Researchers in Schools

# Can we do experiments on a Computer?

Pupil Name

Coursebook Designed by Dr Maeve Kavanagh

# Contents

Timetable and Assignment Submission ..... 1
Timetable – Tutorials ..... 1
Timetable – Homework Assignments ..... 1
Assignment Submission – Lateness and Plagiarism ..... 1
Course Rationale ..... 2
Uni Pathways Mark Scheme 2021 – science-based assignments ..... 3
Baseline Assignment (essay based): Pupil Feedback Report ..... 4
Final Assignment (essay based): Pupil Feedback Report ..... 5
Subject vocabulary glossary: ..... 6
Launch Event ..... 9
Tutorial 1 – Imitating the World Around Us with Models ..... 10
What is the Purpose of Tutorial 1? ..... 10
Tutorial 2 – What do we need to build a model? *Data, Resources and Crystallography* ..... 17
What is the Purpose of Tutorial 2? ..... 17
Tutorial 3 – How does our model work? *Classical mechanics, quantum mechanics and using algorithms…* ..... 22
What is the Purpose of Tutorial 3? ..... 22
Tutorial 4 – Testing our Model. *Spectroscopy and Collaboration* ..... 27
What is the Purpose of Tutorial 4? ..... 27
Tutorial 5 – Thinking like a Computational Chemist. ..... 31
What is the Purpose of Tutorial 5? ..... 31
Tutorial 6 – Feedback tutorial ..... 41
What is the Purpose of Tutorial 6? ..... 41
Final assignment feedback from your Uni Pathways Teacher ..... 41
Tutorial 7 – Final tutorial ..... 43
Appendix 1 – Referencing correctly ..... 45
How do I reference? ..... 46
Notes ..... 47

# Timetable and Assignment Submission

## Timetable – Tutorials

| Tutorial | Date | Time | Location |
|---|---|---|---|
| 1 | | | |
| 2 | | | |
| 3 | | | |
| 4 | | | |
| 5 | | | |
| 6 (Feedback) | | | |
| 7 (Feedback) | | | |

## Timetable – Homework Assignments

| Homework Assignment | Description | Due Date |
|---|---|---|
| Tutorial 1 | | |
| Tutorial 2 | | |
| Tutorial 3 | | |
| Tutorial 4 | | |
| Tutorial 5 | | |

## Assignment Submission – Lateness and Plagiarism

| Lateness | |
|---|---|
| Submission after midnight on 9th August | 10 marks deducted |
| **Plagiarism** | |
| Some plagiarism | 10 marks deducted |
| Moderate plagiarism | 20 marks deducted |
| Extreme plagiarism | Automatic fail |

## Course Rationale

Welcome to your Uni Pathways course, where we will find out how researchers can use nothing more than a computer to do science experiments. This course was designed by Dr Kavanagh, based on her PhD, which she completed at Imperial College in London. Uni Pathways gives you a fun and unique opportunity to see what university work and life would be like.

In this course, you will get the opportunity to expand on your scientific knowledge to tackle questions like a real scientist would, such as: 'What do I want to find out?' and 'How can I plan an experiment that will tell me all the things I want to know?'. You will learn things that are not usually taught at school, giving you a head start in A level science subjects and even university-level learning on these topics. Because of the nature of this project, we will learn some new biology, some new chemistry, *and* some new physics. You will also get to practice your writing in our final assignment, a key skill for any scholar!

In our first tutorial we will talk about what a model is, including where you'll have seen some before. This is key knowledge for your GCSE in science (although we will go into a lot more detail than we have seen in the science classroom before). In tutorial 1 you will also be introduced to a futuristic new field of science called 'Computational Chemistry'. We will talk about some of the topics you have already covered in Biology and ask, 'can we build a model to help us understand what is going on here?'.

Next you will learn what is needed to build a model. Now you're starting to face the questions that a real research scientist would come up against. We will preview some key concepts in Chemistry that you wouldn't usually be thinking about until A-level. And we will throw in some university level Chemistry and learn all about a really useful technique called Crystallography (biologists also really love this technique!).

Lesson three is where we will be diving into Physics. OK so you know how forces work but do you know how electrons move? Welcome to the world of Quantum Mechanics; it's all a bit unexpected! We will also learn about algorithms; these are really crucial for Computer Scientists.

Now you are already pretty good at building models, the most important thing is to know if they are working well. In the fourth tutorial we start to find out how we can tell if the model we have built is up to the task we have set it. How do we test our model to find out if it is any good? One technique that chemists use is called Spectroscopy, you will learn about this in some detail. Of course, we can't do all this work alone, in this lesson we discuss the importance of collaborating with other scientists to make sure we are on the right track.

Our final tutorial, lesson 5, is where you get to show off everything you have learned. You are a Computational Chemist embarking on a quest for new knowledge. How will you apply your scientific reasoning to solving four different problems? How can you write your proposals down like a real scientist? This tutorial will really set you up for writing your final assignment. Good luck!

# Uni Pathways Mark Scheme 2021 – science-based assignments

| | Subject Knowledge | Critical Thinking | Written Communication |
|---|---|---|---|
| 1st | The work shows a depth of knowledge and understanding of key concepts and scientific methods, through engaging with relevant sources. Knowledge is used to build and support highly effective scientific arguments and explanations. | Analyses key scientific evidence, arguments, and reasoning. Interprets meaning and makes connections. Identifies and critically evaluates key scientific arguments and evidence, deciding on their credibility, strength, and relative significance, drawing convincing conclusions. | The work has a coherent flow and is well structured. The writing style is appropriate; scientific language and key scientific terms are used accurately and effectively to support the arguments and explanations made. There are no, or very few, errors in spelling or grammar. Consistent referencing used throughout. |
| 2:1 | The work shows an understanding of key concepts and scientific methods, drawing on relevant sources. Knowledge is used to build and support effective scientific arguments and explanations. | Analyses relevant scientific evidence, arguments, and reasoning. Identifies and critically evaluates relevant scientific arguments and evidence, deciding on their credibility and strength, drawing reasonable conclusions. Shows some understanding of the relative value of evidence and arguments. | The work is well-structured. The writing style is appropriate; scientific language and key terms are used correctly. There are few errors in spelling or grammar. Mostly consistent referencing. |
| 2:2 | The work shows an understanding of key concepts and scientific methods, with no major misconceptions. Beginning to apply this knowledge to build and support effective scientific arguments and explanations. | Identifies and uses basic scientific evidence, arguments, and reasoning. Showing some understanding of the quality of scientific arguments and evidence. Not yet showing understanding of the relative value of evidence and arguments. | The work has some structure. The writing style can sometimes be informal; occasionally scientific language and key terms are not used when it would be appropriate to do so. There are some errors in grammar and spelling do not get in the way of communicating the content. Referencing has some consistency. |
| 3rd | Shows a developing understanding of key concepts and scientific methods, with some misconceptions. Does not yet apply this knowledge to build and support scientific arguments and explanations. | Beginning to analyse scientific evidence, arguments, and reasoning. Describes evidence and arguments, while not yet evaluating them. | The grammar, spelling, style, and structure of the work need improving in order to communicate ideas to the reader. Scientific language, key terms and references are not always used correctly. |

# Baseline Assignment (essay based): Pupil Feedback Report

| | |
|---|---|
| Name of Pupil | |
| Name of School | |
| Name of RIS teacher | |
| Title of Assignment | |

How your assignment is graded:

| Grade | Marks | What this means |
|---|---|---|
| 1st | 70+ | Performing to an excellent standard at A-level |
| 2:1 | 60-69 | Performing to a good standard at A-level |
| 2:2 | 50-59 | Performing to an excellent standard at GCSE |
| 3rd | 40-49 | Performing to a good standard at GCSE |
| Working towards a pass | 0-39 | Performing below a good standard at GCSE |
| Did not submit | DNS | No assignment received by The Brilliant Club |

| Lateness | |
|---|---|
| Any lateness | 10 marks deducted |
| **Plagiarism** | |
| Some plagiarism | 10 marks deducted |
| Moderate plagiarism | 20 marks deducted |
| Extreme plagiarism | Automatic fail |

Marks

| | | | |
|---|---|---|---|
| OVERALL MARK / 100 | | FINAL MARK / 100 (including any deductions) | |
| DEDUCTED MARKS | | FINAL GRADE | |

If marks have been deducted (e.g. late submission, plagiarism) the teacher should give an explanation in this section:

Mark Breakdown and Feedback

| Subject knowledge | |
|---|---|
| | *mark* |
| | |
| | |
| **Critical thinking** | |
| | *mark* |
| | |
| | |
| **Written communication** | |
| | *mark* |
| | |
| | |

# Final Assignment (essay based): Pupil Feedback Report

| | |
|---|---|
| Name of Pupil | |
| Name of School | |
| Name of RIS teacher | |
| Title of Assignment | |

How your assignment is graded:

| Grade | Marks | What this means |
|---|---|---|
| 1st | 70+ | Performing to an excellent standard at A-level |
| 2:1 | 60-69 | Performing to a good standard at A-level |
| 2:2 | 50-59 | Performing to an excellent standard at GCSE |
| 3rd | 40-49 | Performing to a good standard at GCSE |
| Working towards a pass | 0-39 | Performing below a good standard at GCSE |
| Did not submit | DNS | No assignment received by The Brilliant Club |

| Lateness | |
|---|---|
| Any lateness | 10 marks deducted |
| **Plagiarism** | |
| Some plagiarism | 10 marks deducted |
| Moderate plagiarism | 20 marks deducted |
| Extreme plagiarism | Automatic fail |

Marks

| | | | |
|---|---|---|---|
| OVERALL MARK / 100 | | FINAL MARK / 100 (including any deductions) | |
| DEDUCTED MARKS | | FINAL GRADE | |

If marks have been deducted (e.g. late submission, plagiarism) the teacher should give an explanation in this section:

Mark Breakdown and Feedback

| Subject knowledge | |
|---|---|
| | *mark* |
| | |
| | |
| **Critical thinking** | |
| | *mark* |
| | |
| | |
| **Written communication** | |
| | *mark* |
| | |
| | |

## Subject vocabulary glossary:

| Word | Definition | In a sentence |
|---|---|---|
| Ab initio | A method which is based on the theory of quantum mechanics, where every single calculation has to be done by the computer on the spot. | Ab initio methods can only be used to model a small system (just a few atoms) because they are so expensive. |
| Binding | The way that a specific drug attaches to a protein inside our bodies | It is important to model protein binding when you want to develop a new drug |
| Biological system | A chemical system that exists inside a living thing | A protein is a both a biological system and a chemical system |
| Chemical system | An atom, a molecule, a group of molecules or a bulk material. | The molecules in the air are a chemical system |
| Classical mechanics | A theory that tells us how large things (atoms or larger) will move. | Classical mechanics can be used to predict what will happen when you kick a football |
| Computational chemistry | Using computers to build models of chemical systems and study them. | Computational chemistry helps us understand the world around us without having to do costly experiments. |
| Crystallography | An experimental technique that shows us which atoms are where within a chemical system. | Crystallography tells us about the structure of proteins |
| Data | Information that can be collected by doing an experiment or running a simulation. | Wow, look at all this data! |
| Drug | A molecule that can interact with proteins in our bodies and change their behaviour | Computational chemistry is extremely useful in research into new drugs. |
| Electrons | Sub-atomic particles that are found in atoms and molecules | Chemists study the way that electrons interact with light |
| Electronic | Something to do with electrons | Electrons have electronic properties. |
| Empirical | Anything that has been found out using a real-world experiment | Empirical data is data that was generated by experiments. |

| | | |
|---|---|---|
| Experimental | Something that involves doing a real experiment. | Experimental chemists do experiments with real-world materials. |
| Geometry | Where things are in space, in relation to each other | Atoms in a molecule are always moving, they don't have one constant geometry unless we look at a snapshot. |
| Hybrid | A combination of two or more things | Hybrid models involve both quantum mechanics and classical mechanics parts. |
| Method | A particular way of doing something | Scientists need to choose a method that will allow them to answer their research question. |
| Model | An imitation of something in the real world, something you can build. | In year 8 we look at a model of the lungs and chest cavity that is made of a bell jar and some balloons. |
| Molecular Dynamics | A method that uses classical mechanics to predict how atoms will move within a chemical system | Molecular dynamics can be used to model whole proteins. |
| Protein | A huge molecule found inside our bodies that is responsible for the way we function, grow and heal. | Proteins are especially difficult to model because they are so large! |
| Quantum mechanics | A theory that tells us how very small things (smaller than atoms) will move | The theory of quantum mechanics explains strange properties of electrons, such as wave-particle duality. |
| Semi-empirical | A method which is based on ab initio but also includes some information from experiments, so the computer doesn't have to calculate everything as some of the answers are already there. | Semi-empirical models are a lot cheaper than ab initio, but still get reasonable results. |
| Simulated | Produced by a model. | Data can be simulated or can be found through experiments. |
| Simulation | Making a model go, imitating the real world using a model. | For large models, we sometimes have to run simulations that last days or even months! |
| Spectroscopy | An experimental technique which measures a spectrum, produced by shining light on a chemical or material. | Chemists study the way light interacts with matter using spectroscopy |

| | | |
|---|---|---|
| Spectrum | The result you get when you do spectroscopy | In a lab you can produce an experimental spectrum, or you can produce a simulated spectrum using a computational model. |
| Sub-atomic | Something smaller than an atom | Sub-atomic particles include electrons and protons |
| Theoretical | Anything that uses a theory, instead of real-world experiment | Data that is produced by a computer model is theoretical. |
| Theory | A group of ideas that can explain something about the world around us. | Computational chemists use theories to build models that can imitate real-life systems. |
| Wave-Particle duality | A property that we can only see in sub-atomic particles, meaning that they behave like waves and particles at the same time. | Electrons have wave-particle duality |
| | | |
| | | |
| | | |
| | | |
| | | |
| | | |
| | | |

We have left some space for you to add your own words if you would like to.

## Launch Event

The launch event is your opportunity to learn more about this course and Uni Pathways. You will watch some videos, listen to your teacher and have some discussion. Below is some room to make notes for some of the videos you will watch during the event.

**Virtual Campus Tours**

Notes…

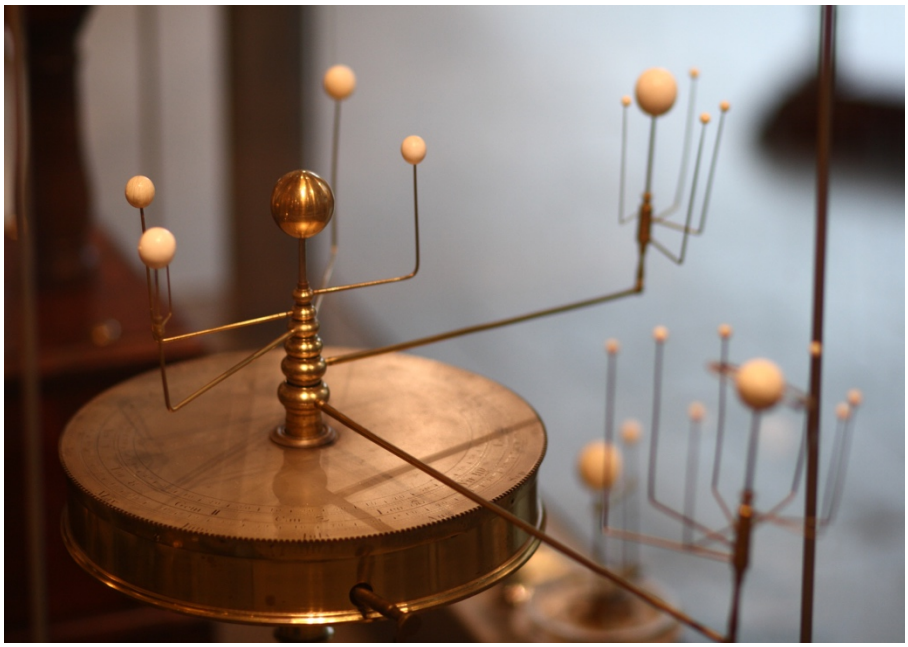
**The Scholars Programme Alumni**

Notes…

**Student Ambassadors**

Notes…

# Tutorial 1 – Imitating the World Around Us with Models



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A model of our solar system

## What is the Purpose of Tutorial 1?

- To be able to define what a model is
- To know what a computational chemist does
- To be able to discuss why biological research is important

### Activity 1

Draw a picture of a scientist in the space below:

If you have finished you may label the equipment that your scientist has, maybe you want to add some of the equipment examples on the board.

**(Blank page for your notes)**

**Activity 2 – What does a computational chemist look like?**

Computational chemists

Look at the picture of the **computational chemists** above, what equipment do computational chemists need? Talk to your partner about what equipment you gave to your scientist on page 9. There is space for some reflections below:

**Activity 3 - What models have you seen before?**

Use the space below to copy down some of your favourite examples of models from the whole class discussion:

**Activity 4 – Quiz**

Choose the correct answer to complete the sentences. Get ready to show your answers on your mini whiteboard:

1. A model is something that you can…
    a. **Build** to imitate a real-world system
    b. **Run** in order to make predictions
    c. **Observe** in the real world

My answer: Correct answer:

2. A simulation is something that you can…
    a. **Build** to imitate a real-world system
    b. **Run** in order to make predictions
    c. **Observe** in the real world

My answer: Correct answer:

3. Models can help us understand the real world by…
    a. Helping us to explain what we can observe
    b. Allowing us to explore unseen scenarios
    c. Showing us a more simple version of what is going on

My answer: Correct answer:

4. Models are:
    a. Cheap and easy to build
    b. Exactly the same as what we can observe
    c. Useful in all fields of science

My answer: Correct answer:

**Activity 5 – What is a model?**

Now use the space below to write down what a model is, use the following key words to help you (**build**, **observe**, **real-world**, **imitate**, **simulate**):

**Activity 6 – Biological Systems**

Some examples of biological systems

What biological system would you like to build a model of?

_____

_____

_____

_____

**Activity 7 – True or False**

Answer the questions by raising your hand to indicate the correct answer:

1. We can make models of diseases like Covid-19 using computational chemistry
2. The particles in the air are a biological system
3. Computational chemists can do science with no equipment
4. A model shows us exactly what is going on in the real world
5. Computational chemistry can help us understand how drugs work

My answers:

Correct answers:

**Activity 8 – Summary: Why do we use computational chemistry to study biological systems?**

Use the space below to write down what computational chemistry is and why it is useful to us, use these key words to help you (**biological system**, **model**, **simulation**, **describe**, **explain**, **predict**):

**Baseline assignment question:**

**You are a computational chemist who has been asked to build a model of a protein. Write an essay (approx. 400 words) describing why computational chemistry is a useful tool to use when doing research into proteins.**

**Details of the assignment:**

**You will write an essay (approximately 400 words long) using the work we have done today to guide you.**

**Success criteria – how to structure your assignment and what to include:**

**A successful essay will include:**

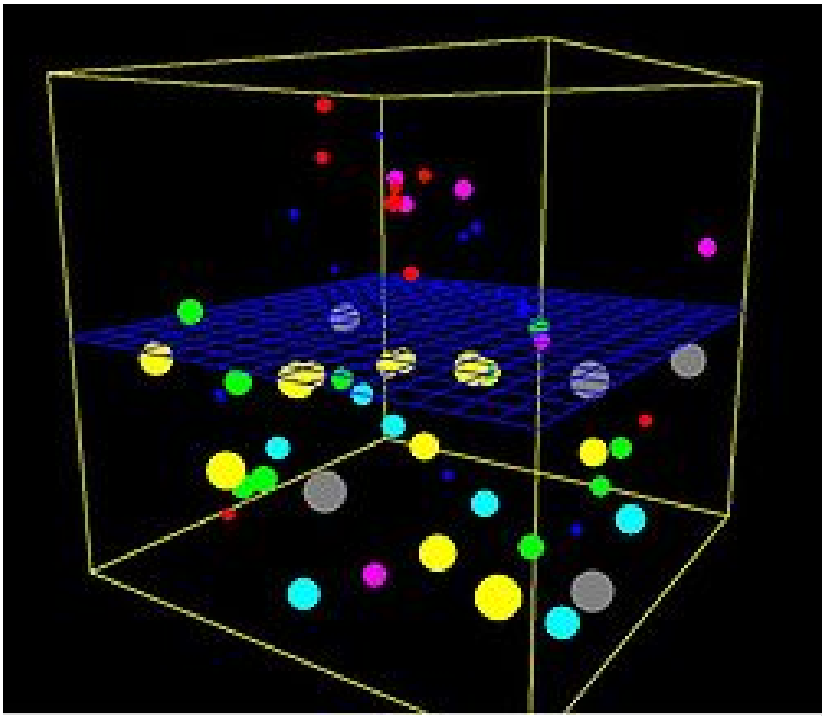
- **An introduction to modelling and its importance to scientists**
- **A description of what computational chemistry is**
- **A discussion of why research into biological systems (such as proteins) is important**
- **A conclusion linking what you have discussed back to the main question (*Why is computational chemistry useful for studying proteins?*)**

**Your notes from today's session will be useful to you.**

**You will use full sentences and proper paragraphs in your writing, paying attention to spelling and grammar. You can refer to the glossary for this course to check the spelling of key words.**

| | |
|---|---|
| In this assignment, show me that you **understand**:<br><br>What computational chemists do and why they do it. | Show me that you **are able to**:<br><br>**Give justifications for why we choose to model proteins using computational chemistry** |

# Tutorial 2 – What do we need to build a model? *Data, Resources and Crystallography*



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What does a computational model of a chemical system look like?

## What is the Purpose of Tutorial 2?

- To know that the behaviour of a chemical system is linked to its structure.
- To know what a computational chemist needs to create a model
- To be able to describe what crystallography is and how it is useful to computational chemists

### Activity 1 – What does a model look like?

Working together with a partner, fill in the end of this sentence to recap from last lesson:

A computational chemist … _____

_____

_____

_____

Now with your partner, use the next page to make notes and draw diagrams of what you think a computational model of a chemical system might look like. What do you think you would be able to see on the computer screen?

**What I think a model might look like** (write any ideas and/or draw what you might see on the computer screen when you looked at your model, use your imagination!)

**Activity 2 – Data and Resources**

Working in pairs sort the words on the board into data and resources, write them in the correct box below:

| Data | Resources |
| --- | --- |
| | |

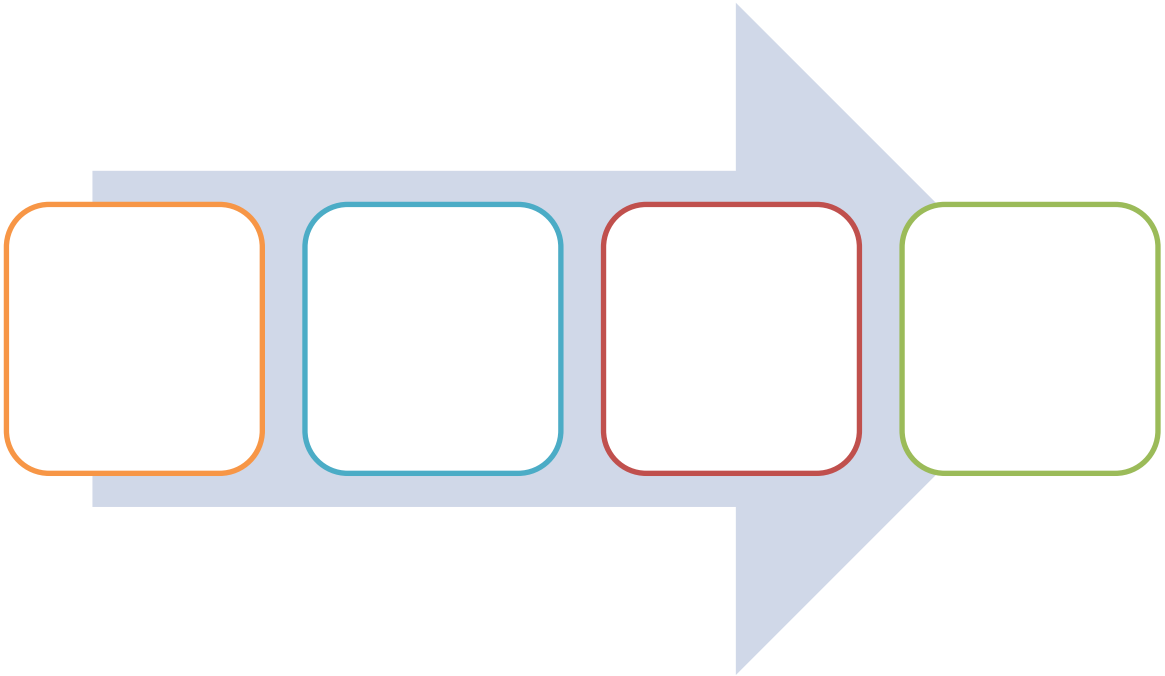
Now can you use these words to label your imaginary model on the previous page? Remember to add to your imaginary model if you left any of these things out.

**Activity 3 – What do you need to build a model?**

Write in your own words below what you need to build a model, think about data and resources. To stretch yourself, write down why you would need each of the items in your list.

**Activity 4 – Steps to building a computational model**

Fill in what steps you would need to take to build a model of a chemical system, check that you have them in the same order as they are on the board.



**Reading together – Crystallography**

So, you want to know where the atoms are in a molecule, protein, new drug or material? But if atoms are way too small to see with a microscope, how can you possibly find this out? One incredible technique is called Crystallography.

Crystals are solid materials in which repeating chemical units (i.e. molecules or proteins) are packed together in a perfectly ordered way. Imagine a kaleidoscope showing the exact same image repeated over and over just rotated in a number of different ways. Now imagine that kaleidoscope is 3 dimensional and the repeating pattern is a protein! Crystals don't have to be made of proteins, in fact mostly we make crystals from very small molecules.

***Fun Fact***
*Great Crystallographers are really sought after in science, some of the most famous published work in the scientific literature is made by crystallographers!*

Anything you can crystallise (make into a crystal) can be studied by crystallography. Crystallography is a way of seeing where atoms are inside your crystal. If we only had one protein or one molecule we could not see where the atoms were, but the power of crystals means that we can use X-rays to discover the repeating arrangement inside them.

X-rays are fired at a crystal and a 3D pattern emerges. The pattern is cleverly analysed by experts called Crystallographers, they can tell which atoms (i.e which chemical elements) are where in the crystal. Once they know this they have the power to tell the world! Luckily for the rest of us scientists, crystal structures (the 3D arrangement of atoms in molecules, proteins, drugs, you name it!) are published freely on the internet.

Crystal structures aren't perfect, there might be some uncertainty around where smaller atoms are inside the crystal. Also consider this; the atoms in molecules are always moving. When we look at crystal structures we can only see a snapshot of where the atoms are in our system. Is that always the best thing?

**Activity 5 – Test your knowledge of crystallography**

Answer true or false for each question, get ready to show your answers on your mini whiteboard:

1. Crystallography can only be used to model small molecules
2. Once they have been found, crystal structures are freely available on the internet
3. Crystal structures give us a perfect picture of where the atoms in a protein are
4. Crystal structures are the only way to find out the structure of a protein
5. You can use crystallography to study systems in any state (solid, liquid or gas)

My answers:

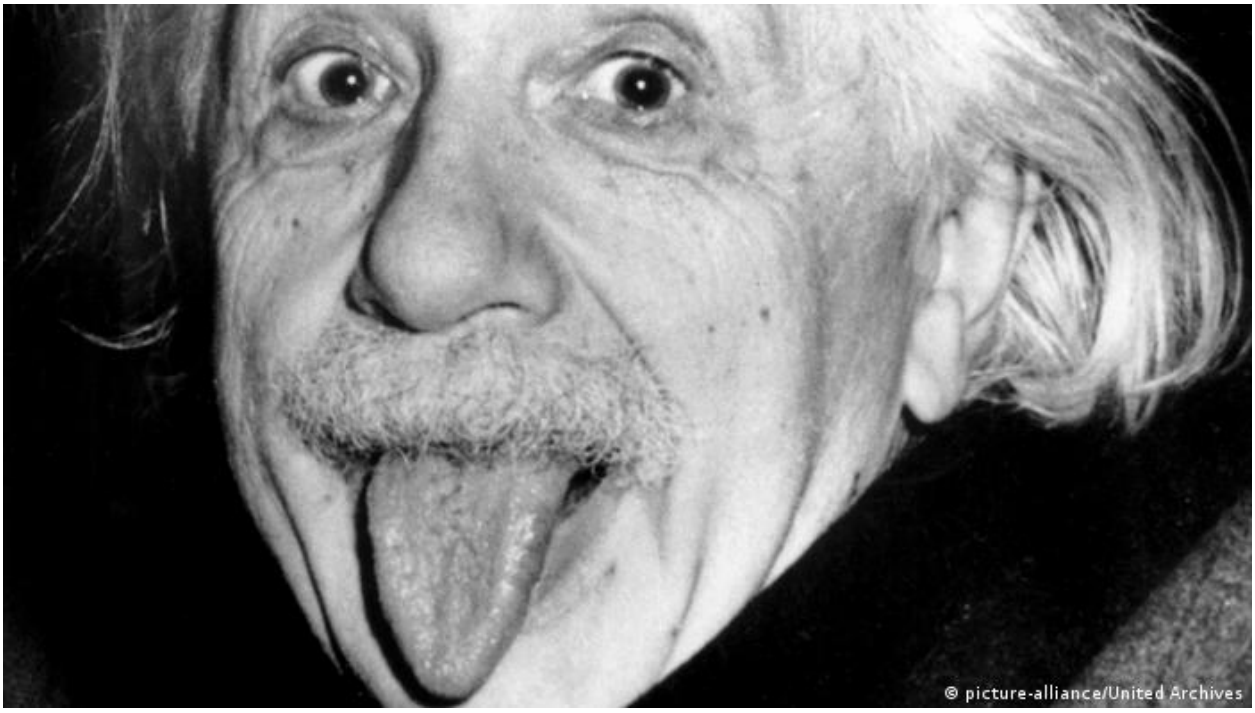
Correct answers:

**Homework – Reflections on the use of crystallography**

Write down your own answer to the following questions.

a) How is crystallography useful to computational chemists?
b) What do we need to be wary of when we use crystal structures to build computational models?

## Tutorial 3 – How does our model work? *Classical mechanics, quantum mechanics and using algorithms…*




Famous Physicist Albert Einstein: Who could never decide which maths to use!

### What is the Purpose of Tutorial 3?

1. Students will be able to distinguish between classical and quantum mechanical systems
2. Students can list four computational chemistry methods: Ab initio, Semi empirical, Molecular Dynamics and Hybrid modelling
3. Students will analyze the cost of computational resources for the four methods in relation to system size (i.e. number of atoms)

**Activity 1 – Making predictions using physics!**

Working together with a partner, fill in the end of this sentence to recap from last lesson:

A computational chemist uses crystallography …_____

_____

_____

_____

Now look at the systems on the board and discuss with your partner, what forces are acting on the objects? Use the space below to write your ideas down…_____

_____

_____

_____

_____

_____

_____

**Activity 2 – Classical Mechanics Quiz**

1. What can Classical Mechanics describe?

a) Objects moving at the speed of light
b) Massive objects such as planets
c) The observable world

2. How can we best explain Classical Mechanics?

a) Maths
b) Diagrams
c) Observations

3. In which subject would you study Classical Mechanics?

a) History
b) Physics
c) Maths

4. What does Classical Mechanics allow us to do?

a) Predict where classical objects will be in the future
b) Predict how objects move
c) Predict how objects interact with each other
d) All of the above

My Answers:

Correct Answers:

**Reading together – Quantum Mechanics**

Long after Newton had told the world about gravity and forces, a new kind of science became very fashionable. Scientists, including a young Albert Einstein, became obsessed with trying to understand some seriously weird new data.

Welcome to the world of quantum mechanics, the unusual mathematics that we use to describe how tiny particles, such as electrons, move and behave. Don't worry if you can't get your head around this, because basically – nobody can! The objects we see and interact with in our daily lives are all way, way larger than electrons. So we can almost never observe quantum mechanics in action, unless we do complicated experiments with tiny, quantum particles.

There are many fascinating and weird things happening when we get down to the size of an electron, which mean that "normal" classical mechanics is not obeyed. Instead, we see strange things going on, such as particles being in two places at once! Sometimes quantum phenomena can be hard to believe because we live in a classical world.

One key property of a quantum particle is wave-particle duality. This means that electrons and other quantum objects are both waves and particles at the same time. But what does that mean? So far, in the Physics and Chemistry that you will have learned at school, you will be used to thinking about electrons as particles (little spheres that live in the shells of atoms) and light as waves (e.g. UV rays that come down to Earth from the Sun). It is still really useful to keep thinking about things in this way. BUT if we look closer at their properties, we see that electrons are also waves, and light is also made of particles (called photons). Weird…

While reliable old classical mechanics will do a fine job of predicting how anything larger than an atom will behave, smaller things <u>must</u> be modelled using quantum mechanics. Choosing which maths to use can be tricky sometimes, especially in chemistry. Did you know that bonding (how atoms are joined together into molecules) and chemical reactions are both all to do with electrons?

**Activity 3 – Quantum or Classical?**

**Which properties are quantum mechanical? Which of these things can be described using classical mechanics? Which must be described using quantum mechanics?**

A. How red blood cells move through your veins
B. Chemical bonds (how atoms are joined together to form molecules)
C. A drug molecule interacting with a large protein
D. How chemical reactions occur
E. How plants absorb sunlight
F. How an embryo starts to develop inside the womb
G. Pouring a cup of tea
H. Electrons moving through electrically conductive material
I. Sugar molecules dissolving into water

My Answers:

Correct Answers:

**Activity 4 – Four Computational Chemistry Methods**

**Fill in the table below:**

| **Method** | **Classical or Quantum** | **Suitable system size** | **Cost** |
|---|---|---|---|
| **Ab initio** | | | |
| **Molecular Dynamics** | | | |
| **Semi Empirical** | | | |
| **Hybrid** | | | |

**Activity 5 – Check your understanding**
**True or False**

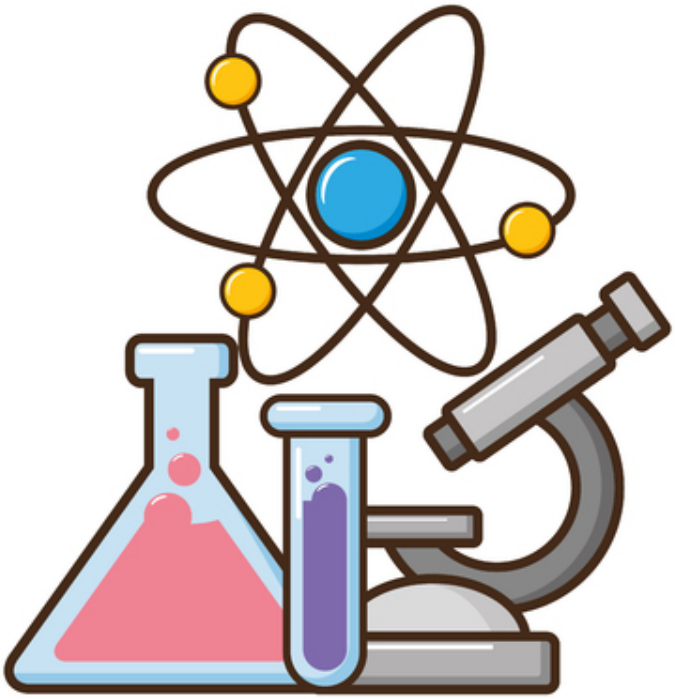
1. Before choosing a modelling method it is important to consider the size of your system
2. Proteins may have up to 1000 atoms
3. Methods that use classical mechanics only do not cost as much as quantum mechanical methods
4. Hybrid models use quantum mechanics only
5. Molecular dynamics uses classical mechanics only

My Answers:

Correct Answers:

**Homework – Summary**
**Write 2-3 paragraphs summarising the four methods you have learned about, including a discussion of when you would use each method**

# Tutorial 4 – Testing our Model. *Spectroscopy and Collaboration*.



## What is the Purpose of Tutorial 4?

1. Students will be able to describe spectroscopy and its uses
2. Students can explain why collaboration between experimental chemists and computational chemists is important
3. Students will be able to assess the suitability of different ways to validate a set of model results

**Activity 1 – Recap**
**Talk to your partner about what you remember learning so far, why is it important that models are checked for accuracy?**

Space for notes: _____
_____
_____
_____

**Activity 2 – Spectroscopy and its uses**

**Fill in the gaps**
Spectroscopy is the study of how _____ (electromagnetic radiation) interacts with matter. Some examples are _____/visible spectroscopy NMR (which stands for _____) and _____ spectroscopy. Spectroscopy is an _____ technique that gives us important information about how atoms are arranged in a compound, for example we can find out about the types of _____ in molecules.

When we study a compound using spectroscopy, we place a sample into our spectrometer and a spectrum is produced. We need skilled experimental collaborators to create and analyse these _____!

**Key Words:** Chemical bonds, Nuclear Magnetic Resonance, Spectra, Infra-red, Ultra-Violet, Light, Experimental,

**Activity 3 – Why do we need collaborators?**
**Complete the group exercise to find out!**

**Activity 4 – Match the data**
**Working in pairs, match the experimental data to the simulated data on the board. Fill in the table with your answers!**

| Experimental Data | Simulated Data |
|---|---|
| | |
| | |
| | |
| | |
| | |

**Notes** _____
_____
_____

**Activity 5 – Check your understanding**

**True or False:**

1. A really good set of simulated data is enough to answer a new scientific research question
2. Spectroscopy is the study of electrons interacting with matter
3. Classical mechanics can be used to create simulated spectra, which can be compared with real experimental spectra
4. Light is actually both a wave and a particle (called a photon)
5. The only experimental data that computational chemists are interested in using is spectroscopic data

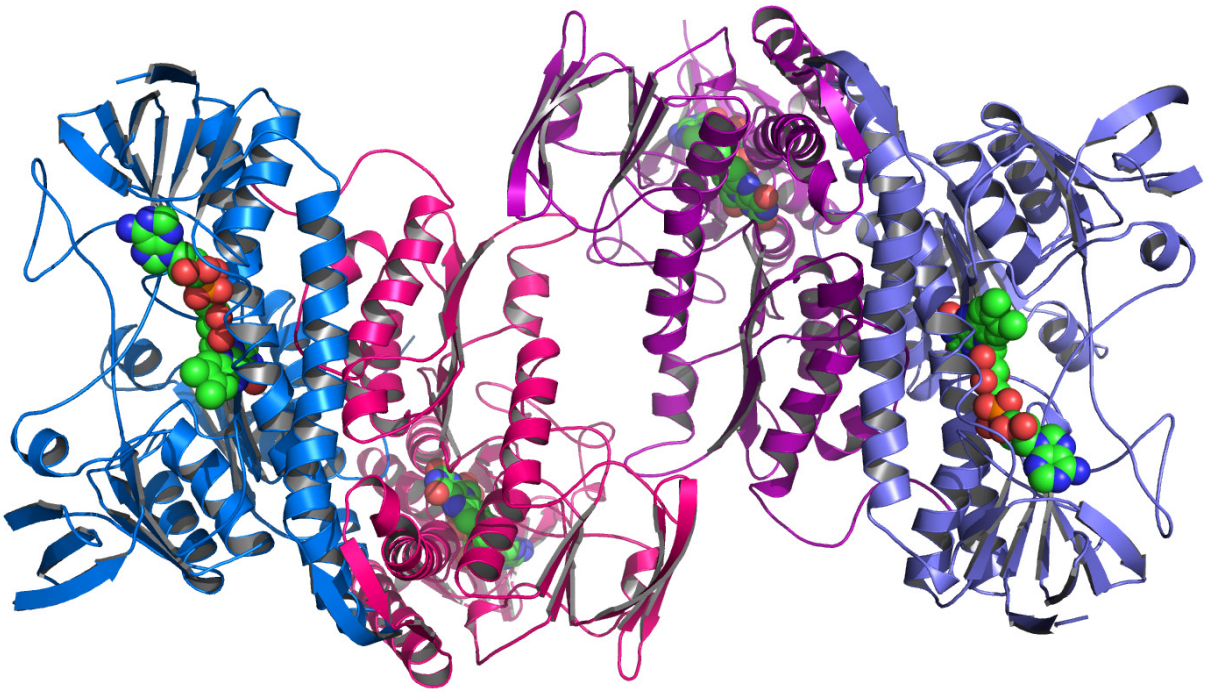
My Answers:

Correct Answers:

**Homework – Collaborators Wanted!**

*You are a computational chemist who has built a computational model of a new protein, you already have some data from your simulations which you need to test by comparing with experimental data.* ***Write a letter appealing to potential collaborators explaining what you need and why it is important for scientists to collaborate.***

# Tutorial 5 – Thinking like a Computational Chemist.



## What is the Purpose of Tutorial 5?

1. Students will discuss four different research questions and be able to choose suitable modelling methods to tackle each one
2. Students will be able to produce references from scientific literature

**Activity 1 – Recap**

**Look back through the booklet to answer these questions.**

**What four methods do computational chemists use?**

_____

_____

**Why do computational chemists want to build models of biological systems?**

_____

_____

_____

_____

**What do we need to build a model?**

_____

_____

_____

**How can we model the behaviour of electrons?**

_____

_____

**How do computational chemists make sure their models are producing valid results?**

_____

_____

_____

**Activity 2 – Case Study 1**
Read the case study below, then watch as the teacher models how they would tackle this research question. Fill in the answers to the questions below and include reasons for each choice that is made.

The research question:
How do plants photosynthesise?
During photosynthesis, a large protein in the leaves of plants is responsible for a key chemical reaction:
Water → Oxygen + Hydrogen
This reaction happens in a relatively small area of the protein that comprises (is made up of) a few hundred atoms. Can you build a model to help us understand how this protein uses the energy from the sun to carry out this reaction?

What will you need to build a model of?

_____

What results would you like to collect?

_____

_____

Description of data required to build our model.

_____

_____

_____

What theory should we use? Why?

_____

_____

_____

_____

What method(s) can we use to evaluate the model?

_____

_____

_____

How can we validate the results?

_____

_____

_____

_____

**Activity 3 – Case Study 2**
Read the case study below and work with your partner to respond to the questions below, include a reason for your choices.

The research question:
How do pollutants break down in the atmosphere?
An environmental protection agency is concerned about a new pollutant that is being released into the atmosphere. The pollutant molecule comprises 23 atoms. Can you help them understand what reactions will take place as it interacts with molecules in the atmosphere by building a model?

What will you need to build a model of?

_____

What results would you like to collect?

_____

_____

Description of data required to build our model.

_____

_____

_____

What theory should we use? Why?

_____

_____

_____

_____

What method(s) can we use to evaluate the model?

_____

_____

_____

How can we validate the results?

_____

_____

_____

_____

**Activity 4 – Case Studies 3 and 4**
Working on your own, read the two case studies below and fill in what choices you would make and the reasons behind them.

**Case Study 3**
The research question:
Have we found a new cure for Cancer?
Collaborators come to you with an idea for a new drug that they can synthesise (make in the lab). They have a suspicion that it will interact with a known protein and slow down the progress of disease on the body. Many thousands of atoms make up the protein and the drug contains around 40 atoms. Can you help them find out what these interactions look like between the drug molecule and the protein by building a model?

What will you need to build a model of?

_____

What results would you like to collect?

_____

_____

Description of data required to build our model.

What theory should we use? Why?

What method(s) can we use to evaluate the model?

How can we validate the results?

Stretch question: Why is it a good idea to test the action of this new drug using a computational model before we test it in humans?

Space for additional notes:

**Case study 4**

The research question:

Testing new Solar materials.

We need more efficient solar power technology, and for this we need materials that can absorb sunlight and generate a current. Can you build a model to test three bulk materials and see which ones are more likely to be useful?

What will you need to build a model of?

What results would you like to collect?

Description of data required to build our model.

What theory should we use? Why?

What method(s) can we use to evaluate the model?

How can we validate the results?

Stretch question: What resources do you need to do this investigation?

Space for additional notes:

**Activity 5 – Referencing Quiz**
Read the section on referencing in the appendix, then look at the reference below and answer the questions:

> Erwin Schrödinger, 'An undulatory theory of the mechanics of atoms and molecules', The Physical Review, (1926)

Who is the author? _____

Which Journal was this published in? _____

In what year was the paper published? _____

What is the title of the article? _____

**Activity 6 – Planning your final assignment**

**Look back through the booklet, what pages will you want to refer back to when writing your final assignment?**
Use this space to note down page numbers or other resources (websites, articles etc.) that you might want to refer to when writing your essay.

**Final assignment question:**

**You are a computational chemist who has been asked to build a model of a chemical system. Describe the different theories you have learned about which may be of use to you and what you will need to consider before building your model.**

**To help you structure your essay, you should discuss the key considerations and most suitable methods for the following research questions:**

- **You want to find out how a pollutant molecule might react with oxygen in the atmosphere**
- **You are simulating the infra-red spectrum of a single water molecule**
- **You need to know whether a new drug molecule will bind to a specific protein**
- **Try coming up with a problem of your own. Use your imagination!**

**For each case think about how large your model would have to be (how many atoms), what data you would need to gather before building your computational model and what you could do to validate the results you produced with your model. Use this information to justify which method you have chosen to use for each system.**

**Details of the assignment:**

**You will write an essay (1,500 words long), using the work we have done so far to help guide you.**

**Success criteria – how to structure your assignment and what to include:**

**A successful essay will include:**

- **an introduction to computational modelling**
- **a discussion of why we choose to model biological systems**
- **a comparison of different theories and methods used by computational chemists**
- **suggestions for how you would validate your model and why this is so important**
- **and an explanation of how we can collaborate with experimental chemists.**

**Wherever possible you should back up your writing with references from throughout the course.**

**You will use full sentences and proper paragraphs in your writing, paying attention to spelling and grammar. You can refer to the glossary for this course to check the spelling of key words.**

| In this assignment, show me that you **understand**: | Show me that you **are able to**: |
| --- | --- |
| What are the benefits and challenges associated with computational modelling of biological and chemical systems.<br><br>What are some of the theories and techniques used by computational chemists. | Think like a theoretical modeller, considering different methods and how they would be suitable to tackle a new research problem. |

# Tutorial 6 – Feedback tutorial

## What is the Purpose of Tutorial 6?

- To receive feedback on your final assignment
- To respond to the feedback from your Uni Pathways teacher
- To write targets for improvement on your final assignment

## Final assignment feedback from your Uni Pathways Teacher

(Remember to look at the mark scheme to help you understand what you have done well so far, and how you can do even better in your final assignment)

| Here are three things that my Uni Pathways Teacher thought I did well in my draft assignment |
| --- |
| • <br><br>• <br><br>• |

| Here are three things that my Uni Pathways Teacher thinks that I could do to get a higher mark in my final assignment |
| --- |
| • <br><br>• <br><br>• |

| Tasks from my Uni Pathways Teacher to do during the feedback tutorial to help me improve |
| --- |
| • <br><br>• <br><br>• |
| My response: |

| Actions I will take to improve my final assignment after this tutorial… |
| --- |
| • <br><br>• <br><br>• |

| Hand in date for my final assignment: | |
| --- | --- |

# Tutorial 7 – Final tutorial

**What is the Purpose of Tutorial 7?**

- To receive feedback and a grade on your final assignment.
- To reflect on the programme including what you enjoyed and what was challenging.
- To ask any questions you may have about university.

**Final assignment feedback from my Uni Pathways Teacher**

| Final mark: | University style grade: |
|---|---|
| Feedback: Here are three things that my Uni Pathways teacher thought I did well in my final assignment<br>•<br>•<br>• | |

| Here are three things that my Uni Pathways teacher thinks I should remember for when I am doing this kind of study in the future |
|---|
| •<br>•<br>• |

**University**

| What questions do you still have about University after taking part in Uni Pathways? |
| --- |
| • <br> • <br> • |

**Reflecting on Uni Pathways**

| What did you most enjoy about Uni Pathways? |
| --- |
| • <br> • <br> • |

| What did you find challenging about the programme? | How did you overcome these challenges? |
| --- | --- |
| • <br> • <br> • | • <br> • <br> • |

## Appendix 1 – Referencing correctly

When you get to university, you will need to include references in the assignments that you write, so we would like you to start getting into the habit of referencing in your Brilliant Club assignment. This is really important, because it will help you to avoid plagiarism. Plagiarism is when you take someone else's work or ideas and pass them off as your own. Whether plagiarism is deliberate or accidental, the consequences can be severe. In order to avoid losing marks in your final assignment, or even failing, you must be careful to reference your sources correctly.

**What is a reference?**

A reference is just a note in your assignment which says if you have referred to or been influenced by another source such as book, website or article. For example, if you use the internet to research a particular subject, and you want to include a specific piece of information from this website, you will need to reference it.

**Why should I reference?**

Referencing is important in your work for the following reasons:

- It gives credit to the authors of any sources you have referred to or been influenced by.
- It supports the arguments you make in your assignments.
- It demonstrates the variety of sources you have used.
- It helps to prevent you losing marks, or failing, due to plagiarism.

**When should you use a reference?**

You should use a reference when you:

- Quote directly from another source.
- Summarise or rephrase another piece of work.
- Include a specific statistic or fact from a source.

## How do I reference?

There are a number of different ways of referencing, and these often vary depending on what subject you are studying. The most important to thing is to be consistent. This means that you need to stick to the same system throughout your whole assignment. Here is a basic system of referencing that you can use, which consists of the following two parts:

1. **A marker in your assignment**: After you have used a reference in your assignment (you have read something and included it in your work as a quote, or re-written it your own words) you should mark this is in your text with a number, e.g. [1]. The next time you use a reference you should use the next number, e.g. [2].
2. **Bibliography**: This is just a list of the references you have used in your assignment. In the bibliography, you list your references by the numbers you have used, and include as much information as you have about the reference. The list below gives what should be included for different sources.

    a. **Websites** – Author (if possible), title of the web page, website address, [date you accessed it, in square brackets].

    E.g. Dan Snow, 'How did so many soldiers survive the trenches?', http://www.bbc.co.uk/guides/z3kgjxs#zg2dtfr [11 July 2014].

    b. **Books** – Author, date published, title of book (in italics), pages where the information came from.

    E.g. S. Dubner and S. Levitt, (2006) *Freakonomics*, 7-9.

    c. **Articles** – Author, 'title of the article' (with quotation marks), *where the article comes from* (newspaper, journal etc.), date of the article.

    E.g. Maeve Kennedy, 'The lights to go out across the UK to mark First World War's centenary', Guardian, 10 July 2014.

## Notes

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