

Structura Moleculară – Aplicații Practice

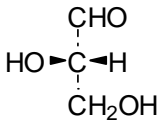
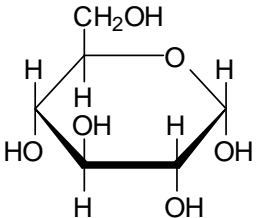
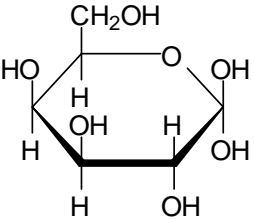
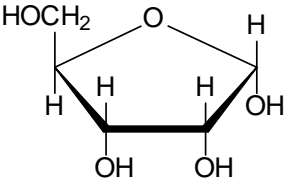
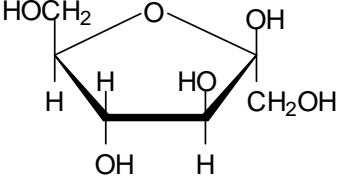
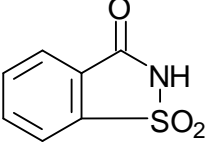
Obiective:

- Desenarea structurilor moleculare. (Problema 1)
- Construirea geometriei moleculare. (Problema 2)
- Calcularea polinomului caracteristic a unui compus pe baza structurii. (Problema 3)
- Utilizarea bazei de date PubChem pentru identificarea structurilor chimice. (Problema 4)

Cerințe

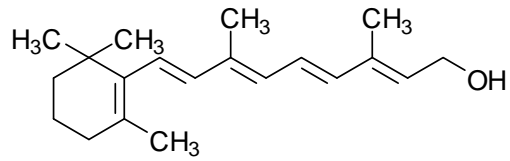
Problema 1. Desenați următoarele clase de molecule în HiperChem:

A. Zaharuri:

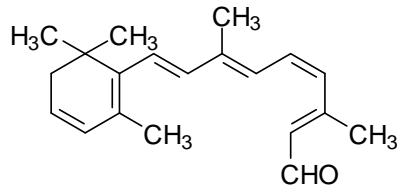
- D-gliceraldehida:

- D-glucoza:

- D-galactoza:

- D-riboza:

- D-fructoza:

- Zaharina:


Salvați moleculele într-un director denumit Zaharuri. Extensia fișierelor trebuie să fie *.hin (ex. fructoza.hin).

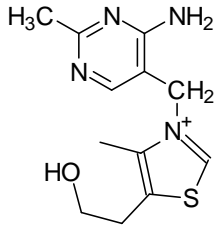
B. Vitamine



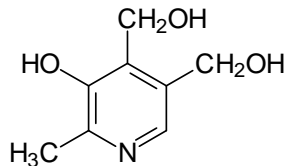
- Vitamina A:



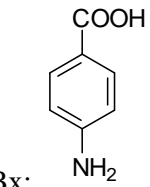
- Vitamina A2:



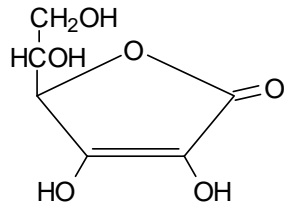
- Vitamina B1:



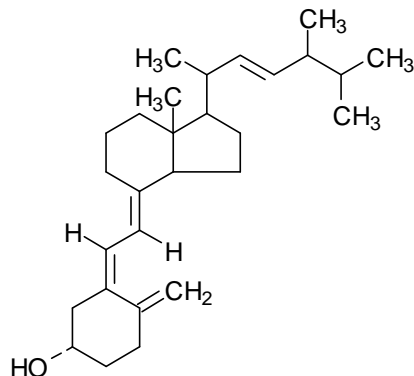
- Vitamina B6:



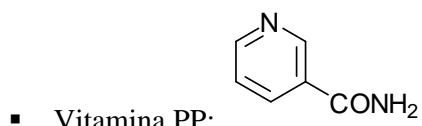
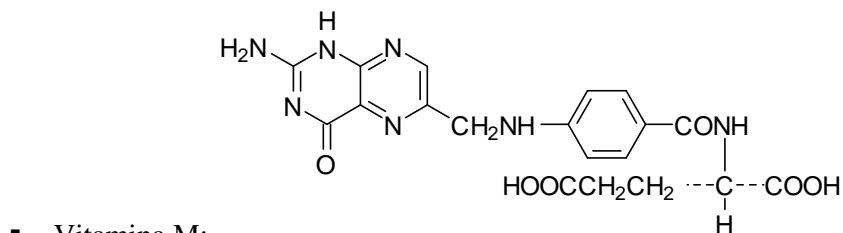
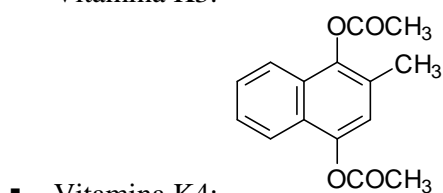
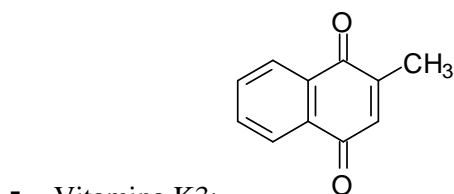
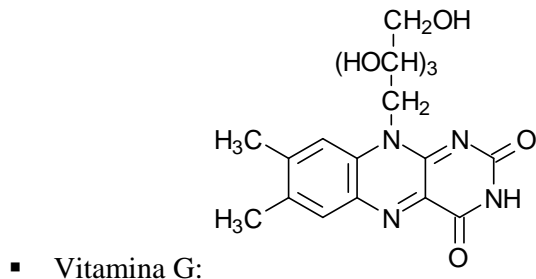
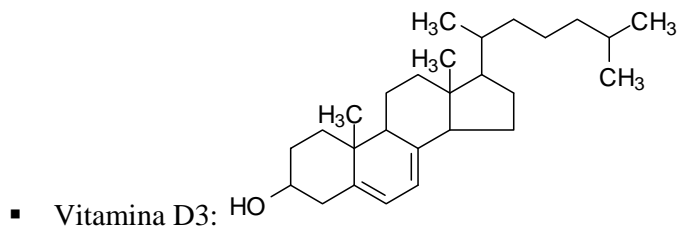
- Provitamina Bx:



- Vitamina C:

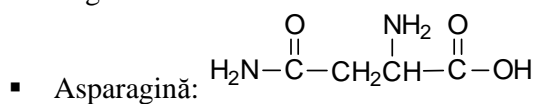
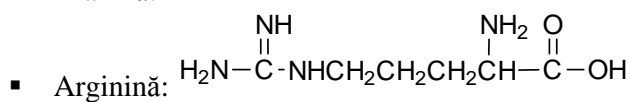
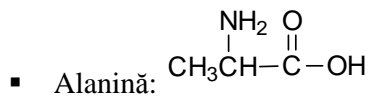


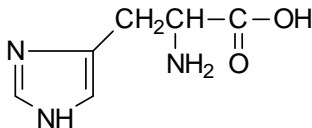
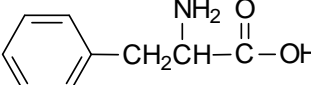
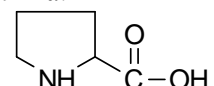
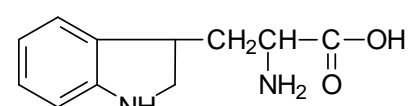
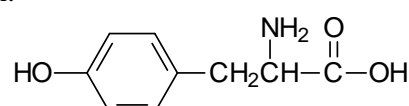
- Vitamina D2:

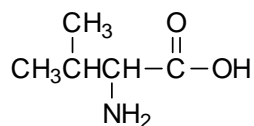


Salvați moleculele într-un director denumit Vitamine. Extensia fișierelor trebuie să fie *.hin (ex. pp.hin).

C. Amino acizi



- Aspartat: $\text{HO}-\overset{\text{O}}{\parallel}{\text{C}}-\text{CH}_2\overset{\text{NH}_2}{\underset{\text{O}}{\parallel}{\text{C}}}-\text{OH}$
- Cisteină: $\text{HSCH}_2\overset{\text{NH}_2}{\underset{\text{O}}{\parallel}{\text{C}}}-\text{OH}$
- Glutamat: $\text{HO}-\overset{\text{O}}{\parallel}{\text{C}}-\text{CH}_2\text{CH}_2\overset{\text{NH}_2}{\underset{\text{O}}{\parallel}{\text{C}}}-\text{OH}$
- Glutamină: $\text{H}_2\text{N}-\overset{\text{O}}{\parallel}{\text{C}}-\text{CH}_2\text{CH}_2\overset{\text{NH}_2}{\underset{\text{O}}{\parallel}{\text{C}}}-\text{OH}$
- Glicină: $\text{H}_2\text{NCH}_2-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH}$
- Histidină: 
- Isoleucină: $\text{CH}_3\text{CH}_2\overset{\text{NH}_2}{\underset{\text{O}}{\parallel}{\text{C}}}-\text{CH}(\text{CH}_3)-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH}$
- Leucină: $\text{CH}_3\overset{\text{CH}_3}{\underset{\text{O}}{\parallel}{\text{C}}}-\text{CH}(\text{CH}_3)\text{CH}_2\overset{\text{NH}_2}{\underset{\text{O}}{\parallel}{\text{C}}}-\text{OH}$
- Lisină: $\text{H}_2\text{NCH}_2\text{CH}_2\text{CH}_2\text{CH}_2\overset{\text{NH}_2}{\underset{\text{O}}{\parallel}{\text{C}}}-\text{OH}$
- Metionină: $\text{CH}_3\text{SCH}_2\text{CH}_2\overset{\text{NH}_2}{\underset{\text{O}}{\parallel}{\text{C}}}-\text{OH}$
- Fenilalanină: 
- Prolină: 
- Serină: $\text{HOCH}_2\overset{\text{NH}_2}{\underset{\text{O}}{\parallel}{\text{C}}}-\text{OH}$
- Treonină: $\text{CH}_3\overset{\text{OHCH}_3}{\underset{\text{O}}{\parallel}{\text{C}}}-\text{CH}(\text{CH}_3)-\overset{\text{O}}{\parallel}{\text{C}}-\text{OH}$
- Triptofan: 
- Tirosină: 



- Valină:

Salvați moleculele într-un director denumit aa. Extensia fișierelor trebuie să fie *.hin (ex. fructoza.hin).

Problema 2. Construiți modelul molecular al structurilor desenate.

Problema 3.

- Calculați pentru zaharuri polinoamele caracteristice asociate structurilor moleculare.
- Care este cea mai bună valoare a lui X care corelează cel mai bine cu valorile zaharurilor (valorile se găsesc în Cursul 2).

Problema 4. Identificați proteine prin utilizarea bazei de date PubChem.

INSTRUCȚIUNI

Problema 1.

- În mod implicit elementul chimic în HiperChem este carbonul (^C^). Pentru a alege alt atom: [Build – Default Element...].
- Nu este necesară desenarea atomilor de hidrogen!
- Salvați structura creată ([File - Save As...]/ CTRL+S) cu denumirea cerută, în folderul asociat fiecărei clase de compuși.

Problema 2.

- Deschideți structura în HiperChem.
- Construiți modelul molecular: [Build – Add H & Model Build].
- Salvați structura.

Problema 3.

- Pentru calcularea polinoamelor caracteristice utilizați resursa online: http://l.academicdirect.org/Fundamentals/Graphs/polynomials/a_characteristic_polynomial_in.php
- Pentru calcularea polinoamelor caracteristice aveți nevoie de structurile *.hin.
- Realizați o foaie de calcul Excel cu următoarele coloane:
 - Denumire compus (7 compuși)
 - Valoare măsurată (vezi Cursul 2).
 - Polinomul caracteristic.
 - X=1
 - X=2
 - X=3 ...

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

- Identificați valoarea lui X care înlocuită în formula polinomului caracteristic corelează cel mai bine cu valorile măsurate. Utilizați resursa online: http://l.academicdirect.org/Statistics/linear_dependence/. Se consideră o corelație pozitivă semnificativă statistic dacă valorile tuturor coeficienților de corelație (Pearson, Spearman, Semi-

Cantitativ, Kendall tau și Gamma) sunt semnificative statistic.

- Salvați fișierul cu denumirea zaharuri.xls în directorul zaharuri.

Problema 4.

- Pentru a identifica structurile chimice utilizați baza de date PubChem (<http://pubchem.ncbi.nlm.nih.gov/>).
- Identificați și salvați într-un director denumit PubChem structurile 3D pentru următorii compuși:

▪ Apigenin	▪ Dihydroxymethoxychlor olefin	▪ Mestranol	▪ Norethynodrel
▪ Aurin	▪ Dimethylstilbestrol	▪ Methyl paraben	▪ Phenolphthalein
▪ Baicalein	▪ Diphenolic acid	▪ Monobenzene	▪ Phenolphthalin
▪ Benzoresorcinol	▪ Doisynoestrol	▪ Monohydroxymethoxychlor	▪ Phenolsulfonphthalein
▪ Benzylparaben	▪ Droloxifene	▪ Monohydroxymethoxychlor olefin	▪ Phloretin
▪ Butyl paraben	▪ Equol	▪ Monomethyl ether diethylstilbestrol	▪ Propyl paraben
▪ Carbonochloridic acid	▪ Estriol	▪ Monomethyl ether hexestrol	▪ Prunetin
▪ Chalcone	▪ Estrone	▪ Moxestrol	▪ Raloxifene
▪ Chlorocresol	▪ Ethylparaben	▪ Myricetin	▪ Sanidril
▪ Clomiphene	▪ Ethynylestradiol	▪ Nafoxidine	▪ Tamoxifen
▪ Coumestrol	▪ Fisetin	▪ Naringenin	▪ Toremifene
▪ Daidzein	▪ Formononetin	▪ Nonylphenol	▪ Triphenylethylene
▪ Dichlorophen	▪ Genistein	▪ Nordihydroguaiaretic acid	▪ Zearalanone
▪ Dienestrol	▪ Hexestrol		▪ Zearalenol
▪ Diethylstilbestrol dimethyl ether	▪ Hydrocinchonine		▪ Zearalenone
▪ Diethylstilbestrol	▪ Kaempferol		
	▪ Kepone		