Report 2 – Choosing a method and in-depth assessment of method in context to a commerical laboratory (40 %)

Background context for report 2

You are working in an IANZ accredited lab; a client has come to the company asking for quantitative data on a particular analyte and matrix (this will be a different analyte and matrix than you previously studied for your oral presentation and report 1) that the laboratory does not currently test for.

The laboratory is well equipped with typical laboratory equipment (2, 4 and 5 figure balances, auto pipettes, ovens etc) and has UV spectrometers, LC-MS, GC-MS, GC-FID, HPLC (UV, RI and fluorescence detection) and ICP-MS instrumentation – you can decide on make and model.

Part A – Choosing a method

Your boss has asked you to review the literature for a suitable method and put forward a proposal for a method that can be validated and accredited for use in the busy commercial laboratory. Your boss wants a clear, concise business case to read to decide whether the lab should proceed with this new testing.

Part B – In-depth analysis of the chosen method
Using the method you have chosen you will look at the price and time to carry out method, steps that are classes as critical, improvements that could be made and suggest a validation plan.

As a starting point, you will be given the references for four articles from the literature on your given analyte and matrix which you need to find. These articles have been selected because they contain various methodology to prepare the sample before analysis and/or different instrument techniques for analysing the analyte. You need to read the four papers in depth. You will also need to source further literature to gain more of an understanding on the analyte, matrix, sample preparation methods and/or instrumentation. You need to include **at least eight** other references of reputable nature in your report.

A marking guide is attached at the bottom of this document with details on distribution of marks.

Report style guidelines
Your reports should be in 11 or 12 point font and have 1.5 line spacing.
Number all pages
Place your name and student ID in the header
Use ACS reference style (super script)

Hints for report
Avoid generalising sweeping statements (e.g. “and so forth”).
Back up your comments with critical analysis, chemistry (e.g. chemical reactions, interactions, solubility etc) and other literature

Refer to the paper outline or Moodle for the due date. Please submit an electronic copy onto Moodle.

Part A– Choosing a Method

Part A of your report should include:

Overview of the analyte and matrix (Introduction)

- State why detection of this analyte in this matrix is important
- Details on the chemical and physical properties of the analyte and expected concentrations (e.g. is it heat/light sensitive, volatile, what is it soluble in?)
- Details on the matrix (e.g. potential interferences, solubility complications. Are there sample size limitations)
- Potential complications in quantifying the analyte (e.g. interactions/interferences in matrix)

Commercial laboratory requirements

- Discuss the parameters and requirements necessary for choosing a suitable method for a commercial laboratory

Methods from prescribed papers

- Summary of sample preparation and analysis methods. Do not just restate the methods from the articles; you should include information such as concentrations of target analyte in solution, dilutions, concentration/ratio of analyte:derivatising agent, concentrations of acids, mass of sample required. Include thoughtful information for why these reagents, concentrations etc have been used (i.e. what is the underlying chemistry?).
- Compare and contrast sample preparation techniques **and** analyte detection methods used in the articles.
- Discuss advantages and disadvantages of the sample preparation **and** instrument analysis of the methods.
- Discuss any novel concepts of sample collection, preparation and/or analysis
- Suggest why the authors chose the sample preparation methodology (i.e. think about interference of other analytes in matrix, concentration of target analyte, toxicity of solvents/analyte, fit for purpose).
- Ensure that you add critical analysis, comparisons and wider reading to your report.

Extended literature search

- Search the literature and comment on if the methods in these articles are common methodology for analysis of this analyte in this matrix.
- Is this analyte present in other matrices and could any of these methods potentially be used? (Justify your answer)

Recommendation

Give your recommendation for which method should be chosen and explain why you have chosen the particular method over other methods.

Notes:

- You have freedom on how to set out the report; the above headings do not necessarily have to be used as your sub-sections
- If your analyte is a broad category (e.g. phenolics, trace elements), choose 1 – 3 specific compounds/elements to focus on. Perhaps one is more difficult to extract/detect than others, which will lead to a better discussion.
- If your matrix is a broad category (e.g. food) you may focus on one food group that is presented in the articles.

Part B – In-depth assessment of chosen method

Following on from Part A, your boss has accepted your recommendation for methodology and wants further information on this method. You need to prepare a business case to your boss for using the chosen methodology. As a guideline this should be prepared in a succinct way that is set out in an easy to read format. You need to carry out due diligence on the method to ensure that it is appropriate for a commercial laboratory.

*****Please note: <u>Do not</u> contact instrument or consumable representatives for quotes. ******
If prices are not available online, use an estimate from an equivalent product. A PDF document is available on Moodle with some items for a price estimate.

Part B of your report will be divided into three parts:

Part 1: Assessment of chosen method

- A breakdown of the time required for sample preparation steps and instrument analysis (how many samples can be analysed in a day?). You may have to estimate some times. State if it is active or passive time.
- Discuss the number of steps for sample preparation and identify the key critical steps (i.e. if a step was missed out, carried out at wrong temperature or for the wrong time would this make a large difference to the results, sample storage, representative sample)
- Equipment, consumables and standards required (e.g. are these stable, readily available)
- Complete a cost analysis of the chosen method (i.e. price per sample). Is it more cost effective if there are more samples? (e.g. price per 100 samples)
  *****Please note: Do not contact instrument or consumable representatives for quotes. Use prices from the PDF document provided to you, or prices that you can find online, or estimate the price based on equivalent consumables/reagents******
- Toxicity of reagents/ chemicals (MSDS)/hazards
- Are the any incompatibilities with other tests/chemicals?

Part 2: Improvements to method

- Make at least one suggestion for method improvement to the sample preparation and justify your suggestion
- Make at least one suggestion for improvement to the instrument method and justify your suggestion
- What step/s could be altered to be quicker, save on consumables/reagents or make the method an greener analysis?
- Recalculate the cost analysis with your method improvements taken into consideration

Part 3: Validation of the method

- Propose a procedure to validate the method that would allow it to be accredited by IANZ. This should include the different validation tests that should be carried out, quality control samples, spike level concentrations etc. Set out how many samples are required, how long this will take, what matrices will be used etc.
- Summary of what is required to implement method in the lab and a suggested timeframe

Report 3– Marking Rubric

Areas report will be graded
CONTENT (35 marks) Report addresses all required elements. Report shows clear understanding and knowledge of subject matter Report shows critical thinking Understanding of the chemistry is discussed.
STYLE (5 marks) The report is clear and concise (Up to 3 marks will be deducted for waffle). Report shows maturity of writing Report takes a range of information and collates it into own words Report takes into consideration the theme/background context
STRUCTURE, GRAMMAR, SPELLING, PUNCTUATION, CHEMICAL NOTATION (5 marks) Report is set out in a logical order, flows well and is well presented. Headings and sub-headings are used. Free of spelling and punctuation errors. Chemical notation is present and correct (including any equations). Tables and figures have captions and also callout in the body of the text.
REFERENCES (5 marks) References have been carefully chosen. References are in ACS format. References are cited correctly throughout the text.
Comments:

*Note: List of items under each heading is not exhaustive, but an indication of what is required.

	Content	**Style**	**Structure etc.**	**References**	**Total**
Mark	/35	/5	/5	/5	**/50**