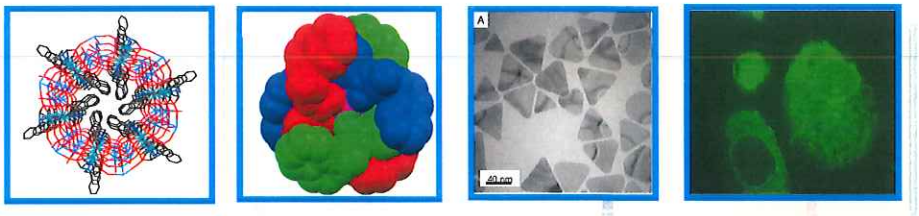
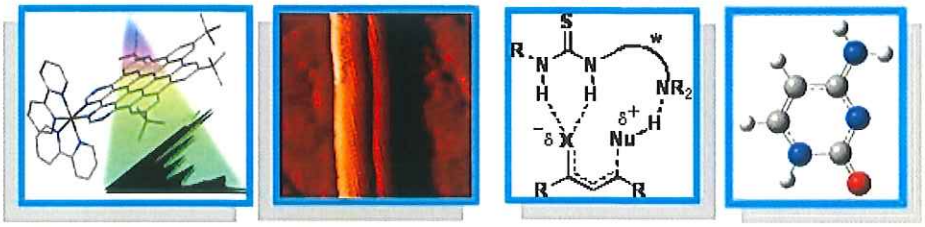
School of Chemistry
Trinity College Dublin

JUNIOR SOPHISTER COURSE BOOKLET FOR MODERATORSHIP IN:

Chemistry,
Medicinal Chemistry
and
Chemistry with Molecular Modelling

2014/2015





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The JS webpage can be found on the School of Chemistry's website at:
http://www.chemistry.tcd.ie/undergraduate/chemistry/js/

Information for all JS Chemistry Students

Junior Sophister 2014/15

Welcome back to the School of Chemistry for your JS year. We hope you have a wonderful experience in a year that is quite a transition from the earlier JF and SF years. The JS and SS years bring about more in-depth chemistry education than you have experienced before, with greater emphasis on theoretical as well as practical education and training. We wish you all the best for this academic year and the staff of the School of Chemistry look forward to working with you. **This year's Course Advisor is Prof. Rachel Evans**.

Introduction to Chemistry at TCD

Chemistry holds a key position among the sciences. It is the study of matter, that is, the composition, structure and properties of substances and the changes they undergo. Life on Earth owes its origin to a series of these chemical changes. Formal chemistry teaching in TCD commenced in August 1711 as part of the new School of Medicine. The main building includes two lecture theatres and four recently refurbished research laboratories. A new suite of teaching laboratories (the Cocker laboratories) was completed in September 1997 and provides facilities for the teaching of preparative inorganic and organic chemistry. The Sami Nasr Institute for Advanced Materials (SNIAM), which was completed in 2000, provides *ca*. 1500 m^2 of accommodation for the School of Chemistry. This includes a Physical Chemistry teaching laboratory and six research laboratories to house *ca*. 40 researchers. This institute also houses the School of Physics. Computational Chemistry research is housed in the Lloyd Institute on a multidisciplinary computational-science floor comprising researchers from Mathematics, Physics, Chemistry and High Performance Computing. In addition, chemists play an important role in interdisciplinary research taking place in two of TCD's newest research institutes: (i) the Nanoscience Institute – The Centre for Research on Adaptive Nanostructures and Nanodevices (CRANN), which was formally opened in January 2008 and (ii) the Trinity Biomedical Sciences Institute (TBSI), which was inaugurated in July 2011.

Moderatorship in Chemistry

The School of Chemistry currently offers four Moderatorships, namely Chemistry, Medicinal Chemistry, Chemistry with Molecular Modelling (CMM), and Nanoscience, Physics and Chemistry of Advanced Materials (NPCAM), which is a joint course offered by the Schools of Physics and Chemistry. All of these courses with the exception of Chemistry have been developed in response to changes in the modern subject and identified needs for graduates with special skills in Ireland.

Staff, Research and Facilities

The School currently has 20 academic staff and 15 technical staff. The School has an active research programme, with approximately 130 postgraduate students and postdoctoral researchers. They study a range of subjects such as organic, inorganic, organometallic, physical, theoretical, medicinal, analytical, material, polymer, environmental, and supramolecular chemistry. Research income is earned from

national, international and commercial sources and the School has held grants in all relevant research programmes funded by the EU.

The College also fosters an interdisciplinary approach to research, with members of the School having strong links with colleagues in the physical, technological and biological sciences both within College, nationally and internationally.

The school is well equipped for its research activities, having an Agilent 800 MHz, and Bruker 600 and 400 MHz high-field multi-nuclear NMR, FTIR, dispersive IR and UV-visible spectrometers, high performance liquid (HPLC) and gas (GC) chromatography equipment, a Rigaku Saturn 724 Diffractometer and Bruker SMART APEX single crystal and Siemens D500 powder diffractometers, Micromass LCT^{TM} (TOF) mass spectrometer, thermogravimetric analysis and differential scanning calorimetry, dynamic light scattering, several spectrofluorimeters for steady-state and time-resolved fluorescence measurements, circular and linear dichroism, and a large range of wave generators and potentiostats for cyclic voltammetry.

Module exam structure

Each taught module is worth 5 ECTS and is examined by four questions split into two sections, of which, two must be answered, one from each section.

Lectures

Lectures should begin on the hour and end ten minutes to the hour. Timetables will be published through my.tcd.ie. These should be checked regularly for changes to the original schedule. Attendance at lectures is recorded. All lectures are complemented by tutorials. Attendance at tutorials will be recorded.

Practicals

In the JS year, practical classes take place over one-and-a-half days. In **Semester 1** there are 7 weeks of organic chemistry and 4 weeks of inorganic chemistry in the Cocker lab; in **Semester 2**, there are 3 weeks of inorganic chemistry in the Cocker lab and 7 weeks of physical chemistry in the SNIAM building. Practical work is assessed in-course, and amounts to a total of 15 ECTS.

Attendance at chemistry practical classes is compulsory for students in all years. Students may be deemed non-satisfactory if they miss more than a third of their course of study or fail to submit a third of the required course work in any semester.

Examinations

Your attention is drawn to the Science examination regulations which prescribe the level of performance you must achieve in order to be permitted to proceed to the Senior Sophister year. A bare pass in the examination is not sufficient. Full details of the Junior Sophister Science (TR071) examination regulations may be found at the end of this booklet.

Prizes

The Dr. George A. Lonergan prize, value €381, is awarded annually to the student who gives the best performance in the Junior Sophister year, provided sufficient merit is shown.

JS Contribution to Final degree mark

The JS Chemistry mark makes up **35%** of the final degree mark.

Senior Sophister year

Semester 1 of the Senior Sophister year is spent working full-time on a research project in TCD, in industry or at a university abroad. The School encourages interested students to go abroad if they wish to do so. Prof. Eoin Scanlan will coordinate these projects and arrangements are made during the JS year.

Careers

Since some students will be away from College during the first semester of the SS year, it is desirable that you make contact with the Careers Office in the JS year. Sarah Ryan, Careers Advisor, will be glad to get your names on her files and will visit the School to explain what the Careers Office can do for you.

Career prospects in Chemistry are good, although you should realise that a primary degree may not be enough to gain immediate employment in research and development; an additional qualification, such as a diploma or higher degree, will be useful.

In addition, the School of Chemistry (in conjunction with the Royal Society of Chemistry) hosts an annual Chemistry Careers event for the Sophister/postgraduate students, in which representatives from national and international employers of chemistry graduates discuss different career pathways.

Library

Much of your regular reading will depend on textbooks in the Hamilton Library. In addition, many of the research journals, collections of data and Chemical Abstracts are now available on-line *via* the Library's website.

Seminars and Special Lectures

You are expected to attend the School's research seminars, which are held at noon on Thursdays. During the year, lectures on various topics will be arranged by the School, the Werner Chemical Society, the Royal Society of Chemistry or the Institute of Chemistry of Ireland. You will find many of them interesting and valuable. Attendance at these lectures is recorded.

School of Chemistry: Scheme for marking of examination answers in Sophister years

Mark Range	Criteria
90-100	IDEAL ANSWER; showing insight and originality and wide knowledge. Logical, accurate and concise presentation. Evidence of reading and thought beyond course content. Contains particularly apt examples. Links materials from lectures, practicals and seminars where appropriate.
80-89	OUTSTANDING ANSWER; falls short of the 'ideal' answer either on aspects of presentation or on evidence of reading and thought beyond the course. Examples, layout and details are all sound.
70-79	MAINLY OUTSTANDING ANSWER; falls short on presentation and reading or thought beyond the course, but retains insight and originality typical of first class work.
65-69	VERY COMPREHENSIVE ANSWER; good understanding of concepts supported by broad knowledge of subject. Notable for synthesis of information rather than originality. Sometimes with evidence of outside reading. Mostly accurate and logical with appropriate examples. Occasionally a lapse in detail.
60-64	LESS COMPREHENSIVE ANSWER; mostly confined to good recall of coursework. Some synthesis of information or ideas. Accurate and logical within a limited scope. Some lapses in detail tolerated.
55-59	SOUND BUT INCOMPLETE ANSWER; based on coursework alone but suffers from a significant omission, error or misunderstanding. Usually lacks synthesis of information or ideas. Mainly logical and accurate within its limited scope and with lapses in detail.
50-54	INCOMPLETE ANSWER; suffers from significant omissions, errors and misunderstandings, but still with understanding of main concepts and showing sound knowledge. Several lapses in detail.
45-49	WEAK ANSWER; limited understanding and knowledge of subject. Serious omissions, errors and misunderstandings, so that answer is no more than adequate.
40-44	VERY WEAK ANSWER; a poor answer, lacking substance but giving some relevant information. Information given may not be in context or well explained, but will contain passages and words that indicate a marginally adequate understanding.
35-39	MARGINAL FAIL; inadequate answer, with no substance or understanding, but with a vague knowledge relevant to the question.
30-34	CLEAR FAILURE; some attempt made to write something relevant to the question. Errors serious but not absurd. Could also be a sound answer to the misinterpretation of a question.
0-29	UTTER FAILURE; with little hint of knowledge and serious errors. Could also be a trivial response to the misinterpretation of a question.

Schedule of Grades	
I	= 70%+
II-1	= 60-69%
II-2	= 50-59%
III	= 40-49%
F-1	= 30-39%
F-2	= 0-29%

Important additional information for all JS-Chemistry Students

DESCRIPTION OF THE EUROPEAN CREDIT TRANSFER SYSTEM (ECTS)

The European Credit Transfer and Accumulation System (ECTS) is an academic credit system based on the estimated student workload required to achieve the objectives of a module or programme of study. It is designed to enable academic recognition for periods of study, to facilitate student mobility and credit accumulation and transfer. The ECTS is the recommended credit system for higher education in Ireland and across the European Higher Education Area.

The ECTS weighting for a module is a **measure of the student input or workload** required for that module, based on factors such as the number of contact hours, the number and length of written or verbally presented assessment exercises, class preparation and private study time, laboratory classes, examinations, clinical attendance, professional training placements, and so on as appropriate. There is no intrinsic relationship between the credit volume of a module and its level of difficulty.

The European **norm for full-time study over one academic year is 60 ECTS**. The Trinity academic year is 40 weeks from the start of Michaelmas Term to the end of the annual examination period 1 ECTS credit represents 20-25 hours estimated student input, so a 10-credit module will be designed to require 200-250 hours of student input including class contact time and assessments.

ECTS credits are awarded to a student only upon successful completion of the course year. Progression from one year to the next is determined by the course regulations. Students who fail a year of their course will not obtain credit for that year even if they have passed certain component courses. Exceptions to this rule are one-year and part-year visiting students, who are awarded credit for individual modules successfully completed.

COLLEGE REGULATION REGARDING PLAGIARISM:
EXTRACT FROM THE COLLEGE CALENDAR 2014-2015

Plagiarism

82 Plagiarism is interpreted by the University as the act of presenting the work of others as one's own work, without acknowledgement.

Plagiarism is considered as academically fraudulent, and an offence against University discipline. The University considers plagiarism to be a major offence, and subject to the disciplinary procedures of the University.

83 Plagiarism can arise from deliberate actions and also through careless thinking and/or methodology. The offence lies not in the attitude or intention of the perpetrator, but in the action and in its consequences.

Plagiarism can arise from actions such as:

(a) copying another student's work;

(b) enlisting another person or persons to complete an assignment on the student's behalf;

(c) quoting directly, without acknowledgement, from books, articles or other sources, either in printed, recorded or electronic format;

(d) paraphrasing, without acknowledgement, the writings of other authors.

Examples (c) and (d) in particular can arise through careless thinking and/or methodology where students:

(i) fail to distinguish between their own ideas and those of others;

(ii) fail to take proper notes during preliminary research and therefore lose track of the sources from which the notes were drawn;

(iii) fail to distinguish between information which needs no acknowledgement because it is firmly in the public domain, and information which might be widely known, but which nevertheless requires some sort of acknowledgement;

(iv) come across a distinctive methodology or idea and fail to record its source.

All the above serve only as examples and are not exhaustive.

Students should submit work done in co-operation with other students only when it is done with the full knowledge and permission of the lecturer concerned. Without this, work submitted which is the product of collusion with other students may be considered to be plagiarism.

84 It is clearly understood that all members of the academic community use and build on the work of others. It is commonly accepted also, however, that we build on the work of others in an open and explicit manner, and with due acknowledgement. Many cases of plagiarism that arise could be avoided by following some simple guidelines:

(i) Any material used in a piece of work, of any form, that is not the original thought of the author should be fully referenced in the work and attributed to its source. The material should either be quoted directly or paraphrased. Either way, an explicit citation of the work referred to should be provided, in the text, in a footnote, or both. Not to do so is to commit plagiarism.

(ii) When taking notes from any source it is very important to record the precise words or ideas that are being used and their precise sources.

(iii) While the Internet often offers a wider range of possibilities for researching particular themes, it also requires particular attention to be paid to the distinction between one's own work and the work of others. Particular care should be taken to keep track of the source of the electronic information obtained from the Internet or other electronic sources and ensure that it is explicitly and correctly acknowledged.

85 It is the responsibility of the author of any work to ensure that he/she does not commit plagiarism.

86 Students should ensure the integrity of their work by seeking advice from their lecturers, tutor or supervisor on avoiding plagiarism. All schools and departments should include, in their handbooks or other literature given to students, advice on the appropriate methodology for the kind of work that students will be expected to undertake.

87 If plagiarism as referred to in §82 above is suspected, in the first instance, the head of school, or designate, will write to the student, and the student's tutor advising them of the concerns raised and inviting them to attend an informal meeting with the head of school, or designate, (The director of teaching and learning (undergraduate) may also attend the meeting as appropriate. As an alternative to their tutor, students may nominate a representative from the Students' Union to accompany them to the meeting) and the lecturer concerned, in order to put their suspicions to the student and give the student the opportunity to respond. The student will be requested to respond in writing stating his/her agreement to attend such a meeting and confirming on which of the suggested dates and times it will be possible for the student to attend. If the student does not in this manner agree to attend such a meeting, the head of school, or designate, may refer the case directly to the Junior Dean, who will interview the student and may implement the procedures as referred to under Conduct and College Regulations §2.

88 If the head of school, or designate, forms the view that plagiarism has taken place, he/she must decide if the offence can be dealt with under the summary procedure set out below. In order for this summary procedure to be followed, all parties attending the informal meeting as noted in §87 above must state their agreement in writing to the head of school, or designate. If the facts of the case are in dispute, or if the head of school, or designate, feels that the penalties provided for under the summary procedure below are inappropriate given the circumstances of the case, he/she will refer the case directly to the Junior Dean, who will interview the student and may implement the procedures as referred to under Conduct and College Regulations §2.

89 If the offence can be dealt with under the summary procedure, the head of school, or designate, will recommend to the Senior Lecturer one of the following penalties:

(a) that the piece of work in question receives a reduced mark, or a mark of zero; or

(b) if satisfactory completion of the piece of work is deemed essential for the student to rise with his/her year or to proceed to the award of a degree, the student may be required to re-submit the work. However the student may not receive more than the minimum pass mark applicable to the piece of work on satisfactory re-submission.

90 Provided that the appropriate procedure has been followed and all parties in §87 above are in agreement with the proposed penalty, the Senior Lecturer may approve the penalty and notify the Junior Dean accordingly. The Junior Dean may nevertheless implement the procedures as referred to under Conduct and College Regulations §2.

Part II College Calendar 2014-2015, Conduct and Regulations

While every effort will be made to give due notice of major changes, the School of Chemistry and Science Course Office reserve the right to suspend, alter or initiate modules, timetables, examinations and regulations at any time.

JS-MODERATORSHIP IN CHEMISTRY

This academic year will be based on the following 60 ECTS:
Core Modules: 40 ECTS
Practical Course: 15 ECTS
Optional Module or Broad Curriculum: 5 ECTS

Examination: Each module is examined by four questions split into two sections, of which, one question from each section must be answered.

Year Coordinator: Prof. Rachel Evans (raevans@tcd.ie; 896 4215)

Core Modules:

Semester 1 (11 weeks)	Semester 2 (11 weeks)
Inorganic Chemistry I CH3103: Organometallics & Coordination Chemistry (5 ECTS) Transition metal organometallics (11L) Transition metal compounds and complexes (11L) Homogeneous catalysis (11L)	**Inorganic Chemistry II** CH3104: Solid State Materials (5 ECTS) Inorganic polymers (11L) Structural inorganic chemistry (7L) Characterisation techniques of solid state materials (9L) Surface science (6L)
Organic Chemistry I CH3203: Synthetic Organic Chemistry I (5 ECTS) Organometallic C-C couplings (9L) Pericyclic reactions, FMO theory & stereoelectronic effects (15L) Physical organic chemistry (9L)	**Organic Chemistry II** CH3204: Synthetic Organic Chemistry II (5 ECTS) Heterocyclic chemistry (9L) Organoheteroatom chemistry (15L) FGI and retrosynthesis (9L)
Physical Chemistry I CH3303: Quantum Mechanical Concepts in Physical Chemistry (5 ECTS) Quantum mechanics (15L) Spectroscopy (9L) Group theory (9L)	**Physical Chemistry II** CH3304: Molecular Thermodynamics and Kinetics (5 ECTS) Molecular thermodynamics & statistical mechanics (15L) Electrochemistry (9L) & Kinetics (9L)
Interdisciplinary Module I CH3403: Analytical Methods (5 ECTS) Analytical chemistry (11L) Organic spectroscopy (11L) Structural methods in inorg. chem. (11L)	**Interdisciplinary Module II** CH3404: Biomaterials and Macromolecules (5 ECTS) Bioorganic chemistry & natural products (11L) Bioinorganic chemistry (11L) Soft matter (11L)
CH3080 Practical Chemistry (15 ECTS) This is a laboratory module broadening the student's knowledge of Physical, Organic and Inorganic Chemistry	

Optional Modules:

CH3441 - Medicinal Chemistry (5 ECTS)
This module covers fundamental medicinal chemistry. It encompasses an introduction to medicinal chemistry, antiviral and anticancer chemistry, and the computational method QSAR.

OR

CH3601 - Computational Chemistry (5 ECTS)
This module covers numerical methods – optimisation, introduction to static and dynamic atomistic simulation, and computational molecular Quantum Chemistry.

OR

CH3602 - Quantitative Methods for Chemists (5 ECTS)
This module encompasses courses on Unix/Linux, Fortran 77 and Fortran 90+. This material is assessed during the year (no end-of-year examination).

OR

Broad Curriculum (5 ECTS; http://www.tcd.ie/Broad_Curriculum/). Please note that you can obtain a registration form for the Broad Curriculum modules from the School Office. If choosing a Broad Curriculum module, you must inform the School Office of the module(s) you are taking.

JS - MODERATORSHIP IN MEDICINAL CHEMISTRY

This academic year will be based on the following 60 ECTS:
Core Modules: 45 ECTS
Practical Course: 15 ECTS
Examination: Each module is examined by four questions split into two sections, of which, one question from each section must be answered.
Course Director: Prof. Mike Southern (southerj@tcd.ie; 896 3411)

Core Modules:

Semester 1 (11 weeks)	Semester 2 (11 weeks)
Inorganic Chemistry I CH3103: Organometallics & Coordination Chemistry (5 ECTS) Transition metal organometallics (11L) Transition metal compounds and complexes (11L) Homogeneous catalysis (11L)	**Physical Chemistry II** CH3304: Molecular Thermodynamics and Kinetics (5 ECTS) Thermodynamics & statistical mechanics (15L) Electrochemistry (9L) Kinetics (9L)
Organic Chemistry I CH3203: Synthetic Organic Chemistry I (5 ECTS) Organometallic C-C couplings (9L) Pericyclic reactions, FMO theory & stereoelectronic effects (15L) Physical organic chemistry (9L)	**Organic Chemistry II** CH3204: Synthetic Organic Chemistry II (5 ECTS) Heterocyclic chemistry (9L) Organoheteroatom chemistry (15L) FGI and retrosynthesis (9L)
Interdisciplinary Module I CH3403: Analytical Methods (5 ECTS) Analytical chemistry (11L) Organic spectroscopy (11L) Structural methods in inorganic chemistry (11L)	**Interdisciplinary Module II** CH3404: Biomaterials and Macromolecules (5 ECTS) Bioorganic chemistry & natural products (11L) Bioinorganic chemistry (11L) Soft matter (11L)
Medicinal Chemistry I - CH3441: Introduction to Medicinal Chemistry (5 ECTS) Introduction to medicinal chemistry (15L) Antiviral, anticancer chemistry and QSAR (18L).	
Medicinal Chemistry II - CH3446: Microbiology and Medicinal Chemistry (5 ECTS) Antimicrobial agents (12L) Anti-infective agents (10L) Antimalarial and industrial medical chemistry (11L) (by partial continuous assessment).	
Medicinal Chemistry III - CH3447: Biochemistry and Pharmacology (5 ECTS) Protein structure, function, activity and regulation (15L) Receptors, drugs and the autonomic nervous system (9L) & Steroids (9L)	
CH3080 Practical Chemistry (15 ECTS) This is a laboratory module broadening the student's knowledge in Physical, Organic and Inorganic Chemistry.	

JS-MODERATORSHIP IN CHEMISTRY WITH MOLECULAR MODELLING

This academic year will be based on the following 60 ECTS:
Core Modules: 45 ECTS
Practical Course: 15 ECTS
Examination: Each module is examined by four questions split into two sections of which you must answer one from each section.
Course Director: Prof. Graeme Watson (watsong@tcd.ie; 896 1357)

Core Modules:

Semester 1 (11 weeks)	Semester 2 (11 weeks)
Inorganic Chemistry I CH3103: Organometallics & Coordination Chemistry (5 ECTS) Transition metal organometallics (11L) Transition metal compounds and complexes (11L) Homogeneous catalysis (11L)	**Inorganic Chemistry II** CH3104: Solid State Materials (5 ECTS) Inorganic polymers (11L) Structural inorganic chemistry (7L) Characterisation techniques of solid state materials (9L) Surface science (6L)
Organic Chemistry I CH3203: Synthetic Organic Chemistry I (5 ECTS) Organometallic C-C couplings (9L) Pericyclic reactions, FMO theory & stereoelectronic effects (15L) Physical organic chemistry (9L)	**Organic Chemistry II** CH3204: Synthetic Organic Chemistry II (5 ECTS) Heterocyclic chemistry (9L) Organoheteroatom chemistry (15L) FGI and retrosynthesis (9L)
Physical Chemistry I CH3303: Quantum Mechanical Concepts in Physical Chemistry (5 ECTS) Quantum mechanics (15L) Spectroscopy (9L) Group theory (9L)	**Physical Chemistry II** CH3304: Molecular Thermodynamics and Kinetics (5 ECTS) Thermodynamics & statistical mechanics (15L) Electrochemistry (9L) Kinetics (9L)
Interdisciplinary Module I CH3403: Analytical Methods (5 ECTS) Analytical chemistry (11L) Organic spectroscopy (11L) Structural methods in inorganic chem. (11L)	**Computational Chemistry I** CH3601: Computational Chemistry (5 ECTS) Numerical methods – optimisation static and dynamic atomistic simulation Computational molecular quantum chemistry
CH3602: Computational Chemistry II (5 ECTS) This module encompasses courses on Unix/Linux, Fortran 77 and Fortran 90+. This material is assessed during the year (no end-of-year examination).	
CH3080: Practical Chemistry (15 ECTS) This is a laboratory module broadening the student's knowledge of Physical, Organic, and Inorganic Chemistry, and of molecular modelling (~40%).	

End of year examinations

R = MODERATORSHIP IN CHEMISTRY
M = MODERATORSHIP IN MEDICINAL CHEMISTRY
C = MODERATORSHIP IN CHEMISTRY WITH MOLECULAR MODELLING
O = OPTIONS

JS Chemistry Exam 1

Module CH3103: Organometallics & Coordination Chemistry (R, C, M)

Module CH3104: Solid State Materials (R, C)

Module CH3446: Microbiology and Medicinal Chemistry (M)

JS Chemistry Exam 2

Module CH3203: Synthetic Organic Chemistry I (R, M, C)

Module CH3204: Synthetic Organic Chemistry II (R, M, C)

JS Chemistry Exam 3

Module CH3303: Quantum Mechanical Concepts (R, C)

Module CH3304: Molecular Thermodynamics and Kinetics (R, C, M)

Module CH3447: Biochemistry and Pharmacology (M)

JS Chemistry Exam 4

Module CH3403: Analytical Methods (R, C, M)

Module CH3404: Biomaterials and Macromolecules (R, M)

JS Chemistry Exam 5

Module CH3441: Medicinal Chemistry (M, O)

Module CH3601: Computational Chemistry (C, O)