

Overview

PART I (Secondary Structure)

- Introduction
 - Motivation.
 - Levels of RNA Structure?
 - Secondary Structure Prediction
 - Representation
- Software
 - Prediction (mfold, vienna, dynalign)
 - Rendering (Annotation s2s, others.)
- Everyones Favorite FIKA!

Overview

PART II (Rigid Block Model)

- Rigid Block Model for Nucleic Acids.

Overview

PART III (Practical Workshop-Tutorial)

- Practical Examples.
 - Using paper and pencil alone do Nussinov algorithm to some sequence. This gives you some structure, not necessarily minimal energy I guess.
 - Use computer to go to mfold, or vienna webserver to do prediction for same sequence. (maybe mfold is better because it gives more cartoons)
 - Make A-DNA, B-DNA, Z-DNA. Chromosomal DNA.

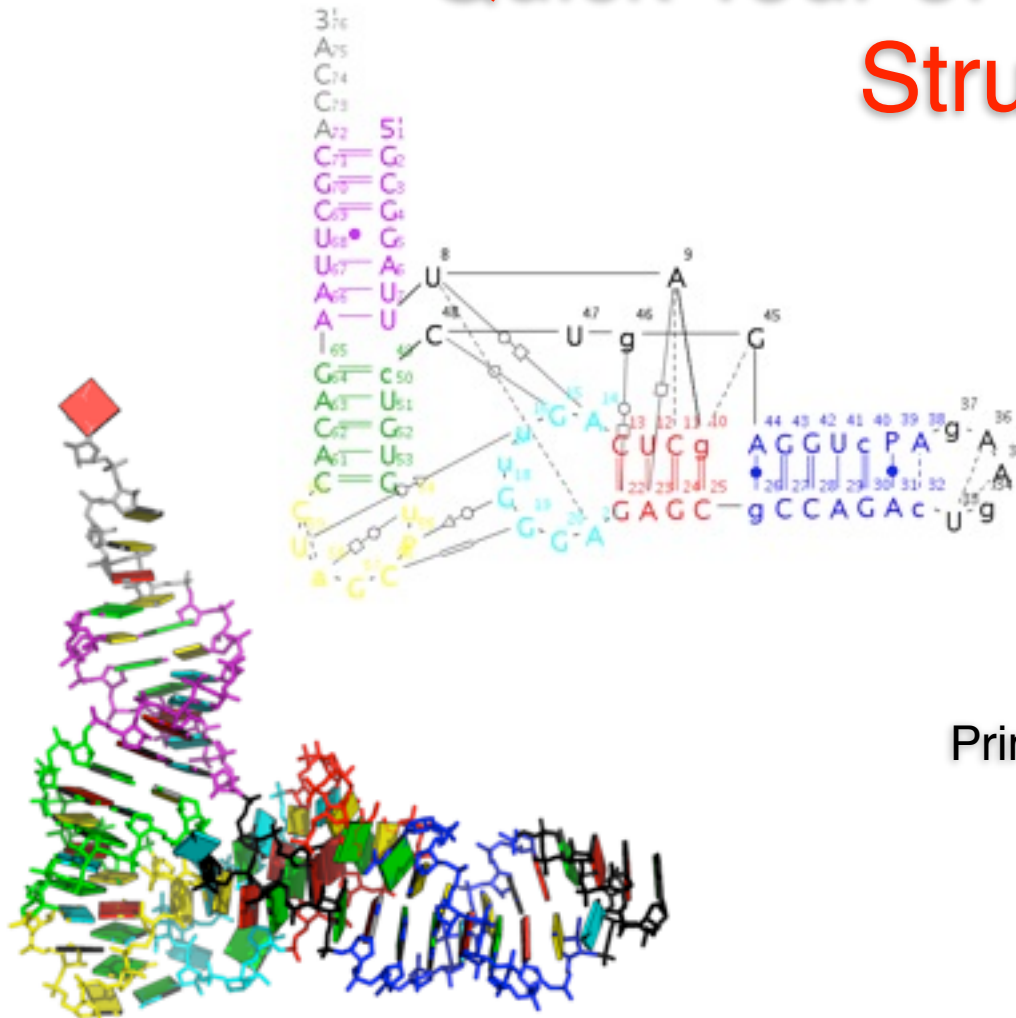
GCGGAUU UA gCUC AGuuGGGA GAGC gCCAGAc UgAAg APcUGGA GgUC cUGUG uPCGaUC CACAG AAUUCGC ACCA
 1234567 89 0123 45678901 2345 6789012 34567 8901234 5678 90123 4567890 12345 6789012 3456

Quick Tour of RNA Secondary Structure Prediction

Mauricio Esguerra Neira

Lennart Nilsson Group

<http://mesguerra.net>



Principles of Nucleic Acid Structure

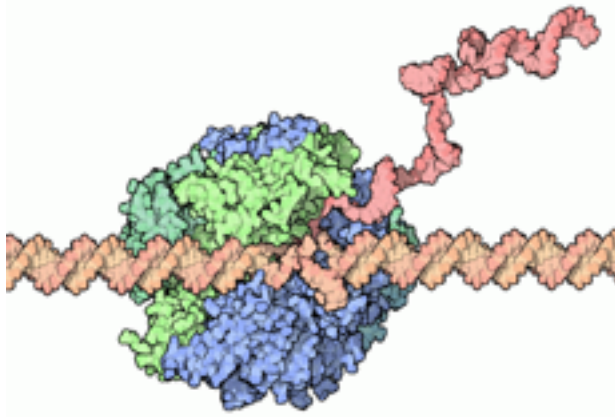
KI Doctoral Course 2430

Torsdag, Februari Två, 2012

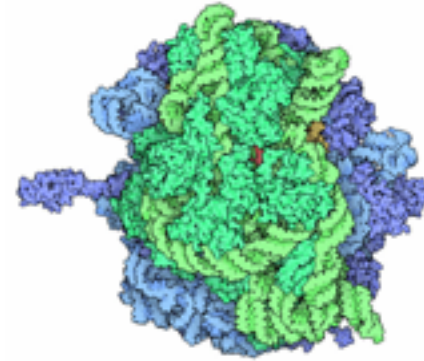
13:00 - 16:00

GENOMICS
PROTEOMICS
POST-GENOMICS
EPIGENETICS
RIBONOMICS

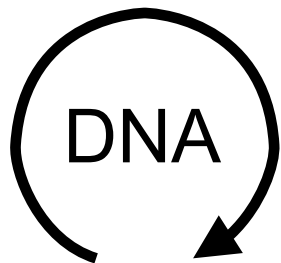
Biology's Central Dogma



TRANSCRIPTION
RNA Pol II



TRANSLATION
Ribosome, aka rRNA



Replication

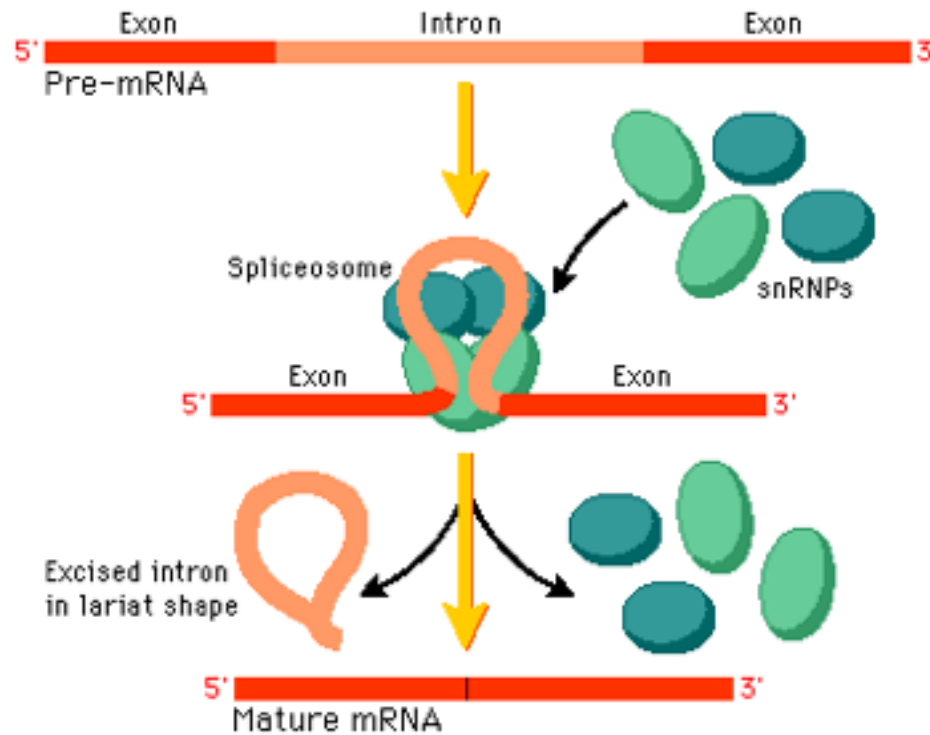


Genotype

**Gene Expression
(Activation, Silencing)**

Phenotype

RNA is spliced by the spliceosome after transcription.



Non-coding RNA's

- RNAPol I rRNA not 5S (~ 50% cell RNA)
- RNAPol II precursors of mRNA and most snRNA and microRNA
- RNAPol III 5S rRNA, tRNA and other small RNAs
- piwiRNA
- siRNA
-

The RNA Zoo

Structure Determines Function

Types of RNA Structure

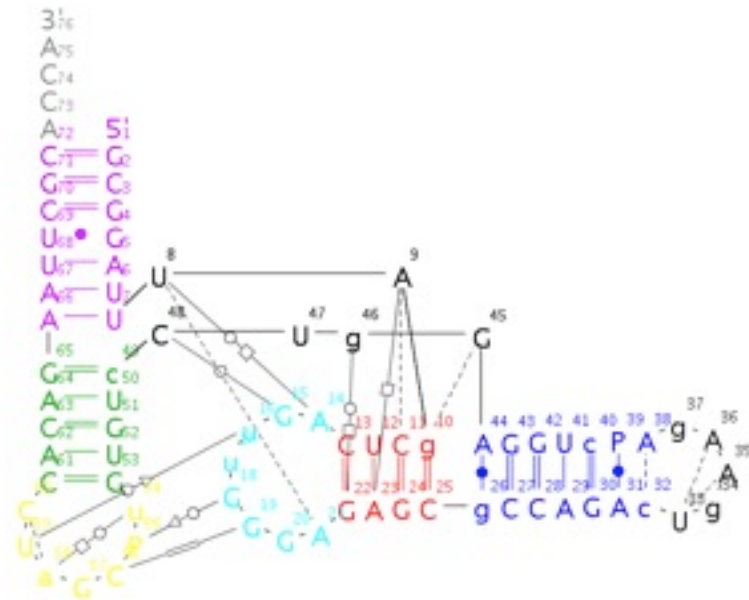
Primary Structure

Backbone covalent linked through phosphodiester group with 5' to 3' sense.

GCGGAUU UA gCUC AGuuGGGA GAGC gCCAGAc UgAAg APcUGGA GgUC cUGUG uPCGaUC CACAG AAUUCGC ACCA
1234567 89 0123 45678901 2345 6789012 34567 8901234 5678 90123 4567890 12345 6789012 3456

Secondary Structure

Hydrogen Bonded Base-Pairs



Two Types of RNA Secondary Structure Prediction

- RNA Sequence Covariation
- RNA Free Energy Minimization (Tinoco-Uhlenbeck)

Sequence Covariation

- Main Idea is:
- Gutell quite successful in getting rRNA.

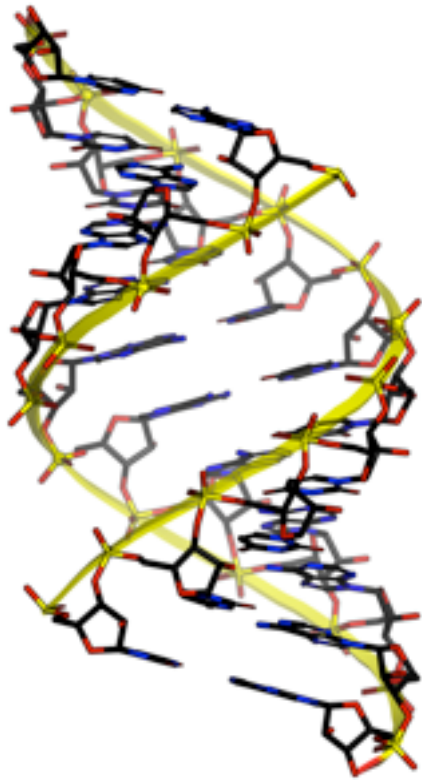
Delta G Minimization

- Tinoco-Uhlenbeck Postulate
- Dynamic Programming Nussinov Algorithm
-

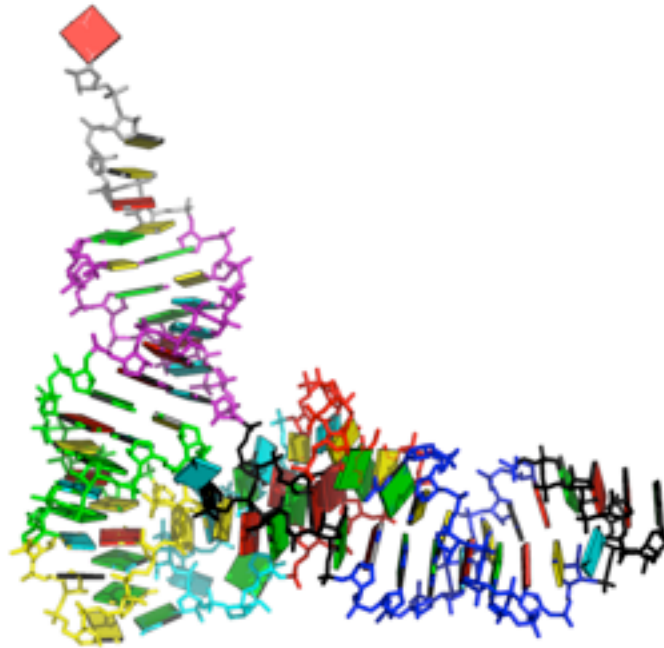
Visualization of Secondary Structure

- Standard
- Circular
- Dot Plot

Tertiary Structure



A-RNA



Nobel Prizes and RNA

Classic Papers on Secondary Structure

- Classics
 - Tinoco - Uhlenbeck Nature 1971
- Books
 - Tinoco's Book
 - Bioinformatics Book Chapter by Mathews
- Online
- Recent Trends
- People

RNA Secondary Structure Prediction Groups

- Doug Turner University of Rochester (Turner Rules)
- David Mathews University of Rochester (Dynalign)
- Michael Zuker Rensselaer Polytechnic Institute (mfold)
- Ivo Hoffacker Wien (vienna)
- Peter Stadler Leipzig (vienna)
- Francois Major Montreal (mc-sym)
- Tamar Schlick NYU (graph-grammars)
- Ruth Nussinov Tel Aviv (1978 dynamic algorithm)
- Nacho Tinoco (1971 free-energy minimization)