RNA结构分析：prediction

意义——

- Ribozymes的功能

  Group I/II introns；Rnase P；ribosome…
  the “RNA world” in the origin of life…

- Aptamers和配体的相互作用

  RNA or DNA molecules that fold into higher-ordered structures and form complexes with specific ligands.（参与代谢通路调节）

- LncRNA（功能多样...）

RNA structure prediction

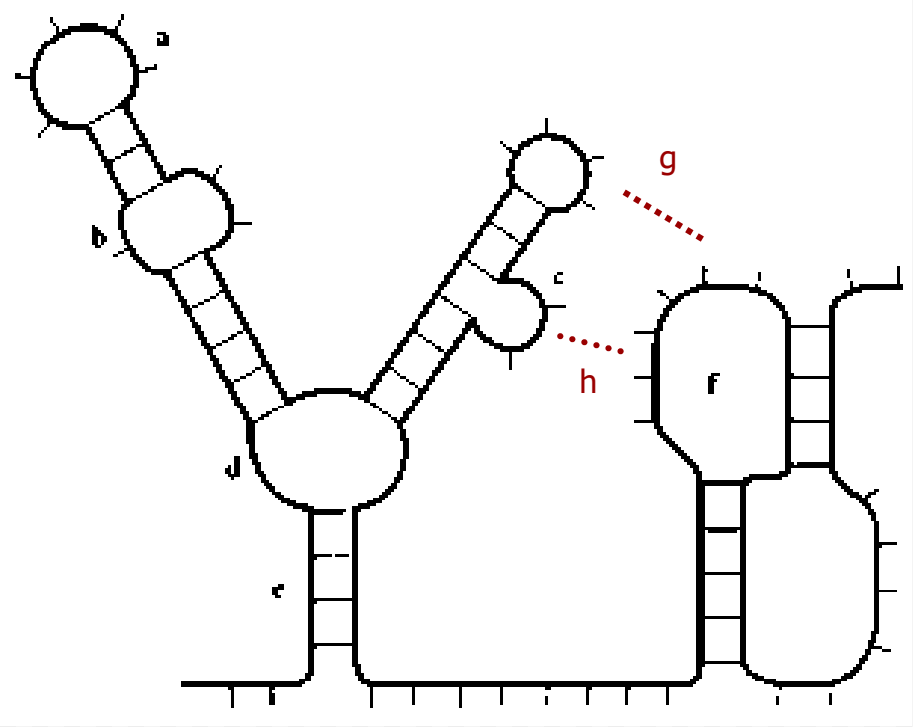
- Secondary structures

  --- AU, CG; GU. (canonical base pairs)

- Tertiary structures

  --- 3D arrangement of the atoms.

RNA secondary structures



a. hairpin loop
b. internal loop
c. bulge loop
d. multibranched loop
e. stem
f. Pseudoknot
g. Kissing hairpins
h. Hairpin-bulge contact

Prediction methods (RNA)

- Ab initio prediction
- Evidence-associated prediction
- Genetic algorithm
- Specific sequences with known structures ~ knowledge-based

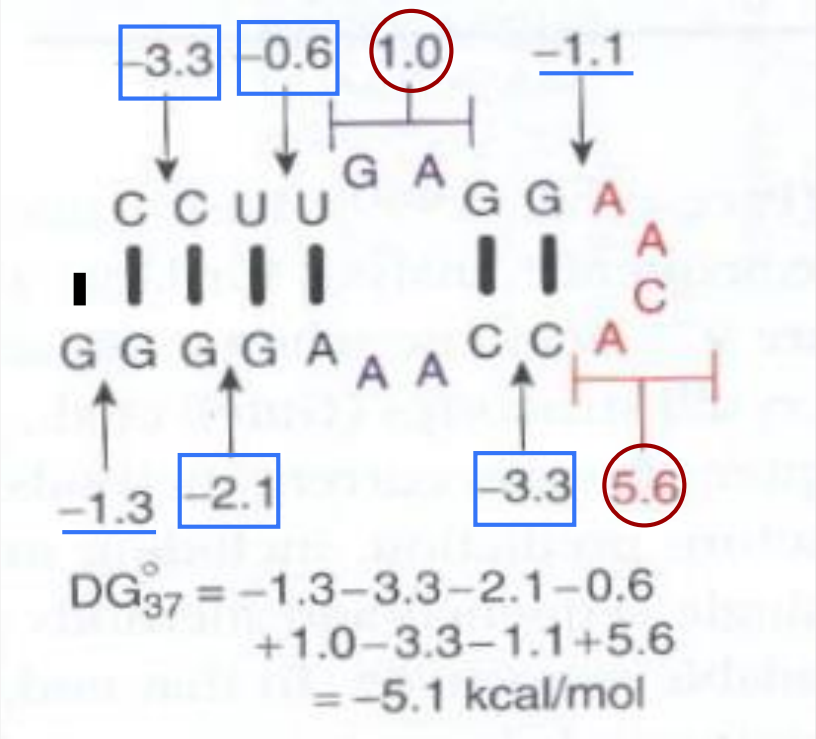
Ab initio prediction

- Choosing the most energetically stable sets from the many possible choices of complementary sequences.
- Limitation: only local effects;

  Pseudoknots --- computation-costly.
- Efficiency and accuracy: 70% structure for a sequence.

Energy estimation

- Stabilizing energy ~ stacking base pairs.
- Destabilzing influence ~ non-paired region.



Algorithm

- Listing all possible secondary structure.

  1.8^N – N, sequence length.

  $1.8^{100} \sim 3 \times 10^{25}$ structures.

  If 10000/sec, 1.6×10^{14} years.

- Dynamic programming （加速）.

  从序列的一小段出发，逐渐向两边加长。一般假设局部不受全局影响，即不考虑假结等。

Prediction methods

- Ab initio prediction
- Evidence-associated prediction
- Genetic algorithm
- Specific sequences with known structures ~ knowledge-based

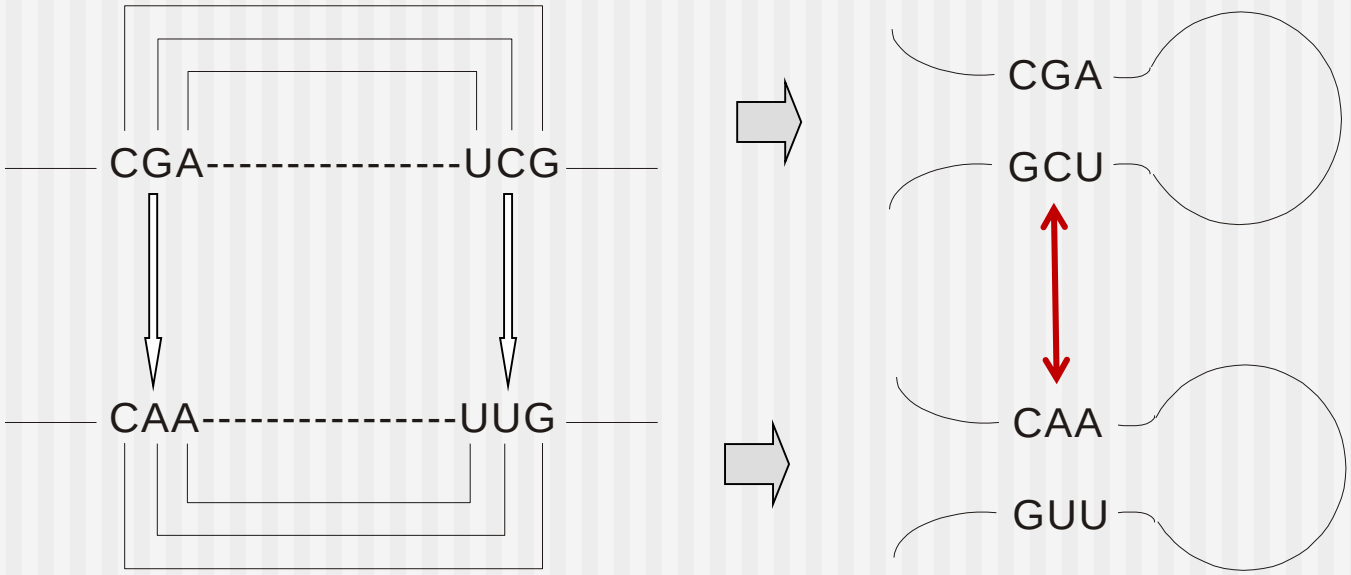
Evidence-associated prediction

- 酶切特异于单或双链;
- 共变异;

……

Covariation prediction

- --- from a set of related sequences.



Covariational bases would be considered reasonable matches in structure.

Prediction methods

- Ab initio prediction
- Evidence-associated prediction
- Genetic algorithm
- Specific sequences with known structures ~ knowledge-based

Genetic Algorithm

- 遗传算法是借鉴生物进化机制而建立的一种搜索算法，从一组“随机解”开始，通过反复的选择和变异等操作来寻找问题的优化解。
- Using random mutations of structure and selecting fit solutions.
- Optimal solution not guaranteed.

  --- providing different results with repeated calculations on the same sequence.

人工智能（Artificial Intelligence）

概率方法（贝叶斯，隐马模型）

进化算法

……

Machine Learning

ANN

Deep Learning

广义AI

狭义AI

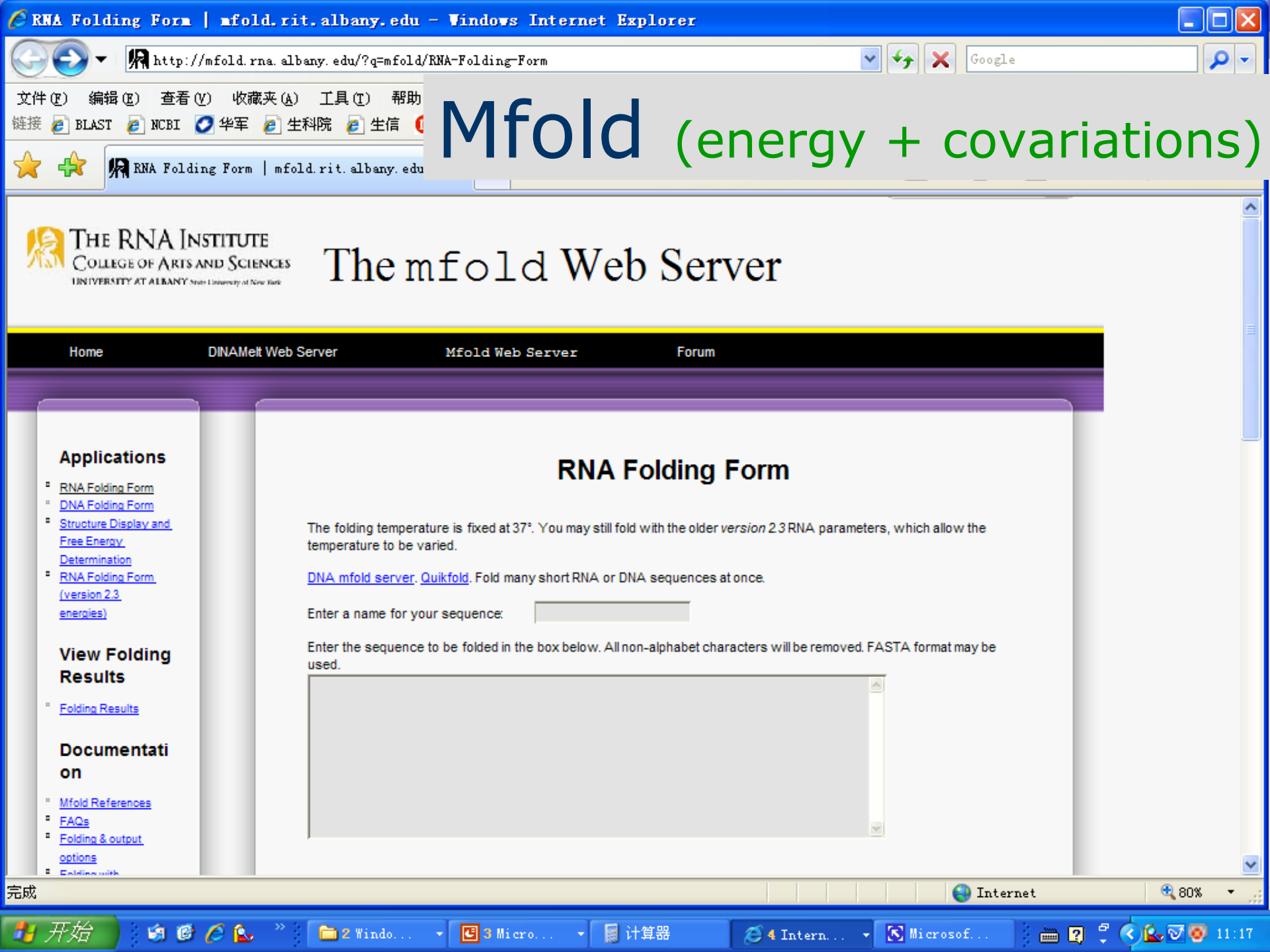
Methods

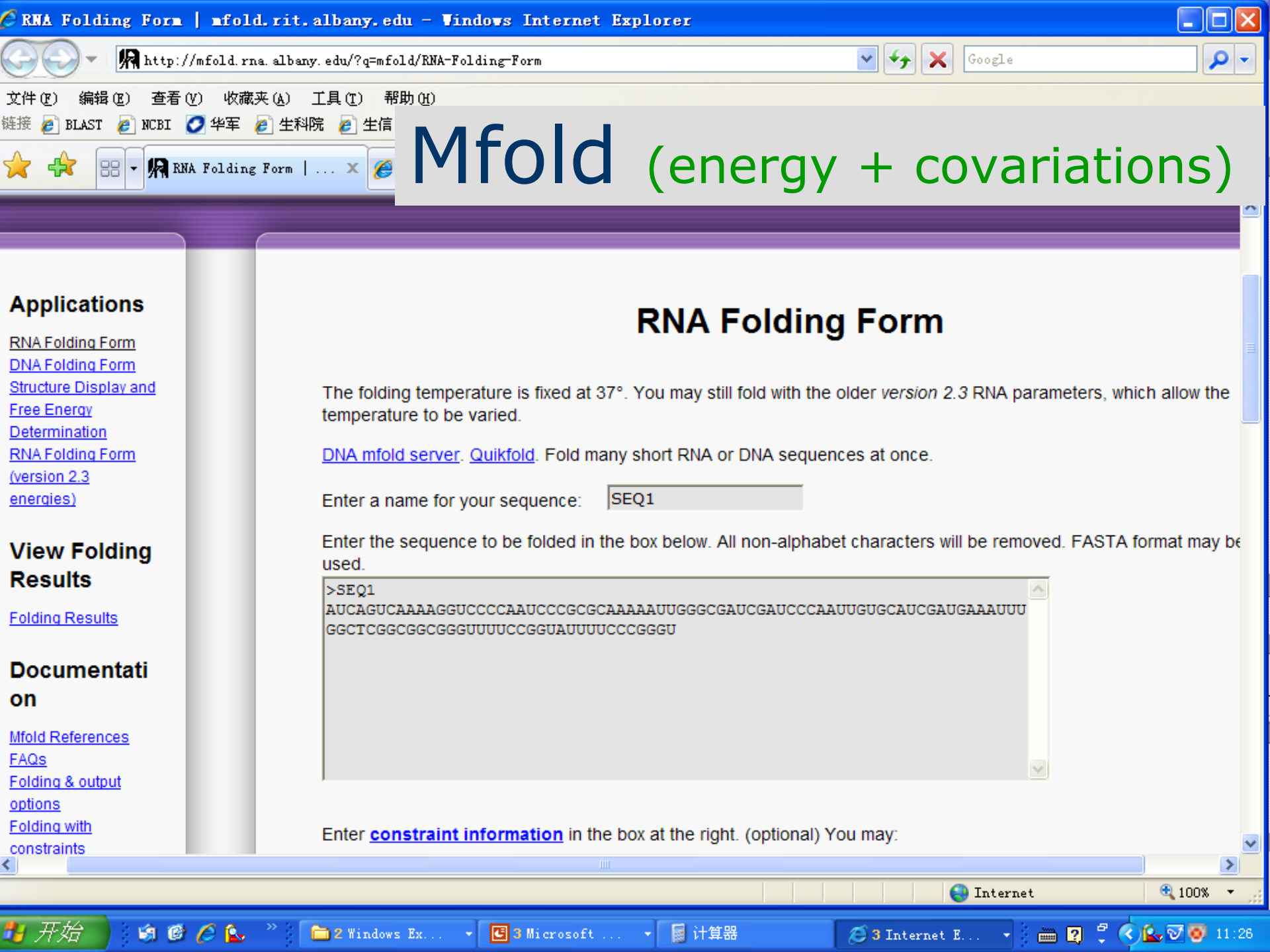
- Ab initio prediction
- Evidence-associated prediction
- Genetic algorithm
- Specific sequences with known structures ~（knowledge-based）

Programs

- Mfold;
- Sfold;
- Vienna RNA;
- RNAstructure;

……


RNA Folding Form | mfold.rit.albany.edu - Windows Internet Explorer
http://mfold.rna.albany.edu/?q=mfold/RNA-Folding-Form
Mfold (energy + covariations)
THE RNA INSTITUTE
COLLEGE OF ARTS AND SCIENCES
UNIVERSITY AT ALBANY
The mfold Web Server
Home
DINAMelt Web Server
Mfold Web Server
Forum
Applications
RNA Folding Form
DNA Folding Form
Structure Display and Free Energy Determination
RNA Folding Form (version 2.3 energies)
View Folding Results
Folding Results
Documentation
Mfold References
FAQs
Folding & output options
RNA Folding Form
The folding temperature is fixed at 37°. You may still fold with the older version 2.3 RNA parameters, which allow the temperature to be varied.
DNA mfold server. Quikfold. Fold many short RNA or DNA sequences at once.
Enter a name for your sequence:
Enter the sequence to be folded in the box below. All non-alphabet characters will be removed. FASTA format may be used.
完成
Internet
80%


RNA Folding Form | mfold.rit.albany.edu - Windows Internet Explorer
http://mfold.rna.albany.edu/?q=mfold/RNA-Folding-Form
Google
文件(F) 编辑(E) 查看(V) 收藏夹(A) 工具(T) 帮助(H)
链接 BLAST NCBI 华军 生科院 生信
RNA Folding Form | ...
Mfold (energy + covariations)
Applications
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DNA Folding Form
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RNA Folding Form (version 2.3 energies)
View Folding Results
Folding Results
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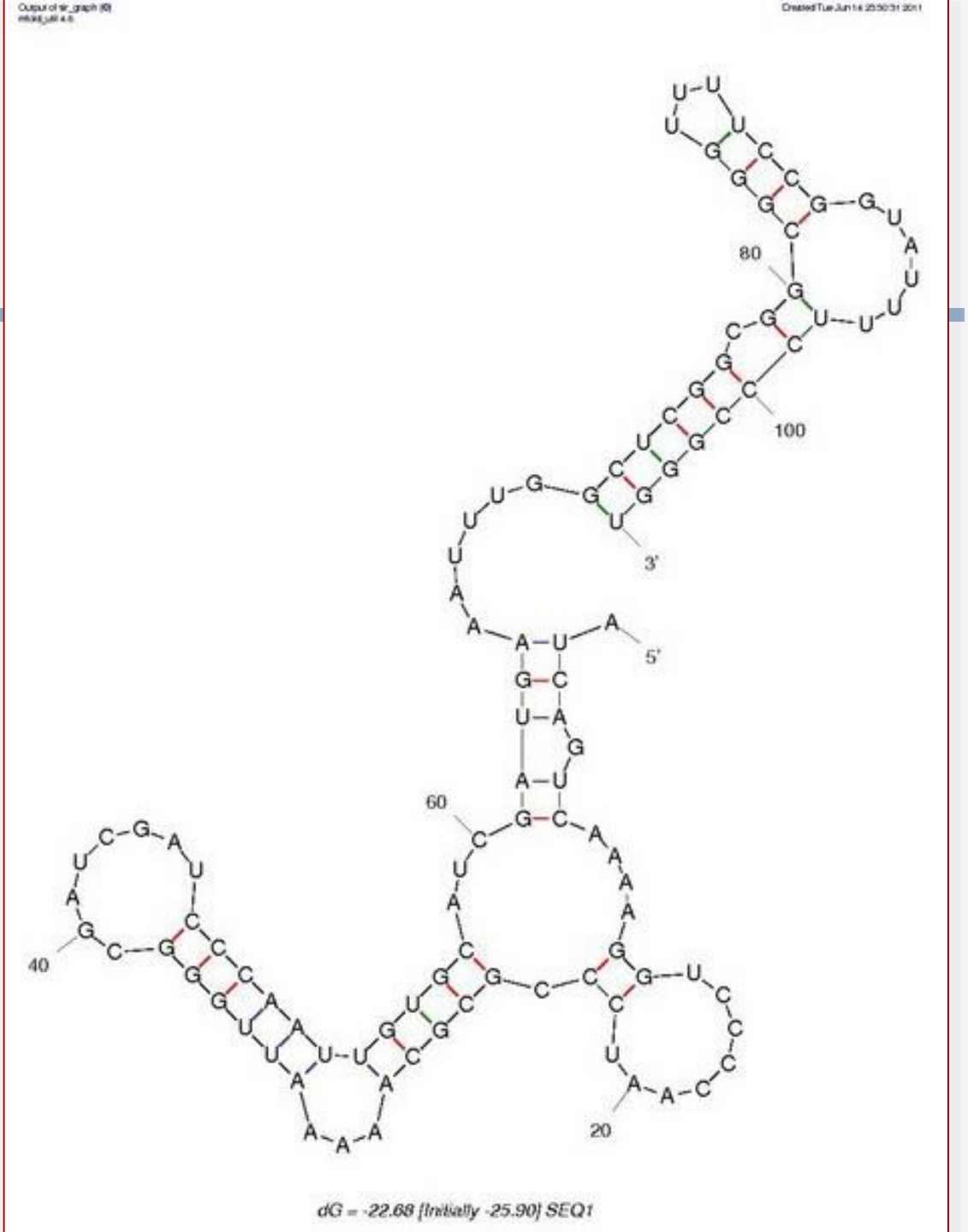
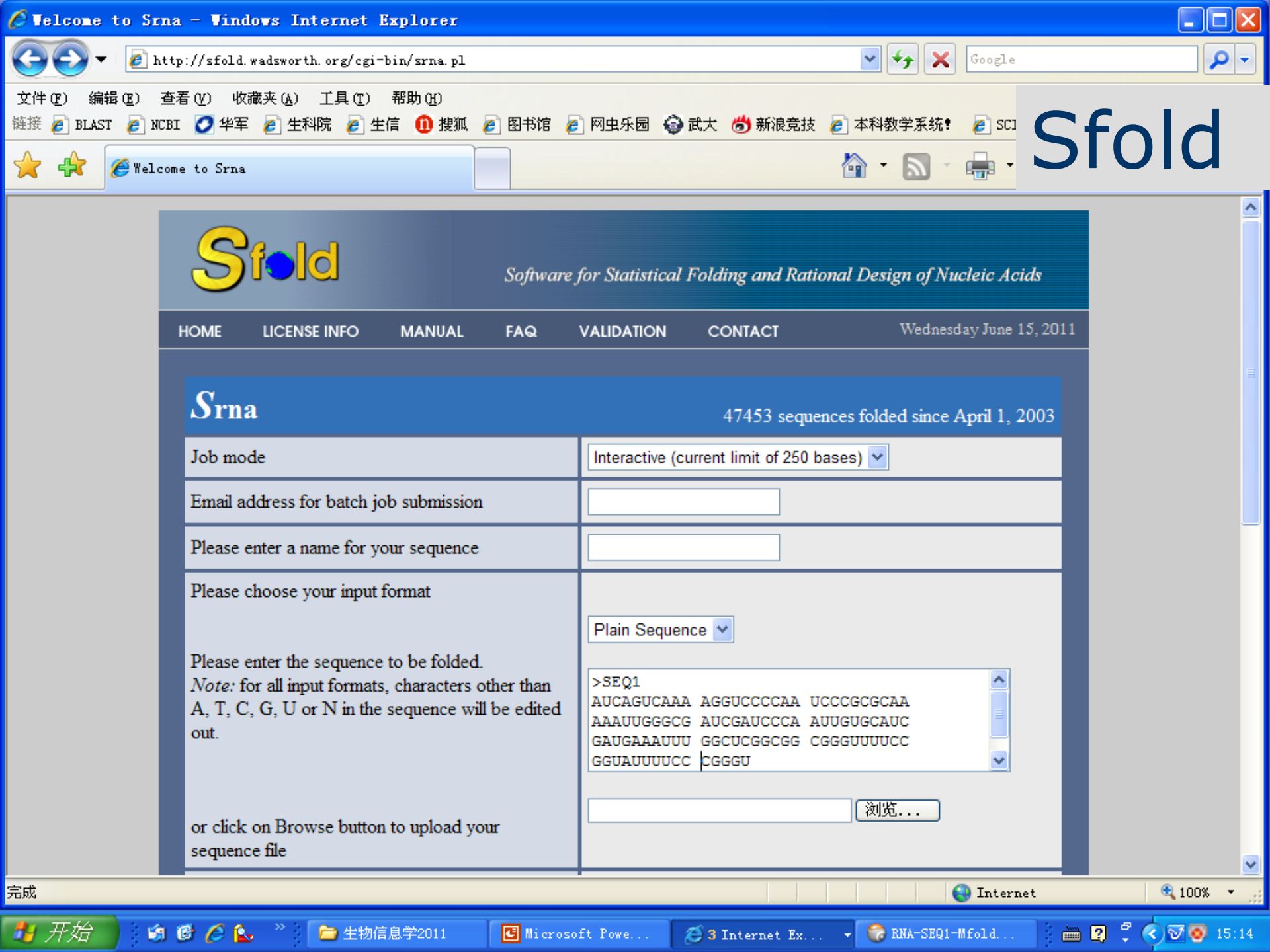
Mfold References
FAQs
Folding & output options
Folding with constraints
RNA Folding Form
The folding temperature is fixed at 37°. You may still fold with the older version 2.3 RNA parameters, which allow the temperature to be varied.
DNA mfold server. Quikfold. Fold many short RNA or DNA sequences at once.
Enter a name for your sequence: SEQ1
Enter the sequence to be folded in the box below. All non-alphabet characters will be removed. FASTA format may be used.
>SEQ1
AUCAGUCAAAAGGUCCCCAAUCCCGCGCAAAAAUUGGGCGAUCGAUCCCAAUUGUGCAUCGAUGAAAUUU
GGCTCGGCGGCGGGUUUUCCGGUAUUUUCCCGGGU
Enter constraint information in the box at the right. (optional) You may:
Internet
100%
开始
2 Windows Ex...
3 Microsoft ...
计算器
3 Internet E...
11:26

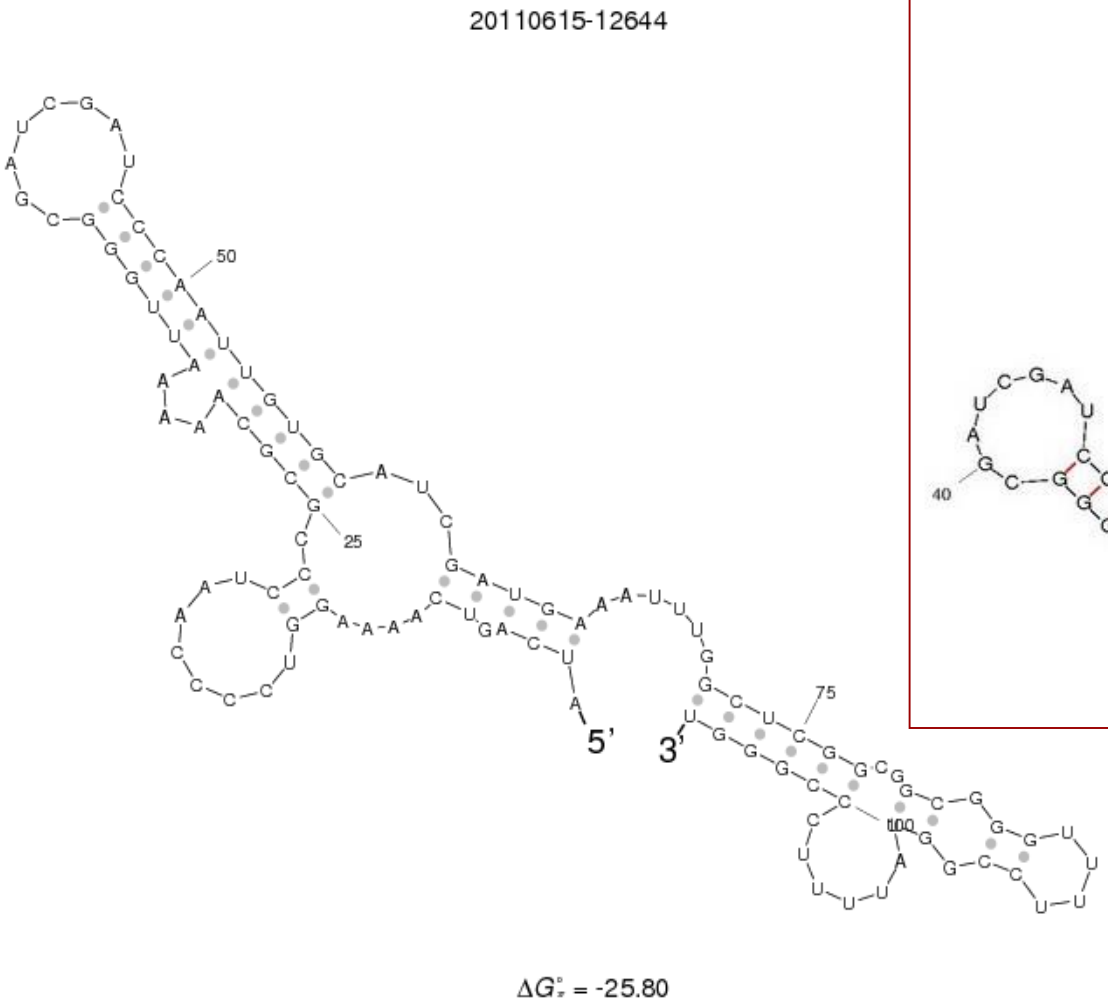


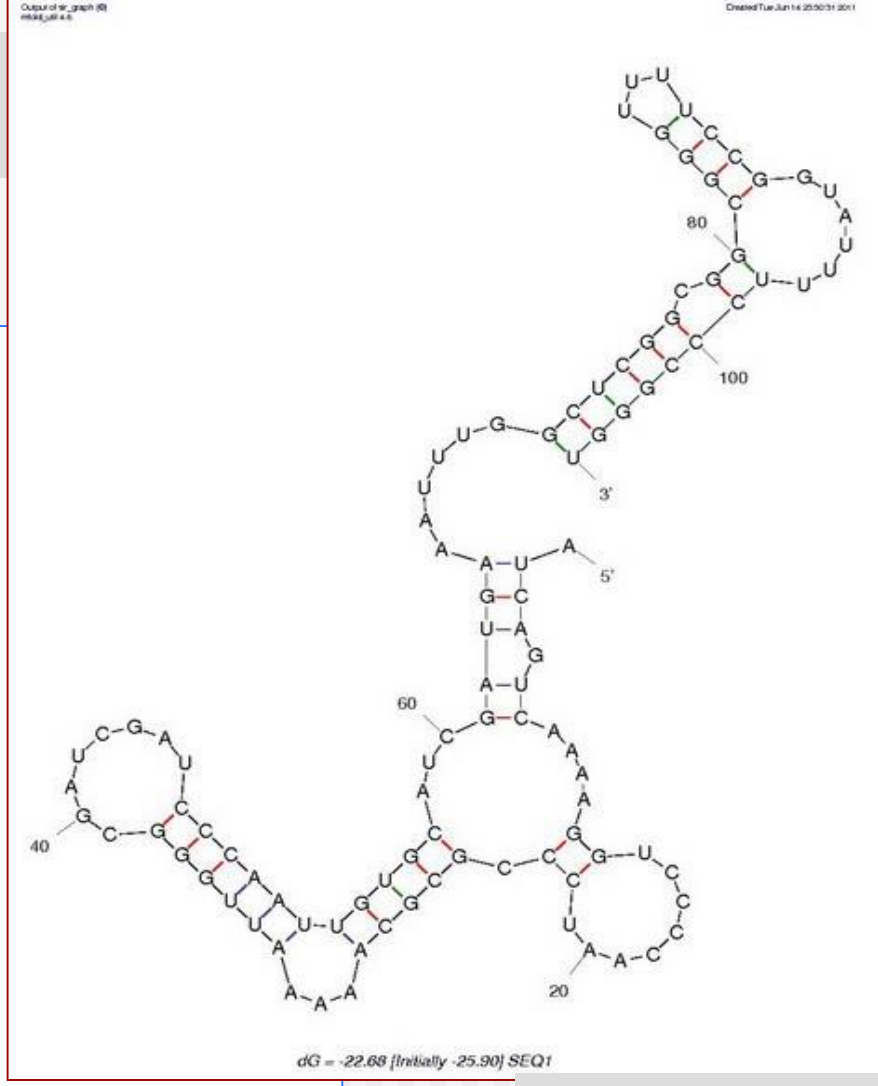
Mfold

(SEQ1---structure)

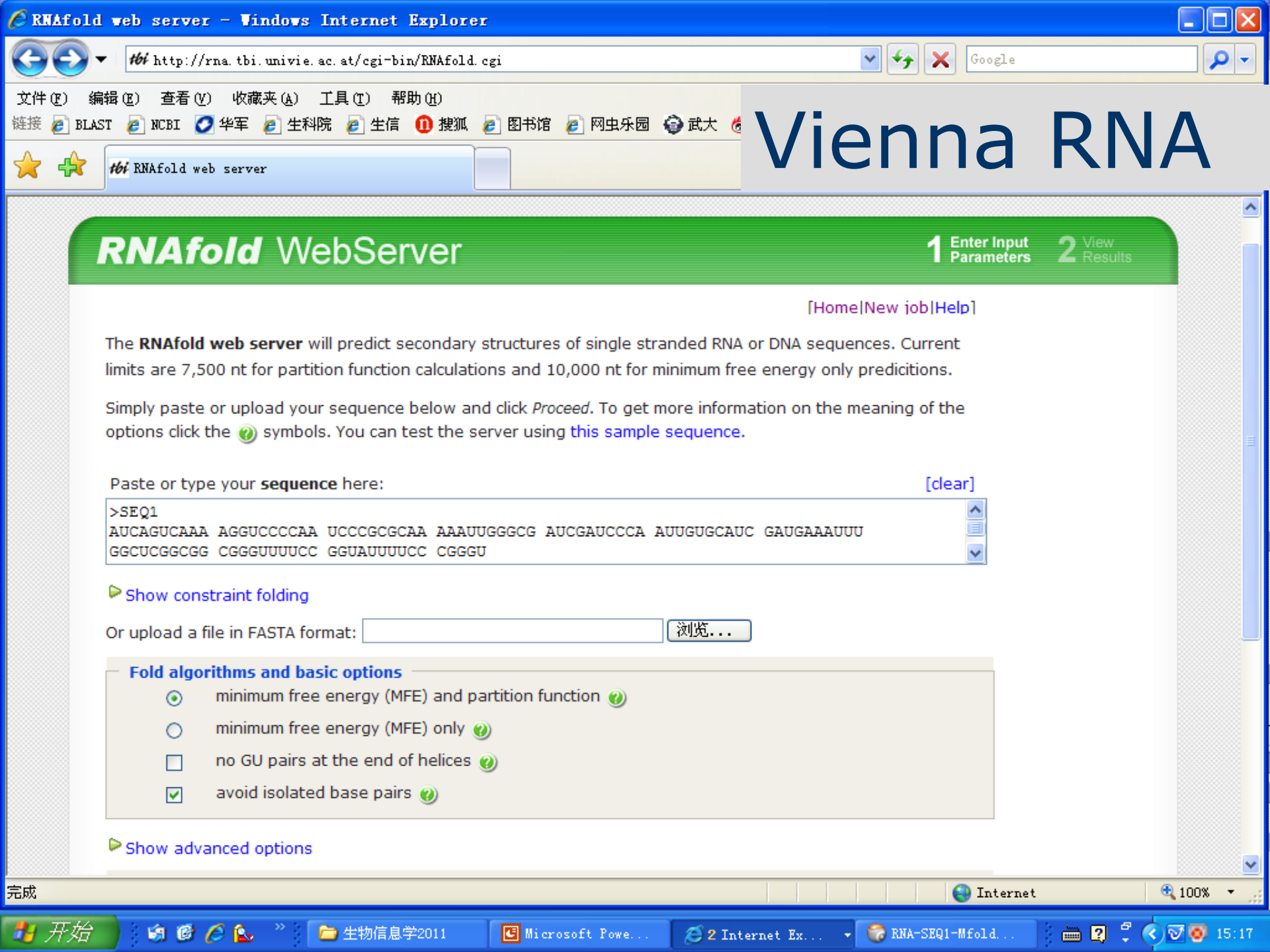

Welcome to Srna - Windows Internet Explorer
http://sfold.wadsworth.org/cgi-bin/srna.pl
Welcome to Srna
Sfold
Sfold
Software for Statistical Folding and Rational Design of Nucleic Acids
HOME
LICENSE INFO
MANUAL
FAQ
VALIDATION
CONTACT
Wednesday June 15, 2011
Srna
47453 sequences folded since April 1, 2003
Job mode
Interactive (current limit of 250 bases)
Email address for batch job submission
Please enter a name for your sequence
Please choose your input format
Plain Sequence
Please enter the sequence to be folded.
Note: for all input formats, characters other than A, T, C, G, U or N in the sequence will be edited out.
>SEQ1
AUCAGUCAAA AGGUCCCCAA UCCCGCGCAA
AAAUUGGGCG AUCGAUCCCA AUUGUGCAUC
GAUGAAAUUU GGCUCGGCGG CGGGUUUUCC
GGUAUUUUCC CGGGU
浏览...
or click on Browse button to upload your sequence file
完成
Internet
100%
开始
生物信息学2011
Microsoft Powe...
3 Internet Ex...
RNA-SEQ1-Mfold...
15:14

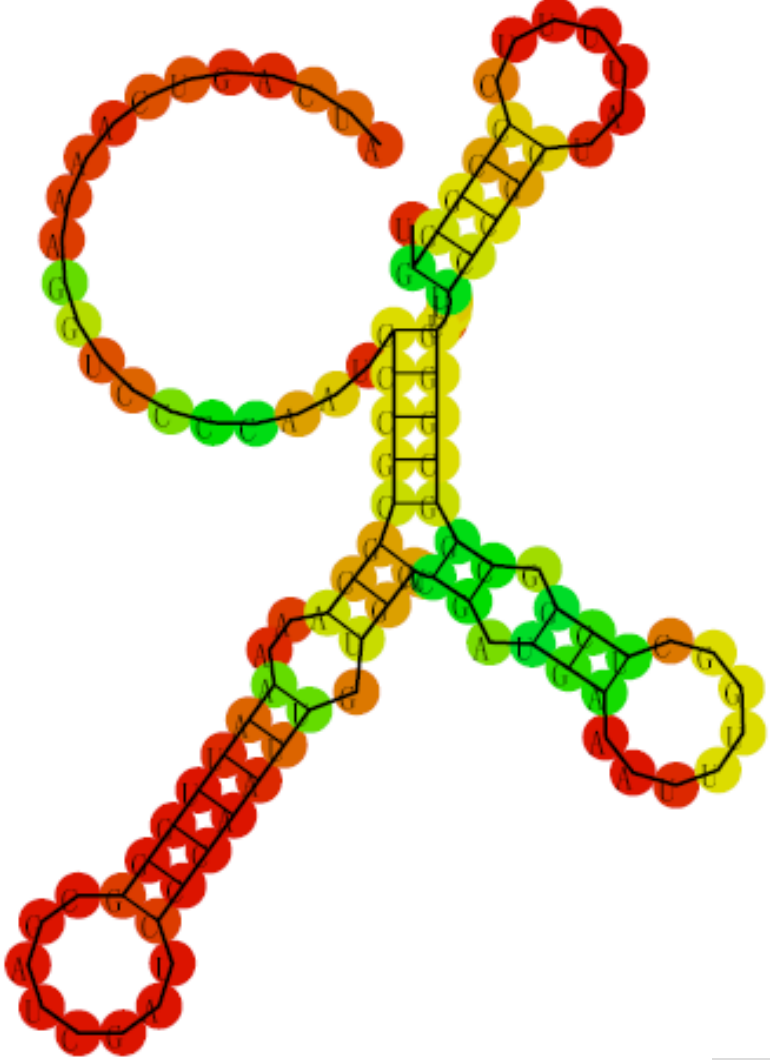
Sfold (SEQ1





Mfold


RNAfold web server - Windows Internet Explorer
http://rna.tbi.univie.ac.at/cgi-bin/RNAfold.cgi
RNAfold web server
Vienna RNA
RNAfold WebServer
1 Enter Input Parameters
2 View Results
[Home|New job|Help]
The RNAfold web server will predict secondary structures of single stranded RNA or DNA sequences. Current limits are 7,500 nt for partition function calculations and 10,000 nt for minimum free energy only predicitions.
Simply paste or upload your sequence below and click Proceed. To get more information on the meaning of the options click the symbols. You can test the server using this sample sequence.
Paste or type your sequence here:
[clear]
>SEQ1
AUCAGUCAAA AGGUCCCCAA UCCCGCGCAA AAAUUGGGCG AUCGAUCCCA AUUGUGCAUC GAUGAAAUUU
GGCUCGGCGG CGGGUUUUCC GGUAUUUUCC CGGGU
Show constraint folding
Or upload a file in FASTA format:
浏览...
Fold algorithms and basic options
minimum free energy (MFE) and partition function
minimum free energy (MFE) only
no GU pairs at the end of helices
avoid isolated base pairs
Show advanced options
完成
Internet
100%
开始
生物信息学2011
Microsoft Powe...
2 Internet Ex...
RNA-SEQ1-Mfold...
15:17



Sequence display options

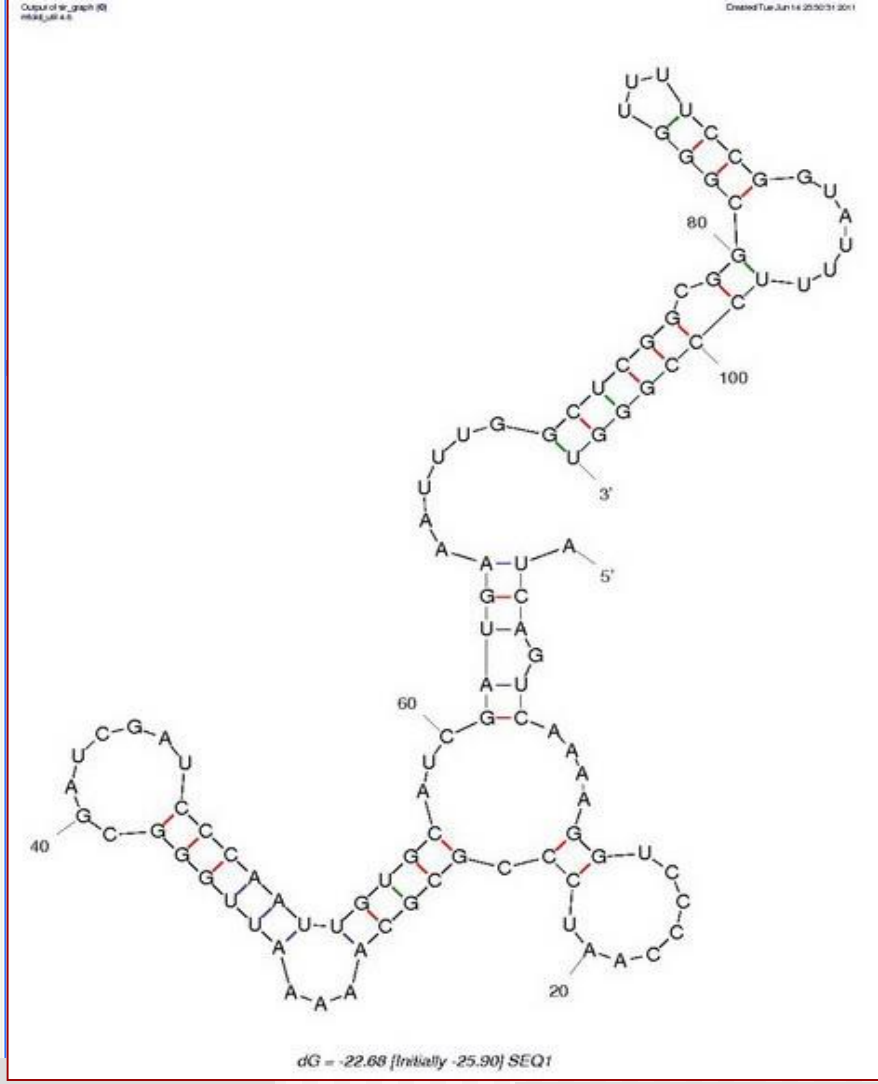
- (•) Plain Sequence
- ( ) No Sequence

MFE secondary structure

Other display options

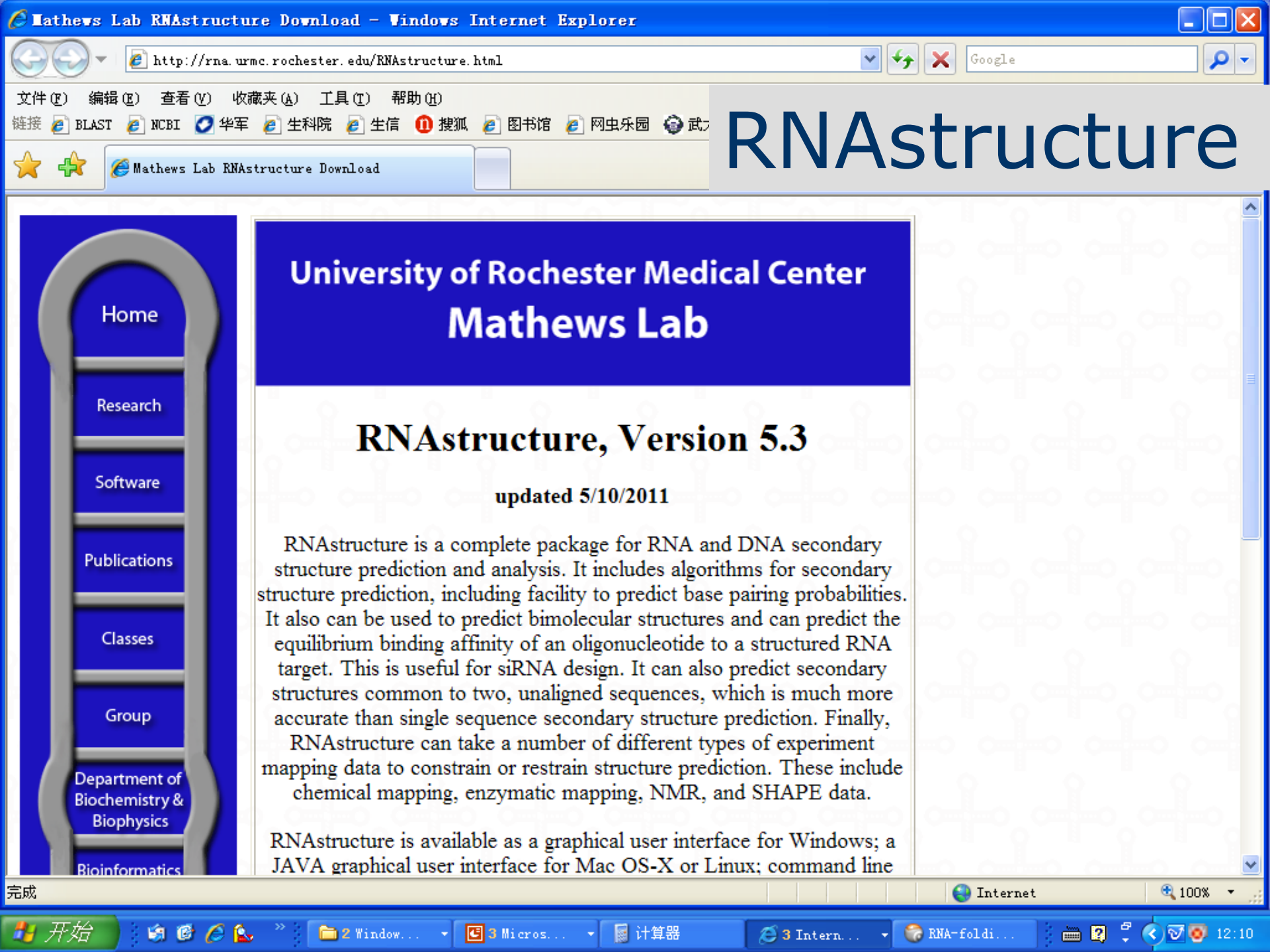
- (•) Base-pair probabilities
- ( ) Positional entropy
- ( ) None

0 — 1



Vienna RNA (SEQ1---structure)

Mfold


Mathews Lab RNAstructure Download - Windows Internet Explorer
http://rna.urmc.rochester.edu/RNAstructure.html
Mathews Lab RNAstructure Download
RNAstructure
Home
Research
Software
Publications
Classes
Group
Department of Biochemistry & Biophysics
Bioinformatics
University of Rochester Medical Center
Mathews Lab
RNAstructure, Version 5.3
updated 5/10/2011
RNAstructure is a complete package for RNA and DNA secondary structure prediction and analysis. It includes algorithms for secondary structure prediction, including facility to predict base pairing probabilities. It also can be used to predict bimolecular structures and can predict the equilibrium binding affinity of an oligonucleotide to a structured RNA target. This is useful for siRNA design. It can also predict secondary structures common to two, unaligned sequences, which is much more accurate than single sequence secondary structure prediction. Finally, RNAstructure can take a number of different types of experiment mapping data to constrain or restrain structure prediction. These include chemical mapping, enzymatic mapping, NMR, and SHAPE data.
RNAstructure is available as a graphical user interface for Windows; a JAVA graphical user interface for Mac OS-X or Linux; command line

三级结构

- Ab initio
- Homology modeling
- …
- …

RNA-PUZZLES 竞赛

RNA-Puzzles

is a collective experiment for blind RNA structure prediction.

Aims of the project

- To determine the capabilities and limitations of current methods of 3D RNA structure prediction based on sequence;
- To find whether and how progress has been made, as well as what has yet to be done to achieve better solutions
- To identify whether there are specific bottlenecks that hold back the field;
- To promote the available methods and guide potential users in the choice of suitable tools for real-world problems;
- To encourage the RNA structure prediction community in their efforts to improve the current tools and to make automated prediction tools available.
- To explore the underlying mechanism of ligand-RNA binding and the conformational changes in riboswitches.

Basic Rules

- Confidential agreement: "I will use the provided sequence data for prediction purposes only. I will not distribute the sequences in any form outside my working group."
- It is strongly recommanded that all the predictions formatted in standard **PDB format**. So that all the modellers could have a fair comparison without considering the file format and prediction region. We provide a python script **here** for generating standard PDB format files, only the coordinates need to be replaced by the predictors.
- RNA chains should be named in alphabetical order. e.g. A for the first chain, B for the second chain.
- Up to **FIVE** prediction models could be predicted as the final results of one problem for each group. It is also recommended to submit ten models.
- Please put all prediction models together in one PDB file as NMR format (Separate models by lines: "MODEL n" and "ENDMDL").
- For submission, please either use our online submission system or send us an email.

RNA-Puzzles

A CASP-like evaluation of RNA three-dimensional structure prediction

Recent Posts

PZ20 Release

Unknown Rfam Puzzles First Round Prediction Release

Unknown Rfam Puzzles First Round Closed

New Domain Name

New RNA-Puzzles Website at Github

GitHub Repos

RNA_assessment
Basic RNA 3D structure comparison metrics in RNA-Puzzles, including INF,

Menu

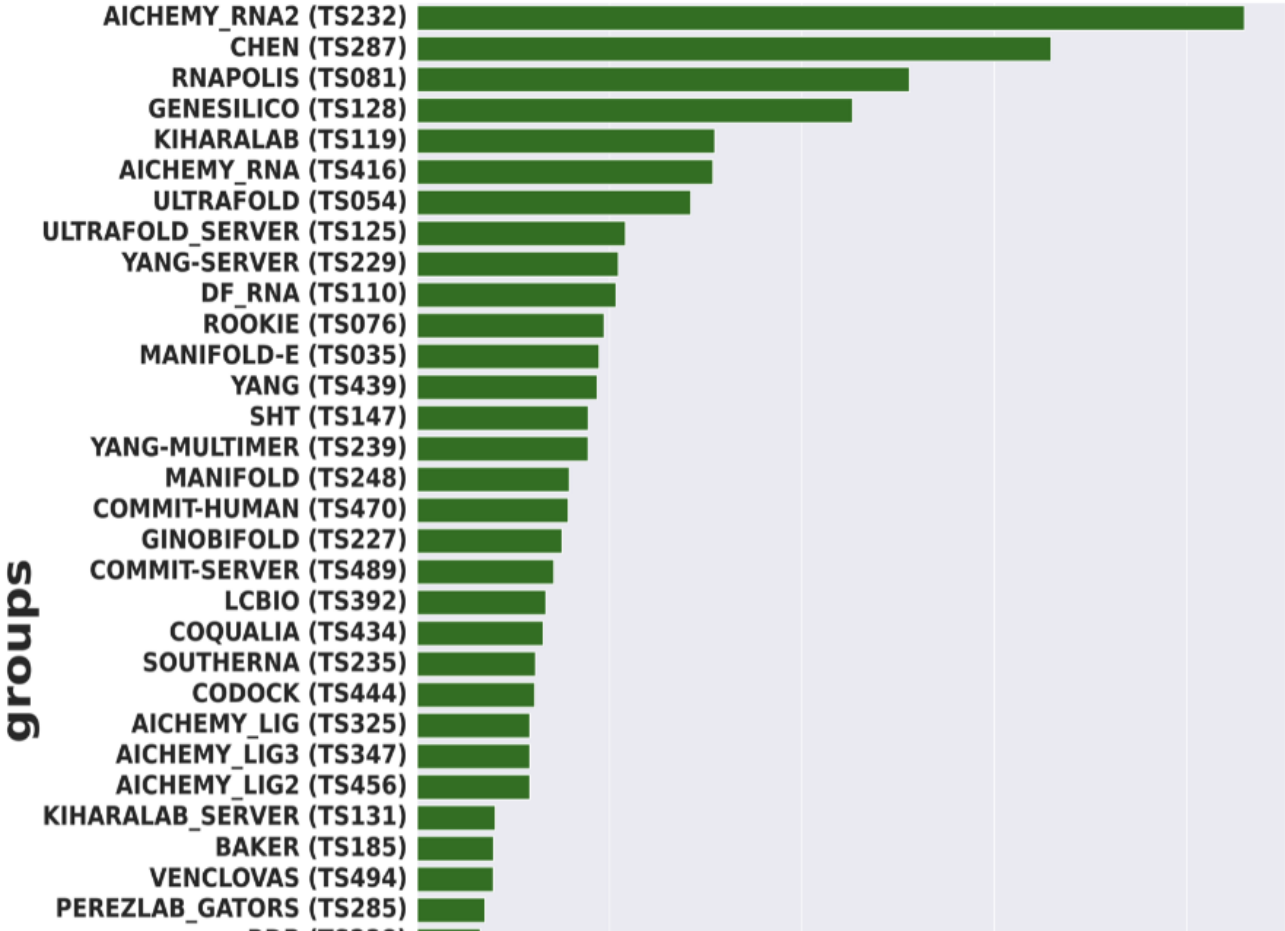
Home
PC Login
PC Registration
CASP Experiments

CASP15 (2022)

CASP14 (2020)
CASP_Commons
(COVID-19,2020)
CASP13 (2018)
CASP12 (2016)
CASP11 (2014)
CASP10 (2012)
CASP9 (2010)
CASP8 (2008)
CASP7 (2006)
CASP6 (2004)
CASP5 (2002)
CASP4 (2000)
CASP3 (1998)
CASP2 (1996)
CASP1 (1994)

Initiatives
Data Archive
Proceedings
CASP Measures

RNA Prediction : Group performance based on combined z-scores

Results Home

$$Z_{RNA} = \frac{1}{3}[Z_{TM} + Z_{GDT-TS}] + \frac{1}{8}[Z_{INF} + Z_{lDDT}] + \frac{1}{12}Z_{clash}$$