

<b>Academic Year</b>	2022/23	<b>Semester</b>	1
<b>Course Coordinator</b>	Richard D. WEBSTER and Alessandra Bonanni		
<b>Course Code</b>	CM2011		
<b>Course Title</b>	Analytical Chemistry		
<b>Pre-requisites</b>	(CM1021 and CM1041) or CM9001/CM5000 or CY1101 or CM1001		
<b>No of AUs</b>	3		
<b>Contact Hours</b>	On-line or face to face lectures - 35 hours Mid-term assessments - 4 hours		
<b>Proposal Date</b>	21 October 2021		

### Course Aims

The lectures provide an introduction to modern analytical methods that are used to quantify species and instrumental methods used to monitor the progress of reactions. The course comprises a mixture of numerical problem solving and descriptive chemical analysis.

### Intended Learning Outcomes (ILO)

By the end of this course, you (as a student) would be able to:

#### 1. Errors and Confidence Interval

- Explain the difference between absolute, relative and percent relative uncertainties.
- Discuss how errors are totaled when numbers (with errors) are combined.
- Apply and calculate the confidence interval.
- Apply the *Q*-test to exclude points.
- Explain when to use the correct number of significant figures and correct rounding.
- Execute the student *t*-test to compare different sets of data for three cases: (a) Comparing a measured result with a 'known' value. (b) Comparison of the means of two methods. (c) Paired *t* test for comparing individual differences

#### 2. Air Pollution Measurements in Singapore

- Identify the differences between Air Quality Index (AQI) and Pollutant Standards Index (PSI).
- Discuss the major pollutants that are measured.
- Discuss how data from the NEA website is interpreted.
- Discuss how to calculate PSI from raw data.
- Explain how "cigarette scale" can be used to understand PM values.
- Describe how the elemental concentrations of PM are measured.

#### 3. Introductory Electrochemistry

- Discuss the concept of ionic strength and how to calculate activities and activity coefficients.
- Analyse activity coefficients to calculate solubility products.
- Explain how to draw an electrochemical cell in shorthand notation.
- Describe how to calculate the cell potential and direction of the spontaneous reaction of two half-cell reactions.
- Explain how the Nernst equation can be used to calculate cell potentials when activities are less than unity.

- 4. Potentiometry**
  - a. Explain how the pH electrode functions, which equilibrium reactions occur, and the importance of ionic strength.
  - b. Discuss how to write an ISE cell in short hand notation.
  - c. Identify all of the potentials that operate in an ISE (interfacial potentials and junction potentials).
  - d. Discuss the operation of the major types of ISEs (glass, single crystal, pressed powder and polymer membrane).
  - e. Describe the practical limitations of ISEs and how to calculate selectivity coefficients.
  
- 5. Molecular Absorption Spectroscopy**
  - a. Explain how to convert between different units of measurement used for spectroscopy.
  - b. Discuss the difference between rotational, vibration and electronic energy levels.
  - c. Explain the calculations based on Beer's law ( $A = \epsilon bc$ ) and Scatchard plots.
  - d. Discuss the different components of an Absorption spectrometer and how they function (excitation source, monochromator, sample holders, detector).
  
- 6. Molecular Florescence (Emission) Spectroscopy**
  - a. Discuss the similarities and differences between molecular fluorescence and absorption instrumentation.
  - b. Describe molecular fluorescence and phosphorescence electronic transitions (vibrational relaxation, internal conversion, intersystem crossing).
  - c. Explain stokes shift.
  - d. Describe the quantum yield.
  - e. Discuss why fluorescence measurements are very sensitive.
  
- 7. Atomic Spectroscopy:**
  - a. Discuss the differences between atomic and molecular spectroscopy.
  - b. Identify the differences between Atomic Absorption Spectroscopy (AAS) and Atomic Emission Spectroscopy (AES).
  - c. Explain how a hollow cathode lamp functions.
  - d. Discuss why AES is more sensitive to temperature than AAS.
  - e. Identify the causes of line broadening.
  
- 8. Extractions**
  - a. Explain how to extract a solute from one phase into another in which it is more soluble.
  - b. Apply the partition coefficient to determine ratio of solute concentrations in each phase at equilibrium.
  - c. Apply distribution coefficient when more than one form of solute exists in each phase at equilibrium.
  - d. Derive equations relating the fraction of solute extracted to the partition or distribution coefficient, volumes, and pH.
  - e. Explain how the number of extractions relate to efficiency of extractions.
  - f. Describe how the metal chelator can extract metal ions from aqueous solutions.
  - g. Explain how crown ethers and salts containing a hydrophobic ion act as phase transfer agents
  
- 9. General Chromatography**
  - a. Describe the equilibration of solute between mobile and stationary phase in adsorption and partition chromatography.
  - b. Describe the stationary phase of packed columns and open tubular columns.
  - c. Explain the separation process in ion-exchange and ion chromatography.

- d. Explain the separation process in molecular exclusion chromatography.
- e. Explain how solutes interact with the stationary phase in affinity chromatography.
- f. Describe the relative retention and adjusted retention times in chromatography.
- g. Describe the retention factor for a single component in chromatography.
- h. Explain how to scale up a separation from a small load to a large load.
- i. Describe the relationship between plate height and band emerging from column.
- j. Describe resolution in terms of average width of peaks and number of plates.
- k. Discuss how relative retention affects chromatographic resolution.
- l. Explain the standard deviation of a diffusing band of solute.
- m. Describe band broadening using the terms in the van Deemter equation.
- n. Discuss band spreading during injection, detection, in connecting tubing, and during passage through the separation column.
- o. Explain the cause of fronting and tailing in chromatography, and how to prevent them.

#### 10. Gas Chromatography

- a. Describe the stationary and mobile phases in gas chromatography.
- b. Explain the resolution from wall-coated, porous and packed columns.
- c. Explain temperature and pressure programming.
- d. Discuss the separation efficiency with respect to hydrogen, helium and nitrogen carrier gases.
- e. Explain split injection, splitless injection and on-column injection and their advantages and disadvantages.
- f. Discuss the use of internal standards in gas chromatography.
- g. Describe thermal conductivity detection, flame ionization detection, electron capture detection.
- h. Discuss the methods in chromatographic development.

#### 11. High-Performance Liquid Chromatography

- a. Describe the stationary and mobile phases in high-performance liquid chromatography (HPLC).
- b. Discuss how the particle size and its polarity affects column efficiency.
- c. Explain the difference between normal-phase and reversed-phase chromatography.
- d. Discuss the polarity of solvent used in HPLC.
- e. Discuss the difference between reversed-phase and hydrophilic interaction columns.
- f. Explain gradient elution process in separation of solutes with different polarities.
- g. Describe the functions of the guard column, pump, oven, and detector in HPLC.
- h. Explain the working principles of ultraviolet detection, refractive index detection, evaporative light scattering detector, electrochemical and fluorescence detectors.

#### Course Content

S/N	Topic	Approx. Lecture Hours
1	<b>Errors and Confidence Interval:</b> Common analytical problems, statistical treatment, accuracy and precision, significant figures, Gaussian distribution, confidence interval, student's <i>t</i> tests and <i>Q</i> test.	3
2	<b>Air Pollution Measurements in Singapore:</b> Pollutants Standards Index (PSI), Air Quality Index (AQI), particles in the atmosphere, PM <sub>2.5</sub> and PM <sub>10</sub> , elemental analysis, platinum and rare earth group elements, local events, haze, enrichment factors and organic pollutants.	2

3A	<b>Introductory Electrochemistry:</b> Fundamentals, ionic strengths, activities and activity coefficients, electrode and cell potentials, the Nernst equation and concentration (activity) dependence.	5
3B	<b>Potentiometry:</b> Chemical sensors, ion-selective electrodes, glass membrane electrodes, liquid junction potentials, inorganic salt membranes, polymer membranes and selectivity coefficients.	3
4A	<b>Molecular Absorption Spectroscopy:</b> Electromagnetic radiation, electronic transitions, Beer-Lambert law and instrumentation.	2
4B	<b>Molecular Fluorescence (Emission) Spectroscopy:</b> Instrumentation, fluorescence and phosphorescence, Stokes shift and quantum yield.	2
4C	<b>Atomic Spectroscopy:</b> Absorption and emission, instrumentation, inductively coupled plasma (ICP), temperature effects and atomic linewidths.	2
5	<b>Extractions:</b> Solvent extractions, efficiency, pH effects, extraction with a metal chelator, transfer agents.	3
6	<b>General Chromatography:</b> Types of chromatography, chromatogram, retention parameters, retention time, partition coefficient, scaling up, resolution, diffusion, plate height, factors affecting resolution, broadening outside the column, plate height equation, longitudinal diffusion, finite equilibration time between phases, multiple flow paths, advantages of open tubular columns, asymmetric peaks.	5
7	<b>Gas Chromatography:</b> Separation process, open tubular columns, common stationary phases, packed columns, retention, temperature and pressure programming, carrier gas, guard columns and retention gaps, sample injection, split injection, splitless injection, on-column injection, detectors, thermal conductivity detector, flame ionization detector, electron capture detector, gas-chromatography-mass spectrometry, sample preparation, method development.	4
8	<b>High-Performance Liquid Chromatography:</b> Chromatographic process, scaling between columns, performance as function of particle diameter, column, stationary phase, elution process, isocratic and gradient elution, hydrophilic interaction chromatography, injection and detection, pumps and injection valves, spectrophotometric detectors, evaporative light-scattering detector, charged aerosol detector, electrochemical detector, refractive index detector, optimization of isocratic retention, pH effects, gradient separations.	4

**Assessment (includes both continuous and summative assessment)**

Component	Course LO Tested	Related Programme LO or Graduate Attributes	Weighting	Team/Individual	Assessment Rubrics
Mid-term Test 1	1-4	Competence and Creativity	20%	Individual	See Appendix 1
Mid-term Test 2	8-10		20%	Individual	
Final Examination	All		60%	Individual	
Total			100%		

### Formative feedback

You will be given feedback in four ways:

1. By response to postings on the course discussion board.
2. Through the marking of the mid-terms.
3. Through one-on-one discussions via appointment with the course instructor
4. General feedback will be provided to the students following the final exam.

### Learning and Teaching approach

Approach	How does this approach support students in achieving the learning outcomes?
Blend of online and face-to-face lectures.	The bulk of the content will be delivered online. This allows (a) extensive use of animations and laboratory videos and (b) use of interactive questions so that students may immediately test their learning. Face to face lectures and experimental demonstrations will be employed for selected topics.

### Reading and References

D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch "Fundamentals of Analytical Chemistry (9th Edition)", Brooks/Cole, Cengage Learning, 2014. ISBN: 9780495558286

Reference textbook: D. C. Harris and C. A. Lucy "Quantitative Chemical Analysis (9th Edition)", W. H. Freeman and Company, 2016. ISBN: 9781319154141

### Course Policies and Student Responsibilities

#### (1) General

You are expected to complete all online activities in good time.

#### (2) Absenteeism

If you miss a lecture, you are expected to make up for the lost learning activities. If you miss one of the mid-term tests with a valid reason and approval (such as a medical certificate), then the total CA will come from the other mid-term test. If you miss both mid-term tests with a valid reason then an additional make-up test will be set to obtain the total CA mark.

### Academic Integrity

Good academic work depends on honesty and ethical behaviour. The quality of your work as a student relies on adhering to the principles of academic integrity and to the NTU Honour Code, a set of values shared by the whole university community. Truth, Trust and Justice are at the core of NTU's shared values.

As a student, it is important that you recognize your responsibilities in understanding and applying the principles of academic integrity in all the work you do at NTU. Not knowing what is involved in maintaining academic integrity does not excuse academic dishonesty. You need to actively equip yourself with strategies to avoid all forms of academic dishonesty, including plagiarism, academic fraud, collusion and cheating. If you are uncertain of the definitions of any of these terms, you should go to the [academic integrity website](#) for more information. Consult your instructor(s) if you need any clarification about the requirements of academic integrity in the course.

### Course Instructors

Instructor	Office Location	Phone	E-mail
Richard WEBSTER	SPMS-CBC-04-06	6316 8793	webster@ntu.edu.sg
Alessandra Bonanni (Dr)	SPMS CBC-04-19	6316 8757	<a href="mailto:a.bonanni@ntu.edu.sg">a.bonanni@ntu.edu.sg</a>

### Planned Weekly Schedule

Week	Topic	Course LO	Readings/ Activities
1	Errors and Statistics	1	Lecture and online
2	Environmental Chemistry	2	Online content
3	Introductory Electrochemistry	3	Online content
4	Introductory Electrochemistry / Chemical sensors	3, 4a to 4c	Online content
5	Chemical sensors	4	Online content
6	Mid-term Test 1 / Molecular Spectrophotometry	5	Lecture and online content
7	Molecular Spectrophotometry / Atomic Spectroscopy	6,7	Online content
8	Extractions	8	Lecture and online
9	General Chromatography	9a to 9g	Lecture and online
10	General Chromatography / Gas Chromatography	9h to 9o, 10a to 10c	Lecture and online
11	Gas Chromatography	10d to 10h	Lecture and online
12	Mid-term Test 2 / High- Performance Liquid Chromatography	11a to 11c	Lecture and online
13	High-Performance Liquid Chromatography	11d to 11i	Lecture and online

The above schedule is for illustrative purposes and is subject to the exigencies of the calendar

## Appendix 1: Assessment Criteria for all components

*Mid-term Test 1 and 2 – MCQ questions (two tests worth 20 marks each).*

<b>Standards</b>		
<b>Fail standard (0-7 marks)</b>	<b>Pass standard (8-15 marks)</b>	<b>High standard (16-20 marks)</b>
Answers to the questions are mostly incorrect.	Answers to the questions are mostly correct.	Answers to the questions are almost always correct.

*Final Examination – short answer questions and calculations (exam worth 60 marks).*

<b>Standards</b>		
<b>Fail standard (0-24 marks)</b>	<b>Pass standard (25-48 marks)</b>	<b>High standard (49 -60 marks)</b>
Answers demonstrate the ability to repeat factual knowledge but not to apply it outside of the lecture context. Answers do not have a strong logical underpinning or maybe attempts to answer both ways at the same time.	Answers to the standard level question are correct and show the ability to apply concepts from the course, but a high level of critical thinking is absent. Answers are reasonably logical, but with gaps.	Answers to all questions show a high and consistent level of critical analysis of the information presented and creative solutions to the problems. Answers are highly logical and demonstrate strong reasoning. Answers are concise and to the point.

## CBC Programme Learning Outcome

The Division of Chemistry and Biological Chemistry (CBC) offers an undergraduate degree major in Chemistry that satisfies the American Chemical Society (ACS) curricular guidelines and equips students with knowledge relevant to the industry. Graduates of the Division of Chemistry and Biological Chemistry should have the following key attributes:

### **1. Competence**

Graduates should be well-versed in the foundational and advanced concepts of chemical science, be able to evaluate chemistry-related information critically and independently, and be able to use complex reasoning to solve emergent chemical problems.

### **2. Creativity**

Graduates should be able to synthesize and integrate multiple ideas across the curriculum, and propose innovative solutions to emergent chemistry-related problems based on their training in chemistry.

### **3. Communication**

Graduates should be able to demonstrate clarity of thought, independent thinking, and sound scientific analysis and reasoning through written and oral reports to audiences with varying technical backgrounds. They should also be able to effectively engage other professional chemists in collaborative endeavours.

### **4. Character**

Graduates should be able to act in responsible ways and uphold the high ethical standards that the society expects of professional chemists.

### **5. Civic-mindedness**

Graduates should be aware of the impact of chemistry on society, and how chemistry can be applied to benefit mankind. They should also be aware of and uphold the best chemical safety practices.