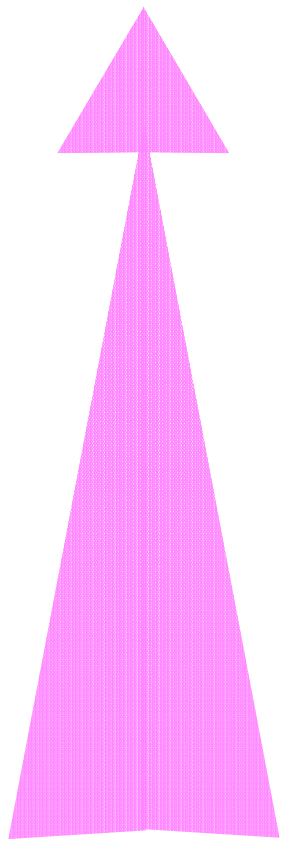
NORCIA,
self organization and emergence,
OVVERO:

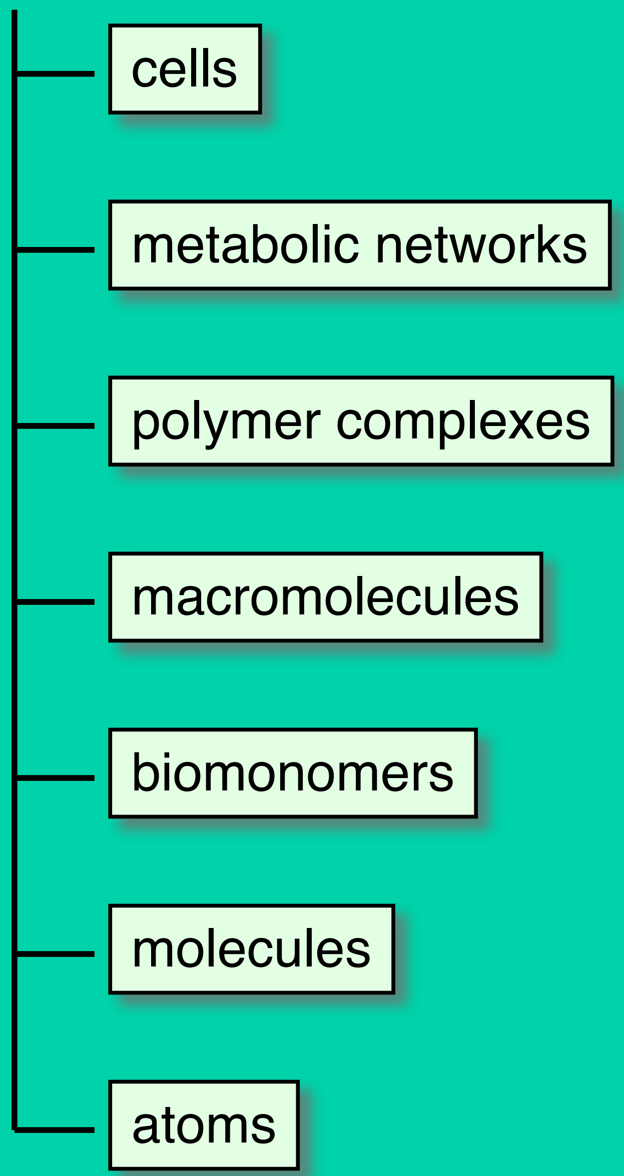
COME SI PUO‘ SPONTANEAMENTE COSTRUIRSI LA COMPLESSITA‘ MOLECOLARE?

LIFE



INANIMATE MATTER

(NON - LIFE)


cells
metabolic networks
polymer complexes
macromolecules
biomonomers
molecules
atoms

THE INCREASE OF COMPLEXITY TOWARDS THE EMERGENCE OF LIFE PROCEEDS

VIA THE INTERPLAY BETWEEN SELF-ORGANIZATION AND EMERGENCE

SELF-ORGANIZATION: THE ACQUISITION OF HIGHER STRUCTURAL ORDER-AS DETERMINED BY THE SYSTEM'S RULES

…under thermodynamic or kinetic control

Self-assembly
Self-organization
Self-replication

What does “self” mean?

SELF: MEANS THAT THE PROCESS IS DETERMINED

BY THE „INTERNAL RULES“ OF THE SYSTEM

and not imposed by external forces

Which of these cases are examples of Self-organization?

The costruction of an ant nest
The assembly of a TV set
The structure of a city
Crystallization
Queing at the post office
Protein folding
The growth of plants from seeds
The assembly of a virus

QUESTION:

When is self-organization under thermodynamic control?

or under kinetic control?

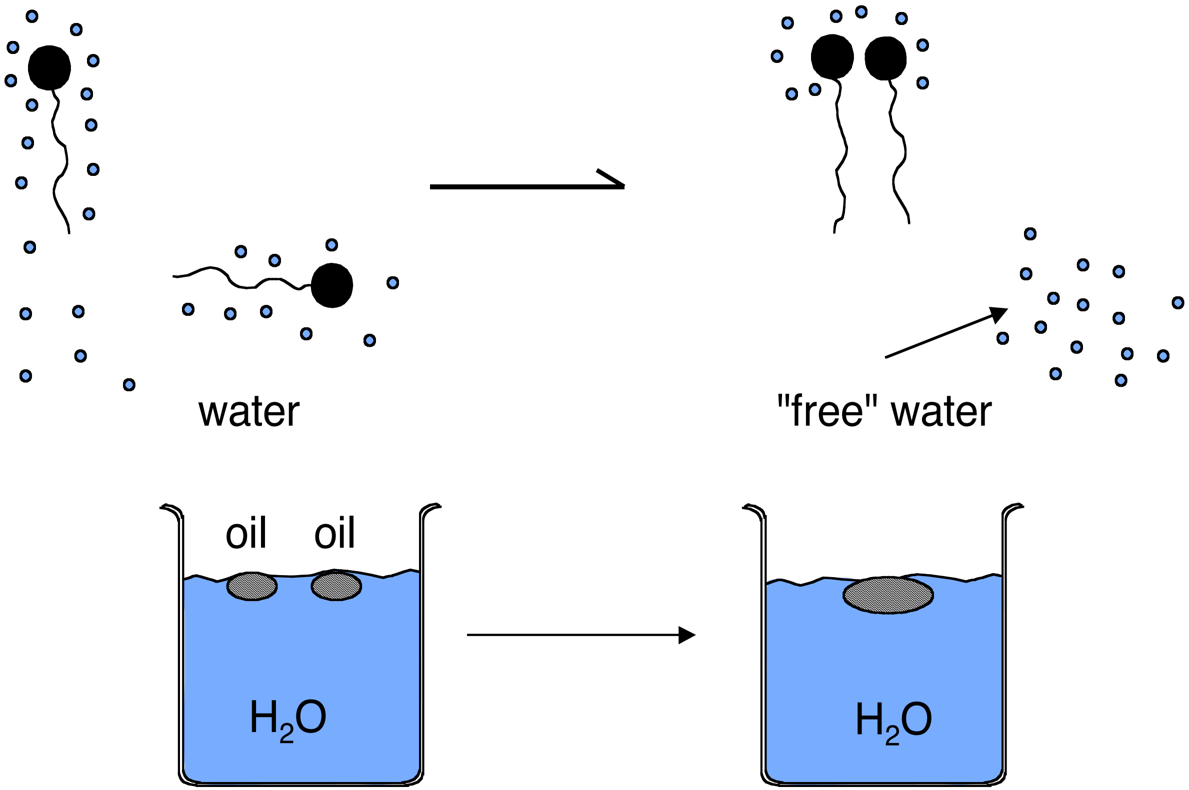
An useful criterium for checking self-organization Under thermodynamic control is the reversibility of the process:

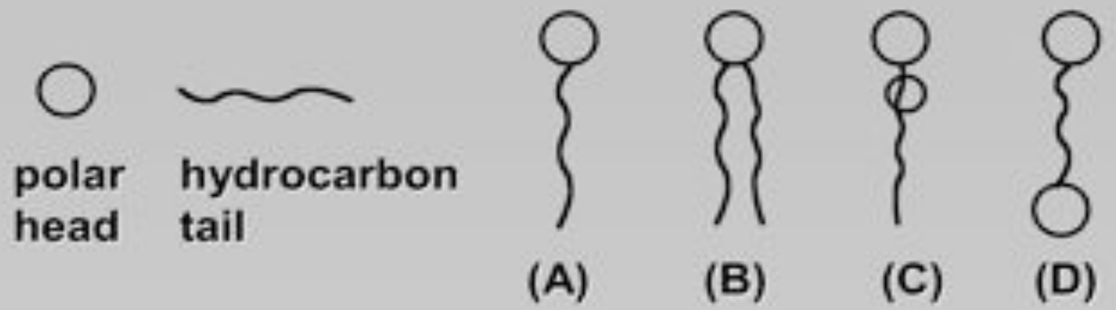
Destroy the structural organization (mildly) and ask: Does it reform again by itself?

However, also chemically irreversible process can be under thermodynamic control. What is determining for the definition is a negative change of free energy

LET US SEE SOME EXAMPLES

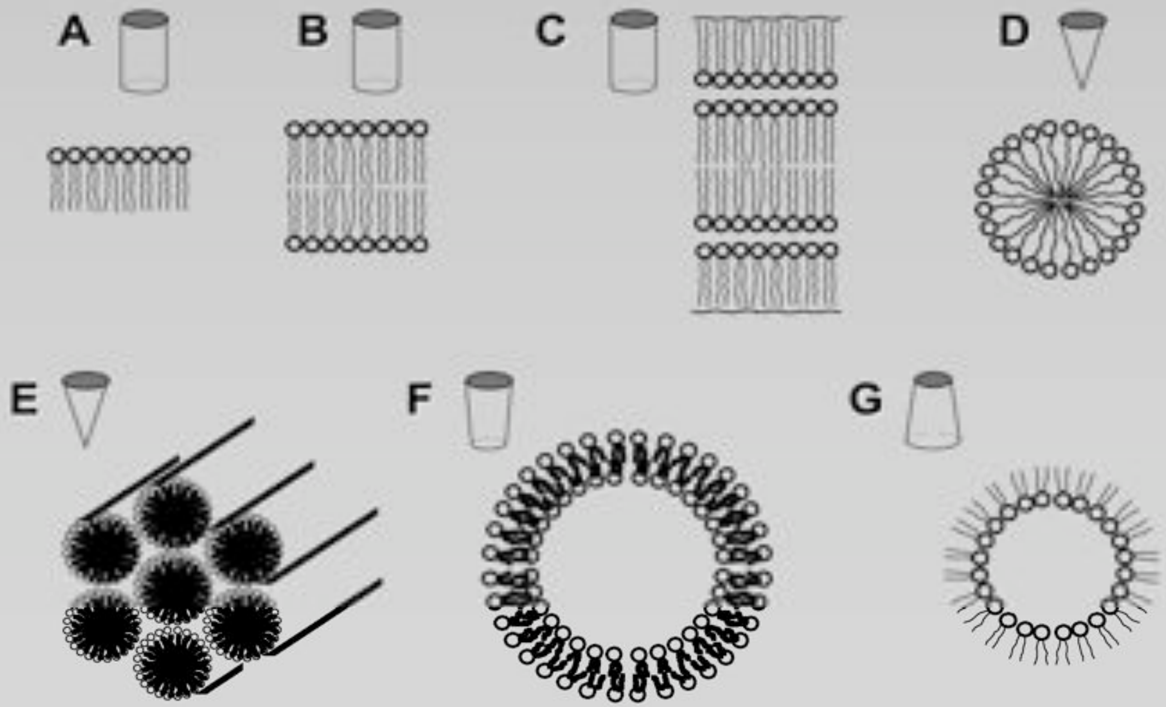
hydrophobic forces as the main factors for the association of surfactant molecules





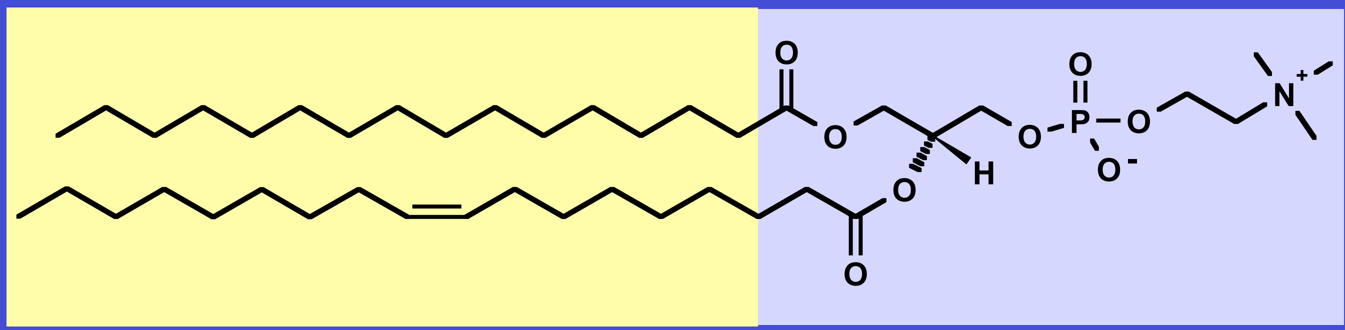
Diagrammatic representation of a detergent molecule

(A) Single tailed
(B) Double tailed
(C) Zwitterionic
(D) Bolamphiphilic

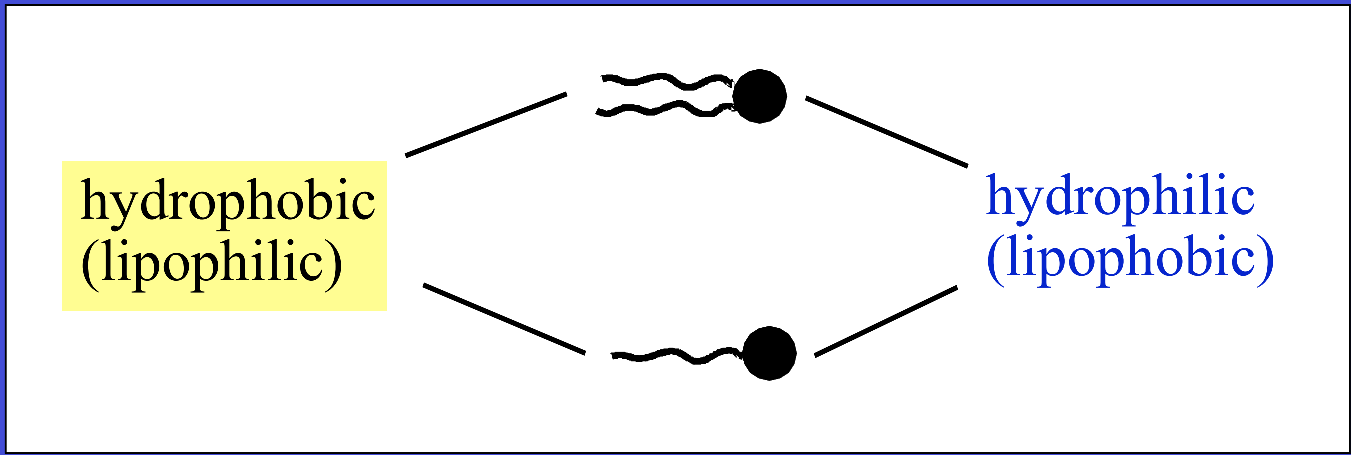


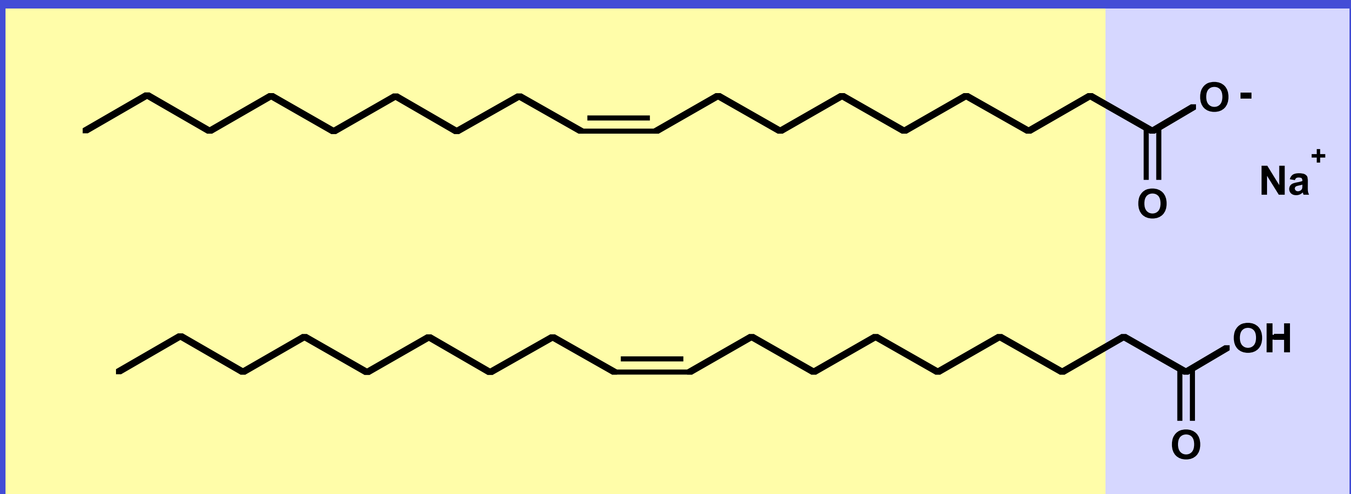
Different types of surfactant aggregates in solution

(A) Monolayer
(B) Bilayer
(C) Liquid-crystallin phase (lamellar)
(D) Normal micelles
(E) Cylindrical micelles (hexagonal)
(F) vesicles (liposomes)
(G) Reversed micelles



POPC



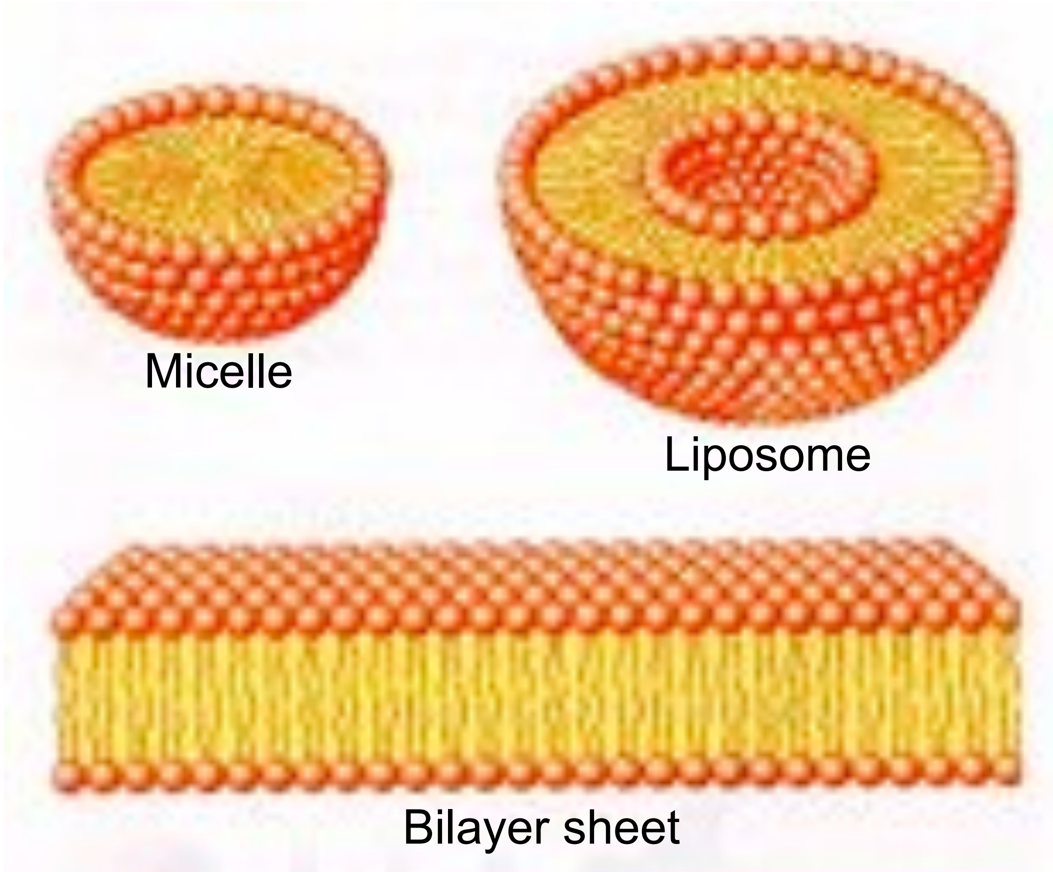


**sodium oleate
+ oleic acid**

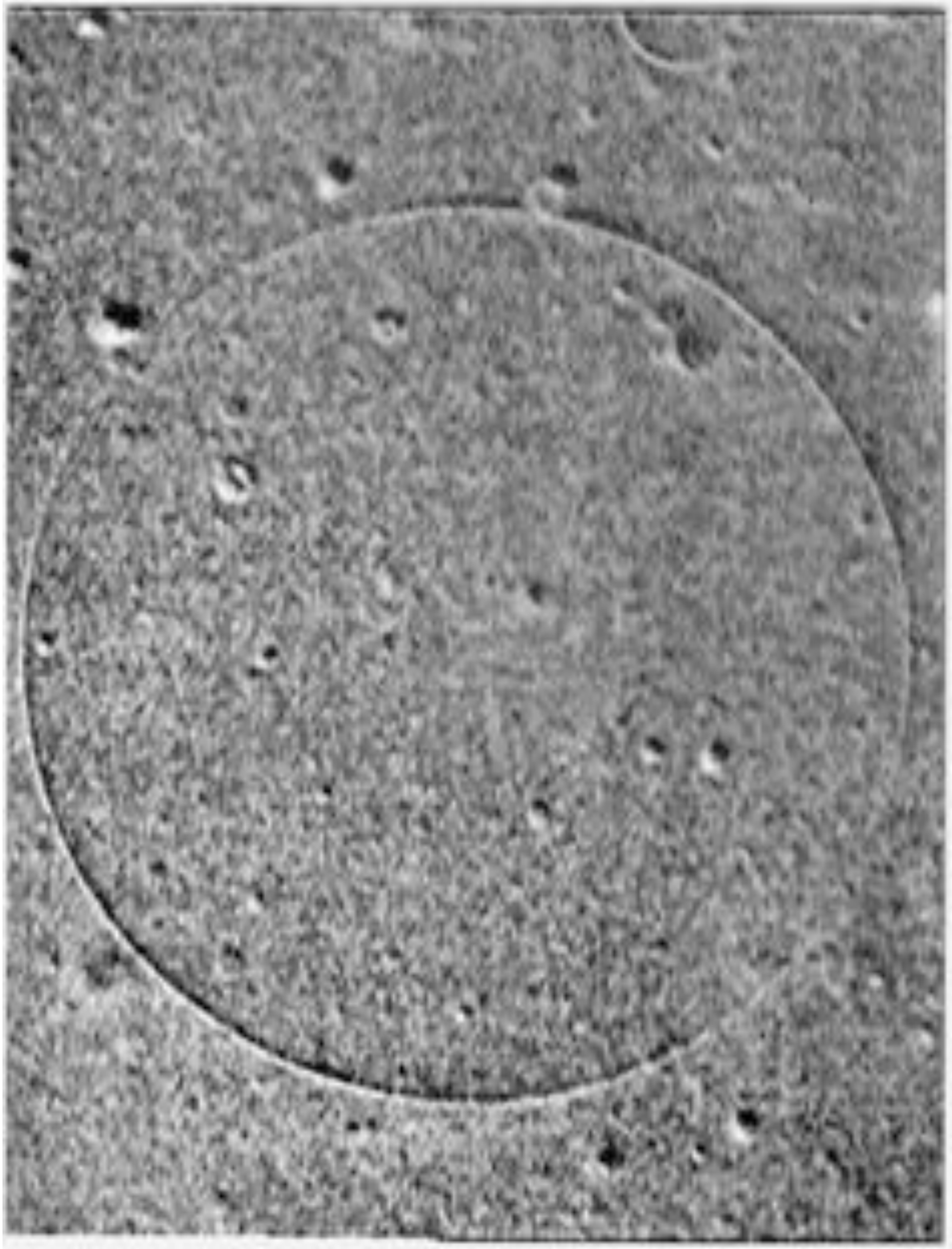
.. A PROCESS WHICH BRINGS ABOUT
ORDER
AND IS ACCOMPANIED BY AN
INCREASE
OF ENTROPY

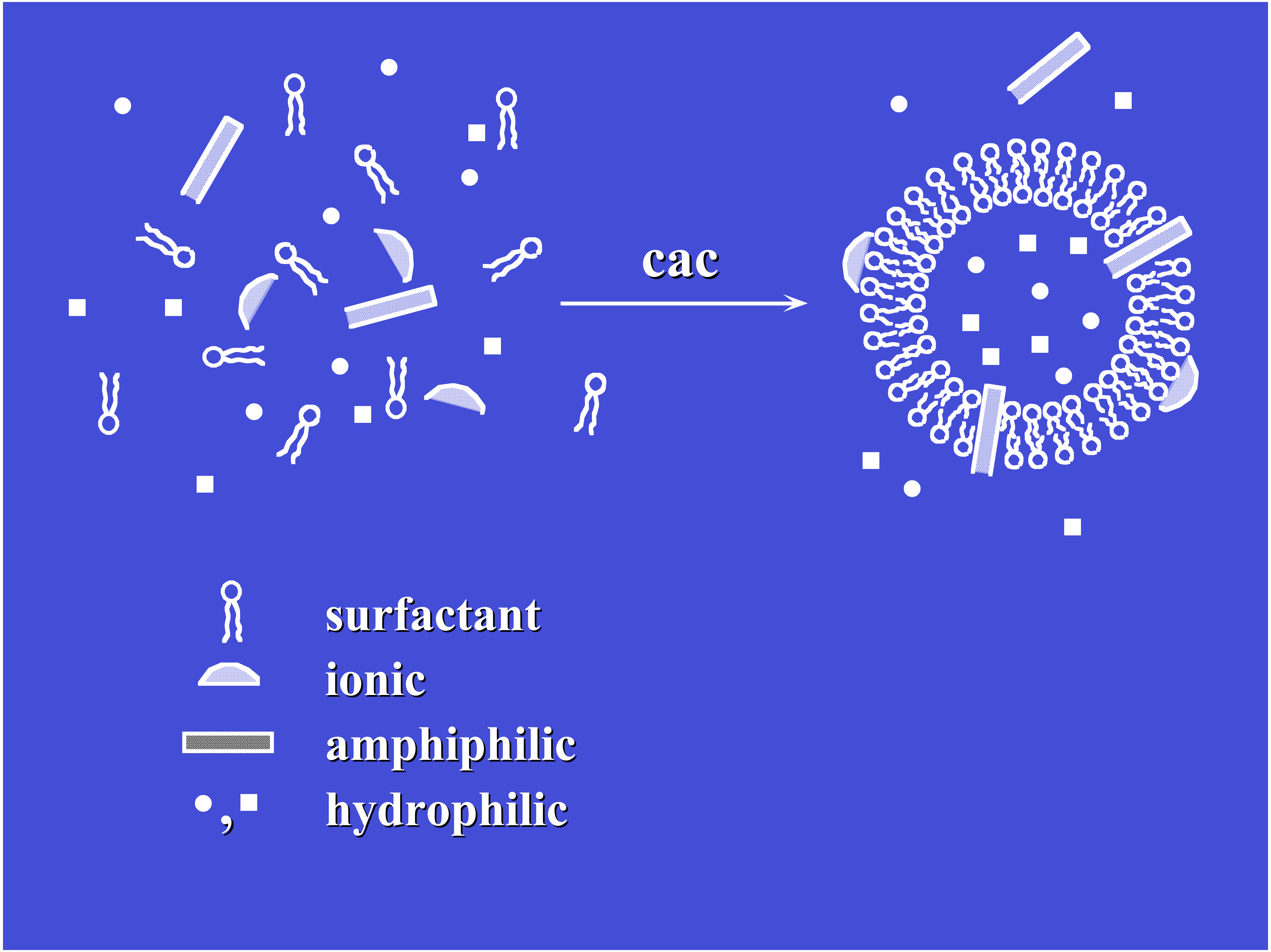
BEING UNDER THERMODYNAMIC CONTROL

Cross-sectional views of the three structures that can be formed by mechanically dispersing a suspension of phospholipids in aqueous solution

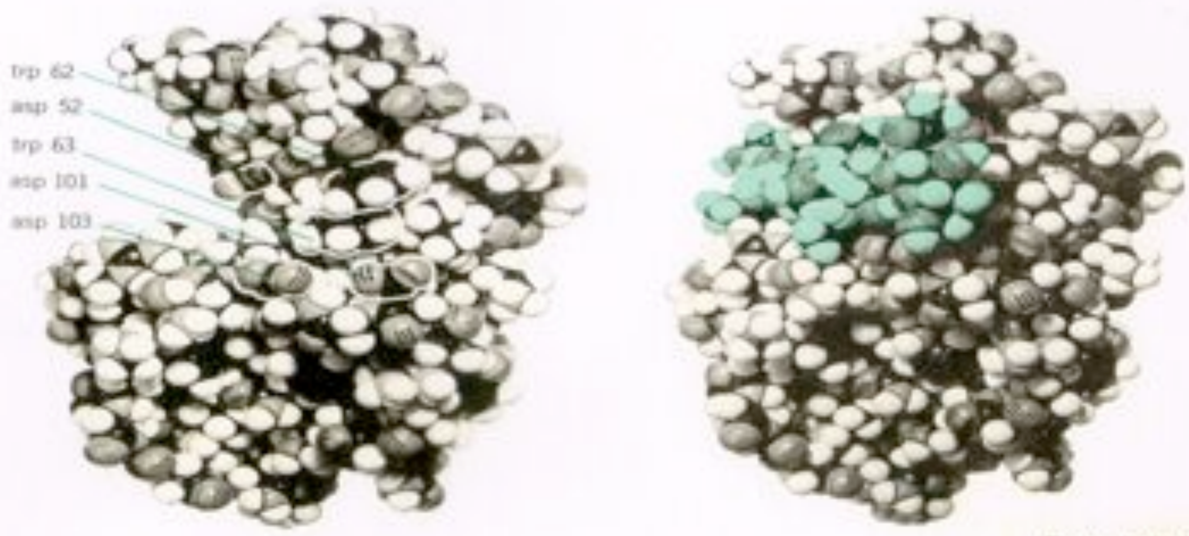


The red circles depict the hydrophilic heads of phospholipids, and the squiggly lines (in the yellow region) the hydrophobic tails.



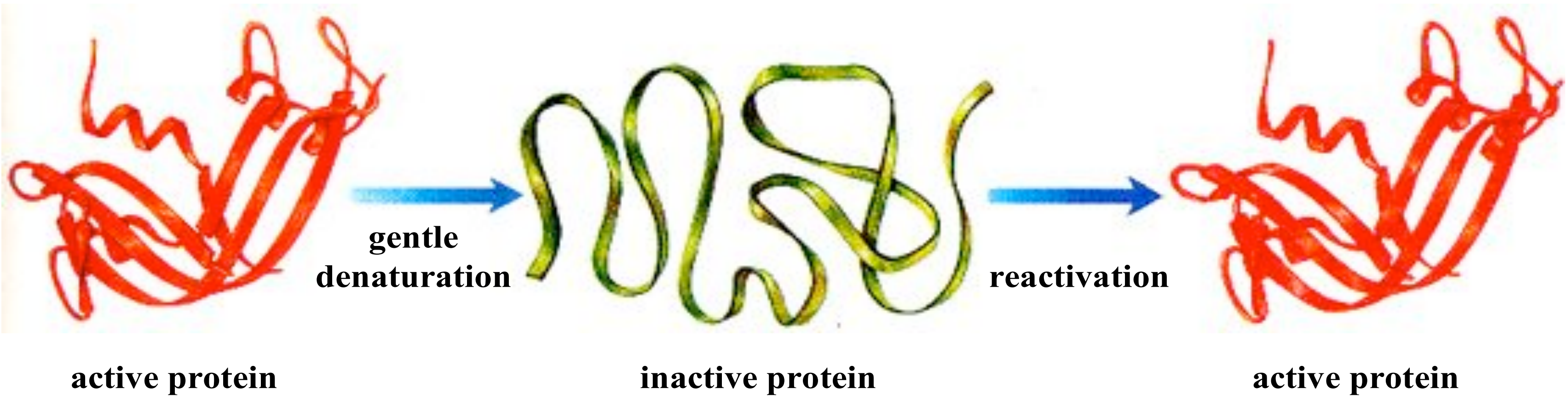

cac
surfactant
ionic
amphiphilic
hydrophilic

PROTEIN FOLDING: AN IMPORTANT CLASS OF BIOLOGICAL SELF-ORGANIZATION



(75)

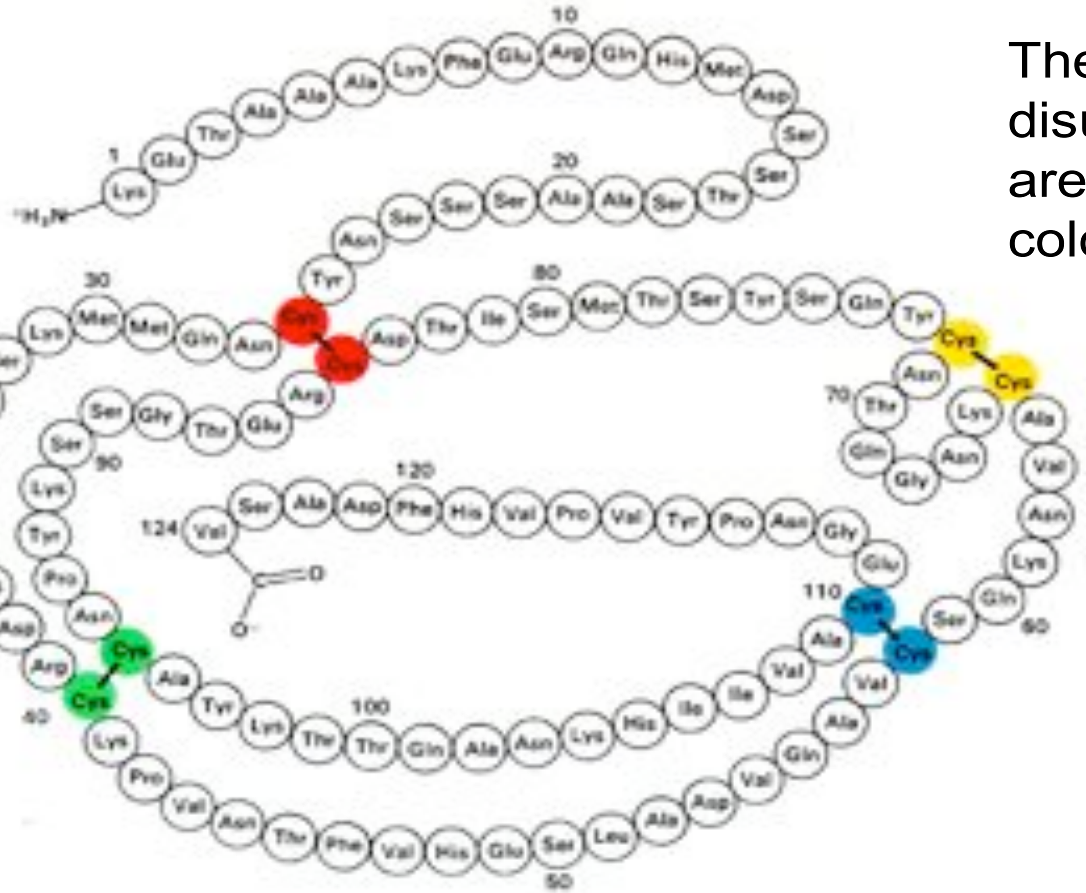
Ein raumfüllendes CPK-Modell von Lysozym. Links: Enzym ohne Substratmolekül; man erkennt das spaltförmige aktive Zentrum. Rechts: Enzym-Substrat-Komplex, Substratmolekül in Farbe



Denaturation and reactivation of the enzyme ribonuclease. When a protein is denatured, it loses its normal shape and activity. If denaturation is gentle and if the conditions are removed, some proteins regain their normal shape. This shows that the normal conformation of the molecule is due to the various interactions among a set sequence of amino acids. Each type of proteins has a particular sequence of amino acids.

(from Biology / S.Mader, 5th ed.)

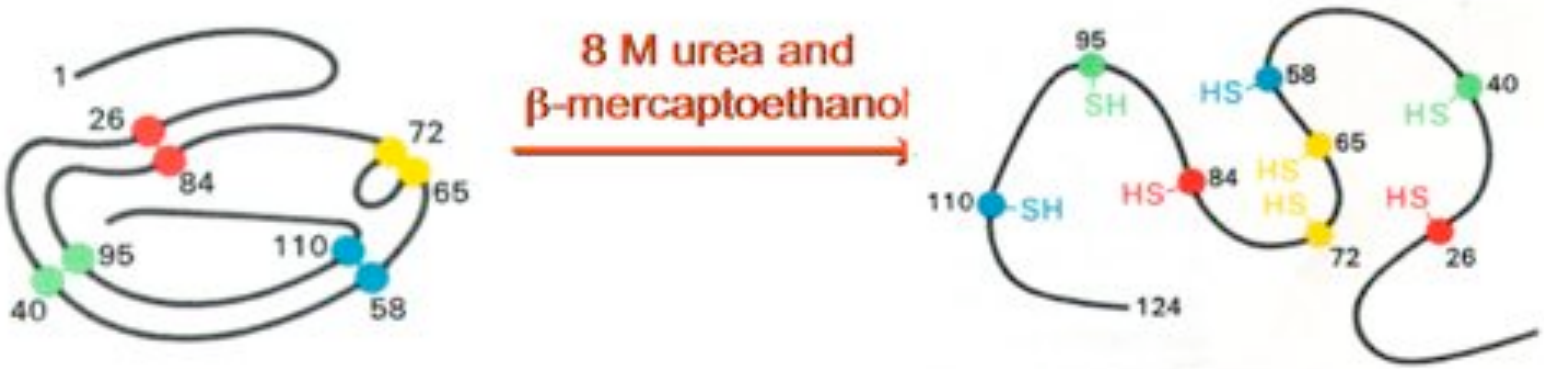
Amino acid sequence of bovine ribonuclease



The four disulfide bonds are shown in color.

(from Biochemistry / L.Stryer)

Reduction and denaturation of ribonuclease



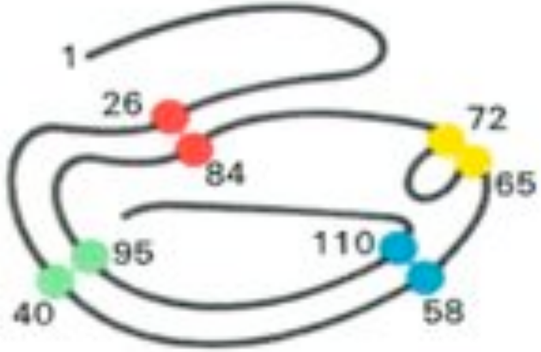
Native ribonuclease

Denatured reduced ribonuclease

(from Biochemistry / L.Stryer)

Renaturation of ribonuclease

Denatured reduced ribonuclease



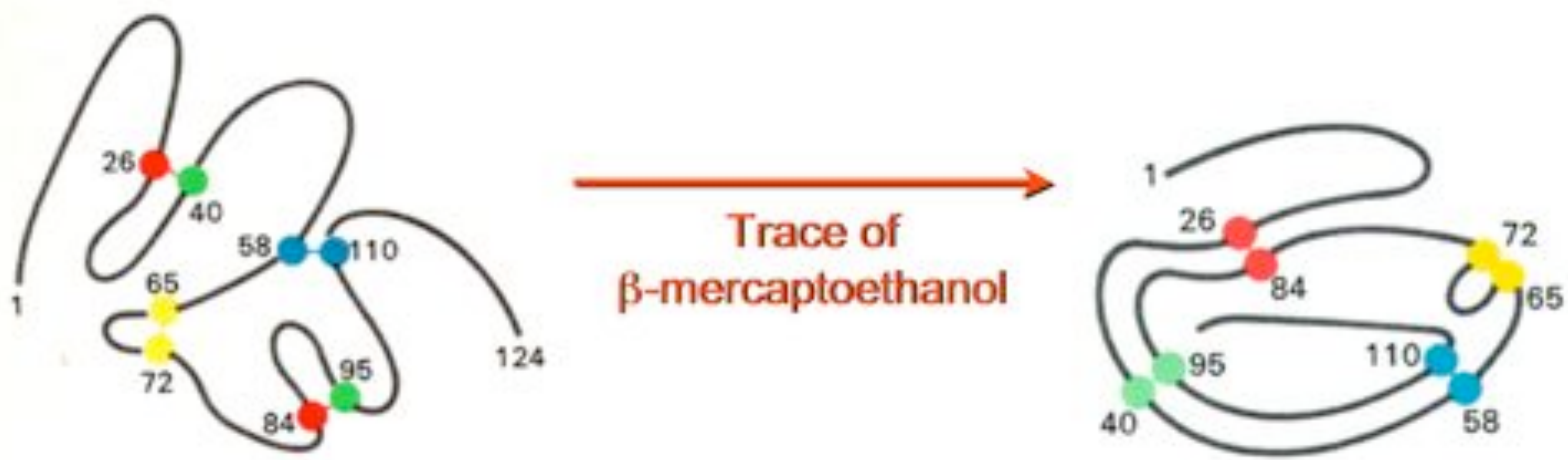
Native ribonuclease

Dialysis to remove urea and β-mercaptoethanol

Air oxidation of the sulfhydryl groups in reduced ribonuclease

(from Biochemistry / L.Stryer)

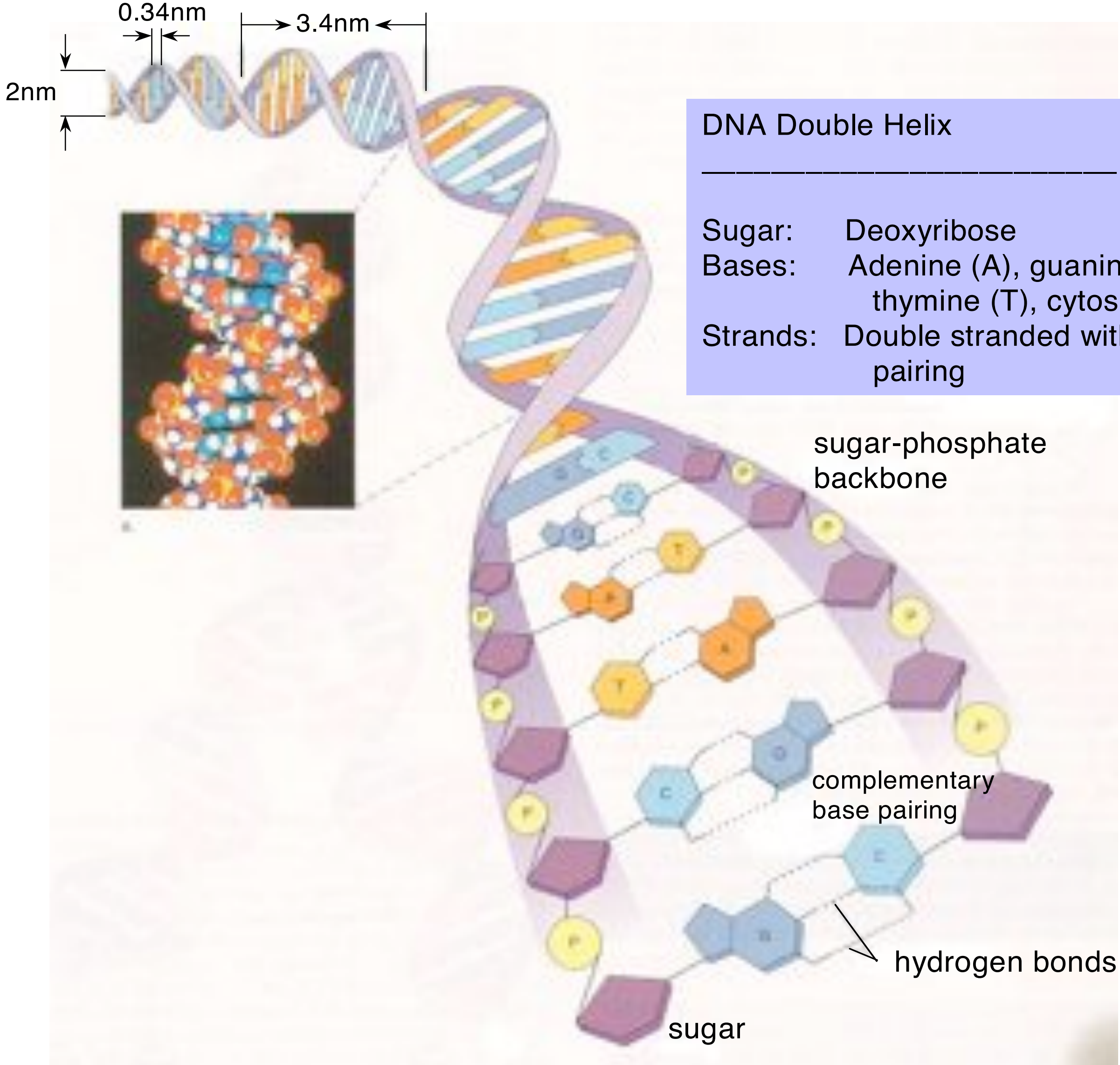
Formation of native ribonuclease from “scambled“ ribonuclease in the presence of a trace of β-mercaptoethanol



“Scrambled“ ribonuclease

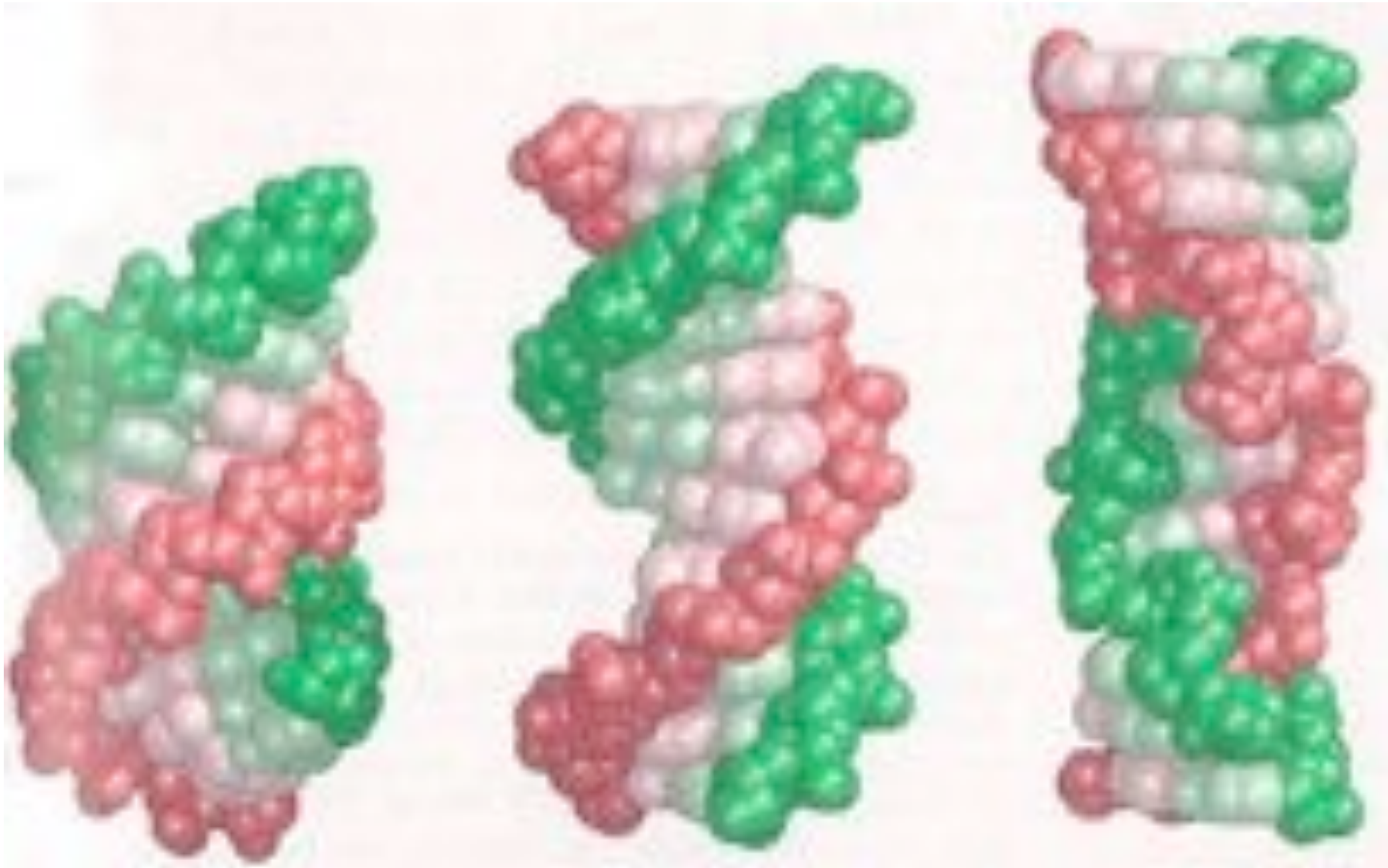
Native ribonuclease

(from Biochemistry / L.Stryer)

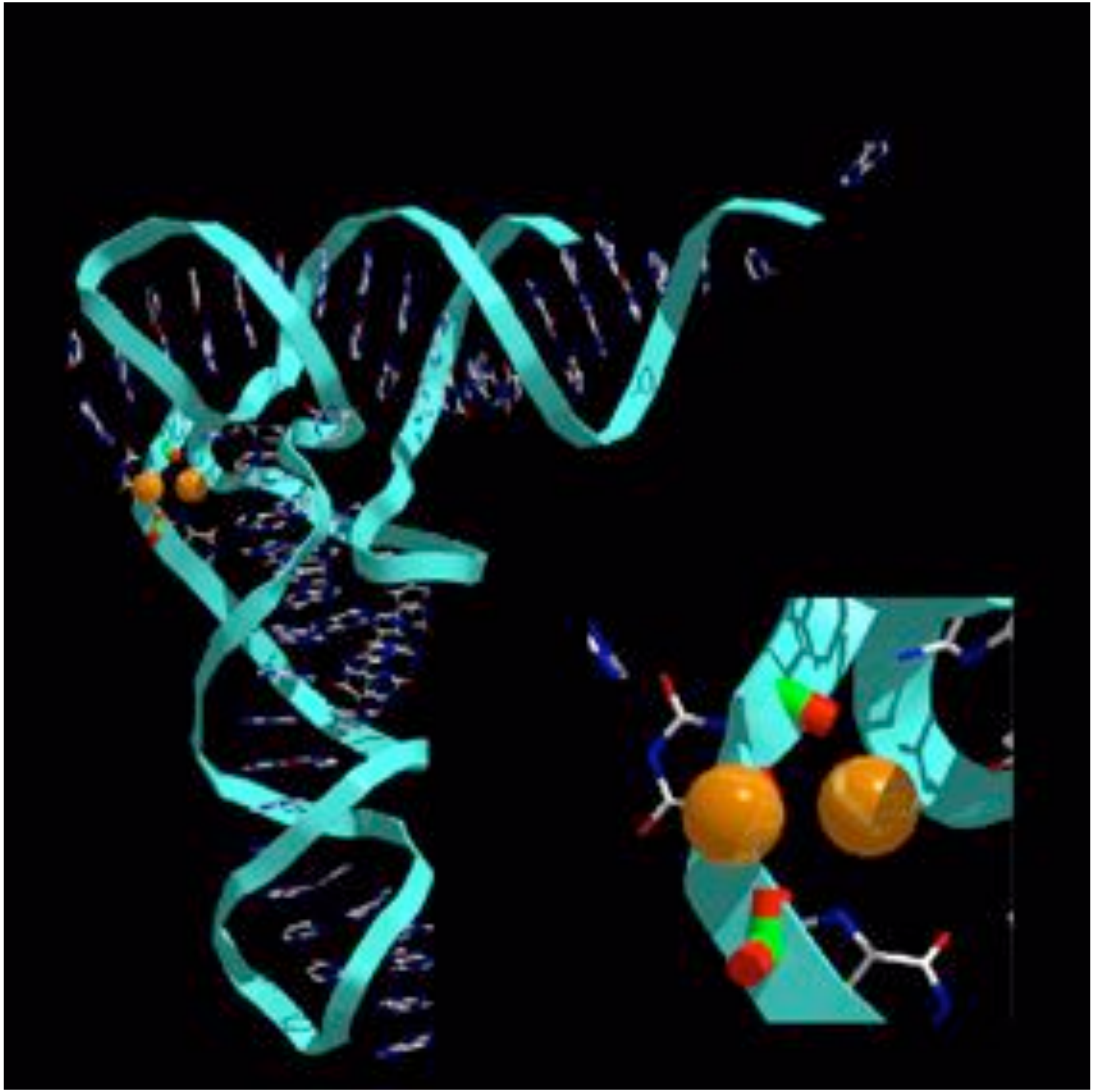


DNA Double Helix

Sugar: Deoxyribose
Bases: Adenine (A), guanine (G) thymine (T), cytosine (C)
Strands: Double stranded with base pairing

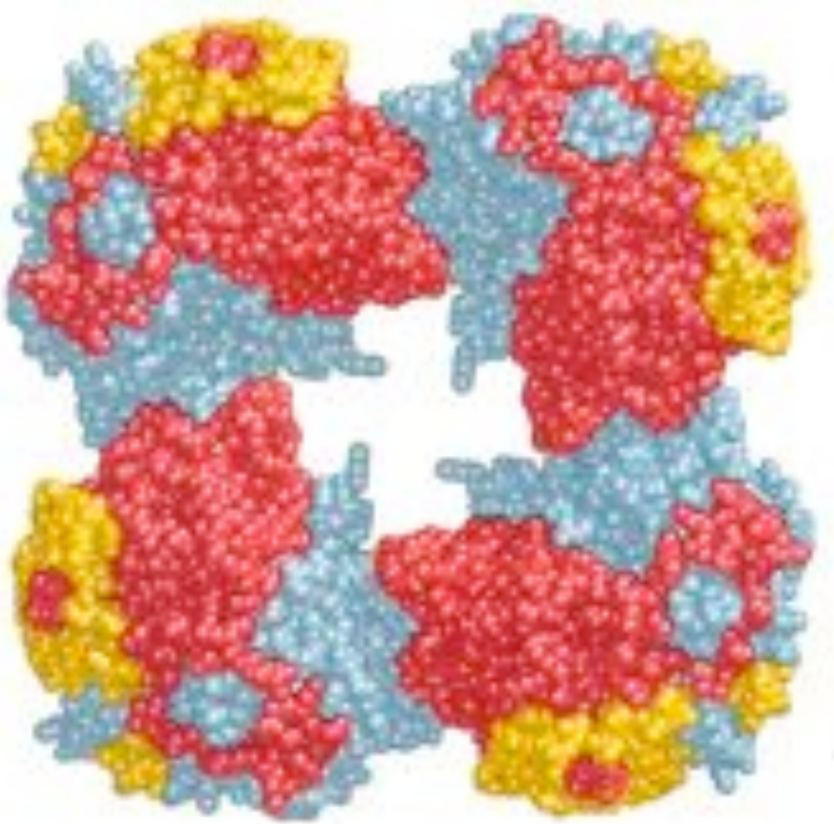


A-DNA **B-DNA** **Z-DNA**



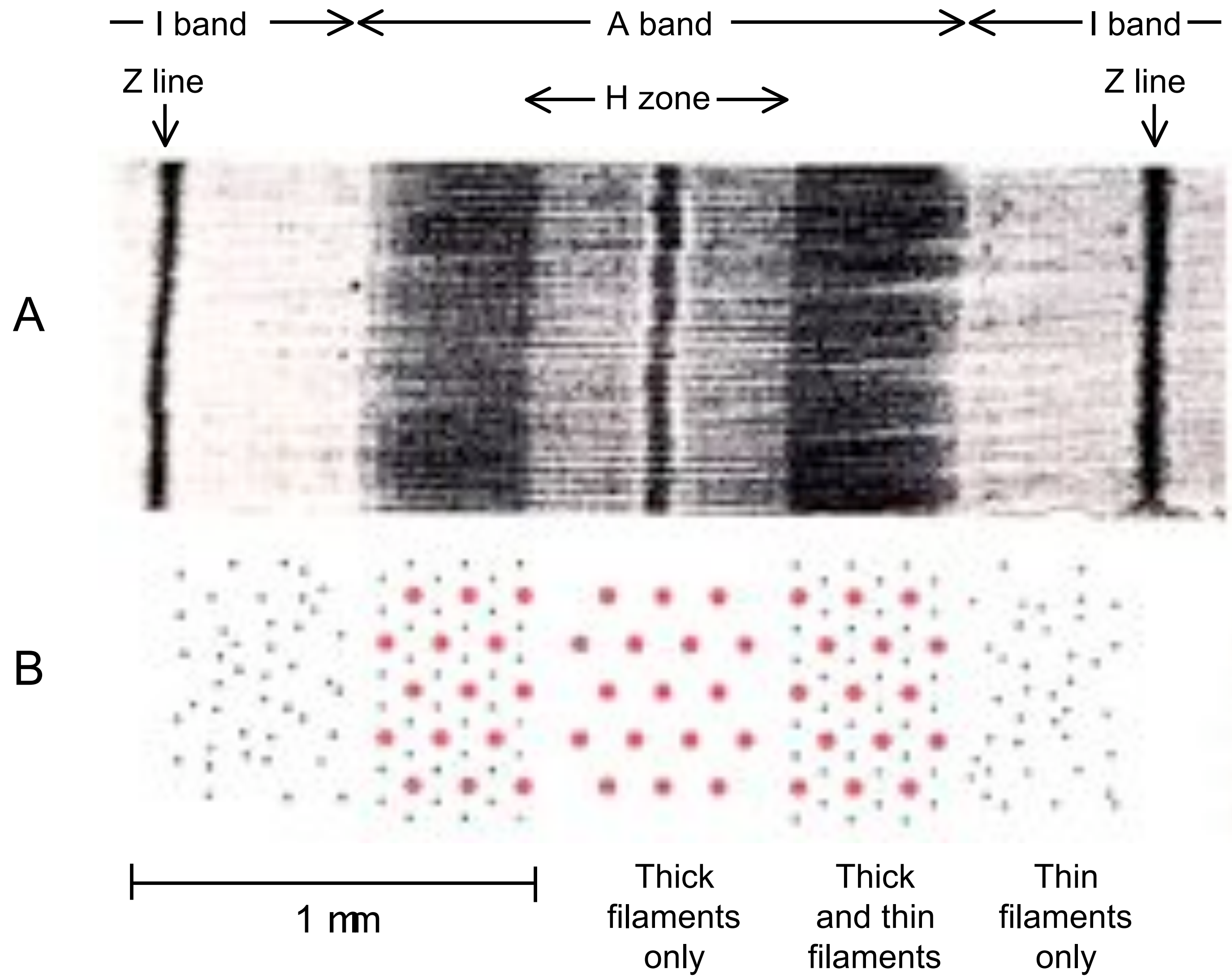

β_2
β_1
α_2
α_1

Metabolic Energy:
Generation and Storage



Structure of the transacetylase core of the pyruvate dehydrogenase complex. This multienzyme assembly catalyzes the irreversible funneling of the product of glycolysis into the critic acid cycle, the final common pathway for the oxidation of fuel molecules. The core consists of 24 identical chains. Four of the eight trimers can be seen in this view.

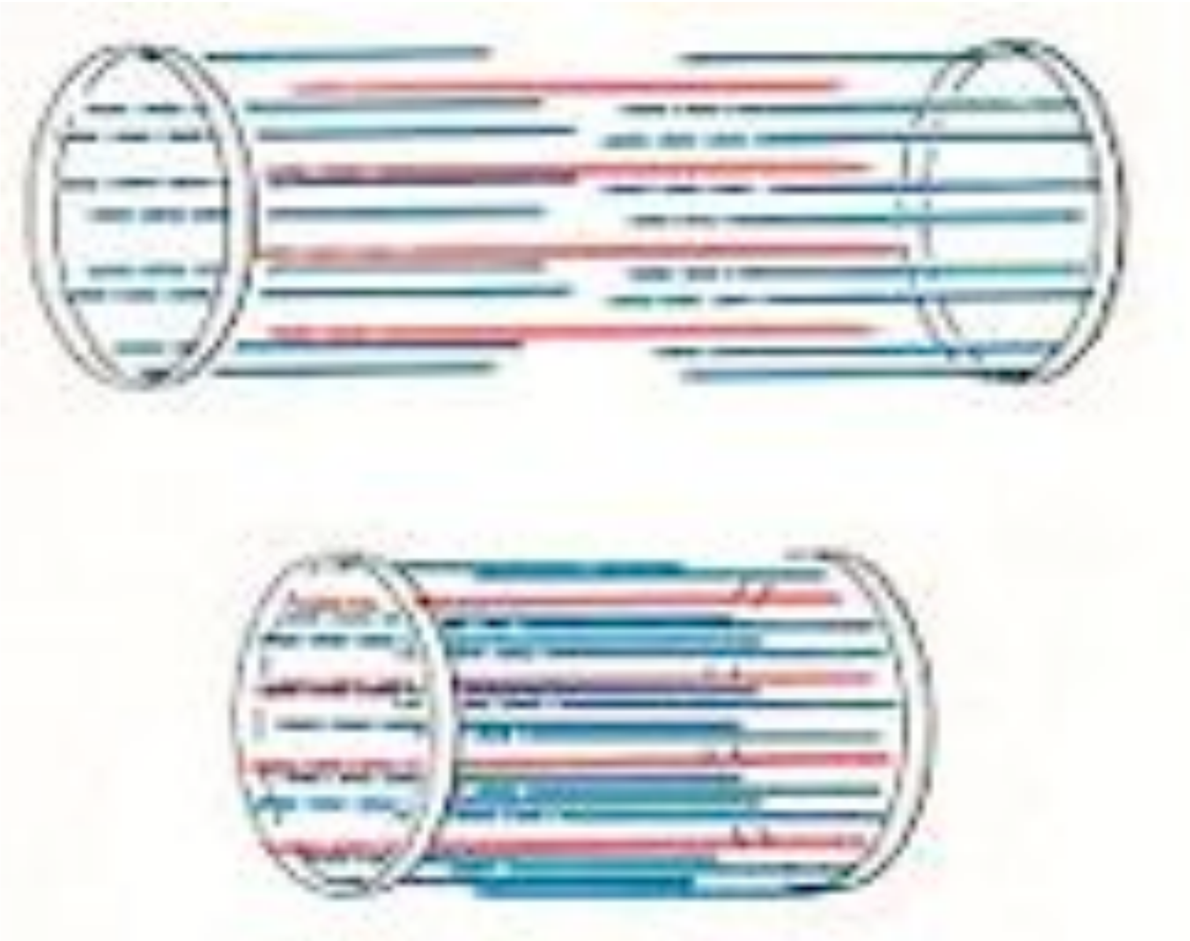
(from Biochemistry / L.Stryer, 4th ed.)



A) **Electron micrograph of a longitudinal section of a skeletal muscle myofibril, showing a single sarcomere.**

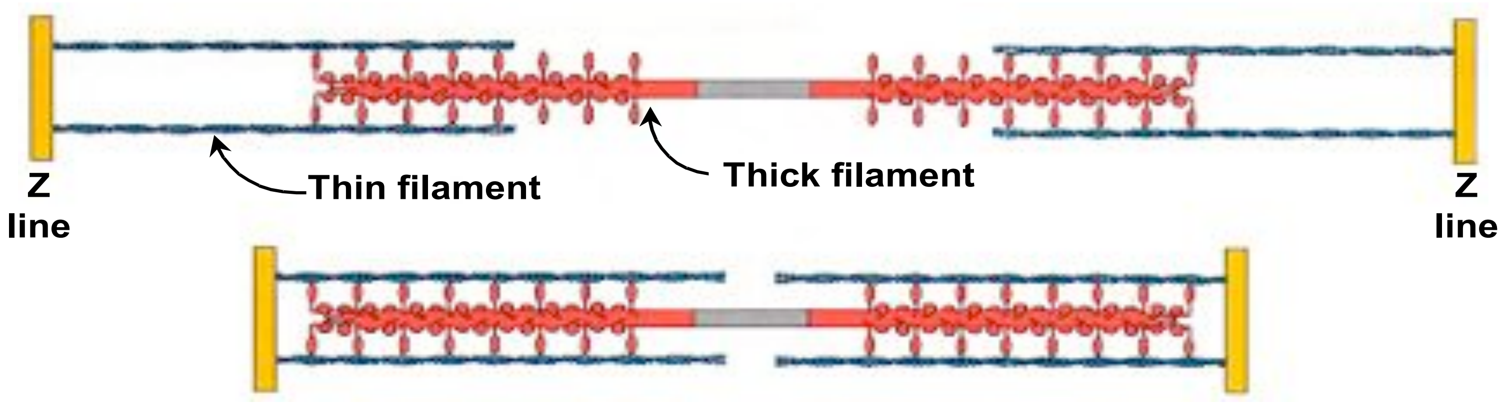
B) **Schematic diagrams of cross sections are shown below the corresponding regions in the micrograph.**

(from Biochemistry / L.Stryer, 4th ed.)



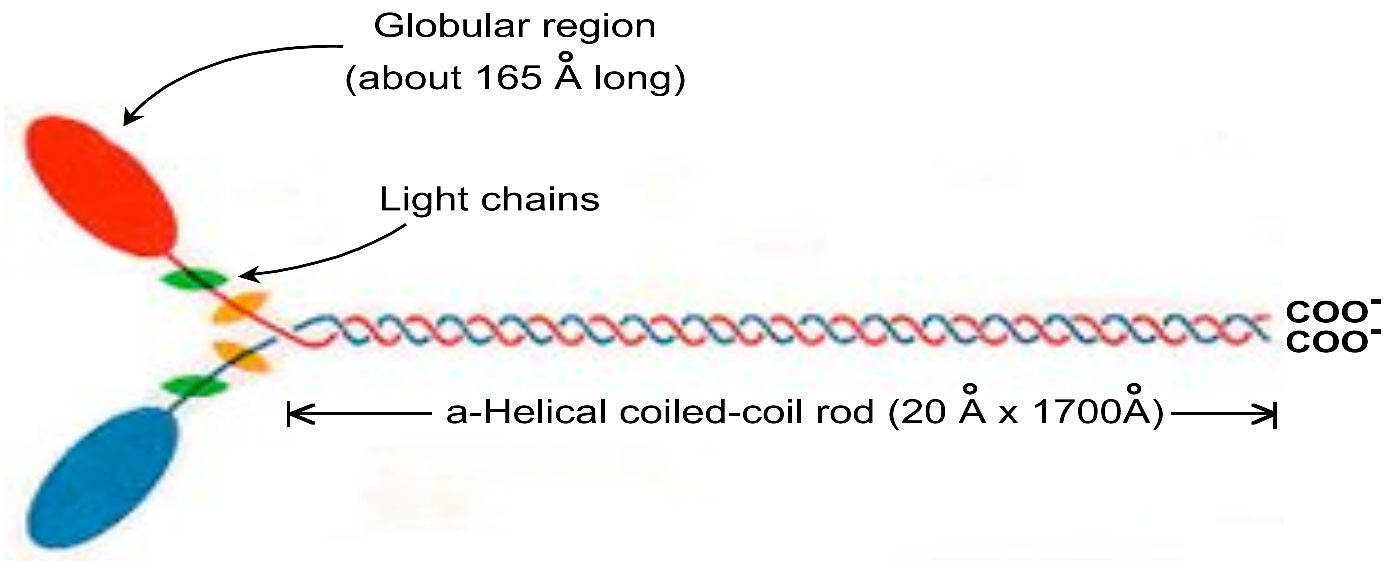
Sliding-filament model

(from Biochemistry / L.Stryer, 4th ed.)



Schematic diagram showing the interaction of thick and thin filaments in skeletal muscle contraction

(from Biochemistry / L.Stryer, 4th ed.)



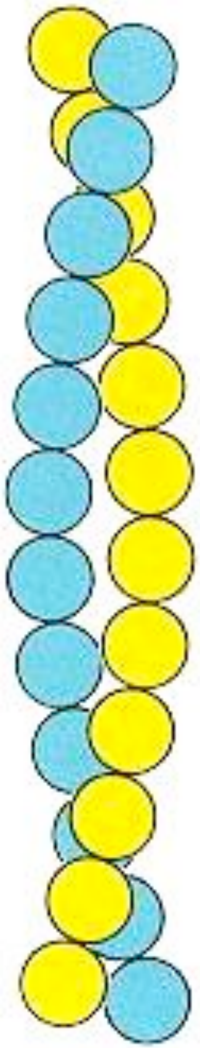
Schematic diagram of a myosin molecule

(from Biochemistry / L.Stryer, 4th ed.)

Proposed model of a thin filament

(from Biochemistry / L.Stryer)

F-actin is a double-stranded helix of actin monomers



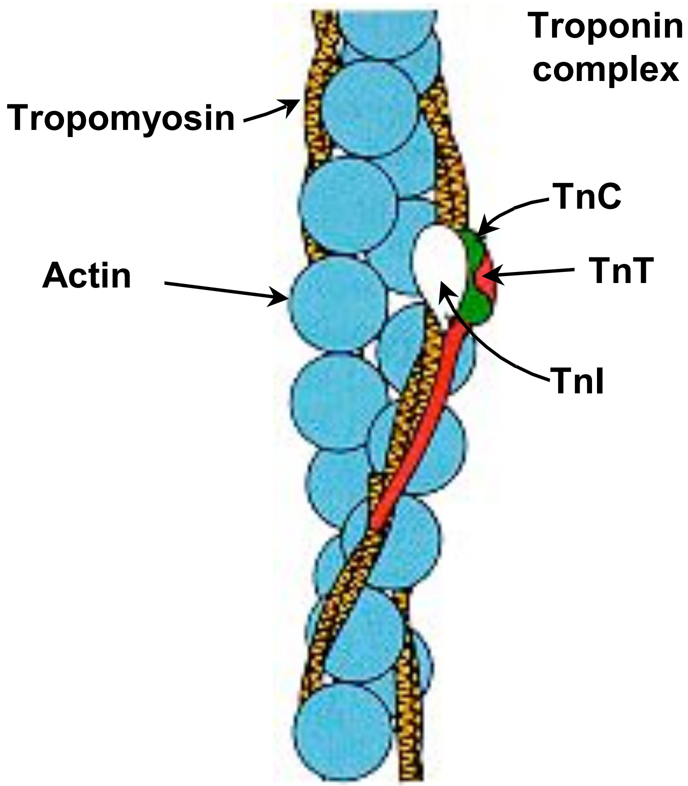
(from Biochemistry / L.Stryer)

Molecular Motors

Structure of F-actin.

The identical subunits of this helical assembly are depicted in several colors to show the interactions of an actin monomer with its our neighbors.
All monomers point in the same direction. The helix repeats after 13 subunits. The myosin-binding sites (dark red) are at the periphery of the filament.

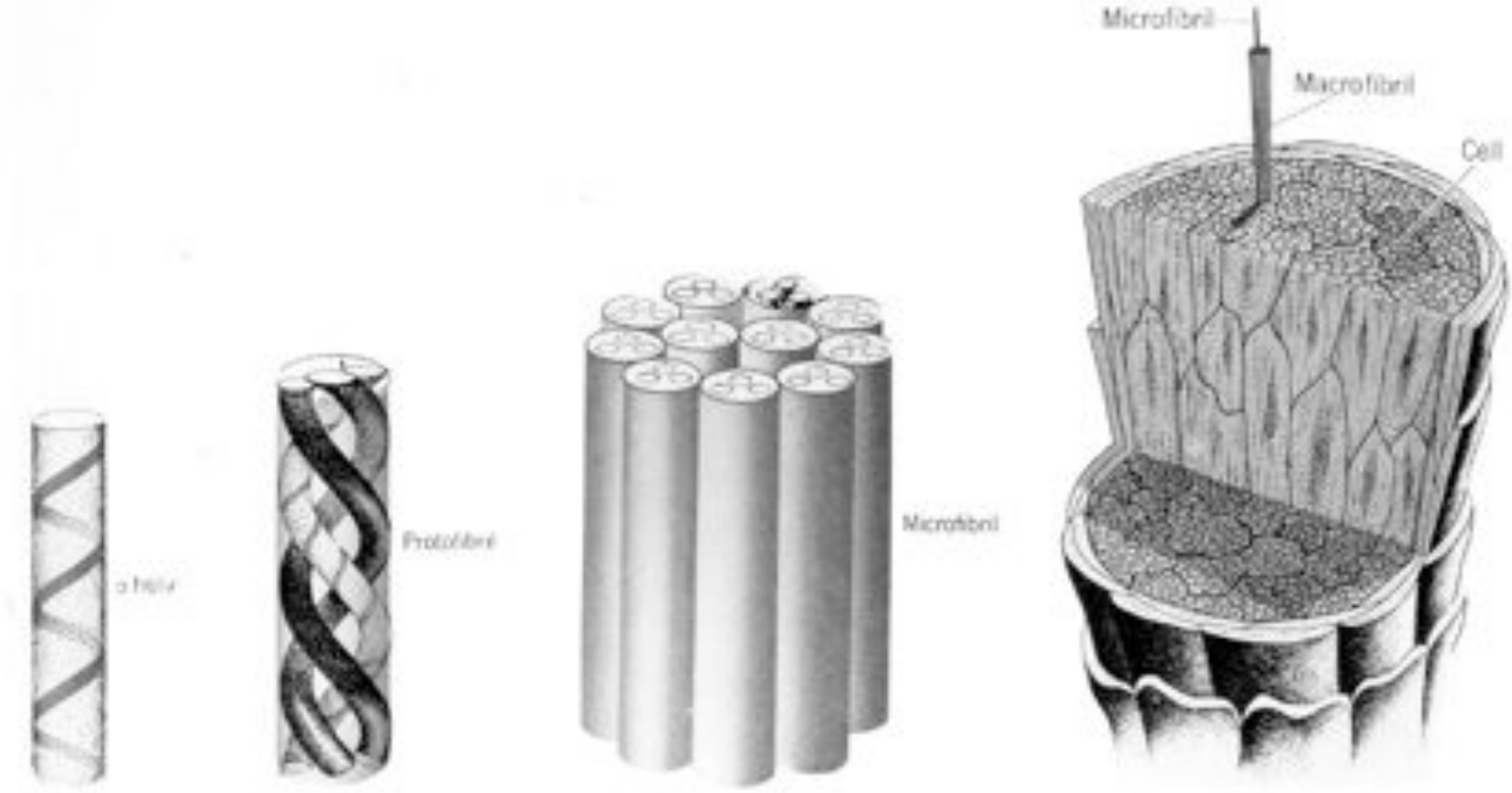
(from Biochemistry / L.Stryer, 4th ed.)

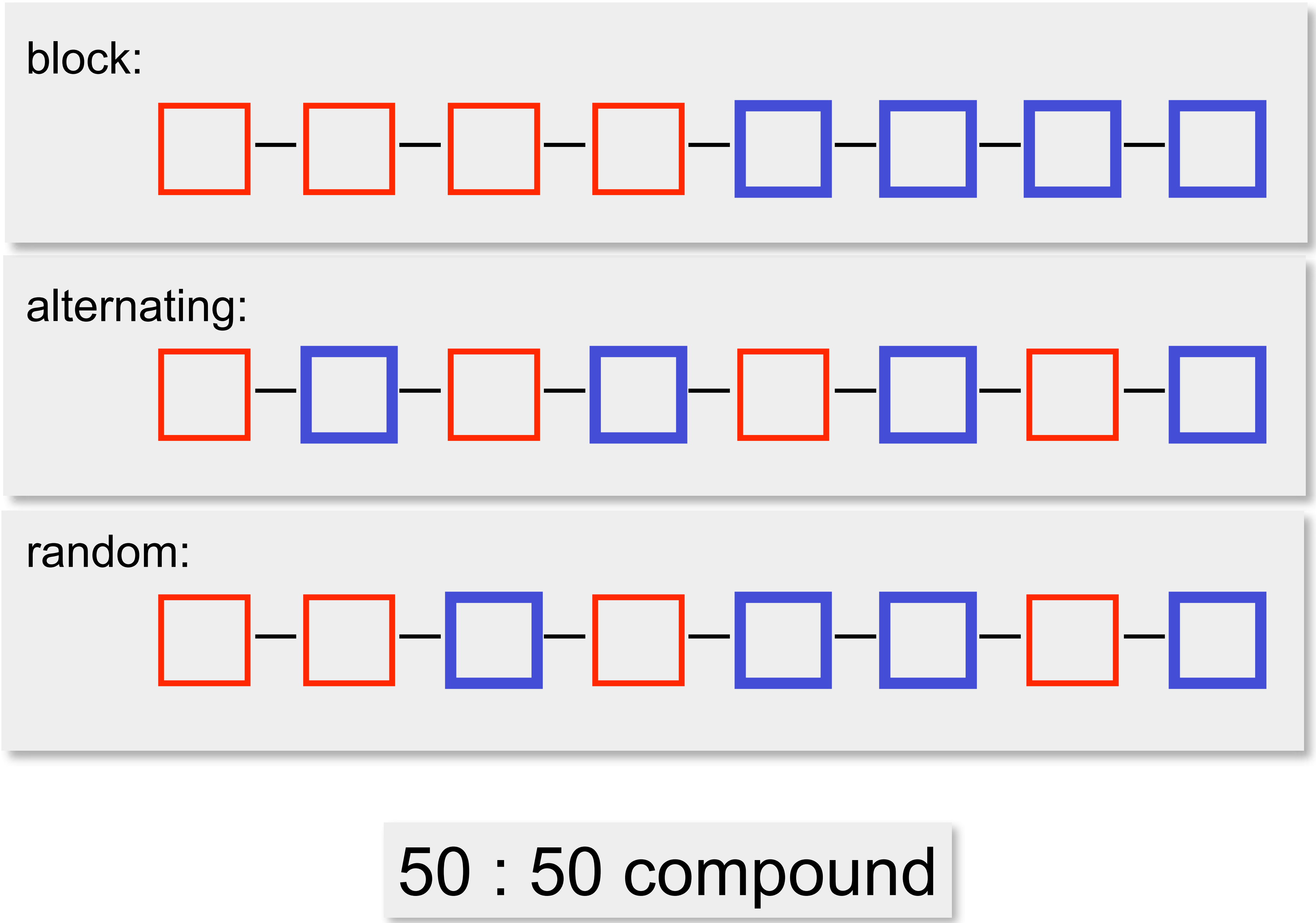


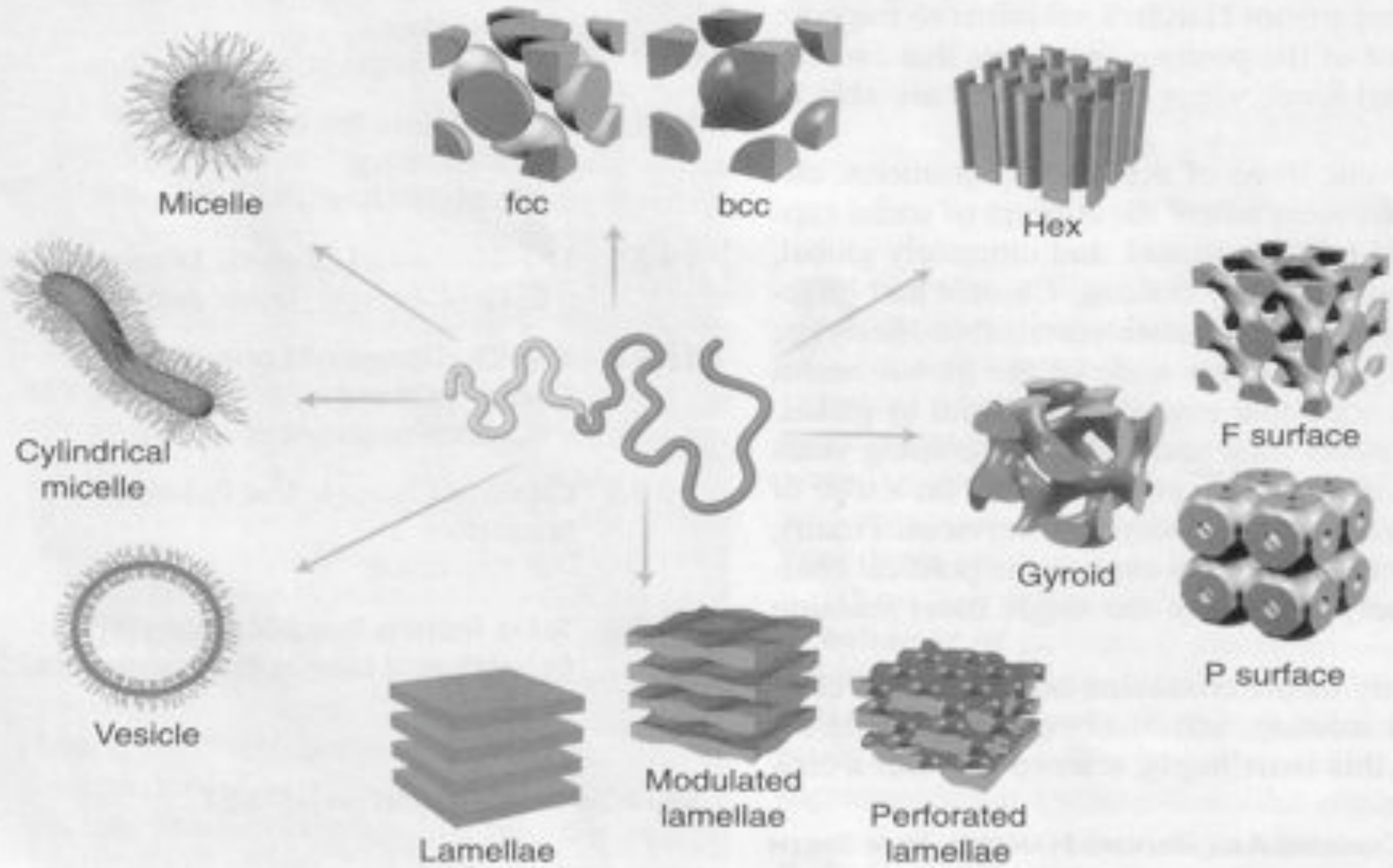
Model of a thin filament

The troponin complex consists of three components: TnI (whith), TnC (green), and TnT (red).
In relaxed muscle (low Ca^{2+}), tropomyosin (yellow) prevents actin from interacting with myosin S1 units.

(from Biochemistry / L.Stryer, 4th ed.)


α helix
Protofibril
Microfibril
Microfibril
Macrofibril
Cell


block:
alternating:
random:
50 : 50 compound



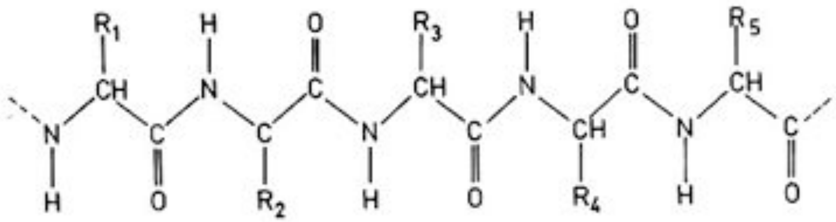
Self-organization of block copolymers. Block copolymers can form spherical and cylindrical micelles, vesicles, spheres with face-centered cubic (fcc) and body-centered cubic (bcc) packing, hexagonally packed cylinders, minimal surfaces (gyroid, F surface, and P surface), simple lamellae, and modulated and perforated lamellae.

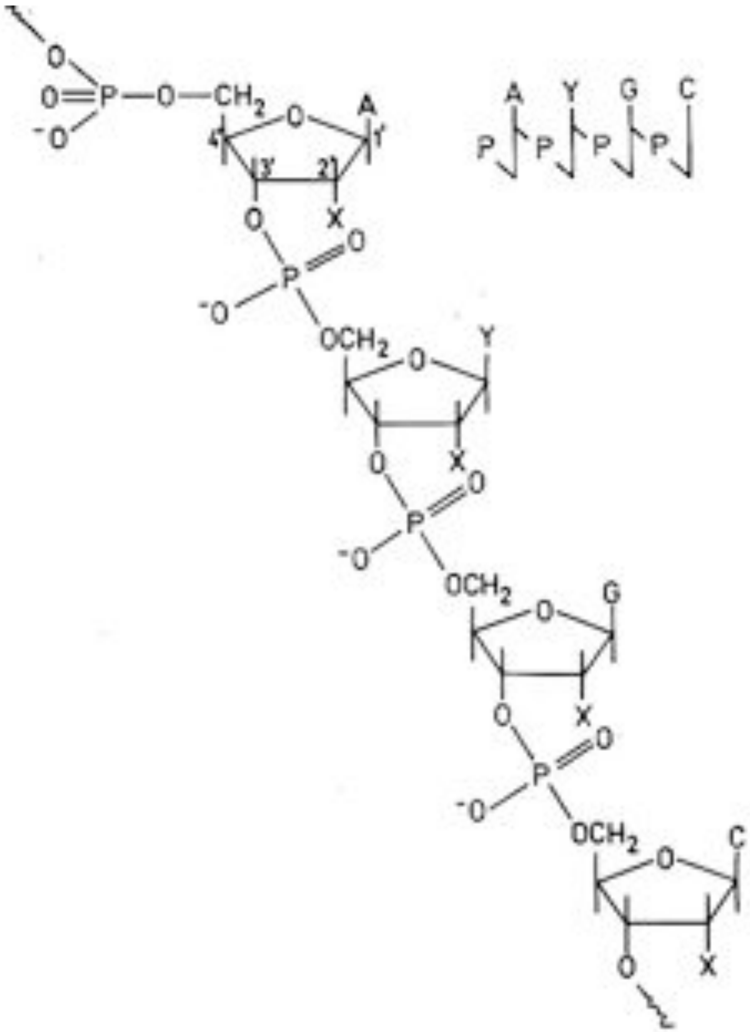
STEREOREGULARITY

AS AN ORDERING PROCESS

IN THE MACROMOLECULES OF LIFE

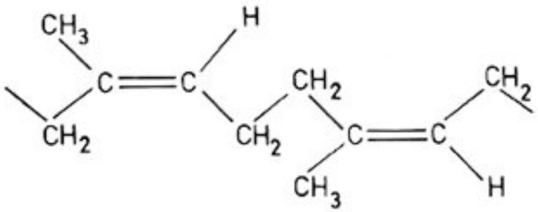
...AND IN SOME SYNTHETIC ONES



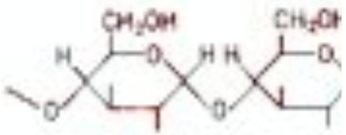


RNA (X=
DNA (X=

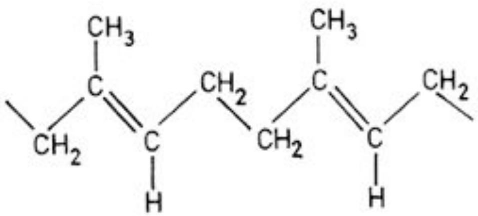
3`-end
("tail")



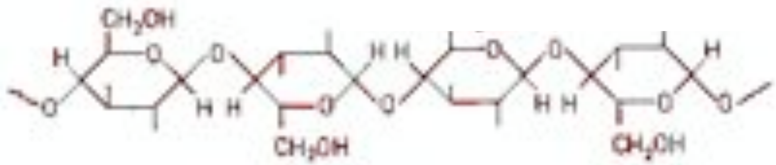
Caoutchouc



Amyl



Guttapercha



Cellulose

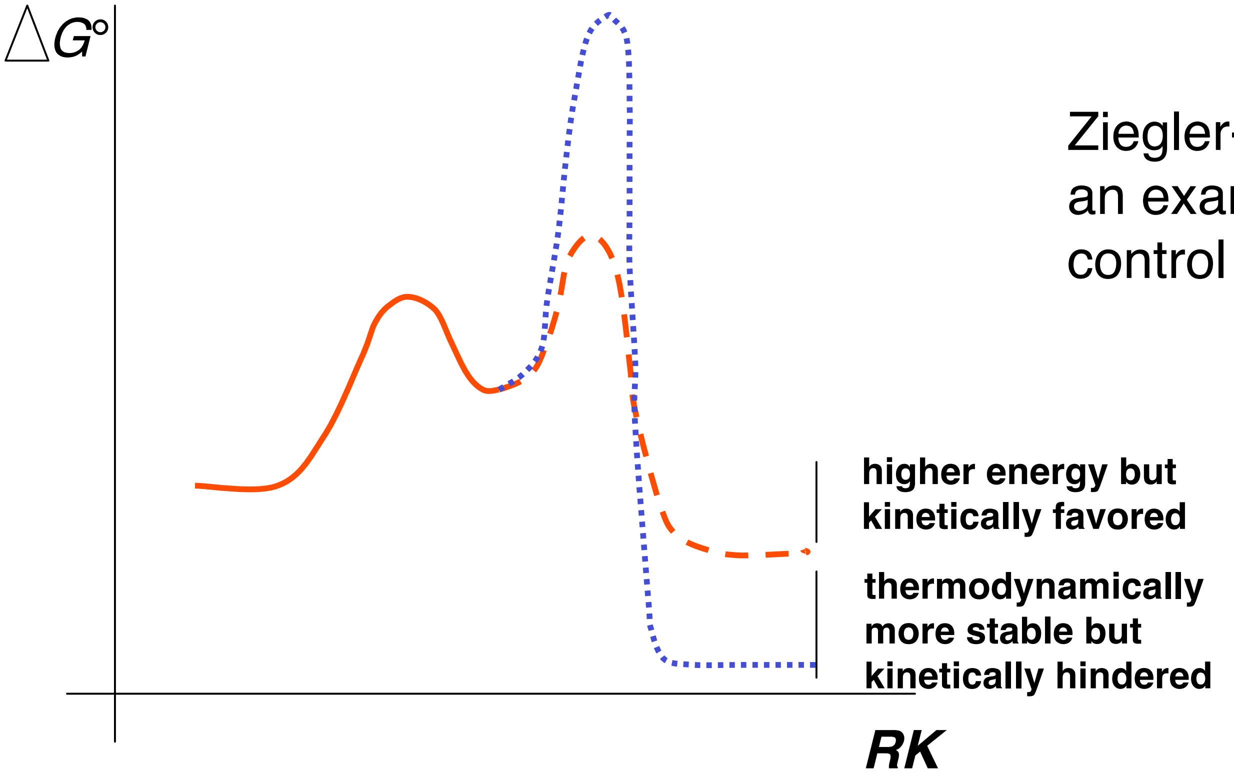
biopolymers

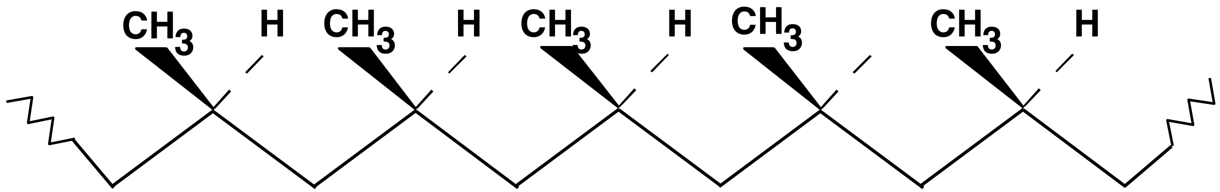
When enzymes are involved in the self-organization process, we are usually dealing with kinetic control

KINETIC CONTROL

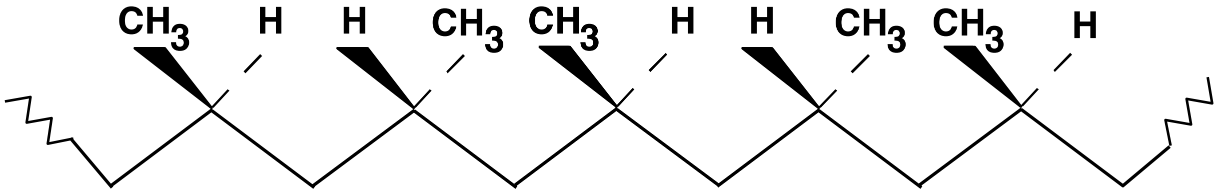
Most enzymatic reactions are kinetically controlled- those for example which lead to stereoregular polymers

Ziegler-Natta reactions as an example of kinetic control in polymerization

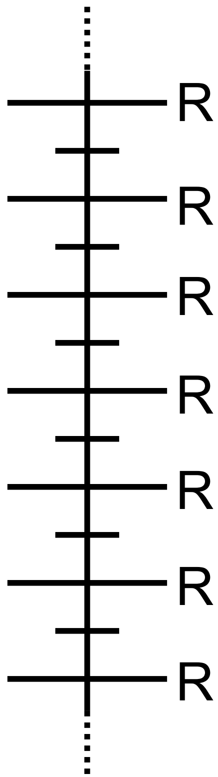




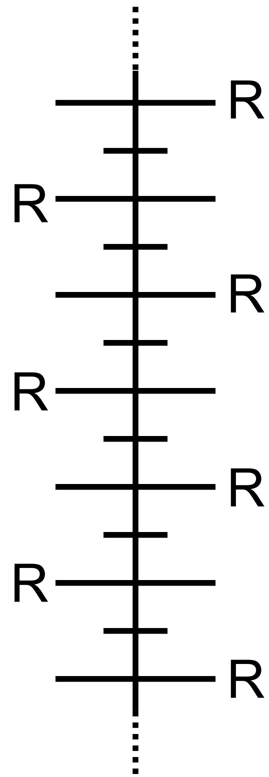
isotactic



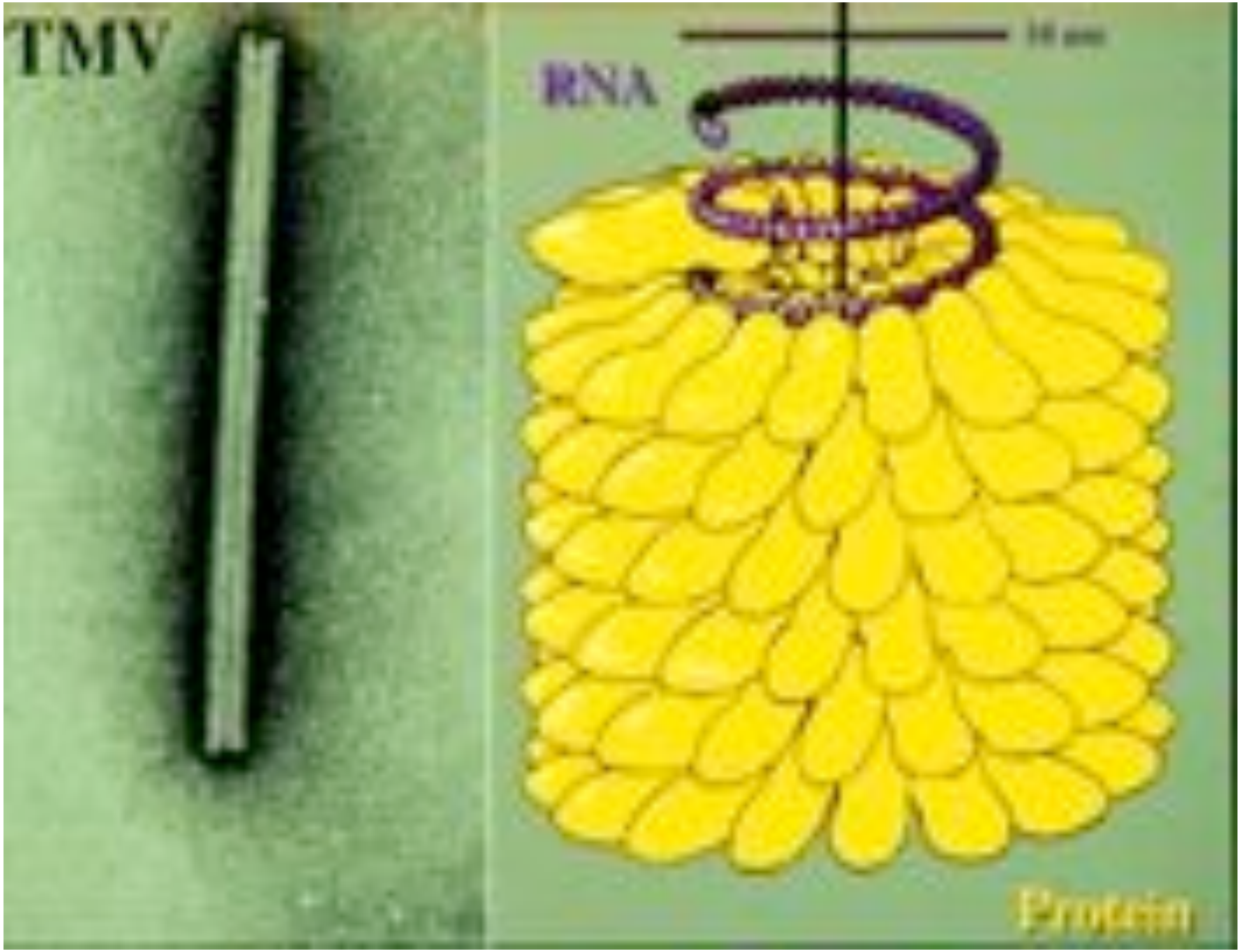
syndiotactic



isotactic

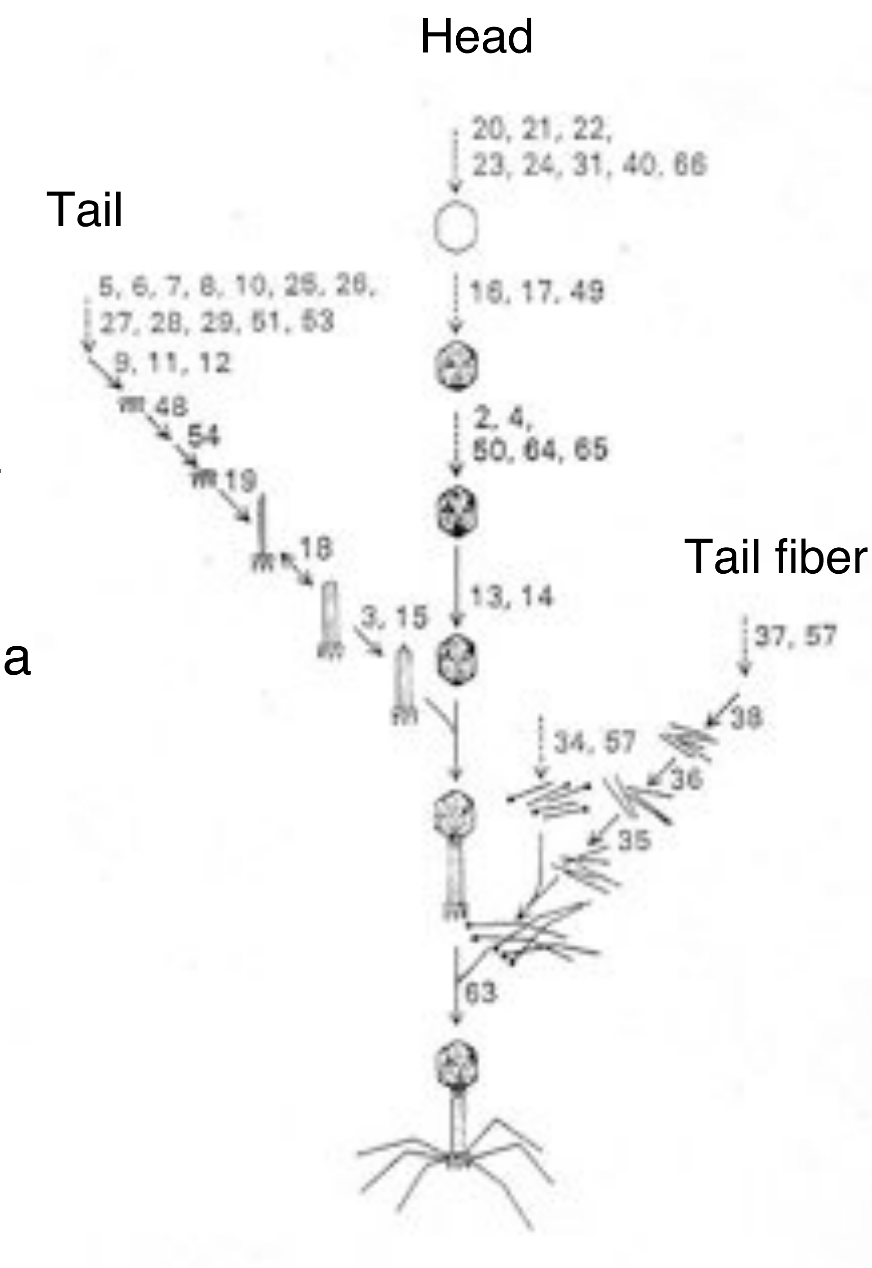


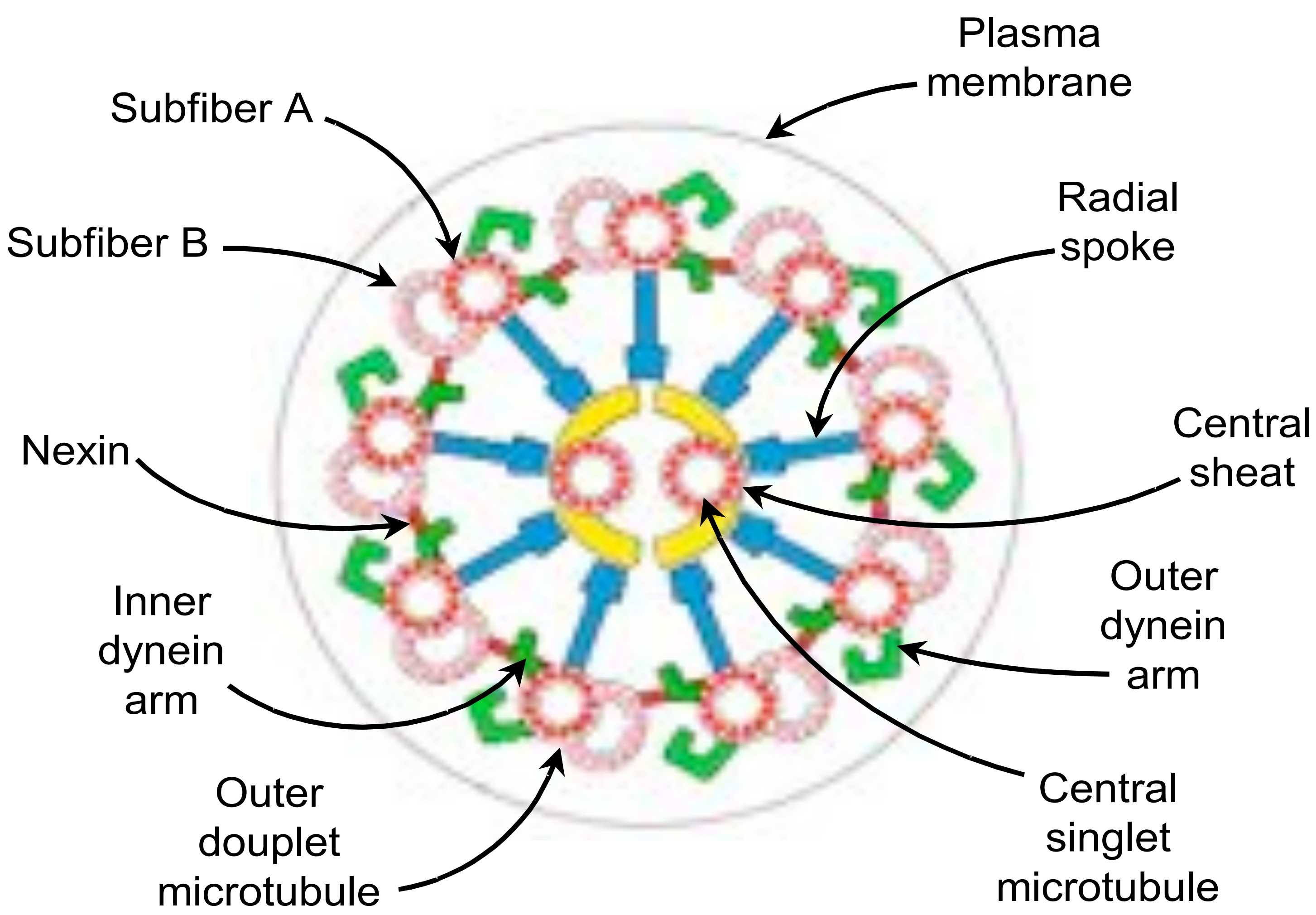
syndiotactic


TMV
RNA
Protein

Morphogenetic pathway of T4 phage. The numbers next to the arrows refer to gene products that are required for a particular step in assembly.

[From W.B. Wood, *Genetic Mechanism of Development*, F.J. Ruddle, ed. (Academic Press, 1973), p.20.]





Schematic diagram of the structure of an axoneme

(from Biochemistry / L.Stryer, 4th ed.)

Emergence:
the formation of a higher complexity level brings about NOVEL properties that are not present in the basic components

..the whole is more
than the sum of
the parts
...holism

The British emergentism:

J.S. Mill, System of logic, 1843,1872 (8.th edit.)

A. Bain, Logic, Book II and III, 1870

S. Alexander, Time and Deity, 1920

C.L. Morgan, Emergent Evolution, 1923

C.D. Broad, the Mind and its Place, 1925

And modern literature, for example:

R.W. Sperry, Philosophy of Science, 1986

W.C. Wimsatt, 1972; 1976

J. Klee, 1984

B.P. McLaughlin, 1992

J.H. Hollnd, 1998

T. O'connor, 1994

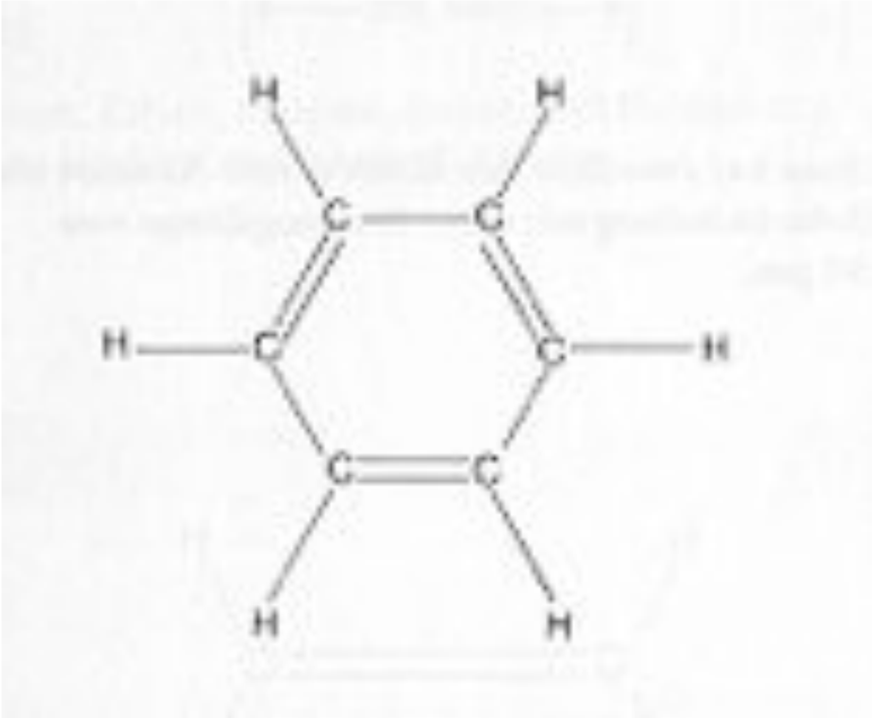
Emergence:
the formation of a higher complexity level brings about NOVEL properties that are not present in the basic components

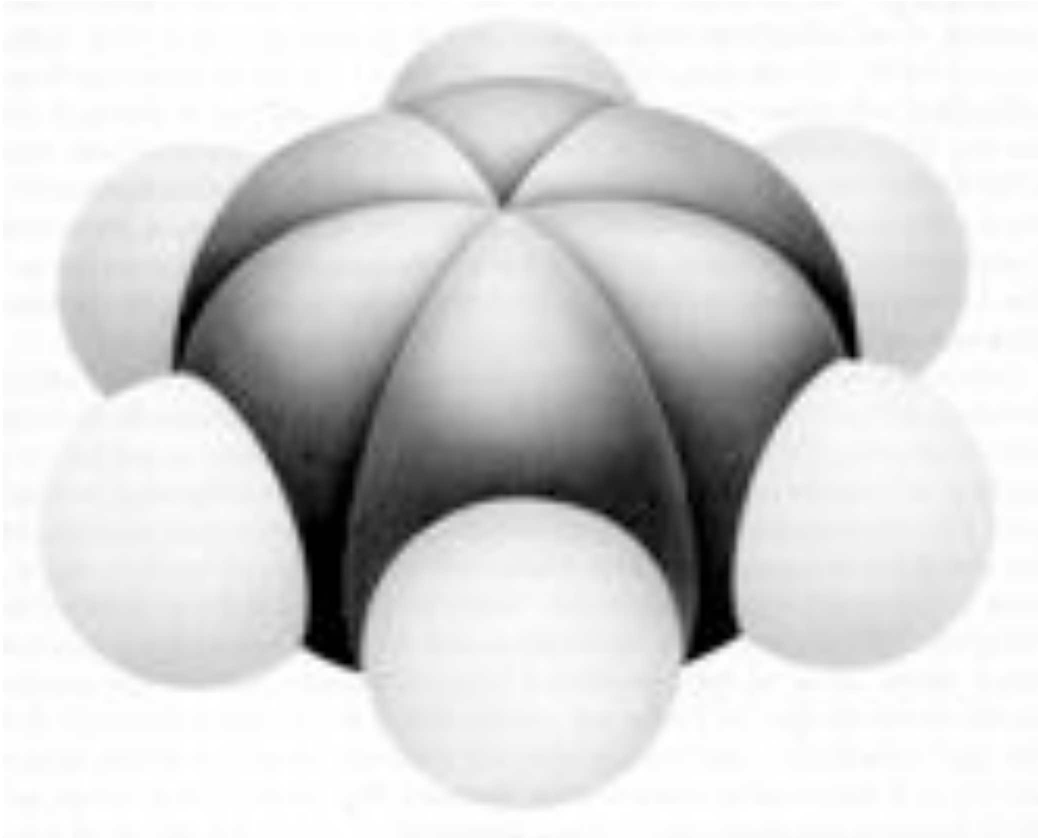
..the whole is more
than the sum of
the parts
...holism

REDUCTIONISM & EMERGENCE

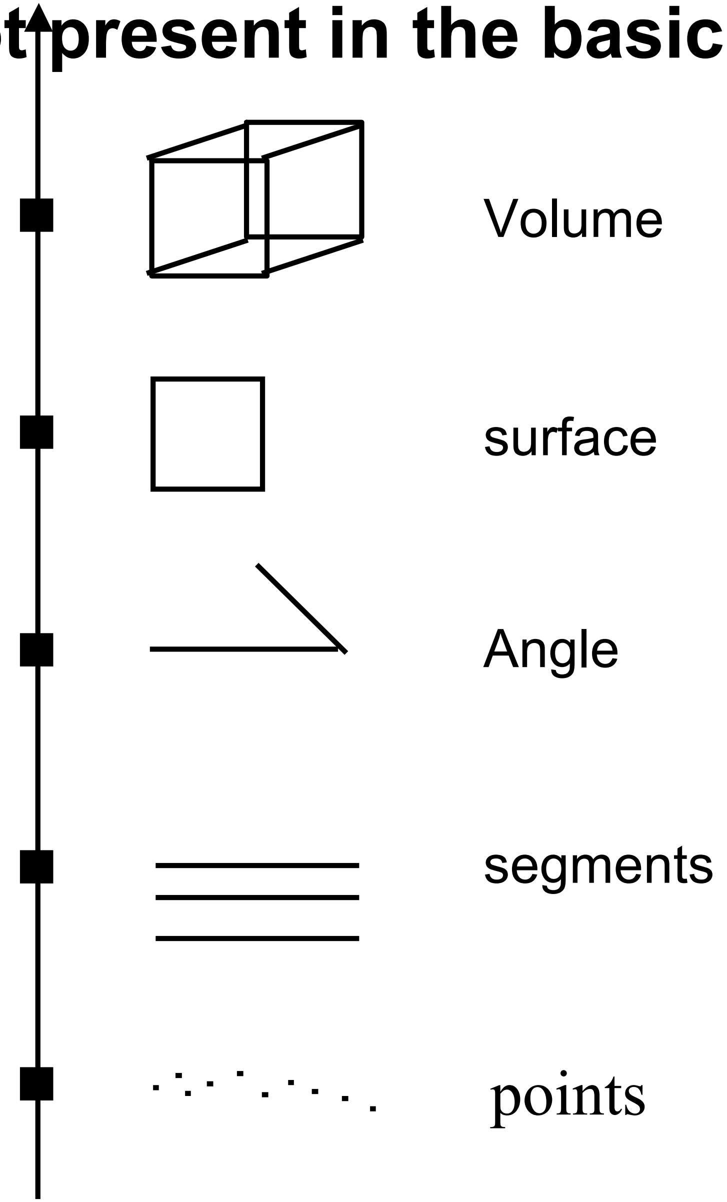
$$H_2 + {}^{1}/_{2}\, O_2 \longrightarrow H_2O$$

structural reductionism and novel emergent properties

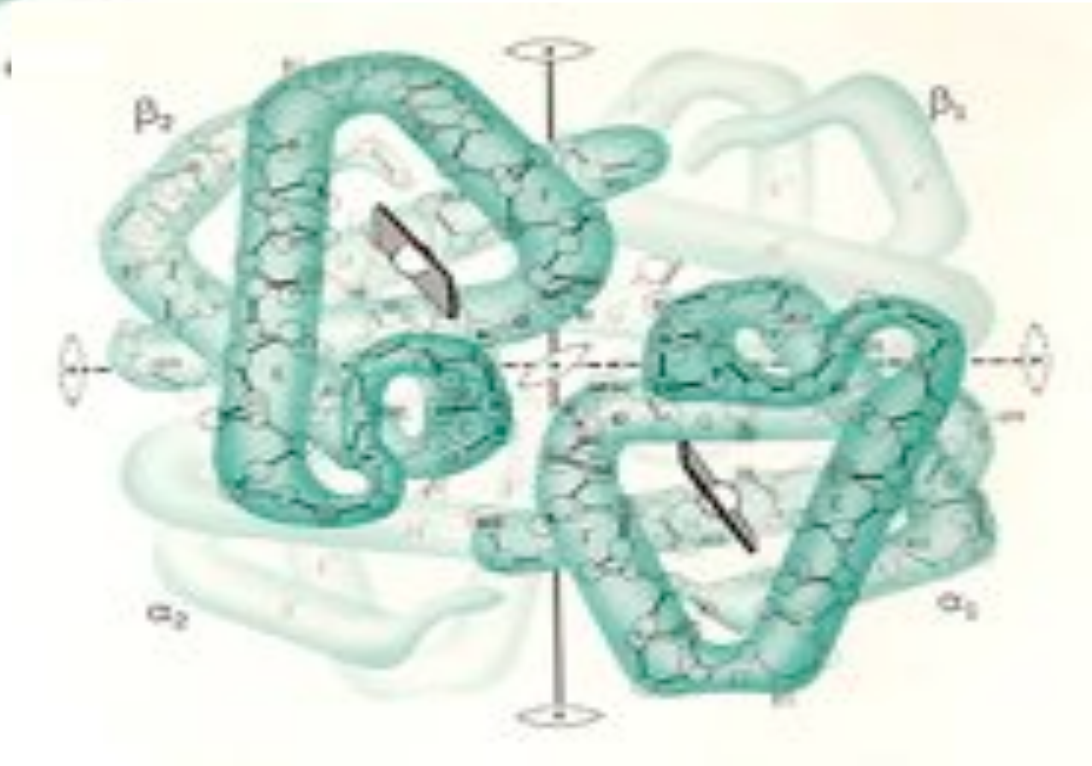


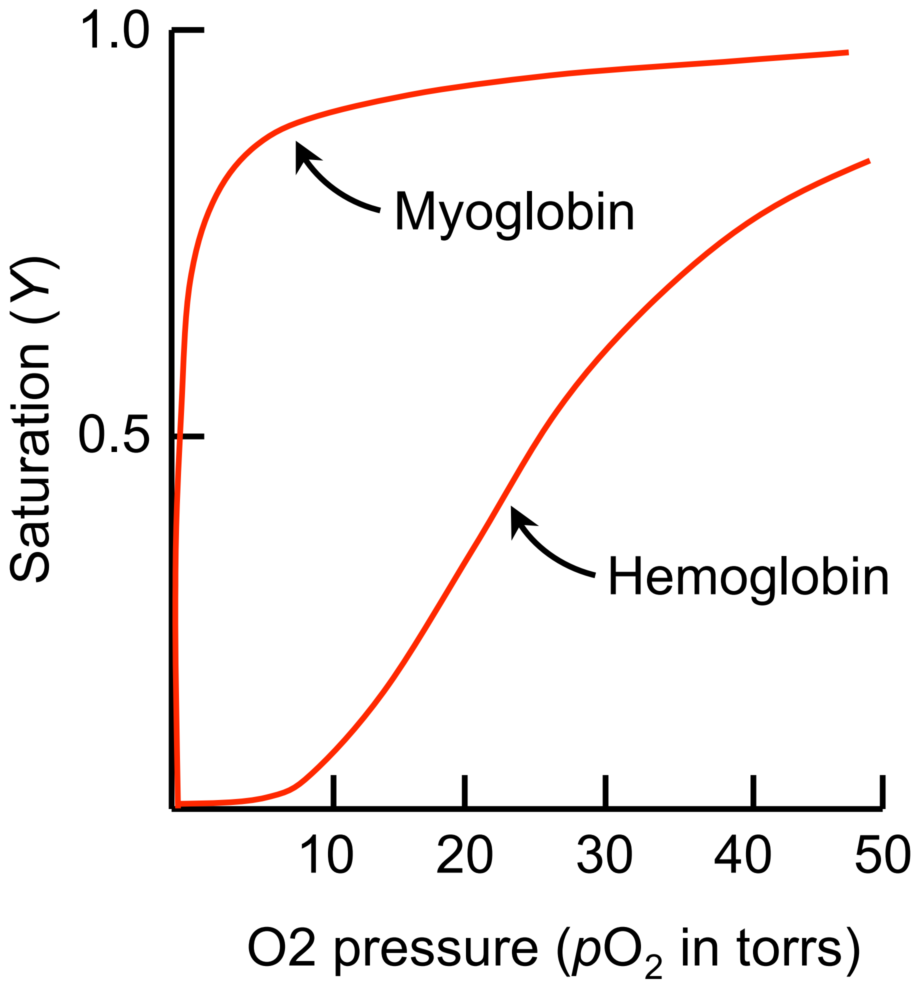


Emergence: the formation of a higher complexity level brings about properties that are not present in the basic components



..the whole is more than the sum of the parts
...holism


β_2
β_1
α_2
α_1



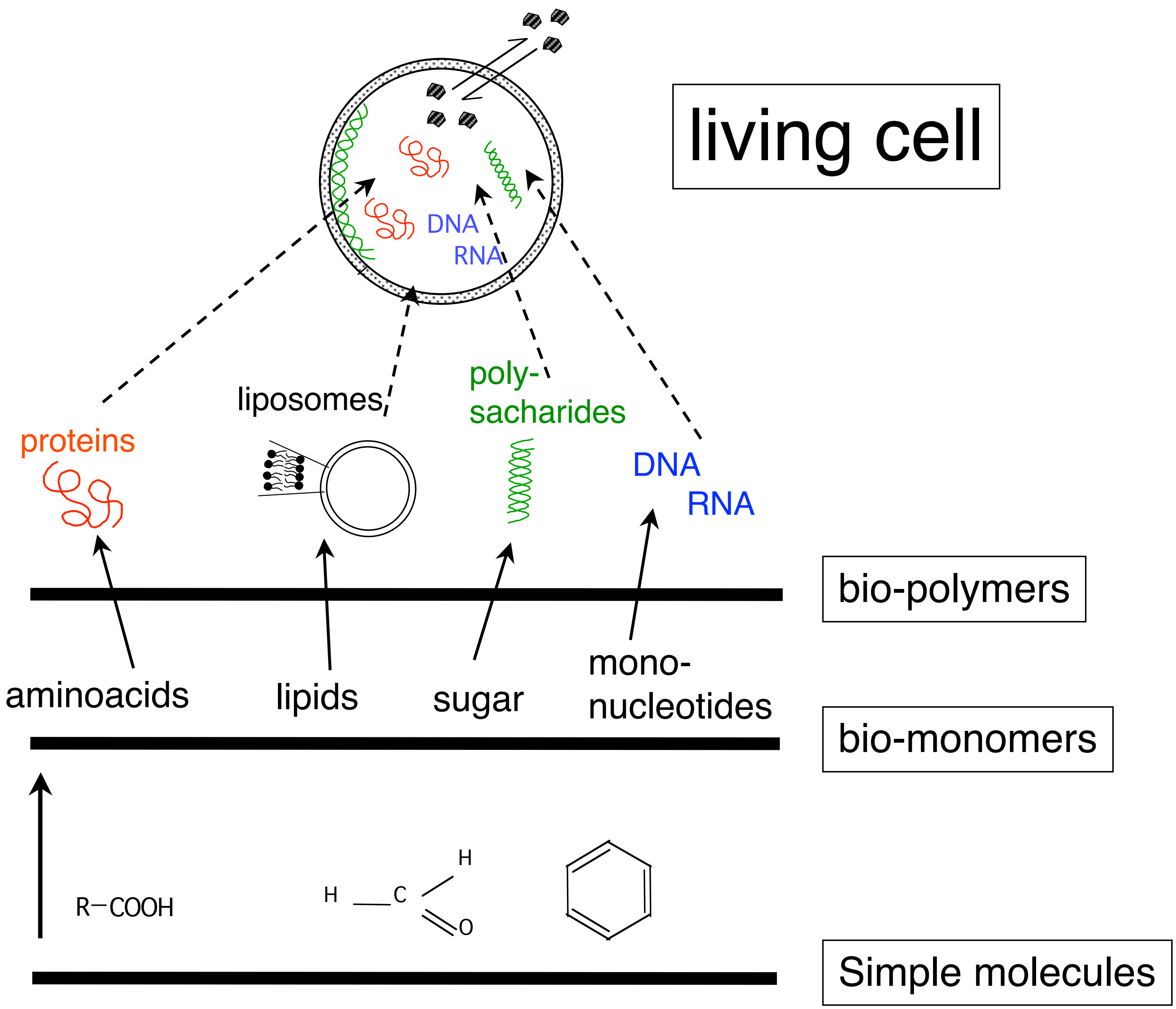
Oxygen dissociation curves of myoglobin and hemoglobin.

Saturation of the oxygen-binding sites is plotted as a function of the partial pressure of oxygen surrounding the solution.

(from Biochemistry / L.Stryer, 4th ed.)

Life is an emergent property:

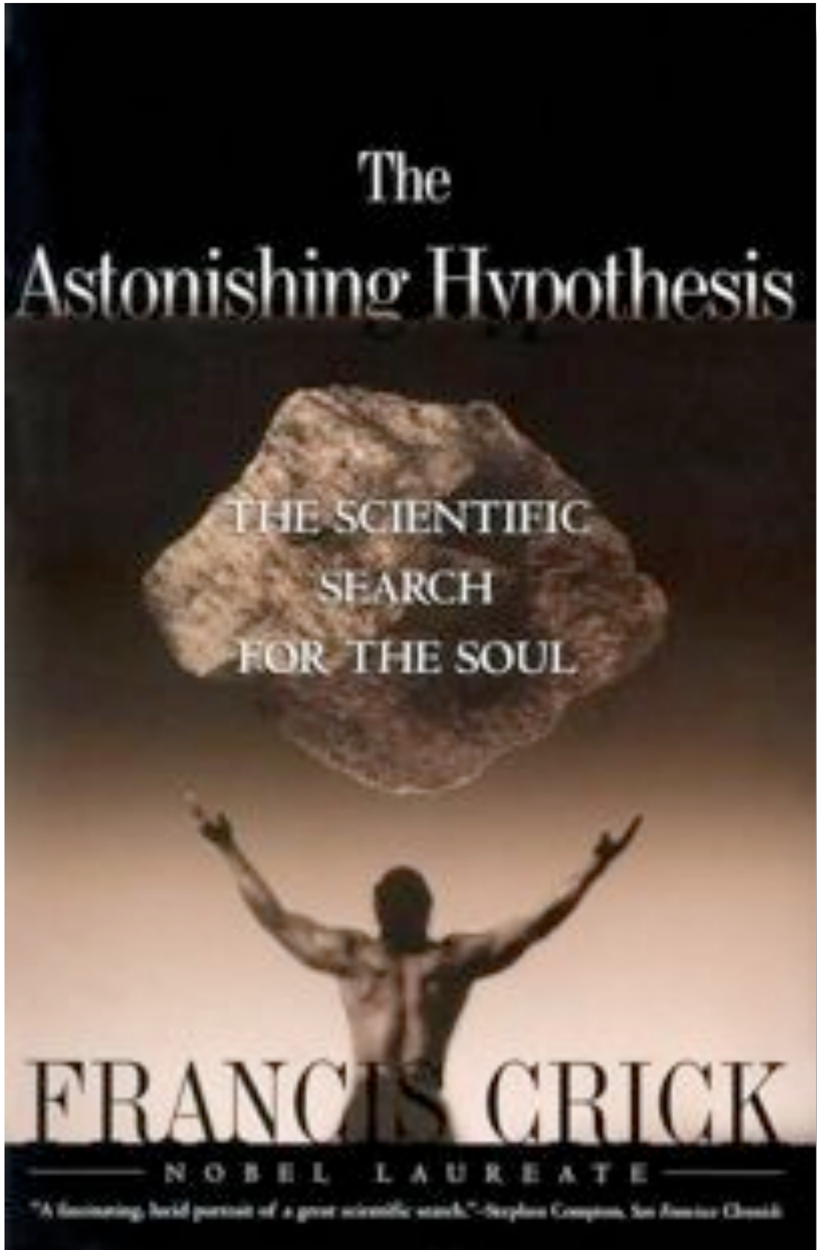
the components (nucleic acids, proteins, lipids, sugars etc) are per se' not living;
When they are assembled together in a particular space/time structure, then life emerges



living cell
DNA
RNA
liposomes
poly-
sacharides
proteins
DNA
RNA
bio-polymers
aminoacids
lipids
sugar
mono-
nucleotides
bio-monomers
R—COOH
H
C
H
O
Simple molecules

Life as a very particular emergent property:
Corresponds to biological autonomy

And to self-referentiality


The
The Astonishing Hypothesis
THE SCIENTIFIC
SEARCH
FOR THE SOUL
FRANCIS CRICK
NOBEL LAUREATE

Questions related to the notion of emergence:

Emergence versus reductionism

Deducibility and predictability

Finality

Downward causation

Emergence and reductionism

This question takes us directly into the relation between emergence and reductionism. This is another complex topic, abundantly discussed in the specialized literature, see Schroeder (1998),or Wimsatt (1972, 1974) and Primas (1985, 1991,1993,1998.

Generally reductionism and emergentism are presented as two opposite fronts

The strongest form of reductionism maintains (according to Ayala (1983) cited by Primas (1998))
“*that organisms are ultimately made up of the same atoms that make up inorganic matter, and of nothing else*”.

Deducibility and predictability

can the emergent properties be deduced from the properties of the components?

The question of deducibility (or „predictability“):

Can the emergent properties be deduced from the properties of the components?

This question has two sides:

1. Can the emergent properties be deduced a posteriori from the lower level properties?
------ reductionism

2. Can the emergent properties be explained a priori? (bottom-up approach)

the relation between emergent properties and the properties of the components has two sides.

One can ask whether the properties of water (or any other molecule), can be **explained *a posteriori*** in terms of the properties of the components; or one can instead pose the question of whether the emergent properties can be **foreseen *a priori*** from the properties of the components

Consider for example **biological evolution**, for example the emergence of flagella in bacteria, or wings in the early birds. The arising of such properties cannot be predicted; however, once they are there, they can be deduced a posteriori from a series of small evolutionary changes.

On the question of predictability:

(bottom to top...)

„strong emergence“

„ the...relation between an emergent property

of a whole and the properties of ist parts

is..one of non-explanatoriness...“

Schroeder, 1998

“weak emergence”

..it is rather so, that the explanation is often

tecnically difficult-no time, no computational

power, no skill

For example A. Bedeau, 1997

One claims that the properties of the higher hierarchic level are *in principle* not deducible from the components of the lower level. This is the so-called "strong emergence" or radical emergence, that demands, as formulated by Schroeder (1998) that: "*the …relation between an emergent property of a whole and the properties of its parts is…one of non-explanatoriness*".

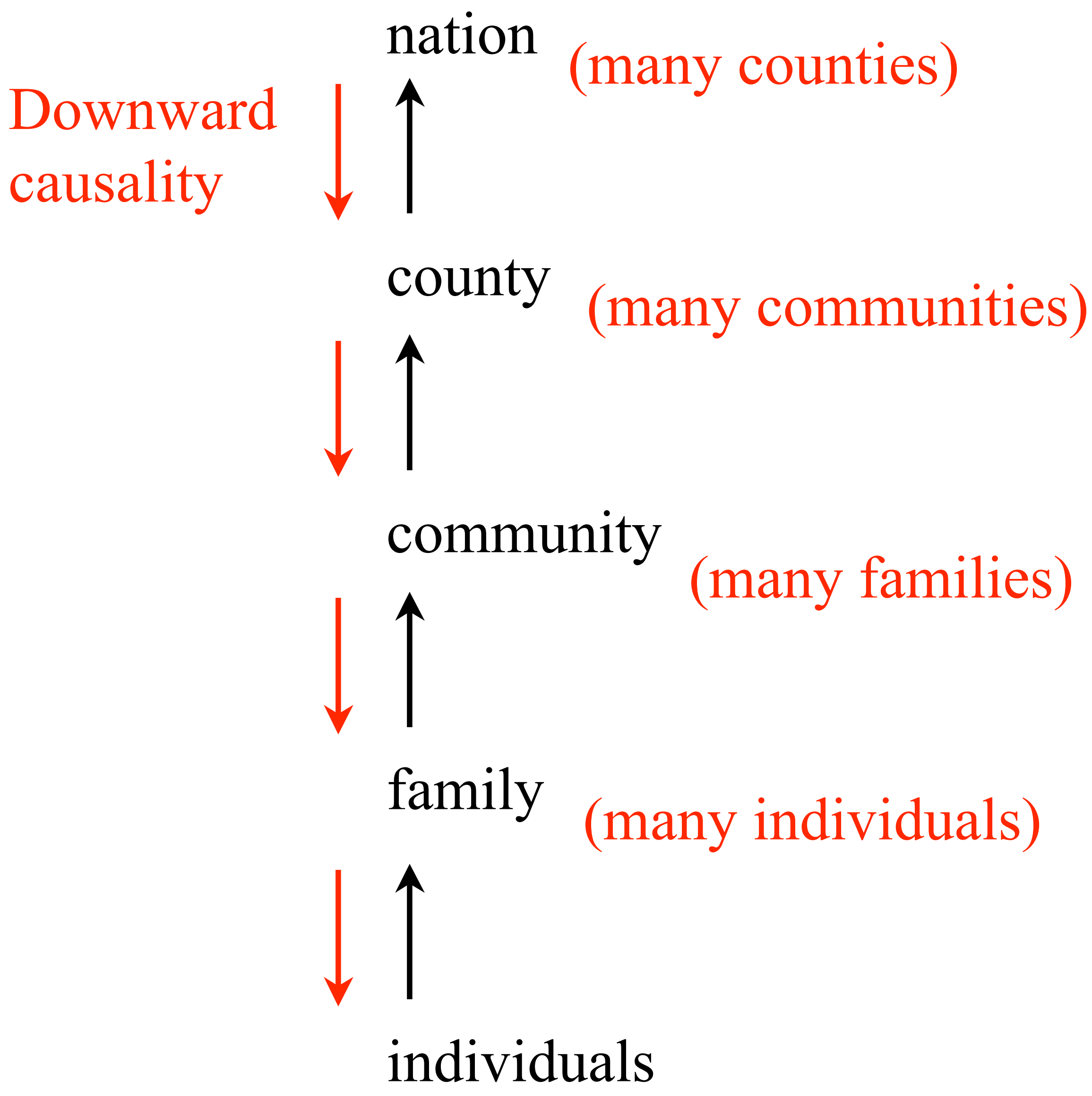
Opposite to this "strong emergence", there is the "weak emergence," a point of view that more pragmatically asserts that the relationship between the whole and the parts may not be established because of technical difficulties

Take the case of myoglobin, with its 143 aminoacid residues. Can the properties of myoglobin be predicted on the basis of the properties of the twenty amino acids?

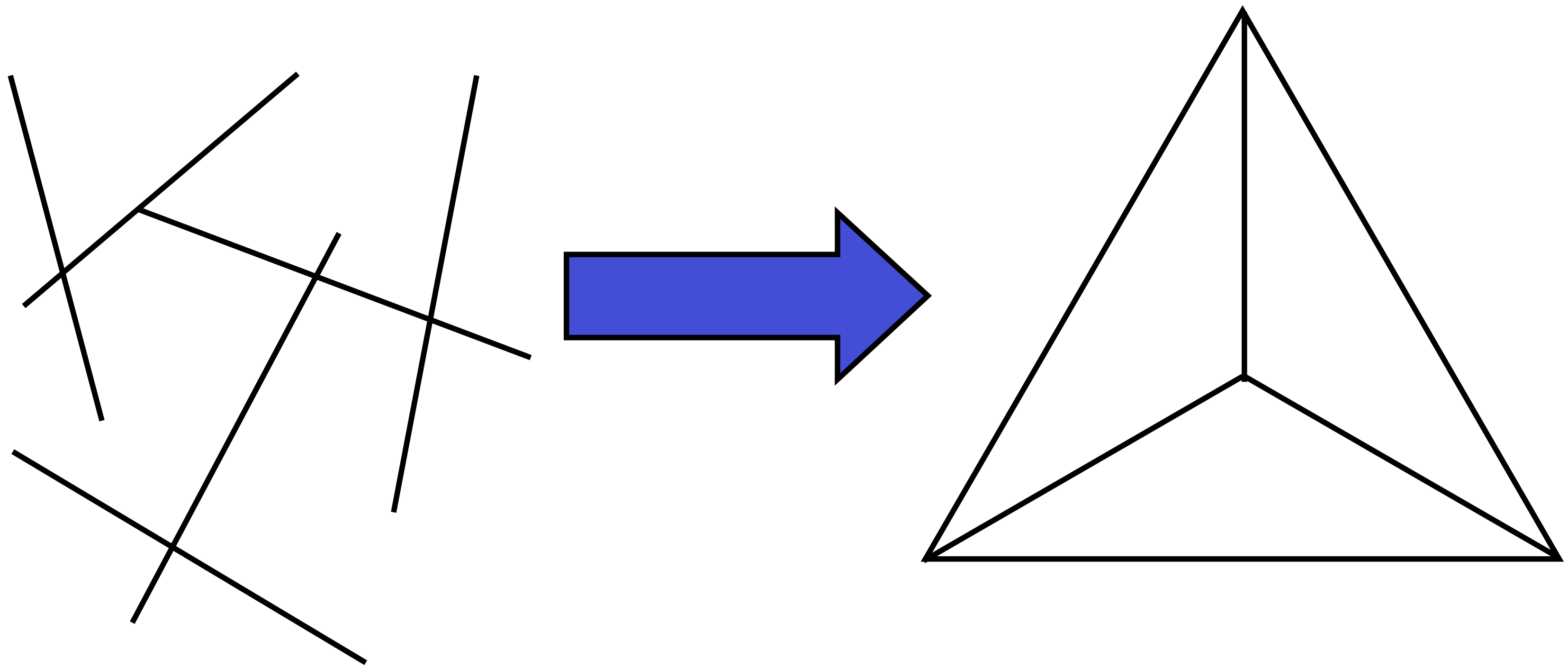
Not only one arrow going up
...but also coming down!

Downward causality

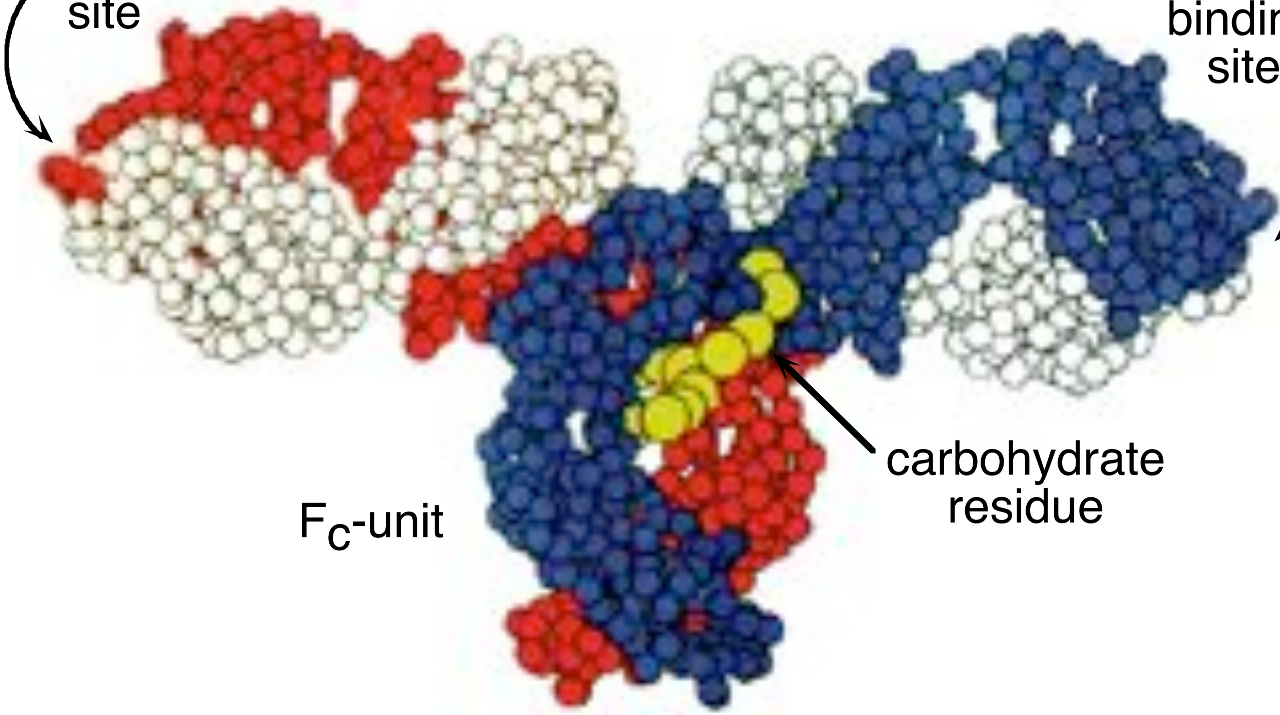
(macrodeterminism)



nation
(many counties)
Downward
causality
county
(many communities)
community
(many families)
family
(many individuals)
individuals



SCHEMATIC REPRESENTATION OF THE THREE-DIMENSIONAL STRUCTURE OF I_gG



Each amino acid residue is represented by a small circle. The H chains are red and the L chains blue. A carbohydrate residue is yellow.

E. W. Silverton, et al. *Proc. Nat. Acad. Sci. 74 (1977); p. 142.*

SWARM INTELLIGENCE

Self-organization and finality

The pictures of the swarm intelligence, an axoneme or an anthill arise an old question-the question of finality. One may in fact argue that these complex biological systems appear to have a a rather specific finality- the question of the relationship between self-organization and *finality* arises.

SELF-ORGANIZATION AND EMERGENCE

IN DYNAMIC SYSTEMS OUT OF EQUILIBRIUM

DISSIPATIVE STRUCTURES

PRIGOGINE, ETC.

According to Capra (2002):

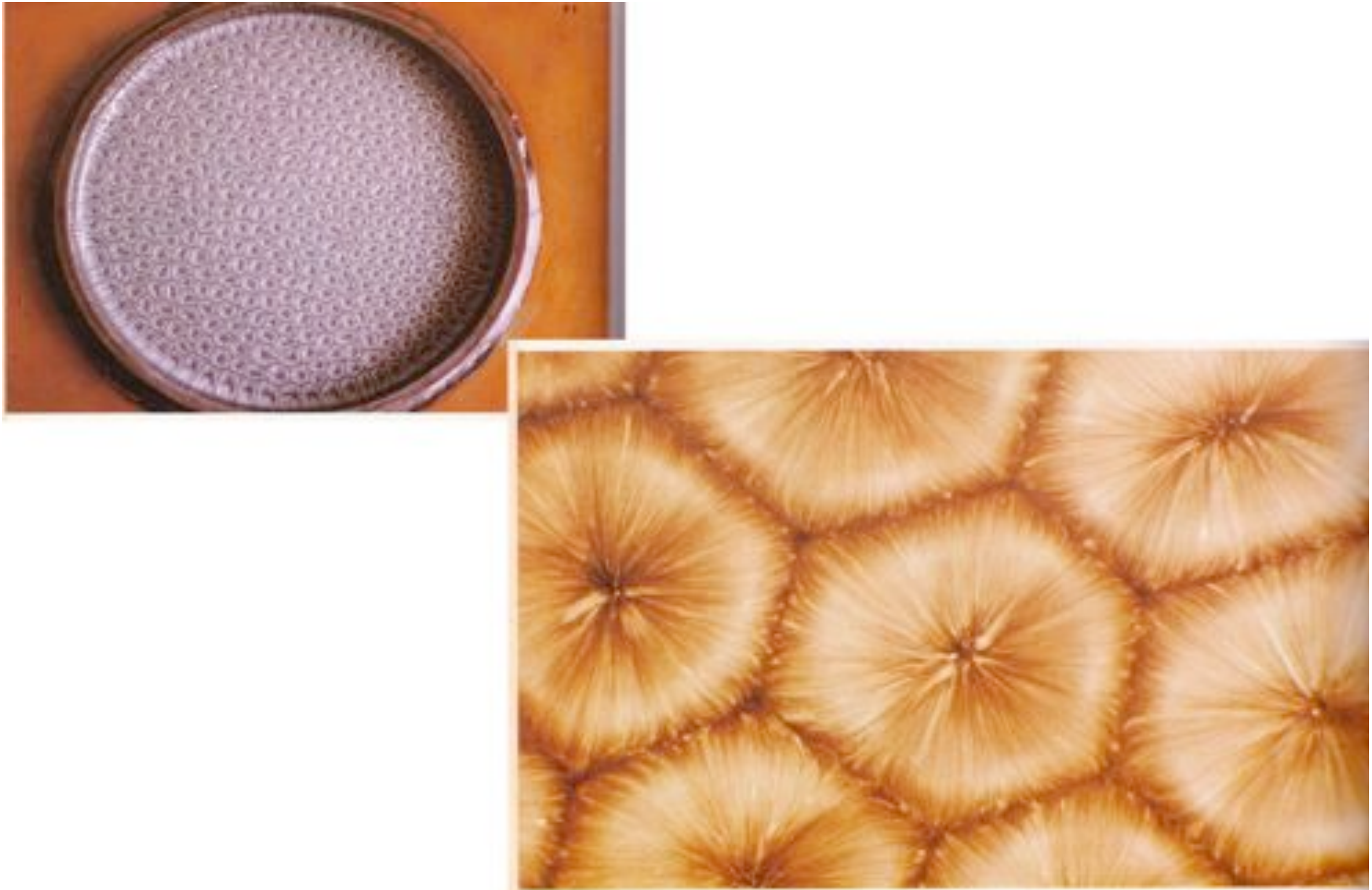
" *the spontaneous emergence of order at critical points of instability is one of the most important concepts of the new understanding of life. It is technically known as self-organization and is often referred to simply as" emergence". It has been recognized as the dynamic origin of development, learning and evolution.*"

Out of equilibrium self-organization

Terms such as chaos and non-linear dynamics, self-organized criticality, self-organization in non equilibrium systems, are typical of such field (C.G. Langton, 1990; P. Bak et al., 1988; R.C. Hilborn, 1994; Nicolis and Prigogine, 1977; S.H. Strogatz, 1994; de Jong and de Boer, 2004).

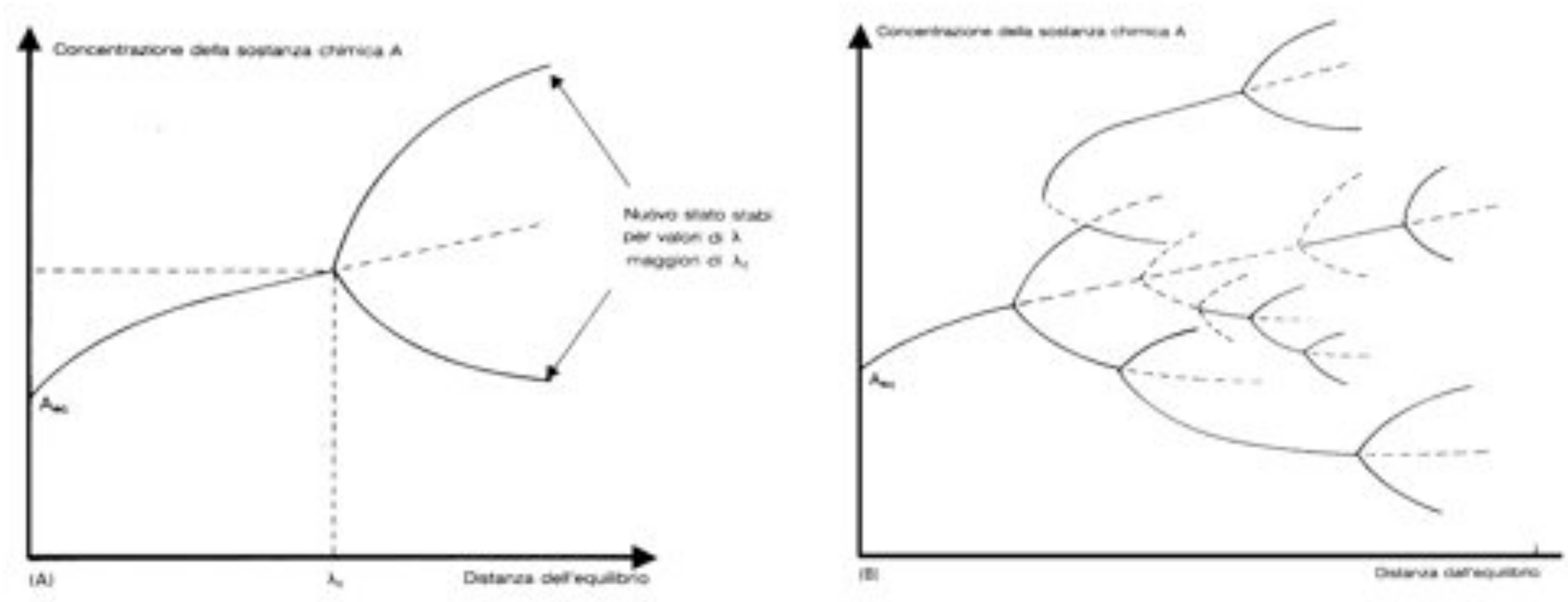
Such dynamical systems are generally out of equilibrium, and at first sight it is counter-intuitive that a system out of equilibrium may form self-organized structures. This is in fact the challenge and beauty of this particular field.

the theoretical background of this dynamic aspect of emergence can be traced to the introduction of the dissipative structures by Prigogine and his school. A dissipative structure in these terms is an open system that is in itself far from equilibrium, maintaining however a form of stability



Veduta complessiva e ingrandimento dello schema esagonale di convezione in uno strato di olio siliconico dello spessore di 1 millimetro.

, depending on the initial conditions and fluctuations of the energy flow, the system in its dynamic behavior may encounter a point of instability- the bifurcation point- at which it can branch off with the emergence of new forms of structure and properties.



Bifurcation far from equilibrium. (A), primary bifurcation. Lc Is the distance from equilibrium, at which the thermodynamic branching of minimal entropy production becomes unstable. The bifurcation point or critical point corresponds to the concentration λc. (B) complete diagram of bifurcations. As the non-linear reaction goes away from equilibrium, the number of possible states increases enormously

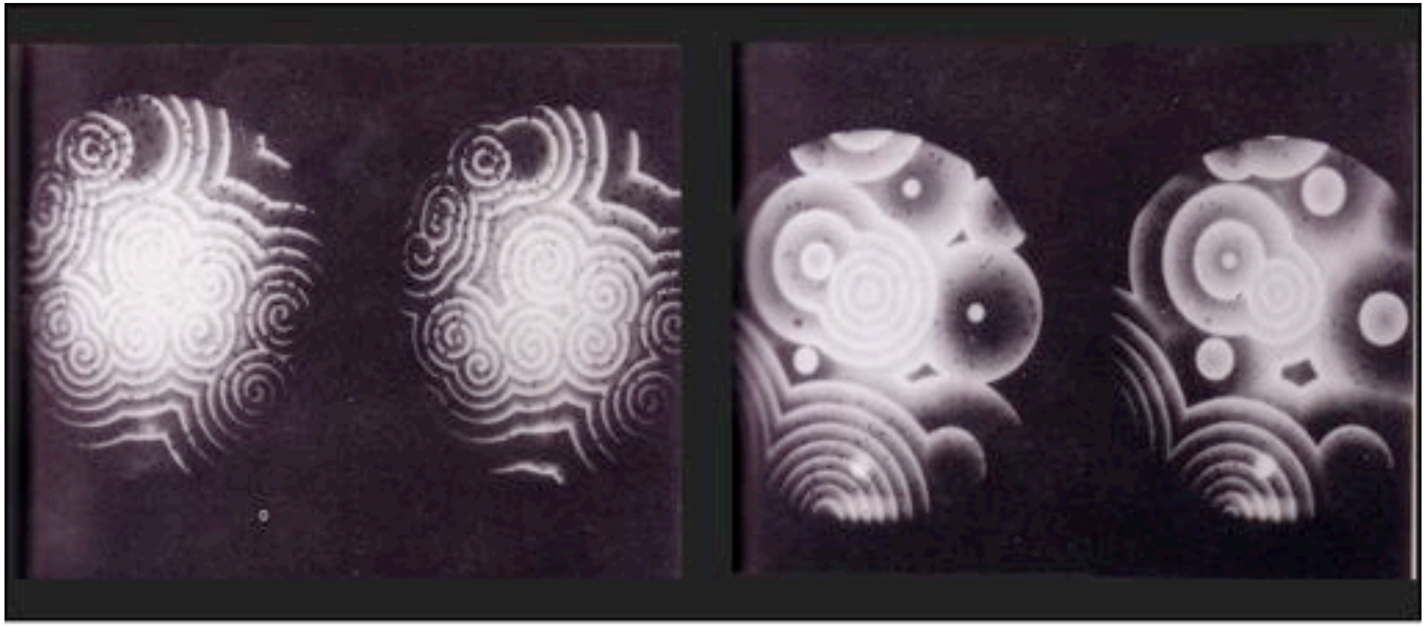
SWARM INTELLIGENCE

, I **would like to cite Francisco Varela in one of his last interviews before his death (in Poerkson, 2004):**

"***Consider, for example, a colony of ants. It is perfectly clear that the local rules manifest themselves in the interaction of innumerable individual ants. At the same time, it is equally clear that the whole anthill, on a global level, has an identity of its own…We can now ask ourselves where this insect colony is located. Where is it? If you stick your hand into the anthill, you will only be able to grasp a number of ants, i.e., the incorporation of local rules. Furthermore, you will realize that a central control unit cannot be localised anywhere because it does not have an independent identity but a relational one. The ants exist as such but their mutual relations produce an emergent entity that is quite real and amenable to direct experience. This mode of existence was unknown before: on the one hand, we perceive a compact identity, on the other, we recognize that it has no determinable substance, no localisable core."***

And this is so also for the SELF, seen as an emergent pattern:

"T*his is one of the key ideas*, *and a stroke of genius in today's cognitive science. There are the different functions and components that combine and together produce a transient, non-localisable, relationally formed self, which nevertheless manifests itself as a perceivable entity. …we will never discover a neuron, a soul, or some core essence that constitutes the emergent self of Francisco Varela or some other person."*



Some aspects of the B-Z reaction

THE INCREASE OF COMPLEXITY TOWARDS THE EMERGENCE OF LIFE PROCEEDS

VIA THE INTERPLAY BETWEEN SELF-ORGANIZATION AND EMERGENCE

System biology **system chemistry**

System theories applied to biology or chemistry

The study of complexity of the entire system

Key words: proteomics, genomics, libraries, combinatorial chemistry, dynamic networks, catalytic networks, neuronal networks; complexity, emergent properties, non-linearity, attractors, fractals, collective properties…

WHAT IS COMPLEXITY? WHEN IS A SYSTEM A COMPLEX SYSTEM?

A simple definition given by Simon (1981)

A COMPLEX SYSTEM IS SEEN AS A
HIERARCHIC SYSTEM, I.E. A SYSTEM
COMPOSED BY SUBSYSTEMS THAT IN TURN
HAVE THEIR OWN SUBSYSTEMS, AND SO ON...
H.A. Simon, The Sciences of the Artificial, MIT Press

Consider for example the progression:
Atom, molecules, molecular complexes, polymeric complexes...
Or
Cell, tissue, organ, organism...

Questions to the reader chapter five

1. **Do you accept the idea that self-organization in prebiotic time was the main driving force for the formation of the first living cells? (And if not, what would you add to the picture?)**

2. Suppose to divide a prokaryotic cell into its components, say ten different fractions, obtained by mild procedures; and then mix them all together. Would the living cell self-organize again? If not, why not? And: which kind of cell would you rather choose to run this kind of experiment?

3. Is the folding of proteins activated by chaperons under thermodynamic – or under kinetic control?

4. Are you convinced of the fact that finality is not an issue in the field of self-organization?

Questions to the reader chapter six (emergence)

1- Do you accept the idea that in the future unimaginable novel properties will emerge from the study of new composite materials or new synthetic complex systems?

Do you accept the idea that human consciousness is an emergent property of a particular neuronal and physical human construct?

After reading this chapter, do you adhere more to the view of "strong emergence" – or "weak emergence"?

PAROLE/DOMANDE CHIAVE

CONCETTO DI „SELF“/AUTO

AUTO-ORGANIZZAZIONE

CONTROLLO TERMODINAMICO E CINETICO

PROPIETA‘ EMERGENTI

AUTOORGANIZZAZIONE COLLETTIVA SENZA CENTRO

STRUTTURE DISSIPATIVE

SISTEMI DINAMICI E AUTO-ORGANIZZANTI

LA VITA COME PROPRIETA‘ EMERGENTE

SI PUO‘ COSTRUIRE LA COMPLESSITA‘ MOLECOLARE DELLA VITA IN QUESTO MODO?