 62(Pt 10):1103-13.
- IX. Aricescu AR, Assenberg R, Bill RM, Busso D, Chang VT, Davis SJ, Dubrovsky A, Gustafsson L, Hedfalk K, Heinemann U, Jones IM, Ksiazek D, Lang C, Maskos K, Messerschmidt A, Macieira S, Peleg Y, Perrakis A, Poterszman A, Schneider G, Sixma TK, Sussman JL, Sutton G, Tarboureich N, Zeev-Ben-Mordehai T, Jones EY. (2006) Eukaryotic expression: developments for structural proteomics. **Acta Crystallogr D Biol Crystallogr** 62(Pt 10):1114-24.
- X. Bahar M, Ballard C, Cohen SX, Cowtan KD, Dodson EJ, Emsley P, Esnouf RM, Keegan R, Lamzin V, Langer G, Levnikov V, Long F, Meier C, Muller A, Murshudov GN, Perrakis A, Siebold C, Stein

- N, Turkenburg MG, Vagin AA, Winn M, Winter G, Wilson KS. (2006) SPINE workshop on automated X-ray analysis: a progress report. **Acta Crystallogr D Biol Crystallogr** 62(Pt 10): 1170-83.
- XI. Banci L, Bertini I, Cusack S, de Jong RN, Heinemann U, Jones EY, Kozielski F, Maskos K, Messerschmidt A, Owens R, Perrakis A, Poterszman A, Schneider G, Siebold C, Silman I, Sixma T, Stewart-Jones G, Sussman JL, Thierry JC, Moras D. (2006) First steps towards effective methods in exploiting high-throughput technologies for the determination of human protein structures of high biomedical value. **Acta Crystallogr D Biol Crystallogr** 62(Pt 10):1208-17.
- XII. Berry IM, Dym O, Esnouf RM, Harlos K, Meged R, Perrakis A, Sussman JL, Walter TS, Wilson J, Messerschmidt A. (2006) SPINE high-throughput crystallization, crystal imaging and recognition techniques: current state, performance analysis, new technologies and future aspects. **Acta Crystallogr D Biol Crystallogr** 62(Pt 10):1137-49.
- XIII. Lamzin, V and Perrakis, A. Current state of automated crystallographic data analysis (2000) **Nature Structural Biology** 7, 978-81.
- XIV. Cusack, S, Belrhali, H, Bram, A, Burghammer, M, Perrakis, A, and Riek, C. (1998) Small is beautiful: protein micro-crystallography. **Nature Structural Biology, Synchrotron Supplement**, 5, 634-637

-Books, or contributions to books

- A. van Beusekom B, Perrakis A, Joosten RP. Data Mining of Macromolecular Structures. (2016) *Methods Mol Biol*. 2016;1415:107-38. doi: 10.1007/978-1-4939-3572-7_6.
- B. Caillat C and Perrakis A*. (2012) Cdt1 and Geminin in DNA Replication Initiation. In *THE EUKARYOTIC REPLISOME: A GUIDE TO PROTEIN STRUCTURE AND FUNCTION*, Subcell Biochem. 2012;62:71-87.
- C. Perrakis A*, Musacchio A, Cusack S, Petosa C. (2011) Investigating a macromolecular complex: The toolkit of methods. *J Struct Biol*. 175(2):106-12
- D. Hilge M, Aelen J, Perrakis A, Vuister GW. (2007) Structural basis for Ca²⁺ regulation in the Na⁺/Ca²⁺ exchanger. *Ann N Y Acad Sci*. 2007 Mar;1099:7-15. Epub 2007 Mar 8.
- E. Morris RJ, Perrakis A, Lamzin VS. (2003) ARP/wARP and automatic interpretation of protein electron density maps *Methods Enzymol*. 374, 229-44
- F. Lamzin, V.S., Perrakis, A and Wilson K.S. The ARP/wARP suite for automated construction and refinement of protein models. *International Tables for Crystallography Vol. IV, Macromolecular Crystallography*
- G. Perrakis, A*, Sixma, T.K., Wilson K.S. and Lamzin, V.S. (1997) The world according to wARP In *Recent advances in phasing*. Proceedings of the CCP4 Study Weekend, SERC Daresbury Laboratory, Daresbury, Warrington, England, pp 87-91.
- H. Vorgias, C.E., Perrakis, A and Tews, I. (1996) Structure-function studies of the chitinolytic enzymes of *Serratia marcescens* chitinase and chitobiase, *Annals of the New York Academy of Sciences* 799, 190-192.
- I. Perrakis, A, Tews, I., Wilson, K.S. and Vorgias, C.E. (1996) Family 18 chitinases: Faraway so close. In *Chitin Enzymology 2*. (R.A.A. Muzzarelli, ed.) , pp 357-369, European Chitin Society, Italy.
- J. Perrakis, A, Ouzounis, C., Wilson, K.S. and Vorgias, C. (1996) Implications of the tertiary structure determination of chitinase A. Similarities with Fibronectin III domains, oviductal proteins and narbonin. In *Advances in Chitin Science*, (Domard, A., Jeuniaux, C., Muzzarelli, R. and Roberts, G. eds.), pp 34-41, Brest, France.
- K. Perrakis, A, Tews, I., Dauter, Z., Wilson, K.S. and Vorgias C.E. (1994) X-ray structure analysis of chitinase A from *Serratia marcescens* In *Chitin World*. (Karnicki, Z.S., Wojtasz-Pajak, A., Brzeski, M.M. and Bykowski, P.J., ed.), pp 408-415, Gdynia, Poland.
- L. Vorgias, C.E., Tews, I., Perrakis, A, Wilson, K.S. and Oppenheim, A. (1993) Purification and characterisation of the recombinant chitin degrading enzymes, Chitinase A and Chitobiase from *Serratia marcescens*. In *Chitin Enzymology* (R.A.A. Muzzarelli, ed.) , pp 417-422, European Chitin Society, Italy.
- M. Perrakis, A, Wilson, K.S., Chet, I., Oppenheim, A. and Vorgias, C.E. (1993) Phylogenetic relationships of chitinases. In *Chitin Enzymology* (R.A.A. Muzzarelli, ed.) , pp 217-232,

European Chitin Society, Italy.

- Commentaries and editorials

- a. iNEXT Consortium. iNEXT: a European facility network to stimulate translational structural biology. FEBS Lett. 2018 May 15. doi: 10.1002/1873-3468.13062. [Epub ahead of print]
- b. Meijers, R., Perrakis, A. (2016) Editorial overview: New constructs and expression of proteins (2016) Current Opinion in Structural Biology, 38, pp. v-vi.
- c. Joosten RP, Soueidan H, Wessels LF, Perrakis A. (2013) Timely deposition of macromolecular structures is necessary for peer review. **Acta Crystallogr D Biol Crystallogr.** 2013;69(Pt 12):2293-5. Epub 2013/12/07.
- d. Perrakis A, Daenke S, Stuart DI, Sussman JL. (2011) From SPINE to SPINE-2 complexes and beyond. **J Struct Biol.** 175(2):105.
- e. Haramis AP, Perrakis A. (2006) Selectivity and promiscuity in Eph receptors. **Structure.** 14, 169-71.
- f. Lamzin, V.S., Perrakis, A., Bricogne, G., Jiang, J., Swaminathan, S. and Sussman, J.L. (2000) Apotheosis, not apocalypse: methods in protein crystallography, **Acta Crystallogr D Biol Crystallogr.** 56, 1510-1