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Objective

Continuing a leadership career in science, software development, and management, emphasizing Magnetic Resonance (NMR) methods, spectroscopy and imaging, drug discovery, database mining, and proteomics.

1991-Present

Consultant - Biophysical and Biomedical Software Applications for Research and Industry

Consultant to leading structural biology laboratories at the National Institutes of Health.

Consultant to major pharmaceutical companies emphasizing structure-based drug design and screening.

Numerous invited presentations, including advanced course instructor for Canada's National High Field NMR Center (NANUC) and the European Molecular Biology Organization (EMBO).

Scientific software advisor to analytical instrument manufacturers, and companies developing and supporting spectral analysis and imaging software.

Commercial projects include software for automated processing, quantification, and multivariate analysis of one-dimensional and two-dimensional spectra as used in drug discovery protocols, and software for visualization and analysis of multivariate spectroscopic images from infrared microscopes.

Software advisor for the Lund University Hospital Image Digitization Project (Sweden), a medical image display and archive project serving 290 clinicians performing 200,000 imaging examinations annually. This included design of a prototype for digital-image based clinical measurement of Hip-Knee Angles (HKA).

1991 - 2006

Special Expert (subsequently Scientist on permanent staff) National Institutes of Health, Section on Biophysical NMR, NIDDK LCP

Principal software scientist for a world-leading Nuclear Magnetic Resonance (NMR) laboratory; invited to this post by Ad Bax, the most cited scientist in the chemical literature. Primary research areas include multidimensional signal processing, automated spectral analysis, high-precision spectral feature measurement, parallel processing, and novel methods for biomolecular structure calculation based primarily on database mining and orientational restraints rather than interatomic distances.

Succeeded in implementing a comprehensive set of software tools for multidimensional NMR. This software, called the NMRPipe System, is now a standard tool for NMR structural biology throughout the world, and enjoys over 3,000 citations. It has been used to help generate roughly one-third of all NMR protein structures which have ever been measured, including 70% of the structures deposited over the last year.

Implemented NMRWish, a spectral analysis environment based on the Tcl/Tk scripting language; its applications include the TALOS program for protein backbone angle prediction from a chemical shift database, an application with over 1,000 citations.

Develop software and the first protocols illustrating the possibility of quantitative determination of protein folds exclusively from database mining with chemical shifts and dipolar couplings, without the use of NMR distance restraints. Most recently, this approach was used to simplify the structure determination of the 177-residue protein Gamma-S crystallin, supplemented only by amide-amide and methyl-methyl distances.

1985-1991

Product Manager

New Methods Research, Inc. (a 1989 Inc 500 Top Small Company)

As leader of a four member group, designed and implemented the NMR2 system for Two-Dimensional NMR processing and analysis; at the time it was the NMR industry's most commercially successful off-line software package, and the company's primary source of profit.

As research investigator, secured two Phase I SBIR software grant awards for development of automated spectral assignment techniques and image analysis methods.

Visited over 50 industrial and academic laboratories in the US, Europe, and Asia, to assess worldwide requirements for NMR analysis software.

As applications expert, led the company in technical commissions earned.

1983-1985

Senior Programmer Analyst

Syracuse University

Implemented a variety of NMR processing techniques for mainframe computers, including digital filters, symmetrization methods, and 2D peak picking.

Conducted research on pattern recognition for NMR spectral analysis.

Ported and maintained very large software systems in a variety of computer environments.

Summers 1982 and 1983

Physical Chemistry Research Assistant

Syracuse University

Conducted research on use of X-ray scattering to characterize properties of supported metal catalysts used in the petrochemical industry.

Invented mathematical models to simulate geometry and X-ray scattering of heterogeneous amorphous solids.

Designed and implemented software for surface area analysis from X-ray scattering data, including model fitting, graphics, and data acquisition.

1982 - 1983

General Chemistry Teaching Assistant

Syracuse University

Laboratory teaching assistant and tutor in general chemistry for non-majors.

Professional Skills

Effective public speaker.

Managed teams of Ph.D. scientists and graduate level programmers.

Skilled in all aspects of scientific software development.

Well versed in NMR, signal processing techniques, and numerical methods.

Over 20 years programming experience, C, UNIX, X11, Tk/TCL, FORTRAN, etc.

Experienced with HTML and Web Design, web server configuration and management.

Emphasize strategies for visual presentation of information to support decision-making.

Education

Syracuse University, 1979-1984
B.A., Dept. of Chemistry

Osaka University, 2000-2001
Ph.D., Graduate Dept. of Pharmaceutical Sciences
Advisor: Prof. Y. Kobayashi, Molecular Biophysics

Invited Presentations

2008 and Pending

EMBO World Practical Course, Beijing China
Quo Vadis Structural Bio Symposium, Harvard
Data Processing Summit, U. Conn.
NANUC NMR Bootcamp, U. Conn.
NIH Advanced NMR Course, Bethesda
LAS NMR Workshops, Japan

2007

LAS NMR Workshops, Japan
EMBO NMR Course, Basel Switzerland
NANUC NMR Bootcamp, Edmonton Canada

2006

University of Maryland
NMRFAM Workshop, University of Wisconsin
Structural Biology Workshop, Univ. Nebraska
Computational NMR Seminar, Univ. Cal. at Irvine
LAS NMR Workshops, Japan

2005

University of Connecticut Health Science Center
University of Copenhagen NMR Course, Denmark
NANUC NMR Course, Edmonton Canada
EMBO NMR Course, Basel Switzerland
NIEHS Bioinformatics Conference, NC
LAS NMR Workshops, Japan

2004

Yale Medical School
Harvard Medical School
Texas A+M University
LAS NMR Workshops, Japan
University of California, Irvine

2003

New York Structural Biology Center
State University of New York, Stony Brook
EMBO NMR Course, Heidelberg Germany
NANUC NMR Course, Edmonton Canada
University of California, Irvine
LAS NMR Workshops, Japan

2002

LAS NMR Workshops, Japan

2001

Genomic Science Center Symposium, Japan
Yokohama NMR Structural Biology Symposium

CCPN Meeting, Edinburgh Scotland
Washington Area NMR Group (WANG)
LAS NMR Workshops, Japan

2000

Nalorac Symposium (ENC)
LAS NMR Workshops, Japan
Texas A+M University
Ontario Cancer Institute
PNL Structural Genomics Workshop

1999

University of Georgia
University of Virginia
CHI Frontiers of NMR
LAS NMR Workshops, Japan
Nalorac Symposium (ENC)
Keystone Symposium, Frontiers of NMR
Gordon Conference, Computational NMR, Italy

1998

Yale University
Center for Advanced Research in Biotechnology
LAS NMR Workshops, Japan

1997-1990

Weizmann Institute of Science, Israel
Tsukuba International NMR Conference, Japan (3)
LAS NMR Workshops, Japan (3)
Karolinska Medical Research Institute, Sweden
ACS NYC Area NMR Meeting
Ontario Cancer Institute, Canada (2)
University of Maryland School of Medicine
Japan Young NMR Scientists Conference (2)
Johns-Hopkins University
Sloan-Kettering Cancer Center
Karolinska Medical Research Institute, Sweden
Glaxo US
Protein Engineering Centers of Excellence, Canada
Astra AB, Sweden
NATO Advanced Research Workshop, Italy

Publications

45. Y. Shen, O. Lange, F. Delaglio, P. Rossi, J.M. Aramini, G. Liu, A. Eletsy, Y. Wu, K. Singarapu, A. Lemak, A. Ignatchenko, C.H. Arrowsmith, T. Szyperski, G.T. Montelione, D. Baker, and A. Bax: Consistent blind protein structure generation from NMR chemical shift data. *Proc. Natl. Acad. Sci.* (submitted).
44. J.H. Chill, J.M. Louis, F. Delaglio and A. Bax: Local and global structure of the monomeric subunit of the potassium channel KcsA probed by NMR. *Biochim. Biophys. Acta - Biomembranes* **1768**, 3260-3270 (2007).
43. Z. Wu, F. Delaglio, K. Wyatt, G. Wistow, and A. Bax: Solution structure of γ S crystallin by molecular fragment replacement NMR. *Protein Science* **14** (12), 3101-3114 (2005).
42. R.M. Venable, F. Delaglio, S.E. Norris, D.I. Freedberg: The utility of residual dipolar couplings in detecting motion in carbohydrates: application to sucrose. *Carbohydrate Research*, **340**, 863-874 (2005).
41. G. Kontaxis, F. Delaglio, and A. Bax: Molecular Fragment Replacement approach for protein structure determination using chemical shift and dipolar coupling homology database mining. *Meth. Enzymol.*, **394**, 42-78 (2004).
40. J.L. Yan, F. Delaglio, A. Kaerner, A.D. Kline, H.P. Mo, M.J. Shapiro, T.A. Smitka, G.A. Stephenson, and E.R. Zartler: Complete relative stereo-chemistry of multiple stereocenters using only residual dipolar couplings. *J. Am. Chem. Soc.*, **126** (15) 5008-5017 (2004).
39. J. Boisbouvier, F. Delaglio, and A. Bax: Direct observation of dipolar couplings between distant protons in weakly aligned nucleic acids *P. Natl. Acad. Sci. USA*, **100** (20): 11333-11338 (2003).
38. Z. Wu, F. Delaglio, N. Tjandra, V.B. Zhurkin, and A. Bax: Overall structure and sugar dynamics of a DNA dodecamer from homoand heteronuclear dipolar couplings and P-31 chemical shift anisotropy. *J. Biomol. NMR*, **26**, 297-315 (2003).
37. T.S. Ulmer, B.E. Ramirez, F. Delaglio, and A. Bax: Evaluation of backbone proton positions and dynamics in a small protein by liquid crystal NMR spectroscopy. *J. Am. Chem. Soc.* **125**, 9179-9191 (2003).
36. J. Boisbouvier, F. Delaglio, and A. Bax: Direct observation of dipolar couplings between distant protons in weakly aligned nucleic acids, *Proc. Natl. Acad. Sci.*, **100**, 11333-11338 (2003).
35. A.T. Petkova, Y. Ishii, J.J. Balbach, O.N. Antzutkin, R.D. Leapman, F. Delaglio, R.P. Tycko: A structural model for Alzheimer's beta-amyloid fibrils based on experimental constraints from solid state NMR, *Natl. Acad. Sci. USA*, **99**, (26) 16742-16747 (2002).
34. F. Delaglio, Z. Wu and A. Bax: Measurement of homonuclear proton couplings from regular 2D COSY spectra, *J. Magn. Reson.*, **149**, 276-281 (2001).
33. J.J. Chou, F. Delaglio, and A. Bax: Measurement of ^{15}N - $^{13}\text{C}'$ dipolar couplings in medium sized proteins. *J. Biomol. NMR*, **18**, 101-105 (2000).
32. F. Delaglio, G. Kontaxis and A. Bax: Protein Structure Determination Using Molecular Fragment Replacement and NMR Dipolar Couplings. *J. Am. Chem. Soc.*, **122**, (9), 2142-2143 (2000).
31. G. Cornilescu, F. Delaglio and A. Bax: Protein backbone angle restraints from searching a database for chemical shift and sequence homology. *J. Biomol. NMR*, **13**, 289-302 (1999).
30. M. Ottiger, F. Delaglio, J.L. Marquardt, N. Tjandra and A. Bax: Measurement of Dipolar Couplings for Methylene and Methyl Sites in Weakly Oriented Macromolecules and their Use in Structure Determination. *J. Magn. Reson.*, **134**, 365-369 (1998).
29. M. Ottiger, F. Delaglio and A. Bax: Measurement of J and dipolar couplings from simplified two dimensional NMR spectra *J. Magn. Reson.*, **131**, 373-378 (1998).
28. F. Delaglio, S. Grzesiek, G. W. Vuister, G. Zhu, J. Pfeifer and A. Bax: NMRPipe: a multidimensional spectral processing system based on UNIX pipes. *J. Biomol. NMR.*, **6**, 277-293 (1995).

27. H. Kuboniwa, S. Grzesiek, F. Delaglio and A. Bax: Measurement of HN-Ha J couplings in calcium free calmodulin using new 2D and 3D water-flip-back methods. *J. Biomol. NMR*, **4**, 871-878 (1994).
26. A. Bax, F. Delaglio, S. Grzesiek and G.W. Vuister: Resonance assignment of methionine methyl groups and c3 angular information from long range proton-carbon J correlation in a calmodulin-peptide complex. *J. Biomol. NMR*, **4**, 787-797 (1994).
25. A. Bax, G.W. Vuister, S. Grzesiek, F. Delaglio, A.C. Wang, R. Tschudin and G. Zhu: Measurement of homo- and heteronuclear J couplings from quantitative J correlation. *Methods in Enzymology*, **239**, 79-105 (1994).
24. J. Anglister, A. Bax, F. Delaglio, S. Grzesiek, and G.W. Vuister: Recent Advances in the Study of Isotopically Enriched Proteins. *Journal of Cellular Biochemistry*, 243-243, Suppl. 17C (1993).
23. J. Qin, F. Delaglio, G.N. La Mar and A. Bax: Distinguishing the effects of cross correlation and J coupling in COSY spectra of paramagnetic proteins. *J. Magn. Reson. B* **102**, 332-336 (1993).
22. L.K. Nicholson, L.E. Kay, F. Delaglio, A. Bax, and D.A. Torchia: Backbone and Side-chain Dynamics of Staphylococcal Nuclease in Solution As Studied by Proton-detected C13 and N15 NMR Spectroscopy. *Biophysical Journal*, **64** (2), A182 (1993).
21. G.W. Vuister, F. Delaglio and A. Bax: The use of $^1J_{CaHa}$ coupling constants as a probe for protein backbone conformation. *J. Biomol. NMR*, **3**, 67-80 (1993).
20. G.W. Vuister, F. Delaglio and A. Bax: An empirical correlation between $^1J_{CaHa}$ and protein backbone conformation. *J. Am. Chem. Soc.*, **114**, 9674-9675 (1992).
19. L.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 mechanism on the measurement of heteronuclear T1 and T2 values in proteins. *J. Magn. Reson.*, **97**, 359-375 (1992).
18. R.E. Hoffman, F. Delaglio, and G.C. Levy: Phase Correction of 2D NMR Spectra Using DISPA. *J. Magn. Reson.*, **98** (2), 231-237 (1992).
17. F. Delaglio, D.A. Torchia and A. Bax: Measurement of nitrogen-15 carbon-13 J couplings in Staphylococcal nuclease. *J. Biomol. NMR*, **1**, 439-446 (1991).
16. A. Bax, F. Delaglio, M. Ikura, L.E. Kay, M. Clore, A. Gronenborn, D. Torchia: Multidimensional NMR of isotopically Enriched Proteins. Abstracts of Papers of the American Chemical Society, **202**, 113-PHYS, Part 2 (1991).
15. H. Grahn, U. Edlund, Y.T. van den Hoogen, C. Altona, F. Delaglio, M.W. Roggenbuck, P.N. Borer: Toward a Computer Assisted Analysis of NOESY Spectra: A Multivariate Data Analysis of an RNA NOESY Spectrum. *J. Biomol. Struct. Dyn.*, **6**, 1135-1150 (1989).
14. H. Grahn, N.M. Szeverenyi, M.W. Roggenbuck, F. Delaglio, P. Geladi: Data Analysis of Multivariate Magnetic Resonance Images. *Chemometrics and Intelligent Laboratory Systems*, **5**, 311-322 (1989).
13. H. Grahn, F. Delaglio, M.A. Delsuc and G.C. Levy: Multivariate Data Analysis for Pattern Recognition in 2D NMR. *J. Magn. Reson.*, **77**, 294-307 (1988).
12. G.C. Levy, F. Delaglio, A. Macur and J. Begemann: NMR2: A Powerful Software System for Processing Multi-Dimensional NMR Data. *Computer Enhanced Spectroscopy*, **3**, 1-12 (1986).
11. P. Sole, F. Delaglio, G.C. Levy: A Segmentation Technique for Automated Contour Selection in 2D NMR Spectroscopy. *J. Magn. Reson.*, **80**, 517-519 (1988).
10. P. Sole, F. Delaglio, A. Macur, and G.C. Levy: Quantitative Analysis of Multivariate Magnetic Resonance Images, *Internat. Labmate*, **14** (1988).
9. P. Sole, F. Delaglio, A. Macur, and G.C. Levy: Multivariate Analysis and Logic Programming in Chemical Data Analysis. *Abstracts of Papers of the American Chemical Society*, **196**, 54-COMP (1988).
8. P. Sole, F. Delaglio, A. Macur, and G.C. Levy: Interactive Image Processing for NMR Imaging and Spectroscopy. *American Laboratory*, August 1988.

7. T.J. Harner, G.C. Levy, E.J. Dudewicz, F. Delaglio, and A. Kumar: Artificial Intelligence, Logic Programming, and Statistics in Magnetic Resonance Imaging and Spectroscopic Analysis. Chapter 26, Artificial Intelligence Applications in Chemistry, ed. T.H. Price, B.A. Hohne, ACS Symposium Series, **306**, 337-349 (1986).

6. F. Delaglio, J. Goodisman and H. Brumberger: A Correlated-Cell Model for Small-Angle X-Ray Scattering of Amorphous Systems, *J. Catalysis*, **99**, 383-390 (1986).

5. J. Goodisman, F. Delaglio and H. Brumberger: Analysis of Slit-Distorted Small-Angle X-Ray Scattering Intensities Without Desmearing. *J. App. Cryst.*, **19**, 243-245 (1986).

4. H. Brumberger, Y.C. Chang, M.G. Phillips, F. Delaglio and J. Goodisman: Sintering of Pt/Al₂O₃ From Continuous Small-Angle X-Ray Scattering. *J. Catalysis*, **97** (1986).

3. H. Brumberger, F. Delaglio, J. Goodisman, and M. Whitfield: Small-Angle X-Ray Scattering Analysis of Catalysts - Comparison and Evaluation of Models. *J. App. Cryst.*, **19**, 287-299, (1986).

2. G.C. Levy, J. Begemann, A. Macur, J. Stanley, and F. Delaglio: Workstation Computers in the Spectroscopic Laboratory. *Abstracts of Papers of the American Chemical Society*, **192**, 9-CSEC (1986).

1. H. Brumberger, F. Delaglio, J. Goodisman, M.G. Phillips, J.A. Schwartz, and P. Sen: Investigation of the SMSI Catalyst Pt/TiO₂ By Small-Angle X-Ray Scattering. *J. Catalysis*, **92** (2), 199-210 (1985).