MACQUARIE University

Tutorial 1

pH and Amino Acids

BMOL2201/6201

General Plan for Tutorials

- Place to:
  - engage with content,
  - check your understanding with your peers, and
  - get feedback from a tutor in a small class setting
- NOT a lecture!
  - May revise some content, but aim is to **engage** with the content, **try out** questions and **get feedback**
- 2 hrs every other week, alternating with practicals
  - Case study – please have a read before coming
  - Tutorial quiz – only 10 minutes, at the end of the tutorial, peer-marked (and tutor moderated!)

Tutorial 1 Aims

- Understand what **pH** is, how to calculate it, and how it's relevant to biochemical systems
- Describe what a **buffer** is, and why buffers are important in the human body
- Identify **amino acids** based on their structures, and understand how amino acids bond together to give **peptides**
- Understand how pH affects the **charge** of a peptide
- Define the **isoelectric point** (pI) of peptides, and how to calculate it for small peptide chains

Introduce yourselves!

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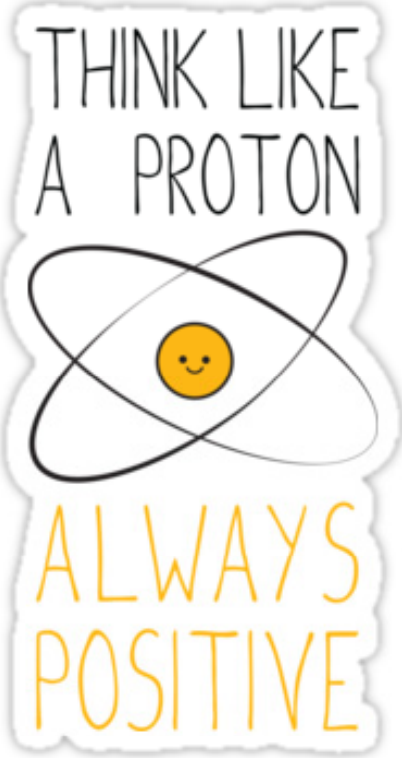
pH – what is that again?

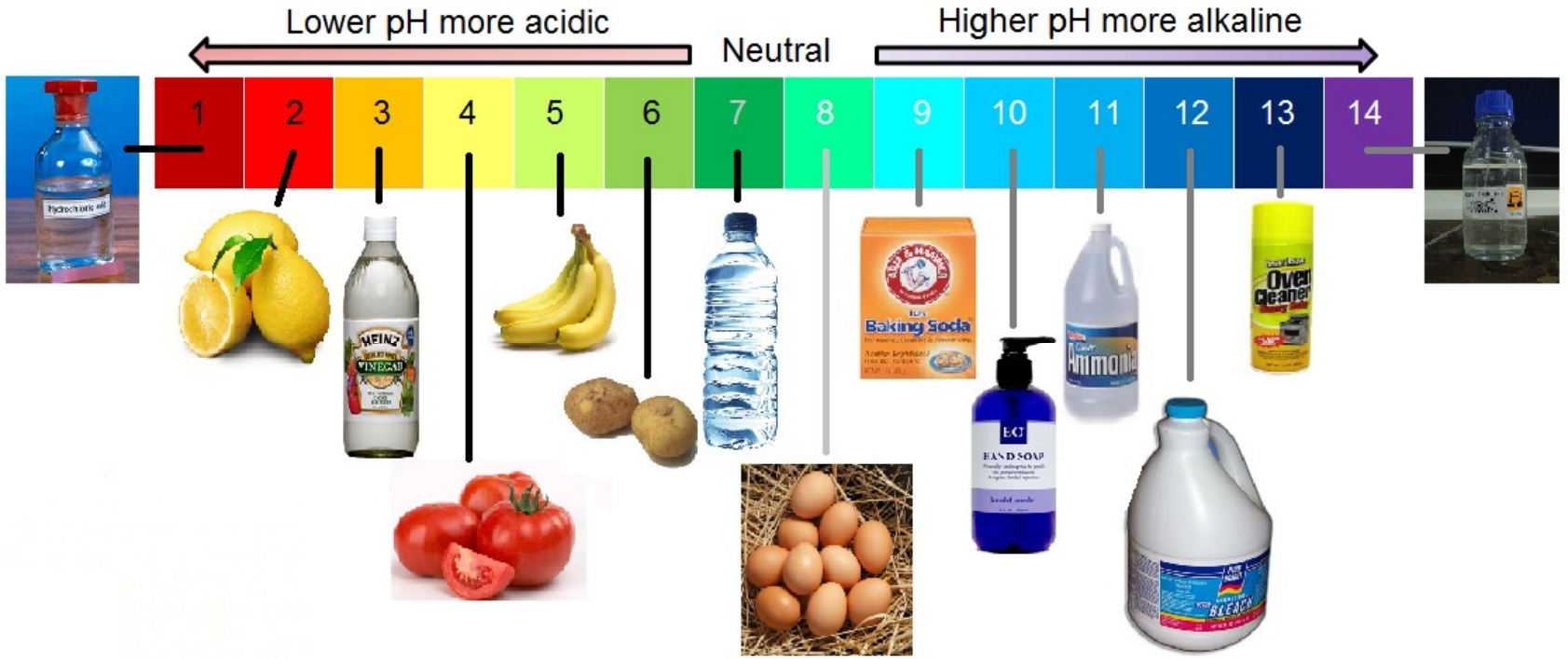
- "Acids and bases are proton donors and acceptors" – Bronsted-Lowry definition
  - "protons" = H^+
  - Concentration of H^+ in solution determines how lots of reactions happen
  - Need something more meaningful than e.g. $[H^+] = 10^{-4}$ mol.L^{-1} – is that a lot??



pH - Definition

$$\mathrm{pH} = -\log_{10}[\mathrm{H}^+]$$

- What that means is:
  - $[H^+] = 10^{-3}$ mol.L^{-1} → pH = 3.0 (acidic – lots of H^+)
  - $[H^+] = 10^{-10}$ mol.L^{-1} → pH = 10.0 (basic – very little H^+)
- Every change in pH of 1 is actually a 10x change in $[H^+]$!
- NB: pH = "power of hydrogen"
  - we often use pX to mean "power of X" for lots of other things too


Lower pH more acidic
Neutral
Higher pH more alkaline
1
2
3
4
5
6
7
8
9
10
11
12
13
14
HEINZ
VINEGAR
Baking Soda
Ammonia
Oven Cleaner
BLEACH

Question 1: pH

a) What is the pH of a solution if $[H^+] = 10^{-4}\ \text{mol.}\,L^{-1}$?

b) Is this acidic or basic?

b) What is the $[H^+]$ concentration of a solution with a pH of 9.0?

pH “neutral”?

- “Neutral” pH is 7.0 – but why?
  - Pure water has $[H^+] = 10^{-7}$ mol.L^{-1} so pH = 7.0
- In the body, a pH of 7.0 is not always desirable
- Normal pH of blood is in the range 7.35 – 7.45
  - Below this range = acidosis; above = alkalosis

Weak Acids and pK_a

- Not all acids give up all their protons instantly - some exist in an equilibrium:

$$HA \rightleftharpoons H^+ + A^-$$

- The equilibrium constant of this reaction determines how much the acid dissociates, and therefore how **strong** it is:

$$K_a = \frac{[H^+][A^-]}{[HA]}$$

- Usually use pK_a instead:

$$pK_a = -\log_{10}(K_a)$$

Most biochemical molecules are weak acids or bases!

Weak Acids and Buffers

- pH = pK_a when there is an equal amount of the acid and base forms of a molecule
  - can use this to work out pK_a values in titrations
- Around this value, the equilibrium **resists changes in pH**
- pH region is usually ± 1 from pK_a value
- Extremely important in maintaining correct pH levels in the body!

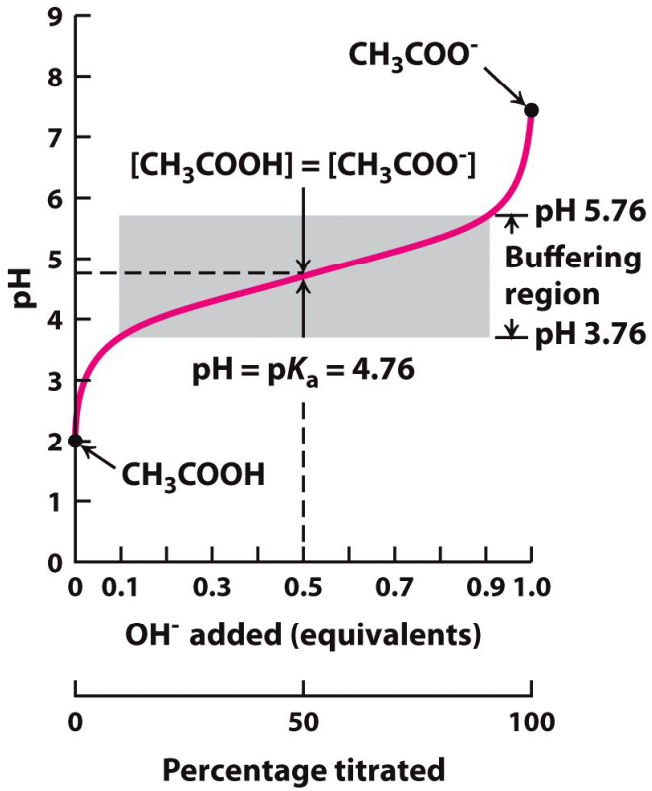


Figure 2.10
Biochemistry: A Short Course, First Edition

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Question 2: Weak Acids and pK_a

We have a solution of a weak acid with a pK_a value of 4.5.

a) If the pH of the solution is **2.0** (i.e. below the pK_a value), is there more of the **protonated** form or the **deprotonated** form?

b) If the pH of the solution is raised to **6.0**, would we have more of the **protonated** form or the **deprotonated** form?

c) What about if the pH is just **4.5**?


Case Study 1: Aspirin!
Team work time!

Case Study Q&A!

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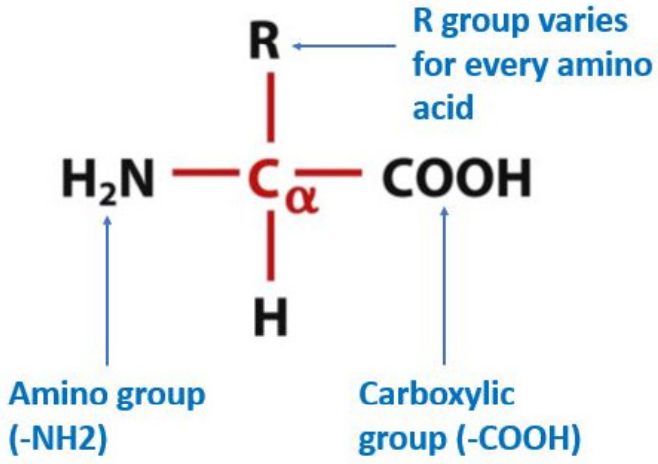
Amino Acids – Cellular LEGO

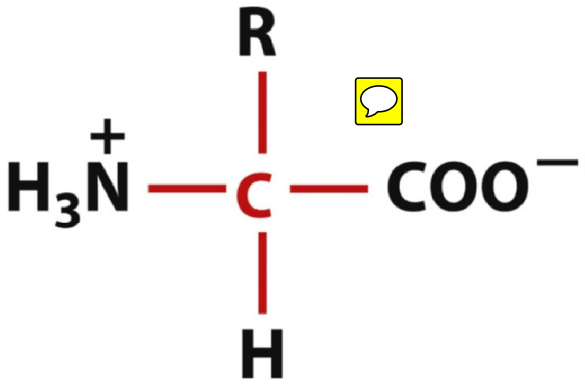
- Building blocks of proteins
- 20 different types in humans, each with unique shape and properties (like LEGO!)
- No need to memorise structures BUT need to understand their properties and identify them!

Amino Acids in Solution

- Every amino acid* has the same main structure, just with a different side chain (R)
- Two functional groups: amino group and carboxy (carboxylic acid) group

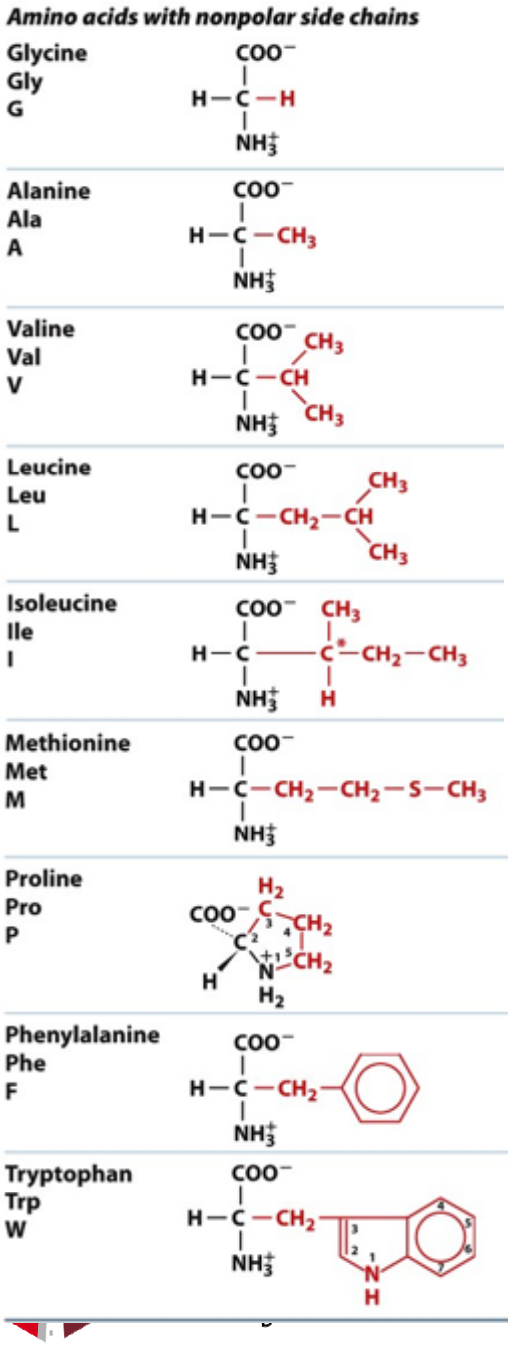


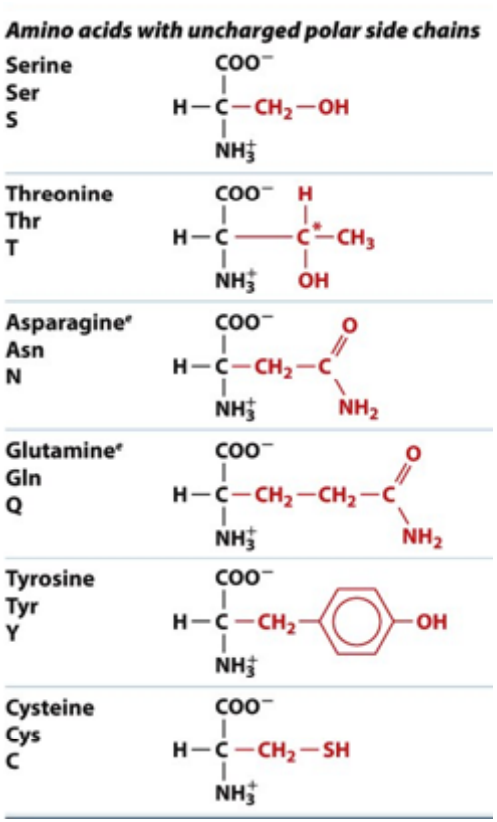
- Amino and carboxy groups can be charged (and usually are!)
  - Both groups charged = neutral charge overall = **zwitterion**



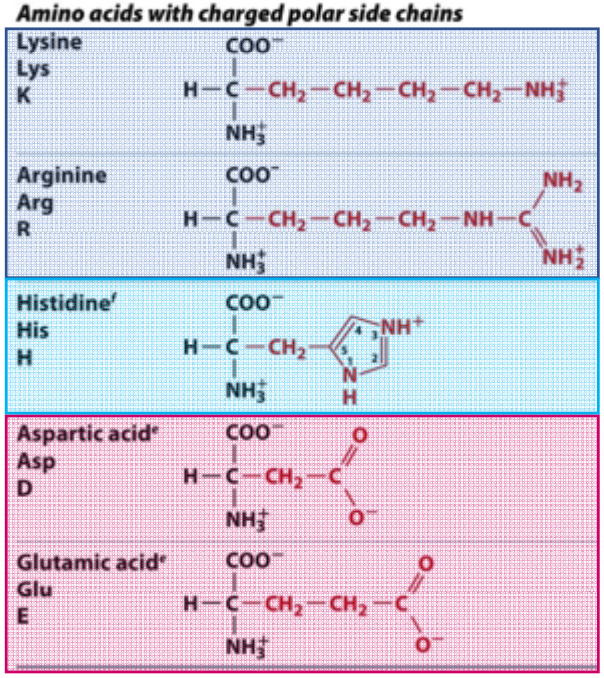
* Except proline – only weird exception!

Amino Acid Side Chain Fun





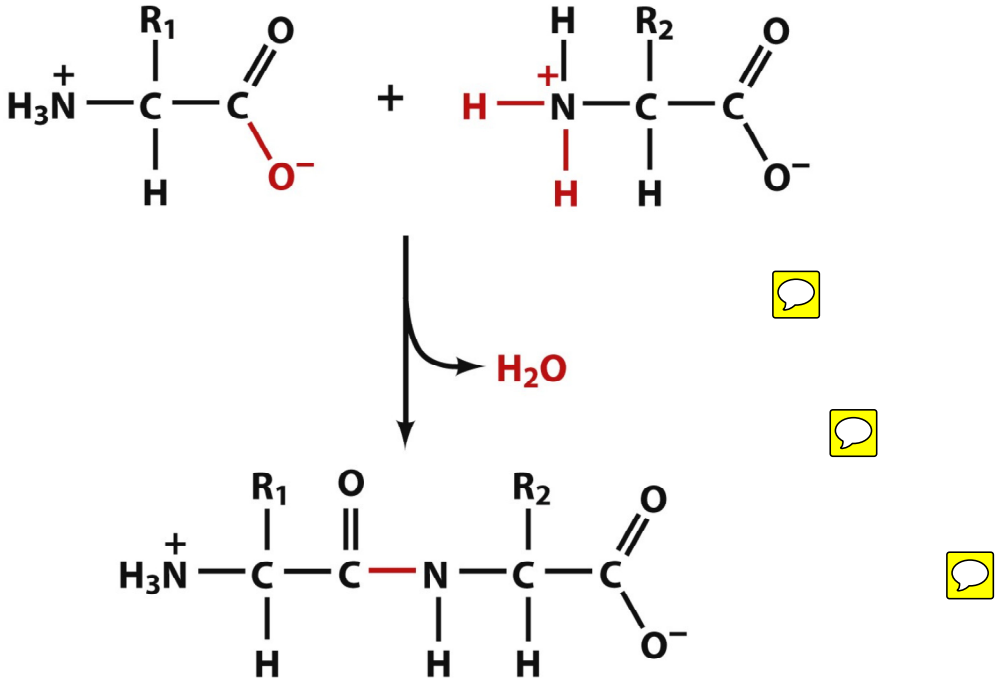
15 are just zwitterions



5 have charged side chains

Peptide Bonds

- Amino and carboxy groups can bond together in a condensation reaction:



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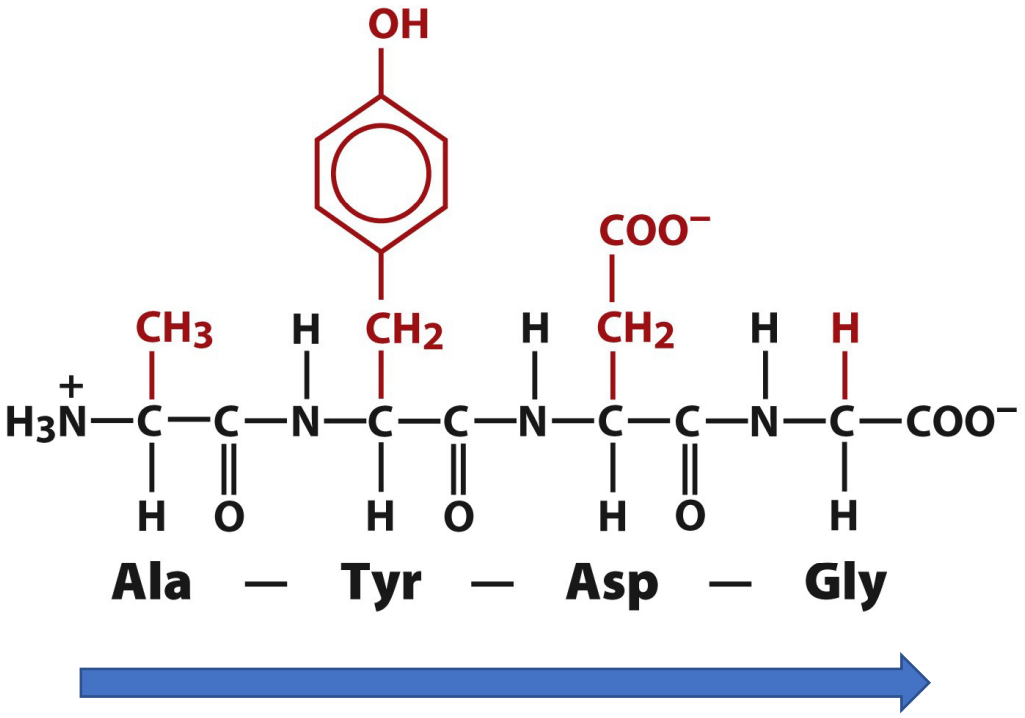
Amino Acid Chains = Peptides

- Start of peptide = AMINO END (N-terminus)
- End of peptide = CARBOXY END (C-terminus)
- When listing names, go from N to C



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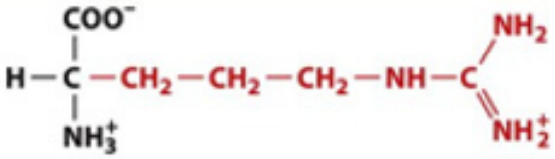
pH and Amino Acid Groups

- pH affects what groups are charged in amino acids, including some side chains
- As pH increases, more and more H^+ are ripped off, making the molecule more NEGATIVE
- Exactly when H^+ starts to get ripped off of a particular group depends on the pK_a
- To calculate the **charge** at a given pH, start from a completely protonated form (super low pH), and work your way up, ripping off one proton at each p*K* value

Question 3: Charge and pH

Arginine
Arg
R



The amino acid arginine has a basic side chain, with pK_1 = 2.0, pK_2 = 10.0 and pK_R of 12.5.

a) Draw the charged structure of arginine at a pH of 1.0 (completely protonated)

b) Next, draw it at a pH of 5.0

c) Next, draw it at a pH of 11.0

d) Finally, draw it at a pH of 14.0 (completely deprotonated)

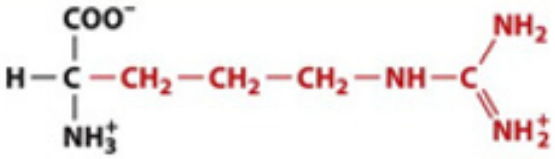
e) What is the **charge** on each of the above molecules?

Isoelectric Point and pI

- The pH at which an amino acid or peptide has zero net charge is called its isoelectric point, or pI
- We can calculate it by working out the charge like before, then using the nearest pK_a values to get an average

Question 4: pI

Arginine
Arg
R



The amino acid arginine has a basic side chain, with pK_1 = 2.0, pK_2 = 10.0 and pK_R of 12.5.

a) Using the information provided and your structures from Question 3, what two p*K* values must the pI of arginine lie between? (i.e. when is it 0?)

b) Calculate the pI by taking the average of the two (i.e. add them, and divide by 2)


See what
you've learnt!
Quiz time