CHEM106 Section 001 Problem Set 2
Due Wednesday, October 3, 2018

Name: Key

Answer all of the following questions and record your answer on the answer sheet. You must show all of your calculations in order for any credit to be given. You must box your final answers on any scratch paper that you include with this Problem Set. If I can't follow your work, you won't receive partial credit.

1. **Km =** 0.502 μM **Vm =** 5.08 nmol/min

2. $[S]_1$ = 16.31 mM $[S]_2$ = 22.93 mM $[S]_3$ = 24.86 mM $[S]_4$ = 31.67 mM

3. **Type of inhibition?** Uncompetitive Inhibition

4. 39.9 mL

5. i) 3.5 ii) 0.054 M iii) 8.00

6. i) 3.5 ii) 0.13 M iii) 6.00

7. i) see key ii) See key

8. **Attach a sheet directly after this sheet.**

9. See key

10. See key

1. The following data were obtained from an enzyme kinetics experiment. Graph the data using a Lineweaver-Burk plot and determine, by inspection of the graph, the values for K_m and V_{max}.

[S] (μM)	V (nmol/min)
0.20	1.43
0.26	1.67
0.33	2.08
1.00	3.33

2. Use the Michaelis-Menton Equation to calculate the missing values of [S] given below if V_{max} = 5 mmol/min. Plot [S] versus V (NOT the reciprocals!). Draw line parallel to the x-axis at V_{max} and extend your plotted line to show its approach to V_{max}.

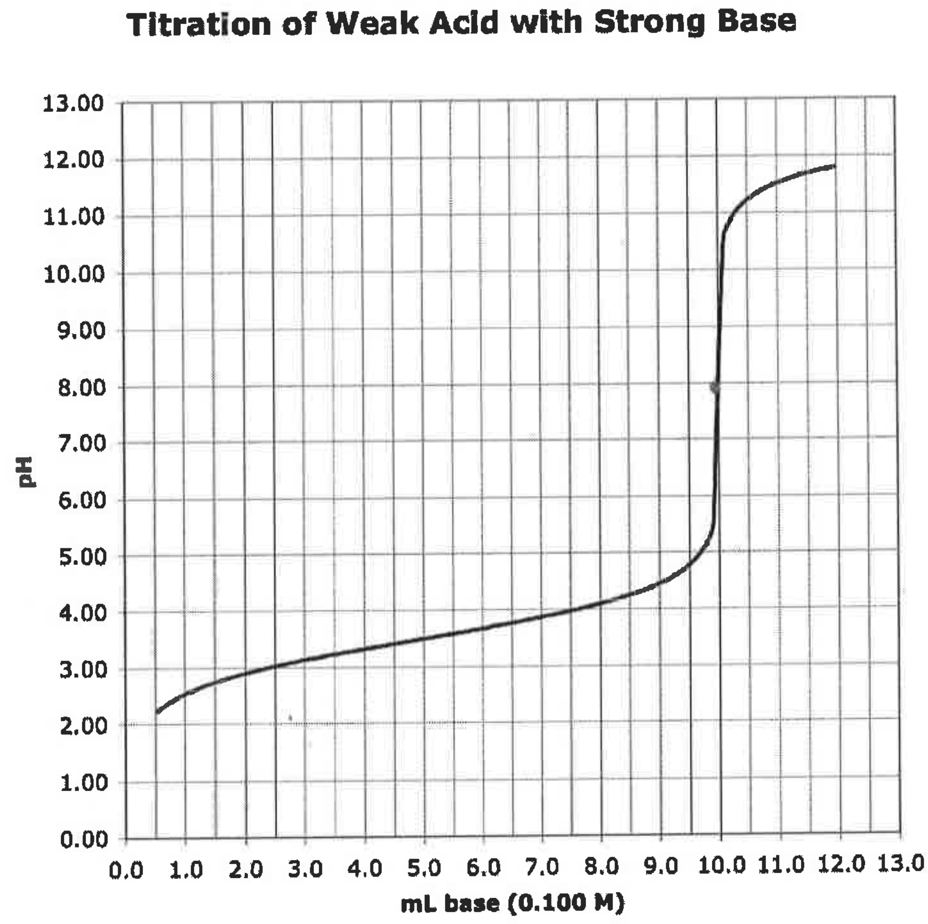
[S] (mM)	V (mmol/min)
10	1.2
$[S]_1$	1.7
$[S]_2$	2.1
$[S]_3$	2.2
$[S]_4$	2.5

3. The effect of an inhibitor on an enzyme was tested and the experiment gave the results below. Plot the data and determine, by inspection of the graph, what type of inhibition is involved.

[S] μM	V (μmol/min) with 0.0 nM Inhibitor	V (μmol/min) with 25 nM Inhibitor	V (μmol/min) with 50 nM Inhibitor
0.4	0.22	0.21	0.20
0.67	0.29	0.26	0.24
1.00	0.32	0.30	0.28
2.00	0.40	0.36	0.32

4. How many ml of a 0.2 M NaOH solution are required to bring the pH of 20 ml of a 0.4 M HCl solution to 7.0?

5. The following questions refer to the figure below. There is enough information in the titration curve to answer the 3 questions below, but you must show your work. Start by writing the equivalence point volume.

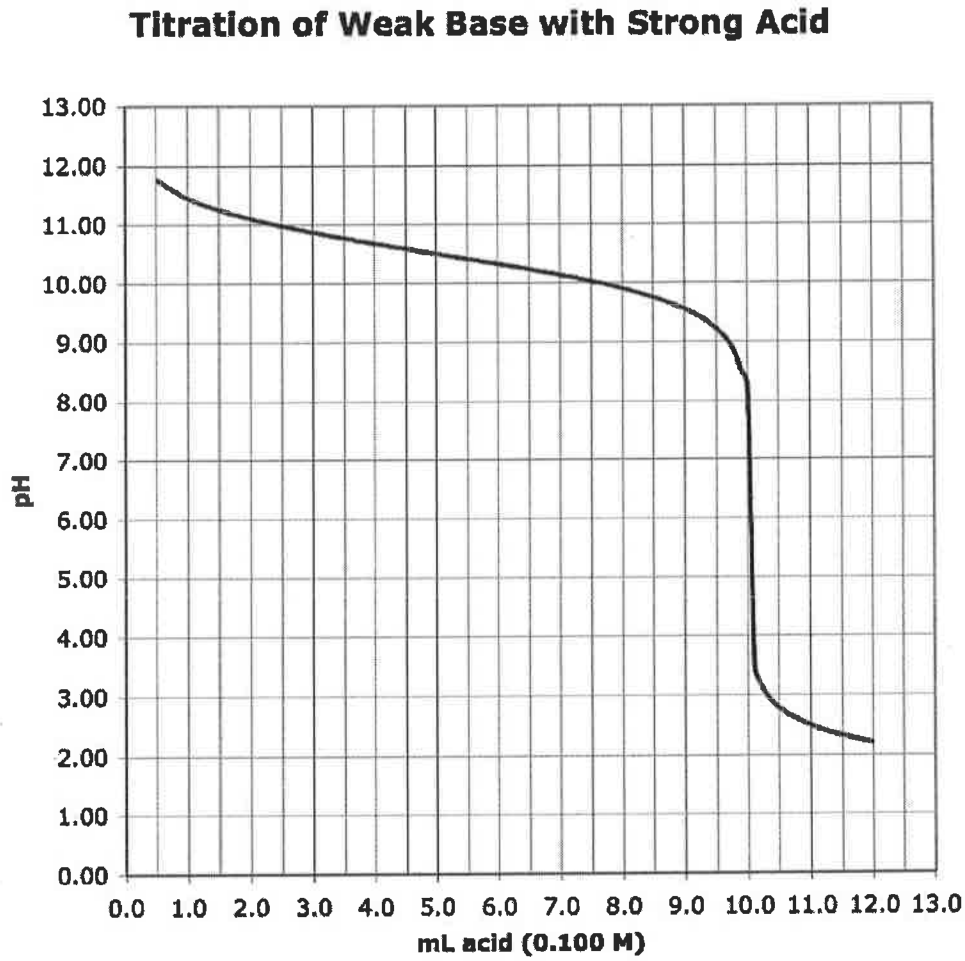


i) What is the pKa of the weak acid?

ii) What was the original concentration of the acid if the starting volume of acid was 18.60 mL?

iii) Calculate the pH at the equivalence point.

6. The following questions refer to the figure below. There is enough information in the titration curve to answer the 3 questions below, but you must show your work. Start by writing the equivalence point volume.



i) What is the pKb of the weak base?

ii) What was the original concentration of the base if the starting volume of base was 7.50 mL?

iii) Calculate the pH at the equivalence point.

7. Answer the following questions.

i) Draw a tripeptide having R groups consisting of methyl, hydroxyl, and phenol groups.

ii) When a protein is dissolved in water, the amino acids found in its interior are likely to have R groups which are:
   a) hydrophilic
   b) charged
   c) highly reduced
   d) polar
   e) all of the above
   f) none of the above

8. Draw the structure of the following compounds:

i) 2,4-dimethyl-3-pentanol
ii) 1-ethyl-3-methylbenzene
iii) 2,6-diaminohexanoic acid
iv) 1-methoxy-3-hexanone
v) benzaldehyde

9. You have 200 mg of aspirin (FW= 180g/mole) dissolved in 50 mL of water. You take 5 mL of this solution and bring it to 200 mL with water. You then take 100 mL of that and bring it to 1000 mL with water. You take 5 mL of that solution and add it to 10 mL of water. What is the molarity of aspirin in the final solution?

10) Write the name, give the one letter symbol and draw the Lewis Structure of:

a) A polar, uncharged amino acid
b) A polar, charged amino acid
c) An acidic amino acid
d) A hydrophobic amino acid
e) A basic amino acid

CHEM 106 Problem Set 2 Key

① you have [S] and V_0 data, so get the $\frac{1}{[S]}$ and $\frac{1}{V_0}$ by taking the reciprocals of each.

$\frac{1}{[S]}$	$\frac{1}{V_0}$
1	0.30
3.03	0.48
3.84	0.59
5	0.699

Create a linear regression plot of the data and you get the equation for the line in the form $1/V_0 = (K_m/V_m)[S] + 1/V_m$

$$\frac{1}{V_0} = 0.0988\left(\frac{1}{[S]}\right) + 0.197$$

from this equation, $\frac{1}{V_m} = 0.197$, so $\boxed{V_m = 5.08 \text{ mmol/min}}$

$\frac{K_m}{V_m} = 0.0988$ and $V_m = 5.08$, so

$K_m = 0.0988(V_m)$

$K_m = 0.0988(5.08)$

$\boxed{K_m = 0.502\ \mu M}$

② In this problem, you are asked for the missing values of [S] using the Michaelis-Menten equation. You are given $V_m = 5$ mmole/min

The first condition gives you [S], V_0 and you know the V_m, so you can solve for Km using the michaelis-menten equation:

$$V_0 = \frac{V_m[S]}{K_m + [S]}$$

$$V_0(K_m + [S]) = V_m[S]$$

$$V_0 K_m + V_0[S] = V_m[S]$$

$$V_0 K_m = V_m[S] - V_0[S]$$

$$V_0 K_m = [S](V_m - V_0)$$

$$K_m = \frac{[S](V_m - V_0)}{V_0}$$

In the first condition, [S] = 10 mM, V_0 = 1.2 mmol/min and V_m is given 5 mmol/min

Therefore: $K_m = \frac{(10)(5 - 1.2)}{1.2}$

$$\boxed{K_m = 31.67\ mM}$$

Now we can go back and rearrange the equation for Km to solve for [S]

$$K_m = \frac{[S](V_m - V_0)}{V_0}$$

$$V_0 K_m = [S](V_m - V_0)$$

$$[S] = \frac{(V_0 K_m)}{(V_m - V_0)}$$

Using this equation, we can plug in the values of V_0, V_m and K_m to determine [S] at each V_0.

$$[S_1] = \frac{V_0 K_m}{V_m - V_0} = \frac{(1.7)(31.67)}{(5-1.7)}$$

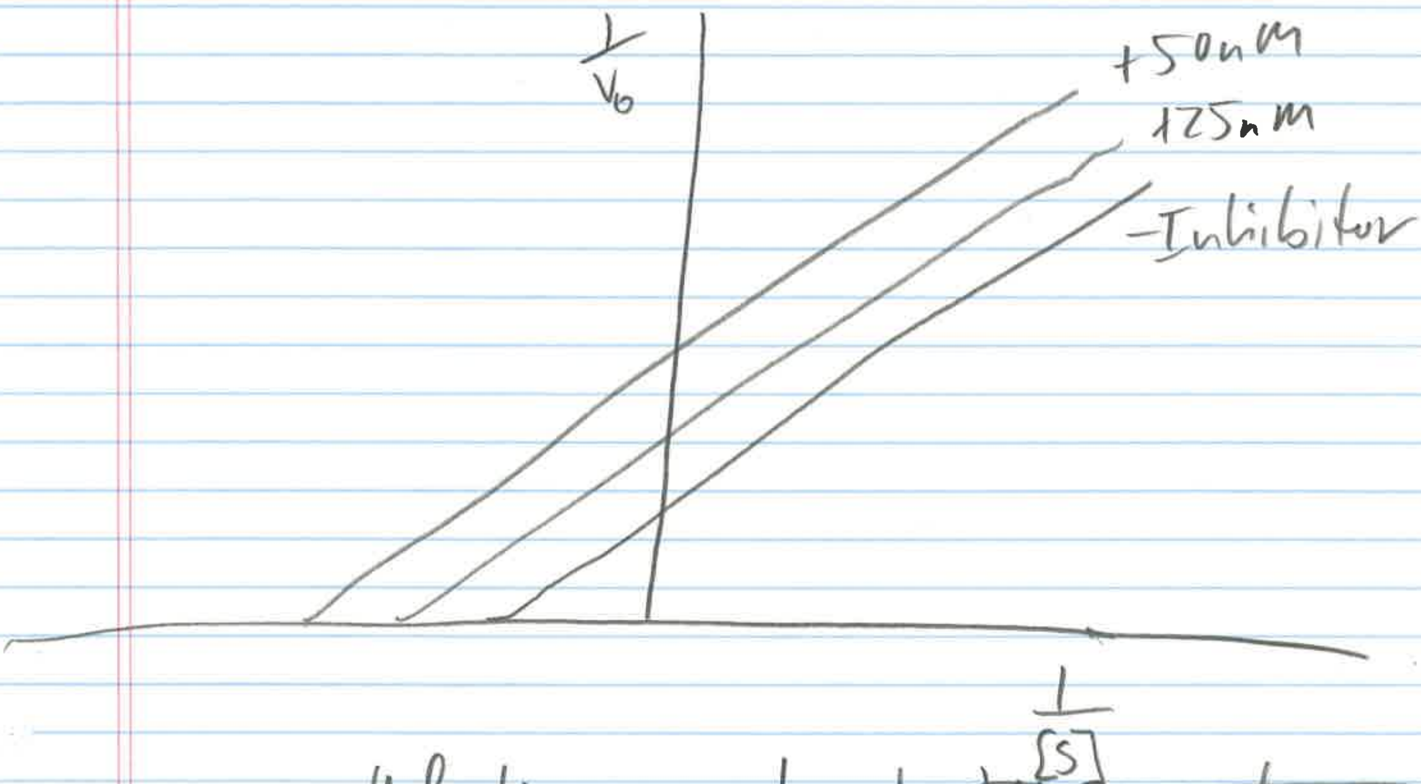
$$\boxed{[S_1] = 16.31\ mM}$$

Similarly, $$\boxed{\begin{aligned}[S_2] &= 22.93\ mM \\ [S_3] &= 24.88\ mM \\ [S_4] &= 31.67\end{aligned}}$$ ← note this is K_m and the V_0 @ this [S] is equal to $0.5\ V_m$!

③ Graph the 3 data sets on the same $\frac{1}{V_o}$ vs $\frac{1}{[S]}$ plot. You should see the following:

[S] (μM)	V_o (−inhibitor)	V_o (+25 nM Inhib)	V_o (+50 nM)
0.4	0.22	0.21	0.20
0.67	0.29	0.26	0.24
1.0	0.32	0.30	0.28
2.0	0.40	0.36	0.32

$\frac{1}{[S]}$	$\frac{1}{V_o}$ (−inhib)	$\frac{1}{V_o}$ (+25 nM)	$\frac{1}{V_o}$ (+50 nM)
0.5	2.5	2.78	3.125
1	3.13	3.33	3.57
1.49	3.49	3.85	4.17
2.5	4.55	4.76	5



3 parallel lines indicates $\boxed{\text{Uncompetitive Inhibition}}$

④ Have: 0.02L of 0.4M HCl

- This is a strong acid, so, it completely ionizes in water

$H_2O + HCl \longrightarrow H_3O^+ + Cl^-$

We have: $0.02L \times \frac{0.4 \text{ moles } H_3O^+}{L} = 8\times10^{-3}$ moles H_3O^+

in 20ml of 0.4M HCl.

Now, the question really is: What are we doing?

We are trying to raise the pH to 7.0. At this pH, the $[H_3O^+] = 1\times10^{-7}$ (take the antilog of 7)

So: We have 8×10^{-3} moles of H_3O^+ @ start
We want 1×10^{-7} moles of H_3O^+ @ end.

8×10^{-3} moles $- 1\times10^{-7}$ moles $= 7.99\times10^{-3}$ moles of H_3O^+ must be reacted off by adding 0.2M NaOH.

The chemical reaction is:

$$\underset{\text{from HCl}}{H_3O^+} + \underset{\text{from NaOH}}{OH^-} \longrightarrow H_2O$$

7.99×10^{-3} moles $H_3O^+ \times \frac{1 \text{ mole } OH^-}{1 \text{ mole } H_3O^+} = 7.99\times10^{-3}$ moles OH^- needed

7.99×10^{-3} moles $OH^- = \frac{0.2M\ NaOH}{L}$ (x)

x = 0.0399L or $\boxed{39.9mL}$ of 0.2M NaOH needed

⑤ The endpoint is reached when the slope of the titration curve is at it's maximum

This is the midpoint of the linear segment @ 10mL. The endpoint of the titration is 10mL

a) 50% of the way through the titration, the moles of conjugate base equals the moles of acid remaining.

If the equivalence/endpoint is 10mL of base added, the 50% would be @ 5mL of base added.

$$pH = pK_A + \log\left(\frac{[A^-]}{[HA]}\right) \rightarrow \text{when } [A^-] = [HA], \text{ the } \log\left(\frac{[A^-]}{[HA]}\right) = \log(1) = 0$$

$$\boxed{pK_A = 3.5}$$

b) It took 10mL of 0.1M base to reach the endpoint, or 1×10^{-3} moles of ^{-}OH. That means there were that many moles of acid at the start, so

$$\frac{1 \times 10^{-3} \text{ moles acid}}{0.0186 \text{ L}} = \boxed{0.054 \text{ M Acid}} \text{ @ start}$$

c) At the equivalence point, the pH is $\boxed{8.00}$

⑥ This is the reverse of the previous problem.
The endpoint is @ 10mL (midway through the linear segment)

a)
When the titration is 50% complete, 5ml of base have been added based on the curve the pK_A is 10.5, so:

$$pK_A + pK_B = 14$$

$$pK_B = 14 - pK_A$$

$$pK_B = 14 - 10.5 = \boxed{3.5}$$

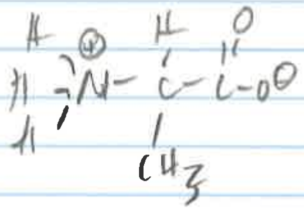
b) To reach the endpoint/equivalencepoint:

10ml of 0.01M acid = 1×10^{-3} moles acid added

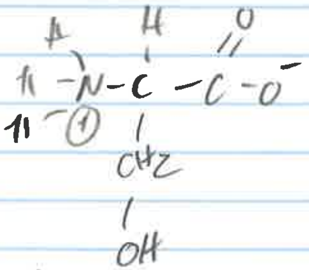
@ the start $\dfrac{1 \times 10^{-3} \text{ moles base}}{0.0075 \text{ L}} = \boxed{0.13M}$

c) Based upon the curve: $\boxed{pH = 6.0}$

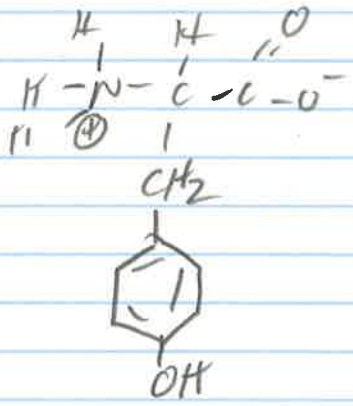
⑨ i) Write the amino acids first, then link them peptide bonds.



Alanine



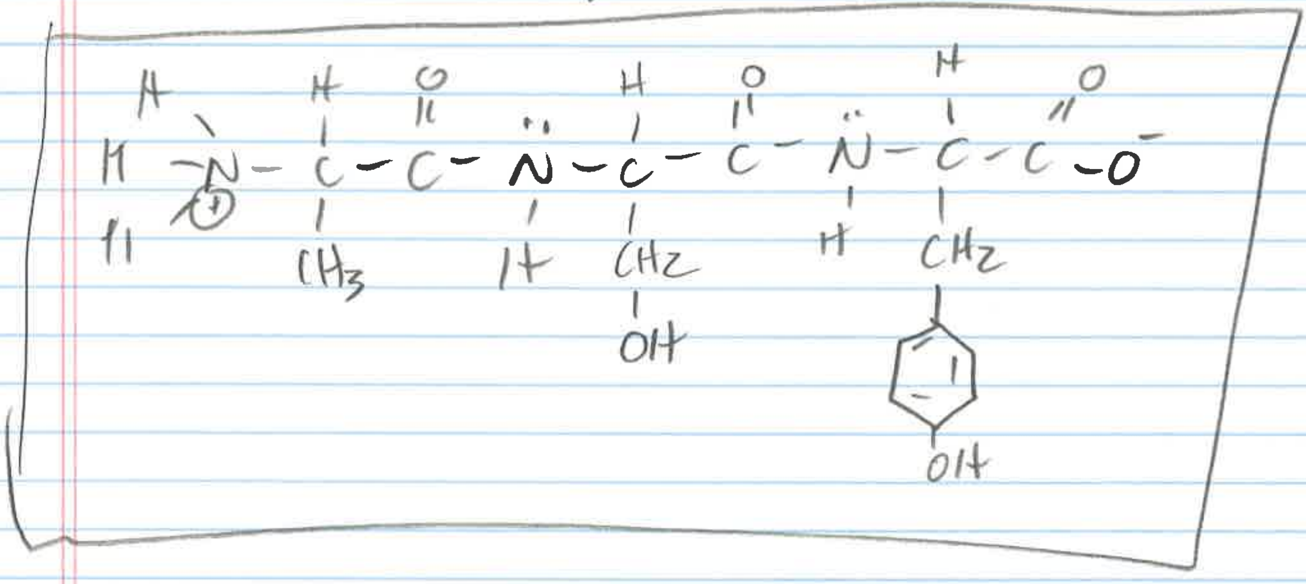
Serine



Tyrosine

Link them and release 2 H_2O

↓

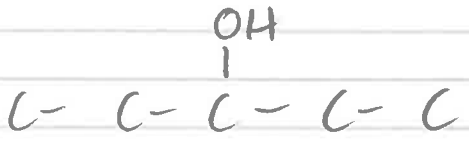


⑦ ii) F

When a globular protein folds in water, the folding process is driven by the entropy increase of the water molecules being released from interacting with hydrophobic amino acids. All globular proteins have hydrophobic amino acids at their cores

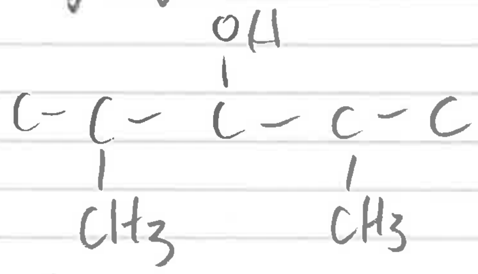
⑧ i) Start with the last part of the name:

3-Pentanol. This means a 5 carbon alcohol with the hydroxyl group on carbon 3, Draw that first



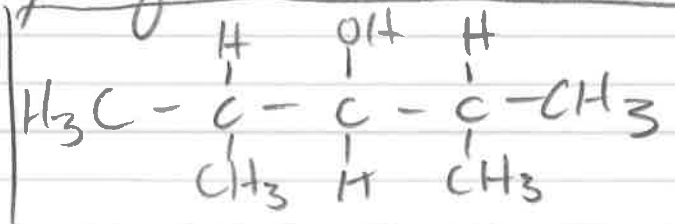
$$\begin{array}{ccccc} & & OH & & \\ & & | & & \\ C- & C- & C- & C- & C \end{array}$$

Then we have 2,4 dimethyl, so add the methyl groups to the molecule



$$\begin{array}{ccccc} & & OH & & \\ & & | & & \\ C- & C- & C- & C- & C \\ & | & & | & \\ & CH_3 & & CH_3 & \end{array}$$

Now add hydrogens so all carbons have 4 bonds.



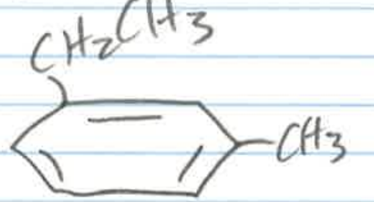
$$\begin{array}{cccc} & H & OH & H \\ & | & | & | \\ H_3C- & C- & C- & C-CH_3 \\ & | & | & | \\ & CH_3 & H & CH_3 \end{array}$$

2,4 Dimethyl-3-pentanol

ii) Start with the last part of the name:

3-methyl benzene (Pick any carbon as #1, it doesn't matter YET)

Now, the 1 ethyl



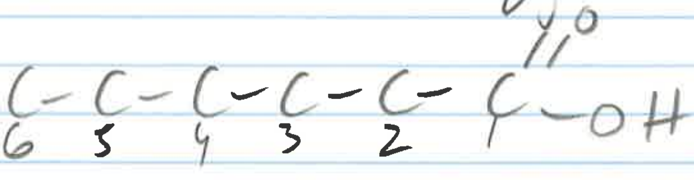
1 ethyl-3 methyl benzene

iii) Start with the last part of the name:

Hexanoic acid

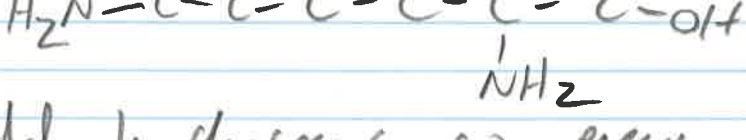
The "-oic acid" tells you it has a carboxylic acid functional group, so...

Six carbons starting with a carboxylic acid



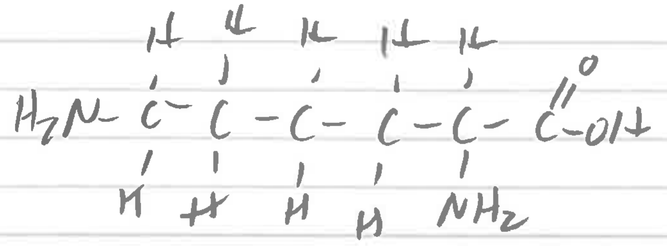
$$\underset{6}{C}-\underset{5}{C}-\underset{4}{C}-\underset{3}{C}-\underset{2}{C}-\underset{1}{\overset{\overset{O}{\|}}{C}}-OH$$

Now: 2,6 diamino. This means that there are two ("di") amino groups (-NH_2) on carbons 2 and 6.



$$H_2N-C-C-C-C-\underset{\underset{NH_2}{|}}{C}-\overset{\overset{O}{\|}}{C}-OH$$

- Add hydrogens so every carbon has 4 bonds



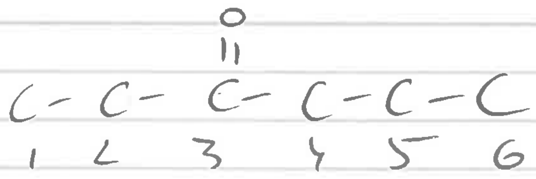
$H_2N-\overset{H}{\underset{H}{C}}-\overset{H}{\underset{H}{C}}-\overset{H}{\underset{H}{C}}-\overset{H}{\underset{H}{C}}-\overset{H}{\underset{NH_2}{C}}-\overset{O}{\overset{\|}{C}}-OH$

2,6-diaminohexanoicacid

iv) 1-methoxy-3-hexanone

Start with the end: 3-hexanone

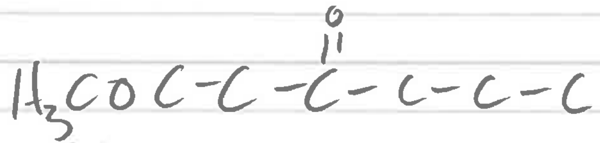
the "-one" suffix means it is a ketone and the 3 tells us which carbon has the carbonyl oxygen attached, so..



$\underset{1}{C}-\underset{2}{C}-\underset{3}{\overset{O}{\overset{\|}{C}}}-\underset{4}{C}-\underset{5}{C}-\underset{6}{C}$

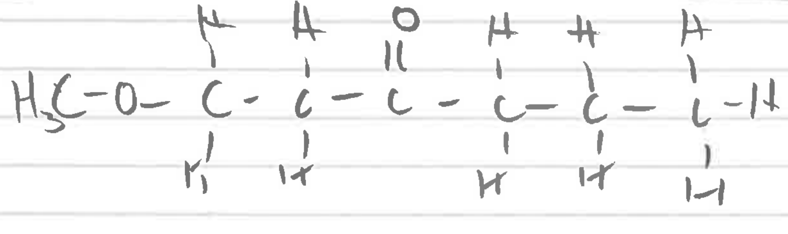
The 1-methoxy implies a methyl ether is attached to carbon 1

methyl ether looks like $-OCH_3$ so add it to carbon 1



$H_3COC-C-\overset{O}{\overset{\|}{C}}-C-C-C$

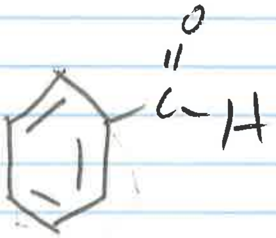
Now add hydrogens so each carbon has 4 bonds



$H_3C-O-\overset{H}{\underset{H}{C}}-\overset{H}{\underset{H}{C}}-\overset{O}{\overset{\|}{C}}-\overset{H}{\underset{H}{C}}-\overset{H}{\underset{H}{C}}-\overset{H}{\underset{H}{C}}-H$

1-methoxyl-3-hexanone

v) Benzene with an aldehyde



Doesn't matter what carbon you stick it to since there's no other functional groups attached.

⑨ Have: 200mg = 0.2g aspirin (FW = 180g/mole)
in 0.05L H_2O

Convert to molarity:

$0.2g \times \frac{1 mole}{180g} = \frac{1.11 \times 10^{-3} mole\ aspirin}{0.05L} = $ 0.022M aspirin @ the start

Now, what are we doing?

Step1: Take 5ml and dilute to 200mL

There are several ways to treat this.
1) Calculate the new molarity by $C_1V_1 = C_2V_2$

$C_1 = 0.022M$ $\quad C_2 = x$
$V_1 = 0.005L$ $\quad V_2 = 0.2L$

$$C_2 = \frac{C_1V_1}{V_2} = \frac{(0.022M)(0.005L)}{(0.2L)}$$

$$\boxed{C_2 = 5.5 \times 10^{-4} M}$$

Alternatively you could calculate the dilution factor

$\frac{200mL}{5mL} =$ 40 times diluted

$$\frac{0.022M}{40} = \boxed{5.5 \times 10^{-4} M}$$

Step 2: $C_1V_1 = C_2V_2$

$C_1 = 5.5 \times 10^{-4} M$ $\quad C_2 \ x$
$V_1 = 0.1L$ $\quad V_2 = 1L$

$$\boxed{C_2 = 5.5 \times 10^{-5} M}$$

or, using dilution factors

$\frac{1000\,mL}{100\,mL} =$ 10 times diluted

$\frac{5.5\times10^{-4}M}{10} = \boxed{5.5\times10^{-5}M}$

Then we :

$C_1 = 5.5\times10^{-5}M$ $\quad$ $C_2 = x$

$V_1 = 5\,mL$ $\quad$ $V_2 = 10\,mL$

$\boxed{C_2 = 2.75\times10^{-5}}$

Or, using dilution factors

$\frac{10\,mL}{5\,mL} = 2$

$\frac{5.5\times10^{-5}M}{2} = \boxed{2.75\times10^{-5}M}$

Final Concentration

⑩ a) Polar uncharged: Asn, Gln, Ser, Cys, Tyr

b) Polar, charged: Asp, Glu, Lys, Arg, sometimes His

c) Acidic Amino Acid: Asp, Glu

d) Hydrophobic: Phe, Tyr, Trp, Leu, Ile, Ala, Pro, Met

e) Basic aminoacids: Lys, Arg