Disorder, Equilibrium, Entropy

class – 10 (11.9.24)
class - 11 (12.9.24)

LS2103 (Autumn 2024)

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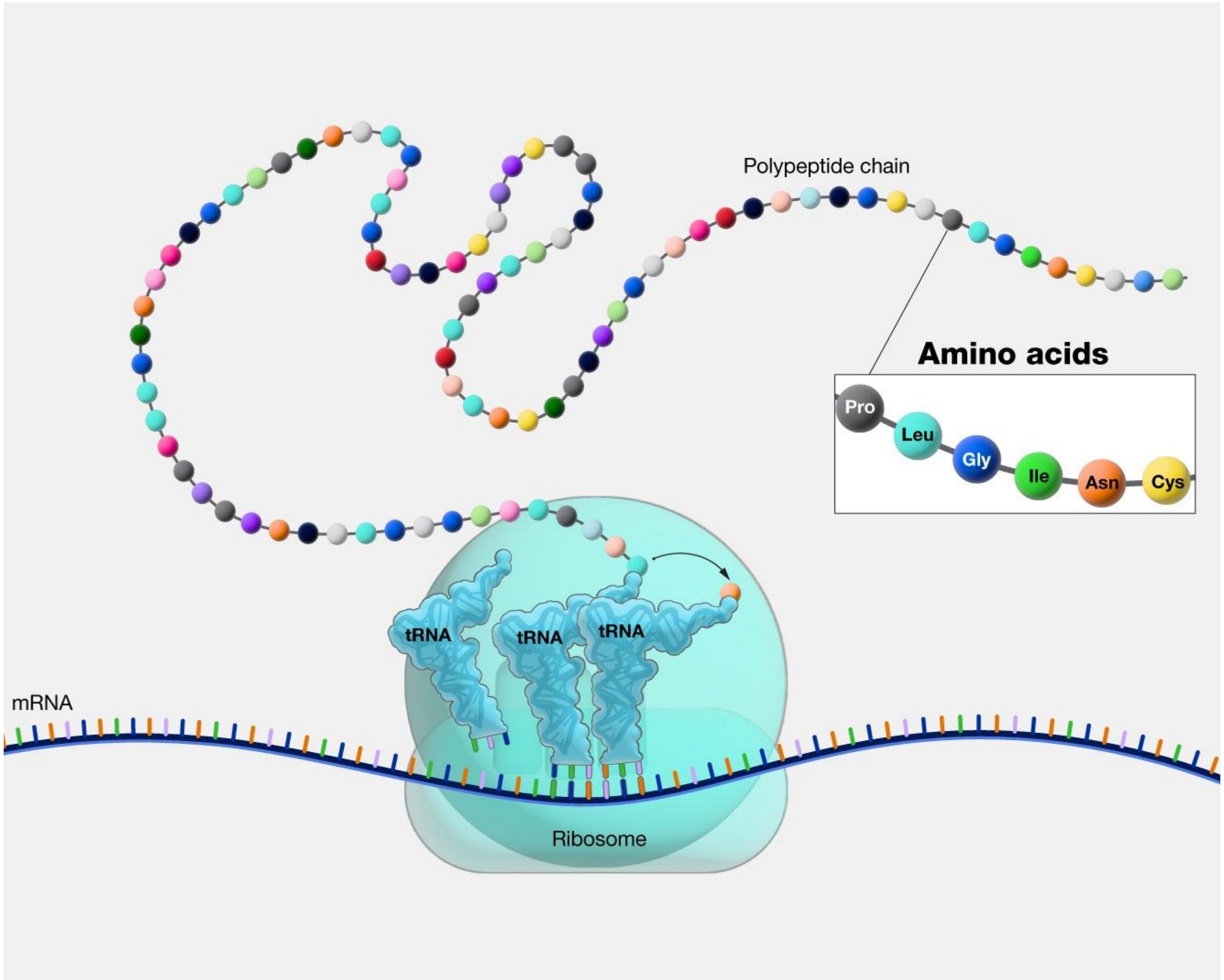
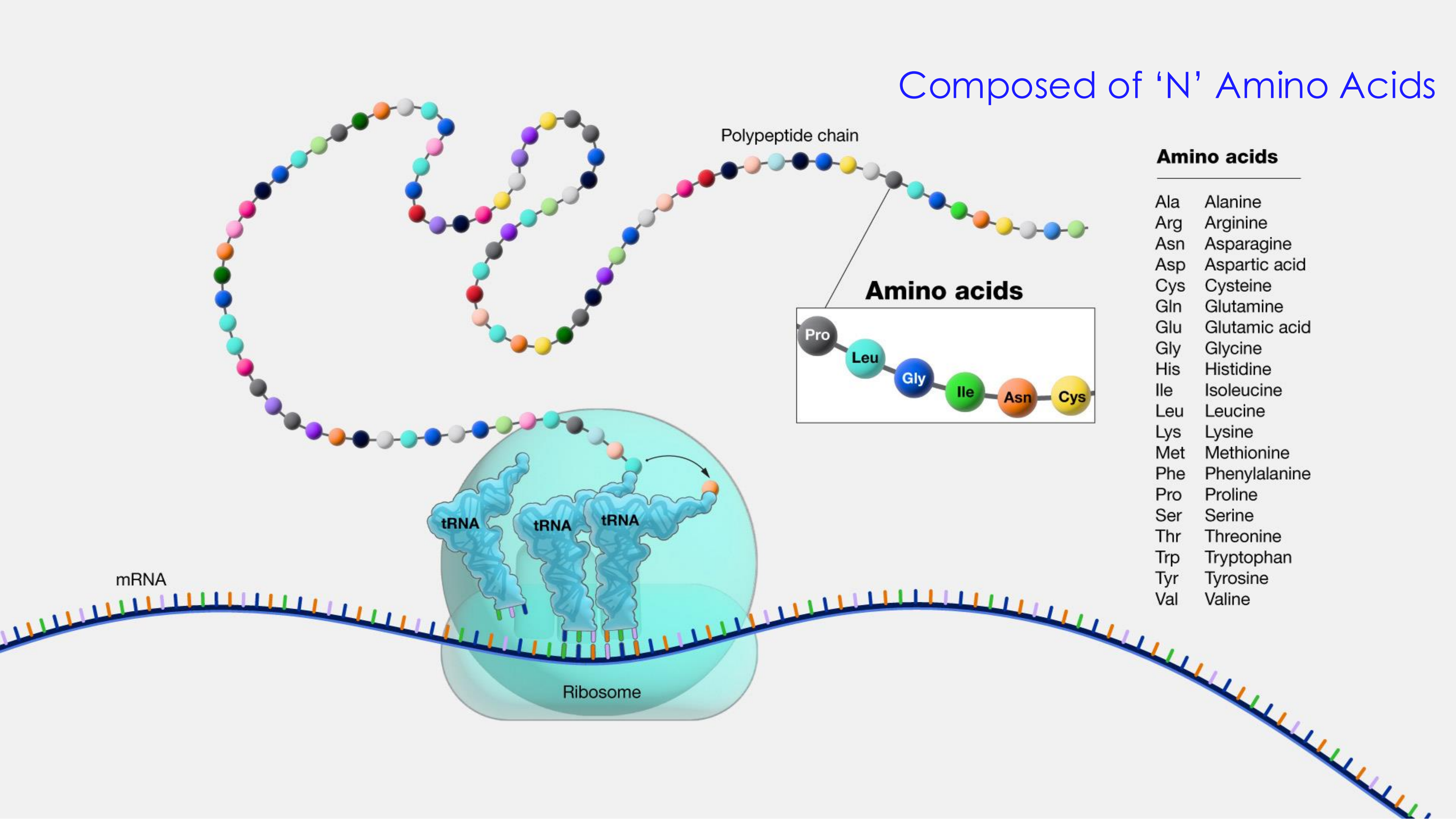
Consider a Protein == Amino Acid Chain of length 'M'



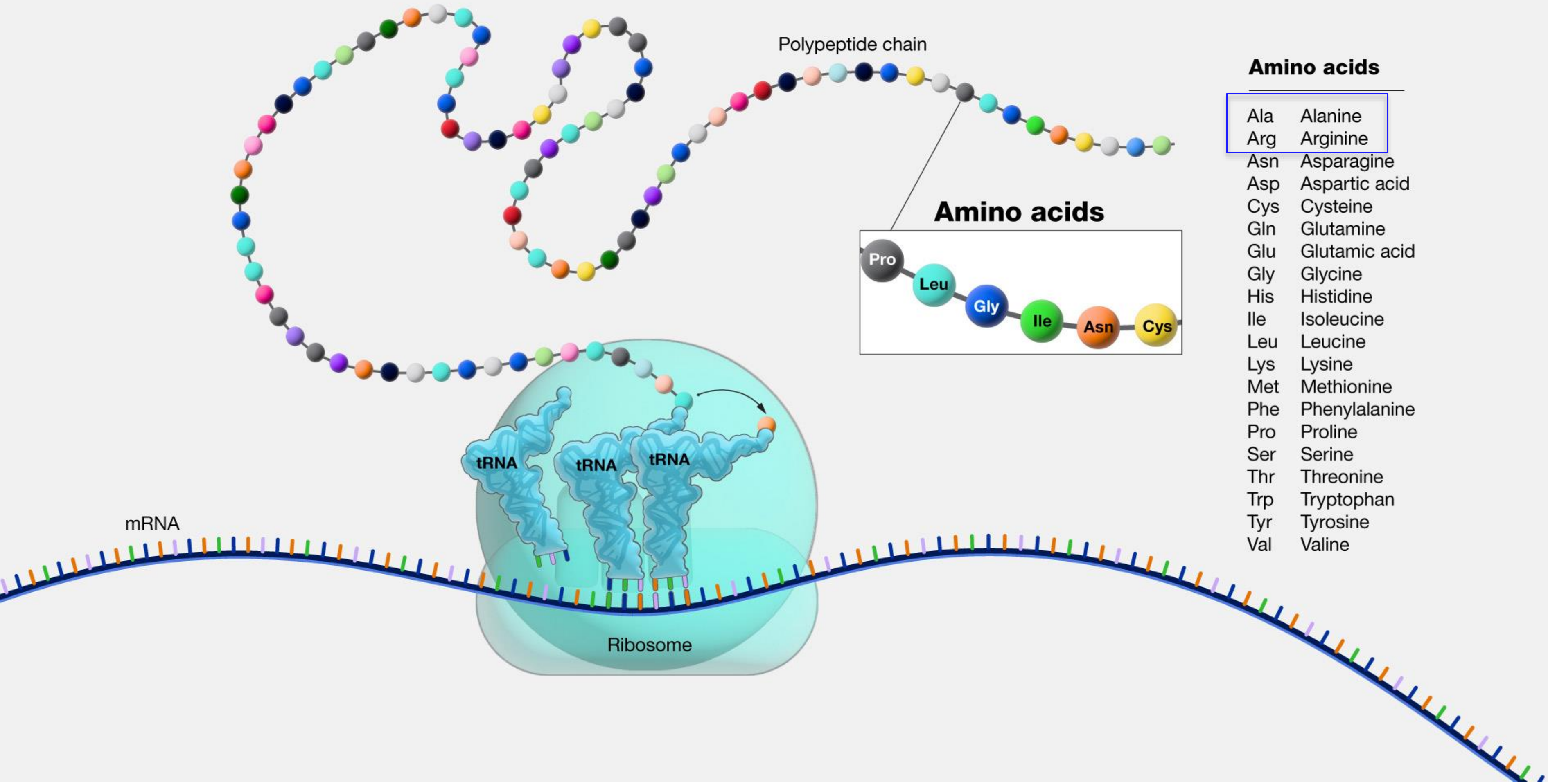
Consider a Protein == Amino Acid Chain of length 'M'

Composed of 'N' Amino Acids



Consider a Protein == Amino Acid Chain of length 'M'

Let us momentarily assume that N = 2



Amino acids

Ala	Alanine
Arg	Arginine
Asn	Asparagine
Asp	Aspartic acid
Cys	Cysteine
Gln	Glutamine
Glu	Glutamic acid
Gly	Glycine
His	Histidine
Ile	Isoleucine
Leu	Leucine
Lys	Lysine
Met	Methionine
Phe	Phenylalanine
Pro	Proline
Ser	Serine
Thr	Threonine
Trp	Tryptophan
Tyr	Tyrosine
Val	Valine

Consider a Protein == Amino Acid Chain of length 'M'

Let us momentarily assume that N = 2

.. such as in a coin toss

Image from BBC Science Focus Article:

https://www.sciencefocus.com/science/are-coin-tosses-really-random

Consider a Protein == Amino Acid Chain of length 'M'

Let us momentarily assume that N = 2

.. such as in a coin toss

Thereby, let us consider the DISORDER in a sequence

Thereby, let us consider the DISORDER in a sequence

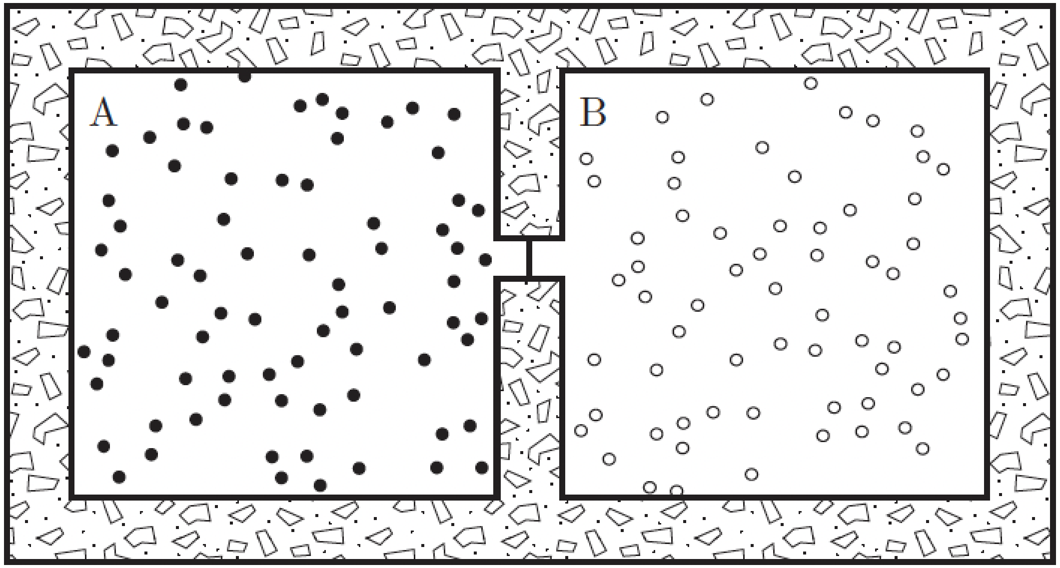
.. and hence the concept of ENTROPY

… and the Statistical Postulate of EQUILIBRIUM:

When an isolated system is left alone long enough,
it evolves to thermal equilibrium.

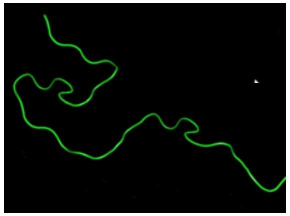
Equilibrium is not one microstate, but rather that *probability distribution of microstates* having the greatest possible disorder allowed by the physical constraints on the system.

Consider a fully insulated system whose total energy is constant, but the energy can be exchanged between the compartments, ‘A’ and ‘B’.

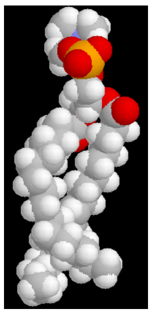


a) How will the total energy be distributed between ‘A’ and B’?
b) What will be their temperature difference?

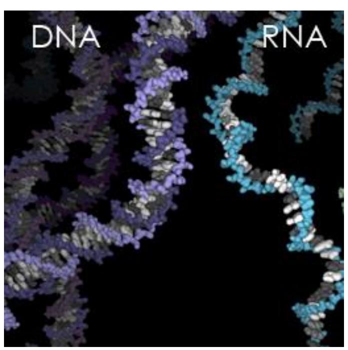
Features of Biological Assembly:



polypeptides



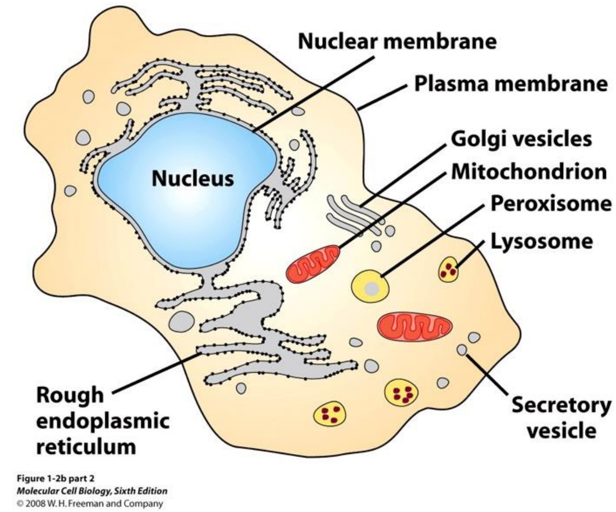
phospholipids

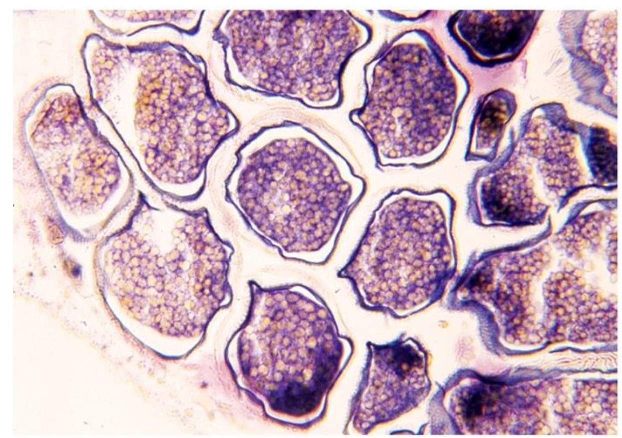


nucleic acids

- **'Soft' systems with large flexibilities**
- **Sensitive to thermal fluctuation**
- **Multi-component, dynamic**
- **Complex interconnectivities**

- **Water is the most common biological milieu**
- **It plays a key role in enabling biomolecular interactions**





Cells and Tissues

Relevant thermodynamic quantities:

Thermodynamic Entropy (S):

$$S = k_B \ln(\Omega)$$

From the 2nd Law of Thermodynamics:

$$S = \frac{\delta Q}{T}$$

$$S_2 - S_1 = \Delta S \geq \int_1^2 \frac{\delta Q}{T}$$

$$\Delta S_{universe} > 0$$

Gibbs Free Energy Change:

$$\Delta G = \Delta H - T\Delta S$$

SPONTANEOUS PROCESS:

$$\Delta G < 0$$

Relevant thermodynamic quantities:

HW:
Identify the variables with their usual units

Entropy (S):

$$S = k_B \ln(\Omega)$$

From the 2nd Law of Thermodynamics:

$$H = E + pV$$

$$S_2 - S_1 = \Delta S \geq \int_1^2 \frac{\delta Q}{T}$$

$$\left.\Delta S_{universe} > 0\right\}$$

At constant (p, V), Helmholtz Free Energy Change:

$$\Delta F = \Delta E - T\Delta S$$

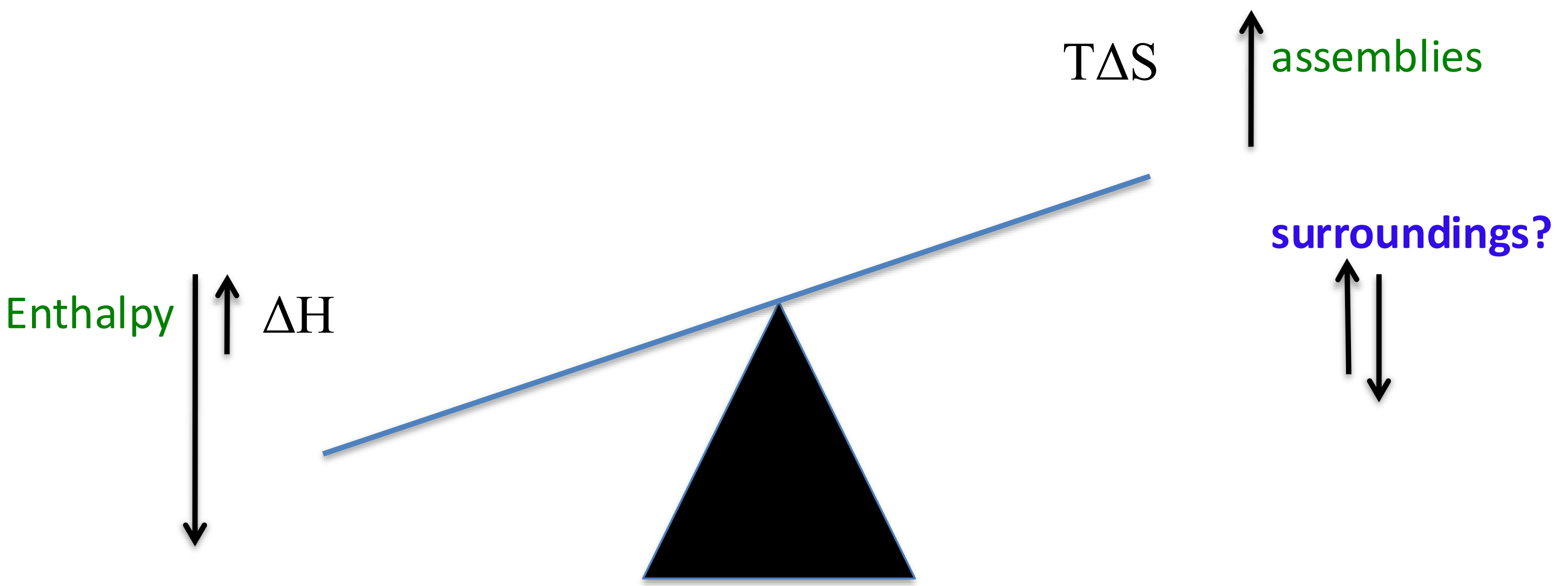
SPONTANEOUS PROCESS:

$$\Delta F < 0$$

Thermodynamic 'Balance' in Biological Assembly

$$\Delta G = \Delta H - T\Delta S$$

During assembly:



The surrounding (often water) plays key roles in the balance

Protein binding on Long DNA strand:

Entropy (S):

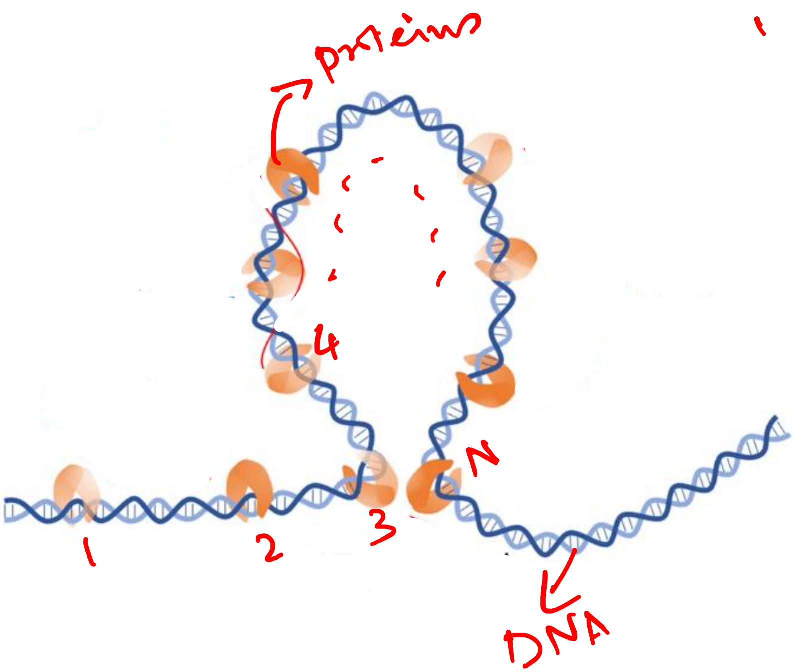
$$S = k_B \ln(\Omega)$$

'N' no. of binding sites on DNA

'N_p' no. of protein molecules

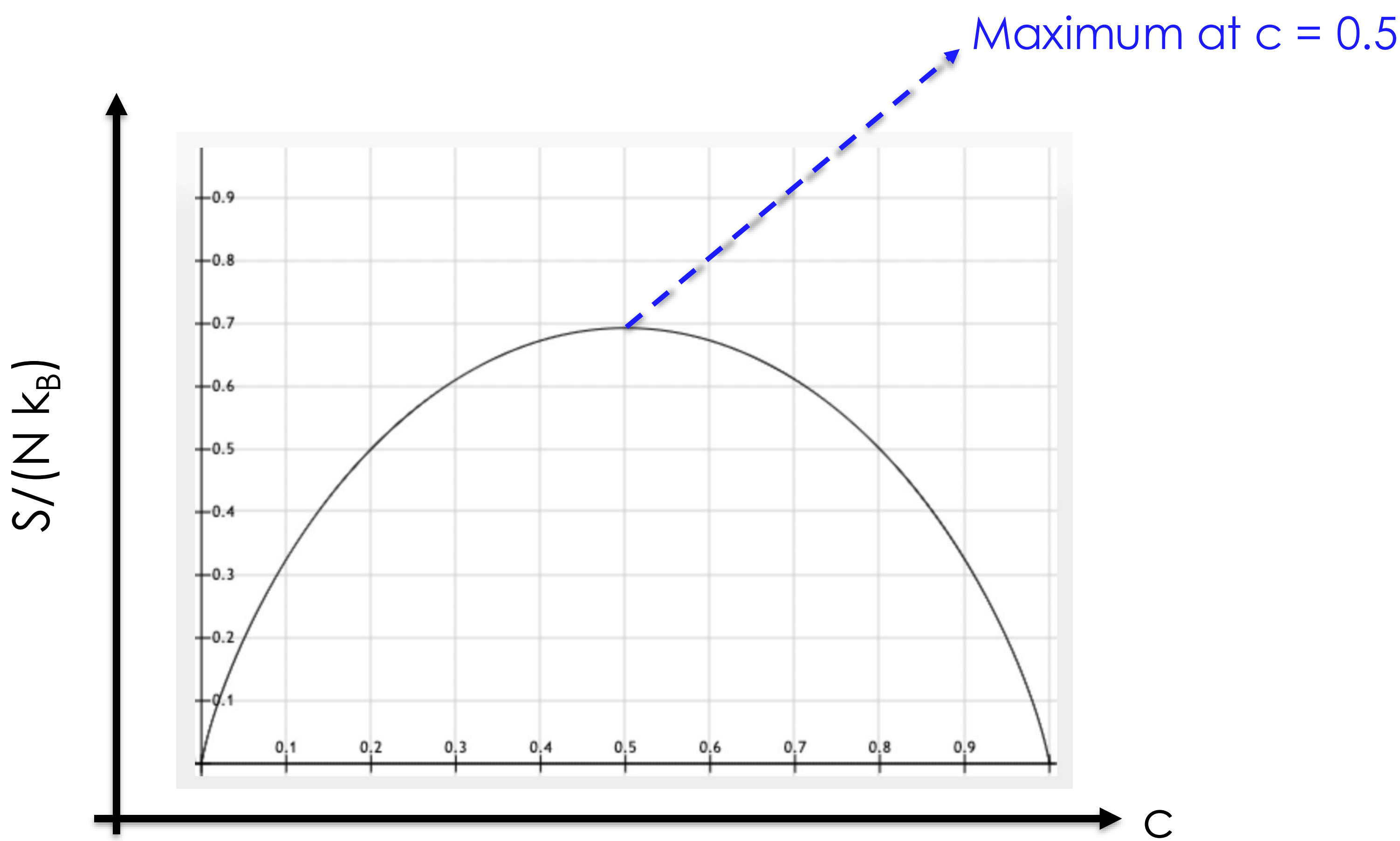
$(N_p < N)$

Protein binding sites on DNA:



Representative image from:
Park et al., J. Korean. Phys. Soc., **78**, 408–426 (2021): review

Protein binding on Long DNA strand:



50% coverage of binding sites maximizes the entropy. Why?