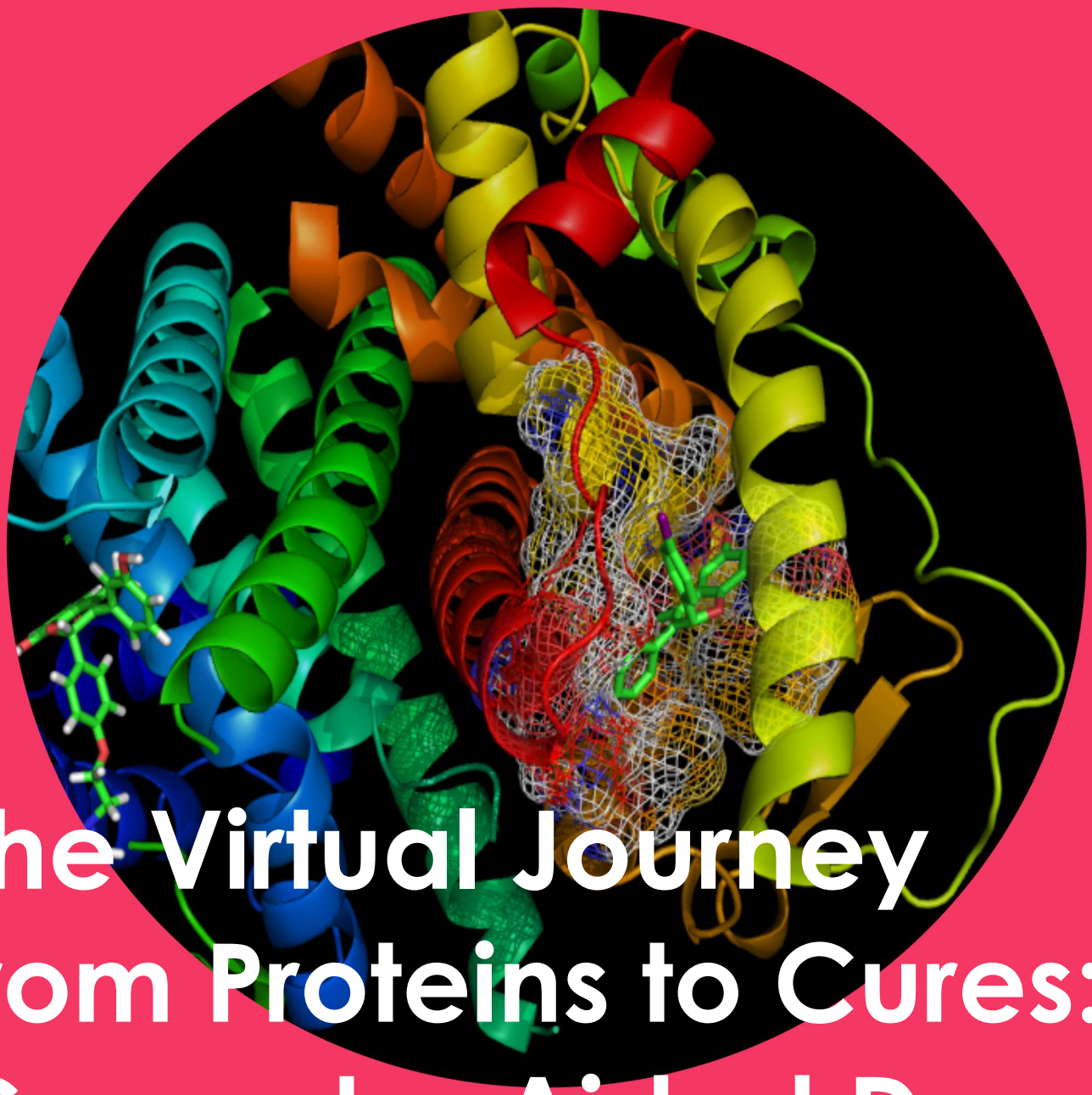
The Scholars Programme



The Virtual Journey from Proteins to Cures: Computer Aided Drug Design

Key Stage 4 Programme

Pupil Name

Coursebook Designed by Léonie Strömich

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THE SCHOLARS PROGRAMME

Timetable and Assignment Submission

Timetable – Tutorials

Tutorial	Date	Time	Location
1 (Launch Trip)	**17th January 2020**		**University of Cambridge**
2			
3			
4			
5			
6 (Draft assignment feedback)			
7 (Final assignment feedback)			

Timetable – Homework Assignments

Homework Assignment	Description	Due Date
Tutorial 1	Baseline assessment	**30.01.2020**
Tutorial 2		
Tutorial 3		
Tutorial 4		
Tutorial 5		
Tutorial 6	Final assignment	**01.04.2020**

Assignment Submission – Lateness and Plagiarism

Lateness	
Submission after midnight on _____**01.04.2020**_____	10 marks deducted
Plagiarism	
Some plagiarism	10 marks deducted
Moderate plagiarism	20 marks deducted
Extreme plagiarism	Automatic fail

KS4 Programme – Pupil Feedback Report

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

Name of PhD Tutor	Léonie Strömich		
Title of Assignment			
Name of Pupil			
Name of School	Dormers Wells High School		
ORIGINAL MARK / 100		FINAL MARK / 100	
DEDUCTED MARKS		FINAL GRADE	

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

Knowledge and Understanding	Research and Evidence
Developing an Argument	**Critical Evaluation**
Structure and Presentation	**Language and Style**

Overall Comments (participation, effort, resilience)

Contents

Course Rationale

Everyone can name a range of illnesses from different cancer types to Alzheimer's. Most of these diseases are based on a malfunctioning of proteins, the so-called molecular machinery in our cells. Consequently, a lot of biological and chemical research focuses on targeting these proteins to find new cures. But often this is a lengthy and expensive process and the development of a new compound can take up to 20 years. This is where computers come into play, by modelling proteins computationally we can aid in developing new medications a lot faster. This course is building a bridge between biology and computing by introducing concepts from bioinformatics. In this course we will explore how computers can aid in predicting and designing new medications by looking at 3D models of proteins and virtual medication screens.

The first tutorial is going to be on the role of proteins in our body, how they are produced and what different classes of proteins there are. Following on from there we will look at examples of diseases where proteins are dysregulated and why this leads to certain disease symptoms. Once the pupils understand the research demand for drug development, we will introduce the computational possibilities we have for designing new medications. We will explore how proteins can be represented in a computer and what virtual drug screens are. The pupils will be able to understand the power of computational methods in research and translate this idea onto medical development. By opening the final assignment to a disease of their choice, we encourage independent research and the usage of computational resources available to the public.

Group Discussions

How do you make the most of a group discussion?

The purpose of discussions is to allow everyone in the group to express their ideas and learn from each other. Often this will involve coming to a group decision about the issue under discussion, though they may of course 'agree to disagree' on certain points.

What we don't want in our tutorials:

Artwork by MiaHague.co.uk

Rules:

1. Pronounce clearly what you are saying
2. Use eye contact and facial expression to help to get your idea across or to support what someone else is saying
3. Speak in a way that is right for a discussion (more formal than a chat between friends)
4. Build on other people's ideas, and summarise your own views and the views of others when necessary
5. Give reasons to support your views and critically examine the views expressed by others
6. Organise the discussion and take turns with others
7. Listen carefully and respond to the views of others

Mark Scheme Table

Skills	1st (70-100)	2:1 (60-69)	2:2 (50-59)	3rd (40-49)	Mark /100
Knowledge and Understanding	o Sophisticated understanding of the course material. o All the content included is relevant to the general topic and final assignment question – this shows clear thought about what to include. o Good evidence of independent thought. o Clear thought about unanswered or unexplored questions. o Very few factual mistakes. o Correct scientific language used, defined when it is useful to do so.	o Good understanding of the course material. o Content included is usually relevant to the general topic and final assignment question. o Some evidence of independent thought. o Some attempt to think about unanswered or unexplored questions. o Very few factual mistakes. o Correct scientific language usually used, defined when it is useful to do so.	o Mostly a good understanding of the course material. o Content included is usually relevant to the general topic and final assignment, but some may have been included without a clear reason. o Some evidence of independent thought. o Little attempt to address unanswered or unexplored questions. o Some factual mistakes. o Sometimes uses the correct scientific language but rarely includes definitions.	o Some understanding of the course material. o Some of the content included is relevant to the general topic and final assignment, but some may have been included without a clear reason. o Little evidence of independent thought. o Does not attempt to address unanswered or unexplored questions. o Some factual mistakes. o Can use the key scientific language, but only uses this correctly occasionally and rarely include definitions.	
Research and Evidence	o Includes research findings from a wide range of sources, beyond what is provided in the tutorials. o Consistently uses scientific evidence to support claims and convince the reader of arguments. o Critically appraises (examines the strengths and weaknesses of) evidence used.	o Includes research findings from different sources from the tutorials and demonstrate some research beyond what is provided in the tutorials. o Often uses scientific evidence to support claims and convince the reader of arguments. o Critically appraises (examines the strengths and weaknesses of) some of the evidence used.	o Make little attempt to research beyond what is provided in the tutorials. o Sometimes uses scientific evidence to support claims and convince the reader of arguments. o Critically appraises (examine the strengths and weaknesses of) some of the evidence used.	o Does not include research or evidence from beyond the tutorials. o Rarely uses scientific evidence to support claims and convince the reader of arguments. o Make no attempt to critically appraise (examine the strengths and weaknesses of) the evidence used.	
Developing an Argument	o Always makes a point of view clear throughout the assignment. o Highlights competing points of view throughout the essay. o Always explains and justifies why certain facts/figures are included and the reader always knows why it is relevant.	o Often makes a point of view clear throughout the assignment. o Often highlights competing points of view. o Explain and justifies why certain facts/figures are included; most of the time the reader knows why it is relevant.	o Tries to make a point of view clear, but sometimes the reader may get confused. o Occasionally highlights competing points of view. o Explain and justifies why certain facts/figures are included but should provide more explanation.	o Tries to make a point of view clear, but sometimes the reader may get confused. o Rarely highlights competing points of view. o Attempts to explain why some facts/figures are included.	

Critical Evaluation	○ Always chooses research evidence that is related to and appropriate for the arguments made. ○ As well as describing the evidence, always explains its value or significance. ○ Often comments on how reliable the sources are, including potential limitations. ○ Evaluation is always clear, easy to follow and explained.	○ Often chooses research evidence that is related to and appropriate for the arguments made. ○ As well as describing the evidence; usually explains its significance. ○ Sometimes suggest why a source is/ is not reliable. ○ Evaluation is usually clear, easy to follow and explained.	○ Sometimes chooses research evidence that is related to and appropriate for the arguments made ○ Consistently describes evidence and sometimes attempts to explain its significance. ○ Can say if a source is reliable or not but does not always explain this. ○ Evaluation is not always clear, easy to follow, or explained.	○ Rarely chooses research evidence that is related to the arguments made. ○ Consistently describes evidence but does not always explain its significance. ○ Can say if a source is reliable or not but does not always explain this. ○ Evaluation is rarely clear, easy to follow, or explained.	
Structure and Presentation	○ Introduction clearly outlines what the assignment will contain. ○ Organises ideas in paragraphs with a logical structure that makes it easy for the reader to follow. ○ Excellent answering of the question. ○ Conclusion summarises all of the main points clearly. ○ Where needed, includes the correct units. ○ Tables and graphs are labelled correctly, including titles and units. ○ Demonstrates an excellent understanding of referencing – all sources are cited in text and referenced in the correct format.	○ Introduction outlines what the assignment will contain. ○ Organises ideas in paragraphs with quite a clear structure that makes it easy for the reader to follow. ○ Good answering of the question. ○ Conclusion summarises most of the main points clearly. ○ Where needed, includes the correct units. ○ Includes most of the appropriate labels for tables and graphs, including titles and units. ○ Demonstrates a good understanding of referencing – most sources are cited in text and referenced in the correct format.	○ Introduction briefly outlines some aspects of the assignment. ○ Organises ideas in paragraphs, but their order could be more logical to make it easier for the reader to follow. ○ Attempts to address all aspects of the question. ○ Conclusion summarises some of the main points. ○ Includes units where needed, but with some errors. ○ Includes some of the appropriate labels for tables and graphs, including titles and units with occasional errors. ○ Demonstrates a developing understanding of referencing – some of sources are cited in text and referenced correctly, but with errors.	○ Introduction mentions the main issue. ○ Usually organises ideas in paragraphs, but their order is not always easy for the reader to follow. ○ Does not address all aspects of the question. ○ Conclusion summarises some of the main points. ○ Often forgets to include the correct units. ○ Sometimes forgets to include the labels needed for tables and graphs, such as titles and units. ○ Has not or only occasionally attempts to reference.	
Language and Style	○ Writing style is consistently clear and appropriate for a scientific document. ○ Spelling, grammar and punctuation are consistently accurate. ○ Worked towards the word limit.	○ Writing style is mostly clear and appropriate for a scientific document. ○ Spelling, grammar and punctuation are usually accurate, with occasional mistakes. ○ Worked towards the word limit.	○ Writing style is sometimes clear and an attempt has been made to make it appropriate for a scientific document. ○ Some errors in spelling/grammar/ punctuation. ○ IWorked towards the word limit.	○ Writing style is often not clear or appropriate for a scientific document. ○ Errors in spelling/grammar/ punctuation. ○ Some attempt to work towards the word limit.	
Overall Mark (average of the 6 marks from the criteria above)					

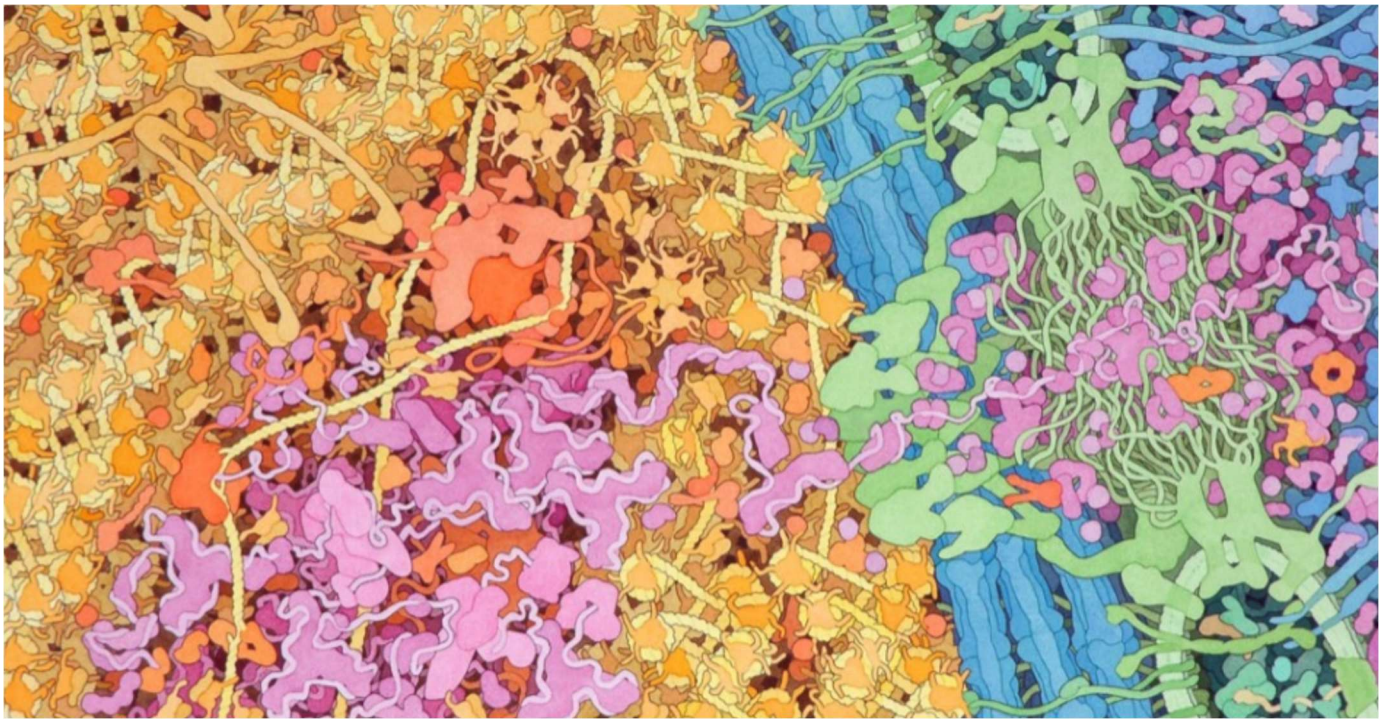
Glossary of Keywords

Word	Definition	In a sentence
Biosynthesis	The production of molecules in biological cells. This can be proteins as well as other small molecules like vitamins or hormones.	
Receptor	A protein which receives a signal often by being able to bind a specific molecule. The receptor initiates further signalling after the ligand is bound.	
Ligand	A small molecule binding to a protein.	
Ribosome	The molecular machinery which synthesis proteins based on messenger RNA.	
Transfer RNA	A type of RNA that is needed to build proteins. One end can recognize a specific sequence on messenger RNA and the other end holds an amino acid.	
Amino acid	The building blocks of proteins. Our bodies are producing 20 different ones.	
Messenger RNA	The link between DNA and proteins. Messenger RNA is a copy of DNA and can be read by ribosomes.	
Antibody	Proteins which are used by our immune system to recognize and neutralize pathogens and other foreign molecules.	
Insulin	A protein that is binding glucose and initiates glucose metabolism.	
Alpha Amylase	A protein which uses a chemical reaction to break down starch.	
Calcium Pump	A protein responsible for the transportation of Calcium ions across membranes.	
Ferritin	A protein in our blood that stores iron.	
Collagen	A protein providing structure for our cells and tissues.	

Proteome	All proteins of a cell or an organism are called proteome.	
Protein inhibition	The process of preventing the normal function of a protein.	
Estrogen receptor	A protein which recognizes estrogen and binds to DNA.	
Estrogen	A hormone found in our bodies which is sometimes referred to as primary female sex hormone.	
Hormone binding domain	The part of a protein where the ligand, in this case a hormone, binds.	
Cystic fibrosis	A disease which leads to thick and sticky mucus which can clog the lungs.	
CFTR	The cystic fibrosis transmembrane conductance regulator (CFTR) is a membrane protein and chloride channel in vertebrates. If it is not working correctly the result is cystic fibrosis.	
Huntington's disease	An inherited disease which leads to the destruction of nerve cells. This leads to a variety of symptoms which can be uncontrolled movement and loss of thinking ability.	
Huntingtin	The protein that causes Huntington's disease if it is mutated.	
Melanoma	A form of cancer which is happening in skin cells.	
B-Raf kinase	A protein which is important in cell signalling and often mal functioning in skin cancer.	
X-ray crystallography	A methodology to solve the 3D structure of proteins. It is based on shooting X-rays at crystals and the resulting diffraction pattern.	
Protein structure	The 3D coordinates of every atom in a protein.	

Protein expression	The production of proteins by cell culture or bacterial cells.	
Protein purification	The process of extracting one protein from a mixture of proteins.	
Protein data bank	The biggest resource of molecular structures on the internet. It is freely accessible to everyone.	
PyMol, Chimera	Molecular visualization tools which can be downloaded and used for scientific purposes.	
EzMol	An online molecular viewer of biostructures.	
CADD	Computer Aided Drug Design. Using computers to make drug discovery more efficient.	
Compound	A small molecule which might bind to a protein.	
Small molecule library	A library of thousands of compounds of which one might be used for drug development.	
Compound screening	The process of trying to find a small molecule which is active against a given protein.	
Molecular docking	Computational methods which are able to fit small molecules into larger structures.	
Binding pose	The position of a small molecule in a protein structure.	

Tutorial 1 – Proteins everywhere



D. Goodsell (2011)

Objectives:

- Understand what proteins are and how they are produced
- Understand the role of proteins in cells

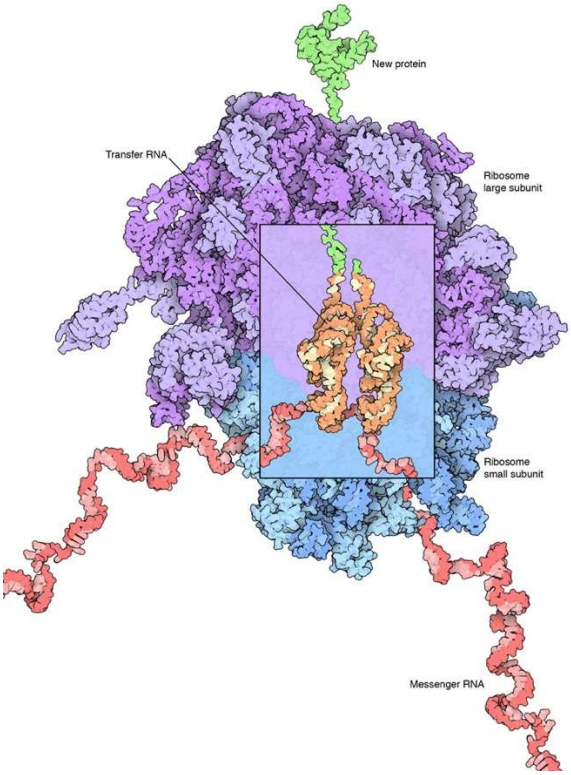
What are proteins?

Have a look at the picture above and have a guess at what we are seeing here.

In partner work, can you figure out what the different colours describe?

Colour	Meaning
Yellow	
Green	
Blue	
Purple	

How are proteins made?



D. Goodsell (2009), The Machinery of Life

The process we are looking at is called protein biosynthesis and can be compared to the process of baking a cake. We need a recipe to know what we are doing; we need ingredients to make up the batter and we need someone to put it all together and bake it to get an edible cake.

Activity: With a partner find the matching pairs and be ready to explain your choices to the group.

Recipe	Ribosome
Ingredients	Protein
Baker	Transfer RNA
Cake	Messenger RNA

What roles do proteins have in cells?

In our body and cells proteins fulfil every task you can think off. Almost all other biomolecules are inert and processed by proteins, which is showing how essential they are. They can be classified according to their field of action as the following:

Protein Class	Role	Example
Defence	To protect our body from foreign pathogens and help in recognizing and destroying them.	Antibodies
Communication	To allow communication between other proteins, different cells or even within the organism.	Insulin
Enzyme	To catalyse chemical reactions to form new molecules by adding or taking away chemical groups.	Alpha Amylase
Transport	To allow controlled transport between different compartments in our body.	Calcium pump
Storage	To store important molecules our body needs like vitamins or metals like iron.	Ferritin
Structure	To provide structural support in our cells.	Collagen

Key definitions:
Proteins are often considered the molecular machinery of a cell because they virtually fulfil all the tasks that are necessary for a cell to live, replicate and communicate.
All proteins in a cell or an organism are called proteome.

Activity: Video time! While we watch a YouTube video on cellular mechanisms, list down the protein classes you recognize from today's tutorial.

Video: The Inner Life of a Cell (https://www.youtube.com/watch?v=wJyUtbn0O5Y)

Homework - Tutorial 1

Your first homework comes in three parts:

1. Watch the following video on YouTube:
   https://www.youtube.com/watch?v=wvTv8TqWC48
   (If the link doesn't work, search this term: What is a protein. Click the first result, which should be a video by the RCSBProteinDataBank)

2. Based on what we learned in tutorial 1 and what you saw in the video, write a **300 - 400 words** essay on the different classes of proteins. Your essay should include the following:
   a. A summary of the different protein classes.
   b. A more detailed explanation of **one** class and an example protein.

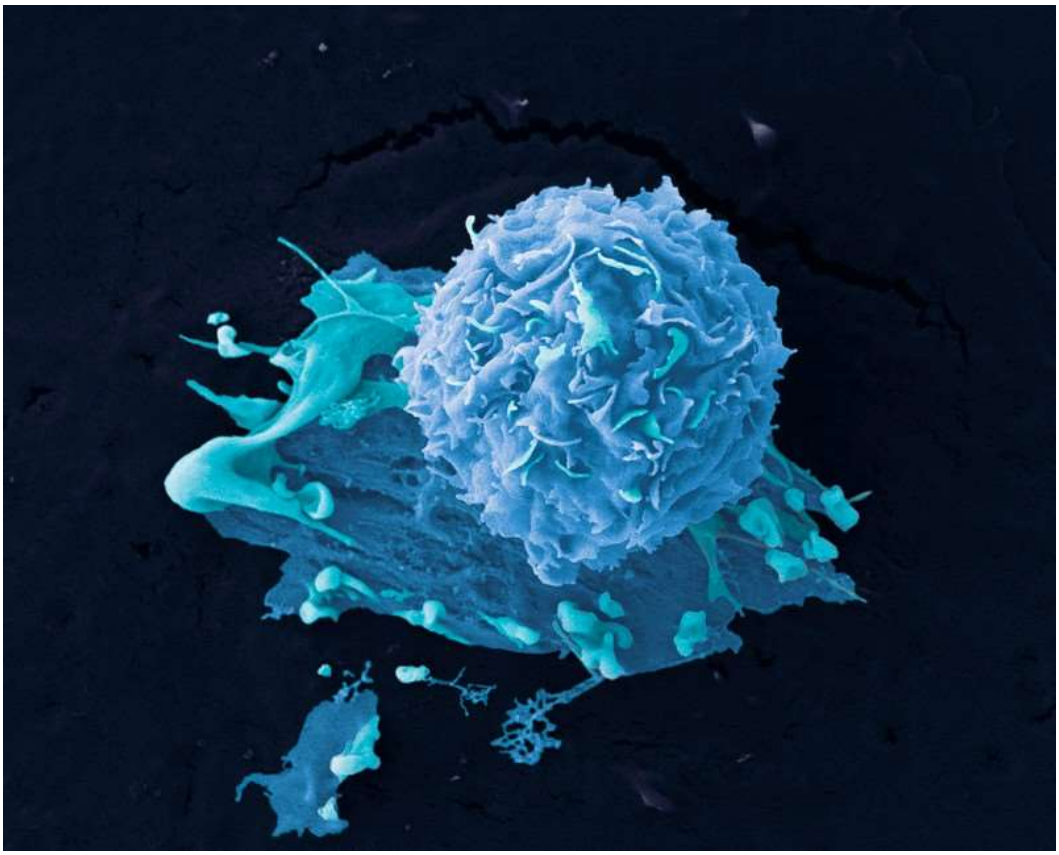
3. Please think about the following question and write **100 – 150 words** answer.
   a. What do you think would happen to our cells if your chosen protein class from above would not work anymore?

This work will be marked along the mark scheme on pages 8-9.
Please also use references if you include additional knowledge from external sources. For a guideline on correct referencing, have a look at Appendix 1.

Please submit your work over the VLE in the Baseline Assignment tab in the Assignments section.
In case you encounter any problems, or you have a question, you can send me a message over the VLE or ask your teacher to send me an email.

Good luck!

Tutorial 2 – When proteins fail



Objectives:

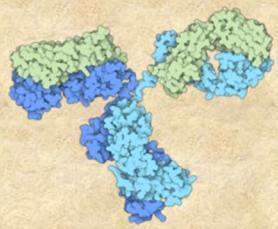
- Understand how a protein can fail
- Understand the implications of a mis functioning protein
- Learn about estrogen receptor alpha and how it is involved in breast cancer

How can a protein fail?

We will investigate the protein examples we looked at in the last tutorial and the homework.
Using our imagination, we want to come up with ideas of how these proteins would not be able to fulfil their function anymore. So, we either want them dead or inhibited.

Activity: With your partner come up with ways of knocking out or inhibiting your two proteins.

WANTED
Dead or Inhibited



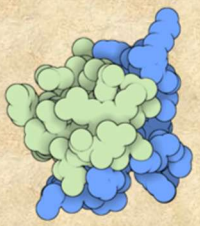
Name: Antibody
Role: Defence
Kill by: _____

_____

_____

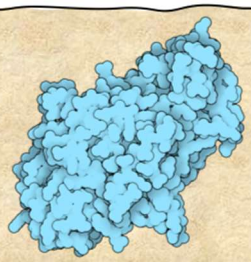
_____

WANTED
Dead or Inhibited



Name: Insulin
Role: Communication
Kill by:

WANTED
Dead or Inhibited

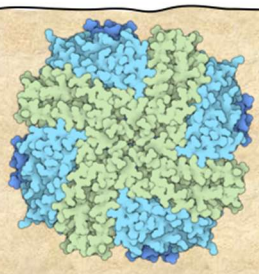


Name: Alpha Amylase
Role: Enzyme
Kill by:

WANTED
Dead or Inhibited

Name: Calcium Pump
Role: Transport
Kill by:

WANTED
Dead or Inhibited



Name: Ferritin
Role: Storage
Kill by:

What happens if a protein fails?

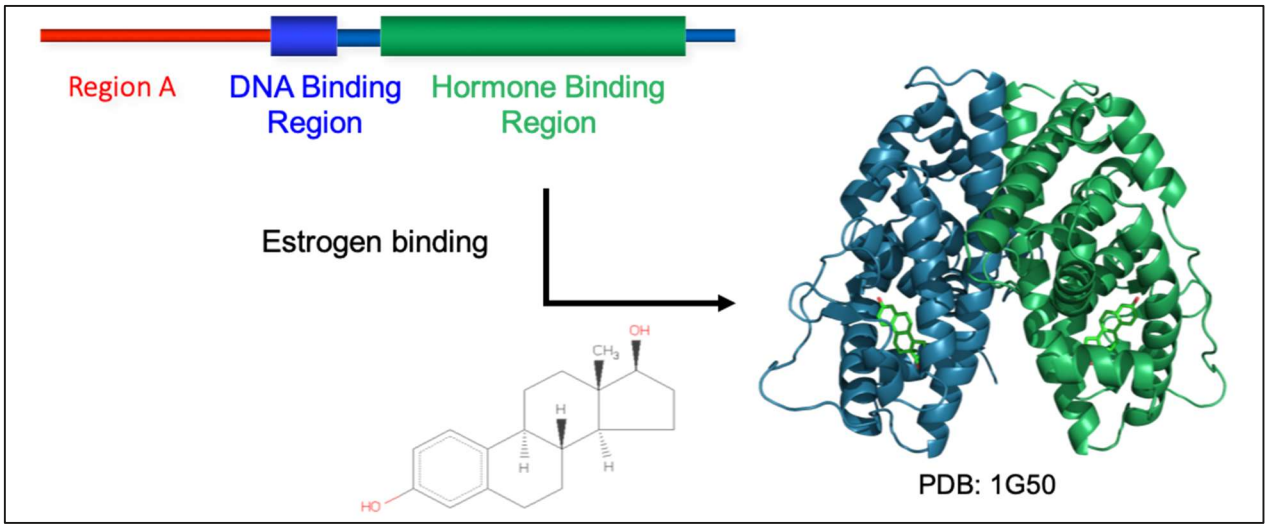
If a protein fails to function how it is supposed to, it will have an impact on the cell, the organ and ultimately the whole body.

Activity: Write in 2 sentences what would happen if your protein class is no longer functioning. Prepare to read these sentences to the group and answer the question whether this would be fatal for the cell.

Chosen protein class	
If this class would fail	
Would the cell be able to survive?	Yes or No?

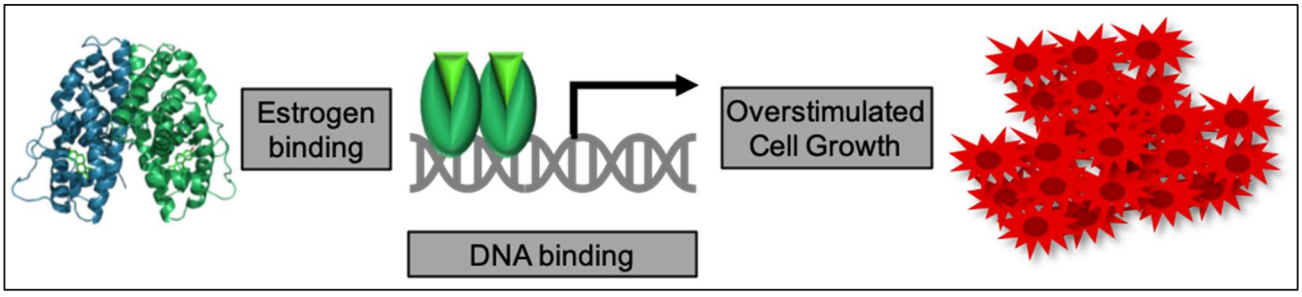
How is breast cancer caused by a protein?

Now we will learn about my field of research: The role of estrogen receptor alpha in breast cancer.



Key definition:
Estrogen receptor alpha is a protein from the nuclear hormone receptor family. These proteins recognize hormones and once a hormone is bound, they enter the cell nucleus to bind to DNA and start the synthesis of more proteins.

How do breast cancer tumours develop?



Activity: Looking back at the different classes of proteins we now know, where would you categorize estrogen receptor alpha?
Discuss with your partner and prepare to explain your decision to the group.

Homework - Tutorial 2

Choose one of the following protein related diseases and conduct some research about it. You can use the internet or primary literature but remember to reference your sources. Prepare a PowerPoint slide or a poster about your disease and be ready to present it in the tutorial next week.
You can either work on your own or as a group on the same disease.

Disease	Protein	Choice
Cystic Fibrosis	Cystic fibrosis transmembrane conductance regulator (CFTR)	
Huntington's disease	Huntingtin	
Melanoma	B-Raf kinase	

Tutorial 3 – Proteins in the computer

Objectives:

- Understand how we get from proteins in our cells to digital representations
- Explore the protein data bank
- Learn how to explore 3D protein data

How are proteins represented as digital data?

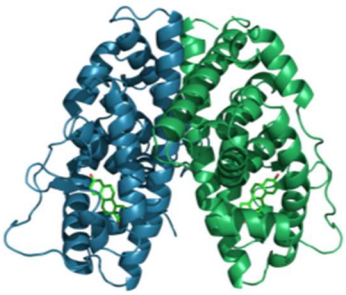
If we want to make use of the continuously increasing computational power, we need to have a computer-based representation of proteins. This data is 3D coordinates of every atom in a protein and the technique used is called x ray crystallography:

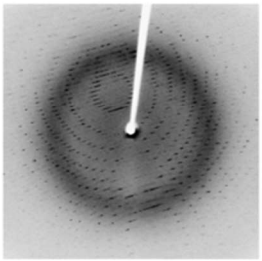
> Key definition:
> "The aim of x ray crystallography is to obtain a three dimensional molecular structure from a crystal. A purified [protein] sample at high concentration is crystallised and the crystals are exposed to an x ray beam. The resulting diffraction patterns can then be processed," to extract 3D coordinates of atoms. (Smyth & Martin, 2000)

To fully solve a protein structure, it often takes several months of laboratory work. From finding the right cells to producing the protein in big cultures over purifying the correct protein to finding the right crystallisation solution to get big crystals.

Activity: Below shows the process from protein to structure. Sort the terms to the pictures below and be ready to discuss your thought process.

protein purification – X-ray diffraction pattern - crystallisation 3D structure - protein expression





Is there a central database for protein structures?

The short answer is – yes! The wonderful protein data bank or short PDB.

Whenever a new structure of a protein or another biomolecule is solved, the data is uploaded in the PDB.
Every entry is freely accessible to scientists around the world over the following link: https://www.rcsb.org

Activity: Search your disease-causing protein in the protein data bank. What information can you gather from the PDB entry of your protein?

PDB ID	
Protein	
Information you found	

How do we explore these protein structures?

There are a range of tools available to make use of 3D data and to investigate protein structures interactively. The most used ones are PyMol and Chimera which can be downloaded for free for educational or scientific purposes.

But there are also some online viewers available which can be used without installation.

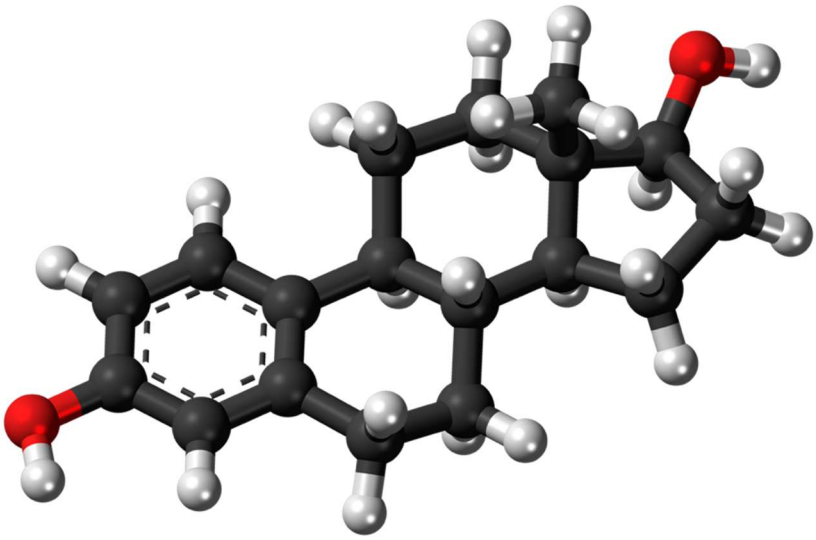
Activity: We will investigate a protein structure interactively using EzMol: http://www.sbg.bio.ic.ac.uk/ezmol/
Upload the entry 1G50 into the viewer and click yourself through the pages.
How can you manipulate the structure you are seeing and what information can you gather? Make a few notes below.

Homework - Tutorial 3

Every PDB entry holds a wide range of additional information and we want to have a closer look at what is available to us.
Have a look at the small molecule section of the PDB entry 1G50:
https://www.rcsb.org/structure/1g50
Which small molecules are present in this PDB file and how do they interact with the protein structure?
Can you figure out which protein residues are in contact with the small molecules?

Protein	
Small molecules	
Information you found	
Protein residues involved in ligand binding	
Picture of ligand interactions	

Tutorial 4 – Computer Aided Drug Design



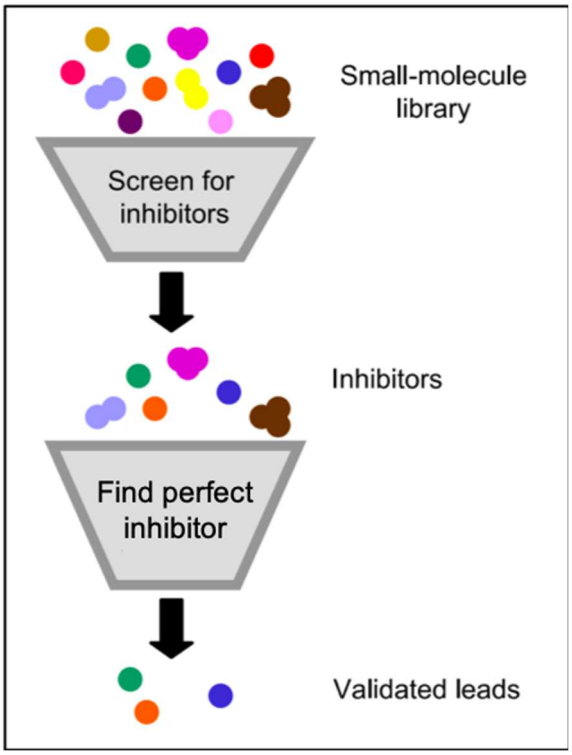
Objectives:

- Understand the purpose of compound screenings to find new drugs
- Understand the power of using computers in the process
- Extra: Understand the advantages of selectivity of a compound

How do scientists find new drugs?

We learned a lot about diseases that are caused by a single protein. To cure one of these diseases, scientist will try to find a drug which inhibits the underlying protein.

This is often achieved by throwing thousands of small molecules, so called compounds, onto the protein and see which one is inhibiting the function of the protein. Once a preliminary inhibitor is found, it is optimized in further experiments.



Adapted from T. Sawyer (2005)

Problem: These laboratory-based compound screenings are often very time and money consuming as every single compound needs to be tested separately.

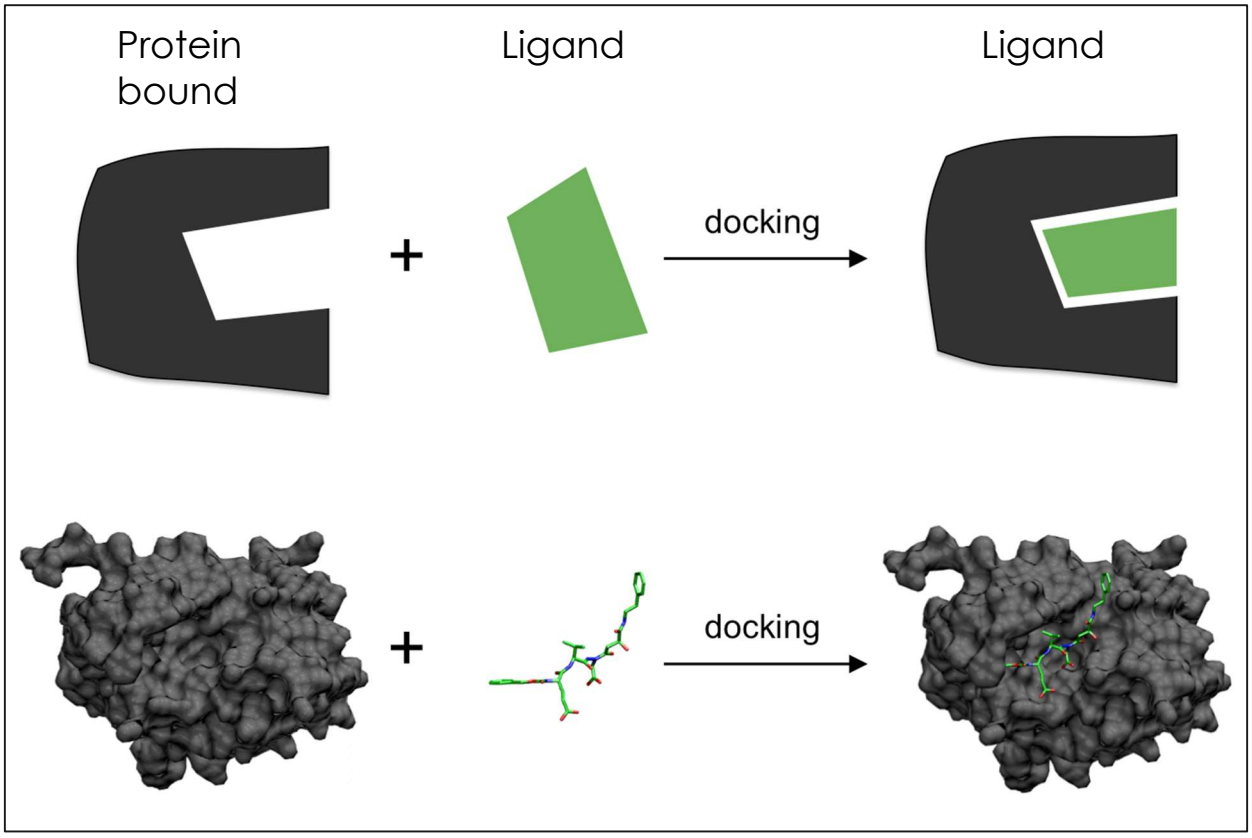
How can computers aid in this process?

As we have access to continuously increasing computational power, it is only logical to use computers to aid in the drug development process. By using computers, we can shorten the time to find a new drug, save a lot of money and make the process more efficient.

> Key definition:
> Computer aided drug design or short CADD is the broad field of using computers to develop new medications against proteins which cause diseases.

The range of computational methods to study proteins and predict new drugs is very broad. All of them mean to make the drug discovery process faster and more specific. We talked about compound screenings before and this can be directly translated into the computer:

> Key definition:
> The process of computationally fitting a small molecule into a protein structure is called molecular docking. There are a range of algorithms available which determine the optimal binding pose and ensure that the ligands do not clash with the structure.



Scigenis (2015)

Activity: Have a think about the following question and come up with answers in partner work.

What kind of data do we need to do a molecular docking experiment?

Which software is used to perform molecular docking?

There are several docking tools out there which all try to optimize the compound position in the structure. All of these tools follow a similar process which ends in giving a score for the final compound binding pose (Pagadala, 2017). This score can then be used to decide which molecule would be best to target a given protein.

As these environments need a lot of time to be set up and quite some experience to manage a molecular docking run, we will now have a go at something a bit more accessible.

Activity: We will have a go at BioBlox2$^1/_2$D, an online game for docking small ligands into protein surfaces. It can be accessed here: http://bioblox.org/

Notes:

Extra Content: What makes a compound a good drug?

To find a new compound which is active against a certain protein is only the start of the drug development process. This lead compound needs to be optimized until it can be used as medication.
This process aims to optimize the following characteristics:

- Affinity
- Selectivity
- Efficacy
- Permeability

Activity: In partner work, try to imagine what these terms describe in the setting of a new drug.

Term	Explanation
Affinity	
Selectivity	
Efficacy	
Permeability	

Homework - Tutorial 4

For your final assignment, you will write an essay about the following:

Explain how computers can aid in developing a new drug against a disease of your choice.

When writing a long essay, it is good practice to make a plan before you start. This will help you keep track of what you need to do. The more detail you include, the easier it will be to write your essay.

Use the prompts below to help you plan your essay.

Topic areas I want to include:

Research I need to do:

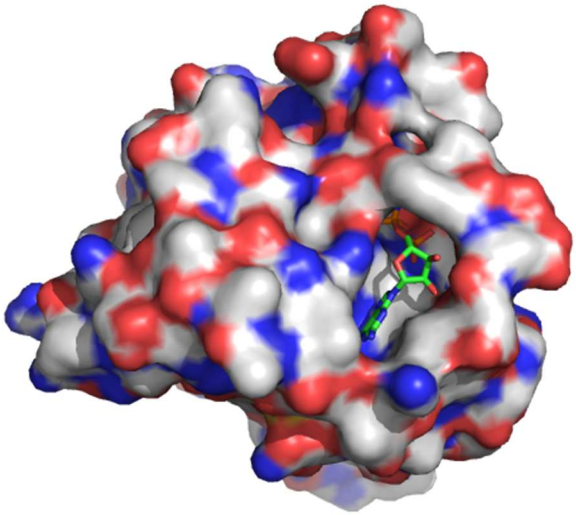
How I will find or make any images or diagrams I need:

Possible problems when writing the essay and how I will solve them:

Questions to ask in the next tutorial:

Other notes to help me plan my essay:

Tutorial 5 – Consolidating Computer Aided Drug Design



Objectives:

- To consolidate the material learnt so far
- To discuss referencing

Consolidation of Computer Aided Drug Design

We did a full journey from proteins in cells to structural data in computers and how to use it to develop new drugs against different diseases. Answer the questions below to have a summary of our tutorial.

What are your key learning points about proteins in cells?

What are your key learning points about dysregulation of proteins?

What are your key learning points about disease mechanisms?

What are your key learning points about the protein data bank?

What are your key learning points about compound screenings?

What are your key learning points about computer aided drug design?

What is referencing?

If writing any sort of scientific work, we need to do some research to find additional information. Whenever you include external information which can be thoughts or knowledge as well as figures or data, you need to note that you have done so.
This is called referencing and means you give credit to the original author. This is good scientific practice and makes your work honest. No one ever comes up with their whole work out of nowhere, we always build our experiments and research on the work of others and by referencing we give them credit.

Key definition:
Not referencing the source of external thoughts and work in your writing is called plagiarism. Plagiarism has serious consequences at universities and in the Brilliant Club I will need to deduct marks from your final assignment.

Activity: Have a look through tutorial 1-4. Can you find examples of referencing?

Page	What was referenced?	How was it referenced?

What is a reliable source?

Here are a few things to consider when choosing sources:

- What is the source, and who created it?
- Why was the source created?
- Is the source suitably recent for my needs, or is it out of date?
- Is the source heavily biased, and in what way if so?

Notes:

For more information about referencing, have a look at appendix 1.

Homework - Tutorial 5

Draft Assignment

For your final assignment, you will be writing an essay of 2,000 words based on the draft you will produce now. The essay will answer the following question:

Explain how computers can aid in developing a new drug against a disease of your choice.

Please have a look at the mark scheme (p. 8-9) as this is what I will use to mark your final essay. Submit your draft assignment as a word or pdf over the VLE in the homework section.
I will give you full feedback on your draft and we can go through what needs improvement for your final essay. Also keep in mind that the more you produce now for you draft, the less you have to do for your final assignment.

The following might help you in setting up your draft:

- Can you give a short summary of proteins and how they are important for our cells?
- Please explain how the disease you chose is the result of a malfunctioning protein and consider how current medication works.
- What computational methods can help in studying this protein and how can we predict a new medication for it?

Below is what I am expecting from your final assignment:

- A 2000 words essay (± 10%)
- An introduction giving an overview over the topic and why it is relevant
- Figures supporting your arguments
- Referencing throughout the assignment
- A conclusion summing up your arguments
- A bibliography

In case you encounter any problems, or you have a question, you can send me a message over the VLE or ask your teacher to send me an email.

Happy writing!

Please also have a look at page 38 and fill in the essay writing reflection

Tutorial 6 – Draft assignment feedback and reflection

What is the Purpose of Tutorial 6?

- To receive feedback on your draft assignment
- To reflect on your essay writing skills
- To identify practical ways to improve your assignment

What three things can you now do to improve your assignment and your essay writing ability?

1

2

3

Essay writing reflection

Use the checklist below to reflect on your essay writing ability at the moment. Read the statements for each skill and then tick the box that most closely fits how you currently feel about your ability to do that skill.

You will use this to help your PhD tutor give you feedback in your next tutorial. They will give you specific advice on how to improve these areas in relation to your draft assignment so be completely honest.

Addressing the question			Using evidence		
I can… • identify what the title or question is asking me to do • select relevant information from the course to answer the title or question • explain why the information I have used is relevant			I can… • select evidence that supports my points • link evidence to my points and ideas • clearly and convincingly explain how my evidence supports my points • use references		
I feel…			I feel…		
Confident	Partially confident	Not confident	Confident	Partially confident	Not confident
☐	☐	☐	☐	☐	☐

Developing an argument			Critical evaluation		
I can… • include a point of view or position in response to the title or question • develop and explain my point of view • argue why my point of view or position is correct			I can… • ensure I analyse events and information rather than just describe them • assess the relevance and significance of the ideas and examples I am writing about		
I feel…			I feel…		
Confident	Partially confident	Not confident	Confident	Partially confident	Not confident
☐	☐	☐	☐	☐	☐

Structuring			Use of language		
I can… • arrange my points in to a logical order • write paragraphs that focus on one idea or point each • write an introduction that explains how I will deal with the issues of the essay • write a conclusion that sums up my main points			I can… • minimise spelling, punctuation and grammar errors • ensure my writing makes the meaning clear and easy to follow • write using and appropriate tone and level of formality		
I feel…			I feel…		
Confident	Partially confident	Not confident	Confident	Partially confident	Not confident
☐	☐	☐	☐	☐	☐

Final Assignment

For your final assignment, you will be writing an essay of 2,000 words based on the draft you will produce now. The essay will answer the following question:

Explain how computers can aid in developing a new drug against a disease of your choice.

The following might help you in setting up your draft:

- Can you give a short summary of proteins and how they are important for our cells?
- Please explain how the disease you chose is the result of a malfunctioning protein and consider how current medication works.
- What computational methods can help in studying this protein and how can we predict a new medication for it?

Please have a look at the mark scheme (p. 8-9) as this is what I will use to mark your final essay. Submit your final assignment as a word or pdf over the VLE in the assignment section.

Below is what I am expecting from your final assignment:

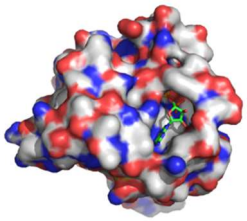
- A 2000 words essay (± 10%)
- An introduction giving an overview over the topic and why it is relevant
- Figures supporting your arguments
- Referencing throughout the assignment
- A conclusion summing up your arguments
- A bibliography
- Submission on time as I will have to deduct marks for late submission

Before you hand in your essay, make sure you have completed the checklist below.

Checklist:

- ☐ I have addressed the question directly and only included relevant information
- ☐ I have only included information from reliable sources
- ☐ I have included references wherever I used information I found somewhere else, and these references are written out fully at the end of my essay
- ☐ I have read through my essay to check for spelling, punctuation and grammar
- ☐ I have included diagrams and images to aid my explanations

Happy writing!



Tutorial 7 – Final assignment feedback and reflection

What is the Purpose of Tutorial 7?

- To receive feedback on final assignments.
- To write targets for improvement in school lessons.
- To reflect on the programme including what was enjoyed and what was challenging.

Final assignment feedback

What I did well…	What I could have improved on…
•	•
•	•
•	•

My target for future work is…

Reflecting on The Scholars Programme

What did you most enjoy about The Scholars Programme?
•
•
•

What did you find challenging about the programme?	How did you overcome these challenges?
•	•
•	•
•	•

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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 I 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:

- **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].
- **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.
- **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].

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