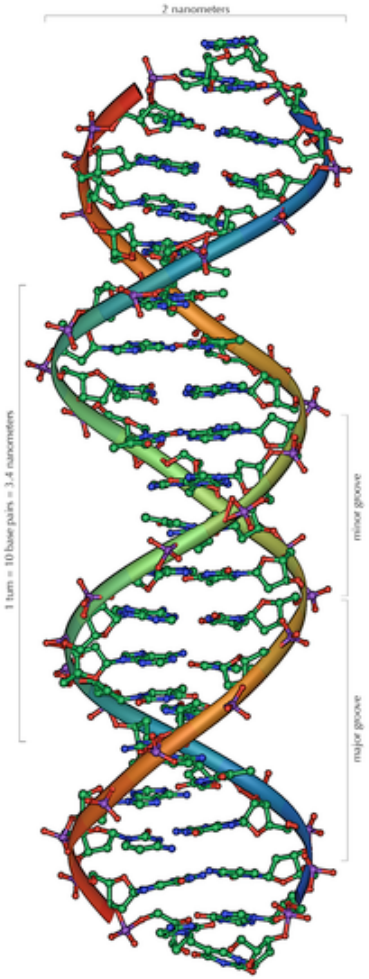
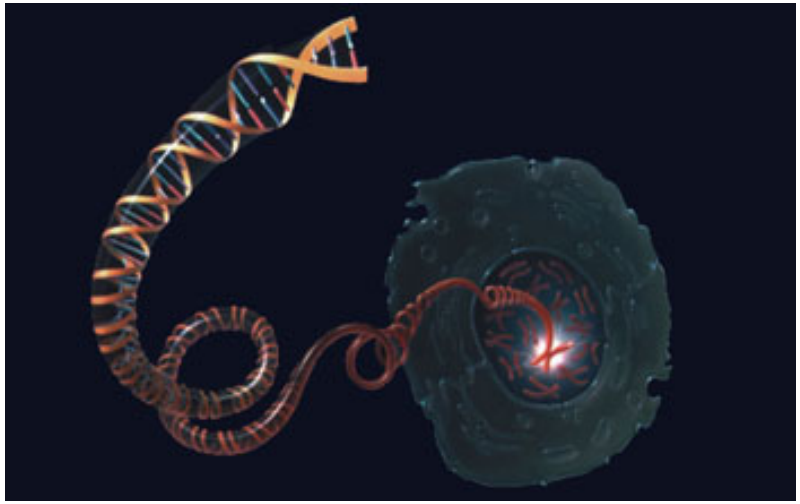
Module 1: Basics of DNA and DNA self-assembly

CSE590: Molecular programming and neural computation

Double-stranded DNA



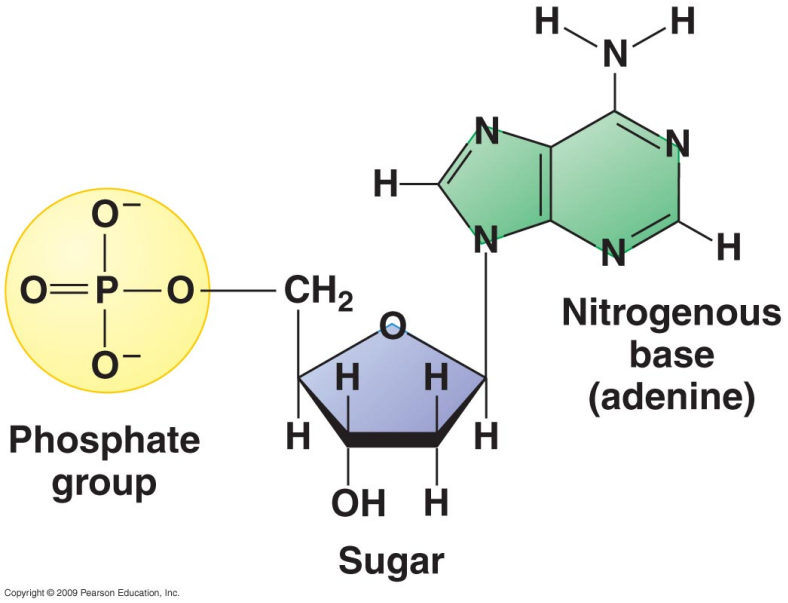


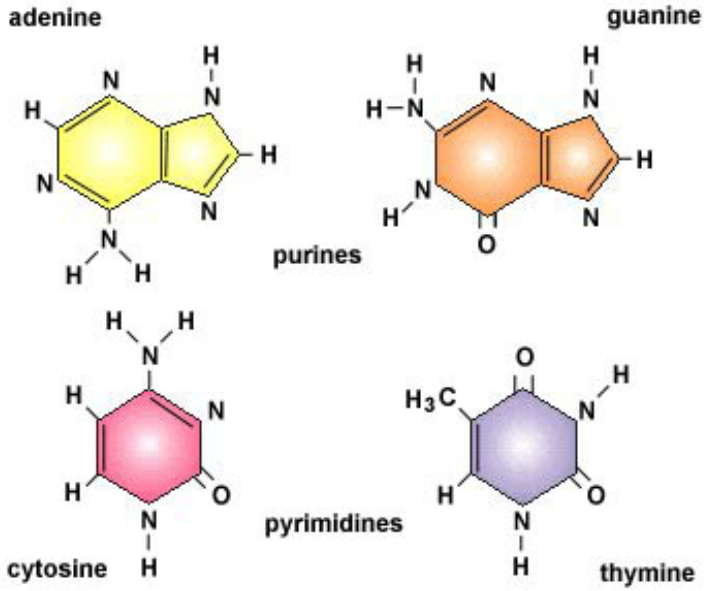
Biological DNA stores hereditary information

Width of the double helix: 2nm
Distance between base pairs: 0.34 nm

Carsonella rudii (smallest non-viral genome): 160,000 bp
Human genome: 3.2 Billion bp
Lungfish (largest vertebrate genome): 130 Billion bp

DNA nucleotides





DNA directionality

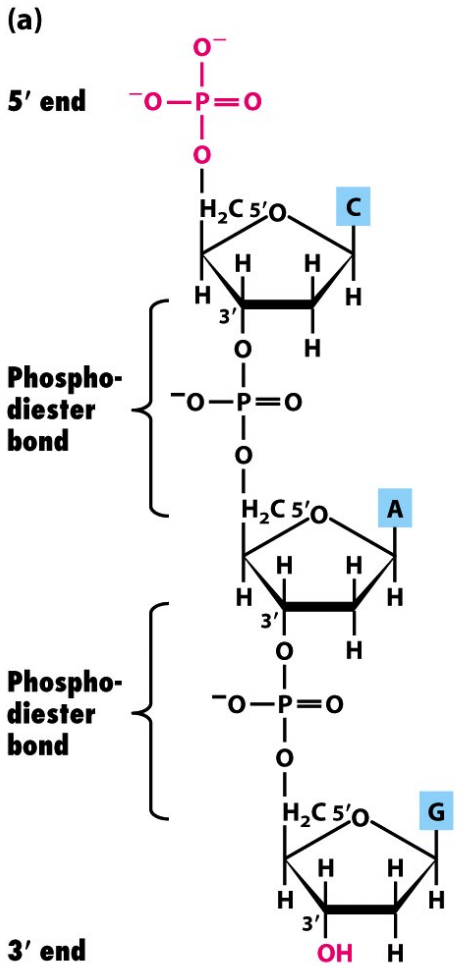


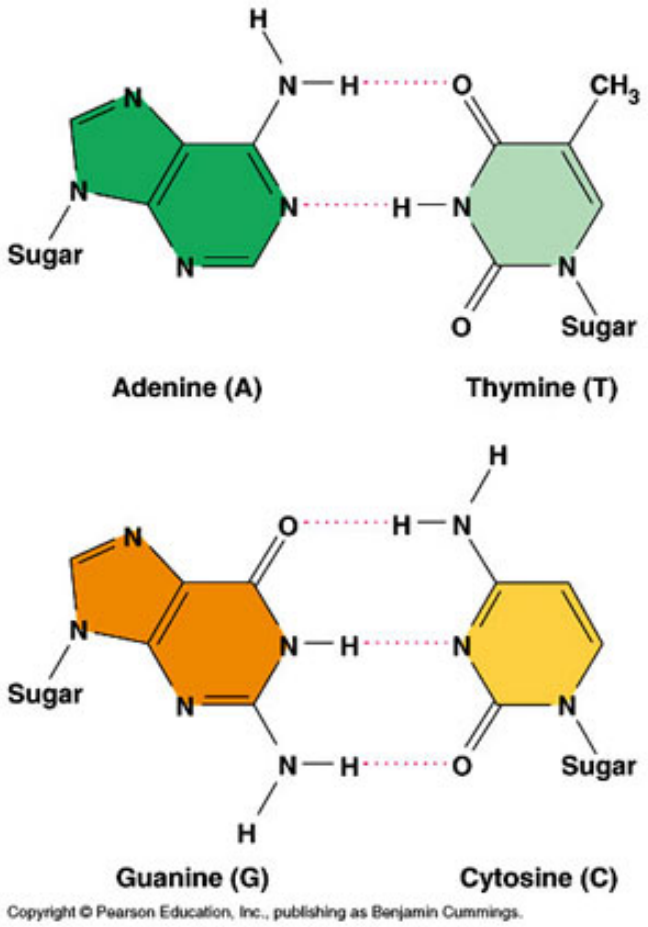
Figure 4-2
Molecular Cell Biology, Sixth Edition

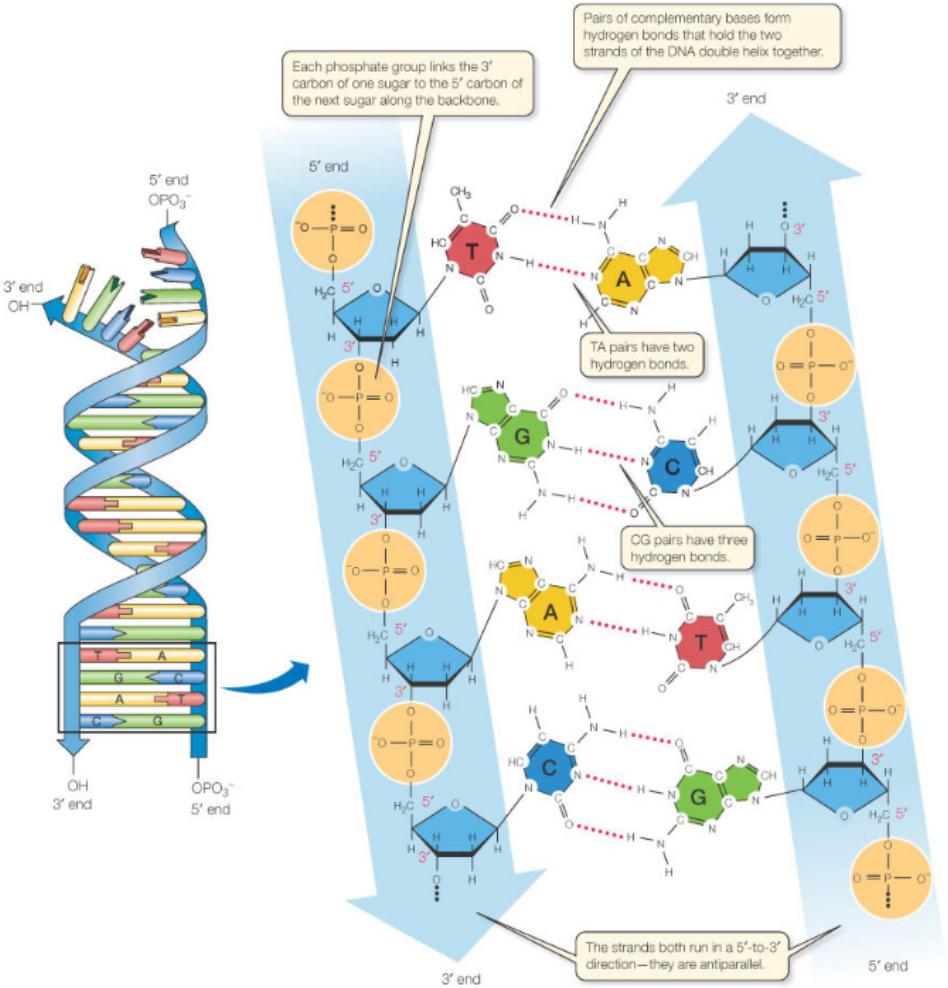
A DNA **strand**

= 5'-CAG-3'

The strand **sequence**

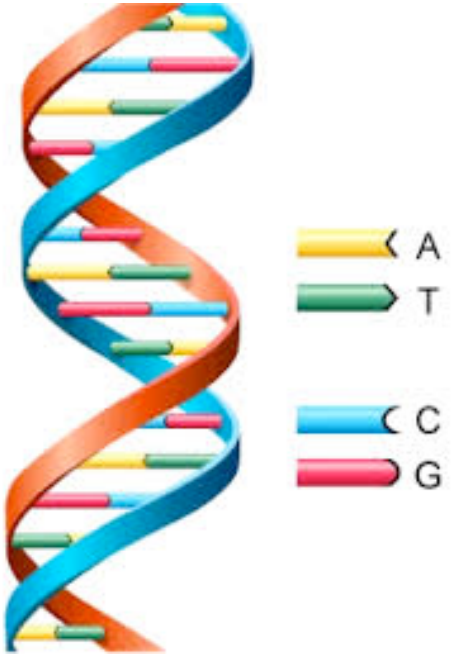
Watson Crick base paring





Double-stranded DNA representations

DNA double helix



=

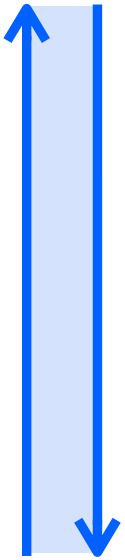
DNA sequence representation

5′ –ATTCAGATCCACC–3′

3′ –TAAGTCTAGGTGG–5′

=

Domain representation



The double helix consists of **two DNA strands with complementary sequences** (base pairs: A:T, C:G) and with opposite orientation

DNA can be commercially synthesized

DNA sequence 1:
5′-ATTCAGATCCACCCAAAGAG-3′

DNA sequence 2:
5′-CTCTTTGGGTTCCCAAATGT-3′

DNA sequence 3:
5′-ACATTTGGGAGGATCTGAAT-3′

Single-stranded DNA with any sequence can be commercially synthesized
length up to ~200 bases, cost: ~50 cents/base, 1 nMole (10^{15}) per order, same-day synthesis

Reverse complementarity

Find the reverse complement of the following sequences:

5′-AAAAA-3′

5′-AACCC-3′

5′-CTGGACTAGAATT-3′

DNA hybridization (binding)

What happens when these strands are mixed in a test tube?

1: 5′-CACACACA-3′

2: 5′-TTTTTTGTGTGTG-3′

3: 5′-GTGTGTGT-3′

DNA hybridization (binding)

What happens when these strands are mixed in a test tube?

1: 5′-TTTTTT-3′

2: 5′-CACACACANNNNNAGAGAGAG-3′

DNA hybridization (binding)

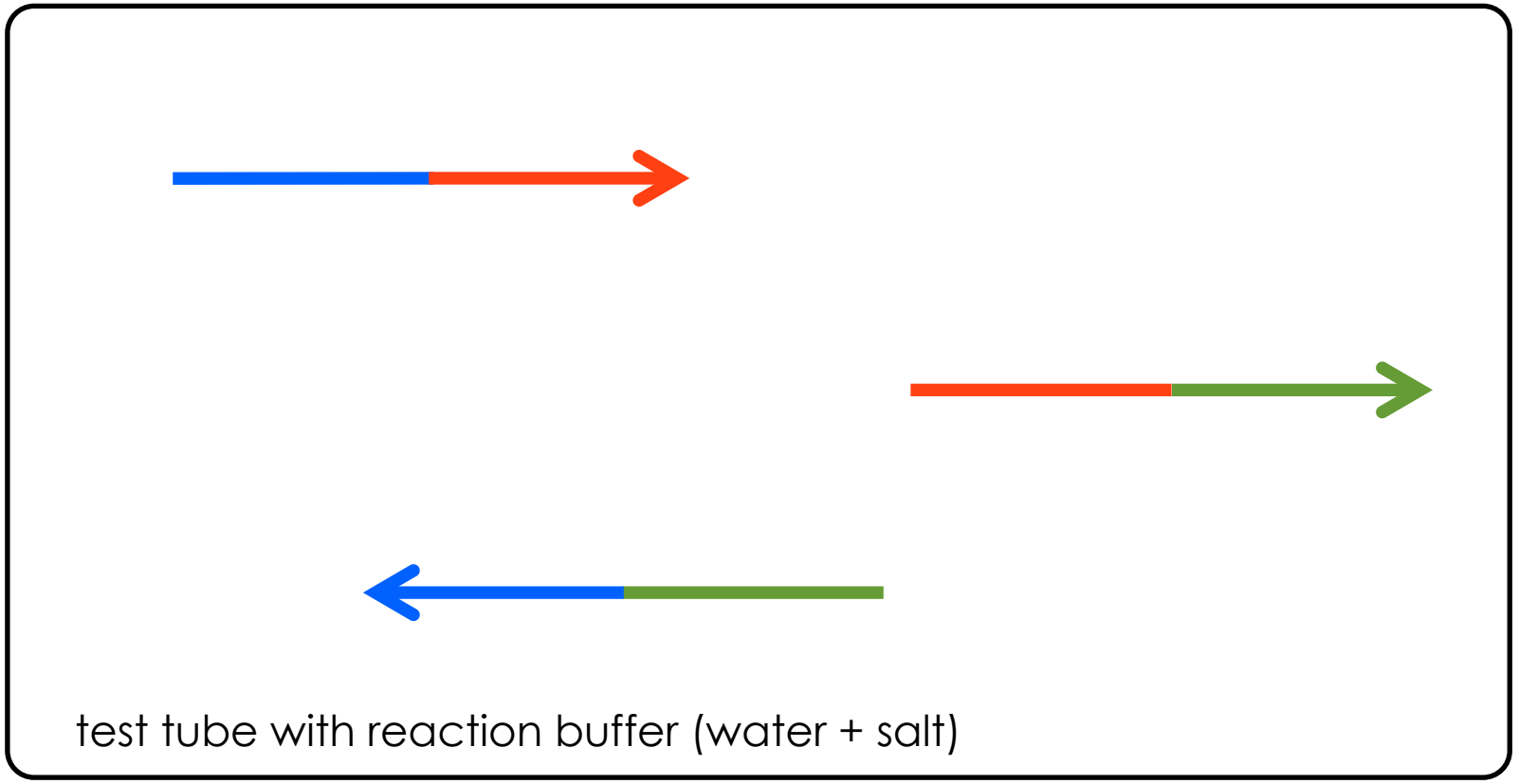
What happens when these strands are mixed in a test tube?

1: 5′-ATTCAGATCCACCCAAAGAG-3′

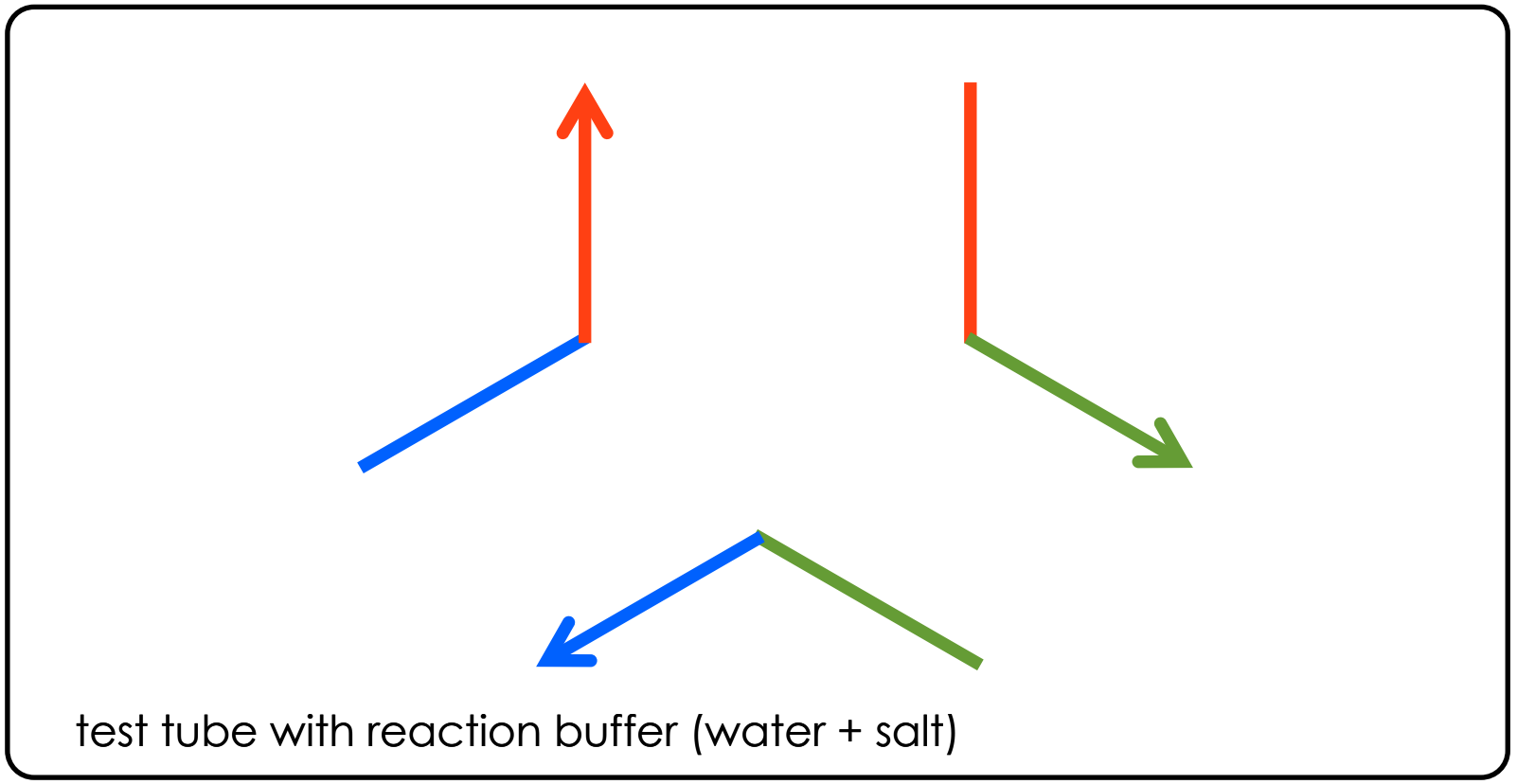
2: 5′-CTCTTTGGGTTCCCAAATGT-3′

3: 5′-ACATTTGGGAGGATCTGAAT-3′

DNA hybridization (binding)

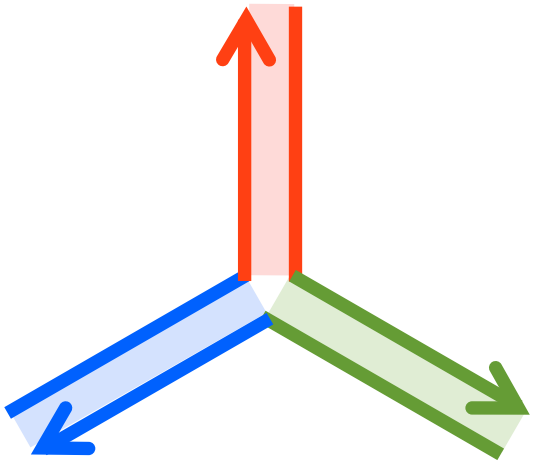


DNA hybridization (binding)



Single-stranded DNA is flexible

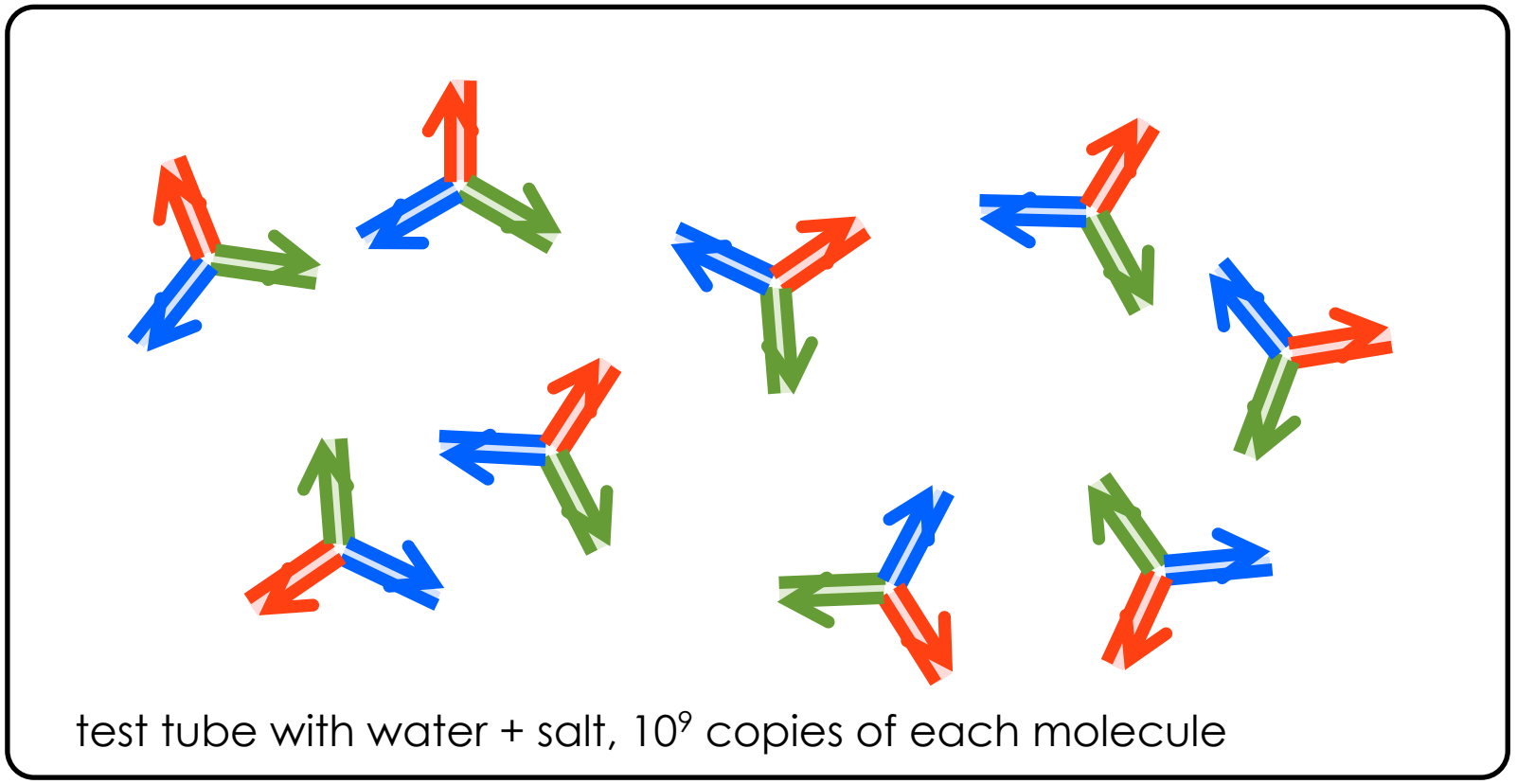
DNA hybridization (binding)



test tube with reaction buffer (water + salt)

Complementary single-stranded domains bind (hybridize) to each other. Formation of base pairs is energetically favorable and drives the reaction forwards

DNA is a programmable material



DNA is programmable: sequence determines interactions

Are we really doing this by hand?

NUPACK nucleic acid package

Analysis | Design | Utilities | Downloads

NUPACK is a growing software suite for the analysis and design of nucleic acid systems.

The NUPACK web application currently enables:

- **Analysis**: thermodynamic analysis of dilute solutions of interacting nucleic acid strands (demos).
- **Design**: single-state and multi-state sequence design for interacting nucleic acid strands (demos).
- **Utilities**: evaluation, display, and annotation of equilibrium properties of a complex of nucleic acid strands (demos).

NUPACK algorithms are formulated in terms of nucleic acid secondary structure. In most cases, pseudoknots are excluded from the structural ensemble.

You are welcome to use NUPACK for your research. Please cite NUPACK algorithms and the NUPACK web application appropriately.

 | Contact | Model | Citation | Funding | Terms of use

www.nupack.org

Analysis | Design | Utilities | Downloads

Input | Demos | Help

Nucleic acid type: (•) RNA ( ) DNA

Temperature: 37.0 °C

Compute melt: ☐

Number of strand species: 1

Maximum complex size: 1 strand

Strand species

strand1 :

Advanced options

Email address:

Analyze

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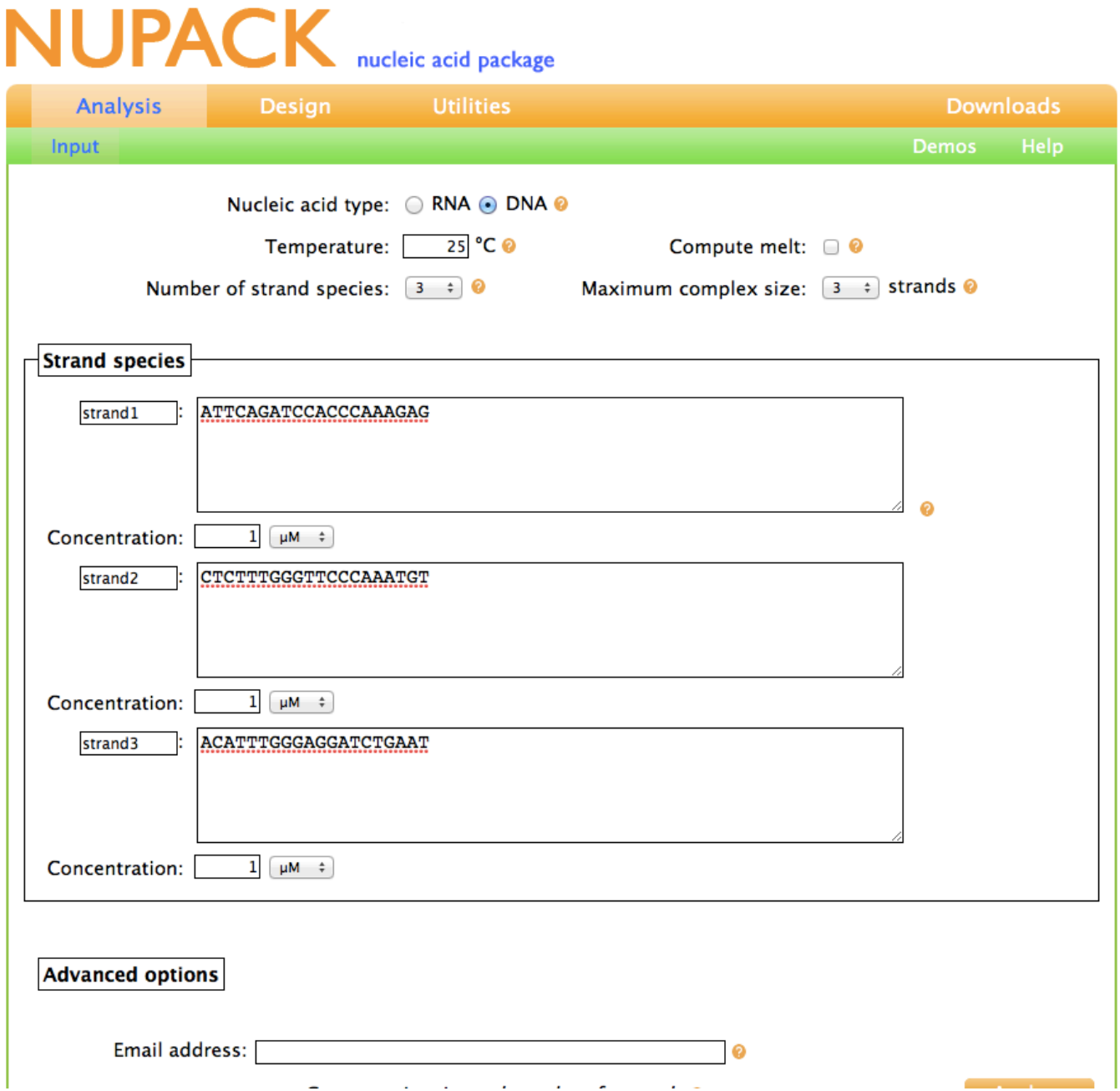
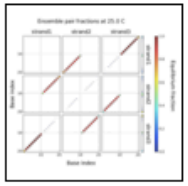

NUPACK
nucleic acid package
Analysis
Design
Utilities
Downloads
Input
Demos
Help
Nucleic acid type: RNA DNA
Temperature: 25 °C
Compute melt:
Number of strand species: 3
Maximum complex size: 3 strands
Strand species
strand1: ATTCAGATCCACCCAAAGAG
Concentration: 1 µM
strand2: CTCTTTGGGTTCCCAAATGT
Concentration: 1 µM
strand3: ACATTTGGGAGGATCTGAAT
Concentration: 1 µM
Advanced options
Email address:

Ensemble pair fractions



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Download data

Equilibrium concentrations

strand1-strand2-strand3
0.88 μM

strand1-strand3
0.12 μM

strand2
0.12 μM

strand2-strand2
0.0011 μM

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Histogram filters

Change strand concentrations

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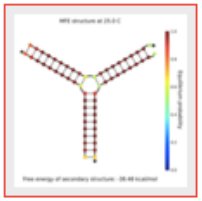
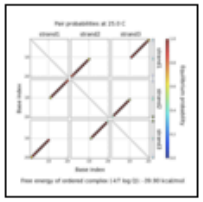
Back to results

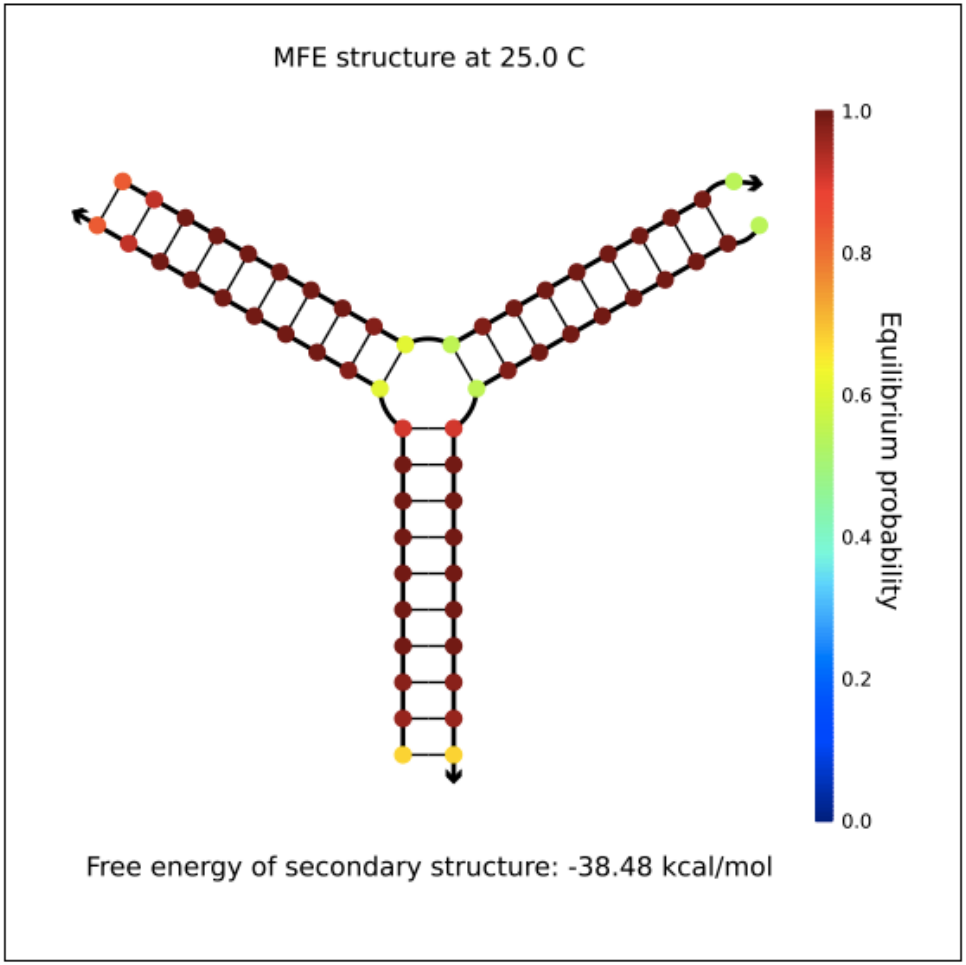
MFE structure



Pair probabilities



Probability shading Identity shading



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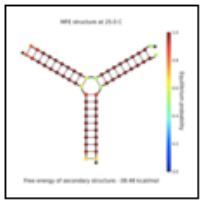
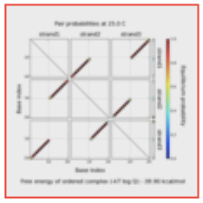
To Design | To Utilities

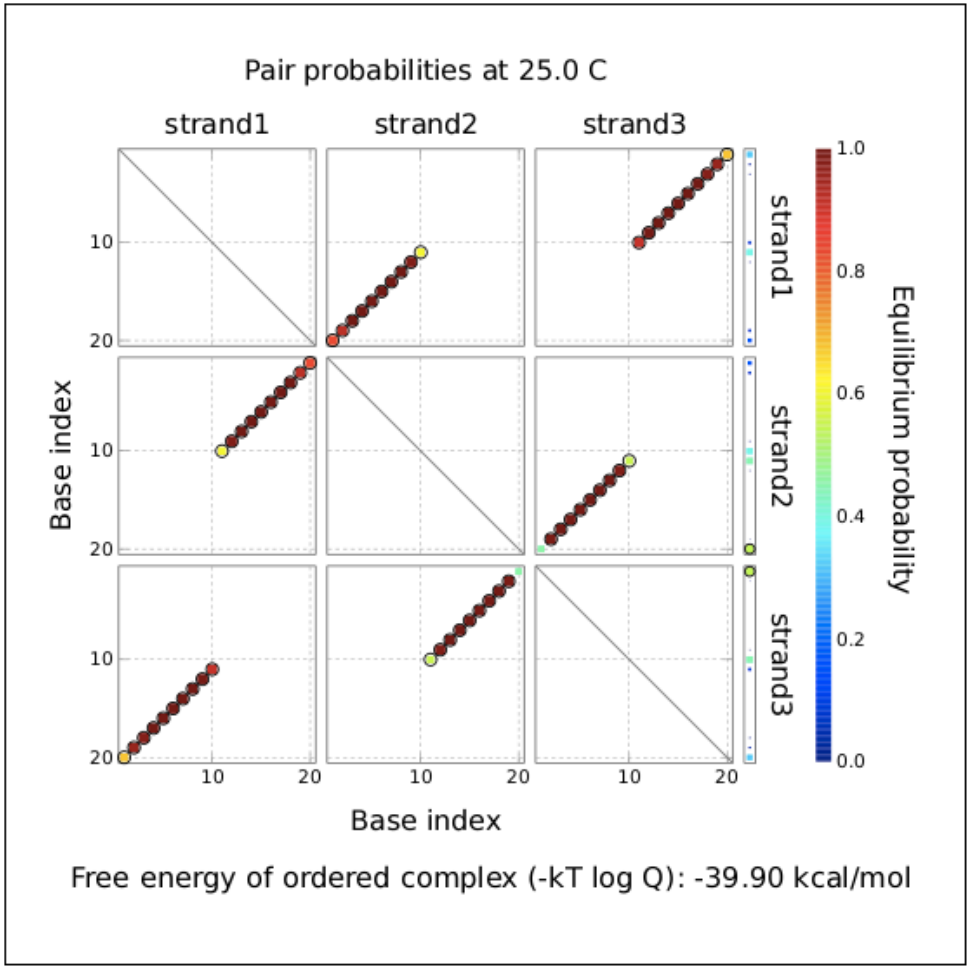
MFE structure



Pair probabilities



Depict MFE structure



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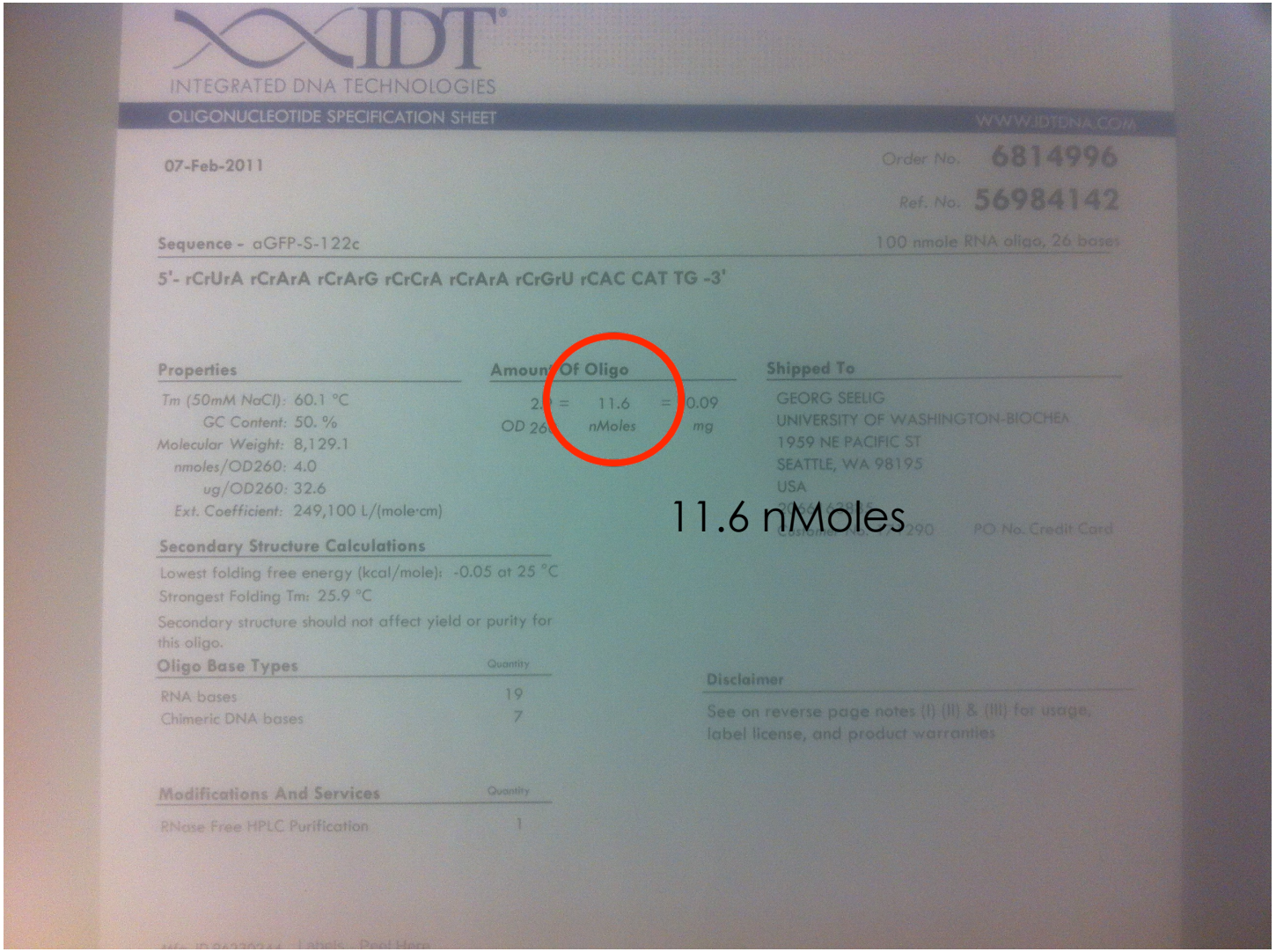
Download data

To Design To Utilities

Amounts and concentrations



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Sequence - aGFP-S-122c

100 nmole RNA oligo, 26 bases

5'- rCrUrA rCrArA rCrArG rCrCrA rCrArA rCrGrU rCAC CAT TG -3'

Properties

Tm (50mM NaCl): 60.1 °C
GC Content: 50. %
Molecular Weight: 8,129.1
nmoles/OD260: 4.0
ug/OD260: 32.6
Ext. Coefficient: 249,100 L/(mole·cm)

Amount Of Oligo

2.9 = 11.6 = 0.09
OD 260 nMoles mg

11.6 nMoles

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Secondary Structure Calculations

Lowest folding free energy (kcal/mole): -0.05 at 25 °C
Strongest Folding Tm: 25.9 °C
Secondary structure should not affect yield or purity for this oligo.

Oligo Base Types	Quantity
RNA bases	19
Chimeric DNA bases	7

Disclaimer

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Modifications And Services	Quantity
RNase Free HPLC Purification	1

Amounts and concentrations

What's a Mole (unit)? 6.02×10^{23} molecules

11.6 nMoles = $11.6 \times 10^{-9} \times 6.02 \times 10^{23}$ molecules

DNA reactions occur in an aqueous solution and it is convenient to think about concentrations rather than amounts.

Concentration=Number/Volume (Unit: M, Molar=Mole/liter)

How much water do you need to add to 11.6 nMoles of DNA to get a 100 uM (micro Molar) concentration?

Outlook: Designing DNA structures

So far, we analyzed sequence that were already given to us. But how can we design the sequences that correspond to a target structure?