CURRICULUM VITAE

Lewis Edward Kay
OC, FRS, FRSC

Department of Molecular Genetics,
Department of Biochemistry
Department of Chemistry
University of Toronto
Medical Sciences Building
1 King's College Circle
Toronto, Ontario, Canada, M5S 1A8

Academic Degrees

1988 PhD in Molecular Biophysics, Yale University, New Haven, Connecticut, USA. Supervisor: Dr. J.H. Prestegard; Thesis: "NMR Methods for Studying Motional and Structural Properties of Molecules in Solution"

1983 BSc in Biochemistry (first class honours), University of Alberta, Edmonton, Alberta, Canada

Employment

1995 - Professor of Molecular Genetics (previously Medical Genetics), Biochemistry and Chemistry, University of Toronto, Toronto, Ontario, Canada
Phone: 416-978-0741, Fax: 416-978-8548, E-mail: kay@pound.med.utoronto.ca

1992 - 1995 Assistant Professor of Molecular Genetics (previously Medical Genetics), Biochemistry and Chemistry, University of Toronto, Toronto, Ontario, Canada

1988 - 1991 Alberta Heritage and Medical Research Council of Canada Post-Doctoral Fellow, Laboratory of Dr. Adrian Bax, Laboratory of Chemical Physics, National Institutes of Health, Bethesda, Maryland, USA

Endowed Lectures (plenary lectures not listed here)

Birss Lecturer, Department of Chemistry, University of Alberta, Edmonton, October 1999.

NIH Director's Wednesday Afternoon Lecture Series, May, 2006.

Wilbur Cross Medal Lecture, Yale University, Oct, 2006.

The Gitte Vold Memorial Lecture, University of California, San Diego, March 2007.

Proctor and Gamble Lecture, Department of Chemistry, UMass Amherst, October 2007

Hartek Lecturer, Department of Chemistry, RPI, October 2007

McDowell Lecture, Department of Chemistry, UBC, October 2009.

Colter Lecture, Department of Biochemistry, University of Alberta, Fall 2011.

Aline U. and James M. Orten Memorial Lecturer, Department of Biochemistry and Molecular Biology, Wayne State University, April 2012.

Sackler Lecturer, Tel Aviv University, 2013-2014.

Sir Rex Richards Lecture, Dept of Chemistry, Oxford, April 2016.

National Lecturer, Biophysical Society of Canada, Winnipeg, Manitoba, June, 2016.

2016 Distinguished Lecturer, Scripps Research Institute, La Jolla, CA, Sept. 2016.

Peng Memorial Lecture, Biophysics, University of Connecticut Health Center, Oct. 2016.

Robert Olson Lecture, Washington University & University of St. Louis, Dec, 2017.

2018 Lemieux Lecture, Dept. of Chemistry, University of Ottawa, May 2018.

Krimm Lecture, Dept. of Biophysics, University of Michigan, April 2019.

John T. Edsall Lecture, Molecular and Cellular Biology, Harvard University, May 2019.

2019 Garner King Lecture, Faculty of Medicine, University of Alberta, June 2019.

Maude Menten Lecture, Western University, October 2019. (Postponed)

Silvestri Lecture, Villanova, December 2020.

Nordin Lecture, U. Mass, Amherst, May 2023.

Honors and Awards

2023	Akutsu Prize, Korean Magnetic Resonance Society, Seoul, Korea
2023	Honorary Doctorate of Science, University of Ottawa
2020	Ranked #2 in biophysics category of 2020 Stanford List of the world's top scientists
2020	Elected International Member of the National Academy of Sciences, USA
2019	Honorary Doctorate of Science, University of British Columbia
2018	Nakanishi Prize, American Chemical Society
2018	Gerhard Herzberg Canada Gold Medal for Science and Engineering
2017	Protein Society Christian B Anfinson Award
2017	Canada Gairdner Foundation International Award
2017	Fellow of the Biophysical Society Award
2016	Appointed Officer of the Order of Canada
2016	Fellow of the Biophysical Society of Canada
2013	E. W. R. Steacie Award, Canadian Society for Chemistry
2012	University Professor, University of Toronto
2012	Khorana Prize, Royal Society of Chemistry, UK
2010	Election to the Royal Society of London
2009	Distinguished Alumni Award, University of Alberta
2008	Premier's Discovery Award, Province of Ontario
2008	Elected as one of the initial fellows of the International Society of Magnetic Resonance
2007	Dales Prize, Faculty of Medicine, University of Toronto
2006	Election to the Royal Society of Canada

2006	Wilbur Cross Medal of the Yale University Graduate School.
2005	Listed in ISI's database of Highly Cited Researchers; top 0.5% of most cited chemists in the world.
2004	Gunther Laukien Prize, Experimental NMR Conference.
2002	Founders Medal from the International Society of Magnetic Resonance in Biological Systems
2002	Flavelle Medal from the Royal Society of Canada
2000	Canada Research Chair, Tier 1
1999	Premier's Research Excellence Award, Province of Ontario
1999	Steacie Prize from the National Research Council of Canada
1999	Medical Research Council of Canada Scientist Award (1999-2000)
1998	University of Toronto McLean Award
1998	Canada's Top 40 Under 40 Award
1997	Member Editorial Board of Journal of Biomolecular NMR (- current)
1997	International Research Scholar of the Howard Hughes Medical Institute (1997-2002)
1996	Member Editorial Advisory Board of Biochemistry (-current)
1996	Merck Frosst Award
1995	Alfred P. Sloan Research Fellow (1995-1997)
1994 - 1999	MRC (Medical Research Council of Canada) Scholarship
1994	Editorial Board of Concepts in Magnetic Resonance (1994-1999)
1994	Appointed to the Faculty of NMR Concepts, Rhode Island, USA (1994-1999)
1993 -	Editorial Board of the Journal of Magnetic Resonance (-current)
1990 - 1992	MRC (Medical Research Council of Canada) Centennial Fellowship
1988 - 1991	Alberta Heritage Post-Doctoral Fellowship

1988 - 1989 MRC (Medical Research Council of Canada) Post-Doctoral Fellowship

1983 - 1987 NSERC (Natural Science and Engineering Council of Canada) 1967 Science and Engineering Scholarship for Graduate Education

1983 - 1985 Sir James Lougheed Award of Distinction

1982 - 1983 Society of Chemical Industry Merit Award

1982 - 1983 Lieutenant Governor's Gold Medal - Highest Academic Achievement in graduating class of the Faculty of Science (fix tabs)

1978 - 1979 Highest Honors Standing in Grade XII in the Edmonton Public School System

Outreach and Mentoring of High School Students and Undergraduates

Through the Canada Gairdner Foundation I have travelled extensively throughout Canada giving science lectures to high school students and meeting with them to discuss why science is something that they may wish to consider career-wise. The lectures describe simple concepts of biophysics and how physics can inform on how biomolecules function. Independently I mentor a series of high school students and undergraduates that I have met through these lectures, keeping in touch electronically. I discuss careers in science with them and assist with selection of courses that would best meet their needs and satisfy their interests. A sampling of cities where I have met with high school students includes: Lethbridge, Edmonton, Calgary, Winnipeg, Montreal, St. John's, Toronto, Ottawa, Thunder Bay, Charlottetown, Halifax, Fredricton.

In the past 12 months I have been a speaker at:

(1) StAR (Student Advancement Research), which is a paid 6-week internship program for Black, Indigenous, and Filipino students to get some lab experience.
(2) SSuRe (SickKids Summer Undergraduate Research), which is a paid 3-month internship for students to gain research insights.
(3) Toronto local high schools
(4) Exploring by the Seat of your Pants, "Unlocking the Mysteries of Life with Dr. Lewis Kay"

Publications

1. J. Gariépy, Lewis E. Kay, I.D. Kuntz, B.D. Sykes and R.S. Hodges. Nuclear Magnetic Resonance Determination of Metal-Proton Distances in a Synthetic Calcium Binding Site of Rabbit Skeletal Troponin-C. *Biochemistry* **24**, 544-550 (1985). doi:10.1021/bi00323a045.

2. D.C. Corson, T.C. Williams, Lewis E. Kay and B.D. Sykes. ^{1}H NMR Spectroscopic Studies of Calcium Binding Proteins: 1: Stepwise Proteolysis of the C-Terminal α-Helix of a Helix-Loop-Helix Metal-Ion-Binding Domain. *Biochemistry* **25**, 1817-1826 (1986). doi:10.1021/bi00355a055.

3. Lewis E. Kay and J.H. Prestegard. An Application of Pulse-Gradient Double Quantum Spin Echoes to Diffusion Measurements on Molecules with Scalar-Coupled Spins. *J. Magn. Reson.* **67**, 103-113 (1986). doi:10.1016/0022-2364(86)90413-0.

4. Lewis E. Kay, J.N. Scarsdale, D.R. Hare and J.H. Prestegard. Simulation of Two-Dimensional Cross-Relaxation Spectra in Strongly Coupled Spin Systems. *J. Magn. Reson.* **68**, 515-525 (1986). doi:10.1016/0022-2364(86)90340-9.

5. Lewis E. Kay, T.A. Holak, B.A. Johnson, I.M. Armitage and J.H. Prestegard. Second-Order Effects in Two-Dimensional Cross-Relaxation Spectra of Proteins: Investigation of Glycine Spin Systems. *J. Am. Chem. Soc.* **108**, 4242-4244 (1986). doi:10.1021/ja00274a076.

6. Lewis E. Kay, M. Pascone, B.D. Sykes and J.W. Shriver. ^{19}F Nuclear Magnetic Resonance as a Probe of Structural Transitions and Cooperative Interactions in Heavy Meromyosin. *J. Biol. Chem.* **262**, 1984-1988 (1987). doi:10.1016/S0021-9258(18)61608-4.

7. Lewis E. Kay and J.H. Prestegard. Methyl Group Dynamics from Relaxation of Double Quantum Filtered NMR Signals: Application to Deoxycholate. *J. Am. Chem. Soc.* **109**, 3829-3835 (1987). doi:10.1021/ja00247a002.

8. Lewis E. Kay, P.-J. Jones and J.H. Prestegard. Strong Coupling Effects in the Homonuclear RELAY Experiment, with Applications to Leucine Spin Systems of Octanoyl-Acyl Carrier Protein. *J. Magn. Reson.* **72**, 392-396 (1987). doi:10.1016/0022-2364(87)90307-6.

9. Lewis E. Kay, T.L. Jue, B. Bangerter and P.C. Demou. Sensitivity Enhancement of ^{13}C T_1 Measurements Via Polarization Transfer. *J. Magn. Reson.* **73**, 558-564 (1987). doi:10.1016/0022-2364(87)90024-2.

10. Lewis E. Kay and R.E.D. McClung. A Product Operator Description of AB and ABX Spin Systems. *J. Magn. Reson.* **77**, 258-273 (1988). doi:10.1016/0022-2364(88)90177-1.

11. Lewis E. Kay, T.A. Holak and J.H. Prestegard. AX_3 Spin System Dynamics from Forbidden Cross Peak Intensities in Double Quantum Spectra, with Application to Acyl Carrier Protein. *J. Magn. Reson.* **76**, 30-40 (1988). doi:10.1016/0022-2364(88)90198-9.

12. Lewis E. Kay and J.H. Prestegard. Spin-Lattice Relaxation Rates of Coupled Spins from 2D Accordion Spectroscopy. *J. Magn. Reson.* **77**, 599-605 (1988). doi:10.1016/0022-2364(88)90021-2.

13. Lewis E. Kay and J.H. Prestegard. Simultaneous Measurement of ^{13}C Multiplicities and ^{1}H and ^{13}C Chemical Shifts. *J. Magn. Reson.* **78**, 172-177 (1988). doi:10.1016/0022-2364(88)90170-9.

14. A.F. Frederick, Lewis E. Kay and J.H. Prestegard. Location of Divalent Ion Sites in Acyl Carrier Protein Using Relaxation Perturbed 2D NMR. *FEBS Lett.* **238**, 43-48 (1988). doi:10.1016/0014-5793(88)80222-9.

15. D.M. LeMaster, Lewis E. Kay, A.T. Brünger and J.H. Prestegard. Protein Dynamics and Distance Determination by NOE Measurements. *FEBS Lett.* **236**, 71-76 (1988). doi:10.1016/0014-5793(88)80287-4.

16. Lewis E. Kay, D.S. Thomson and J.H. Prestegard. Extraction of ^{1}H-^{1}H and ^{1}H-^{13}C Dipolar Couplings from Spectra Acquired in Inhomogeneous Magnetic Fields. *Magn. Reson. Chem.* **26**, 860-866 (1988). doi:10.1002/mrc.1260261010.

17. A. Bax, Lewis E. Kay, S.W. Sparks and D.A. Torchia. Line Narrowing of Amide Proton Resonances in 2D NMR Spectra of Proteins. *J. Am. Chem. Soc.* **111**, 408-409 (1989). doi:10.1021/ja00183a082.

18. D. Marion, Lewis E. Kay, S.W. Sparks, D.A. Torchia and A. Bax. Three-Dimensional Heteronuclear NMR of ^{15}N Labeled Proteins. *J. Am. Chem. Soc.* **111**, 1515-1517 (1989). doi:10.1021/ja00186a066.

19. Lewis E. Kay, D. Marion and A. Bax. Practical Aspects of 3D Heteronuclear NMR of Proteins. *J. Magn. Reson.* **84**, 72-84 (1989). doi:10.1016/0022-2364(89)90006-1.

20. Lewis E. Kay and A. Bax. Separation of NH and NH_2 Resonances in ^{1}H-Detected Heteronuclear Multiple-Quantum Correlation Spectra. *J. Magn. Reson.* **84**, 598-603 (1989). doi:10.1016/0022-2364(89)90125-X.

21. Lewis E. Kay, B. Brooks, S.W. Sparks, D.A. Torchia and A. Bax. Measurement of NH-CαH Coupling Constants in Staphylococcal Nuclease by Two-Dimensional NMR and Comparison with X-ray Crystallographic Results. *J. Am. Chem. Soc.* **111**, 5488-5490 (1989). doi:10.1021/ja00196a078.

22. D. Marion, P.C. Driscoll, Lewis E. Kay, P.T. Wingfield, A. Bax, A.M. Gronenborn and G.M. Clore. Overcoming the Overlap Problem in the Assignment of ^{1}H NMR Spectra of Larger Proteins by Use of Three-Dimensional Heteronuclear ^{1}H-^{15}N Hartmann-Hahn-Multiple Quantum Coherence and Nuclear Overhauser-Multiple Quantum Coherence Spectroscopy: Application to Interleukin 1ß. Biochemistry **28**, 6150-6156 (1989). doi:10.1021/bi00441a004.

23. Lewis E. Kay, D.A. Torchia and A. Bax. Backbone Dynamics of Proteins as Studied by ^{15}N Inverse Detected Heteronuclear NMR Spectroscopy: Application to Staphylococcal Nuclease. Biochemistry 28, 8972-8979 (1989). doi:10.1021/bi00449a003.

24. Lewis E. Kay and A. Bax. New Methods for the Measurement of NH-CαH Coupling Constants of ^{15}N-Labeled Proteins. *J. Magn. Reson.* **86**, 110-126 (1990). doi:10.1016/0022-2364(90)90215-U.

25. J.D. Forman-Kay, A.M. Gronenborn, Lewis E. Kay, P.T. Wingfield and G.M. Clore. Studies on the Solution Conformation of Human Thioredoxin using Heteronuclear ^{15}N-^{1}H Nuclear Magnetic Resonance Spectroscopy. *Biochemistry* **29**, 1566-1572 (1990). doi:10.1021/bi00458a030.

26. A. Bax, M. Ikura, Lewis E. Kay, D.A. Torchia and R. Tschudin. Comparison of Different Modes of Two-Dimensional Reverse-Correlation NMR for the Study of Proteins. *J. Magn. Reson.* **86**, 304-318 (1990). doi:10.1016/0022-2364(90)90262-8.

27. M. Ikura, Lewis E. Kay, R. Tschudin and A. Bax. Three-Dimensional NOESY-HMQC Spectroscopy of a ^{13}C-Labeled Protein. *J. Magn. Reson.* **86**, 204-209 (1990). doi:10.1016/0022-2364(90)90227-Z.

28. Lewis E. Kay, M. Ikura and A. Bax. Proton-Proton Correlation via Carbon-Carbon Couplings: A Three-Dimensional NMR Approach for the Assignment of Aliphatic Resonances in Proteins Labeled with Carbon-13. *J. Am. Chem. Soc.* **112**, 888-889 (1990). doi:10.1021/ja00158a070.

29. D.A. Torchia, S.W. Sparks, H.B.R. Cole, D.M. Baldisseri, Lewis E. Kay, D. Marion and A. Bax. Assignments, Structure and Dynamics of Staphylococcal Nuclease. *Polymer Preprints* **91**, 2618-2619 (1990).

30. M. Ikura, Lewis E. Kay, D.A. Torchia, C. Klee and A. Bax. Novel Approaches for Obtaining Resonance Assignments of Larger Proteins. *Polymer Preprints* **91**, (1990).

31. M. Ikura, D. Marion, Lewis E. Kay, H. Shih, M. Krinks, C.B. Klee and A. Bax. Heteronuclear 3D NMR and Isotopic Labeling of Calmodulin: Towards the Complete Assignment of the ^{1}H NMR Spectrum. *Biochem. Pharmacol.* **40**, 153-160 (1990). doi:10.1016/0006-2952(90)90190-V.

32. M. Ikura, Lewis E. Kay and A. Bax. A Novel Approach for Sequential Assignment of ^{1}H, ^{13}C, and ^{15}N Spectra of Larger Proteins: Heteronuclear Triple Resonance 3D NMR Spectroscopy. Application to Calmodulin. *Biochemistry* **29**, 4659-4667 (1990). doi:10.1021/bi00471a022.

33. A. Bax, G.M. Clore, P.C. Driscoll, A.M. Gronenborn, P.C. Driscoll, M. Ikura and Lewis E. Kay. Practical Aspects of Proton-Carbon-Carbon-Proton Three-Dimensional Correlation Spectroscopy of ^{13}C Labeled Proteins. *J. Magn. Reson.* **87**, 620-627 (1990). doi.org:10.1016/0022-2364(90)90320-9.

34. G.M. Clore, A. Szabo, A. Bax, Lewis E. Kay, P.C. Driscoll and A.M. Gronenborn. Deviations from the Simple Two Parameter Model-Free Approach to the Interpretation of Nitrogen-15 Nuclear Magnetic Relaxation of Proteins. *J. Am. Chem. Soc.* **112**, 4989-4991 (1990). doi:10.1021/ja00168a070.

35. Lewis E. Kay, M. Ikura, R. Tschudin and A. Bax. Three-Dimensional Triple-Resonance NMR Spectroscopy of Isotopically Labelled Proteins. *J. Magn. Reson.* **89**, 496-514 (1990). doi:10.1016/j.jmr.2011.09.004.

36. Lewis E. Kay, G.M. Clore, A. Bax and A.M. Gronenborn. Four-Dimensional Heteronuclear Triple-Resonance Spectroscopy of a Protein in Solution. Application to Interleukin-1β in Solution. *Science* **249**, 411-414 (1990). doi:10.1126/science.2377896.

37. G.M. Clore, Lewis E. Kay, A. Bax and A.M. Gronenborn. Four-Dimensional $^{13}C/^{13}C$-Edited Nuclear Overhauser Enhancement Spectroscopy of a Protein in Solution: Application to Interleukin-1β. *Biochemistry* **30**, 12-18 (1991). doi.org:10.1021/bi00215a002.

38. A. Bax, M. Ikura, Lewis E. Kay and G. Zhu. Removal of F_1 Baseline Distortion and Optimization of Folding in Multidimensional NMR Spectra. *J. Magn. Reson.* **91**, 174-178 (1991). doi:10.1016/0022-2364(91)90422-P.

39. Lewis E. Kay, M. Ikura and A. Bax. The Design and Optimization of Complex NMR Experiments: Application to a Triple-Resonance Pulse Scheme Correlating Hα, NH and ^{15}N Chemical Shifts in ^{15}N-^{13}C Labeled Proteins. *J. Magn. Reson.* **91**, 84-92 (1991). doi:10.1016/0022-2364(91)90410-U.

40. Lewis E. Kay, M. Ikura, G. Zhu and A. Bax. Four-Dimensional Heteronuclear Triple-Resonance NMR of Isotopically Enriched Proteins for Sequential Assignment of Backbone Atoms. *J. Magn. Reson.* **91**, 422-428 (1991). doi:10.1016/0022-2364(91)90208-B.

41. R. Boelens, C. Griesinger, Lewis E. Kay, D. Marion and E.R.P. Zuiderweg. Applicability and Limitations of Three-Dimensional NMR Spectroscopy for the Study of Proteins in Solution. In "Computational Aspects of the Study of Biological Macromolecules." Vol 225, pp 127-150, NATO ASI Series, Eds. J.C. Hoch, F.M. Poulsen, C. Redfield; Springer, Boston, MA (1991). doi:10.1007/978-1-4757-9794-7_9.

42. Lewis E. Kay, J.D. Forman-Kay, W.D. McCubbin and C.M. Kay. Solution Structure of a Polypeptide Dimer Comprising the Fourth Ca^{2+}-Binding Site of Troponin C by Nuclear Magnetic Resonance Spectroscopy. *Biochemistry* **30**, 4323-4333 (1991). doi:10.1021/bi00231a031.

43. M. Ikura, Lewis E. Kay, M. Krinks and A. Bax. A Triple-Resonance Multidimensional NMR Study of Calmodulin Complexed with the Binding Domain of Myosin Light-Chain Kinase: Indication of a Conformational Change in the Central Helix. *Biochemistry* **30**, 5498-5504 (1991). doi:10.1021/bi00236a024.

44. Lewis E. Kay and D.A. Torchia. The Effects of Dipolar Cross Correlation on ^{13}C Methyl-Carbon T_1, T_2 and NOE Measurements in Macromolecules. *J. Magn. Reson.* **95**, 536-547 (1991). doi:10.1016/0022-2364(91)90167-R.

45. M. Ikura, S. Spera, G. Barbato, Lewis E. Kay, M. Krinks and A. Bax. Secondary Structure and Side-Chain ^{1}H and ^{13}C Resonance Assignments of Calmodulin by Heteronuclear Multidimensional NMR Spectroscopy. *Biochemistry* **30**, 9216-9228 (1991). doi.org:10.1021/bi00102a013.

46. M. Ikura, Lewis E. Kay and A. Bax. Improved Three-Dimensional ^{1}H-^{13}C-^{1}H Correlation Spectroscopy of a ^{13}C Labeled Protein Using Constant-Time Evolution. *J. Biomol. NMR.* **1**, 299-304, (1991). doi.org:10.1007/bf01875522.

47. A. Bax, M. Ikura, Lewis E. Kay, G. Barbato and S. Spera. Multidimensional Triple Resonance NMR Spectroscopy of Isotopically Uniformly Enriched Proteins: A Powerful New Strategy for Structure Determination. In "Protein Conformation." pp 108-134, Ciba Foundation Symposium 161, Eds. D.J. Chadwick, K. Widdows, Wiley, Chichester (1991). doi:10.1002/9780470514146.ch8.

48. L.K. Nicholson, Lewis E. Kay, D.M. Baldisseri, J. Arango, P.E. Young, A. Bax and D.A. Torchia. Dynamics of Methyl Groups in Proteins as Studied by Proton-Detected ^{13}C NMR Spectroscopy. Application to the Leucine Residues of Staphylococcal Nuclease. *Biochemistry* **31**, 5253-5263 (1992). doi:10.1021/bi00138a003.

49. Lewis E. Kay, L.K. Nicholson, F. Delaglio, A. Bax and D.A. Torchia. Pulse Sequences for Removal of the Effects of Cross Correlation Between Dipolar and Chemical-Shift Anisotropy Relaxation Mechanisms on the Measurement of Heteronuclear T_1 and T_2 Values in Proteins. *J. Magn. Reson.* **97**, 359-375 (1992). doi:10.1016/0022-2364(92)90320-7.

50. G. Barbato, M. Ikura, Lewis E. Kay, R.W. Pastor and A. Bax. Backbone Dynamics of Calmodulin Studied by ^{15}N Relaxation Using Inverse Detected Two-Dimensional NMR Spectroscopy: The Central Helix is Flexible. *Biochemistry* **31**, 5269-5278 (1992). doi:10.1021/bi00138a005.

51. Lewis E. Kay, T.E. Bull, L.K. Nicholson, C. Griesinger, H. Scwalbe, A. Bax and D.A. Torchia. The Measurement of Heteronuclear Transverse Relaxation Times in AX_3 Spin Systems via Polarization Transfer Techniques. *J. Magn. Reson.* **100**, 538-558 (1992). doi:10.1016/0022-2364(92)90058-F.

52. Lewis E. Kay and T.E. Bull. Heteronuclear Transverse Relaxation in AMX, AX_2 and AX_3 Spin Systems. *J. Magn. Reson.* **99**, 615-622 (1992). doi:10.1016/0022-2364(92)90218-V.

53. Lewis E. Kay, M. Wittekind, M.A. McCoy, M.S. Friedrichs and L. Mueller. 4D Triple-Resonance Experiments for Assignment of Protein Backbone Nuclei Using Constant-Time Evolution Periods. *J. Magn. Reson.* **98**, 443-450 (1992). doi:10.1016/0022-2364(92)90146-X.

54. Lewis E. Kay, M. Ikura, A.A. Grey and D.R. Muhandiram. Three-Dimensional NMR Experiments for the Separation of Side-Chain Correlations in Proteins via the Carbonyl Chemical Shift. *J. Magn. Reson.* **99**, 652-659 (1992). doi:10.1016/0022-2364(92)90223-T.

55. Lewis E. Kay. A Three-Dimensional NMR Experiment for the Separation of Aliphatic Carbon Chemical Shifts via the Carbonyl Chemical Shift in ^{15}N, ^{13}C Labeled Proteins. *J. Magn. Reson. Series B* **101**, 110-113 (1993). doi:10.1006/jmrb.1993.1018.

56. M. Görlach, M. Wittekind, B.T. Farmer II, Lewis E. Kay and L. Mueller. Measurement of $^{3}J_{HN\alpha}$ Vicinal Coupling Constants in Proteins. *J. Magn. Reson. Series B* **101**, 194-197 (1993). doi:10.1006/jmrb.1993.1031.

57. Lewis E. Kay, P. Keifer and T. Saarinen. Pure Absorption Gradient Enhanced Heteronuclear Single Quantum Correlation Spectroscopy with Improved Sensitivity. *J. Am. Chem. Soc.* **114**, 10663-10665 (1992). doi:10.1021/ja00052a088.

58. D.A. Torchia, L.K. Nicholson, H.B.R. Cole and Lewis E. Kay. Heteronuclear NMR Studies of the Molecular Dynamics of Staphylococcal Nuclease. In "Topics in Molecular and Structural Biology Series: NMR of Proteins." pp 190-219, Eds. G.M. Clore and A.M. Gronenborn; The Macmillan Press Ltd (1993). doi.org:10.1007/978-1-349-12749-8_7.

59. Lewis E. Kay. A Pulsed-Field Gradient-Enhanced Three-Dimensional NMR Experiment for Correlating ^{13}Cα/^{13}Cβ, ^{13}C', ^{1}Hα Chemical Shifts in Uniformly ^{13}C-Labeled Proteins Dissolved in H_2O. *J. Am. Chem. Soc.* **115**, 2055-2057 (1993). doi:10.1021/ja00058a072.

60. Lewis E. Kay, G.-Y. Xu, A.U. Singer, D.R. Muhandiram and J.D. Forman-Kay. A Gradient-Enhanced HCCH-TOCSY Experiment for Recording Side-Chain ^{1}H and ^{13}C Correlations in H_2O Samples of Proteins. *J. Magn. Reson. Series B* **101**, 333-337 (1993). doi:10.1006/jmrb.1993.1053.

61. D.R. Muhandiram, G.Y. Xu and Lewis E. Kay. An Enhanced-Sensitivity Pure Absorption Gradient 4D ^{15}N-,^{13}C-Edited NOESY Experiment. *J. Biol. NMR* **3**, 463-470 (1993). doi:10.1007/BF00176011.

62. D.R. Muhandiram, N.A. Farrow, G.-Y. Xu, S. H. Smallcombe and Lewis E. Kay. A Gradient ^{13}C NOESY-HSQC Experiment for Recording NOESY Spectra of ^{13}C-Labeled Proteins Dissolved in H_2O. *J. Magn. Reson. Series B* **102**, 317-321 (1993). doi:10.1006/jmrb.1993.1102.

63. T. Yamazaki, J.D. Forman-Kay and Lewis E. Kay. Two-Dimensional NMR Experiments for Correlating ^{13}Cβ-^{1}Hδ/ε Chemical Shifts of Aromatic Residues in ^{13}C Labeled Proteins via Scalar Couplings. *J. Am. Chem. Soc.* **115**, 11054-11055 (1993). doi:10.1021/ja00076a099.

64. D.R. Muhandiram and Lewis E. Kay. Gradient-Enhanced Triple-Resonance Three-Dimensional NMR Experiments with Improved Sensitivity. *J. Magn. Reson. Series B* **103**, 203-216 (1994). doi:10.1006/jmrb.1994.1032.

65. S.M. Pascal, D.R. Muhandiram, T. Yamazaki, J.D. Forman-Kay and Lewis E. Kay. Simultaneous Acquisition of ^{15}N- and ^{13}C-Edited NOE Spectra of Proteins Dissolved in H_2O. *J. Magn. Reson.Series B* **103**, 197-201 (1994). doi:10.1006/jmrb.1994.1031.

66. S. Bagby, T.S. Harvey, Lewis E. Kay, S.G. Eagle, S. Inouye and M. Ikura. Unusual Helix-Containing Greek Keys in Development-Specific Ca^{2+}-Binding Protein S. ^{1}H, ^{15}N and ^{13}C Assignments and Secondary Structure Determined with the Use of Multidimensional Double and Triple Resonance Heteronuclear NMR Spectroscopy. *Biochemistry* **33**, 2409-2421 (1994). doi:10.1021/bi00175a009.

67. N.A. Farrow, R. Muhandiram, A.U. Singer, S.M. Pascal, C.M. Kay, G. Gish, S.E. Shoelson, T. Pawson, J.D. Forman-Kay and Lewis E. Kay. Backbone Dynamics of a Free and Phosphopeptide-Complexed Src Homology 2 Domain Studied by ^{15}N NMR Relaxation. *Biochemistry* **33**, 5984-6003 (1994). doi:10.1021/bi00185a040

68. T. Yamazaki, D.R. Muhandiram and Lewis E. Kay. NMR Experiments for the Measurement of Carbon Relaxation Properties in Highly Enriched, Uniformly ^{13}C, ^{15}N Labeled Proteins: Application to $^{13}C^{\alpha}$ Carbons. *J. Am. Chem. Soc.* **116**, 8266-8278 (1994). doi:10.1021/ja00097a037.

69. Lewis E. Kay, G.Y. Xu and T. Yamazaki. Enhanced Sensitivity Triple-Resonance Spectroscopy with Minimal H_2O Saturation. *J. Magn. Reson. Series A* **109**, 129-133 (1994). doi.org:10.1006/jmra.1994.1145.

70. S.M. Pascal, A.U. Singer, G. Gish, S.E. Shoelson, T. Pawson, Lewis E. Kay and J.D. Forman-Kay. Nuclear Magnetic Structure of an SH2 Domain of Phospholipase C-γ1 Complexed with a High Affinity Binding Peptide. *Cell* **77**, 461-472 (1994). doi:10.1016/0092-8674(94)90160-0.

71. T. Yamazaki, W. Lee, M. Revington, D.L. Mattiello, F.W. Dahlquist, C.H. Arrowsmith and Lewis E. Kay. An HNCA Pulse Scheme for the Backbone Assignment of ^{15}N, ^{13}C, ^{2}H Labeled Proteins: Application to a 37-kDa *Trp* Repressor-DNA Complex. *J. Am. Chem. Soc.* **116**, 6464-6465 (1994). doi:10.1021/ja00093a069.

72. N.A. Farrow, O. Zhang, J.D. Forman-Kay and Lewis E. Kay. A Heteronuclear Correlation Experiment for Simultaneous Determination of ^{15}N Longitudinal Decay and Chemical Exchange Rates of Systems in Slow Equilibrium. *J. Biomol. NMR* **4**, 727-734 (1994). doi:10.1007/bf00404280.

73. W. Lee, M.J. Revington, C.H. Arrowsmith and Lewis E. Kay. A Pulsed Field Gradient Isotope-Filtered 3D ^{13}C HMQC-NOESY Experiment for Extracting Intermolecular NOE Contacts in Molecular Complexes. *FEBS Lett.* **350**, 87-90 (1994). doi:10.1016/0014-5793(94)00740-3.

74. O. Zhang, Lewis E. Kay, J.P. Olivier and J.D. Forman-Kay. Backbone ^{1}H and ^{15}N Resonance Assignments of the N-terminal SH3 Domain of Drk in Folded and Unfolded States

using Enhanced-Sensitivity Pulsed Field Gradient NMR Techniques. *J. Biomol. NMR* **4**, 845-858 (1994). doi:10.1007/bf00398413.

75. T. Yamazaki, W. Lee, C.H. Arrowsmith, D.R. Muhandiram and Lewis E. Kay. A Suite of Triple Resonance NMR Experiments for the Backbone Assignment of ^{15}N, ^{13}C, ^{2}H Labeled Proteins with High Sensitivity. *J. Am. Chem. Soc.* **116**, 11655-11666 (1994). doi:10.1021/ja00105a005.

76. C.H. Arrowsmith, W. Lee, M. Revington, T. Yamazaki and Lewis E. Kay. Toward the Solution Structure of Large (> 30 kDa) Proteins and Macromolecular Complexes. In "Techniques in Protein Chemistry" Ed. J.W. Crabb; Academic Press, vol 6, pp 503-510 (1995). doi.org:10.1016/S1080-8914(06)80061-X.

77. N.A. Farrow, O. Zhang, J.D. Forman-Kay and Lewis E. Kay. Comparison of the Backbone Dynamics of a Folded and an Unfolded SH3 Domain Existing in Equilibrium in Aqueous Buffer. *Biochemistry* **34**, 868-878 (1995). doi:10.1021/bi00003a021.

78. T. Yamazaki, S.M. Pascal, A.U. Singer, J.D. Forman-Kay and Lewis E. Kay. NMR Pulse Schemes for the Sequence-Specific Assignment of Arginine Guanidino ^{15}N and ^{1}H Chemical Shifts in Proteins. *J. Am. Chem. Soc.* **117**, 3556-3564 (1995). doi:10.1021/ja00117a025.

79. M.K. Rosen, T. Yamazaki, G.D. Gish, C.M. Kay, T. Pawson and Lewis E. Kay. Direct Demonstration of an Intramolecular SH2-Phosphotyrosine Interaction in the Crk Protein. *Nature* **374**, 477-479 (1995). doi.org:10.1038/374477a0.

80. N.A. Farrow, O. Zhang, A. Szabo, D.A. Torchia and Lewis E. Kay. Mapping Spectral Density Functions from ^{15}N Relaxation Data Exclusively. *J. Biomol. NMR* **6**, 153-162 (1995). doi:10.1007/bf00211779.

81. G.-Y. Xu, E. Ong, N.R. Gilkes, D.G. Kilburn, D.R. Muhandiram, M. Harris-Brandts, J.P. Carver, Lewis E. Kay and T.S. Harvey. Solution Structure of a Cellulose-Binding Domain from *Cellulomonas fimi* by Nuclear Magnetic Resonance Spectroscopy. *Biochemistry* **34**, 6993-7009 (1995). doi.org:10.1021/bi00021a011.

82. Lewis. E. Kay. Pulsed Field Gradient Multi-Dimensional NMR Methods for the Study of Protein Structure and Dynamics in Solution. *Prog. Biophys. Molec. Biol.* **63**, 277-299 (1995). doi:10.1016/0079-6107(95)00007-0.

83. D.R. Muhandiram, T. Yamazaki, B.D. Sykes and Lewis E. Kay. Measurement of ^{2}H T_1 and $T_{1\rho}$ Relaxation Times in Uniformly ^{13}C Labeled and Fractionally ^{2}H Labeled Proteins in Solution. *J. Am. Chem. Soc.* **117**, 11536-11544 (1995). doi:10.1021/ja00151a018.

84. Lewis E. Kay. Field Gradient Techniques in NMR Spectroscopy. *Curr. Opin. Struct. Biol.* **5**, 674-681 (1995). doi:10.1016/0959-440x(95)80061-1.

85. M.M. McEvoy, H. Zhou, A.F. Roth, D.F. Lowry, T.B. Morrison, Lewis E. Kay and F.W. Dahlquist. Nuclear Magnetic Resonance Assignments and Global Fold of a CheY-binding Domain in CheA, the Chemotaxis-Specific Kinase of *Escherichia coli*. *Biochemistry* **34**, 13871-13880 (1995). doi:10.1021/bi00042a019.

86. S.M. Pascal, T. Yamazaki, A.U. Singer, Lewis E. Kay and J.D. Forman-Kay. Structural and Dynamic Characterization of the Phosphotyrosine Binding Region of a Src Homology 2 Domain-Phoshopeptide Complex by NMR Relaxation, Proton Exchange, and Chemical Shift Approaches. *Biochemistry* **34**, 11353-11362 (1995). doi.org:10.1021/bi00036a008.

87. S.M. Pascal, A.U. Singer, T. Yamazaki, Lewis E. Kay and J.D. Forman-Kay. Structural and Dynamic Characterization of an SH2 Domain-Phosphopeptide Complex by NMR Approaches. *Biochem. Soc. Trans.* **23**, 729-733 (1995). doi.org:10.1042/bst0230729.

88. L.K. Nicholson, Lewis E. Kay and D.A. Torchia. Protein Dynamics as Studied by Solution NMR Techniques (Chapter 5). In "NMR Spectroscopy and Its Applications to Biomedical Research." Ed. S.K. Sarkar; Elsevier, Amsterdam (1996). doi:10.1016/B978-044489410-6/50007-6.

89. D.R. Muhandiram and Lewis E. Kay. Three Dimensional HMQC-NOESY, NOESY-HMQC and NOESY-HSQC. In "Encyclopedia of Nuclear Magnetic Resonance." John Wiley and Sons, Baffins Lane, Chichester, West Sussex (1996).

90. J.D. Forman-Kay, S.M. Pascal, A.U. Singer, T. Yamazaki, O. Zhang, N.A. Farrow and Lewis E. Kay. Structural, Dynamic and Folding Studies of SH2 and SH3 Domains. In "NMR as a Structural Tool for Macromolecules: Current Status and Future Directions." pp 35-47, Eds. B.D.N. Rao, M.D. Kemple; Plenum, NY (1996). doi:10.1007/978-1-4613-0387-9_3.

91. Lewis E. Kay, D.R Muhandiram, N.A. Farrow, Y. Aubin and J.D. Forman-Kay. Correlation between Dynamics and High Affinity Binding in an SH2 Domain Interaction. *Biochemistry* (Accelerated) **35**, 361-368 (1996). doi:10.1021/bi9522312.

92. D. Yang and Lewis E. Kay. The Effects of Cross Correlation and Cross Relaxation on the Measurement of Deuterium T_1 and $T_1\rho$ Relaxation Times in $^{13}CH_2D$ Spin Systems. *J. Magn. Reson. Series B* **110**, 213-218 (1996). doi.org:10.1006/jmrb.1996.0035.

93. K.A. Williams, N.A. Farrow, C.M. Deber and Lewis E. Kay. Structure and Dynamics of Bacteriophage IKe Major Coat Protein in MPG Micelles by Solution NMR. *Biochemistry* **35**, 5145-5157 (1996). doi:10.1021/bi952897w.

94. M.M. McEvoy, D.R. Muhandiram, Lewis E. Kay and F.W. Dahlquist. Structure and Dynamics of a CheY-binding Domain of the Chemotaxis Kinase CheA Determined by Nuclear Magnetic Resonance Spectroscopy. *Biochemistry* **35**, 5633-5640 (1996). doi:10.1021/bi952707h.

95. M. Anafi, M.K. Rosen, G.D. Gish, Lewis E. Kay and T. Pawson. An Potential SH3-Binding in the Crk SH2 Domain. *J. Biol. Chem.* **271**, 21365-21374 (1996). doi:10.1074/jbc.271.35.21365.

96. X. Shan, K.H. Gardner, D.R. Muhandiram, N.S. Rao, C.H. Arrowsmith and Lewis E. Kay. Assignment of ^{15}N, $^{13}C^{\alpha}$, $^{13}C^{\beta}$ and HN Resonances in an ^{15}N, ^{13}C, ^{2}H Labeled 64 kDa Trp Repressor-Operator Complex Using Triple Resonance NMR Spectroscopy and ^{2}H-Decoupling. *J. Am. Chem. Soc.* **118**, 6570-6579 (1996). doi:10.1021/ja960627a.

97. D. Yang and Lewis E. Kay. Contributions to Conformational Entropy Arising from Bond Vector Fluctuations Measured from NMR Derived Order Parameter: Application to Protein Folding. *J. Mol. Biol.* **263**, 369-382 (1996). doi:10.1006/jmbi.1996.0581.

98. G.-Yi Xu, J. Hong, T. McDonagh, M. Stahl, Lewis E. Kay, J. Seehra and D.A. Cumming. Complete ^{1}H, ^{15}N and ^{13}C Assignments, Secondary Structure, and Topology of Recombinant Human Interleukin-6, *J. Biomol. NMR* **8**, 123-135 (1996). doi.org:10.1007/bf00211159.

99. M.K. Rosen, K.H. Gardner, R.C. Willis, W.E. Parris, T. Pawson and Lewis E. Kay. Selective Methyl Protonation of Perdeuterated Proteins. *J. Mol. Biol.* **263**, 627-636 (1996). doi:10.1006/jmbi.1996.0603.

100. K.H. Gardner, R. Konrat, M.K. Rosen and Lewis E. Kay, A (H)C(CO)NH-TOCSY Pulse Scheme for Sequential Assignment of Protonated Methyl Groups in Otherwise Deuterated ^{15}N, ^{13}C-Labeled Proteins. *J. Biomol. NMR* **8**, 351-356 (1996). doi:10.1007/bf00410333.

101. J.L. Battiste, H. Mao, N.S. Rao, R. Tan, D.R. Muhandiram, Lewis E. Kay, A.D. Frankel and J.R. Williamson. α-Helix-RNA Major Groove Recognition in an HIV-1 Peptide-RRE RNA Complex. *Science* **273**, 1547-1551 (1996). doi.org:10.1126/science.273.5281.1547.

102. O. Zhang, J.D. Forman-Kay, D. Shortle and Lewis E. Kay. Triple-Resonance NOESY-Based Experiments with Improved Spectral Resolution: Applications to Structural Characterization of Unfolded, Partially Folded and Folded Proteins. *J. Biomol. NMR* **9**, 181-200 (1997). doi:10.1023/a:1018658305040.

103. G.-Yi Xu, H.-A. Yu, J. Hong, M. Stahl, T. McDonagh, Lewis E. Kay and D.A. Cumming. Solution Structure of Recombinant Human Interleukin-6. *J. Mol. Biol.* **268**, 468-481 (1997). doi:10.1006/jmbi.1997.0933.

104. K.H. Gardner, M.K. Rosen and Lewis E. Kay. Global Folds of Highly Deuterated, Methyl-Protonated Proteins by Multidimensional NMR. *Biochemistry* **36**, 1389-1401 (1997). doi:10.1021/bi9624806.

105. N.A. Farrow, O. Zhang, J.D. Forman-Kay and Lewis E. Kay. Characterization of the Backbone Dynamics of Folded and Denatured States of an SH3 Domain. *Biochemistry* **36**, 2390-2402 (1997). doi.org:10.1021/bi962548h.

106. N.S. Rao, P. Legault, D.R. Muhandiram, J. Greenblatt, J.L. Battiste, J.R. Williamson and Lewis E. Kay. NMR Pulse Schemes for the Sequential Assignment of Arginine Sidechain H^{ε} Protons. *J. Magn. Reson. Series B* **113**, 272-276 (1996). doi:10.1006/jmrb.1996.0188.

107. R. Konrat, D.R. Muhandiram, N.A. Farrow and Lewis E. Kay. Pulse Schemes for the Measurement of $^{3}J_{C'C\gamma}$ and $^{3}J_{NC\gamma}$ Scalar Couplings in ^{15}N, ^{13}C Uniformly Labeled Proteins. *J. Biomol. NMR* **9**, 409-422 (1997). doi:10.1023/a:1018354712430.

108. Lewis E. Kay. NMR Methods for the Study of Protein Structure and Dynamics. *Biochem. Cell Biol.* **75**, 1-15 (1997). doi:10.1139/o97-023.

109. C. Zwahlen, P. Legault, S.J.F. Vincent, J. Greenblatt, R. Konrat and Lewis E. Kay. Methods for Measurement of Intermolecular NOEs by Multinuclear NMR Spectroscopy: Application to a Bacteriophage λ N-peptide/*boxB* RNA Complex. *J. Am. Chem. Soc.* **119**, 6711-6721 (1997). doi:10.1021/ja970224q.

110. L.P. McIntosh, E. Brun and Lewis E. Kay. Stereospecific Assignment of the $^{15}NH_2$ Resonances from the Primary Amides of Asparagine and Glutamine Side Chains in Isotopically Labeled Proteins. *J. Biomol. NMR* **9**, 306-312 (1997). doi:10.1023/a:1018635110491.

111. K.H. Gardner and Lewis E. Kay. Production and Incorporation of ^{15}N, ^{13}C, ^{2}H (^{1}H-δ1 methyl) Isoleucine into Proteins for Multidimensional NMR Studies. *J. Am. Chem. Soc.* **119**, 7599-7600 (1997). doi.org:10.1021/ja9706514.

112. S. Li, Z. Songyang, S.J.F. Vincent, C. Zwahlen, S. Wiley, L. Cantley, Lewis E. Kay, J.D. Forman-Kay and T. Pawson. High-Affinity Binding of the *Drosophila* Numb Phoshotyrosine-Binding Domain to Peptides Containing a Gly-Pro-(p)Tyr Motif. *Proc. Natl. Acad. USA* **94**, 7204-7209 (1997). doi:10.1073/pnas.94.14.7204.

113. O. Zhang, Lewis E. Kay, D. Shortle and J.D. Forman-Kay. Comprehensive NOE Characterization of a Partially Folded Large Fragment of Staphylococcal Nuclease, Δ131Δ, Using NMR Methods with Improved Resolution. *J. Mol. Biol.* **272**, 9-20 (1997). doi:10.1006/jmbi.1997.1219.

114. L. Spyracopoulos, S.M. Gagné, W. Gronwald, Lewis E. Kay and B.D. Sykes. NMR Studies of Protein Sidechain Dynamics: Examples from Antifreeze and Calcium-regulatory Proteins. In "Proceedings for the International School of Structural Biology and Magnetic Resonance, 3rd Course on Protein Dynamics, Function and Design." Vol 301, pp147-162, Eds. O. Jardetzky, J.F Lefèvre, R.E. Holbrook; Plenum Press, NY (1998). doi:10.1007/978-1-4615-4895-9_10.

115. D. Yang, Y.-K. Mok, J.D. Forman-Kay, N.A. Farrow and Lewis E. Kay. Contributions to Protein Entropy and Heat Capacity from Bond Vector Motions Measured by NMR Spin Relaxation. *J. Mol. Biol.* **272**,790-804 (1997). doi:10.1006/jmbi.1997.1285.

116. Lewis E. Kay and K.H. Gardner. Solution NMR Spectroscopy Beyond 25 kDa. *Curr. Opin. Struct. Biol.* **7**, 722-731 (1997). doi:10.1016/s0959-440x(97)80084-x.

117. D.R. Muhandiram, P.E. Johnson, D. Yang, O. Zhang, L.P. McIntosh and Lewis E. Kay. Specific ^{15}N, NH Correlations for Residues in ^{15}N, ^{13}C and Fractionally Deuterated Proteins that

Immediately Follow Methyl-Containing Amino Acids. *J. Biomol. NMR* **10**, 283-288 (1997). doi:10.1023/a:1018301818803.

118. D. Yang, R. Konrat and Lewis E. Kay. A Multidimensional NMR Experiment for Measurement of the Protein Dihedral angle ψ Based on Cross-Correlated Relaxation Between $^{1}H^{\alpha}$-$^{13}C^{\alpha}$ Dipolar and $^{13}C'$ (Carbonyl) Chemical Shift Anisotropy Mechanisms. *J. Am. Chem. Soc.* **119**, 11938-11940 (1997). doi:10.1021/ja972329z.

119. Lewis E. Kay. The Development of NMR Methods to Study Protein Structure and Dynamics. In "New Methods for the Study of Biomolecular Complexes." NATO ASI Series. vol 510, pp 285-293, Eds. W. Ens, K.G. Standing, I.V. Chernushevich; Kluwer Academic Publishers (1998). doi.org:10.1007/978-94-015-9046-4_22.

120. K.H. Gardner and Lewis E. Kay. The Use of ^{2}H, ^{13}C, ^{15}N Multidimensional NMR to Study the Structure and Dynamics of Proteins. *Annu. Rev. Biophys. Biomol. Struct.* **27**, 357-406 (1998). doi:10.1146/annurev.biophys.27.1.357.

121. C. Zwahlen, S.J.F. Vincent and Lewis E. Kay. Analytical Description of the Effect of Adiabatic Pulses in IS, I_2S and I_3S Spin Systems. *J. Magn. Reson.* **130**, 169-175 (1998). doi:10.1006/jmre.1997.1289.

122. X. Shan, K.H. Gardner, D.R. Muhandiram, Lewis E. Kay and C.H. Arrowsmith. Subunit-Specific Backbone NMR Assignments of a 64 kDa *trp* Repressor/DNA Complex: A Role for N-Terminal Residues in Tandem Binding. *J. Biomol. NMR* **11**, 307-318 (1998). doi:10.1023/a:1008257803130.

123. Lewis E. Kay, D.R. Muhandiram, G. Wolf, S.E. Shoelson and J.D. Forman-Kay. Correlation Between Binding and Dynamics at SH2 Domain Interfaces. *Nat. Struct. Biol.* **5**, 156-163 (1998). doi:10.1038/nsb0298-156.

124. D. Yang, A. Mittermaier, Y.-K. Mok and Lewis E. Kay. A Study of Protein Side-Chain Dynamics from ^{2}H Auto-Correlation and ^{13}C Cross-Correlation NMR Spectroscopy: Application to the N-terminal SH3 Domain of Drk. *J. Mol. Biol.* **276**, 939-954 (1998). Doi:10.1006/jmbi.1997.1588.

125. J. Mogridge, P. Legault, J. Li, M.D. Van Oene, Lewis E. Kay and J. Greenblatt. Independent Ligand-Induced Folding of the RNA-Binding Domain and Two Functionally Distinct Antitermination Regions in the Phage λ N Protein. *Mol. Cell* **1**, 265-275 (1998). doi:10.1016/s1097-2765(00)80027-1.

126. D. Yang, K.H. Gardner and Lewis E. Kay. A Sensitive Pulse Scheme for Measuring the Backbone Dihedral Angle ψ Based on Cross-Correlation Between $^{13}C^{\alpha}$-$^{1}H^{\alpha}$ Dipolar and Carbonyl Chemical Shift Anisotropy Relaxation Interactions. *J. Biomol. NMR* **11**, 213-220 (1998). doi:10.1023/a:1008284315816.

127. S. Gagné, S. Tsuda, L. Spyracopoulos, Lewis E. Kay and B.D. Sykes. Backbone and Methyl Dynamics of the Regulatory Domain of Troponin C: Anisotropic Rotational Diffusion and Contribution of Conformational Entropy to Calcium Affinity. *J. Mol. Biol.* **278**, 667-686 (1998). doi:10.1006/jmbi.1998.1723.

128. C. Zwahlen, S.J.F. Vincent, K.H. Gardner and Lewis E. Kay. Significantly Improved Resolution for NOE Correlations from Valine and Isoleucine ($C^{\gamma 2}$) Methyl Groups in ^{15}N, ^{13}C and ^{15}N, ^{13}C, ^{2}H-Labeled Proteins. *J. Am. Chem. Soc.* **120**, 4825-4831 (1998). doi:10.1021/ja9742601.

129. P. Legault, J. Li, J. Mogridge, Lewis E. Kay and J. Greenblatt. NMR Structure of the Bacteriophage λ N-Peptide/*boxB* RNA Complex: Recognition of a GNRA Fold by an Arginine-Rich Motif. *Cell* **93**, 289-299 (1998). doi:10.1016/s0092-8674(00)81579-2.

130. D. Yang, J.R. Tolman, N.K. Goto and Lewis E. Kay. An HNCO-based Pulse Scheme for the Measurement of $^{13}C^{\alpha}$-$^{1}H^{\alpha}$ One-Bond Dipolar Couplings in ^{15}N, ^{13}C Labeled Proteins. *J. Biomol. NMR* **12**, 325-332 (1998). doi:10.1023/a:1008223017233.

131a. Lewis E. Kay. Protein Dynamics from NMR. *Nat. Struct. Biol.* **5**, 513-517 (1998). doi:10.1038/755.
131b. Lewis E. Kay. Protein Dynamics from NMR. *Biochem. Cell Biol.* **76**, 145-152 (1998). doi:10.1139/bcb-76-2-3-145.

132. C. Zwahlen, K.H. Gardner, S.P. Sarma, D.A. Horita, R.A. Byrd and Lewis E. Kay. An NMR Experiment for Measuring Methyl-Methyl NOEs in ^{13}C-Labeled Proteins with High Resolution. *J. Am. Chem. Soc.* **120**, 7617-7625 (1998). doi:10.1021/ja981205z.

133. S.-C. Li, C. Zwahlen, S.J.F. Vincent, C.J. McGlade, Lewis E. Kay, T. Pawson and J.D. Forman-Kay. Structure of a Numb PTB Domain-Peptide Complex Suggests a Basis for Diverse Binding Specificity. *Nat. Struct. Biol.* **5**, 1075-1083 (1998). doi:10.1038/4185.

134. V. Kanelis, N.A. Farrow, Lewis E. Kay, D. Rotin and J.D. Forman-Kay. NMR Studies of Tandem WW Domains of Nedd4 in Complex with a PY Motif-Containing Region of the Epithelial Sodium Channel. *Biochem. Cell Biol.* **76**, 341-350 (1998). doi:10.1139/bcb-76-2-3-341.

135. K.H. Gardner, X. Zhang, K. Gehring and Lewis E. Kay. Solution NMR Studies of a 42 kDa *Escherichia coli* Maltose Binding Protein/β-Cyclodextrin Complex: Chemical Shift Assignments and Analysis. *J. Am. Chem. Soc.* **120**, 11738-11748 (1998). doi:10.1021/ja982019w.

136. J. Greenblatt, T.F. Mah, P. Legault, J. Morgridge, J. Li and Lewis E. Kay. Structure and Mechanism in Transcriptional Antitermination by the Bacteriophage λ N Protein. Symposia on Quantitative Biology. CSH Laboratory. vol 63, pp 327-336 (1998). doi:10.1101/sqb.1998.63.327.

137. D. Yang and Lewis E. Kay. Determination of the Protein Backbone Dihedral Angle ψ From a Combination of NMR-Derived Cross-Correlation Spin Relaxation Rates. *J. Am. Chem. Soc.* **120**, 9880-9887 (1998). doi:10.1021/ja981873k.

138. D. Liu, R. Ishima, K.I. Tong, S. Bagby, T. Kokubo, D.R. Muhandiram, Lewis E. Kay, Y. Natakani and M. Ikura. Solution Structure of a TBP-$TAF_{II}230$ Complex: Protein Mimicry of the Minor Groove Surface of the TATA Box Unwound by TBP. *Cell* **94**, 573-583 (1998). doi:10.1016/s0092-8674(00)81599-8.

139. K. H. Gardner and Lewis E. Kay. Multidimensional ^{2}H-Based Methods for Resonance Assignment, Structure Determination, and the Study of Protein Dynamics. In "Modern Techniques in Protein NMR", Biological Magnetic Resonance. Vol. 16, pp 27-74; Eds. N.R. Krishna, L.J. Berliner, Kluwer/Plenum, New York (1998).

140. D. Yang and Lewis E. Kay. Improved ^{1}HN-detected Triple Resonance TROSY-Based Experiments. *J. Biomol. NMR* **13**, 3-10 (1999). doi:10.1023/a:1008329230975.

141. A. Mittermaier, Lewis E. Kay and J.D. Forman-Kay. Analysis of Deuterium Relaxation-Derived Methyl Axis Order Parameters and Correlation with Local Structure. *J. Biomol. NMR* **13**, 181-185 (1998). doi:10.1023/a:1008387715167.

142. D. Yang and Lewis E. Kay. TROSY Triple-Resonance Four-Dimensional NMR Spectroscopy of a 46 ns Tumbling Protein. *J. Am. Chem. Soc.* **121**, 2571-2575 (1999). doi:10.1021/ja984056t.

143. N.K. Goto, K.H. Gardner, G.A. Mueller, R.C. Willis and Lewis E. Kay. A Robust and Cost-Effective Method for the Production of Val, Leu and Ile (δ1) Methyl Protonated ^{15}N-, ^{13}C-, ^{2}H-Labeled Proteins. *J. Biomol. NMR* **13**, 369-374 (1999). doi:10.1023/a:1008393201236.

144. D. Yang, Y.-K. Mok, D.R. Muhandiram, J.D. Forman-Kay and Lewis E. Kay. ^{1}H-^{13}C Dipole-Dipole Cross-Correlated Spin Relaxation as a Probe of Dynamics in Unfolded Proteins: Application to the DrkN SH3 Domain. *J. Am. Chem. Soc.* **121**, 3555-3556 (1999). doi:10.1021/ja9900914.

145. Y.-K. Mok, C.M. Kay, Lewis E. Kay and J.D. Forman-Kay. NOE Data Demonstrating a Compact Unfolded State for an SH3 Domain Under Non-Denaturing Conditions. *J. Mol. Biol.* **289**, 619-638 (1999). doi:10.1006/jmbi.1999.2769.

146. D. Yang and Lewis E. Kay. Improved Lineshape and Sensitivity in the HNCO-Family of Triple-Resonance Experiments. *J. Biomol. NMR* **14**, 273-276 (1999). doi:10.1023/A:1008381929212.

147. D. Yang, R.A. Venters, G.A. Mueller, W.Y. Choy and Lewis E. Kay. TROSY-Based HNCO Pulse Sequences for the Measurement of ^{1}HN-^{15}N, ^{15}N-^{13}CO, ^{1}HN-^{13}CO, ^{13}CO-$^{13}C^{\alpha}$ and ^{1}HN-$^{13}C^{\alpha}$ Dipolar Couplings in ^{15}N, ^{13}C, ^{2}H Labeled Proteins. *J. Biomol. NMR* **14**, 333-343 (1999). doi:10.1023/A:1008314803561.

148. A. Mittermaier, L. Varani, D.R. Muhandiram, Lewis E. Kay and G. Varani. Changes in Side-Chain and Backbone Dynamics Identify Determinants of Specificity in RNA Recognition by Human U1A Protein. *J. Mol. Biol.* **294**, 967-979 (1999). doi:10.1006/jmbi.1999.3311.

149. A. Mittermaier and Lewis E. Kay. Measurement of Methyl ^{2}H Quadrupolar Couplings in Oriented Proteins. How Uniform is the Quadrupolar Coupling Constant? *J. Am. Chem. Soc.* **121**, 10608-10613 (1999). doi:10.1021/ja9925047.

150. R. Konrat, D. Yang and Lewis E. Kay. A 4D TROSY-Based Scheme for Correlating $^{1}HN_{i}$, $^{15}N_{i}$, $^{13}C^{\alpha}_{i}$,$^{13}C'_{i-1}$ Chemical Shifts in High Molecular Weight, ^{15}N, ^{13}C, ^{2}H Labeled Proteins. *J. Biomol. NMR* **15**, 309-313 (1999). doi:10.1023/a:1008310617047.

151. S.-C. Li, G. Gish, D. Yang, A.J. Coffey, J.D. Forman-Kay, I. Ernberg, Lewis E. Kay and T. Pawson. Novel Mode of Ligand Binding by the SH2 Domain of the Human XLP Disease Gene Product SAP/SH2D1A. *Curr. Biol.* **9**, 1355-1362 (1999). doi.org:10.1016/s0960-9822(00)80080-9.

152. N.R. Skrynnikov, N.K. Goto, D. Yang, W.-Y. Choy, J.R. Tolman, G.A. Mueller and Lewis E. Kay. Orienting Domains in Proteins Using Dipolar Couplings Measured by Liquid-State NMR: Differences in Solution and Crystal Forms of Maltodextrin Binding Protein Loaded with β-Cyclodextrin. *J. Mol. Biol.* **295**, 1265-1273 (2000). doi:10.1006/jmbi.1999.3430.

153. C. Zwahlen, S.-C. Li, Lewis E. Kay, T. Pawson and J.D. Forman-Kay. Multiple Modes of Peptide Recognition by the PTB Domain of the Cell Fate Determinant Numb. *EMBO J.* **19**, 1505-1515 (2000). doi.org:10.1093/emboj/19.7.1505.

154. T. Kortemme, M.J.S. Kelly, Lewis E. Kay, J.D. Forman-Kay and L. Serrano. Similarities Between the Spectrin SH3 Domain Denatured State Resembles its Folding Transition State. *J. Mol. Biol.* **297**, 1217-1229 (2000). doi:10.1006/jmbi.2000.3618.

155. L. Varani, S.I. Gunderson, I.W. Mattaj, Lewis E. Kay, D. Neuhaus and G. Varani. The NMR Structure of the 38 kDa U1A Protein-PIE RNA Complex Reveals the Basis of Cooperativity in Regulation of Polyadenylation by Human U1A Protein. *Nat. Struct. Biol.* **7**, 329-335 (2000). doi:10.1038/74101.

156. V. Kanelis, L. Donaldson, D.R. Muhandiram, D. Rotin, J.D. Forman-Kay and Lewis E. Kay. Sequential Assignment of Proline-Rich Regions in Proteins: Application to Modular Binding Domain Complexes. *J. Biomol. NMR* **16**, 253-259 (2000). doi:10.1023/a:1008355012528.

157. N.R. Skrynnikov, R. Konrat, D.R. Muhandiram and Lewis E. Kay. Relative Orientation of Peptide Planes is Reflected in Carbonyl-Carbonyl Chemical Shift Anisotropy Cross-Correlated Spin Relaxation. *J. Am. Chem. Soc.* **122**, 7059-7071 (2000). doi:10.1021/ja0000201.

158. G.A. Mueller, W.Y. Choy, D. Yang, J.D. Forman-Kay, R.A. Venters and Lewis E. Kay. Global Folds of Proteins with Low Densities of NOEs Using Residual Dipolar Couplings: Application to the 370 Residue Maltodextrin-Binding Proteins. *J. Mol. Biol.* **300**, 197-212 (2000). doi:10.1006/jmbi.2000.3842.

159. F.A.A. Mulder, A. Ayed, D. Yang, C.H. Arrowsmith and Lewis E. Kay. Assignment of $^{1}H^{N}$, ^{15}N, $^{13}C^{\alpha}$ and $^{13}C^{\beta}$ Resonances in a 67 kDa p53 Dimer using 4D-TROSY NMR Spectroscopy. *J.Biomol. NMR* **18**, 173-176 (2000). doi:10.1023/a:1008317825976.

160. N.K. Goto and Lewis E. Kay. New Developments in Isotope Labeling Strategies for Protein Solution NMR Spectroscopy. *Curr. Opin. Struct. Biol.* **10**, 585-592 (2000). doi:10.1016/s0959-440x(00)00135-4.

161. F.A.A. Mulder, B. Hon, D.R. Muhandiram, F.W. Dahlquist and Lewis E. Kay. Flexibility and Ligand Exchange in a Buried Cavity Mutant of T4 Lysozyme Studied by Multinuclear NMR. *Biochemistry* **39**, 12614-12622 (2000). doi:10.1021/bi001351t.

162. G.A. Mueller, W.Y. Choy, N.R. Skrynnikov and Lewis E. Kay. A Method for Incorporating Dipolar Couplings into Structure Calculations in Cases of (Near) Axial Symmetry of Alignment. *J. Biomol. NMR* **18**, 183-188 (2000). doi:10.1023/a:1026788430236.

163. N.R. Skrynnikov and Lewis E. Kay. Assessment of Molecular Structure Using Frame-Independent Orientational Restraints Derived from Residual Dipolar Couplings. *J. Biomol. NMR* **18**, 239-252 (2000). doi:10.1023/a:1026501101716.

164. Lewis E. Kay. NMR Methods for the Study of High Molecular Weight Proteins: A Study Involving a Complex of Maltose Binding Protein and β-cyclodextrin. *Methods Enzymol.* **339**, 174-203, (2001). doi:10.1016/s0076-6879(01)39314-x.

165. J.R. Tolman, H.M. Al-Hashimi, Lewis E. Kay and J.H. Prestegard. Structural and Dynamic Analysis of Residual Dipolar Coupling Data for Proteins. *J. Am. Chem. Soc.* **123**, 1416-1424 (2001). doi:10.1021/ja002500y.

166. F.A.A. Mulder, N.R. Skrynnikov, B. Hon, F.W. Dahlquist and Lewis E. Kay. Measurement of Slow (μs-ms) Timescale Dynamics in Protein Side Chains by ^{15}N Relaxation Dispersion NMR Spectroscopy: Application to Asn and Gln Residues in a Cavity Mutant of T4 Lysozyme. *J. Am. Chem. Soc.* **123**, 967-975 (2001). doi:10.1021/ja003447g.

167. J. Evenäs, A. Mittermaier, D. Yang and Lewis E. Kay. Measurement of $^{13}C^{\alpha}$-$^{13}C^{\beta}$ Dipolar Couplings in ^{15}N, ^{13}C, ^{2}H-Labeled Proteins: Application to Domain Orientation in Maltose Binding Protein. *J. Am. Chem. Soc.* **123**, 2858-2864 (2001). Doi:10.1021/ja003833y.

168. N.R. Skrynnikov, F.A.A. Mulder, B. Hon, F.W. Dahlquist and Lewis E. Kay. Probing Slow Timescale Dynamics at Methyl-Containing Sidechains in Proteins by Relaxation Dispersion NMR Measurements: Application to Methionine Residues in a Cavity Mutant of T4 Lysozyme. *J. Am. Chem. Soc.* **123**, 4556-4566 (2001). doi:10.1021/ja004179p.

169. N.K. Goto, N.R. Skrynnikov, F.W. Dahlquist and Lewis E. Kay. What is the Average Conformation of T4 Lysozyme in Solution? A Domain Orientation Study Using Dipolar Couplings Measured by Solution NMR. *J. Mol. Biol.* **308**, 745-764 (2001). doi:10.1006/jmbi.2001.4614.

170. P. M. Hwang, N. R. Skrynnikov and Lewis E. Kay. Domain Orientation in β-Cyclodextrin-Loaded Maltose Binding Protein: Diffusion Anisotropy Measurements Confirm the Results of a Dipolar Coupling Study. *J. Biomol. NMR*. **20**, 83-88 (2001). doi:10.1023/a:1011226512421.

171. J. Evenäs, V. Tugarinov, N.R. Skrynnikov, N.K. Goto, R. Muhandiram and Lewis E. Kay. Ligand-Induced Structural Changes to Maltodextrin-Binding Protein as Studied by Solution NMR Spectroscopy. *J. Mol. Biol*. **309**, 961-974 (2001). doi:10.1006/jmbi.2001.4695.

172. A. Mittermaier and Lewis E. Kay. χ_1 Torsion Angle Dynamics in Protein from Dipolar Couplings. *J. Am. Chem. Soc*. **123**, 6892-6903 (2001). doi:10.1021/ja010595d.

173. W.-Y. Choy, M. Tollinger, G.A. Mueller and Lewis E. Kay. Direct Structure Refinement of High Molecular Weight Proteins Against Residual Dipolar Couplings and Carbonyl Chemical Shift Changes Upon Alignment: An Application of Maltose Binding Protein. *J. Biomol. NMR*. **21**, 31-40 (2001). doi:10.1023/a:1011933020122.

174. A. Ayad, F.A.A. Mulder, G.-S. Yi, Y. Lu, Lewis E. Kay and C. H. Arrowsmith. Latent and Active p53 are Identical in Conformation. *Nat. Struct. Biol*. **8**, 755-760 (2001). doi:10.1038/nsb0901-756.

175. L.W. Donaldson, N.R. Skrynnikov, W.-Y. Choy, D.R. Muhandiram, B. Sarkar, J D. Forman-Kay and Lewis E. Kay. Structural Characterization of Proteins with an Attached ATCUN Motif by Paramagnetic Relaxation Enhancement NMR Spectroscopy. *J. Am. Chem. Soc*. **123**, 9843-9847 (2001). doi:10.1021/ja011241p.

176. Lewis E. Kay and G.A. Petsko. Editorial Overview: Biophysical Methods. *Curr. Opin. Struct. Biol*., **11**, 513-515 (2001). doi:10.1016/S0959-440X(00)00244-X.

177. M. Tollinger, N.R. Skrynnikov, F.A.A. Mulder, J.D. Forman-Kay and Lewis E. Kay. Slow Dynamics in Folded and Unfolded States of an SH3 Domain. *J. Am. Chem. Soc*. **123**, 11341-11352 (2001). doi:10.1021/ja011300z.

178. F.A.A. Mulder, A. Mittermaier, B. Hon, F.W. Dahlquist and Lewis E. Kay. Studying Excited States of Proteins by Relaxation Dispersion NMR Spectroscopy. *Nat. Struct. Biol*. **8**, 932-935 (2001). doi:10.1038/nsb1101-932.

179. F.A.A. Mulder, B. Hon, A. Mittermaier, F.W. Dahlquist and Lewis E. Kay. Slow Internal Dynamics in Proteins: Application of NMR Relaxation Dispersion Spectroscopy to Methyl Groups in a Cavity Mutant of T4 Lysozyme. *J. Am. Chem. Soc*. **124**, 1443-1451 (2001). doi:10.1021/ja0119806.

180. P.M. Hwang, C. Li, M. Morra, J. Lillywhite, D.R. Muhandiram, F. Gertler, C. Terhorst, Lewis E. Kay, T. Pawson, J. D. Forman-Kay and S-C. Li. A 'Three-Pronged' Binding Mechanism for the SAP/SH2D1A SH2 Domain: Structural Basis and Relevance to the XLP Syndrome. *EMBO* **21**, 314-323 (2002). doi:10.1093/emboj/21.3.314.

181. V. Kanelis, J.D. Forman-Kay and Lewis E. Kay. Multidimensional NMR Methods for Protein Structure Determination. *IUBMB Life* **52**, 291-302 (2001). doi:10.1080/152165401317291147.

182. W.-Y. Choy, F.A.A. Mulder, K.A. Crowhurst, D.R. Muhandiram, I.S. Millet, S. Doniach, J.D. Forman-Kay and Lewis E. Kay. Distribution of Molecular Size Within an Unfolded State Ensemble Using Small-Angle X-ray Scattering and Pulsed Field Gradient NMR Techniques. *J. Mol. Biol.* **316**, 101-112 (2002). doi:10.1006/jmbi.2001.5328.

183. O. Millet, D.R. Muhandiram, N.R. Skrynnikov and Lewis E. Kay. Deuterium Spin Probes of Side-Chain Dynamics in Proteins. I. Measurement of Five Relaxation Rates per Deuteron in ^{13}C-Labeled and Fractionally ^{2}H-Enriched Proteins in Solution. *J. Am. Chem. Soc.* **124**, 6439-6448 (2002). doi:10.1021/ja012497y.

184. N.R. Skrynnikov, O. Millet, and Lewis E. Kay. Deuterium Spin Probes of Sidechain Dynamics in Proteins II. Spectral Density Mapping and Identification of Nanosecond Time-Scale Side-Chain motions. *J. Am. Chem. Soc.* **124**, 6449-6460 (2002). doi:10.1021/ja012498q.

185. M. Tollinger, J.D. Forman-Kay and Lewis E. Kay. Measurement of Side-Chain Carboxyl p*K*a values of Glutamate and Aspartate Residues in an Unfolded Protein by Multinuclear NMR Spectroscopy. *J. Am. Chem. Soc.* **124**, 5714-5717 (2002). doi:10.1021/ja020066p.

186. A. Mittermaier and Lewis E. Kay. Effect of Deuteration on Some Structural Parameters of Methyl Groups in Proteins as Evaluated by Residual Dipolar Couplings. *J. Biomol. NMR.* **23** 35-45 (2002). doi:10.1023/a:1015368803552.

187. L.W. Donaldson, T. Pawson, Lewis E. Kay and J.D. Forman-Kay. Structure of a Regulatory Complex Involving the Abl SH3 Domain, the Crk SH2 Domain, and a Crk-Derived Phosphopeptide. *Proc. Nalt. Acad. Sci. USA* **99**, 14053-14058 (2002). doi:10.1073/pnas.212518799.

188. D.M. Korzhnev, N.R. Skrynnikov, O. Millet, D.A. Torchia and Lewis E. Kay. An NMR Experiment for the Accurate Measurement of Heteronuclear Spin-Lock Relaxation Rates. *J. Am. Chem. Soc.* **124**, 10743-10753 (2002). doi:10.1021/ja0204776.

189. V. Tugarinov, D.R. Muhandiram, A. Ayed and Lewis E. Kay. Four-Dimensional NMR Spectroscopy of a 723-Residue Protein: Chemical Shift Assignment and Secondary Structure of Malate Synthase G. *J. Am. Chem. Soc.* **124**, 10025-10035 (2002). doi:10.1021/ja0205636.

190. N.R. Skrynnikov, F.W. Dahlquist and Lewis E. Kay. Reconstructing NMR Spectra of "Invisible" Excited Protein States using HSQC and HMQC Experiments. *J. Am. Chem. Soc.* **124**, 12352-12360 (2002). doi:10.1021/ja0207089.

191. P.M. Hwang, W.-Y. Choy, E.I. Lo, L. Chen, J.D. Forman-Kay, C.R.H. Raetz, G.G. Privé, R.E. Bishop and Lewis E. Kay. Solution Structure and Dynamics of the Outer Membrane Enzyme PagP by NMR. *Proc. Natl. Acad. Sci. USA* **99**, 13560-13565 (2002). doi:10.1073/pnas.212344499.

192. T.K. Mal, M. Ikura and Lewis E. Kay. The ATCUN Domain as a Probe of Intermolecular Interactions: Application to Calmodulin-Peptide Complexes. *J. Am. Chem. Soc.* **124**, 14002-14003 (2002). doi:10.1021/ja028109p.

193. T.K. Mal, N.R. Skrynnikov, K.L. Yap, Lewis E. Kay and M. Ikura. Detecting Protein Kinase Recognition Modes of Calmodulin by Residual Dipolar Couplings in Solution NMR. *Biochemistry* (Accelerated) **41**, 12899-12906 (2002). doi:10.1021/bi0264162.

194. W.-Y. Choy, D. Shortle and Lewis E. Kay. Side Chain Dynamics in Unfolded Protein States: An NMR Based ^{2}H Spin Relaxation Study of Δ131Δ. *J. Am. Chem. Soc.* **125**, 1748-1758 (2003). doi:10.1021/ja021179b.

195. M. Tollinger, K.A. Crowhurst, Lewis. E. Kay and J.D. Forman-Kay. Site-specific Contributions to the pH Dependence of Protein Stability. *Proc. Natl. Acad. Sci. USA* **100**, 4545-4550 (2003). doi:10.1073/pnas.0736600100.

196. V. Tugarinov and Lewis E. Kay. Quantitative NMR Studies of High Molecular Weight Proteins: Application to Domain Orientation and Ligand Binding in the 723 Residue Enzyme Malate Synthase G. *J. Mol. Biol.* **327**, 1121-1133 (2003). doi:10.1016/s0022-2836(03)00238-9.

197. W.-Y. Choy and Lewis E. Kay. Model Selection for the Interpretation of Protein Side Chain Methyl Dynamics. *J. Biomol. NMR* **25**, 325-333 (2003). doi:10.1023/a:1023065310430.

198. D.M. Korzhnev, V.Y. Orekhov, F.W. Dahlquist and Lewis E. Kay. Off-resonance $R_{1\rho}$ Relaxation Outside of the Fast Exchange Limit: An experimental Study of a Cavity Mutant of T4 Lysozyme. *J. Biomol. NMR* **26**, 39-48 (2003). doi:10.1023/a:1023039902737.

199. V. Tugarinov and Lewis E. Kay. Side Chain Assignments of Ile δ1 Methyl Groups in High Molecular Weight Proteins: An Application to a 46 ns Tumbling Molecule. *J. Am. Chem. Soc.* **125** 5701-5706 (2003). doi:10.1021/ja021452+.

200. O. Millet, A. Mittermaier, D. Baker and Lewis E. Kay. The Effects of Mutations on the Motions of Side-Chains in Protein L Studied by ^{2}H NMR Dynamics and Scalar Couplings. *J. Mol. Biol.* **329** 551-563 (2003). doi:10.1016/s0022-2836(03)00471-6.

201. J. E. Ollerenshaw, D.A. Lidar and Lewis E. Kay. A Magnetic Resonance Realization of Decoherence-Free Quantum Computation. *Phys. Rev. Lett.* **91**, 17904 (2003). doi:10.1103/physrevlett.91.217904.

202. A. Mittermaier, A. R. Davidson and Lewis E. Kay. Correlation Between ^{2}H NMR Side-Chain Order Parameters and Sequence Conservation in Globular Proteins. *J. Am. Chem. Soc.* **125**, 9004-9005 (2003). doi:10.1021/ja034856q.

203. V. Tugarinov, P.M. Hwang, J.E. Ollerenshaw and Lewis E. Kay. Cross-Correlated Relaxation Enhanced ^{1}H-^{13}C NMR Spectroscopy of Methyl Groups in Very High Molecular Weight Proteins and Protein Complexes. *J. Am. Chem. Soc.* **125**, 10420-10428 (2003). doi:10.1021/ja030153x.

204. J. E. Ollerenshaw, V. Tugarinov and Lewis E. Kay. Methyl TROSY: Explanation and Experimental Verification. *Magn. Reson. Chem.* **41**, 843-852 (2003). doi:10.1002/mrc.1256.

205. E. Kupce, D.R. Muhandiram and Lewis E. Kay. A Combined HNCA/HNCO Experiment for ^{15}N Labeled Proteins with ^{13}C at Natural Abundance. *J. Biomol. NMR* **27**, 175-179 (2003). doi:10.1023/a:1024985219764.

206. W.-Y. Choy and Lewis E. Kay. Probing Residual Interactions in Unfolded Protein States Using NMR Spin Relaxation Techniques: An Application to Δ131Δ. *J. Am. Chem. Soc.* **125**, 11988-11992 (2003). doi:10.1021/ja035705q.

207. V. Tugarinov and Lewis E. Kay. Ile, Leu, and Val Methyl Assignments of the 723-Residue Malate Synthase G Using a New Labeling Strategy and Novel NMR Methods. *J. Am. Chem. Soc.* **125** 13868-13878 (2003). Doi:10.1021/ja030345s.

208. V. Tugarinov and Lewis E. Kay. An Isotope Labeling Strategy for Methyl TROSY Spectroscopy. *J. Biomol. NMR* **28**, 165-172 (2004). doi:10.1023/b:jnmr.0000013824.93994.1f.

209. O. Millet, R.P. Hudson and Lewis E. Kay. The Energetic Cost of Domain Reorientation in Maltose-Binding Protein as Studied by NMR and Fluorescence Spectroscopy. *Proc. Natl. Acad. Sci. USA* (Track II) **100**, 12700-12705 (2003). doi:10.1073/pnas.2134311100.

210. A. Mittermaier and Lewis E. Kay. The Response of Internal Dynamics to Hydrophobic Core Mutations in the SH3 Domain from the Fyn Tyrosine Kinase. *Protein Sci.* **13**, 1088-1099 (2004). doi:10.1110/ps.03502504.

211. V.Y. Orekhov, D.M. Korzhnev and Lewis E. Kay. Double- and Zero-Quantum Relaxation Dispersion Experiments Sampling Millisecond Time-Scale Dynamics in Proteins. *J. Am. Chem. Soc.* **126**, 1886-1891 (2004). doi.org:10.1021/ja038620y.

212. V. Tugarinov, P.M. Hwang and Lewis E. Kay, Nuclear Magnetic Resonance Spectroscopy of High Molecular Weight Proteins. *Annu. Rev. Biochem.* **73**, 107-146 (2004). doi:10.1146/annurev.biochem.73.011303.074004.

213. V.E. Ahn, E.I. Lo, C.K. Engel, L. Chen, P.M. Hwang, Lewis E. Kay, R.E. Bishop and G. G. Privé, A Hydrocarbon Ruler Measures Palmitate in the Enzymatic Acylation of Endotoxin. *EMBO J.* **23**, 2931-2941 (2004). doi:10.1038/sj.emboj.7600320.

214. A.A. Di Nardo, D.M. Korzhnev, P.J. Stogios, A. Zarrine-Afsar, Lewis E. Kay, and A.R. Davidson. Dramatic Acceleration of Protein Folding by Stabilization of a Nonnative Backbone Conformation. *Proc. Natl. Acad. Sci. USA* (Track II) **101**, 7954-7959 (2004). doi:10.1073/pnas.0400550101.

215. D.M. Korzhnev, X. Salvatella, M. Vendruscolo, A.A. Di Nardo, A.R. Davidson, C.M. Dobson and Lewis E. Kay. Low-Populated Folding Intermediates of Fyn SH3 Characterized by Relaxation Dispersion NMR Spectroscopy. *Nature* **430**, 586-590 (2004). doi:10.1038/nature02655.

216. D.M. Korzhnev, K. Kloiber and Lewis E. Kay. Multiple-Quantum Relaxation Dispersion NMR Spectroscopy Probing Millisecond Time-Scale Dynamics in Proteins: Theory and Application. *J. Am. Chem. Soc.* **126**, 7320-7329 (2004). doi:10.1021/ja049968b.

217. D.M. Korzhnev, K. Kloiber, V. Kanelis, V. Tugarinov and Lewis E. Kay. Probing Slow Dynamics in High Molecular Weight Proteins by Methyl-TROSY NMR Spectroscopy: Application to a 723 Residue Protein. *J. Am. Chem. Soc.* **126**, 3964-3973 (2004). doi:10.1021/ja039587i.

218. V. Tugarinov and Lewis E. Kay. $^{1}H,^{13}C$-$^{1}H,^{1}H$ Dipolar Cross-Correlated Spin Relaxation in Methyl Groups. *J. Biomol. NMR*. **29**, 369-376 (2004). doi:10.1023/b:jnmr.0000032562.07475.7f.

219. V. Tugarinov, R. Sprangers and Lewis E. Kay. Line Narrowing in Methyl-TROSY Using Zero-Quantum ^{1}H-^{13}C NMR Spectroscopy. *J. Am. Chem. Soc.* **126**, 4921-4925 (2004). doi:10.1021/ja039732s.

220. V. Tugarinov and Lewis E. Kay. Stereospecific NMR Assignments of Prochiral Methyls, Rotameric States and Dynamics of Valine Residues in Malate Synthase G. *J. Am. Chem. Soc.* **126**, 9827-9836 (2004). doi:10.1021/ja048738u.

221. P.M. Hwang, R.E. Bishop and Lewis E. Kay. The Integral Membrane Enzyme PagP Alternates Between Two Dynamically Distinct States. *Proc. Natl. Acad. Sci. USA* (Track II) **101**, 9618-9623 (2004). doi:10.1073/pnas.0402324101.

222. P.M. Hwang and Lewis E. Kay. Solution Structure and Dynamics of Integral Membrane Proteins by NMR: A Case Study Involving the Enzyme PagP. *Methods Enzymol.* **394**, 335-350 (2005). doi:10.1016/s0076-6879(05)94013-5.

223. V. Tugarinov, W.-Y. Choy, E. Kupče and Lewis E. Kay. Addressing the Overlap Problem in the Quantitative Analysis of Two Dimensional NMR Spectra: Application to ^{15}N Relaxation Experiments. *J. Biomol. NMR* **30**, 347-352 (2004). doi:10.1007/s10858-005-1549-y.

224. J.E. Ollerenshaw, H. Kaya, H.S. Chan and Lewis E. Kay. Sparsely Populated Folding Intermediates of the Fyn SH3 Domain: Matching Native-Centric Essential Dynamics and

Experiment. *Proc. Natl. Acad. Sci.* (Track II) **101**, 14748-14753 (2004). doi:10.1073/pnas.0404436101

225. P.J. Finerty Jr., A.K. Mittermaier, R. Muhandiram, Lewis E. Kay and J.D. Forman-Kay. NMR Dynamics-Derived Insights into the Binding Properties of a Peptide Interacting with an SH2 Domain. *Biochemistry* **44**, 694-703 (2005). doi:10.1021/bi048641k.

226. V. Tugarinov, C. Scheurer, R. Brüschweiler and Lewis E. Kay. Estimates of Methyl ^{13}C and ^{1}H CSA Values ($\Delta\sigma$) in Proteins from Cross-Correlated Spin Relaxation. *J. Biomol. NMR* **30**, 397-406 (2004). doi:10.1007/s10858-004-4349-x.

227. J. Xu, O. Millet, Lewis E. Kay and N.R. Skrynnikov. A New Spin Probe of Protein Dynamics: Nitrogen Relaxation in ^{15}N-^{2}H Amide Groups. *J. Am. Chem. Soc.* **127**, 3220-3229 (2005). doi:10.1021/ja040215z.

228. D.M. Korzhnev, V.Y. Orekhov and Lewis E. Kay. Off-resonance $R_{1\rho}$ NMR Studies of Exchange Dynamics in Proteins with Low Spin-Lock Fields: An Application to a Fyn SH3 Domain. *J. Am. Chem. Soc.* **127**, 713-721 (2005). doi:10.1021/ja0446855.

229. V. Tugarinov, Lewis E. Kay, I. Ibraghimov and V.Y. Orekhov. High-Resolution Four-Dimensional ^{1}H-^{13}C NOE Spectroscopy Using Methyl-TROSY, Sparse Data Acquisition, and Multidimensional Decomposition. *J. Am. Chem. Soc.* **127**, 2765-2775 (2005). doi:10.1021/ja044032o.

230. V. Tugarinov, W.-Y. Choy, V.Y. Orekhov and Lewis E. Kay. Solution NMR-Derived Global Fold of a Monomeric 82 kDa Protein. *Proc. Natl. Acad. Sci. USA* (Track II) **102**, 622-627 (2005). doi:10.1073/pnas.0407792102.

231. Lewis E. Kay. NMR Studies of Protein Structure and Dynamics. *J. Magn. Reson.* **173**, 193-207 (2005). doi:10.1016/j.jmr.2004.11.021.

232. P. Vallurupalli and Lewis E. Kay. A Suite of ^{2}H NMR Spin Relaxation Experiments for the Measurement of RNA Dynamics. *J. Am. Chem. Soc.* **127**, 6893-6901 (2005). doi:10.1021/ja0427799.

233. W.-Y. Choy, Z. Zhou, Y. Bai and Lewis E. Kay. An ^{15}N NMR Spin Relaxation Dispersion Study of the Folding of a Pair of Engineered Mutants of Apocytochrome b_{562}. *J. Am. Chem. Soc.* **127**, 5066-5072 (2005). doi:10.1021/ja042560u.

234. D.M. Korzhnev, A.K. Mittermaier and Lewis E. Kay. Cross-Correlated Spin Relaxation Effects in ^{1}H Methyl CPMG-Based Relaxation Dispersion Experiments: Complications and a Simple Solution. *J. Biomol. NMR* **31**, 337-342 (2005). doi:10.1007/s10858-005-2468-7.

235. M.A. Pufall, G.M. Lee, M.L. Nelson, H.-S. Kang, A. Velyvis, Lewis E. Kay, L.P. McIntosh and B.J. Graves. Variable Control of Ets-1 DNA Binding by Multiple Phosphates in an Unstructured Region. *Science* **309**, 142-145 (2005). doi:10.1126/science.1111915.

236. V. Tugarinov and Lewis E. Kay. Methyl Groups as Probes of Structure and Dynamics in NMR Studies of High-Molecular-Weight Proteins. *Chembiochem* **6**, 1567-1577 (2005). doi:10.1021/ja051942c.

237. M. Tollinger, Lewis E. Kay and J.D. Forman-Kay. Measuring p*K*a Values in Protein Folding Transition State Ensembles by NMR Spectroscopy. *J. Am. Chem. Soc*. **127**, 8904-8905 (2005). doi:10.1021/ja051942c.

238. V. Tugarinov, J.E. Ollerenshaw and Lewis E. Kay. Probing Side-Chain Dynamics in High Molecular Weight Proteins by Deuterium NMR Spin Relaxation: An Application to an 82-kDa Enzyme *J. Am. Chem. Soc*. **127**, 8214-8225 (2005). doi:10.1021/ja0508830.

239. J.E. Ollerenshaw, V. Tugarinov and Lewis E. Kay. Comparison of $^{13}CH_3$, $^{13}CH_2D$, and $^{13}CHD_2$ Methyl Labeling Strategies in Proteins. *J. Biomol. NMR* **33**, 25-41 (2005). doi:10.1007/s10858-005-2614-2.

240. E.Z. Eisenmesser, O. Millet, W. Labeikovsky, D.M. Korzhnev, M. Wolf-Watz, D.A. Bosco, J.J. Skalicky, Lewis E. Kay and D. Kern. Intrinsic Dynamics of an Enzyme Underlies Catalysis. *Nature* **438**, 117-121 (2005). doi:10.1038/nature04105.

241. R. Sprangers, A, Gribun, P.M. Hwang, W.A. Houry and Lewis E. Kay. Quantitative NMR Spectroscopy of Supramolecular Complexes: Dynamic Side Pores in ClpP are Important for Product Release. *Proc. Natl. Acad. Sci. USA (Track II)* **102**, 16678-16683 (2005). doi:10.1073/pnas.0507370102.

242. D.M. Korzhnev, P. Neudecker, A. Mittermaier, V.Y. Orhekov and Lewis E. Kay. Multiple-Site Exchange in Proteins Studied with a Suite of Six NMR Relaxation Dispersion Experiments: An Application to the Folding of a Fyn SH3 Domain Mutant. *J. Am. Chem. Soc*. **127**, 15602-15611 (2005). doi:10.1021/ja054550e.

243. A. Mittermaier, D.M. Korzhnev and Lewis E. Kay. Side-Chain Interactions in the Folding Pathway of a Fyn SH3 Domain Mutant Studied by Relaxation Dispersion NMR Spectroscopy. *Biochemistry* (Accelerated) **44**, 15430-15436 (2005). doi:10.1021/bi051771o.

244. V. Tugarinov and Lewis E. Kay. Quantitative ^{13}C and ^{2}H NMR Studies of the 723-Residue Enzyme Malate Synthase G Reveal a Highly Dynamic Binding Interface. *Biochemistry* (Accelerated) **44**, 15970-15977 (2005). doi:10.1021/bi0519809.

245. A. Zarrine-Afsar, A. Mittermaier, Lewis E. Kay and A.R. Davidson. Protein Stabilization by Specific Binding of Guanidinium to a Functional Arginine-Binding Surface on an SH3 Domain. *Protein Sci*. **15**, 162-170 (2006). doi:10.1110/ps.051829106.

246. P. Neudecker, D.M. Korzhnev and Lewis E. Kay. An Assessment of the Effects of Increased Relaxation Dispersion Data on the Extraction of 3-Site Exchange Parameters

Characterizing the Unfolding of an SH3 Domain. *J. Biomol NMR* **34**, 129-135 (2006). doi:10.1007/s10858-006-0001-2.

247. U. Brath, M. Akke, D. Yang, Lewis E. Kay and F.A.A. Mulder. Functional Dynamics of Human FKBP12 Revealed by Methyl ^{13}C Rotating Frame Relaxation Dispersion NMR Spectroscopy. *J. Am. Chem. Soc.* **128**, 5718-5727 (2006). doi:10.1021/ja0570279.

248. V. Tugarinov, J. E. Ollerenshaw and Lewis E. Kay. Dipolar Dynamic Frequency Shifts in Multiple Quantum Spectra of Methyl Groups in Proteins: Correlation with Side-Chain Motion. *Magn. Reson. Chem.* **44**, S122-S129 (2006). doi:10.1002/mrc.1819.

249. V. Tugarinov and Lewis E. Kay. Relaxation Rates of Degenerate ^{1}H Transitions in Methyl Groups of Proteins as Reporters of Side-Chain Dynamics. *J. Am. Chem. Soc.* **128**, 7299-7308 (2006). doi:10.1021/ja060817d.

250. D.M. Korzhnev, I. Bezsonova, F. Evanics, N. Taulier, Z. Zhou, Y. Bai, T.V. Chalikian, R.S. Prosser and Lewis E. Kay. Probing the Transition State Ensemble of a Protein Folding Reaction by Pressure Dependent NMR Relaxation Dispersions. *J. Am. Chem. Soc.* **128**, 5262-5269 (2006). doi:10.1021/ja0601540.

251. I. Bezsonova, D.M. Korzhnev, R.S. Prosser, J.D. Forman-Kay and Lewis E. Kay. Hydration and Packing Along the Folding Pathway of SH3 Domains by Pressure-Dependent NMR. *Biochemistry* (Accelerated) **45**, 4711-4719 (2006). doi:10.1021/bi060177r.

252. M. Tollinger, C. Neale, Lewis E. Kay and J.D. Forman-Kay. Characterization of the Hydrodynamic Properties of the Folding Transition State of an SH3 Domain by Magnetization Transfer NMR Spectroscopy. *Biochemistry* **45**, 6434-6445 (2006). doi:10.1021/bi060268o.

253. A. Mittermaier and Lewis E. Kay. New Tools Provide New Insights in NMR Studies of Protein Dynamics. *Science* **312**, 224-228 (2006). doi:10.1126/science.1124964.

254. F. Evanics, P.M. Hwang, Y. Cheng, Lewis E. Kay, and R.S. Prosser. Topology of an Outer-Membrane Enzyme: Measuring Oxygen and Water Contacts in Solution NMR Studies of PagP. *J. Am. Chem. Soc.* **128**, 8256-8264 (2006). doi:10.1021/ja0610075.

255. P. Vallurupalli and Lewis E. Kay. Complementarity of Ensemble and Single-Molecule Measures of Protein Motion: A Relaxation Dispersion NMR Study of an Enzyme System. *Proc. Natl. Acad. Sci. USA*, (Track 2), **103**, 11910-11915 (2006). doi:10.1073/pnas.0602310103.

256. V. Tugarinov and Lewis E. Kay. A ^{2}H NMR Experiment for the Measurement of the Time Scale of Methyl Side-Chain Dynamics in Large Proteins. *J. Am. Chem. Soc.* **128**, 12484-12489 (2006). doi:10.1021/ja063071s.

257. V. Tugarinov, V. Kanelis and Lewis E. Kay. Isotope Labeling Strategies for the Study of High Molecular Weight Proteins by Solution NMR Spectroscopy. *Nature Protocols* **1**, 749-754 (2006). Epub 13 July 2006. doi:10.1038/nprot.2006.101.

258. P. Vallurupalli, L. Scott. M. Hennig, J.R. Williamson and Lewis E. Kay. New RNA Labeling Methods Offer Dramatic Sensitivity Enhancements in ^{2}H Relaxation Spectra. *J. Am. Chem. Soc.* **128**, 9346-9347 (2006). doi:10.1021/ja0632512.

259. D.M. Korzhnev, P. Neudecker, A. Zarrine-Afsar, A.R. Davidson and Lewis E. Kay, Abp1p and Fyn SH3 Domains Fold Through Similar Low-Populated Intermediate States. *Biochemistry* (Accelerated) **45**, 10175-10183 (2006). doi:10.1021/bi0611560.

260. P. Neudecker, A. Zarrine-Afsar, W.-Y. Choy, D.R. Muhandiram, A.R. Davidson and Lewis E. Kay. Identification of a Collapsed Intermediate with Non-Native Long-Range Interactions on the Folding Pathway of a Pair of Fyn SH3 Domain Mutants by NMR Relaxation Dispersion Spectroscopy. *J. Mol. Biol.* **363**, 958-976 (2006). doi:10.1016/j.jmb.2006.08.047.

261. R. Sprangers and Lewis E. Kay. Quantitative Dynamics and Binding Studies of the 20S Proteasome by NMR. *Nature*. **445**, 618-622 (2007). doi:10.1038/nature05512.

262. V. Tugarinov, R. Sprangers and Lewis E. Kay, Probing Side-Chain Dynamics in the Proteasome by Relaxation Violated Coherence Transfer NMR. *J. Am. Chem. Soc.* **129**, 1743-1750 (2007). Epub 24 Jan 2007. doi:10.1021/ja067827z.

263. D.F. Hansen and Lewis E. Kay. Improved Magnetization Alignment Schemes for Spin-Lock Relaxation Experiments. *J. Biomol. NMR*. **37**, 245-255 (2007). Epub 20 Feb 2007. doi:10.1007/s10858-006-9126-6.

264. Lewis E. Kay. The Molecular Dance of a Protein Molecule Allows a Chemist's Secret Wish to Come True. *Nature* **444**, 657 (2006). doi:10.1038/444656a.

265. A. Zhuravleva, D.M. Korzhnev, S.B. Nolde, Lewis E. Kay, A.S. Arseniev, M. Billeter and V.Y. Orekhov. Propagation of Dynamic Changes in Barnase upon Binding Barstar: An NMR and Computational Study. *J. Mol. Biol.* **367**, 1079-1092 (2007). Epub 24 Jan 2007. doi:10.1016/j.jmb.2007.01.051.

266. P. Vallurupalli, L. Scott, J.R. Williamson and Lewis E. Kay. Strong Coupling Effects During X-Pulse CPMG Experiments: Artifacts and a Simple Solution. *J Biomol. NMR* **38**, 41-46 (2007). Epub 3 Mar 2007. doi:10.1007/s10858-006-9139-1.

267. P. Lündstrom, P. Vallurupalli, T. Religa, F.W. Dahlquist and Lewis E. Kay. A Single-Quantum Methyl ^{13}C-Relaxation Dispersion Experiment with Improved Sensitivity. *J. Biomol. NMR* **38**, 79-88 (2007). Epub 27 Apr 2007. doi:10.1007/s10858-007-9149-7.

268. P. Lündstrom, K. Teilum, T. Carstensen, I. Bezsonova, S. Wiesner, D.F. Hansen, T.L. Reglia, M. Akke and Lewis E. Kay. Fractional ^{13}C Enrichment of Isolated Carbons Using [1-^{13}C]- or [2-^{13}C]-Glucose Facilitates the Accurate Measurement of Dynamics at Backbone C^{α} and Side-Chain Methyl Positions in Proteins. *J. Biomol. NMR* **38**, 199-212 (2007). Epub 7 Jun 2007. doi:10.1007/s10858-007-9158-6.

269. R. Sprangers, A. Velyvis and Lewis E. Kay. Solution NMR Studies of Supramolecular Complexes: New Insights into Function. *Nat. Methods* **4**, 697-703 (2007). Epub 30 Aug 2007. doi:10.1038/nmeth1080.

270. A. Velyvis, Y.R. Yang, H.K. Schachman and Lewis E. Kay. A Solution NMR Study Showing that Active Site Ligands and Nucleotides Directly Perturb the Allosteric Equilibrium in Aspartate Transcarbamoylase. *Proc. Natl. Acad. Sci. USA* (*Track II*), **104**, 8815-8820 (2007). Epub 14 May 2007. doi:10.1073/pnas.0703347104.

271. V. Tugarinov and Lewis E. Kay. Separating Degenerate ^{1}H Transitions in Methyl Group Probes for Single-Quantum ^{1}H-CPMG Relaxation Dispersion NMR Spectroscopy. *J. Am. Chem. Soc.* **129**, 9514-9521 (2007). Epub 12 Jul 2007. doi:10.1021/ja0726456.

272. D.F. Hansen, D. Yang, H. Feng, Z. Zhou, S. Wiesner, Y. Bai and Lewis E. Kay. An Exchange-Free Measure of ^{15}N Transverse Relaxation: An NMR Spectroscopy Application to the Study of a Folding Intermediate with Pervasive Chemical Exchange Contributions. *J. Am. Chem. Soc.* **129**, 11468-11479 (2007). Epub 28 Aug 2007. doi:10.1021/ja072717t.

273. D.M. Korzhnev, T.L. Religa, P. Lündstrom, A.R. Fersht and Lewis E. Kay. The Folding Pathway of an FF Domain: Characterization of an On-Pathway Intermediate State Under Folding Conditions by ^{15}N, ^{13}C$^{\alpha}$ and ^{13}C-Methyl Relaxation Dispersion and ^{1}H/^{2}H-exchange NMR Spectroscopy. *J. Mol. Biol.* **372**, 497-512 (2007). Epub 9 Jun 2007. doi:10.1016/j.jmb.2007.06.012.

274. J.M. Murphy, D.M. Korzhnev, D.F. Ceccarelli, A. Zarrine-Afsar, F. Sicheri, Lewis E. Kay and T. Pawson. Conformational Instability of the MARK3 UBA Domain Compromises Ubiquitin Recognition and Promotes Interaction with the Adjacent Kinase Domain. *Proc. Natl. Acad. Sci. USA* (*Track II*) **104**, 14336-14341 (2007). Epub 28 Aug 2007. doi:10.1073/pnas.0703012104.

275. P. Neudecker, A. Zarrine-Afsar, A.R. Davidson and Lewis E. Kay. Φ-Value Analysis of a Three-State Protein Folding Pathway by Relaxation Dispersion NMR Spectroscopy. *Proc. Natl. Acad. Sci. USA* (*Track II*) **104**, 15717-15722 (2007). Epub 26 Sep 2007. doi:10.1073/pnas.0705097104.

276. P. Vallurupalli, D.F. Hansen, E. Stollar, E. Meirovitch and Lewis E. Kay. Measurement of Bond Vector Orientations in Invisible Excited States of Proteins. *Proc. Natl. Acad. Sci. USA* (Track II) **104**, 18473-18477 (2007). Epub 15 Nov 2007. doi:10.1073/pnas.0708296104.

277. R. Sprangers and Lewis E. Kay. Probing SupraMolecular Structure from Measurement of Methyl ^{1}H-^{13}C Residual Dipolar Couplings. *J. Am. Chem. Soc.* **129**, 12668-12669 (2007). Epub 2 Oct 2007. doi:10.1021/ja075846i.

278. D.F. Hansen, P. Vallurupalli and Lewis E. Kay. An Improved ^{15}N Relaxation Dispersion Experiment for the Measurement of Millisecond Time-Scale Dynamics in Proteins. *J. Phys. Chem. B*. **112**, 5898-5904 (2008). Epub 15 Nov 2007. doi:10.1021/jp074793o.

279. A. Grishaev, V. Tugarinov, Lewis E. Kay, J. Trewhella and Ad Bax. Refined Solution Structure of the 82-kDa Enzyme Malate Synthase G from Joint NMR and Synchrotron SAXS Restraints. *J. Biomol. NMR* **40**, 95-106 (2008). Epub 16 Nov 2007. doi:10.1007/s10858-007-9211-5.

280. Z. Zhou, H. Feng, D.F. Hansen, E. Luk, H. Kato, D.I. Freedberg, Lewis E. Kay, C. Wu and Y. Bai. NMR Structure of Chaperone Chz1 Complexed with Histones H2A.Z-H2B. *Nat. Struct. Biol.* **15**, 868-869 (2008). Epub 20 Jul 2008. doi:10.1038/nsmb.1465.

281. D.M. Korzhnev and Lewis E. Kay. Probing Invisible, Low-Populated States of Protein Molecules by Relaxation Dispersion NMR Spectroscopy: An Application to Protein Folding. *Acc. Chem. Res.* **41**, 442-451 (2008). Epub 15 Feb 2008. doi:10.1021/ar700189y.

282. T. Mittag, S. Orlicky, W.-Y. Choy, X. Tang, H. Lin, F. Sicheri, Lewis E. Kay, M. Tyers and J.D. Forman-Kay. Dynamic Equilibrium Engagement of a Polyvalent Ligand with a Single-Site Receptor. *Proc. Natl. Acad. Sci. USA* **105**, 17772-17777 (2008). Epub 13 Nov 2008. doi:10.1073/pnas.0809222105.

283. D.F. Hansen, P. Vallurupalli, P. Lundström, P. Neudecker and Lewis. E. Kay. Probing Chemical Shifts of Invisible States of Proteins with Relaxation Dispersion NMR Spectroscopy: How Well Can We Do? *J. Am. Chem. Soc.* **130**, 2667-2675 (2008). Epub 1 Feb 2008. doi:10.1021/ja078337p.

284. P. Vallurupalli, D.F. Hansen and Lewis. E. Kay. Probing Structure in Invisible Protein States with Anisotropic NMR Chemical Shifts. *J. Am. Chem. Soc.* **130**, 2734-2735 (2008). Epub 8 Feb 2008. doi:10.1021/ja710817g.

285. D.F. Hansen, P. Vallurupalli and Lewis E. Kay. Quantifying Two-Bond ^{1}HN-^{13}CO and One-Bond $^{1}H\alpha$-$^{13}C\alpha$ Dipolar Couplings of Invisible Protein States by Spin-State Selective Relaxation Dispersion NMR Spectroscopy. *J. Am. Chem. Soc.* **130**, 8397-8405 (2008). Epub 3 Jun 2008. doi:10.1021/ja801005n.

286. M.A.S. Hass, D.F. Hansen, H.E.M. Christensen, J.J. Led and Lewis E. Kay. Characterization of Conformational Exchange of a Histidine Side Chain: Protonation, Rotamerization, and Tautomerization of His 61 in Plasotcyanin from *Anabaena variabilis*. *J. Am. Chem. Soc.* **130**, 8460-8470 (2008). 7 Jun 2008. doi:10.1021/ja801330h.

287. R. Sprangers, X. Li, X. Mao, J.L. Rubinstein, A.D. Schimmer and Lewis E. Kay. TROSY-Based NMR Evidence for a Novel Class of 20S Proteasome Inhibitor. *Biochemistry* (Accelerated) **47**, 6727-6734 (2008). Epub 10 Jun 2008. doi:10.1021/bi8005913.

288. X. Mao, X. Li, R. Sprangers, X. Wang, A. Vengopal, T. Wood, Y, Zhang, D.A. Kuntz, E. Coe, S. Trudel, D. Rose, R.A. Batey, Lewis E. Kay and A.D. Schimmer. Clioquinol Inhibits the Proteosome and Displays Preclinical Activity in Leukemia and Myeloma. *Leukemia*, **23**, 585-590 (2009). Epub 28 Aug 2008. doi:10.1038/leu.2008.232.

289. D. F. Hansen, P. Vallurupalli and Lewis E. Kay. Using Relaxation Dispersion NMR Spectroscopy to Determine Structures of Excited, Invisible Protein States. *J. Biomol. NMR*. **41**, 113-120 (2008). Epub 24 Jun 2008. doi:10.1007/s10858-008-9251-5.

290. P. Vallurupalli, D. F. Hansen and Lewis E. Kay. Structures of Invisible, Excited Protein States by Relaxation Dispersion NMR Spectroscopy. *Proc. Natl. Acad. Sci.* USA (Track II) **105**, 11766-11771 (2008). Epub 13 Aug 2008. doi:10.1073/pnas.0804221105.

291. P. Lundström, D.F. Hansen and Lewis E. Kay. Measurement of Carbonyl Chemical Shifts of Excited Protein States by Relaxation Dispersion NMR spectroscopy: Comparison Between Uniformly and Selectively ^{13}C Labeled Samples. *J. Biomol NMR* (2008) **42**, 35-47. Epub 2 Sep 2008. doi:10.1007/s10858-008-9260-4.

292. P. Fillippakopoulos, M. Kofler, O. Hantschel, G.D. Gish, F. Grebien, E. Salah, P. Neudecker, Lewis E. Kay, B.E. Turk, G. Superti-Furga, T. Pawson and S. Knapp. Structural Coupling of SH2-kinase Domains Links Fes and Abl Substrate Recognition and Kinase Activation. *Cell* **134**, 793-803 (2008). doi:10.1016/j.cell.2008.07.047.

293. P. Lundström, D.F. Hansen, P. Vallurupalli and Lewis E. Kay. Accurate Measurement of Alpha Proton Chemical Shifts of Excited Protein States by Relaxation Dispersion NMR Spectroscopy. *J. Am. Chem. Soc.* **131**, 1915-1926 (2009). Epub 11 Feb 2009. doi:10.1021/ja807796a.

294. D.M. Korzhnev, I. Bezsonova, S. Lee, T.V. Chalikian, and Lewis E. Kay. Alternate Binding Modes for a Ubiquitin-SH3 Domain Interaction Studied by NMR Spectroscopy. *J. Mol. Biol.* **386**, 391-405 (2009). Epub 6 Dec 2008. doi:10.1016/j.jmb.2008.11.055.

295. D.F. Hansen, Z. Zhou, H. Feng, L.M.M. Jenkins, Y. Bai and Lewis E. Kay. Binding Kinetics of Histone Chaperone Chz1 and Variant Histone H2A.Z-H2B by Relaxation Dispersion NMR Spectroscopy. *J. Mol. Biol.* **387**, 1-9 (2009). Doi:10.1016/j.jmb.2009.01.009.

296. P. Neudecker, P. Lundström and Lewis E. Kay. Relaxation Dispersion NMR Spectroscopy as a Tool for Detailed Studies of Protein Folding. *Biophys. J.* **96**, 2045-2054 (2009). doi:/10.1016/j.bpj.2008.12.3907.

297. A. Velyvis, H.K. Schachman and Lewis E. Kay. Application of Methyl-TROSY NMR to Test Allosteric Models Describing Effects of Nucleotide Binding to Aspartate Transcarbamoylase. *J. Mol. Biol.* **387**, 540-547 (2009). Epub 4 Feb 2009. doi:10.1016/j.jmb.2009.01.066.

298. P. Vallurupalli, D.F. Hansen, P. Lundström and Lewis E. Kay. CPMG Relaxation Dispersion NMR Experiments Measuring Glycine ^{1}H$^{\alpha}$ and ^{13}C$^{\alpha}$ Chemical Shifts in the 'Invisible'

Excited States of Proteins. *J. Biomol. NMR* **45**, 45-55 (2009). Epub 25 Mar 2009. doi:10.1007/s10858-009-9310-6.

299. P. Lundström and Lewis E. Kay. Measuring $^{13}C^{\beta}$ Chemical Shifts of Invisible Excited States in Protein by Relaxation Dispersion NMR Spectroscopy. *J. Biomol. NMR* **44**, 139-155 (2009). Epub 16 May 2009. doi:10.1007/s10858-009-9321-3.

300. D.F. Hansen, P. Vallurupalli and Lewis E. Kay. Measurement of Methyl Group Motional Parameters of Invisible, Excited Protein States by NMR Spectroscopy. *J. Am. Chem. Soc.* **131**, 12745-12754 (2009). Epub 17 Aug 2009. doi:10.1021/ja903897e.

301. T. Mittag, Lewis E. Kay and J.D. Forman-Kay. Protein Dynamics and Conformational Disorder in Molecular Recognition. *J. Mol. Recognit.* **23**, 105-116 (2010). Epub 7 Jul 2009. doi:10.1002/jmr.961.

302. H. van Ingen, D.M. Korzhnev and Lewis E. Kay. An Analysis of the Effects of $^{1}H^{N}$-$^{1}H^{N}$ Dipolar Couplings on the Measurement of Amide Bond Vector Orientations in Invisible Protein States by Relaxation Dispersion NMR. *J. Phys. Chem. B.* **113**, 9968-9977 (2009). Epub 1 July 2009. doi:10.1021/jp902793y.

303. R. Auer, P. Neudecker, D.R. Muhandiram, P. Lundström, D.F. Hansen, R. Konrat and Lewis E. Kay. Measuring the Signs of $^{1}H^{\alpha}$ Chemical Shift Differences Between Ground and Excited Protein States by Off-Resonance Spin-Lock $R_{1\rho}$ NMR Spectroscopy. *J. Am. Chem. Soc.* **131**, 10832-10833 (2009). Epub 16 Jul 2009. doi:10.1021/ja904315m.

304. A.J. Baldwin, D.F. Hansen, P. Vallurupalli and Lewis E. Kay. Measurement of Methyl Axis Orientations in Invisible, Excited States of Proteins by Relaxation Dispersion NMR Spectroscopy. *J. Am. Chem. Soc.* **131**, 11939-11948 (2009). Epub 24 Jul 2009. doi:10.1021/ja903896p.

305. P. Lundström, P. Vallurupalli, D.F. Hansen and Lewis E. Kay. Isotope Labeling Methods for Studies of Excited Protein States by Relaxation Dispersion NMR Spectroscopy. *Nat. Protoc.* **4**, 1641-1648 (2009). Epub 22 Oct 2009. doi:10.1038/nprot.2009.118.

306. J.M. Murphy, D.F. Hansen, S. Wiesner, D.R. Muhandiram, M. Borg, M.J. Smith, F. Sicheri, Lewis E. Kay, J.D. Forman-Kay and T. Pawson. Structural Studies of FF Domains of the Transcription Factor CA150 Provide Insights into the Organization of FF Domain Tandem Arrays. *J. Mol. Biol.* **393**, 409-424 (2009). Epub 26 Aug 2009. doi:10.1016/j.jmb.2009.08.049.

307. A.K. Mittermaier and Lewis E. Kay. Observing Biological Dynamics at Atomic Resolution Using NMR. *Trends Bciochem. Sci.* **34**, 601-611 (2009). Epub 19 Oct 2009. Doi:10.1016/j.tibs.2009.07.004.

308. A.J. Baldwin and Lewis E. Kay. NMR Spectroscopy Brings Invisible Protein States into Focus. *Nat. Chem. Biol.* 5, 808-814 (2009). Epub 19 Oct 2009. doi:/10.1038/nchembio.238.

309. A.M. Ruschak and Lewis E. Kay. Methyl Groups as Probes of Supra-Molecular Structure, Dynamics and Function. *J. Biomol. NMR* **46**, 75087 (2010). Epub 27 Sept 2009. doi:10.1007/s10858-009-9376-1.

310. D.F. Hansen, H. Feng, Z. Zhou, Y. Bai and Lewis E. Kay. Selective Characterization of Microsecond Motions in Proteins by NMR Relaxation. *J. Am. Chem. Soc.* **131**, 16257-16265 (2009). Epub 20 Oct 2009. doi:10.1021/ja906842s.

311. A. Velyvis, H.K. Schachman and Lewis E. Kay. Assignment of Ile, Leu, and Val Methyl Correlations in Supra-Molecular Systems: An Application to Aspartate Transcarbamoylase. *J. Am. Chem. Soc.* **131**, 16534-16543 (2009). Epub 27 Oct 2009. doi:10.1021/ja906978r.

312. F. Stengel, A.J. Baldwin, A.J. Painter, N. Jaya, E. Basha, Lewis E. Kay, E. Vierling, C.V. Robinson and J.L. Benesch. Quaternary Dynamics and Plasticity Underlie Small Heat Shock Chaperone Function. *Proc. Natl. Acad. Sci USA* (*Track II*) **107**, 2007-2012 (2010). Epub 2 Feb 2010. doi:10.1073/pnas.0910126107.

313. R. Auer, D.F. Hansen, P. Neudecker, D.M. Korzhnev, D.R. Muhandiram, R. Konrat and Lewis E. Kay. Measurement of Signs of Chemical Shift Differences Between Ground and Excited Protein States: A Comparison Between H(S/M)QC and $R_{1\rho}$ Methods. *J. Biomol. NMR* **46**, 205-216 (2010). Epub 22 Dec 2009. doi:10.1007/s10858-009-9394-z.

314. D.F. Hansen, P. Neudecker, P. Vallurupalli, F.A.A. Muder and Lewis E. Kay. Determination of Leu Side-Chain Conformations in Excited Protein States by NMR Relaxation Dispersion. *J. Am. Chem. Soc.* **132**, 42-43 (2010). Epub 11 Dec 2009. doi:10.1021/ja909294n.

315. T.L. Religa, R. Sprangers and Lewis E. Kay. Dynamic Regulation of Archaeal Proteasome Gate Opening as Studied by TROSY NMR. *Science* **328**, 98-102 (2010). doi:10.1126/science.1184991.

316. M. Dey, A. Velyvis, J.J. Li, E. Chiu, D. Chiovitti, Lewis E. Kay, F. Sicheri, and T.E. Dever. Requirement for Kinase-Induced Conformational Change in Eukaryotic Initiation Factor 2α (eIF2α) Restricts Phosphorylation of Ser51. *Proc. Natl. Acad. Sci. USA* **108**, 4316-4321 (2011). Epub 28 Feb 2011. doi:10.1073/pnas.1014872108.

317. Lewis E. Kay. Structure and Dynamics of Proteins: Big and Small. *eMagRes*. Epub 15 Sep 2010. doi:10.1002/9780470034590.emrhp1027.

318. T.L. Religa and Lewis E. Kay. Optimal Methyl Labeling for Studies of Supra-Molecular Systems. *J. Biomol. NMR* **47**, 163-169 (2010). Epub 27 Apr 2010. doi:10.1007/s10858-010-9419-7.

319. G. Bouvignies, D.M. Korznev, P. Neudecker, D.F. Hansen, M.H.J. Cordes and Lewis E. Kay. A Simple Method for Measuring Signs of $^{1}H^{N}$ Chemical Shift Differences Between Ground and Excited Protein States. *J. Biomol. NMR* **47**, 135-141 (2010). Epub 29 Apr 2010. doi:10.1007/s10858-010-9418-8.

320. D.F. Hansen, P. Neudecker and Lewis E. Kay. Determination of Isoleucine Side-Chain Conformations in Ground and Excited States of Proteins from Chemical Shifts. *J. Am. Chem. Soc.* **132**, 7589-7591 (2010). Epub 13 May 2010. doi:10.1021/ja102090z.

321. A.M. Ruschak, T.L. Religa, S. Breuer, S. Witt and Lewis E. Kay. The Proteasome Antechamber Maintains Substrates in an Unfolded State. *Nature* **467**, 868-871 (2010). Epub 13 Oct 2010. doi:10.1038/nature09444.

322. D.M. Korzhnev, T.L. Religa, W.J. Banachewicz, A.R. Fersht and Lewis E. Kay. A Transient and Low-Populated Protein-Folding Intermediate at Atomic Resolution. *Science* **329**, 1311-1316 (2010). doi:10.1126/science.1191723.

323. X. Li, T.E. Wood, R. Sprangers, G. Jansen, N.E. Franke, X. Mao, X. Wang, Y. Zhang, S.E. Verbrugge, H. Adomat, Z. Li, S. Trudel, C. Chen, T.L. Religa, N. Jamal, H. Messner, J. Cloos, D.R. Rose, A. Navon, R.a. Batey, Lewis E. Kay and A.D. Schimmer. Effect of Noncompetitive Proteasome Inhibition Bortezomib Resistance. *J. Natl. Cancer Inst.* **102**, 1069-1082 (2010). Epub 26 May 2010. doi:10.1093/jnci/djq198.

324. A.J. Baldwin, T.L. Religa, D.F. Hansen, G. Bouvignies and Lewis E. Kay. $^{13}CHD_2$ Methyl Group Probes of Millisecond Time Scale Exchange in Proteins by ^{1}H Relaxation Dispersion: An Application to Proteasome Gating Residue Dynamics. *J. Am. Chem. Soc.* **132**, 10992-10995 (2010). Epub 23 Jul 2010. doi:10.1021/ja104578n.

325. A.M. Ruschak, A. Velyvis and Lewis E. Kay. A Simple Strategy for $^{13}C,^{1}H$ Labeling at the Ilg-γ2 Methyl Position in Highly Deuterated Proteins. *J. Biomol. NMR* **48**, 129-135 (2010). Epub 14 Oct 2010. Doi:10.1007/s10858-010-9449-1.

326. E. Kupče, Lewis E. Kay and R. Freeman. Detecting the "Afterglow" of ^{13}C NMR in Proteins Using Multiple Receivers. *J. Am. Chem. Soc.* **132**, 18008-18011 (2010). Epub 2 Dec 2010. doi:10.1021/ja1080025.

327. A.M. Ruschak, M. Slassi, Lewis E. Kay and A.D. Schimmer. Novel Proteasome Inhibitors to Overcome Bortezomib Resistance. *J. Natl. Cancer Inst.* **103**, 1007-1017 (2011). Epub 23 May 2011. doi:10.1093/jnci/djr160.

328. G. Bouvignies, D.F. Hansen, P. Vallurupalli and Lewis E. Kay. Divided-Evolution-Based Pulse Scheme for Quantifying Exchange Processes in Proteins: Powerful Complement to Relaxation Dispersion Experiments. *J. Am. Chem. Soc.* **133**, 1935-1945 (2011). Epub 18 Jan 2011. doi:10.1021/ja109589y.

329. G. Bouvignies, P. Vallurupalli, M.H.J. Cordes, D.F. Hansen and Lewis E. Kay. Measuring $^{1}H^{N}$ Temperature Coefficients in Invisible Protein States by Relaxation Dispersion NMR Spectroscopy. *J. Biomol. NMR* **50**, 13-18 (2011). Epub 18 Mar 2011. doi:10.1007/s10858-011-9498-0.

330. A.J. Baldwin, H. Lioe, C.V. Robinson, Lewis E. Kay and J.L.P. Benesch. αB-Crystallin Polydispersity is a Consequence of Quaternary Dynamics. *J. Mol. Biol.* **413**, 297-309 (2011). Epub 3 Aug 2011. doi:10.1016/j.jmb.2011.07.016.

331. A.J. Baldwin, G.R. Hilton, H. Lioe, C. Bagnéris, J.L.P. Benesch and Lewis E. Kay. Quaternary Dynamics of αB-Crystallin as a Direct Consequence of Local Fluctuations in the C-Terminus. *J. Mol. Biol.* **413**, 310-320 (2011). Epub 3 Aug 2011. doi:10.1016/j.jmb.2011.07.017.

332. H. Kato, H. van Ingen, B.-R. Zhou, H. Feng, M. Bustin, Lewis E. Kay and Y. Bai. Architecture of the High Mobility Group Nucleosomal Protein 2-Nucleosome Complex as Revealed Methyl-Based NMR. *Proc. Natl. Acad. Sci.* **10**8, 12283-12288 (2011). Epub 5 Jul 2011. doi:10.1073/pnas.1105848108.

333. Lewis E. Kay. Solution NMR Spectroscopy of Supra-Molecular Systems, Why Bother? A Methyl-TORSY View. *J. Magn. Reson.* **210**, 159-170 (2011). Epub 8 Mar 2011. doi:10.1016/j.jmr.2011.03.008.

334. D.M. Korzhnev, R.M. Vernon, T.L. Religa, A.L. Hansen, D. Baker, A.R. Fersht and Lewis E. Kay. Nonnative Interactions in the FF Domain Folding Pathway from an Atomic Resolution Structure of a Sparsely Populated Intermediate An NMR Relaxation Dispersion Study. *J. Am. Chem. Soc.* **133**, 10974-10982 (2011). Epub 28 Jun 2011. doi:10.1021/ja203686t.

335. D.F. Hansen and Lewis E. Kay. Determining Valine Side-Chain Rotamer Conformations in Protein from Methyl ^{13}C Chemical Shifts: Application to the 360 kDa Half-Proteasome. *J. Am. Chem. Soc.* **133**, 8272-8281 (2011). Epub 5 May 2011. doi:10.1021/ja2014532.

336. G. Bouvignies, P. Vallurupalli, D.F. Hansen, B.E. Correia, O. Lange, A. Bah, R.M. Vernon, F.W. Dahlquist, D. Baker and Lewis E. Kay. Solution Structure of a Minor and Transiently Formed State of a T4 Lysozyme Mutant. *Nature* **477**, 111-114 (2011). Epub 21 Aug 2021. doi:10.1038/nature10349.

337. T.L. Religa, A.M. Ruschak, R. Rosenzweig and Lewis E. Kay. Site-Directed Methyl Group Labeling as a Probe of Structure and Dynamics in Supramolecular Protein Systems: Applications to the Proteasome and to the ClpP Protease. *J. Am. Chem. Soc.* **133**, 9063-9068 (2011). Epub 20 May 2011. doi:10.1021/ja202259a.

338. A.L. Hansen and Lewis E. Kay. Quantifying Millisecond Time-Scale Exchange in Proteins by CPMG Relaxation Dispersion Spectroscopy of Side-Chain Carbonyl Groups. *J. Biomol. NMR* **50**, 347-355 (2011). Epub 18 Jun 2011. doi:10.1007/s10858-011-9520-6.

339. Lewis E. Kay. NMR Studies of Protein Structure and Dynamics – A Look Backwards and Forwards. *J. Magn. Reson.* **213**, 492-494 (2011). Epub 31 Aug 2011. doi:10.1016/j.jmr.2011.08.010.

340. A.J. Baldwin, H. Lioe, G.R. Hilton, L.A. Baker, J.L. Rubinstein, Lewis E. Kay and J.L.P. Benesch. The Polydispersity of αB-Crystallin is Rationalized by an Interconverting Polyhedral Architecture. *Structure* **19**, 1855-1863 (2011). doi:10.1016/j.str.2011.09.015.

341. P. Vallurupalli, G. Bouvignies and Lewis E. Kay. Increasing the Exchange Time-Scale that can be Probed by CPMG Relaxation Dispersion NMR. *J. Phys. Chem. B* **115**, 14891-14900 (2011). Epub 11 Nov 2011. doi:10.1021/jp209610v.

342. J. Barette, A.Velyvis, T.L. Religa, D.M. Korzhnev and Lewis E. Kay. Cross-Validation of the Structure of a Transiently Formed and Low Populated FF Domain Folding Intermediate Determined by Relaxation Dispersion NMR and CS-Rosetta. *J. Phys. Chem B* **116**, 6637-6644 (2012). Epub 23 Dec 2011. doi:10.1021/jp209974f.

343. Lewis E. Kay. The Importance of Dynamics in Structural Biology. *Nat. Struct. Mol. Biol.* **18**, 1308 (2011). Epub 5 Dec 2011. doi:10.1038/nsmb1211-1304.

344. H. Sun, Lewis E. Kay and V. Turgarinov. An Optimized Relaxation-Based Coherence Transfer NMR Experiment for the Measurement of Side-Chain Order in Methyl-Protonated, Highly Deuterated Proteins. *J. Phys. Chem. B* **115**, 14878-14884 (2011). Epub 15 Nov 2011. doi:10.1021/jp209049k.

345. A.L. Hansen, P. Lundström, A. Velyvis and Lewis E. Kay. Quantifying Millisecond Exchange Dynamics in Protein by CPMG Relaxation Dispersion NMR Using Side-Chain ^{1}H Probes. *J. Am. Chem. Soc.* **134**, 3178-3189 (2012). Epub 2 Feb 2012. doi:10.1021/ja210711v.

346. P. Neudecker, P. Robustelli, A. Cavalli, P. Walsh, P. Lundström, A. Zarrine-Afsar, S. Sharpe, M. Vendruscolo and Lewis E. Kay. Structure of an Intermediate State in Protein Folding and Aggregation. *Science* **336**, 362-366 (2012). doi:10.1126/science.1214203.

347. A.J. Baldwin and Lewis E. Kay. Measurement of the Signs of methyl ^{13}C Chemical Shift Differences between Interconverting Ground and Excited Protein States by $R_{1\rho}$: An Application to αB-Crystallin. *J. Biomol. NMR* **53**, 1-12 (2012). Epub 5 Apr 2012. doi:10.1007/s10858-012-9617-6.

348. P. Vallurupalli, G. Bouvignies and Lewis E. Kay. Studying "Invisible" Excited Protein States in Slow Exchange with a Major State Conformation. *J. Am. Chem. Soc.* **134**, 8148-8161 (2012). Epub 3 May 2012. doi:10.1021/ja3001419.

349. D.M. Korzhnev, T.L. Religa and Lewis E. Kay. A Transiently Populated Intermediate Functions as a Branching Point of the FF Domain Folding Pathway. *Proc. Natl. Acad. Sci. USA* **109**, 17777-17782 (2012). Epub 30 May 2012. doi:10.1073/pnas.1201799109.

350. G. Bouvignies and Lewis E. Kay. A 2D ^{13}C-CEST Experiment for Studying Slowly Exchanging Protein Systems Using Methyl Probes: An Application to Protein Folding. *J. Biomol. NMR* **53**, 303-310 (2012). Epub 12 Jun 2012. doi:10.1007/s10858-012-9640-7.

351. A.J. Baldwin, P. Walsh, D.F. Hansen, G. Hilton, J.L.P. Benesch, S. Sharpe and Lewis E. Kay. Probing Dynamic Conformations of the High Molecular Weight αB-Crystallin Heat Shock Protein Ensemble by NMR Spectroscopy. *J. Am. Chem. Soc.* **134**, 15343-50 (2012). Epub 7 Sep 2012. doi:10.1021/ja307874r.

352. E. Kupče and Lewis E. Kay. Parallel Acquisition of Multi-Dimensional Spectra in Protein NMR. *J. Biomol. NMR* **54**, 1-7 (2012). Epub 17 Jul 2012. doi:10.1007/s10858-012-9646-1.

353. A.J. Baldwin and Lewis E. Kay. Structural Biology: Dynamic Binding. *Nature* **488**, 165-166 (2012). Epub 8 Aug 2012. doi:10.1038/488165a.

354. J.L. Markley et al. In Support of the BMRB. *Nat. Struct. Mol. Biol.* **19**, 854-860 (2012).

355. A. Velyvis, A.M. Ruschak and Lewis E. Kay. An Economical Method for Production of $^{2}H,^{13}CH_3$-Threonine for Solution NMR Studies of Large Protein Complexes: Application to the 670 kDa Proteasome. *PloS One* **7**, e43725 (2012). Epub 11 Sept 2012. doi:/10.1371/journal.pone.0043725.

356. A. Sekhar, P. Vallurupalli and Lewis E. Kay. Folding of the Four-Helix Bundle FF Domain from a Compact On-Pathway Intermediate State is Governed Predominantly by Water Motion. *Proc. Natl. Acad. Sci. USA* **109**, 19268-19273 (2012). 5 Nov 2012. doi:10.1073/pnas.1212036109.

357. A.J. Baldwin and Lewis E. Kay. An $R_{1\rho}$ Expression for a Spin in Chemical Exchange between Two Sites with Unequal Transverse Relaxation Rates. *J. Biomol. NMR* **55**, 211-218 (2013). Epub 23 Jan 2013. doi:10.1007/s10858-012-9694-6.

358. A.M. Ruschak and Lewis E. Kay. Proteasome Allostery as a Population Shift between Interchanging Conformers. *Proc. Natl. Acad. Sci. USA* **109**, E3454-3462. Epub 12 Nov 2012. doi:10.1073/pnas.1213640109 (2012).

359. M.P. Latham and Lewis E. Kay. Is Buffer a Good Proxy for a Crowded Cell-Like Environment? A Comparative Study of Calmodulin Side-Chain Dynamics in Buffer and *E. coli* Lysate. *Plos One* **7**, e48226 (2012). Epub 30 Oct 2012. doi:10.1371/journal.pone.0048226.

360. G. Bouvignies and Lewis E. Kay. Measurement of Proton Chemical Shifts in Invisible States of Slowly Exchanging Protein Systems by Chemical Exchange Saturation Transfer. *J. Phys. Chem. B* **116**, 14311-14317 (2012). Epub 29 Nov 2012. doi:10.1021/jp311109u.

361. A. Mainz, T.L. Religa, R. Sprangers, R. Linser, Lewis E. Kay and B. Rief. NMR Spectroscopy of Soluble Protein Complexes at One Mega-Dalton and Beyond. *Angew. Chem. Int. Ed. Engl.* **52**, 8746-8751 (2013). Epub 19 Jul 2013. doi:10.1002/anie.201301215.

362. M.P. Latham and Lewis E. Kay, Probing Non-Specific Interactions of Ca^{2+}-Calmodulin in *E. coli* Lysate. *J. Biomol. NMR* **55**, 211-218 (2013). Epub 17 Jan 2013. doi:10.1007/s10858-013-9705-2.

363. A.L. Hansen, G. Bouvignies and Lewis E. Kay. Probing Slowly Exchanging Protein Systems via $^{13}C^{\alpha}$-CEST: Monitoring Folding of the Im7 Protein. *J. Biomol. NMR* **55**, 279-289 (2013). Epub 6 Feb 2013. doi:10.1007/s10858-013-9711-4.

364. P. Vallurupalli and Lewis E. Kay. Probing Slow Chemical Exchange at Carbonyl Sites in Proteins via Chemical exchange Saturation Transfer NMR Spectroscopy. *Angew. Chem. Int. Ed. Eng.* **52**, 4156-4159 (2013). Epub 28 Feb 2013. doi:10.1002/anie.201209118.

365. M.T. Mazhab-Jafari, C.B. Marshall, P.B. Stathopulos, Y. Kobashigawa, V. Stambolic, Lewis E. Kay, F. Inagaki and M. Ikura. Membrane-Dependent Modulation of the mTOR Activator Rheb: NMR Observations of a GTPase Tethered to a Lipid-Bilayer Nanodisc. J. *Am. Chem. Soc.* **135**, 3367-3370 (2013). Epub 20 Feb 2013. doi:10.1021/ja312508w.

366. R. Rosenzweig, S. Moradi, A. Zarrine-Afsar, J.R. Glover and Lewis E. Kay. Unraveling the Mechanism of Protein Disaggregation Through ClpB-DnaK Interaction. *Science* **339**, 1080-1083 (2013). Epub 7 Feb 2013. doi:10.1126/science.1233066.

367. V. Tugarinov and Lewis E. Kay. Estimating Side-Chain Order in [U-^{2}H;$^{13}CH_3$]-Labeled High Molecular Weight Proteins from Analysis of HMQC/HSQC Spectra. *J. Phys. Chem. B* **117**, 3571-3577 (2013). Epub 25 Mar 2013. doi:10.1021/jp401088c.

368. A. Sekhar, P. Vallurupalli and Lewis E. Kay. Defining a Length Scale for Millisecond-Timescale Protein Conformational Exchange. *Proc. Natl. Acad. Sci. USA* **110**, 11391-11396 (2013). Epub 25 Jun 2013. doi:10.1073/pnas.1303273110.

369 A. Sekhar and Lewis E. Kay. NMR Paves the Way for Atomic Level Descriptions of Sparsely Populated, Transiently Formed Biomolecular Conformers. *Proc. Natl. Acad. Sci. USA* **110**, 12867-12874 (2013). Epub 18 Jul 2013. doi:10.1073/pnas.1305688110.

370. A. Velyvis and Lewis E. Kay. Measurement of Active Site Ionization Equilibria in the 670 kDa Proteasome Core Particle Using Methyl-TROSY NMR. *J. Am. Chem. Soc.* **135**, 9259-9262 (2013). Epub 2 May 2013. doi:10.1021/ja403091c.

371. P. Vallurupalli, G. Bouvignies and Lewis E. Kay. A Computational Study of the Effects of ^{13}C-^{13}C Scalar Couplings on ^{13}C CEST NMR Spectra: Towards Studies on a Uniformly ^{13}C-Labeled Protein. *Chembiochem* **14**, 1709-1713 (2013). Epub 19 Jun 2013. doi:10.1002/cbic.201300230.

372. G. Bouvignies, P. Vallurupalli and Lewis E. Kay. Visualizing Side Chains of Invisible Protein Conformers by Solution NMR. *J. Mol. Biol.* **426**, 763-774 (2014). Epub 8 Nov 2013. doi:10.1016/j.jmb.2013.10.041.

373. D. Long, C.B. Marshall, G. Bouvignies. M.T. Mazhab-Jafari, M.J. Smith, M. Ikura and Lewis E. Kay. A Comparative CEST NMR Study of Slow Conformational Dynamics of Small GTPases Complexed with GTP and GTP Analogues. *Angew. Chem. Int. Ed. Engl.* **52**, 10771-10774 (2013). Epub 22 Aug 2013. doi:10.1002/anie.201305434.

374. C.L. Pocanschi, S. Ehsani, M. Mehrabian, H. Wille, W. Reginold, W.S. Trimble, H. Wang, A. Yee, C.H. Arrowsmith, Z. Bozóky, Lewis E. Kay, J.D. Forman-Kay, J.M. Rini and G. Schmitt-Ulms. The ZIP5 Ectodomain Co-Localizes with PrP and May Acquire a Prp-Like Fold That Assembles into a Dimer. *Plos One* **8**, e72446 (2013). Epub 6 Sep (2013). doi:10.1371/journal.pone.0072446.

375. R. Rosenzweig and Lewis E. Kay. Bringing Dynamic Molecular Machines into Focus by Methyl-TROSY NMR. *Annu. Rev. Biochem.* **83**, 291-315 (2014). doi:10.1146/annurev-biochem-060713-035829.

376. L. Shi and Lewis E. Kay. Tracing an Allosteric Pathway Regulating the Activity of the HslV Protease. *Proc. Nat. Acad. Sci. USA* **111**, 2140-2145 (2014). 27 Jan 2014. doi:10.1073/pnas.1318476111.

377. X. Wang, P. Vallurupalli, A. Vu, K. Lee, S. Sun, W.-J. Bai, C. Wu, H. Zhou, J. Shea, Lewis E. Kay and F. W. Dahlquist. The Linker Between the Dimerization and Catalytic Domains of the CheA Histidine Kinase Propagates Changes in Structure and Dynamics That are Important for Enzymatic Activity. *Biochemistry* **53**, 855-861 (2014). Epub 28 Jan 2014. doi:10.1021/bi4012379.

378. M.P. Latham, A. Sekhar and Lewis E. Kay. Understanding the Mechanism of Proteasome 20S Core Particle Gating. *Proc. Natl. Acad. Sci. USA* **111**, 5532-5537 (2014). Epub 31 Mar 2014. doi:10.1073/pnas.1322079111.

379. A. Sekhar, M.P. Latham, P. Vallurupalli and Lewis E. Kay. Viscosity-Dependent Kinetics of Protein Conformational Exchange: Microviscosity Effects and the Need for a Small Viscogen. *J. Phys. Chem. B* **118**, 4546-4551 (2014). Epub 18 Apr 2014. doi:10.1021/jp501583t.

380. L. E. Kay and L. Frydman. A Special "JMR" Perspectives Issue: Foresights in Biomolecular Solution-State NMR Spectroscopy: From Spin Gymnastics to Structure and Dynamics. *J. Magn. Reson.* **241**, 1-2 (2014). doi:10.1016/j.jmr.2014.01.010.

381. A.L. Hansen and Lewis E. Kay. Measurement of Histidine pKa values and Tautomer Populations in Invisible Protein States. *Proc. Natl. Acad. Sci. USA* **111**, E1705-1712 (2014), Epub 14 Apr 2014. doi:10.1073/pnas.1400577111.

382. C. Sanchez-Medina, A. Sekhar, P. Vallurupalli, M. Cerminara, V. Muñoz and Lewis E. Kay. Probing the Free Energy Landscape of the Fast-Folding gpW Protein by Relaxation Dispersion NMR. *J. Am. Chem. Soc.* **136**, 7444-7451 (2014). Epub 8 May 2014. doi:10.1021/ja502705y.

383. D. Long, G. Bouvignies and Lewis E. Kay. Measuring Hydrogen Exchange Rates in Invisible Protein Excited States. *Proc. Natl. Acad. Sci. U S A.* **111**, 8820-8825 (2014). Epub 2 Jun 2014. doi:10.1073/pnas.140501111.

384. A. Bah, R.M. Vernon, Z. Siddiqui, M. Krzeminski, R. Muhandiram, C. Zhao , N. Sonenberg, Lewis E. Kay and J.D. Forman-Kay. Folding of an Intrinsically Disordered Protein

by Phosphorylation as a Regulatory Switch. *Nature* **519**, 106-109 (2015). Epub 22 Dec 2014. doi10.1038/nature13999.

385. M.P. Latham and Lewis E. Kay. A Similar *In Vitro* and In Cell Lysate Folding Intermediate for the FF Domain. *J. Mol. Biol.* **426**, 3214-3220 (2014). Epub 30 Jul 2014. doi10.1016/j.jmb.2014.07.019.

386. D. Long, A. Sekhar and Lewis E. Kay. Triple Resonance-Based $^{13}C^{\alpha}$ and $^{13}C^{\beta}$ CEST Experiments for Studies of ms Timescale Dynamics in Proteins. *J. Biomol. NMR* **60**, 203-208 (2014). Epub 28 Oct 2014. doi:10.1007/s10858-014-9868-5.

387. M.T. Mazhab-Jafari, C.B. Marshall, M.J. Smith, G.M.C. Gasmi-Seabrook, P.B. Stathopoulos, F. Inagaki, Lewis E. Kay, B.G. Neel, and M Ikura. Oncogenic and RASopathy-Associated K-RAS Mutations Relieve a Membrane-Dependent Occlusion of the Effector-Binding Site. *Proc. Natl. Acad. Sci USA*. **112**, 6625-6630 (2015). Epub 4 May 2015. doi:10.1073/pnas.1419895112.

388. A. Ahlner, C. Andresen, S.N. Khan, Lewis E. Kay and P. Lundström. Fractional Enrichment of Proteins using [2-^{13}C]-glycerol as the Carbon Source Facilitates Measurement of Excited State $^{13}C\alpha$ Chemical Shifts with Improved Sensitivity. *J. Biomol. NMR* **62**, 341-351 (2015). 20 May 2015. doi:10.1007/s10858-015-9948-1.

389. A. Sekhar, J.A.O. Rumfeldt, H.R. Broom, C.M. Doyle, G. Bouvignies, E.M. Meiering and Lewis E. Kay. Thermal Fluctuations of Immature SOD1 Lead to Separate Folding and Misfolding Pathways. *Elife* **4**, e07296 (2015). Epub 23 Jun 2015. doi:10.7554/eLife.07296.

390. D. Long, F. Delaglio, A. Sekhar and Lewis E. Kay. Probing Invisible, Excited Protein States by Non-Uniformly Sampled Pseudo-4D CEST Spectroscopy. *Angew. Chem. Int. Ed. Engl.* **54**, 10507-10511 (2015). Epub 15 Jul 2015. doi:10.1002/anie.201504070.

391. A. Sekhar, R. Rosenzweig, G. Bouvignies and Lewis E. Kay. Mapping the Conformation of a Client Protein through the Hsp70 Functional Cycle. *Proc. Natl. Acad. Sci. USA*. **112**, 10395-103400 (2015). Epub 3 Aug 2015.doi:10.1073/pnas.1508504112.

392. A. Sekhar, A.D. Bain, J.A.O. Rumfeldt, E.M. Meiering and Lewis E. Kay. Evolution of Magnetization Due to Asymmetric Dimerization: Theoretical Considerations and Application to Aberrant Oligomers Formed by apoSOD1^{2SH}. *Phys Chem. Chem. Phys*. **18**, 5720-5728 (2016). Epub 9 Jul 2015. doi:10.1039/c5cp03044g.

393. Z. Wang, P. Dove, A. Shamas-Din, Z. Li, A. Nachman, Y.J. Oh, R. Hurren, A. Ruschak, S. Climie, B. Press, C. Griffin, E. Undzys, A. Aman, R. Al-awar, Lewis E. Kay, D. O'Neill, S. Trudel, M. Slassi and A.D. Schimmer. FV-162 is a Novel, Orally Bioavailable, Irreversible Proteasome Inhibitor with Improved Pharmacokinetics Displaying Preclinical Efficacy with Continuous Daily Dosing. *Cell Death Dis.* 2015 **6**, e1815 (2015). Epub 9 Jul 2015. doi:10.1038/cddis.2015.187.

394. R. Rosenzweig, P. Farber, A. Veylvis, E. Rennella, M.P. Latham and Lewis E. Kay. The ClpB N-Terminal Domain Plays a Regulatory Role in Protein Disaggregation. *Proc. Natl. Acad. Sci. USA* **112**, E6872-E6881 (2015). Epub 30 Nov 2015. doi:10.1073/pnas.1512783112.

395. E. Rennella, R. Huang, A. Velyvis and Lewis E. Kay. $^{13}CHD_2$-CEST NMR Spectroscopy Provides an Avenue for Studies of Conformational Exchange in High Molecular Weight Proteins. *J. Biomol. NMR* **63**,187-199 (2015). Epub 14 Aug 2015. doi:10.1007/s10858-015-9974-z.

396. Lewis E. Kay. New Views of Functionally Dynamic Proteins by Solution NMR Spectroscopy. *J. Mol. Biol.* **428**, 323-331 (2016). Epub 19 Dec 2015. doi:10.1016/j.jmb.2015.11.028.

397. P. Vallurupalli, N. Chakrabarti, R. Pomès and Lewis E. Kay. Atomistic Picture of Conformational Exchange in a T4 Lysozyme Cavity Mutant: An Experiment-Guided Molecular Dynamics Study. *Chem. Sci.* **7**, 3602-3613 (2016). Epub 7 Jan 2016. doi:10.1039/c5sc03886c.

398. R. Rosenzweig and Lewis E. Kay. NMR Spectroscopy Provides an Avenue for the Study of Functionally Dynamic Molecular Machines: The Example of Protein Disaggregation. *J. Am. Chem. Soc.* **138**, 1466-1477 (2016). Epub 29 Dec 2015. doi:10.1021/jacs.5b11346.

399. C.M. Doyle, J.A. Rumfeldt, H.R. Broom, A. Sekhar, Lewis E. Kay and E.M. Meiering. Concurrent Increases and Decreases in Local Stability and Conformational Heterogeneity in Cu, Zn Superoxide Dismutase Variants Revealed by Temperature-Dependence of Amide Chemical Shifts. *Biochemistry* **55**, 1346-61 (2016). Epub 22 Feb 2016. doi:10.1021/acs.biochem.5b01133.

400. A. Sekhar, R. Rosenzweig, G. Bouvignies and Lewis E. Kay. Hsp70 Biases the Folding Pathways of Client Proteins. *Proc. Natl. Acad. Sci. USA* **113**, E2794-E2801 (2016). Epub 2 May 2016. doi:10.1073/pnas.1601846113.

401. S.W.S. Chan, J. Yau, C. Ing, K. Liu, P. Farber, A. Won, V. Bhandari, N. Kara-Yacoubian, T.V. Seraphim, N. Chakrabarti, Lewis E. Kay, C. Yip, R. Pomès, S. Sharpe and W.A. Houry. Mechanism of Amyloidogenesis of a Bacterial AAA+ Chaperone. *Structure* **24**, 1095-1109 (2016). Epub 2 Jun 2016. doi:10.1016/j.str.2016.05.002.

402. R. Huang, Z.A. Ripstein, R. Augustyniak, M. Laznieswki, K. Ginalski, Lewis E. Kay and J.L. Rubinstein. Unfolding the Mechanism of the AAA+ Unfoldase VAT by a Combined Cryo-EM, Solution NMR Study. *Proc. Natl. Acad. Sci. USA* **113**, E4190-4199 (2016). Epub 11 Jul 2016. doi:10.1073/pnas.1603980113.

403. E. Rennella, A.K. Schuetz and Lewis E. Kay. Quantitative Measurement of Exchange Dynamics in Proteins via ^{13}C Relaxation Dispersion of $^{13}CHD_2$-Labeled Samples. *J. Biomol. NMR* **65**, 59-64 (2016). Epub 1 Jun 2016. doi:10.1007/s10858-016-0038-9.

404. A.N. Borkar, P. Vallurupalli, C. Camilloni, Lewis E. Kay and M. Vendruscolo. Simultaneous NMR Characterization of Multiple Minima in the Free Energy Landscape of the

RNA UUCG Tetraloop. *Phys. Chem. Chem. Phys.* **19**, 2797-2804 (2017). Epub 20 Dec 2016. doi:10.1039/c6cp08313g.

405. T. Yuwen, A. Sekhar and Lewis E. Kay. Evaluating the Influence of Initial Magnetization Conditions on Extracted Exchange Parameters in NMR Relaxation Experiments: Applications to CPMG and CEST. *J. Biomol. NMR* **65**, 143-156 (2016). Epub 29 Jul 2016. doi:10.1007/s10858-016-0045-x.

406. A.K. Schutz and Lewis E. Kay. A Dynamic Molecular Basis for Malfunction in Disease Mutations of p97/VCP. *Elife* **5**, e20143 (2016). Epub 9 Nov 2016. doi:10.7554/eLife.20143.

407. T. Yuwen, P. Vallurupalli and Lewis E. Kay. Enhancing the Sensitivity of CPMG Relaxation Dispersion to Conformational Exchange Processes via Multiple-Quantum Spectroscopy. *Angew. Chem. Int. Ed. Engl.* **55**, 11490-11494 (2016). Epub 16 Aug 2016. doi:10.1002/anie.201605843.

408. A Sekhar, J.A.O. Rumfeldt, H.R. Broom, C.M. Doyle, R.E. Sobering, E.M. Meiering and Lewis E. Kay. Probing the Free Energy Landscapes of ALS Disease Mutants of SOD1 by NMR Spectroscopy. *Proc. Natl. Acad. Sci. USA* **113**, E6939-E6945 (2016). Epu 24 Oct 2016. doi:10.1073/pnas.1611418113.

409. T. Yuwen, A. Sekhar and Lewis E. Kay. Separating Dipolar and Chemical Exchange Magnetization Transfer in ^{1}H-CEST. *Angew. Chem. Int. Ed. Engl.* **56***,* 6122-6125 (2016). Epub 30 Dec 2016. doi:10.1002/anie.201610759.

410. E. Rennella, A. Sekhar and Lewis E. Kay. Self-Assembly of Human Profilin-1 Detected by Carr-Purcell-Meiboom-Gill Nuclear Magnetic Resonance (CPMG NMR) Spectroscopy. *Biochemistry* **56**, 692-703 (2017). Epub 20 Jan 2017. doi:10.1021/acs.biochem.6b01263

411. P. Vallurupalli, A. Sekhar, T. Yuwen and Lewis E. Kay. Probing Conformational Dynamics in Biomolecules via Chemical Exchange Saturation Transfer: A Primer. *J. Biomol. NMR* **67**, 243-271 (2017). Epub 19 Mar 2017. doi:10.1007/s10858-017-0099-4.

412. J. Kitevski-LeBlanc, A. Fradet-Turcotte, P. Kukic, M.D. Wilson, G. Portella, T. Yuwen, S. Panier, S. Duan, M.D. Canny, H. van Ingen, C.H. Arrowsmith, J.L. Rubinstein, M. Vendruscolo, D. Durocher and Lewis E. Kay. The RNF168 Paralog RNF169 Defines a New Class of Ubiquitylated Histone Reader Involved in the Response to DNA Damage. *Elife* **6**, e23872. Epub 13 Apr 2017. doi:10.7554/eLife.23872.

413. T. Yuwen and Lewis E. Kay. Longitudinal Relaxation Optimized ^{1}H-CEST Experiments for Studying Slow Chemical Exchange Processes in Fully Protonated Proteins. *J. Biomol. NMR* **67**, 295-307 (2017). Epub 29 Mar 2017. doi:10.1007/s10858-017-0104-y.

414. T. Yuwen, R. Huang and Lewis E. Kay. Probing Slow Timescale Dynamics in Proteins Using Methyl ^{1}H-CEST. *J Biomol. NMR* **68**, 215-224 (2017). Epub 24 Jun 2017. doi:10.1007/s10858-017-0121-x.

415. Z.A. Ripstein, R. Huang, R. Augustyniak, Lewis E. Kay and J.L. Rubinstein. Structure of a AAA+ Unfoldase in the Process of Unfolding Substrate. *Elife* **6**, e25754. Epub 8 Apr 2017. doi:10.7554/eLife.25754.

416. A. Malevanets, P.A. Chong, D.F. Hansen, P. Rizk, Y. Sun, H. Lin, R. Muhandiram, A. Chakrabartty, Lewis E. Kay, J. D. Forman-Kay and S.J. Wodak. Interplay of Buried Histidine Protonation and Protein Stability in Prion Misfolding. *Sci. Rep.* 2017 **7**, 882. Epub 13 Apr 2017. doi:10.1038/s41598-017-00954-7.

417. M. Chojnacki, W. Mansour, D.S. Hameed, R.K. Singh, F. El Oualid, R. Rosenzweig, M.A. Nakasone, Z. Yu, F. Glaser, Lewis E. Kay, D, Fushman, H. Ovaa and M.H. Glickman. Polyubiquitin-Photoactivatable Crosslinking Reagents for Mapping Ubiquitin Interactome Identify Rpn1 as a Proteasome Ubiquitin-Associating Subunit. *Cell Chem. Biol.* **24**, 443-457 (2017). Epub 16 Mar 2017. doi:10.1016/j.chembiol.2017.02.013.

418. R. Rosenzweig, A. Sekhar, J. Nagesh and Lewis E. Kay. Promiscuous Binding by Hsp70 Results in Conformational Heterogeneity and Fuzzy Chaperone-Substrate Ensembles. *Elife* **6**, e28030 (2017). Epub 14 Jul 2017. doi:10.7554/eLife.28030.

419. R. Huang, J.P. Brady, A. Sekhar, T. Yuwen and Lewis E. Kay. An Enhanced Sensitivity Methyl ^{1}H Triple-Quantum Pulse Scheme for Measuring Diffusion Constants of Macromolecules. *J Biomol. NMR* **68**, 249-255 (2017). Epub 17 Jul 2017. doi:10.1007/s10858-017-0122-9.

420. A.K. Schutz, E. Rennella and Lewis E. Kay. Exploiting Conformational Plasticity in the AAA+ Protein VCP/p97 to Modify Function. *Proc. Nat. Acad. Sci. USA* **114**, E6822-E6829 (2017). Epub 31 Jul 2017. doi:10.1073/pnas.1707974114.

421. A. Sekhar, J. Nagesh, R. Rosenzweig and Lewis E. Kay. Conformational Heterogeneity in the Hsp70 Chaperone-Substrate Ensemble Identified from Analysis of NMR-Detected Titration Data. *Protein Sci.* **26**, 2207-2220 (2017). Epub 18 Sept 2017. doi:10.1002/pro.3276.

422. J.P. Brady, P.J. Farber, A. Sekhar, Y.-H. Lin, R. Huang, A. Bah, T.J. Nott, H.S. Chan, A.J. Baldwin, J.D. Forman-Kay and Lewis E. Kay. Structural and Hydrodynamic Properties of an Intrinsically Disordered Region of a Germ Cell-Specific Protein on Phase Separation. *Proc. Nat. Acad. Sci. USA* **114**, E8194-E8203 (2017). Epub 11 Sep 2017. doi:10.1073/pnas.1706197114.

423. R. Huang, F. Pérez and Lewis E. Kay. Probing the Cooperativity of *Thermoplasma acidophilum* Proteasome Core Particle Gating by NMR Spectroscopy. *Proc. Nat. Acad. Sci. USA* **114**, E9846-E9854. Epub 30 Oct 2017. doi:10.1073/pnas.1712297114.

424. T. Yuwen, J.P. Brady and Lewis E. Kay. Probing Conformational Exchange in Weakly Interacting, Slowly Exchanging Systems via Off-Resonance $R_{1\rho}$ Experiments: Application to Studies of Protein Phase Separation. *J. Am. Chem. Soc.* **140**, 2115-2126 (2018). Epub 31 Jan 2018. doi:10.1021/jacs.7b09576.

425. A. Sekhar, A. Velyvis, G. Zoltsman, R. Rosenzweig, G. Bouvignies and Lewis E. Kay. Conserved Conformational Selection Mechanism of Hsp70 Chaperone-Substrate Interactions. *Elife* **7**, e32764 (2018). Epub 20 Feb 2018. doi:10.7554/eLife.32764.

426. T. Yuwen and Lewis E. Kay. A New Class of CEST Experiment Based on Selecting Different Magnetization Components at the Start and End of the CEST Relaxation Element: An Application to ^{1}H CEST. *J Biomol. NMR* **70**, 93-102 (2018). Epub 19 Jan 2018. doi:10.1007/s10858-017-0161-2.

427. R.M. Culik, A. Sekhar, J. Nagesh, H. Deol, J.A.O. Rumfeldt, E.M. Meiering and Lewis E. Kay. The Effects of Maturation on the Conformational Free-Energy Landscape of SOD1. *Proc. Nat. Acad. Sci USA* **115**, E2546-E2555 (2018). Epub 26 Feb 2018. doi;10.1073/pnas.1721022115.

428. J. Mondal, N. Ahalawat, S. Pandit, Lewis E. Kay and P. Vallurupalli, Atomic Resolution Mechanism of Ligand Binding to a Solvent Inaccessible Cavity in T4 Lysozyme. *PLoS Comput. Biol.* **14**, e1006180 (2018). Epub 18 May 2018. doi:10.1371/journal.pcbi.1006180.

429. R. Augustyniak and Lewis E Kay. Cotranslational Processing of the Protein Substrate Calmodulin by a AAA+ Unfoldase Occurs via Unfolding and Refolding Intermediates. *Proc. Natl. Acad. Sci USA* **115**, E4786-E4795 (2018). Epub 7 May 2018doi:10.1073/pnas.1721811115.

430. J.L. Kitevski-LeBlanc, T. Yuwen, P.N. Dyer, J. Rudolph, K. Lugar and Lewis E. Kay. Investigating the Dynamics of Destabilized Nucleosomes Using Methyl-TROSY NMR. *J. Am. Chem. Soc.* **140**, 4774-4777 (2018). Epub 28 Mar 2018. doi:10.1021/jacs.8b00931.

431. Lewis E. Kay. A Magnetic Moment Silenced: A Tribute to My Friend and Mentor Alex D. Bain. *Concepts Magn. Reson.* **45A**, e21420. doi: 10.1002/cmr.a.21420.

432. T. Yuwen, Lewis E. Kay, G. Bouvignies. Dramatic Decrease in CEST Measurement Times Uisng Multi-Site Excitation. *Chemphyschem*. **19**, 1707-1710 (2018). Epub 24 May 2018. doi:10.1002/cphc.201800249.

433. T. Yuwen, G. Bouvignies and Lewis E. Kay. Exploring Methods to Expedite the Recording of CEST Datasets Using Selective Pulse Excitation. *J. Magn. Reson.* **292**, 1-7. Epub 26 Apr 2018. doi:10.1016/j.jmr.2018.04.013.

434. S. Vahidi, Z.A. Ripstein, M. Bonomi, T. Yuwen, M.F. Mabanglo, J.B. Juravsky, K. Rizzolo, A. Velyvis, W.A. Houry, M. Vendruscolo, J.L. Rubinstein and Lewis E. Kay. Reversible Inhibition of the ClpP Protease via an N-Terminal Conformational Switch. *Proc. Natl. Acad. Sci. USA* **115**, E6447-E6456. Epub 25 Jun 2018. doi:10.1073/pnas.1805125115.

435. J. Boisbouvier and Lewis E. Kay. Advanced Isotopic Labeling for the NMR Investigation of Challenging Proteins and Nucleic Acids. *J. Biomol. NMR* **7**, 115-117 (2018). doi:10.1007/s10858-018-0199-9.

436. A.B. Gopalan, T. Yuwen, Lewis E. Kay and P. Vallurupalli. A Methyl ^{1}H Double Quantum CPMG Experiment to Study Protein Conformational Exchange. *J. Biomol. NMR* **72**, 79-91 (2018). Epub 1 Oct 2018. doi:10.1007/s10858-018-0208-z.

437. T. Yuwen, A. Bah, J.P. Brady, F. Ferrage, G. Bouvignies and Lewis E. Kay. Measuring Solvent Hydrogen Exchange Rates by Multifrequency Excitation ^{15}N CEST: Application to Protein Phase Separation. *J. Phys. Chem. B* **122**, 11206-11217 (2018). Epub 19 Sep 2018. doi:10.1021/acs.jpcb.8b06820.

438. T. Yuwen, A. Sekhar, A.J. Baldwin, P. Vallurupalli and Lewis E. Kay. Measuring Diffusion Constants of Invisible Protein Conformers by Triple-Quantum ^{1}H CPMG Relaxation Dispersion. *Angew. Chem. Int. Ed. Engl.* **57**, 16777-16780. Epub 21 Nov 2018. doi:10.1002/anie.201810868.

439. R. Huang, Z.A. Ripstein, J.L. Rubinstein and Lewis E. Kay. Cooperative Subunit Dynamics Modulate p97 Function. *Proc. Natl. Acad. Sci. USA* **116**, 158-167 (2019). Epub 24 Dec 2018. doi:10.1073/pnas.1815495116.

440. E. Rennella, G.J. Morgan, J.W. Kelly and Lewis E. Kay. Role of Domain Interactions in the Aggregation of Full-Length Immunoglobulin Light Chains. *Proc Natl Acad Sci USA* **116**, 854-863 (2019). Epub Dec 31 2018. doi:10.1073/pnas.1817538116.

441. A. Sekhar and Lewis E. Kay. An NMR View of Protein Dynamics in Health and Disease. *Annu. Rev. Biophys.* **48**, 297-319 (2019). Epub 22 Mar 2019. doi:10.1146/annurev-biophys-052118-115647.

442. Lewis E. Kay. Artifacts Can Emerge in Spectra Recorded with Even the Simplest of Pulse Schemes: an HMQC Case Study. *J. Biomol. NMR* **73**, 423-427. Epub 23 Feb 2019. doi:10.1007/s10858-019-00227-7.

443. T. Yuwen, R. Huang, P. Vallurupalli and Lewis E. Kay. A Methyl-TROSY-Based ^{1}H Relaxation Dispersion Experiment for Studies of Conformational Exchange in High Molecular Weight Proteins. *Angew. Chem. Int. Ed. Engl.* **58**, 6250-6254 (2019). Epub 4 Apr 2019. doi:10.1002/anie.201900241.

444. G.J. Morgan, N.L. Yan, D.E. Mortenson, E. Rennella, J.M. Blundon, R.M. Gwin, C.-Y. Lin, R.L. Stanfield, S.J. Brown, H. Rosen, T.P. Spicer, V. Fernandez-Vega, G. Merlini, Lewis E. Kay, I.A. Wilson and J.W. Kelly. Stabilization of Amyloidogenic Immunoglobulin Light Chains by Small Molecules. *Proc. Natl. Acad. Sci. USA* **116**, 8360-8369. Epub 10 Apr 2019. doi:10.1073/pnas.1817567116.

445. Lewis E. Kay. The Evolution of Solution State NMR Pulse Sequences Through the 'Eyes' of Triple-Resonance Spectroscopy. *J. Magn. Reson.* **306**, 48-54 (2019). Epub 12 Jul 2019. doi:10.1016/j.jmr.2019.07.035.

446. E. Rennella, G.J. Morgan, N. Yan, J.W. Kelly and Lewis E. Kay. The Role of Protein Thermodynamics and Primary Structure in Fibrillogenesis of Variable Domains from Immunolglobulin Light Chains. *J. Am. Chem. Soc.* **141**, 13562-13571 (2019). Epub 14 Aug 2019. doi: 10.1021/jacs.9b05499.

447. T.H. Kim, B. Tsang, R.M. Vernon, N. Sonenberg, Lewis E. Kay and J.D. Forman-Kay. Phospho-Dependent Phase Separation of FMRP and CAPRIN1 Recapitulates Regulation of Translation and Deadenylation. *Science* **365**, 825-829 (2019). doi:10.1126/science.aax4240.

448. T.R. Alderson and Lewis E. Kay. Unveiling Invisible Protein States with NMR Spectroscopy. *Curr. Opin. Struct. Biol.* **60**, 39-49 (2019). Epub 11 Dec 2019. doi:10.1016/j.sbi.2019.10.008.

449. T. Yuwen and Lewis E. Kay. Revisiting $^{1}H^{N}$ CPMG Relaxation Dispersion Experiments: a Simple Modification Can Eliminate Large Artifacts. *J. Biomol. NMR.* **73**, 641-650 (2019). Epub 23 Oct 2019. doi:10.1007/s10858-019-00276-y.

450. Z.A. Ripstein, S. Vahidi, W.A. Houry, J.L. Rubinstein and Lewis E Kay. A Processive Rotary Mechanism Couples Substrate Unfolding and Proteolysis in the ClpXP Degradation Machinery. *Elife* **9**, e52158 (2020). Epub 9 Jan 2020. doi:10.7554/eLife.52158.

451. Lewis E. Kay. A Tribute to James H. Prestegard – 75 Years Young! *J. Magn. Reson.* **310**, 106616 (2020). Epub 8 Oct 2019. doi:10.1016/j.jmr.2019.106616.

452. L.E. Wong, T.H. Kim, D.R. Muhandiram, J.D. Forman-Kay, and Lewis E. Kay. NMR Experiments for Studies of Dilute and Condensed Protein Phases: Application to the Phase-Separating Protein CAPRIN1. *J. Am. Chem. Soc.* **142**, 2471-2489 (2020). Epub 21 Jan 2020. doi:10.1021/jacs.9b12208.

453. M.F. Mabanglo, E. Leung, S. Vahidi, T.V. Seraphim, B.T. Eger, S. Bryson, V. Bhandari, J.L. Zhou, Y.-Q. Mao, K. Rizzolo, M.M. Barghash, J.D. Goodreid, S. Phanse, M. Babu, L.R.S. Barbosa, C.H.I. Ramos, R.A. Batey, Lewis E. Kay, E.F. Pai and W.A. Houry. ClpP Protease Activation of the Electrostatic Interaction Networks at the Entrance Pores. *Commun. Biol.* 2019 **2**, 410 (2019). Epub 13 Nov 2019. doi:10.1038/s42003-019-0656-3. eCollection 2019.

454. E. Rennella, R. Huang, Z. Yu and Lewis E. Kay. Exploring Long-Range Cooperativity in the 20S Proteasome Core Particle from *Thermoplasma Acidophilum* using Methyl-TROSY-Based NMR. *Proc. Natl. Acad. Sci. USA* **117**, 5298-5309 (2020). Epub 24 Feb 2020. doi:10.1073/pnas.1920770117.

455. S. Vahidi, Z.A. Ripstein, J.B. Juravsky, E. Rennella, A.L. Goldberg, A.K. Mittermaier, J.L. Rubinstein, and Lewis E. Kay. An Allosteric Switch Regulates *Mycobacterium Tuberculosis* ClpP1P2 Protease Function as Established by Cryo-EM and Methyl-TROSY NMR. *Proc. Natl. Acad. Sci. USA* **117**, 5895-5906 (2020). Epub 2 Mar 2020. doi:10.1073/pnas.1921630117.

456. N. Kessler, S.R. Akabayov, A. Moseri, L.S. Cohn, D. Sakhapov, D. Bolton, B. Fridman, Lewis E. Kay, F. Naider and J. Anglister. Allovalency Observed by Transferred-NOE:

Interactions of Sulfated Tyrosine Residues in the N-Terminal Segment of CCR5 with CCL5 Chemokine. *FEBS J.* **288**, 1648-1663 (2021). Epub 8 Sep 2020. doi:10.1111/febs.15503.

457. L.E. Wong, T.H. Kim, E. Rennella, P. Vallurupalli, and Lewis E. Kay. Confronting the Invisible: Assignment of Protein $^{1}H^{N}$ Chemical Shifts in Cases of Extreme Broadening. *J. Phys. Chem. Lett.* 2020 **11**, 3384-3389. Epub 17 Apr 2020. doi:10.1021/acs.jpclett.0c00747.

458. G. Abramov, A. Velyvis, E. Rennella, L.E. Wong and Lewis E. Kay. A Methyl-TROSY Approach for NMR Studies of High Molecular Weight DNA with Application to the Nucleosome Core Particle. *Proc. Natl. Acad. Sci. USA* **117**, 12836-12846 (2020). Epub 26 May 2020. doi:10.1073/pnas.2004317117.

459. S. Kumar, S.R. Akabayov, N. Kessler, L.S. Cohen, J. Solanki, F. Naider, Lewis E. Kay and J. Anglister. The Methyl ^{13}C-Edited/^{13}C-Filtered Transferred NOE for Studying Protein Interactions with Short Linear Motifs. *J. Biomol. NMR* **74**, 681-693 (2020). Epub 30 Sep 2020. doi:10.1007/s10858-020-00340-y.

460. N. Yan, D. Santos-Martins, E. Rennella, B.B. Sanchez, J.S. Chen, Lewis E. Kay, I.A. Wilson, G.J. Morgan, S. Forli, J.W. Kelly. Structural Basis for the Stabilization of Amyloidogenic Immunoglobulin Light Chains by Hydantoins. *Bioorg. Med. Chem. Lett.* **30**, 127356 (2020). Epub 16 Jun 2020. doi:10.1016/j.bmcl.2020.127356.

461. R.W. Harkness, Y. Toyama, and Lewis E. Kay. Analyzing Multi-Step Ligand Reactions for Oligomeric Proteins by NMR: Theoretical and Computations Considerations. *J. Magn. Reson.* **318**, 106802 (2020). Epub 4 Aug 2020. doi:10.1016/j.jmr.2020.106802.

462. A.E. Conicella, R. Huang, Z.A. Ripstein, A. Nguyen, E. Wang, T. Löhr, P. Schuck, M. Vendruscolo, J.L. Rubinstein and Lewis E. Kay. An Intrinsically Disordered Motif Regulates the Interaction between the p47 Adaptor and the p97 AAA+ ATPase. *Proc. Natl. Acad. Sci. USA* **117**, 26226-26236. Epub 7 Oct 2020. doi:10.1073/pnas.2013920117.

463. R. Huang, Z.A. Ripstein, J.L. Rubinstein and Lewis E. Kay. Probing Cooperativity of N-Terminal Domain Orientations in the p97 Molecular Machine: Synergy between NMR and cryo-EM. *Angew. Chem. Int. Ed. Engl.* **59**, 22423-22426 (2020). Epub 6 Oct 2020. doi:10.1002/anie.202009767.

464. Z.A. Ripstein, S. Vahidi, J.L. Rubinstein and Lewis E. Kay. A pH-Dependent Conformational Switch Controls *N. meningitidis* ClpP Protease Function. *J. Am. Chem. Soc.* **142**, 20519-20523 (2020). Epub 24 Nov 2020. doi:10.1021/jacs.0c09474.

465. T.R. Alderson and Lewis E. Kay. NMR Spectroscopy Captures the Essential Role of Dynamics in Regulating Biomolecular Function. *Cell* 184, 577- 595 (2021). doi:10.1016/j.cell.2020.12.034

466. Y. Toyama, R.W. Harkness, T.Y.T. Lee, J.T. Maynes and Lewis E. Kay. Oligomeric Assembly Regulating Mitochondrial HtrA2 Function as Examined by Methyl-TROSY NMR. *Proc. Natl. Acad. Sci. USA* **118**, e2025022118 (2021). Epub 10 Mar 2021. doi:10.1073/pnas.2025022118.

467. Lewis E Kay. A Life Writ Large: Chris Dobson 1949-2019. *J. Magn. Reson.* **326**, 106947 (2021). Epub 18 Feb 2018. doi:10.1016/j.jmr.2021.106947.

468. A. Parupudi, S.K. Chaturvedi, R. Adão, R.W. Harkness, S. Dragulin-Otto, Lewis E. Kay, R. Esfandiary, H. Zhao and P Schuck. Global Multi-method Analysis of Interaction Parameters for Reversibly Self-Associating Macromolecules at High Concentrations. *Sci. Rep.* **11**, 741. Epub 11 Mar 2021. doi:10.1038/s41598-021-84946-8.

469. T.H. Kim, B.J. Payliss, M.L. Nosella, I.T.W. Lee, Y. Toyama, J.D. Forman-Kay and Lewis E. Kay. Interaction Hot Spots for Phase Separation Revealed by NMR Studies of a CAPRIN1 Condensed Phase. *Proc. Natl. Acad. Sci. USA* **118**, e2104897118. Epub 31 May 2021. doi:10.1073/pnas.2104897118.

470. C.R. Knoverek, U.L. Mallimadugula, S Singh, E. Rennella, T.E. Frederick, T. Yuwen, S. Raavicharla, Lewis E. Kay and G.R. Bowman. Opening of a Cryptic Pocket in β-lactamase Increases Penicillinase Activity. *Proc Natl. Acad. Sci. USA* 2021 **118**, e2106473118 (2021). Epub 19 Nov 2021. doi:10.1073/pnas.2106473118.

471. R.W. Harkness, Y. Toyama, Z.A. Ripstein, H. Zhao, A.I.M. Server, Q. Luan, J.P. Brady, P.L. Clark, P. Schuck and Lewis E. Kay. Competing Stress-Dependent Oligomerization Pathways Regulate Self-Assembly of the Periplasmic Protease-Chaperone DegP. *Proc. Natl. Acad. Sci. USA* **118**, e2109732118 (2021). Epub 6 Aug 2021. doi:10.1073/pnas.2109732118.

472. Y. Toyama, R.W. Harkness and Lewis E. Kay Dissecting the Role of Interprotomer Cooperativity in the Activation of Oligomeric High-Temperature Requirement A2 protein. *Proc. Natl. Acad. Sci. USA* **118**, e2111257118 (2021). Epub 26 Aug 2021. doi:10.1073/pnas.2111257118.

473. V.P. Tiwari, Y. Toyama, D. De, Lewis E. Kay and P. Vallurupalli. The A39G FF Domain Folds on a Volcano-Shaped Free Energy Surface via Separate Pathways. *Proc. Natl. Acad. Sci. USA* **118**, e2115113118 (2021). Epub 10 Nov 2021. doi:10.1073/pnas.2115113118.

474. Y. Toyama and Lewis E. Kay. Probing Allosteric Interactions in Homo-Oligomeric Molecular Machines using Solution NMR Spectroscopy. *Proc. Natl. Acad. Sci. USA* **118**, e2116325118 (2021). Epub 10 Dec 2021. doi: 10.1073/pnas.2116325118.

475. Y. Toyama, R.W. Harkness and Lewis E Kay. Structural Basis of Protein Substrate Processing by Human Mitochondrial High-Temperature Requirement A2 Protease. *Proc. Natl. Acad. Sci. USA* **119**, e2203172119. Epub 22 Apr 2022. doi: 10.1073/pnas.2203172119.

476. G. Karunanity, T. Yuwen, Lewis E. Kay and D.F. Hansen. Towards Autonomous Analysis of Chemical Exchange Saturation Transfer Experiments using Deep Neural Networks. *J. Biomol. NMR* **76**, 75-86 (2022). Epub 27 May 2022. doi:10.1007/s10858-022-00395-z.

477. Y. Toyama and Lewis E. Kay. Revisiting Dipolar Relaxation of a Homonuclear Spin Pair in the Presence of a Radio Frequency Field: A Tutorial. *J. Mag. Reson. Open* **12-13**, 1000065 (2022). Epub 15 Jul 2022. doi:10.1016/j.jmro.2022.100065.

478. Y. Toyama, A.K. Rangadurai, and Lewis E. Kay. Measurement of $^{1}H^{\alpha}$ Transverse Relaxation Rates in Proteins: Application to Solvent PREs. *J. Biomol. NMR* **76**, 137-152 (2022). Epub 26 Aug 2022. doi:10.1007/s10858-022-00401-4.

479. N. Bolik-Coulon, D.F. Hansen, and Lewis E. Kay. Optimizing Frequency Sampling in CEST Experiments. *J Biomol NMR* **76**, 167-183 (2022). Epub 4 Oct 2022. doi:10.1007/s10858-022-00403-2.

480. Y. Toyama, A.K. Rangadurai, J.D. Forman-Kay and Lewis E. Kay. Mapping the Per-Residue Surface Electrostatic Potential of CAPRIN1 During its Phase-Separation Trajectory. *Proc. Natl. Acad. Sci. USA* **119**, e2210492119 (2022). Epub 30 Aug 2022. doi:10.1073/pnas.2210492119.

481. Lewis E. Kay and T. Carlomagno. Editorial for Kurt Wuthrich JMR Celebratory Issue. *J. Magn Reson.* **343**, 107296. Epub 5 Sep 2022. doi:10.1016/j.jmr.2022.107296.

482. N. Bolik-Coulon, A.I.M. Sever, R.W. Harkness, J.M. Aramini, Y. Toyama, D.F. Hansen and Lewis E. Kay. Less is more: A Simple Methyl-TROSY Based Pulse Scheme Offers Improved Sensitivity in Applications to High Molecular Weight Complexes. *J. Magn. Reson.* **349**, 107400. Epub 9 Nov 2022. doi:10.1016/j.jmr.2022.107326.

483. Y. Toyama, A.K. Rangadurai, J.D. Forman-Kay and Lewis E. Kay. Surface Electrostatics Dictate RNA-Binding CAPRIN1 Condensate Concentration and Hydrodynamic Properties. *J. Biol. Chem.* **299**, 107326 (2023). Epub 7 Dec 2022. doi:10.1016/j.jbc.2022.102776.

484. A.K. Rangadurai, Y. Toyama, and Lewis E. Kay. Practical Considerations for the Measurement of Near-Surface Electrostatics based on Solvent Paramagnetic Relaxation Enhancements. *J. Magn. Reson.* **349**, 107400 (2023). Epub 9 Feb 2023. doi:10.1016/j.jmr.2023.107400.

485. A.K. Rangadurai, Y. Toyama, and Lewis E. Kay. Sometimes Pulses Just Have to be Perfect – An Example Based on the Measurement of Amide Proton Transverse Relaxation Rates in Proteins. *J. Magn. Reson.* **349**, 107412 (2023). Epub 2 Mar 2023. doi:10.1016/j.jmr.2023.107412.

486. S. Nim, D.M. O'Hara, C. Corbi-Verge, A. Perez-Riba, K. Fujisawa, M. Kapadia, H. Chau, F. Albanese, G. Pawar, M.L. De Snoo, S.G. Ngana, J. Kim, O.M.A. El-Agnaf, E. Rennella, Lewis E. Kay, S.K. Kalia, L.V. Kalia and P. Kim. Disrupting the α-synuclein-ESCRT Interaction with a Peptide Inhibitor Mitigates Neurodegeneration in Preclinical Models of Parkinson's Disease. *Nat. Commun.* 14, 2150 (2023). Epub 19 Apr 2023. doi:10.1038/s41467-023-37464-2.

487. R. W. Harkness, Z. A. Ripstein, J. M. D. Trani and Lewis E Kay. Flexible Client-Dependent Cages in the Assembly Landscape of the Periplasmic Protease-Chaperone DegP. *J. Am. Chem. Soc.* 145, 13015-13026 (2023). Epub 7 Jun 2023. doi: 10.1021/jacs.2c11849.

488. T.H. Kim, M.L. Nosella, N. Bolik-Coulon, R.W. Harkness, S.K. Huang and Lewis E. Kay. Correlating Histone Acetylation with Nucleosome Core Particle Dynamics and Function. *Proc. Natl Acad Sci USA* **120**, e2301063120 (2023). Epub 3 Apr 2023. doi:10.1073/pnas.2301063120.

489. D. D. Sahtoe, E. A. Andrzejewska, H. L. Han, E. Rennella, M. M. Schneider, G. Meisl, H. Choi, M. Ahlrichs, J. Decarreau, H. Nguyen, X. Li, A. K. Bera, Lewis E. Kay, T. P.J. Knowles, D. Baker. Design of Amyloidogenic Peptide Traps. *Nat. Chem. Biol*. **20**, 981-990 (2024). Epub 19 Mar 2024. doi: doi.org/10.1038/s41589-024-01578-5.

490. E. Rennella, D. D. Sahtoe, D. Baker and Lewis E. Kay. Exploiting Conformation Dynamics to Modulate the Function of Designed Proteins. *Proc. Natl. Acad. Sci. USA*. 2023 May 2;120(18):e2303149120. doi: 10.1073/pnas.2303149120. Epub 24 Apr 2023. doi:10.1073/pnas.2303149120.

491. A. I. M. Sever, T. R. Alderson, E. Rennella, J. M. Aramini, Z. H. Liu, R. W. Harkness, and Lewis E. Kay. Activation of caspase-9 on the apoptosome as studied by methyl-TROSY NMR. *Proc Natl Acad Sci USA*. 2023 Dec 19;120(51):e2310944120. doi: 10.1073/pnas.231094412

492. V. P. Tiwari, D. De, N. Thapliyal, Lewis E. Kay, and P. Vallurupalli. Beyond Slow Two-Site Protein Conformational Exchange using CEST: Applications to Three-State Protein Interconversion on the Millisecond Timescale. *J Biomol NMR*. 2024 Jan 3. doi: 10.1007/s10858-023-00431-6.

493. M. L. Nosella, T. H. Kim, S. K. Huang, R. W. Harkness, M. Goncalves, A. Pan, M. Tereshchenko, S. Vahidi, J. L. Rubinstein, H. O. Lee, J. D. Forman-Kay, and Lewis E. Kay. Poly(ADP-ribosyl)ation Enhances Nucleosome Dynamics and Organizes DNA Damage Repair Components within Biomolecular Condensates. *Mol Cell.* 2024 Feb 1;84(3):429-446.e17. doi: 10.1016/j.molcel.2023.12.019. Epub 2024 Jan 11. PMID: 38215753.

494. Y. Jin, Y. Cui, Lewis E. Kay, and T. Yuwen. Optimization of TROSY and anti-TROSY-based ^{15}N CPMG Relaxation Dispersion Experiments through Phase Cycling. *J. Magn. Reson*. 2024 Apr;361:107629. doi: 10.1016/j.jmr.2024.107629. Epub 2024 Feb 2.

495. R. W. Harkness, H. Zhao, Y. Toyama, P. Schuck, and Lewis E. Kay. Exploring Host-Gues Interactions Within a 600 kDa DegP Protease Cage Complex Using Hydrodynamics Measurements and Methyl-TROSY NMR. *J. Am. Chem. Soc*. 2024, Mar 27;146(12):8242-8259. doi: 10.1021/jacs.3c13247. Epub 2024 Mar 13.

496. S. K. Huang, J. L. Rubinstein, and Lewis E. Kay. Cryo-EM of the Nucleosome Core Particle Bound to Ran-RCC1 Reveals a Dynamic Complex. *Biochemistry*. 2024 Apr 2;63(7):880-892. doi: 10.1021/acs.biochem.3c00724. Epub 2024 Mar 19.

497. Y. Dong, J. P. Bonin, P. Devant, Z. Liang, A. I. M Sever, J. Mintseris, J. M. Aramini, S. P. Gygi, J. Kagan, Lewis E. Kay, and H. Wu. Structural Transitions Enable Il-18 Maturation and Signaling. *Immunity*. 2024 Jul 9;57(7):1533-1548.e10. doi: 10.1016/j.immuni.2024.04.015. Epub 2024 May 10.

498. Y. H. Lin, T. H. Kim, S. Das, T. Pal, J. Wessen, A. K. Rangadurai, Lewis E. Kay, J. D. Forman-Kay, and H. S. Chan. Electrostatics of Salt-Dependent Reentrant Phase Behaviors Highlights Diverse Roles of ATP in Biomolecular Condensates. *eLife*, In Press.

499. J. P. Bonin, J. M. Aramini, Y. Dong, H. Wu, and Lewis E. Kay. AlphaFold2 as a Replacement for Solution NMR Structure Determination of Small Proteins: Not So Fast! 2024 Jul;364:107725. doi: 10.1016/j.jmr.2024.107725. Epub 2024 Jun 19.

500. R. Ahmed, A. K. Rangadurai, L. Ruetz, M. Tollinger, C. Kreutz, and Lewis E. Kay. A Delayed Decoupling Methyl-TROSY Pulse Sequence for Atomic Resolution Studies of Folded Proteins and RNA in Condensates. *J Magn Reson*. 2024 May;362:107667. doi: 10.1016/j.jmr.2024.107667. Epub 2024 Mar 28.

501. A. K. Rangadurai, L. Ruetz, R. Ahmed, K. Lo, M. Tollinger, J. D. Forman-Kay, C. Kreutz and Lewis E. Kay. Phase Separation Modulates the Thermodynamics and Kinetics of RNA Hybridization. *J Am Chem Soc*. 2024 Jul 24;146(29):19686-19689. doi: 10.1021/jacs.4c06530. Epub 2024 Jul 11.

502. B. Yu, N. Bolik-Coulon, A. K. Rangadurai, Lewis E. Kay, J. Iwahara. Gadolinium-Based Spin Relaxation Measurements of Near-Surface Electrostatic Potentials of Biomolecules. *J Am Chem Soc*. 2024 Jul 19;146(30):20788-20801. doi: 10.1021/jacs.4c04433. Epub 2024 Jul 19.

503. R. Ahmed, M. Liang, R. P. Hudson, A. T. Rangadurai, S. K. Huang, J. D. Forman-Kay and Lewis E. Kay. Atomic Resolution Map of the Solvent Interactions Driving SOD1 Unfolding in CAPRIN1 Condensates. *Proc. Natl. Acad. Sci. USA*. 2024 Aug 27;121(35):e2408554121.doi: 10.1073/ pnas.2408554121. Epub 22 Aug 2024.

TEACHING

Undergraduate coordinator of Molecular Biophysics BSc program offered through the Department of Physics.

1) Chemistry 1455H, NMR Spectroscopy 1: Introduction to NMR: Theory and Application.

2) Chemistry 1456H, NMR Spectroscopy 2: Advanced Theory and Application.

3) MMG 1012Y Protein Structure and Function.

4) MMG 1014Y. Macromolecular Biology. Special Topics Course.

5) Biochemistry 2021.

6) BCH 2024H Biomolecular Dynamics and Function.

ORGANIZATION OF NATIONAL AND INTERNATIONAL MEETINGS

"Frontiers in Structural Biology Symposium" June 1993.

2) "NMR of Biomolecules" for the Canadian Society of ChemistryMay 1995.

3) Minisymposium on Biomolecular NMR, Canadian Society for Biochemistry and Molecular and Cellular Biology. June 1996.

4) International Society of Magnetic Resonance in Biological Systems Conference, Toronto, August 2002.

RESEARCH TRAINING

1) Ouwan Zhang, Graduate Student (PhD) in Chemistry with Dr. Julie Forman-Kay, June 1992 - April 1997.

2) Neil Farrow, Post-Doctoral Associate, September 1992 - July 1997.

3) Steven Pascal, Post-Doctoral Associate, March 1993 - July 1996.

4) Toshio Yamazaki, Post-Doctoral Associate, April 1993 - April 1995.

5) Yves Aubin, Post-Doctoral Associate, September 1993 - October 1995.

6) Mike Rosen, Post-Doctoral Associate, October 1993 - January 1996.

7) Ping Xu, Post-Doctoral Associate, January 1994 - September 1994.

8) Li-Lin Tay, Graduate Student (MSc) in Chemistry with Dr. Bill Reynolds. September 1994 - November 1996.

9) N. Rao, Post-Doctoral Associate, April 1995 - October 1996.

10) D. Yang, Post-Doctoral Associate, May 1995 – May 2001.

11) Kevin Gardner, Post-Doctoral Associate, August 1995 - July 1998.

12) Pascale Legault, Post-Doctoral Associate, September 1995 - July 1998.

13) Sebastian Vincent, Post-Doctoral Associate, May 1996 - September 1997.

14) Catherine Zwahlen, Post-Doctoral Associate, May 1996 - December 1998.

15) Joel Tolman, Post-Doctoral Associate, December 1997 - September 1999.

16) Logan Donaldson, Post-Doctoral Associate, July 1998 - September 2000.

17) Geoff Mueller, Post-Doctoral Associate, September 1998 – May 2001.

18) James Choy, Post-Doctoral Associate, October 1998 – Nov 2005.

19) Nikolai Skrynnikov, Post-Doctoral Associate, January 1998 – Sept. 2002.

20) Frans Mulder, Post-Doctoral Associate, February 1998 – July 2001.

21) Johan Evenäs, Post-Doctoral Associate, July 1999 – February 2001.

22) Tony Mittermaier, Graduate Student, September 1997 – Jan 2004.

23) Natalie Goto, Graduate Student, September 1997 - February 2001.

24) Peter Hwang, Graduate Student, September 1999 – Nov 2005.

25) Jason Ollerenshaw, Graduate Student, September 2000 – Sept 2005.

26) Vitali Tugarinov, Post-Doctoral Associate, December 2000 – July 2007.

27) Oscar Millet, Post-Doctoral Associate, September 2000 – April 2004.

28) Dimitry Korzhnev, Post-Doctoral Associate, September 2001-Sept 2010.

29) Irina Bezsonova, Graduate Student, September 2001-Sept. 2008

30) Karen Kloibler, Post-Doctoral Associate, September 2001-Jan 2004.

31) Pramodh Vallurupalli, Post-Doctoral Associate, Oct 2002-June 2009.

32) Remco Sprangers, Post-Doctoral Associate, April 2003-March 2008.

33) Algirdas Velyvis, Post-Doctoral Associate, April 2003-2009.

34) Philipp Neudecker, Post-Doctoral Associate, April 2004-Oct. 2010.

35) Jason Malthrop, Graduate Student, Sept. 2004-February 2008.

36) Flemming Hansen, Post-Doctoral Associate, Sept 2005-Sept 2010.

37) Patrik Lundström, Post-Doctoral Associate, Oct 2005-February 2009.

38) Eugene V. Tischenko, Post-Doctoral Associate, Oct 2005-August 2009.

39) Tomasz Religa, Post-Doctoral Associate, August 2008-October 2011.

40) Andy Baldwin, Post-Doctoral Associate, May 2008-July 2012.

41) Amy Ruschak, Post-Doctoral Associate, June 2008-April 2012.

42) Michael Latham, Post-Doctoral Associate, July 2008-Nov 2014.

43) Hugo van Ingen, Post-Doctoral Associate, August 2008-Dec 2010.

44) Guillaume Bouvignies, Post-Doctoral Associate, August 2008-November 2013.

45) Julia Barette, Graduate Student, January 2009, August 2011.

46) Alex Hansen, Post-doctoral Fellow, January 2009-February 2014.

47) Rina Rosenzweig, Post-Doctoral Associate, September 2010-June 2016.

48) Lichi Shi, Post-Doctoral Associate, Jan 2011-Sept 2014.

49) Julianne Kitevski, Post-Doctoral Associate, July 2013-June 2017.

50) Ashok Sekhar, Post-Doctoral Associate, July 2011-August 2017.

51) Rafal Augustyniak, Post-Doctoral Associate, May 2012-June 2018.

52) Dong Long, Post-Doctoral Associate, Oct 2012-May 2015.

53) Anne Schuetz, Post-Doctoral Associate, August 2013-May 2017.

54) Enrico Rennella, Post-Doctoral Associate / Senior Research Associate, June 2014-Present.

55) Rui Hwang, Post-Doctoral Associate, Sept 2014-May 2020.

56) Rob Culik, Post-Doctoral Associate, Sept 2014-August 2017.

57) Siavash Vahidi, Post-Doctoral Associate, Sept 2015-May 2020.

58) Zev Ripstein, Graduate Student, Sept 2015-Oct 2020

59) Tairan Yuwen, Post-Doctoral Associate, Nov 2015-Nov 2019

60) Jacob Brady, Post-Doctoral Associate, Nov 2015-Nov 2019.

61) Tae Hun Kim, Post-Doctoral Associate, Dec 2016-Dec 2022.

62) Gili Abramov, Post-Doctoral Associate, Jan 2018-Feb 2022.

63) Rob Harkness, Post-Doctoral Associate, July 2018-March 2024.

64) Alex Conicella, Post-Doctoral Associate, July 2018-Feb 2021.

65) Leo Wong, Post-Doctoral Associate, November 2018-July 2020.

66) T. Reid Alderson, Post-Doctoral Associate, February 2019-Feb 2022.

67) Yuki Toyama, Post-Doctoral Associate, April 2019-Sept 2022.

68) Zev Ripstein, Post-Doctoral Associate, Oct 2020-Aug 2021.

69) Alex Server, Graduate Student, Sept 2020-Present.

70) Rashik Ahmed, Post-Doctoral Associate, Nov. 1, 2021-Present.

71) Atul Kaushik Rangadurai, Post-Doctoral Associate, Nov. 1, 2021-Aug 2024

72) Nicolas BolikCoulon, Post-Doctoral Associate, Dec. 1, 2021-Present.

73) Jeff Paul Bonin, Post-Doctoral Associate, July 1, 2022-Present.

74) Philipp Roessler, Post-Doctoral Associate, Jan 1, 2023 – Present.

75) Aidan Estelle, Post-Doctoral Associate, April 15, 2023-Present.

Current statistics show that only about 10% of trainees go on to independent research careers – yet 40 of 57 trainees who have left the Kay laboratory are on faculty at major research-intensive universities, an additional 5 are scientists in government laboratories and 6 are in industry. My trainees are now professors at University of Toronto, Université de Montréal, McGill University, University of Ottawa, York University, Guelph University, University of Manitoba, and other academic centers, group leaders at Health Canada and industrial sites. Other trainees have established careers at universities throughout the U.S., Europe, Israel and Asia at sites as diverse as Singapore, Dallas, New York, London and Hyderabad. Included in this list are a very significant number of women.

Listed below are former trainees that are now on faculty across the world: Steven Pascal, Professor, Massey University, New Zealand; Toshio Yamazaki, Professor, Osaka University, Japan; Mike Rosen, Professor, Southwestern Medical Center and Howard Hughes Investigator, USA; Daiwen Yang, Professor, National University of Singapore, Singapore; Kevin Gardner, Professor, Southwestern Medical Center, USA; Pascale Legault, Professor, University of Montreal, Canada; Joel Tolman, Professor, Johns Hopkins University, USA; Logan Donaldson, Professor, York University, Canada; James Choy, Professor, University of Western Ontario, Canada; Nikolai Skrynnikov, Professor, Purdue University, USA; Frans Mulder, Professor, University of Groningen, Netherlands; Tony Mittermaier, Professor, McGill University, Canada; Natalie Goto, Professor, University of Ottawa, Canada; Oscar Millet, Professor, University of Bilbao, Spain; Voula Kanelis, Professor, University of Toronto, Canada; Remco Sprangers, Group Leader, Max Planck, Tuebingen, Germany; Patrik Lundstrum, Professor, Linköping University, Sweden; Vitali Turgarinov, Professor, University of Maryland, USA; Flemming Hansen, Professor, Imperial College, London, UK; Dmitry Korzhnev, Professor, University of Connecticut; Tomasz Religa, Professor, Case Western Reserve, Cleveland, USA; Amy Ruschak, Professor, Case Western Reserve, Cleveland, USA; Philipp Neudecker, Professor. Julich Institutes; Pramodh Vallurupalli, Professor, Hyderabad, India; Andy Baldwin, Professor Oxford, Alex Hansen, Research Professor Ohio State, USA; Guillaume Bouvignies, Assistant Professor, CNRS Grenoble France; Irina Bezsonova, Professor, University of Connecticut; Don Long, Professor, University of Science and Technology, China; Michael Latham, Professor, Texas Tech University; Peter Hwang, Professor, University of Alberta; Rina Rosenzweig, Professor Weizmann Institute, Israel; Ashok Sekhar, Professor, Indian Institute of Science, Bengaluru, India; Rafael Augustyniak, Assistant Professor, University of Warsaw, Poland; Anne Schuetz, Professor, University of Munich, Germany; Tairan Yuwen, Assistant Professor, Peking University, China; Rui Hwang, Assistant Professor, University of Guelph, Canada; Siavash Vahidi, Assistant Professor, University of Guelph; Leo Wong, Shenzhen Institute of Advanced Technology (SIAT) in Shenzhen, China; Zev Ripstein, Assistant Professor, University of Manitoba, Canada. Reid Alderson, Assistant Professor, University of Graz, Austria. Tae Hun Kim, Assistant Professor, Case Western Reserve University, Canada. Robert Harkness, Assistant Professor, University of Guelph, Canada. Several trainees have pursued industry related careers: Yves Aubin, Merck Frosst, Canada; Neil Farrow, Berringer-Manheim, USA; Sebastian Vincent, Nestle, Switzerland; Johan Evenas, Astra Zeneca, Sweden as well as independent positions in government laboratories: Ping Xu, NRC, Canada; Geoff Mueller, National Cancer Institute, North Carolina, USA. Eugene Tishchenko, JEOL, USA.

RESEARCH INTERESTS

Research focuses on the development of NMR techniques for studying macromolecular structure and dynamics and the application of NMR techniques to problems of biological and clinical importance. In particular the research is divided into the following areas:

1) *Methodological Developments*. Research is focused on developing ^{15}N, ^{13}C, ^{2}H multi-dimensional NMR spectroscopy and gradient enhanced spectroscopy to increase the molecular weight limitations currently imposed on protein structure determination using conventional techniques. A second area relates to the development of ^{15}N and ^{13}C relaxation techniques for the study of protein dynamics in solution.

2) *Dynamics Studies of Supra-molecular Complexes*. In particular, we are studying the proteasome as well as protein machines involved in disaggregation and the nucleosome. The work builds on our methodological developments that facilitate studies of protein complexes in the MDa molecular weight range.

3) *Protein Dynamics*. Methods are developed and applied to study backbone and sidechain protein dynamics and how dynamic properties change upon ligand binding or folding. Relationships between dynamics and thermodynamics are being developed and applied to binding and folding events.

4) *Protein Folding*. Methods are developed and applied to study protein folding and misfolding, residual structure in unfolded and partially folded states and dynamic properties of these molecules.

5) *Studies of Excited State Protein Conformers*. We are developing the framework to study sparsely populated, transiently formed conformations of proteins that are implicated in function and in disease. The methodology is applied to a wide spectrum of protein systems.