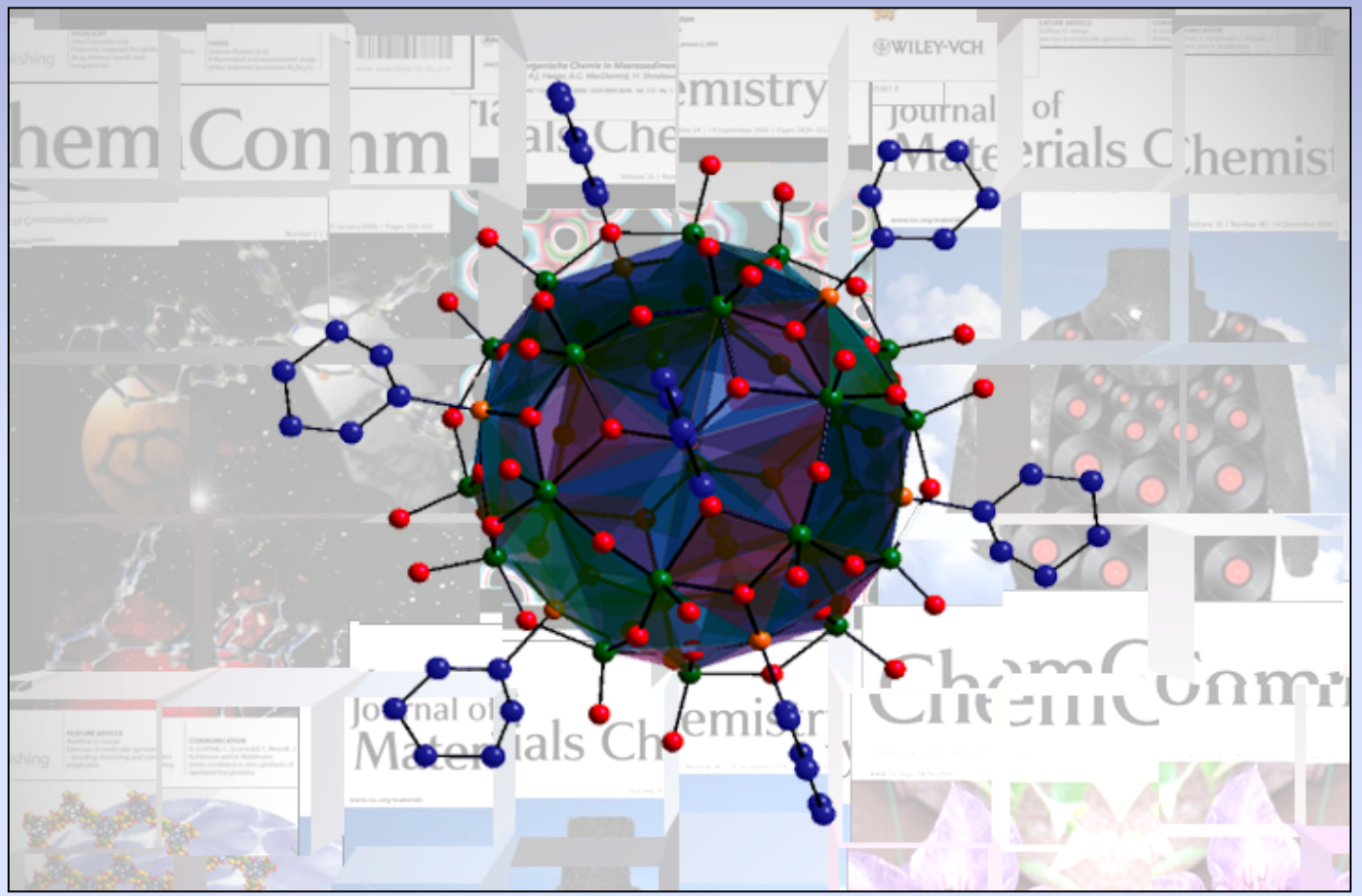
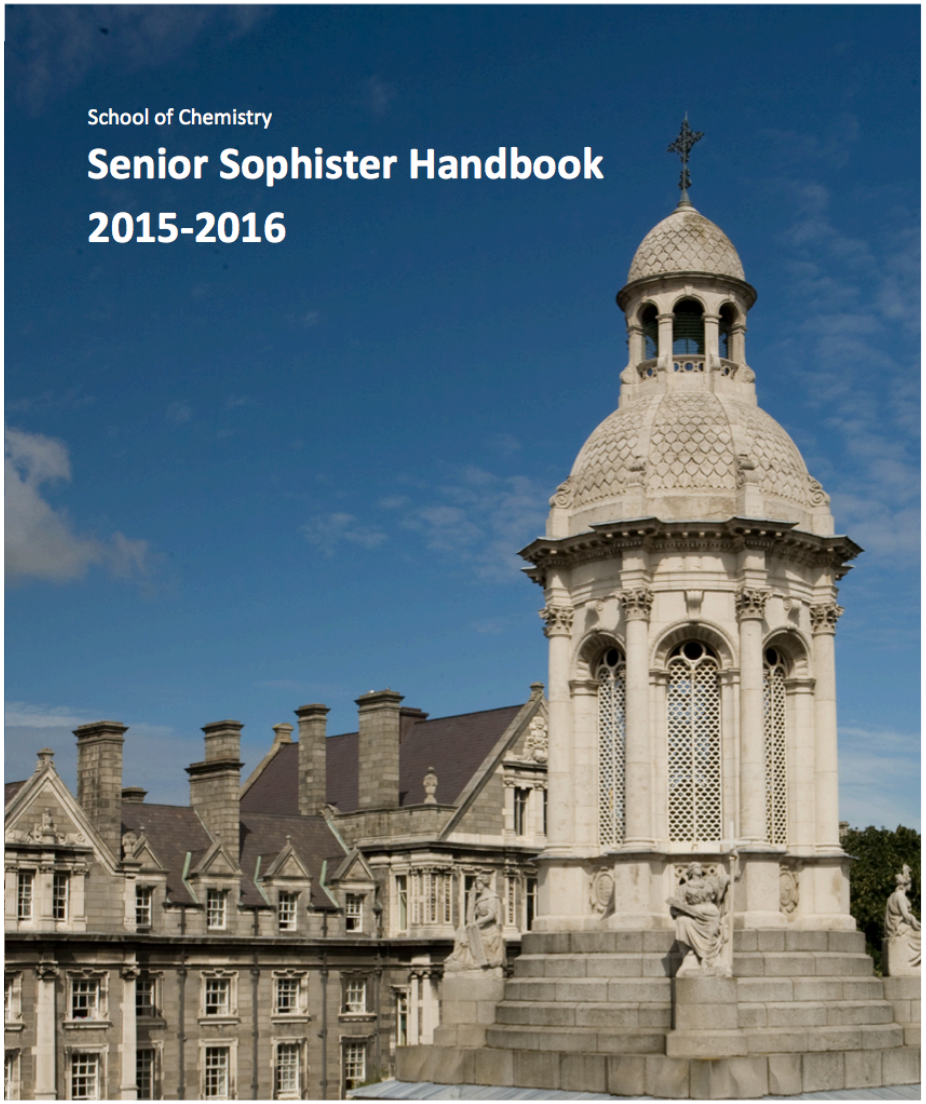
Trinity College Dublin – School of Chemistry



Senior Sophister 2015-2016

Trinity College Dublin
Coláiste na Tríonóide, Baile Átha Cliath
The University of Dublin

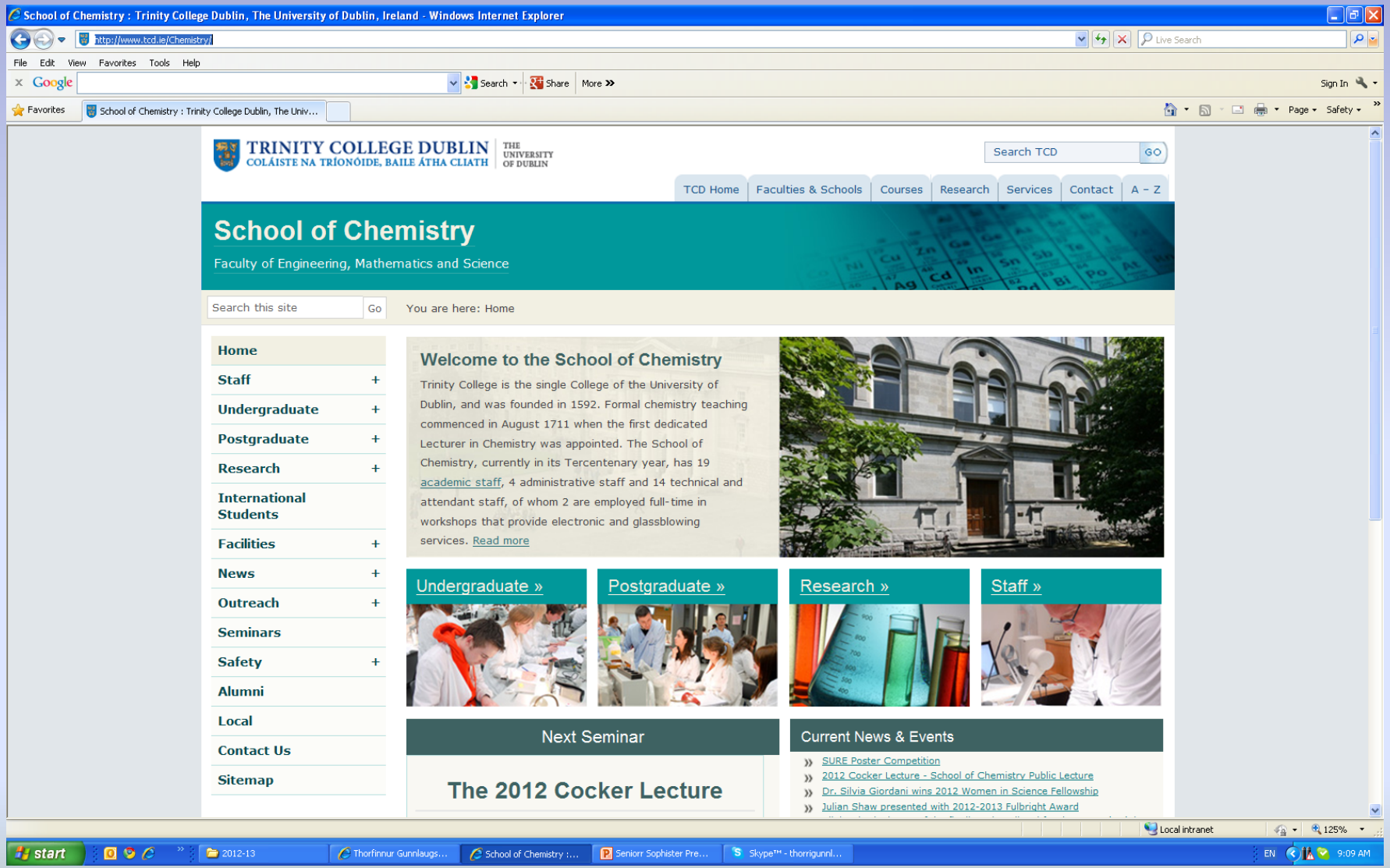


School of Chemistry

Senior Sophister Handbook

2015-2016

Trinity College Dublin – School of Chemistry



Trinity College Dublin – School of Chemistry

School of Chemistry
Trinity College Dublin

Research Project (20 credits) – Important Dates

Start of the Project: **September 14 th 2015**

Duration: 12 weeks (teaching week 8)
Safety workshop 15th of September

Electronic Submission of Report: **16.30 on 4th December 2015**

In an attempt to create a fair evaluation method and to keep with college guidelines on plagiarism it has been decided to make use of the software "**TurnItIn**" provided by CAPSL for electronic report submission. Details and guidance on how to use this software will be sent out to you later.

Submission of 2 hard Copies : **4.30 on Monday 7th December 2015.**

Make sure you have shown your supervisor your 'final copy' by 20th of November

Examination: **The week of 14-18th of December 2015**

Research Project – Structure of the Report

Discuss the structure and content of the report with your supervisor.

- The report must be typed with **font size 12**, **1.5-2 line spaced**, bound, and **not longer than 30 pages** in length.

- Your laboratory notebooks together with appendices of spectra *etc*. if appropriate must also be handed in at this time.

- It is crucial that you allow sufficient time for the completion of your report. NB. *Your supervisor must receive a draft copy of your report* ***by November 20th 2015 (Friday)***. **Discuss the writing with him/her! Know what is expected of you…..**

Again….All students should submit their final project report electronically by no later than 16:30 on Friday 4 December 2015. Two hard copies of the identical report should be handed in to the School Office by no later than 16:30 on Monday 7 December 2015.

15 September: Safety workshop

Research Project – Assessment

Project Assessment: Your project work will be assessed by:
three examiners:

Supervisor: will submit a written report on the work conducted.

Two other assessors: will mark the project report and conduct a formal assessment involving a **10 min. presentation** by the student followed by a **question & answer session in which the work and underlying theoretical concepts will be discussed**.

Dates for presentations: between **Monday 14th December and Friday 18th December 2015.** You have to be here that week!

Marks for your project contribute **33% to your SS year mark** (20 credits for project), and will be allotted on the basis of **quality of content**, **presentation**, **effort made**, and **performance** during the oral examination….

SCHOOL OF CHEMISTRY, TCD

REPORT ON FINAL YEAR PROJECT
SENIOR SOPHISTER 2013-2014
EXAMINER FORM

Name of student:

Name of Examiner:

Place where project was carried out:

Title of Thesis:

Comments on Thesis:

Style, appearance, structure and English usage. Organisation of data/results - *max 15*

Clarity of introduction – originality and appropriateness of references and setting the project in context - *max 15*

Results and discussion - *max 25*

Conclusions, suggestions for future work - *max 5*

Comments on presentation and Viva Voce examination* - *max 40

(Please refer to the Guidelines and add comments to justify the mark given)

	Examiner
The Thesis	
Style, appearance, structure and English usage. Organisation of data/results - *max 15*	
Clarity of introduction – originality and appropriateness of references and setting the project in context - *max 15*	
Results and discussion *max 25*	
Conclusions, suggestions for future work - *max 5*	
Presentation and Viva Voce examination	
Presentation of results, thesis defence and general knowledge - *max 40*	
Final Mark	

Signature (Examiner): …….…… Date: ……

Research Project – Structure of the Report

1. Introduction and Objectives of the Project: Identifies the scientific aims of the project and set this in context with other current and recent work.

2. Results and Discussion: The experiments conducted and results are set out and described. Results should be discussed and set in context with the recent literature so that their significance is evident. A clear story should be developed so that the reader is lead through the project, understanding why experiments were performed and the relevance of the results at each stage. The R&D section should lead on from the introduction, and into the conclusion, building on ideas from the introduction and clearly highlighting key results for the conclusion.

3/4. Experimental Sections/Materials and Methods: Experimental work should be described so that the experiments and results can be reproduced by other researchers. Appropriate characterisations and analyses need to be provided in order to provide evidence for the claims in the R&D section.

3/4. Conclusions and Future Work: The conclusions should be fully supported by the results. The conclusions should be discussed and set in the context of current and recent literature. The conclusions should be used to suggest a series of experiments highly likely to lead to further useful results which extend the current study into new and important areas.

5. References: related work and underlying concepts should be referenced; the references should obey the format of a recognised scientific journal (format of *Angewandte Chemie*, *J. Am. Chem. Soc.*, (ACS) *Chem. Commun*. (RSC) and etc.

3. Experimental Sections/Materials and Methods:

5. Procedure

This section is written in the 3rd person past passive voice and is a *concise* summary of what you did. It should contain the *actual procedure* you carried out in the course of the experiment, not the one written in the manual, which you will need to note in the lab as you go along. It should include any modifications you had to make to the method or reagents written in the manual, and your observations, for example of solution colours, the evolution of heat or gas etc. It is never written as a series of numbered points.

e.g. A solution of $CrCl_3.6H_2O$ (10.0 g, 0.038 mol) in HCl (40ml, 5:3 *conc*.HCl:H_2O) was added to granulated zinc (10.0 g, 0.153 mol) under a nitrogen atmosphere and the solution was allowed to stand for 2 h until a pale blue colour was observed.

Note – the formula or IUPAC name of each reagent is written out along with the number of grams and number of moles this corresponds to.

For further examples of this style, look in a synthetic paper of a chemical journal, for example the Journal of Inorganic Chemistry.

IR spectroscopy

List the major peaks, labelling them as strong (s), medium (m) or weak (w). Assign any peaks which are important in identifying the product. Note: IR data are quoted to the nearest whole number.

e.g. IR (KBr disk) $\bar{\nu}$/cm^{-1} 3413 m (H_2O), 3000 m (CH_{Ph}), 2014 w (RuH), 1921 s (C≡O), 1305 s, 1153 m, 1078 s (CH def), 740 m.

UV-vis spectroscopy

The wavelength and usually the extinction coefficient must be listed for each peak in the spectrum (sh = shoulder). The extinction coefficient can be calculated using the Beer-Lambert law ($A = \varepsilon\ c\ l$). Some maxima are not automatically labelled by the machine. Since these usually turn out to be the most interesting ones, it is usually worth magnifying and labelling these absorptions.

e.g. UV-vis λ_{max} / nm (ε_{max} / dm^3 mol^{-1} cm^{-1}) 275 (30 000), 410 (850)

NMR spectroscopy

It is important to include the nucleus (e.g. ^{1}H, ^{13}C, ^{31}P), the frequency of the spectrometer (e.g. 250 MHz, 400 MHz), the solvent (e.g. $CDCl_3$, D_2O) and the identity of the signal if it is known. The order of the signals is from high to low field, *ie.* from large to small ppm. For proton spectra, the number of protons (the signal integration), the peak multiplicity, the coupling constant *J in Hertz* are also included. Peak multiplicities are described as s = singlet, d = doublet, t = triplet, dd = doublet of doublets, dt = doublet of triplets, m = multiplet. Remember that for proton signals the coupling constant is the interval between peaks in ppm multiplied by the frequency of the field in MHz.

e.g. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31-7.02 (45 H, m, H^{Ph}), -7.15 (H, dt, $J_{HP(trans)}$ 105.4 Hz, $J_{HP(cis)}$ 24.9 Hz, H^{H^-}).

or as a table:

δ (ppm)	multiplicity	integration	*J* (Hz)	signal
7.31-7.02	m	45 H		Phenyl Hs
-7.15	dt	1 H	105.4 *trans* 24.9 *cis*	hydride

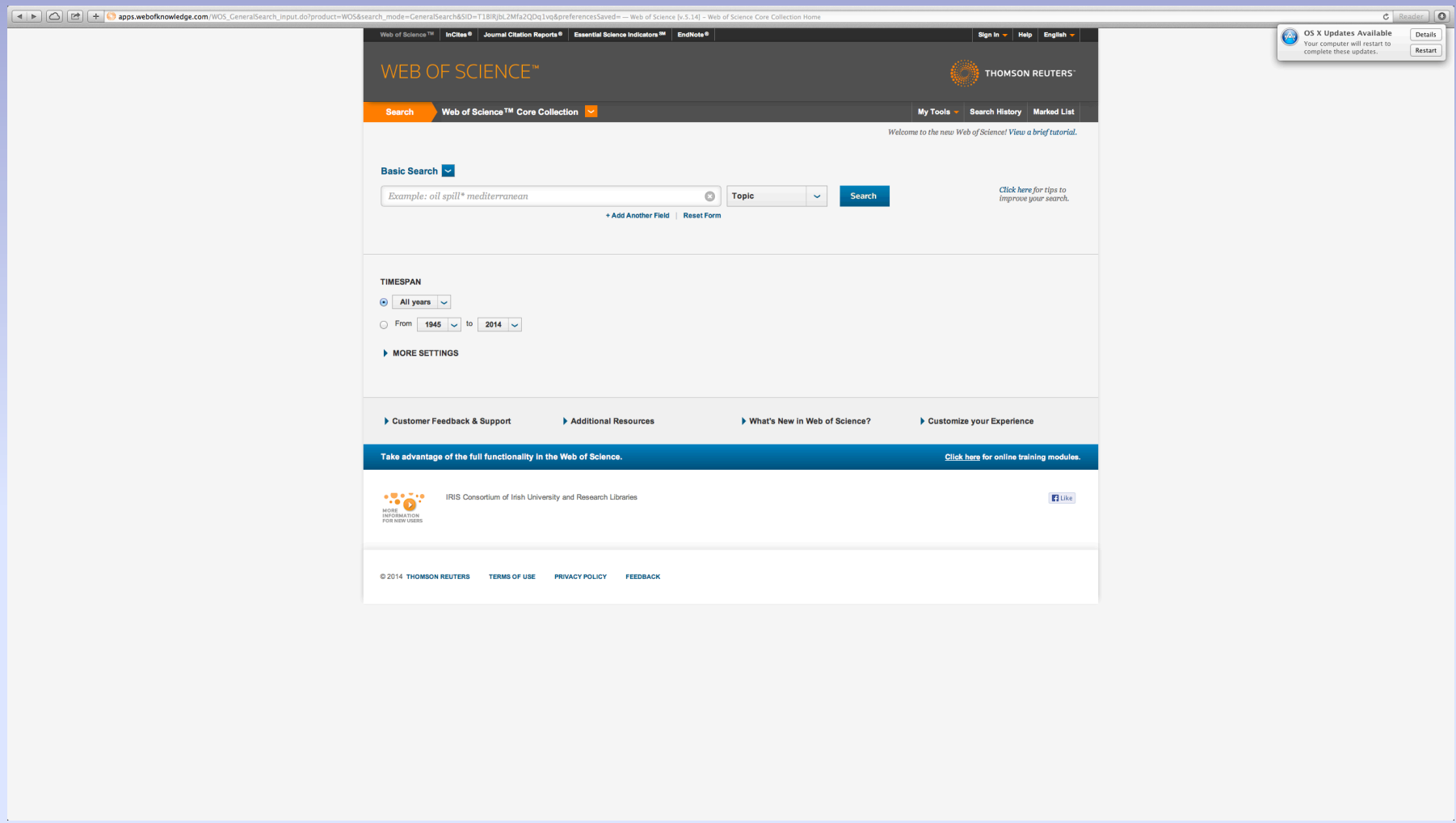
3. Experimental Sections/Materials and Methods (organic):

***N*-[1-Methyl-pyprazino-ethyl]-4-nitro-1,8-naphthalimide,** (8) Compound **8** was synthesised by reacting 1-(2-aminoethyl)-4-methylpiperazine (2.47 g, 2.58 mL, 17.2 mmol, 1.4 eq.) with 4-nitro-1,8-naphthalic anhydride (3.0 g, 12.3 mmol, 1 eq.) and Et_3N (2.5 g, 3.56 mL, 24.6 mmol, 2 eq.) in anhydrous toluene (200 ml), to yield the product as a brown solid (3.50 g, 77%) after a recrystallisation from MeOH. m.p. 109 - 111 ºC; HRMS: 369.1554 ($[M + H]^+$. $C_{19}H_{21}N_4O_4$ requires 369.1563); δ_H (400 MHz, $CDCl_3$), 8.85 (1H, d, *J* = 9.0 Hz, Ar-H7), 8.74 (1H, d, *J* = 7.5 Hz, Ar-H5), 8.70 (1H, d, *J* = 8.0 Hz, Ar-H2), 8.42 (1H, d, *J* = 8.0 Hz, Ar-H3), 8.00 (1H, t, *J* = 8.0 Hz, Ar-H6), 4.36 (2H, t, *J* = 7.0 Hz, $NCH_2CH_2N(CH_2CH_2)_2NCH_3$), 2.73 (2H, t, *J* = 7.0 Hz, $NCH_2CH_2N(CH_2CH_2)_2NCH_3$), 2.65(4H, s, $NCH_2CH_2N(CH_2CH_2)_2NCH_3$), 2.44 (4H, br. s, $NCH_2CH_2N(CH_2CH_2)_2NCH_3$), 2.28 (3H, s, $NCH_2CH_2N(CH_2CH_2)_2NCH_3$); δc (100 MHz, $CDCl_3$), 162.7, 161.9, 149.0, 131.8, 129.4, 129.2, 128.7, 128.5, 126.4,123.4, 123.1, 122.4, 54.9, 54.6, 52.7, 45.5, 45.5, 37.3; *m/z*: 369 $(M + H)^+$; ν_{max} (neat sample)/cm^{-1} 3078, 2928, 2793, 2757, 1655, 1522,1339, 824, 761.

Project - Safety

- Standard safety regulations also apply to research laboratories: Lab-coats and safety glasses must be worn; eating and drinking is not allowed in the laboratories.
- Project students should get a safety tour by supervisors; familiarise yourself with the locations of fire extinguishers, fire blankets, safety exits, showers
- Plan your experiments well in advance; familiarise yourself with risks associated with starting materials, products (MSDS), instruments and etc.
- Consult with supervisors/advisors to discuss safety aspects before starting the experiments
- Overnight experiments need to be signed off by your supervisor.
- College Emergency Number: Ext. 1999

1 Day Safety Workshop given by Dr. Bridge and Dr. Baker
15th of September 2015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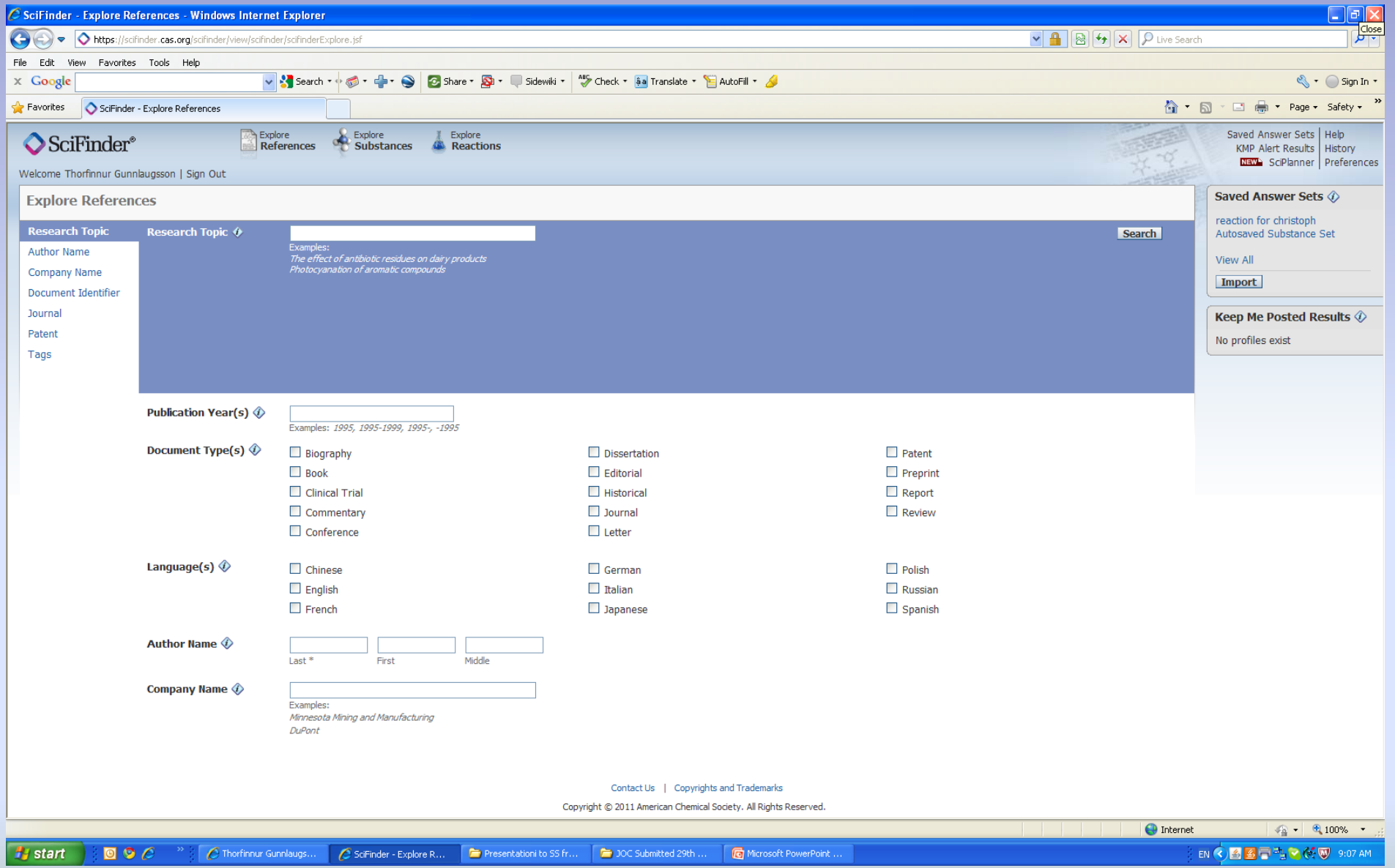
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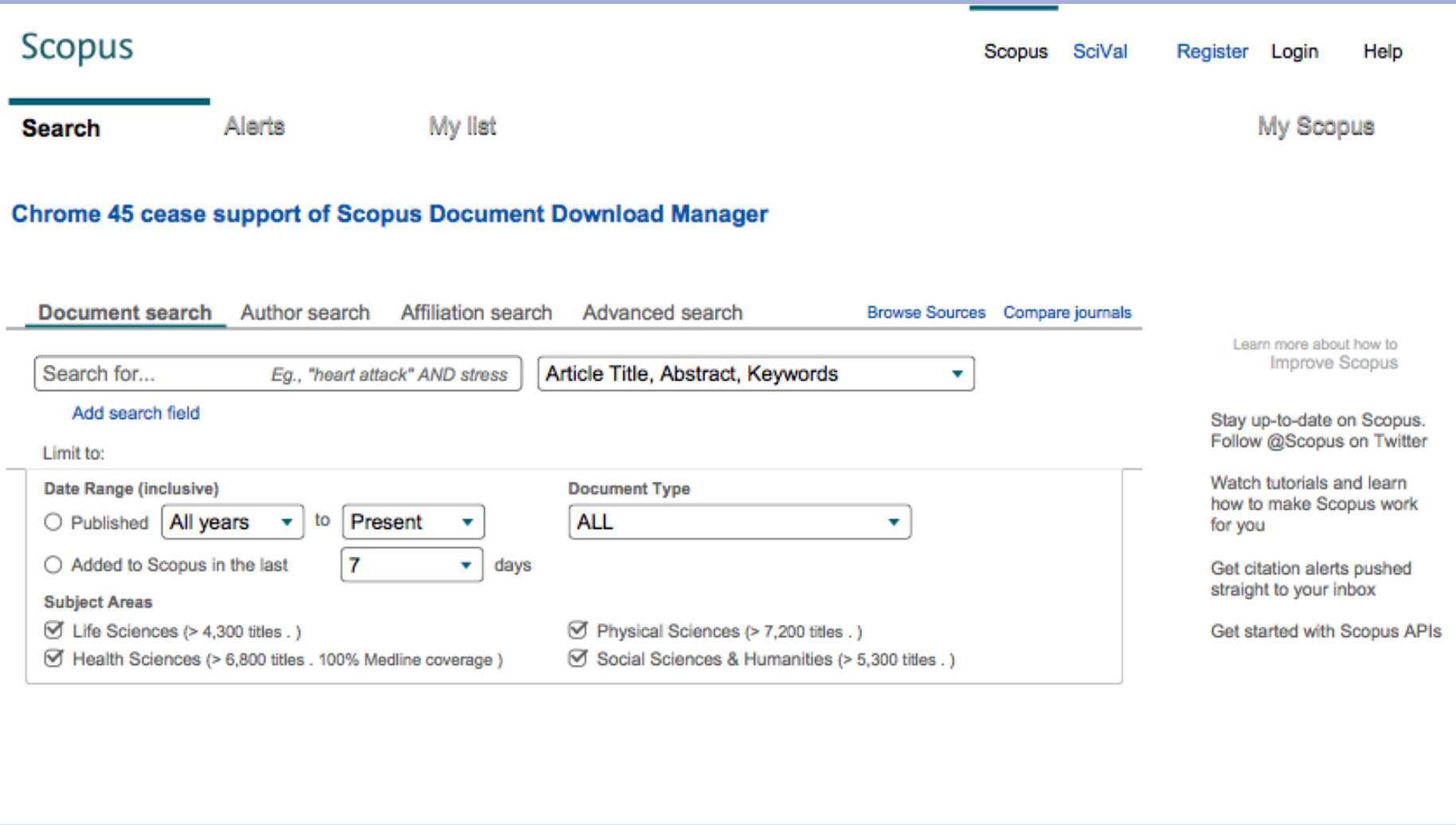
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Lectures and Seminars

Lectures will be given during the first 8 teaching weeks of semester 2. You must attend all those lectures listed as core courses.

Moderatorships: Chemistry and Chemistry with Molecular Modelling

+ 4 Option Courses

full list of available options course will be circulated later in the year and you must notify the School office electronically of your choice of four optional courses by **7th December 2015.**

Moderatorship: Medicinal Chemistry

+ 4 Short Course Lectures

(Supramolecular chemistry, Organic synthetic methods II, DNA Structure and drug DNA complexes, Bio-organic chemistry)

All students are expected to attend the School Research Seminars (Thursday noon!)

Moderatorship Examinations

The Final degree mark: 35% from JS Mark and 65% from the SS year.

Project mark :	20 credits	≈ 33%
Examinations:	40 credits	≈ 67%

Provisional Dates for Moderatorship Examinations:

Will be informed about that later in the year….but in 2014 it was

Paper I:	29th April	Paper II:	1st May
Paper III:	3rd May	Paper IV:	6th May
Paper V:	8th May		

External examiners: The external examiner for the Moderatorship Chemistry with Molecular Modelling will be appointed later in the year.

The external examiners will be in the School in early June (provisional date 6-7th) and they may request a viva voce with any candidate.

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