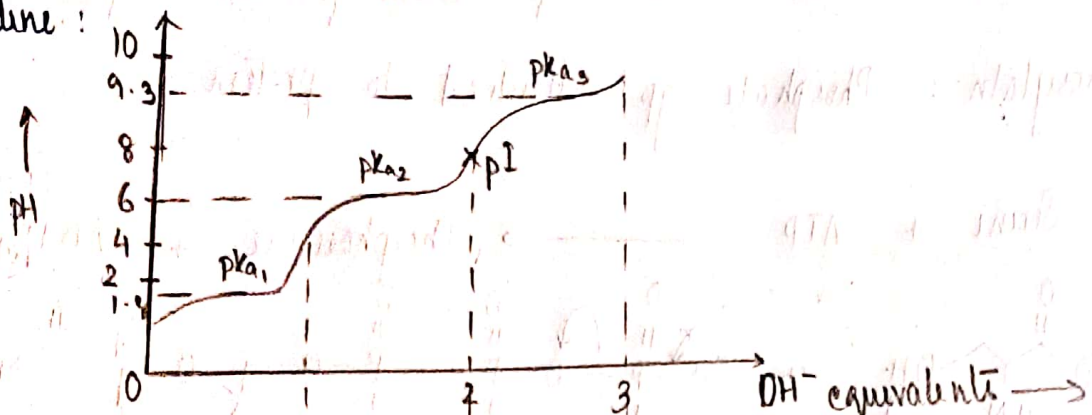
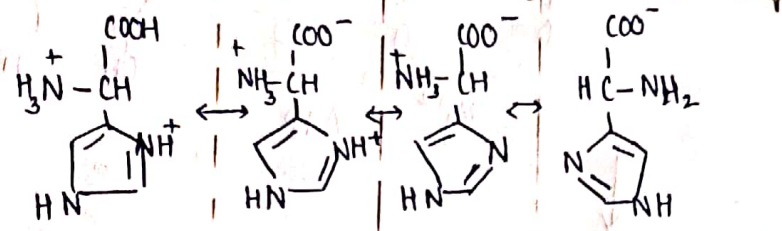
SHREEVA
2018113011

Biomolecular Structures

Assignment 1

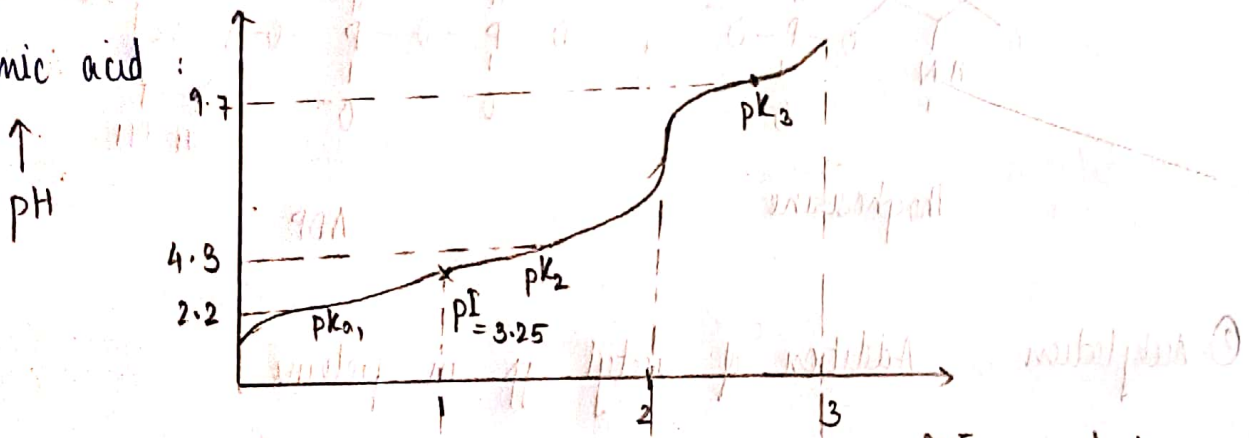
1) Histidine :

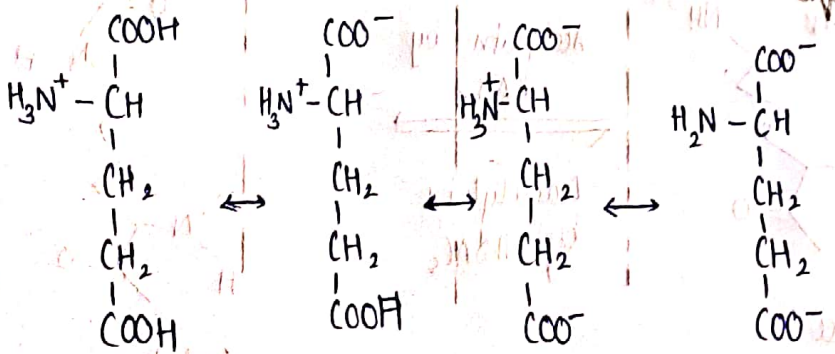




(Below 1.8) (pH 1.8–6.0) (pH 6–9.3) (pH 9.3 above)

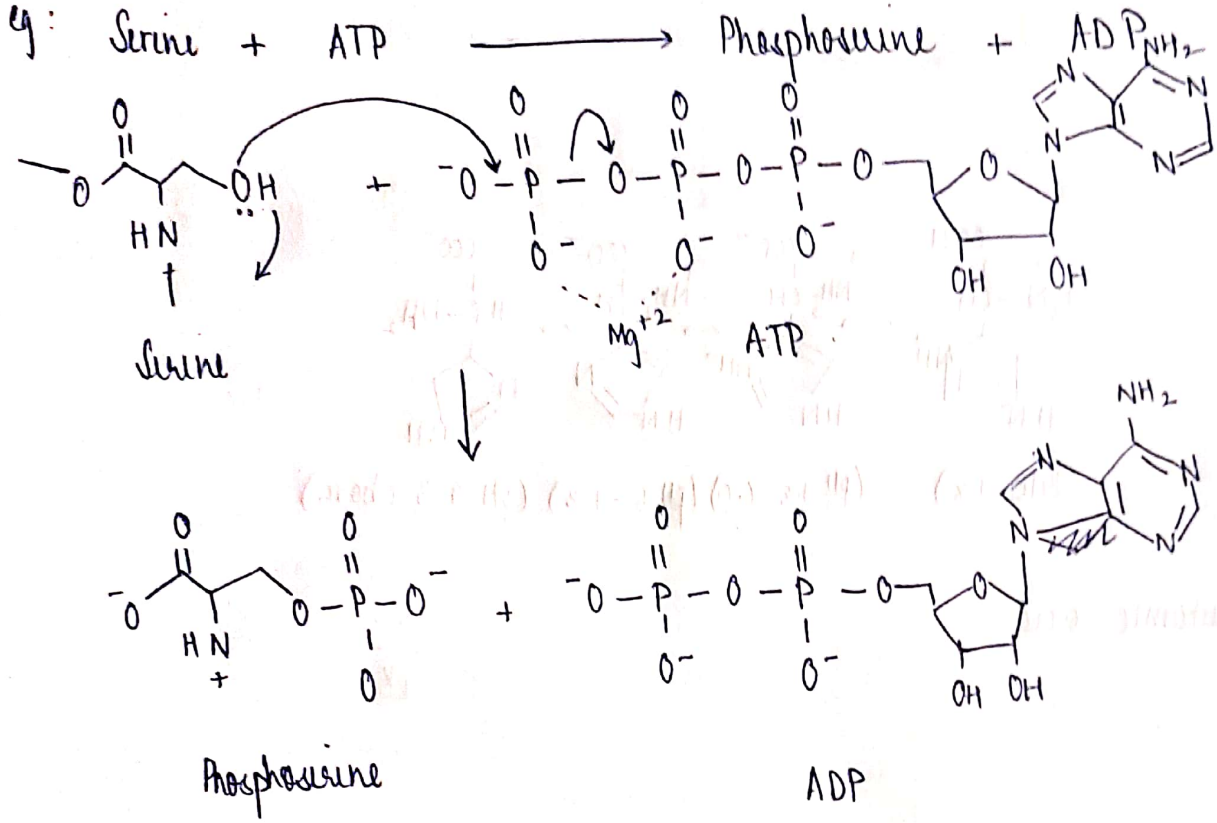
Glutamic acid :



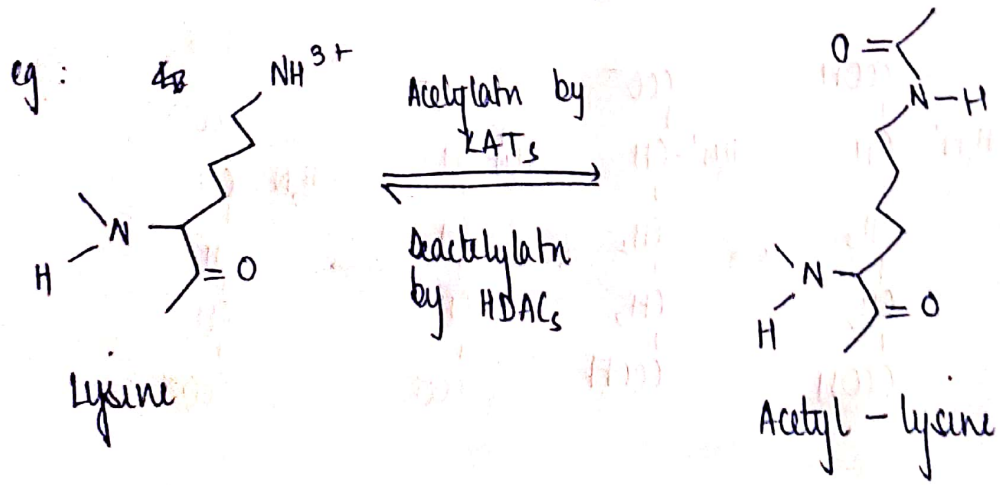


2) The chemical changes in a protein that occur after a protein has been produced, are called post-translational modifications (PTMs). It is the covalent addition of certain functional gps to proteins

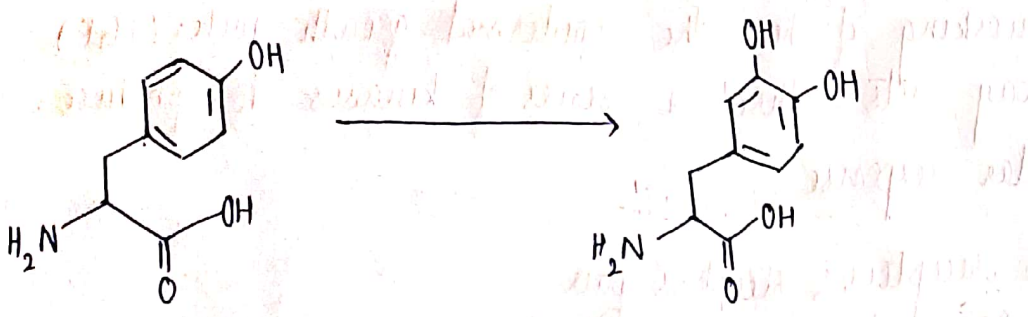
① Phosphorylation : Phosphate gp attached to protein



② Acetylation : Addition of acetyl gp in proteins.

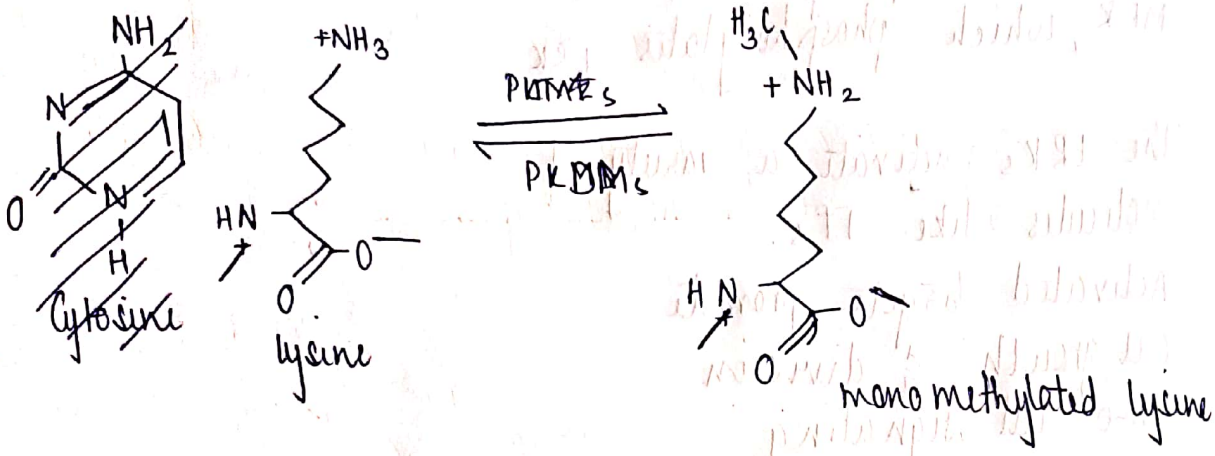


③ Hydroxylatn : Addition of hydroxyl group :



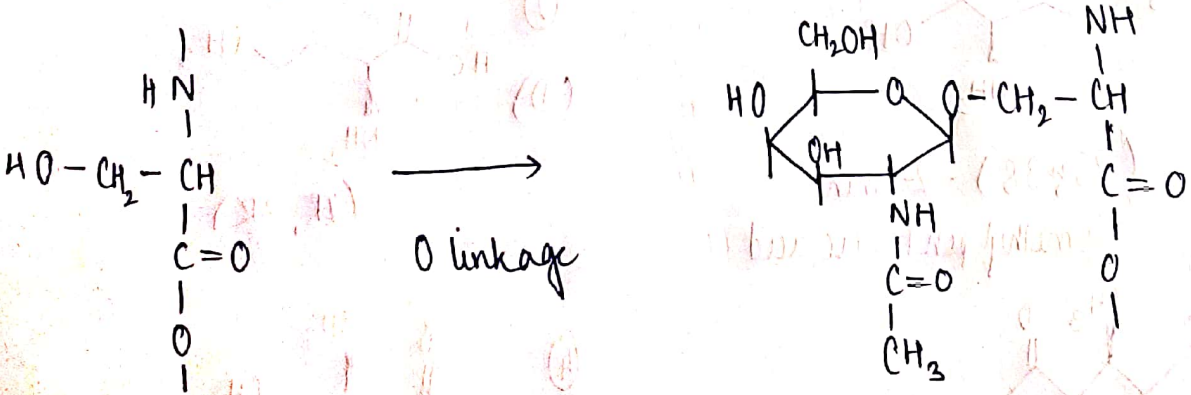
Tyrosine — Tyrosine hydroxylase

④ Methylatn : Addition of methyl gp



Cytosine — lysine — mono methylated lysine

⑤ Glycosylation : Sugar is attached thro' a oxygen on a hydroxyl group (OH) to serine (O-linkage)



Serine

(N-acetylgalactosamine linked to serine)

3) MAP K signaling cascade (Phosphorylation):

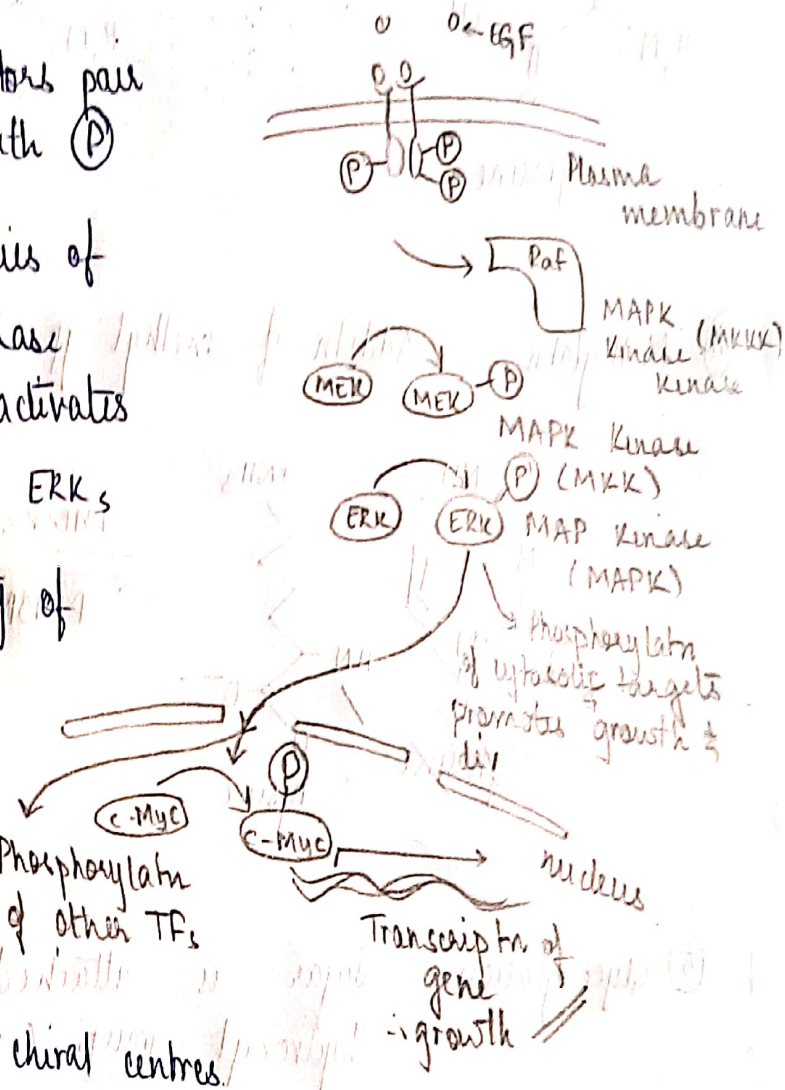
The working of how the epidermal growth factor (EGF) pathway acts thro' a series of kinases to produce cellular response.

① GF bind to receptors, receptors pair up & act as kinases with (P)

② Activated receptors trigger series of events & activate Raf kinase

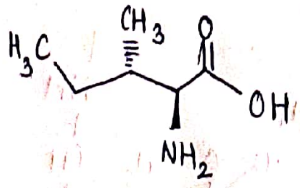
③ Active Raf phosphorylates & activates MEK, which phosphorylates ERKs

④ The ERKs activate a variety of molecules like TFs.
∴ Activated targets promote cell growth & division thro' cell signaling using phosphorylation.



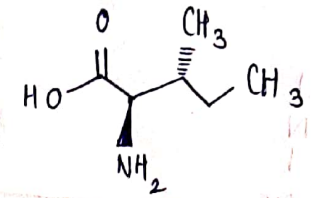
4) (I) Isoleucine: C_2, C_3 are chiral centres. (Cx)

① (L)



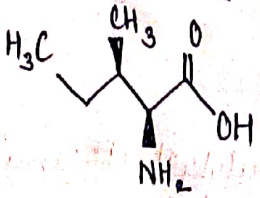
(2S,3S) - 2-amino-3 methyl pentanoic acid

② (D)



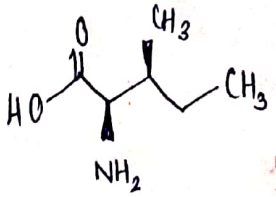
(2R, 3R)

③



(2S, 3R)

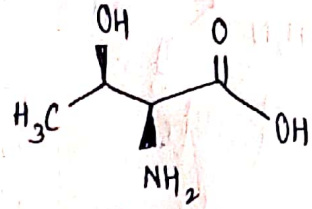
④



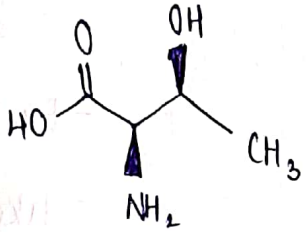
(2R, 3S)

(II) Threonine : C_2, C_3 are chiral centres. (Ch)

(1) (L)



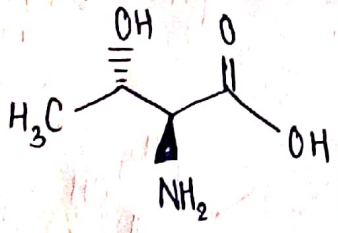
(2) (D)



(2S, 3R) – 2-amino – 3hydroxy butanoic acid

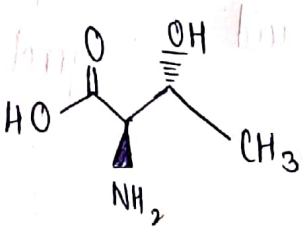
(2R, 3S)

(3)



(2S, 3S)

(4)



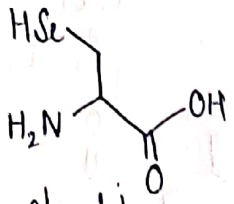
(2R, 3R)

5) Essential amino acids : Cannot be made by the human body & hence must be retrieved from outside (diet)

Non essential " " : Can be made within the body.

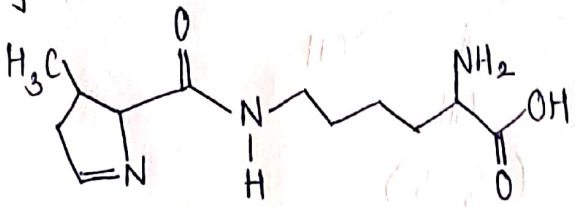
Non essential (11)	Essential (9)
(1) ALA	(1) HIS
(2) ARG	(2) ILE
(3) ASN	(3) LEU
(4) ASP	(4) LYS
(5) CYS	(5) MET
(6) GLY	(6) PHE
(7) PRO	(7) THR
(8) SER	(8) TRP
(9) TYR	(9) VAL
(10) GLN	
(11) GLU	

6) 21st Amino acid : - Selenocystine (Sec)



- Exists in all 3 domains of life (codon : UGA)
- Like all amino acids has its own tRNA.
- Selenium analogue of Cystine (Se replaces S).
- Imp for fundamental cellular process (metabolic rate reg.)

22nd amino acid : - Pyrrolysine (Pyl)



- Like all amino acids has its own tRNA & aminoacyl-tRNA synthase (aaRS) (codon : UAG)
- Very rare, found in 7 organisms

) This is because carbon atoms make up the backbone of many important molecules in our body like DNA, RNA sugars, proteins & fats. i.e organic molecules. Since carbon is the only element that can form 4 chem. bonds to other atoms ∴ its the right size. to accomodate (4 valency) [unlike Si atoms ∵ large]. Along with this it has the ability to form long C-C chains, straight & branched (complex). C atom can form = & ≡ bonds also. Chains & rings can also be used to form bonds ∴ millions of org. comp. exist with C as main atom.

8) Isoionic pt : pt is the pH at which zwitterion molecule has equal no. of +ve & -ve charges & no adherent ionic species

→ Isoionic pt of 0.1 M ALA :

$$[H] = \sqrt{\frac{k_1 k_2 C + k_1 k_w}{k_1 + C}}$$

$k_1 = 10^{-2.34}$
$k_2 = 10^{-9.69}$
$k_w = 10^{-14}$
$C = 0.1$

$$= \sqrt{\frac{10^{-2.34 + -9.69 - 1} + 10^{-2.34 - 14}}{10^{-2.34} + 10^{-1}}}$$

$$= 9.45 \times 10^{-7}$$

$\therefore pH = -\log [H^+]$

$= 6.02$

$\therefore$ Isoionic pt $= \underline{\underline{6.02}}$

9) a) 2.27 ribbon : - Similar to ξ also called α_{II} ribbon (α_{II} struct.)
- N-H ··· O L^us differ from st. Lk by 60° - 66°
- L^k btw N-H & N···O are 40° - 48°
- Unacceptable structure all over.
- N···O distance is > 0.1 A° shorter than reliable value → (= 2.56 Å)

b) ① Left handed polyproline II : (PP II)

- $\phi = -78°$, $\psi = +146°$.
- Most are shorter than 5 residues
- Have perfect 3-fold & rotational sym.
- correlatn btw hydrophobicity of residues i & i+3

② Left handed polyglycine II : (PG II)

~~- Basis of Gly : Gly differ~~
- Do not form a self contained H bonding network (same for PP II)
- $\phi = -77°$, $\psi = +145°$
- An extended 3, helix is hydrogen bonded to 6 neighbouring chains packed in hexagonal array.
- CO & NH H-bond stabilise (inter molecular)

c) Collagen triple helix :

- Confers strict amino acid seq. constraints requiring a $(Gly-X-Y)_n$ repeating pattern
- Requires high content of imino acids.
- Has supercoiled triple helix structure.
- X & Y were found to be usually hydroxy proline (OH gp of this stabilises the collagen helix stabilising proline via stereo electronic effects & does not participate in H bonding.)

10) α helix :

$5.4\ A^\circ \longrightarrow 3.6$ residues (one turn)

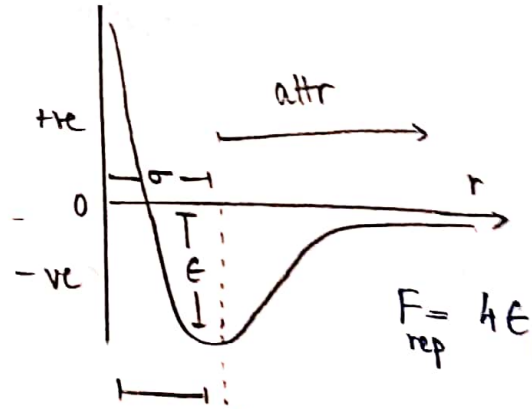
$x \longrightarrow 30$ residues

$$x = \frac{30 \times 5.4}{3.6}$$

$$= 45\ A^\circ$$

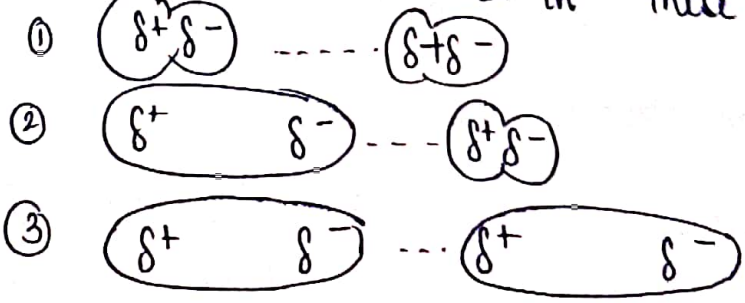
11) - Vanderwalls forces are the cum total of non covalent forces that depend on distance btw entities
- They can be repulsive or attr based on dist & the interacting nonbonded atoms/molecules.
- Vanderwaal f are weak electrostatic & are mainly attractive.

- attr when interatn btw entities are induced dipoles
- repulsion when clouds overlap or too close



$$F_{rep} = 4\epsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right)$$

& Since VDW forces exist btw in these following cases :



& are weak electrostatic f ∴ mostly attr.

Columbic forces on the other hand are much stronger & develop btw charged atoms (already charged) or ions.

& $F = \frac{Q_1 Q_2}{4\pi\epsilon_0 r^2}$: - Nature & mgn depend on signs of charges, medium, distance btw the entities involved. (btw mols)

$\therefore$ $Q_1 > 0$ $Q_2 > 0$ or $Q_1 < 0$ $Q_2 < 0$

$\Rightarrow F = +ve$ $\therefore$ repulsion

$Q_1 < 0$ & $Q_2 < 0$ or vice versa

$\Rightarrow F = -ve$ $\therefore$ attr.

Sources

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butane.chem.uiuc.edu/cyerkes/chem104A-507/Lecture_Notes-104/lect27c.html

2) Science direct – Posttranslational modifications
   ① Thermo Fisher Scientific
   ② Cayman Chemical.
   ③ Public Library of Science
   ④ Epigenetics
   ⑤ ~~PRIE~~ PREMIER Biosoft-

3) Khan academy – cell signaling – signal relay pathways.

4) Isoleucine stereoisomers on the Earth – (Research paper – Harvard)

5) Researchgate (Diff. btw essential & non essential amino acids)

6) ncbi.nlm.gov/pmc/articles/PMC1976440/
   Yale Scientific – Expanding the genetic code discovery of 2 new amino acids

7) Khanacademy – Carbon & hydrocarbons
   Science.jrank.org – Why carbon special

8) iubmb.onlinelibrary.wiley.com/doi/pdf/10.1016/0307-4412(78)90164-4

9) a) JSTOR : Journal Article – Hydrogen Bonded Helical config of polypeptide
   b) ~~Research gate~~ – publicatn – A survey of left-handed polyproline II chains
      ① PubMed.
      ② J Phys Chem B – Raman Studies of Soln polyglycine helices
         Nature – Structure of PG II
      ③ PubMed – Paper – Molecular Structure of collgen triple helix.

11) Science Direct - Van Der Waals Force & knowing