

**Phospholipid Bilayer Membrane** helping material for research of molecules in address:

<http://aris.gusc.lv/06Daugavpils/Engl/LipdBiLayerMembran.pdf> **A. Task** for practical research works:  
<http://aris.gusc.lv/06Daugavpils/Engl/PhosphLipidBilayerMembran.pdf> for Interactive Molecule viewers:



Chemscape MDL **MDL** ISIS Draw **ISIS** RasMol **RasMol** FireFox 3.5.5v **B task** To the molecule structure lunch the Riga Stradin's University assistant professor **Aris Kaksis 2019**. prepared **Phospholipid Bilayer Membrane** molecules experimental research practical work 1: <http://aris.gusc.lv/ChemFiles/BilipidCholine/Membrane/Membrane/membrane/Membrane.html> **Phosphatidyl**

**Choline, Lecithin:** Hydrophobic & Hydrophilic molecule Biphilic in the **CPK** color scheme:

at Display conditions: **Stick** (on Menu Stripe) **Ball & Stick** **Spacefill**

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

the **CPK** color scheme 1965

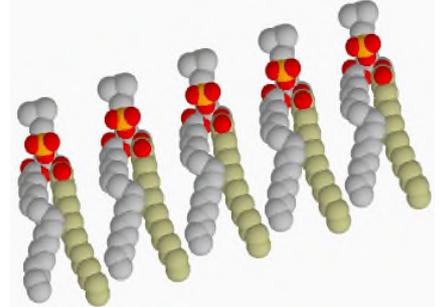
**Nature Journal**

publication of scientists

**Corey, Pauling, Koltun**

for atomic modeling

Positive(+) and negative(-) charge



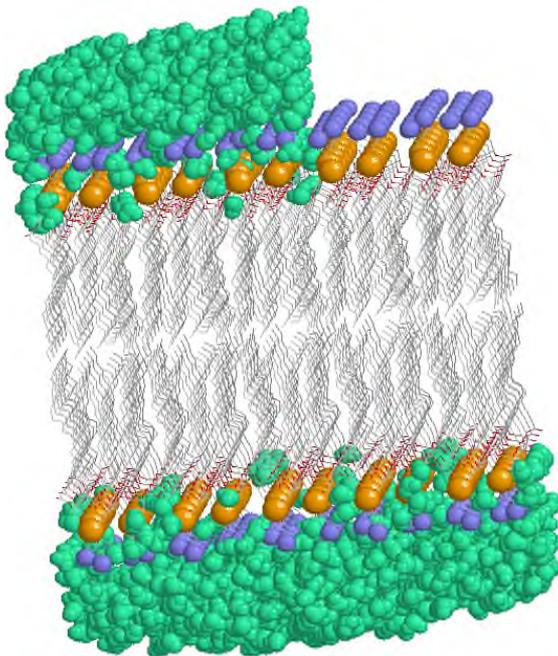
Hydrophobic non polar molecule part

**1. Write the main Physiological function of **Phospholipid Bilayer Membranes** in Life?**

**Membrane waterless Interior** is impermeable for **water** molecules and **water solutes**..... so work as .....

**2. What the Structure Properties has Interior, Exterior. What the biological destiny has cells wall building in liposomes, organelles and **Monolayer** in lipoprotein vesicles. **Water medium green**.**

**3. Draw Phosphatidyl Choline-Lecithin Structure Formula and water **H<sub>2</sub>O** 1,4 Å size dipole molecule!**



Choline, Phosphate, Glycerol, Palmitate **C16:0**

ω number are unsaturated account from tail methyl group **-CH<sub>3</sub>**  
 Essential omega Fatty Acids :  
 ω=6 and ω =3

**4. Show Choline , Phosphate, Glycerol, Palmitate, Oleate ester bonds 7 carbon contact points with**

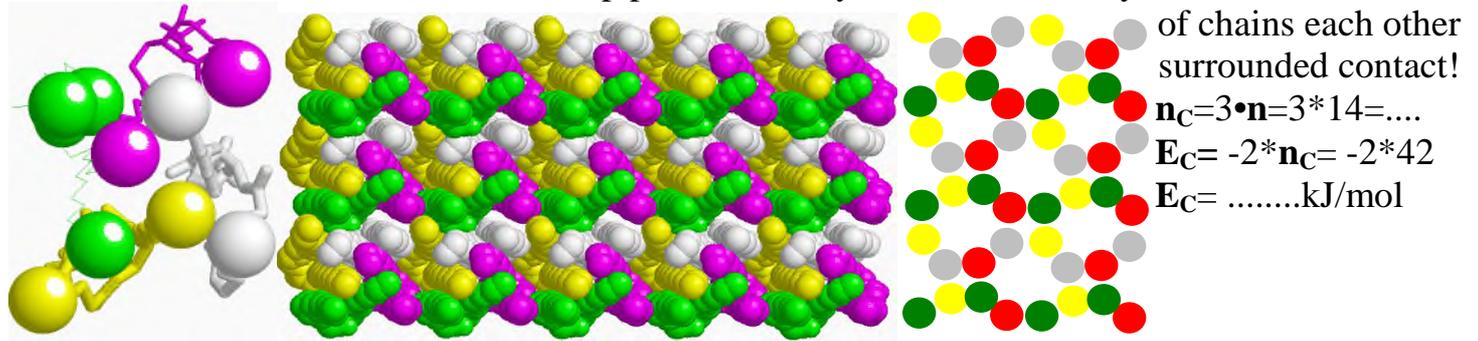
5. Draw essential Fatty Acid Salts at pH=7.36 :  $\omega=6$  C18:2 and  $\omega=3$  C18:3

linoleic acid salt

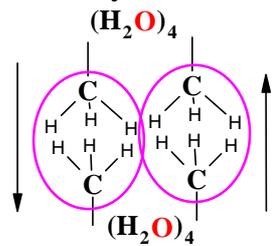
$\alpha$ -linolenic acid salt

6. Calculate accumulate London Forces -2 kJ/mol Bonding Energy between two hydrogen contacts at each of 7 carbon methylene -CH<sub>2</sub>- on Palmitate & Oleate chains contact  $n=7 \cdot 2=$ .. points!  $E = -2 \cdot 7 \cdot 2 = -2 \cdot n = -2 \cdot 14 = \dots\dots$  kJ/mol

7. On drawn tetramer -CH<sub>3</sub> structure top pattern of fatty acids chains Bilayer detect Number 3



8. What is London Forces made Energy  $E_L$  of Phosphatidyl Choline molecule having two Fatty Acid hydrocarbon chains?  $n_L = 2 * n_C = 2 * 42 = \dots\dots$  contacts  $E_L = -2 * n_L = \dots\dots$ kJ/mol



9. What Hydrophobic interaction Forces -10kJ Energy  $E_H$  are per one Phosphatidyl Choline of both side **Water** tetramer structures (H<sub>2</sub>O)<sub>4</sub> as detected number six contact points for two methyl group's hydrogens -CH<sub>3</sub> for two chains Palmitate C16 and Oleate C18:1 in two Phosphatidyl Choline molecules opposite Bilayer contacts  $n_H = 2 \cdot 3 = \dots\dots$  and energy for one Phosphatidyl Choline molecule  $E_H = -10 \cdot 3 / 2 = -60 / 2 = \dots\dots$ kJ/mol?

10. What total Bonding Force Energy per one Bilayer **Phosphatidyl Choline** molecule? Each single phospholipid in membrane distributed London Forces -2 kJ/mol for 84 contact points -168 kJ/mol adds **hydrophobic** interactions Energy -30 kJ/mol forming total sum on Phosphatidyl Choline.  $E_{Bond} = -168 + (-30) = \dots\dots\dots$ kJ/mol

11. Measure the thickness of **Phospholipid Bilayer Membrane** using right button click on interactive picture and in menu chose "select", "Mouse Click Action", "Distance". Experimentally measure the thickness of **Membrane** performing by mouse two clicks: 1) on **blue nitrogen** atom one side and following click on **blue nitrogen** atom opposite side of **Membrane**. On status bar is shown distance value in angstroms  $\dots\dots\dots \text{\AA}$ . Get the average size of Membrane thickness as mean  $Dist_{mean} = \dots\dots\dots \text{\AA}$  as  $\dots\dots\dots$  nm !

12. What number of 1.4 Å size water molecules cover the distance 56 Å?  $56 / 1.4 = \dots\dots$  times

13. What would be thickness in meters of home buildings walls if human average tall size is 1.75 meters?  $\dots\dots\dots$  So wall (membrane) cross channel would be  $1.75 \cdot 40 = \dots\dots\dots$  meters long .

14. What kind of pure Phosphatidyl Choline bilayer membrane physical state is liquid or solid?.....

15. What mass fraction constitute the Phosphatidyl Choline molecules in cellular membranes total mass 100%?  $\dots\dots\dots$

- I) 1/3 part constitute **Phospholipids** which mass fraction of **Membranes** to make **33.3%** of total mass 100%;
  - II) second 1/3 part **Cholesterols** which mass fraction of **Membranes** to make **33.3%** of total mass 100%;
  - III) third 1/3 part **Membranes integral Proteins** which mass fraction to make 33.3% of total mass 100%
- Bulk mass fraction **20%** goes to **Aquaporins** for other remains **13.3%** are constitute four type **Proteins**:

The **Cholesterol/PhosphoLipid** C/PL mole ratio of human red cell membranes ranges from a normal value of 0.9–1.0 (Journal of Cellular Biochemistry 2004 V8, 4, p 413-430). 1 mol cholesterol against 1 mol Phospholipid.

**C. Task Cholesterol Steroid Lipid** All atoms **C27** **H46** **O** colored **CPK** labels in work2:

<http://aris.gusc.lv/ChemFiles/BilipidCholine/Membrane/Cholesterol/CholesterolMembran.html>;

1. Draw in Cholesterol four carbon rings **A,B,C & D** solid frame structure

2. Draw four cyclic rings Structure of **Cholesterin** with **linoleate fatty acid** ester!

Call the four cyclic rings Structure of **Cholesterin** with linoleate **C18:2** hydro carbon chain!

stabilized by double bond between carbon atoms  $>C=C<$  5 and 6, alcohol **HO-** at carbon 3, angular methyl groups  $-CH_3$  labeled 18 and 19, flexible tail 3 splinter  $-CH_3$ , fork, rod are good clutch fixing chains of hydrocarbon mechanically in phosphatidyl choline bilayer **membrane**.

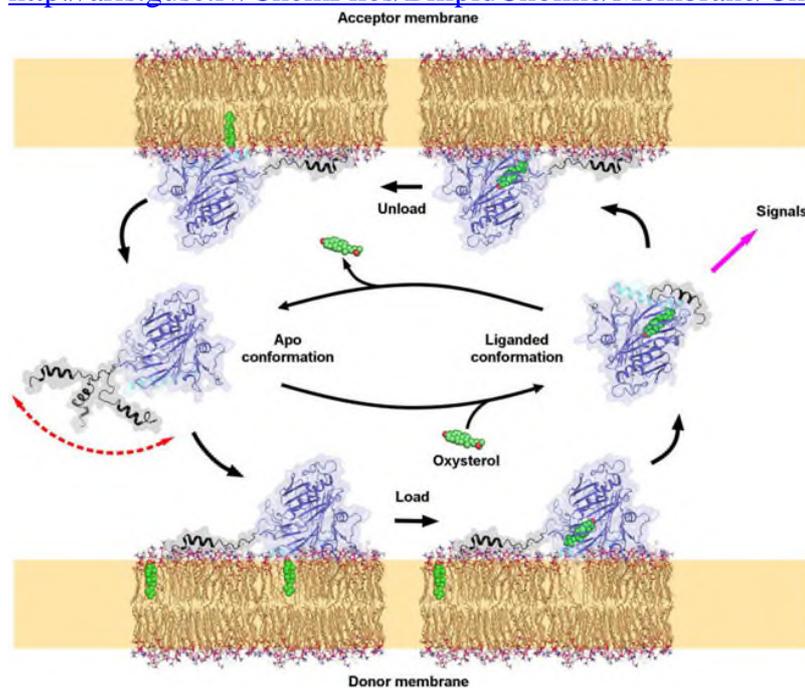
**Cholesterol/Phospho Lipid** mole ratio of human membranes a normal value of 0.9–1.0.

3. What three Cholesterol functions of Human body? .....

4. What is Cholesterol 1/3 mass fraction eukaryote membranes of total 100%?.....

5. Cholesterol/Phospholipid rate in erythrocyte membranes .....!published in 1978.Year

<http://aris.gusc.lv/ChemFiles/BilipidCholine/Membrane/Cholest5ene3-20diol/Cholesterol5Membran.html>;



**OSBP** oxi-sterol transport protein involved in cholesterol metabolic transport through membranes surface, that keep 33.3% mass fraction 1/3 100% membrane mass. Cholesterol upload and unload from to membranes. **Lipocalins** mechanism like **OSBP**, retinol **ORPs** and other **Lipocalins** A,K,E,D vitamin transport proteins. Human organism has 12 **OSBP** iso forms. To investigate **Osh4** human protein iso form **OSBP4** for steroids:

**Cholesterol CRL.pdb**,

20-hidroksiholessterols HC2\_ideal.pdb,

25-hidroksiholessterols HC3\_ideal.pdb,

7-hidroksiholessterols HCR\_ideal.pdb

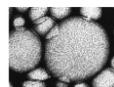
6. What name molecules which in human transport cholesterol, A, K, E, D vitamins, hormones fats and fatty acids? .....

7. Writ lipids five transport forms in lipoproteins! Aggregates, structure, localization, geometry, content of forming parts! .....

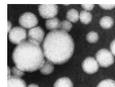
**Lipoproteins...**

**Albumin** .....

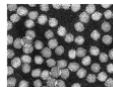
80...200 nm



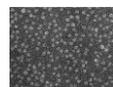
28...70 nm



20...25 nm



8...12 nm



8. Writ two transport forms of lipocalins! .....

9. What three mass fractions 1/3,1/3,1/3 constitute cell **membranes** 100% mass?.....