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Digital Filtering with a Sinusoidal Window Function: An Alternative Technique for Resolution Enhancement in FT NMR

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As an alternative to convolution difference techniques for resolution enhancement in the ^{1}H NMR spectra of proteins, digital filtering of the FID with a sinusoidal window function is suggested. As an illustration, this "sine bell routine" was applied to the high-field region of the ^{1}H NMR spectrum at 360 MHz of the basic pancreatic trypsin inhibitor.

Even with the highest currently available magnetic fields, the spectral resolution in the ^{1}H NMR spectra of proteins and other macromolecules is limited by the mutual overlap of the resonance lines of individual groups of protons (Fig. 1A). In FT NMR,

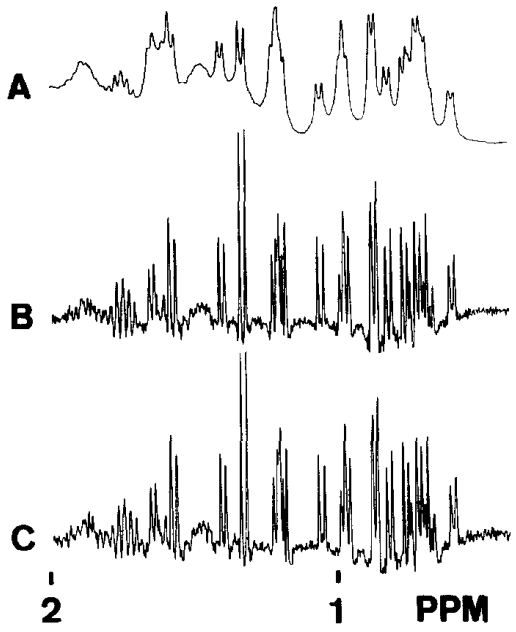

FIG. 1. Aliphatic region of the FT ^{1}H NMR spectrum at 360 MHz of the basic pancreatic trypsin inhibitor, 0.01 M solution in D_2O, 225 scans, 4000 Hz spectral width, 2 sec acquisition time, 16K of memory in the time domain. (A) Normal spectrum. The natural linewidth $\Delta\omega_{1/2}$ is approximately 20 rad sec^{-1}. (B) Same spectrum as (A) after digital filtering of the FID with the sine bell routine. (C) Same spectrum as (A) after application of the convolution difference routine with $\tau_1 = \infty$, $\tau_2 = 0.31$ sec, $K = 1$.

MONTE VERITA`

ASCONA

Centro Stefano Franscini

Swiss Federal Institute of Technology Zurich

Associazione Antonio De Marco

Milan, Italy

Workshop on

NMR Spectroscopy and the Protein Folding Problem

September 28 - October 3, 1997

The ways by which a polypeptide chain, with its genetically determined amino acid sequence, assumes its three-dimensional structure is one of the big unsolved problems of biology. Nuclear magnetic resonance (NMR) spectroscopy enables structural studies of proteins in non-crystalline milieus similar to those where protein folding occurs. In this workshop the potentialities of NMR applications for studies of the protein folding problem will be discussed.

Organizers: *Prof. Henriette Molinari* (University of Verona, Italy), *Prof. Kurt Wüthrich* (Swiss Federal Institute of Technology, Zurich), *Dr. Lucia Zetta* (CNR, Milan, Italy)

The conference is sponsored by the Swiss National Science Foundation (Berne), Swiss Academy of Sciences, the CSF (Swiss Federal Institute of Technology Zurich) and the Associazione Antonio De Marco (Milan)

Symposium "NMR Spectroscopy and the Protein Folding Problem"

September 28-October 3, 1997, Ascona, Switzerland

Scientific Program

Sunday, September 28

18.00 Welcome Apero
19.00 Dinner

Opening session Chairperson: L. Zetta.

20.30-2045 Welcome and Information on the "Associazione Antonio De Marco".
20.45-21.45 Keynote Lecture I: R. Jaenicke
Protein Folding in Vitro and in Vivo

Monday, September 29

Morning session Chairperson: K. Wüthrich

09.00-10.00 Keynote Lecture II: A. Fersht
Protein Folding: the New View from NMR and Protein Engineering
10.00-10.30 Coffee
10.30-11.10 A. Plückthun
The Protein Folding Pathway and Antibody Fragments: a Model for Two-Domain Proteins
11.10-11.50 R. Zahn
Molecular Chaperone-Activity Analysed by Amide Proton Exchange
11.50-12.20 General Discussion

12.30 Lunch

Afternoon session Chairperson: A. Gräslund

16.30-17.00 Coffee
17.00-17.40 L. Serrano
Design and Structural Characterization of Structured Monomeric Peptides. Implications for Protein Folding and Thermostability
17.40-18.20 A. Tramontano
Advantages and Pitfalls of Molecular Modelling: the Hepatitis C Serine Proteinase
18.20-18.40 General Discussion

19.00 Dinner

Evening session Chairperson: H. Molinari

20.30-21.10 H. Roder
Structural and Kinetic Description of Submillisecond Folding Events
21.10-21.50 T. Oas
Use of Dynamic NMR to Measure Ultrafast Protein Folding Rates
21.50-22.10 General Discussion

Tuesday, September 30

Morning session Chairperson: H. Senn

09.00-09.50 C. Dobson
Mapping the energy landscapes for Protein Folding
09.50-10.30 Y. Goto
Folding of β-Lactoglobulin, a Predominantly β-Sheet Protein with High Helical Propensity
10.30-11.00 Coffee
11.00-11.40 L. Gierasch
Folding of Cellular Retinoic Acid Binding Protein, a Predominantly Beta-Sheet Protein with an Internal Cavity
11.40-12.10 General discussion

12.15 Lunch

Afternoon session

16.30-17.00 Coffee
17.00-18.45 Posters and informal discussions

Evening session Chairperson: C. Dobson

20.30-21.10 M. Rossi
Protein Assisted Folding at High Temperature

21.10-21.50 K. Akasaka
Effect of Pressure on Protein Structure and Folding

21.50-22.10 General Discussion

Wednesday, October 1

Morning session Chairperson: F. Poulsen

09.00-09.50 P. Wright
Characterization of the Structure and Dynamics of Unfolded States and Folding Intermediates

09.50-10.30 G. Wider
Characterization of Unfolded States of Proteins in Solution

10.30-11.00 Coffee

11.00-11.40 D. Shortle
Characterization of the Residual Structure in the Denatured State of Staphylococcal Nuclease

11.40-12.10 General Discussion

12.15 Lunch

Afternoon and evening: Excursion

Thursday, October 2

Morning session Chairperson: L. Gierasch

09.00-09.50 R.Glockshuber
Random Approaches to Study Protein Folding

09.50-10.30 P. Temussi
Conformational Preferences of Proteins and Peptides in Viscous Media

10.30-11.00 Coffee

11.00-11.40 J. Dyson
Exploration of the Folding Pathways of Proteins Using Mutants

11.40-12.10 General Discussion

12.15 Lunch

Afternoon session

16.30-17.00 Coffee

17.00-18.45 Posters and informal discussions

19.00 Dinner

Evening session Chairperson: F. Toma

20.30-21.10 A. Fontana
Probing Partly Folded States of Proteins by Limited Proteolysis

21.10-21.50 K. Wüthrich
Protein Folding in Transmissible Spongiform Encephalopathies

21.50-22.10 General Discussion

Friday, October 2

Morning session Chairperson: J. Dyson

09.00-09.40 A. Alexandrescu
NMR Studies of Structure Formation in Proteins that Share a Common Fold

09.40-10.20 T. Szyperski
Unfolding of the Valyl-Rich α-Helix of SP-C Studied by NMR, CD and FTIR

10.20-10.40 General Discussion

10.40 -11.10 Coffee

11.10-12.10 Closing lecture: R. Baldwin
Nature of the pH4 Folding Intermediate of Apomyoglobin

12.15 Farewell, Lunch, Departure

"Giornata di Studio della Divisione di Chimica dei Sistemi Biologici della Società Chimica Italiana"

Co-Organised with

Istituto di Biocatalisi e Riconoscimento Molecolare - CNR
and
Fondazione Antonio De Marco

Modelling and Computational Methods: New perspectives in the study of folding and binding mechanisms of biomolecules

29th March 2001, Sala Convegni, Area della Ricerca CNR, Via Ampère 56, Milano

9.15 Opening remarks: Henriette Molinari President of the "Divisione di Chimica dei Sistemi Biologici"

Chairperson:	Giacomo Carrea (IBRM-CNR of Milano)	
9.30- 10.30	**Herman Berendsen**	(University of Groningen , The Netherlands) Detection of 'foldons' in proteins and simulation of the folding of a peptide fragment. Comparison with NMR measurements
10.30-11.05	**Rita Casadio**	(University of Bologna) From sequence to 3D structure: the prediction of contact maps of proteins
11.05.11.30	Coffee break	
Chairperson:	Herman Berendsen	(University of Groningen, The Netherlands)
11.30-12.05	**Federico Fogolari**	(University of Verona) Simulation of electrostatics in biomolecular systems
12.05-12.40	**Giorgio Colombo**	(IBRM-CNR of Milano and University of Groningen) Molecular dynamics simulations of beta-sheet peptide folding
12.40-13.15	**Anna Bernardi**	(University of Milano) Design and synthesis of GM1 mimics as binders for Cholera toxin
13.15-14.30	Lunch	
Chairperson:	Henriette Molinari	(University of Verona)
14.30-15.05	**Lucia Zetta**	(ICM-CNR of Milano) Unfolding studies of the extreme heat- and pressure-resistant Sso7d protein from *Sulfolobus solfataricus*
15.05-15.40	**Luigi Casella**	(University of Pavia) Phenol nitration catalyzed by heme proteins in the presence of nitrite/hydrogen peroxide: a potential mechanism of nitric oxide-dependent toxicity
15.40-16.15	**Hugo Monaco**	(University of Verona) The liver (basic) fatty acid-binding proteins
16.15-16.30	Concluding remarks	