Method Sheet 113

Advice for writing up - Antibiotic discovery data analysis projects

Overview

Congratulations on the completion of your data analysis! Now comes the writing up phase. Giving as much care and attention to this process as your data analysis phase is essential to help you score the highest possible mark for your final report or dissertation. This document offers some generic advice on how to begin writing up your project report or dissertation. Please check with your university supervisor if this advice is suitable for your own, specific project.

Structuring your report or dissertation

Different universities have slightly different requirements for the structure of a BSc or MSc project dissertation. You should follow the guidelines of your own institution. However, a final report at this level typically comprises the following major elements, in the following order:

- **Title page**
- **Abstract**
- **Acknowledgements**
- **Table of Contents**
- **Abbreviations**
- **Introduction**
- **Materials and methods**
- **Results**
- **Discussion**
- **References**
- **(Appendices - optional extra section)**

Advice on word count

The overall word limit for your final project writeup varies greatly between institutions. However, regardless of the overall length, you will still have to decide how much space to give to each section of your report. Suggestions for word counts for each section that might work for this type of project are shown in the table below, broken down by common total word count limits for typical BSc and MSc research project dissertations. These suggestions assume that your word count limit does not include the references list at the end of the document, or the data contained within tables of the results section.

Please note that these figures are just a guide - they are very flexible. Feel free to alter the lengths of each section to meet your own institution's requirements and project-specific needs. Please check with your supervisor if they will be appropriate for your project.

Section	4,000 word limit	8,000 word limit	12,000 word limit
Abstract	200	250	250
1. Introduction	1,600	3,750	6,000
2. Methods	700	1,000	1,500
3. Results	700	1,500	2,000
4. Discussion	800	1,500	2,250

Advice for the Title page

This will be the front page of your dissertation. Here you should give the title to your project, your name (in most institutions) and your student identification number. Keep your title concise, and be sure to include the name of the micro-organism(s) you studied. Insert a 'page break' just after the text of this page so that the text from the rest of your document does not overlap onto this front page.

Advice for the Acknowledgements section

This can be a short section of several sentences to offer your thanks to those who have helped you in your project. Unlike the rest of the document, it can be quite personal. For example, you can thank your supervisor, friends and family here. Make sure to use 'Page breaks' to present this section on a separate page from the rest of the report.

Advice for section numbering and the Table of contents

This adds a layer of professionalism to your report that may help win additional marks. Method sheet 28 shows how to easily insert a table of contents for your report using a Microsoft Word automated function.

We recommend that you number your major sections as follows:

1. Introduction

2. Methods

3. Results

4, Discussion

5. References

You should split each of these major sections into smaller subsections, each covering a specific topic and with their own subheading with appropriate second level numbering. For example: 1.1 Background to antimicrobial resistance, 1.2 Mechanisms of antibiotic resistance, etc.

Advice for the abstract

The abstract is a standalone summary of your project, typically between 200 and 300 words (check your institution's guidelines for your specific word limit). It must explain *why* you did the work, *how* you did it, *what* you found, and *why* it matters. The following is a suggested structure for your abstract, we advise you to give one or two sentences for each of the following:

- **Context**: Introduce the "Big Picture", mentioning the threat of Antimicrobial Resistance (AMR) and the scale of the problem.
- **The gap in knowledge**: Explain why your specific project is necessary. For example, you could mention that there is a requirement to discover new antibiotics, and that natural products could represent a useful resource for this.
- **The aim**: State the objective clearly and concisely, in no more than one sentence.
- **Key results**: Give space only to the most relevant findings, and no space to minutiae. Be concise and quantitative. For example, instead of saying "some extracts worked", say instead, "Three extracts inhibited bacterial growth by more than 50% at 256 µg/ml, and the most potent extract (#102, *Cinnamomum verum*) yielded an IC_{50} of 25 µg/ml."
- **Conclusion/Impact**: Try to summarise the benefits your findings bring to the field in a single sentence, and perhaps (very briefly) where to go next with the work.

How to improve your abstract:

- **Do** remember to write in the past tense and the passive voice. For example, instead of saying “I will test 400 samples for antimicrobial properties”, say instead, “400 samples were screened for their capacity to inhibit growth of *Micrococcus luteus*”.
- **Don’t** write the abstract first. You should only write the abstract after you have completed the rest of your report, so you can summarise it accurately.
- **Don’t** make conclusions beyond what is clearly supported by your data. For example, do not “over-reach” by claiming that you have discovered a new antibiotic, or that it will work well in human studies.

Advice for the introduction

A high-scoring introduction for a BSc or MSc dissertation is not just a summary of facts; it is a persuasive argument that explains to the reader a key knowledge gap in the field, and why your project is necessary to address it. Examiners of project reports give the highest marks for the "Inverted Pyramid" structure in an introduction. This is where you begin with a broad overview of the field, and progressively narrow down the focus to eventually reach your specific research area.

We recommend giving space to at least the following topics in your introduction, in the following order:

1.1 Background to antibiotic resistance

Explain why AMR is a challenge in the clinic today. Support these statements by referring to studies and statistics from reputable sources (e.g. UN or NHS studies). Explain how AMR arises, and why it has become increasingly common in our hospitals over the last century. Give some examples of human behaviours that have increased the prevalence of AMR in recent years.

1.2 Mechanisms of action of existing antibiotics

Explain how the major classes of antibiotic work. You don’t have to cover every single antibiotic, but do give at least one example for each of the major mechanisms of action.

1.3 Mechanisms of antibiotic resistance in (Gram-negative or Gram-positive) bacteria

Explain how Gram-negative or Gram-positive bacteria (select one to match the type of bacteria you chose to study in your own project) resist existing antibiotics. Explain how resistance is spread between bacteria and in which environmental niches this most commonly occurs.

1.4 Reasons for the recent slowdown in antibiotic discovery

Explain how we used to discover antibiotics in the past, the golden age of antibiotic discovery, and why that source has dried up recently. Give some examples of approaches currently being explored by researchers to get past the present bottleneck in discovery.

1.5 Natural products as structural leads for the development of new drugs

Give a brief overview of the historical successes of natural products in drugs used today, including examples of some drugs in use today that derive from a natural origin.

1.6 Advantages and disadvantages of natural product screening in drug discovery

Explain that natural product screening typically offers a higher hit rate than synthetic compound screening, and often yields molecules with better toxicity / ADMET profiles. Discuss also the disadvantages of natural product screening, such as confounding from pigments or viscosity of extracts, and the requirement for activity guided separation to isolate the active compound. Mention that more work is necessary to figure out how to synthesise natural products and that they are therefore more difficult and time-consuming to patent. Explain why big pharma moved away from natural products to synthetic compound discovery in the early 1990s, and the impact that had on drug discovery. Explain here also the key principles of the Nagoya Protocol.

1.7 Hypothesis and aims

Keep this section very short and simple. The hypothesis (that screening a natural product library may reveal novel inhibitors of bacterial growth) and each of the aims (maximum 3-4) should be one sentence only. The aims should match the overarching objective of each of the experimental approaches you took.

How to improve your introduction:

- **Do** start simple, and then introduce more complex concepts one at a time
- **Do** cite key articles in the field which support the major points of your introduction, inserting these at the end of the sentence where you make the point
- **Do** give preference to citation of more recent articles, and those which report primary research rather than review articles
- **Do** give space to discussing the pros and cons of various schools of thought if there is controversy in the area you aim to study
- **Do** steer the narrative towards key questions that remain unanswered in the field, specifically those that could be addressed by your project
- **Do** include diagrams which explain the key cellular or molecular mechanisms of the areas you intend to study; we suggest ~1 figure per 500 words of introductory text
- **Do** draw your own diagrams for the introduction - copying an image from the internet will score less marks than if you draw something yourself in PowerPoint or Biorender. (If you do copy an image from elsewhere, remember you must cite the source of the image in the figure legend).

Advice for the methods section

The goal of the Methods section is to enable another scientist reading your report to critically assess how you did the work, and if necessary repeat the analyses you have performed to replicate your processes exactly. High scoring methods sections will be precise, technically accurate and free of minutiae. We recommend structuring your methods section using subsection titles similar to the following:

2.1. Source of primary data

Explain where you obtained the primary data sets for your study, including the URL, specific file names and the date the files were accessed. Briefly explain the types of experiment that were performed to create the primary data sets, and the format of the data as presented in the original download files.

2.2 Background correction and normalisation

Explain how you performed the background correction and normalisation processes, why this was necessary, and which software you used for this process.

2.3 Calculation of Z' factor values

Give the equation used to calculate Z' factor values for each of your plates, and which software you used for this process.

2.4 Hit criteria and selection

Explain the criteria you used to define a "hit" in the primary screen.

2.5 Correlation analyses

Explain which statistical approach you used to perform correlation analyses on the data.

2.6 Four parameter logistic curve fitting and calculation of IC50

Explain how you performed four parameter logistic curve fitting and calculation of IC50 for the dose response data you have, and which software you used for this process.

2.6 Statistical analyses

It is essential to include a section on how you performed your statistical analyses - missing this out or explaining it poorly greatly hurts the mark. Mention the main data analysis techniques, and which software you used for each different step of the analysis (e.g. Excel, GraphPad Prism or R). State what type of statistical test you used to analyse each different type of data (i.e. for the primary screening data, correlation analyses, dose curve data). State the p-value cutoff chosen for statistical significance.

How to improve your Methods section

- **Do** remember to write in the past tense and the passive voice (e.g. do not say "I did a T-test in Excel", say instead, "Student's T-tests were performed using Microsoft Excel").
- **Do** be precise with quantities and concentrations (e.g. do not say "A small amount of extract was added to each well", say instead, "1 µl of extract was added to 99 µl of culture in each well to yield a final extract concentration of 100 µg/ml."
- **Do** be very clear on how you did your statistical analyses.
- **Don't** give space to the minutiae, which means content that is either not directly relevant to your project, or would be obvious to someone with basic competence in the field. For example, there is no requirement to explain how a pipette works or how to prepare a dilution series - just give the final concentration achieved.
- **Don't** repeat the same content more than once.

Advice for the results section

The results section is where you present summaries of the results of your data analysis, presented in a way that is best able to help the reader understand them. This section will include all of your charts, tables and results of statistical analyses. In the main text of the results section, you should only describe what you saw in the analysis, highlighting only the most relevant findings in the text. Do not give any space to interpretation of what the findings mean in terms of mechanism, relevance to the field, limitations or comparisons to earlier studies in this section. Those comments are necessary, but they belong in the following discussion section and must be put there.

A high scoring results section will present high quality charts and tables with appropriate description of the main findings and summary statistics in the main body of the text between each figure and table.

Results to report in this type of project

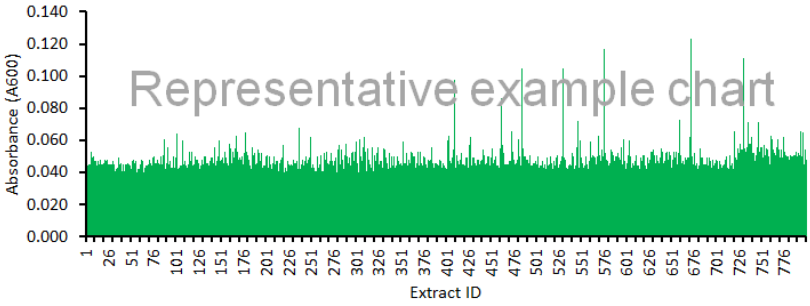
For a basic *Phytotitre* antibiotic discovery data analysis project, we recommend that you should present the following results in the order shown:

Figure #	Data to report
Figure 3.1	Column chart of absorbance values of diluted *Phytotitre* extracts
Figure 3.2	Scatter plot of *Phytotitre E. coli* screen (A: 8 hours, B: 21 hours)
Figure 3.3	Scatter plot of *Phytotitre S. aureus* screen (A: 8 hours, B: 21 hours)
Table 3.1	Z' factor values obtained for primary *Phytotitre* screens
Figure 3.4	Bar chart of *E. coli* hits at 8 hours (A) and 21 hours (B)
Figure 3.5	Bar chart of *S. aureus* hits at 8 hours (A) and 21 hours (B)
Figure 3.6	Scatter plot of 8 hour vs 21 hour *E. coli* screen results
Figure 3.7	Scatter plot of 8 hour vs 21 hour *S. aureus* screen results
Figure 3.8	Scatter plot of 21 hour *E. coli* vs 21 hour *S. aureus* screen results
Figure 3.9	Column chart of absorbance values of diluted *Puretitre* compounds
Figure 3.10	Scatter plot of *Puretitre E. coli* screen (A: 12 hours, B: 24 hours)
Figure 3.11	Scatter plot of *Puretitre M. luteus* screen (A: 12 hours, B: 24 hours)
Table 3.2	Z' factor values obtained for primary *Puretitre* screens
Figure 3.12	Bar chart of *Puretitre E. coli* hits at 12 hours (A) and 24 hours (B)
Figure 3.13	Bar chart of *Puretitre M. luteus* hits at 12 hours (A) and 24 hours (B)
Figure 3.14	Scatter plot of *Puretitre* 12 hour vs 24 hour *E. coli* screen results
Figure 3.15	Scatter plot of *Puretitre* 12 hour vs 24 hour *M. luteus* screen results
Figure 3.16	Scatter plot of *Puretitre* 24 hour *E. coli* vs 24 hour *M. luteus* screen results
Table 3.3	R^2 and p-values for correlations between compound structure and activity
Figure 3.17	Scatter plot to show ONE correlation between structure and activity
Figure 3.18	Dose response curve of *E. coli* growth with dihydroartemisinin (DHA)
Figure 3.19	Example of 4PL curve fitting for IC50 calculation
Figure 3.x-y	(*Optional: Data from any additional experiments you performed*)

<u>Interference arising from absorbance of diluted plant extracts</u>

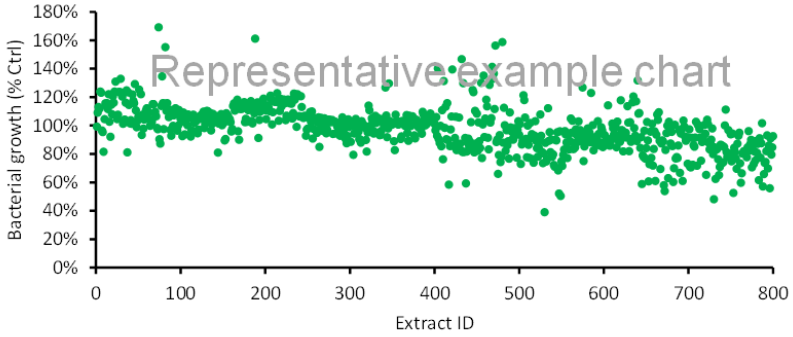
The first chart you should show is a simple column chart of the raw absorbance values of every well containing extract at time = 0 - in other words, the raw data of the plate read just after plating. These data should not be background corrected or normalised. Showing the raw absorbance values indicates how many of the extracts absorb light at the wavelength used in the assay, and to what extent, and therefore helps explain to the reader why you had to perform background correction for baseline absorbance in the next

steps. This figure would be numbered 3.1, as it is the first figure of your third major section (i.e. the Results section). Your chart should look something like this:



Results of the primary screen

Next, you should present the background corrected and normalised results from the primary screens. This should be done by showing a simple scatter plot in which the data are ordered by the Extract ID number, and the chart plots the Extract ID number on the x-axis and the response you measured on the y-axis, but with no error bars. You should do this first for the *E. coli* 8 hour data set. It should look something like this:



This type of chart is typically favoured in the reporting of drug discovery screening results as it gives an easy visualisation of how variable the responses were across the tested extracts and also the extent of inhibition achieved by the top 'hits' from the screen.

Next, you should present the *E. coli* data for the 21 hour timepoint in the same way. You can show this chart in the same figure (3.2) on the same page, but label the 8 hour timepoint chart as 'A' and the 21 hour timepoint chart as 'B'. Then, in a separate figure (3.3), show the data for the *S. aureus* screen at the 8 hour and 21 hour timepoints.

Explain in the main text of this section which extracts you chose to take forward as "hits" from your primary screen and why.

Table of Z' factors for each plate you measured

Make a list of all the Z' factor values you calculated for each plate of the 8 hour timepoint data for the *E. coli* screen. Align these values in a single column, then order these by value to find the maximum value, the minimum value, and the average Z' factor value. Now do the same for the 21 hour timepoint *E. coli* data, then the 8 hour and 21 hour *S. aureus* data.

Present these values in your report in a table with 4 columns and 5 rows. The top row should contain the headings and the first column the sources of each batch of

experimental data. Type the Z' factors from each of your lists into the relevant boxes to three decimal places. Remember to give a table number, title and footnote.

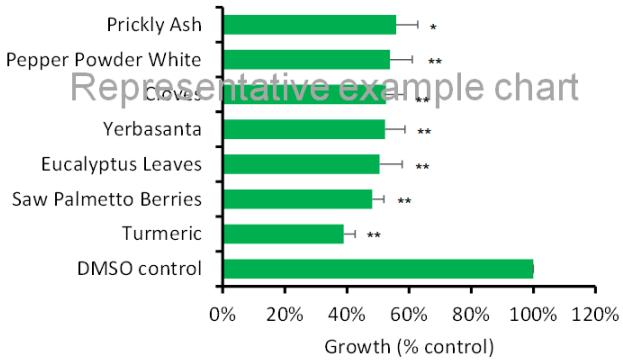
For example, your table might look like this (please note, the numbers shown are not the correct values, so you will have to insert your own calculations):

Table 3.1: Range of Z' factor values obtained from primary screens

Data source	Min	Max	Average
E. coli 8 hour data	0.201	0.701	0.501
E. coli 21 hour data	0.201	0.701	0.501
S. aureus 8 hour data	0.201	0.701	0.501
S. aureus 21 hour data	0.201	0.701	0.501

Bar chart of top hits

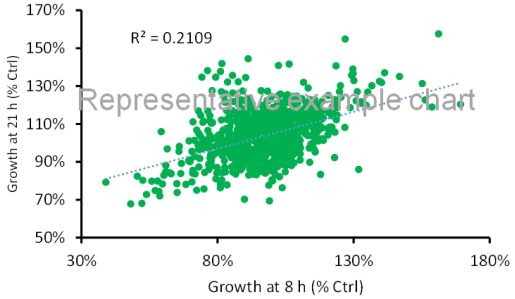
Align your normalised data for each timepoint, including the SD for all 3 plate measurements, and order by average growth, with the lowest growth values at the top of your table. Create a bar chart of the top 7 hits, with the names of the plant extracts yielding those values on the y-axis. Add error bars and stars for the results of ANOVA statistical analysis to your chart to indicate the level of variation between the three experiments. Your chart should look something like this:



Now do the same for the *E. coli* 21 hour timepoint, and the *S. aureus* 8 hour and 21 hour timepoints, presenting each as a separate chart.

Seek correlations within the primary screening dataset

Order the normalised screen results by Extract ID to align the 8 hour and 24 hour data for *E. coli*. Prepare a scatter plot of the growth at both timepoints (i.e. results from one timepoint on the x-axis and results from the other timepoint on the y-axis). This will be helpful to establish if any extracts work well at early timepoints but lose their inhibition at later timepoints. Add a trendline and R^2 value. The chart should look something like this:



Now prepare a scatter plot of the 8 h vs 21 timepoint data for *S. aureus*, and also a third scatter plot chart, charting the results for *E. coli* at 21 h against the results for *S. aureus* at 21 h. This plot will help to show if any extracts have activity against both different types of bacteria simiultaneously.

Report the results of linear regression of these scatter plots by giving the 'r' value and the p-value in the main text of the results section.

Prepare the same charts for the *Puretitre* screening data

Now repeat the same processes listed above for the *Phytotitre* data sets using your analyses of the *Puretitre* data sets. It may be helpful to number these according to the table of figures shown at the start of this section.

Seek correlations with physicochemical properties of *Puretitre* compounds

Prepare scatter plots to determine which of the major *Puretitre* compound properties correlate significantly with inhibition of *E. coli* growth. Obtain an R^2 value from each chart and use it to create a table, which you should show in your dissertation, of the R^2 value, r value, n (number of compounds), t statistic and p-value for each of the following physical features: Molecular weight, LogP, Hydrogen Bond Donor Count, Hydrogen Bond Acceptor Count, Rotatable Bond Count, Topological Polar Surface Area. Your table should look something like this (note, the numbers shown as examples are not all correct, you will have to input values from your own calculations):

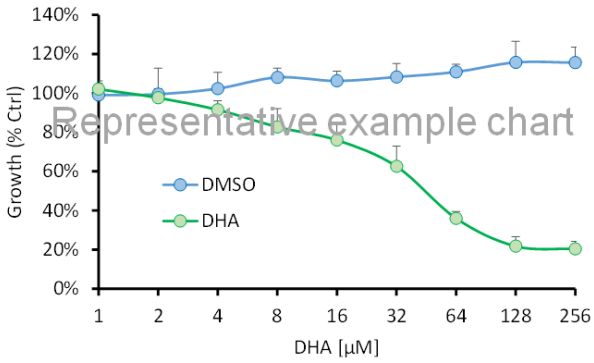
Table 3.3: Correlations between *Puretitre* compound physical features and inhibition of *E. coli* growth

Structural property	R^2	r	n	t	p-value
Mwt	0.0022	0.047	200	0.66	0.508
LogP	0.0022	0.047	200	0.66	0.508
Hydrogen Bond Donor Count	0.0022	0.047	200	0.66	0.508
Hydrogen Bond Acceptor Count	0.0022	0.047	200	0.66	0.508
Rotatable Bond Count	0.0022	0.047	200	0.66	0.508
Topological Polar Surface Area	0.0022	0.047	200	0.66	0.508

Do the same thing for the *M. luteus Puretitre* screen, inserting this as a separate table. Mention in the table footnote what the threshold for p-value significance should be after Bonferoni correction for multiple testing. You can then insert ONE scatter plot to show the correlation between bacterial growth and the physical feature that yields the lowest of all the p-values you found in these two tables (i.e. the most significant correlation).

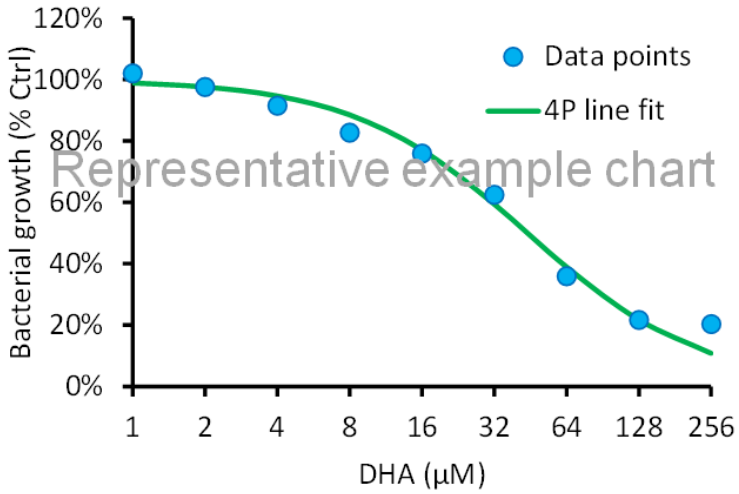
Replication dose curves of a top hit

Plot the results of the experiments measuring *E. coli* growth in the presence of various concentrations of dihydroartemisinin (DHA), as a scatter plot of concentration on the x-axis and the mean bacterial growth from the four experiments on the y-axis, plus SD or SEM error bars in the y-axis direction. Use a log scale with base 2 on the x-axis, but normal (non-log) scale on the y-axis. Remember to plot the results of both the compound and the DMSO control dilution series on the same chart to enable easy visualisation of any dfferences between them. Place asterisks (*) above any data point on the DHA line that is significantly higher or lower than the control (DMSO) growth condition (see Method sheet 25). Your chart should look something like this:



Calculation of IC50 value for *E. coli* growth in the presence of DHA

Prepare a similar scatter plot to the example given above but with the DHA compound data only. Follow the advice given in Method sheet 112 to add a 4-PL curve fit to the chart and calculate the IC_{50} value for the compound. Your 4-PL curve fit chart should look something like this:



Report the IC_{50} value obtained from your line fit for the compound DHA in the Results section of your report.

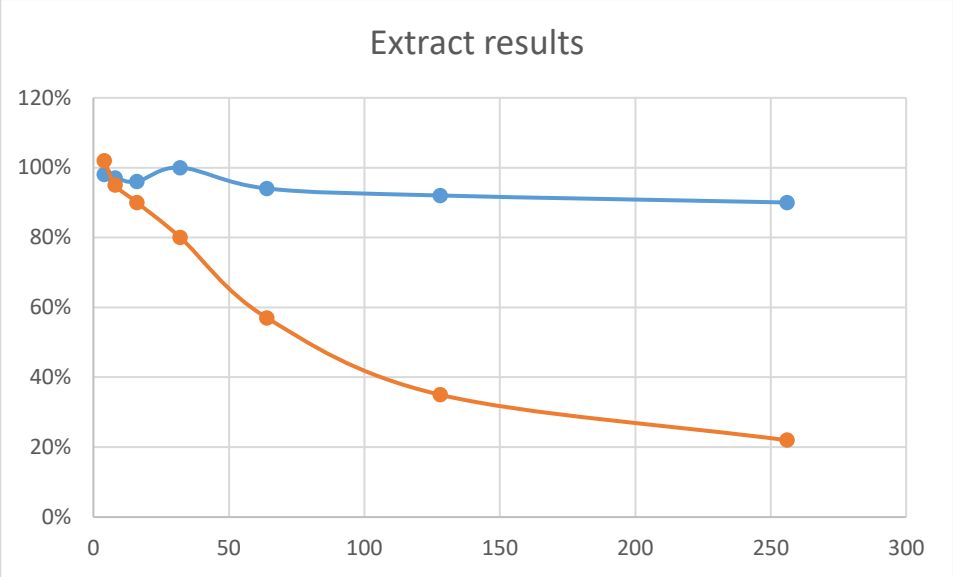
Advice for presentation of results of extended (e.g. MSc) projects

If you have performed additional experiments beyond those suggested in the basic version of the *Phytotitre* project, remember to present these as additional figures following the guidelines shown above.

What makes a good chart?

Good quality charts are essential both for publication of manuscripts in Life Science journals, and for obtaining a high mark in student dissertations. The hallmark of a well-presented chart is one that is clear, uncluttered, and shows the information necessary for easy visualisation of the data. Journals have specific guidelines for chart formatting to meet their requirements for quality. Following these rules in the preparation of your own charts should help lift the mark for your own dissertation significantly.

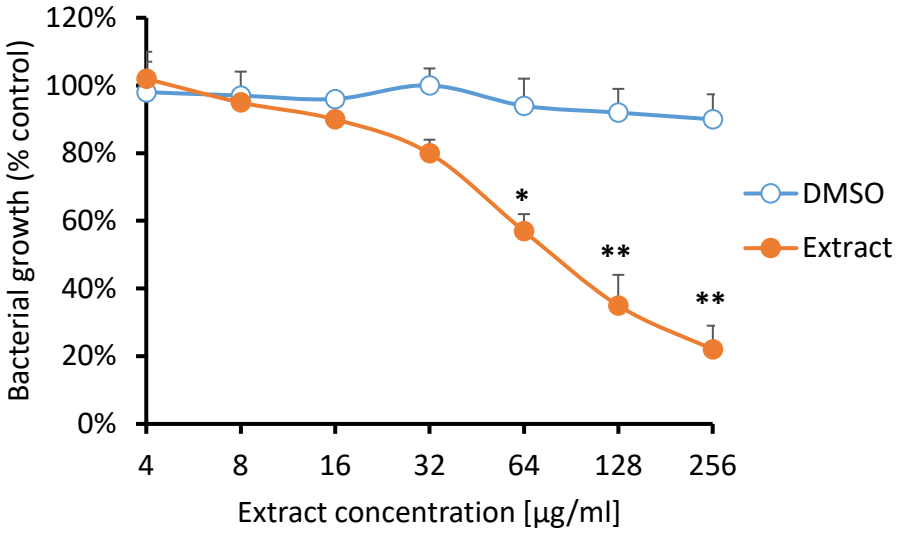
Let's examine what a poorly formatted chart looks like, using a chart prepared with the default settings Microsoft Excel applies to a scatter-plot chart before correct formatting (see below).



Reasons why the above example is a **poorly formatted chart**:

- There are no x-axis or y-axis labels
- There is a title at the top of the chart (Excel inserts these by default)
- There are no error bars to indicate the variability between experiments
- The x-axis is on a linear scale, when it should be on a log scale for dilution curves
- There is no legend on the chart to explain what the different colours of line represent
- There are horizontal and vertical gridlines
- There is a border around the outer perimeter of the chart area
- The font is light grey, a little too small, and difficult to read clearly
- The axis lines are light grey and too thin (insufficient line weight)
- There are no tick marks on the axes
- No asterisks are present to indicate values significantly different from control

Now let's have a look at a well formatted chart plotted from the same data (see example below).



Reasons why the above example is a **well-formatted chart**:

- X-axis and y-axis labels are both present and indicate the correct units
- There is no title at the top of the chart (this will go in the text below your chart)
- Error bars indicating the standard deviation are present
- The x-axis is on a log scale in base 2, which is correct for doubling dilutions
- A legend is present on the chart to explain what the different colours of line represent
- The horizontal and vertical gridlines have been removed
- The border around the outer perimeter has been removed
- The font is solid black, a little larger, and now easier to read
- The axis lines are solid black and 1.5 line weight
- Tick marks are present on both axes
- Asterisks are present to indicate p-values on values significantly different from control

Use the above as a checklist to ensure your charts meet the same level of quality. Your examiners will be looking for all of these things in charts of a high scoring Results section.

What to include in your figure titles and legends

Every figure in your report must have a number, a title and a legend. These must also be formatted correctly to score well. The figure title and legend will appear directly below the chart in your report, not above. They should be in a font or style that is slightly different from the main text to help distinguish the title and legend text from the rest of the document. An example of a poor figure title and legend is shown below:

> Figure: Antibiotic effects of extract
>
> The results are shown in the above chart.

Reasons why this is a poor title and legend:

- There is no figure number
- The title is vague and non-descriptive
- There is no clear explanation of how the experiment was performed
- The legend lacks essential information on experimental replicates ('n'), statistical tests, error bars and p-value thresholds

Now let's look at an example of a good figure title and legend:

> Figure 3.2: Dose-dependent inhibition of growth of *Micrococcus luteus* by extract of *Cinnamomum verum*
>
> *M. luteus* cultures were grown for 18 h in the presence of indicated concentrations of *C. verum* extract or equivalent content of vehicle control (DMSO). Growth was measured by absorbance at 600 nm. Means of 3 independent experiments ± SD are shown. Statistical significance was determined using a two-way ANOVA followed by Sidak's post-hoc test, comparing each extract dose to the corresponding vehicle control (* $p < 0.05$, ** $p < 0.01$).

Reasons why this is a good title and legend:

- There is a figure number (3.1) and a descriptive but concise title that explains clearly what is shown
- The legend gives sufficient explanation of what was done in the experiment so a reader can understand the basics of what is shown without having to refer to the main text
- The identity of the control is made clear
- The number of independent experiments performed to collect the data is shown clearly (it is essential to always report this 'n' value in your legends)
- The fact that error bars represent standard deviation is explained
- The type of statistical test used, and the comparator condition, is clearly explained (this too, is essential)
- The meaning of the one star and two star marking on the chart is explained in terms of the p-value thresholds they represent

How to improve your Results section

- **Do** make sure every figure is numbered and cited in the main text by its number
- **Do** check whether your data are parametric or non-parametric before choosing a statistical test to apply
- **Do** explain clearly which statistical test you chose for analysis of each type of data and why
- **Do** present the results in an order that follows a logical progression and tells a story beginning with your hypothesis and following your thought process through each experiment
- **Do** prepare your figures to a high standard as explained in the section above
- **Do** mention any problems you may have seen in your experiments if they may affect the results (e.g. unusual cell morphology, low reproducibility, unexpected results, edge effect etc.), but leave discussion of those issue to the next section of the report
- **Do** show evidence of good reproducibility of experimental work (e.g. small error bars)
- **Do** include appropriate controls in all your experiments (e.g. vehicle alone etc)
- **Do** remember to insert a space between number and unit every time (e.g. 1 µg/ml, not 1µg/ml)
- **Don't** show the raw data - only show the summary data after processing and analysis of data from all experiments of the same type combined
- **Don't** give a chart for each individual experiment - give only a single chart combining all the data from all experiments of the same type combined
- **Don't** show the results from individual experiments - only show the means of multiple repeat experiments post analysis (the exception to this is where you show an image of an agar plate or a microscope field or similar, in which case you should clearly indicate in the figure legend that the image shown is "a representative result from 'n' independent experiments")
- **Don't** give space to description of the minutiae - stick to the main findings and key observations

Advice for the discussion section

Here, the examiner will be assessing your understanding of the project, how it fits in with past work in the field and your understanding of what the results show and mean more broadly. Your results section is where you **describe** the findings. The discussion section is where you **interpret** the findings and **compare** them with earlier studies. You should structure your discussion section in the following order:

1) **Brief recap**: Why was your project necessary for the field?
2) **Interpretation**: What do your results mean and can you explain the observations?
3) **Context**: How do your findings compare to previous studies?
4) **Limitations**: What were the weaknesses of your study?
5) **Future Work**: What should be done to take this work forward?
6) **Conclusion**: What is the final "take-home" message?

The brief recap should be at most 1-3 sentences, explaining why your project was necessary. Make sure you link back to your original hypothesis here.

Then try to explain what factors may be responsible for the main findings of your project. Give space particularly to why you think any extracts did, or did not, inhibit the readout chosen for your screen. If you saw any unusual results that are difficult to explain, this is where you will raise the point and offer some possible explanations.

Next, you should discuss what others have reported in terms of the effects of the same herb in previous studies, particularly if those studies look at the same phenotype you did. Give space to discussion of the likely toxicity of the plant - has it been trialled in human or animal studies previously? Mention any active compounds that others have previously reported to be present in the extract, and if these compounds have activity similar to what you have seen.

Then you should discuss the advantages and limitations of your own study. Give space to the pros and cons of natural extract and compound screening. Then mention any specific issues you found in your own project (e.g. the edge effect, contamination issues, etc.).

Insert a paragraph or two on future work. This is where you suggest what direction you would like to take the work forward if you had sufficient funding. Focus specifically on which types of follow-on experiments or development programmes you think would be most valuable for the field.

Finish with a clearly defined ‘Conclusion’ section. This should sum up the broad picture of what your work found and how it contributes to the field. Also mention the potential value to society if you have found some potentially useful bioactivity. But do not over-reach - make sure your claims are entirely supported by your own data. If you speculate that your extract could have therapeutic potential in future, make clear that this is a speculative point and will require further work to validate. Do not introduce any new information or discussion into this closing section - it should be quite brief and mainly a summary of what you have said previously. Some institutions prefer this to be a standalone section after the discussion (e.g. 5. Conclusions) - follow their guidelines if that is the case.

How to improve your Discussion section:

- **Do** cite a wide range of relevant references
- **Do** explain how your work addresses an unanswered problem in the field, and how your approach relates to studies of previous workers

- **Do** give space to discussion of both the advantages and limitations of the experimental approaches you have taken
- **Do** mention the key limitation that your work is *in vitro* only, and that the results may not be applicable to an infection *in vivo*
- **Do** give space to discussion of evidence from earlier studies which support or refute your own observations
- **Do** mention the possibility of activity guided separation as the next step in identifying any active compounds of interest that may be present in your hit extracts
- **Do** explain that progressing to isolation of a natural compound and developing it as a candidate drug in future work will require careful consideration of the Nagoya Protocol
- **Don't** simply repeat the minutiae of the results again, a brief summary of a key finding is fine, but leave most of the numerical results in the results section
- **Don't** be afraid to express your view if your findings challenge existing thought in the field - just be sure to explain clearly why you think you are right and they are wrong
- **Don't** simply ignore any unusual results, or those that are difficult to explain - offering plausible explanations for these can actually win extra marks
- **Don't** be afraid of "negative results" - remember that two projects will score exactly the same mark if they are performed and written up to the same standard, regardless of whether one makes an amazing discovery and the other does not - this is not what you are being assessed on

Advice for the references section

Here, your examiner will assess your grasp of the literature in the field relevant to your project, and your ability to cite previous works correctly. Different institutions prefer different referencing styles. However, most UK universities require you to use either the **Harvard** or **Vancouver** styles. These styles have some key differences you should be aware of. Harvard style involves giving the first author surname and year of publication in the in-text citations (e.g. Smith et al., 2019). Vancouver style replaces this with a simple number, often in square brackets (e.g. [1]). Make sure you format your own references in the main text and in the reference list according to the style favoured by your own institution. These can be inserted and sorted by hand, but using a software application to manage your references will save a lot of time and effort in this process.

Examples of the Harvard and Vancouver referencing styles:

Style	In-text citation	Reference list
Harvard	(Wilson et al., 2020)	Wilson, B.A.P., Thornburg, C.C., Henrich, C.J., Grkovic, T. and O'Keefe, B.R. (2020) 'Creating and screening natural product libraries', Natural Product Reports, 37(7), pp. 893–918.
Vancouver	[1]	Wilson BAP, Thornburg CC, Henrich CJ, Grkovic T, O'Keefe BR. Creating and screening natural product libraries. Nat Prod Rep. 2020;37(7):893-918.

What references should you include?

Cite articles that support the major claims you are making, primarily in the introduction and discussion sections. It is better, where possible, to cite peer-reviewed journals over websites, and primary research articles over review articles. Remember to insert your citations at the end of the same sentence in which you have made a major claim that refers to or requires support from earlier work.

Here are some examples of journal articles that you could read to help you get started with this specific project:

1) Wilson BAP, Thornburg CC, Henrich CJ, Grkovic T, O'Keefe BR. Creating and screening natural product libraries. Nat Prod Rep 37:893-918 (2020)
2) Martínez-Fructuoso L, Arends SJR, Freire VF, Evans JR, DeVries S, Peyser BD, Akee RK, Thornburg CC, Kumar R, Ensel S, Morgan GM, McConachie GD, Veeder N, Duncan LR, Grkovic T, O'Keefe BR. Screen for new antimicrobial natural products from the NCI program for natural product discovery prefractionated extract library. ACS Infect Dis 9:1245-1256 (2023)
3) Atanasov AG, Zotchev SB, Dirsch VM; International Natural Product Sciences Taskforce; Supuran CT. Natural products in drug discovery: advances and opportunities. Nat Rev Drug Discov 20:200-216 (2021)

How to improve your citations and referencing

- **Do** cite previous works that are most relevant to the area of interest, the methods you have chosen, and the overall aim of your project
- **Do** cite studies in reputable, peer-reviewed journals
- **Do** cite mostly primary research articles, with only a handful of review articles
- **Do** place your in text citations at the end of the same sentence where you make a claim or statement, don’t save them up to the end of the paragraph or section
- **Do** favour citation of journal articles over textbooks
- **Don’t** cite studies that report results that are far beyond the scope of your own project
- **Don’t** cite studies from disreputable sources (e.g. unofficial websites, wiki pages etc.)
- **Don’t** forget to order your reference list alphabetically if you choose to use Harvard referencing

General advice for your dissertation write-up

- Your writing should be clear, well organised and with excellent grammar and spelling
- Present your work to a high standard in terms of the formatting and presentation of the report (e.g. consistent font style and size for each level of heading, consistent formatting of charts and legends, etc.)
- Use hierarchical numbering for sections and subsection headings (e.g. 1. for Introduction, then 1.1 for the first subheading in your introduction, etc.)
- Use the Microsoft Word headings function to prepare a table of contents page just after your acknowledgements section
- Where possible, draw your own diagrams for explanatory figures in the introduction (e.g. using PowerPoint or BioRender)
- If you do copy an image from elsewhere to use it in your thesis, make sure to cite the source of the image clearly in the figure legend
- Introduce your facts in a logical order that makes sense for the reader
- Sections which jump about randomly between topics without a clear thread score low marks
- Use italics for all genus and species names (e.g. *Escherichia coli*)
- Remember to also use italics for all other Latin terms, such as *et al*., *in vitro* and *in vivo*
- For abbreviations, give the full term at first use explaining the acronym in brackets straight after, then use the acronym on every occasion thereafter (e.g. polymerase chain reaction (PCR) at first use, then simply PCR at every point in the document after that)
- Remember to include the abbreviations you have used in the list near the start of your report
- Unlike the Introduction, Methods, Results and Discussion sections, which are all numbered (1-4), the Abstract, Acknowledgements and References sections do not receive a number
- Use the ‘Page break’ function to ensure every figure is on the same page as its title and legend (which should be placed just beneath it)
- Also insert a ‘Page break’ just before each of the major sections to prevent cluttering