

Complete Curriculum Vitae and Bibliography

G. Marius Clore BSc, MD, PhD, DSc., MAE, FRSC, FRS

NIH Distinguished Investigator
 Chief, Molecular and Structural Biophysics Section
 Laboratory of Chemical Physics, National Institute of Diabetes and Digestive and Kidney Diseases, National Institutes of Health, Bethesda, MD 20892-0520, U.S.A.
 Tel: (301) 496 0782; Fax: (301) 496 0825
 e-mail: mariusc@mail.nih.gov
 web: <https://spin.niddk.nih.gov/clore> (lab home page)
<http://www.nasonline.org/member-directory/members/20033168.html> (National Academy of Sciences web page)
<https://royalsociety.org/people/G-Marius-Clore-25341/> (Royal Society web page)
http://www.ae-info.org/ae/User/Clore_G_Marius (Academia Europaea web page)
https://en.wikipedia.org/wiki/G._Marius_Clore (Wikipedia profile)

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

2021-: Chief, Molecular and Structural Biophysics Section (renamed from Protein NMR Section)
 2011-: Appointed NIH Distinguished Investigator
 2005-: Appointed to Title 42f, Band IV.
 1996-2005: Senior Biomedical Research Service (SBRS)
 1991-2021: Chief, Protein NMR Section
 1988-: Senior Investigator, Laboratory of Chemical Physics, National Institute of Diabetes and Digestive and Kidney Diseases (NIDDK), National Institutes of Health (NIH), Bethesda, Maryland, U.S.A.
 1984-1988: Head of the Biological NMR Group, Max-Planck Institute for Biochemistry, Martinsried, Germany
 1980-1984: Member of the Scientific Staff of the MRC at the National Institute for Medical Research, London, U.K.
 1980: House Surgeon (general surgery), St. Charles Hospital (St. Mary's Hospital Group), London, U.K.
 1979: House Physician (gastroenterology), University College Hospital, London, U.K.

Honors and Awards

2021: [Biopolymers Murray Goodman Memorial Prize](#)
 2021: [Khorana Prize of the Royal Society of Chemistry](#)
 2021: [Awarded Honorary Doctor of Science \(DSc.\) from University College London \(U.K.\)](#)
 2021: NIDDK Nancy Nossal Mentorship Award
 2020: [Elected Fellow of the Royal Society \(FRS\)](#)
 2020: NIDDK Director's Scientific Award (Scientific)
 2020: [Biophysical Society Innovation Award](#)
 2015: [Elected Foreign Member of Academia Europaea \(MAE\)](#)
 2014: [Elected Member, United States National Academy of Sciences](#)
 2013: [Biochemical Society 2013 Centenary Award](#) (previously known as the Jubilee Medal) and Sir Frederick Gowland Hopkins Memorial Lecture (U.K.)

Honors and Awards (cont.)

- 2011: Royal Society of Chemistry Centenary Prize
 2011: NIH Distinguished Investigator
 2010: Elected Fellow of the American Academy of Arts and Sciences
 2010: Hillebrand Award of the Washington Chapter of the American Chemical Society
 2009: Elected Fellow of the Biophysical Society
 2009: NIDDK Nancy Nossal Scientific Mentorship Award
 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 (Biology and Biochemistry 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: 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 (U.K.)
 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 and assembly, 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; 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; transient interactions involving the very earliest stages in the formation of huntingtin protofibrils; and transient interdomain interactions and transient oligomerization of the Hsp40 chaperone DNAJB6b.

Membership of Editorial Boards

- 2022 - : Co-Editor-in-Chief of Current Opinions in Structural Biology
 2009-2014: Member of the Editorial Board of the Journal of Biological Chemistry
 2003-: Member of the Editorial Board of PEDS (Protein Engineering, Design and Selection; previously Protein Engineering)

Membership of Editorial Boards (cont.)

- 2003-2013: Series Editor for the Structural Biology, Chemical Biology and Informatics Section of the Royal Society of Chemistry Biomolecular Biosciences Book Series.
- 2002-2007: Member of the Editorial Board of the Journal of Biological Chemistry
- 1998-2018: Member of the Editorial Board of the Journal of Magnetic Resonance
- 1996-2001: Member of the Editorial Board of the Journal of Biological Chemistry
- 1994-1999: Member of the Editorial Board of Protein Science
- 1993-1997: Associate Editor of Protein and Peptide Letters
- 1993-: Member of the Editorial Board of Structure
- 1987-2003: Member of the Editorial Board of Protein Engineering

Membership of Societies

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

Service

- 2022-: 2022 - : Co-Editor-in-Chief of Current Opinions in Structural Biology
- 2021: Reviewer for the National Academies report on “Radioactive Sources: Applications and Alternative Technologies” from the National Academies’ Nuclear and Radiation Studies Board
- 2020: Reviewer for NIGMS National and Regional Resource (R24) Applications
- 2020-: Reviewer for the National Academy of Sciences BBCSS report on “Consideration of Generational Issues in Workforce Management and Employment Practices”
- 2020-: NAS Reviewer Pool for Consensus Study Reports of the National Academies of Science, Engineering and Medicine.
- 2020-: Director, NIDDK Computational Biomolecular Magnetic Resonance Core.
- 2018-2020: European Science Foundation, College of Experts Reviewers
- 2017-2018: Member of the Macromolecular Dynamics Canvassing Committee of the Biophysics and Computational Biology Section (Class II, Section 29) of the National Academy of Sciences.
- 2016: Selection Committee for the Raymond and Beverley Sackler International Prize in the Physical Sciences.
- 2016-2018: Member of the NIH Intramural AIDS Targeted Antiviral Program Scientific Review Committee.
- 2009: Member of the UCLA-DOE Institute for Genomics and Proteomics Cooperative Agreement Review Panel.
- 2009: Member of Ad Hoc NIH Review Panel for High End NMR Shared Instrumentation Grants. 1989- Adviser in the U.S. National Research Council (NRC) Research Associateship Program.
- 2007-: Member, Executive Committee of the NIH/Oxford/Cambridge Scholars Program.
- 2006-2011: Member of the Scientific Advisory Board of the Institute of Biotechnology at the University of Helsinki, Finland.
- 2005-2010: Member, RCSB (PDB-BMRB) Task Group on NMR
- 2002: Member, Special Emphasis Panel on 900 MHz NMR Spectrometers, Center for Scientific Review, NIGMS, NIH.
- 1998-2003: Member of NMR Task Force of the Research Collaboratory for Structural Bioinformatics.

Service (cont.)

- 1998-2004: Reviewer for the quinquennial assessment of the MRC Center for Protein Engineering at the University of Cambridge, U.K.
- 1998-2001: Co-Chair, Intramural NIH-Wide Structural Biology Interest Group.
- 1997-: Member of Review Panel for the John Sealy Memorial Endowment Fund for Biomedical Research.
- 1997: NIH Special Emphasis Panel on Structural Biology of AIDS Related Proteins.
- 1996-: Preceptorship in the Pharmacology Research Associate (PRAT) Program of the National Institute for General Medical Sciences.
- 1996-1998: Member, Membership Committee, Protein Society
- 1994-2000: Chairman, NIH-Wide Tenure and Promotions Committee for Computer Scientists.
- 1994: Special Reviewer, Biophysical Chemistry (BCCB) Study Section, NIH
- 1992: Subcommittee on Structural Biology of the Health and Environmental Research Advisory Committee of the Department of Energy.
- 1989: Special Study Section of the Division of Research Resources, Biomedical Research Technology Program, NIH.

Grant peer review for the following agencies:

National Science Foundation, National Institutes of Health, Medical Research Council (U.K.), Biotechnology and Biological Sciences Research Council (U.K.), Wellcome 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, French National Research Agency (ANR), European Research Council, Japanese Society for the Promotion of Science.

Mentoring

My overarching goal is to train my post-doctoral fellows to successfully make the transition from graduate student to fully independent principal investigator capable of running a successful and productive research group in academia or industry. Of my 51 former trainees, 28 are currently principal investigators (at the full, associate and assistant professor levels) at major research universities or institutions (both in the US and Europe), one has just been elected a Fellow of the Royal Society and another a Member of Academia Europaea. The remainder hold either senior positions in pharma/biotech (9), are staff scientists at the NIH or in Academia (10), science administrators (3) or work for National Public Radio as chief science editor (1).

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 lectures

Approximately 200 invited lectures at national and international conferences.

25 most significant publications (out of a total of 537 publications)

Total citation count: > 85,600 (Google scholar)

***h* index (number of papers *h* cited *h* or more times): 140 (Google Scholar)**

- Oschkinat, H., Griesinger, C., Kraulis, P.J., Sørensen, O.W., Ernst, R.R., Gronenborn, A.M. & **Clore, G.M.** (1988) Three-dimensional NMR spectroscopy of a protein in solution. *Nature* 332, 374-376.
- Clore, G.M.** & Gronenborn, A.M. (1991) Structures of larger proteins in solution: three- and four-dimensional heteronuclear NMR spectroscopy. *Science* 252, 1390-1399.
- Lodi, P.J., Garrett, D.S., Kuszewski, J., Tsang, M.L.S., Weatherbee, J.A., Leonard, W.J., Gronenborn, A.M. & **Clore, G.M.** (1994) High resolution solution structure of the β chemokine hMIP-1 β by multi-dimensional NMR. *Science* 263, 1762-1767.
- Garrett, D.S., Seok, Y.-J., Peterkofsky, A., Gronenborn, A.M. & **Clore, G.M.** (1999) Solution structure of the 40,000 M_r phosphoryl transfer complex between Enzyme I and HPr. *Nature Struct. Biol.* 6, 166-173.

25 most significant publications (cont.)

- Williams, D.C., Cai, M. & **Clore, G.M.** (2004) Molecular basis for synergistic transcriptional activation by Oct1 and Sox2 revealed from the solution structure of the 42 kDa Oct1·Sox·*Hoxb1*-DNA ternary transcription factor complex. *J. Biol. Chem.* 279, 1449-1457.
- Iwahara, J. & **Clore, G. M.** (2006) Detecting transient intermediates in macromolecular binding by paramagnetic NMR. *Nature* 440, 1227-1230.
- Iwahara, J., Zwecksetter, M. & **Clore, G.M.** (2006) NMR structural and kinetic characterization of a homeodomain diffusing and hopping on non-specific DNA. *Proc. Natl. Acad. Sci. U.S.A.* 103, 15062-15067.
- Tang, C., Iwahara, J. & **Clore, G.M.** (2006) Visualization of transient encounter complexes in protein-protein association. *Nature* 444, 383-386.
- Tang, C., Schwieters, C.D. & **Clore, G.M.** (2007) Open to closed transition in apo maltose-binding protein visualized by paramagnetic NMR. *Nature* 449, 1878-1882.
- Tang, C., Louis, J.M., Aniana, A., Suh, J.-Y. & **Clore, G.M.** (2008) Visualizing transient events in amino-terminal auto-processing of HIV-1 protease. *Nature* 455, 693-696.
- Clore, G.M.** & Iwahara, J. (2009) Theory, practice and applications of paramagnetic relaxation enhancement for the characterization of transient low-population states of biological macromolecules and their complexes. *Chem. Rev.* 109, 4108-4139.
- Schwieters, C.D., Suh, J.-Y., Grishaev, A., Ghirlando, R., Takayama, Y. & **Clore, G.M.** (2010) Solution structure of the 128 kDa Enzyme I dimer from *Escherichia coli* and its 146 kDa complex with HPr using residual dipolar couplings and small and wide angle X-ray scattering. *J. Am. Chem. Soc.* 133, 13026-13045.
- Fawzi, N.L., Doucleff, M., Suh, J.-Y. & **Clore, G.M.** (2010) Mechanistic details of a protein-protein association pathway revealed by paramagnetic relaxation enhancement titration measurements. *Proc. Natl. Acad. Sci. U. S. A.* 107, 1379-1384.
- Fawzi, N.L., Ying, J., Ghirlando, R., Torchia, D.A. & **Clore, G.M.** (2011) Atomic resolution dynamics on the surface of amyloid β protofibrils probed by solution NMR. *Nature* 480, 268-272.
- Libich, D.S., Tugarinov, V. & **Clore, G.M.** Intrinsic unfoldase/foldase activity of the chaperonin GroEL directly demonstrated using multinuclear relaxation-based NMR. (2015) *Proc. Natl. Acad. Sci. U. S. A.* 112, 8817-8823.
- Schmidt, T. Wälti, M.A., Baber, J.L., Hustedt, E.J. & **Clore, G.M.** (2016) Long distance measurements up to 160 Å in the GroEL tetradecamer using Q-band DEER EPR spectroscopy. *Angewandte Chemie Int. Ed.* 55, 15905-15909.
- Deshmukh, L., Louis, J.M., Ghirlando, R. & **Clore, G.M.** (2016) Transient Gag-protease interactions revealed by paramagnetic NMR suggest origins of compensatory drug resistance mutations in HIV-1. *Proc. Natl. Acad. Sci. U. S. A.* 113, 12456-12461.
- Libich, D.S., Tugarinov, V., Ghirlando, R. & **Clore, G.M.** (2017) Confinement and stabilization of Fyn SH3 folding intermediate mimetics within the cavity of the chaperonin GroEL demonstrated by relaxation-based NMR. *Biochemistry* 56, 903-906.
- Kotler, S.A., Tugarinov, V., Schmidt, T., Cecon, A., Libich, D.S., Ghirlando, R., Schwieters, C.D. and **Clore, G.M.** (2019) Probing initial transient oligomerization events facilitating Huntingtin fibril nucleation at atomic resolution by relaxation-based NMR. *Proc. Natl. Acad. Sci. U. S. A.* 116, 3562-3571.
- Karamanos, T.K., Tugarinov, V. & **Clore, G.M.** (2019) Unraveling the structure and dynamics of the human DNAJB6b chaperone by NMR reveals insights into Hsp40-mediated proteostasis. *Proc. Natl. Acad. Sci. U.S.A.* 116, 21529-21538.
- Cecon, A., Tugarinov, V., Ghirlando, R. & **Clore, G.M.** (2020) Abrogation of pre-nucleation, transient oligomerization of the Huntingtin exon-1 protein by human profilin-I. *Proc. Natl. Acad. Sci. U.S.A.* 117, 5844-5852.
- Okuno, Y., Szabo, A. & **Clore, G.M.** (2020) Quantitative interpretation of solvent paramagnetic relaxation for probing protein-cosolute interactions. *J. Am. Chem. Soc.* 142, 8281-8290.

25 most significant publications (cont.)

- Ceccon, A., Tugarinov, V. & **Clore, G.M.** (2021) Quantitative exchange NMR-based analysis of huntingtin-SH3 interactions suggests an allosteric mechanism of inhibition of huntingtin aggregation. *J. Am. Chem. Soc.* *143*, 9672-9681.
- Okuno, Y., Yoo, J., Schwieters, C.D., Best, R.B., Chung, H.-S., **Clore, G.M.** (2021) Atomic view of cosolute-induced protein denaturation probed by NMR solvent paramagnetic relaxation enhancement. *Proc. Natl. Acad. Sci. U.S.A.* *118*, e2112021118.
- Schmidt, T., Heon, J., Ya, W.M., Schwieters, C.D., Tycko, R. & **Clore, G.M.** (2022) Time-resolved DEER EPR and solid-state NMR afford kinetic and structural elucidation of substrate binding to Ca²⁺-ligated calmodulin. *Proc. Natl. Acad. Sci. U.S.A.* *119*, e2122308119.

Former Trainees

- **Alberto Ceccon, PhD** (Post-doc, 2015-2021, Nancy Nossal Fellow): Associate Professor, Department of Chemistry, Free University of Bozen-Bolzano, Italy (from May 2022).
- **Marielle Wälti, PhD** (Post-doc, 2015-2021, Nancy Nossal Fellow and K99 Awardee): Assistant Professor, Department of Chemistry and Biochemistry, University of Arizona, Tucson (from March 2022).
- **Thomas Schmidt PhD** (Post-doc, 2015-2020): Staff Scientist, Laboratory of Chemical Physics, NIDDK, NIH.
- **Theodoros Karamanos PhD** (Post-doc and Nancy Nossal Fellow, 2017-2020): Assistant Professor, Astbury Center for Structural Biology, University of Leeds (U.K.).
- **Sam Kotler, PhD** (Post-doc and PRAT Fellow, 2015-2018): Staff Scientist, National Centre for Advancing Translational Sciences (NCATS), National Institutes of Health.
- **Lalit Deshmukh PhD** (Post-doc and Nancy Nossal Fellow, 2011-2017): Assistant Professor, Department of Chemistry, University of California San Diego (UCSD).
- **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.
- **Vincenzo Venditti PhD** (Post-doc 2009-2014): Assistant Professor, Department of Chemistry, Iowa State 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);
- **Nicolas Fawzi PhD** (Post-doc 2008-2012 and Nancy Nossal Fellow): Associate Professor, Department of Molecular Pharmacology, Physiology and Biotechnology, Brown University.
- **Yuki Takayama PhD** (Post-doc 2009-2012): Senior Scientist, Kyowa Kirin Company, Japan; previously Assistant Professor, Department of System Sciences, Kyoto University, Japan.
- **Young-Sang Jung PhD** (Post-doc 2006-2010): Senior Scientist, Department of Medicinal Chemistry, Chong Kun Dang Pharmaceutical Corporation, South Korea; previously Assistant Professor, Korea Basic Science Institute, South 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).
- **Jeong-Yong Suh, PhD** (Post-doc 2003-2008): Associate Professor, Seoul National University, Korea.
- **Kaifeng Hu, PhD** (Post-doc 2004-2008): Full Professor, Kunmin Institute of Botany, Chinese Academy of Sciences, Yunnan, China.
- **Jun Hu, PhD** (Post-doc 2004-2007): Senior Scientist, AstraZeneca, Waltham, Massachusetts.
- **Chun Tang, PhD** (Post-Doc 2003-2008): Distinguished Professor, Peking University and Chinese Academy of Sciences; previously Full Professor and HHMI International Scholar, Wuhan Institute of Physics and Mathematics, Chinese Academy of Sciences, Wuhan, China.

Former trainees (cont.)

- **Junji Iwahara, PhD** (Post-Doc 2002-2006): Full Professor, Department of Biochemistry and Molecular Biology, University of Texas Medical Branch, Galveston, Texas.
- **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
- **Michal Komlos, PhD** (Post-doc, 2001-2004): Staff scientist, NICHD, NIH.
- **Gabriel Cornilescu, PhD** (Post-doc and PRAT Fellow, 2000-2002): Senior Scientist, Leidos Biomedical Research Inc. at Frederick National Laboratory for Cancer Research; previously Associate Researcher, Nuclear Magnetic Resonance Facility (NMRFAM), University of Wisconsin, Madison.
- **Gus Wang, PhD** (Post-doc 1998-2002): Associate Professor, Department of Pathology and Microbiology, Eppley Cancer Institute, University of Nebraska Medical Center.
- **Elliott Gozansky, MD, PhD** (Post-Doc, 1998-2000): Clinical Associate Professor in Cardiothoracic Radiology at NYU Langone Health.
- **Demetrios Braddock, MD, PhD** (Post-doc and Pathology Resident, NCI 1997-2000): Associate Professor, Department of Pathology, Yale University.
- **Elizabeth Murphy, PhD** (Graduate student 1995-1999): Chief, Clinical Informatics Section, Office of the Clinical Director, National Eye Institute, NIH.
- **Kai Huang, PhD** (Post-doc 1997-1999): NMR facility manager, Structural Biology NMR Facility, Northwestern University.
- **Michael Caffrey, PhD** (Post-doc, 1996-1999) Associate Professor, University of Illinois at Chicago.
- **Carole Bewley, PhD** (Post-doc and Cancer Research Institute Fellow, 1995-1999): Senior Investigator, Section Chief and Laboratory Chief, Laboratory of Bioorganic Chemistry, NIDDK.
- **Silke Schumaker, PhD** (Post-doc 1995-1997): CEO, Anadys Pharmaceuticals GmbH, Heidelberg, Germany.
- **Mats Wikström, PhD** (Post-doc 1995-1997): Senior Scientist, Amgen, Thousand Oaks, California; previously Full Professor, Faculty of Health Sciences, University of Copenhagen.
- **Mary Starich, PhD** (Post-doc 1995-1998): Staff scientist, Laboratory of Structural Biophysics, NHLBI.
- **John Kuszewski, PhD** (graduate student 1994-1998, Post-doc 1998-2001): Staff scientist, Center for Information Technology, NIH.
- **Logan Donaldson, PhD** (Post-doc 1996-1998): Full Professor, Department of Biology, York University, Toronto, Canada.
- **Mengli Cai, PhD** (Post-doc, 1996-1998): Staff scientist, Laboratory of Chemical Physics, NIDDK (2001-); senior scientist, Abbott Laboratories (1999-2001).
- **Jeff Huth, MD, PhD** (Post-doc, 1994-1997): Founder and CEO of ScopiaRx, LLC, Ohio. Previously, Senior Scientist, Abbott Laboratories.
- **Wm. Dexter Kennedy, MD** (Post-doc 1994-1996): Senior Director, Alios BioPharma, San Francisco.
- **James Ernst, PhD** (Pre-doctoral student, 1994-1995): Senior Scientist, Genentech, San Francisco.
- **Robert Clubb, PhD** (Post-doc and Leukemia Society of America Fellow, 1993-1996): Full Professor, Department of Chemistry and Biochemistry, UCLA, Los Angeles.
- **Jun Qin, PhD** (Post-doc, 1993-1996): Full Professor of Molecular Medicine, Lerner Research Institute, Cleveland Clinic Foundation, Cleveland.
- **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).
- **Patricia Lodi LiWang, PhD** (Post-doc and Cancer Research Institute Fellow, 1991-1995): Full Professor, University of California Merced.
- **Bruce Grasberger, PhD** (Post-doc, 1989-1993): Senior Scientist, Johnson & Johnson, New Brunswick, Pennsylvania.
- **James Omichinski, PhD** (Post-doc, Staff fellow and Senior Staff fellow, 1989-1997): Full Professor, University of Montreal, Canada.
- **Dan Garrett, PhD** (Post-doc 1990-1995): Staff scientist, Laboratory of Chemical Physics, NIDDK.
- **Bob Powers, PhD** (Post-doc 1990-1993): Full Professor, University of Nebraska.

Former trainees (cont.)

- **Mark Robien, MD** (Howard Hughes medical student, 1990-1992): Medical Officer, Division of Allergy, Immunology and Transplantation, NIAID, NIH.
- **Julie Forman-Kay, PhD, FRS** (Graduate student 1989-1992; Post-doc 1992-1993): Full Professor, Department of Biochemistry, University of Toronto and Scientific Staff, Hospital for Sick Children, Toronto.
- **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.
- **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).
- **Hartmut Oschkinat, PhD** (Post-doc 1987-1989): Full Professor, Institute for Molecular Pharmacology, University of Berlin, Germany.
- **Michael Nilges, PhD, MAE** (Graduate student 1985-1987; Post-doc 1987-1989): Chair, Department of Structural Biology and Chemistry, Institut Pasteur, Paris, France.

Complete Bibliography

G. Marius CLORE FRS

Contents

A. Complete Bibliography (1977 – 2022)

B. List of highly cited publications (citations \geq 100)

- **Total citation count for articles published during the period Jan 1977 to June 2021: >84,300 from Google Scholar (https://scholar.google.com/citations?user=5KmWmkEAA_AAJ&hl=en).**
- ***h*-index: **140**** 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
- **8th 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 in 2011** [[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>

A. Complete Bibliography (1977-2022)

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, α 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. & Holloway, 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_C 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 a₃ and Cu_B 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., Holloway, 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) ¹³C-NMR evidence for three slowly interconverting conformations of the dihydrofolate reductase-NADP⁺-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 ^1H -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 ^1H and ^{195}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^+ 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.
31. Takahashi, M., Gronenborn, A.M., Clore, G.M., Blazy, B. & Baudras, B. (1982) DNA binding of cAMP receptor protein and its N-terminal core stabilizes the double helix and is modulated by cAMP. *FEBS Lett.* *139*, 37-40.
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 ^1H -NMR. *FEBS Lett.* *145*, 197-202.
35. Clore, G.M., Gronenborn, A.M., Mitchinson, C. & Green, N.M. (1982) ^1H -NMR studies on nucleotide binding to the sarcoplasmic reticulum Ca^{2+} -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) ^1H , ^{13}C and ^{31}P NMR studies of the dihydrofolate reductase-NADP $^+$ -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-¹H-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) ¹⁹F-NMR studies of 3',5'-difluoromethotrexate binding to *Lactobacillus casei* dihydrofoate reductase: molecular motion and coenzyme induced conformational changes. *Biochem. J.* 217, 659-666.
50. Gronenborn, A.M., Papadopoulos, P. & Clore, G.M. (1984) Immunochemical evidence for extensive ligand induced conformational changes in *Lactobacillus casei* dihydrofolate reductase. *J. Biol. Chem.* 259, 1082-1085.
51. Antonjuk, D.J., Birdsall, B.M., Chang, H.T.A., Clore, G.M., Feeney, J., Gronenborn, A.M., Roberts, G.C.K. & Tran, T.Q. (1984) A ¹H-NMR study of the role of the glutamate moiety in the binding of methotrexate to *Lactobacillus casei* dihydrofolate reductase. *Bri. J. Pharmacol.* 81, 309-315.

52. Gronenborn, A.M., Clore, G.M. & Jeffery, J. (1984) An unusual conformation of NAD⁺ bound to sorbitol dehydrogenase: a time dependent transferred nuclear Overhauser effect study. *J. Mol. Biol.* *172*, 559-572.
53. Clore, G.M., Gronenborn, A.M. & McLaughlin, L.W. (1984) The structure of the ribotrinucleoside diphosphate codon UpUpC bound to tRNA^{Phe} from yeast: a time dependent transferred nuclear Overhauser effect study. *J. Mol. Biol.* *174*, 163-173.
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.
55. Gronenborn, A.M., Clore, G.M. & Kimber, B.J. (1984) An investigation into the solution structures of two self-complementary DNA oligonucleotides 5'd-CGTACG and 5'd-ACGCGCGT by means of nuclear Overhauser enhancement measurements. *Biochem. J.* *221*, 723-736.
56. Clore, G.M., Gronenborn, A.M., Piper, E.A., McLaughlin, L.W., Graeser, E. & van Boom, J.H. (1984) The solution structure of a RNA pentadecamer comprising the anticodon loop and stem of yeast tRNA^{Phe}: a 500 MHz ¹H-NMR study. *Biochem. J.* *221*, 737-751.
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-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, ³¹P-NMR, oxygen equilibrium and molecular modelling study. *J. Mol. Biol.* *178*, 731-742.
59. Clore, G.M. & Gronenborn, A.M. (1984) An investigation into the solution structure of the single stranded DNA undecamer 5'd-AAGTGTGATAT by means of nuclear Overhauser enhancement measurements. *Eur. Biophys. J.* *11*, 95-102.
60. Clore, G.M. & Gronenborn, A.M. (1984) Internal mobility in a double stranded B DNA hexamer and undecamer: a time dependent proton-proton nuclear Overhauser enhancement study. *FEBS Lett.* *172*, 219-225.
61. Clore, G.M. & Gronenborn, A.M. (1984) Interproton distance measurements in solution for a double stranded DNA undecamer comprising a portion of the specific target site for the cyclic AMP receptor protein in the *gal* operon: a nuclear Overhauser enhancement study. *FEBS Lett.* *175*, 117-123.
62. Gronenborn, A.M., Clore, G.M., McLaughlin, L.W., Graeser, E., Lorber, B. & Giege, R. (1984) Yeast tRNA^{Asp} - Codon and wobble codon-anticodon interactions: a transferred nuclear Overhauser enhancement study. *Eur. J. Biochem.* *145*, 359-364.
63. Gronenborn, A.M., Clore, G.M., Hobbs, L. & Jeffery, J. (1984) Glucose-6-phosphate dehydrogenase: a transferred nuclear Overhauser effect study of NADP⁺ conformations in enzyme-coenzyme binary complexes. *Eur. J. Biochem.* *145*, 365-371.
64. Clore, G.M., Lauble, H., Frenkiel, T.A. & Gronenborn, A.M. (1984) A two-dimensional NMR study of the solution structure of a DNA dodecamer comprising the consensus sequence for the specific DNA binding sites of the glucocorticoid receptor protein. *Eur. J. Biochem.* *145*, 629-636.

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.
67. Clore, G.M. & Gronenborn, A.M. (1985) Probing the three-dimensional structures of DNA and RNA oligonucleotides in solution by nuclear Overhauser enhancement measurements. *FEBS Lett.* 179, 187-198.
68. Gronenborn, A.M. & Clore, G.M. (1985) Investigations into the solution structures of short nucleic acid fragments by means of nuclear Overhauser enhancement measurements. *Progr. Nucl. Magn. Reson. Spectroscopy* 17, 1-32.
69. Andrews, J., Clore, G.M., Davies, R.W., Gronenborn, A.M., Gronenborn, B., Kalderon, D., Papadopoulos, P.C., Schafer, S., Sims, P.F.G. & Stancombe, R. (1985) Nucleotide sequence of the dihydrofolate reductase gene of methotrexate resistant *Lactobacillus casei*. *Gene* 35, 217-222.
70. Perutz, M.F., Gronenborn, A.M., Clore, G.M., Hogg, J.H. & Shi, T. (1985) The pK_a's of two histidines in human haemoglobin, the Bohr effect and the dipole moment of α -helices. *J. Mol. Biol.* 183, 491-498.
71. Perutz, M.F., Gronenborn, A.M., Clore, G.M., Shi, T. & Craescu, C.T. (1985) Comparison of histidine proton magnetic resonances of human carbonmonoxy haemoglobin in different buffers. *J. Mol. Biol.* 186, 471-473.
72. Clore, G.M. & Gronenborn, A.M. (1985) The solution structure of a B-DNA undecamer comprising a portion of the specific target site for the cyclic AMP receptor protein in the *gal* operon: refinement on the basis of interproton distance data. *EMBO J.* 4, 829-835.
73. Clore, G.M., Gronenborn, A.M., Moss, D.S. & Tickle, I.J. (1985) Refinement of the solution structure of the B-DNA hexamer 5'd(CGTACG)₂ on the basis of interproton distance data. *J. Mol. Biol.* 185, 219-226.
74. Clore, G.M., Gronenborn, A.M. & McLaughlin, L.W. (1985) The structure of the double stranded RNA pentamer 5'(CACAG).5'(CUGUG) by nuclear Overhauser enhancement measurements: interproton distance determination and structure refinement on the basis of X-ray coordinates. *Eur. J. Biochem.* 151, 153-165.
75. Clore, G.M., Gronenborn, A.M., Brunger, A.T. & Karplus, M. (1985) The solution conformation of a heptadecapeptide comprising the DNA binding helix F of the cyclic AMP receptor protein of *Escherichia coli*: combined use of ¹H-nuclear magnetic resonance and restrained molecular dynamics. *J. Mol. Biol.* 186, 435-455.

1986

76. Clore, G.M. & Gronenborn, A.M. (1986) Determination of three-dimensional structures of oligonucleotides in solution: combined use of nuclear Overhauser enhancement measurements and restrained least squares refinement. In *Biomolecular Stereodynamics IV* (Sarma, R.H., ed.) pp. 139-155, Adenine Press, New York.

77. Gronenborn, A.M. & Clore, G.M. (1986) The solution structure of RNA fragments by nuclear Overhauser enhancement measurements. *In Structure and Dynamics of RNA*, (van Knippenberg, R.H. & Hilbers, C.W., eds.) pp. 137-150, NATO ASI series, Plenum Press, New York.
78. Gronenborn, A.M. & Clore, G.M. (1986) Overproduction of the cAMP receptor protein of *Escherichia coli* and expression of the engineered carboxy-terminal DNA binding domain. *Biochem. J.* 236, 643-649.
79. Clore, G.M., Gronenborn, A.M., Greipel, J. & Maass, G. (1986) The conformation of the single stranded DNA undecamer 5'd(AAGTGTGATAT) bound to single stranded DNA binding protein of *Escherichia coli*: a time dependent transferred nuclear Overhauser enhancement study. *J. Mol. Biol.* 187, 119-124.
80. Nilsson, L., Clore, G.M., Gronenborn, A.M., Brunger, A.T. & Karplus, M. (1986) Structure refinement of oligonucleotides by molecular dynamics with NOE interproton distance restraints: application to 5'd(CGTACG)₂. *J. Mol. Biol.* 188, 455-475.
81. Clore, G.M., Gronenborn, A.M., Carlson, G. & Meyer, E.F. (1986) Stereochemistry of binding of the tetrapeptide Acetyl-Pro-Ala-Pro-TyrNH₂ to porcine pancreatic elastase: combined use of two-dimensional transferred nuclear Overhauser enhancement measurements, restrained molecular dynamics, X-ray crystallography and molecular modelling. *J. Mol. Biol.* 190, 259-267.
82. Brunger, A.T., Clore, G.M., Gronenborn, A.M. & Karplus, M. (1986) Three-dimensional structures of proteins determined by molecular dynamics with interproton distance restraints: application to crambin. *Proc. Natl. Acad. Sci. U.S.A.* 83, 3801-3805.
83. Clore, G.M., Brunger, A.T., Karplus, M. & Gronenborn, A.M. (1986) Application of molecular dynamics with interproton distance restraints to three-dimensional protein structure determination: a model study of crambin. *J. Mol. Biol.* 191, 523-551.
84. Clore, G.M., Martin, S.R. & Gronenborn, A.M. (1986) The solution structure of human growth hormone releasing factor: combined use of circular dichroism and nuclear magnetic resonance spectroscopy. *J. Mol. Biol.* 191, 553-561.
85. Gronenborn, A.M., Clore, G.M., Schmeissner, U. & Wingfield, P.T. (1986) Sequence specific assignments of aromatic residues in the ¹H-NMR spectrum of human interleukin-1 β using site directed mutant proteins. *Eur. J. Biochem.* 161, 37-43.
86. Zarbock, J., Clore, G.M. & Gronenborn, A.M. (1986) Nuclear magnetic resonance study of the globular domain of chicken histone H5: resonance assignment and secondary structure. *Proc. Natl. Acad. Sci. U.S.A.* 23, 7628-7632.
87. Minter, S.J., Clore, G.M., Gronenborn, A.M. & Davies, R.W. (1986) Cooperative DNA binding by lambda integration protein - a key component of specificity. *Eur. J. Biochem.* 161, 727-731.
88. Clore, G.M., Nilges, M., Sukumaran, D.K., Brunger, A.T., Karplus, M. & Gronenborn, A.M. (1986) The three-dimensional structure of α 1-purothionin in solution: combined use of nuclear magnetic resonance, distance geometry and restrained molecular dynamics. *EMBO J.* 5, 2729-2735.
89. MacDonald, H.R., Wingfield, P., Schmeissner, U., Shaw, A., Clore, G.M. & Gronenborn, A.M. (1986) Point mutations of human interleukin-1 with decreased receptor binding affinity. *FEBS Lett.* 209, 295-298.

1987

90. Clore, G.M., Sukumaran, D.K., Gronenborn, A.M., Teeter, M.M., Whitlow, M. & Jones, B.L. (1987) A nuclear magnetic resonance study of the solution structure of α 1-purothionin: sequential resonance assignment, secondary structure and low resolution tertiary structure. *J. Mol. Biol.* 193, 571-578.
91. Gent, M., Gronenborn, A.M., Davies, R.W. & Clore, G.M. (1987) Probing the sequence specific interaction of the cAMP receptor protein with DNA by site directed mutagenesis. *Biochem. J.* 242, 645-653.
92. Sukumaran, D.K., Clore, G.M., Preuss, A., Zarbock, J. & Gronenborn, A.M. (1987) A proton nuclear magnetic resonance study of hirudin: resonance assignment and secondary structure. *Biochemistry* 26, 333-338.
93. Clore, G.M., Sukumaran, D.K., Nilges, M. & Gronenborn, A.M. (1987) The three-dimensional structure of phoratoxin in solution: combined use of nuclear magnetic resonance, distance geometry and restrained molecular dynamics. *Biochemistry* 26, 1732-1745.
94. Brünger, A.T., Campbell, R.L., Clore, G.M., Gronenborn, A.M., Karplus, M., Petsko, G.A. & Teeter, M.M. (1987) Solution of a protein crystal structure with a model obtained from NMR interproton distance restraints. *Science* 235, 1049-1053.
95. Clore, G.M., Sukumaran, D.K., Nilges, M., Zarbock, J. & Gronenborn, A.M. (1987) The conformations of hirudin in solution: a study using nuclear magnetic resonance, distance geometry and restrained molecular dynamics. *EMBO J.* 6, 529-537.
96. Clore, G.M., Nilges, M., Brünger, A.T., Karplus, M. & Gronenborn, A.M. (1987) A comparison of the restrained molecular dynamics and distance geometry methods for determining three-dimensional structures of proteins on the basis of interproton distance restraints. *FEBS Lett.* 213, 269-277.
97. Gronenborn, A.M., Bovermann, G. & Clore, G.M. (1987) A ^1H -NMR study of the solution conformation of secretin: resonance assignment and secondary structure. *FEBS Lett.* 215, 88-94.
98. Clore, G.M., Gronenborn, A.M., Nilges, M., Sukumaran, D.K. & Zarbock, J. (1987) The polypeptide fold of the globular domain of histone H5 in solution: a study using nuclear magnetic resonance, distance geometry and restrained molecular dynamics. *EMBO J.* 6, 1833-1842.
99. Nilges, M., Clore, G.M., Gronenborn, A.M., Brünger, A.T., Karplus, M. & Nilsson, L. (1987) Refinement of the solution structure of the DNA hexamer 5'd(GCATGC)₂: combined use of nuclear magnetic resonance and restrained molecular dynamics. *Biochemistry* 26, 3718-3733.
100. Nilges, M., Clore, G.M., Gronenborn, A.M., Piel, N. & McLaughlin, L.W. (1987) Refinement of the solution structure of the DNA decamer 5'd(CTGGATCCAG)₂: combined use of nuclear magnetic resonance and restrained molecular dynamics. *Biochemistry* 26, 3734-3744.
101. Gent, M.E., Gartner, S., Gronenborn, A.M., Sandulache, R. & Clore, G.M. (1987) Site-directed mutants of the cAMP receptor protein - DNA binding of five mutant proteins. *Protein Engineering* 3, 201-203.
102. Shih, D.T., Perutz, F., Gronenborn, A.M. & Clore, G.M. (1987) Histidine proton resonances of carbonmonoxyhaemoglobins A and Cowtown in Chloride-free buffer. *J. Mol. Biol.* 195, 453-455.
103. Clore, G.M., Gronenborn, A.M., Nilges, M. & Ryan, C.A. (1987) The three-dimensional structure of potato carboxypeptidase inhibitor in solution: a study using nuclear magnetic resonance, distance geometry and restrained molecular dynamics. *Biochemistry* 26, 8012-8023.

104. Jansen, C., Gronenborn, A.M. & Clore, G.M. (1987) The binding of the cAMP receptor protein to synthetic DNA sites containing permutations in the consensus sequence TGTGA. *Biochem. J.* 246, 227-232.
105. Nilges, M., Clore, G.M. & Gronenborn, A.M. (1987) A simple method for delineating well-defined and variable regions in protein structures determined from interproton distance data. *FEBS Lett.* 219, 11-16.
106. Clore, G.M., Gronenborn, A.M., Kjær, M. & Poulsen, F.M. (1987) The determination of the three-dimensional structure of barley serine proteinase inhibitor 2 by nuclear magnetic resonance, distance geometry and restrained molecular dynamics. *Protein Engineering* 1, 305-311.
107. Clore, G.M., Gronenborn, A.M., James, M.N.G., Kjær, M., McPhalen, C.A. & Poulsen, F.M. (1987) Comparison of the solution and X-ray structures of barley serine proteinase inhibitor 2. *Protein Engineering* 1, 313-318.
108. Clore, G.M. & Gronenborn, A.M. (1987) Determination of three-dimensional structures of proteins in solution by nuclear magnetic resonance spectroscopy. *Protein Engineering* 1, 275-288.
109. Wingfield, P., Mattaliano, R., MacDonald, H.R., Craig, S., Clore, G.M., Gronenborn, A.M. & Schmeissner, U. (1987) Recombinant derived interleukin-1 α stabilized against specific deamidation. *Protein Engineering* 5, 413-417.
110. Bax, A., Sklenar, V., Clore, G.M. & Gronenborn, A.M. (1987) Water suppression in two-dimensional spin-locked NMR experiments using a novel phase cycling procedure. *J. Am. Chem. Soc.* 109, 6511-6513.
111. Brünger, A.T., Clore, G.M., Gronenborn, A.M. & Karplus, M. (1987) Solution conformations of human growth hormone releasing factor: comparison of the restrained molecular dynamics and distance geometry methods for a system without long range distance data. *Protein Engineering* 1, 399-406.
112. Oschkinat, H., Clore, G.M., Nilges, M. & Gronenborn, A.M. (1987) Application of the z-COSY technique to macromolecules: measuring coupling constants with a modified pulse sequence. *J. Magn. Reson.* 75, 534-539.

1988

113. Meyer, E.F., Clore, G.M., Gronenborn, A.M. & Hansen, H.A.S. (1988) Analysis of an enzyme-substrate complex by X-ray crystallography and transferred nuclear Overhauser enhancement measurements: porcine pancreatic elastase and a hexapeptide. *Biochemistry* 27, 725-730.
114. Clore, G.M., Nilges, M., Brünger, A.T. & Gronenborn, A.M. (1988) Determination of the backbone conformation of secretin by restrained molecular dynamics on the basis of interproton distance data. *Eur. J. Biochem.* 171, 479-484.
115. Scalfi Happ, C., Happ, E., Nilges, M., Gronenborn, A.M. & Clore, G.M. (1988) Refinement of the solution structure of the ribonucleotide 5'r(GCAUGC)₂: combined use of nuclear magnetic resonance and restrained molecular dynamics. *Biochemistry* 27, 1735-1743.
116. Clore, G.M., Oschkinat, H., McLaughlin, L.W., Benseler, F., Scalfi Happ, C., Happ, E. & Gronenborn, A.M. (1988) Refinement of the solution structure of the DNA dodecamer 5'd(CGCGPATTCGCG)₂ containing a stable purine-thymine base pair: combined use of nuclear magnetic resonance and restrained molecular dynamics. *Biochemistry* 27, 4185-4197.

117. Allet, B., Payton, M., Mattaliano, R.J., Gronenborn, A.M., Clore, G.M. & Wingfield, P.T. (1988) The purification and characterization of the bacteriophage Mu DNA-binding protein *ner*. *Gene* 65, 259-268.
118. Gronenborn, A.M., Sandulache, R., Gärtner, S. & Clore, G.M. (1988) Mutations in the cyclic AMP binding site of the cyclic AMP receptor protein of *Escherichia coli*. *Biochem. J.* 253, 801-807.
119. Cieslar, C., Clore, G.M. & Gronenborn, A.M. (1988) Automatic phasing of pure phase absorption two-dimensional NMR spectra. *J. Magn. Reson.* 79, 154-157.
120. Cieslar, C., Clore, G.M. & Gronenborn, A.M. (1988) Computer aided sequential assignment of protein ^1H -NMR spectra. *J. Magn. Reson.* 80, 119-127.
121. Nilges, M., Clore, G.M. and Gronenborn, A.M. (1988) Determination of three-dimensional structures of proteins from interproton distance data by hybrid distance geometry-dynamical simulated annealing calculations. *FEBS Lett* 229, 317-324.
122. Oschkinat, H., Griesinger, C., Kraulis, P.J., Sørensen, O.W., Ernst, R.R., Gronenborn, A.M. & Clore, G.M. (1988) Three-dimensional NMR spectroscopy of a protein in solution. *Nature* 332, 374-376.
123. Nilges, M., Gronenborn, A.M., Brünger, A.T. & Clore, G.M. (1988) Determination of three-dimensional structures of proteins by simulated annealing with interproton distance restraints: application to crambin, potato carboxypeptidase inhibitor and barley serine proteinase inhibitor 2. *Protein Engineering* 2, 27-38.
124. Oschkinat, H., Clore, G.M. & Gronenborn, A.M. (1988) A two-dimensional nuclear Overhauser enhancement experiment using semiselective soft pulses and its applications to proteins. *J. Magn. Reson.* 78, 371-375.
125. Holak, T.A., Engström, Å, Kraulis, P.J., Lindeberg, G., Bennich, H., Jones, T.A., Gronenborn, A.M. & Clore, G.M. (1988) The solution conformation of the antibacterial peptide cecropin A: a nuclear magnetic resonance and dynamical simulated annealing study. *Biochemistry* 27, 7620-7629.
126. Holak, T.A., Nilges, M., Prestegard, H., Gronenborn, A.M. & Clore, G.M. (1988) Three-dimensional structure of acyl carrier protein in solution determined by nuclear magnetic resonance and the combined use of dynamical simulated annealing and distance geometry. *Eur. J. Biochem.* 175, 9-15.
127. Gronenborn, A.M., Wingfield, P.T., McDonald, H.R., Schmeissner, U. & Clore, G.M. (1988) Site directed mutants of human interleukin- 1α : a ^1H -NMR and receptor binding study. *FEBS Lett.* 231, 135-138
128. Scalfi Happ, C., Happ, E., Clore, G.M. & Gronenborn, A.M. (1988) Refinement of the solution structure of the RNA-DNA hybrid $5'[\text{r}(\text{GCA})\text{d}(\text{TGC})]_2$: combined use of nuclear magnetic resonance and restrained molecular dynamics. *FEBS Lett.* 236, 62-70.
129. Clore, G.M., Bax, A., Wingfield, P.T. & Gronenborn, A.M. (1988) Long range ^{15}N - ^1H correlation as an aid to sequential proton resonance assignment of proteins: application to the DNA binding protein *ner* from phage Mu. *FEBS Letters* 238, 17-21.
130. Zarbock, J., Gennaro, R., Romeo, D., Clore, G.M. & Gronenborn, A.M. (1988) A proton nuclear magnetic resonance study of the conformation of bovine anaphylatoxin C5a in solution. *FEBS Letters* 238, 289-294.

131. Nilges, M., Clore, G.M. & Gronenborn, A.M. (1988) Determination of three-dimensional structures of proteins from interproton distance data by dynamical simulated annealing from a random array of atoms. *FEBS Letters* 239, 129-136.
132. Garin, J., Vignais, P.V., Gronenborn, A.M., Clore, G.M., Gao, Z. & Baeuerlein, E. (1988) ¹H-NMR studies on nucleotide binding to the catalytic sites of bovine mitochondrial F₁-ATPase. *FEBS Letters* 242, 178-182.

1989

133. Driscoll, P.C., Clore, G.M., Beress, L. & Gronenborn, A.M. (1989) A proton nuclear magnetic resonance study of the anti-hypertensive and anti-viral protein BDS-I from the sea anemone *Anemonia sulcata*: sequential and stereospecific assignment and secondary structure. *Biochemistry* 28, 2178-2187.
134. Driscoll, P.C., Gronenborn, A.M., Beress, L. & Clore, G.M. (1989) Determination of the three-dimensional structure of the anti-hypertensive and anti-viral protein BDS-I from the sea anemone *Anemonia sulcata*: a study using nuclear magnetic resonance and hybrid distance geometry-dynamical simulated annealing. *Biochemistry* 28, 2188-2198.
135. Oschkinat, H., Cieslar, C., Gronenborn, A.M. & Clore, G.M. (1989) Three-dimensional homonuclear Hartmann Hahn-Nuclear Overhauser enhancement spectroscopy in H₂O and its application to proteins. *J. Magn. Reson.* 81, 212-216.
136. Folkers, P.J.M., Clore, G.M., Driscoll, P.C., Dodt, J., Köhler, S. & Gronenborn, A.M. (1989) The solution structure of recombinant hirudin and the Lys-47→Glu mutant: a nuclear magnetic resonance and hybrid distance geometry-dynamical simulated annealing study. *Biochemistry* 28, 2601-2617.
137. Gronenborn, A.M., Bax, A., Wingfield, P.T. & Clore, G.M. (1989) A powerful method of sequential proton resonance assignment in proteins using relayed ¹⁵N-¹H multiple quantum coherence spectroscopy. *FEBS Letters* 243, 93-98.
138. Driscoll, P.C., Gronenborn, A.M. & Clore, G.M. (1989) The influence of stereospecific assignments on the determination of three-dimensional structures of proteins by nuclear magnetic resonance spectroscopy: application to the sea anemone protein BDS-I. *FEBS Lett.* 243, 223-233.
139. Clore, G.M. & Gronenborn, A.M. (1989) Determination of three-dimensional structures of proteins and nucleic acids in solution by nuclear magnetic resonance spectroscopy. *CRC Critical Reviews in Biochemistry and Molecular Biology* 24, 479-564.
140. Clore, G.M., Nilges, M. & Gronenborn, A.M. (1989) Determination of three-dimensional structures of proteins in solution by dynamical simulated annealing with interproton distances derived from nuclear magnetic resonance spectroscopy. In *Computer-Aided Molecular Design* (Richards, W.G., ed.), pp. 203-219, IBC Technical Services, London.
141. Wingfield, P.T., Graber, P., Shaw, A.R., Gronenborn, A.M., Clore, G.M. & McDonald, H.R. (1989) Preparation, characterization and biochemical application of mutant interleukin-1β's with surface accessible cysteine residues. *Eur. J. Biochem.* 179, 565-571.
142. Oschkinat, H., Cieslar, C., Holak, T.A., Clore, G.M. & Gronenborn, A.M. (1989) Practical and theoretical aspects of three-dimensional homonuclear Hartmann Hahn-nuclear Overhauser enhancement spectroscopy of proteins. *J. Magn. Reson.* 83, 450-472.

143. Gronenborn, A. M., Wingfield, P. T. & Clore, G. M. (1989) Determination of the secondary structure of the DNA binding protein Ner from phage Mu using ^1H homonuclear and ^{15}N - ^1H heteronuclear NMR spectroscopy. *Biochemistry* 28, 5081-5089.
144. Gronenborn, A.M. & Clore, G.M. (1989) Analysis of the relative contributions of the nuclear Overhauser interproton distance restraints and the empirical energy function in the calculation of oligonucleotide structures using restrained molecular dynamics. *Biochemistry* 28, 5978-5984.
145. Forman-Kay, J.D., Clore, G.M., Driscoll, P.C., Wingfield, P.T., Richards, F.M. & Gronenborn, A.M. (1989) A proton nuclear magnetic resonance assignment and secondary structure determination of recombinant human thioredoxin. *Biochemistry* 28, 7088-7097.
146. Kraulis, P.J., Clore, G.M., Nilges, M., Jones, T.A., Pettersson, G., Knowles, J. & Gronenborn, A.M. (1989) Determination of the three-dimensional solution structure of the C-terminal domain of cellobiohydrolase I from *Trichoderma reesei*: a study using nuclear magnetic resonance and hybrid distance geometry-dynamical simulated annealing. *Biochemistry* 28, 7241-7257.
147. Clore, G.M. & Gronenborn, A.M. (1989) How accurately can interproton distances in macromolecules really be determined by full relaxation matrix analysis of nuclear Overhauser enhancement data? *J. Magn. Reson.* 84, 398-409.
148. Marion, D., Driscoll, P.C., Kay, L.E., Wingfield, P.T., Bax, A., Gronenborn, A.M. & Clore, G.M. (1989) Overcoming the overlap problem in the assignment of ^1H -NMR spectra of larger proteins using three-dimensional heteronuclear ^1H - ^{15}N Hartmann-Hahn and nuclear Overhauser - multiple quantum coherence spectroscopy: application to interleukin- 1β . *Biochemistry* 28, 6150-6156.
149. Clore, G.M., Appella, E., Yamada, M., Matsushima, K. & Gronenborn, A.M. (1989) Determination of the secondary structure of interleukin-8 by nuclear magnetic resonance spectroscopy. *J. Biol. Chem.* 264, 18907-18911.

1990

150. Gronenborn, A.M., Nilges, M., Peanasky, R.J. & Clore, G.M. (1990) Sequential resonance assignment and secondary structure determination of the *Ascaris* trypsin inhibitor, a member of a novel class of proteinases inhibitors. *Biochemistry* 29, 183-189.
151. Nilges, M., Clore, G.M. & Gronenborn, A.M. (1990) ^1H -NMR stereospecific assignments by conformational database searches. *Biopolymers* 29, 813-822.
152. Clore, G.M. & Gronenborn, A.M. (1990) Extending the limits of protein structure determination by NMR. In *Theoretical Biochemistry and Molecular Biophysics: a Comprehensive Survey*, (Beveridge, D.L. and Lavery, L., eds.), vol. 2, pp. 1-16, Adenine Press, New York.
153. Forman-Kay, J.D., Gronenborn, A.M., Kay, L.E., Wingfield, P.T. & Clore, G.M. (1990) Studies on the solution conformation of human thioredoxin using heteronuclear ^{15}N - ^1H nuclear magnetic resonance spectroscopy. *Biochemistry* 29, 1566-1572.
154. Gronenborn, A.M. & Clore, G.M. (1990) Protein structure determination in solution by two-dimensional and three-dimensional nuclear magnetic resonance spectroscopy. *Analytical Chemistry* 62, 2-15.

155. Driscoll, P.C., Clore, G.M., Marion, D., Wingfield, P.T. & Gronenborn, A.M. (1990) Complete resonance assignment for the polypeptide backbone of interleukin-1 β using three-dimensional heteronuclear NMR spectroscopy. *Biochemistry* 29, 3542-3556.
156. Driscoll, P.C., Gronenborn, A.M., Wingfield, P.T. & Clore, G.M. (1990) Determination of the secondary structure and molecular topology of interleukin-1 β using two- and three-dimensional heteronuclear ^{15}N - ^1H NMR spectroscopy. *Biochemistry* 29, 4468-4682.
157. Clore, G.M., Appella, E., Yamada, M., Matsushima, K. & Gronenborn, A.M. (1990) The three-dimensional structure of interleukin-8 in solution. *Biochemistry* 29, 1689-1696.
158. Bax, A., Clore, G.M., Driscoll, P.C., Gronenborn, A.M., Ikura, M. & Kay, L.E. (1990) Practical aspects of proton-carbon-carbon-proton three-dimensional correlation spectroscopy of ^{13}C -labeled proteins. *J. Magn. Reson.* 87, 620-628.
159. Bax, A., Clore, G.M. & Gronenborn, A.M. (1990) ^1H - ^1H correlation via isotropic mixing of ^{13}C magnetization: a new three-dimensional approach for assigning ^1H and ^{13}C spectra of ^{13}C -enriched proteins. *J. Magn. Reson.* 88, 425-431.
160. Clore, G.M., Szabo, A., Bax, A., Kay, L.E., Driscoll, P.C. & Gronenborn, A.M. (1990) Deviations from the simple two parameter model free approach to the interpretation of ^{15}N nuclear magnetic relaxation of proteins. *J. Am. Chem. Soc.* 112, 4989-4991.
161. Clore, G.M., Driscoll, P.C., Wingfield, P.T. & Gronenborn, A.M. (1990) Low resolution structure of interleukin-1 β in solution derived from ^1H - ^{15}N heteronuclear three-dimensional NMR spectroscopy. *J. Mol. Biol.* 214, 811-817.
162. Clore, G.M., Driscoll, P.C., Wingfield, P.T. & Gronenborn, A.M. (1990) Analysis of backbone dynamics of interleukin-1 β using two-dimensional inverse detected heteronuclear ^{15}N - ^1H NMR spectroscopy. *Biochemistry* 29, 7387-7401.
163. Clore, G.M., Bax, A., Wingfield, P.T. & Gronenborn, A.M. (1990) Identification and localization of bound internal water in the solution structure of interleukin-1 β by heteronuclear three-dimensional ^1H rotating frame Overhauser ^{15}N - ^1H multiple quantum coherence NMR spectroscopy. *Biochemistry* 29, 5671-5676.
164. Clore, G.M., Bax, A., Driscoll, P.C., Wingfield, P.T. & Gronenborn, A.M. (1990) Assignment of the side chain ^1H and ^{13}C resonance of interleukin-1 β using double and triple resonance heteronuclear three-dimensional NMR spectroscopy. *Biochemistry* 29, 8172-8184.
165. Kay, L.E., Clore, G.M., Bax, A. & Gronenborn, A.M. (1990) Four-dimensional heteronuclear triple resonance NMR spectroscopy of interleukin-1 β in solution. *Science* 249, 411-414.
166. Omichinski, J., Clore, G.M., Appella, E., Sakaguchi, K. & Gronenborn, A.M. (1990) High resolution three-dimensional solution structure of a single zinc finger from a human enhancer binding protein in solution. *Biochemistry* 29, 9324-9334.
167. Becerra, S.P., Clore, G.M., Gronenborn, A.M., Karlström, A., Stahl, S.J., Wilson, S.H. & Wingfield, P.T. (1990) Purification and characterization of the RNase H domain of HIV-1 reverse transcriptase expressed in recombinant Escherichia coli. *FEBS Lett.* 270, 76-80.
168. Ikura, M., Bax, A., Clore, G.M. & Gronenborn, A.M. (1990) Detection of nuclear Overhauser effects between degenerate amide proton resonances by heteronuclear three-dimensional NMR spectroscopy. *J. Am. Chem. Soc.* 112, 9020-9022.

1991

169. Clore, G.M., Kay, L.E., Bax, A. & Gronenborn, A.M. (1991) Four dimensional $^{13}\text{C}/^{13}\text{C}$ -edited nuclear Overhauser enhancement spectroscopy of a protein in solution: application to interleukin-1 β . *Biochemistry* 30, 12-18.
170. Clore, G.M. & Gronenborn, A.M. (1991) Two, three and four dimensional NMR methods for obtaining larger and more precise three-dimensional structures of proteins in solution. *Ann. Rev. Biophys. Biophys. Chem.* 20, 29-63.
171. Clore, G.M. & Gronenborn, A.M. (1991) Comparison of NMR and X-ray structures of hirudin. In *Computational Aspects of the Study of Biological Macromolecules by Nuclear Magnetic Resonance Spectroscopy*, (ed. Hoch, J.C.), pp. 57-66, NATO ASI Series, Plenum Press.
172. Forman-Kay, J.D., Clore, G.M., Wingfield, P.T. & Gronenborn, A.M. (1991) The high resolution three-dimensional structure of reduced recombinant human thioredoxin in solution. *Biochemistry* 30, 2685-2698.
173. Baldwin, E.T., Weber, I.T., St. Charles, R., Xuan, J.C., Appella, E., Yamada, M., Matsushima, K., Edwards, B.F.P., Clore, G.M., Gronenborn, A.M. & Wlodawer, A. (1991) Crystal structure of interleukin-8: symbiosis of NMR and crystallography. *Proc. Natl. Acad. Sci. U.S.A.* 88, 502-506.
174. Clore, G.M. & Gronenborn, A.M. (1991) Comparison of the solution nuclear magnetic resonance and crystal structures of interleukin-8: possible implications for the mechanism of receptor binding. *J. Mol. Biol.* 217, 611-620.
175. Gronenborn, A.M. & Clore, G.M. (1991) Modeling the three-dimensional structure of the monocyte chemoattractant and activating protein MCAF/MCP-1 on the basis of the solution structure of interleukin-8. *Protein Engineering* 4, 263-269.
176. Clore, G.M., Bax, A. & Gronenborn, A.M. (1991) Stereospecific assignment of β -methylene protons in larger proteins using three-dimensional ^{15}N -separated Hartmann-Hahn and ^{13}C -separated rotating frame Overhauser spectroscopy. *J. Biomol. NMR* 1, 13-22.
177. Clore, G.M., Wingfield, P.T. & Gronenborn, A.M. (1991) High resolution three dimensional structure of interleukin-1 β in solution by three and four dimensional nuclear magnetic resonance spectroscopy. *Biochemistry* 30, 2315-2323.
178. Clore, G.M. & Gronenborn, A.M. (1991) NMR and X-ray analysis of the three-dimensional structure of interleukin-8. In *Neutrophil-Activating Peptides and other Chemotactic Cytokines*, (Baggiolini, M. & Sorg, C., eds.) 4, 18-40, S. Karger, Basel.
179. Clore, G.M. & Gronenborn, A.M. (1991) Applications of three- and four-dimensional heteronuclear NMR spectroscopy to protein structure determination. *Progr. Nucl. Magn. Reson. Spectroscopy* 23, 43-92.
180. Sakaguchi, K., Appella, E., Omichinski, J.G., Clore, G.M. & Gronenborn, A.M. (1991) Specific DNA binding to an MHC enhancer sequence by a synthetic 57-residue double zinc finger peptide from a human enhancer binding protein. *J. Biol. Chem.* 266, 7306-7311.
181. Clore, G.M., Omichinski, J.G. & Gronenborn, A.M. (1991) Slow conformational dynamics at the metal coordination site of a zinc finger. *J. Am. Chem. Soc.* 113, 4350-4351.

182. Clore, G.M. & Gronenborn, A.M. (1991) Structures of larger proteins in solution: three- and four-dimensional heteronuclear NMR spectroscopy. *Science* 252, 1390-1399.
183. Forman-Kay, J.D., Gronenborn, A.M., Wingfield, P.T. & Clore, G.M. (1991) Determination of the positions of bound water in the solution structure of reduced human thioredoxin by heteronuclear three-dimensional nuclear magnetic resonance spectroscopy. *J. Mol. Biol.* 220, 209-216.
184. Clore, G.M. & Gronenborn, A.M. (1991) Comparison of the solution nuclear magnetic resonance and X-ray crystal structures of human recombinant interleukin-1 β . *J. Mol. Biol.* 221, 47-53.
185. Powers, R., Gronenborn, A.M., Clore, G.M. & Bax, A. (1991) Three-dimensional triple resonance NMR of $^{13}\text{C}/^{15}\text{N}$ enriched proteins using constant-time evolution. *J. Magn. Reson.* 94, 209-213.
186. Gronenborn, A.M., Filpula, D.R., Essig, N.Z., Achari, A., Whitlow, M., Wingfield, P.T. & Clore, G.M. (1991) A novel highly stable fold of the immunoglobulin binding domain of Streptococcal protein G. *Science* 253, 657-661.
187. Powers, R., Clore, G.M., Bax, A., Garrett, D.S., Stahl, S.J., Wingfield, P.T. & Gronenborn, A.M. (1991) Secondary structure of the ribonuclease H domain of the human immunodeficiency virus reverse transcriptase in solution using three-dimensional double and triple resonance heteronuclear magnetic resonance spectroscopy. *J. Mol. Biol.* 221, 1081-1090.
188. Garrett, D.S., Powers, R., Gronenborn, A.M. & Clore, G.M. (1991) A common sense approach to peak picking two-, three- and four-dimensional spectra using automatic computer analysis of contour diagrams. *J. Magn. Reson.* 95, 214-220.
189. Omichinski, J.G., Clore, G.M., Sakaguchi, K., Appella, E. & Gronenborn, A.M. (1991) Structural characterization of a 39-residue synthetic peptide containing the two zinc binding domains from the HIV-1 p7 nucleocapsid protein by CD and NMR spectroscopy. *FEBS Lett.* 292, 25-30.
190. Gronenborn, A.M. & Clore, G.M. (1991) Similarity of Protein G and Ubiquitin. *Science* 254, 581-582.

1992

191. Clore, G.M. & Gronenborn, A.M. (1992) Localization of bound water in the solution structure of the immunoglobulin binding domain of Streptococcal protein G: evidence for solvent induced helical distortions in solution. *J. Mol. Biol.* 223, 853-856.
192. Grzesiek, S., Ikura, M., Clore, G.M., Gronenborn, A.M. & Bax, A. (1992) A 3D triple resonance NMR technique for qualitative measurement of carbonyl-H β J couplings in isotopically enriched proteins. *J. Magn. Reson.* 96, 215-221.
193. Clore, G.M. & Gronenborn, A.M. (1992) Practical aspects of two, three and four-dimensional nuclear magnetic resonance spectroscopy applied to the study of protein structure. In *Protein Engineering - a Practical Approach*, (eds. Rees, A.R., Wetzel, R. & Sternberg, M.J.E.), pp. 33-56, Oxford University Press.
194. Lozier, R.H., Xie, A., Hofrichter, J. & Clore, G.M. (1992) Reversible steps in the bacteriorhodopsin photocycle. *Proc. Natl. Acad. Sci.* 89, 3610-3614.
195. Omichinski, J.G., Clore, G.M., Robien, M., Sakaguchi, K., Appella, E. & Gronenborn, A.M. (1992) High resolution solution structure of the double Cys $_2$ His $_2$ zinc finger from the human enhancer binding protein MBP-1. *Biochemistry* 31, 3907-3917.

196. Forman-Kay, J.D., Clore, G.M. & Gronenborn, A.M. (1992) The relationship between electrostatics and redox function in human thioredoxin: characterization of pH titration shifts using two-dimensional homo- and heteronuclear NMR. *Biochemistry* 31, 3442-3452.
197. Robien, M.A., Clore, G.M., Omichinski, J.G., Perham, R.N., Appella, E., Sakaguchi, K. & Gronenborn, A.M. (1992) Three-dimensional solution structure of the E3-binding domain of the dihydrolipoamide succinyltransferase core from the 2-oxoglutarate dehydrogenase multienzyme complex of *Escherichia coli*. *Biochemistry* 31, 3463-3471.
198. Powers, R., Garrett, D.S., March, C.J., Frieden, E.A., Gronenborn, A.M. & Clore, G.M. (1992) ^1H , ^{15}N , ^{13}C and ^{13}CO assignments of human interleukin-4 using three-dimensional double and triple resonance heteronuclear magnetic resonance spectroscopy. *Biochemistry* 31, 4334-4347.
199. Garrett, D.S., Powers, R., March, C.J., Frieden, E.A., Clore, G.M. & Gronenborn, A.M. (1992) Determination of the secondary structure and folding topology of human interleukin-4 using three-dimensional heteronuclear magnetic resonance spectroscopy. *Biochemistry* 31, 4347-4353.
200. Chandrasasekhar, I., Clore, G.M., Szabo, A., Gronenborn, A.M. & Brooks, B.R. (1992) A 500 ps molecular dynamics simulation study of interleukin-1 β in water: correlation with nuclear magnetic resonance spectroscopy and crystallography. *J. Mol. Biol.* 226, 239-250.
201. Ikura, M., Clore, G.M., Gronenborn, A.M., Zhu, G., Klee, C.B. & Bax, A. (1992) Solution structure of a calmodulin-target peptide complex by multi-dimensional NMR. *Science* 256, 632-638.
202. Powers, R., Garrett, D.S., March, C.J., Frieden, E.A., Gronenborn, A.M. & Clore, G.M. (1992) Three-dimensional solution structure of human interleukin-4 by multi-dimensional heteronuclear magnetic resonance spectroscopy. *Science* 256, 1673-1677.
203. Forman-Kay, J.D., Clore, G.M., Stahl, S.J. & Gronenborn, A.M. (1992) ^1H and ^{15}N resonance assignments and secondary structure of the human thioredoxin C62A, C69A, C73A mutant. *J. Biomolec. NMR* 2, 431-445.
204. Achari, A., Hale, S.P., Howard, A.J., Clore, G.M., Gronenborn, A.M., Hardman, K.D. & Whitlow, M. (1992) The 1.67 Å X-ray structure of the B2 immunoglobulin domain of streptococcal protein G and comparison to the NMR structure of the B1 domain. *Biochemistry* 31, 10449-10457.
205. Shaanan, B., Gronenborn, A.M., Cohen, G.H., Gilliland, G.L., Veerapandian, B., Davies, D.R. & Clore, G.M. (1992) Combining experimental information from crystal and solution studies: joint X-ray and NMR refinement. *Science* 257, 961-964.
206. Rose, K., Simona, M.G., Savoy, L.A., Regamey, P.O., Green, B.N., Clore, G.M., Gronenborn, A.M. & Wingfield, P.T. (1992) Pyruvic acid is attached through its central carbon atom to the amino terminus of the recombinant-DNA derived DNA-binding protein Ner of bacteriophage Mu. *J. Biol. Chem.* 267, 19101-19106.
207. Powers, R., Clore, G.M., Stahl, S.J., Wingfield, P.T. & Gronenborn, A.M. (1992) Analysis of the backbone dynamics of the ribonuclease H domain of the human immunodeficiency virus reverse transcriptase using ^{15}N relaxation measurements. *Biochemistry* 31, 9150-9157.

1993

208. Omichinski, J.G., Trainor, C., Evans, T., Gronenborn, A.M., Clore, G.M. & Felsenfeld, G. (1993) A small single-'finger' peptide from the erythroid factor GATA-1 binds specifically to DNA as a zinc or iron complex. *Proc. Natl. Acad. Sci. U.S.A.* 90, 1676-1680.

209. Grasberger, B.L., Gronenborn, A.M. & Clore, G.M. (1993) Analysis of the backbone dynamics of interleukin-8 by ^{15}N relaxation measurements. *J. Mol. Biol.* 230, 364-372.
210. Clore, G.M., Robien, M.A. & Gronenborn, A.M. (1993) Exploring the limits of precision and accuracy of protein structures determined by nuclear magnetic resonance spectroscopy. *J. Mol. Biol.* 231, 82-102.
211. Vuister, G.W., Clore, G.M., Gronenborn, A.M., Powers, R., Garrett, D.S., Tschudin, R. & Bax, A. (1993) Increased resolution and improved spectral quality in four-dimensional $^{13}\text{C}/^{13}\text{C}$ -separated HMQC-NOE-HMQC spectra using pulsed field gradients. *J. Magn. Reson. Series B* 101, 210-213.
212. Sakaguchi, K., Zambrano, N., Baldwin, E.T., Shapiro, B.A., Erickson, J.W., J.G. Omichinski, G.M. Clore, A.M. Gronenborn & E. Appella (1993) Identification of a binding site for the human immunodeficiency virus type I nucleocapsid protein. *Proc. Natl. Acad. Sci. U.S.A.* 90, 5219-5223.
213. Varley, P., Gronenborn, A.M., Christensen, H., Wingfield, P.T., Pain, R.H. & Clore, G.M. (1993) Kinetics of folding of the all β -sheet protein interleukin-1 β studied by nuclear magnetic resonance, circular dichroism and fluorescence. *Science* 240, 1110-1113.
214. Powers, R., Clore, G.M., Garrett, D.S. & Gronenborn, A.M. (1993) Relationships between the precision of high resolution protein NMR structures, solution order parameters and crystallographic B factors. *J. Magn. Reson. Series B* 101, 325-327.
215. Gronenborn, A.M. & Clore, G.M. (1993) Structural studies of immunoglobulin binding domains of Streptococcal Protein G. *ImmunoMethods* 2, 3-8.
216. Powers, R., Garrett, D.S., March, C.J., Frieden, E.A., Gronenborn, A.M. & Clore, G.M. (1993) The high resolution three-dimensional solution structure of human interleukin-4 determined by multi-dimensional heteronuclear magnetic resonance spectroscopy. *Biochemistry* 32, 6744-6762.
217. Gronenborn, A.M. & Clore, G.M. (1993) Identification of the contact surface of a Streptococcal protein G domain complexed with a human Fc fragment. *J. Mol. Biol.* 233, 331-335.
218. Clore, G.M. & Gronenborn, A.M. (1993) Structural studies of interleukin-1 β , interleukin-4 and interleukin-8, *ImmunoMethods* 3, 56-81.
219. Brünger, A.T., Clore, G.M., Gronenborn, A.M., Saffrich, R. & Nilges, M. (1993) Assessing the quality of solution nuclear magnetic resonance structures by complete cross-validation. *Science* 261, 328-331.
220. Omichinski, J.G., Clore, G.M., Schaad, O., Felsenfeld, G., Trainor, C., Appella, E., Stahl, S.J. & Gronenborn, A.M. (1993) NMR structure of a specific DNA complex of a Zn-containing DNA binding domain of GATA-1. *Science* 261, 438-446.
221. Clore, G.M., Bax, A., Ikura, M. & Gronenborn, A.M. (1993) Structure of calmodulin-target peptide complexes. *Current Opinion in Structural Biology* 3, 838-845.

1994

222. Bax, A., Grzesiek, S., Gronenborn, A.M. & Clore, G.M. (1994) Isotope-filtered 2D HOHAHA spectroscopy of a peptide-protein complex using heteronuclear Hartmann-Hahn dephasing. *J. Magn. Reson.* 106 Series A, 269-273.

223. Gronenborn, A.M. & Clore, G.M. (1994) Experimental support for the "hydrophobic zipper" hypothesis of protein folding. *Science* 263, 536.
224. Barchi, J.J., Grasberger, B., Gronenborn, A.M. & Clore, G.M. (1994) Investigation of the backbone dynamics of the IgG-binding domain of Streptococcal Protein G by heteronuclear two-dimensional ^1H - ^{15}N nuclear magnetic resonance spectroscopy. *Protein Science* 3, 15-21.
225. Clore, G.M., Bax, A., Omichinski, J.G. & Gronenborn, A.M. (1994) Localization of bound water in the solution structure of the specific complex of the erythroid transcription factor GATA-1 with DNA by water selective two-dimensional heteronuclear magnetic resonance spectroscopy. *Structure* 2, 89-94.
226. Clubb, R.T., Omichinski, J.G., Clore, G.M. & Gronenborn, A.M. (1994) Mapping the binding surface of interleukin-8 complexed with an N-terminal fragment of the type I human interleukin-8 receptor. *FEBS Lett.* 338, 93-97.
227. Garrett, D.S., Lodi, P.J., Shamoo, Y., Williams, K.R., Clore, G.M. & Gronenborn, A.M. (1994) Determination of the secondary structure and folding topology of a RNA binding domain of the mammalian hnRNP A1 protein using three-dimensional heteronuclear magnetic resonance spectroscopy. *Biochemistry* 33, 2852-2858.
228. Clore, G.M. & Gronenborn, A.M. (1994) Structures of larger proteins, protein-ligand and protein-DNA complexes by multi-dimensional heteronuclear NMR. *Protein Science* 3, 372-390.
Progr. Biophys. Mol. Biol. 62, 153-184.
In Encyclopedia of Nuclear Magnetic Resonance, vol. 7, pp. 4602-4622, (eds. Grant, D.M. & Harris, R.K.), John Wiley & Sons, New York (1996).
229. Rozwarski, D.A., Gronenborn, A.M., Clore, G.M., Bazan, J.F., Bohm, A., Wlodawer, A., Hatada, M. & Karplus, P.A. (1994) Structural comparison among the short-chain helical cytokines. *Structure* 2, 159-173.
230. Lodi, P.J., Garrett, D.S., Kuszewski, J., Tsang, M.L.S., Weatherbee, J.A., Leonard, W.J., Gronenborn, A.M. & Clore, G.M. (1994) High resolution solution structure of the β chemokine hMIP-1 β by multi-dimensional NMR. *Science* 263, 1762-1767.
231. Garrett, D.S., Kuszewski, J., Hancock, T.J., Lodi, P.J., Vuister, G.W., Gronenborn, A.M. & Clore, G.M. (1994) The impact of direct refinement against three-bond $\text{HN-C}^{\alpha}\text{H}$ coupling constants on protein structure determination by NMR. *J. Magn. Reson. Series B* 104, 99-103.
232. Gronenborn, A.M. & Clore, G.M. (1994) Identification of N-terminal helix capping boxes by means of ^{13}C chemical shifts. *J. Biomol. NMR* 4, 455-458.
233. Smith, L.J., Redfield, C., Smith, R.A.G., Dobson, C.M., Clore, G.M., Gronenborn, A.M., Walter, M.R., Naganbushan, T.L. & Wlodawer, A. (1994) Comparison of four independently determined structures of human recombinant interleukin-4. *Nature Struct. Biol.* 1, 301-310.
234. Werner, M.H., Clore, G.M., Gronenborn, A.M., Kondoh, A. & Fisher, R.J. (1994) Refolding proteins by gel filtration chromatography. *FEBS Lett.* 345, 125-130.
235. Qin, J., Clore, G.M. & Gronenborn, A.M. (1994) The high resolution three-dimensional solution structure of the oxidized and reduced states of human thioredoxin: delineation of conformational differences between the two redox states. *Structure* 2, 503-522.
236. Werner, M.W., Clore, G.M., Gronenborn, A.M. & Nash, H.A. (1994) Symmetry and asymmetry in the function of Escherichia coli integration host factor. *Current Biology* 4, 477-487.

237. Grasberger, B.L., Clore, G.M. & Gronenborn, A.M. (1994) High-resolution structure of *Ascaris* trypsin inhibitor in solution: direct evidence for a pH induced conformational transition in the reactive site. *Structure* 2, 669-678.
238. Makhatadze, G.I., Clore, G.M., Gronenborn, A.M. & Privalov, P.L. (1994) Thermodynamics of unfolding of the all β -sheet protein interleukin-1 β . *Biochemistry* 33, 9327-9332
239. Clore, G.M. & Gronenborn, A.M. (1994) Multidimensional heteronuclear nuclear magnetic resonance of proteins. *Meth. Enzymol.* 239, 349-363.
Spectroscopy 10, 32-38 (1995).
In Encyclopedia of Nuclear Magnetic Resonance, vol. 7, pp. 4744-4752, (eds. Grant, D.M. & Harris, R.K.), John Wiley & Sons, New York (1996).
240. Gronenborn, A.M. & Clore, G.M. (1994) Where is NMR taking us. *Proteins: Struct. Funct. Genet.* 19, 273-276.
241. Clore, G.M., Omichinski, J.G., Sakaguchi, K., Zambrano, N., Sakamoto, H., Appella, E. & Gronenborn, A.M. (1994) High-resolution solution structure of the oligomerization domain of p53 by multi-dimensional NMR. *Science* 265, 386-391.
242. Wang, A.C., Lodi, P.J., Qin, J., Vuister, G.W., Gronenborn, A.M. & Clore, G.M. (1994) An efficient triple-resonance experiment for proton-directed sequential backbone assignment of medium-sized proteins. *J. Magn. Reson. Series B* 105, 196-198.
243. Gronenborn, A.M. & Clore, G.M. (1994) Structural studies of interleukin-8 and interleukin-4. *In Structural Biology: The State of the Art*, (Sarma, R.H. & Sarma, M.H., eds.) pp. 19-42, Adenine Press, New York.
244. Covell, D.G., Smythers, G.W., Gronenborn, A.M. & Clore, G.M. (1994) Analysis of hydrophobicity in the α and β chemokine families and its relevance to dimerization. *Protein Science* 3, 2064-2072.
245. Kuszewski, J., Clore, G.M. & Gronenborn, A.M. (1994) Fast folding of a prototypic polypeptide: the immunoglobulin binding domain of Streptococcal Protein G. *Protein Science* 3, 1945-1952.
246. Clubb, R.T., Omichinski, J.G., Savilahti, H., Mizuuchi, K., Gronenborn, A.M. & Clore, G.M. (1994) A novel class of winged helix-turn-helix protein - the DNA binding domain of Mu transposase. *Structure* 2, 1041-1048.

1995

247. Clore, G.M. & Gronenborn, A.M. (1995) Three-dimensional structures of α and β chemokines. *FASEB Journal* 9, 57-62.
248. Kuszewski, J., Qin, J., Gronenborn, A.M. & Clore, G.M. (1995) The impact of direct refinement against $^{13}\text{C}^\alpha$ and $^{13}\text{C}^\beta$ chemical shifts on protein structure determination by NMR. *J. Magn. Reson Series B* 106, 92-96.
249. Ernst, J.A., Clubb, R.T., Zhou, H.-X., Gronenborn, A.M. & Clore, G.M. (1995) Demonstration of positionally disordered water within a protein hydrophobic cavity by NMR. *Science* 267, 1813-1817.

250. Clore, G.M., Omichinski, J.G., Sakaguchi, K., Zambrano, N., Sakamoto, H., Appella, E. & Gronenborn, A.M. (1995) Interhelical angles in the solution structure of the oligomerization domain of the tumour suppressor p53. *Science* 267, 1515-1516.
251. Strzelecka, T.E., Hayes, J.J., Clore, G.M. & Gronenborn, A.M. (1995) DNA binding specificity of the Mu Ner protein. *Biochemistry* 34, 2946-2955.
252. Qin, J., Clore, G.M. Kennedy, W.M.P., Huth, J.R. & Gronenborn, A.M. (1995) Solution structure of human thioredoxin in a mixed disulfide intermediate complex with its target peptide from the transcription factor NFκB. *Structure* 3, 289-297.
253. Clore, G.M., Ernst, J., Clubb, R.T., Omichinski, J.G., Kennedy, W.M.P., Sakaguchi, K., Appella, E. & Gronenborn, A.M. (1995) Refined solution structure of the oligomerization domain of the tumour suppressor p53. *Nature Struct. Biol.* 2, 321-332.
254. Clubb, R.T., Omichinski, J.G., Sakaguchi, K., Appella, E., Gronenborn, A.M. & Clore, G.M. (1995) Backbone dynamics of the oligomerization domain of p53 determined from ¹⁵N NMR relaxation measurements. *Protein Science* 4, 855-862.
255. Kuszewski, J., Gronenborn, A.M. & Clore, G.M. (1995) The impact of direct refinement against proton chemical shifts in protein structure determination by NMR. *J. Magn. Reson. Series B* 107, 293-297.
256. Werner, M.H., Huth, J.R., Gronenborn, A.M. & Clore, G.M. (1995) Molecular basis of human 46X,Y sex reversal revealed from the three-dimensional solution structure of the human SRY-DNA complex. *Cell* 81, 705-714.
257. Balagurumoorthy, P., Sakamoto, K., Lewis, M.S., Zambrano, N., Clore, G.M., Gronenborn, A.M., Appella, E. & Harrington, R.E. (1995) Four p53 DNA binding domains bind natural p53 response elements and bend the DNA. *Proc. Natl. Acad. Sci. U.S.A.* 92, 8591-8585.
258. Lodi, P.J., Ernst, J.A., Kuszewski, J., Hickman, A.B., Engelman, A., Craigie, R., Clore, G.M. & Gronenborn, A.M. (1995) Solution structure of the DNA binding domain of HIV-1 integrase. *Biochemistry* 34, 9826-9833.
259. Makhatadze, G.I., Clore, G.M. & Gronenborn, A.M. (1995) Solvent isotope effect and protein stability. *Nature Struct. Biol.* 2, 852-855.
260. Werner, M.H., Bianchi, M.E., Gronenborn, A.M. & Clore, G.M. (1995) NMR spectroscopic analysis of the DNA conformation induced by the human testis determining factor SRY. *Biochemistry* 34, 11998-12004.
261. Strzelecka, T.E., Clore, G.M. & Gronenborn, A.M. (1995) The solution structure of the Mu Ner protein reveals a helix-turn-helix DNA recognition motif. *Structure* 3, 1087-1095.
262. Gronenborn, A.M. & Clore, G.M. (1995) Structures of protein complexes by multidimensional heteronuclear magnetic resonance spectroscopy. *CRC Crit. Rev. Biochem. Mol. Biol.* 30, 351-385.
263. Werner, M.H., Clore, G.M., Fisher, C.L., Fisher, R.J., Trinh, L., Shiloach, J. & Gronenborn, A.M. (1995) The solution structure of the human ETS1/DNA complex reveals a novel mode of binding and true sidechain intercalation. *Cell* 83, 761-771.
Erratum: *Cell* 87, issue No. 2 (1996).
Correction of the NMR structure of the ETS1/DNA complex. *J. Biomol. NMR* 10, 317-328 (1997).

264. Frank, M.K., Clore, G.M. & Gronenborn, A.M. (1995) Structural and dynamic characterization of the urea denatured state of the immunoglobulin binding domain of Streptococcal protein G. *Protein Science* 4, 2605-2615.

1996

265. Clubb, R.T., Mizuuchi, M., Huth, J.R., Omichinski, J.G., Savilahti, H., Mizuuchi, K., Clore, G.M. & Gronenborn, A.M. (1996) The wing of the enhancer binding domain of Mu phase transposase is flexible and essential for efficient transposition. *Proc. Natl. Acad. Sci. U.S.A.* 93, 1146-1150.
266. Qin, J., Clore, G.M. & Gronenborn, A.M. (1996) Ionization equilibria for the side chain carboxyl groups in oxidized and reduced human thioredoxin and in the complex with its target peptide from the transcription factor NFκB. *Biochemistry* 35, 7-13.
267. Gronenborn, A.M. & Clore, G.M. (1996) Rapid screening for structural integrity of expressed proteins by heteronuclear NMR spectroscopy. *Protein Science* 5, 174-177.
268. Pedone, P.V., Ghirlando, R., Clore, G.M., Gronenborn, A.M., Felsenfeld, G. & Omichinski, J.G. (1996) The single Cys₂His₂ zinc finger domain of the GAGA protein flanked by basic residues is sufficient for high affinity DNA binding. *Proc. Natl. Acad. Sci. U.S.A.* 93, 2822-2826.
269. Werner, M.H., Gronenborn, A.M. & Clore, G.M. (1996) Intercalation, DNA kinking and the control of transcription. *Science* 271, 778-784.
270. Grzesiek, S., Bax, A., Clore, G.M., Gronenborn, A.M., Hu, J.-H., Kaufman, J., Palmer, I., Stahl, S.J. & Wingfield, P.T. (1996) The solution structure of HIV-1 Nef reveals an unexpected fold and permits delineation of the binding surface for the SH3 domain of Hck tyrosine protein kinase. *Nature Struct. Biol.* 3, 340-345.
271. Clore, G.M., Werner, M.H., Huth, J.R. & Gronenborn, A.M. (1996) Understanding 46X,Y sex reversal at the atomic level.
In Biological Structure and Dynamics, (eds. Sarma, R.H. & Sarma, M.H.), Vol. 1, pp. 35-40, Adenine press, New York.
In Mechanisms in Transcription, Nucleic Acids and Molecular Biology, (ed., Ecsktein, F. & Lilley, D.M.J.), vol. 11, pp. 265-273, Springer-Verlag, Berlin.
272. Trainor, C.D., Omichinski, J.G., Vandergon, T.L., Gronenborn, A.M., Clore, G.M. & Felsenfeld, G. (1996) A palindromic regulatory site with vertebrate GATA-1 promoters requires both zinc fingers of the GATA-1 DNA binding domain for high affinity interaction. *Mol. Cell. Biol.* 16, 2238-2247.
273. Qin, J., Clore, G.M., Kennedy W.P., Kuszewski, J. & Gronenborn, A.M. (1996) The solution structure of human thioredoxin complexed with its target from Ref-1 reveals peptide chain reversal. *Structure* 4, 613-620.
274. Kuszewski, J., Gronenborn, A.M. & Clore, G.M. (1996) Improving the quality of NMR and crystallographic protein structures by means of a conformational database potential derived from structure databases. *Protein Science* 5, 1067-1080.
275. Werner, M.H., Huth, J.R., Gronenborn, A.M. & Clore, G.M. (1996) Molecular determinants of mammalian sex. *Trends in Biochem.* 21, 302-308.

276. Kuszewski, J., Gronenborn, A.M. & Clore, G.M. (1996) A potential involving multiple proton chemical shift restraints for non-stereospecifically assigned methyl and methylene protons. *J. Magn. Reson. Series B* 112, 79-81.
277. Gronenborn, A.M., Frank, M.K. & Clore, G.M. (1996) Core mutants of the immunoglobulin binding domain of Streptococcal protein G: stability and structural integrity. *FEBS Lett.* 398, 312-316.
278. Miller, M., Lubkowski, J., Rao, M.J.K., Danishefsky, A.T., Omichinski, J.G., Sakaguchi, K., Sakamoto, H., Appella, E., Gronenborn, A.M. & Clore, G.M. (1996) The oligomerization domain of p53: crystal structure of the trigonal form. *FEBS Lett.* 399, 166-170.

1997

279. Clore, G.M. & Gronenborn, A.M. (1997) Dissecting intrinsic chaperonin activity. *Proc. Natl. Acad. Sci. U.S.A.* 94, 7-8.
280. Omichinski, J.G., Pedone, P.V., Felsenfeld, G., Gronenborn, A.M. & Clore, G.M. (1997) The solution structure of a specific GAGA factor/DNA complex reveals a modular binding mode. *Nature Struct. Biol.* 4, 122-132.
281. Garrett, D.S., Seok, Y.J., Liao, D.I., Peterkofsky, A., Gronenborn, A.M. & Clore, G.M. (1997) Solution structure of the 30 kDa N-terminal domain of Enzyme I of the *Escherichia coli* phosphoenolpyruvate:sugar phosphotransferase system by multidimensional NMR. *Biochemistry* 36, 2517-2530.
282. Kuszewski, J., Gronenborn, A.M. & Clore, G.M. (1997) Improvements and extensions in the conformational database potential for the refinement of NMR and X-ray structures of proteins and nucleic acids. *J. Magn. Reson.* 125, 171-177.
283. Pedone, P.V., Omichinski, J.G., Nony, P., Trainor, C., Gronenborn, A.M., Clore, G.M. & Felsenfeld, G. (1997) The N-terminal fingers of cGATA-2 and cGATA-3 are independent sequence-specific DNA binding domains. *EMBO J.* 16, 2874-2882.
284. Garrett, D.S., Seok, Y.J., Peterkofsky, A., Clore, G.M. & Gronenborn, A.M. (1997) Identification by NMR of the binding surface for the histidine-containing phosphocarrier protein HPr on the N-terminal domain of enzyme I of the *Escherichia coli* phosphotransferase system. *Biochemistry* 36, 4393-4398.
285. Gronenborn, A.M. & Clore, G.M. (1997) Water in and around proteins. *The Biochemist* 19, issue 3, 18-21.
286. Tjandra, N., Garrett, D.S., Gronenborn, A.M., Bax, A. & Clore, G.M. (1997) Defining long range order in NMR structure determination from the dependence of heteronuclear relaxation times on rotational diffusion anisotropy. *Nature Struct. Biol.* 4, 443-449.
287. Nagaich, A.K., Zhurkin, V.B., Sakamoto, H., Gorin, A.A., Clore, G.M., Gronenborn, A.M., Appella, E. & Harrington, R.E. (1997) Architectural accommodation in the complex of four p53 DNA binding domain peptides with the *p21/Waf1/Cip1* DNA response element. *J. Biol. Chem.* 272, 14830-14841.
288. Wingfield, P.T., Stahl, S.J., Kaufman, J., Zlotnick, A., Hyde, C.C., Gronenborn, A.M. & Clore, G.M. (1997) The extracellular domain of immunodeficiency virus gp41 protein: expression in *Escherichia coli*, purification and crystallization. *Protein Sci.* 6, 1653-1660.

289. Cai, M., Zheng, R., Caffrey, M., Craigie, R., Clore, G.M. & Gronenborn, A.M. (1997) Solution structure of the N-terminal zinc binding domain of HIV-1 integrase. *Nature Struct. Biol.* 4, 567-577.
290. Tjandra, N., Omichinski, J.G., Gronenborn, A.M., Clore, G.M. & Bax, A. (1997) Use of dipolar ^{15}N - ^1H and ^{13}C - ^1H couplings in the structure determination of magnetically oriented macromolecules in solution. *Nature Struct. Biol.* 4, 732-738.
291. Huth, J.R., Bewley, C.A., Nissen, M.S., Evans, J.N.S., Reeves, R., Gronenborn, A.M. & Clore, G.M. (1997) The solution structure of an HMG-I(Y)/DNA complex defines a new architectural minor groove binding motif. *Nature Struct. Biol.* 4, 657-665.
292. Caffrey, M., Cai, M., Kaufman, J., Stahl, S.J., Wingfield, P.T., Gronenborn, A.M. & Clore, G.M. (1997) Determination of the secondary structure and global topology of the 44 kDa ectodomain of gp41 of the simian immunodeficiency virus by multidimensional nuclear magnetic resonance spectroscopy. *J. Mol. Biol.* 271, 819-826.
293. Clore, G.M. & Gronenborn, A.M. (1997) NMR structures of proteins and protein complexes beyond 20,000 Mr. *Nature Struct. Biol.* 4, 849-853 (1997)
Current Opinions in Chemical Biology 2, 564-570 (1998).
294. Clubb, R.T., Schumaker, S., Mizuuchi, K., Gronenborn, A.M. & Clore, G.M. (1997) Solution structure of the I γ subdomain of the Mu end DNA binding domain of Mu phage transposase. *J. Mol. Biol.* 273, 19-25.
295. Huth, J.R., Bewley, C.A., Jackson, B.M., Hinnebusch, A.G., Clore, G.M. & Gronenborn, A.M. (1997) Design of an expression system for detecting folded protein domains and mapping macromolecular interactions by NMR. *Protein Sci.* 6, 2359-2364.
296. Schumacher, S., Clubb, R.T., Cai, M., Mizuuchi, K., Clore, G.M. & Gronenborn, A.M. (1997) Solution structure of the Mu end DNA binding I β subdomain of phage Mu transposase: modular DNA recognition by two tethered domains. *EMBO J.* 16, 7532-7541.

1998

297. Clore, G.M. & Gronenborn, A.M. (1998) Determining structures of large proteins and protein complexes by NMR. *Trends in Biotechnology* 16, 22-34.
In Modern Techniques in Protein NMR, Biological Magnetic Resonance Vol. 16 (eds. Krishnan, R.N. & Berliner, L.J.), Plenum, New York (1999).
298. Bewley, C.A., Gronenborn, A.M. & Clore, G.M. (1998) Minor-groove binding architectural proteins: structure, function and DNA recognition. *Ann. Rev. Biophys. Biomolec. Struct.* 27, 105-131.
299. Cai, M., Huang, Y., Sakaguchi, K., Clore, G.M., Gronenborn, A.M. & Craigie, R. (1998) An efficient and cost-effective isotope labeling protocol for proteins expressed in *Escherichia coli*. *J. Biomol. NMR* 11, 97-102.
300. Louis, J.M., Martin, R., Clore, G.M. & Gronenborn, A.M. (1998) Preparation of uniformly isotope labeled DNA oligonucleotides for NMR spectroscopy. *J. Biol. Chem.* 273, 2374-2378.
301. Clore, G.M. & Gronenborn, A. M. (1998) New methods of structure refinement for macromolecular structure determination by NMR. *Proc. Natl. Acad. Sci. U.S.A.* 95, 5891-5898.

302. Clore, G.M., Gronenborn, A.M. & Tjandra, N. (1998) Direct refinement against residual dipolar couplings in the presence of rhombicity of unknown magnitude. *J. Magn. Reson.* 131, 159-162.
303. Garrett, D.S., Seok, Y.-J., Peterkofsky, A., Clore, G.M. & Gronenborn, A.M. (1998) Tautomeric state and pK_a of the phosphorylated active site histidine in the N-terminal domain of Enzyme I of the *Escherichia coli* phosphoenolpyruvate:sugar phosphotransferase system. *Protein Science* 7, 789-793.
304. Starich, M.R., Wikström, M., Arst, H.N., Clore, G.M. & Gronenborn, A.M. (1998) The solution structure of a fungal AREA protein-DNA complex: an alternative binding mode for the basic carboxyl tail of GATA factors. *J. Mol. Biol.* 277, 605-620.
305. Starich, M.R., Wikström, M., Schumacher, S., Arst, H.N., Gronenborn, A.M. & Clore, G.M. (1998) The solution structure of the Leu22→Val mutant of the AREA DNA binding domain complexed with a TGATA core element defines a role for hydrophobic packing in the determination of specificity. *J. Mol. Biol.* 277, 621-634.
306. Brünger, A.T., Adams, P.D., Clore, G.M., DeLano, W.L., Gros, P., Grosse-Kunsteleve, R.W., Jiang, J.-S., Kuszewski, J., Nilges, M., Pannu, N.S., Read, R.J., Rice, L.M., Simonson, T. & Warren, G.L. (1998) Crystallography and NMR system (CNS): a new software suite for macromolecular structure determination. *Acta Cryst. Series D* 54, 901-921.
307. Clore, G.M., Gronenborn, A.M. & Bax, A. (1998) A robust method for determining the magnitude of the fully asymmetric alignment tensor of oriented macromolecules in the absence of structural information. *J. Magn. Reson.* 133, 216-221.
308. Clore, G.M., Gronenborn, A.M., Szabo, A. & Tjandra, N. (1998) Determining the magnitude of the fully asymmetric diffusion tensor from heteronuclear relaxation data in the absence of structural information. *J. Am. Chem. Soc.* 120, 4889-4890.
309. Clore, G.M., Murphy, E.C., Gronenborn, A.M. & Bax, A. (1998) Determination of three-bond ¹H3'-³¹P couplings in nucleic acids and protein-nucleic acid complexes by quantitative J correlation spectroscopy. *J. Magn. Reson.* 134, 164-167.
310. Bewley, C.A., Gustafson, K.R., Boyd, M.R., Covell, D.G., Bax, A., Clore, G.M. & Gronenborn, A.M. (1998) Solution structure of cyanovirin-N, a potent HIV-inactivating protein. *Nature Struct. Biol.* 5, 571-578.
311. Caffrey, M., Cai, M., Kaufman, J., Stahl, S.J., Wingfield, P.T., Covell, D.G., Gronenborn, A.M. & Clore, G.M. (1998) Three-dimensional solution structure of the 44 kDa ectodomain of SIV gp41. *EMBO J.* 17, 4572-4584.
312. Caffrey, M., Kaufman, J., Stahl, S.J., Wingfield, P.T., Gronenborn, A.M. & Clore, G.M. (1998) 3D NMR experiments for measuring ¹⁵N relaxation data of large proteins: application to the 44 kDa ectodomain of SIV gp41. *J. Magn. Reson.* 135, 368-372.
313. Cai, M., Huang, Y., Zheng, R., Wei, S.-Q., Ghirlando, R., Lee, M.S., Craigie, R., Gronenborn, A.M. & Clore, G.M. (1998) Solution structure of the cellular factor BAF responsible for protecting retroviral DNA from autointegration. *Nature Struct. Biol.* 5, 903-909.
314. Cai, M., Huang, Y., Caffrey, M., Zheng, R., Craigie, R., Clore, G.M. & Gronenborn, A.M. (1998) Solution structure of the His12→Cys mutant of the N-terminal zinc binding domain of HIV-1 integrase complexed to cadmium. *Protein Sci.* 7, 2669-2674.

315. Clore, G.M., Starich, M.R., Gronenborn, A.M. (1998) Measurement of residual dipolar couplings of macromolecules aligned in the nematic phase of a colloidal suspension of rod-shaped viruses. *J. Am. Chem. Soc.* *120*, 10571-10572.

1999

316. Yu, B., Blaber, M., Gronenborn, A.M., Clore, G.M. & Caspar, D.L.D. (1999) Disordered water within a hydrophobic cavity visualized by X-ray crystallography. *Proc. Natl. Acad. Sci. U.S.A.* *96*, 103-108.
317. Gronenborn, A.M., Clore, G.M., Louis, J.M. & Wingfield, P.T. (1999) Is human thioredoxin monomeric or dimeric? *Protein Sci.* *8*, 426-429.
318. Garrett, D.S., Seok, Y.-J., Peterkofsky, A., Gronenborn, A.M. & Clore, G.M. (1999) Solution structure of the 40,000 M_r phosphoryl transfer complex between Enzyme I and HPr. *Nature Struct. Biol.* *6*, 166-173.
319. Kuszewski, J., Gronenborn, A.M. & Clore, G.M. (1999) Improving the packing and accuracy of NMR structures with a pseudopotential for the radius of gyration. *J. Am. Chem. Soc.* *121*, 2337-2338.
320. Yang, F., Bewley, C.A., Louis, J.M., Gustafson, K.R., Boyd, M.R., Gronenborn, A.M., Clore, G.M. & Wlodawer, A. (1999) Crystal structure of cyanovirin-N, a potent HIV-inactivating protein, shows unexpected domain swapping. *J. Mol. Biol.* *288*, 403-412.
321. Cornilescu, G., Ramirez, B.E., Frank, M.K., Clore, G.M., Gronenborn, A.M. & Bax, A. (1999) Correlation between ³hJ_{NC'} and hydrogen bond length in proteins. *J. Am. Chem. Soc.* *121*, 6275-6279.
322. Caffrey, M., Kaufman, J., Stahl, S.J., Wingfield, P.T., Gronenborn, A.M. & Clore, G.M. (1999) Monomer-trimer equilibrium of the ectodomain of SIV gp41: insight into the mechanism of peptide inhibition of HIV infection. *Protein Sci.* *8*, 1904-1907.
323. Louis, J.M., Clore, G.M. & Gronenborn, A.M. (1999) Regulation of HIV-1 protease: autoprocessing is tightly coupled to protein folding. *Nature Struct. Biol.* *6*, 868-875.
324. Clore, G.M., Starich, M.R., Bewley, C.A., Cai, M. & Kuszewski, J. (1999) Impact of residual dipolar couplings on the accuracy of NMR structures determined from a minimal number of NOE restraints. *J. Am. Chem. Soc.* *121*, 6513-6514.
325. Clore, G.M. & Garrett, D.S. (1999) R-factor, Free R and complete cross-validation for dipolar coupling refinement of NMR structures. *J. Am. Chem. Soc.* *121*, 9008-9012.

2000

326. Kontaxis, G., Clore, G.M. & Bax, A. (2000) Evaluation of cross-relaxation effects and measurement of one-bond couplings in proteins with short transverse relaxation times. *J. Magn. Reson.* *143*, 184-196.
327. Tjandra, N., J. Marquardt, J. & Clore, G.M. (2000) Direct refinement against proton-proton dipolar couplings in NMR structure determination of macromolecules. *J. Magn. Reson.* *142*, 393-396.
328. Louis, J.M., Weber, I.T., Tözser, J., Clore, G.M. & Gronenborn, A.M. (2000) HIV-1 protease: maturation, enzyme specificity and drug resistance. *Adv. Pharmacol.* *49*, 111-146.

329. Caffrey, M., Braddock, D.T., Louis, J.M., Abu-Asab, M.A., Kingma, D., Liotta, L., Tsokos, M., Tresser, N., Pannell, L.K., Watts, N., Steven, A.C., Simon, M.N., Stahl, S.J., Wingfield, P.T. & Clore, G.M. (2000) Biophysical characterization of gp41 aggregates suggests a model for the molecular mechanism of HIV-associated neurological damage and dementia. *J. Biol. Chem.* 275, 19877-19882.
330. Wang, G., Sondej, M., Garrett, D.S., Peterkofsky, A. & Clore, G.M. (2000) A common interface on HPr for interaction with its partner proteins. *J. Biol. Chem.* 275, 16401-16403.
331. Huang, K., Louis, J.M., Donaldson, L., Lim, F.-L., Sharrocks, A.D. & Clore, G.M. (2000) Solution structure of the MEF2A-DNA complex: structural basis for the modulation of DNA bending and specificity by MADS-box transcription factors. *EMBO J.* 19, 2615-2628.
332. Clore, G.M. (2000) Accurate and rapid docking of protein-protein complexes on the basis of intermolecular nuclear Overhauser enhancement data and dipolar couplings by rigid body minimization. *Proc. Natl. Acad. Sci. U.S.A.* 97, 9021-9025.
333. Bewley, C.A. & Clore, G.M. (2000) Determination of the relative orientation of the two halves of the domain-swapped dimer of cyanovirin-N in solution using dipolar couplings and rigid body minimization. *J. Am. Chem. Soc.* 122, 6009-6016.
334. Kuszewski, J. & Clore, G.M. (2000) Source of and solutions to problems in the refinement of protein NMR structures against torsion angle potentials of mean force. *J. Magn. Reson.* 146, 249-254.
335. Chen, Y.W. & Clore, G.M. (2000) A systematic case study on using NMR models for molecular replacement: p53 tetramerization domain revisited. *Acta Cryst. D56*, 1535-1540.
336. Wang, G., Louis, J.M., Sondej, M., Seok, Y.-J., Peterkofsky, A. & Clore, G.M. (2000) Solution structure of the phosphoryl transfer complex between the signal transducing protein HPr and IIA^{Glucose} of the *Escherichia coli* phosphoenolpyruvate:sugar phosphotransferase system. *EMBO J.* 19, 5635-5649.
337. Wang, G., Peterkofsky, A. & Clore, G.M. (2000) A novel membrane anchor function for the N-terminal amphipathic sequence of the signal transducing protein IIA^{Glucose} of the *Escherichia coli* phosphotransferase system. *J. Biol. Chem.* 275, 39811-39814.

2001

338. Schwieters, C.D. & Clore, G.M. (2001) The VMD-XPLOR visualization package for NMR structure refinement. *J. Magn. Reson.* 149, 239-244.
339. Peterkofsky, A., Wang, G., Garrett, D.S., Lee, B.R. & Clore, G.M. (2001) Three-dimensional structures of protein-protein complexes in the *E. coli* PTS. *J. Mol. Microbiol. Biotechnol.* 3, 347-354. (Symposium on PTS).
340. Kuszewski, J., Schwieters, C.D. & Clore, G.M. (2001) Improving the accuracy of NMR structures of DNA by means of a database potential of mean force describing base-base positional interactions. *J. Am. Chem. Soc.* 123, 3903-3918.
341. Louis, J.M., Bewley, C.A. & Clore, G.M. (2001) Design and properties of N_{CCG}-gp41, a chimeric gp41 molecule with nanomolar HIV-fusion inhibitory activity. *J. Biol. Chem.* 276, 29485-29489.
342. Cai, M., Huang, Y., Ghirlando, R., Wilson, K.L., Craigie, R. and Clore, G.M. (2001) Solution structure of the constant region of nuclear envelope protein LAP2 reveals two LEM-domain structures: one binds BAF and the other binds DNA. *EMBO J.* 20, 4399-4407.

343. Braddock, D.T., Cai, M., Baber, J.L., Huang, Y. & Clore, G.M. (2001) Rapid identification of medium to large scale interdomain motion in modular proteins using dipolar couplings. *J. Am. Chem. Soc.* *123*, 8634-8635.
344. Cai, M., Huang, Y. & Clore, G.M. (2001) Accurate orientation of the functional groups of asparagine and glutamine side-chains using one- and two-bond dipolar couplings. *J. Am. Chem. Soc.* *123*, 8642-8643.
345. Schwieters, C.D. & Clore, G.M. (2001) Internal coordinates for molecular dynamics and minimization in structure determination and refinement. *J. Magn. Reson.* *152*, 288-302.
346. Murphy, E.C., Zhurkin, V.B., Louis, J.M., Cornilescu, G. and Clore, G.M. (2001) Structural basis for SRY-dependent 46-X,Y sex reversal: modulation of DNA bending by a naturally occurring point mutation. *J. Mol. Biol.* *312*, 481-499.

2002

347. Clore, G.M. & Bewley, C.A. (2002) Using conjoined rigid body / torsion angle simulated annealing to determine the relative orientation of covalently linked protein domains from dipolar couplings. *J. Magn. Reson.* *154*, 329-335.
348. Clore, G.M. & Schwieters, C.D. (2002) Theoretical and Computational Advances in Biomolecular NMR. *Curr. Op. Struct. Biol.* *12*, 146-153.
349. Braddock, D.T., Louis, J.M., Baber, J.L., Levens, D. & Clore, G.M. (2002) Structure and dynamics of KH domains from FBP bound to single-stranded DNA. *Nature* *415*, 1051-1056.
350. Clore, G.M. & Kuszewski, J. (2002) χ_1 rotamer populations and angles of mobile surface side chains are accurately predicted by a torsion angle database potential of mean force. *J. Am. Chem. Soc.* *124*, 28666-2867.
351. Bewley, C.A., Louis, J.M., Ghirlando, R. & Clore, G.M. (2002) Design of a novel peptide inhibitor of HIV fusion that disrupts the internal trimeric coiled-coil of gp41. *J. Biol. Chem.* *277*, 14238-14245.
352. Braddock, D.T., Baber, J.L., Levens, D. & Clore, G.M. (2002) Molecular basis of sequence specific single-stranded DNA recognition by KH domains: solution structure of a complex between hnRNP K KH3 and single-stranded DNA. *EMBO J.* *21*, 3476-3485.
353. Schwieters, C.D. & Clore, G.M. (2002) Reweighted atomic densities to represent ensembles of NMR structures. *J. Biomol. NMR* *23*, 221-225.
354. Cornilescu, G., Lee, B.R., Cornilescu, C.C., Wang, G., Peterkofsky, A. & Clore, G.M. (2002) Solution structure of the phosphoryl transfer complex between the cytoplasmic A domain of the mannitol transporter Π^{Mannitol} and HPr of the *Escherichia coli* phosphotransferase system. *J. Biol. Chem.* *277*, 42289-42298.

2003

355. Schwieters, C.D., Kuszewski, J., Tjandra, N. & Clore, G.M. (2003) The Xplor-NIH NMR molecular structure determination package. *J. Magn. Reson.* *160*, 66-74.

356. Clore, G.M. & Kuszewski, J. (2003) Improving the accuracy of NMR structures of RNA by means of conformational database potentials of mean force as assessed by complete dipolar coupling cross-validation. *J. Am. Chem. Soc.* 125, 1518-1525.
357. Clore, G.M. & Schwieters, C.D. (2003) Docking of protein-protein complexes on the basis of highly ambiguous intermolecular distance restraints derived from $^1\text{H}_\text{N}/^{15}\text{N}$ chemical shift mapping and backbone ^{15}N - ^1H residual dipolar couplings using conjoined rigid body/torsion angle dynamics. *J. Am. Chem. Soc.* 125, 2902-2912.
358. Louis, J.M., Nesheiwat, I., Chang, L.C., Clore, G.M. & Bewley, C.A. (2003) Covalent trimers of the internal N-terminal trimeric coiled-coil of gp41 and antibodies directed against them are potent inhibitors of HIV envelope-mediated cell fusion. *J. Biol. Chem.* 278, 20278-20285.
359. Iwahara, J., Anderson, D.E., Murphy, E.C. & Clore, G.M. (2003) EDTA-derivatized deoxythymidine as a tool for rapid determination of protein binding polarity to DNA by intermolecular paramagnetic relaxation enhancement. *J. Am. Chem. Soc.* 125, 6634-6635.
360. Cai, M., Williams, D.C., Wang, G., Lee, B.R., Peterkofsky, A. & Clore, G.M. (2003) Solution structure of the phosphoryl transfer complex between the signal transducing protein IIA^{Glucose} and the cytoplasmic domain of the glucose transporter IICB^{Glucose} of the *Escherichia coli* glucose phosphotransferase system. *J. Biol. Chem.* 278, 25191-25206.

2004

361. Williams, D.C., Cai, M. & Clore, G.M. (2004) Molecular basis for synergistic transcriptional activation by Oct1 and Sox2 revealed from the solution structure of the 42 kDa Oct1·Sox·Hoxb1-DNA ternary transcription factor complex. *J. Biol. Chem.* 279, 1449-1457.
362. Clore, G.M. & Schwieters, C.D. (2004) How much backbone motion in ubiquitin is required to be consistent with dipolar coupling data measured in multiple alignment media as assessed by independent cross-validation. *J. Am. Chem. Soc.* 126, 2923-2938.
363. Schulz, D.M., Ihling, C., Clore, G.M. & Sinz, A. (2004) Mapping the topology and determination of a low resolution three-dimensional structure of the calmodulin-mellitin complex by chemical cross-linking and high resolution FTICR mass spectrometry. *Biochemistry* 43, 4703-4715.
364. Iwahara, J., Schwieters, C.D. & Clore, G.M. (2004) Ensemble approach for NMR structure refinement against ^1H paramagnetic relaxation enhancement data arising from a flexible paramagnetic group attached to a macromolecule. *J. Am. Chem. Soc.* 126, 5879-5896.
365. Kuszewski, J., Schwieters, C.D., Garrett, D.S., Byrd, R.A., Tjandra, N. & Clore, G.M. (2004) Completely automated, highly error tolerant macromolecular structure determination from multidimensional nuclear Overhauser enhancement spectra and chemical shift assignments. *J. Am. Chem. Soc.* 126, 6258-6273.
366. Gallo, S.A., Clore, G.M., Louis, J.M., Bewley, C.A. & Blumenthal, R. (2004) Temperature-dependent intermediates in HIV-1 envelope glycoprotein-mediated fusion revealed by inhibitors that target N-terminal and C-terminal helical regions of HIV-1 gp41. *Biochemistry* 43, 8230-8233.
367. Miclet, E., Williams, D.C., Clore, G.M., Boisbouvier, J. & Bax, A. (2004) Relaxation-optimized NMR spectroscopy of methylene groups in proteins and nucleic acids. *J. Am. Chem. Soc.* 126, 10560-10570.

368. Clore, G.M. & Schwieters, C. D. (2004) Amplitudes of protein backbone dynamics and correlated motions in a small α/β protein: correspondence of dipolar coupling and heteronuclear relaxation measurements. *Biochemistry* 43, 10678-10691.
369. Huth, J.R., Yu, L., Collins, I., Mack, J., Mendoza, R., Isaac, B., Braddock, D.T., Muchmore, S.W., Comess, K.M., Fesik, S.W., Clore, G.M., Levens, D. & Hajduk, P.J. (2004) Benzoylanthranilic acid inhibitors of FBP binding to the *c-myc* promoter. *J. Med. Chem.* 47, 4851-4857.
370. Legler, P. M., Cai, M., Peterkofsky, A. & Clore, G. M. (2004) Three-dimensional solution structure of the cytoplasmic B domain of the mannitol transporter Π^{Mannitol} of the *Escherichia coli* phosphotransferase system. *J. Biol. Chem.* 279, 39115-39121.
371. Iwahara, J., Schwieters, C.D. & Clore, G.M. (2004) Characterization of non-specific protein-DNA interactions by ^1H paramagnetic relaxation enhancement. *J. Am. Chem. Soc.* 126, 12800-12808.

2005

372. Gozansky, E.K., Louis, J.M., Caffrey, M. & Clore, G.M. (2005) Mapping the binding of the N-terminal extracellular tail of the CXCR4 receptor to stromal cell-derived factor-1 α . *J. Mol. Biol.* 345, 651-658.
373. Gutschina, E., Hummer, G., Bewley, C.A & Clore, G.M. (2005) Differential inhibition of HIV-1 and SIV envelope-mediated cell fusion by C34 peptides derived from the C-terminal heptad repeat of gp41 from diverse strains of HIV-1, HIV-2 and SIV. *J. Med. Chem.* 48, 3036-3044.
374. Tang, C., Williams, D.C., Ghirlando, R. & Clore, G.M. (2005) Solution structure of enzyme IIA^{Chitobiose} from the N,N'-diacetylchitobiose branch of the *Escherichia coli* phosphotransferase system. *J. Biol. Chem.* 280, 11770-11780.
375. Williams, D.C., Cai, M., Suh, J.-Y., Peterkofsky, A. & Clore, G.M. (2005) Solution NMR structure of the 48 kDa IIA^{Mannose}-HPr complex of the *Escherichia coli* mannose phosphotransferase system. *J. Biol. Chem.* 280, 20775-20784.
376. Williams, D.C., Lee, J. Y., Cai, M., Bewley, C.A. & Clore, G.M. (2005) Crystal structures of the HIV-1 inhibitory cyanobacterial protein MVL free and bound to Man₃GlcNac₂: structural basis for specificity and high-affinity binding to the core pentasaccharide from N-linked oligomannoside. *J. Biol. Chem.* 280, 29269-29276.
377. Tang, C., Iwahara, J. & Clore, G.M. (2005) Accurate determination of leucine and valine side-chain conformations using U- $^{15}\text{N}/^{13}\text{C}/^2\text{H}$ /[^1H -methyl/methine]-Leu/Val isotope labeling, NOE pattern recognition and methine C γ -H γ /C β -H β residual dipolar couplings: application to the 34 kDa enzyme IIA^{Chitobiose}. *J. Biomol. NMR.* 33, 105-121.
378. Dimitrov, A.S., Louis, J.M., Bewley, C.A., Clore, G.M. & Blumenthal, R. (2005) Conformational changes in HIV-1 gp41 in the course of HIV-1 Env-mediated fusion and inactivation. *Biochemistry* 44, 12471-12479.
379. Suh, J.-Y., Tang, C., Cai, M. & Clore, G.M. (2005) Visualization of the phosphorylated active site loop of the cytoplasmic B domain of the mannitol transporter Π^{Mannitol} of the *Escherichia coli* phosphotransferase system by NMR spectroscopy and residual dipolar couplings. *J. Mol. Biol.* 353, 1129-1136.

380. Louis, J.M., Bewley, C.A., Gustchina, E., Aniana, A. & Clore, G.M. (2005) Characterization and HIV-1 fusion inhibitory properties of monoclonal Fabs obtained from a human non-immune phage library selected against diverse epitopes of the ectodomain of HIV-1 gp41. *J.Mol. Biol.* 353, 945-951.

2006

381. Schwieters, C. D., Kuszewski, J. J. & Clore, G.M. (2006) Using Xplor-NIH for NMR molecular structure determination. *Progr. NMR Spectroscopy.* 48, 47-62.
382. Clore, G.M. & Schwieters, C. D. (2006) Concordance of residual dipolar couplings, backbone order parameters and crystallographic B-factors for a small α/β protein: a unified picture of high probability, fast atomic motions in proteins. *J. Mol. Biol.* 355, 879-886.
383. Iwahara, J. & Clore, G. M. (2006) Direct observation of enhanced translocation of a homeodomain between DNA cognate sites by NMR exchange spectroscopy. *J. Am. Chem. Soc.* 128, 404-405.
384. Suh, J.-Y., Cai, M., Williams, D.C. & Clore, G.M. (2006) Solution structure of a post-transition state analog of the phosphotransfer reaction between the A and B cytoplasmic domains of the mannitol transporter II^{Mannitol} of the *Escherichia coli* phosphotransferase system. *J. Biol. Chem.* 281, 8939-8949.
385. Clore, G.M. (2006) Structural proteomics by NMR. In *Proteomics for Biological Discovery* (Veenstra, T.D. & Yates, J.R., eds.), pp. 171-185, John Wiley & Sons, New York.
386. Iwahara, J. & Clore, G. M. (2006) Detecting transient intermediates in macromolecular binding by paramagnetic NMR. *Nature* 440, 1227-1230.
387. Hu, K., Vögeli, B & Clore, G.M. (2006) Interference between transverse cross-correlated relaxation and longitudinal relaxation affects apparent *J*-coupling and transverse cross-correlated relaxation. *Chem. Phys. Lett.* 423, 123-125.
388. Tang, C. & Clore, G.M. (2006) A simple and reliable approach to docking protein-protein complexes from very sparse NOE-derived intermolecular distance restraints. *J. Biomol. NMR* 36, 37-44.
389. Iwahara, J., Zwecksetter, M. & Clore, G.M. (2006) NMR structural and kinetic characterization of a homeodomain diffusing and hopping on non-specific DNA. *Proc. Natl. Acad. Sci. U.S.A.* 103, 15062-15067.
390. Tang, C., Iwahara, J. & Clore, G.M. (2006) Visualization of transient encounter complexes in protein-protein association. *Nature* 444, 383-386.
(News & Views: Blundell & Fernandez-Recio, Brief encounters bolster contacts, *Nature* 444, 279-280).
(Leading Edge Molecular Biology Selects, Brief encounters lead to a lasting bond, *Cell* 127, 653, 2006)
391. Gustchina, E., Louis, J.M., Bewley, C.A. & Clore, G.M. (2006) Synergistic inhibition of HIV-1 envelope-mediated membrane fusion by inhibitors targeting the N- and C-terminal heptad repeats of gp41. *J. Mol. Biol.* 364, 283-289.
392. Iwahara, J. & Clore, G.M. (2006) Sensitivity improvement for correlations involving arginine side-chain N ϵ /H ϵ resonances in multi-dimensional NMR experiments using broadband ¹⁵N 180° pulses. *J. Biomol. NMR* 36, 251-257.
393. Hu, K., Vögeli, B. & Clore, G.M. (2006) ¹³C-detected HN(CA)C and HMCNC experiments using a single methyl-reprotonated sample for unambiguous methyl resonance assignment. *J. Biomol. NMR* 36, 259-266.

2007

394. Iwahara, J., Tang, C. & Clore, G.M. (2007) Practical aspects of ^1H transverse paramagnetic relaxation enhancement measurements on macromolecules. *J. Magn. Reson.* 184, 185-195.
395. Schwieters, C.D. & Clore, G.M. (2007) A physical picture of atomic motions within the Dickerson DNA dodecamer in solution derived from joint ensemble refinement against NMR and large angle X-ray scattering data. *Biochemistry* 46, 1152-1166
396. Suh, J.-Y., Iwahara, J. & Clore, G.M. (2007) Intramolecular domain-domain association/ dissociation and phosphoryl transfer in the mannitol transporter of *Escherichia coli* are not coupled. *Proc. Natl. Acad. Sci. U.S.A.* 104, 3153-3158.
397. Iwahara, J., Jung, Y.-S., & Clore, G.M. (2007) Heteronuclear NMR spectroscopy for lysine NH_3 groups in proteins: unique effect of water-exchange on ^{15}N transverse relaxation. *J. Am. Chem. Soc.* 129, 2971-2980.
398. Hu, K., Vögeli, B. & Clore, G.M. (2007) Spin state selective carbon-detected HNC0 with TROSY optimization in all dimensions and double echo-antiecho sensitivity enhancement in both indirect dimensions. *J. Am. Chem. Soc.* 129, 5484-5491.
399. Cai, M., Huang, Y., Suh, J.-Y., Louis, J.M., Ghirlando, R., Craigie, R. & Clore, G.M. (2007) Solution NMR structure of the Barrier-to-Autointegration Factor/Emerin complex. *J. Biol. Chem.* 282, 14525-14535.
400. Tang, C., Schwieters, C.D. & Clore, G.M. (2007) Open to closed transition in apo maltose-binding protein visualized by paramagnetic NMR. *Nature* 449, 1878-1882.
401. Clore, G.M., Tang, C. & Iwahara, J. (2007) Elucidating transient macromolecular interactions using paramagnetic relaxation enhancement. *Curr. Op. Struct. Biol.* 17, 603-616.
402. Gustchina, E., Louis, J. M., Lam, S.N., Bewley, C.A. & Clore, G.M. (2007) A monoclonal Fab derived from a human non-immune phage library reveals a new epitope on gp41 and neutralizes diverse HIV-1 strains. *J. Virol.* 81, 12946-12953.
403. Sahu, D., Clore, G.M. & Iwahara, J. (2007) TROSY-based z -exchange spectroscopy: application to the determination of the activation energy for intermolecular protein translocation between specific sites on different DNA molecules. *J. Am. Chem. Soc.* 129, 13232-13237.
404. Suh, J.-Y., Tang, C. & Clore, G.M. (2007) Role of electrostatic interactions in transient encounter complexes in protein-protein association investigated by paramagnetic relaxation enhancement. *J. Am. Chem. Soc.* 129, 12954-12955.

2008

405. Schwieters, C.D. & Clore, G.M. (2008) A pseudopotential for improving the packing of ellipsoidal protein structures determined by NMR. *J. Phys. Chem. B* 112, 6070-6073.
406. Tang, C., Ghirlando, R. & Clore, G. M. (2008) Visualization of transient ultra-weak protein self-association in solution using paramagnetic relaxation enhancement. *J. Am. Chem. Soc.* 130, 4048-4056.
407. Hu, J., Hu, K., Williams, D.C., Komlosh, M., Cai, M. & Clore, G.M. (2008) Solution NMR structures of productive and non-productive complexes between the A and B domains of the cytoplasmic subunit of the mannose transporter of the *Escherichia coli* phosphotransferase system. *J. Biol. Chem.* 283, 11024-11037.

408. Nelson, J.D., Kinkead, H., Brunel, F.M., Leaman, D., Jensen, R., Louis, J.M., Maruyama, T., Bewley, C.A., Bowdish, K., Clore, G.M., Dawson, P.E., Frederickson, S., Mage, R.G., Richman, D.D., Burton, D.R. & Zwick, M.B. (2008) Antibody elicited against the gp41 N-heptad repeat (NHR) coiled-coil can neutralize HIV-1 with modest potency but non-neutralizing antibodies also bind to NHR mimetics. *Virology* 377, 170-183.
409. Suh, J.-Y., Cai, M. & Clore, G. M. (2008) Impact of phosphorylation on the structure and thermodynamics of the interaction between the N-terminal domain of Enzyme I and the histidine phosphocarrier protein of the bacterial phosphotransferase system. *J. Biol. Chem.* 283, 18980-18989.
410. Kim, Y.C., Tang, C., Clore, G.M. & Hummer, G. (2008) Replica exchange simulations of transient encounter complexes in protein-protein association. *Proc. Natl. Acad. Sci. U. S. A.* 105, 12855-12860.
411. Kuszewski, J., Thottungal, R.A., Clore, G. M. & Schwieters, C.D. (2008) Automated error-tolerant macromolecular structure determination from multidimensional nuclear Overhauser enhancement spectra and chemical shift assignments: improved robustness and performance of the PASD algorithm. *J. Biomol. NMR*, 41, 221-239.
412. Clore, G.M. (2008) Visualizing lowly-populated regions of the free energy landscape of macromolecular complexes by paramagnetic relaxation enhancement. *Molecular BioSystems* 4, 1058-1069.
413. Doucleff, M. & Clore, G.M. (2008) Global jumping and domain-specific intersegment transfer between DNA cognate sites of the multi-domain transcription factor Oct-1. *Proc. Natl. Acad. Sci. U. S. A.* 105, 13871-13876.
414. Gustchina, E., Bewley, C.A. & Clore, G.M. (2008) Sequestering the pre-hairpin intermediate of gp41 by peptide N36^{Mut(e,g)} potentiates the human immunodeficiency virus type 1 neutralizing activity of monoclonal antibodies directed against the N-terminal helical repeat of gp41. *J. Virol.* 82 10032-10041.
415. Tang, C., Louis, J.M., Aniana, A., Suh, J.-Y. & Clore, G.M (2008) Visualizing transient events in amino-terminal auto-processing of HIV-1 protease. *Nature* 455, 693-696.

2009

416. Clore, G.M. (2009) NMR in Structural Biology, in *Imaging Life: Biological Systems from Atoms to Tissues*, pp. 51-73, ed. G.C.Howard, W.E. Brown & M. Auer, Oxford University Press (published 2014).
417. Clore, G.M. & Iwahara, J. (2009) Theory, practice and applications of paramagnetic relaxation enhancement for the characterization of transient low-population states of biological macromolecules and their complexes. *Chem. Rev.* 109, 4108-4139.
418. Ryabov, Y., Suh, J.-Y., Grishaev, A., Clore, G.M. & Schwieters, C.D. (2009) Using the experimentally determined components of the overall rotational diffusion tensor to restrain molecular shape and size in NMR structure determination of globular proteins and protein-protein complexes. *J. Am. Chem. Soc.* 131, 9522-9531.
419. Hu, K., Doucleff, M. & Clore, G.M. (2009) Using multiple quantum coherence to increase the ¹⁵N resolution in a three-dimensional TROSY HNC0 experiment for accurate PRE and RDC measurements. *J. Magn. Reson.* 200, 173-178.

420. Gustchina, E., Louis, J.M., Frisch, C., Ylera, F., Lechner, A., Bewley, C.A. & Clore, G.M. (2009) Affinity maturation by targeted diversification of the CDR-H2 loop of a monoclonal Fab derived from a synthetic naïve human antibody library and directed against the internal trimeric coiled-coil of gp41 yields a set of Fabs with improved HIV-1 neutralization potency and breadth. *Virology* 393, 112-119.

2010

421. Fawzi, N.L., Doucleff, M., Suh, J.-Y. & Clore, G.M. (2010) Mechanistic details of a protein-protein association pathway revealed by paramagnetic relaxation enhancement titration measurements. *Proc. Natl. Acad. Sci. U. S. A.* 107, 1379-1384.
422. Yung, Y.-S., Cai, M. & Clore, G.M. (2010) Solution structure of the IIA^{Chitobiose}-IIB^{Chitobiose} complex of the *N,N'*-diacetylchitobiose branch of the *Escherichia coli* phosphotransferase system. *J. Biol. Chem.* 285, 4173-4184.
423. Ryabov, Y., Clore, G.M. & Schwieters, C.D. (2010) Direct use of ¹⁵N relaxation rates as experimental restraints on molecular shape and orientation for docking of protein-protein complexes. *J. Am. Chem. Soc.* 132, 5987-5989
424. Fawzi, N., Ying, J., Torchia, D, A., Clore, G. M. (2010) Kinetics of amyloid β monomer to oligomer exchange by NMR relaxation. *J. Am. Chem. Soc.* 132, 9948-9951.
425. Schwieters, C.D., Suh, J.-Y., Grishaev, A., Ghirlando, R., Takayama, Y. & Clore, G.M. (2010) Solution structure of the 128 kDa Enzyme I dimer from *Escherichia coli* and its 146 kDa complex with HPr using residual dipolar couplings and small and wide angle X-ray scattering. *J. Am. Chem. Soc.* 133, 13026-13045.
426. Iwahara, J. & Clore, G.M. (2010) Structure-independent analysis of the breadth of the positional distribution of disordered groups in macromolecules from order parameters for long variable-length vectors using NMR paramagnetic relaxation enhancement. *J. Am. Chem. Soc.* 132, 13346-13356.
427. Gustchina, E., Li, M., Louis, J.M., Anderson, D.E., Lloyd, J., Frisch, C., Bewley, C.A., Gustchina, A., Wlodawer, A. & Clore, G.M. (2010) Structural basis of HIV-1 neutralization by affinity matured Fabs directed against the internal trimeric coiled-coil of gp41. *PLoS Pathogens* 6, e1001182.
428. Yin, H., Feng, G., Clore, G.M., Hummer, G. & Rasaiah, J.C. (2010) Water in the polar and non-polar cavities of the protein interleukin-1 β . *J. Phys. Chem.* 114, 16290-16297.
429. Cai, M., Huang, Y., Craigie, R. & Clore, G.M. (2010) Structural basis of the association of HIV-1 matrix protein with DNA. *PloS ONE* 5, e15675.

2011

430. Clore, G.M. (2011) Exploring sparsely-populated states of macromolecules by diamagnetic and paramagnetic NMR relaxation. *Protein Sci.* 20, 229-246.
431. Takayama, Y., Schwieters, C.D., Grishaev, A., Ghirlando, R. & Clore, G.M. (2011) Combined use of residual dipolar couplings and solution X-ray scattering to rapidly probe rigid body conformational transitions in a non-phosphorylatable active site mutant of the 128 kDa enzyme I dimer. *J. Am. Chem. Soc.* 133, 424-427.

432. Clore, G.M. (2011) Adventures in Biomolecular NMR, in *Encyclopedia of Magnetic Resonance, Historical Perspectives*, (Becker, E.D., ed.; Harris, R.K. & Wasylishen, R.E., editors-in-chief), John Wiley & Sons (Chichester), DOI:10.1002/9780470034590.emrhp1008.
433. Shahzad-ul-Hussan, S., Gustchina, E., Ghirlando, R., Clore, G.M. & Bewley, C.A. (2011) Solution structure of the monovalent lectin microvirin in complex with Man α (1-2)Man provides a basis for anti-HIV activity with low toxicity. *J. Biol. Chem.* 286, 20788-20796.
434. Takayama, Y. & Clore, G.M. (2011) Intra- and intermolecular translocation of the bi-domain transcription factor Oct1 characterized by liquid crystal and paramagnetic NMR. *Proc. Natl. Acad. Sci. U. S. A.* 108, E169-E176.
435. Ryabov, Y., Schwieters, C.D. & Clore, G.M. (2011) Impact of ^{15}N R_2/R_1 relaxation restraints on molecular size, shape and bond vector orientation for NMR protein structure determination with sparse distance restraints. *J. Am. Chem. Soc.* 133, 6154-6157.
436. Fawzi, N.L., Fleissner, M.R., Anthis, N.J., Kalai, T., Hideg, K., Hubbell, W.L. & Clore, G.M. (2011) A rigid disulfide-linked nitroxide side chain simplifies the quantitative analysis of PRE data. *J. Biomol. NMR* 51, 105-114.
437. Clore, G.M. (2011) Exploring translocation of proteins on DNA by NMR. *J. Biomol. NMR* 51, 201-219.
438. Venditti, V., Fawzi, N.L. & Clore, G.M. (2011) Automated sequence- and stereo-specific assignment of methyl-labeled proteins by paramagnetic relaxation and methyl-methyl nuclear Overhauser enhancement spectroscopy. *J. Biomol. NMR* 51, 319-328.
439. Huang, Y., Cai, M., Clore, G.M. & Craigie, R. (2011) No interaction of barrier-to-autointegration factor (BAF) with HIV-1 MA, cone-rode homeobox (Crx or MAN1-C in absence of DNA. *PloS ONE* 6, e25123.
440. Fawzi, N.L., Ying, J., Ghirlando, R., Torchia, D.A. & Clore, G.M. (2011) Atomic resolution dynamics on the surface of amyloid β protofibrils probed by solution NMR. *Nature* 480, 268-272.
441. Anthis, N.J., Doucleff, M. & Clore, G.M. (2011) Transient sparsely-populated compact states of apo and calcium-loaded calmodulin probed by paramagnetic relaxation enhancement: interplay of conformational selection and induced fit. *J. Am. Chem. Soc.* 133, 18976-18974.

2012

442. Ryabov, R., Clore, G.M. & Schwieters, C.D. (2011) Coupling between internal dynamics and rotational diffusion in the presence of exchange between discrete molecular conformations. *J. Chem. Phys.* 136, 01348.
443. Venditti, V., Fawzi, N.L. & Clore, G.M. (2012) An efficient protocol for incorporation of an unnatural amino acid in perdeuterated recombinant proteins using glucose-based media. *J. Biomol. NMR* 52, 191-195.
444. Dogo-Isonagie, C., Lam, S., Gustchina, E., Acharya, P., Yang, Y., Shahzad-ul-Hussan, S., Clore, G.M., Kwong, P.D. & Bewley, C.A. (2012) Peptides from the second extracellular loop of the C-C chemokine receptor type 5 (CCR5) inhibit diverse strains of HIV-1. *J. Biol. Chem.* 287, 15076-15086.
445. Takayama, Y. & Clore, G.M. (2012) Interplay between minor and major groove-binding transcription factors Sox2 and Oct1 in translocation on DNA studied by paramagnetic and diamagnetic NMR. *J. Biol. Chem.* 287, 14349-14363.

446. Arredondo, S.A., Cai, M., Takayama, Y., MacDonald, N.J., Anderson, D.E., Aravind, L., Clore, G.M. & Miller, L.H. (2012) Structure of the Plasmodium 6-cysteine s48/s46 domain. *Proc. Natl. Acad. Sci. U.S.A.* *109*, 6692-6697.
447. Fawzi, N.L., Ying, J., Torchia, D.A. & Clore, G.M. (2012) Probing exchange kinetics and atomic resolution dynamics in high molecular weight complexes: dark-state exchange saturation transfer NMR spectroscopy. *Nature Protocols* *7*, 1523-1533.
448. Jung, Y.-S., Cai, M. & Clore, G.M. (2012) Solution structure of the IIA^{Chitobiose}-HPr complex of the N,N'-diacetylchitobiose branch of the *Escherichia coli* phosphotransferase system. *J. Biol. Chem.* *287*, 23819-23829
449. Takayama, Y. & Clore, G.M. (2012) Impact of protein-protein interactions on global intermolecular translocation rates of the transcription factors Sox2 and Oct1 between DNA cognate sites studied by z-exchange NMR spectroscopy. *J. Biol. Chem.* *287*, 26962-26970.
450. Venditti, V. & Clore, G.M. (2012) Conformational selection and substrate binding regulate the monomer/dimer equilibrium of the C-terminal domain of *Escherichia coli* Enzyme I. *J. Biol. Chem.* *287*, 26989-26998.
451. Grishaev, A., Anthis, N.J. & Clore, G.M. (2012) Contrast-matched small angle X-ray scattering from a heavy atom-labeled protein in structure determination: application to a lead-substituted calmodulin-peptide complex. *J. Am. Chem. Soc.* *134*, 14686-14689.
452. Bermejo, G. A., Clore, G.M. & Schwieters, C.D. (2012) Smooth statistical torsion angle potential derived from a large conformational database via adaptive kernel density estimation improves the quality of NMR protein structures. *Protein Sci.* *21*, 1824-1836.
- 2013**
453. Anthis, N.J. & Clore, G.M. (2013) Sequence-specific determination of protein and peptide concentrations by absorbance at 205 nm. *Protein Sci.* *22*, 581-588
454. Venditti, V., Ghirlando, R. & Clore, G.M. (2013) Structural basis for Enzyme I inhibition by α -ketoglutarate. *ACS Chem. Biol.* *8*, 1232-1240.
455. Clore, G.M. (2013) Generating accurate contact maps of transient long-range interactions in intrinsically disordered proteins by paramagnetic relaxation enhancement. *Biophys. J.* *104*, 1635-1636.
456. Libich, D.S., Fawzi, N.L., Ying, J. & Clore, G.M. (2013) Probing the transient 'dark-state' of substrate binding to GroEL by relaxation-based solution NMR. *Proc. Natl. Acad. Sci. U.S.A.* *110*, 11361-11366.
457. Anthis, N.J. & Clore, G.M. (2013) The length of the calmodulin linker determines the extent of transient interdomain association and target affinity. *J. Am. Chem. Soc.* *135*, 9648-9651.
458. Clore, G.M. & Venditti, V. (2013) Structure, dynamics and biophysics of the cytoplasmic protein-protein complexes of the bacterial phosphoenolpyruvate:sugar phosphotransferase system. *Trends Biochem.* *38*, 515-530.
459. Gustchina, E., Ghirlando, R., Schuck, P., Louis, J.M., Pierson, J., Rao, P., Subramaniam, S., Gustchina, A., Clore, G.M. & Wlodawer, A. (2013) Complexes of neutralizing and non-neutralizing affinity matured Fabs with a mimetic of the internal trimeric coiled-coil of HIV-1 gp41. *PLoS One* *8*, e78187

460. Deshmukh, L., Schwieters, C.D., Grishaev, A., Ghirlando, R., Baber, J.L. & Clore, G.M. (2013) Structure and dynamics of full length HIV-1 capsid protein in solution. *J. Am. Chem. Soc.* *135*, 16133-16147.
461. Clore, G.M. (2013) Seeing the invisible by paramagnetic and diamagnetic NMR. Centenary Award and Frederick Gowland Hopkins Memorial Lecture. *Biochem. Soc. Trans.* *41*, 1343-1354.

2014

462. Clore, G.M. (2014) Interplay between conformational selection and induced fit in multidomain protein-ligand binding probed by paramagnetic relaxation enhancement. *Biophysical Chemistry*, *186*, 3-12.
463. Deshmukh, L., Ghirlando, R. & Clore, G.M. (2014) Investigation of the structure and dynamics of the capsid-spacer peptide 1–nucleocapsid fragment of the HIV-1 Gag polyprotein by solution NMR spectroscopy. *Angewandte Chemie Int. Ed.* *53*, 1025-1028
464. Tugarinov, V., Venditti, V. & Clore, G.M. (2014) A NMR experiment for simultaneous correlations of valine and leucine/isoleucine methyls with carbonyl chemical shifts in proteins. *J. Biomol. NMR* *58*, 1-8.
465. Kozakov, D., Lee, K., Hall, D.R., Beglov, D., Zheng, J., Vakili, P., Schueler-Furman, O., Paschalidis, I.C., Clore, G.M. & Vajda, S. (2014) Encounter complexes and dimensionality reduction in protein-protein association. *eLife* *3*:e01370
466. Schwieters, C.D. & Clore, G.M. (2014) Using small angle solution scattering data in Xplor-NIH structure calculations. *Progr. Nucl. Magn. Reson. Spectroscopy.* *80*, 1-11.
467. Louis, J.M., Aniana, A., Lohith, K., Sayer, J.M., Roche, J., Bewley, C.A. & Clore, G.M. (2014) Binding of HIV-1 gp41-directed neutralizing and non-neutralizing fragment antibody binding domain (Fab) and single chain variable fragment (ScFv) antibodies to the ectodomain of gp41 in the pre-hairpin and six-helix bundle conformations. *Plos One* *9*, e104683.
468. Fawzi, N.L., Libich, D.S., Ying, J., Tugarinov, V. & Clore, G.M. (2014) Characterizing methyl-bearing side chain contacts and dynamics mediating amyloid β protofibril interactions using $^{13}\text{C}_{\text{methyl}}$ -DEST and lifetime line broadening. *Angewandte Chemie* *53*, 10345-10349.
469. Ryu, K.-S., Tugarinov, V. & Clore, G.M. (2014) Probing the rate limiting step for intramolecular transfer of a transcription factor between specific sites on the same DNA molecule by $^{15}\text{N}_z$ -exchange NMR spectroscopy. *J. Am. Chem. Soc.* *136*, 14369-14372.

2015

470. Venditti, V., Tugarinov, V., Schwieters, C.D., Grishaev, A. & Clore, G.M. (2015) Large interdomain rearrangement triggered by suppression of micro- to millisecond dynamics in bacterial Enzyme I. *Nature Communications* *6*, 5960.
471. Anthis, N.J. & Clore, G.M. (2015) Visualizing transient dark states by NMR spectroscopy. *Q. Rev. Biophys.* *48*, 35-116.
472. Clore, G.M. (2015) Dynamics of Sox2 interactions with DNA. In *Sox2: Biology and Role in Development and Disease*, pp. 225-41, eds. Kondoh, H. & Lovell-Badge, R., Elsevier, Amsterdam.

473. Deshmukh, L., Ghirlando, R. & Clore, G.M. (2015) Conformation and dynamics of the Gag polyprotein of the human immunodeficiency virus 1 studied by NMR spectroscopy. *Proc. Natl. Acad. Sci. U. S. A.* *112*, 3374-3379.
474. Baber, J.L., Louis, J.M. & Clore, G.M. (2015) Dependence of distance distributions derived from double electron-electron resonance pulsed EPR spectroscopy on pulse-sequence time. *Angewandte Chemie Int. Ed.* *56*, 5336-5339.
475. Libich, D.S., Tugarinov, V. & Clore, G.M. (2015) Intrinsic unfoldase/foldase activity of the chaperonin GroEL directly demonstrated using multinuclear relaxation-based NMR. *Proc. Natl. Acad. Sci. U. S. A.* *112*, 8817-8823.
476. Clore, G.M. (2015) Practical aspects of paramagnetic relaxation enhancement in biological macromolecules. *Meth. Enzymol.* *564*, 485-497.
477. Tugarinov, V., Libich, D.S., Meyer, V., Roche, J. & Clore, G.M. (2015) The energetics of a three-state protein folding system probed by high-pressure relaxation dispersion NMR spectroscopy. *Angewandte Chemie Int. Ed.* *54*, 11157-11161.
478. Venditti, V., Schwieters, C.D., Grishaev, A. & Clore, G.M. (2015) Dynamic equilibrium between closed and partially-closed states of the bacterial Enzyme I unveiled by solution NMR and X-ray scattering. *Proc. Natl. Acad. Sci. U. S. A.* *112*, 11565-11570.
479. Louis, J.M., Deshmukh, L., Sayer, J., Anania, A. & Clore, G.M. (2015) Mutations proximal to sites of autoproteolysis and the α -helix which co-evolve under drug pressure modulate autoproteolysis and vitality of HIV-1 protease. *Biochemistry* *54*, 5414-5424.
480. Clore, G.M. (2015) NMR in structural and cell biology. In *Encyclopedia of Cell Biology* (eds. Bradshaw, R.A. and Stahl, P.D.), vol. 1, pp. 98-107, Academic Press, Waltham, MA. doi:10.1016/B978-0-12-394447-4.10019-7.
481. Louis, J.M., Baber, J.L. & Clore, G.M. (2015) The C34 peptide fusion inhibitor binds to the 6-helix bundle core domain of HIV-1 gp41 by displacement of the C-terminal helical repeat region. *Biochemistry* *54*, 6796-6805.
482. Libich, D.S., Tugarinov, V & Clore, G.M. (2015) Flux analysis of GroEL-assisted folding/unfolding. *Proc. Natl. Acad. Sci. U. S. A.* *112*, E6833-6844.

2016

483. Clore, G.M. (2016) Structure determination of large macromolecular complexes using NMR. In *Encyclopedia of Spectroscopy and Spectrometry*, 3rd ed., 3rd ed., (ed. Lindon, J.C., Tranter G.E. & Koppenaal, D.W.), vol. 4, pp. 316-318, Oxford, Elsevier. <http://dx.doi.org/10.1016/B978-0-12-409547-2.12131-6>.
484. Venditti, V., Egner, T.K. & Clore, G.M. (2016) Hybrid approaches to structural characterization of conformational ensembles of complex macromolecular systems combining NMR residual dipolar couplings and solution X-ray scattering. *Chem. Rev.* *11*, 6305-6322.
485. Bermejo, G., Clore, G.M. & Schwieters, C.D. (2016) Improving NMR structures of RNA. *Structure* *24*, 806-815.

486. Deshmukh, L., Schweiters, C.D., Grishaev, A. & Clore, G.M. (2016) Quantitative characterization of configurational space sampled by HIV-1 nucleocapsid using solution NMR, X-ray scattering and protein engineering. *ChemPhysChem* 17, 1548-1552.
487. Cecon, A., Tugarinov, V., Bax, A. & Clore, G.M. (2016) Global dynamics and exchange kinetics of a protein on the surface of nanoparticles revealed by relaxation-based solution NMR spectroscopy. *J. Am. Chem. Soc.* 138, 5789-5792.
488. Schmidt, T., Ghirlando, R., Baber, J. & Clore, G.M. (2016) Quantitative resolution of monomer-dimer populations by inversion modulated DEER EPR spectroscopy. *ChemPhysChem* 17, 2987-2991.
489. Cai, M., Huang, Y., Yang, R., Craigie, R. & Clore, G.M. (2016) A simple and robust protocol for high-yield expression of perdeuterated proteins in *Escherichia coli* grown in shaker flasks. *J. Biomol. NMR* 66, 85-91.
490. Cecon, A., Clore, G.M. & Tugarinov, V. (2016) Towards interpretation of intermolecular paramagnetic relaxation enhancement outside the fast exchange limit. *J. Biomol. NMR* 66, 1-7.
491. Deshmukh, L., Louis, J.M., Ghirlando, R. & Clore, G.M. (2016) Transient Gag-protease interactions revealed by paramagnetic NMR suggest origins of compensatory drug resistance mutations in HIV-1. *Proc. Natl. Acad. Sci. U. S. A.* 113, 12456-12461.
492. Schmidt, T., Wälti, M.A., Baber, J.L., Hustedt, E.J. & Clore, G.M. (2016) Long distance measurements up to 160 Å in the GroEL tetradecamer using Q-band DEER EPR spectroscopy. *Angewandte Chemie Int. Ed.* 55, 15905-15909.
- 2017**
493. Libich, D.S., Tugarinov, V., Ghirlando, R. & Clore, G.M. (2017) Confinement and stabilization of Fyn SH3 folding intermediate mimetics within the cavity of the chaperonin GroEL demonstrated by relaxation-based NMR. *Biochemistry* 56, 903-906.
494. Cecon, A., Tugarinov, V., Boughton, A. J., Fushman, D. & Clore, G.M. (2017) Probing the binding modes of a multidomain protein to lipid-based nanoparticles by relaxation-based NMR. *J. Chem. Phys. Lett.* 8, 2535-2540.
495. Wälti, M., Schmidt, T., Murray, D.T., Wang, H., Hinshaw, J.E. & Clore, G.M. (2017) The chaperonin GroEL accelerates profibril formation and decorates fibrils of the Het-s prion protein. *Proc. Natl. Acad. Sci. U. S. A.* 114, 9104-9109.
496. Wälti, M.A. & Clore, G.M. (2017) Disassembly/reassembly strategy for the production of highly pure GroEL, a tetradecameric supramolecular machine, suitable for quantitative NMR, EPR and mutational studies. *Protein Expression and Purification* 142, 8-15.
497. Deshmukh, L., Tugarinov, V., Louis, J.M. & Clore, G.M. (2017) Binding kinetics and substrate selectivity in HIV-1 protease-Gag interactions probed at atomic resolution by chemical exchange NMR. *Proc. Natl. Acad. Sci. U. S. A.* 114, E9855-E9862.
- 2018**
498. Schwieters, C.D., Bermejo, G.A. & Clore, G.M. (2018) Xplor-NIH for molecular structure determination from NMR and other data sources. *Protein Sci.* 27, 26-40.

499. Schmidt, T., Lian, T. & Clore, G.M. (2018) Probing conformational states of the finger and thumb subdomains of HIV-1 reverse transcriptase using double electron-electron resonance EPR spectroscopy. *Biochemistry* 55, 489-493.
500. Deshmukh, L., Tugarinov, V., Appella, D.H. & Clore, G.M. (2018) Targeting a dark excited state of HIV-1 nucleocapsid by anti-retroviral thioesters revealed by NMR. *Angewandte Chemie Int. Ed.* 57, 2687-2691.
501. Cecon, A., Schmidt, T., Tugarinov, V., Kotler, S.A., Schwieters, C.D. & Clore, G.M. (2018) Interaction of Huntingtin Exon-1 peptides with lipid-based micellar nanoparticles probed by solution NMR and Q-band pulsed EPR. *J. Am. Chem. Soc.* 140, 6199-6202.
502. Wälti, M., Libich, D.S. & Clore, G.M. (2018) Extensive sampling of the cavity of the GroEL nanomachine by protein substrates probed by paramagnetic relaxation enhancement. *J. Phys. Chem. Lett.* 9, 3368-3371.
503. Cecon, A., Clore, G.M. & Tugarinov, V. (2018) Decorrelating kinetic and relaxation parameters in exchange saturation transfer NMR: a case study of N-terminal huntingtin peptides binding to unilamellar lipid vesicles. *J. Phys. Chem. B.* 122, 11271-11278.
504. Wälti, M.A., Steiner, J., Meng, F., Chung, H. S., Louis, J.M., Ghirlando, R., Tugarinov, V., Nath, A. & Clore, G.M. (2018) Probing the mechanism of inhibition of amyloid $\beta(1-42)$ induced neurotoxicity by the chaperonin GroEL. *Proc. Natl. Acad. Sci. U. S. A.* 115, E11924-E11932.

2019

505. Cecon, A., Tugarinov, V. & Clore, G.M. (2019) TiO₂ nanoparticles catalyze oxidation of Huntingtin exon 1-derived peptides impeding aggregation: a quantitative NMR study of binding and kinetics. *J. Am. Chem. Soc.* 141, 94-97.
506. Kotler, S.A., Tugarinov, V., Schmidt, T., Cecon, A., Libich, D.S., Ghirlando, R., Schwieters, C.D. and Clore, G.M. (2019) Probing initial transient oligomerization events facilitating Huntingtin fibril nucleation at atomic resolution by relaxation-based NMR. *Proc. Natl. Acad. Sci. U. S. A.* 116, 3562-3571.
507. Tugarinov, V. & Clore, G.M. (2019) Exchange saturation transfer and associated NMR techniques for studies of protein interactions involving high molecular weight systems. *J. Biomol. NMR* 73, 461-469.
508. Miller-Henkins, L., Paine, E.L., Deshmukh, L., Nikolayevskiy, H., Lyons, G.C., Scerba, M.T., Gorge-Rosenker, K., Luecke, H., Louis, J.M. Chertova, E., Gorelick, R.J., Ott, D.E., Clore, G.M. & Appella, D.H. (2019) Inhibition of HIV maturation via selective unfolding and crosslinking of Gag polyprotein by a mercaptobenzamide acetylator. *J. Am. Chem. Soc.* 141, 8327-8338.
509. Bax, A. & Clore, G.M. (2019) Protein NMR: boundless opportunities. *J. Magn. Reson.* 306, 187-191
510. Schmidt, T., Schwieters, C.D. & Clore, G.M. (2019) Spatial domain organization in the HIV-1 reverse transcriptase p66 homodimer precursor probed by double electron-electron resonance EPR. *Proc. Natl. Acad. Sci. U. S. A.* 116, 17809-17816.
511. Karamanos, T.K., Tugarinov, V. & Clore, G.M. (2019) Unraveling the structure and dynamics of the human DNAJB6b chaperone by NMR reveals insights into Hsp40-mediated proteostasis. *Proc. Natl. Acad. Sci. U.S.A.* 116, 21529-21538.

512. Cai, M., Huang, Y., Craigie, R. & Clore, G.M. (2019) A simple protocol for expression of isotope-labeled proteins in *Escherichia coli* grown in shaker flasks at high cell density. *J. Biomol. NMR* 73, 743-748.
513. Cai, M., Huang, Y., Shen, Y., Li, M., Mizuuchi, M., Ghirlando, R., Mizuuchi, K. & Clore, G.M. (2019) Probing transient excited states of the bacterial cell division regulator MinE by relaxation dispersion NMR spectroscopy. *Proc. Natl. Acad. Sci. U.S.A.* 116, 25446-25455.

2020

514. Schwieters, C.D., Bermejo, G.A. & Clore, G.M. (2020) A three-dimensional potential of mean force to improve hydrogen bond geometry in Xplor-NIH protein structure determination. *Protein Sci.* 29, 100-110.
515. Garrett, D.S., Cai, M. & Clore, G.M. (2020) XIPP – Multi-dimensional NMR analysis software. *J. Biomol. NMR* 74, 9-25.
516. Tugarinov, V., Karamanos, T.K. & Clore, G.M. (2020) Optimized NMR experiments for the isolation of $I = \frac{1}{2}$ manifold transitions in methyl groups of proteins. *ChemPhysChem* 21, 13-19.
517. Karamanos, T.K., Tugarinov, V. & Clore, G.M. (2020) Determining methyl sidechain conformations in a CS-ROSETTA model using ^1H - ^{13}C residual dipolar couplings. *J. Biomol. NMR* 74, 111-118.
518. Cecon, A., Tugarinov, V., Ghirlando, R. & Clore, G.M. (2020) Abrogation of pre-nucleation, transient oligomerization of the Huntingtin exon-1 protein by human profilin-I. *Proc. Natl. Acad. Sci. U.S.A.* 117, 5844-5852.
519. Tugarinov, V., Karamanos, T.K. & Clore, G.M. (2020) Magic-angle-pulse driven separation of degenerate ^1H transitions in methyl groups of proteins: application to studies of methyl axis dynamics. *ChemPhysChem*. 21, 1087-1091.
520. Okuno, Y., Szabo, A. & Clore, G.M. (2020) Quantitative interpretation of solvent paramagnetic relaxation for probing protein-cosolute interactions. *J. Am. Chem. Soc.* 142, 8281-8290.
521. Schmidt, T., Jeon, J., Okuno, Y., Chiliveri, S.C. & Clore, G.M. (2020) Sub-millisecond freezing permits cryoprotectant-free EPR double electron-electron resonance spectroscopy. *ChemPhysChem*. 21, 1224-1229.
522. Schmidt, T., Louis, J.M. & Clore, G.M. (2020) Probing the interaction between HIV-1 protease and the homodimeric p66/p66' reverse transcriptase precursor by double electron-electron resonance EPR spectroscopy. *ChemBioChem* 21, 3051-3055.
523. Cecon, A., Tugarinov, V. & Clore, G.M. (2020) Kinetics of fast tetramerization of the huntingtin exon 1 protein probed by concentration-dependent on-resonance $R_{1\rho}$ measurements. *J. Phys. Chem. Lett.* 11, 5643-5648.
524. Schmidt, T. & Clore, G.M. (2020) T_m filtering by ^1H -methyl labeling in a deuterated protein for pulsed double electron-electron resonance EPR. *Chem. Commun.* 56, 10890-10893.
525. Tugarinov, V., Karamanos, T.K. & Clore, G.M. (2020) Optimized selection of slow-relaxing ^{13}C transitions in methyl groups of proteins: application to relaxation dispersion. *J. Biomol. NMR* 74, 673-680.

526. Karamanos, T.K., Tugarinov, V. & Clore, G.M. (2020) An S/T motif controls reversible oligomerization of the Hsp40 chaperone DNAJB6b through subtle reorganization of a β -sheet backbone. *Proc. Natl. Acad. Sci. U.S.A.* *117*, 30441-30450.

2021

527. Cai, M., Huang, Y., Lloyd, J., Craigie, R. & Clore, G.M. (2021) A simple and cost-effective protocol for high-yield expression of deuterated and selectively isoleucine/leucine/valine methyl protonated proteins in *Escherichia coli* grown in shake flasks. *J. Biomol. NMR* *75*, 83-87.
528. Wälti, M.A., Kotler, S.A. & Clore, G.M. (2021) Probing the interaction of huntingtin exon-1 polypeptides with the chaperonin nanomachine GroEL. *ChemBioChem* *22*, 1985-1991.
529. Tugarinov, V., Ceccon, A. & Clore, G.M. (2021) Probing side-chain dynamics in proteins by NMR relaxation of isolated ^{13}C magnetization modes in $^{13}\text{CH}_3$ methyl groups. *J. Phys. Chem. B* *125*, 3343-3352.
530. Ceccon, A., Tugarinov, V. & Clore, G.M. (2021) Quantitative exchange NMR-based analysis of huntingtin-SH3 interactions suggests an allosteric mechanism of inhibition of huntingtin aggregation. *J. Am. Chem. Soc.* *143*, 9672-9681.
531. Tugarinov, V. & Clore, G.M. (2021) The measurement of relaxation rates of degenerate ^1H transitions in methyl groups of proteins using acute angle radiofrequency pulses. *J. Magn. Reson. Epub ahead of print* doi:10.1016/j.jmr.107034.
532. Okuno, Y., Yoo, J., Schwieters, C.D., Best, R.B., Chung, H.-S., Clore, G.M. (2021) Atomic view of cosolute-induced protein denaturation probed by NMR solvent paramagnetic relaxation enhancement. *Proc. Natl. Acad. Sci. U.S.A.* *118*, e2112021118.
533. Wälti, M., Canagarajah, B., Schwieters, C.D. & Clore, G.M. (2021) Visualization of sparsely-populated lower oligomeric states of human mitochondrial Hsp60 by cryo-electron microscopy. *J. Mol. Biol.* *433*, 167322.

2022

533. Karamanos, T.K. & Clore, G.M. (2022) Large chaperone complexes through the lens of NMR spectroscopy. *Ann. Rev. Biophys.* *51*, 223-246.
535. Tugarinov, V., Ceccon, A. & Clore, G.M. (2022) NMR methods for exploring 'dark' states in ligand binding and protein-protein interactions. *Progr. Nucl. Magn. Reson. Spectr.* *128*, 1-24.
536. Schmidt, T., Heon, J., Ya, W.M., Schwieters, C.D., Tycko, R. & Clore, G.M. (2022) Time-resolved DEER EPR and solid-state NMR afford kinetic and structural elucidation of substrate binding to Ca^{2+} -ligated calmodulin. *Proc. Natl. Acad. Sci. U.S.A.* *119*, e2122308119.
537. Cawood, E.M., Clore, G.M. & Karamanos, T.K. (2022) Microsecond backbone motions modulate the oligomerization of the DNAJB6 chaperone. *Angewandte Chemie Int. Ed.* e202116403.

Books

- Clore, G.M. & Gronenborn, A.M. (1993) *NMR of Proteins*, Topics in Molecular and Structural Biology, MacMillan Press, Ltd. (London).
- Clore, G.M. & Potts, J. (2012) *Recent Developments in Biomolecular NMR*, RSC Biomolecular Sciences Series, Royal Society of Chemistry Publishing (Cambridge). doi:10.1039/9781849735391
- Chill, J. & Clore, G.M. (2021) Biophysical Methods (editors), *Current Opinion in Structural Biology*, Vol. 70, <https://www.sciencedirect.com/journal/current-opinion-in-structural-biology/vol/70/suppl/C>. Editorial. Seing is believing. doi:10.1016/j.sbi.2021.08.005

Patents

1. Clore, G.M., Bewley-Clore, C. A.; Medabalimi, J.L. GP41 inhibitors. US Provisional Application No. 60/339,751 (filed Dec 17, 2001); International Application No. PCT/US02/40684 (filed Dec 17, 2002)
2. Clore, G.M., Bewley-Clore, C. A.; Medabalimi, J.L. Novel peptide inhibitor of HIV fusion that disrupts the internal trimeric coiled-coil of gp41. US Provisional Patent Application No. 60/480,070 (filed February 11, 2003). PCT Patent application No. PCT/US04/003794 (filed February 10, 2004)
3. Clore, G.M., Bewley-Clore, C. A.; Medabalimi, J.L. Tightly binding antibodies directed against the internal trimeric coiled-coil of gp41 inhibit HIV-envelope mediated cell fusion. US Provisional Patent Application No. 60/480,070 (filed June 20, 2003).

B. Highly Cited Publications (≥ 100 citations)

Greater than 1000 citations

- Marion, D., Driscoll, P.C., Kay, L.E., Wingfield, P.T., Bax, A., Gronenborn, A.M. & Clore, G.M. (1989) Overcoming the overlap problem in the assignment of ^1H -NMR spectra of larger proteins using three-dimensional heteronuclear ^1H - ^{15}N Hartmann-Hahn and nuclear Overhauser - multiple quantum coherence spectroscopy: application to interleukin- 1β . *Biochemistry* 28, 6150-6156.
- Clore, G.M., Szabo, A., Bax, A., Kay, L.E., Driscoll, P.C. & Gronenborn, A.M. (1990) Deviations from the simple two parameter model free approach to the interpretation of ^{15}N nuclear magnetic relaxation of proteins. *J. Am. Chem. Soc.* 112, 4989-4991.
- Ikura, M., Clore, G.M., Gronenborn, A.M., Zhu, G., Klee, C.B. & Bax, A. (1992) Solution structure of a calmodulin-target peptide complex by multi-dimensional NMR. *Science* 256, 632-638.
- Brünger, A.T., Adams, P.D., Clore, G.M., DeLano, W.L., Gros, P., Grosse-Kunstleve, R.W., Jiang, J.-S., Kuszewski, J., Nilges, M., Pannu, N.S., Read, R.J., Rice, L.M., Simonson, T. & Warren, G.L. (1998) Crystallography and NMR system (CNS): a new software suite for macromolecular structure determination. *Acta Cryst. Series D* 54, 901-921.
- Schwieters, C.D., Kuszewski, J., Tjandra, N. & Clore, G.M. (2003) The Xplor-NIH NMR molecular structure determination package. *J. Magn. Reson.* 160, 65-73.

500-1000 citations

- 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.
- Nilges, M., Clore, G.M. and Gronenborn, A.M. (1988) Determination of three-dimensional structures of proteins from interproton distance data by hybrid distance geometry-dynamical simulated annealing calculations. *FEBS Lett* 229, 317-324.
- Nilges, M., Clore, G.M. & Gronenborn, A.M. (1988) Determination of three-dimensional structures of proteins from interproton distance data by dynamical simulated annealing from a random array of atoms. *FEBS Letters* 239, 129-136.
- Nilges, M., Gronenborn, A.M., Brünger, A.T. & Clore, G.M. (1988) Determination of three-dimensional structures of proteins by simulated annealing with interproton distance restraints: application to crambin, potato carboxypeptidase inhibitor and barley serine proteinase inhibitor 2. *Protein Engineering* 2, 27-38.
- Kraulis, P.J., Clore, G.M., Nilges, M., Jones, T.A., Pettersson, G., Knowles, J. & Gronenborn, A.M. (1989) Determination of the three-dimensional solution structure of the C-terminal domain of cellobiohydrolase I from *Trichoderma reesei*: a study using nuclear magnetic resonance and hybrid distance geometry-dynamical simulated annealing. *Biochemistry* 28, 7241-7257.
- Clore, G.M., Driscoll, P.C., Wingfield, P.T. & Gronenborn, A.M. (1990) Analysis of backbone dynamics of interleukin- 1β using two-dimensional inverse detected heteronuclear ^{15}N - ^1H NMR spectroscopy. *Biochemistry* 29, 7387-7401.
- Clore, G.M., Appella, E., Yamada, M., Matsushima, K. & Gronenborn, A.M. (1990) The three-dimensional structure of interleukin-8 in solution. *Biochemistry* 29, 1689-1696.

500-1000 citations (cont.)

- Bax, A., Clore, G.M. & Gronenborn, A.M. (1990) ^1H - ^1H correlation via isotropic mixing of ^{13}C magnetization: a new three-dimensional approach for assigning ^1H and ^{13}C spectra of ^{13}C -enriched proteins. *J. Magn. Reson.* 88, 425-431.
- Gronenborn, A.M., Filpula, D.R., Essig, N.Z., Achari, A., Whitlow, M., Wingfield, P.T. & Clore, G.M. (1991) A novel highly stable fold of the immunoglobulin binding domain of Streptococcal protein G. *Science* 253, 657-661.
- Garrett, D.S., Powers, R., Gronenborn, A.M. & Clore, G.M. (1991) A common sense approach to peak picking two-, three- and four-dimensional spectra using automatic computer analysis of contour diagrams. *J. Magn. Reson.* 95, 214-220.
- Clore, G.M. & Gronenborn, A.M. (1991) Structures of larger proteins in solution: three- and four-dimensional heteronuclear NMR spectroscopy. *Science* 252, 1390-1399.
- Werner, M.H., Huth, J.R., Gronenborn, A.M. & Clore, G.M. (1995) Molecular basis of human 46X,Y sex reversal revealed from the three-dimensional solution structure of the human SRY-DNA complex. *Cell* 81, 705-714.
- Tjandra, N., Omichinski, J.G., Gronenborn, A.M., Clore, G.M. & Bax, A. (1997) Use of dipolar ^{15}N - ^1H and ^{13}C - ^1H couplings in the structure determination of magnetically oriented macromolecules in solution. *Nature Struct. Biol.* 4, 732-738.
- Garrett, D.S., Seok, Y.-J., Peterkofsky, A., Clore, G.M. & Gronenborn, A.M. (1997) Identification by NMR of the binding surface for the histidine-containing phosphocarrier protein HPr on the N-terminal domain of Enzyme I of the Escherichia coli phosphotransferase system. *Biochemistry* 36, 4393-4398.
- Caffrey, M., Cai, M., Kaufman, J., Stahl, S.J., Wingfield, P.T., Covell, D.G., Gronenborn, A.M. & Clore, G.M. (1998) Three-dimensional solution structure of the 44 kDa ectodomain of SIV gp41. *EMBO J.* 17, 4572-4584.
- Schwieters, C. D., Kuszewski, J. J. & Clore, G.M. (2006) Using Xplor-NIH for NMR molecular structure determination. *Progr. NMR Spectroscopy.* 48, 47-62.
- Clore, G.M. & Iwahara, J. (2009) Theory, practice and applications of paramagnetic relaxation enhancement for the characterization of transient low-population states of biological macromolecules and their complexes. *Chem. Rev.* 109, 4108-4139.

200-500 citations

- Clore, G.M., Gronenborn, A.M., Brunger, A.T. & Karplus, M. (1985) The solution conformation of a heptadecapeptide comprising the DNA binding helix F of the cyclic AMP receptor protein of *Escherichia coli*: combined use of ^1H -nuclear magnetic resonance and restrained molecular dynamics. *J. Mol. Biol.* 186, 435-455.
- 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.

200-500 citations (cont.)

- Brünger, A.T., Clore, G.M., Gronenborn, A.M. & Karplus, M. (1986) Three-dimensional structures of proteins determined by molecular dynamics with interproton distance restraints: application to crambin. *Proc. Natl. Acad. Sci. U.S.A.* 83, 3801-3805.
- Clore, G.M., Brünger, A.T., Karplus, M. & Gronenborn, A.M. (1986) Application of molecular dynamics with interproton distance restraints to three-dimensional protein structure determination: a model study of crambin. *J. Mol. Biol.* 191, 523-551.
- Clore, G.M., Nilges, M., Sukumaran, D.K., Brünger, A.T., Karplus, M. & Gronenborn, A.M. (1986) The three-dimensional structure of α 1-purothionin in solution: combined use of nuclear magnetic resonance, distance geometry and restrained molecular dynamics. *EMBO J.* 5, 2729-2735.
- Clore, G.M., Gronenborn, A.M., Nilges, M. & Ryan, C.A. (1987) The three-dimensional structure of potato carboxypeptidase inhibitor in solution: a study using nuclear magnetic resonance, distance geometry and restrained molecular dynamics. *Biochemistry* 26, 8012-8023.
- Oschkinat, H., Griesinger, C., Kraulis, P.J., Sørensen, O.W., Ernst, R.R., Gronenborn, A.M. & Clore, G.M. (1988) Three-dimensional NMR spectroscopy of a protein in solution. *Nature* 332, 374-376.
- Holak, T.A., Engström, Å, Kraulis, P.J., Lindeberg, G., Bennich, H., Jones, T.A., Gronenborn, A.M. & Clore, G.M. (1988) The solution conformation of the antibacterial peptide cecropin A: a nuclear magnetic resonance and dynamical simulated annealing study. *Biochemistry* 27, 7620-7629.
- Clore, G.M. & Gronenborn, A.M. (1989) Determination of three-dimensional structures of proteins and nucleic acids in solution by nuclear magnetic resonance spectroscopy. *CRC Critical Reviews in Biochemistry and Molecular Biology* 24, 479-564.
- Gronenborn, A.M., Bax, A., Wingfield, P.T. & Clore, G.M. (1989) A powerful method of sequential proton resonance assignment in proteins using relayed ^{15}N - ^1H multiple quantum coherence spectroscopy. *FEBS Letters* 243, 93-98.
- Bax, A., Clore, G.M., Driscoll, P.C., Gronenborn, A.M., Ikura, M. & Kay, L.E. (1990) Practical aspects of proton-carbon-carbon-proton three-dimensional correlation spectroscopy of ^{13}C -labeled proteins. *J. Magn. Reson.* 87, 620-628.
- Clore, G.M., Bax, A., Driscoll, P.C., Wingfield, P.T. & Gronenborn, A.M. (1990) Assignment of the side chain ^1H and ^{13}C resonance of interleukin-1 β using double and triple resonance heteronuclear three-dimensional NMR spectroscopy. *Biochemistry* 29, 8172-8184.
- Kay, L.E., Clore, G.M., Bax, A. & Gronenborn, A.M. (1990) Four-dimensional heteronuclear triple resonance NMR spectroscopy of interleukin-1 β in solution. *Science* 249, 411-414.
- Ikura, M., Bax, A., Clore, G.M. & Gronenborn, A.M. (1990) Detection of nuclear Overhauser effects between degenerate amide proton resonances by heteronuclear three-dimensional NMR spectroscopy. *J. Am. Chem. Soc.* 112, 9020-9022.
- Clore, G.M., Wingfield, P.T. & Gronenborn, A.M. (1991) High resolution three dimensional structure of interleukin-1 β in solution by three and four dimensional nuclear magnetic resonance spectroscopy. *Biochemistry* 30, 2315-2323.

200-500 citations (cont.)

- Clore, G.M., Kay, L.E., Bax, A. & Gronenborn, A.M. (1991) Four-dimensional $^{13}\text{C}/^{13}\text{C}$ -edited nuclear Overhauser enhancement spectroscopy of a protein in solution: application to interleukin-1 β . *Biochemistry* 30, 12-18.
- Clore, G.M. & Gronenborn, A.M. (1991) Applications of three- and four-dimensional heteronuclear NMR spectroscopy to protein structure determination. *Progr. Nucl. Magn. Reson. Spectroscopy* 23, 43-92.
- Clore, G.M. & Gronenborn, A.M. (1991) Two, three and four dimensional NMR methods for obtaining larger and more precise three-dimensional structures of proteins in solution. *Ann. Rev. Biophys. Biophys. Chem.* 20, 29-63.
- Baldwin, E.T., Weber, I.T., St. Charles, R., Xuan, J.C., Appella, E., Yamada, M., Matsushima, K., Edwards, B.F.P., Clore, G.M., Gronenborn, A.M. & Wlodawer, A. (1991) Crystal structure of interleukin-8: symbiosis of NMR and crystallography. *Proc. Natl. Acad. Sci. U.S.A.* 88, 502-506.
- Omichinski, J.G., Clore, G.M., Schaad, O., Felsenfeld, G., Trainor, C., Appella, E., Stahl, S.J. & Gronenborn, A.M. (1993) NMR structure of a specific DNA complex of Zn-containing DNA binding domain of GATA-1. *Science* 261, 438-446.
- Vuister, G.W., Clore, G.M., Gronenborn, A.M., Powers, R., Garrett, D.S., Tschudin, R. & Bax, A. (1993) Increased resolution and improved spectral quality in four-dimensional $^{13}\text{C}/^{13}\text{C}$ -separated HMQC-NOE-HMQC spectra using pulsed field gradients. *J. Magn. Reson. Series B* 101, 210-213.
- Clore, G.M., Omichinski, J.G., Sakaguchi, K., Zambrano, N., Sakamoto, H., Appella, E. & Gronenborn, A.M. (1994) High-resolution solution structure of the oligomerization domain of p53 by multi-dimensional NMR. *Science* 265, 386-391.
- Clore, G.M. & Gronenborn, A.M. (1994) Multidimensional heteronuclear nuclear magnetic resonance of proteins. *Meth. Enzymol.* 239, 349-363.
- Lodi, P.J., Garrett, D.S., Kuszewski, J., Tsang, M.L.S., Weatherbee, J.A., Leonard, W.J., Gronenborn, A.M. & Clore, G.M. (1994) High resolution solution structure of the β chemokine hMIP-1 β by multi-dimensional NMR. *Science* 263, 1762-1767.
- Lodi, P.J., Ernst, J.A., Kuszewski, J., Hickman, A.B., Engelman, A., Craigie, R., Clore, G.M. & Gronenborn, A.M. (1995) Solution structure of the DNA binding domain of HIV-1 integrase. *Biochemistry* 34, 9826-9833.
- Qin, J., Clore, G.M. Kennedy, W.M.P., Huth, J.R. & Gronenborn, A.M. (1995) Solution structure of human thioredoxin in a mixed disulfide intermediate complex with its target peptide from the transcription factor NF κ B. *Structure* 3, 289-297.
- Ernst, J.A., Clubb, R.T., Zhou, H.-X., Gronenborn, A.M. & Clore, G.M. (1995) Demonstration of positionally disordered water within a protein hydrophobic cavity by NMR. *Science* 267, 1813-1817.
- Makhatadze, G.I., Clore, G.M. & Gronenborn, A.M. (1995) Solvent isotope effect and protein stability. *Nature Struct. Biol.* 2, 852-855.
- Clore, G.M., Ernst, J., Clubb, R.T., Omichinski, J.G., Kennedy, W.M.P., Sakaguchi, K., Appella, E. & Gronenborn, A.M. (1995) Refined solution structure of the oligomerization domain of the tumour suppressor p53. *Nature Struct. Biol.* 2, 321-332.

200-500 citations (cont.)

- Grzesiek, S., Bax, A., Clore, G.M., Gronenborn, A.M., Hu, J.-H., Kaufman, J., Palmer, I., Stahl, S.J. & Wingfield, P.T. (1996) The solution structure of HIV-1 Nef reveals an unexpected fold and permits delineation of the binding surface for the SH3 domain of Hck tyrosine protein kinase. *Nature Struct. Biol.* 3, 340-345.
- Werner, M.H., Gronenborn, A.M. & Clore, G.M. (1996) Intercalation, DNA kinking and the control of transcription. *Science* 271, 778-784.
- Trainor, C.D., Omichinski, J.G., Vandergon, T.L., Gronenborn, A.M., Clore, G.M. & Felsenfeld, G. (1996) A palindromic regulatory site with vertebrate GATA-1 promoters requires both zinc fingers of the GATA-1 DNA binding domain for high affinity interaction. *Mol. Cell. Biol.* 16, 2238-2247.
- Kuszewski, J., Gronenborn, A.M. & Clore, G.M. (1996) Improving the quality of NMR and crystallographic protein structures by means of a conformational database potential derived from structure databases. *Protein Science* 5, 1067-1080.
- Huth, J.R., Bewley, C.A., Nissen, M.S., Evans, J.N.S., Reeves, R., Gronenborn, A.M. & Clore, G.M. (1997) The solution structure of an HMG-I(Y)/DNA complex defines a new architectural minor groove binding motif. *Nature Struct. Biol.* 4, 657-665.
- Cai, M., Zheng, R., Caffrey, M., Craigie, R., Clore, G.M. & Gronenborn, A.M. (1997) Solution structure of the N-terminal zinc binding domain of HIV-1 integrase. *Nature Struct. Biol.* 4, 567-577.
- Omichinski, J.G., Pedone, P.V., Felsenfeld, G., Gronenborn, A.M. & Clore, G.M. (1997) The solution structure of a specific GAGA factor/DNA complex reveals a modular binding mode. *Nature Struct. Biol.* 4, 122-132.
- Tjandra, N., Garrett, D.S., Gronenborn, A.M., Bax, A. & Clore, G.M. (1997) Defining long range order in NMR structure determination from the dependence of heteronuclear relaxation times on rotational diffusion anisotropy. *Nature Struct. Biol.* 4, 443-449.
- Kuszewski, J., Gronenborn, A.M. & Clore, G.M. (1997) Improvements and extensions in the conformational database potential for the refinement of NMR and X-ray structures of proteins and nucleic acids. *J. Magn. Reson.* 125, 171-177.
- Clore, G.M. & Gronenborn, A.M. (1997) NMR structures of proteins and protein complexes larger than 20 kDa. *Curr. Op. Chem. Biol.* 2, 564-570 (1998).
- Huth, J.R., Bewley, C.A., Jackson, B.M., Hinnebusch, A.G., Clore, G.M. & Gronenborn, A.M. (1997) Design of an expression system for detecting folded protein domains and mapping macromolecular interactions by NMR. *Protein Sci.* 6, 2359-2364.
- Bewley, C.A., Gustafson, K.R., Boyd, M.R., Covell, D.G., Bax, A., Clore, G.M. & Gronenborn, A.M. (1998) Solution structure of cyanovirin-N, a potent HIV-inactivating protein. *Nature Struct. Biol.* 5, 571-578.
- Bewley, C.A., Gronenborn, A.M. & Clore, G.M. (1998) Minor-groove binding architectural proteins: structure, function and DNA recognition. *Ann. Rev. Biophys. Biomolec. Struct.* 27, 105-131.
- Clore, G.M. & Gronenborn, A.M. (1998) Determining structures of large proteins and protein complexes by NMR. *Trends in Biotechnology* 16, 22-34.

200-500 citations (cont.)

- Clore, G.M., Gronenborn, A.M. & Tjandra, N. (1998) Direct refinement against residual dipolar couplings in the presence of rhombicity of unknown magnitude. *J. Magn. Reson.* *131*, 159-162.
- Clore, G.M., Gronenborn, A.M. & Bax, A. (1998) A robust method for determining the magnitude of the fully asymmetric alignment tensor of oriented macromolecules in the absence of structural information. *J. Magn. Reson.* *133*, 216-221.
- Clore, G.M. & Gronenborn, A. M. (1998) New methods of structure refinement for macromolecular structure determination by NMR. *Proc. Natl. Acad. Sci. U.S.A.* *95*, 5891-5898.
- Clore, G.M., Starich, M.R., Gronenborn, A.M. (1998) Measurement of residual dipolar couplings of macromolecules aligned in the nematic phase of a colloidal suspension of rod-shaped viruses. *J. Am. Chem. Soc.* *120*, 10571-10572.
- Cai, M., Huang, Y., Sakaguchi, K., Clore, G.M., Gronenborn, A.M. & Craigie, R. (1998) An efficient and cost-effective isotope labeling protocol for proteins expressed in *Escherichia coli*. *J. Biomol. NMR* *11*, 97-102.
- Kuszewski, J., Gronenborn, A.M. & Clore, G.M. (1999) Improving the packing and accuracy of NMR structures with a pseudopotential for the radius of gyration. *J. Am. Chem. Soc.* *121*, 2337-2338.
- Cornilescu, G., Ramirez, B.E., Frank, M.K., Clore, G.M., Gronenborn, A.M. & Bax, A. (1999) Correlation between $^3\text{J}_{\text{NC}}$ and hydrogen bond length in proteins. *J. Am. Chem. Soc.* *121*, 6275-6279.
- Garrett, D.S., Seok, Y.-J., Peterkofsky, A., Gronenborn, A.M. & Clore, G.M. (1999) Solution structure of the 40,000 M_r phosphoryl transfer complex between Enzyme I and HPr. *Nature Struct. Biol.* *6*, 166-173.
- Clore, G.M. & Garrett, D.S. (1999) R-factor, Free R and complete cross-validation for dipolar coupling refinement of NMR structures. *J. Am. Chem. Soc.* *121*, 9008-9012.
- Clore, G.M. (2000) Accurate and rapid docking of protein-protein complexes on the basis of intermolecular nuclear Overhauser enhancement data and dipolar couplings by rigid body minimization. *Proc. Natl. Acad. Sci. U.S.A.* *97*, 9021-9025.
- Cai, M., Huang, Y., Ghirlando, R., Wilson, K.L., Craigie, R. and Clore, G.M. (2001) Solution structure of the constant region of nuclear envelope protein LAP2 reveals two LEM-domain structures: one binds BAF and the other binds DNA. *EMBO J.* *20*, 4399-4407.
- Iwahara, J., Schwieters, C.D. & Clore, G.M. (2004) Ensemble approach for NMR structure refinement against ^1H paramagnetic relaxation enhancement data arising from a flexible paramagnetic group attached to a macromolecule. *J. Am. Chem. Soc.* *126*, 5879-5896.
- Clore, G.M. & Schwieters, C.D. (2004) How much backbone motion in ubiquitin is required to be consistent with dipolar coupling data measured in multiple alignment media as assessed by independent cross-validation. *J. Am. Chem. Soc.* *126*, 2923-2938.
- Iwahara, J. & Clore, G. M. (2006) Detecting transient intermediates in macromolecular binding by paramagnetic NMR. *Nature* *440*, 1227-1230.
- Tang, C., Iwahara, J. & Clore, G.M. (2006) Visualization of transient encounter complexes in protein-protein association. *Nature* *444*, 383-386.

200-500 citations (cont.)

- Tang, C., Schwieters, C.D. & Clore, G.M. (2007) Open-to-closed transition in apo maltose-binding protein visualized by paramagnetic NMR. *Nature* 449, 1878-1882.
- Clore, G.M., Tang, C. & Iwahara, J. (2007) Elucidating transient macromolecular interactions using paramagnetic relaxation enhancement. *Curr. Op. Struct. Biol.* 17, 603-616.
- Iwahara, J., Tang, C. & Clore, G.M. (2007) Practical aspects of ¹H transverse paramagnetic relaxation enhancement measurements on macromolecules. *J. Magn. Reson.* 184, 185-195.
- Fawzi, N.L., Ying, J., Ghirlando, R., Torchia, D.A. & Clore, G.M. (2011) Atomic resolution dynamics on the surface of amyloid β protofibrils probed by solution NMR. *Nature* 480, 268-272.
- Anthis, N.J. & Clore, G.M. (2013) Sequence-specific determination of protein and peptide concentrations by absorbance at 205 nm. *Protein Sci.* 22, 581-588

100-200 Citations

- Clore, G.M., Andreasson, L.E., Karlsson, B., Aasa, R. & Malstrom, 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.
- Clore, G.M., Andreasson, L.E., Karlsson, B., Aasa, R. & Malstrom, 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.
- 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-¹H-NMR. *J. Magn. Reson.* 54, 170-173.
- Gronenborn, A.M. & Clore, G.M. (1985) Investigations into the solution structures of short nucleic acid fragments by means of nuclear Overhauser enhancement measurements. *Progr. Nucl. Magn. Reson. Spectroscopy* 17, 1-32.
- Perutz, M.F., Gronenborn, A.M., Clore, G.M., Hogg, J.H. & Shi, T. (1985) The pK_a's of two histidines in human haemoglobin, the Bohr effect and the dipole moment of α -helices. *J. Mol. Biol.* 183, 491-498.
- 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.
- Clore, G.M., Gronenborn, A.M., Carlson, G. & Meyer, E.F. (1986) Stereochemistry of binding of the tetrapeptide Acetyl-Pro-Ala-Pro-TyrNH₂ to porcine pancreatic elastase: combined use of two-dimensional transferred nuclear Overhauser enhancement measurements, restrained molecular dynamics, X-ray crystallography and molecular modelling. *J. Mol. Biol.* 190, 259-267.
- Nilsson, L., Clore, G.M., Gronenborn, A.M., Brunger, A.T. & Karplus, M. (1986) Structure refinement of oligonucleotides by molecular dynamics with NOE interproton distance restraints: application to 5'd(CGTACG)₂. *J. Mol. Biol.* 188, 455-475.

100-200 Citations (cont.)

- Clore, G.M., Martin, S.R. & Gronenborn, A.M. (1986) The solution structure of human growth hormone releasing factor: combined use of circular dichroism and nuclear magnetic resonance spectroscopy. *J. Mol. Biol.* 191, 553-561.
- Clore, G.M. & Gronenborn, A.M. (1987) Determination of three-dimensional structures of proteins in solution by nuclear magnetic resonance spectroscopy. *Protein Engineering* 1, 275-288.
- Bax, A., Sklenar, V., Clore, G.M. & Gronenborn, A.M. (1987) Water suppression in two-dimensional spin-locked NMR experiments using a novel phase cycling procedure. *J. Am. Chem. Soc.* 109, 6511-6513.
- Clore, G.M., Sukumaran, D.K., Nilges, M., Zarbock, J. & Gronenborn, A.M. (1987) The conformations of hirudin in solution: a study using nuclear magnetic resonance, distance geometry and restrained molecular dynamics. *EMBO J.* 6, 529-537.
- Clore, G.M., Gronenborn, A.M., Nilges, M., Sukumaran, D.K. & Zarbock, J. (1987) The polypeptide fold of the globular domain of histone H5 in solution: a study using nuclear magnetic resonance, distance geometry and restrained molecular dynamics. *EMBO J.* 6, 1833-1842.
- Holak, T.A., Nilges, M., Prestegard, H., Gronenborn, A.M. & Clore, G.M. (1988) Three-dimensional structure of acyl carrier protein in solution determined by nuclear magnetic resonance and the combined use of dynamical simulated annealing and distance geometry. *Eur. J. Biochem.* 175, 9-15.
- Driscoll, P.C., Clore, G.M., Beress, L. & Gronenborn, A.M. (1989) A proton nuclear magnetic resonance study of the anti-hypertensive and anti-viral protein BDS-I from the sea anemone *Anemonia sulcata*: sequential and stereospecific assignment and secondary structure. *Biochemistry* 28, 2178-2187.
- Driscoll, P.C., Gronenborn, A.M., Beress, L. & Clore, G.M. (1989) Determination of the three-dimensional structure of the anti-hypertensive and anti-viral protein BDS-I from the sea anemone *Anemonia sulcata*: a study using nuclear magnetic resonance and hybrid distance geometry-dynamical simulated annealing. *Biochemistry* 28, 2188-2198.
- Folkers, P.J.M., Clore, G.M., Driscoll, P.C., Dodt, J., Köhler, S. & Gronenborn, A.M. (1989) The solution structure of recombinant hirudin and the Lys-47/Glu mutant: a nuclear magnetic resonance and hybrid distance geometry-dynamical simulated annealing study. *Biochemistry* 28, 2601-2617.
- Clore, G.M., Appella, E., Yamada, M., Matsushima, K. & Gronenborn, A.M. (1989) Determination of the secondary structure of interleukin-8 by nuclear magnetic resonance spectroscopy. *J. Biol. Chem.* 264, 18907-18911.
- Driscoll, P.C., Clore, G.M., Marion, D., Wingfield, P.T. & Gronenborn, A.M. (1990) Complete resonance assignment for the polypeptide backbone of interleukin-1 β using three-dimensional heteronuclear NMR spectroscopy. *Biochemistry* 29, 3542-3556.
- Clore, G.M., Bax, A., Wingfield, P.T. & Gronenborn, A.M. (1990) Identification and localization of bound internal water in the solution structure of interleukin-1 β by heteronuclear three-dimensional ^1H rotating frame Overhauser ^{15}N - ^1H multiple quantum coherence NMR spectroscopy. *Biochemistry* 29, 5671-5676.
- Omichinski, J., Clore, G.M., Appella, E., Sakaguchi, K. & Gronenborn, A.M. (1990) High resolution three-dimensional solution structure of a single zinc finger from a human enhancer binding protein in solution. *Biochemistry* 29, 9324-9334.

100-200 Citations (cont.)

- Nilges, M., Clore, G.M. & Gronenborn, A.M. (1990) ^1H -NMR stereospecific assignments by conformational database searches. *Biopolymers* 29, 813-822.
- Clore, G.M., Bax, A. & Gronenborn, A.M. (1991) Stereospecific assignment of β -methylene protons in larger proteins using three-dimensional ^{15}N -separated Hartmann-Hahn and ^{13}C -separated rotating frame Overhauser spectroscopy. *J. Biomol. NMR* 1, 13-22.
- Forman-Kay, J.D., Clore, G.M., Wingfield, P.T. & Gronenborn, A.M. (1991) The high resolution three-dimensional structure of reduced recombinant human thioredoxin in solution. *Biochemistry* 30, 2685-2698.
- Omichinski, J.G., Clore, G.M., Sakaguchi, K., Appella, E. & Gronenborn, A.M. (1991) Structural characterization of a 39-residue synthetic peptide containing the two zinc binding domains from the HIV-1 p7 nucleocapsid protein by CD and NMR spectroscopy. *FEBS Lett.* 292, 25-30.
- Powers, R., Gronenborn, A.M., Clore, G.M. & Bax, A. (1991) Three-dimensional triple resonance NMR of $^{13}\text{C}/^{15}\text{N}$ enriched proteins using constant-time evolution. *J. Magn. Reson.* 94, 209-213.
- Robien, M.A., Clore, G.M., Omichinski, J.G., Perham, R.N., Appella, E., Sakaguchi, K. & Gronenborn, A.M. (1992) Three-dimensional solution structure of the E3-binding domain of the dihydrolipoamide succinyltransferase core from the 2-oxoglutarate dehydrogenase multienzyme complex of *Escherichia coli*. *Biochemistry* 31, 3463-3471.
- Forman-Kay, J.D., Clore, G.M. & Gronenborn, A.M. (1992) The relationship between electrostatics and redox function in human thioredoxin: characterization of pH titration shifts using two-dimensional homo- and heteronuclear NMR. *Biochemistry* 31, 3442-3452.
- Powers, R., Garrett, D.S., March, C.J., Frieden, E.A., Gronenborn, A.M. & Clore, G.M. (1992) Three-dimensional solution structure of human interleukin-4 by multi-dimensional heteronuclear magnetic resonance spectroscopy. *Science* 256, 1673-1677.
- Chandrasasekhar, I., Clore, G.M., Szabo, A., Gronenborn, A.M. & Brooks, B.R. (1992) A 500 ps molecular dynamics simulation study of interleukin-1 β in water: correlation with nuclear magnetic resonance spectroscopy and crystallography. *J. Mol. Biol.* 226, 239-250.
- Achari, A., Hale, S.P., Howard, A.J., Clore, G.M., Gronenborn, A.M., Hardman, K.D. & Whitlow, M. (1992) The 1.67 Å X-ray structure of the B2 immunoglobulin domain of streptococcal protein G and comparison to the NMR structure of the B1 domain. *Biochemistry* 31, 10449-10457.
- Varley, P., Gronenborn, A.M., Christensen, H., Wingfield, P.T., Pain, R.H. & Clore, G.M. (1993) Kinetics of folding of the all β -sheet protein interleukin-1 β studied by nuclear magnetic resonance, circular dichroism and fluorescence. *Science* 240, 1110-1113.
- Brünger, A.T., Clore, G.M., Gronenborn, A.M., Saffrich, R. & Nilges, M. (1993) Assessing the quality of solution nuclear magnetic resonance structures by complete cross-validation. *Science* 261, 328-331.
- Sakaguchi, K., Zambrano, N., Baldwin, E.T., Shapiro, B.A., Erickson, J.W., J.G. Omichinski, G.M. Clore, A.M. Gronenborn & E. Appella (1993) Identification of a binding site for the human immunodeficiency virus type I nucleocapsid protein. *Proc. Natl. Acad. Sci. U.S.A.* 90, 5219-5223.

100-200 Citations (cont.)

- Powers, R., Garrett, D.S., March, C.J., Frieden, E.A., Gronenborn, A.M. & Clore, G.M. (1993) The high resolution three-dimensional solution structure of human interleukin-4 determined by multi-dimensional heteronuclear magnetic resonance spectroscopy. *Biochemistry* 32, 6744-6762.
- Clore, G.M., Robien, M.A. & Gronenborn, A.M. (1993) Exploring the limits of precision and accuracy of protein structures determined by nuclear magnetic resonance spectroscopy. *J. Mol. Biol.* 231, 82-102.
- Gronenborn, A.M. & Clore, G.M. (1993) Identification of the contact surface of a Streptococcal protein G domain complexed with a human Fc fragment. *J. Mol. Biol.* 233, 331-335.
- Omichinski, J.G., Trainor, C., Evans, T., Gronenborn, A.M., Clore, G.M. & Felsenfeld, G. (1993) A small single-'finger' peptide from the erythroid factor GATA-1 binds specifically to DNA as a zinc or iron complex. *Proc. Natl. Acad. Sci. U.S.A.* 90, 1676-1680.
- Clubb, R.T., Omichinski, J.G., Clore, G.M. & Gronenborn, A.M. (1994) Mapping the binding surface of interleukin-8 complexed with an N-terminal fragment of the type I human interleukin-8 receptor. *FEBS Lett.* 338, 93-97.
- Garrett, D.S., Kuszewski, J., Hancock, T.J., Lodi, P.J., Vuister, G.W., Gronenborn, A.M. & Clore, G.M. (1994) The impact of direct refinement against three-bond HN-C α H coupling constants on protein structure determination by NMR. *J. Magn. Reson. Series B* 104, 99-103.
- Qin, J., Clore, G.M. & Gronenborn, A.M. (1994) The high resolution three-dimensional solution structure of the oxidized and reduced states of human thioredoxin: delineation of conformational differences between the two redox states. *Structure* 2, 503-522.
- Werner, M.H., Clore, G.M., Gronenborn, A.M., Kondoh, A. & Fisher, R.J. (1994) Refolding proteins by gel filtration chromatography. *FEBS Lett.* 345, 125-130.
- Rozwarski, D.A., Gronenborn, A.M., Clore, G.M., Bazan, J.F., Bohm, A., Wlodawer, A., Hatada, M. & Karplus, P.A. (1994) Structural comparison among the short-chain helical cytokines. *Structure* 2, 159-173.
- Kuszewski, J., Clore, G.M. & Gronenborn, A.M. (1994) Fast folding of a prototypic polypeptide: the immunoglobulin binding domain of Streptococcal Protein G. *Protein Science* 3, 1945-1952.
- Kuszewski, J., Qin, J., Gronenborn, A.M. & Clore, G.M. (1995) The impact of direct refinement against $^{13}\text{C}\alpha$ and $^{13}\text{C}\beta$ chemical shifts on protein structure determination by NMR. *J. Magn. Reson Series B* 106, 92-96.
- Kuszewski, J., Gronenborn, A.M. & Clore, G.M. (1995) The impact of direct refinement against proton chemical shifts in protein structure determination by NMR. *J. Magn. Reson. Series B* 107, 293-297.
- Frank, M.K., Clore, G.M. & Gronenborn, A.M. (1995) Structural and dynamic characterization of the urea denatured state of the immunoglobulin binding domain of Streptococcal protein G. *Protein Science* 4, 2605-2615.
- Balagurumorthy, P., Sakamoto, K., Lewis, M.S., Zambrano, N., Clore, G.M., Gronenborn, A.M., Appella, E. & Harrington, R.E. (1995) Four p53 DNA binding domains bind natural p53 response elements and bend the DNA. *Proc. Natl. Acad. Sci. U.S.A.* 92, 8591-8585.

100-200 Citations (cont.)

- Clore, G.M. & Gronenborn, A.M. (1995) Three-dimensional structures of α and β chemokines. *FASEB Journal* 9, 57-62.
- Qin, J., Clore, G.M., Kennedy W.P., Kuszewski, J. & Gronenborn, A.M. (1996) The solution structure of human thioredoxin complexed with its target from Ref-1 reveals peptide chain reversal. *Structure* 4, 613-620.
- Pedone, P.V., Ghirlando, R., Clore, G.M., Gronenborn, A.M., Felsenfeld, G. & Omichinski, J.G. (1996) The single Cys₂His₂ zinc finger domain of the GAGA protein flanked by basic residues is sufficient for high affinity DNA binding. *Proc. Natl. Acad. Sci. U.S.A.* 93, 2822-2826.
- Pedone, P.V., Omichinski, J.G., Nony, P., Trainor, C., Gronenborn, A.M., Clore, G.M. & Felsenfeld, G. (1997) The N-terminal fingers of cGATA-2 and cGATA-3 are independent sequence-specific DNA binding domains. *EMBO J.* 16, 2874-2882.
- Garrett, D.S., Seok, Y.J., Liao, D.I., Peterkofsky, A., Gronenborn, A.M. & Clore, G.M. (1997) Solution structure of the 30 kDa N-terminal domain of Enzyme I of the *Escherichia coli* phosphoenolpyruvate:sugar phosphotransferase system by multidimensional NMR. *Biochemistry* 36, 2517-2530.
- Cai, M., Huang, Y., Zheng, R., Wei, S.-Q., Guirlando, R., Lee, M.S., Craigie, R., Gronenborn, A.M. & Clore, G.M. (1998) Solution structure of the cellular factor BAF responsible for protecting retroviral DNA from autointegration. *Nature Struct. Biol.* 5, 903-909.
- Louis, J.M., Clore, G.M. & Gronenborn, A.M. (1999) Regulation of HIV-1 protease: autoprocessing is tightly coupled to protein folding. *Nature Struct. Biol.* 6, 868-875.
- Yang, F., Bewley, C.A., Louis, J.M., Gustafson, K.R., Boyd, M.R., Gronenborn, A.M., Clore, G.M. & Wlodawer, A. (1999) Crystal structure of cyanovirin-N, a potent HIV-inactivating protein, shows unexpected domain swapping. *J. Mol. Biol.* 288, 403-412.
- Yu, B., Blaber, M., Gronenborn, A.M., Clore, G.M. & Caspar, D.L.D. (1999) Disordered water within a hydrophobic cavity visualized by X-ray crystallography. *Proc. Natl. Acad. Sci. U.S.A.* 96, 103-108.
- Clore, G.M., Starich, M.R., Bewley, C.A., Cai, M. & Kuszewski, J. (1999) Impact of residual dipolar couplings on the accuracy of NMR structures determined from a minimal number of NOE restraints. *J. Am. Chem. Soc.* 121, 6513-6514.
- Huang, K., Louis, J.M., Donaldson, L., Lim, F.-L., Sharrocks, A.D. & Clore, G.M. (2000) Solution structure of the MEF2A-DNA complex: structural basis for the modulation of DNA bending and specificity by MADS-box transcription factors. *EMBO J.* 19, 2615-2628.
- Kuszewski, J. & Clore, G.M. (2000) Source of and solutions to problems in the refinement of protein NMR structures against torsion angle potentials of mean force. *J. Magn. Reson.* 146, 249-254.
- Kontaxis, G., Clore, G.M. & Bax, A. (2000) Evaluation of cross-relaxation effects and measurement of one-bond couplings in proteins with short transverse relaxation times. *J. Magn. Reson.* 143, 184-196.
- Wang, G.S., Louis, J.M., Sondej, M., Seok, Y.-J., Peterkofsky, A. & Clore, G.M. (2000) Solution structure of the phosphoryl transfer complex between the signal transducing protein HPr and IIA^{Glucose} of the *Escherichia coli* phosphoenolpyruvate:sugar phosphotransferase system. *EMBO J.* 19, 5635-5649.

100-200 Citations (cont.)

- Schwieters, C.D. & Clore, G.M. (2001) Internal coordinates for molecular dynamics and minimization in structure determination and refinement. *J. Magn. Reson.* 152, 288-302.
- Schwieters, C.D. & Clore, G.M. (2001) The VMD-XPLOR visualization package for NMR structure refinement. *J. Magn. Reson.* 149, 239-244.
- Murphy, E.C., Zhurkin, V.B., Louis, J.M., Cornilescu, G. and Clore, G.M. (2001) Structural basis for SRY-dependent 46-X,Y sex reversal: modulation of DNA bending by a naturally occurring point mutation. *J. Mol. Biol.* 312, 481-499.
- Louis, J.M., Bewley, C.A. & Clore, G.M. (2001) Design and properties of N_{CCG}-gp41, a chimeric gp41 molecule with nanomolar HIV-fusion inhibitory activity. *J. Biol. Chem.* 276, 29485-29489.
- Bewley, C.A., Louis, J.M., Ghirlando, R. & Clore, G.M. (2002) Design of a novel peptide inhibitor of HIV fusion that disrupts the internal trimeric coiled-coil of gp41. *J. Biol. Chem.* 277, 14238-14245.
- Braddock, D.T., Louis, J.M., Baber, J.L., Levens, D. & Clore, G.M. (2002) Structure and dynamics of KH domains from FBP bound to single-stranded DNA. *Nature* 415, 1051-1056.
- Braddock, D.T., Baber, J.L., Levens, D. & Clore, G.M. (2002) Molecular basis of sequence specific single-stranded DNA recognition by KH domains: solution structure of a complex between hnRNP K KH3 and single-stranded DNA. *EMBO J.* 21, 3476-3485.
- Clore, G.M. & Schwieters, C.D. (2003) Docking of protein-protein complexes on the basis of highly ambiguous intermolecular distance restraints derived from ¹H_N/¹⁵N chemical shift mapping and backbone ¹⁵N-¹H residual dipolar couplings using conjoined rigid body/torsion angle dynamics. *J. Am. Chem. Soc.* 125, 2902-2912.
- Louis, J.M., Nesheiwat, I., Chang, L.C., Clore, G.M. & Bewley, C.A. (2003) Covalent trimers of the internal N-terminal trimeric coiled-coil of gp41 and antibodies directed against them are potent inhibitors of HIV envelope-mediated cell fusion. *J. Biol. Chem.* 278, 20278-20285.
- Williams, D.C., Cai, M. & Clore, G.M. (2004) Molecular basis for synergistic transcriptional activation by Oct1 and Sox2 revealed from the solution structure of the 42 kDa Oct1·Sox·Hoxb1-DNA ternary transcription factor complex. *J. Biol. Chem.* 279, 1449-1457.
- Schulz, D.M., Ihlung, C., Clore, G.M. & Sinz, A. (2004) Mapping the topology and determination of a low-resolution three-dimensional structure of the calmodulin-mellitin complex by chemical cross-linking and high resolution FTICR mass spectrometry. *Biochemistry* 43, 4703-4715.
- Clore, G.M. & Schwieters, C. D. (2004) Amplitudes of protein backbone dynamics and correlated motions in a small α/β protein: correspondence of dipolar coupling and heteronuclear relaxation measurements. *Biochemistry* 43, 10678-10691.
- Clore, G.M. & Schwieters, C. D. (2006) Concordance of residual dipolar couplings, backbone order parameters and crystallographic B-factors for a small α/β protein: a unified picture of high probability, fast atomic motions in proteins. *J. Mol. Biol.* 355, 879-886.
- Iwahara, J., Zwecksetter, M. & Clore, G.M. (2006) NMR structural and kinetic characterization of a homeodomain diffusing and hopping on non-specific DNA. *Proc. Natl. Acad. Sci. U.S.A.* 103, 15062-15067.

100-200 Citations (cont.)

- Tang, C., Louis, J.M., Aniana, A., Suh, J.-Y., & Clore, G.M. (2008) Visualizing transient events in amino-terminal autoprocessing of HIV-1 protease. *Nature* 455, 693-696.
- Kim, Y.C., Tang, C., Clore, G.M. & Hummer, G. (2008) Replica exchange simulations of transient encounter complexes in protein-protein association. *Proc. Natl. Acad. Sci. U.S.A.* 105, 12855-12860.
- Fawzi, N., Ying, J., Torchia, D, A., Clore, G. M. (2010) Kinetics of amyloid β monomer to oligomer exchange by NMR relaxation. *J. Am. Chem. Soc.* 132, 9948-9951.
- Schwieters, C.D., Suh, J.-Y., Grishaev, A., Ghirlando, R., Takayama, Y. & Clore, G.M. (2010) Structure of the 128 kDa enzyme I dimer from *Escherichia coli* and its 146 kDa complex with HPr using residual dipolar couplings and small- and wide-angle solution X-ray scattering. *J. Am. Chem. Soc.* 132, 13026-13045.
- Anthis, N.J., Doucleff, M. & Clore, G.M. (2011) Transient, sparsely populated compact states of apo and calcium-loaded calmodulin probed by paramagnetic relaxation enhancement: interplay of conformational selection and induced fit. *J. Am. Chem. Soc.* 133, 18966-18974.
- Deshmukh, L., Schwiewers, C.D., Grishaev, A., Ghirlando, R., Baber, K.L. & Clore, G.M. (2013) Structure and dynamics of full length HIV-1 capsid protein in solution. *J. Am. Chem. Soc.* 135, 16133-16147
- Anthis, N.J. & Clore, G.M. (2015) Visualizing transient dark states by NMR spectroscopy. *Q. Rev. Biophys.* 48, 35-116.
- Schmidt, T, Wälti, M.A., Baber, J.L., Hustedt, E.J. & Clore, G.M. (2016) Long distance measurements up to 160 Å in the GroEL tetradecamer using Q-band DEER EPR spectroscopy. *Angewandte Chemie Int. Ed.* 55, 15905-15909.
- Schwieters, C.D., Bermejo, G.A. & Clore, G.M. (2018) Xplor-NIH for molecular structure determination from NMR and other data sources. *Protein Sci.* 27, 26-40.