

Structura moleculară.

§1.2. Structura moleculară: primară, secundară, terțiară, cuaternară;

Sunt o mare varietate de compuși chimici de dimensiuni mari în sistemele vii, cum sunt:

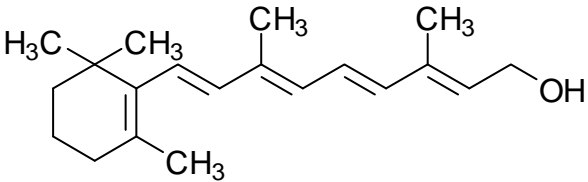
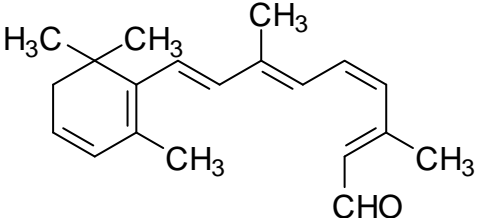
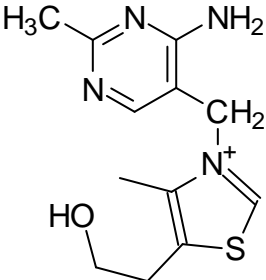
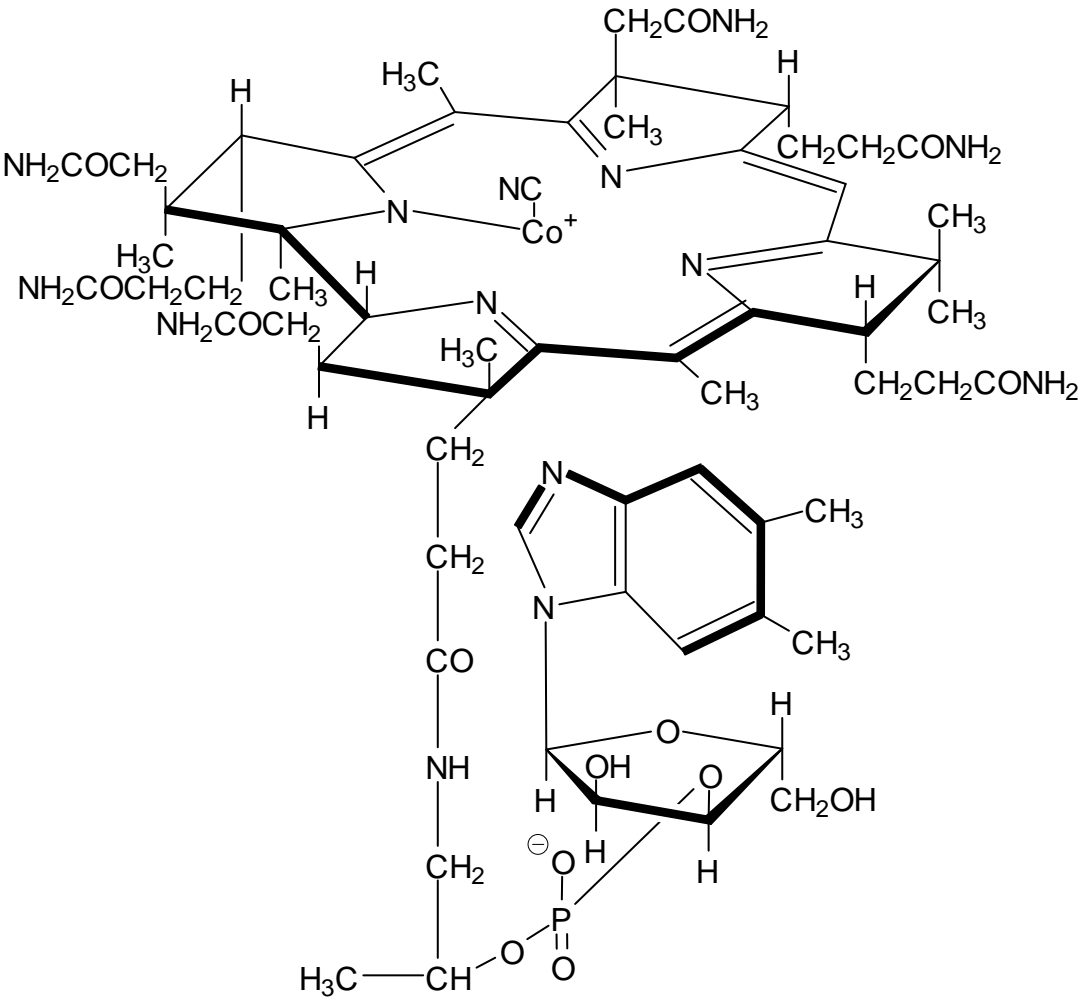
- ÷ **carbohidrați**: asigură energia celulei, structura și servesc la recunoașterea moleculară; conțin C, H și O, au formula generală $C_x(H_2O)_y$ având toți grupări C=O și -OH; se clasifică după dimensiunea bazei carbonice din șir, numărul de unități de zahăr, localizarea legăturii C=O (aldoze, cu legătura C=O la capăt de șir și cetoze, cu legătura C=O în mijlocul lanțului carbonic) și stereochimie; carbohidrați: monozaharide (cu o singură unitate de zahăr); dizaharide (două unități de zahăr); oligozaharide (2-10 unități de zahăr); polizaharide (>10 unități de zahăr);
exemple de monozaharide:

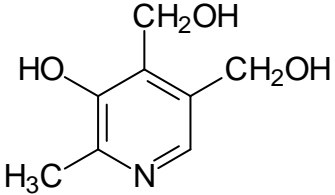
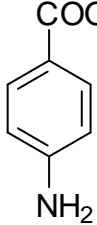
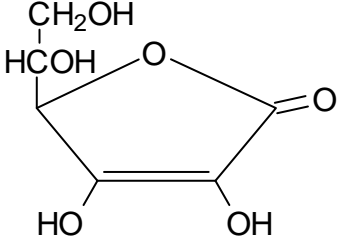
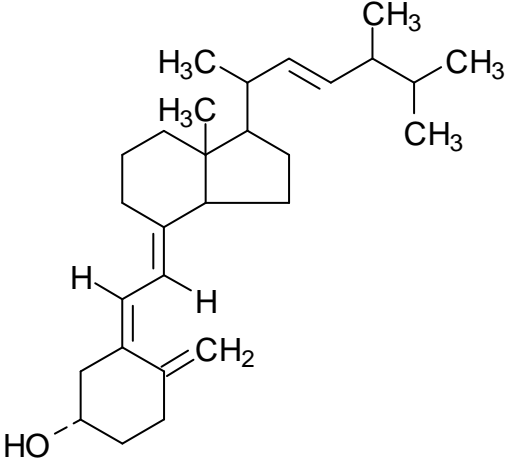
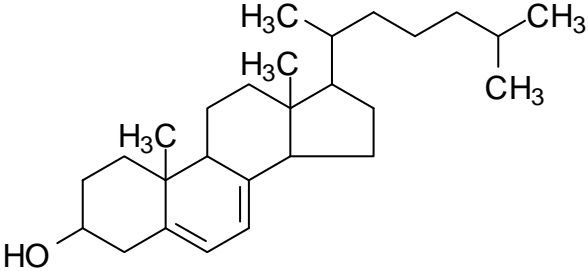
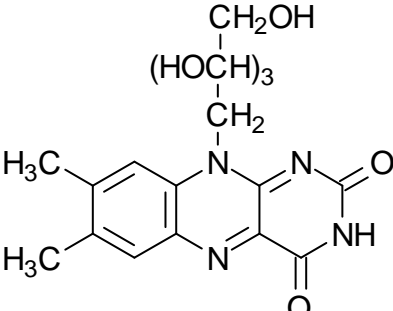
$\begin{array}{c} \text{CHO} \\ \\ \text{HO} \blacktriangleright \text{C} \blacktriangleleft \text{H} \\ \\ \text{CH}_2\text{OH} \end{array}$	D-gliceraldehida	cel mai simplu zahăr
	D-glucoza	cel mai important zahăr în dietă
	D-galactoza	parte a zahărului din lapte
	D-riboza	folosit în construcția RNA
	D-fructoza	cel mai dulce dintre toate zaharurile naturale
	Zaharina	îndulcitor artificial

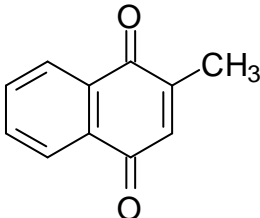
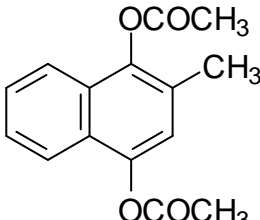
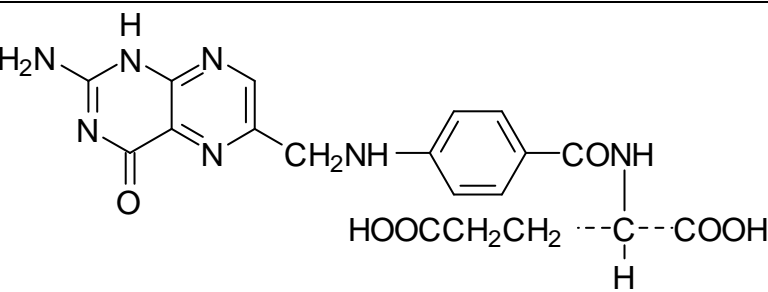
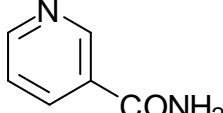
Cât de dulci sunt zaharurile (calitățile gustative ale monozaharidelor):

Zahăr	lactoză	galactoză	maltoză	sucroză	fructoză	aspartam	zaharină
Relativ la sucroză	0.16	0.32	0.33	1.00	1.73	180	450

÷ **vitamine**: amestec de compuși care joacă multe roluri și sunt părți esențiale ale altor biomoleculă; **exemple de vitamine**:

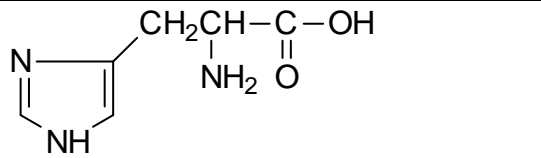
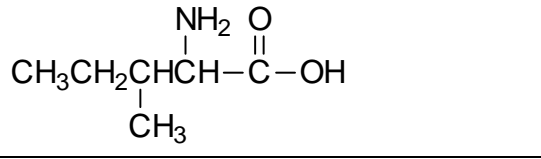
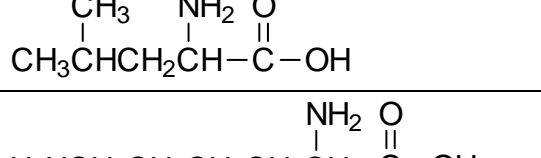
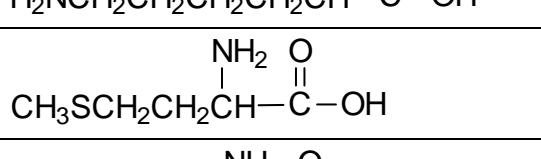
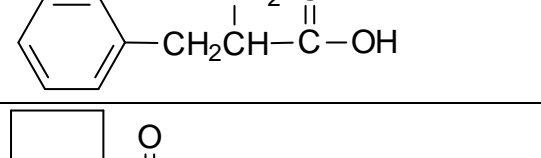
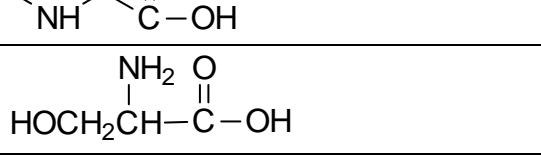
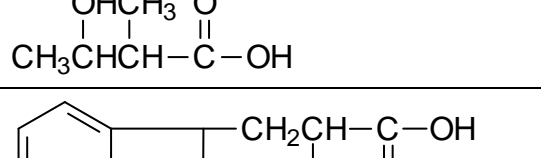
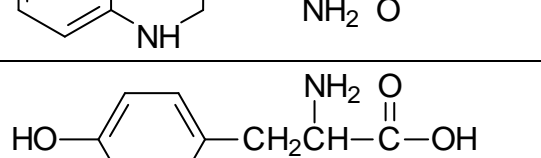
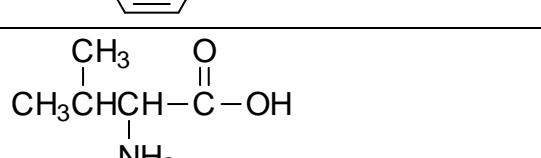
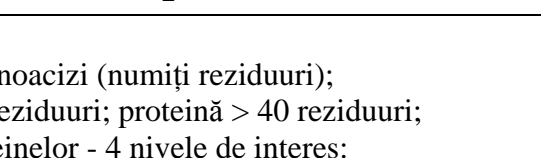
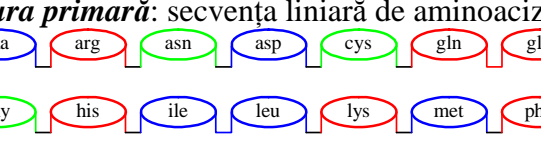
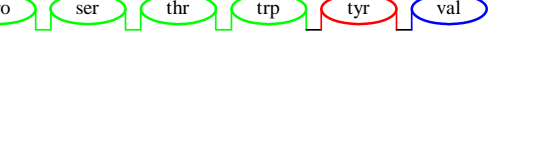
	Vitamina A
	Vitamina A2
	Vitamina B1
	Vitamina B12

	Vitamina B6
	Provitamina Bx
	Vitamina C
	Vitamina D2
	Vitamina D3
	Vitamina G

	Vitamina K3
	Vitamina K4
	Vitamina M
	Vitamina PP

÷ **aminoacizi**: blocurile constructive din proteine; **exemple**:

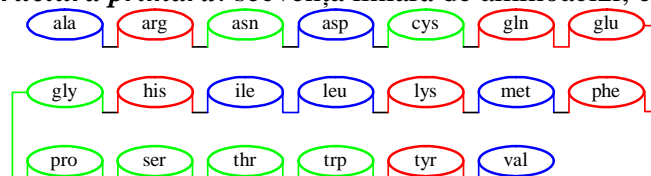
Aminoacid	Simbol	Formulă structurală	Formulă moleculară
Alanină	Ala A	$\begin{array}{c} \text{NH}_2 \quad \text{O} \\ \quad \\ \text{CH}_3\text{CH}-\text{C}-\text{OH} \end{array}$	$\text{C}_3\text{H}_7\text{NO}_2$
Arginină	Arg R	$\begin{array}{c} \text{NH} \quad \quad \quad \text{NH}_2 \quad \text{O} \\ \quad \quad \quad \quad \\ \text{H}_2\text{N}-\text{C}-\text{NHCH}_2\text{CH}_2\text{CH}_2\text{CH}-\text{C}-\text{OH} \end{array}$	$\text{C}_6\text{H}_{14}\text{N}_4\text{O}_2$
Asparagină	Asn N	$\begin{array}{c} \text{O} \quad \quad \quad \text{NH}_2 \quad \text{O} \\ \quad \quad \quad \quad \\ \text{H}_2\text{N}-\text{C}-\text{CH}_2\text{CH}-\text{C}-\text{OH} \end{array}$	$\text{C}_4\text{H}_8\text{N}_2\text{O}_3$
Aspartat	Asp D	$\begin{array}{c} \text{O} \quad \quad \quad \text{NH}_2 \quad \text{O} \\ \quad \quad \quad \quad \\ \text{HO}-\text{C}-\text{CH}_2\text{CH}-\text{C}-\text{OH} \end{array}$	$\text{C}_4\text{H}_7\text{NO}_4$
Cisteină	Cys C	$\begin{array}{c} \text{NH}_2 \quad \text{O} \\ \quad \\ \text{HSCH}_2\text{CH}-\text{C}-\text{OH} \end{array}$	$\text{C}_3\text{H}_7\text{NO}_2\text{S}$
Glutamat	Glu E	$\begin{array}{c} \text{O} \quad \quad \quad \text{NH}_2 \quad \text{O} \\ \quad \quad \quad \quad \\ \text{HO}-\text{C}-\text{CH}_2\text{CH}_2\text{CH}-\text{C}-\text{OH} \end{array}$	$\text{C}_5\text{H}_9\text{NO}_4$
Glutamină	Gln Q	$\begin{array}{c} \text{O} \quad \quad \quad \text{NH}_2 \quad \text{O} \\ \quad \quad \quad \quad \\ \text{H}_2\text{N}-\text{C}-\text{CH}_2\text{CH}_2\text{CH}-\text{C}-\text{OH} \end{array}$	$\text{C}_5\text{H}_{10}\text{N}_2\text{O}_3$
Glicină	Gly G	$\begin{array}{c} \text{O} \\ \\ \text{H}_2\text{NCH}_2-\text{C}-\text{OH} \end{array}$	$\text{C}_2\text{H}_5\text{NO}_2$

Histidină	His	H		C ₆ H ₉ N ₃ O ₂
Izoleucină	Ile	I		C ₆ H ₁₃ NO ₂
Leucină	Leu	L		C ₆ H ₁₃ NO ₂
Lisină	Lys	K		C ₆ H ₁₄ N ₂ O ₂
Metionină	Met	M		C ₅ H ₁₁ NO ₂ S
Fenilalanină	Phe	F		C ₉ H ₁₁ NO ₂
Prolină	Pro	P		C ₅ H ₉ NO ₂
Serină	Ser	S		C ₃ H ₇ NO ₃
Treonină	The	T		C ₄ H ₉ NO ₃
Triptofan	Trp	W		C ₁₁ H ₁₂ N ₂ O ₂
Tirosină	Tyr	Y		C ₉ H ₁₁ NO ₃
Valină	Val	V		C ₅ H ₁₁ NO ₂

÷ **proteine:**

- lanțuri de aminoacizi (numiți reziduuri);
- peptidă ≤ 40 reziduuri; proteină > 40 reziduuri;
- structura proteinelor - 4 nivele de interes:

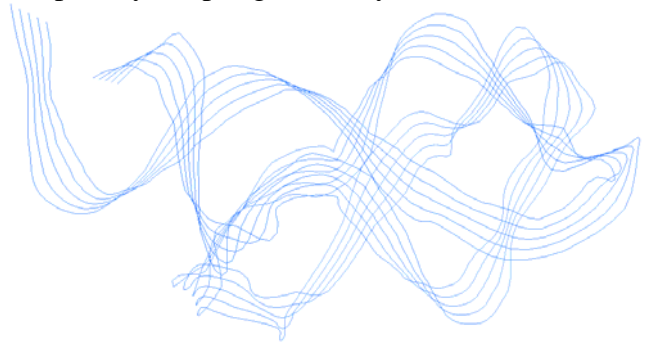
▪ **structura primară:** secvența liniară de aminoacizi; exemplu:



- **structura secundară:** referă lanțuri de aminoacizi care au o formă regulată (peptide) obținută în urma stabilirii de legături de hidrogen care saturează toți donorii și acceptorii de astfel de legături; două forme de structuri regulate sunt adoptate: spirala "α" și fibra "β"; cu However, a protein never keep a strictly linear form. The energy in the hydrogen bonds, disulfide bridges, the attraction between positive and negative charges, and radicals hydrophobic or hydrophilic, require a protein secondary structure, mainly helix or sheet. The molecules become more compact by adopting a tertiary structure



3dqb.pdb (spirale "α")



1y26.pdb (fibre "β")

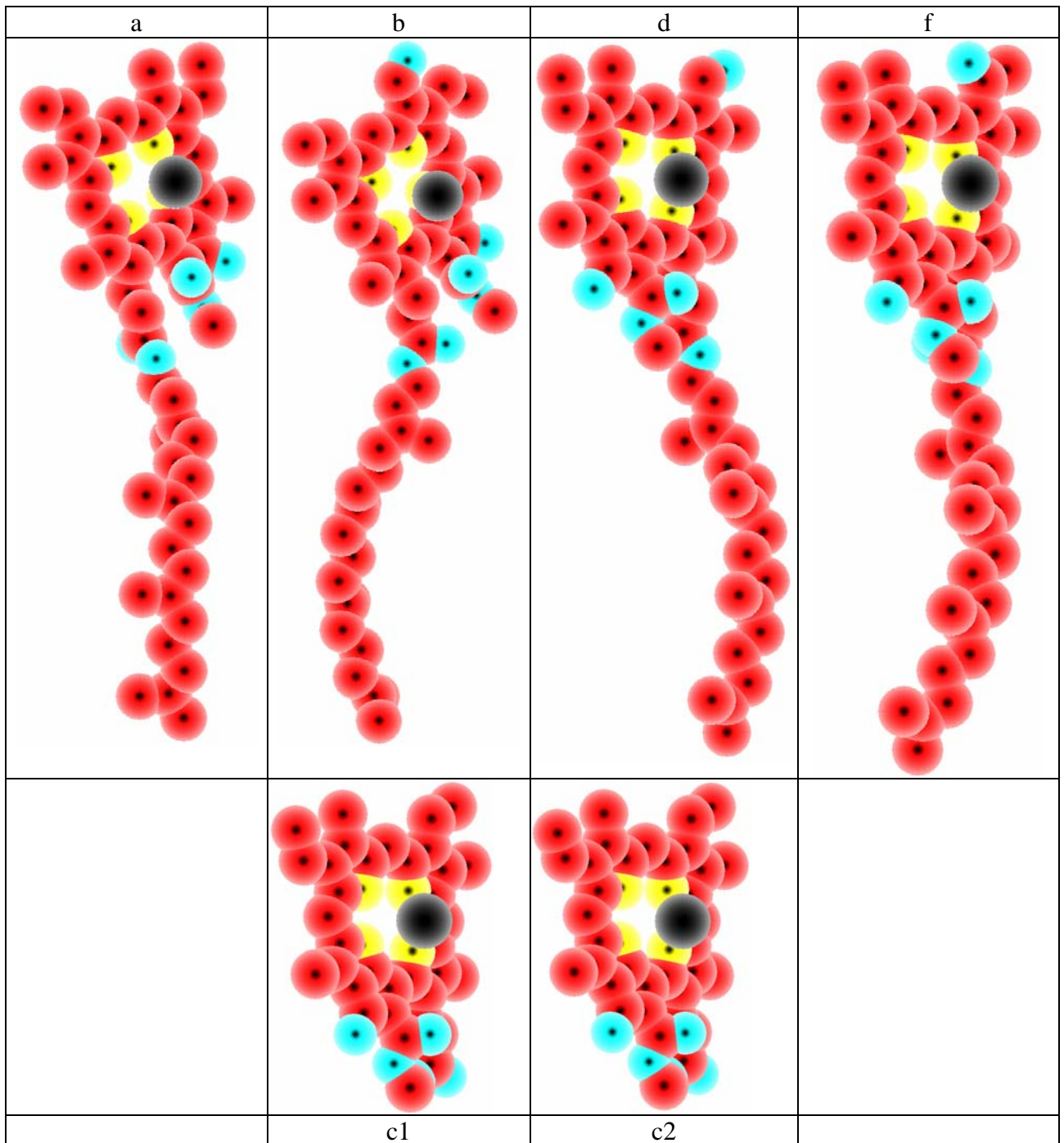
- **structura terțiară:** spiralele "α" și/sau fibrele "β" se împachetează compact (ca în figurile de mai sus); următoarele împachetări sunt frecvente:
 - **globulare:** împachetare prin "sechestrarea" de reziduuri hidrofobe de aminoacizi în nucleul proteic;
 - **de secreție:** împachetare prin punți -S-S- din cisteine;
 - **spirale spiralate:** între de la 2 la 7 spirale "α" (ca în "3ddb.pdb") stabilizate de forțe atractive între dipoli formați de alternanța aminoacizilor hidrofobi;
- **structura cuaternară:** reprezintă aranjamente cu rol funcțional de două sau mai multe proteine fixate steric; **exemplu:** hemoglobina, polimeraza ADN;



1gzx.pdb (șirul "α" al hemoglobinei):

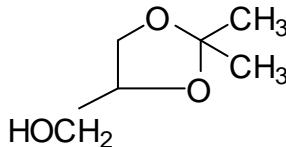
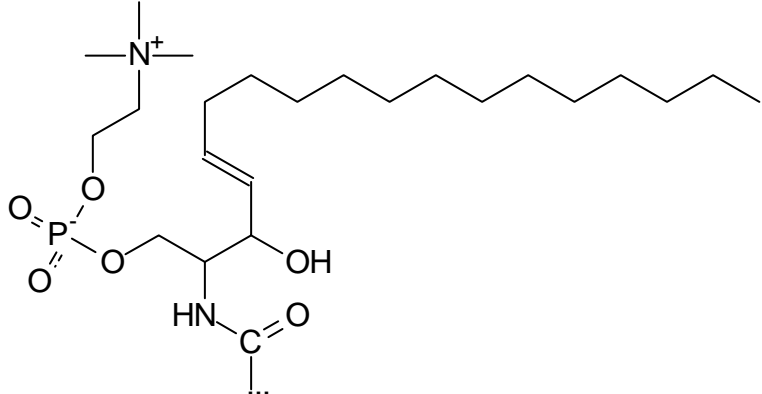
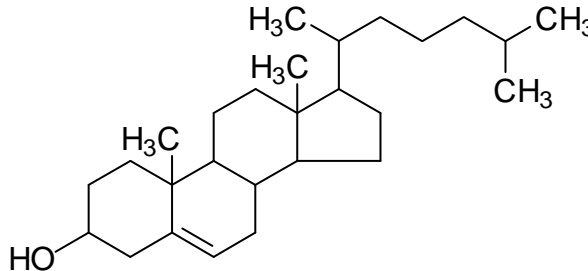
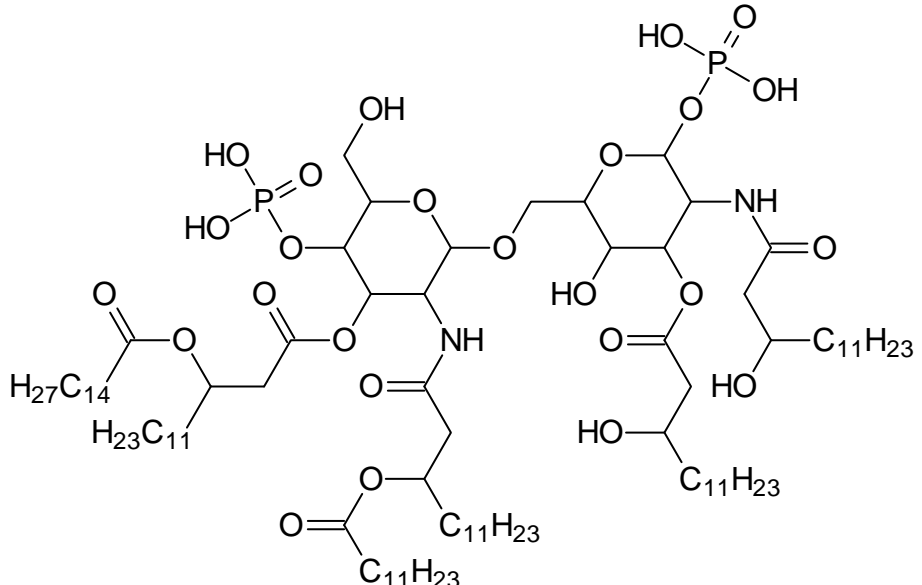
÷ **inele de porfirină:** specii ca hemul și clorofila; **exemplu - clorofila:**

Clorofila	Formula molec.	Prezentă în	Energie (fără/cu Mg/dif)		
a	C ₅₅ H ₇₂ O ₅ N ₄ Mg	Universal	91.523	89.711	1.812
b	C ₅₅ H ₇₀ O ₆ N ₄ Mg	Multe plante	93.617	91.819	1.798
c1	C ₃₅ H ₃₀ O ₅ N ₄ Mg	Diferite alge	96.225	94.456	1.769
c2	C ₃₅ H ₂₈ O ₅ N ₄ Mg	Diferite alge	95.285	93.516	1.769
d	C ₅₄ H ₇₀ O ₆ N ₄ Mg	Ciano-bacterii	94.596	92.865	1.731
f	C ₅₅ H ₇₀ O ₆ N ₄ Mg	Ciano-bacterii	95.140	93.403	1.737



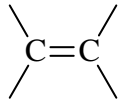
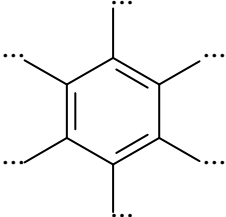
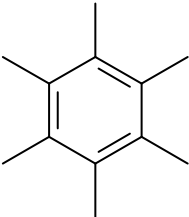
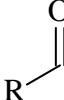
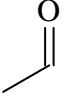
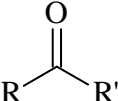
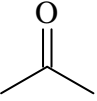
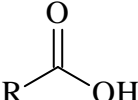
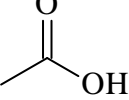
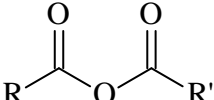
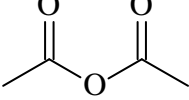
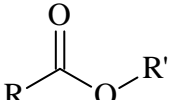
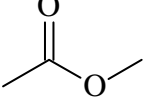
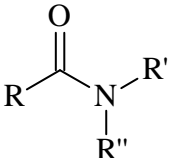
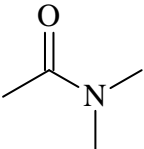
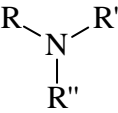

÷ **lipide**: asigură energia celulei, constituent de bază al membranei celulare, intră în compoziția hormonilor; se împart în mai multe categorii, dintre care: acizi grași, fosfolipide, glicerolipide, sfingolipide, , steroli, zaharolipide; **exemple**:

denumire	categorie	structură
acid n-dodecanoic	acid gras	
fosfatidilserina	fosfolipide	

acetonglicerol	glicerolipide	
sfingomielina	sfingolipide	
colesterol	sterol	
lipida "A" din E. coli	zaharolipide	

Grupuri funcționale: sunt grupuri specifice de atomi din interiorul moleculelor care sunt responsabile pentru reacțiile chimice în care sunt implicate moleculele. **Exemple:**

Clasă	Structură	Grup	Exemplu
Alcani	R—H	-	butan: C ₄ H ₁₀
Haloalcani	R—X X = F, Cl, Br, I	—X	iodoetan: C ₂ H ₅ I
Alcooli	R—OH	—OH	propanol: C ₃ H ₇ O
Eteri	R—O—R'	—O—	metoxietan: C ₃ H ₈ O
Tioli	R—SH	—SH	etantiol: C ₂ H ₆ S

Alchene	$\begin{array}{c} \text{(H)R} \quad \text{R'(H)} \\ \diagdown \quad / \\ \text{C}=\text{C} \\ / \quad \diagdown \\ \text{(H)R}'''' \quad \text{R}''(\text{H}) \end{array}$		dimetilpropenă: C ₄ H ₈
Arene			metilbenzen (toluen): C ₇ H ₈
Aldehyde			propanal: C ₃ H ₆ O
Cetone			pentanonă: C ₅ H ₁₀ O
Acizi carboxilici			acid propanoic: C ₃ H ₆ O ₂
Anhidride			anhidrida propanoică: (C ₃ H ₅ O) ₂ O
Esteri			metil etanoat (acetat de metil): C ₃ H ₆ O ₂
Amide			butanamidă: C ₄ H ₉ NO
Nitrili	R—C≡N	—C≡N	etannitril: C ₂ H ₃ N
Amine			trimetilamină: C ₃ H ₉ N