



Frank Delaglio, Ph.D.

delaglio@nih.gov

406 Pensacola Drive
Gaithersburg MD 20878
Tel: 301 806-0867
Fax: 301 947-3390

Objective

Continuing a leadership career in scientific software development and computational analysis for commercial and research applications, emphasizing multidimensional spectroscopy, drug discovery, database mining, and proteomics.

1991-Present

Special Expert (now Scientist on permanent staff)

National Institutes of Health, Section on Biophysical NMR, NIDDK LCP

Principal software scientist for a world-leading multidimensional 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 support of NMR biomolecular structure determination.

Succeeded in implementing a comprehensive set of multidimensional spectral processing and analysis software tools, supporting both routine and research-oriented applications. This software, called the NMRPipe System, is used in over 400 academic and commercial sites in the Americas, Europe, and Asia. Implemented NMRWish, a spectral analysis environment based on the Tcl/Tk scripting language; applications include protein backbone angle prediction from a chemical shift database (the widely used TALOS program), and automated processing, quantification, and multivariate analysis of 1D STD and 2D HSQC spectral series as used in drug discovery protocols.

Current research emphasizes novel approaches to improve the speed and effectiveness of protein structure determination using homology based on NMR observables. An aspect of this work is development of a new software system for simulated annealing, structure calculation, and homology search. This system, called DYNAMO, was used to develop the first protocols illustrating the possibility of determination of protein folds exclusively from database mining with chemical shift and dipolar couplings, without the use of NMR distance restraints.

1991-Present

Software Science Consultant

Software applications consultant to numerous leading pharmaceutical companies emphasizing structure-based drug design.

Scientific software advisor to companies developing and supporting spectral analysis and imaging software.

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.

Extended NMRPipe for visualization and analysis of multivariate infrared spectroscopic images. Adapted the UNIX-based NMRPipe for commercial use on WindowsNT/2002/XP platforms.

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, X11, Tk/TCL, FORTRAN, etc.

Experienced with HTML and Web Design, currently NMR group's webmaster.

Education

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

Osaka University, 2000-2001
Ph.D., Graduate Dept. of Pharmaceutical Sciences

Invited Presentations

2004

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, Edinburg 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
Osaka University
University of Tokyo
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

Weizmann Institute of Science, Israel
Tsukuba International NMR Conference, Japan
LAS NMR Workshops, Japan
Karolinska Medical Research Institute, Sweden

1996

ACS NYC Area NMR Meeting
Ontario Cancer Institute, Canada
LAS NMR Workshops, Japan
University of Maryland School of Medicine
Tsukuba International NMR Conference, Japan

1995

Japan Young NMR Scientists Conference
LAS NMR Workshops, Japan
Johns-Hopkins University
Tsukuba International NMR Conference, Japan

1994

Japan Young NMR Scientists Conference
Sloan-Kettering Cancer Center
Karolinska Medical Research Institute, Sweden
Glaxo US

1993

Protein Engineering Centers of Excellence, Canada
LAS NMR Workshops, Japan
Ontario Cancer Institute, Canada

1992

LAS NMR Workshops, Japan
Ontario Cancer Institute, Canada

1991

JTC NMR Workshops, Japan
Astra AB, Sweden

1990

NATO Advanced Research Workshop, Italy.

Publications

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.*, in press (2004).

J.L. Yan, F. Delaglio, A. Kaerner, A.D. Kline, H.P. Mo, M.J. Shapiro, T.A. Smitka, G.A. Stephenson, E.R. Zartler: Complete relative stereochemistry of multiple stereocenters using only residual dipolar couplings. *J. Am. Chem. Soc.*, **126** (15) 5008-5017 (2004).

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).

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).

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).

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).

F. Delaglio, Z. Wu and A. Bax: Measurement of homonuclear proton couplings from regular 2D COSY spectra, *J. Magn. Reson.*, **149**, 276-281 (2001).

J.J. Chou, F. Delaglio, and A. Bax: Measurement of ¹⁵N-¹³C' dipolar couplings in medium sized proteins. *J. Biomol. NMR*, **18**, 101-105 (2000).

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).

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).

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).

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).

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).

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).

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).

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).

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).

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).

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 ¹³C and ¹⁵N NMR Spectroscopy. *Biophysical Journal*, **64** (2), A182 (1993).

- 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).
- 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).
- 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).
- 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).
- 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).
- 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).
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- 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).
- 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).
- 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).
- P. Sole, F. Delaglio, A. Macur, and G.C. Levy: Quantitative Analysis of Multivariate Magnetic Resonance Images, *Internat. Labmate*, **14** (1988).
- 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).
- P. Sole, F. Delaglio, A. Macur, and G.C. Levy: Interactive Image Processing for NMR Imaging and Spectroscopy. *American Laboratory*, August 1988.
- 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).
- 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).
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- 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).
- 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).