

**Gaetano T. Montelione, Ph.D.**  
Constellation Chair of Structural Bioinformatics and Professor  
Center for Biotechnology and Interdisciplinary Studies  
Department of Chemistry and Chemical Biology  
Rensselaer Polytechnic Institute

**EDUCATION**

- 1974-1976 Marine Biology  
Southampton College, Long Island University, Southampton NY
- 1977-1980 **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  
Advisor: Prof. Harold A. Scheraga, Co-Advisor: Prof. Kurt Wüthrich

**POSTGRADUATE TRAINING**

- 1987-1988 **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 – 2019 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 – 2019 Adjunct Professor, Department of Biochemistry, Robert Wood Johnson Medical School
- 2005 – 2019 Distinguished Professor, Rutgers University
- 2007 – 2018 Foreign Expert Advisor, Jiangnan University, Wuxi, PEOPLES REPUBLIC OF CHINA
- 2010 – 2019 Jerome and Lorraine Aresty Chair, Rutgers University
- 2019 – present Professor of Chemistry and Chemical Biology, Rensselaer Polytechnic Institute
- 2019 – present Constellation Chair of Structural Bioinformatics, Rensselaer Polytechnic Institute
- 2019 Visiting Professor, University of Florence, Florence ITALY

**INDUSTRY 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 and Founder, Nexomics Biosciences, 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  
2019 – present Member, International Society for HDX with Mass Spectrometry (IS-HDXMS)

**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 Appointed Jerome and Lorraine Aresty Endowed Chair by Rutgers University Board of Trustees  
2014 Rutgers Football Award for Academic Excellence  
2019 Appointed Rensselaer Polytechnic Institute Constellation Chair in Structural Bioinformatics

**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  
2018 – present KUSCO (Korea-US. Science Cooperation Center), National Research Foundation of Korea  
2018 Czech National Science Foundation  
2018 The Lise Meitner-Programme of the Austrian Science Fund (FWF)  
2020 – 2021 Austrian Science Foundation

United States 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
2019	NIH Special Study Section: NIGMS Maximizing Investigators' Research Award (R35)
2019	Ralph E Power Junior Faculty Enhancement Awards Review Panel – Oak Ridge Natl Labs

## 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 – 2018	Rutgers University Committee on Academic Promotions and Tenure (AP&T) – Distinguished Professor Rank
2014 – 2018	Member, Rutgers University Presidential Advisory Committee on Academic Planning and Review (CAPR)
2017 – 2018	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
2019	Molecular Biology and Biochemistry Faculty Recruitment 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> , Section of Integrative Methods for Structural Biology

### 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 Bioinformatics  
2011 – present. Advisor, New Jersey American Chemical Society (NJACS) NMR Topical Group and Annual Symposium  
2013 – 2018 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 (Ph.D.) 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 (Ph.D.) 2012 – 2016 Co-advisor w/ V. Nanda, Rutgers University  
Yisha Yao (M.S.) 2014 - 2017  
Ryan Woltz (Ph.D.) 2014 – 2019

**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  
Dr. Khushboo Banfa 2019 - present

## 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 – 2019

Byrne Seminar Astrobiology, Can Life Evolve on Other Planets (15 contact hours). 2012 - 2019

### 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, Rutgers Biomedical Health Sciences.

Anastasia Chernyatina, 2014. Visiting postdoctoral trainee from KU Leuven University, Brussels, BELGIUM

## GRANT SUPPORT

***Prof. Montelione brought more than \$120 million in federal funding to Rutgers University and subcontract institutes 1990 - 2019.***

### Active Grant Funding

#### As Principal Investigator

1. *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
2. *Constellation Endowed Chair in Structural Bioinformatics.* 2019 – ongoing. ~ \$30,000 per year.

#### As Co-Investigator

1. *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).
2. *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. *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 – 9/30/19. \$60,000 total award.
2. *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.

3. 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).
4. 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.
5. 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.
6. 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)
7. NIH ORIP "600 MHz NMR RF Console with <sup>19</sup>F NMR Probe" (S10 OD018207) 04/01/2014 - 03/31/2015. \$439,792 G.T. Montelione, PI; M. Roth, Co-PI; V. Nanda, Co-PI
8. 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)
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 "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.
11. CINJ "CINJ Protein Production and Structural Genomics Project" 02/01/04 – 01/31/06. G.T. Montelione, PI. \$70,000 annual direct cost
12. 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)
13. Merck Research Foundation. "Structure-based Functional Genomics of Strongly-Conserved Microbial Gene Families. 9/98 - 9/00. Direct costs: \$306,000 over two years.
14. 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.
15. NIH "Structures of RNA-binding Proteins from Influenza Virus". (R01-GM-47014). 4/97 - 4/02. Direct costs: ~ \$712,440 over 5 years.
16. Geneformatics Inc. "Improved Methods for Automated Analysis of Protein Structure from NMR Data." 01/01 – 12/02. Direct costs: \$400,000 total direct cost.
17. Camille and Henry Dreyfus Teacher Scholar Award. 5/95 - 5/00. Direct costs: \$55,000 over five years.
18. 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.
19. 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.
20. 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).
21. NIH NIRR "Purchase of 600 MHz NMR and Upgrade of Existing NMR Facilities". 09/95 Direct costs: \$400,000. (G. Montelione and J. Baum).
22. 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).
23. Wyeth Ayerst Pharmaceutical Company. "Improved Software for NMR Analysis". 7/97 - 7/99. Direct costs: \$75,000 over two years.
24. 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.).
25. NSF "Improved Technologies for Protein Structure Determination by NMR." (DIR-9019313 / MCB-9407569). 7/91-7/98. Direct costs: \$463,000 over 6 years.
26. NIH "Improved Technologies for Protein Structure Determination by NMR." (R01-GM-47014). 1992-1997.

### As Co-Investigator

1. NIH-NIGMS. "Interactions of MuLV IN with Host Proteins and DNA". 05/01/16 – 04/30/19. M. Roth. PI. (Montelione Lab share of total support: \$183,125).
2. NSF BRAIN EAGER "The Molecular Interactome of Synaptogenesis" (MCB 1450895) 09/01/14 – 08/31/16 \$43,387 (Montelione portion) (Montelione & Comoletti, coPIs)
3. NIH/NIGMS "Structural Basis of Protein Homeostasis" (U01 GM098254-03) 09/30/12 – 07/31/15 \$100,000 annual direct (Montelione portion).
4. 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).
5. 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)
6. 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).
7. 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).
8. 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).
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 360 peer-reviewed scientific articles and book chapters. His Google citation H-index is 78 as of Dec 28, 2021, see <https://scholar.google.com/citations?user=mrtpF44AAAAJ&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 1,136 PDB depositions, including more than 480 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.**, Wüthrich, 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,  $^1\text{H}$ -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  $^1\text{H}$ -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  $^1\text{H}$ -NMR assignments and identification of two small antiparallel  $\beta$ -sheets in the solution structure of recombinant human transforming growth factor  $\alpha$ . *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  $^1\text{H}$  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  $^1\text{H}$ - $^{13}\text{C}$ - $^{15}\text{N}$  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  $^3\text{J}(\text{H}\alpha - \text{H}\beta)$  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



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## PATENTS

### Issued Patents

1. United States Patent 6,210,655 Date of Issue: April 3, 2001.  
"Site-specific <sup>13</sup>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.*

13. *United States Patent 10,131,915 B2 Date of Issue: Nov. 20, 2018*

*"Independently Inducible System of Gene Expression"*

*Inventors: Roth M, Schneider W, Montelione GT, Inouye M, Tang, Y..*

14. *United States Patent 10,385,350B2 Date of Issue: Aug 20, 2019*

*"System for High-level Production of Proteins and Protein Domains"*

*Inventors: Acton TB, Anderson S, Montelione, GT, Huang YJ, Provisional Filed 11/10/11. PCT Filed 11/09/12. Serial No: 61/558,277. Rutgers Tech ID: 2012-056*

#### Pending Patents

1. *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.*

2. *Klessig D, Park S-W., Montelione GT, Hamilton K, Gurla S, Bianchi ME. “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 US patent filed 6/2013. PCT filed 6/2014. Rutgers Tech ID: 2013-114.*

3. **Montelione GT**, Bafna K, Krug RM, Garcia-Sastre A, White K. "Protein inhibitors for inhibition of SARS-CoV2 virus". Provisional US Patent filed 7/31/20. Attorney Docket: 104576-100. Updated 10/05/20 Attorney Docket: 104576-200.

## 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

*CASP13 – Experimental-Guided Prediction*  
Cancun, MEXICO.  
CASP Co-organizer 2018

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, "12<sup>th</sup> 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, "5<sup>th</sup> 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, "2<sup>nd</sup> 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". Critical Assessment of Protein Structure Prediction 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 7<sup>th</sup> 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. School of Biotechnology. 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 International Meeting. Pairaso Mayo, Playa de Carmen, MEXICO. December 1 - 7, 2014.

*Invited Speaker*, “Hybrid Approaches for Protein Structure Determination Combining Computational Modeling with Sparse NMR Restraints”. 56<sup>th</sup> 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”. 14<sup>th</sup> Upstate New York NMR and Structural Biology Symposium. Syracuse, New York, USA. October 20, 2015.

*Invited Speaker*. “Hybrid Approaches for Protein Structure Determination Combining Computational Modeling with Sparse NMR Restraints”. Symposium on Enzymes for Chirality: Protein Engineering and Molecular Design, School of Biotechnology, 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”. 16<sup>th</sup> Korean Institute for Advanced Study (KIAS) Protein Folding Winter School. Seoul, KOREA. January 16 – 20, 2017. Three lectures.

*Invited Speaker*. “Protein NMR Structure Validation”. 61<sup>st</sup> Annual Meeting of the Biophysical Society. New Orleans, USA. February 11-15, 2017.

*Lead 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”. 17<sup>th</sup> KIAS Conference on Protein Structure and Function. Korean Institute for Advanced Study, Seoul, SOUTH 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, WEST INDIES. 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.*

*Invited Speaker.* "Hybrid Methods for Protein Structure Determination Combining Computational Modeling with Evolutionary Co-Variance and NMR Data". *Gordon Research Conference on Structure Elucidation in Pharmaceutical Industry. Newby, Maine, USA. August 13, 2018.*

*Invited Speaker.* "Proteins Flex to Function: The Role of Conformational Plasticity in Molecular Recognition". *Department of Biological Sciences, Rensselaer Polytechnic Institute. Troy, New York, USA. October 11, 2018*

*Invited Speaker.* "Proteins Flex to Function: The Role of Conformational Plasticity in Molecular Recognition". *Centro di Risonanze Magnetiche CERM, University of Florence, Sesto Fiorentino, ITALY. October 22, 2018.*

*Plenary Speaker.* "Proteins Flex to Function: The Role of Conformational Plasticity in Molecular Recognition". *2018 Symposium on Protein Engineering and Molecular Design of Industrial Enzymes. School of Biotechnology, Jiangnan University, Wuxi, PEOPLES REPUBLIC OF CHINA. November 7, 2018.*

*Plenary Speaker.* "Proteins Flex to Function: The Role of Conformational Plasticity in Molecular Recognition". *The 18<sup>th</sup> KIAS Conference on Protein Structure and Function. Korean Institute for Advanced Study, Seoul, SOUTH KOREA. November 16, 2018*

*Plenary Speaker.* "Data-Assisted Protein Prediction in CASP13". *Critical Assessment of Protein Structure Prediction CASP 13 International Meeting. Pairaso Mayo, Playa de Carmen, MEXICO. December 3, 2018.*

*Invited Speaker.* "Proteins Flex to Function: The Role of Conformational Plasticity in Molecular Recognition". *Institute for Bioscience and Biotechnology Research, National Institutes of Standard and Technologies, Rockville, Maryland USA. February 4, 2019.*

*Invited Speaker.* "The wwPDB NMR Structure Validation Project". *Biophysical Society Satellite Workshop: Working Towards Federated Structural Models". Baltimore Maryland USA. March 1, 2019.*

*Invited Speaker.* "Proteins Flex to Function: The Role of Conformational Plasticity in Molecular Recognition". *University of Calgary, Calgary CANADA. May 21, 2019.*

*Invited Speaker.* "HDX-MS in CASP – Critical Assessment of Protein Structure Prediction" *Second International Meeting in Biomolecular Hydrogen-Deuterium Exchange with Mass Spectroscopy. Banff, CANADA. May 23, 2019.*

*Sabbatical Lectures in Bioinformatics and Protein NMR. University of Florence, Florence, ITALY. November and December 2019.*

*Invited Speaker. "The Hepatitis C Virus Protease Inhibitor Grazoprevir Synergizes with SARS-CoV2 Polymerase Inhibitor Remdesivir to Suppress Virus Replication". Western New York American Chemical Society. New York, USA (by zoom) November 11, 2020*

*Invited Speaker. "Proteins Flex to Function: The Role of Conformational Plasticity in Molecular Recognition". Center for Quantitative Biology (formally Center for Theoretical Biology). Peking University, Beijing PEOPLES REPUBLIC OF CHINA (by zoom). December 14, 2020*

## 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.

**1. 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 lead 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.

Zimmerman, D.E.; Kulikowski, C.A.; Huang, Y.J.; Feng, W.; Tashiro, M.; Shimotakahara, S.; Chien, C.; Powers, R.; Montelione, G.T. *J. Mol. Biol.* 1997, 269: 592-610. Automated analysis of protein NMR assignments using methods from artificial intelligence.

Baran, M.C.; Huang, Y.J.; Moseley, H.N.; Montelione, G.T. *Chemical Reviews* 2004, 104: 3451-3555. Automated analysis of protein NMR assignments and structures.

Huang, Y.J.; Powers, R.; Montelione, G.T. *J. Am. Chem. Soc.* 2005 127: 1665-1674. Protein NMR recall, precision, and F-measure scores (RPF scores): Structure quality assessment measures based on information retrieval statistics.

Raman, S.; Lange, O.F.; Rossi, P.; Tyka, M.; Wang, X.; Prestegard, J.; Montelione, G.T.; Baker, D. *Science* 2010 327, 1014-8. NMR structure determination for larger proteins using backbone-only data. PMC2909653.

Lange, O.F.; Rossi, P.; Sgourakis, N.; Song, Y.; Lee, H.-W.; Aramini, J.M.; Ertekin, A.; Xiao, R.; Acton, T.B.; Montelione, G.T.; Baker, D. *Proc. Natl. Acad. Sci. U.S.A.* 2012, 109: 10873 - 10878. Determination of solution structures of proteins up to 40 kDa using CS-Rosetta with sparse NMR data from deuterated samples. PMC3390869

Mao, B.; Tejero, R.; Baker, D.; Montelione, G.T. *J. Amer. Chem. Soc.* 2014, 136: 1893 - 1906. Protein NMR structures refined with Rosetta have higher accuracy relative to corresponding X-ray crystal structures. PMC4129517

Montelione, G.T.; Nilges, M.; Bax, A.; Güntert, P.; Herrmann, T.; Richardso J.S.; Schwieters, C.; Vranken, W.F.; Vuister, G.W.; Wishart, D.S.; Berman, H.; Kleywegt, G.J.; Markley, J.L. *Structure* 2013, 21: 1563 - 1570. Recommendations of the wwPDB NMR Validation Task Force. PMC3884077.

Mao, B.; Guan, R.; Montelione, G.T. *Structure* 2011, 19: 757 - 766. Improved technologies now routinely provide protein NMR structures useful for molecular replacement. PMC3612016.

Tang, Y.; Huang, Y.P.; Hopf, T.A.; Sanders, C.; Marks, D.S.; Montelione, G.T. *Nature Methods* 2015, 12: 751-754. Protein structure determination by combining sparse NMR spectroscopy data with evolutionary couplings. PMC4521990.

**2. 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  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{15}\text{N}$  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.

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

- Montelione, G.T.; Winkler, M.E.; Rauenbuehler, P.; Wagner, G. *J. Magn. Resonance* 1989, 82: 198-204. Accurate measurements of long-range heteronuclear coupling constants from homonuclear 2D NMR Spectra of isotope-enriched proteins.
- Montelione, G.T.; Wagner, G. *J. Amer. Chem. Soc.* 1989, 111: 5474 - 5475. Accurate measurements of homonuclear HN-H $\alpha$  coupling constants in polypeptides using heteronuclear 2D NMR experiments.
- Montelione, G.T.; Wagner, G. *J. Magn. Reson.* 1990, 87: 183 - 188. Conformation-independent sequential NMR connections in isotope-enriched polypeptides by  $^1\text{H}$ - $^{13}\text{C}$ - $^{15}\text{N}$  triple-resonance experiments.
- Montelione, G.T.; Lyons, B.A.; Emerson, S.D.; Tashiro, M. *J. Amer. Chem. Soc.* 1992, 114: 10974 - 10975. An efficient triple resonance experiment using carbon-13 isotropic mixing for determining sequence-specific resonance assignments of isotopically enriched proteins.
- Emerson, S.D.; Montelione, G.T. *J. Am. Chem. Soc.* 1992, 114: 354-356. Accurate measurements of proton scalar coupling-constants using C-13 isotropic mixing spectroscopy.
- Lyons, B.A.; Montelione, G.T. *J. Magn. Resonance Series B.* 1993, 101: 206-209. A HCCNH triple-resonance experiment using C-13 isotropic mixing for correlating backbone amide and side-chain aliphatic resonances in isotopically enriched proteins.
- Shang, Z.G.; Swapna, G.V.T.; Rios, C.B.; Montelione, G.T. *J. Am. Chem. Soc.* 1997, 119: 9274-9278. Sensitivity enhancement of triple-resonance protein NMR spectra by proton evolution of multiple-quantum coherences using a simultaneous  $^1\text{H}$  and  $^{13}\text{C}$  constant-time evolution period.

**3. 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.

- Montelione, G.T.; Anderson, S. *Nature Struct. Biology*, 1999, 6: 11-12. Structural genomics: Keystone for a Human Proteome Project;
- Montelione, G.T.; Zheng, D.; Huang, Y.J.; Gunsalus, K.C; Szyperski, T. *Nature Struct. Biol.* 2000, 7: 982 - 985. Protein NMR spectroscopy in structural genomics.
- Acton, T.B.; Xiao, R.; Anderson, S.; Aramini, J.M.; ... Zhao, L.; Montelione, G.T. *Meth. Enzymology* 2011, 493: 21 - 60. Preparation of protein samples for NMR structure, function, and small molecule screening studies. PMC4110644.
- Montelione, G.T. *F1000 Biology Reports*, 2012, 4: 7. The Protein Structure Initiative: Achievements and visions for the future.

Koga, N.; Tatsumi-Koga, R.; Liu, G.; Xiao, R.; Acton, T.B.; Montelione, G.T.; Baker, D. *Nature* 2012, 491: 222 - 227. Principles for designing ideal protein structures. PMC3705962.

Boël, G.; Letso, R.; Neely, H.; Price, W.N.; Wong, K.H.; Su, M.; Luff, J.; Valecha, M.; Everett, J.; Acton, T.B.; Xiao, R.; Montelione, G.T.; Aalberts, D.P.; Hunt, J.F. *Nature* 2016, 529: 358 - 363. Codon influence on protein expression in *E. coli* correlates to mRNA levels. PMC5054687

**4. 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- $\alpha$  transforming growth factor, and allosteric mechanisms of molecular recognition of HRAS by the RAS-binding domain of the BRAF kinase.

Montelione, G.T.; Wüthrich, K.; Nice, E.C.; Burgess, A.W.; Scheraga, H.A. *Proc. Natl. Acad. Sci. U.S.A.* 1987, 84: 5226-5230. Solution structure of murine epidermal growth factor: determination of the polypeptide backbone chain-fold by nuclear magnetic resonance and distance geometry.

Huang, Y.J.; Hang, D.; Lu, L.J.; Tong, L.; Gerstein, M.B.; Montelione, G.T. *Mol. Cell. Proteomics* 2008, 7: 2048 - 2060. Targeting the human cancer pathway protein interaction network by structural genomics. PMC2559933

Ertekin, A.; Aramini, J.M.; Rossi, P.; Leonard, P.G.; Janjua, H.; Xiao, R.; Maglaqui, M.; Lee, H.-W.; Prestegard, J.H.; Montelione, G.T. *J. Biol. Chem.* 2012, 287: 16541 - 16549.

Human cyclin dependent kinase 2 associated protein 1 is dimeric in its disulfide-reduced state, with natively disordered N-terminal region. PMC3351331.

Aramini, J.M.; Vorobiev, S.M.; Tuberty, L.M.; Janjua, H.; Campbell, E.T.; Seethraman, J.; Su, M.; Huang, Y.P.; Acton, T.B.; Xiao, R.; Tong, L.; Montelione, G.T. *Structure* 2015, 23: 1 - 12. The RAS-binding domain of human BRAF protein serine/threonine kinase exhibits allosteric conformational changes upon binding HRAS. PMC4963008.

Song, F.; Li, M.; Li, G.; Swapna, G.V.T.; Daigham, N.S.; Xia, B.; Montelione, G.T.; Bunting, S.F. *Biochemistry* 2018 57:6581-6591. Antiparallel coiled-coil interactions mediate homodimerization of the DNA damage repair protein, PALB2.

**5. 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)

Chien, C.-Y.; Tejero, R.; Huang, Y.; Zimmerman, D.E.; Krug, R.M.; Montelione, G.T. *Nature Struct. Biol.* 1997, 4: 891 - 895. A novel RNA-binding motif in influenza A non-structural protein 1.



- Yin, C.; Khan, J.A.; Swapna, G.V.T.; Krug, R.M.; Tong, L.; Montelione, G.T. *J. Biol. Chem.* 2007, 282: 20584 -20592. Conserved surface features form the double-stranded RNA-binding site of non-structural protein 1 (NS1) from influenza A and B viruses.
- Das, K.; Ma, L-C.; Xiao, R.; Radvansky, B.; Aramini, J.; Zhao, L.; Marklund, J.; Kuo, R-L.; Twu, K.Y.; Arnold, E.; Krug, R.M.; Montelione, G.T. *Proc. Natl. Acad. Sci. U.S.A.* 2008, 105: 13092 - 13097. Structural basis for suppression by influenza A virus of a host antiviral response. PMC2522260.
- Guan, R.; Ma, L-C.; Leonard, P.G.; Amer, B.R.; Sridharan, H.; Zhao, C.; Krug, R.M.; Montelione, G.T. *Proc. Natl. Acad. Sci. U.S.A.* 2011, 108: 13468 – 13473. Structural basis for the sequence-specific recognition of human ISG15 by the NS1 protein of influenza B virus. PMC3158222.
- Aramini, J.M.; Hamilton, K.; Ma, L.C.; Swapna, G.V.; Leonard, P.G.;Ladbury, J.E.; Krug, R.M.; Montelione, G.T. *Structure* 2014, 22: 515-525. <sup>19</sup>F NMR reveals multiple conformations at the dimer interface of the nonstructural protein 1 effector domain from influenza A virus.
- Ma, L-C.; Guan, R.; Hamilton, K.; Aramini, J.; Mao, L.; Wang, S.; Krug, R.M.; Montelione, G.T. *Structure* 2016, 24: 1562-1572. A second RNA-binding site in the NS1 protein of influenza B virus.