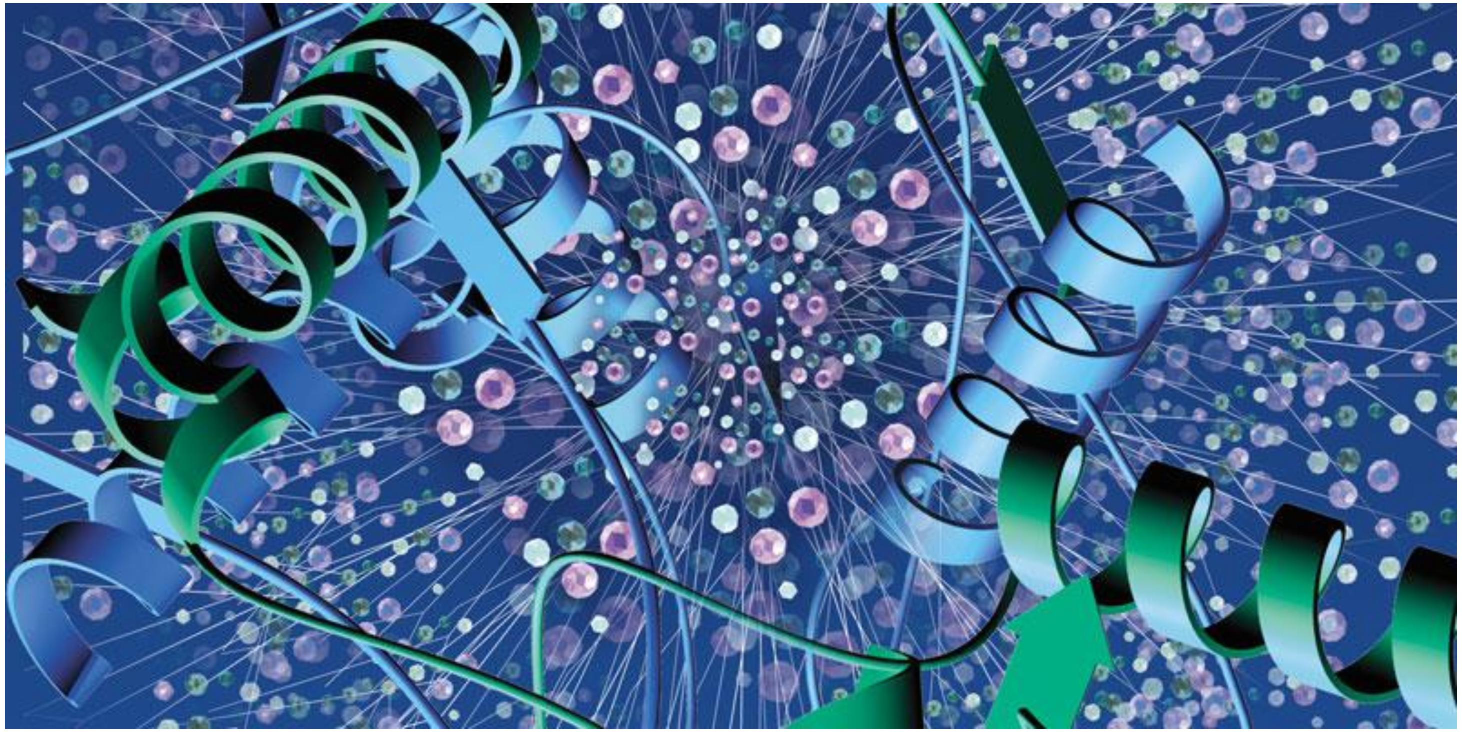
Physics of biological systems
From DNA and dipeptides to cells



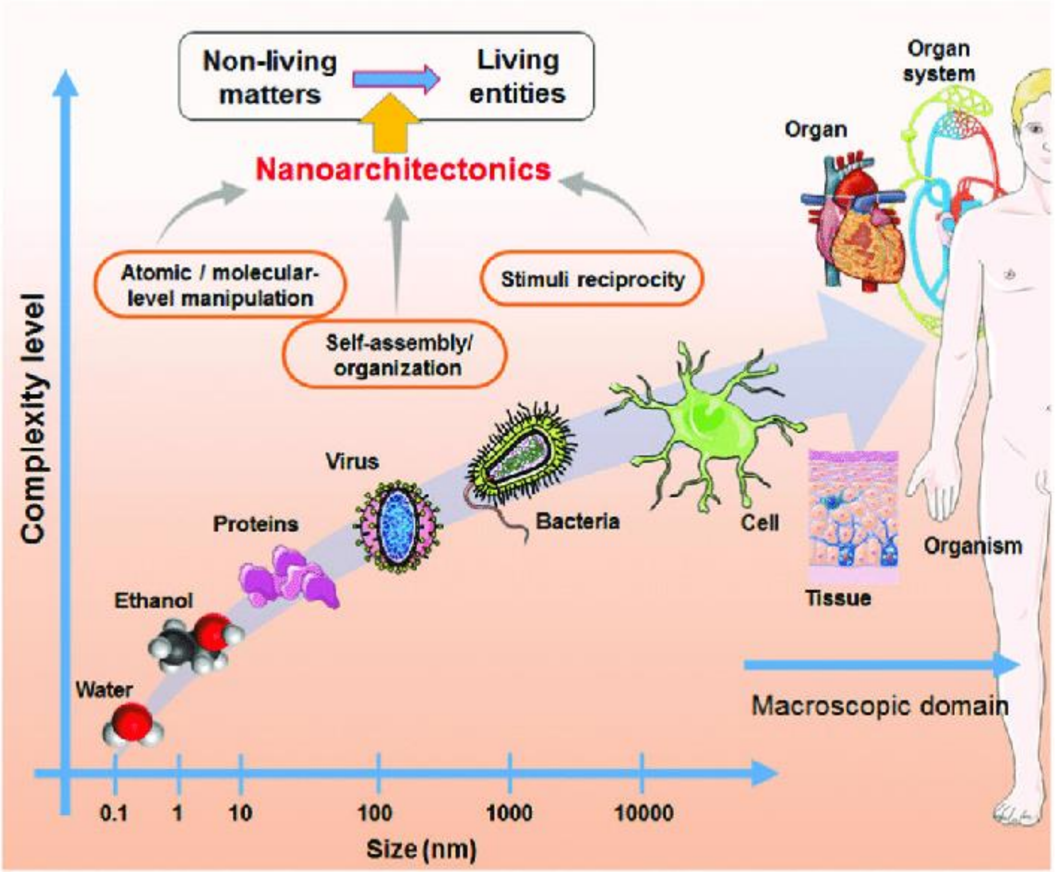
Giornate di orientamento per le tesi, Corso di Laurea in Fisica, 23/03/2023,
alessandro.paciaroni@unipg.it

Biological systems

Multiscale (space/time)

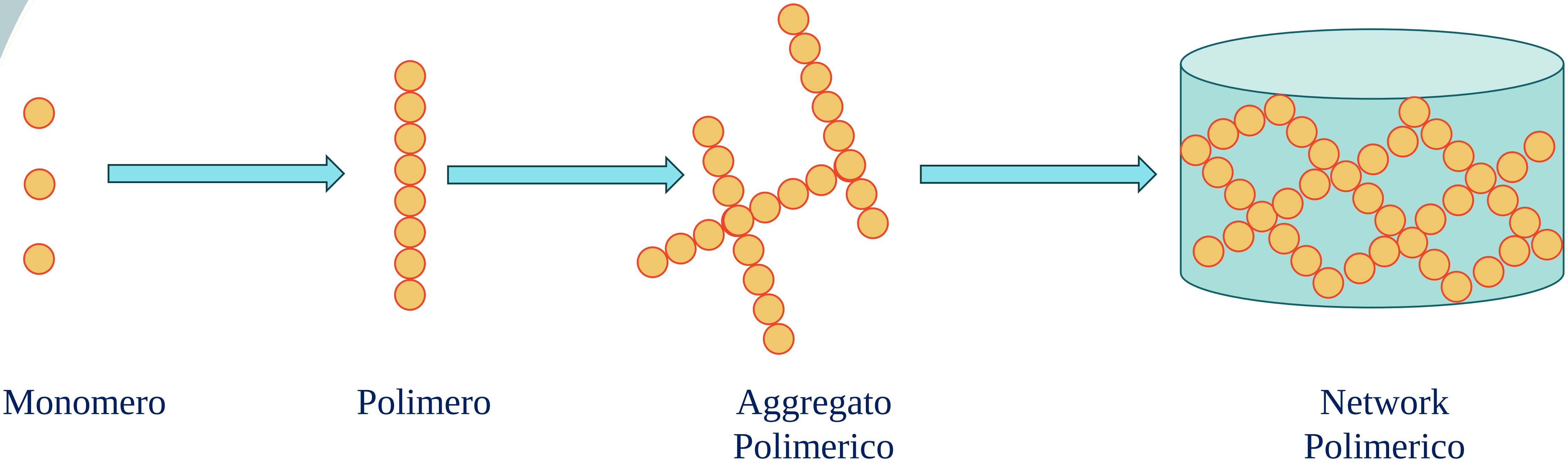
Complexity (more is different*)

Multidisciplinary
Multitechnique
Multipurpose



*A complex system is composed of **many parts** which interact with each other in multiple ways, culminating in a higher order of **emergence** greater than the sum of its parts (synchronized double pendulum from Huygens)

Aggregazione gerarchica delle biomolecole: dal monomero al network polimerico



Appel, E.A., et al., Chemical Society Reviews. 2012

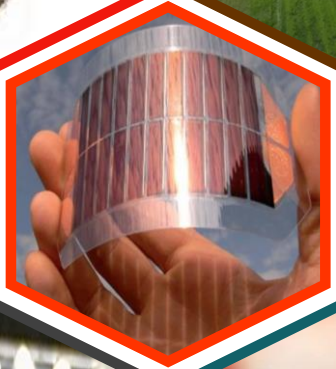
Nano-aggregati e idrogel: applicazioni

Agricoltura

W.E. Rudzinski et al., Des. Monomers Pol. 2002

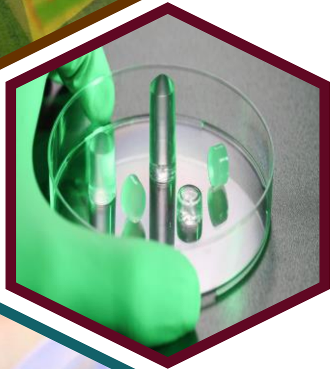
Industria Alimentare

X. Zhu et al., J. Adv. Res. 2022



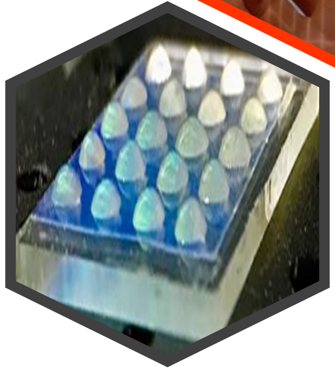
Fotovoltaico

E. Meneghin et al., J. Phys. Chem. Lett. 2020



Trasporto dei farmaci

N.A. Peppas et al., Eur. J. Pharm. Biopharm. 2000



Biosensori

Y.S. Zhang et al., Science 2017

Ingegneria Tissutale

Q. Zou et al., J. Am. Chem. Soc. 2017

Medicina rigenerativa

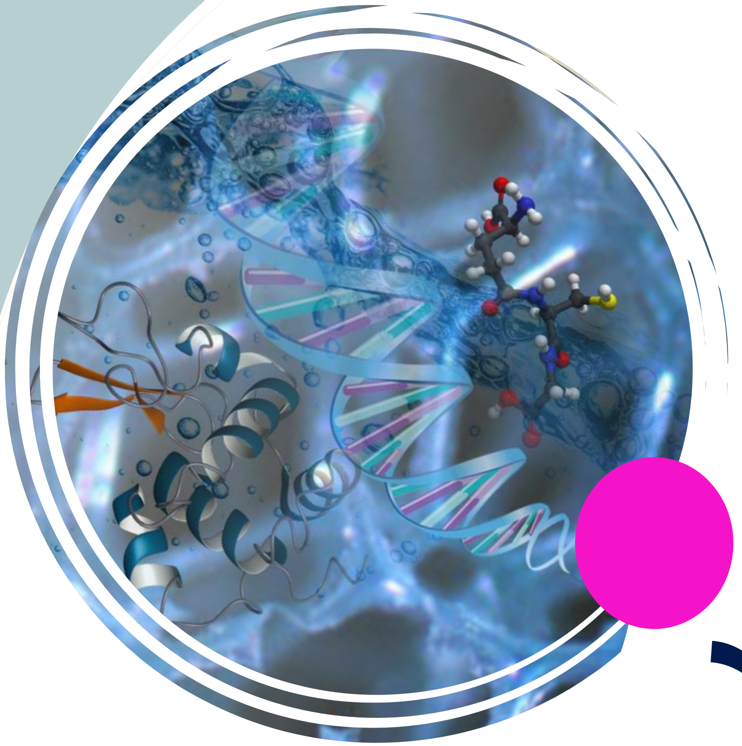
B.V. Slaughter et al., Adv. Mater. 2009

Scaffold cellulari

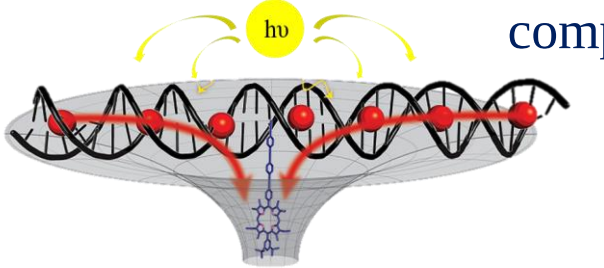
Q. Hu et al., Mater. Today Chem. 2022

Sistemi fotosintetici bio-inspirati

Sfruttando la capacità delle **biomolecole** di **auto-aggregare** vogliamo riprodurre artificialmente dei sistemi in grado di **trasferire energia**, prendendo ispirazione dai complessi proteici fotosintetici.

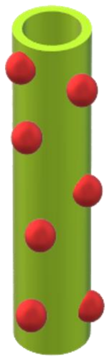


DNA



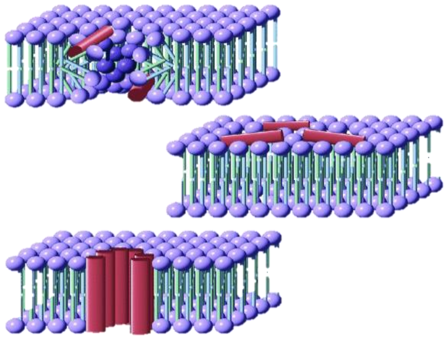
J.G. Woller et al., J. Am. Chem. Soc. 2013

PEPTIDI



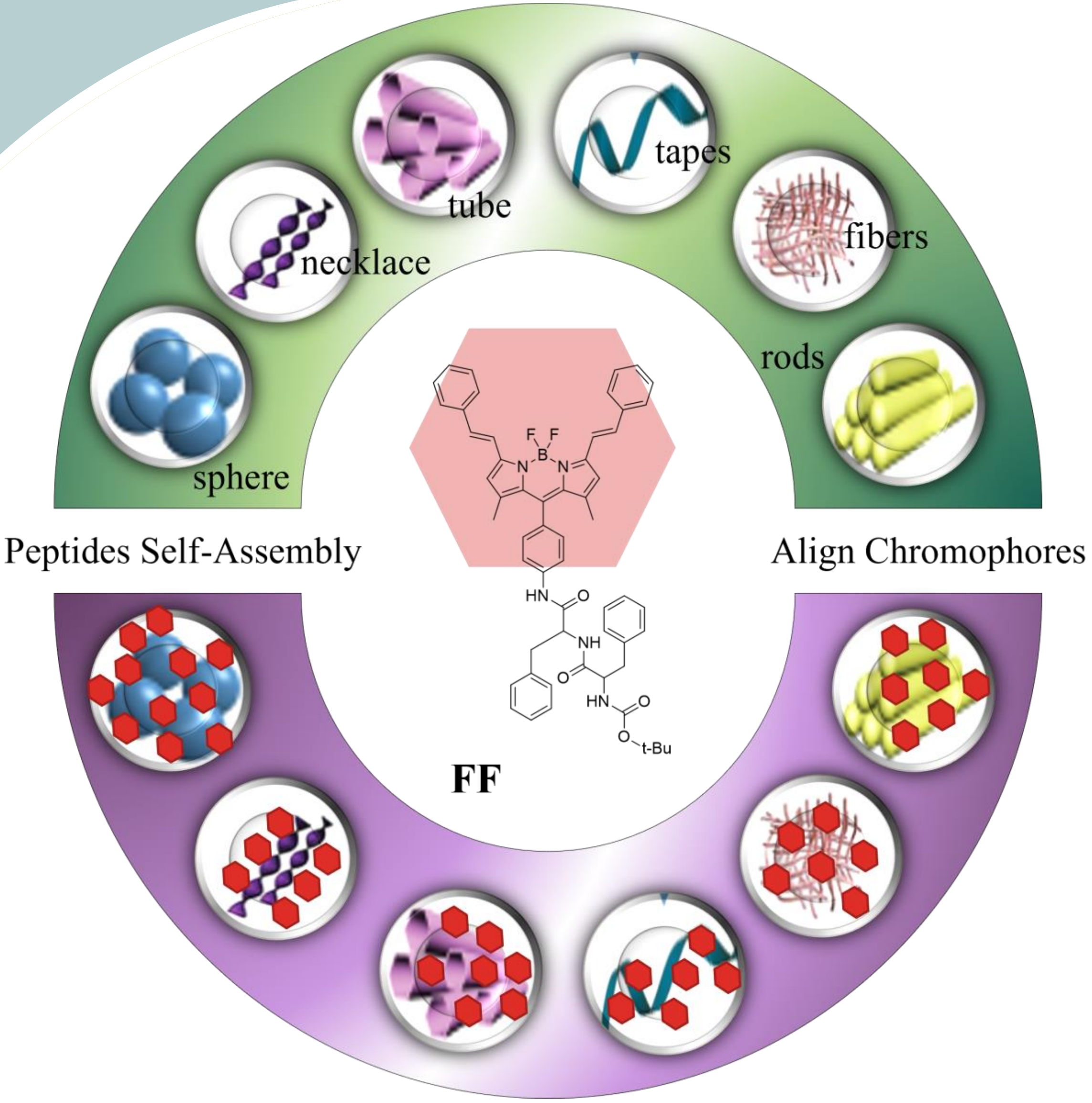
Q. Zou et al., Adv. Mater. 2016

LIPIDI



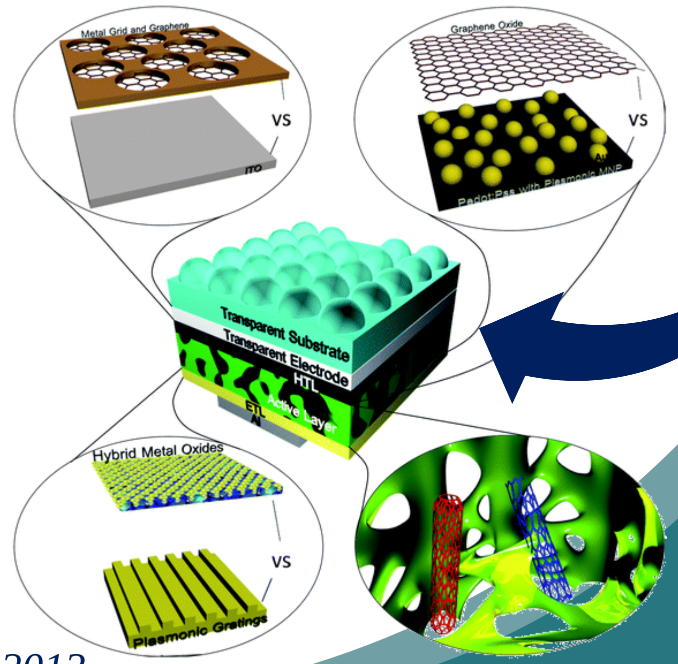
Mura, F., et al., Dyes and Pigments. 2020

Nano-aggregati formati attraverso l'auto-aggregazione di peptidi corti



Attraverso il controllo della **struttura** e della **morfologia** degli aggregati peptidici si può controllare la **spaziatura** e l'**orientazione** tra i cromofori, entrambi sono parametri essenziali per avere il **trasferimento di energia**.

Lo scopo è quello di produrre degli **strati attivi** efficienti per lo sviluppo di **celle solari ibride** di nuova generazione.

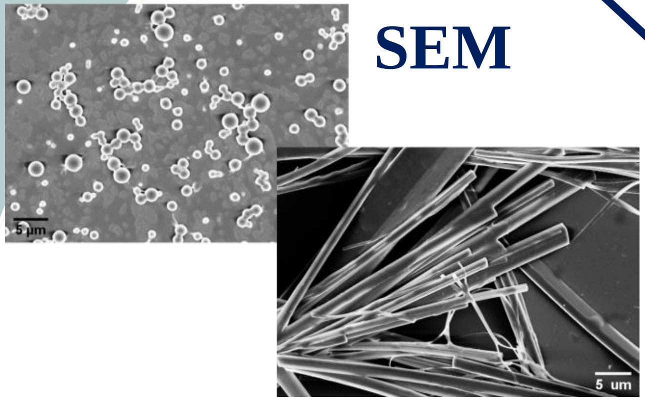


Jayawardena, K.I., et al. Nanoscale. 2013

Studio multiscala attraverso un approccio multitecnica

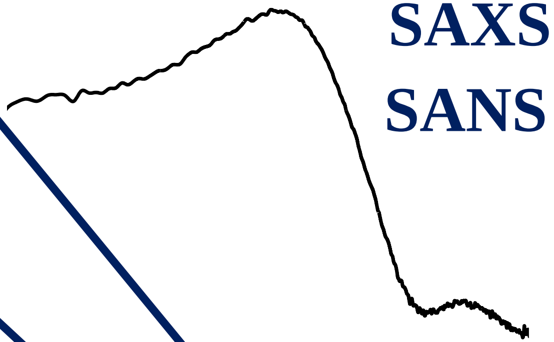
❑ MORFOLOGIA

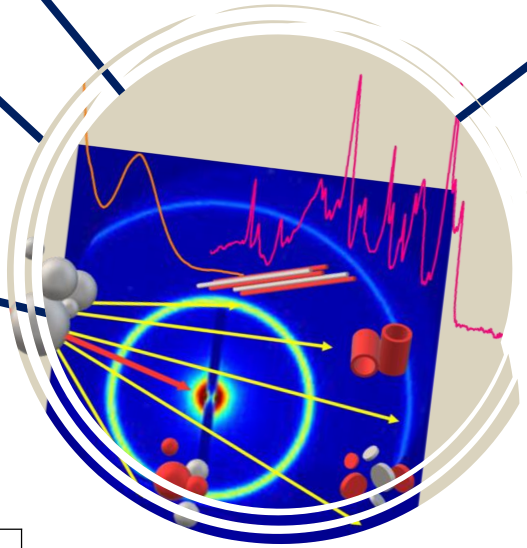
SEM



❑ STRUTTURA

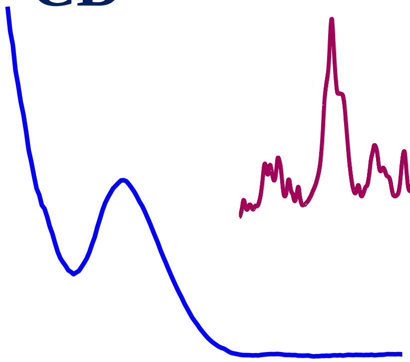
SAXS
SANS





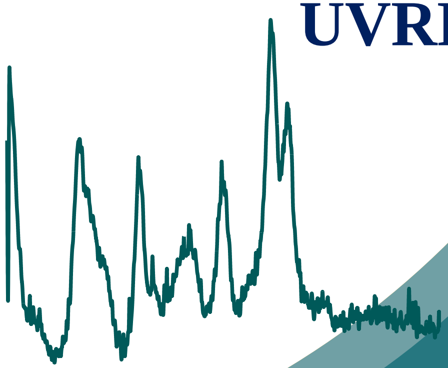
❑ CONFORMAZIONE

CD



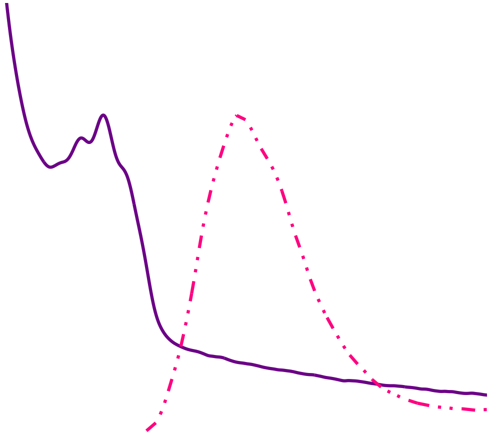
ATR-IR

UVRR

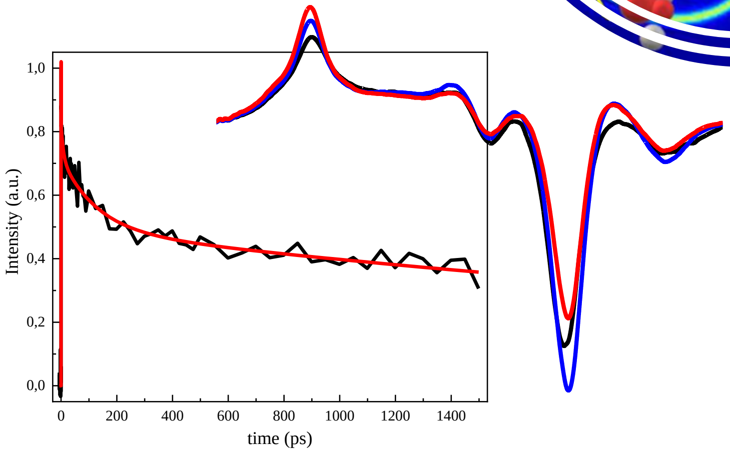


❑ PROPRIETÀ FOTOFISICHE

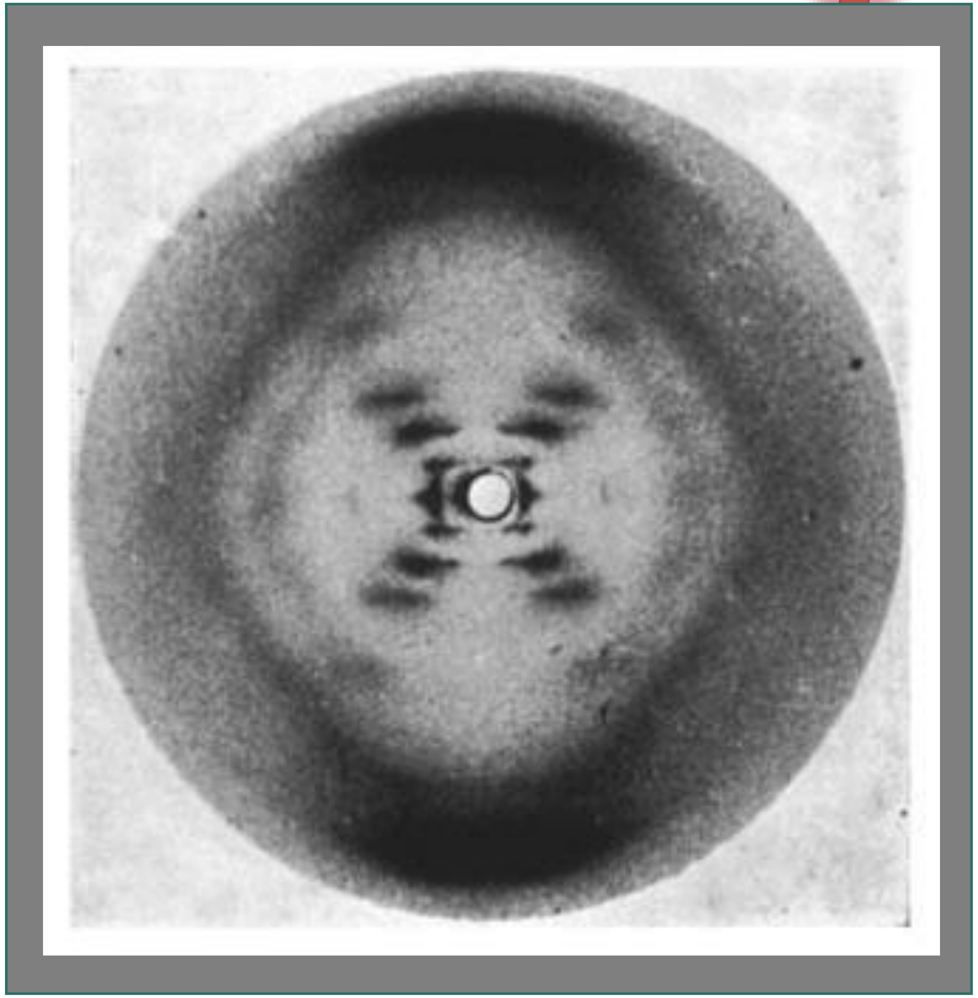
ABS. & FLUO.
STAZIONARIE



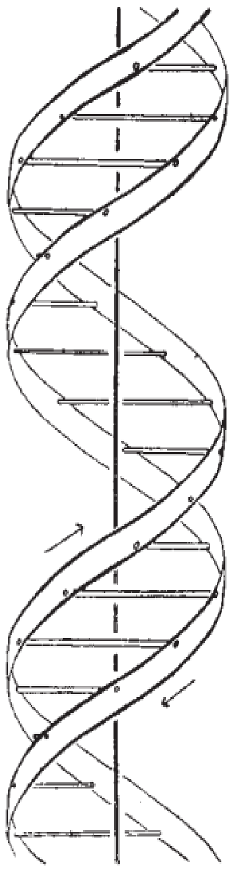
TAS
RISOLTE IN TEMPO



1953

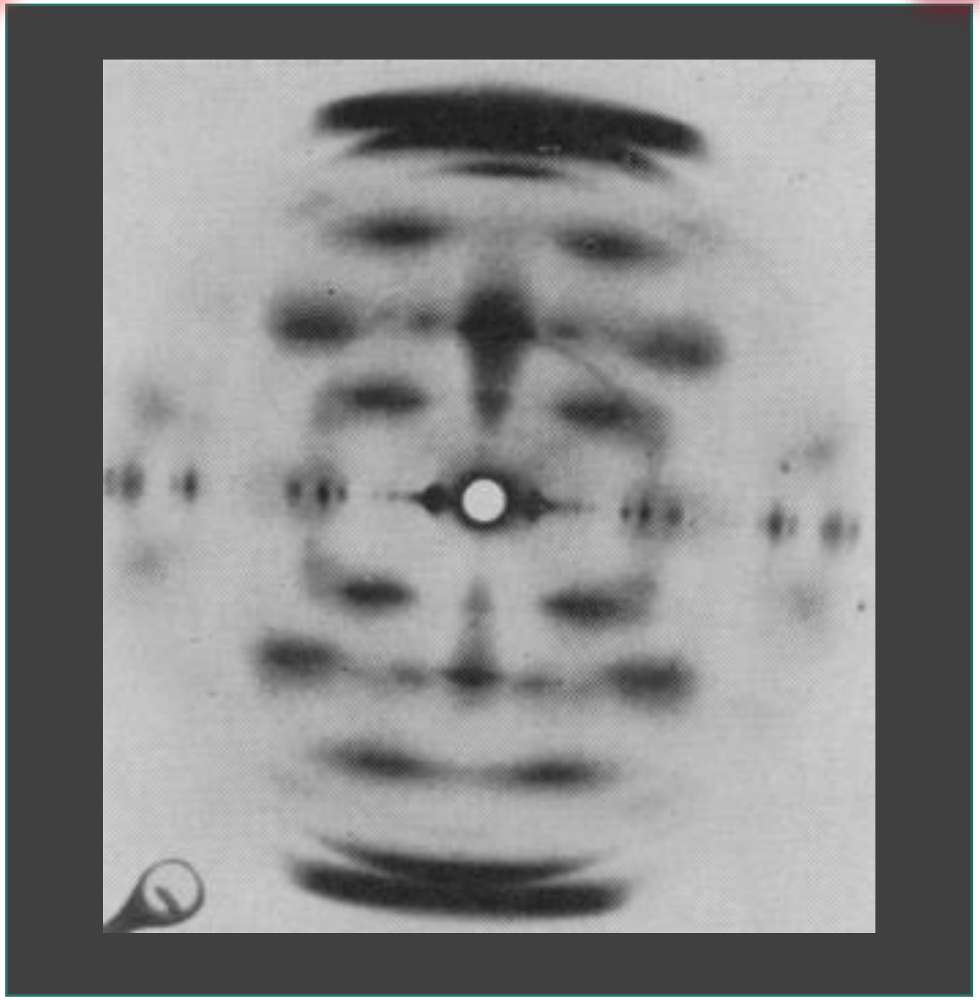


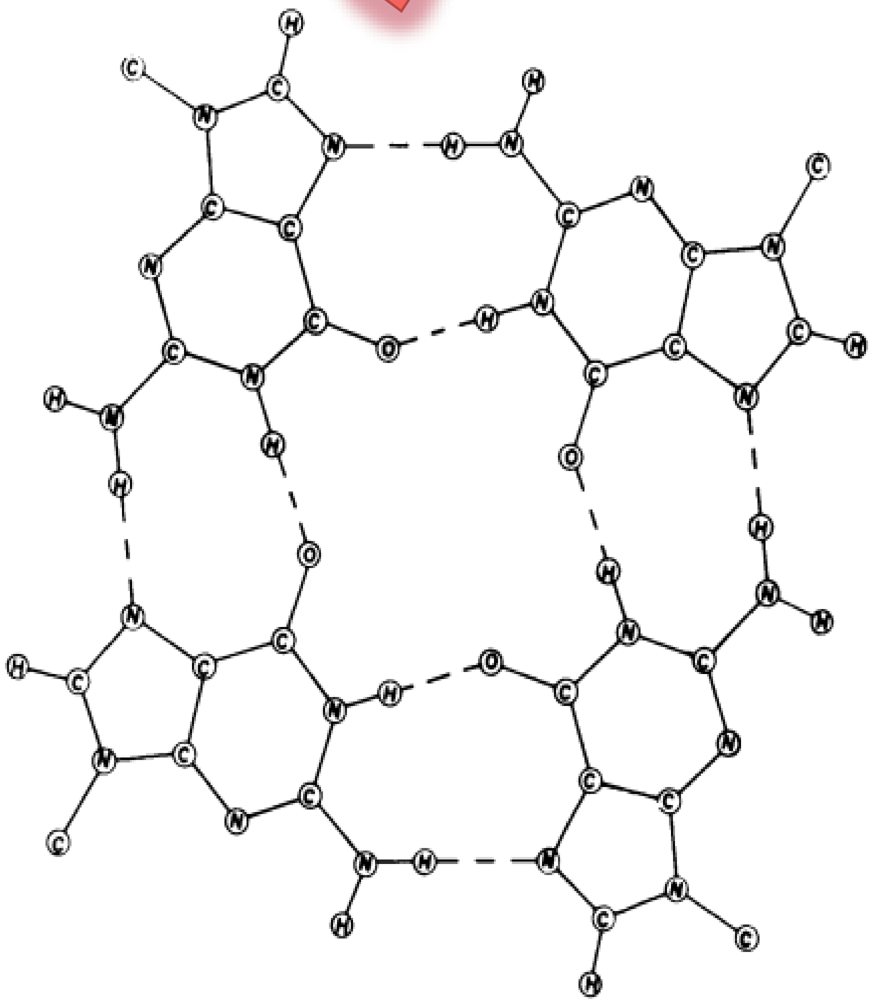
«Photograph 51»
Franklin and Gosling



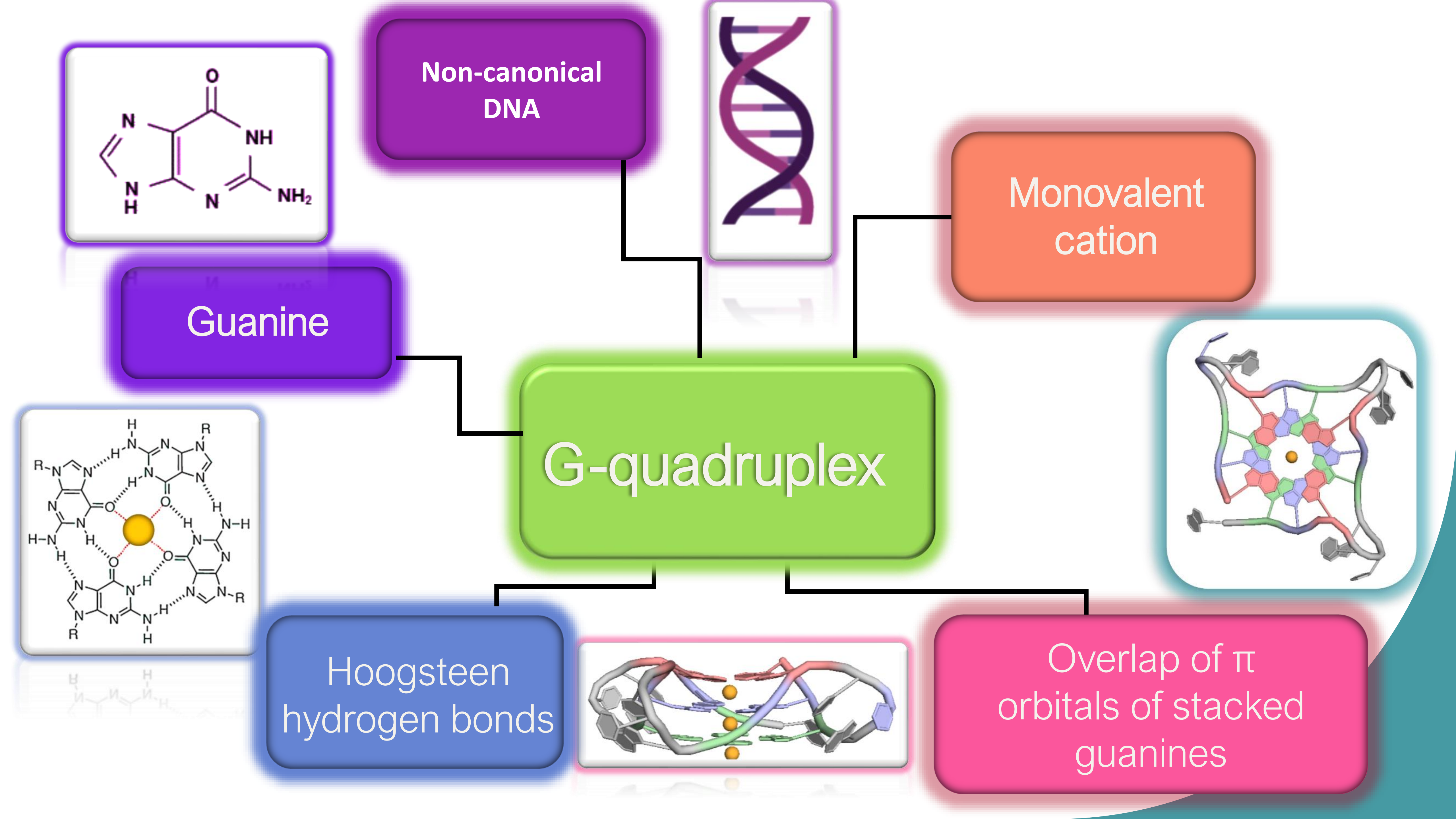
Watson and Crick
"Molecular structure of nucleic acids: a structure for deoxyribose nucleic acid". Nature 1953 171.4356, 737–738.

1962





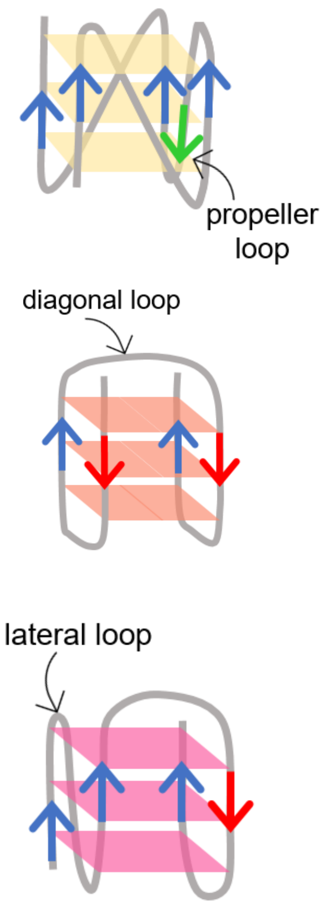
Gellert, Lipsett, and Davies.
"Helix formation by guanylic acid".
Proceedings of the National Academy of Sciences
1962 48.12,2013–2018


Non-canonical DNA
Guanine
Monovalent cation
G-quadruplex
Hoogsteen hydrogen bonds
Overlap of π orbitals of stacked guanines

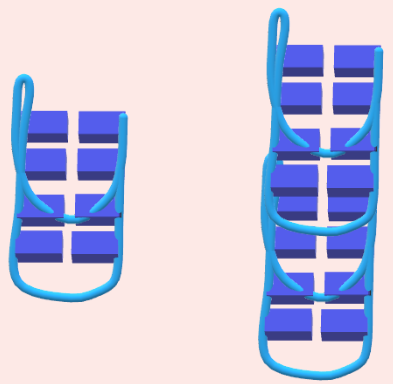
G-quadruplex secondary structure topologies

G4 topologies

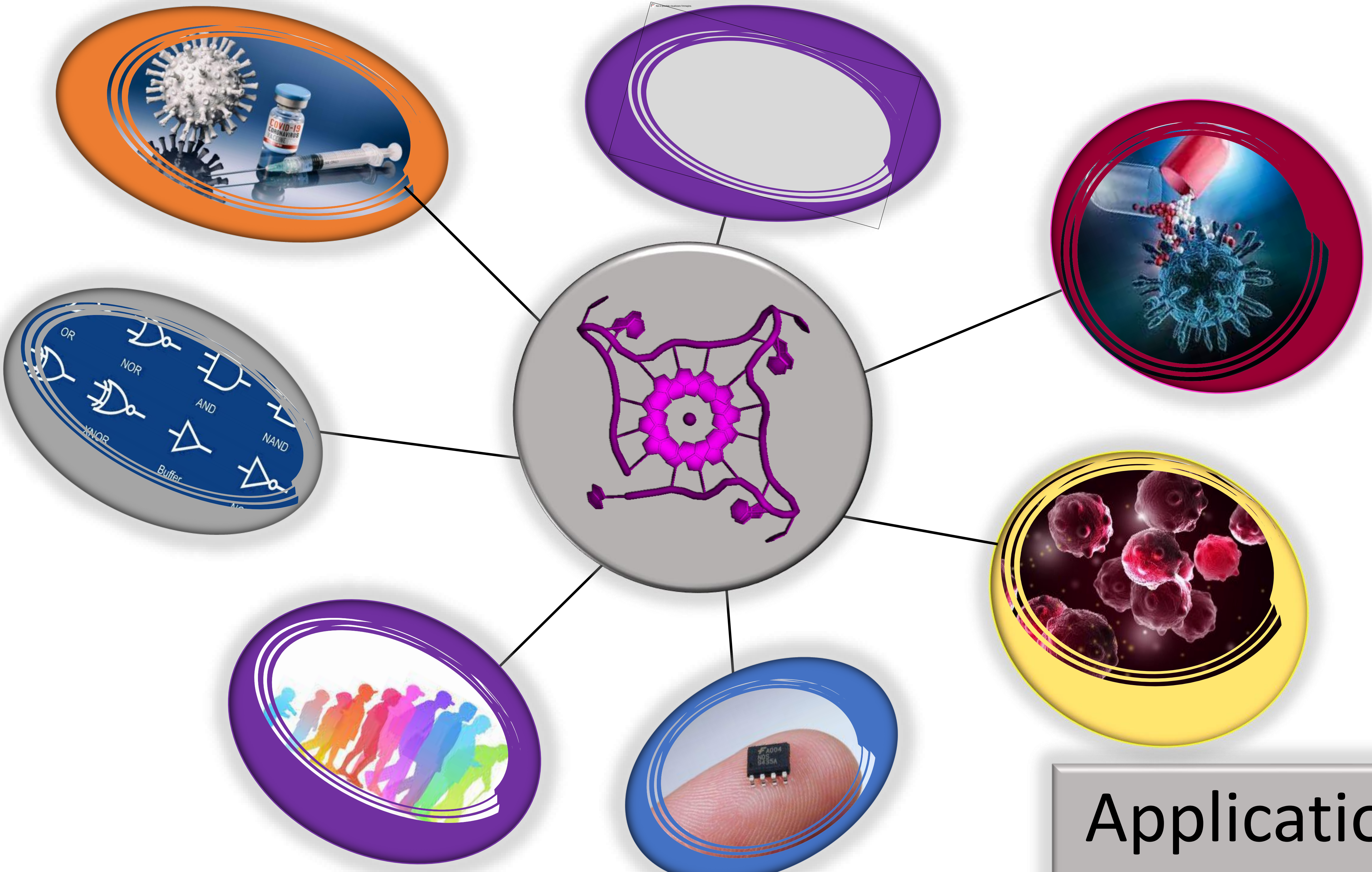
- Parallel
- Antiparallel
- Hybrid



Multimerization



G4 structure and stability depend on various factors: sequence, loop length, flanking nucleotides, concentration, and the presence of cations



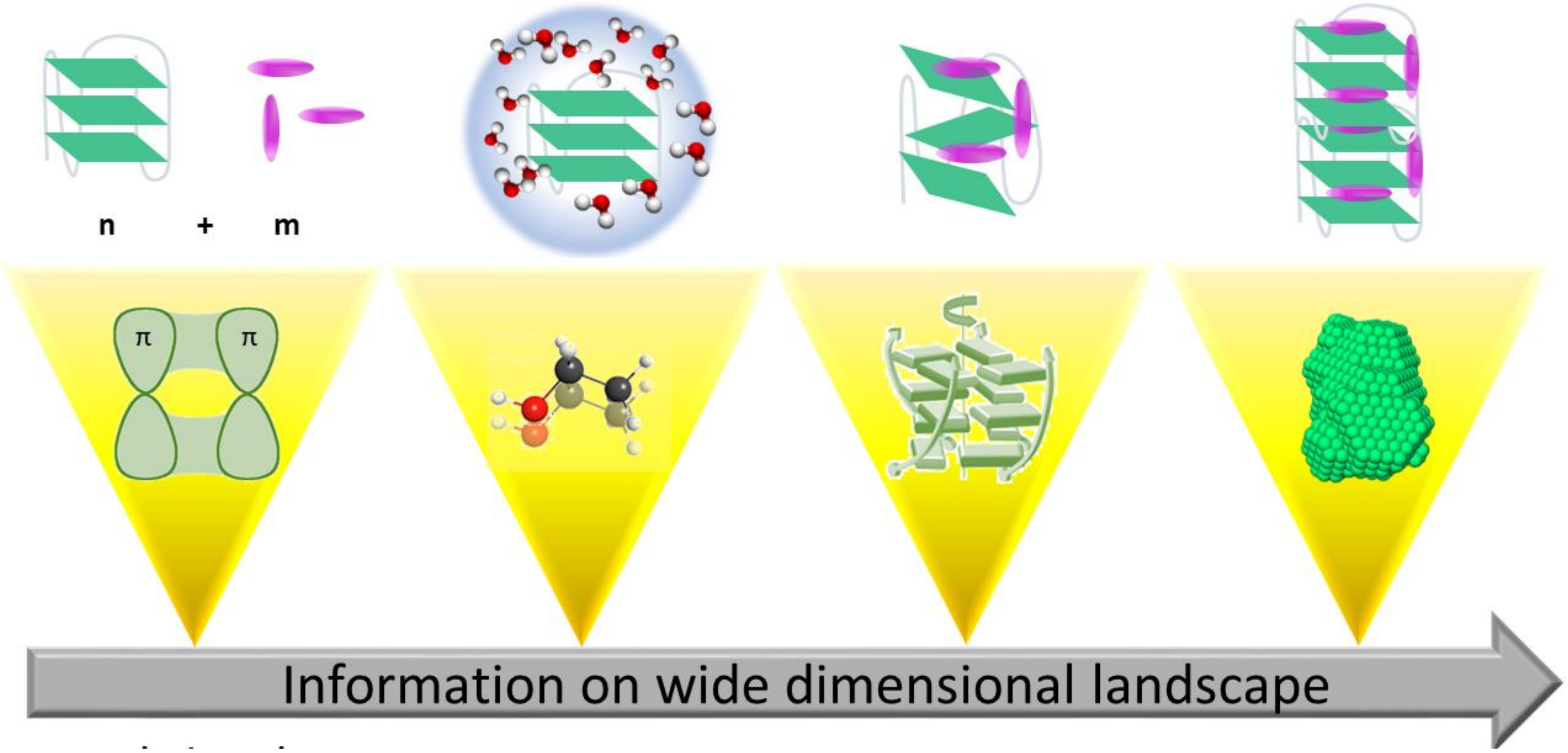
Applications

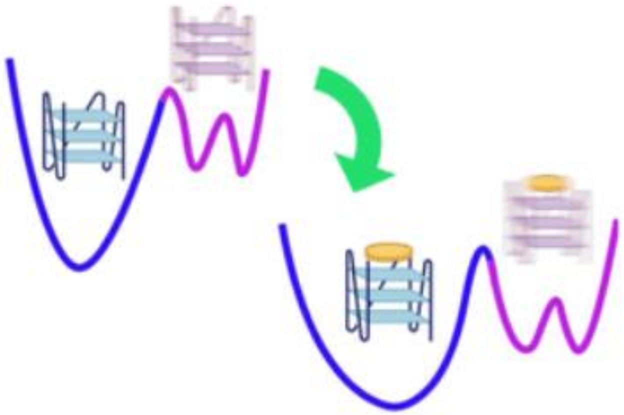
What ?

Structure

Interaction

Dynamics

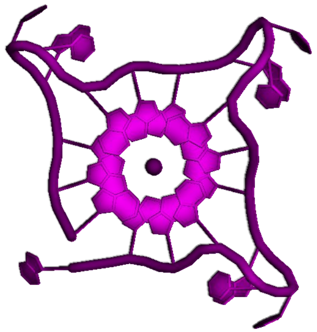


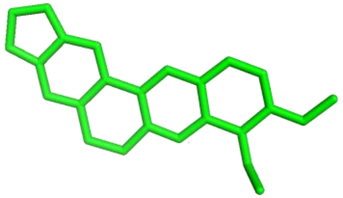


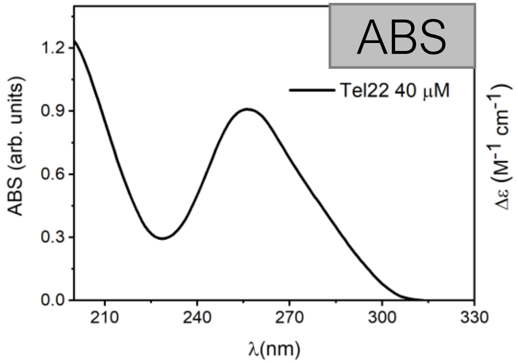
How? Where?

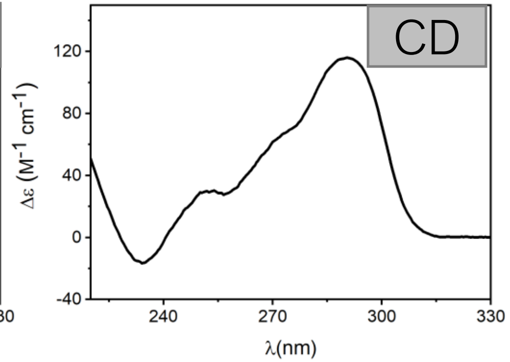
In-house

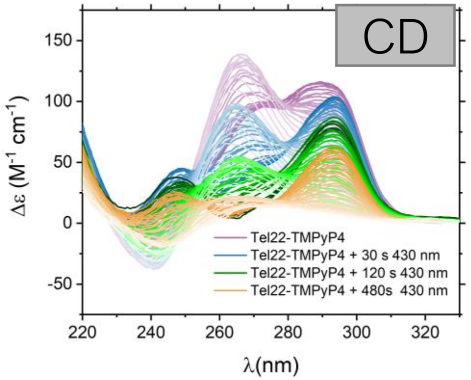
- ❑ Sample preparation
- ❑ UV-Vis absorption spectroscopy (ABS)
- ❑ Circular dichroism spectroscopy (CD)
- ❑ Infrared spectroscopy (IR)
- ❑ Fluorescence spectroscopy (Fluo) (Sapienza, Rome)

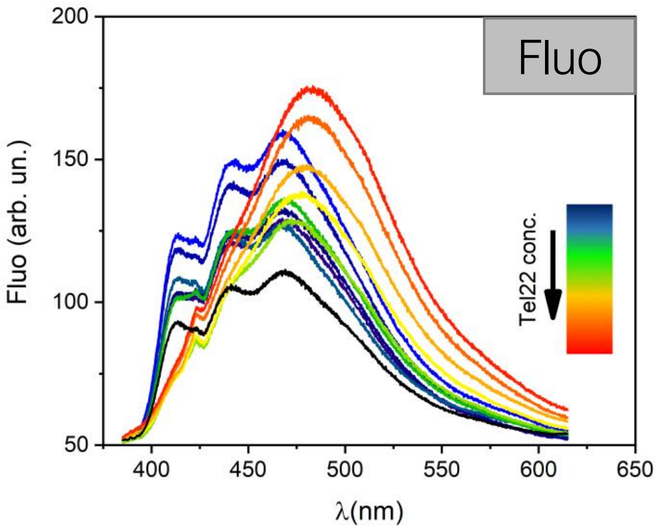


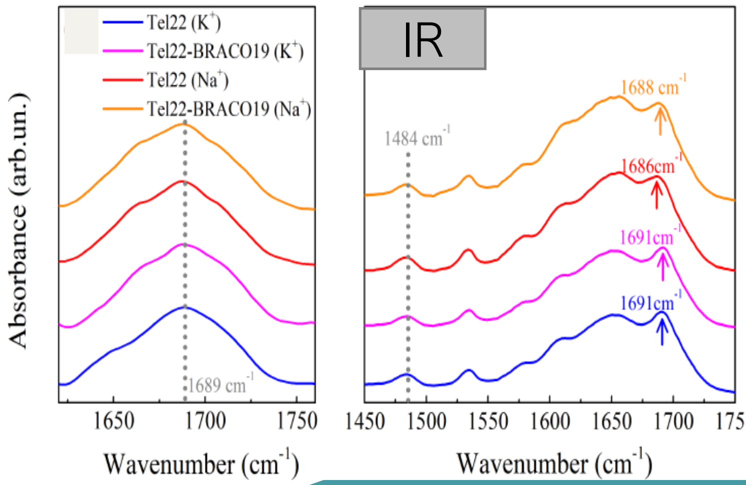








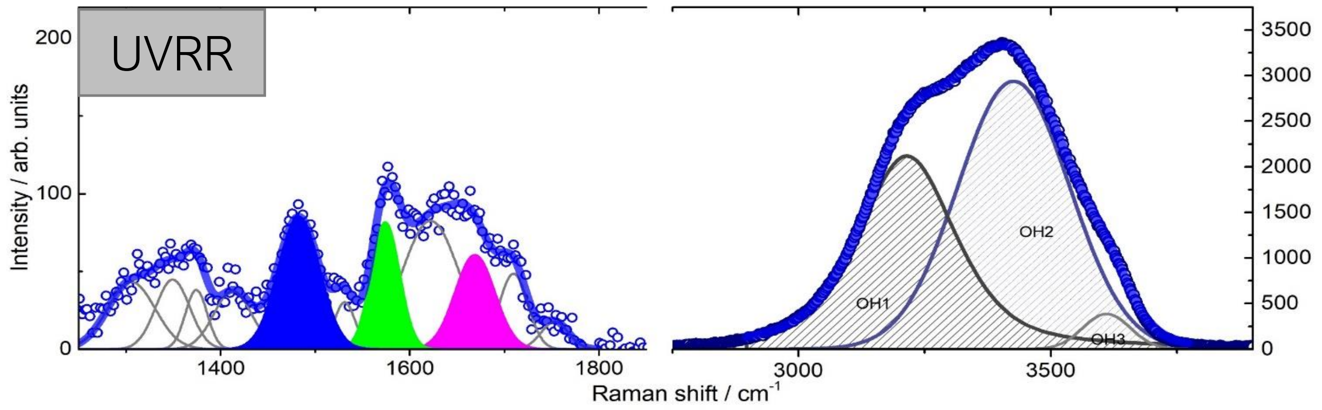


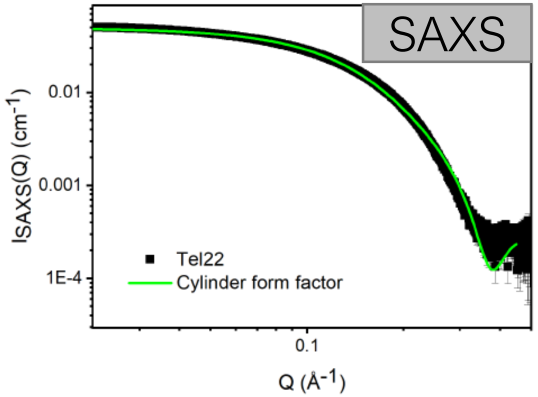


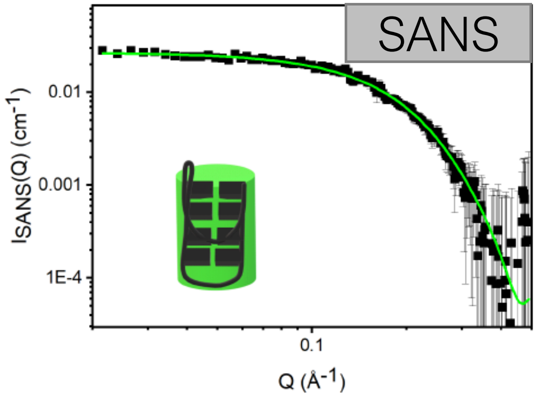
How? Where?

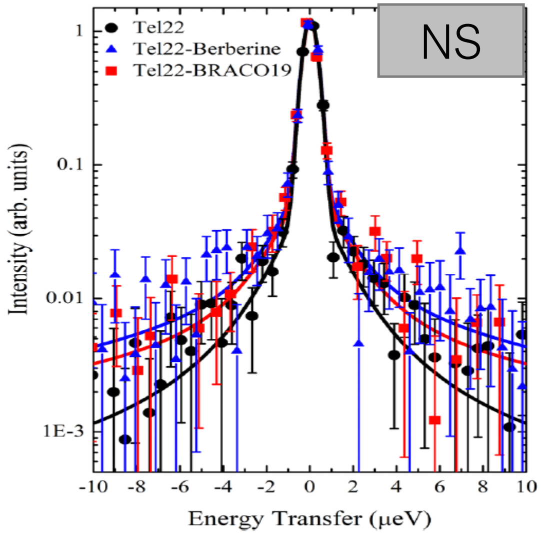
Large scale facilities

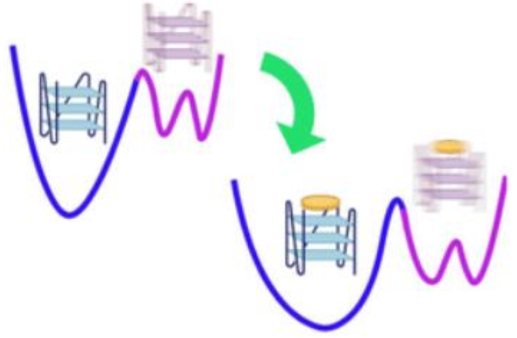
- ❑ UV-Resonant Raman (UVRR) (Elettra synchrotron Trieste)
- ❑ Small Angle Neutron Scattering (SANS) (ILL Grenoble)
- ❑ Small Angle X-ray Scattering (SAXS) (ESRF synchrotron Grenoble)
- ❑ Neutron Scattering (NS) (ILL Grenoble)







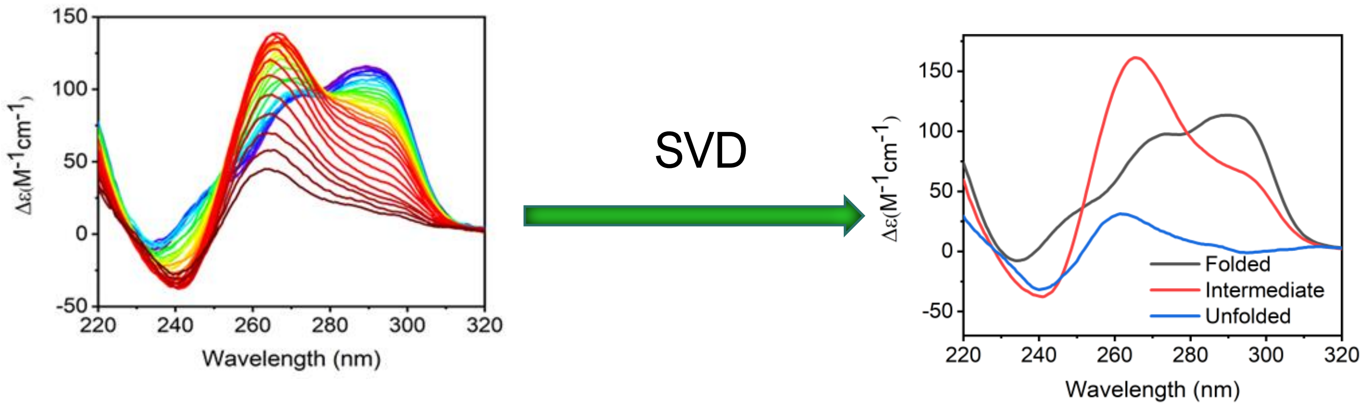


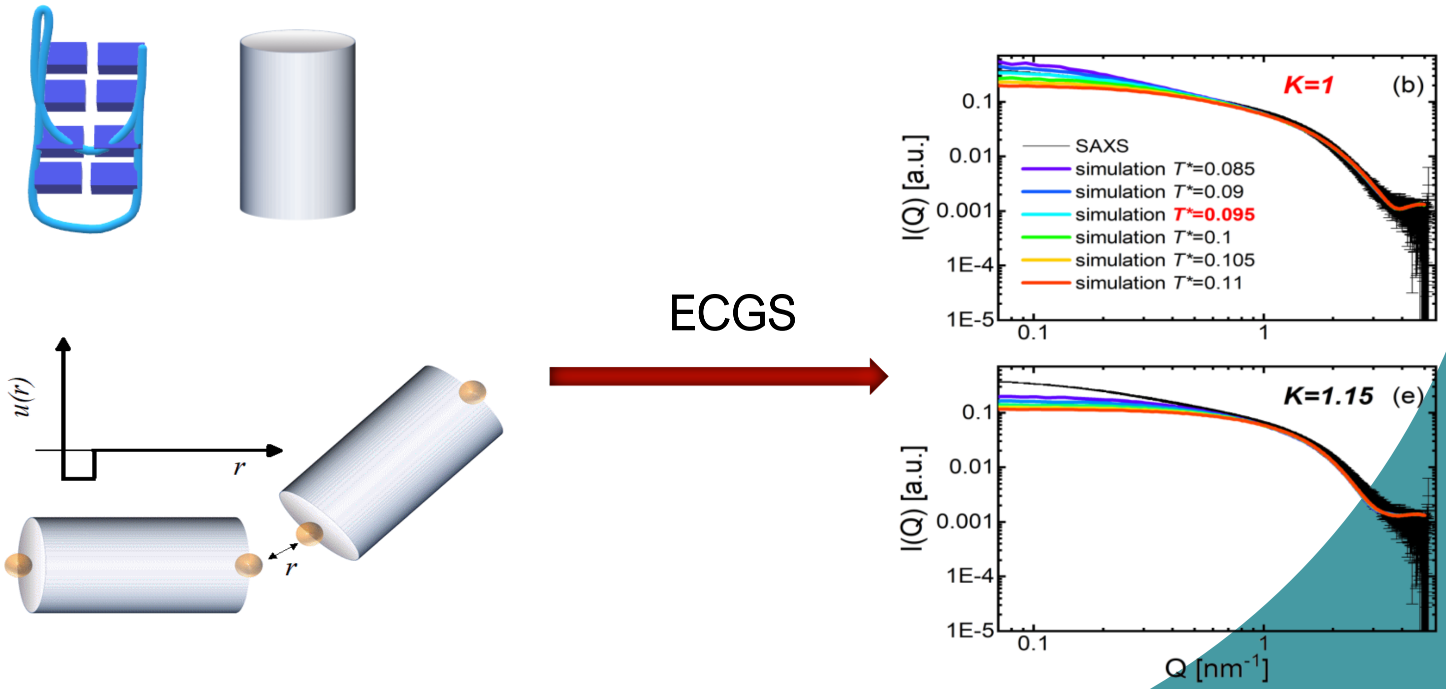


How?

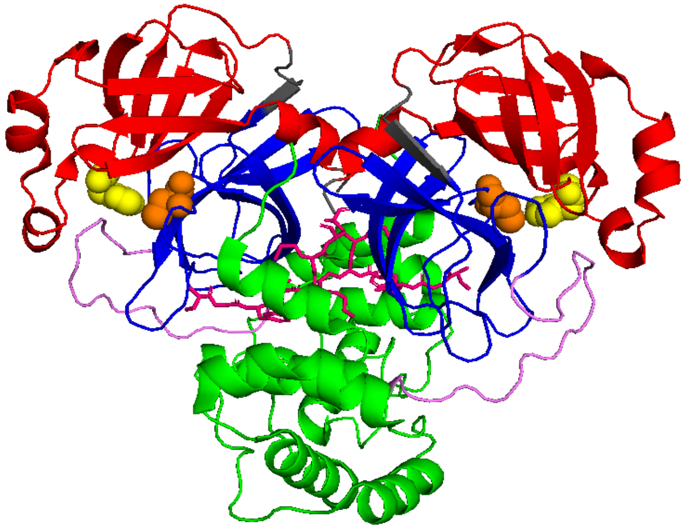
❑ Singular Value Decomposition (SVD)

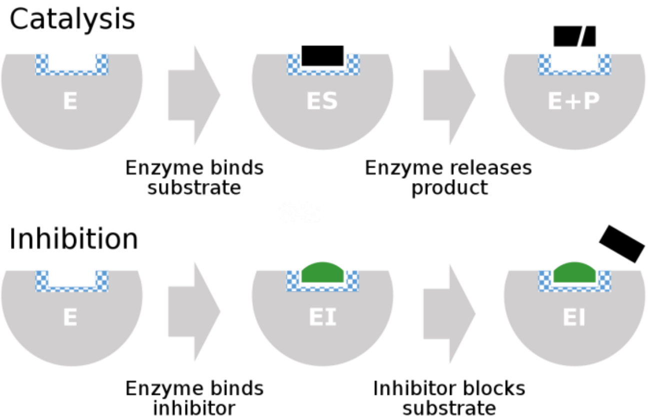
❑ Extremely coarse-grained simulations (ECGS)

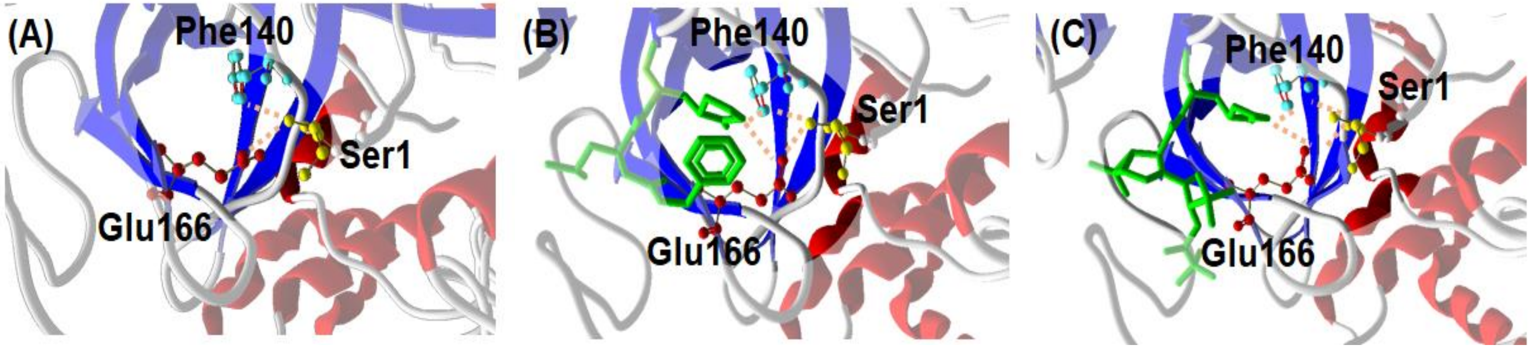




Main protease from SARS-CoV-2



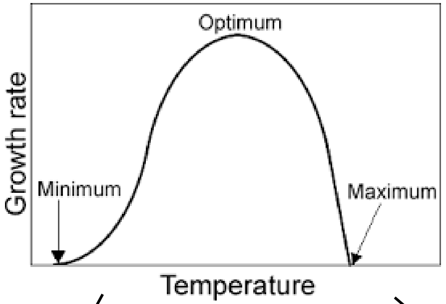




Life at extreme conditions

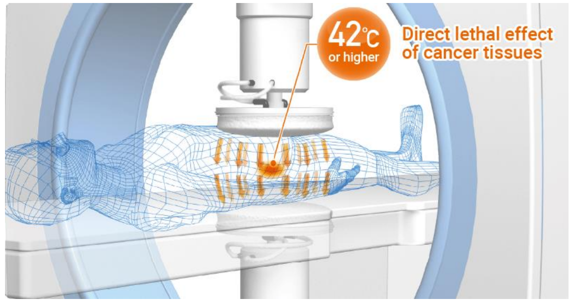
Heat as an epigenetic factor

Thermal regulation of immunity in vertebrates

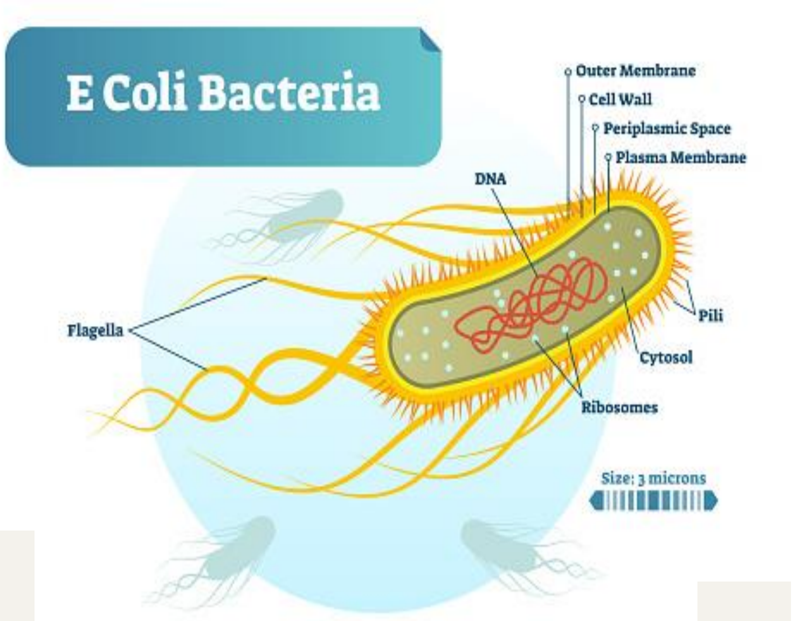


Sterilization in biotechnology

Hyperthermia Treatment of Cancer

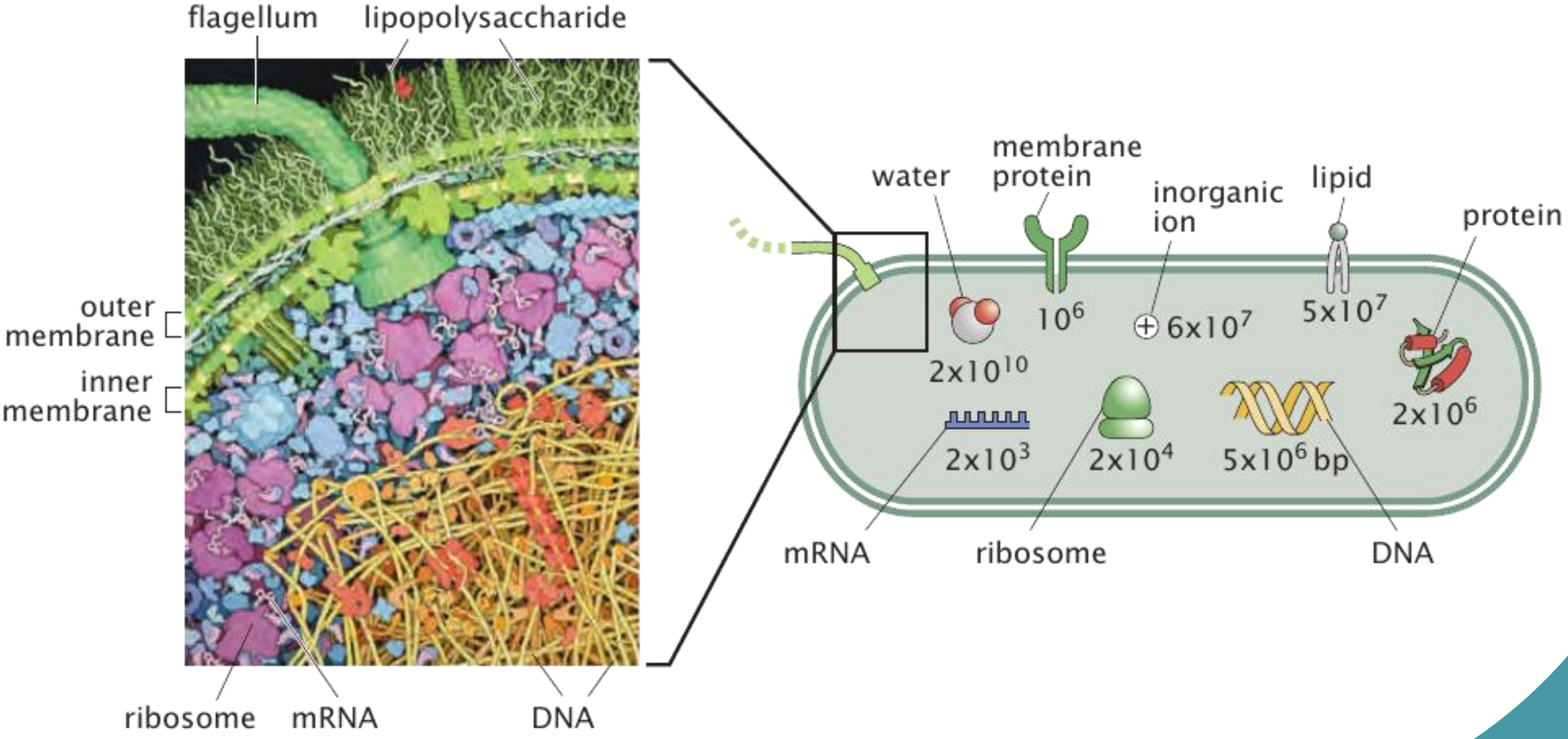


The hydrogen atom of microbiology

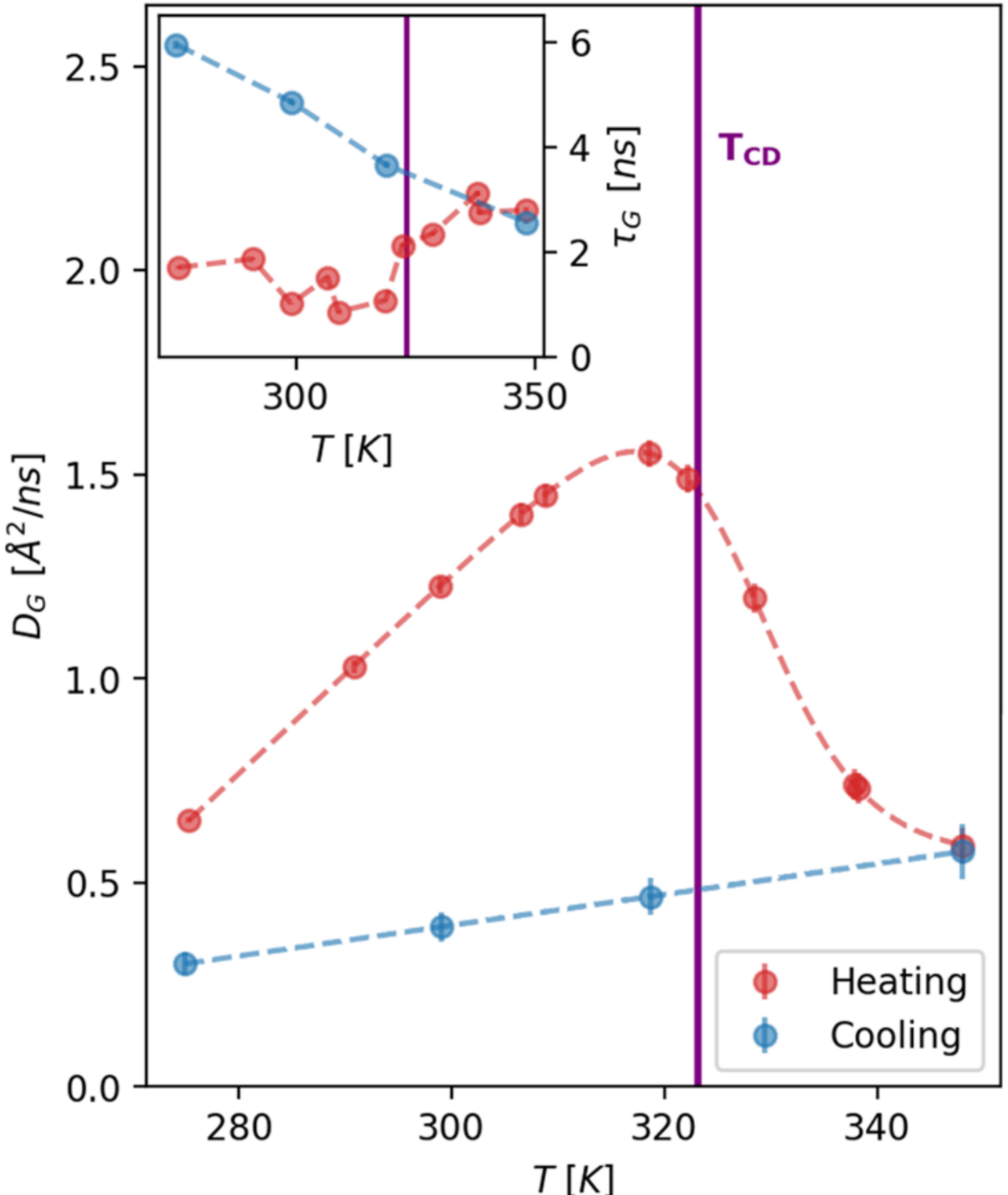


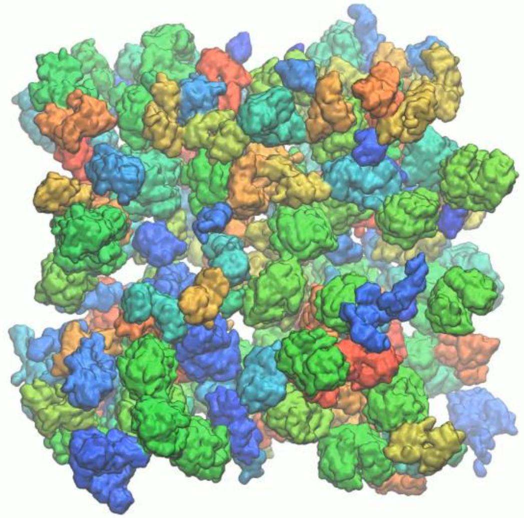
Substance	% of total dry weight	Number of molecules
Macromolecules		
Protein	55.0	2.4×10^6
RNA	20.4	
23S RNA	10.6	19,000
16S RNA	5.5	19,000
5S RNA	0.4	19,000
Transfer RNA (4S)	2.9	200,000
Messenger RNA	0.8	1,400
Phospholipid	9.1	22×10^6
Lipopolysaccharide (outer membrane)	3.4	1.2×10^6
DNA	3.1	2
Murein (cell wall)	2.5	1
Glycogen (sugar storage)	2.5	4,360
Total macromolecules	**96.1**	
Small molecules		
Metabolites, building blocks, etc.	2.9	
Inorganic ions	1.0	
Total small molecules	**3.9**	

Crowded E. coli



Global proteome dynamics





Who?

- Prof. Alessandro Paciaroni
- Dr. Lucia Comez
- Prof. Andrea Orecchini
- Prof. Francesco Sacchetti
- Prof. Caterina Petrillo
- Prof. Silvia Corezzi
- Dr. Alessandra Luchini
- Dr. Francesca Ripanti
- Dr. Sara Catalini
- Valeria Libera (PhD)
- Luca Bertini (PhD)
- Beatrice Caviglia (PhD)

Thanks!