

LOSCHMIDT
LABORATORIES

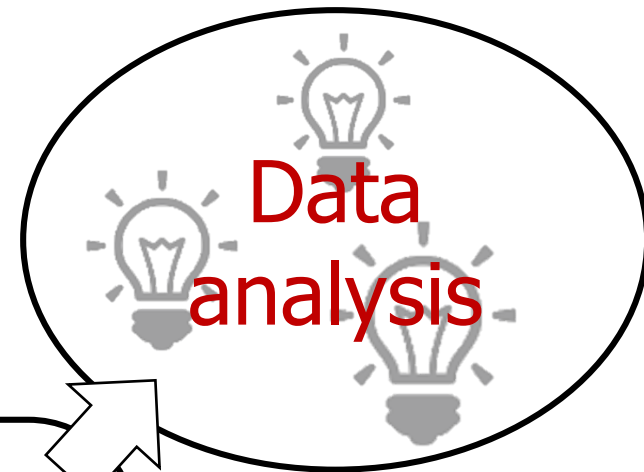


Bi1051: Loschmidt Laboratories

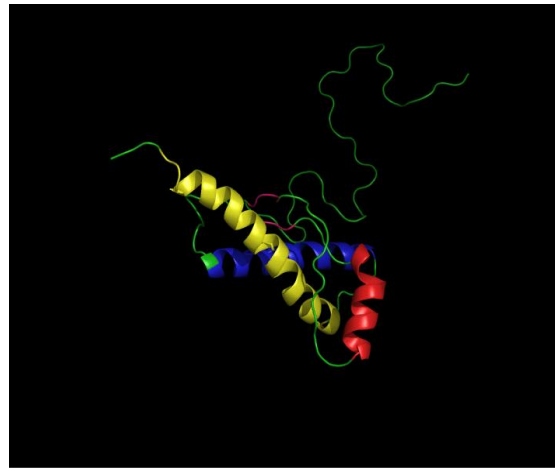
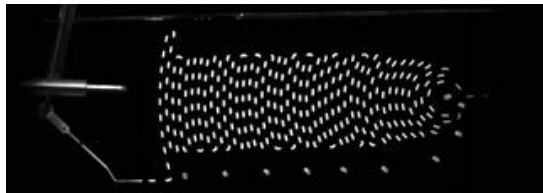
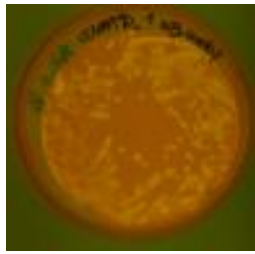
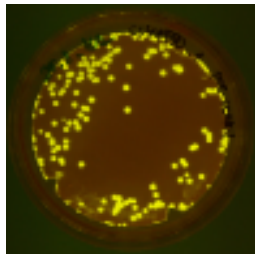
Stanislav Mazurenko, PhD

11/05/2020

Motivation



Experiments

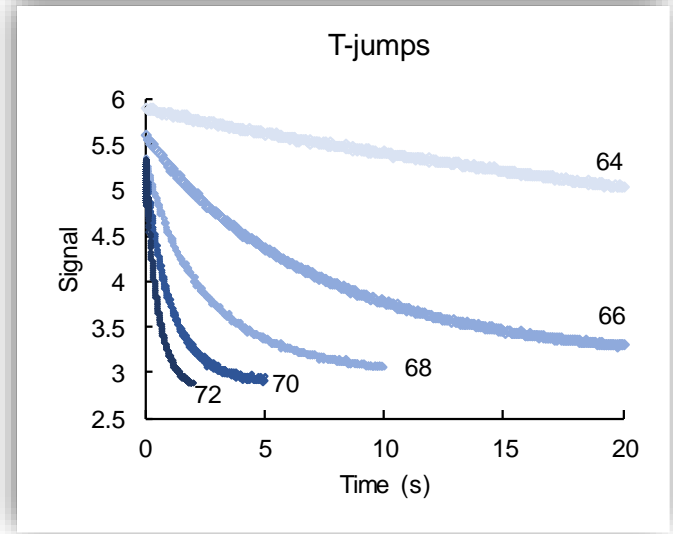
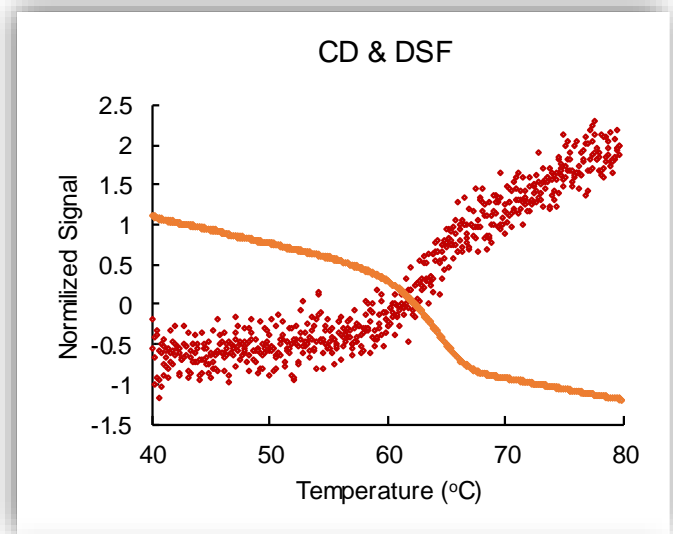
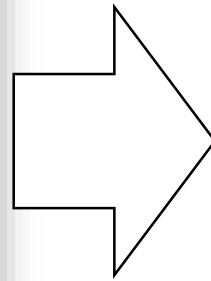


0.2 ns



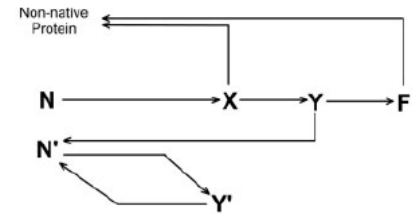
Analysis for Protein Denaturation

Input



Data analysis

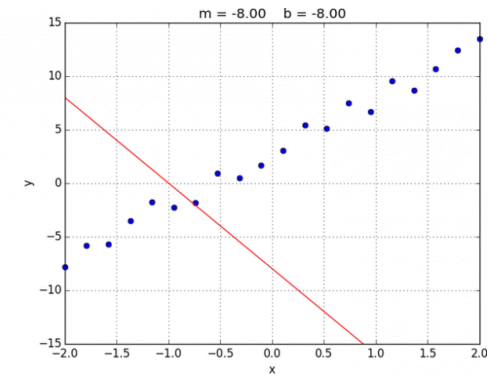
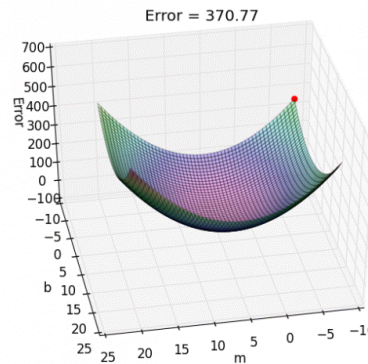
- Graphs



- Dynamical systems

$$\begin{cases} \frac{dx_N}{dt} = -k_1 x_N + k_{-1} x_I, \\ \frac{dx_I}{dt} = k_1 x_N - (k_{-1} + k_2) x_I, \\ \frac{dx_D}{dt} = k_2 x_I, \\ x_N + x_I + x_D = 1, \end{cases}$$

- Optimization



Results



v1.3

Analysis of protein thermal denaturation data



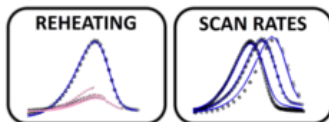
Submit job Help Example

Job ID: e.g. xxxxxx

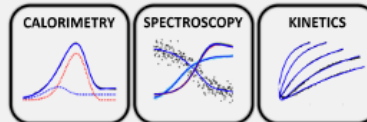
Find job

SELECT TYPE OF INPUT DATA

DSC FIT



GLOBAL FIT



Load example

Add new calorimetry data file

Add new spectroscopy data file

Add new kinetics data file

DATA FILE #1 (CALORIMETRY)

Remove data file

Add new dataset

Data preview

name	temperature	heat capacity	scan rate	
Dataset 1.1	1.0 (T)	1.0 (CP)	1	⬆️ ⬆️ ⬇️
Dataset 1.2	2.0 (T)	2.0 (CP)	2	⬆️ ⬆️ ⬇️
Dataset 1.3	3.0 (T)	3.0 (CP)	0.5	⬆️ ⬆️ ⬇️

temperature: °C

heat capacity: cal/T/mol

REFERENCE

Mazurenko, S., Stourac, J., Kunka, A., Nedeljkovic, S., Bednar, D., Prokop, Z., Damborsky, J., 2018: CalFitter: A Web Server for Analysis of Protein Thermal Denaturation Data. *Nucleic Acids Research* 46 (W1): W344-W349.



USER STATISTICS

Number of visitors: 2133

266

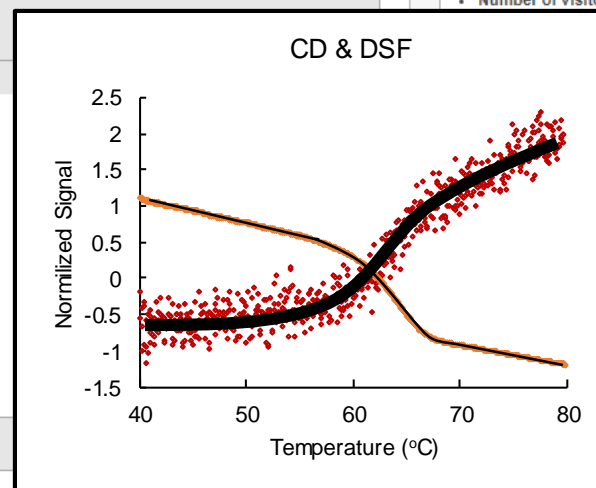
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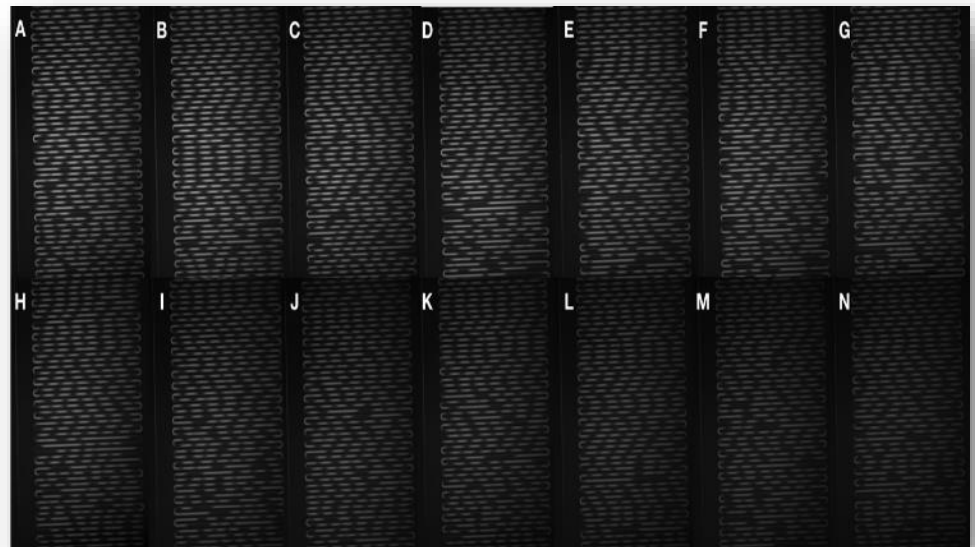
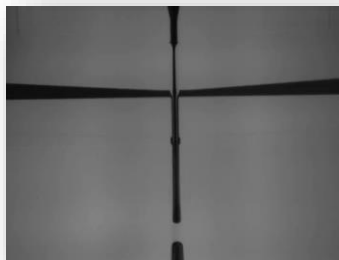
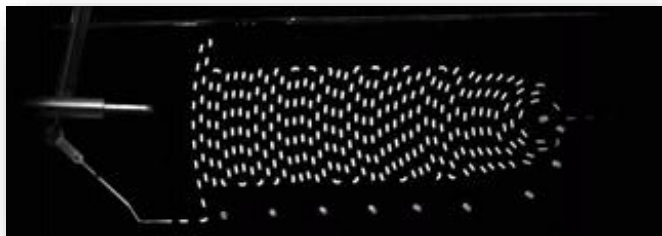
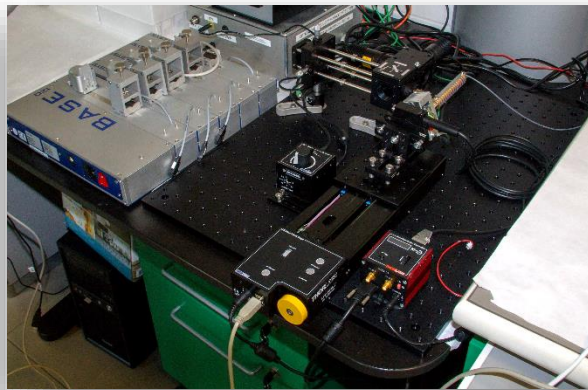
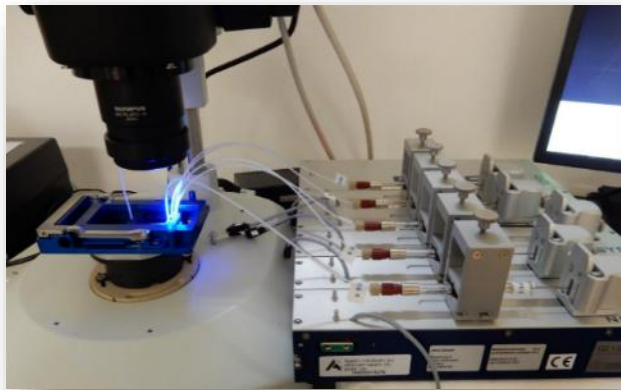
4Sys



A blue-tinted image showing a network of interconnected microfluidic channels or a porous structure, likely a microfluidic chip or a porous medium, used for fluid flow and analysis.

Analysis for Microfluidics

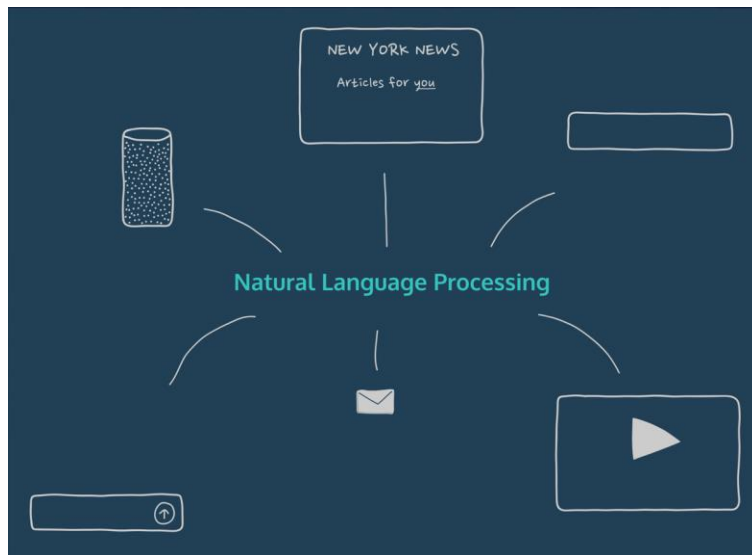
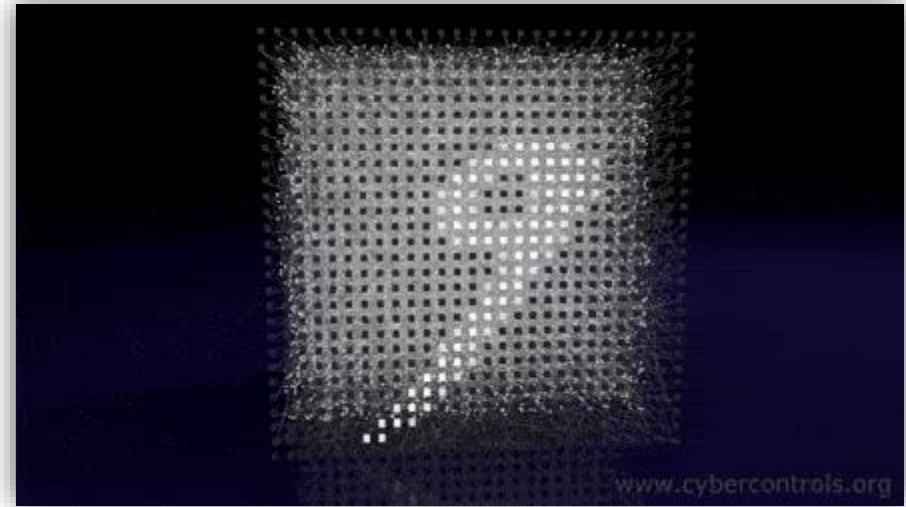
Microfluidics





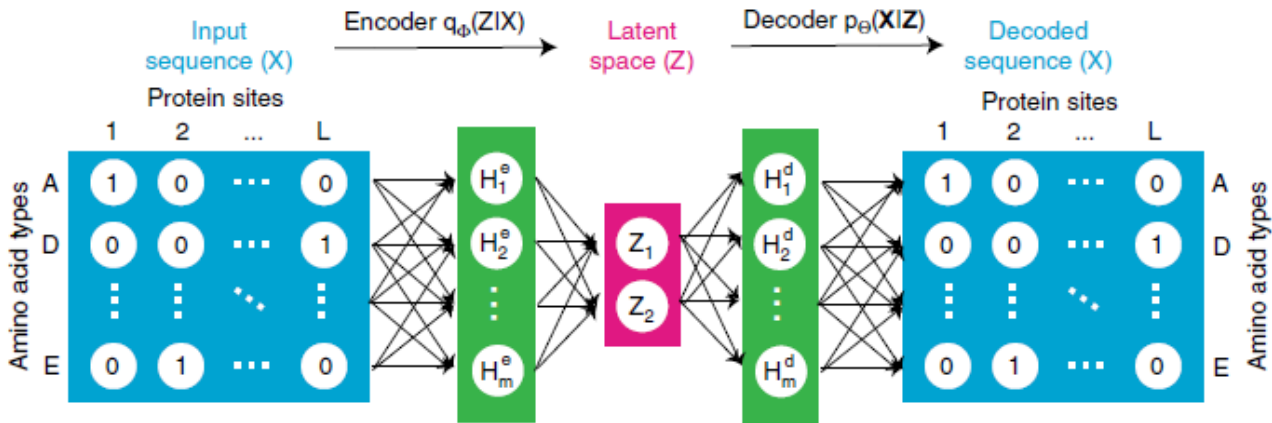
Machine Learning for Protein Engineering

Artificial Intelligence



Predicting protein stability

Protein 1: LTLEEIIGIGGFGKV... stable
 Protein 2: WIGDEVAVKAARH... unstable
 Protein 3: IENVRIGIKLFAML... stable
 ...
 KLAAPPSIGIEPFM... stable



Further reading

- Articles:

Musil M, Konegger H, Hon J, Bednar D, Damborsky J. Computational design of stable and soluble biocatalysts. [ACS Catalysis. 2018](#)

Mazurenko S, Prokop Z, Damborský J. Machine Learning in Enzyme Engineering. [ACS Catalysis. 2019](#)

Mazurenko S, Stourac J, Kunka A, Nedeljković S, Bednar D, Prokop Z, Damborsky J. CalFitter: a web server for analysis of protein thermal denaturation data. [Nucleic acids research. 2018](#)

- Courses:

[Bi9410](#) Structural Biology

[Bi7430](#) Molecular biotechnology

[Bi9680en](#) Artificial Intelligence in Biology, Chemistry, and Bioengineering