

# Trace Analysis

## INSTRUCTOR

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- As target for medicine must be as pure as possible
- Try to identify techniques to remove traces
- NMR is not good for trace analysis because you have to look for higher concentrations.
- Mass-spec, atomic absorption, X-ray fluorescence (XRF) → The are suitable for TA
- If I don't have a protective group, my rxn could be affected

## Seminars:

- Via zoom → Wednesdays 12m
- Mandatory
- 1, 2 / month

## Lab Notebook

- Open Webware

## Article Interpretation

- Extract information from articles
- Example of sample prep techniques

## Instrument SOP

- Learn how to use an SOP (lab steps)
- Analyse and interpret SOP
- Measure trace analysis

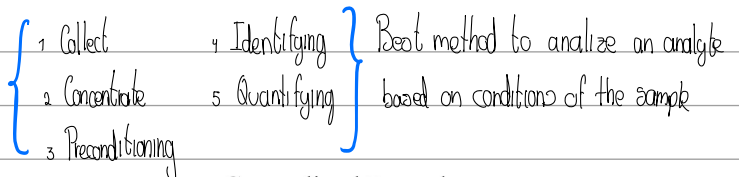
## Lab reports

- Calculations and answers to questions

Week	Date	Topic	Chapter
1	Jan 13	Introduction / Statistics/Electrochemistry	1
2	Jan 20	Bracht Seminar <b>Genomics</b> / Statistics/Electrochemistry	
3	Jan 27	Connaughton Seminar Zebrafish/Fluorescence Optics	3, 4
4	Feb 3	LAB: Fluorescence	
5	Feb 10	Sampling / Protein analysis/Separations	8, 10
6	Feb 17	DNA analysis / Concentration methods/Chromatography	11, 6
7	Feb 24	LAB: Electrochemistry	
8	Mar 3	Microscopy / X-ray methods/Chromatographic Methods	15
9	Mar 10	No Class – Spring Break	
10	Mar 17	Isotopic methods / Capillary Electrophoresis	7, 9, 14
11	Mar 24	LAB: GC-MS	
12	Mar 31	Speciation / Statistical analysis	12, 2
13	Apr 7	Electrochemical methods	handout

## Analyte decision tree

for trace material



- TA is characterization of compounds < 0.01% of a sample
- Report as mass ratio, mass concentration or mole ratio
- ppm, ppb, ppt NOT reported
- Limit of detection LOD →  $ex = \sqrt{\frac{\sum (y_i - \bar{y})^2}{n-1}}$  (Measurement value / Average # of measurements)
- Smaller concentration, greater the uncertainty
- Improve accuracy? multiple measurements
- Results trapped → lower concentration under the variation

## Factors reducing precision

- Large excess of other compounds
- Use of multistep analytical procedure
- Contamination of an analyte
- Interference of other compounds.
- Low precision of instrumentation.

## Generalized Procedure

- Select and validate appropriate sample preparation
- Select and validate appropriate analysis method
- Maintain and upgrade analytical instruments
- Ensure good record keeping
- Ensure quality of data
- Maintain high quality lab performance