

smr1316/Programme

Speakers and dates in alphabetic order.

Amzel 13

Evaluation of Entropy Changes in Binding and Folding

Bastolla 21

Connectivity of neutral networks and the substitution process in protein evolution (15 min talk)

Broglia 12

Reading the three--dimensional structure of lattice model designed proteins from their amino acid sequence

Bruscolini 21

Nonpolar compounds and polymers hydration: a simple hydration model, a lattice mean field technique, and experimental result (15 min talk)

Butt 15

Protein Composition of Spring Wheats Grown in Pakistan (15 min talk)

Carlioni 20

Ab Initio Approach to Drug-Target Interactions

Cassia-Moura 13

Memory Effect on Biomembrane-Protein (15 min talk)

Cecconi 14

Molecular Dynamics Studies on HIV-1 Protease: Drug Resistance and Folding Pathways

Chan 11, 12

1. Polymer Principles of Protein Calorimetric Two-State Cooperativity
2. Towards a Consistent Modelling of Protein Thermodynamics and Kinetic Cooperativity

Chang 20

A Route to a Solution of the Protein Threading Problem by Learning

Chen 21

Stochastic Dynamics Simulation of Proteins with Full Poisson-Boltzmann Electrostatics (15 min talk)

Clementi 11

Topology and energetics in protein folding: beyond the Go-like approach

Dadlez 12

Folding initiation sites as detected by disulfide formation kinetics I

De Los Rios 12

Protein Design with Explicit Solvent (15 min talk)

DesJarlais 12, 15

1. Protein Design: Predicting Sequence from Structure
2. Determinants of Conformational Change

Dill 14, 18

1. A Simple Model of Water, the Hydrophobic Effect
2. Ion Solvation

Dokholyan 14, 15

1. Understanding hierarchical protein evolution from the first principles
2. Direct observation of folding transition state ensemble of C-Src SH3 domain in molecular dynamics simulations

Doniach 18, 21

1. Protein folding and misfolding
2. Protein folding and misfolding

Domany 14

- Part A. Automated Protein Structure Classification
- Part B. Do Contact Vectors Determine a Protein's Structure?

Eaton 15, 19

1. Fast processes in protein folding
2. Simple models for protein folding Simple models for protein folding

Ejtehadi 14

The ground states in HP lattice models

Garcia 14, 21

1. Atomic Simulations of Helix-Coil Transition in Peptides
2. Water Penetration in Proteins

Godzik 19

Goldstein 18, 21, 22

1. Evolutionary Perspectives on Protein Folding, Stability, and Function
2. Evolutionary Perspectives on Protein Folding, Stability, and Function
3. Evolutionary Perspectives on Protein Folding, Stability, and Function

Hackl 21

Irback 18

Folding Thermodynamics of Small Helical Proteins: A Model Study

Jernigan 15, 18

1. Extracting Functional Motions from Protein Structures
2. Strong Packing Regularities in Proteins

L Kuhn 18, 20

1. Protein Unfolding Pathways and Folding Nucleation Sites Predicted by Graph Theory
2. Modeling Protein and Small Molecule Flexibility in Ligand Screening and Docking

Lesk 19, 22

1. Prediction of Protein Function from Structure.
2. Conformational Changes in Proteins.

Maddocks 13

Modelling of the Folding Twisting and Bending of DNA

Matthews: 11, 13, 14

1. (Introductory Talk): Challenges and Opportunities in Experimental Protein Folding
2. Rough Energy Landscapes: Early Commitments Can Have Long-lasting Consequences
3. Conserved Folding Mechanisms in Homologous Proteins: Are Mechanisms better Conserved than Sequences?

Mai 13

Side Chain Effect on Protein Folding

Micheletti 14

Protein-like structures emerging from general variational principles

Mirny 19

What Evolution Can Tell us about Protein-DNA Interactions.

Molinari 15

Folding and interaction studies of beta-lactoglobulins

Mozzarelli 15

Unfolding of PLP-Dependent Enzymes

Oliveberg 19, 20

Plaxco 20

The convergence of theory and experiment in the folding of the simplest proteins

Privalov 12, 15

1. Climbing the Hierarchy of Protein Structure
2. Climbing the Hierarchy of Protein Structure

Settanni 14

The Role of Topology in the Stabilization of Intracellular Ig Domains

Shifman 11

Redesign of Calmodulin Receptor Directed Towards Improving its Binding Specificity (15 min talk)

Simon 13, 19

1. Topology of Transmembrane Proteins
2. Stabilization Centers and Protein Stability

Srivastava 21

Orthogonalization of vectors

Thorpe 18, 20

1. Ligand and Protein Flexibility using Constraint Theory
2. Protein Unfolding: Rigidity Lost

Tiana 12

Statistical analysis of contact formation in model proteins

Tramontano 20

Advancements and pitfalls in protein comparative modelling

Trinh 14

Sequencing of folding events in model proteins (15 min talk)

Vaiana 12

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Protein Conformation vs Aggregation: Interaction Between Processes in Two Cases of Different Complexity

Vendruscolo 19

Structural Determination of Partially Folded States of Proteins from Residue-Specific Experimental Data

Vishveshwara 13

Insights on Structure and Topology of Proteins from Graph Spectral Method

White 11, 13

1. Energetics of Folding Proteins into Membranes
2. Global Statistics of Protein Sequences

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PROGRAM OF THE WORKSHOP " PROTEIN FOLDING, STRUCTURE AND DESIGN"

@@@@@@@@@@@@@@@@@@@@@ WEEK I @@@@@@@@@@@@@@@@@@@@@@

***** MONDAY June 11 *****

8:30 REGISTRATION

9:45 C R Matthews

Introductory Talk: Challenges and Opportunities in Experimental Protein Folding I

10:30 COFFEE BREAK

11:00 H S Chan

Polymer Principles of Protein Calorimetric Two-State Cooperativity

11:45 S White

Global Statistics of Protein Sequences I

12:30 LUNCH

14:00 C Clementi

Topology and energetics in protein folding: beyond the Go-like approach

14:45 M R Ejtehadi

The ground states in HP lattice models

15:30 COFFEE BREAK

16:00 J M Shifman

Redesign of Calmodulin Receptor Directed Towards Improving its Binding Specificity

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16:15 End

***** TUESDAY June 12 *****

9:00 P Privalov
Climbing the Hierarchy of Protein Structure I

9:45 J DesJarlais
Protein Design: Predicting Sequence from Structure I

10:30 COFFEE BREAK

11:00 M Dadlez
Protein Folding Initiation Structures as Detected by the Disulphide
Formation Kinetics Studies.

11:45 H S Chan
Towards a Consistent Modelling of Protein Thermodynamics and Kinetic
Cooperativity

12:30 LUNCH

14:00 G Tiana
Statistical analysis of contact formation in model proteins

14:45 R Broglia
Reading the three--dimensional structure of lattice
model designed proteins from their amino acid sequence

15:30 COFFEE BREAK

16:00 S Vaiana
Protein Conformation vs Aggregation: Interaction Between
Processes in Two Cases of Different Complexity

16:15 P De Los Rios
Protein Design with Explicit Solvent

16:30 End

***** WEDNESDAY June 13 *****

9:00 C R Matthews
Rough Energy Landscapes: Early Commitments Can Have
Long-lasting Consequences II

9:45 M Amzel
Evaluation of Entropy Changes in Binding and Folding

10:30 COFFEE BREAK

11:00 S Vishveshwara
Insights on Structure and Topology of Proteins from Graph Spectral
Method.

11:45 J Maddocks
Modelling of the Folding Twisting and Bending of DNA

12:30 LUNCH

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14:00 I Simon
Topology of Transmembrane Proteins I

14:45 S H White
Energetics of Folding Proteins into Membranes II

15:30 COFFEE BREAK

16:00 R Cassia-Moura
Memory Effect on Biomembrane Protein

16:15 S L Mai
Side Chain Effect on Protein Folding

16:30 End

***** THURSDAY June 14 *****

9:00 C R Matthews:
Conserved Folding Mechanisms in Homologous Proteins: Are
Mechanisms Better Conserved than Sequences? III

9:45 E Domany
Part A. Automated Protein Structure Classification
Part B. Do Contact Vectors Determine a Protein's Structure?

10:30 COFFEE BREAK

11:00 K Dill
A Simple Model of Water, the Hydrophobic Effect I

11:45 N V Dokholyan
Understanding hierarchical protein evolution from the first principles I

12:30 LUNCH

14:00 A Garcia
Atomic Simulations of Helix-Coil Transition in Peptides

14:45 C Micheletti
Geometrical Aspects of Protein Folding

15:30 COFFEE BREAK

16:00 G Settanni
The Role of Topology in the Stabilization of Intracellular Ig Domains

16:15 F Cecconi
Molecular Dynamics Studies on HIV-1 Protease: Drug Resistance and
Folding Pathways

16:30 H X Trinh
Sequencing of folding events in model proteins

16:45 POSTER SECTION I

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***** FRIDAY June 15 *****

9:00 W A Eaton
Fast processes in protein folding I

9:45 J DesJarlais
Determinants of Conformational Change II

10:30 COFFEE BREAK

11:00 P Privalov
Climbing the Hierarchy of Protein Structure II

11:45 R. Jernigan
Extracting Functional Motions from Protein Structures I

12:30 LUNCH

14:00 H Molinari
Folding and interaction studies of beta-lactoglobulins

14:45 N Dokholyan
Direct observation of folding transition state ensemble of
C-Src SH3 domain in molecular dynamics simulations II

15:30 COFFEE BREAK

16:00 A Mozzarelli
Unfolding of PLP-Dependent Enzymes

16:45 End

@@@@@@@@@@@@@@@@@@@@ II WEEK @@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@@

***** MONDAY June 18 *****

9:00 M F Thorpe
Ligand and Protein Flexibility using Constraint Theory I

9:45 L Kuhn
Protein Unfolding Pathways and Folding Nucleation
Sites Predicted by Graph Theory I

10:30 COFFEE BREAK

11:00 Doniach
Protein Folding and Misfolding I

11:45 K Dill
Ion Solvation II

12:30 LUNCH

14:00 R. Goldstein
Evolutionary Perspectives on Protein Folding, Stability and Function I

14:45 R Jernigan
Strong Packing Regularities in Proteins II

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15:30 COFFEE BREAK

16:00 A Irback
Folding Thermodynamics of Small Helical Proteins: A Model Study

16:45 End

***** TUESDAY June 19 *****

9:00 W A Eaton
Simple models for protein folding II

9:45 I Simon
Stabilization Centers and Protein Stability II

10:30 COFFEE BREAK

11:00 A M Lesk
Prediction of Protein Function from Structure I

11:45 M Oliveberg
Protein engineering analysis of two-state folding I

12:30 LUNCH

14:00 L Mirny
What Evolution Can Tell us about Protein-DNA Interactions

14:45 M Vendruscolo
Structural Determination of Partially Folded States of Proteins
from Residue-Specific Experimental Data

15:30 COFFEE BREAK

16:00 Godzik
??????????(to be communicated)

16:45 M S Butt
Protein Composition of Spring Wheats Grown in Pakistan

17:00 End

***** WEDNESDAY June 20 *****

9:00 A Tramontano
Advancements and pitfalls in protein comparative modelling

9:45 M Oliveberg
Folding gate keepers: experimental evidence for anti-design II

10:30 COFFEE BREAK

11:00 Plaxco
The convergence of theory and experiment in the folding of the

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simplest proteins

11:45 M F Thorpe
Protein Unfolding: Rigidity Lost II

12:30 LUNCH

14:00 L Kuhn
Modeling Protein and Small Molecule Flexibility in
Ligand Screening and Docking II

14:45 I Chang
A Route to a Solution of the Protein Threading Problem by Learning

15:30 COFFEE BREAK

16:00 P Carloni
Ab Initio Approach to Drug-Target Interactions

16:45 POSTER SECTION II

***** THURSDAY June 21 *****

9:00 S Doniach
Protein folding and misfolding II

9:45 A Garcia
Water Penetration in Proteins II

10:30 COFFEE BREAK

11:00

11:45 R Goldstein
Evolutionary Perspectives on Protein Folding, Stability and Function II

12:30 LUNCH

14:00 V Srivastava
Orthogonalization of vectors

14:45 E Hackl
??????? (to be communicated)

15:30 COFFEE BREAK

16:00 P Bruscolini
Nonpolar compounds and polymers hydration: a simple hydration model, a
lattice mean field technique, and experimental results

16:15 W Chen
Stochastic Dynamics Simulation of Proteins with Full Poisson-Boltzmann
Electrostatics

16:30 U. Bastolla
Connectivity of neutral networks and the substitution process in

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protein evolution

16:45 End

***** FRIDAY June 22 *****

9:00 A M Lesk

Conformational Changes in Proteins II

9:45 R Goldstein

Evolutionary Perspectives on Protein Folding, Stability and Function III

10:30 COFFEE BREAK

11:00 Closing talk

11:45 END

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