

Gaetano T. Montelione, Ph.D.

Jerome and Lorraine Aresty Chair and Distinguished Professor
 Center for Advanced Biotechnology and Medicine
 Department of Molecular Biology and Biochemistry
 Rutgers, The State University of New Jersey

EDUCATION

- 1974-1976 Marine Biology
 Southampton College, Long Island University, Southampton NY
- 1977-1990 **B.S.**, Biochemistry, with Highest Honors
 Cornell University, Ithaca NY
- 1980-1981 Physical Chemistry
 University of Oregon, Eugene OR
- 1981-1983 **M.A.**, Physical Chemistry
 Cornell University, Ithaca, NY
- 1983-1987 **Ph.D.**, Physical Chemistry
 Cornell University, Ithaca NY
 with studies at ETH Zurich Switzerland
 Physical Chemistry
 Advisor: Prof. Harold A. Scheraga, Co-Advisor: Prof. Kurt Wüthrich

POSTGRADUATE TRAINING

- 1987-1989 **Ph.D.**, Postdoctoral Appointment, Molecular Biophysics
 University of Michigan, Ann Arbor, MI
 Advisor: Prof. Gerhard Wagner

ACADEMIC APPOINTMENTS

- 1988 – 1989 Research Assistant Professor, University of Michigan
- 1989 – present Resident Faculty, Center for Advanced Biotechnology and Medicine
- 1989 Assistant Professor, Rutgers University
- 1995 Associate Professor, Rutgers University
- 1997 Visiting Professor, Department of Physical Chemistry, University of Valencia, Spain
- 1998 – 2005 Professor, Rutgers University
- 2000 – present Member, Rutgers Cancer Institute of New Jersey
- 2000 – 2016 Director, Northeast Structural Genomics Consortium, NIH NIGMS Protein Structure Initiative
- 2001 – present Adjunct Professor, Department of Biochemistry, Robert Wood Johnson Medical School
- 2005 – present Distinguished Professor, Rutgers University
- 2010 – present Jerome and Lorraine Aresty Chair, Rutgers University
- 2007 – present Foreign Expert and Visiting Professor, Jiangan University, Wuxi, Peoples Republic of China

CONSULTING

- 1990 – 1997 Consultant, Pharmacia, A.B., Stockholm, Sweden
- 1990 – 1999 Consultant, Chiron Corp., Emeryville, CA
- 1993 Visiting Scientist, Pharmacia, A.B., Stockholm, Sweden
- 1993 – 1999 Consultant, Wyeth-Ayerst Research Laboratories, Princeton, NJ
- 1995 – 2003 Consultant, Novartis Pharmaceutical Corp., East Hanover, NJ
- 1996 – 1999 Consultant, Eli Lilly and Co., Indianapolis, IN
- 2000 – 2002 Scientific Advisory Board and Consultant, GeneFormatics, San Diego, CA
- 2006 – 2008 Scientific Advisory Board and Consultant, Influmedics, Philadelphia, PA

2007 – present Scientific Advisory Board, Founder, and Consultant, Nexomics Biosciences,
North Brunswick, NJ

MEMBERSHIPS and OFFICES IN PROFESSIONAL SOCIETIES

1992 – 1998 Treasurer, Experimental NMR Conference (ENC)
1995 – present Member, American Association for the Advancement of Science (AAAS)
2000 – present Member, Biophysical Society
2000 – present Member, American Chemical Society
2006 – present Member, International Structural Genomics Organization
2006 – 2014 Treasurer, International Structural Genomics Organization

HONORS AND AWARDS

1981 – 1984 National Science Foundation Graduate Fellowship, National Science Foundation,
1981 – 1982 Sage Graduate Research Fellowship, Cornell University, Ithaca NY,
1987 Outstanding Chemistry Graduate Student, Cornell University, Ithaca NY,
1988 – 1989 Damon Runyon-Walter Winchell Cancer Research Fund Postdoctoral Fellowship
1989 Searle Scholar Award Searle Scholars Program,
1990 Johnson & Johnson Research Discovery Award, Johnson & Johnson, New Brunswick NJ,
1992, 1994 American Cyanamid Award in Physical and Analytical Chemistry, American Cyanamid
Company, Wayne NJ,
1993 – 1998 National Science Foundation Young Investigator Award, National Science Foundation,
1994 – 1997 Proctor and Gamble Young Investigator Award, The Proctor & Gamble Fund
1995 – 1997 Camille and Henry Dreyfus Teacher-Scholar Award
1995 Rutgers University Board of Trustees Award for Research and Scholarly Excellence
1999 Michael and Kate Bárány Young Investigator Award Biophysical Society
2006 Elected Fellow, American Association for the Advancement of Science
2010 – present Jerome and Lorraine Aresty Endowed Chair
2014 Rutgers Football Award for Academic Excellence

SCIENTIFIC ADVISORY BOARDS / DIRECTOR POSITIONS

2007 – 2016 Nexomics Bioscience Inc. – Sole Director, Board of Directors
2016 – present Nexomics Biosciences Inc. – Chair, Scientific Advisory Board
2014 – 2016 New York Protein Biologics – Board of Directors

SERVICE ON NATIONAL GRANT REVIEW PANELS, STUDY SECTIONS, COMMITTEES

International Grant Reviews

1990 Swedish Research Council for Engineering
2015 START Programme of the Austrian Science Fund (FWF)
2017 Swiss National Science Foundation
2017 Japan Society for the Promotion of Science

National Grant Review Panels

1990 – 2005 NIH Research Resources Program, Ad Hoc
1990 – 2005 NIH, National Cancer Institute, Ad Hoc
1990 The Arthritis Foundation,
1995 – 1999 National Science Foundation Molecular Biophysics Study Section Panel
1997 – present National Science Foundation Ad Hoc Grant Reviews,
2005 NIH Special Study Section: NIGMS Postdoctoral Fellowship Program
2005 NIH Special Study Section: NIGMS Membrane Protein Structure Initiative,
2010 National Science Foundation Committee of Visitors – Molecular and Cellular Biology,
2011 – 2015 National Science Foundation Advisory Committee for the Biological Sciences Directorate,

2013	National Science Foundation Committee of Visitors – Plant Genomics
2014	National Science Foundation Committee of Visitors – Molecular and Cellular Biology
2017	NIH, National Cancer Institute, Macromolecular Crystallography and Structural Biophysics Intramural Review Committee, NCI Fredrick Maryland Site.
2018	NIH Special Emphasis Panel/Scientific Review Group 2018/05 ZRG1 BCMB-D

SERVICE ON MAJOR COMMITTEES

International

2003 – 2016	Advisory Board, International Structural Genomics Organization (ISGO)
2006 – present	NMR Advisory Committee, Worldwide Protein Data Bank (wwPDB)
2007 – 2010	Advisory Committee, International BioMagResDataBase (BioMagResDB)
2007 – 2016	Advisory Committee, European E-NMR International Computational Grid Project
2011 – present	co-Chair, wwPDB Task Force on NMR Structure Validation

National

1999 – 2003	Advisory Committee, National Magnetic Resonance Facility Madison WI (NMRFAM)
2017 -present	Scientific Advisory Board, Seattle Structural Genomics Center for Infectious Disease (SSGCID) and Midwest Center for Structural Genomics of Infectious Diseases (CSGID)

Rutgers University and Rutgers Robert Wood Johnson Medical School

2005 – 2012	Director, Cancer Institute of New Jersey Protein Structural Analysis and Modeling Facility
2006 – 2008	Executive Committee, Rutgers University Proteomics Building Planning Committee
2014 – present	Rutgers University Committee on Academic Promotions and Tenure (AP&T) – Distinguished Professor Rank
2014 – present	Member, Rutgers University Presidential Advisory Committee on Academic Planning and Review (CAPR)
2017 – present	Member, CABM Executive Director Faculty Search Committee

Rutgers Graduate School Committees

1998 – 2000	Co-Director, Rutgers Computational Molecular Biology Program
1995 – 2000	Member, NIH Biotechnology Training Program Executive Committee

Departmental Committees

2000 – present	Center for Advanced Biotechnology and Medicine Computer Committee
2016 – present	Center for Advanced Biotechnology and Medicine Peer Evaluation Committee

Editorial Boards of Scientific Journals

2000 – 2007	Editor, <i>J. Structural and Functional Genomics</i>
2007 – 2016	Associate Editor, <i>J. Structural and Functional Genomics</i>
2000 – 2007	Associate Editor, <i>PROTEINS: Structure, Functional, Genetics</i>
2007 – present	Editorial Board Member, <i>PROTEINS: Structure, Functional, Genetics</i>
2001 - present	Associate Editor, <i>Faculty of 1000</i> , Sections of Structural Genomics

Reviewer for Scientific Journal Articles

Science, Nature, Proceedings of the National Academy of Science USA, Nature Methods, Nature Communications, Nature Structural Molecular Biology, Structure (Cell Journal), Angewandte Chemie International Edition, Biochemistry, FEBS Letters, Journal of American Chemical Society, Journal of Biological Chemistry, Journal of Biomolecular NMR, Journal of Magnetic Resonance, Journal of Molecular Biology, Protein Science, PROTEINS: Structure, Function, Bioinformatics, J. Structural and Functional Genomics

Service to the General Scientific Community

1998 – 2003	Director, New Jersey Commission on Science and Technology Initiative in Structural Genomics and Bioinformatics
2011 – present.	Advisor, New Jersey American Chemical Society (NJACS) NMR Topical Group and Annual Symposium

2013 – present Director, Rutgers University – Jiangnan University Summer Biotechnology Training Program,

SPONSORSHIP (Primary Mentorship) OF CANDIDATES FOR POSTGRADUATE DEGREE

Yuchin Li (Ph.D.) 1989 – 1994
 Clelia Biamonte (Ph.D.) 1990 – 1996
 Franklin Moy (Ph.D.) 1990 – 1993 Co-advisor w/ H.A. Scheraga, Cornell University
 Sakurako Shimotakahara 1994 – 1996 Co-advisor w/ H. A. Scheraga, Cornell University
 Wenqing (Wendy) Feng (Ph.D.) 1993 – 1997
 David Yorio, (M.S.) 1997 – 1998
 Subir Kumedan (M.S.) 1997 – 1999
 Chen-ya Chen (Ph.D.) 1994 – 1999
 Ying Xiong (M.S.) 1997 – 2000
 Yuanpeng (Janet) Huang (Ph.D.) 1997 - 2001
 Elisabet Wahlberg (M.S.) 1999 – 2001
 Deyou Zheng (Ph.D.), 1999 – 2003
 Michael Baran (Ph.D.) 2000 – 2005
 Gregory Kornhaber (Ph.D.) 2000 – 2005
 Cuifeng Yin (Ph.D.) 2000 – 2005
 Aneerban Bhattacharya (Ph.D.), 2000 – 2006
 David Snyder (Ph.D.) 2000 – 2006
 John Everett (Ph.D.) 2000 – 2006
 Asli Ertekin (Ph.D.) 2005 – 2011
 Binchen Mao (Ph.D.) 2006 – 2013
 Patrick Nosker 2012 – 2016 Co-advisor w/ V. Nanda, Rutgers University
 Yisha Yao (M.S.) – 2014 - 2017
 Ryan Woltz (Ph.D.) 2014 – present

SPONSORSHIP (Primary Mentorship) OF POSTDOCTORAL FELLOWS

Dr. Barbara A. Lyons 1990 – 1993
 Dr. Donald Emerson 1991 – 1993
 Dr. Keith Newkirk 1992 – 1994
 Dr. Mitsuru Tashiro 1992 – 1996
 Dr. Carlos Rios 1993 – 1997
 Dr. Zhigang Shang 1993 – 1997
 Dr. Diane Zimmerman 1994 – 1998
 Dr. Sakurako Shimotakahara 1997
 Dr. Michael Andrec 1997 – 1999
 Dr. Kristin Gunsalus 1997 – 2000
 Dr. Parag Sahasrabudhe 1997 – 2000
 Dr. Bonnie Dixon 1998 – 2000
 Dr. Daniel Monleon 1999 – 2002
 Dr. Hunter Moseley 1998 – 2002
 Dr. Dehua Hang 2006 - 2007
 Dr. Yuefeng Tang 2006 – 2014
 Dr. Rajeswari Mani 2007 – 2010
 Dr. Fei Xu 2013 - 2014
 Dr. Fei Song 2013 – 2016

TEACHING

The Montelione Laboratory has trained more than 100 Rutgers undergraduate students in independent research projects. For a complete list see: <http://www-nmr.cabm.rutgers.edu/>

Undergraduate Courses (hours indicated for the current year unless otherwise noted)

MBB 407 Molecular Biology and Biochemistry (20 contact hrs). 1995-2003

MBB 412 Proteomics and Functional Genomics (25 contact hrs). 2004 – present

Byrne Seminar Astrobiology, Can Life Evolve on Other Planets (15 contact hours). 2012-present

Graduate Courses

Rutgers University Bootcamp in Molecular Biophysics (6 contact hours). 2014, 2015

16:695:539 Experimental Methods in Molecular Biosciences (4 contact hours). 2015

Research Training (other than Primary Mentorship)

David Pantoja, 2000 – 2001. Visiting Ph.D. candidate from Madrid, Spain

Sriram Aiyer, 2010 – 2014. Co-advisor with M. Roth, Biochemistry, Rutgers Robert Wood Johnson Medical School.

Anastasia Chernyatina. 2014. Visiting postdoc from Brussels Belgium.

GRANT SUPPORT

Prof. Montelione has brought more than \$120 million in federal funding to Rutgers University and subcontract institutes 1990 - 2018.

Active Grant Funding

As Principal Investigator

1. *Rutgers Biomedical Health Sciences Program. "Targeting Protein Complexes Mediating DNA Repair with Computationally Designed Peptides". 06/01/14 – 12/31/17. \$40,000 total award (shared with 5 co-investigators)*
2. *NIH R01-GM120574. "Membrane Protein Structure Using Evolutionary Couplings and Sparse NMR Data." G.T. Montelione, PI (w co-investigators/ M. Inouye, C. Sander, D. Marks). 09/01/17 – 6/30/21. \$2,022,000 total*
3. *Rutgers Cancer Institute of New Jersey and National Institute of Cancer Research Precision Medicine Award. "Targeted Proteomics of Clinically Relevant Mutations Driving Human Cancers" J. Drake and G.T. Montelione, coPIs. 10/01/17 – 9/30/18. \$60,000 total award.*

As Co-Investigator

1. *NIH-NIGMS. "Interactions of MuLV IN with Host Proteins and DNA". 05/01/16 – 04/30/18. M. Roth. PI. (Montelione Lab share of total support: \$183,125).*
2. *NIH-NIGMS. "Targeting retroviral and virus-like particles for gene and protein delivery". 09/30/17 – 08/31/22. M. Roth. PI. (Montelione Lab share of total support: \$420,609).*
3. *NASA Astrobiology Institute. "ENIGMA: Evolution of Nanomachines In Geospheres and Microbial Ancestors". P. Falkowski, PI (multiple coPIs including G.T. Montelione).*

Completed Grant Funding

As Principal Investigator

1. *NIH NIAID "A Novel RNA Recognition Site on the Influenza B Virus NS1 Protein" (R21 AI117510) 01/01/15 – 12/31/17. G.T. Montelione, PI. \$534,312 total costs.*
2. *Rutgers University Office of Global Advancement and International Affairs. "International Collaborative Research Project in Protein Dynamics and Industrial Enzyme Engineering". G.T. Montelione, PI. 03/1/16 – 12/31/16. \$8,000 total award.*
3. *Rutgers University China Office. "CABM Summer Training Program with Jiangnan University, Wuxi, China. 4/1/15 – 3/31/16. G.T. Montelione, PI. \$6,000 total award.*
4. *NIH NIGMS Center for High-Throughput Structure Determination "PSI:Biology - Structural Genomics of Eukaryotic Domain Families" (U54 GM094597) 09/01/10 – 06/30/16 G.T. Montelione, PI. ~38,000,000 total costs (shared with 8 Consortium institutions)*
5. *NIH ORIP "600 MHz NMR RF Console with ¹⁹F NMR Probe" (S10 OD018207) 04/01/2014 - 03/31/2015. \$439,792 G.T. Montelione, PI; M. Roth, Co-PI; V. Nanda, Co-PI*

6. National Science Foundation BRAIN EAGER "The Molecular Interactome of Synaptogenesis" (MCB 1450895) 09/01/14 – 08/31/16. G.T. Montelione and D. Comeletti, coPIs. \$43,387 annual direct (Montelione portion)
7. NIH-NIGMS "Instrumentation for Protein Production and Structural Genomics." Supplement to P50 GM62413. 9/02 – 1/03. G.T. Montelione, PI. Direct costs: \$1,500,000 over 1 year.
8. CINJ "CINJ Protein Production and Structural Genomics Project" 02/01/04 – 01/31/06. G.T. Montelione, PI. \$70,000 annual direct cost
9. NIH-NIGMS "Structural Genomics of Eukaryotic Model Organisms (U54-GM074958) 07/01/05 – 06/30/10. G.T. Montelione, PI. \$51,000,000 total cost (shared with 9 Consortium institutions).
10. NIH-NIGMS "Structural Genomics of Eukaryotic Model Organisms" (P50-GM62413) 09/30/00 – 8/31/05 \$31,800,000 total cost (shared with 8 Consortium institutions)
11. Merck Research Foundation. "Structure-based Functional Genomics of Strongly-Conserved Microbial Gene Families. 9/98 - 9/00. Direct costs: \$306,000 over two years.
12. NIH Center for Research Resources "Acquisition of 800 MHz NMR System with Cryogenic Probe" (S10 RR019928) 07/01/04 – 06/30/06 \$760,000 direct cost.
13. NIH "Structures of RNA-binding Proteins from Influenza Virus". (R01-GM-47014). 4/97 - 4/02. Direct costs: ~ \$712,440 over 5 years.
14. Geneformatics Inc. "Improved Methods for Automated Analysis of Protein Structure from NMR Data." 01/01 – 12/02. Direct costs: \$400,000 total direct cost.
15. Camille and Henry Dreyfus Teacher Scholar Award. 5/95 - 5/00. Direct costs: \$55,000 over five years.
16. Hoffmann-LaRoche, Inc., Nutley, NJ. "Development of NMR as a Tool for Structural Bioinformatics". 1/97 - 12/97. Direct costs: \$30,000 over 1 year.
17. AGENE Research Institute Co., Ltd., Kanagawa, JAPAN. "Solution Structures of Genes Identified by Positional Cloning Methods". 1/97 - 12/99. Direct costs: \$100,000 over three years.
18. NIH "Biophysics of Serine Protease-Kunitz Inhibitor Complexes". (R01-GM-50733). 2/97 - 2/02. Direct costs: ~ \$982,167 over 5 years. (G.T. Montelione, S. Anderson).
19. NIH Postdoctoral Grant. "Analysis of Protein NMR Spectra Using Artificial Intelligence." 9/94 - 8/97. Direct costs: \$90,000 over 3 years. (NIH Postdoctoral Grant with Dr. D. Zimmerman).
20. Wyeth Ayerst Pharmaceutical Company. "Improved Software for NMR Analysis". 7/97 - 7/99. Direct costs: \$75,000 over two years.
21. NSF Young Investigator Award. (MCB-9357526). 8/93 - 7/98. Direct costs: \$500,000 over 5 years (including industrial matching funds from Chiron Corp., Proctor & Gamble Co., Schering-Plough, Inc. and Novartis Pharmaceutical Corp.).
22. NSF "Improved Technologies for Protein Structure Determination by NMR." (DIR-9019313 / MCB-9407569). 7/91-7/98. Direct costs: \$463,000 over 6 years.
23. NIH "Improved Technologies for Protein Structure Determination by NMR." (R01-GM-47014). 1992-1997.

As Co-Investigator

1. NSF BRAIN EAGER "The Molecular Interactome of Synaptogenesis" (MCB 1450895) 09/01/14 – 08/31/16 \$43,387 (Montelione portion) (Montelione & Comoletti, coPIs)
2. NIH/NIGMS "Structural Basis of Protein Homeostasis" (U01 GM098254-03) 09/30/12 – 07/31/15 \$100,000 annual direct (Montelione portion).
3. NIH/NIDCD "Human Transcription Factor Immunogens: Generation of a Complete Set" 09/23/10 – 08/31/15 ~\$350,000 total costs (G. Montelione share) (Anderson, PI; Montelione co-PI).
4. NIH Training Program: New Interdisciplinary Workforce "Training for Integrative Proteomics Technologies" (RFA-RM-04-015) 09/30/04 – 09/29/05 \$2,967,942 total cost for 5 years (Levy, Montelione, Berman, Rutgers/RWJMS)
5. NJCST R&D Excellence Program "An Initiative in Structural Bioinformatics -- Connecting Gene Sequence to Function by 3D Structure Determination: A New Paradigm for Drug Discovery". 10/97 – 9/02 Direct costs: \$3,00,000 over one year. (G. Montelione, S. Anderson, E. Arnold, C. Kulikowski, P. Lobel, S. Stein, A. Stock).
6. New Jersey State Higher Education Leasing Fund - Jointly funded by Rutgers University and UMDNJ.

- "Purchase of 600 MHz NMR and Upgrade of Existing NMR Facilities". 1993 Direct costs: \$985,000. (G. Montelione and J. Baum).
7. NSF "Acquisition of a 600 MHz NMR Spectrometer and Upgrade of Existing NMR Facilities at Rutgers University and at the University of Medicine and Dentistry of New Jersey". 09/94 Direct costs: \$571,000. (J. Baum, G. Montelione, S. Anderson, and R. Jones).
 8. NIH NIRR "Purchase of 600 MHz NMR and Upgrade of Existing NMR Facilities". 09/95 Direct costs: \$400,000. (G. Montelione and J. Baum).
 9. WM Keck Foundation "Establishment of the W.M. Keck Laboratory for Computational Chemistry and Molecular Graphics." 07/94 Direct costs: \$500,000. (E. Arnold, G. Montelione, and A. Stock).

PUBLICATIONS

Montelione has published more than 350 peer-reviewed scientific articles and book chapters, and has contribute more than 1,100 protein structure to the Protein Data Bank. His Google H-index is 71 as of June 7, 2018. see <https://scholar.google.com/citations?user=mrtpF44AAAAAJ&hl=en> and <http://www-nmr.cabm.rutgers.edu/publications/index.htm>

Protein Structures Deposited in the Protein Data Bank (PDB).

Montelione is co-author of more than 1,130 PDB depositions, including more than 470 structures determined by NMR spectroscopy methods.

Refereed Original Articles in Scientific Journals

1. **Montelione, G.T.**, Callahan, S., and Podleski, T.R. Physical and chemical characterization of the major lactose-blockable lectin activity from fetal calf skeletal muscle. **Biochim. Biophys. Acta** 1981, 670: 110 - 123.
2. Stimson, E.R., **Montelione, G.T.**, Meinwald, Y.C., Rudolph, R.K. and Scheraga, H.A.; Equilibrium ratios of cis- and trans-proline conformers in fragments of ribonuclease A from nuclear magnetic resonance spectra of adjacent tyrosine ring resonances; **Biochemistry**, 21: 5252-5262, 1982.
3. **Montelione, G.T.**, Arnold, E., Meinwald, Y.C., Stimson, E.R., Denton, J.B., Huang, S.G., Clardy, J. and Scheraga, H.A.; Chain-folding initiation structures in ribonuclease-A: Conformational analysis of trans-Ac-Asn-Pro-Tyr-NHMe and trans-Ac-Tyr-Pro-Asn-NHMe in water and in the solid-state; **J. Am. Chem. Soc.**, 106: 7946-7958, 1984.
4. Oka, M., **Montelione, G.T.** and Scheraga, H.A.; Chain-folding initiation structures in ribonuclease-A: Conformational free-energy calculations on Ac-Asn-Pro-Tyr-NHMe, Ac-Tyr-Pro-Asn-NHMe, and related peptides; **J. Am. Chem. Soc.**, 106: 7959-7969, 1984.
5. Swadesh, J.K., **Montelione, G.T.**, Thannhauser, T.W. and Scheraga, H.A.; Local structure involving histidine-12 in reduced S-sulfonated ribonuclease A detected by proton NMR spectroscopy under folding conditions; **Proc. Natl. Acad. Sci. U.S.A.**, 81: 4606-4610, 1984.
6. **Montelione, G.T.**, Hughes, P., Clardy, J. and Scheraga, H.A.; Conformational properties of 2,4-methanoproline (2-carboxy-2,4-methanopyrrolidine) in peptides: Determination of preferred peptide-bond conformation in aqueous-solution by proton Overhauser measurements; **J. Am. Chem. Soc.**, 108: 6765-6773, 1986.
7. **Montelione, G.T.**, Wuthrich, K., Nice, E.C., Burgess, A.W. and Scheraga, H.A.; Identification of two anti-parallel beta-sheet conformations in the solution structure of murine epidermal growth factor by proton magnetic resonance; **Proc. Natl. Acad. Sci. U.S.A.**, 83: 8594-8598, 1986.
8. Stimson, E.R., Meinwald, Y.C., **Montelione, G.T.** and Scheraga, H.A.; Conformational properties of trans Ac-Asn-Pro-Tyr-NHMe and trans Ac-Tyr-Pro-Asn-NHMe in dimethylsulfoxide and in water determined by multinuclear NMR spectroscopy; **Int. J. Pept. Protein Res.**, 27: 569-582, 1986.
9. Haas, E., **Montelione, G.T.**, McWherter, C.A. and Scheraga, H.A.; Local structure in a tryptic fragment of performic acid oxidized ribonuclease A corresponding to a proposed polypeptide chain-folding initiation site detected by tyrosine fluorescence lifetime and proton magnetic resonance measurements; **Biochemistry**, 26: 1672-1683, 1987.
10. **Montelione, G.T.**, Wüthrich, K., Nice, E.C., Burgess, A.W. and Scheraga, H.A.; Solution structure of murine epidermal growth factor: determination of the polypeptide backbone chain-fold by nuclear magnetic

resonance and distance geometry; *Proc. Natl. Acad. Sci. U.S.A.*, 84: 5226-5230, 1987.

11. Talluri, S., **Montelione, G.T.**, Vanduyne, G., Piela, L., Clardy, J. and Scheraga, H.A.; Conformational properties of 2,4-methanoproline (2-carboxy-2,4-methanopyrrolidine) in peptides: Evidence for 2,4-methanopyrrolidine asymmetry based on solid-state x-ray crystallography, ^1H -NMR in aqueous-solution, and CNDO/2 conformational energy calculations; *J. Am. Chem. Soc.*, 109: 4473-4477, 1987.

12. **Montelione, G.T.**, Wüthrich, K. and Scheraga, H.A.; Sequence-specific ^1H -NMR assignments and identification of slowly exchanging amide protons in murine epidermal growth factor; *Biochemistry*, 27: 2235-2243, 1988.

13. Ray, P., Moy, F.J., **Montelione, G.T.**, Liu, J.F., Narang, S.A., Scheraga, H.A. and Wu, R.; Structure-function studies of murine epidermal growth factor: Expression and site-directed mutagenesis of epidermal growth factor gene; *Biochemistry*, 27: 7289-7295, 1988.

14. **Montelione, G.T.** and Scheraga, H.A.; Formation of local structures in protein folding; *Accounts Chemical Research*, 22: 70-76, 1989.

15. **Montelione, G.T.** and Wagner, G.; Accurate measurements of homonuclear $\text{H}^{\text{N}}-\text{H}^{\alpha}$ coupling-constants in polypeptides using heteronuclear 2D NMR experiments; *J. Am. Chem. Soc.*, 111: 5474-5475, 1989.

16. **Montelione, G.T.** and Wagner, G.; 2D chemical-exchange NMR Spectroscopy by proton-detected heteronuclear correlation; *J. Am. Chem. Soc.*, 111: 3096-3098, 1989.

17. **Montelione, G.T.**, Winkler, M.E., Burton, L.E., Rinderknecht, E., Sporn, M.B. and Wagner, G.; Sequence-specific ^1H -NMR assignments and identification of two small antiparallel β -sheets in the solution structure of recombinant human transforming growth factor α ; *Proc. Natl. Acad. Sci. U.S.A.*, 86: 1519-1523, 1989.

18. **Montelione, G.T.**, Winkler, M.E., Rauenbuehler, P. and Wagner, G.; Accurate measurements of long-range heteronuclear coupling constants from homonuclear 2D NMR Spectra of isotope-enriched proteins; *J. Magn. Resonance*, 82: 198-204, 1989.

19. Moy, F.J., Scheraga, H.A., Liu, J.F., Wu, R. and **Montelione, G.T.**; Conformational characterization of a single-site mutant of murine epidermal growth factor (EGF) by ^1H NMR provides evidence that leucine-47 is involved in the interactions with the EGF receptor; *Proc. Natl. Acad. Sci. U.S.A.*, 86: 9836-9840, 1989.

20. Engler, D.A., **Montelione, G.T.** and Niyogi, S.K.; Human epidermal growth factor: Distinct roles of tyrosine 37 and arginine 41 in receptor binding as determined by site-directed mutagenesis and nuclear magnetic resonance spectroscopy; *FEBS Letters*, 271: 47-50, 1990.

21. **Montelione, G.T.** and Wagner, G.; Conformation-independent sequential NMR connections in isotope-enriched polypeptides by ^1H - ^{13}C - ^{15}N triple-resonance experiments; *J. Magn. Resonance*, 87: 183-188, 1990.

22. Emerson, S.D. and **Montelione, G.T.**; 2D-HCCH and 3D-HCCH TOCSY experiments for determining $^3J(\text{H}\alpha - \text{H}\beta)$ coupling-constants of amino-acid-residues; *J. Magn. Resonance*, 99: 413-420, 1992.

23. Emerson, S.D. and **Montelione, G.T.**; Accurate measurements of proton scalar coupling-constants using C-13 isotropic mixing spectroscopy; *J. Am. Chem. Soc.*, 114: 354-356, 1992.

24. **Montelione, G.T.**, Emerson, S.D. and Lyons, B.A.; A general approach for determining scalar coupling constants in polypeptides and proteins; *Biopolymers*, 32: 327-334, 1992.

25. **Montelione, G.T.**, Lyons, B.A., Emerson, S.D. and Tashiro, M.; An efficient triple resonance experiment using C-13 isotropic mixing for determining sequence-specific resonance assignments of isotopically-enriched proteins; *J. Am. Chem. Soc.*, 114: 10974-10975, 1992.

26. **Montelione, G.T.**, Wüthrich, K., Burgess, A.W., Nice, E.C., Wagner, G., Gibson, K.D. and Scheraga, H.A.; Solution structure of murine epidermal growth factor determined by NMR spectroscopy and refined by energy minimization with restraints; *Biochemistry*, 31: 236-249, 1992.

27. Moy, F.J., Scheraga, H.A., Patt, S.L. and **Montelione, G.T.**; Application of frequency-shifted shaped pulses for overcoming solvent-saturation transfer and preirradiation-associated spin-diffusion effects in aqueous-solutions of peptides and proteins; *J. Magn. Resonance*, 98: 451-457, 1992.

28. Campion, S.R., Biamonti, C., **Montelione, G.T.** and Niyogi, S.K.; The role of asparagine-32 in forming the receptor-binding epitope of human epidermal growth factor; *Protein Engineering*, 6: 651-659, 1993.

29. Celda, B. and **Montelione, G.T.**; Total correlation spectroscopy (TOCSY) of proteins using coaddition of spectra recorded with several mixing times; *J. Magn. Resonance Series B*, 101: 189-193, 1993.

30. Li, Y.C. and **Montelione, G.T.**; Solvent saturation-transfer effects in pulsed-field-gradient heteronuclear single-quantum coherence (PFG-HSQC) spectra of polypeptides and proteins; *J. Magn. Resonance Series B*, 101: 315-319, 1993.

31. Lyons, B.A. and **Montelione, G.T.**; An HCCNH triple-resonance experiment using C-13 isotropic mixing for correlating backbone amide and side-chain aliphatic resonances in isotopically enriched proteins; *J. Magn. Resonance Series B*, 101: 206-209, 1993.

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333. Zhang, M., Yu, X-W., Xu, Y., Jouhten, P., Swapna, G.V.T., Glaser, R.W., Hunt, J.F., **Montelione, G.T.**, Maaheimo, H., Szyperski, T. ¹³C metabolic flux profiling of *Pichia pastoris* grown in aerobic batch cultures on glucose revealed high relative anabolic use of TCA cycle and limited incorporation of provided precursors of branched-chain amino acids. *FEBS Letts.* 18: 3100-3111, 2017.
334. Alasadi, A., Chen, M., Swapna, G.V.T., Tao, H., Guo, J., Collantes, J., Fadhil, N.; **Montelione, G.T.**, Jin, S.V. Effect of mitochondrial uncouplers niclosamide ethanolamine (NEN) and oxyclozanide on hepatic metastasis of colon cancer. *Cell Death and Disease* 9: 215, 2018. PMC5833462
335. Zhang, M., Yu, X-W., Swapna, G.V.T., Liu, G., Xiao, R., Xu, Y., **Montelione, G.T.** Backbone and Ile- δ 1, Leu, Val methyl 1H, 15N, and 13C, chemical shift assignments for *Rhizopus chinensis* lipase. *Biomol NMR Assign* 2018, 12: 63 - 68.
336. Gibbs, A.C., Steele, R., Liu, G, Tounge, B.A., **Montelione, G.T.** Inhibitor bound dengue NS2B-NS3pro reveals multiple dynamic binding modes. *Biochemistry* 2018, 57: 1591 - 1602.
337. Venkataraman, A., Yang, K., Irizarry, J., Mackiewicz, M., Mita, P., Kuang, Z., Xue, L., Ghosh, D.; Liu, S.; Ramos, P.; Hu, S.; Bayron, D.; Keegan, S.; Saul, R.; Colantonio, S.; Zhang, H.; Behn, F.P.; Song, G.; Albino, E.; Asencio, L.; Ramos, L.; Lugo, L.; Morell, G.; Rivera, J.; Ruiz, K.; Almodovar, R.; Nazario, L.; Murphy, K.; Vargas, I.; Rivera-Pacheco, Z.A.; Rosa, C.; Vargas, M.; McDade, J.; Clark, B.S.; Yoo, S.; Khambadkone, S.G.; de Melo, J.; Stevanovic, M.; Jiang, L.; Li, Y.; Yap, W.Y.; Jones, B.; Tandon, A.; Campbell, E.; **Montelione, G.T.**; Anderson, S.; Myers, R.M.; Boeke, J.D.; Fenyö, D.; Whiteley, G.; Bader, J.S.; Pino, I.; Eichinger D.J.; Zhu, H.; Blackshaw, S. . A toolbox of immunoprecipitation-grade monoclonal antibodies to human transcription factors. *Nature Methods* 2018, 15: 303 - 338

338. Zhang, Z., Wang, D., Szyperski, T., **Montelione, G.T.**, Hunt, J.F. Co-lyophilization with detergent strongly stimulates ester synthesis activity of lipases. **Green Chemistry** 2018, (submitted)
339. Nie, Y., Wang, S., Xu, Y., Luo, S., Zhao, Y-L., Xiao, R., **Montelione, G.T.**; Hunt, J., Szyperski, T. Enzyme engineering based on X-ray structures and kinetic profiling of substrate libraries: alcohol dehydrogenases for stereospecific synthesis of a broad range of chiral alcohols. **ACS Catalysis** 2018. (epub ahead of print).

Books, Monographs and Chapters

1. Wagner, G., Nirmala, N.R., **Montelione, G.T.** and Hyberts, S.; Static and dynamic aspects of protein structure; **Frontiers of NMR in Molecular Biology**, 129-143, 1990.
2. Biamonti, C., Rios, C., Lyons, B. and **Montelione, G.T.**; Multidimensional NMR experiments and analysis techniques for determining homo- and heteronuclear scalar coupling constants in proteins and nucleic acids; **Advances in Biophysical Chemistry**, 4: 51-120, 1994.
3. Moseley, H.N., Monleon, D. and **Montelione, G.T.**; Chapter 6 Automatic determination of protein backbone resonance assignments from triple resonance nuclear magnetic resonance data; **Methods in Enzymology**, Vol. 339 Eds. T.J. James, V. Dotsch and U. Schmitz; Academic Press; San Diego, CA, 2001.
4. Acton, T.B., Gunsalus, K.C., Xiao, R., Ma, L.C., Aramini, J., Baran, M.C., Chiang, Y.W., Climent, T., Cooper, B., Denissova, N.G., Douglas, S.M., Everett, J.K., Ho, C.K., Macapagal, D., Rajan, P.K., Shastry, R., Shih, L.Y., Swapna, G.V., Wilson, M., Wu, M., Gerstein, M., Inouye, M., Hunt, J.F. and **Montelione, G.T.**; Chapter 8 Robotic cloning and Protein Production Platform of the Northeast Structural Genomics Consortium; **Methods in Enzymology**, Vol. 394; Ed. TJ James; Academic Press; San Diego, CA, 2005.
5. Huang, Y.J., Moseley, H.N., Baran, M.C., Arrowsmith, C., Powers, R., Tejero, R., Szyperski, T. and **Montelione, G.T.**; Chapter 5 An integrated platform for automated analysis of protein NMR structures; **Methods in Enzymology**, Vol. 394; Ed. TJ James, Academic Press; San Diego, CA, 2005.
6. **Montelione, G.T.** and Szyperski, T.; Advances in NMR-based structural genomics spectroscopy; **Advances in BioNMR Spectroscopy**, Editors A.J. Dingley and S.M. Pascal. IOS Press, 2010.
7. Acton, T.B., Xiao, R., Anderson, S., Aramini, J., Buchwald, W.A., Ciccocanti, C., Conover, K., Everett, J., Hamilton, K., Huang, Y.J., Janjua, H., Kornhaber, G., Lau, J., Lee, D.Y., Liu, G., Maglaqui, M., Ma, L., Mao, L., Patel, D., Rossi, P., Sahdev, S., Shastry, R., Swapna, G.V., Tang, Y., Tong, S., Wang, D., Wang, H., Zhao, L. and **Montelione, G.T.**; Chapter 2 Preparation of protein samples for NMR structure, function, and small-molecule screening studies; **Methods in Enzymology**, Vol. 493; Ed. LC Kuo; Academic Press; San Diego, CA, 2011.
8. Huang, Y.J., Acton, T.B. and **Montelione, G.T.**; Chapter 1. DisMeta: A meta server for construct design and optimization; **Methods in Molecular Biology, Structural Biology**, Vol. 1091; Ed. JM Walker, Humana Press; New York, NY, 2014.
9. Boël, G., **Montelione, G.T.**, Aalberts, D.P., Hunt, J.F. Codon optimization for high level protein production in *E. coli*. **Cell Systems**, 2: 60 - 64. Principles of Systems Biology, No. 2. 2016
10. Huang, Y. J., Brock, K., Sander, C., Marks, D.S., **Montelione, G.T.** A hybrid approach for protein structure determination combining sparse NMR with evolutionary coupling sequence data, in **Integrative Structural Biology with Hybrid Methods** 2018, (in press) in JL Markley, S. Burley, H. Nakamura, G. Kleywegt. [Eds.] Springer Singapore

Published Abstracts

1. Greenfield, N.J., **Montelione, G.T.**, Tsao, J., Stein, S., Smiley, E. and Bonadio, J.; Conformational transitions of a collagen fragment studied by circular dichroism and ^1H -NMR spectroscopy; **Biophysical Journal**, 57: A422, 1990.
2. Bonadio, J., Smiley, E., Bole, D., Greenfield, N.J. and **Montelione, G.**; Structure-function relationships in collagen subdomains; **FASAB Journal**, 5: A445-A445, 1991.
3. Greenfield, N.J., Biamonti, C., Campion, S.R., Engler, D.A., Nyogi, S.K. and **Montelione, G.T.**; Structural analysis of single-site mutants in human epidermal growth-factor by NMR; **FASAB Journal**, 6: A269, 1992.
4. Celda, B., Arnau, M.J. and **Montelione, G.T.**; Sequence-specific C-13 resonance assignments for murine epidermal growth-factor at natural isotope abundance - correlation between secondary structure and Ca chemical-shifts; **J. Cellular Biochemistry**, 291, 1993.
5. Emerson, S.D. and **Montelione, G.T.**; Accurate measurements of vicinal $^3\text{J}(\text{C}13'\text{-H}\beta)$ coupling-constants from J1-resolved heteronuclear e-COSY multiplets; **J. Cellular Biochemistry**, 252, 1993.
6. **Montelione, G.T.**, Zimmerman, D., Kulikowski, C., Rios, C., Tashiro, M., Feng, W.Q., Chien, C.Y., Shang, Z.G. and Biamonti, C.; Automated analysis of resonance assignments for proteins using triple-resonance NMR and

methods from artificial-intelligence; **J. Cellular Biochemistry**, 21, 1995.

7. **Montelione, G.T.**, Anderson, S., Bruccoleri, R., Chien, A., Dixon, B., Feng, W., Gunsalus, K., Huang, Y., Kulikowski, C., Mani, R., Sahasrabudhe, P., Swapna, G.V.T. and Zimmerman, D.; Prognosis for automated analysis of protein structures from NMR data: Applications in structural and functional genomics; **Biophysical Journal**, 76: A265, 1999.

8. Greenfield, N.J., Palm, T., Monleon, D., **Montelione, G.T.** and Hitchcock-DeGregori, S.E.; 3D NMR studies of the N-terminus of short alpha-tropomyosins.; **Biophysical Journal**, 78: 399A, 2000.

9. **Montelione, G.T.**, Anderson, S., Palacios, D., Dixon, B., Gunsalus, K., Huang, Y., Li, E., Mani, R., Moseley, H., Monleon, D., Paranj, R., Sahasrabudhe, P., Sahota, G., Swapna, G.V.T., Tejero, R., Xiao, R. and Zheng, D.; Protein NMR and structural genomics; **Biophysical Journal**, 78: 20A, 2000.

10. Greenfield, N.J., Swapna, G.V.T., **Montelione, G.T.** and Hitchcock-DeGregori, S.E.; Non-cooperative folding of a coiled-coil peptide containing the N-terminus of short alpha-tropomyosin - A heteronuclear NMR study; **Biophysical Journal**, 80: 559A, 2001.

11. Greenfield, N.J., Swapna, G.V.T., Huang, Y.P.J., Palm, T., Graboski, S., **Montelione, G.T.** and Hitchcock-DeGregori, S.E.; The C-terminal domain of striated α -tropomyosin contains an unusual structure with parallel, non-coiled coil α -helices.; **Biophysical Journal**, 84: 250A-250A, 2003.

12. Bachhawat, P., Gurla, S.G.V.T.S., **Montelione, G.T.** and Stock, A.M.; Mechanism of activation in the OmpR/PhoB family of response regulators; **Biophysical Journal**, 86: 76A-76A, 2004.

13. MacCallum, J.L., Tang, Y., Huang, J., **Montelione, G.T.** Automatic protein structure determination from sparse NMR spectroscopy data. **Biophysical Journal**, 110: 153a. 2016.

PATENTS

Issued Patents

1. United States Patent 6,210,655 Date of Issue: April 3, 2001.
"Site-specific ^{13}C -Enriched Reagents for Diagnostic Medicine by Magnetic Resonance Imaging"
Inventors: Stein S., **Montelione G.T.**

2. United Kingdom Patent Patent Issued 2006
"Linking Gene Sequence to Gene Function by 3D Structure Determination"
Inventors: **Montelione G.T.**, Anderson S., Huang Y.P.
European Patent Application No: 99935746.0-2402. Publication No: 1104488.

3. United States Patent 7,709,190. Date of Issue: May 4, 2010.
"Influenza A Virus Vaccines and Inhibitors"
Inventors: **Montelione G.T.**, Das K., Arnold E., Ma L.-C., Xiao R., Krug R.M., Twu K.Y., Kuo R.-L.

4. United States Patent 8,450,085. Date of Issue: May 28, 2013.
"Labeled Biomolecular Compositions and Methods for the Production and Uses Thereof".
Inventors: **Montelione G.T.**, Inouye M., Tang Y., Roth M., Schneider W.

5. United States Patent 8,455,621. Date of Issue: June 4, 2013.
"Influenza A Virus Vaccines and Inhibitors".
Inventors: **Montelione G.T.**, Krug R.M., Twu K.Y., Kuo, R.-L., Arnold E., Das K, Ma, L.-C., Xiao R.

6. Peoples Republic of China Patent #: 2014051400411580
Date of Issue: 5/28/2014
Application Number: CN 102482649 B
Title: Stereospecific Carbonyl Reductases; 立体专一性羰基还原酶

Inventors: **Montelione G.T.**, Xiao R., Nie Y., Xu Y.
盖塔诺 蒙泰莱奥, 肖荣 聂尧 徐岩

7. United States Patent 8,796,008 Date of issue: Aug 5, 2014
"Influenza A Virus Vaccines and Inhibitors".
Inventors: **Montelione G.T.**, Krug R., Das K., Arnold E.; Ma L.-C., Xiao R., Kuo R.-L., Twu K.Y.

8. United States Patent 8,916,519 Date of issue: Dec 23, 2014
"Influenza A Virus Vaccines and Inhibitors".
Inventors: **Montelione G.T.**, Das K., Arnold E.; Ma L.-C.; Xiao R., Krug R.M., Twu, K.Y., Kuo, R.-L.

9. United States Patent 9,119,810 Date of Issue: Sept. 1, 2015
"Novel Compositions and Vaccines Against Influenza A and Influenza B Infection".
Inventors: **Montelione G.T.**, Krug R., Ma L.-C., Yin C.

10. United States Patent 9,228,368 Date of Issue: Jan. 5, 2016.
"Labeled Biomolecular Compositions and Methods for the Production and Uses Thereof".
Inventors: **Montelione G.T.**, Inouye M., Tang Y., Roth M., Schneider W.

11. United States Patent 9,328,217 Date of Issue: May 3, 2016.
"Labeled Biomolecular Compositions and Methods for the Production and Uses Thereof".
Inventors: **Montelione G.T.**, Inouye M., Tang Y., Roth M., Schneider W.

12. United States Patent 9,422,583 Date of Issue: Aug. 23, 2016.
"Stereospecific Carbonyl Reductases".
Inventors: **Montelione G.T.**, Xiao R., Nei Y., Xu Y.

Published Pending Patents

1. Roth M, Schneider W, Montelione G, Inouye M, "Independently Inducible System of Gene Expression".
Nationalized PCT – United States. Filed 4/4/11. Serial No: 13/122,547. Publication No: 2011-0306751 A1A1.
Rutgers Tech ID: 2009-088.

2. Hunt JF, Price WM, Acton TB, Montelione GT, "Methods for Altering Polypeptide Expression". Provisional US
Patent filed 2/9/2010 Appl No 61/320.805. Provisional Filed 9/22/2011. Nationalized PCT – United States.
Nationalized PCT – Europe. Filed 2/9/2010 PCT/US2011024251. Nationalized PCT – China. Rutgers Tech ID:
2010-133.

3. Acton TB, Anderson S, Montelione, GT, Huang YJ, System for High-level Production of Proteins and Protein
Domains. Provisional Filed 11/10/11. PCT Filed 11/09/12. Serial No: 61/558,277. Rutgers Tech ID: 2012-056.

4. Klessig, D, Park, S-W., Montelione, G.T., Hamilton, K., Gurla, S., Bianchi, M.E. "Structure and Function of The
Salicylic Acid Binding Sites on Human HMGB1 and Methods and Use Thereof for the Rational Design of Both
Salicylic Acid Analogs and Other Agents that Alter Animal and Plant HMGBs Activities. Provisional patent filed
6/2013. PCT files 6/2014. Rutgers Tech ID: 2013-114.

CONFERENCE and WORKSHOP ORGANIZATION

International Meetings and Conferences

Experimental NMR Conference (ENC)
 Monterey, California, USA
 Executive Committee, 1992 – 1998

Proteins That Bind RNA International Conference
 Avalon, New Jersey, USA. Austin, Texas, USA.
 Co-organizer, 1998, 2001

Structure-based Functional Genomics Workshop
 Avalon, New Jersey. USA.
 Lead Organizer, 1998

Keystone Symposia in Structural Genomics, From Gene Sequencing to Function
 Breckenridge, Colorado, USA.
 Lead Organizer, 2002

Third International Conference in Structural Genomics
 Washington, D.C. USA.
 Lead Organizer, 2004

Keystone Symposia Structural Genomics, Workshop: Structural Genomics and Functional Proteomics of Biological Macromolecules
 Keystone, Colorado, USA.
 Lead Organizer, 2010

CASP10 – Template Based Modeling
 Gaeta, ITALY.
 CASP Co-organizer 2012

CASP11 – Contact Assisted Prediction – NMR Data
 Cancun, MEXICO.
 CASP Co-organizer 2014

wwPDB Workshop on Protein NMR Structure Validation
 Protein Science Center, Osaka, JAPAN,
 Co-organizer 2016.

wwPDB NMR Validation Task Force
 Newby, Maine
 Organizer, 2017

National Meetings and Conferences

Structural Genomics in the Pharmaceutical Industry
 Rutgers University, Piscataway NJ
 Lead Organizer, 1999

Structural and Functional Genomics in the Pharmaceutical Industry
 Princeton Forrestal Center, Princeton NJ
 Lead Organizer, 2001

Workshop on Protein Production for Structural Genomics
 National Institutes of Health, Bethesda, MD
 Co-Organizer, 2002-2013.
Workshop on NMR and Structural Genomics
 National Institutes of Health, Bethesda, MD
 Co-Organizer, 2002

Workshop on Protein Crystallization for Structural Genomics
 National Institutes of Health, Bethesda, MD
 Co-Organizer, 2003

NJACS NMR Annual Symposium
 Princeton University, Princeton NJ
 Co-Organizer, 2015

INVITED LECTURES (partial listing)

Prof. Montelione has presented approximately 70 invited lectures since 2000, including:

Invited Speaker, "Structural and Functional Genomics in Pharmaceutical Design". Princeton, NJ, October 24 - 25, 2001.

Invited Speaker, "International Keystone Meeting: Structural Genomics: From Gene Sequence to Function". Breckenridge CO. January 5 - 10, 2002.

Invited Speaker, "Workshop in Protein Production for Structural Genomics". NIGMS, NIH, Bethesda, MD, March 7 - 8, 2002.

Invited Speaker, "Workshop in NMR and Structural Genomics". University of Wisconsin at Madison, Madison, WI, June 22, 2002.

Invited Speaker, "Second International Conference in Structural Genomics". International Structural Genomics Organization (ISGO) Conference, Berlin, GERMANY, October 10 - 13, 2002.

Invited Speaker, "Bruker NMR Technology Development Group". Bruker BioSpin, Karlsruhe, GERMANY, October 15, 2002.

Invited Speaker, "International Meeting for European High Field NMR Network". Montecatini, ITALY, October 17, 2002.

Invited Speaker, "Alberta Synchrotron Institute Meeting in Structural Genomics". Banff, Alberta, CANADA, October 24, 2002.

Invited Speaker, "Workshop on Protein Production and Crystallization for Structural Genomics". NIGMS, NIH, Bethesda, MD, April 9 - 11, 2003.

Invited Speaker, "European Science Foundation: NMR in Structural Biology", Strasbourg, FRANCE. Sept. 7 - 12, 2003.

Invited Speaker, "CABM Symposium: Functional Genomics". Piscataway, NJ. October, 2003.

Invited Speaker, "International Keystone Meeting: Frontiers of NMR in Structural Biology". Taos, New Mexico, USA January, 2003.

Invited Speaker, "International Keystone Meeting: Structural Genomics: From Gene Sequence to Function". Snowbird, Utah, USA. April 13-20, 2004.

Invited Speaker, "International Keystone Meeting: Frontiers of NMR in Structural Biology". Banff, British Columbia, CANADA. January 29 - Feb 5, 2005.

Invited Speaker, "International Symposium on Cell Free Protein Production". Matsuyama, JAPAN. October 22 – 25, 2005.

Invited Speaker, "International Keystone Meeting: Structural Genomics: From Gene Sequence to Function" Keystone, Colorado, USA. January 28 – February 4, 2006.

Invited Speaker, "12th Bijvoet Symposium: Protein Structure in relation to dynamics and interactions" Utrecht, THE NETHERLANDS. April 6 – 7, 2006.

Invited Speaker, University of Florence, Florence, ITALY, September 23, 2006.

Invited Speaker, "Computational Aspects – "Biomolecular NMR Gordon Research Conference", Aussois, FRANCE September 24-29, 2006

Invited Speaker, "CABM Symposium: Molecular Aspects of Human Disease". Piscataway, NJ, USA. October 16, 2006.

Invited Speaker, "International Structural Genomics Organization Workshop on Automated Methods for Protein NMR Data Analysis". Yokohama, JAPAN. October 18, 2006.

Invited Speaker, "Third International Conference on Structural Genomics". Beijing, PEOPLES REPUBLIC OF CHINA, October 18 – 22, 2006.

Invited Speaker, "Jiangnan University", Wuxi, PEOPLES REPUBLIC OF CHINA. October 30, 2006.

Invited Speaker, "Eastern Analytical Society", Somerset, NJ, USA. November 13, 2006.

Invited Speaker, "NIH Protein Structure Initiative Annual Meeting", Bethesda, Maryland, USA. December 7, 2006.

Invited Speaker, "Keystone Meeting on Frontiers of NMR in Structural Biology". Snowbird, Utah, USA. January 4 – 11, 2007.

Invited Speaker, "NIH Workshop on Overcoming Bottlenecks in Structural Genomics". Bethesda, Maryland, USA. March 19 - 20, 2007

Invited Speaker. "NIH Protein Structure Initiative, Annual Meeting". Bethesda, Maryland, USA December 5 – 6, 2007.

Invited Speaker, "Keystone Meeting on Structural Genomics in Biology and Medicine". Steamboat Springs, Colorado, USA. January 7 – 11, 2008.

Invited Speaker, "PSI Workshop on Functional Annotation for Structural Genomics", San Diego, California, USA, March 7 – 8, 2008.

Invited Speaker, "PSI Workshop on Homology Modeling for Biology", San Francisco, California, USA, July 10 – 12, 2008.

Organizer and Speaker, "PSI Workshop on Visions for Structural Genomics", Bethesda, Maryland, USA, July 28 - 29, 2008

Invited Speaker, "5th International Meeting in Structural Genomics", Oxford, England, UNITED KINGDOM, September 20 - 23, 2008.

Invited Speaker, Department of Biochemistry, Cambridge, England, UNITED KINGDOM, September 24, 2008.

Invited Speaker. “NIH Protein Structure Initiative, Annual Meeting”. Bethesda, Maryland, USA, December 10 – 12, 2008.

Invited Speaker, “ENMR Workshop on Automated Structure Analysis”. Florence, ITALY. May 4, 2009.

Invited Speaker, “Structural Genomics in Drug Discovery”. Tsin-Jin, PEOPLES REPUBLIC OF CHINA. June 2009.

Invited Speaker, “NIH Protein Structure Initiative, Annual Meeting”. Bethesda Maryland, USA, December 9-10, 2009.

Invited Speaker, “2nd Annual ENMR Workshop on Automated Structure Analysis”. Florence, ITALY. May 6, 2010.

Invited Speaker, “International Structural Genomics Conference”. Toronto, CANADA. May 9 – 13, 2011.

Invited Speaker, “Gordon Research Conference in Computational Methods for NMR Spectroscopy”. Barga, ITALY. May 29 – June 2, 2011.

Invited Speaker, “Functional Roles of Intrinsic Dynamics in Proteins: Some Lessons from Structural Genomics”. University of Michigan, Ann Arbor, Michigan, USA. October 11, 2011.

Invited Speaker, “Structural Genomics”. Cornell University, Ithaca, New York, USA. October 19, 2011.

Invited Speaker. “Template-based Modeling Assessment”. CASP10 International Meeting. Gaeta, ITALY. December 9 - 12. 2012

Invited Speaker, “Evolutionary Couplings in Protein NMR”. Gordon Research Conference in Computational Methods for NMR. Mt. Snow, Vermont, USA. June 2-7, 2013.

Invited Speaker, Structural Life Science 7th International Conference on Structural Genomics, Sapporo, JAPAN. July 29, 2013.

Invited Speaker, “Function Discovery by Structural Genomics”. Inauguration Symposium for Princeton Chemistry Department NMR Laboratory, Princeton University, Princeton, New Jersey, USA. September 26, 2013.

Invited Speaker, “A Structure-Based Inhibitor Discovery Process Applied to Influenza Non-structural Protein 1 (NS1)” ICMol, University of Valencia, Valencia, SPAIN. October 8, 2014.

Keynote Speaker, "Developing NMR for Studies of Larger Proteins and Enzymes. Application to *R. chinensis* Lipase". 2014 Symposium on Lipase Biotechnology and its Application Trends. Jiangnan University. Wuxi, PEOPLES REPUBLIC OF CHINA. Oct 23, 2014.

Invited Speaker, “Sparse NMR Contacts for Modeling Protein Structures”. Critical Assessment of Protein Structure Prediction CASP 11. Pairaso Mayo, MEXICO. December 1 - 7, 2014.

Invited Speaker, “Hybrid Approaches for Protein Structure Determination Combining Computational Modeling with Sparse NMR Restraints”. 56th Experimental NMR Meeting (ENC). Asilomar, California, USA. April 19 – 24, 2015.

Keynote Speaker. “Hybrid Approaches for Protein Structure Determination Combining Computational Modeling with Sparse NMR Restraints”. 14th Upstate New York NMR and Structural Biology Symposium. Syracuse, New York, USA. October 20, 2015.

- Invited Speaker. Symposium on Enzymes for Chirality: Protein Engineering and Molecular Design, Jiangnan University, Wuxi, PEOPLES REPUBLIC OF CHINA. November 6, 2015.*
- Invited Speaker. "Protein Structure Determination Combining Computational Modeling with Sparse NMR Restraints". Eastern Analytical Symposium. Somerset, New Jersey, USA. November 16-18, 2015.*
- Invited Speaker. "Synergies of Molecular Modeling Calculations and Protein NMR Spectroscopy". National Science Foundation / Rice University Workshop in Modeling and Dynamics in Molecular Biophysics. Arlington, Virginia, USA. January 27-28, 2016.*
- Invited Speaker. "Hybrid Approaches for Protein Structure Determination Combining Computational Modeling with Sparse NMR Restraints". Gordon Research Conference on Molecular Structure Elucidation. Mt. Snow, Vermont, USA. August 12-17, 2016.*
- Invited Speaker. "Protein NMR Structure Validation: Model vs Data Validation Metrics". wwPDB Protein NMR Validation Task Force Meeting. Osaka, JAPAN. August 26-27, 2016.*
- Invited Speaker. "Protein NMR". 16th Korean Institute for Advanced Study (KIAS) Protein Folding Winter School. Seoul, KOREA. January 16 – 20, 2017. Three lectures.*
- Invited Speaker. "Protein NMR Structure Validation". 61st Annual Meeting of the Biophysical Society. New Orleans, USA. February 11-15, 2017.*
- Organizer and Speaker. "Protein NMR Structure Validation". wwPDB Protein NMR Validation Task Force Meeting. Newby, Maine, USA. June 17, 2017.*
- Plenary Lecture. "Hybrid Approaches for Protein Structure Determination Combining Computational Modeling with Sparse NMR Restraints". 17th KIAS Conference on Protein Structure and Function. Seoul, KOREA. September 22, 2017.*
- Invited Speaker. "Structural Biology of Innate Immune Suppression by Influenza Viruses". i3D Retreat Rutgers New Jersey Medical School, Newark, NJ USA October 25, 2017*
- Plenary Lecture. "Hybrid Methods for Protein Structure Determination Combining NMR Data, Evolutionary Co-Variance Data, and Conformational Modeling." 4th International Conference on Protein and RNA Structure Prediction. Montego Bay, JAMAICA, W.I. December 6, 2017.*
- Invited Speaker. "Hybrid Methods for Protein Structure Determination Combining NMR Data, Evolutionary Co-Variance Data, and Conformational Modeling." 2018 Biophysical Society Meeting: Memorial Symposium to Honor Dr. Kamal Shukla. San Francisco, California, USA. February 16, 2018.*
- Invited Speaker. "Structural Biology of Innate Immune Suppression by Influenza Viruses". Lawrence Berkeley National Laboratories. Berkeley, California. USA. February 22, 2018.*

RESEARCH AND DISCOVERIES

Gaetano Montelione is an internationally recognized expert and innovator in the fields of structural biology and protein NMR. He served as Director of the NIH Northeast Structural Genomics Consortium (NESG) (2000 – 2016), which developed a successful high-throughput pipeline for protein sample and 3D structure production. The NESG program involved extensive efforts in new technology development for protein sample production, NMR, X-ray crystallography, and structural bioinformatics. More than 1,300 structures were determined by the NESG team, lead by Montelione, using crystallography and NMR. Most of these were the first structures determined from large protein families, providing the basis for modeling of hundreds of thousands of

homologous proteins. With Prof. G. Wagner (Michigan), Montelione carried out pioneering work on NMR pulse sequence development, including the design and implementation of the first triple-resonance protein NMR experiments, as well as the high-impact ZZ-exchange and J1-resolved E_COSY experiments. At Rutgers, he followed up this work by development of the HCCNH-TOCSY, HCCoNH-TOCSY, and related widely-adopted triple-resonance NMR experiments. Montelione has made key contributions in computational NMR methods development, including the development of software for automated analysis of protein resonance assignments, automated analysis of 3D structures, and for protein NMR model quality assessment. The group's biomedical focus areas include structure-function studies of proteins and complexes involved in cancer biology and influenza virus infection. Work with R. Krug on the influenza A non-structural protein 1 (NS1) has provided the basis for creation of attenuated virus vaccines, that are now in clinical trials. The lab's current methods-development focus involves combining evolutionary sequence co-variance restraints from bioinformatics together with sparse NMR data to determine the 3D structures of challenging proteins, including membrane proteins associated with cancer biology. Montelione has also directed a few dozen crystallography projects, and integrative projects combining NMR, crystallography, SAXS, and molecular modeling. As an advisor to the world-wide Protein Data Bank, Montelione leads efforts to standardize methods for protein NMR model validation. Montelione is also a member of several academic and commercial structural biology advisory groups, co-chair of the international wwPDB Task Force on NMR Structure Validation, member of the Organizing Committee for the Critical Assessment of Protein Structure Prediction (CASP), and Foreign Expert Advisor in Protein Engineering to the Key Laboratory of Biotechnology at Jiangnan University, Wuxi, China.

Development of computational methods for analysis of protein NMR assignments and structures. The Montelione laboratory has developed widely used computational NMR methods and software for analysis of protein structures and dynamics. Early work developing triple-resonance NMR led us to the hypothesis that these data could be used for fully automated analysis of protein structures from NMR data. This goal, initiated in a collaboration with computer scientists Drs. D. Zimmerman, Y. Huang, and C. Kulikowski in the mid 1990's, was realized with the development of the AutoAssign and AutoStructure (now called ASDP) expert systems for largely automated analysis of NMR resonance assignments and structures. This work continued in collaborations with computer scientist Dr. Y. Huang to develop robust automated NOESY analysis and structure validation tools, and in collaborations with Prof. David Baker (Univ. of Washington) and Chris Sander (Harvard University) to explore hybrid methods combining automated NMR data analysis with sophisticated computational modeling and bioinformatics methods. Montelione also interacts extensively with the global community of participants in the Critical Assessment of Protein Structure Prediction (CASP) experiment, to explore synergies between protein prediction methods and NMR data, and to drive the field of data-guided protein structure prediction using NMR, SAXS, and other experimental data.

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NMR Pulse sequence design, including Triple Resonance NMR. Montelione's postdoctoral work with Prof. G. Wagner was focused on the creation of new NMR experiments, which have had significant impact in the field of biomolecular NMR. These pulse sequences provide some of the key tools of modern protein NMR, including ZZ-exchange spectroscopy, the J1-resolved E.COSY experiment for measuring scalar coupling constants, and the first ^1H , ^{13}C , ^{15}N triple resonance NMR experiments (HNCH and HCNH) for determining resonance assignments in proteins. This work was followed up at Rutgers by invention of the HCCNH-TOCSY, HcoCCNH-TOCSY experiments, and several other widely used triple-resonance NMR experiments. Triple-resonance NMR is now the standard approach for determining NMR resonance assignments of proteins. This work has had high impact on the field of biomolecular NMR.

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Development of technologies enabling structural genomics. As Director of the Northeast Structural Genomics Consortium (NESG) for 16 years (2000 – 2016), Montelione developed a successful high-throughput pipeline for protein sample and structure production. This program involved extensive efforts in new technology development for protein sample production, as well as for NMR, X-ray, crystallography, and structural bioinformatics. This work resulted in more than 350 peer reviewed publications by the consortium. As part of this project the team targeted large, structurally-uncharacterized domain families, and protein interaction networks involved in human cancer biology. They successfully developed a platform of integrated technology for efficient protein sample and structure production, which has been adopted by industrial structural biology groups. The team developed and refined technologies for codon optimization, construct design and optimization, isotope enrichment using efficient single-protein production systems, automated NMR and X-ray crystallography data analysis, and structure quality assessment metrics. More than 1,300 new structures were deposited in the PDB, and extensive data on protein expression and sample production was

archived. More than 500 NMR structures, representing ~ 5% of all NMR structures in the PDB, were determined by the NESG consortium.

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Structure – function studies of cancer-associated proteins of the Human Cancer Protein Interaction

Network. Montelione has used bioinformatics analysis to characterize networks of protein-protein interactions involved in cancer biology. Several hundred of these cancer-associated proteins were produced by the NESG Protein Production Pipeline, and more than 100 3D structures have been determined and deposited in the PDB. These studies provide novel insights into the structures and functions of oncogenes and tumor suppressors, including structure-function relationships in epidermal growth factor, type- α transforming growth factor, and allosteric mechanisms of molecular recognition of HRAS by the RAS-binding domain of the BRAF kinase.

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Structure – function studies of the non-structural protein 1 (NS1) from influenza virus. Together with virologist Prof. R. Krug (Univ. of Texas), Montelione made fundamental discoveries regarding structure-function relationships of the NS1 protein, which functions to suppress the host innate immune response to viral infection. The collaboration has provided 3D structures of several critical complexes formed between NS1 and human host proteins using both NMR and X-ray crystallography, and discovered the structural basis for one of the key mechanisms by which NS1 contributes to the unique human / primate host range of influenza B viruses. These studies have provided the basis for the invention of patented approaches for rational design of influenza virus inhibitors and attenuated vaccines. For example, mutations of key RNA-binding residues Arg38 and Ly41 in NS1, first characterized by Montelione and Krug, provide the basis for live attenuated influenza vaccines that are being evaluated for human clinical trials (Du et al. 2018 Science 359: 290-6)

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