



Cell and Molecular

IF3211 Domain Specific Computation

School of Electrical Engineering and Informatics ITB

Content

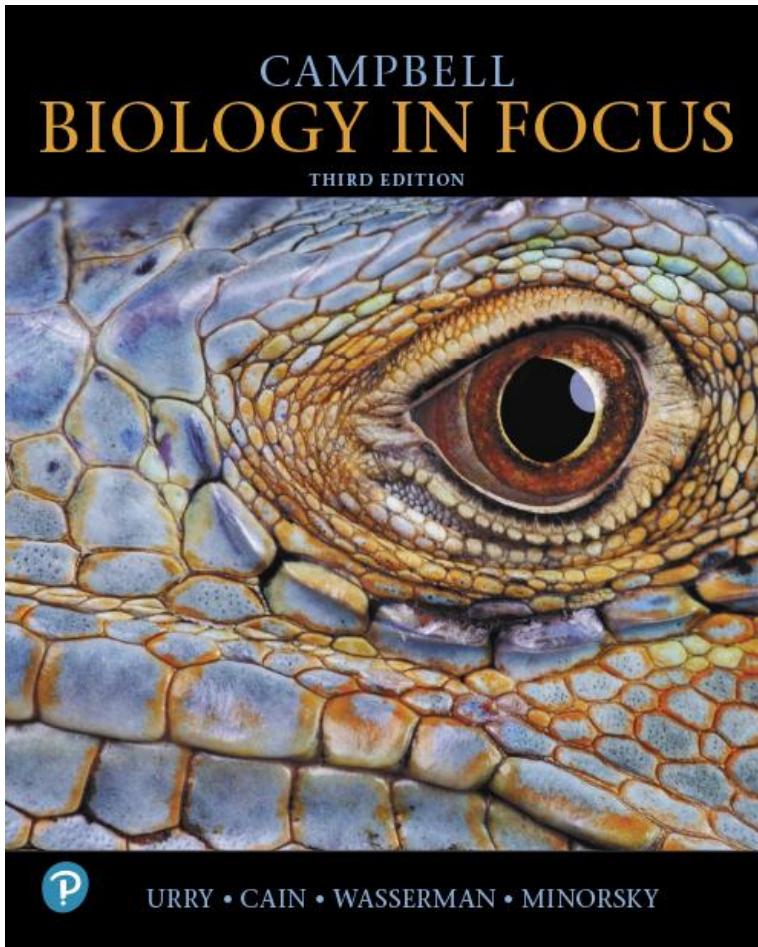
- Cell Molecular
- Cell Structure
- Cell Function
- Cell biology and application



Cell Molecular

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Chapter 4

A Tour of the Cell

Lecture Presentations by
Kathleen Fitzpatrick and Nicole Tunbridge,
Simon Fraser University

Overview: The Fundamental Units of Life

- All organisms are made of cells
- The cell is the simplest collection of matter that can be alive
- All cells are related by their descent from earlier cells
- Though cells can differ substantially from one another, they share common features

Concept 4.1: Biologists Use Microscopes and the Tools of Biochemistry to Study Cells

- Most cells are too small to be seen by the unaided eye

Figure 4.2

The Size Range of Cells

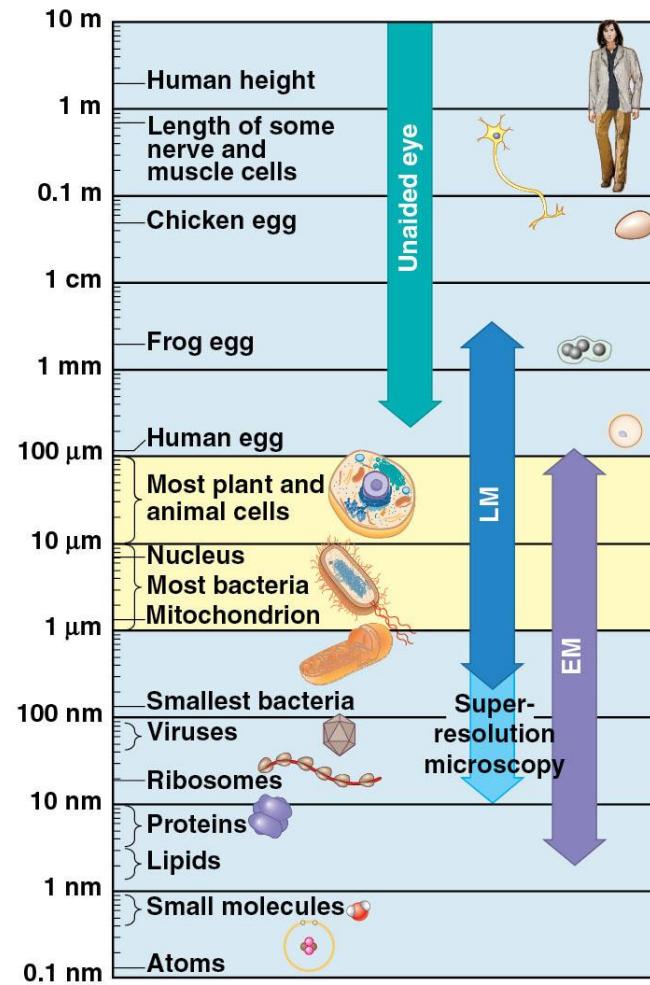
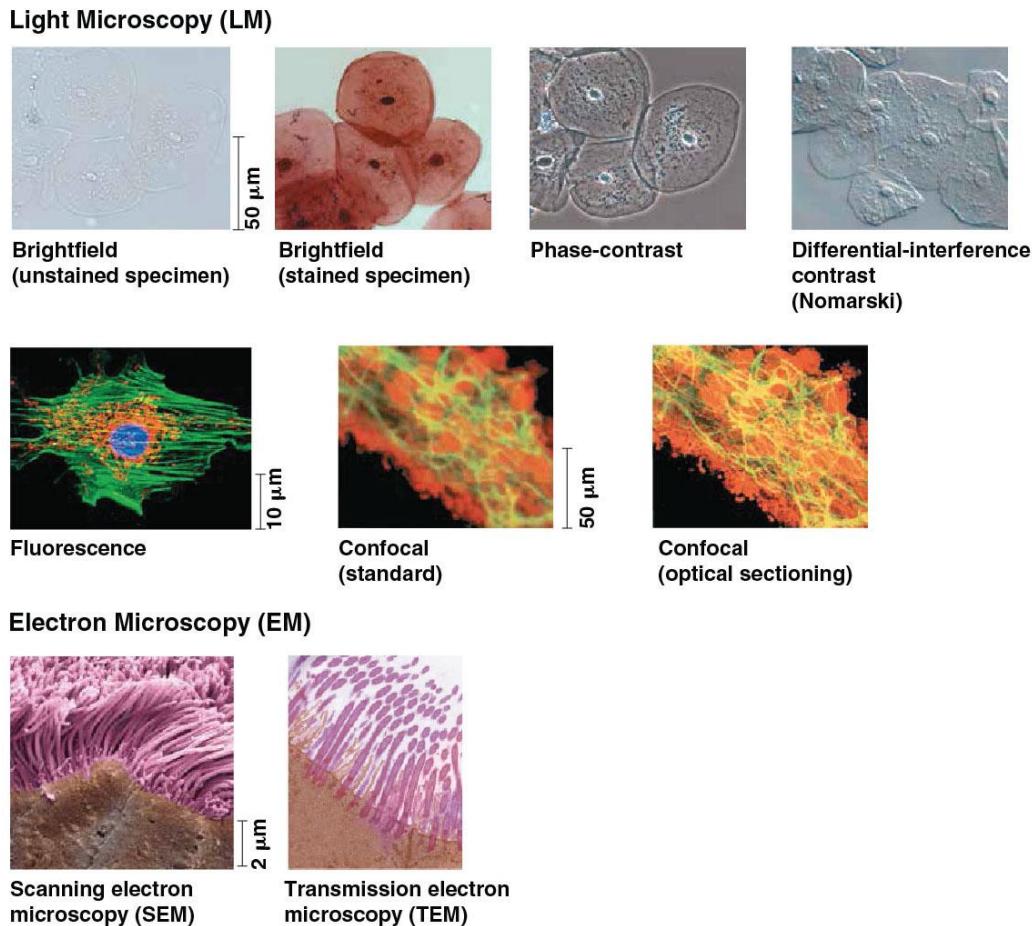


Figure 4.3

Exploring Microscopy



Concept 4.2: Eukaryotic Cells Have Internal Membranes That Compartmentalize Their Functions

- The basic structural and functional unit of every organism is one of two types of cells: prokaryotic or eukaryotic
- Organisms of the domains Bacteria and Archaea consist of prokaryotic cells
- Protists, fungi, animals, and plants all consist of eukaryotic cells

Comparing Prokaryotic and Eukaryotic Cells (1 of 5)

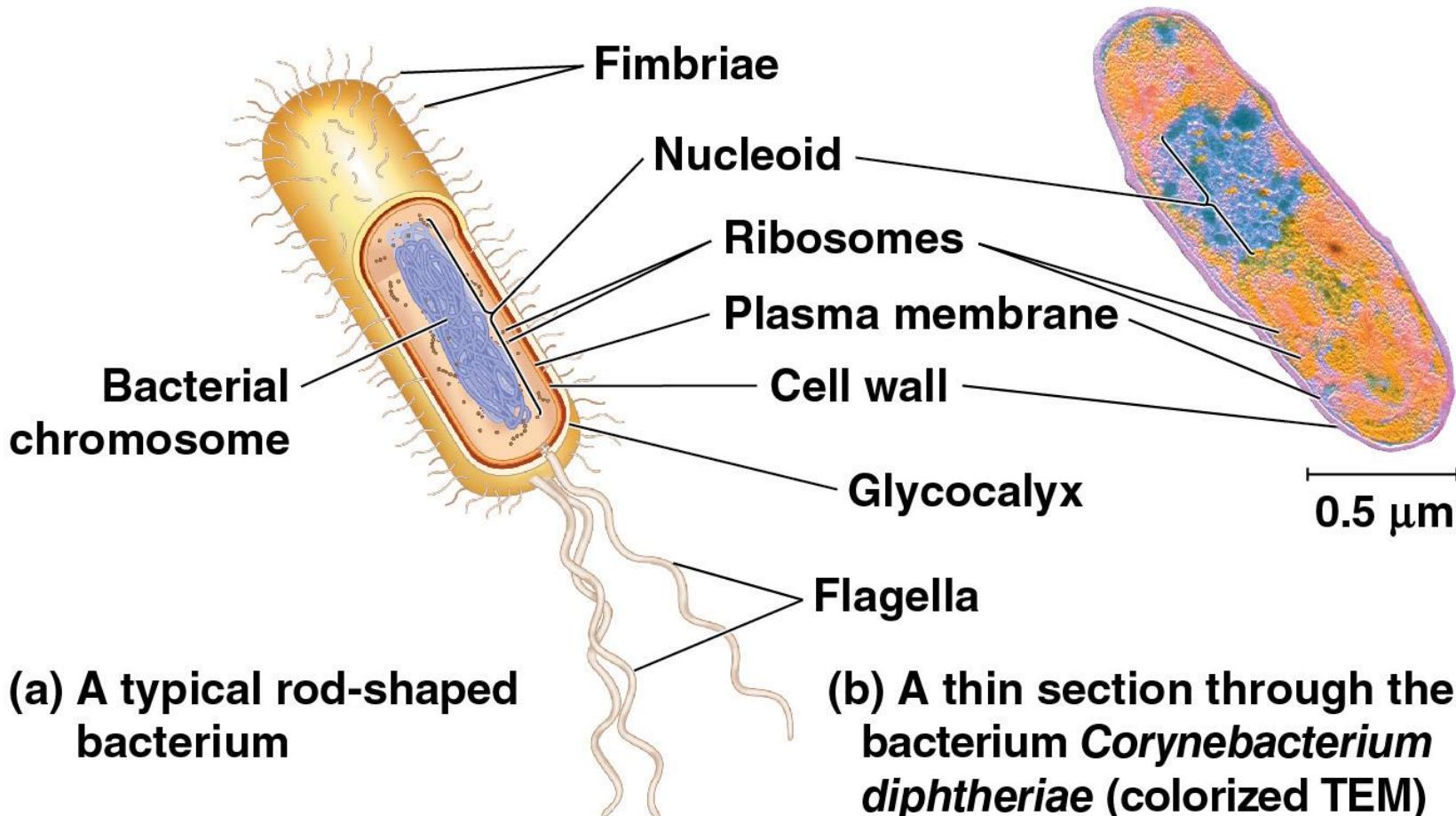
- Basic features of all cells
 - Plasma membrane
 - Semifluid substance called **cytosol**
 - Chromosomes (carry genes)
 - Ribosomes (make proteins)

Comparing Prokaryotic and Eukaryotic Cells (2 of 5)

- In a **eukaryotic cell** most of the DNA is in the nucleus, an organelle that is bounded by a double membrane
- **Prokaryotic cells** are characterized by having
 - No nucleus
 - DNA in an unenclosed region called the **nucleoid**
 - No membrane-enclosed organelles
- Both types of cells contain **cytoplasm** bounded by the plasma membrane

Figure 4.4

A Prokaryotic Cell



Comparing Prokaryotic and Eukaryotic Cells (3 of 5)

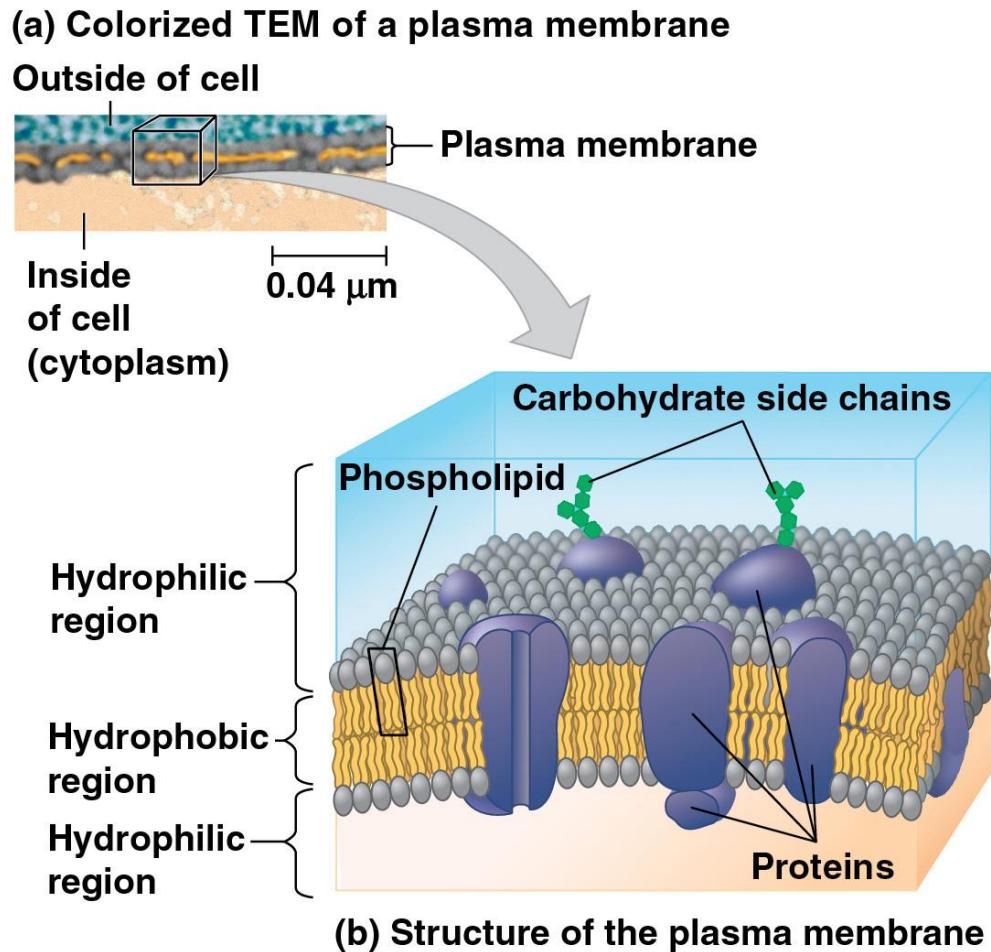
- Eukaryotic cells are generally much larger than prokaryotic cells
- Typical bacteria are $1\text{--}5 \mu\text{m}$ in diameter
- Eukaryotic cells are typically $10\text{--}100 \mu\text{m}$ in diameter

Comparing Prokaryotic and Eukaryotic Cells (4 of 5)

- The **plasma membrane** is a selective barrier that allows passage of oxygen, nutrients, and waste to service the volume of every cell
- The general structure of a biological membrane is a double layer of phospholipids

Figure 4.5

The Plasma Membrane



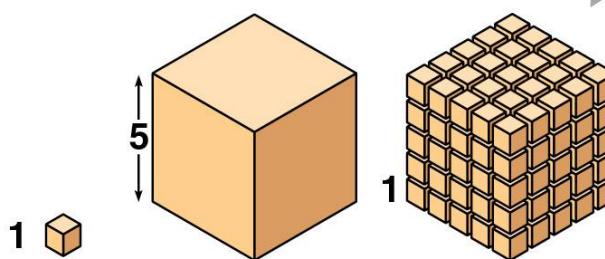
Comparing Prokaryotic and Eukaryotic Cells (5 of 5)

- Metabolic requirements set upper limits on the size of cells
- The ratio of surface area to volume of a cell is critical
- As cell size increases, the surface area increases proportional to the square of the linear dimension, which volume increases proportional to the cube of the linear dimension
- Small cells have a greater surface area to volume ratio

Figure 4.6

Geometric Relationships Between Surface Area and Volume

Surface area increases while total volume remains constant



Total surface area [(height × width of 1 side) × 6 sides × number of cells]	6 units ²	150 units ²	750 units ²
Total volume [(height × width × length of 1 cell) × number of cells]	1 unit ³	125 units ³	125 units ³
Surface area-to-volume ratio [surface area ÷ volume]	6	1.2	6

Figure 4.7 (1 of 2)

Exploring Eukaryotic Cells

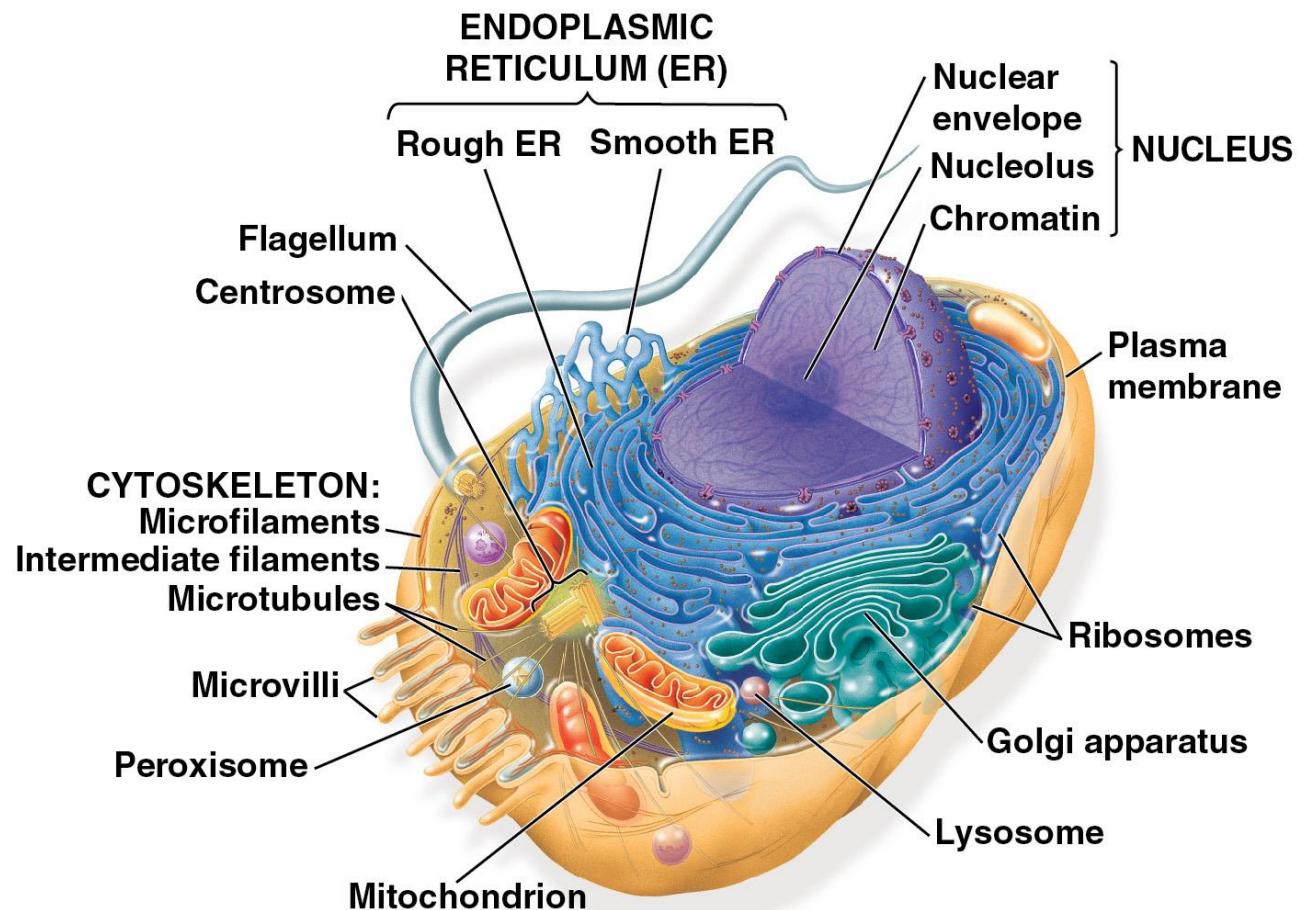
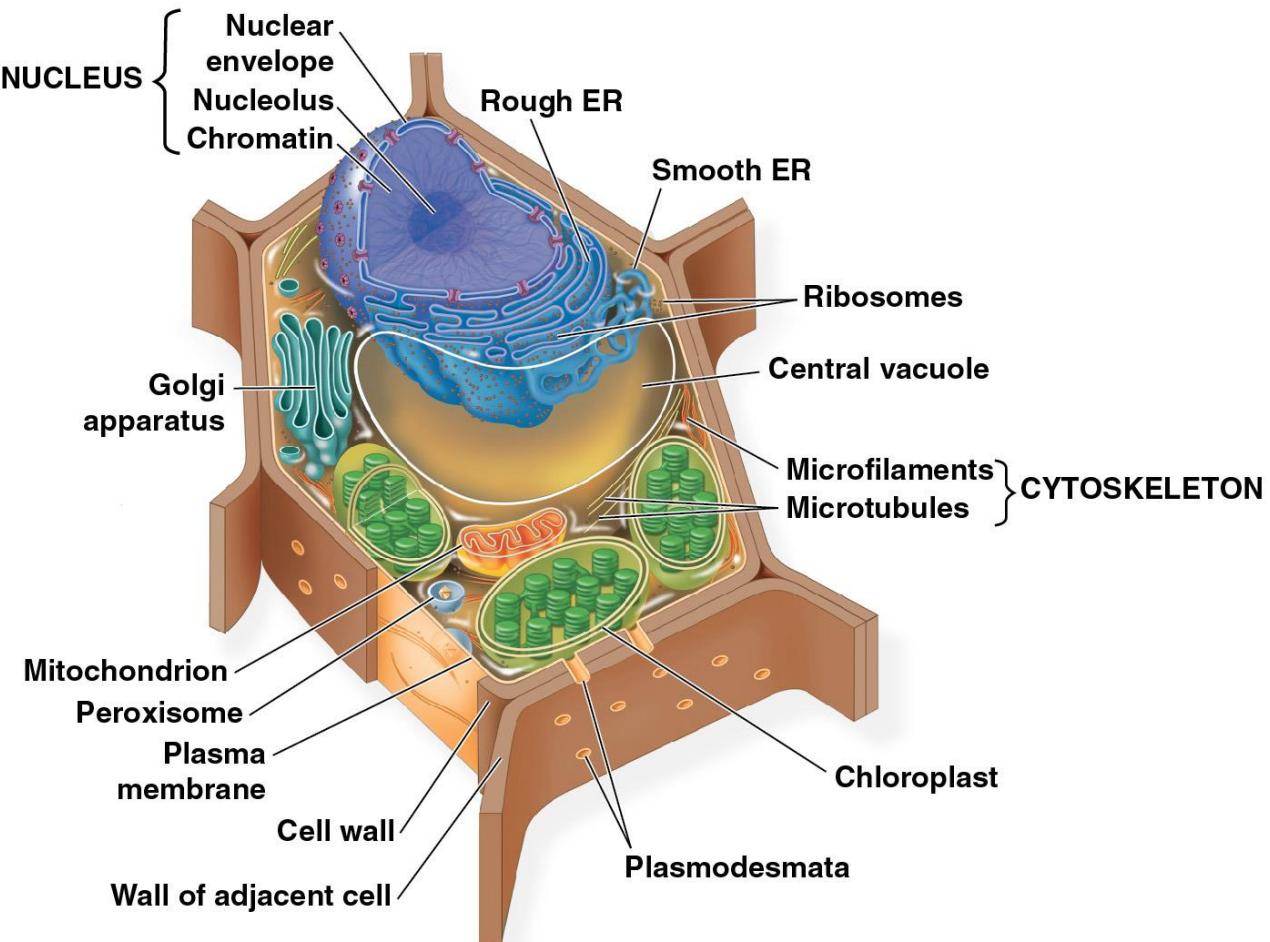


Figure 4.7 (2 of 2)

Exploring Eukaryotic Cells



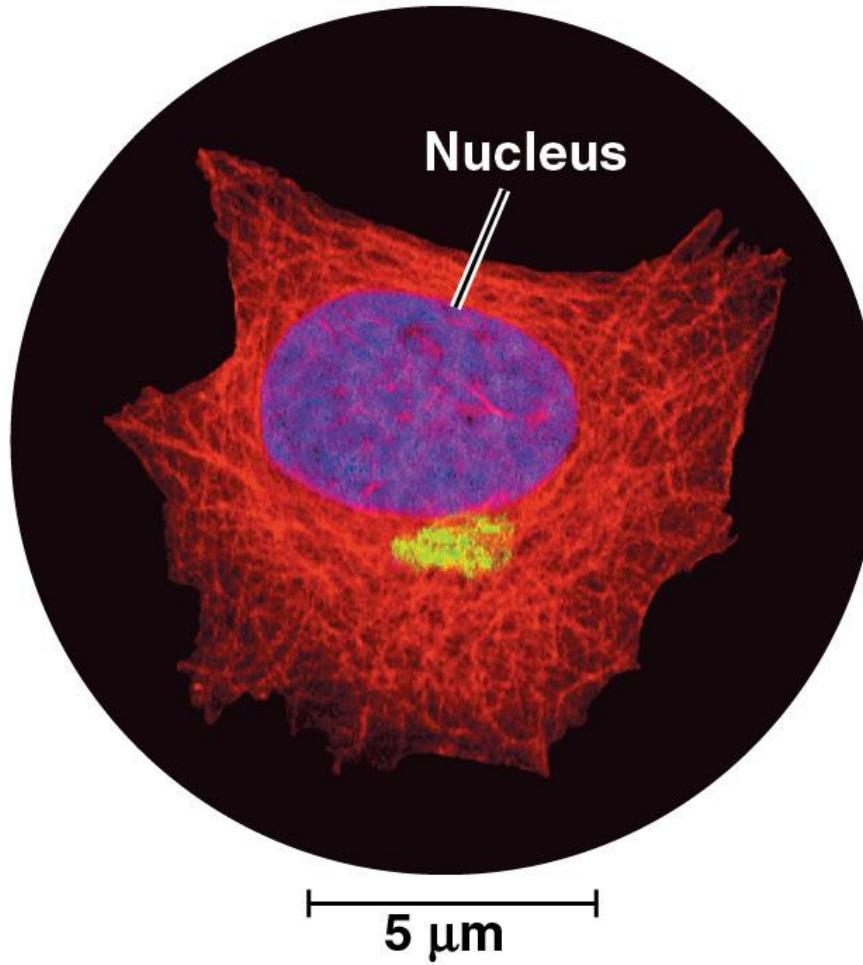
Concept 4.3: The Eukaryotic Cell's Genetic Instructions Are Housed in the Nucleus and Carried out by the Ribosomes

- The nucleus contains most of the DNA in a eukaryotic cell
- Ribosomes use the information from the DNA to make proteins

The Nucleus: Information Central (1 of 3)

- The **nucleus** contains most of the cell's genes and is usually the most conspicuous organelle
- The **nuclear envelope** encloses the nucleus, separating it from the cytoplasm
- The nuclear membrane is a double membrane; each membrane consists of a lipid bilayer

Figure: Nucleus

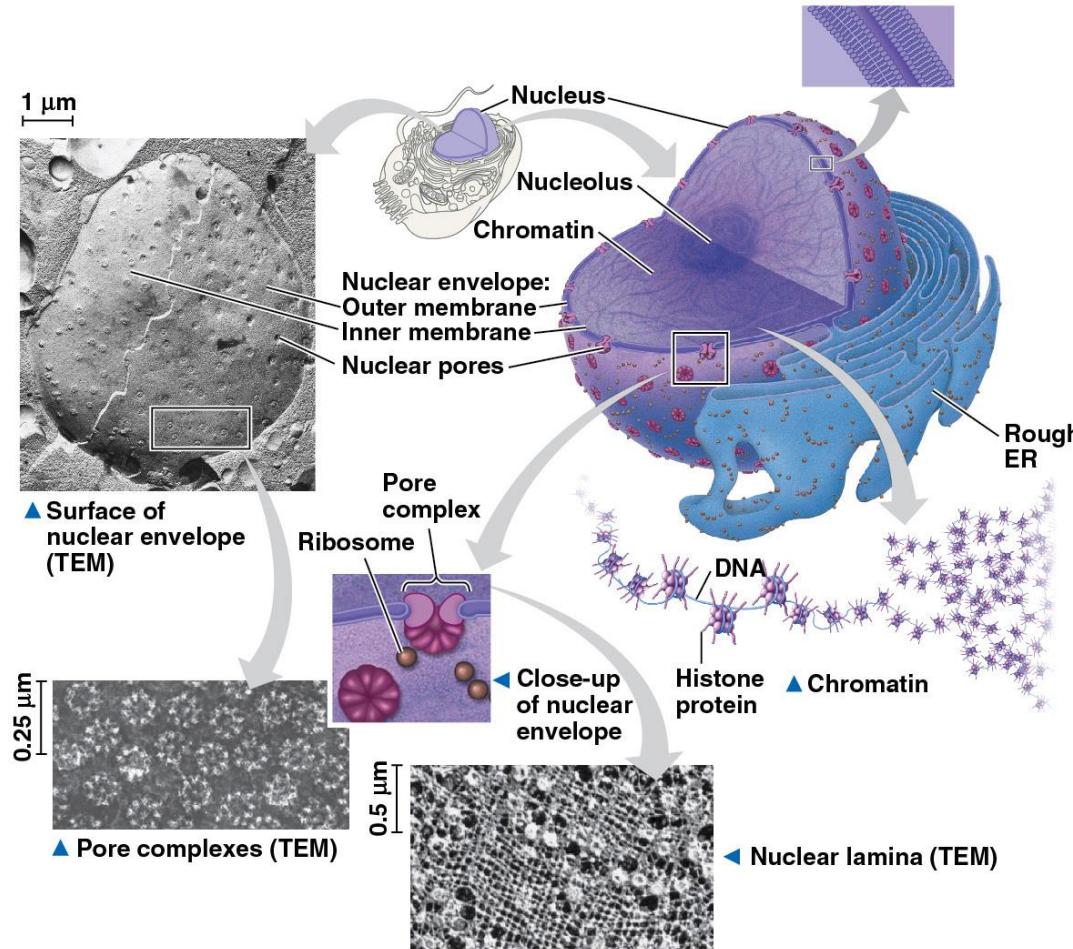


The Nucleus: Information Central (2 of 3)

- Nuclear pores regulate the entry and exit of molecules
- The shape of the nucleus is maintained by the **nuclear lamina**, which is composed of protein filaments

Figure 4.8

The Nucleus and Its Envelope



The Nucleus: Information Central (3 of 3)

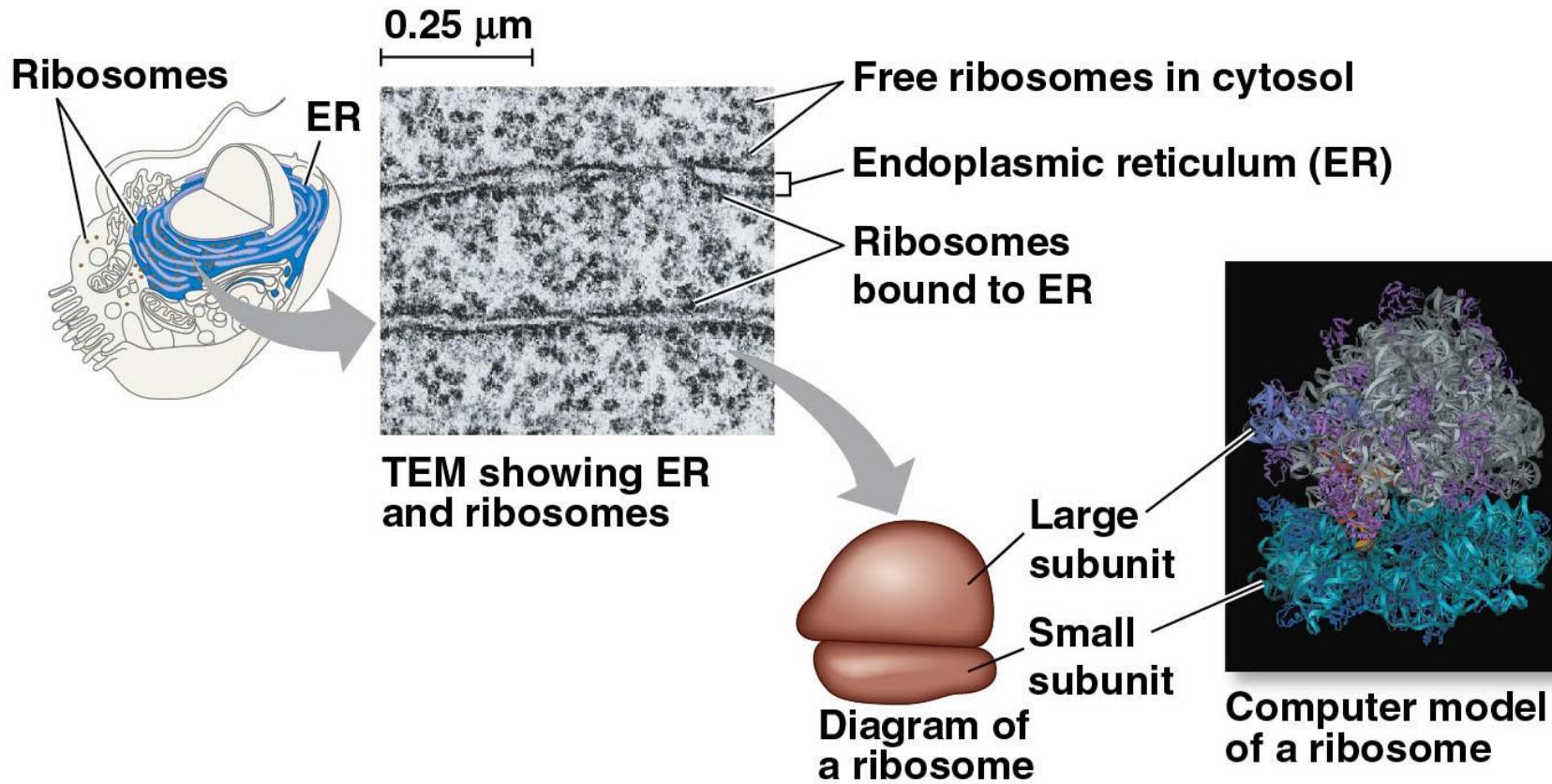
- In the nucleus, DNA is organized into discrete units called **chromosomes**
- Each chromosome is one long DNA molecule associated with proteins
- The DNA and proteins of chromosomes together are called **chromatin**
- Chromatin condenses to form discrete chromosomes as a cell prepares to divide
- The **nucleolus** is located within the nucleus and is the site of ribosomal RNA (rRNA) synthesis

Ribosomes: Protein Factories

- **Ribosomes** are complexes of ribosomal RNA and protein
- Ribosomes carry out protein synthesis in two locations
 - In the cytosol (free ribosomes)
 - On the outside of the endoplasmic reticulum or the nuclear envelope (bound ribosomes)

Figure 4.9

Ribosomes



Concept 4.4: The Endomembrane System Regulates Protein Traffic and Performs Metabolic Functions

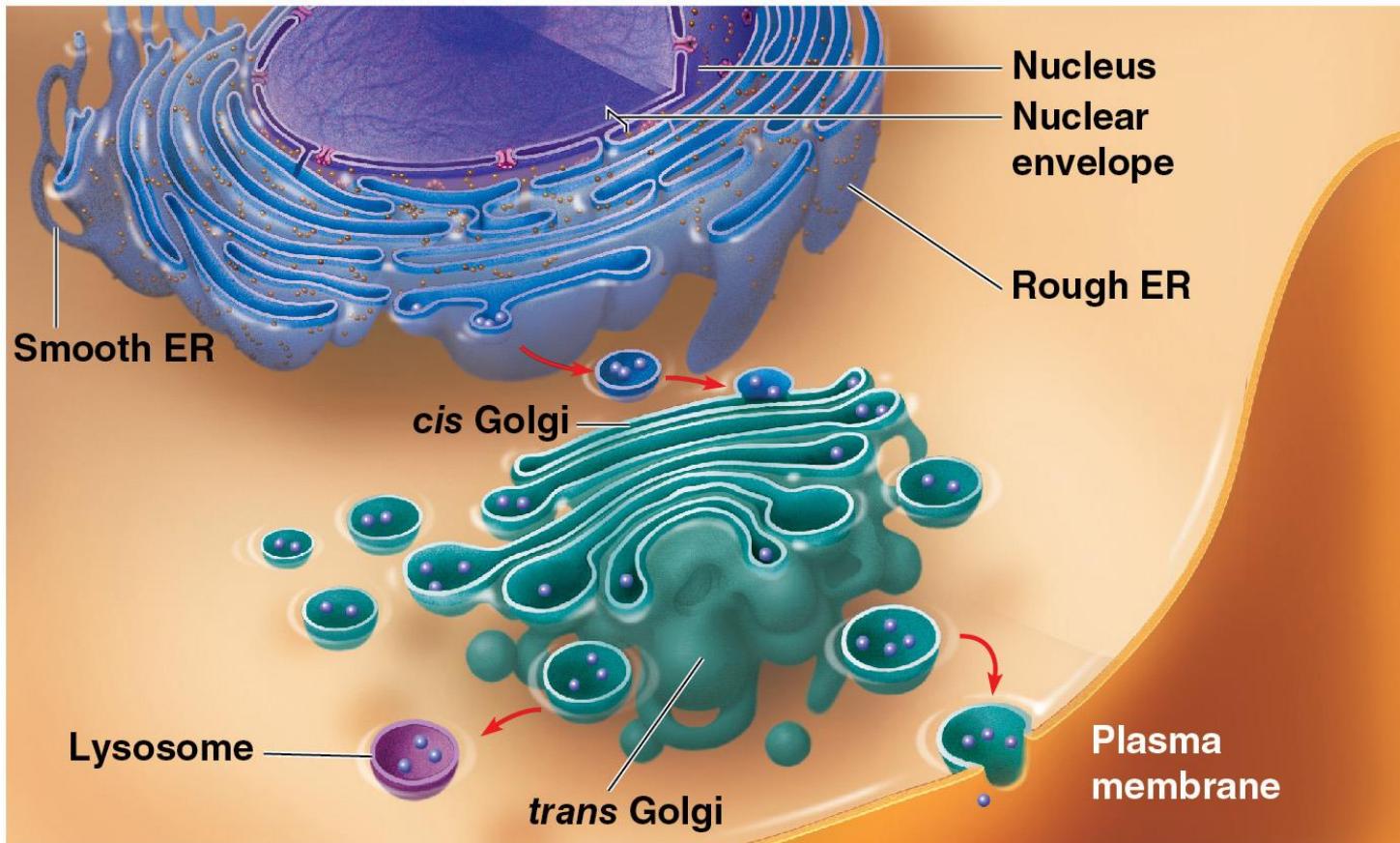
- Components of the **endomembrane system**
 - Nuclear envelope
 - Endoplasmic reticulum
 - Golgi apparatus
 - Lysosomes
 - Vacuoles
 - Plasma membrane
- These components are either continuous or connected through transfer by **vesicles**

The Endomembrane System: A Review

- The endomembrane system is a complex and dynamic player in the cell's compartmental organization

Figure 4.15

Review: Relationships Among Organelles of the Endomembrane System



Concept 4.5: Mitochondria and Chloroplasts Change Energy from One Form to Another

- **Mitochondria** are the sites of cellular respiration, a metabolic process that uses oxygen to generate ATP
- **Chloroplasts**, found in plants and algae, are the sites of photosynthesis
- Peroxisomes are oxidative organelles

The Evolutionary Origins of Mitochondria and Chloroplasts (1 of 2)

- Mitochondria and chloroplasts display the following similarities with bacteria that led to the **endosymbiont theory**:
 - Enveloped by a double membrane
 - Contain ribosomes and multiple circular DNA molecules
 - Grow and reproduce somewhat independently in cells

The Evolutionary Origins of Mitochondria and Chloroplasts (2 of 2)

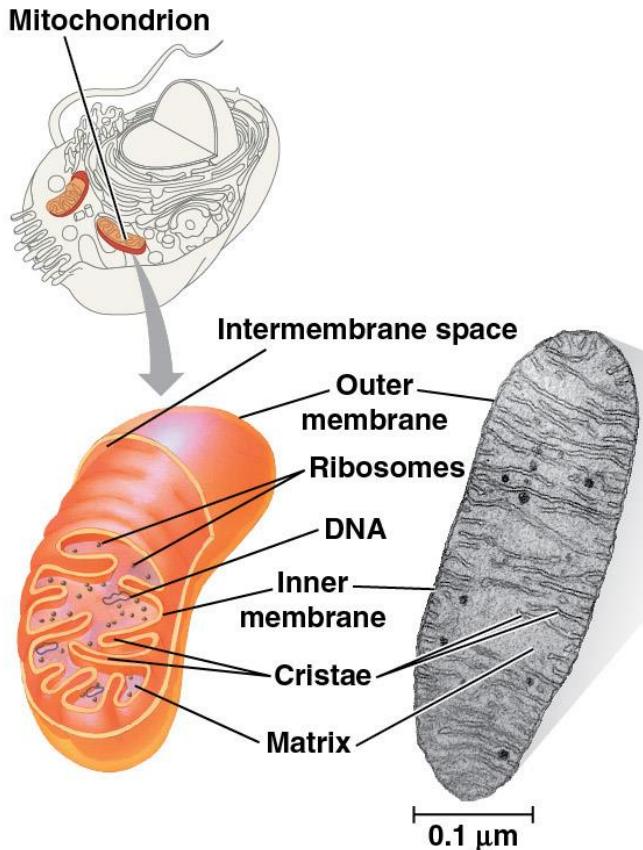
- The endosymbiont theory is widely accepted:
 - An early ancestor of eukaryotic cells engulfed a nonphotosynthetic prokaryotic cell, which formed a relationship with its host
 - The host cell and endosymbiont merged into a single organism, a eukaryotic cell with a mitochondrion
 - At least one of these cells may have then taken up a photosynthetic prokaryote, becoming the ancestor of cells that contain chloroplasts

Mitochondria: Chemical Energy Conversion

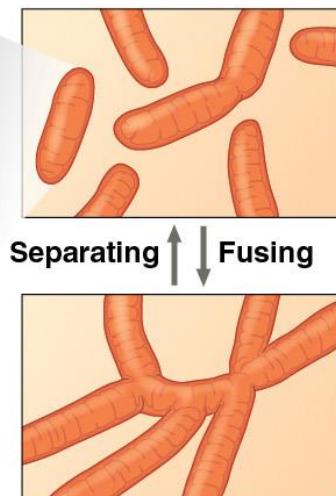
- Mitochondria are in nearly all eukaryotic cells
- They have a smooth outer membrane and an inner membrane folded into **cristae**
- The inner membrane creates two compartments: the intermembrane space and the **mitochondrial matrix**
- Some metabolic steps of cellular respiration are catalyzed in the mitochondrial matrix
- Cristae present a large surface area for enzymes that synthesize ATP

Figure 4.17

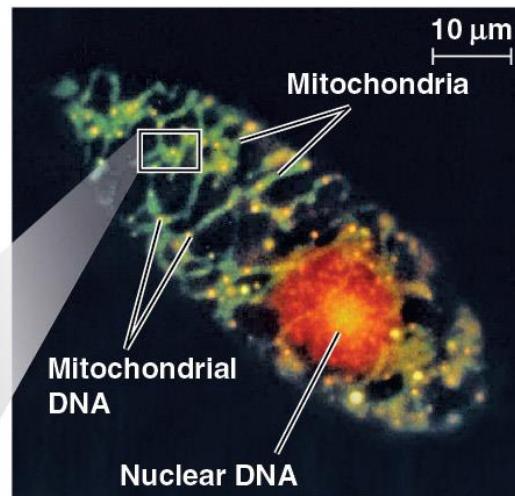
The Mitochondrion, Site of Cellular Respiration



(a) Diagram and TEM of mitochondrion



(b) Dynamic nature of mitochondrial networks



(c) Network of mitochondria in *Euglena* (LM)

Chloroplasts: Capture of Light Energy (1 of 2)

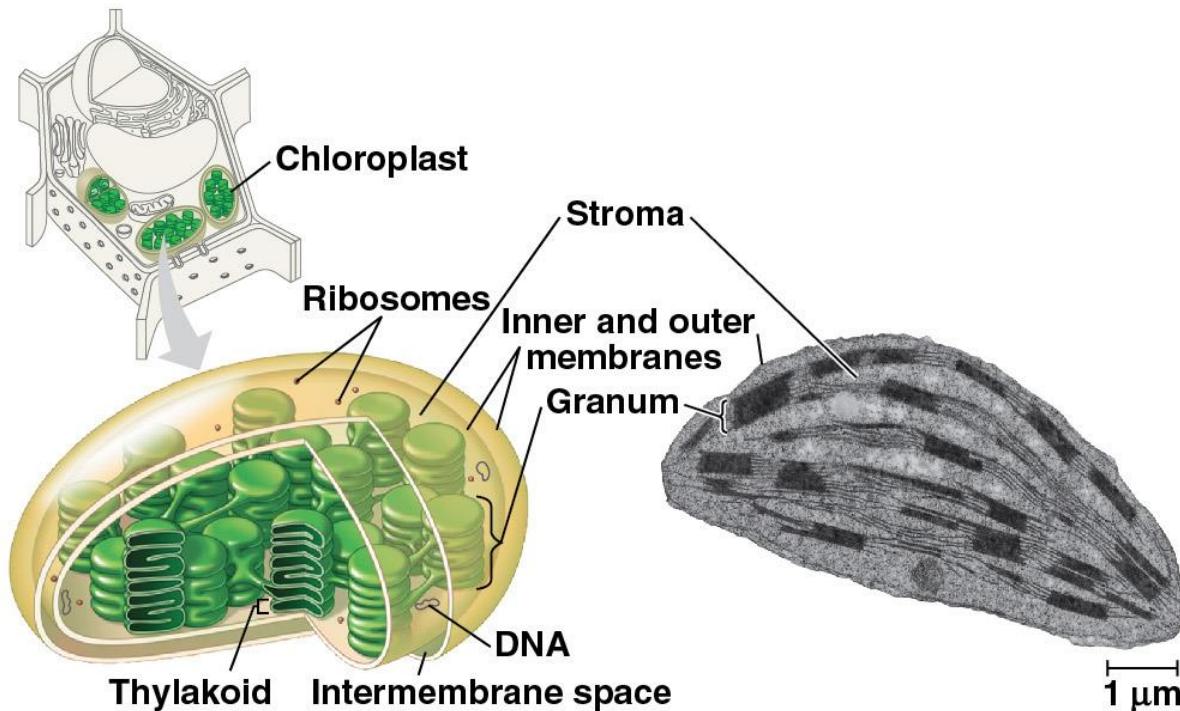
- Chloroplasts contain the green pigment chlorophyll, as well as enzymes and other molecules that function in photosynthesis
- They are found in leaves and other green organs of plants and in algae

Chloroplasts: Capture of Light Energy (2 of 2)

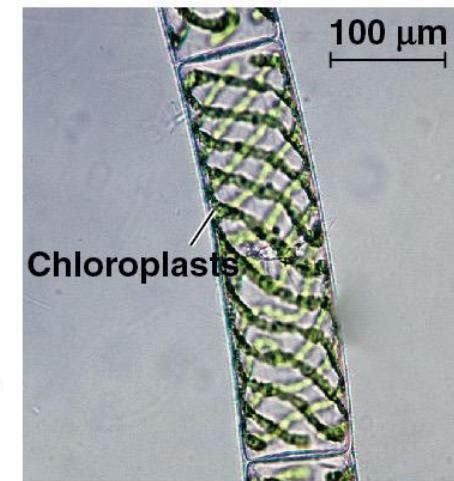
- Chloroplast structure includes
 - **Thylakoids**, membranous sacs, stacked to form a **grana**
 - **Stroma**, the internal fluid
- The chloroplast is one of a group of plant organelles called **plastids**

Figure 4.18

The Chloroplast, Site of Photosynthesis



(a) Diagram and TEM of chloroplast

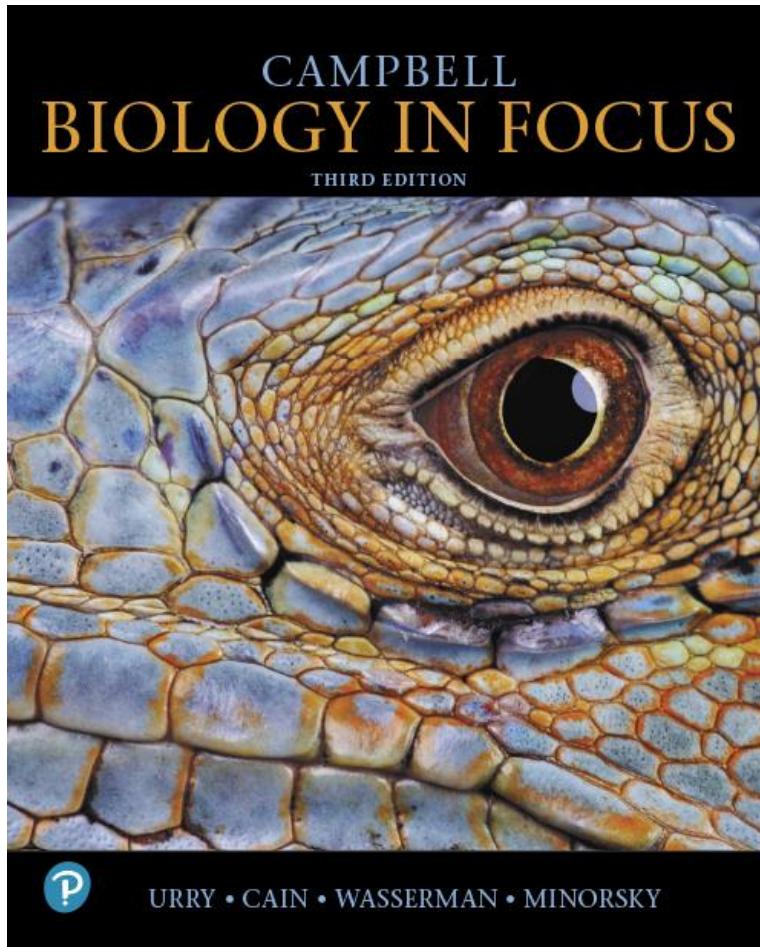


(b) Chloroplasts in an algal cell

Cell Structure

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Chapter 5

Membrane Transport and Cell
Signaling

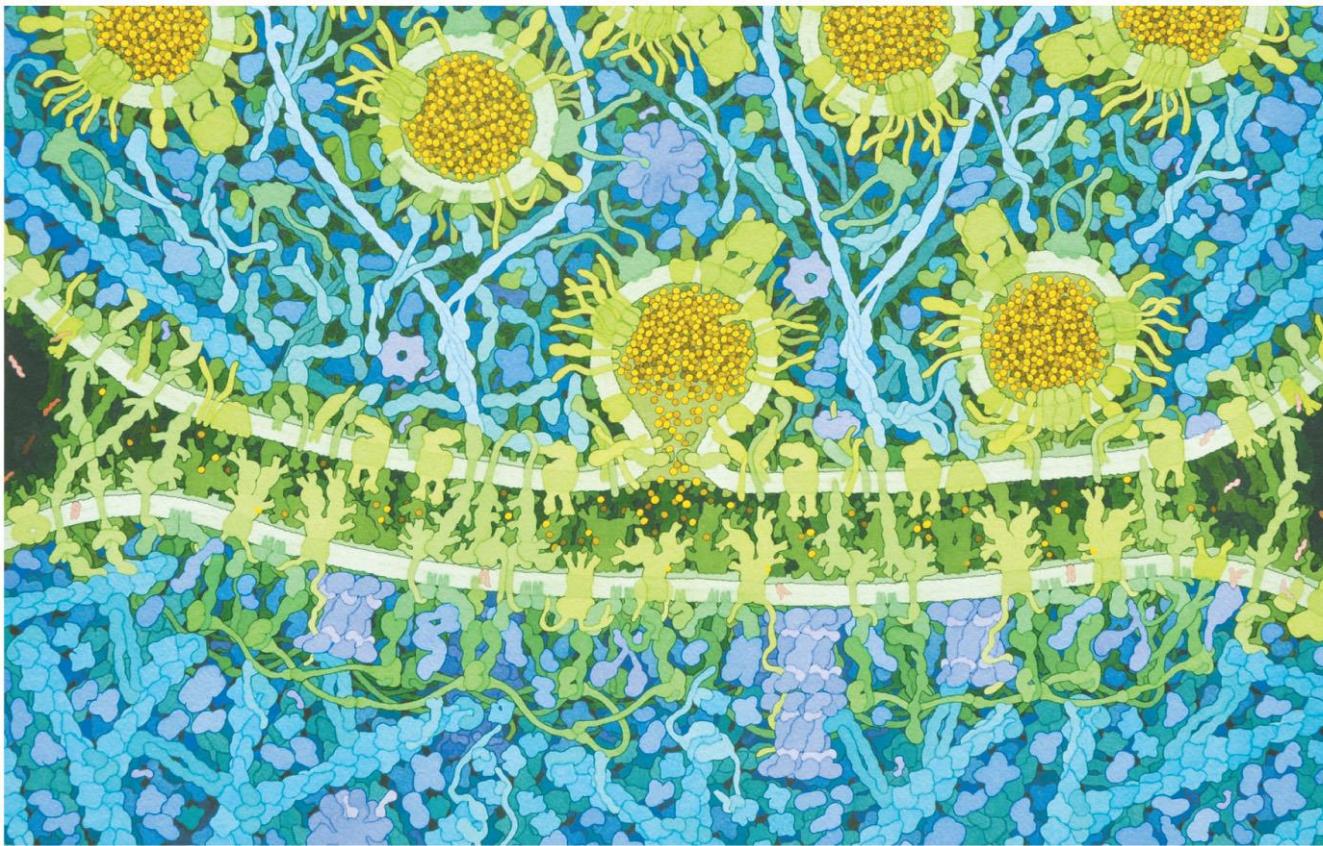
Lecture Presentations by
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Simon Fraser University

Overview: Life at the Edge

- The plasma membrane separates the living cell from its surroundings
- The plasma membrane exhibits **selective permeability**, allowing some substances to cross it more easily than others

Figure 5.1

How Do Brain Cells Communicate with Each Other When You Are Learning?



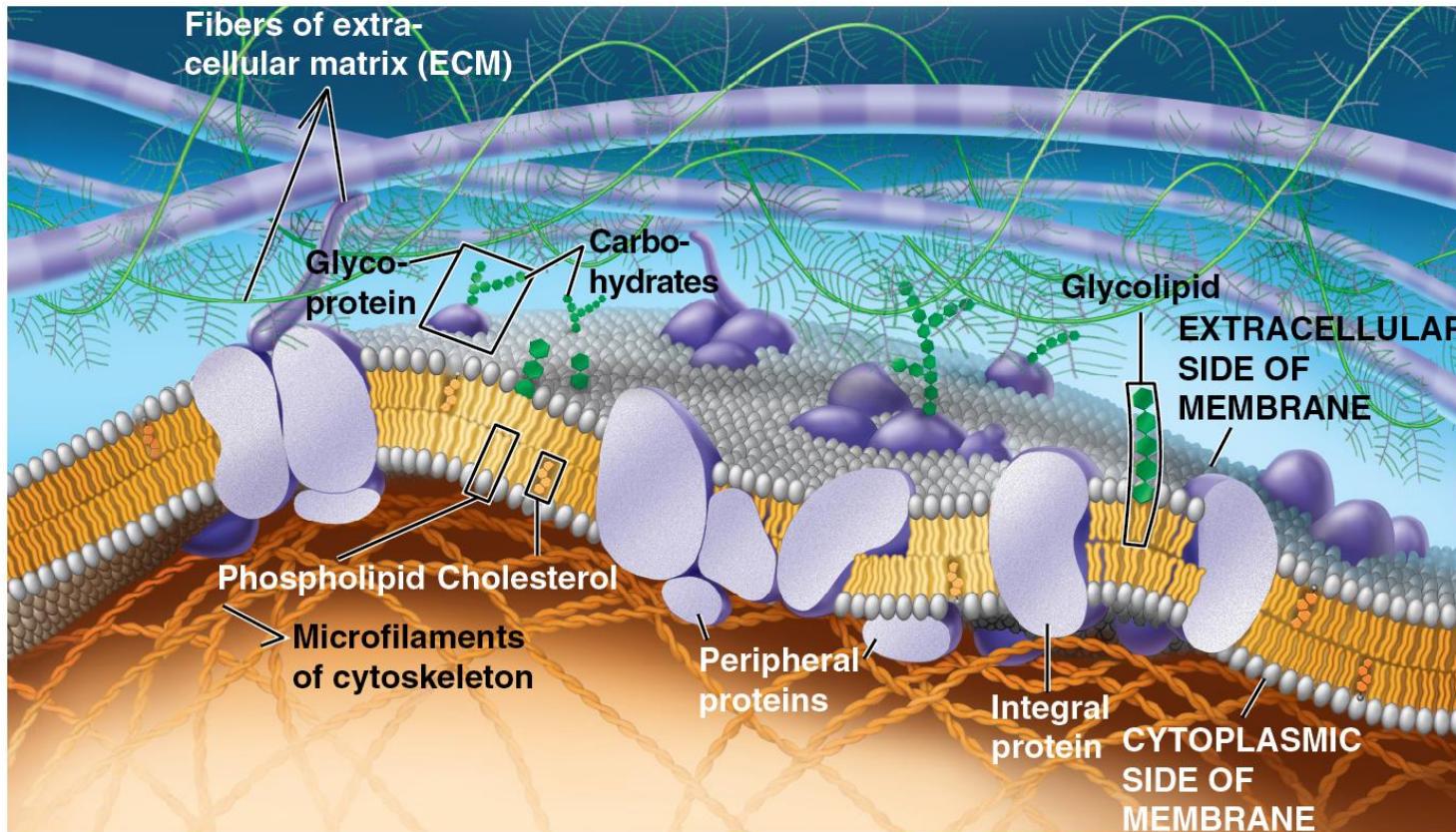
Concept 5.1: Cellular Membranes Are Fluid Mosaics of Lipids and Proteins

(1 of 2)

- Phospholipids are the most abundant lipids in most membranes
- Phospholipids are **amphipathic** molecules, containing hydrophobic and hydrophilic regions
- A phospholipid bilayer can exist as a stable boundary between two aqueous compartments

Figure 5.2

Current Model of an Animal Cell's Plasma Membrane (Cutaway View)



Membrane Proteins and Their Functions (1 of 3)

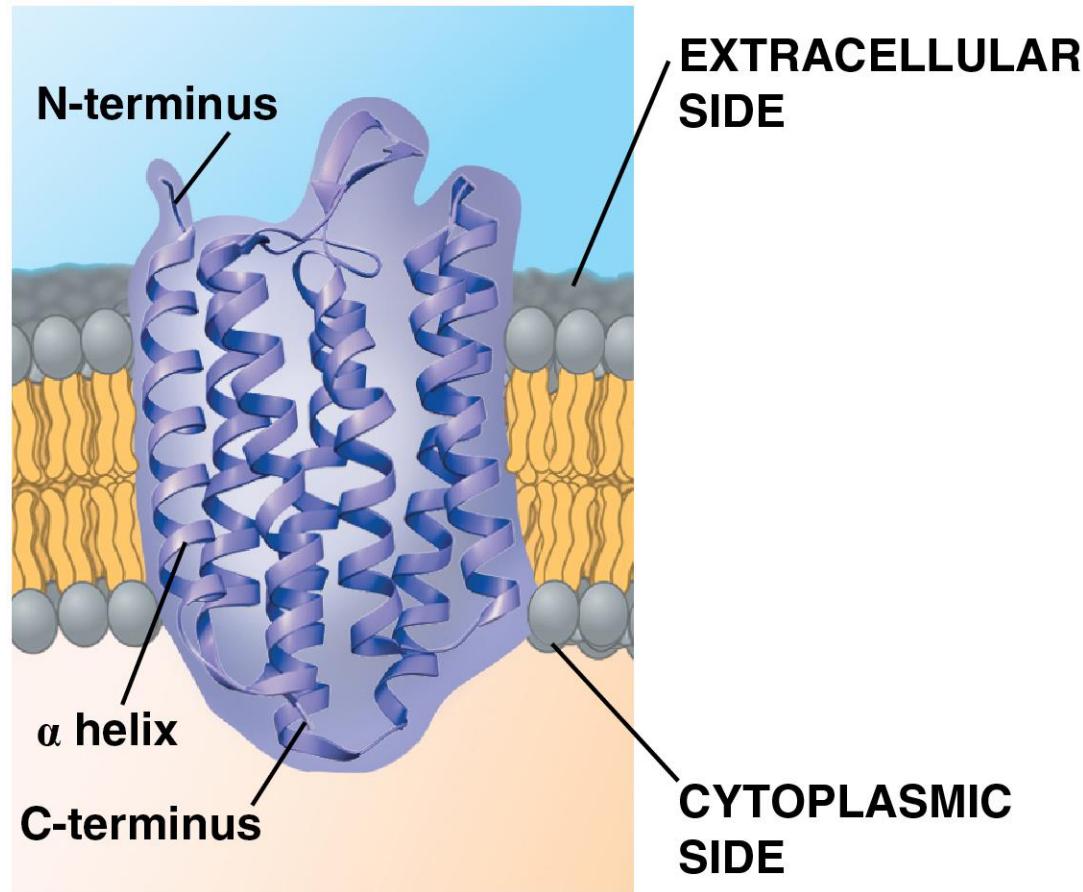
- A membrane is a collage of different proteins embedded in the fluid matrix of the lipid bilayer
- Proteins determine most of the membrane's specific functions

Membrane Proteins and Their Functions (2 of 3)

- **Integral proteins** penetrate the hydrophobic interior of the lipid bilayer
- The majority of these span the membrane and are called transmembrane proteins
- The hydrophobic regions of an integral protein consist of one or more stretches of nonpolar amino acids, often coiled into α helices
- **Peripheral proteins** are loosely bound to the surface of the membrane

Figure 5.6

The Structure of a Transmembrane Protein

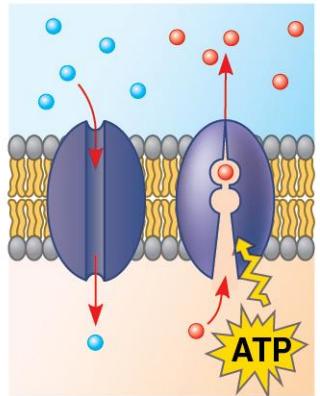


Membrane Proteins and Their Functions (3 of 3)

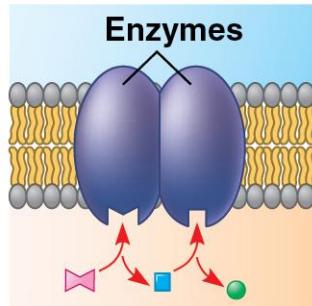
- Six major functions of membrane proteins
 - Transport
 - Enzymatic activity
 - Signal transduction
 - Cell-cell recognition
 - Intercellular joining
 - Attachment to the cytoskeleton and extracellular matrix (EC M)

Figure 5.7

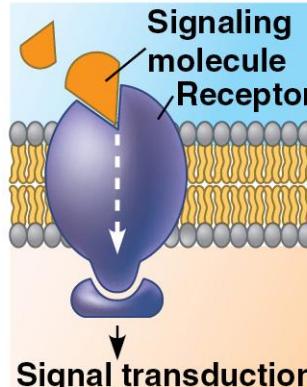
Some Functions of Membrane Proteins



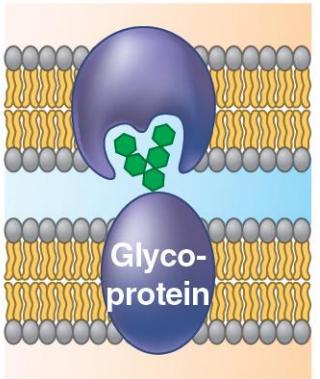
(a) Transport



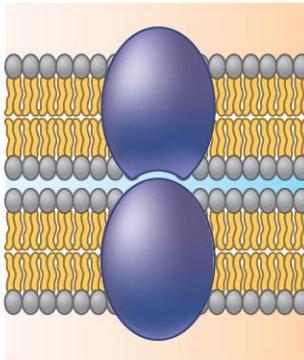
(b) Enzymatic activity



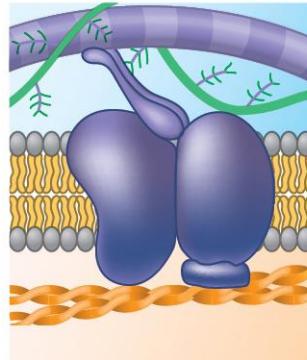
(c) Signal transduction



(d) Cell-cell
recognition



(e) Intercellular
joining



(f) Attachment to the
cytoskeleton and
extracellular matrix (ECM)

Concept 5.2: Membrane Structure Results in Selective Permeability

- A cell must regulate transport of substances across cellular boundaries
- Plasma membranes are selectively permeable, regulating the cell's molecular traffic

The Permeability of the Lipid Bilayer

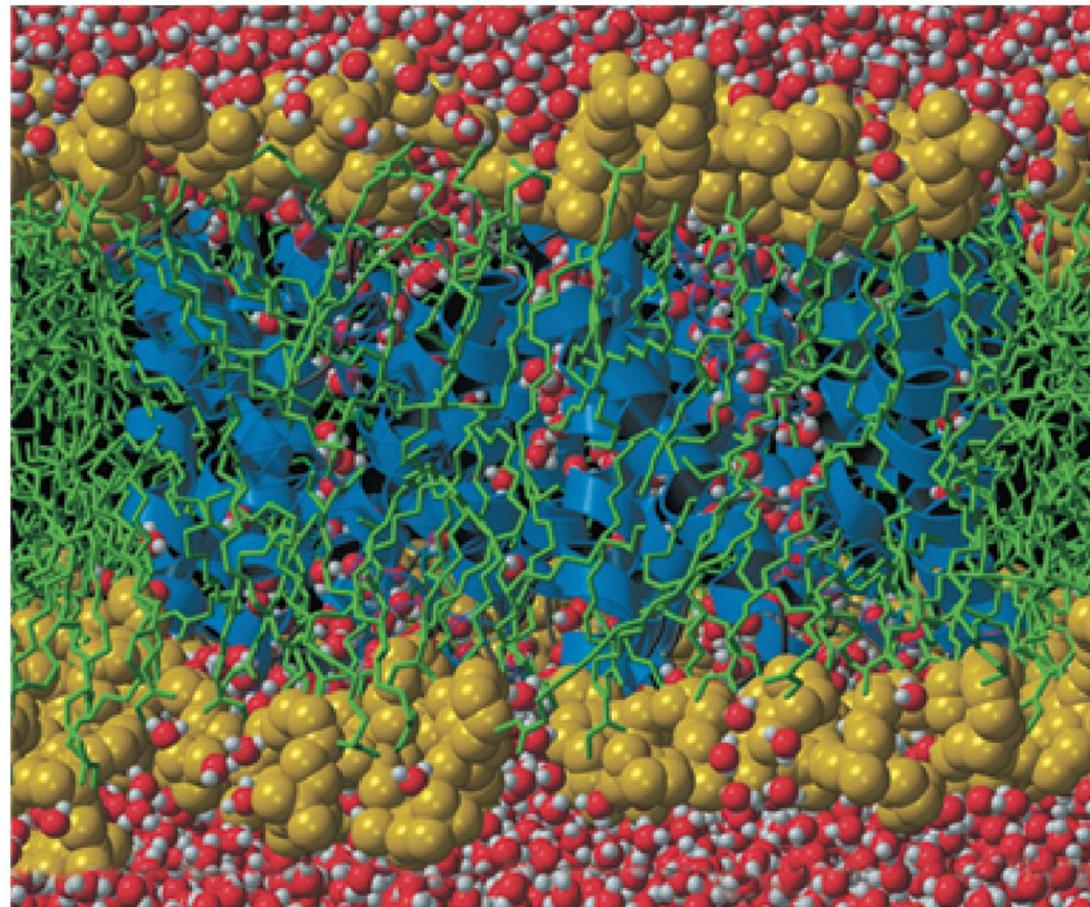
- Hydrophobic (nonpolar) molecules, such as hydrocarbons, can dissolve in the lipid bilayer of the membrane and cross it easily
- Polar molecules, such as sugars, do not cross the membrane easily
- Even water does not cross easily compared to nonpolar molecules

Transport Proteins (1 of 2)

- **Transport proteins** allow passage of hydrophilic substances across the membrane
- Some transport proteins, called channel proteins, have a hydrophilic channel that certain molecules or ions can use as a tunnel
- Channel proteins called **aquaporins** facilitate the passage of water

Figure 5.9

An Aquaporin

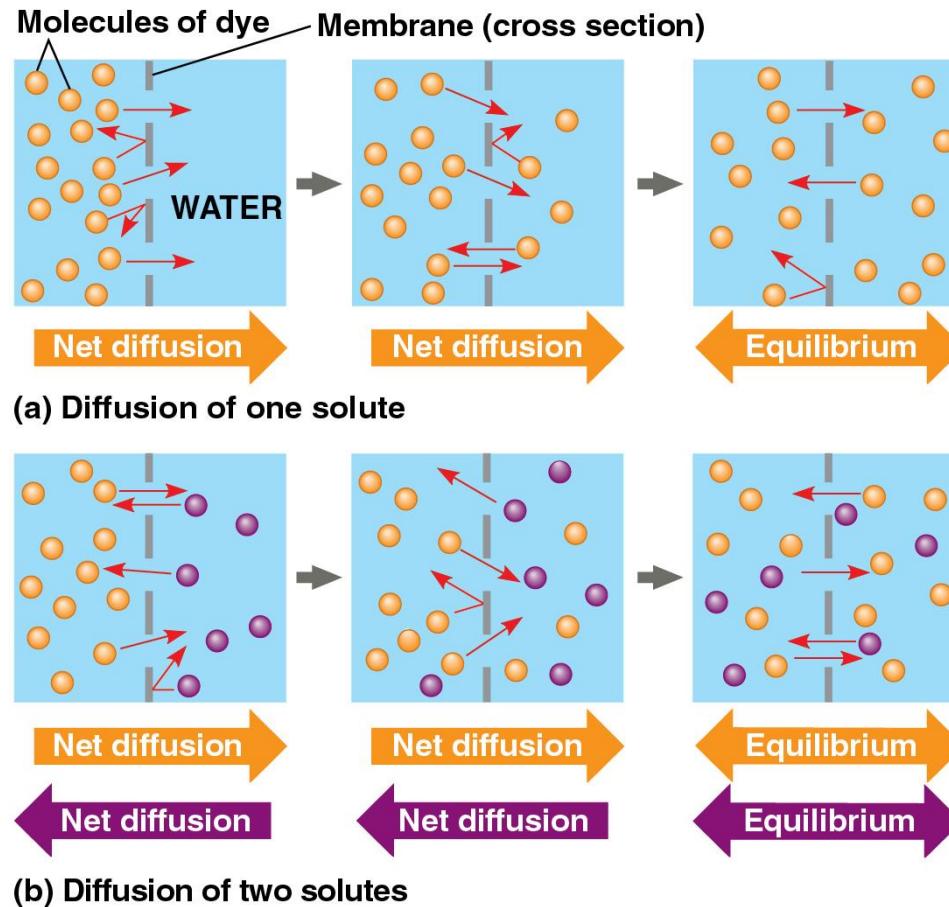


Concept 5.3: Passive Transport Is Diffusion of a Substance Across a Membrane with No Energy Investment (1 of 2)

- **Diffusion** is the tendency for molecules to spread out evenly into the available space
- Although each molecule moves randomly, diffusion of a population of molecules may be directional
- At dynamic equilibrium, as many molecules cross the membrane in one direction as in the other

Figure 5.10

Diffusion of Solutes Across a Synthetic Membrane



Concept 5.3: Passive Transport Is Diffusion of a Substance Across a Membrane with No Energy Investment (2 of 2)

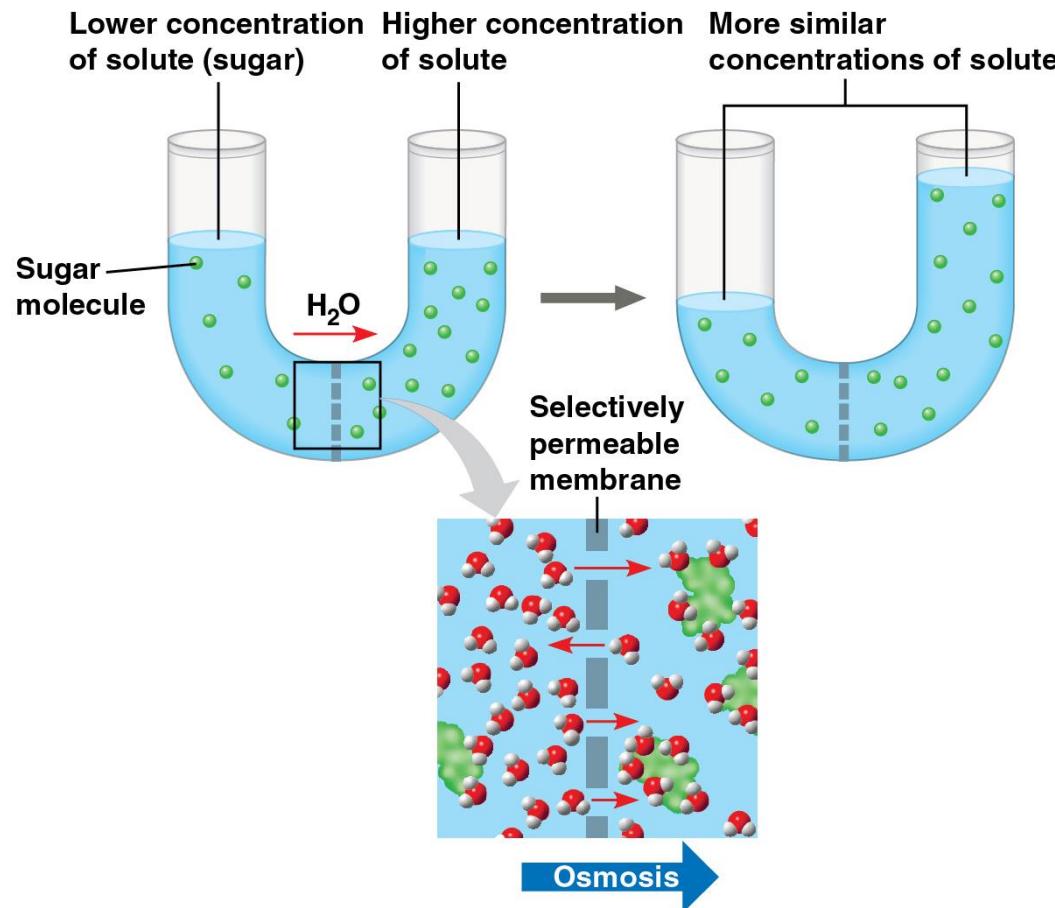
- Substances diffuse down their **concentration gradient**, from where it is more concentrated to where it is less concentrated
- Substances move down their own concentration gradient, unaffected by concentration gradients of other substances
- The diffusion of a substance across a biological membrane is **passive transport** because no energy is expended by the cell to make it happen

Effects of Osmosis on Water Balance

- **Osmosis** is the diffusion of free water across a selectively permeable membrane
- Water diffuses across a membrane from the region of lower solute concentration to the region of higher solute concentration until the solute concentration is equal on both sides

Figure 5.11

Osmosis

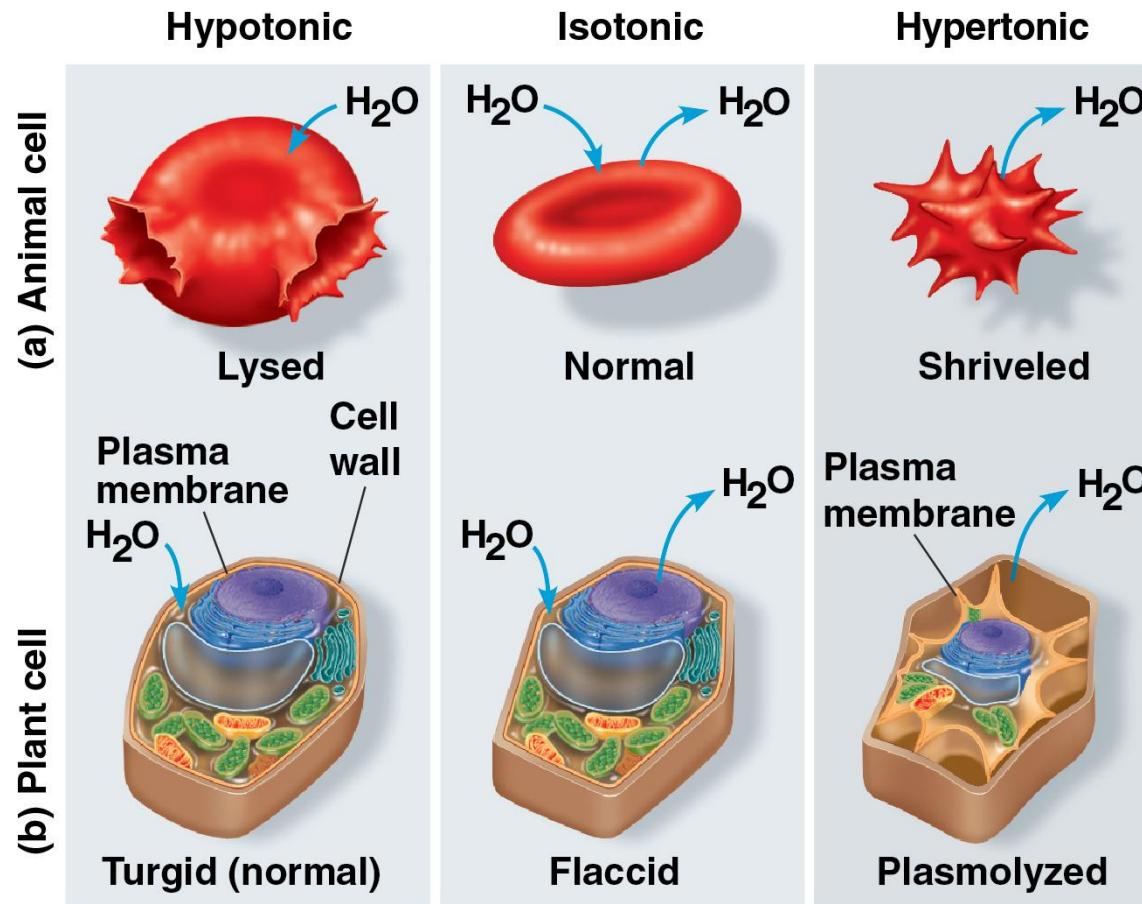


Water Balance of Cells without Cell Walls (1 of 2)

- **Tonicity** is the ability of a surrounding solution to cause a cell to gain or lose water
- **Isotonic solution:** Solute concentration is the same as inside the cell; no net water movement across the plasma membrane
- **Hypertonic solution:** Solute concentration is greater than that inside the cell; cell loses water
- **Hypotonic solution:** Solute concentration is less than that inside the cell; cell gains water

Figure 5.12

The Water Balance of Living Cells



Facilitated Diffusion: Passive Transport Aided by Proteins (1 of 2)

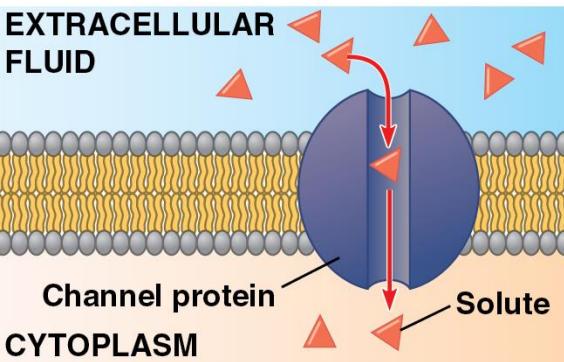
- In **facilitated diffusion**, transport proteins speed the passive movement of specific molecules across the plasma membrane
- Channel proteins provide corridors that allow a specific molecule or ion to cross the membrane
- Channel proteins include
 - Aquaporins, for facilitated diffusion of water
 - **Ion channels** that open or close in response to a stimulus (**gated channels**)

Facilitated Diffusion: Passive Transport Aided by Proteins (2 of 2)

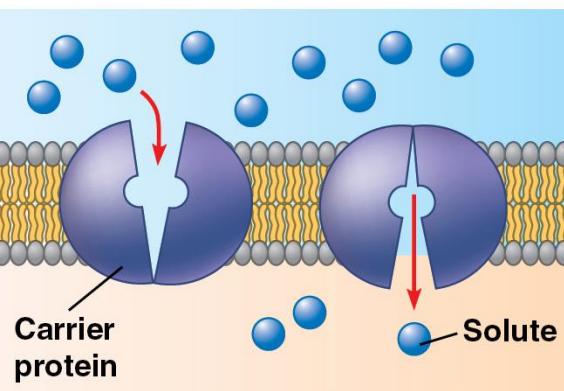
- Carrier proteins undergo a subtle change in shape that translocates the solute-binding site across the membrane
- The shape change may be triggered by binding and release of the transported molecule
- No net energy input is required

Figure 5.14

Two Types of Transport Proteins That Carry out Facilitated Diffusion



(a) A channel protein



(b) A carrier protein

Concept 5.4: Active Transport Uses Energy to Move Solutes Against Their Gradients

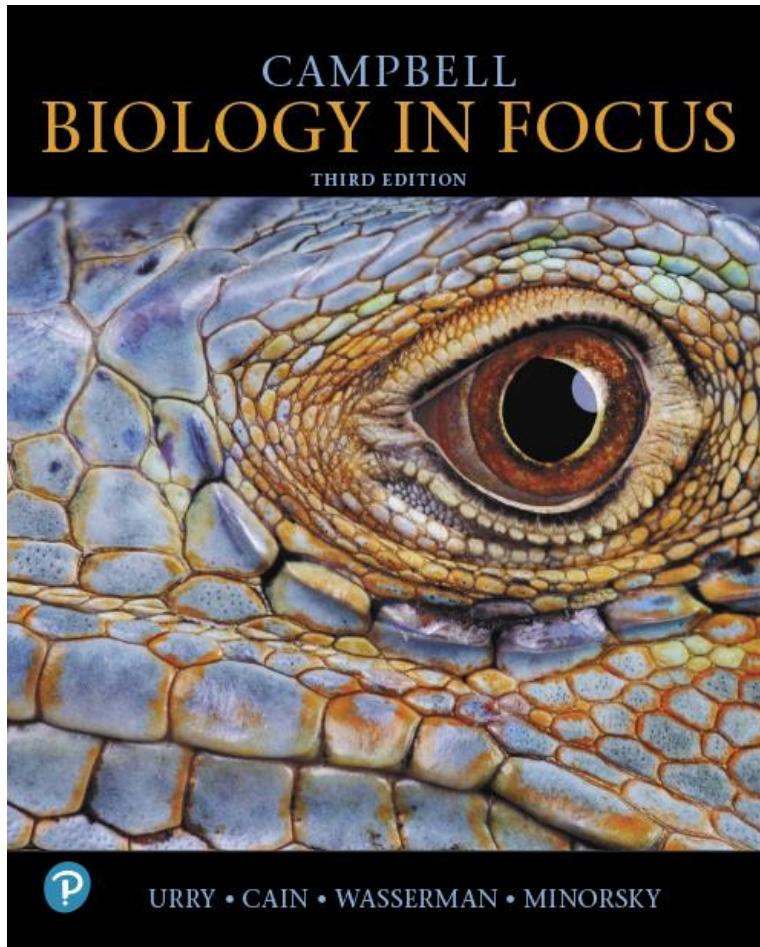
- Facilitated diffusion speeds transport of a solute by providing efficient passage through the membrane but does not alter the direction of transport
- Some transport proteins, however, can move solutes against their concentration gradients



Cell Function

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Chapter 6

An Introduction to Metabolism

Lecture Presentations by
Kathleen Fitzpatrick and Nicole Tunbridge,
Simon Fraser University

Overview: The Energy of Life

- The living cell is a miniature chemical factory where thousands of reactions occur
- Cells extract energy from sugars using cellular respiration and apply that energy to perform work
- Some organisms, such as the firefly, even convert chemical energy to light, a process called bioluminescence

Concept 6.1: An Organism's Metabolism Transforms Matter and Energy

- The totality of an organism's chemical reactions is called **metabolism**
- Metabolism is an emergent property that arises from orderly interactions between molecules

Forms of Energy (2 of 3)

- **Kinetic energy** is energy associated with motion
- **Thermal energy** is kinetic energy associated with random movement of atoms or molecules
- **Heat** is thermal energy in transfer from one object to another
- Light is another type of energy that can be harnessed to perform work

Forms of Energy (3 of 3)

- **Potential energy** is energy that matter possesses because of its location or structure
- **Chemical energy** is potential energy available for release in a chemical reaction
- Energy can be converted from one form to another

Figure 6.2

Transformations Between Potential Energy and Kinetic Energy

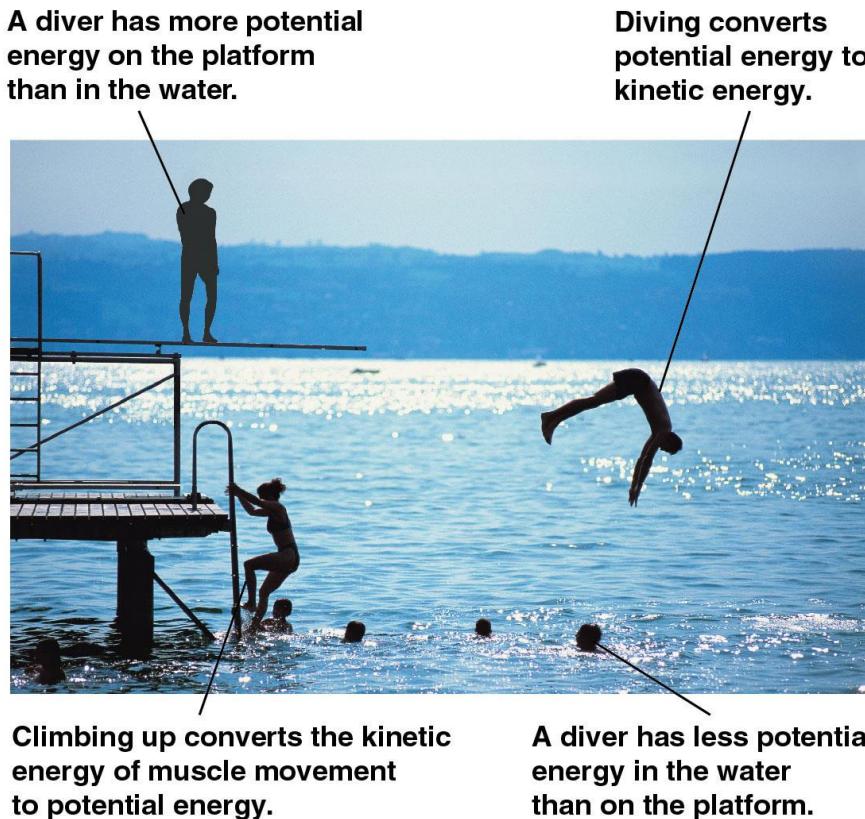


Figure 6.3

The Two Laws of Thermodynamics



(a) First law of thermodynamics

(b) Second law of thermodynamics

Concept 6.2: The Free-Energy Change of a Reaction Tells Us Whether or Not the Reaction Occurs Spontaneously

- Biologists measure changes in free energy to help them understand the chemical reactions of life

Free-Energy Change (ΔG), Stability, and Equilibrium (1 of 4)

- **Free energy** is the portion of a system's energy that can do work when temperature and pressure are uniform throughout, as in a living cell

Free-Energy Change (ΔG), Stability, and Equilibrium (2 of 4)

- The change in free energy (ΔG) during a chemical reaction is the difference between the free energy of the final state and the free energy of the initial state

$$\Delta G = G_{\text{final state}} - G_{\text{initial state}}$$

- Only reactions with a negative ΔG are spontaneous
- Spontaneous reactions can be harnessed to perform cellular work

Free-Energy Change (ΔG), Stability, and Equilibrium (3 of 4)

- Free energy is a measure of a system's instability, its tendency to change to a more stable state
- During a spontaneous change, free energy decreases and the stability of a system increases
- Unstable systems (higher G) tend to change such that they become more stable (lower G)

Figure 6.5

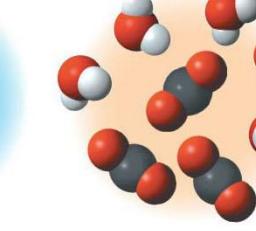
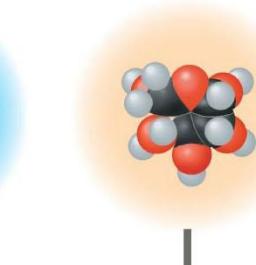
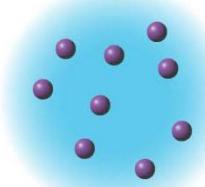
The Relationship of Free Energy to Stability, Work Capacity, and Spontaneous Change

- More free energy (higher G)
- Less stable
- Greater work capacity

In a spontaneous change

- The free energy of the system decreases ($\Delta G < 0$)
- The system becomes more stable
- The released free energy can be harnessed to do work

- Less free energy (lower G)
- More stable
- Less work capacity



(a) Gravitational motion

(b) Diffusion

(c) Chemical reaction

Free-Energy Change (ΔG), Stability, and Equilibrium (4 of 4)

- At chemical equilibrium, forward and reverse reactions occur at the same rate; it is a state of maximum stability
 - **A process is spontaneous and can perform work only when it is moving toward equilibrium**

Free Energy and Metabolism

- The concept of free energy can be applied to the chemistry of life's processes

Concept 6.3: ATP Powers Cellular Work by Coupling Exergonic Reactions to Endergonic Reactions (1 of 2)

- A cell does three main kinds of work
 - Chemical
 - Transport
 - Mechanical

Concept 6.3: ATP Powers Cellular Work by Coupling Exergonic Reactions to Endergonic Reactions (2 of 2)

- To do work, cells manage energy resources by **energy coupling**, the use of an exergonic process to drive an endergonic one
- Most energy coupling in cells is mediated by ATP

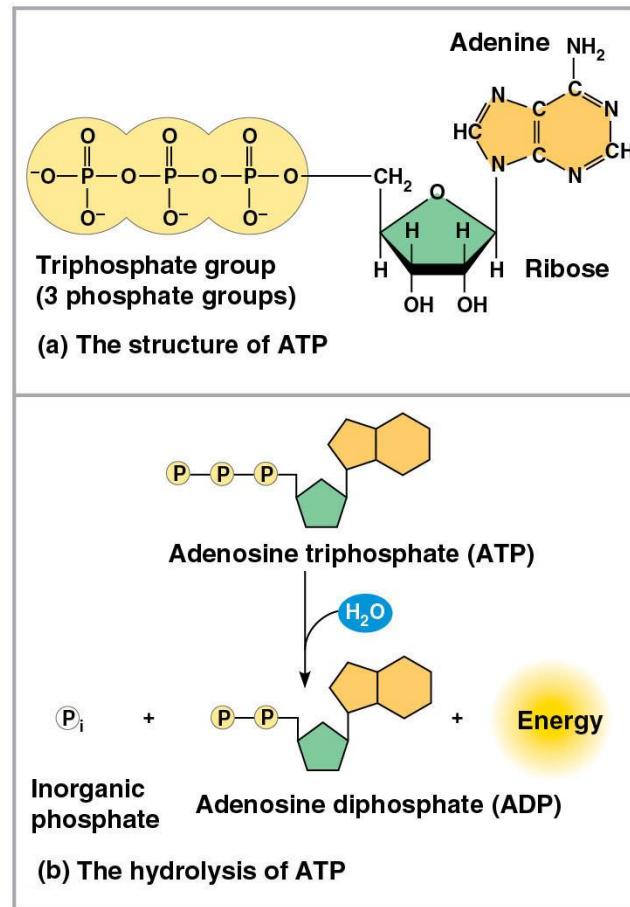
The Structure and Hydrolysis of ATP

(1 of 3)

- **ATP (adenosine triphosphate)** is composed of ribose (a sugar), adenine (a nitrogenous base), and a chain of three phosphate groups
- In addition to its role in energy coupling, ATP is also used to make RNA

Figure 6.8

The Structure and Hydrolysis of Adenosine Triphosphate (ATP)



How ATP Works (1 of 3)

- The chemical work in a cell is powered by ATP hydrolysis
- The energy released by the exergonic reaction of ATP hydrolysis is used to drive endergonic reactions

How ATP Works (2 of 3)

- ATP drives endergonic reactions by phosphorylation, transferring a phosphate group to another molecule, such as a reactant
- The recipient molecule is now called a **phosphorylated intermediate**
- Overall, the coupled reactions are exergonic

Figure 6.9

How ATP Drives Chemical Work: Energy Coupling Using ATP Hydrolysis

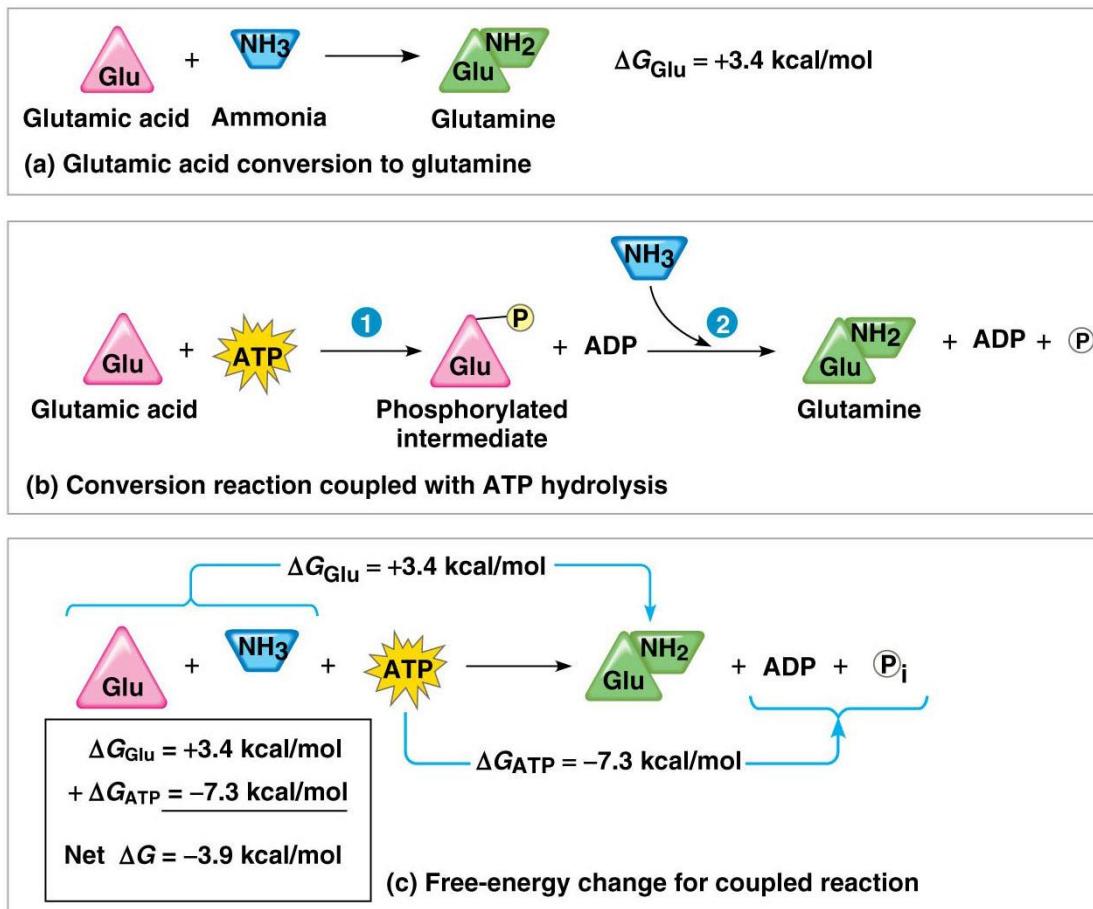
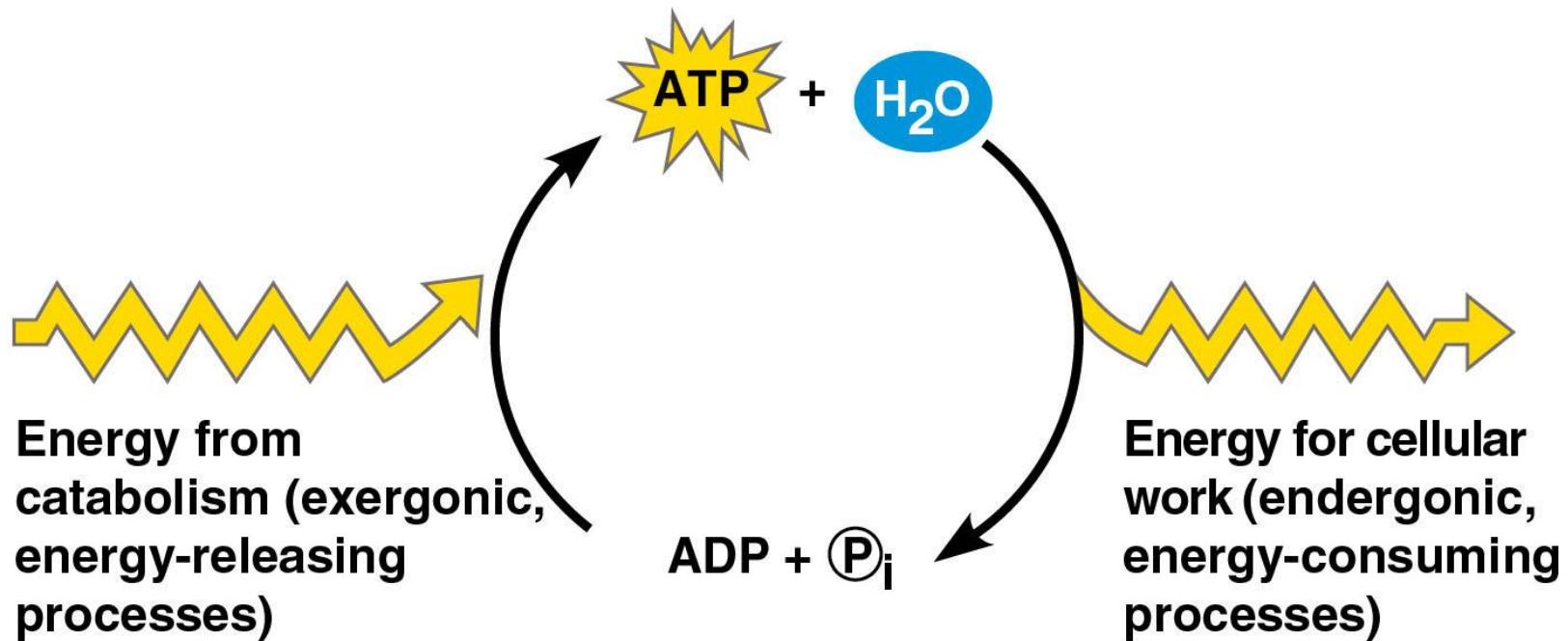


Figure 6.11

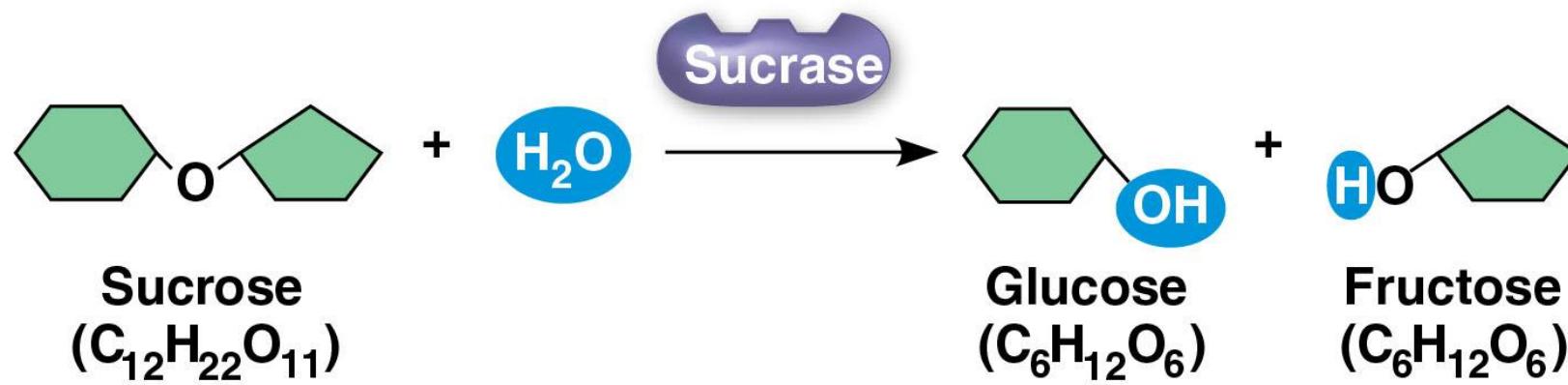
The ATP Cycle



Concept 6.4: Enzymes Speed up Metabolic Reactions by Lowering Energy Barriers

- A **catalyst** is a chemical agent that speeds up a reaction without being consumed by the reaction
- An **enzyme** is a macromolecule that acts as a catalyst; most enzymes are proteins
 - For example, the enzyme sucrase catalyzes the hydrolysis of sucrose

Hydrolysis of Sucrose to Glucose and Fructose



The Activation Energy Barrier

- Every chemical reaction between molecules involves both bond breaking and bond forming
- **Activation energy** (E_A) is the energy required to start a reaction by breaking bonds in the reactant molecules
- Activation energy is often supplied by heat in the form of thermal energy that reactant molecules absorb from the surroundings

Figure 6.12

Energy Profile of an Exergonic Reaction

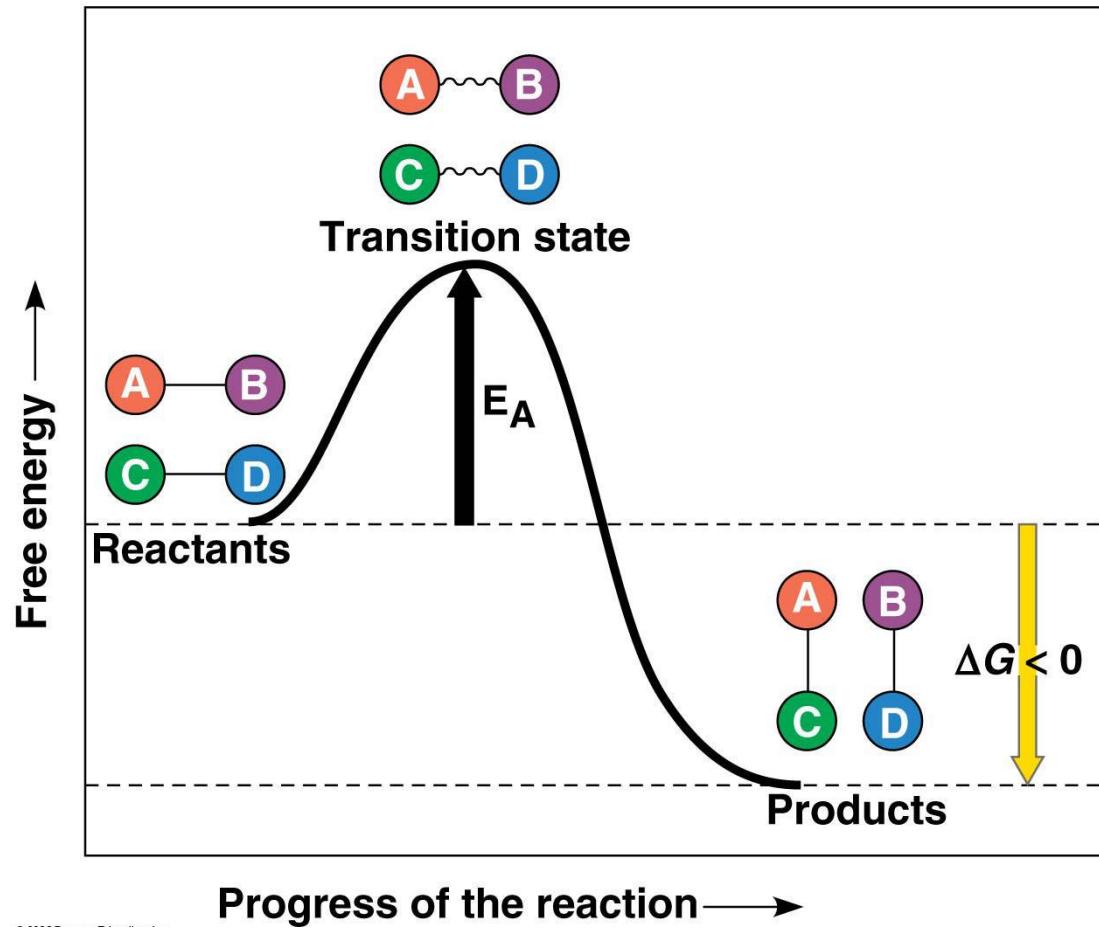
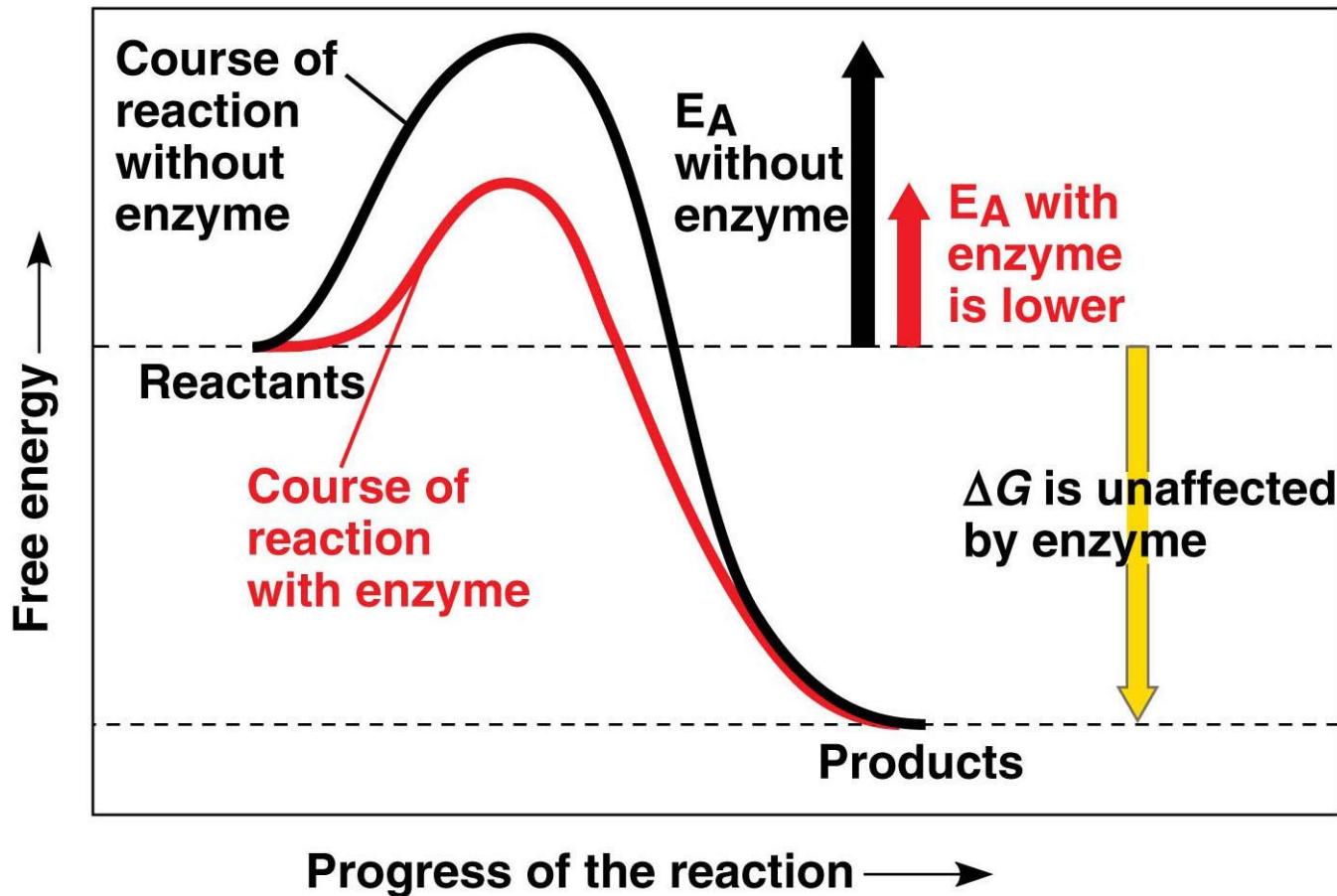


Figure 6.13

The Effect of an Enzyme on Activation Energy



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Cell Biology and Applications

Computing in Cell Biology [1]

- **Protein Modeling and Molecular Structure**

Proteins perform biological functions in cells, and their 3D structures determine how they work.

Computational Processes:

Protein folding: Predicting the 3D shape of proteins from amino acid sequences.

Simulating protein interactions with ligands or drug molecules.

- **Cellular Image Analysis**

Description: Cellular images are produced through microscopy to study cell structures and functions.

Computational Processes:

Segmentation: Separating cell components in images (e.g., nucleus and cytoplasm).

Pattern recognition to detect cell abnormalities, such as cancer.

Computing in Cell Biology [2]

- **Modeling Biochemical Pathways and Signaling**

Biochemical pathways regulate intercellular communication and metabolic processes.

Computational Processes:

Simulating metabolic pathways to study energy production.

Analyzing signaling pathways to understand molecular interactions in cellular responses.

- **Big Data in Cell Biology**

Cell biology studies generate large amounts of data, including genomic, proteomic, and cellular imaging data.

Computational Processes:

Data storage in biological databases.

Data analysis using machine learning algorithms to identify patterns.

Computing Tasks

- Machine Learning for prediction/detection, analysis, pattern recognition
- Simulation and modeling
- Optimization

Machine Learning in Cell Biology

1. Using AI to analyze microscopy images:
 - segmentation of cytoplasm
 - determine live or dead cells
 - differentiate apoptosis and ferroptosis
 - selection of effective drug candidate for breast cancer cells
 - cell counting
 - segmentation of nucleus

2. Predicting cell behavior based on historical data.

Segmentation of cytoplasm

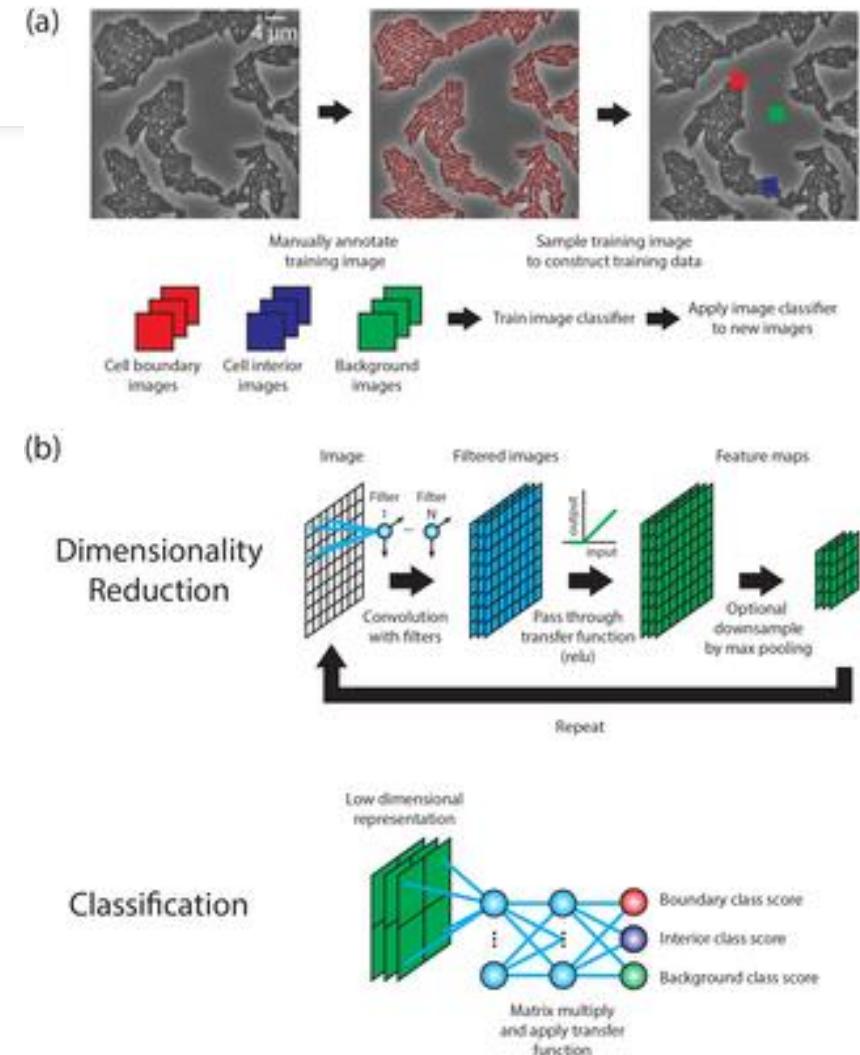
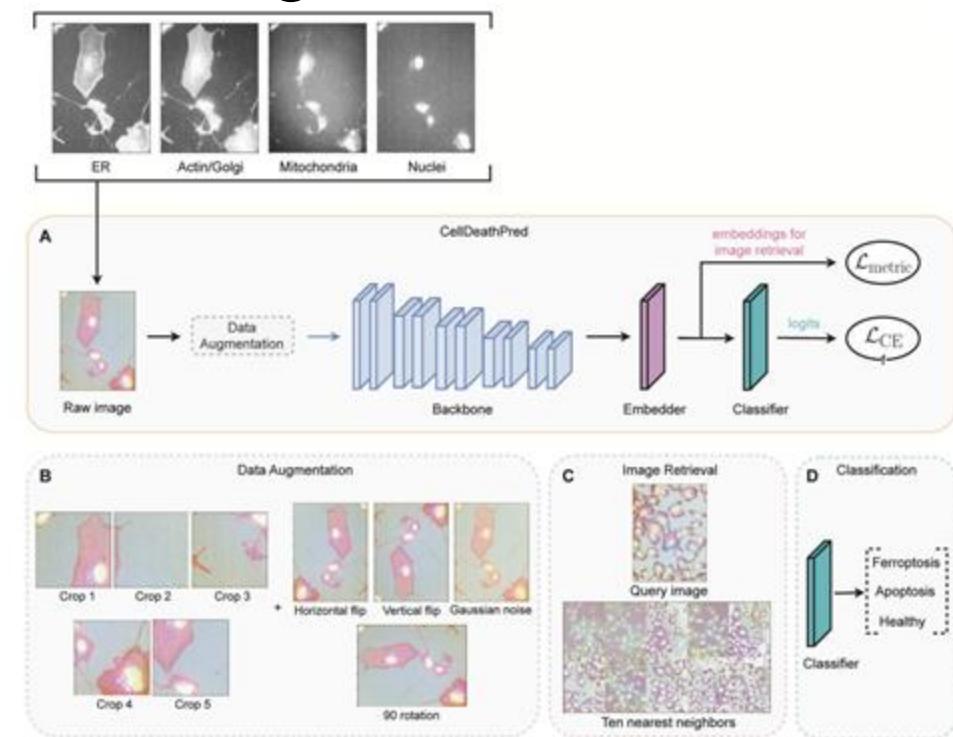


Fig 1. Performing image segmentation with deep convolutional neural networks.
(a) Image segmentation can be recast as an image classification task that is amenable to a supervised machine learning approach. A manually annotated image is converted into a training dataset by sampling regions around boundary, interior, and background pixels. These sample images are then used to train an image classifier that can then be applied to new images. (b) The mathematical structure of a conv-net. A conv-net can be broken down into two components. The first component is dimensionality reduction through the iterative application of three operations—convolutions, a transfer function, and down sampling. The second component is a classifier that uses the representation and outputs scores for each class.

Determine live or dead cells

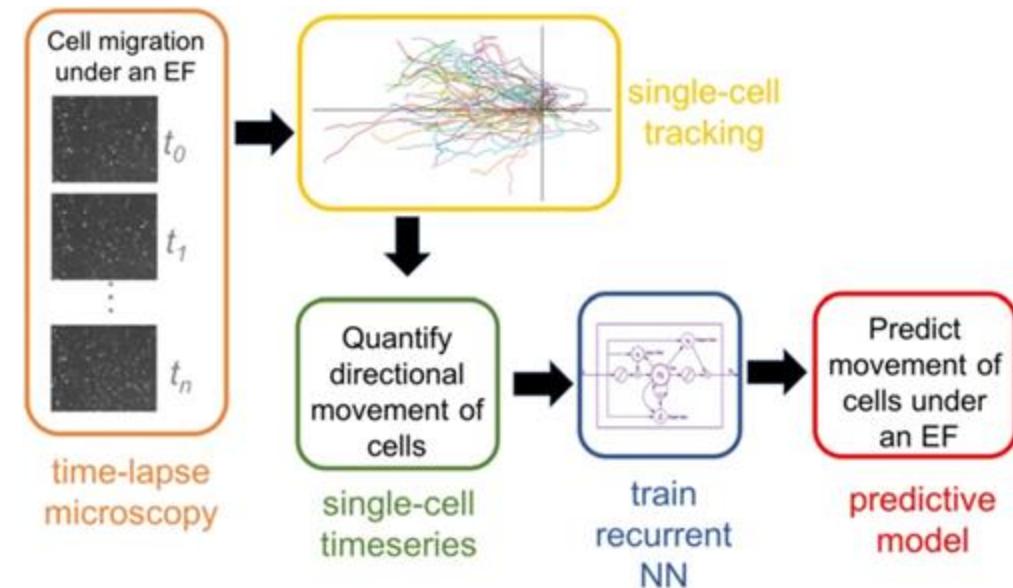
Learning Deep Features for Dead and Living Breast Cancer Cell Classification without Staining

Figure 8. (A) The neural network receives four images as input: ER, Actin/Golgi, Mitochondria, and Nuclei. It can predict whether the medication employed in the experiment causes DMSO-induced apoptosis or ferroptosis. The architecture has four stages. A pre-trained network called Efficientnet-b0 is the backbone model. (1) Data augmentation is used to make the model robust during training. (2) A series of fully connected layers called an embedder is applied to create low-dimensional data. (3) A classifier composed of fully connected layers predicts the modality as output. (B) Data augmentations applied consisted of 512×512 crops, four corner crops, and one center crop. Amplification was implemented for every crop. (C) An illustration of a retrieval image. Ten closest neighbors in the embedding space for a query image. (D) The model's final layer, which has three nodes. Predictions about the classification of the three classes. The orange color represents the deep learning framework, while gray highlights the data augmentation section. Pink indicates image retrieval and embeddings, and blue represents classification outputs. The pinkish cells with a blue-gray background mimic real microscopic images for biological relevance. Reprinted from [178] under CC BY license.



Predicting cell behavior based on historical data

A machine learning based model accurately predicts cellular response to electric fields in multiple cell types

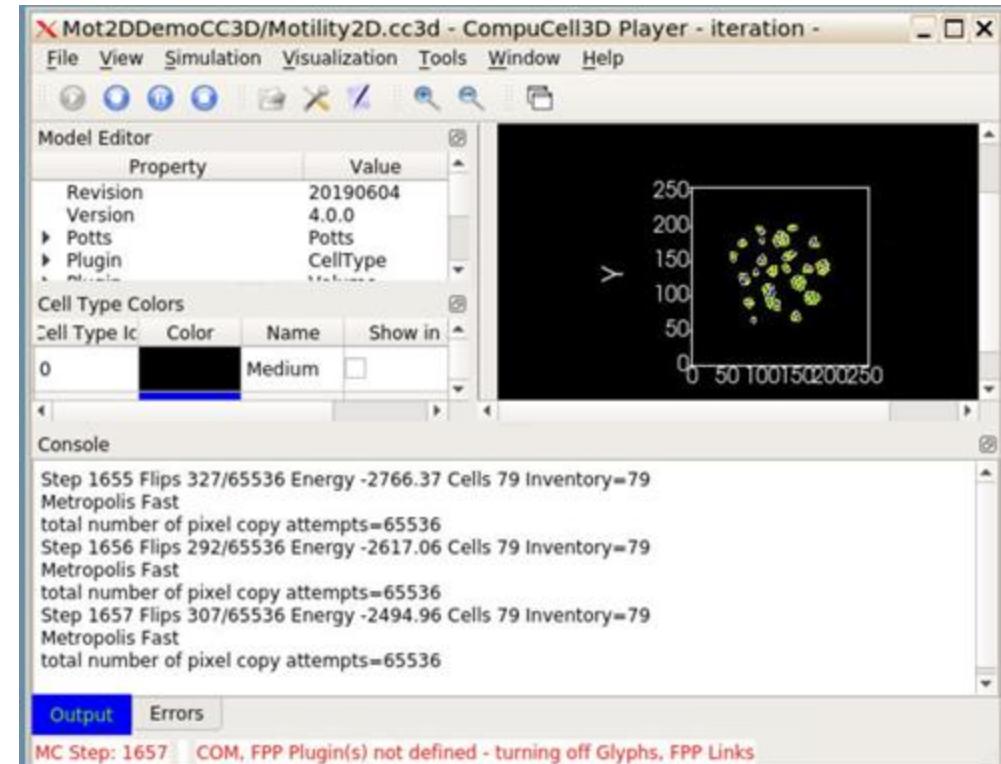


The image processing and cell directedness prediction pipeline. Time-lapse microscope images are used to manually track a number of cells. The tracking data is used to create timeseries of our two features (cell directedness and EF), which are used as inputs to our blackbox LSTM model to make predictions about the next directedness value.

Cellular Simulations

Computational modeling of cell processes (e.g., metabolism, signaling pathways).

- Simulating cell growth and division.
(<https://compuccell3d.org/>)
- Cells Alive! Interactive Cell Models
(http://www.cellsalive.com/cells/cell_model.htm)



Optimization

Molecular docking with multi-objective Particle Swarm Optimization

Tool Exploration [1]

Cells Alive! Interactive Cell Models

1. Explore the Interactive Models:

- Visit the Cells Alive! website (<https://www.cellsalive.com>).
- Explore the interactive models related to cells (e.g., Animal Cell, Plant Cell, Bacteria Cell).
- Understand each organelle and its function as displayed in the simulation.

2. Analyze Differences and Similarities Between Cells:

- Compare the structures of animal, plant, and bacterial cells based on the tool's information.
- Identify at least three major differences and three major similarities among these cell types.

Tool Exploration [2]

3. Computational Biology Applications:

- Explain how these simulations and interactive models aid research and education in *Computational Biology*.
- Provide an example of how similar technologies can be used in bioinformatics or related fields.

4. Exploration Report:

- Prepare a short report (2-3 pages) including:
 - A summary of the interactive model exploration.
 - The results of the cell comparison.
 - An analysis of the benefits of this tool in *Computational Biology*.
 - Write your criticism and suggestions for this tool. Provide sufficient justification.
- Include screenshots if necessary to support the report. Maximum 2 images with proportional size.

Deadline: 1 week, 05/03/2025

Submission Format: PDF, submitted via Edunex.

The use of generative-AI tools in any form is not permitted.

References

- Ali, M., Benfante, V., Basirinia, G., Alongi, P., Sperandeo, A., Quattrocchi, A., Giannone, A. G., Cabibi, D., Yezzi, A., Di Raimondo, D., Tuttolomondo, A., & Comelli, A. (2025). Applications of Artificial Intelligence, Deep Learning, and Machine Learning to Support the Analysis of Microscopic Images of Cells and Tissues. *Journal of Imaging*, 11(2), 59. <https://doi.org/10.3390/jimaging11020059>
- Sargent, B., Jafari, M., Marquez, G. et al. A machine learning based model accurately predicts cellular response to electric fields in multiple cell types. *Sci Rep* 12, 9912 (2022). <https://doi.org/10.1038/s41598-022-13925-4>
- Schorpp, K., Bessadok, A., Bilbosunov, A. et al. CellDeathPred: a deep learning framework for ferroptosis and apoptosis prediction based on cell painting. *Cell Death Discov.* 9, 277 (2023). <https://doi.org/10.1038/s41420-023-01559-y>
- Pattarone, G., Acion, L., Simian, M. et al. Learning deep features for dead and living breast cancer cell classification without staining. *Sci Rep* 11, 10304 (2021). <https://doi.org/10.1038/s41598-021-89895-w>
- Van Valen DA, Kudo T, Lane KM, Macklin DN, Quach NT, DeFelice MM, et al. (2016) Deep Learning Automates the Quantitative Analysis of Individual Cells in Live-Cell Imaging Experiments. *PLoS Comput Biol* 12(11): e1005177. <https://doi.org/10.1371/journal.pcbi.1005177>
- Ali, R., Balamurali, M., & Varamini, P. (2022). Deep Learning-Based Artificial Intelligence to Investigate Targeted Nanoparticles' Uptake in TNBC Cells. *International Journal of Molecular Sciences*, 23(24), 16070. <https://doi.org/10.3390/ijms232416070>
- Ferreira, E.K.G.D., Silveira, G.F. Classification and counting of cells in brightfield microscopy images: an application of convolutional neural networks. *Sci Rep* 14, 9031 (2024). <https://doi.org/10.1038/s41598-024-59625-z>
- Fabian Hörst, Moritz Rempe, Lukas Heine, Constantin Seibold, Julius Keyl, Giulia Baldini, Selma Ugurel, Jens Siveke, Barbara Grünwald, Jan Egger, Jens Kleesiek, CellViT: Vision Transformers for precise cell segmentation and classification, *Medical Image Analysis*, Volume 94, 2024, 103143, ISSN 1361-8415, <https://doi.org/10.1016/j.media.2024.103143>
- Stefan Janson, Daniel Merkle, Martin Middendorf, Molecular docking with multi-objective Particle Swarm Optimization, *Applied Soft Computing*, Volume 8, Issue 1, 2008, Pages 666-675, ISSN 1568-4946, <https://doi.org/10.1016/j.asoc.2007.05.005>.