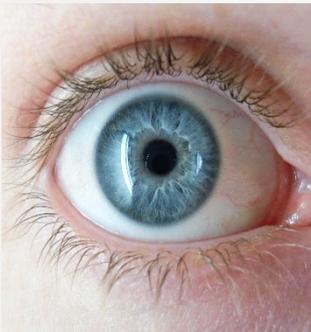


INTRODUCERE ÎN BIOINFORMATICĂ
sau
BIOINFORMATICĂ APLICATĂ ÎN BIOLOGIA
STRUCTURALĂ

Seminar I
**Dimensiuni și numere în biologia
structurală**

Niveluri de observare și unități de măsură

Observațiile în biologie pot fi la nivel:



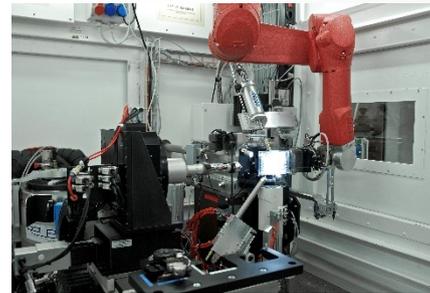
Macroscopic

Obiecte, fenomene observabile cu ochiul liber



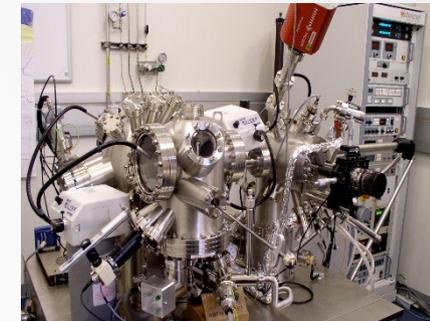
Microscopic

Obiecte, fenomene observabile cu ajutorul microscopului (optic sau electronic)



Molecular

Microscop electronic
Cristalografie raze X
Rezonanță magnetică nucleară



Atomic

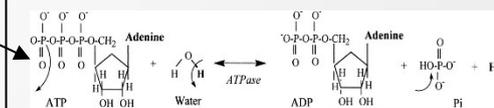
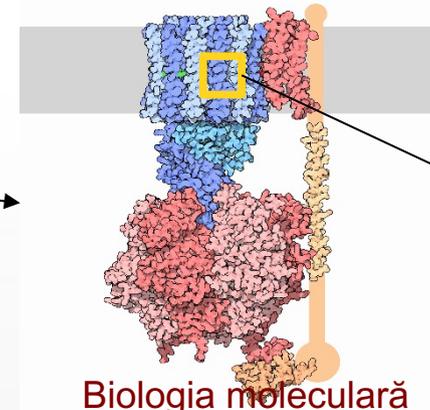
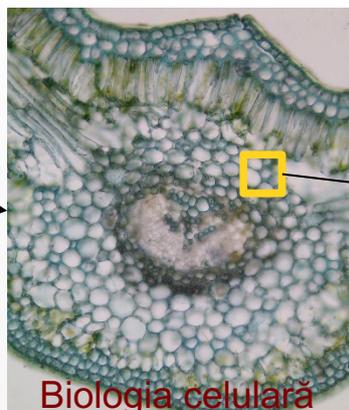
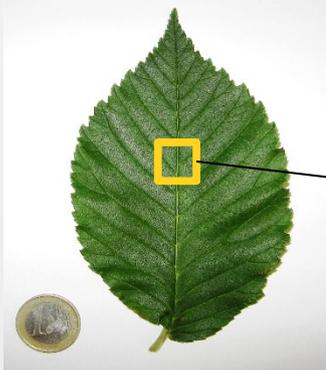
Microscop cuantic
Modelare

Metru – m
dm (10^{-1}), cm (10^{-2}), mm (10^{-3})

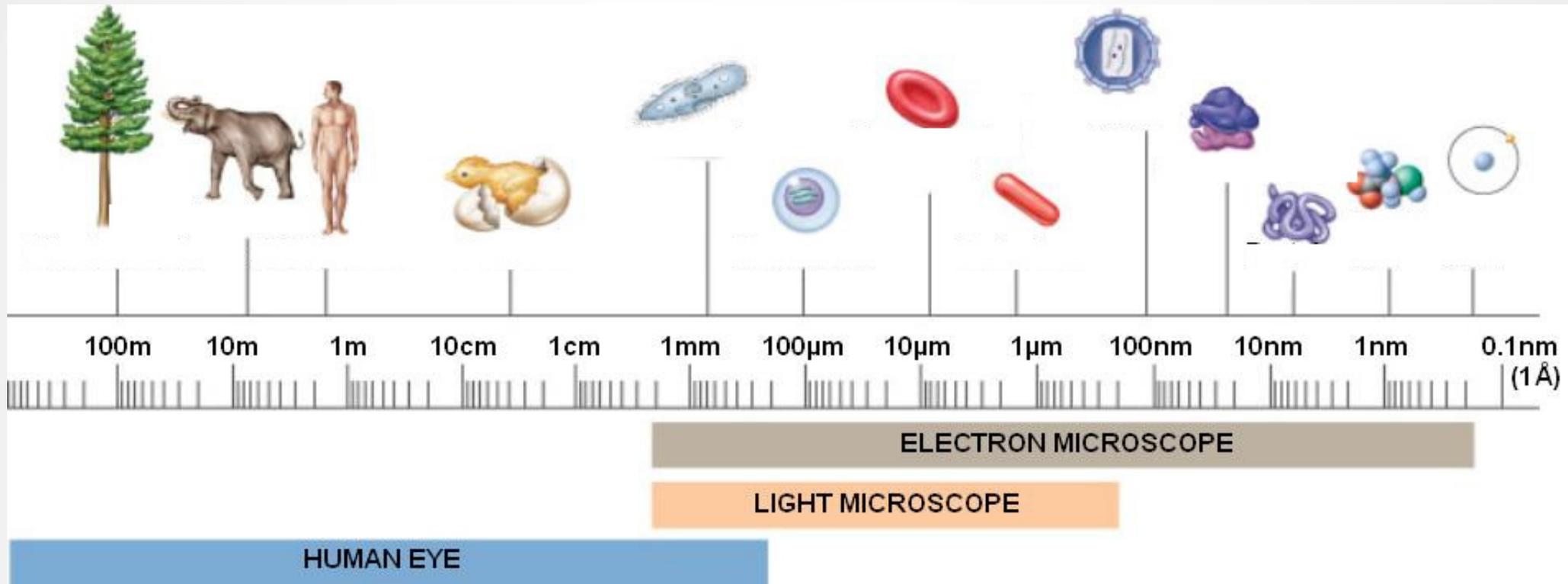
Micronul – μm 10^{-6} m

Nanometrul – nm 10^{-9} m
Angstrom-ul – Å - 10^{-10} m

Angstrom-ul – Å - 10^{-10} m
Picometrul – pm 10^{-12} m



Chimia, Biochimia

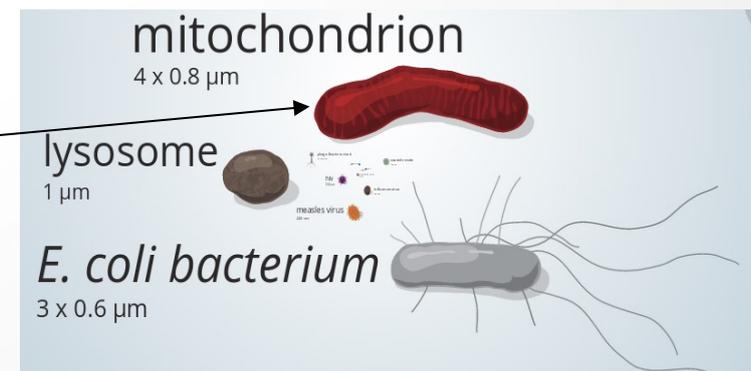
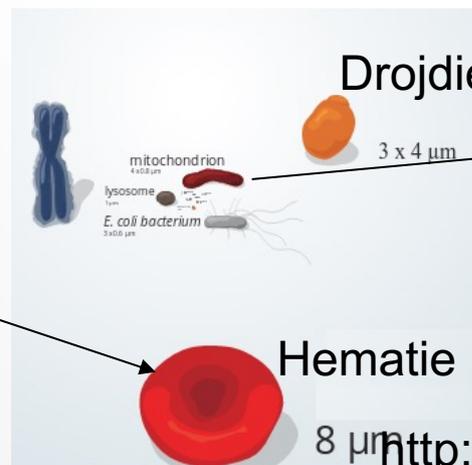
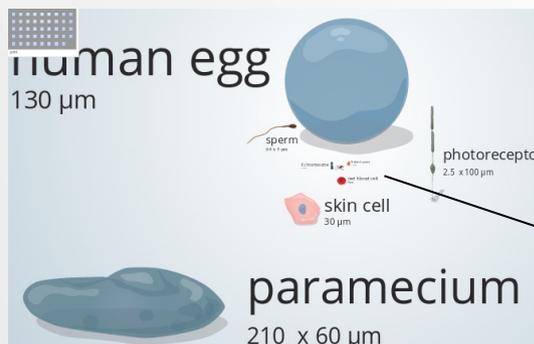


Dimensiunea celulelor

- Observabile în domeniul microscopic (microni)
- Dimensiuni variate, functie de tip (procariot, eucariot) și rol (neuroni – peste 1 m lungime)

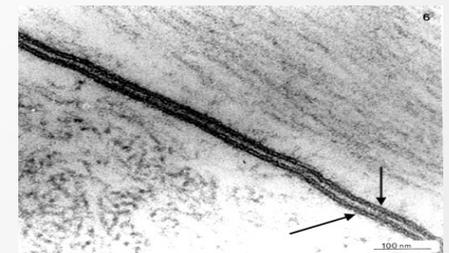
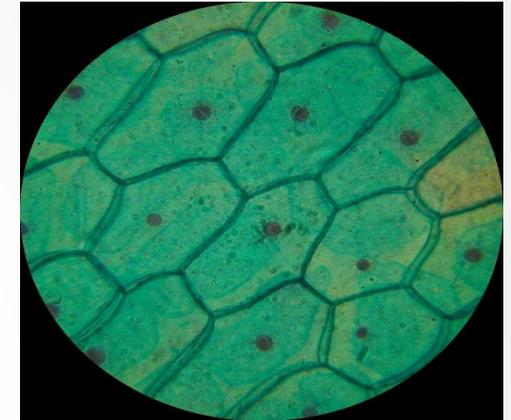
Tip celula	Bacterie	Celula vegetală	Celulă animală
Diametru (μm)	1	10-100	20
Lungime (μm)	2	-	-
Volum (μm^{-3})	0.5-5	-	2000
Greutate (fg)	0.95	-	-

Submultipli			Multipli		
Factor	Nume	Simbol	Factor	Nume	Simbol
10^{-1}	decimetru	dm	10^1	decametru	dam
10^{-2}	centimetru	cm	10^2	hectometru	hm
10^{-3}	milimetru	mm	10^3	kilometru	km
10^{-6}	micrometru (micron)	μm	10^6	megametru	Mm
10^{-9}	nanometru	nm	10^9	gigametru	Gm
10^{-12}	picometru	pm	10^{12}	terametru	Tm
10^{-15}	femtometru (fermi)	fm	10^{15}	petametru	Pm
10^{-18}	attometru	am	10^{18}	exametru	Em
10^{-21}	zeptometru	zm	10^{21}	zettametru	Zm
10^{-24}	yoctometru	ym	10^{24}	yottametru	Ym



Rapoarte dimensionale între organele celulare

	Dimensiuni (μm)	Scala Umana (m)
Celula	30	
Nucleul	2.5	
Mitocondria	6 x 1	
Cloroplast	5 x 2	
Vacuola	Variaza (15 x 20)	
Ribozom / om	0.025	1.5
Membrana celulară	0.01	
Peretele celular	0.07	



Molecular Machinery: A Tour of the Protein Data Bank

Cells build many complex molecular machines that perform the biological jobs needed for life. Some of these machines are molecular scissors that cut food into digestible pieces. Others then use these pieces to build new molecules when cells grow or tissues need to be repaired. Some molecular machines form sturdy beams that support cells, and others are motors that use energy to crawl along these beams. Some recognize attackers and mobilize defenses against infection.

Researchers around the world are studying these molecules at the atomic level. These 3D structures are freely available at the Protein Data Bank (PDB), the central storehouse of biomolecular structures. A few examples from the ~100,000 structures held in the PDB are shown here at a magnification of about 3,500,000 times, with each atom represented as a small sphere. The enormous range of molecular sizes is illustrated here, from the water molecule (H₂O) with only three atoms (shown at the left) to the ribosomal subunits with hundreds of thousands of atoms.

Digestive Enzymes: breaking food into small nutrient molecules

1. Amylase 1am1
2. Phospholipase 1lpoe
4. Lysozyme 1lzl
5. Pepsin 5pep
6. Trypsin 2tpe
7. Carboxypeptidase 3cpa
8. Ribonuclease 5rsa

Blood Plasma Proteins: transporting nutrients and defending against injury

9. Factor X 1xka, 1xod
10. Thrombin 1tpb
11. Fibrin 1fmj, 2baf
12. Serum Albumin 1e7i

Viruses and Antibodies: engaging in constant battle in the bloodstream

13. Antibody 1igt
14. Rhinovirus 4rhv

Hormones: carrying molecular messages through blood

15. Glucagon 1gcg
16. Insulin 2ihu
17. Epidermal Growth Factor 1egf

Channels, Pumps and Receptors: getting back and forth across the membrane

18. Ras Protein 5p2l
19. Beta-Adrenergic Receptor/Cs Protein 3an6
20. Acetylcholine Receptor 2b9g
21. Epidermal Growth Factor Receptor 1ivo, 2jwa, 2g56
22. Rhodopsin 1rh8
23. Polychromatin 3p6l
24. Potassium Channel 3lat
25. Calcium Pump 1s4d
26. Cyclooxygenase 1prh

Photosynthesis: harvesting energy from the sun

27. Photosystem II 1ssi
28. Light-harvesting Complex 1mvt
29. Photosynthetic Reaction Center 1prc

Enzymes: cutting and joining the molecules of life

30. Fatty Acid Synthase 2uiv, 2uvc
31. RuBisCo Ribulose Biphosphate Carboxylase/Oxygenase 1rbc
41. Green Fluorescent Protein 1gfl
42. Luciferase 2d1s
43. Glutamine Synthase 2gls
44. Alcohol Dehydrogenase 2ahx
45. Dihydrofolate Reductase 1dhf
46. Nitrogenase 1niz
47. Leucine Aminopeptidase 1lap
48. beta-Lactamase 4blm
49. Catalase 1cqw
50. Thymidylate Synthase 2tsc
51. Tryptophan Synthase 1wsv
52. Aspartate Carboxyltransferase 4att
53. Hexokinase 1djk
54. Phosphoglucose isomerase 1hox
55. Phosphofruktokinase 4pki
56. Aldolase 4ald
57. Inosophosphate isomerase 2ipi
58. Glyceraldehyde-3-phosphate Dehydrogenase 3gpd
59. Phosphoglycerate Kinase 3pgk
60. Phosphoglycerate Mutase 3pgm
61. Endolase 5entl
62. Pyruvate Kinase 1a5w

Scale:
1nm 5nm 10nm
1nm (nanometer) = 10⁻⁹ millimeters

Energy Production: powering the processes of the cell

30. Cytochrome c Oxidase (Complex IV) 1oxa
31. Cytochrome c 3cyt
32. Cytochrome bc₁ (Complex III) 1bcy
33. Succinate Dehydrogenase (Complex II) 1hck
34. NADH-Quinone Oxidoreductase (Complex I) 3nbs, 3nfo
35. ATP Synthase 1a79, 1c17, 1l2p, 2a7u
36. Myoglobin 1mbd
37. Hemoglobin 4hhb

Storage: containing nutrients for future consumption

38. Ferritin 1ftr

Infrastructure: supporting and moving cells

63. Actin 1mbq
64. Myosin 1mbq
65. Microtubule Tub
66. Collagen 1blv (for left)

Protein Synthesis: building new molecular machines

67. Transfer RNA 4tra
68. ValM tRNA Synthetase 1gax
69. Threonyl tRNA Synthetase 1tq6
70. Glutamyl tRNA Synthetase 1euq
71. Isoleucyl tRNA Synthetase 1lly
72. Phenylalanyl tRNA Synthetase 1eiy
73. Aspartyl tRNA Synthetase 1asy
74. Ribosome 1j3e, 1j3z
75. Elongation factor uRNA 1ttt
76. Elongation factor G 1dar
77. Elongation factor Is and Iu 1efu
78. Prokatin 1pk
79. Chaperonin GroEL/ES 1oon
80. Proline cis/trans isomerase 2cpl
81. Heat Shock Protein 1ap90 2c9g
82. Proteasome 4btv
83. Ubiquitin 1ubq

DNA: storing and reading genetic information

84. DNA 1bna
85. Restriction Endonuclease EcoRI 1eri
86. DNA Helicase 1hez
87. Topoisomerase 1a36
88. RNA Polymerase 2e2i
89. Lac Repressor 1lra, 1ela
90. Catabolite Gene Activator Protein 1cga
91. TATA-binding Protein/ Transcription Factor IIB 1tas
92. DNA Helicase 4esv
93. DNA Polymerase 1tau
94. Nucleosome 1aci
95. HU Protein 1p5l
96. Single-stranded DNA-binding Protein 3a5u

Rapoarte dimensionale între molecule

	Dimensiuni medii (nm)	Scala Umana (m)
H ₂ O	0.28	
Glucosa (liniară)	1.5	
DNA (diametru/grosime)	2.04	
Proteina (medie) / om	2	1,5
Ribozom	21	
Membrana celulară (grosime)	10	
Peretele celular (grosime)	70	
Mitocondria	500	
Celula	30000	

