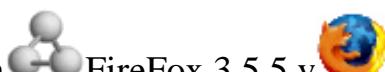


Name Surname: _Teaccher_, Teacher_ Group № ____ Data _Teacher_ 2025 Year

A. RSU Protocol of Task to Student:<http://aris.gusc.lv/06Daugavpils/Research/NucleoSomeAS.pdf>

B. Task for student practical introduction for the use of Interactive Molecule viewers:



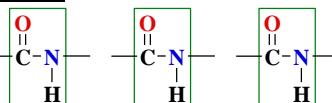
Chemscape **RasWin** FireFox 3.5.5.v lunch the application California Lutheran University professor **David Marcey** 2003. prepared **DNA binding proteins Histones**

Octamere molecules <http://aris.gusc.lv/ChemFiles/CLUnucleosome/nucleosome.htm> created by assistant professor **Aris Kaksis 2025** for practical work at Riga Stradin's University.

To investigate the atoms making up the molecule structure using the **CPK** color scheme 1965 at Display conditions: **Stick** (on Menu Stripe) **Ball & Stick** **Spacefill**

| Atom Name | Symbol | Color | Valence Number |
|---------------|------------------|-----------------------|--------------------------------------|
| Carbon | C | Gray lightly or Black | 4 |
| Hydrogen | H | White | 1 |
| Oxygen | O | Red | 2 (donor acceptor ligand up to 4) |
| Nitrogen | N | Bluish | 3 + 1(donor acceptor ligand up to 4) |
| Sulfur | S | Yellow | -2, +6 |
| Phosphor | P | Yellow Intensive dark | 5 (& 3) |
| Sodium ion | Na ⁺ | Blue | +1 (coordination up to 6) |
| Magnesium ion | Mg ²⁺ | Green | +2 (coordination up to 6) |
| Calcium ion | Ca ²⁺ | Gray Dark | +2 (coordination up to 6) |
| Iron ion | Fe ²⁺ | Yellow Gray | +2 (coordination up to 6) |
| Iron ion | Fe ³⁺ | Yellow Gray | +3 (coordination up to 6) |

USA patent Journal publication of scientists **Corey, Pauling, Koltun** for atomic modeling
Protein Backbone is **Cα trace**



Polypeptide of Amino Acids
Side chains: **Hydrophobic**
Polar pH=7.36
Acidic-COO⁻ negative
Basic-NH₃⁺ positive

3. Call 8 **Histones** the Nucleosome core Particle quaternary structure eight Protein subunits?
4. Explain eight **Histone** proteins similarity pattern! 2*H2A, 2*H2B, 2*H3 and 2*H4.....
5. Which are copies each to other? H2A+H2A, H2B+H2B, H3+H3, H4+H4.....

H3 tails said strand modification shapes in DNA functions for human **HOMEOSTASIS**

Acetyl transferases link acetyl group, -CO-CH₃; Me, methylation enzymes of =N- or -O-CH₃:

Ac, acetylation enzymes:
Deacetylases remove Acyl;
P, Phosphorylation -OP₃²⁻
enzymes=kinases, phosphate hydroxyl group ester formation or remove;
Ub, ubiquitination enzymes
Ligases polypeptide chain cleavage and remove for degrading

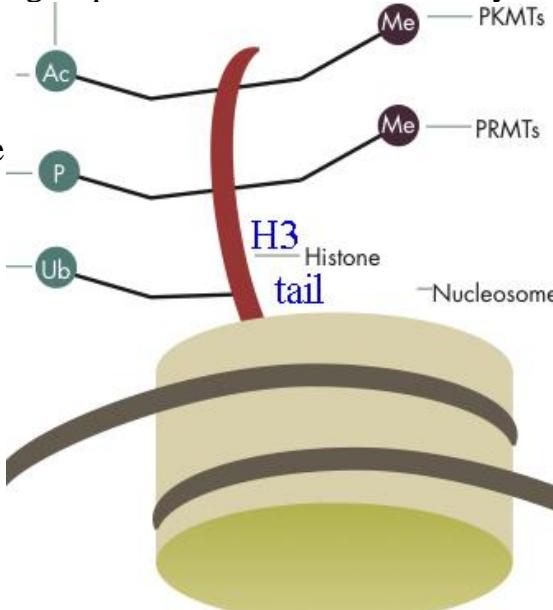
HEALTH ENDPOINTS:

Cancer

Autoimmune disease

Mental disorders

Diabetes



PKMT: Lysine (K) Lys methyl transferase;
PRMT: Arginine (R) Arg methyl transferase;
Methylation, Demethylation
H2A, H2B, H3, H4

EPIGENETIC FACTORS

The binding of epigenetic factors to histone "tails" alters the extent to which DNA is wrapped around histones and the availability of genes in the DNA to be activated for expression.

6. What geometric meaning has the octameric disk? Draw core of 8 subunit disk picture!
7. What six amino acid residues on histone tail polypeptide chain epigenetic markers linkage site endpoints are targets for: Thr22-OH,Lys23-N⁺H₃,Arg26-N⁺H₃,Lys27-N⁺H₃, Ser28-OH,Thr32-OH.....
7. 1. acetylation, -CO-CH₃ amino AA -N⁺H₃ groups of residues for amino acids -HN-CO-CH₃ acyl group?Lys23-N⁺H₃,Arg26-N⁺H₃,Lys27-N⁺H₃
7. 2. phosphorylation, HOP₃²⁻ at AA-OH hydroxyl groups of residues for amino acids AA-OPO₃²⁻?Thr22-OH,Ser28-OH,Thr32-OH.....
- 7.3 methylation -CH₃ positions at amino AA-N⁺H₃ groups of residues for AA-HN-CH₃ methyl group?Lys23-N⁺H₃,Arg26-N⁺H₃,Lys27-N⁺H₃
8. What kind secondary structure motifs comprise each Histone tertiary structure fold protein?

Name Surname: _Teaccher_,_Teacher_ Group № ____ Data _Teacher_ 2025 Year

..... alpha1-loop1-alpha2-loop2- alpha3.....

9. What two hetero dimmers constitute the Histone disk?two each of H3-H4 and H2A-H2B

10. How many hetero dimers of 2 protein subunits make up Histone disk–Nucleosome core Particle?.....two each of H3-H4 and H2A-H2B

11. What is size of Nucleosome core Particle **Histone** in angstroms Å along the symmetry axis? Select “Distance” and make five measurements of histone disk diameter in angstroms Å!

.....67.9Å.....67.3Å.....67.0Å.....73.1Å.....67.9Å.....

12. Which four helices of H3 and H4 Histones form the four-helix bundle **tetramer**?

..... alpha2-loop2- alpha3+alpha2-loop2- alpha3.....

13. With which **dimmer tetramer** begins association the DNA in the **first step of Nucleosome assembly, DNA packaging** in the nucleus of Cells about **Chromosomes**? (H3-H4)₂

14. What three intermolecular forces (underline those) bind in hetero dimmers like H3-H4 arrangement with two monomers of totally known in medical chemistry five intermolecular forces?

What three intermolecular forces (underline those) bind the four-helix bundle **tetramer** and how hetero dimmers H2A-H2B binds to **tetramer** (H3-H4)₂ if each **quaternary structure hetero dimmer** binds to the **tetramer** via another, homologous, four-helix bundle (alpha2 and alpha3 from both H2B and H4), joining the H2B and H4 histone folds of totally known in medical chemistry five intermolecular forces?

1.Hydrogen,2.Hydrophobic,3.Salt bridge,4.sulfur -S-S- disulfide bridge,5.coordinative donor-acceptor bond

15. Draw structural molecular units of three chosen intermolecular bonds which binds to **tetramer** (H3-H4)₂ two **dimers** H2A-H2B:



16. How many double helical DNA base pairs are wrapped around the quaternary structure of histone octa mere disk in a DNA super helix two turns?

.....146 bp of double helical DNA are wrapped around histone octa mere disk.....

17. What three intermolecular forces (underline those) bind to the histone octa mere in a DNA super helix two turns around?

1 Hydrogen,2Hydrophobic,3Salt bridges,4sulfur-S-S-disulfide bridges,5coordinative donor-acceptor bonds

18. Draw structural molecular units of three chosen intermolecular bonds **DNA & Histones**:



19. What is the DNA two fold diameter size in angstroms Å around octa mere of the symmetric **quaternary structure with DNA 146 bp** fragment?

Select “Distance” and make five measurements of DNA disk diameter in angstroms Å!

.....101,2Å.....100.4Å.....101.2Å.....103.2Å.....104.0Å.....

20. What times wraps DNA super helix around histone octamere core disk?

...DNA super helix wraps around the histone octamere core disk in **1.65turns**.....

21. What **base pairs** are half coil around nucleosome?.....each half 73 base pairs.....

22. Are left-handed (clock wise) or right-handed (counter clock wise)?

..... **left-handed DNA super helix** wraps around the histone core

23. Human DNA total length is 2.1meters

constitute **4 934 582 000±5000**base pairs

with two type base pairing **adenine**=**thymine** with two hydrogen bonds and **guanine**=**cytosine** with three hydrogen bonds as human **DNA** total size!

24. What the number of histone octamere nucleosomes are necessary in cell division process to synthesize human chromosomes if in one set 23 chromosomes contain **DNA** with content

..... **4 934 587 000 base pairs** ?

..... 4934587000/146*2=2*33798541=67.6 million nucleosomes.....