




Phospholipids Bilayer Membrane composite materials for compartmentation of organelles:

Task for practical research works: for Interactive Molecule:

Chemscape MDL  ISIS Draw  RasMol  FireFox 3.5.5v **B** task to lunch the Riga Stradin's University Aris Kaksis 2023rd prepared **Phospholipids Bilayer Membrane**

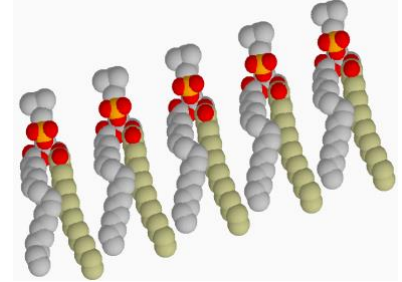
experimental research practical work :

htdocsLocal <http://aris.gusc.lv/ChemFiles/BilipidCholine/Membrane/Membrane/membrane/Membrane.html>

Phosphatidyl Choline, Lecithin: molecule Biphilic Hydrophobic & Hydrophilic **CPK** color scheme 1965:

at Display conditions: **Stick** (on Menu Stripe) **Ball & Stick** **Spacefill** In Nature **Journal Corey, Pauling, Koltun** publication for atomic modeling Positive(+) **N⁺** and negative(-) **O⁻** charge

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)



Hydrophobic non polar molecule part

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

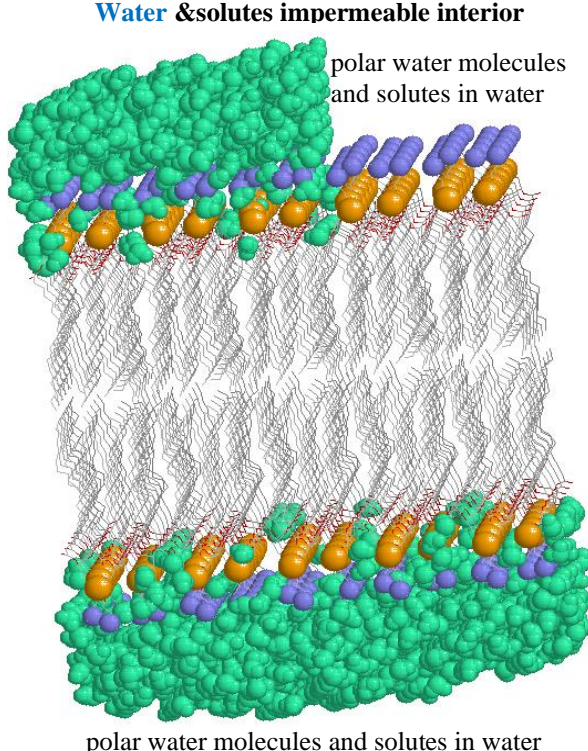
Membrane Interior is impermeable forand **water**.....

so work as **isolating cellular wall** for **compartment**

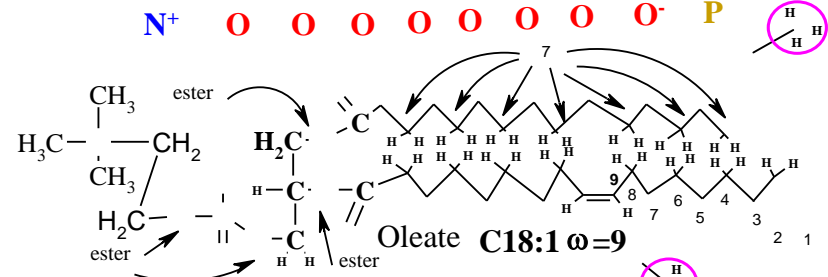
2. What the Structure Properties has Interior, Exterior. What the biological destiny has **cells wall** building in **liposomes, organelles** and **Monolayer** in lipoprotein **vesicles**. **Water medium green**.

Components exterior can not cross membrane Interior

3. Put in phosphatidyl holine structure!

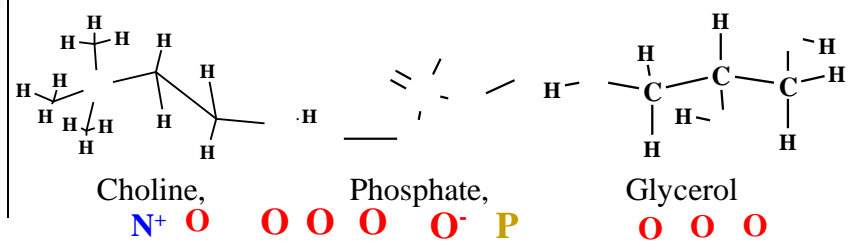
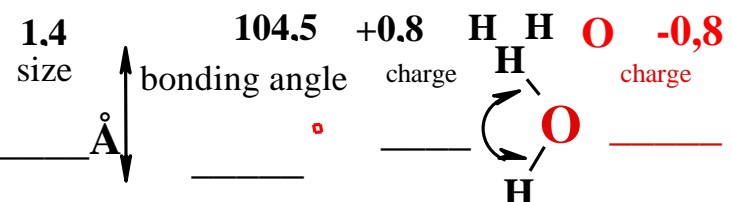


4.B Put atoms for: water size, angle, charge, Choline, Phosphate, Glycerol!

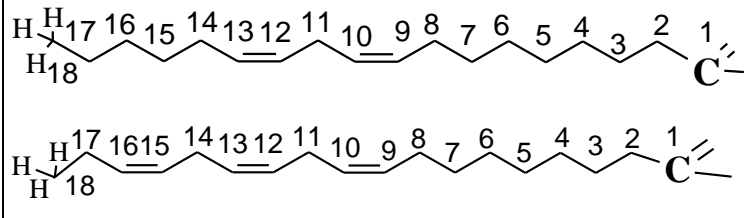


ω number are double bond from methyl group -CH₃
Essential omega Fatty Acids : ω=6 and ω=3

4.A Put in water molecule proper parameters



5. Put in essential Fatty Acid Salts oxygen atoms at pH=7.36 : C18:2 ω=..... and C18:3 ω=.....



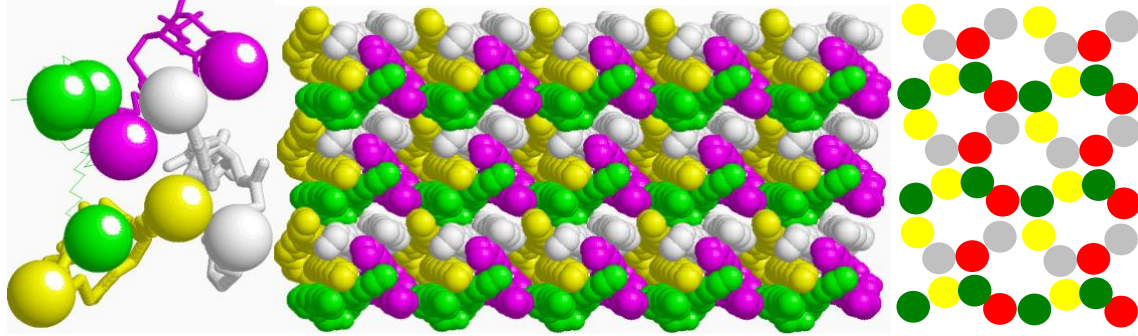
O O⁻
linoleate

O O⁻
α-linolenate

6. Calculate accumulate London Forces -2 kJ/mol Bonding Energy between two hydrogen contacts at each of 7 carbon methylene $-\text{CH}_2-$ on Palmitate & Oleate chains contact $n=7 \cdot 2=...$ points!

$$E = -2 \cdot 7 \cdot 2 = -2 \cdot n = -2 \cdot 14 = \dots \text{ kJ/mol}$$

7. On drawn tetramer $-\text{CH}_3$ structure top pattern of fatty acids chains Bilayer detect Number 3



of chains each other surrounded contact!

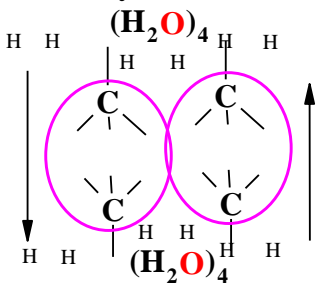
London Forces per one chain is

$$E_C = 3 \cdot E = ;$$

$$E_C = 3 \cdot 28 = \dots \text{ kJ/mol}$$

$$E_C = \dots \text{ kJ/mol}$$

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



9. Calculate hydrophobic contact -10 kJ/mol energy E_H for **water** tetramer structure $(\text{H}_2\text{O})_4$ with six contact points in two methyl groups $-\text{CH}_3$ palmitate **C16** and oleate **C18:1** between two phosphatidyl choline molecules on interface membrane interior of bilayer contacts $n_H = 2 \cdot 3 = 6$ for one phosphatidyl choline molecule $E_H = -10 \cdot 3 / 2 = -60 / 2 = \dots \text{ kJ/mol}$?

9.a Put in structure 12 H given atoms for six hydrophobic bonds!

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. $E_{\text{Bond}} = -168 + (-30) = \dots \text{ kJ/mol}$

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 $\dots \text{ \AA}$. Get the average size of Membrane thickness as mean $\text{Dist}_{\text{mean}} = \dots \text{ \AA}$ as nanometers $\dots \text{ nm}$!

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

13. What would be thickness in meters of home buildings walls if human tall size is 1.75 meters?

So wall (membrane) cross channel would be $1.75 \cdot 40 = \dots \text{ m}$ meters long .

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

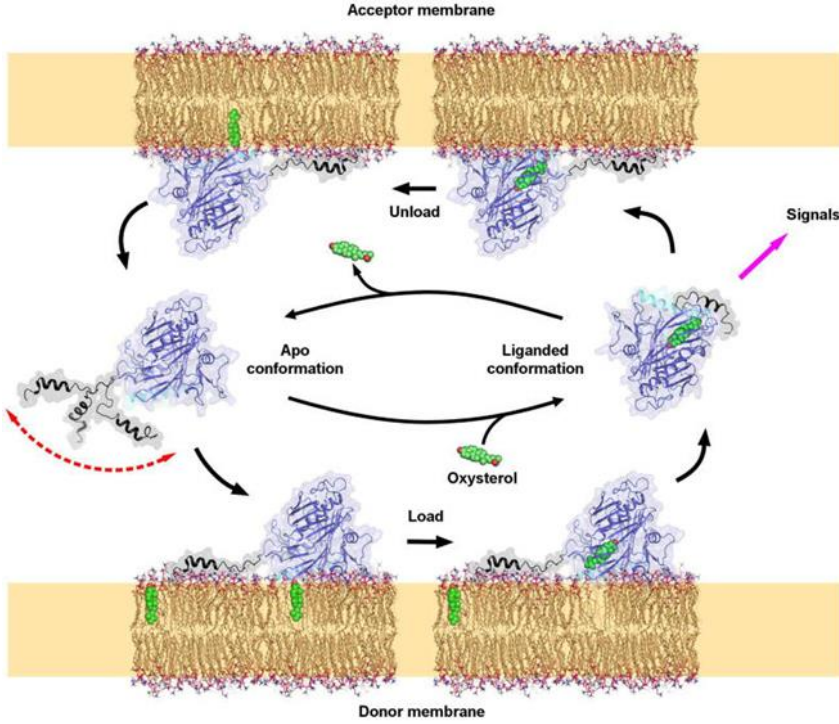
15. What mass fraction the Phosphatidyl Choline molecules in cellular membranes total mass 100%? Phosphatidyl Choline in **Membrane** constitute 1/3 part \dots of **Membranes** mass 100%.

I) 1/3 part **Phospholipids** which mass fraction of **Membranes** to make \dots % of total mass 100%;

II) second 1/3 part **Cholesterols** mass fraction of **Membranes** to make \dots % of total mass 100%;

III) third 1/3 part **Membranes integral Proteins** mass fraction to make \dots % of total mass 100%

Bulk mass fraction 20% goes to **Aquaporins** \nd for other **Proteins** remains \dots % :



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. In **Osh4** protein **1ZHYMarz.pdb** at Display **Backbone**, Termini to determine domain **N-terminus** amino acid...MET... and **C-terminus** amino acid LEU.....!

7. Count amino acids in **OSBP** sterol membrane-membrane transport polypeptide chains primary structure of **1ZHY.pdb**, **1ZHW.pdb**, **1ZHX.pdb**, **1ZHT.pdb** from 1 to 434=>.....?

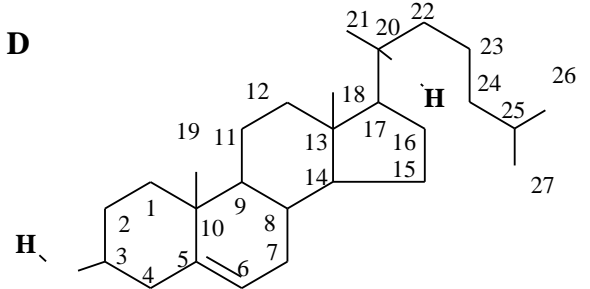
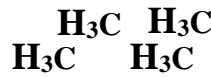
8. Put in **oxy-sterol** four circle symbols
two oxygen atoms

angular **-CH₃** groups C18, C19 :

and 3 metil groups **-CH₃**:

as splinter, fork, rod on flexible tail **C H₃**

A B C D
O O



9. Count hydroxyl groups **-OH** in cholesterol and 20-hydroxicholesterol? 1.....un 2.....

10. Put in 25-hydroxicholesterol

four circle symbols:

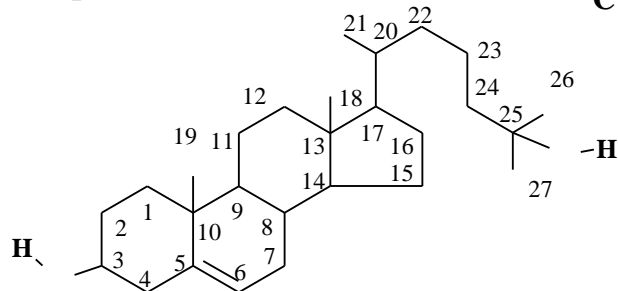
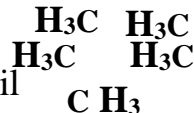
two oxygen atoms

angular **-CH₃** groups C18, C19 :

and 3 metil groups **-CH₃**:

as splinter, fork, rod on flexible tail **C H₃**

A B C D
O O



11. Put in 7-hidroksiholessterolā

four circle symbols:

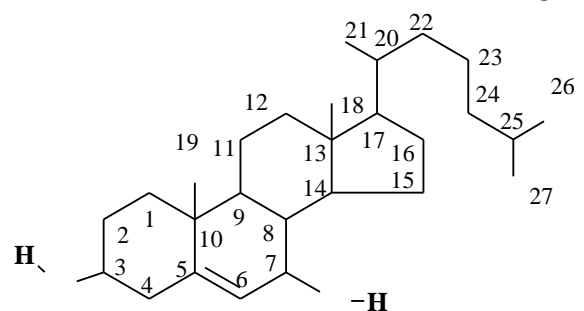
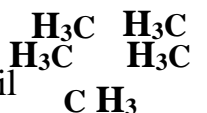
two oxygen atoms

angular **-CH₃** groups C18, C19 :

and 3 metil groups **-CH₃**:

as splinter, fork, rod on flexible tail **C H₃**

A B C D
O O



12. What molecules are in human body transporting cholesterol, A vitamins, hormones fats un fatty acids?;..... transport proteins
.....transport proteins

12.1-12.5 1ZHY.pdb KES1 isoelectric point IEP=pH=pK_{a-mean} at physiologic pH=7,36 .
 Determine at solution pH with KES1 concentration C=10^{-7,286} M (mol/Liter)!
1ZHY.pdb oxysterol-binding protein 4 homolog 49,493 kDa concentration 10^{-7,286} M

<http://aris.gusc.lv/ChemFiles/START/1ZHZpIStudS.doc> ; <http://aris.gusc.lv/ChemFiles/START/1ZHZpI.xls>

SQ SEQUENCE 434 >1ZHZ:A|PDBID|CHAIN|SEQUENCE: RLBP1+Retinal -1-434 (1-434)
 MSQYASSSSWTSFLKSIASFNGDLSSLSAPPFILSPISLTEFSQYWAHEPELFLEPSFINDDNYKEHCLIDPEVESPELA
 RMLAVTKWFISTLKSQYCSRNESLGSEKKPLNPFLGELFVGKVENKEHPEFGETVLLSEQVSHHPPVTAFSIFNDKNKVK
 LQGYNQIKASFTKSLMLTVKQFGHTMLDIKDESYLVTPPLHIEGILVASPFVELEGKSYIQSSTGLLCVIEFSGRGYFS
 GKKNFSFKARIYKDSKDSKDKKALYTISGQWSGSSKIIKANKKEESRLFYDAARIPAEHLNVKPLEEQHPLESRKAWYDV
 AGAIKLGDFNLIAKTKTELEETQRELKKEEAKGISWQRRWFKDFDYSVTPEEGALVPEKDDTLKLLASALNLSTKNAPS
 GTLVGDKEDRKEDLSSIHWRFRQRELWDEEKEIVL IEP=7,4338926 ; sum=1107,65 ; 149 protolytic constants

Protolytic average constant isoelectric point IEP=pK_{a-mean} calculate of side chains ΣpK_{aRside} group.. pK_{aNterminal}NH₃ and pK_{aCterminal}COO-constants sum divide with number of acid groups NpK_a:

$$IEP=pK_{a_mean}=(\Sigma pK_{aRside\ group}+pK_{aNterminal}+pK_{aCterminal})/NpK_a$$

Calculate Yeast KES1 49,493-kDa molecule concentration 10^{-7,286} M

12.1. Acid groups sum NpK_a=Sum of 147 + 2 = pK_a values in table:

434 amino acids of them protolytic constants pK_a for side groups 147+2 ,
 N-terminal methionine M pK_{aNterminal}=9.21 and C-terminal aspartate D pK_{aCterminal}=1.88 .

12.2 Sum are calculate as ΣpK_{aRside} group+pK_{aNterminal}+pK_{aCterminal} =

Average acid group constant **ISOELEKTRIC POINT** pK_{mean}=IEP=1107,65/149=.....

At pH value of amino acid and protein on isoelectric point pH=IEP **total charge** is zero „0”
 0—— plus (+) acidic———zero charge „0” IEP=pH——— minus (-) basic———→ 14 pH scale
 -COOH & -NH₃⁺ positive charge-COO⁻ & -NH₃⁺.....charge is negative -COO⁻ & -NH₂
Underline and determine existing: positive (+) or zero or negative (-)!

12.3 Determine KES1 molecule charge sign (+). zero „0” or (-) at physiologic pH=7.36

Underline existing:

-COOH & -NH₃⁺ positive (+) charge pH=7.36 < IEP=7.43 charge negative(-) -COO⁻ & -NH₂.

12.4 Determine KES1 molecule charge sign (+). zero „0” or (-) at **electrophoresis** pH 8.8

Underline existing:

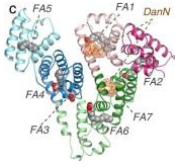
-COOH & -NH₃⁺ positive (+) charge IEP=7.43< pH=8.8 charge negative(-) -COO⁻ & -NH₂.

12.5 Calculate C = 10^{-7,0794} M KES1 solution pH by *Ostwald dilution law* in logarithm of C:

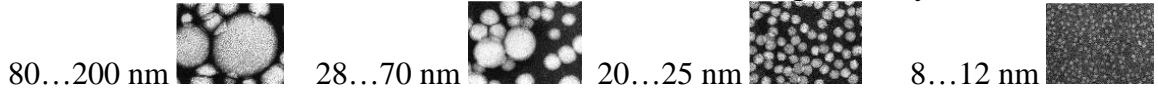
$$pH = \frac{pK_a - \log C}{2} = \frac{7,4338926 - \log 10^{-7,2861074}}{2} = \frac{7,4338926 + 7,2861074}{2} = 14,72 / 2 = \dots\dots$$

7,36 Attractor YEAST_KES1 concentration is C=.....M .

13. Write five lipids transport forms for lipoprotein aggregates under photography!



HDL join esterify outstanding cam Cholesterol molecule which protrude on membrane surface as insoluble. So avoid atherosclerosis and keep healthy cardiovascular state.



14. What compounds transport lipoproteins enclosed interior!

.....;.....;.....;.....;
; Fat soluble
 and;..... other

15. Write two transport forms of lipocalins! and

16. What three mass fractions 1/3,1/3,1/3 form cell **membranes** 100% mass?

17. What secondary structures comprise **OSBP4 1ZHY.pdb**? **alpha helixes**.....
beta half-barrel of and
 **beta sheets** from **strands** in each

18. What 6 nonpolar amino acids **OSBP4** protein closing lid on **N-terminus** helix **H2**
 serve as support floor for cholesterol tail methyl groups **-CH₃** of carbons C26 and C27?
 Trp.....,Phe.....,Leu.....,Ile.....,Leu.....,Ala.....

19. Which 3 water molecules **H₂O** bound buried C3 hydroxyl group **-OH**?
H₂O....., **H₂O**....., **H₂O**.....

20. What inter molecular bonds bound hydroxyl group **-OH** with water molecules on bottom
 of tunnel?..... bonds.....

21. What 5 amino acids bind with hydrogen bonds buried C3 hydroxyl group **-OH** and three
 ...water molecules **H₂O**2003, **H₂O**2004, **H₂O**2018?.....
 Gln.....,Trp.....,Tyr.....,Asn.....,Gln.....

24. What 7 amino acids of 20 proteino genic form hydrophobic pocket tunnel bottom interior....
 ... envelope together 38 non polar amino acids buried in tunnel lipid molecule closing.....
 ... with lid helix **H2**? =>,,,,,,

10: Pro...,Ala...,Leu...,Leu...,Ala...,Pro...,Ile...,Leu...,Phe...,Leu...,

6: Gly...,Pro...,Leu..., Pro...,Pro..., Val...,

8: Ala...,Ile...,Ala...,Phe...,Leu...,Leu...,Val...,Phe...,

8: Pro...,Pro...,Pro..., Val...,Pro...,Pro...,Ile...,Ile...,

6: Leu..., Val...,Ala...,Pro...,Phe...,Val.....

5: Leu...,Leu...,Pro...,Leu...,Ala**25**. Where disposed **C-terminus** polypeptide chain residues
 from 308 to 434 amino acids in

protein?,where enclosed buried lipid

26. What 10 basic amino acids outside on **OSBP4 H2** lid surface are positively charged?.....

Lys.....,Lys.....,Lys.....,Arg.....,Arg.....,

Lys.....,Lys.....,Lys.....,Arg.....,Lys.....