

## CURRICULUM VITAE

### G. Marius Clore BSc., MD, PhD, FRSC, FRS

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 Sciences web page)  
<https://royalsociety.org/people/G-Marius-Clore-25341/> (Royal Society web page)  
[http://www.ae-info.org/ae/Member/Clore\\_G\\_Marius](http://www.ae-info.org/ae/Member/Clore_G_Marius) (Academia Europaea web page)  
[https://en.wikipedia.org/wiki/G\\_Marius\\_Clore](https://en.wikipedia.org/wiki/G_Marius_Clore) (Wikipedia profile)

**Born:** 6<sup>th</sup> June 1955, London (U.K.)

**Citizenship:** Dual US and British

#### Education

1976: BSc. in Biochemistry (1st Class Honors), University College London. "  
 1979: MD, University College Hospital Medical School, London. "  
 1982: PhD in Physical Biochemistry, MRC National Institute for Medical Research, London. "

#### Positions held

2011-: Appointed NIH Distinguished Investigator  
 2005-: Appointed to Title 42f, Band IV, NIH, Bethesda.  
 1996-2005: Appointed to Senior Biomedical Research Service (SBRS), NIH, Bethesda  
 1991-: Chief, Protein NMR Section, NIDDK, NIH, Bethesda  
 1988-: Senior Investigator (Federal grade equivalent to Full Professor), Laboratory of Chemical  
 Physics, NIDDK, NIH, Bethesda.  
 1984-1988: Head of the Biological NMR Group, Max-Planck Institute for Biochemistry, Martinsried,  
 Munich, Germany.  
 1980-1984: Member of the Scientific Staff at the MRC National Institute for Medical Research,  
 London.  
 1980: House Surgeon, St. Charles Hospital (St. Mary's Hospital Group), London.  
 1979: House Physician, University College Hospital, London.  
 1978-1980: Honorary Research Fellow, Department of Biochemistry, University College London.

#### Honors

2020: Elected Fellow of the Royal Society (FRS)  
 2020: Biophysical Society Innovation Award for "Seminal contributions to the development of  
 NMR for determining three-dimensional structures of macromolecules in solution  
 and for the development of paramagnetic and relaxation-based NMR experiments to  
 characterize rare, transient, heretofore invisible states of macromolecules".  
 2015: Elected Foreign Member of Academia Europaea (MAE)  
 2014: Elected Member, United States National Academy of Sciences  
 2012: Biochemical Society 2013 Centenary Award (previously known as the Jubilee Medal)  
 and Sir Frederick Gowland Hopkins Memorial Lecture (U.K.)  
 2011: Centenary Prize, Royal Society of Chemistry (U.K.)  
 2011: Distinguished NIH Investigator

**Honors (cont.)**

- 2011: Elected a Fellow of the International Society of Magnetic Resonance for "Seminal contributions in the field of biological NMR"
- 2010: Elected Fellow of the American Academy of Arts and Sciences.
- 2010: Hillebrand Prize, Washington DC Chapter of the American Chemical Society.
- 2009: NIDDK Nancy Nossal Scientific Mentorship Award.
- 2009: Elected Fellow of the Biophysical Society for "Pioneering contributions in the development of NMR spectroscopy for structural characterization of biological macromolecules".
- 2007: American Society for Biochemistry and Molecular Biology Citation for Distinguished Service in recognition of 10 years as a member of the Editorial Board of the Journal of Biological Chemistry.
- 2003: Elected Member, Lister Institute for Preventive Medicine (U.K.).
- 2001: Original member, Institute for Scientific Information (ISI) Highly Cited Researchers Database (in Biochemistry and Biology Section and Chemistry Section).
- 1999: Elected Fellow of the American Association for the Advancement of Science (AAAS).
- 1996: The Harrington Lecture, National Institute for Medical Research (U.K.)
- 1993: Dupont-Merck Young Investigator Award of the Protein Society.
- 1993: 1993 National Institutes of Health Lecture.
- 1992: National Institutes of Health Director's Award.
- 1991: Elected Fellow of the Washington Academy of Sciences.
- 1990: Distinguished Young Scientist Award of the Maryland Academy of Sciences.
- 1990: Scientific Achievement Award (Biological Sciences) of the Washington Academy of Sciences.
- 1990: Elected Fellow of the Royal Society of Chemistry (FRSC).
- 1982-1984: Lister Institute Research Fellow.
- 1977: Francis Walsche Neurology Prize, University College Hospital Medical School, London.

**Summary of Research Interests**

My research is centered upon the development and application of nuclear magnetic resonance (NMR) to study the structure and dynamics of biological macromolecules and their complexes in solution. Particular emphasis is being placed on novel approaches to extending NMR to larger and more complex systems, especially complexes involved in signal transduction and transcriptional regulation, and exploring fundamental questions associated with protein dynamics, macromolecular interactions and recognition processes. Currently we are exploiting the unique properties of NMR to detect and characterize sparsely-populated states of macromolecules. Many important biological processes proceed through transient intermediate states that comprise only a small fraction of the overall population of a molecular system at equilibrium, and, as a result, are invisible (i.e. dark) to conventional biophysical techniques (including crystallography, cryo-electron microscopy and single molecule spectroscopies). These studies, which have provided new insights into macromolecular recognition, rely on the ability of NMR to amplify, through exchange phenomena, the effect of the invisible "dark" state on some NMR observable (generally a relaxation property) so that its footprint is readily observed in measurements on the NMR visible species. Examples of such phenomena that we have studied include the search processes whereby transcription factors locate their specific DNA binding site within an overwhelming sea of non-specific DNA; the role of encounter complexes in protein-protein association; the interplay of conformational selection and induced fit in protein-ligand interactions; and transient interactions of intrinsically disordered and partially folded polypeptides with large megadalton macromolecular assemblies including highly heterogeneous aggregates involved in amyloid protofibril formation and the GroEL chaperonin molecular machine.

**Membership of Societies**

- 1976-: Biochemical Society (U.K.)  
 1976-: Royal Society of Chemistry (U.K.).  
 1989-: American Chemical Society  
 1990-: Protein Society  
 1991-: Washington Academy of Sciences  
 1991-: American Society for Biochemistry and Molecular Biology  
 1999-: American Association for the Advancement of Science  
 2008-: Biophysical Society  
 2010-: American Academy of Arts and Sciences  
 2014-: National Academy of Sciences  
 2015-: Academia Europaea  
 2020-: The Royal Society

**Editorial work**

- 1987-2003: Member of the Editorial Board of Protein Engineering. "  
 1993-: Member of the Editorial Board of Structure. "  
 1993-1997: Associate Editor of Protein and Peptide Letters. "  
 1994-1999: Member of the Editorial Board of Protein Science. "  
 1996-2001 Member of the Editorial Board of the Journal of Biological Chemistry. "  
 1998-: Member of the Editorial Board of the Journal of Magnetic Resonance.  
 2002-2007: Member of the Editorial Board of the Journal of Biological Chemistry.  
 2003-2013: Series Editor for the Structural Biology, Chemical Biology and Informatics Section of "  
                   the Royal Society of Chemistry Biomolecular Biosciences Book Series.  
 2003-: Member of the Editorial Board of PEDS (Protein Engineering, Design and Selection).  
 2009-2014: Member of the Editorial Board of the Journal of Biological Chemistry.

**Peer review**

*Refereeing of papers for a number of journals including:*

Nature, Science, Cell, Mol. Cell, Proc. Natl. Acad. Sci., J. Biol. Chem., J. Mol. Biol., Biochemistry, J. Am. Chem. Soc., Structure, Nature Struct. Mol. Biol., Nature Methods, EMBO Journal, Nucleic Acids " Research, Proteins, Prot. Sci., Prot. Eng., J. Magn. Reson., J. Biomol. NMR, PEDS, RSC Mol. " Biosystems, Angewandte Chemie. "

*Refereeing of grants for the following agencies: "*

National Science Foundation, National Institutes of Health, Medical Research Council (U.K.), " Welcome Trust (U.K.), Cancer Research U.K., Swiss National Foundation for the Advancement of " Scientific Research, Belgium Incentive Program for Fundamental Research in the Life Sciences, " Swedish Natural Science Research Council, Australian Research Council, Israel Science Foundation, " United States-Israel Binational Science Foundation, ACS Petroleum Research Fund, Georgian National Science Foundation, French National Research Agency (ANR), European Research Council, Japanese Society for the Promotion of Science. "

**Service**

- 1989-: Adviser in the U.S. National Research Council (NRC) Research Associateship Program.  
 1989: Special Study Section of the Division of Research Resources, Biomedical Research Technology Program, NIH.  
 1992: Subcommittee on Structural Biology of the Health and Environmental Research Advisory Committee of the Department of Energy.  
 1994: Special Reviewer, Biophysical Chemistry (BBCB) Study Section, NIH  
 1994: External Scientific Reviewer, H.E.J. Research Institute of Chemistry, University of Karachi, Pakistan.  
 1994-2000: Chairman, NIH-Wide Tenure and Promotions Committee for Computer Scientists.

**Service (cont.)**

- 1996-1998: Member, Membership Committee, Protein Society
- 1996-: Preceptorship in the Pharmacology Research Associate (PRAT) Program of the National Institute for General Medical Sciences.
- 1997: NIH Special Emphasis Panel on Structural Biology of AIDS Related Proteins.
- 1997: Member of Review Panel for the John Sealy Memorial Endowment Fund for Biomedical Research.
- 1998-2001: Co-Chair, Intramural NIH-Wide Structural Biology Interest Group.
- 1998: Reviewer for the qinquennial assessment (1994-1998) of the MRC Center for Protein Engineering at the University of Cambridge, U.K.
- 1998: Member of NMR Task Force of the Research Collaboratory for Structural Bioinformatics.
- 2002: Member, Special Emphasis Panel on 900 MHz NMR Spectrometers, Center for Scientific Review, NIGMS, NIH.
- 2004: Reviewer for the qinquennial assessment (1999-2003) of the MRC Center for Protein Engineering at the University of Cambridge, U.K.
- 2005-2009: Member, RCSB (PDB-BMRB) Task Group on NMR
- 2006-2011: Member of the Scientific Advisory Board of the Institute of Biotechnology at the University of Helsinki, Finland.
- 2007-2012: Member, Executive Committee of the NIH/Oxford/Cambridge Scholars Program.
- 2009: Member of Ad Hoc NIH Review Panel for High End NMR Shared Instrumentation Grants.
- 2009: Member of the UCLA-DOE Institute for Genomics and Proteomics Cooperative Agreement Review Panel.
- 2016: Selection Committee for the Raymond and Beverley Sackler International Prize in the Physical Sciences
- 2016-: Member of the NIH Intramural AIDS Targeted Antiviral Program Scientific Review Committee.
- 2018-2020: European Science Foundation, College of Experts Reviewers
- 2020-: Ad Hoc reviewer for Consensus Study Reports of the National Academies of Science, Engineering and Medicine.
- 2020-: Director, NIDDK Computational Biomolecular Magnetic Resonance Core.
- 2020-: Ad Hoc reviewer for the National Academy of Sciences BBCSS report on “Consideration of Generational Issues in Workforce Management and Employment Practices”

**Competitive Grants**

- 1985-1989: Deutsche Forschungsgemeinschaft (DFG) Grant No. Gr 658/3-1 and Gr 658/3-2. Protein engineering: biochemical and molecular approaches in the study of DNA-protein interactions at the atomic level - The cAMP receptor protein (CRP or CAP) of *Escherichia coli*.
- 1985-1987: Deutsche Forschungsgemeinschaft (DFG) Grant No. Cl 86/1-1. Determination of three-dimensional structures of oligonucleotides and proteins in solution by NMR spectroscopy: refinement using restrained least squares minimization and restrained molecular dynamics.
- 1986-1988: Deutsche Forschungsgemeinschaft (DFG) Grant No. Gr 658/4-1. Stereochemistry and conformational flexibility of the binding of peptide inhibitors to serine and aspartyl proteases: combined use of two-dimensional transferred nuclear Overhauser enhancement spectroscopy, restrained molecular dynamics and computer graphics.
- 1987-1989: Bundesministerium für Forschung und Technologie (BMFT) Grant No. 321-4003-0318909A (30/3003/68327). Eureka Project: Determination of three-dimensional structures of proteins, nucleic acids and their complexes in solution (DM 6.712 million).

**Competitive grants (cont.)**

- 1987-1990: AIDS Intramural Program of the Office of the Director of the NIH: Structural studies of viral proteins and their complexes with drugs and ligands by nuclear magnetic resonance (\$1.0 million).
- 1991-1992: AIDS Intramural Program of the Office of the Director of the NIH: Structural Studies of AIDS proteins and other related proteins by Nuclear Magnetic Resonance (\$1.0 million).
- 1993-1994: AIDS Intramural Program of the Office of the Director of the NIH: Structural Studies of AIDS proteins and other related proteins by Nuclear Magnetic Resonance (\$1.1 million).
- 1995-1996: AIDS Intramural Program of the Office of the Director of the NIH: Structural Studies of AIDS proteins and other related proteins by Nuclear Magnetic Resonance (\$2.15 million).
- 1997-1998: AIDS Intramural Program of the Office of the Director of the NIH: Structural Studies of AIDS proteins and other related proteins by Nuclear Magnetic Resonance (\$1.225 million).
- 1999-2000: AIDS Intramural Program of the Office of the Director of the NIH: NMR Structural Studies of HIV Proteins Related to Fusion and Integration (\$1.064 million).
- 2001-2002: AIDS Intramural Program of the Office of the Director of the NIH: NMR Structural Studies of HIV Proteins Related to Fusion and Integration (\$890,000).
- 2003-2004: AIDS Intramural Program of the Office of the Director of the NIH: Structural and Biophysical Studies Aimed at Targeting HIV-1 gp41 and Integrase (\$600,000).
- 2005-2006: AIDS Intramural Program of the Office of the Director of the NIH: Structural, Biophysical and Biochemical Studies Related to HIV-1 Fusion, HIV-1 Protease and HIV-1 Integrase (\$520,000).
- 2007-2008: AIDS Intramural Program of the Office of the Director of the NIH: Structural and Biophysical Studies of AIDS and AIDS Related Systems. (\$877,200).
- 2009-2010: AIDS Intramural Program of the Office of the Director of the NIH: Structural and Biophysical Studies of AIDS and AIDS Related Systems. (\$1.077 million).
- 2011-2012: AIDS Intramural Program of the Office of the Director of the NIH: NMR, EPR and X-ray scattering studies of HIV and HIV related proteins (\$701,000)
- 2013-2014: AIDS Intramural Program of the Office of the Director of the NIH: NMR, EPR and X-ray scattering studies of HIV and HIV related proteins (\$434,000)
- 2015-2016: AIDS Intramural Program of the Office of the Director of the NIH: NMR, EPR and X-ray scattering studies of HIV-1 Gag, reverse transcriptase and gp41 (\$880,225)
- 2017-2018: AIDS Intramural Program of the Office of the Director of the NIH: Structure, dynamics and interactions of HIV-1 proteins by NMR and EPR (\$929,000).
- 2019-2020: Office of AIDS Research NIH Strategic Funds: Structure, dynamics and interactions of HIV-1 reverse transcriptase and mechanism of viral entry by NMR and EPR spectroscopy (\$2.6 million)

**Invited speaker at conferences****1978**

Japanese-American Symposium on Cytochrome Oxidase, Kyoto, Japan (June).

**1980**

Second Priestley Conference on Oxygen and Life, Birmingham, U.K. (Sept.).

**1985**

German Biophysical Society Meeting on Molecular Biophysics, Hunfeld, Germany (April).

Sixth Delaware NMR Symposium, University of Delaware (June).

Fourth Conversation in Biomolecular Sterodynamics, State University of New York at Albany (June). "

**Invited speaker at conferences (cont.)**

DGF Colloquium on Biophysics of Cellular Organization, Konstanz, Germany (Oct.)  
 Fourteenth Aharon Katzir-Katchalsky Conference on the Biological Significance of Conformational Changes in DNA and DNA-Protein Complexes, University of Bielefeld, Germany (Oct.)

**1986**

British Biophysical Society Meeting on DNA Structure and Gene Expression, University of Kent, U.K. (April).  
 DFG Colloquium on Non-Covalent Interactions, Darmstadt, Germany (April).

International Workshop on Structure and Dynamics of Proteins, INSERM and CNRS, Paris, France (July).

Marcus Wallenberg Symposium of the European Biophysical Societies Association on Structure, Dynamics and Function of Biomolecules, Satsjobaden, Stockholm, Sweden (July).

**1987**

Molecular Graphics Society Meeting on the Generation of Three-Dimensional Structures from Distance Information, University of York, U.K. (Jan.).

Protein Engineering '87, Oxford, U.K. (April).

35th International Colloquium on Protides of the Biological Fluids, Brussels, Belgium (April).

Protein Engineering Workshop, National Research Council Canada, Montreal (May).

CECAM workshop on Force Fields for Simulations of Macromolecules, Paris, France (July).

EMBO Course on Protein Crystallography, Uppsala, Sweden (Sept.).

Fourth European Seminar on Computer Aided Molecular Design, Helsingor, Denmark. (Oct.).

**1988**

Western Winter Workshop, Frontiers of NMR, UCLA Symposia on Molecular and Cellular Biology, Lake Tahoe, California (March).

Mosbach Colloquium of the Deutsche Gesellschaft für Biologische Chemie on Protein Structure and Enzyme Catalysis, Mosbach, Germany (April).

9th European Experimental NMR Conference, Bad Aussee, Austria (May).

Colloquium of the German Chemical Society on Molecular and Cellular Recognition, Irsee, Germany (April).

Meeting of the American Crystallographic Association, Philadelphia (July).

13th International Conference on Magnetic Resonance in Biological Systems, University of Wisconsin, Madison (Aug.).

Sixth Annual Smith, Kline & French Research Symposium on Protein Design and the Development of New Therapeutics and Vaccines, King of Prussia, Pennsylvania (Nov.).

16th Aharon Katzir-Katchalsky Conference on Dynamics in Molecular and Cellular Biology, Brussels, Belgium (Nov.).

**1989**

Symposium on Experimental and Theoretical Aspects of the Interactions that Determine Protein Conformation, National Institutes of Health, Bethesda (Jan.).

UCLA Colloquium on Frontiers of NMR in Molecular Biology, Park City, U.S.A. (Jan.).

Symposium sponsored by the Drug Information Association on Research Perspectives in Structural Biology and Chemistry, San Francisco (Jan.).

30th Experimental Nuclear Magnetic Resonance Conference, Asilomar, California (April).

19th FEBS Meeting, Rome, Italy (July).

2nd Symposium of Protein Engineering, Kobe, Japan (Aug.).

Spetsai Summer School on Molecular and Cellular Biology, "Protein and Genetic Engineering", Island of Spetsai, Greece (Sept.).

3rd Missouri Magnetic Resonance Symposium, University of Missouri, Columbia (Oct.).

**Invited speaker at conferences (cont.)****1990**

34th Annual Meeting of the Biophysical Society, Baltimore, Maryland (Feb.).

The Second York Meeting on the Generation of Structures from Distance Information, University of York, U.K. (April).

NATO Advance Research Workshop on Computational Aspects of the Study of Biological Macromolecules by NMR, Il Ciocco, Italy (June).

Whistler Conference on Expanding Frontiers in Polypeptide and Protein Structural Research, British Columbia, Canada (July).

14th International Conference of Magnetic Resonance in Biological Systems, University of Warwick, U.K. (Sept.)

2nd Nordic Protein Engineering Conference in Helsingør, Denmark (Oct.).

29th Eastern Analytical Symposium on 3D and other Novel Approaches in Protein NMR Spectroscopy, Somerset, New Jersey (Nov.).

**1991**

Keystone Meeting on Frontiers of NMR in Molecular Biology, Colorado (April).

Symposium on the Symbiosis of NMR, X-ray Crystallographic and Computational Techniques at American Society for Biochemistry and Molecular Biology Meeting, Atlanta, Georgia (also symposium organizer) (April).

Conference on Aspects of Drug Design, Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign (June).

Conference on New Developments in Drug Discovery and Drug Design, IBC Conferences, Philadelphia (Oct.).

30th Eastern Analytical Symposium on NMR Methods for Peptides and Proteins, Somerset, New Jersey (Nov.).

**1992**

33rd Experimental Nuclear Magnetic Resonance Conference, Asilomar, California (March).

Mid-Atlantic Protein Crystallography workshop, Center for Advanced Research in Biotechnology, Maryland (May).

Conference on 2D, 3D and 4D NMR: Developments and Applications, Wissembourg, France (May).

XV International Conference on Magnetic Resonance in Biological Systems, Jerusalem, Israel (Aug.).

Symposium on Structural Biology, NIH Research Festival 1992, Bethesda (Sept.).

Southeastern Magnetic Resonance Conference, North Carolina State University (Oct.).

Macromolecular Crystallography, Cold Spring Harbor, New York (Oct.).

**1993**

Symposium on Structure and Function of Growth Factors, University of British Columbia, Vancouver, Canada (Jan.).

Biophysical Society Workshop on Single-Stranded Nucleic Acid-Binding Proteins, Washington D.C. (Feb.).

Keystone Meeting on Frontiers of NMR in Molecular Biology, Taos, New Mexico (March).

Protein Society Meeting, San Diego (July).

Workshop on Structural Biology and Respiratory Enzymes: Crystallography and NMR of Membrane Proteins, National Institutes of Health, Maryland (Aug.).

8th International Lymphokine Workshop and 4th International Workshop on Cytokines, Osaka, Japan (Oct.).

Cyanamid International Analytical Conference, Princeton, New Jersey (Oct.).

Macromolecular Crystallography, Cold Spring Harbor, New York (Oct.).

**Invited speaker at conferences (cont.)****1994**

Gordon Research Conference on Isotopes in Chemistry and the Life Sciences, Oxnard, California (March).  
 Symposium on Cytokine and Cytokine Receptor Structures and Structure/Function Relationships, FASEB Experimental Biology '94 Meeting, Anaheim, California (April).  
 Symposium on NMR of Biomolecules and Macromolecular Interactions, 28th Middle Atlantic Regional Meeting of the American Chemical Society (May).  
 XVIth International Conference on Magnetic Resonance in Biological Systems, Veldhoven, The Netherlands (Aug.).  
 10th International Conference on Methods in Protein Structure Analysis, Utah (Sept).  
 7th International Conference of the Inflammation Research Association, Pennsylvania (Sept.).  
 IBC Conference on Chemokines: Research for Therapeutics and Drug Development, Washington DC (Sept.).  
 International Symposium on NMR as a Structural Tool for Macromolecules: Current Status and Future Directions, Indiana University, Indianapolis (Oct.).  
 Macromolecular Crystallography, Cold Spring Harbor, New York (Oct.).

**1995**

Symposium on p53 and the Cell Cycle, University of York, U.K. (April).  
 Keystone Meeting on Frontiers of NMR in Molecular Biology IV, Keystone, Colorado (April).  
 Ninth Symposium on the Structure of AIDS related systems and their application to targeted drug design, National Institute of General Medical Sciences, Bethesda, Maryland (June).  
 Ninth Conversation in Biomolecular Stereodynamics, Albany, New York (June).  
 Proteins Gordon Conference, New Hampshire (June).  
 International NMR Meeting of the Royal Society of Chemistry, Manchester, U.K. (July).  
 Symposium on Biomolecular Structure and Function at the Silver Anniversary of the Northeast Regional Meeting of the American Chemical Society, Rochester, New York (Oct.).  
 Macromolecular Crystallography, Cold Spring Harbor, New York (Oct.).  
 American Association for Cancer Research Conference on "The Molecular Basis of Gene Transcription", San Diego (Dec.).

**1996**

Symposium on Advanced NMR Techniques and Biomolecular Structure, International Congress of the Pacific Basin Societies, Honolulu (Dec.).  
 Second International Symposium on Reversible Associations in Structural and Molecular Biology, Bethesda, Maryland (Feb.).  
 Science Innovation Symposium on Structural Biology, 1996 Annual Meeting of the American Association for the Advancement of Science (AAAS), Baltimore (Feb.).  
 International Symposium on Perspectives on Protein Engineering, Montpelier, France (March).  
 Symposium on the Biology and Biochemistry of Chemokines and Their Receptors, Frederick, Maryland (May).  
 Symposium entitled "Database III, 25 years of the PDB" at the XVII Congress and General Assembly of the International Union of Crystallography, Seattle (Aug.).  
 XVII International Conference on Magnetic Resonance in Biological Systems, Keystone, Colorado (Aug.).  
 Karolinska Institute 6th Summer School on "Understanding Protein Structure Determination", Stockholm, Sweden (Sept.).  
 Macromolecular Crystallography, Cold Spring Harbor, New York (Oct.).

**1997**

Keystone Symposium on Frontiers of NMR in Molecular Biology V, Taos, New Mexico (Feb.).  
 Gordon Conference on Protons and Membrane Reactions, California (Feb.).

**Invited speaker at conferences (cont.)**

5th Annual Advances in NMR Applications Symposium, Orlando, Florida (March).  
 2nd Joint Symposium of the Strategic Program for Innovative Research on AIDS Treatment and the National Cooperative Drug Discovery Groups for the Treatment of HIV Infection on "New Opportunities for HIV Therapy: From Discovery to Clinical Proof-of-Concept", Vienna, Virginia (June).  
 6th International Conference on Perspectives in Protein Engineering, Norwich, U.K. (June).  
 Gordon Conference on Proteins, Holderness, New Hampshire (June).  
 Conference on Rational Drug Design, National Managed Health Care Congress, Washington DC (Sept).  
 Sixth International Symposium on the Synthesis and Applications of Isotopes and Isotopically Labeled Compounds, Philadelphia (Sept.).  
 Workshop on Future Developments of CNS (Crystallography and NMR System) for Macromolecular Structure Determination, Cold Spring Harbor, New York (Nov.).  
 1st Meeting of the HIV Drug Resistance Program, NCI, Frederick, Maryland (Dec.).

**1998**

Novartis Workshop on "Structure Based Drug Design", Summit, New Jersey (March).  
 Symposium on NMR Studies of Biological Macromolecules, Danish NMR Center Copenhagen, Denmark (March).  
 Pharmacia-Upjohn Symposium on "NMR of Biological Macromolecules", Stockholm, Sweden (May).  
 NIGMS AIDS Symposium, Bethesda, Maryland (June).  
 18th International Conference on Magnetic Resonance in Biological Systems, Tokyo, Japan (Aug.).  
 1st Annual Bruker Atlantic Coast Conference, University of Maryland, Baltimore County (Oct.).

**1999**

Keystone Symposium on Frontiers of NMR in Molecular Biology VI, Breckenridge, Colorado (Jan.).  
 2nd HIV Drug Resistance Program Think Tank Meeting, NCI, Frederick (Feb.).  
 Proteins Gordon Research Conference, Holderness School, New Hampshire (June).  
 European Science Foundation Meeting on NMR in Molecular Biology, Granada, Spain (July).  
 Tsukuba NMR 99 Meeting, Tsukuba, Japan (Oct.).  
 6th Peptide Seminar, Osaka, Japan (Oct.). "

**2000**

Symposium on "Frontiers of Protein Structure and Function" at the Year 2000 ACS Meeting, San Francisco (March).  
 2nd Frederick Workshop on the Cell Biology of Viral Entry, NCI-FCRDC, Frederick, Maryland (May).  
 Workshop on the Role of HMG Proteins in Chromatin Structure, Gene Expression and Neoplasia, National Institutes of Health, Bethesda, Maryland (May).  
 NIGMS AIDS Symposium, Bethesda, Maryland (June).  
 gp160 Think Tank, organized by the Vaccine Research Center (NIH), MIT Endicott House, Massachusetts (Aug.).  
 Symposium on "Understanding Phage Display: Structure, Biology and Applications", Simon Fraser University, Vancouver (Sept.).

**2001**

Keystone Symposium on Frontiers of NMR in Molecular Biology VII, Big Sky, Montana (Jan.).  
 Gordon Conference on Computational Aspects of Biomolecular NMR, Il Cioco, Italy (May).  
 12<sup>th</sup> Conversation in Biomolecular Stereodynamics, Albany (June).  
 Saul Roseman's 80th Birthday Symposium, Johns Hopkins, Baltimore (June).  
 Proteomics Plenary Session, NIH Research Festival, Bethesda (Oct.).  
 Second HIV Drug Resistance Symposium, Chantilly, Virginia (Dec.). "

**Invited speaker at conferences (cont.)****2002**

HIV Drug Resistance Program 2002 Think Tank Meeting, Frederick, Maryland (March).  
 NIGMS 16th Annual Meeting on the Structure of AIDS-Related Systems and their Applications to Targeted Drug Design., Bethesda, Maryland (June).  
 XXth International Conference on Magnetic Resonance in Biological Systems, Toronto (Aug.).  
 West Coast Retrovirus Meeting, Palm Spring, California (Oct.).

**2003**

2003 HIV Drug Resistance Program Workshop, Frederick, Maryland (March).  
 NIGMS 16th Annual Meeting on the Structure of AIDS-Related Systems and their Applications to Targeted Drug Design., Bethesda, Maryland (June).  
 Eastern Analytical Symposium, Somerset, New Jersey (Nov.).

**2004**

Washington Area NMR Group Meeting, Bethesda, Maryland (Feb.).  
 Keystone Symposium on Frontiers in Structural Biology, Snowbird, Colorado (April).  
 45th ENC (Experimental NMR Conference), Asilomar, California (April).  
 Protein Structure, Catalysis and Dynamics: Molecular Assemblies Symposium at the 8th IUBMB Conference and Annual American Society for Biochemistry and Molecular Biology Meeting, Boston (June).  
 NIGMS Symposium on Pharmacology and Therapeutics: The Road to Identification of Molecular Targets and their Structures, Bethesda (Sept.).  
 15<sup>th</sup> International Society of Magnetic Resonance (ISMAR) meeting, Florida (Oct.).

**2006**

NMR Symposium on "NMR as a Tool in Biotechnology", Center for Advanced Research in Biotechnology, Maryland. (May).  
 22nd International Conference on Magnetic Resonance in Biological Systems (ICMRBS), Gottingen, Germany (Aug.).  
 CECAM Workshop on Protein Folding and Misfolding: Bringing Theory Close to Experiment, Lyon, France (Sept.).  
 Gordon Conference on "Computational Aspects of Biomolecular NMR", Aussois, France (Sept.).

**2007**

Keystone Symposium on Frontiers of NMR in Molecular Biology X, Snowbird, Utah (January).  
 2007 Danish NMR Symposium, Copenhagen (June).  
 16th Triennial Conference of the International Society of Magnetic Resonance, Taiwan (October). "

**2008**

2nd International Conference on Molecular Perspectives on Protein-Protein Interactions, Dubrovnic, Croatia (June).  
 Structure Determination of Biological Macromolecules by Solution NMR, National Institutes of Health (Aug.).  
 23rd International Conference on Magnetic Resonance in Biological Systems, San Diego (Aug.).

**2009**

HIV Protease and Beyond: the Past, Present and Future of HIV Structural Biology, NCI, Frederick (Jan).  
 Mesilla Chemistry Workshop on Multi-Scale Modeling of Biological Molecules, Mesilla, New Mexico (Feb.).  
 Keystone Symposium on Frontiers of NMR in Molecular Biology XI, Santa Fe, New Mexico (Feb.).  
 VIII European Symposium of the Protein Society, Zurich (June).

**Invited speaker at conferences (cont.)**

16th Albany Conversation, Albany (June).  
 Keystone Symposium on Protein Dynamics, Allostery and Function, Keystone (June).  
 ACS Symposium on Protein Dynamics and Function, ACS National Meeting, Washington DC (Aug.)  
 3rd Asian-Pacific NMR Symposium, Korea (Oct.) "

**2010**

Gordon Conference on Biomolecular Interactions and Methods, Galveston, Texas (Jan.). "  
 Keystone Symposium on Structural Biology, Breckenridge, Colorado (Jan.) "  
 CMC Strategy Forum, Bethesda (Jan).  
 4th CARB NMR symposium, Center for Advanced Research in Biotechnology, Maryland. (May). "  
 Joint Euromar 2010 and 17th ISMAR Conference, Florence, Italy (July)  
 24th International Conference on Magnetic Resonance in Biological Systems, Cairns, Australia (Aug.) "  
 3rd International Meeting on Molecular Perspectives on Protein-Protein Interactions, Coasta Brava, "  
 Spain (Nov.)

**2011**

Keystone Symposium on Frontiers of NMR in Biology, Big Sky, Montana (January) "  
 16th Structural Biology Symposium, University of Texas Medical Branch, Galveston, Texas (April) "  
 52nd Experimental NMR Conference (ENC), Asilomar (April) "  
 Gordon Conference on Computational Aspects of Biomolecular NMR, Il Ciocco, Italy (May)  
 Symposium on Combined Techniques for Determining Structures of Proteins and RNA Complexes and "  
 RNA in Solution, American Crystallographic Association Annual Meeting, New Orleans (June)  
 Symposium on Macromolecular Structure and Dynamics, Seoul, South Korea (June)  
 Symposium on "DNA Search: from Biophysics to Cell Biology", Safed Israel (September)  
 Barcelona Biomed Conference on Macromolecular Dynamics, Spain (October)  
 Saul Roseman Memorial Symposium, Johns Hopkins, Baltimore (December)

**2012**

ChemComm-RSC Prizes and Awards Symposium, Imperial College London (Feb.) "  
 12<sup>th</sup> Chianti workshop on BioNMR, Tuscany, Italy (June). "  
 25th International Conference on Magnetic Resonance in Biological Systems, Lyons, France (Aug.) "  
 Special Symposium on Protein Structure and Function, University of Kansas (Oct.)  
 51<sup>st</sup> Annual Meeting of the Nuclear Magnetic Resonance Society of Japan, Nagoya, Japan (Nov.) "  
 Biochemical Society (U.K.) Awards Symposium, Cambridge (Dec.) "

**2013**

Keystone Symposium on Frontiers of NMR in Biology, Snowbird (January) "  
 NMR Symposium at the Institute of Bioscience and Biotechnology Research, Maryland (May) "

**2014**

25 years of Chaperone Research: Protein Folding In and Out of Anfinsen's Cage, Arolla, Switzerland (January) "  
 Mini-symposium for NIH's newest members of the National Academy of Sciences, Bethesda (June) "  
 Euromar Meeting, ETH Zurich (June/July) "  
 26<sup>th</sup> International Conference on Magnetic Resonance in Biological Systems, Dulles, Texas (Aug.) "

**2015**

5<sup>th</sup> International Conference on Molecular Perspectives on Protein-Protein Interactions, Ontario (May)  
 Proteins Gordon Conference, Holderness School, New Hampshire (June)

**Invited speaker at conferences (cont.)****2016**

Symposium on Understanding Enzymatic Catalysis across Multiple Timescales: Experiment and Theory, Spring 2016 National ACS Meeting, San Diego (March)

57<sup>th</sup> Experimental NMR Conference (ENC), Pittsburgh (April)

Symposium on Biomolecular Structure, Dynamics and Function, Brown University, Providence, Rhode Island (April)

27<sup>th</sup> International Conference on Magnetic Resonance in Biological Systems, Kyoto, Japan (Aug.)

Symposium on Intrinsically Disordered Proteins. Summer 2016 National ACS Meeting, Philadelphia (Aug.)

**2017**

International Society of Magnetic Resonance International Meeting, Quebec City, (July)

**2018**

Protein folding: Biophysics, Biology & Beyond, University of Maryland (May)

7<sup>th</sup> Biennial NMR Symposium, Institute for Bioscience and Biotechnology Research (IBBR), Maryland (May)

28<sup>th</sup> International Conference on Magnetic Resonance in Biological Systems, Dublin, Ireland (Aug.)

**2019**

NIH Biophysical Methods Boot Camp, Bethesda, Maryland (May) "

Gordon Conference on Computational Aspects – Biomolecular NMR, Les Diableret, Switzerland (June) "

**2020**

Biophysical Society Annual Meeting Awards Symposium, San Diego (February)

Symposium on Structure and Dynamics of Amyloids and Precursors by NMR, 259<sup>th</sup> Annual Meeting of the American Chemical Society, Philadelphia (March)

Symposium on "Dynamic Ensembles Cell Signaling and Drug Discovery in honor of Ruth Nussinov", American Chemical Society National Meeting, San Francisco (August).

## Former trainees

- Michael Nilges, PhD (Graduate student 1985-1987; Post-doc 1987-1989): Chair, Department of Structural Biology and Chemistry, Institut Pasteur, Paris, France.
- Hartmut Oschkinat, PhD (Post-doc 1987-1989): Full Professor, Institute for Molecular Pharmacology, University of Berlin, Germany.
- Tad Holak, PhD (Post-doc 1988-1989): Full Professor, Uniwersytet Jagiellonski, Krakow, Poland (2016-present). Previously group leader, Max-Planck Institute for Biochemistry, Martinsried, Munich, Germany (1990-2015).
- Paul Driscoll, PhD (Post-doc 1987-1990): Full Professor, Department of Biochemistry, University College London (U.K.) and Member of Scientific Staff, MRC National Institute for Medical Research, London.
- July Forman-Kay, PhD (Graduate student 1989-1992; Post-doc 1992-1993): Full Professor, Department of Biochemistry, University of Toronto and Scientific Staff, Hospital for Sick Children, Toronto.
- Mark Robien, MD (Howard Hughes medical student, 1990-1992): Medical Officer, Division of Allergy, Immunology and Transplantation, NIAID, NIH.
- Bob Powers, PhD (Post-doc 1990-1993): Full Professor, University of Nebraska.
- Dan Garrett, PhD (Post-doc 1990-1995): Staff scientist, Laboratory of Chemical Physics, NIDDK.
- James Omichinski, PhD (Post-doc, Staff fellow and Senior Staff fellow, 1989-1997): Full Professor, University of Montreal, Canada.
- Bruce Grasberger, PhD (Post-doc, 1989-1993): Senior Scientist, Johnson & Johnson, New Brunswick, Pennsylvania.
- Patricia Lodi LiWang, PhD (Post-doc and Cancer Research Institute Fellow, 1991-1995): Full Professor, University of California Merced.
- Milton Werner, PhD (Post-doc, 1991-1996): Founder, President and CEO, Inhibikase Therapeutics, Inc, Atlanta, Georgia (2008-present). Previously, Associate Professor, Rockefeller University (1996-2007); and Vice President, Discovery Research, Celtaxsys Inc, Georgia (2007-2008).
- Jun Qin, PhD (Post-doc, 1993-1996): Full Professor of Molecular Medicine, Lerner Research Institute, Cleveland Clinic Foundation, Cleveland.
- Robert Clubb, PhD (Post-doc and Leukemia Society of America Fellow, 1993-1996): Full Professor, Department of Chemistry and Biochemistry, UCLA, Los Angeles.
- James Ernst, PhD (Pre-doctoral student, 1994-1995): Senior Scientist, Genentech, San Francisco.
- Wm. Dexter Kennedy, MD (Post-doc 1994-1996): Senior Director, Alios BioPharma, San Francisco.
- Jeff Huth, MD, PhD (Post-doc, 1994-1997): Founder and CEO of ScopiaRx, LLC, Ohio. Previously, Senior Scientist, Abbott Laboratories.
- Mengli Cai, PhD (Post-doc, 1996-1998): Staff scientist, Laboratory of Chemical Physics, NIDDK.
- Logan Donaldson, PhD (Post-doc 1996-1998): Full Professor, Department of Biology, York University, Toronto, Canada.
- John Kuszewski, PhD (graduate student 1994-1998, Post-doc 1998-2001): Staff scientist, Center for Information Technology, NIH.
- Mary Starich, PhD (Post-doc 1995-1998): Staff scientist, Structural Biophysics Laboratory, NCI.
- Mats Wikström, PhD (Post-doc 1995-1997): Senior Scientist, Amgen, Thousand Oaks, California. Previously Full Professor, Faculty of Health Sciences, University of Copenhagen.
- Silke Schumaker, PhD (Post-doc 1995-1997): CEO, Anadys Pharmaceuticals GmbH, Heidelberg, Germany.
- Carole Bewley, PhD (Post-doc and Cancer Research Institute Fellow, 1995-1999): Senior Investigator, Section Chief and Deputy Laboratory Chief, Laboratory of Bioorganic Chemistry, NIDDK.
- Michael Caffrey, PhD (Post-doc, 1996-1999) Associate Professor, University of Illinois at Chicago.
- Kai Huang, PhD (Post-doc 1997-1999): NMR facility manager, Structural Biology NMR Facility, Northwestern University.
- Elizabeth Murphy, PhD (Graduate student 1995-1999): Chief, Clinical Informatics Section, Office of the Clinical Director, National Eye Institute, NIH.

**Former trainees (cont.)**

- Demetrios Braddock, MD, PhD (Post-doc and Pathology Resident, NCI 1997-2000): Associate Professor, Department of Pathology, Yale University.
- Elliott Gozansky, MD, PhD (Post-Doc, 1998-2000): Assistant Professor, Department of Radiology, Thoracic Imaging Division, University of Pittsburgh Medical Center, Pittsburgh, Pennsylvania.
- Gus Wang, PhD (Post-doc 1998-2002): Associate Professor, Department of Pathology and Microbiology, Eppley Cancer Institute, University of Nebraska Medical Center.
- Gabriel Cornilescu, PhD (Post-doc and PRAT Fellow, 2000-2002): Associate Researcher, Nuclear Magnetic Resonance Facility (NMRFAM), University of Wisconsin, Madison.
- Michal Komlosch, PhD (Post-doc, 2001-2004): Staff scientist, NICHD, NIH.
- David Williams, MD, PhD (Post-doc and PRAT Fellow, 2001-2005): Associate Professor, Department of Pathology and Laboratory Medicine, University of North Carolina School of Medicine, Chapel Hill
- Junji Iwahara, PhD (Post-Doc 2002-2006): Associate Professor, Department of Biochemistry and Molecular Biology, University of Texas Medical Branch, Galveston, Texas.
- Chun Tang, PhD (Post-Doc 2003-2008): Full Professor and HHMI International Scholar, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, Wuhan, China.
- Jun Hu, PhD (Post-doc 2004-2007): Senior Scientist, AstraZeneca, Waltham, Massachusetts.
- Kaifeng Hu, PhD (Post-doc 2004-2008): Full Professor, Kunmin Institute of Botany, Chinese Academy of Sciences, Yunnan, China.
- Jeong-Yong Suh, PhD (Post-doc 2003-2008): Associate Professor, Seoul National University, Korea.
- Michaeleen Doucleff, PhD (Post-doc and Nancy Nossal Fellow, 2007-2009): Editor and reporter for the Science Desk at National Public Radio (2011-). Previously, Scientific Editor, Cell, Cambridge, MA (2009-2011);
- Young-Sang Jung PhD (Post-doc 2006-2010): Assistant Professor, Korea Basic Science Institute, Korea.
- Yuki Takayama PhD (Post-doc 2009-2012): Assistant Professor, Department of System Sciences, Kyoto University, Japan.
- Nicolas Fawzi PhD (Post-doc 2008-2012): Assistant Professor, Department of Molecular Pharmacology, Physiology and Biotechnology, Brown University.
- Nicholas Anthis, PhD (Post-doc and Nancy Nossal Fellow, 2009-2014): Program Officer, University of California Research Initiatives, Research Grants Program Office, University of California Office of the President (2016-). Previously, AAAS Science and Technology Policy Fellow, US Agency for International Development, Washington DC (2014-2016);
- Vincenzo Venditti PhD (Post-doc 2009-2014): Assistant Professor, Department of Chemistry, Iowa State University.
- David Libich PhD (Post-doc and Nancy Nossal Fellow 2011-2017): Assistant Professor, Department of Biochemistry, University of Texas Health Science Center at San Antonio.
- Lalit Deshmukh PhD (Post-doc and Nancy Nossal Fellow, 2011-2017): Assistant Professor, Department of Chemistry, University of California San Diego (UCSD).
- Sam Kotler, PhD (Post-doc and PRAT Fellow, 2015-2018): Staff Scientist, National Centre for Advancing Translational Sciences (NCATS), National Institutes of Health.

## G. Marius CLORE - Complete Bibliography #

- **Total citation count for articles published during the period Jan 1977 to November 2019: >78,500** from Google Scholar.
- ***h*-index: 133** from Google Scholar (the *h*-index is defined as the number of papers *h* having  $\geq h$  citations; J. E. Hirsch (2005) *Proc. Natl. Acad. Sci. U.S.A.* 102, 16569-16572; P. Ball (2005) *Nature* 436, 900).
- Original Member, ISI Highly Cited Researchers Database in Biology & Biochemistry and Chemistry Sections
- **8<sup>th</sup> most cited scientist in Chemistry over period Jan 1, 1998 to June 30, 2008** (ISI Essential Science Indicators)
- **Top 35 in list of *h*-index rankings of living chemists** [[http://www.rsc.org/images/H-index%20ranking%20of%20living%20chemists\(December%202011\)\\_tcm18-211414.pdf](http://www.rsc.org/images/H-index%20ranking%20of%20living%20chemists(December%202011)_tcm18-211414.pdf)], published by the Royal Society of Chemistry in Chemistry World)

PDF files of all publications are available to download at <http://spin.niddk.nih.gov/clore>

### 1977

1. " Clore, G.M. & Chance, E.M. (1977) A computer analysis of cyanide stimulated oxygen uptake in *Chlorella protothecoides*. *FEBS Lett.* 79, 353-356.

### 1978

2. " Clore, G.M. & Shephard, E.P. (1978) Exact solution of the mass transfer equations of gel filtration chromatography by means of a formal inversion of the Laplace transform, and the derivation on an equation for the time spent by a molecule in the gel phase. *J. Chromatogr.* 152, 1-10.
3. " Clore, G.M. & Chance, E.M. (1978) The mechanism of the reaction of fully reduced membrane bound cytochrome oxidase with oxygen at 176 K. *Biochem. J.* 173, 799-810.
4. " Clore, G.M. & Chance, E.M. (1978) The kinetics of the reaction of ferricyanide pretreated mixed valence state membrane bound cytochrome oxidase with oxygen at 173 K. *Biochem. J.* 173, 811-820.
5. " Clore, E.M. & Chance, E.M. (1978) The kinetics and thermodynamics of the reaction of solid state fully reduced membrane bound cytochrome oxidase with carbon monoxide as studied by dual wavelength multichannel spectroscopy and flash photolysis. *Biochem. J.* 175, 709-725.

### 1979

6. " Clore, E.M. & Chance, E.M. (1979) Low temperature kinetics of the reaction of fully reduced membrane bound cytochrome oxidase with oxygen in the Soret,  $\alpha$  and near infrared regions. *Biochem. J.* 177, 613-621.
7. " Clore, G.M. (1979) The mechanism of the fully reduced and mixed valence state membrane bound cytochrome oxidase-oxygen reactions in the 173-176 K temperature range. In *Cytochrome Oxidase* (King, T.E., Orii, Y., Chance, B. and Okunuki, K., eds.) pp. 341-352, North Holland Elsevier, Amsterdam.

8. " Denis, M. & Clore, G.M. (1979) A temperature induced absorption band centered in the region of 666 nm related to the configuration of the active site in frozen cytochrome oxidase. *Biochim. Biophys. Acta* 545, 483-495.
9. " Karlsson, B., Andreasson, L.E., Aasa, R., Malmstrom, B.G. & Clore, G.M. (1979) Studies of the reaction of cytochrome c oxidase with oxygen at low temperature. *Acta Chem. Scand. Ser. B* 33, 615-618.

## 1980

10. " Clore, G.M., Andreasson, L.E., Karlsson, B., Aasa, R. & Malmstrom, B.G. (1980) Characterization of the low temperature intermediates of the reaction of fully reduced soluble cytochrome oxidase with oxygen by electron paramagnetic resonance and optical spectroscopy. *Biochem. J.* 185, 139-154.
11. " Clore, G.M., Andreasson, L.E., Karlsson, B., Aasa, R. & Malmstrom, B.G. (1980) Characterization of the intermediates in the reaction of mixed valence state soluble cytochrome oxidase with oxygen at low temperatures by optical and electron paramagnetic resonance spectroscopy. *Biochem. J.* 185, 155-167.
12. " Clore, G.M. (1980) Characterization of the intermediates in the reaction of membrane bound mixed valence state cytochrome oxidase with oxygen at low temperatures by optical spectroscopy in the visible region. *Biochem. J.* 187, 617-622
13. " Clore, G.M. (1980) The mechanism of reduction of dioxygen by fully reduced cytochrome oxidase: correlation of room and low temperature studies. *Rev. Inorg. Chem.* 2, 343-360.
14. " Clore, G.M. & Chance, E.M. (1980) CO binding to mitochondrial mixed valence state cytochrome oxidase at low temperatures. *Biochim. Biophys. Acta* 590, 34-49.
15. " Campbell, J.R., Clark, R.J.H., Clore, G.M. & Lane, A.N. (1980) Characterization of the electronic properties and geometric environment of the iron atom in the 'myoglobin-hydrogen peroxide' complex by Soret-excited resonance Raman spectroscopy. *Inorg. Chim. Acta* 46, 77-84.
16. " Clore, G.M., Lane, A.N. & Hollaway, M.R. (1980) The kinetics of the reaction of aquo Fe(III) myoglobin with hydrogen peroxide at pH 8. *Inorg. Chim. Acta* 46, 139-146.

## 1981

17. " Clore, G.M. (1981) A re-evaluation of the low temperature kinetics of the reaction of fully reduced mitochondrial cytochrome oxidase with carbon monoxide and the spectral characterization of species I<sub>C</sub> in the Soret and visible regions. *Biochim. Biophys Acta* 634, 129-139.
18. " Chance, E.M., Clore, G.M., Curtis, A.R. & Shephard, E.P. (1981) Numerical solution of the Hodgkin-Huxley equations in a moving coordinate system: simulation of nerve impulse transmission over long distances. *J. Comp. Phys.* 40, 318-326.
19. " Clore, G.M. & Denis, M. (1981) Spectroscopic evidence for an oxygen bridge between the iron atom of cytochrome a<sub>3</sub> and Cu<sub>B</sub> in the Class C group of compounds formed in the reaction of mixed valence state cytochrome oxidase with oxygen. *Inorg. Chim. Acta* 55, L47-L49.
20. " Denis, N. & Clore, G.M. (1981) The reaction of mixed valence state cytochrome oxidase with oxygen in plant mitochondria: a study by low temperature flash photolysis and rapid wavelength scanning optical spectroscopy. *Plant Physiol.* 68, 229-235.

21. " Clore, G.M. (1981) The mechanism of the reaction of fully reduced cytochrome oxidase with oxygen at low temperatures: a kinetic study by electron paramagnetic resonance and optical spectroscopy. *In Oxygen and Life*, Royal Society of Chemistry Special Publications No. 39, pp. 189-198, The Royal Society of Chemistry, London.
22. " Clore, G.M., Hollaway, M.R., Orengo, C., Peterson, J. & Wilson, M. (1981) The mechanism of the reactions of low spin ferric haem undecapeptide with hydrogen peroxide. *Inorg. Chim. Acta* 56, 143-148.
23. " Birdsall, B., Gronenborn, A.M., Clore, G.M., Roberts, G.C.K., Feeney, J. & Burgen, A.S.V. (1981) <sup>13</sup>C-NMR evidence for three slowly interconverting conformations of the dihydrofolate reductase-NADP<sup>+</sup>-folate complex. *Biochem. Biophys. Res. Commun.* 101, 1139-1141.
24. " Gronenborn, A.M., Clore, G.M. & Davies, R.W. (1981) Modulation of specific binding of *Lactobacillus casei* dihydrofolate reductase to DNA by folinic acid. *FEBS Lett.* 133, 92-94.
25. " Clore, G.M., Roberts, G.C.K., Gronenborn, A.M., Birdsall, B & Feeney, J. (1981) Transfer of saturation NMR studies of protein-ligand complexes: the case of three-site exchange. *J. Magn. Reson.* 45, 143-148.
26. " Gronenborn, A.M., Clore, G.M., Blazy, B. & Baudras, A. (1981) Conformational selection of syn-cAMP upon binding to the cAMP receptor protein: a <sup>1</sup>H-NMR study. *FEBS Lett.* 136, 160-164.

## 1982

27. " Clore, G.M. & Gronenborn, A.M. (1982) Kinetic and structural studies on the intermediates formed in the reactions of 5'-adenosine monophosphate and 5'-guanosine monophosphate with cis-dichlorodiammineplatinum II using <sup>1</sup>H and <sup>195</sup>Pt magnetic resonance spectroscopy. *J. Am. Chem. Soc.* 104, 1369-1375.
28. " Clore, G.M., Gronenborn, A.M. & Davies, R.W. (1982) Theoretical aspects of specific and non-specific equilibrium binding of a protein to DNA as studied by the nitrocellulose filter binding assay: cooperative and non-cooperative binding to a one-dimensional lattice. *J. Mol. Biol.* 155, 447-466.
29. " Clore, G.M. & Gronenborn, A.M. (1982) Theory and applications of the transferred nuclear Overhauser effect to the study of the conformations of small ligands bound to proteins. *J. Magn. Reson.* 48, 402-417.
30. " Gronenborn, A.M. & Clore, G.M. (1982) Conformation of NAD<sup>+</sup> bound to yeast and horse liver alcohol dehydrogenase in solution: the use of the proton-proton transferred nuclear Overhauser enhancement. *J. Mol. Biol.* 157, 155-160.
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32. " Gronenborn, A.M. & Clore, G.M. (1982) Proton nuclear magnetic resonance studies on cyclic nucleotide binding to the *Escherichia coli* adenosine 3',5'-phosphate receptor protein. *Biochemistry* 21, 4040-4048.

33. " Clore, G.M. & Gronenborn, A.M. (1982) A proton nuclear magnetic resonance study of the histidine residues of the *Escherichia coli* adenosine 3',5'-phosphate receptor protein: pH titration behaviour, deuterium exchange and partial assignments. *Biochemistry* 21, 4048-4053.
34. " Clore, G.M. & Gronenborn, A.M. (1982) Determination of the conformations of cyclic nucleotides bound to the N-terminal core of the cyclic AMP receptor protein of *Escherichia coli* by <sup>1</sup>H-NMR. *FEBS Lett.* 145, 197-202.
35. " Clore, G.M., Gronenborn, A.M., Mitchinson, C. & Green, N.M. (1982) <sup>1</sup>H-NMR studies on nucleotide binding to the sarcoplasmic reticulum Ca<sup>2+</sup>ATPase: determination of the conformations of bound nucleotides by the measurement of proton-proton transferred nuclear Overhauser enhancements. *Eur. J. Biochem.* 128, 113-117.
36. " Birdsall, B., Gronenborn, A.M., Hyde, E.I., Clore, G.M., Roberts, G.C.K., Feeney, J. & Burgen, A.S.V. (1982) <sup>1</sup>H, <sup>13</sup>C and <sup>31</sup>P NMR studies of the dihydrofolate reductase-NADP<sup>+</sup>-folate complex: characterization of three coexisting conformational states. *Biochemistry* 21, 5831-5838.

### 1983

37. " Clore, G.M. (1983) Computer analysis of transient kinetic data. *In Computing in Biological Science* (Geisow, M.J. & Barrett, A.N., eds.) pp. 313-348, Elsevier North-Holland, Amsterdam.
38. " Unger, B., Clore, G.M., Gronenborn, A.M. & Hillen, W. (1983) Specific DNA binding of the cyclic AMP receptor protein with the *lac* operon stabilizes double stranded DNA in the presence of cAMP. *EMBO J.* 2, 289-293.
39. " Gronenborn, A.M., Clore, G.M. & Gronenborn, B. (1983) Protection against nuclease cleavage of pBR 322 DNA by the cyclic AMP receptor protein of *Escherichia coli*. *J. Mol. Biol.* 166, 93-98.
40. " Gronenborn, A.M. & Clore, G.M. (1983) Characterization of the DNA binding region recognized by dihydrofolate reductase from *Lactobacillus casei*. *J. Biol. Chem.* 258, 11256-11259.
41. " Clore, G.M. & Gronenborn, A.M. (1983) Theory of the time dependent transferred nuclear Overhauser effect: application to the structural analysis of ligand-protein complexes in solution. *J. Magn. Reson.* 53, 423-442.
42. " Clore, G.M., Kimber, B.J. & Gronenborn, A.M. (1983) The 1-1 hard pulse: a novel, simple and effective method of water resonance suppression in FT-<sup>1</sup>H-NMR. *J. Magn. Reson.* 54, 170-173.
43. " Barrett, A.N., Roberts, G.C.K., Burgen, A.S.V. & Clore, G.M. (1983) Ab initio molecular orbital calculations of electron distribution in the tetramethylammonium ion. *Molec. Pharmacol.* 24, 443-448.
44. " Martin, S.R., Gronenborn, A.M. & Clore, G.M. (1983) Specific DNA binding of the cAMP receptor protein to a synthetic oligodeoxyribonucleotide: a circular dichroism study. *FEBS Lett.* 159, 102-106.
45. " Gronenborn, A.M., Kimber, B.J., Clore, G.M. & McLaughlin, L.W. (1983) A nuclear magnetic resonance study of the ribotrinucleoside diphosphate UpUpC. *Nucl. Magn. Res.* 11, 5691-5699.
46. " Clore, G.M., Gronenborn, A.M. & Davies, R.W. (1983) Cooperative non-specific DNA binding of the N-terminal core of the cyclic AMP receptor protein of *Escherichia coli* and its modulation by cyclic AMP. *FEBS Lett.* 164, 57-612.

47. " Clore, G.M. & Gronenborn, A.M. (1983) Sequence dependent structural variations in two right handed alternating pyrimidine-purine DNA oligomers in solution determined by nuclear Overhauser enhancement measurements. *EMBO J.* 2, 2109-2115.

## 1984

48. " Gronenborn, A.M., Clore, G.M., Jones, M.B. & Jiricny, J. (1984) A nuclear Overhauser enhancement study on the imino proton resonances of a DNA pentadecamer comprising the specific target site of the cyclic AMP receptor protein in the *ara* BAD operon. *FEBS Lett.* 165, 216-222.
49. " Clore, G.M., Gronenborn, A.M., Birdsall, B.M., Feeney, J. & Roberts, G.C.K. (1984)  $^{19}\text{F}$ -NMR studies of 3',5'-difluoromethotrexate binding to *Lactobacillus casei* dihydrofoate reductase: molecular motion and coenzyme induced conformational changes. *Biochem. J.* 217, 659-666.
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54. " Clore, G.M. & Gronenborn, A.M. (1984) A Nuclear Overhauser enhancement study of the solution structure of a double stranded DNA undecamer comprising a portion of the specific target site for the cyclic AMP receptor protein in the *gal* operon: sequential resonance assignment. *Eur. J. Biochem.* 141, 119-129.
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57. " Birdsall, B.M., Bevan, A.W., Pascual, C., Roberts, G.C.K., Feeney, J., Gronenborn, A.M. & Clore, G.M. (1984) Multinuclear NMR characterization of two coexisting conformational states of the *Lactobacillus casei* dihydrofolate reductase-trimethoprim- $\text{NADP}^+$  complex. *Biochemistry* 23, 4733-4742.
58. " Gronenborn, A.M., Clore, G.M., Brunori, M., Giardina, B., Falcioni, G. & Perutz, M.F. (1984) Stereochemistry of ATP and GTP bound to fish haemoglobins: a transferred nuclear Overhauser enhancement,  $^{31}\text{P}$ -NMR, oxygen equilibrium and molecular modelling study. *J. Mol. Biol.* 178, 731-742.

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63. " Gronenborn, A.M., Clore, G.M., Hobbs, L. & Jeffery, J. (1984) Glucose-6-phosphate dehydrogenase: a transferred nuclear Overhauser effect study of NADP<sup>+</sup> conformations in enzyme-coenzyme binary complexes. *Eur. J. Biochem.* 145, 365-371.
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65. " Gronenborn, A.M., Nermut, M.V., Eason, P. & Clore, G.M. (1984) Visualization of cAMP receptor protein induced DNA kinking by electron microscopy. *J. Mol. Biol.* 179, 751-757.

## 1985

66. " Clore, G.M. & Gronenborn, A.M. (1985) Assessment of errors involved in the determination of interproton distance ratios and distances by means of one- and two-dimensional NOE measurements. *J. Magn. Reson.* 61, 158-164.
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## G. Marius Clore – Highly Cited Publications ( $\geq 100$ citations)

### Greater than 1000 citations

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