Name Surname: _____,_____ Group Nº ____ Data _____ 2018. Year

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

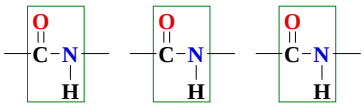
B. Task for student practical introduction for the use of Interactive Molecule viewers:

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 2018** 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** **USA** patent **Journal** publication of scientists **Corey, Pauling, Koltun** for atomic modeling

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)

Protein **Backbone** is **Cα** trace



Polypeptide of Amino Acids

Side chains: **Hydrophobic** **Polar pH=7.36** **Acidic-COO^- negative** **Basic–NH_3^+ positive**

3. Call 8 **Histones** the Nucleosome core Particle quaternary structure eight Protein subunits?

4. Explain eight **Histone** proteins similarity pattern! .....

5. Which are copies each to other? .....

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

Acetyl Acetyl transferases link acetyl group, **-CO-CH_3**; Me, methylation enzymes of **=N-** or **-O-CH_3**:

Ac, acetylation enzymes: Deacetylases remove Acyl;

P, Phosphorylation **-OPO_3^{2-}** enzymes=kinases, phosphate hydroxyl group ester formation or remove;

Ub, ubiquitination enzymes Ligases polypeptide chain cleavage and remove for degrading

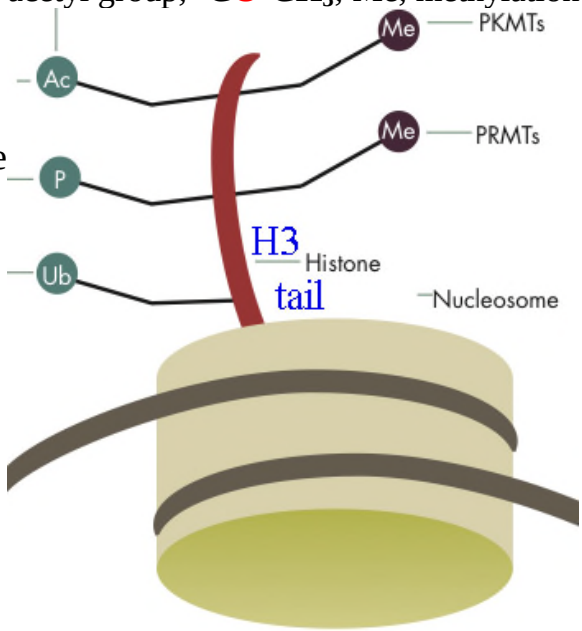
HEALTH ENDPOINTS:

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:.....

7. 1. acetylation, **-CO-CH_3** amino **AA-N^+H_3** groups of residues for amino acids **-HN-CO-CH_3** acyl group? ....

7. 2. phosphorilation, **$HOPO_3^{2-}$** at **AA-OH** hydroxyl groups of residues for amino acids **AA-OPO_3^{2-}** ? ....

7. 3. methylation **-CH_3** positions at amino **AA-N^+H_3** groups of residues for **AA-HN-CH_3** methyl group? ....

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8. What kind **secondary structure** motifs comprise each Histone tertiary structure fold protein?
.....

9. What two hetero dimmers constitute the Histone disk?.....

10. Haw many hetero dimmers of 2 protein subunits make up Histone disk–Nucleosome core Particle?.....

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**!
.....**Å**.....**Å**.....**Å**.....**Å**.....**Å**.....

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

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**? .....

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** $(H3\text{-}H4)_2$ 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** $(H3\text{-}H4)_2$ two **dimers** H2A-H2B:
1.... **2**..... **3**... .....

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?
.....

17. What three intermolecular forces (underline those) bind to the histone octa mere in a **DNA** super helix two turns?
1 **Hydrogen**,2**Hydrophobic**,3**Salt bridges**,4**sulfur**-**S**-**S**-**disulfide bridges**,5**coordinative** donor-acceptor **bonds**

18. Draw structural molecular units of three chosen intermolecular bonds **DNA** & **Histones**:
1.... **2**.... **3**.

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**!
.....**Å**.....**Å**.....**Å**.....**Å**.....**Å**.....

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

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

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

23. Human **DNA** total length is .....meters constitute .....**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=.....million nucleosomes.....