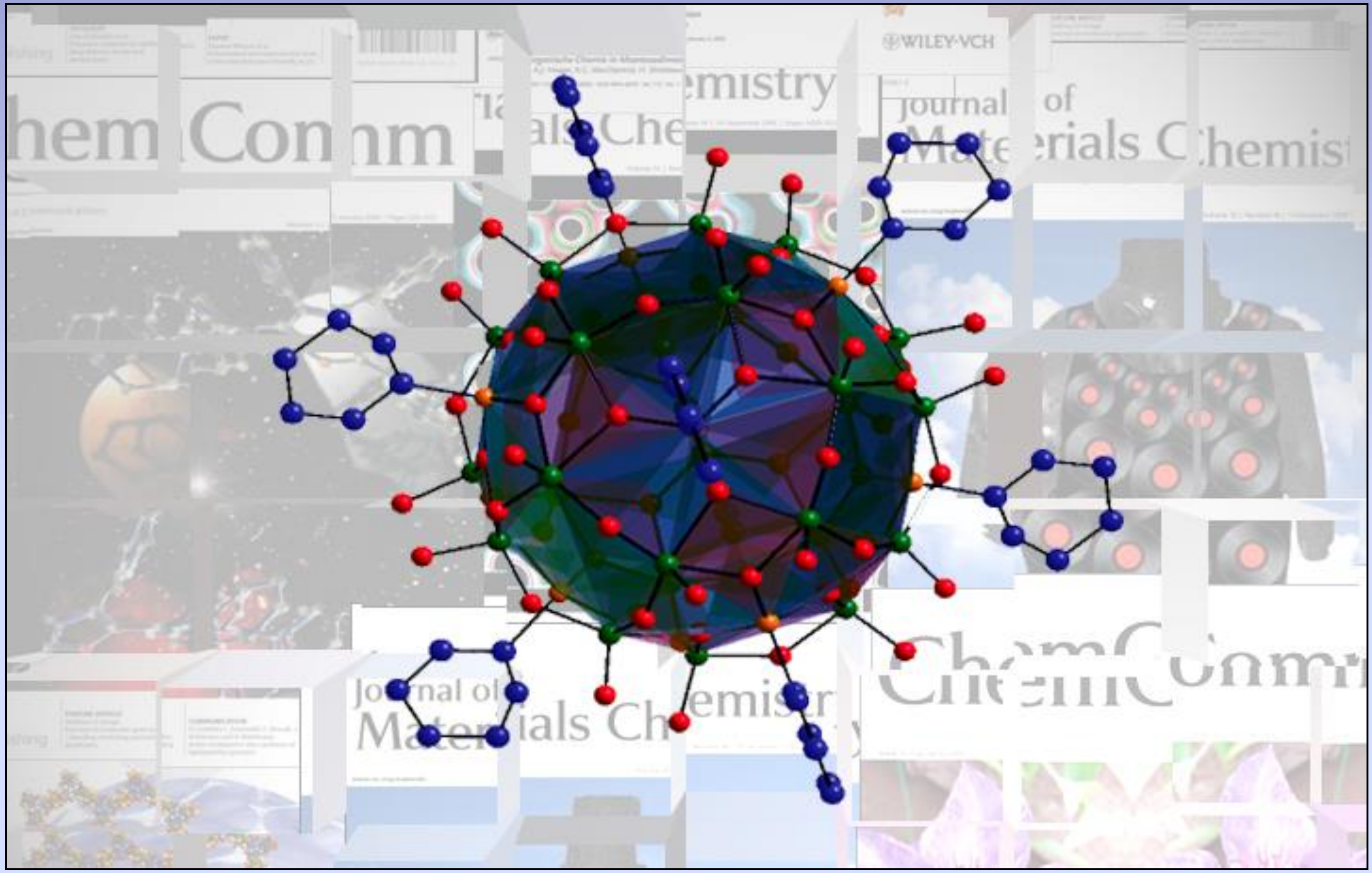
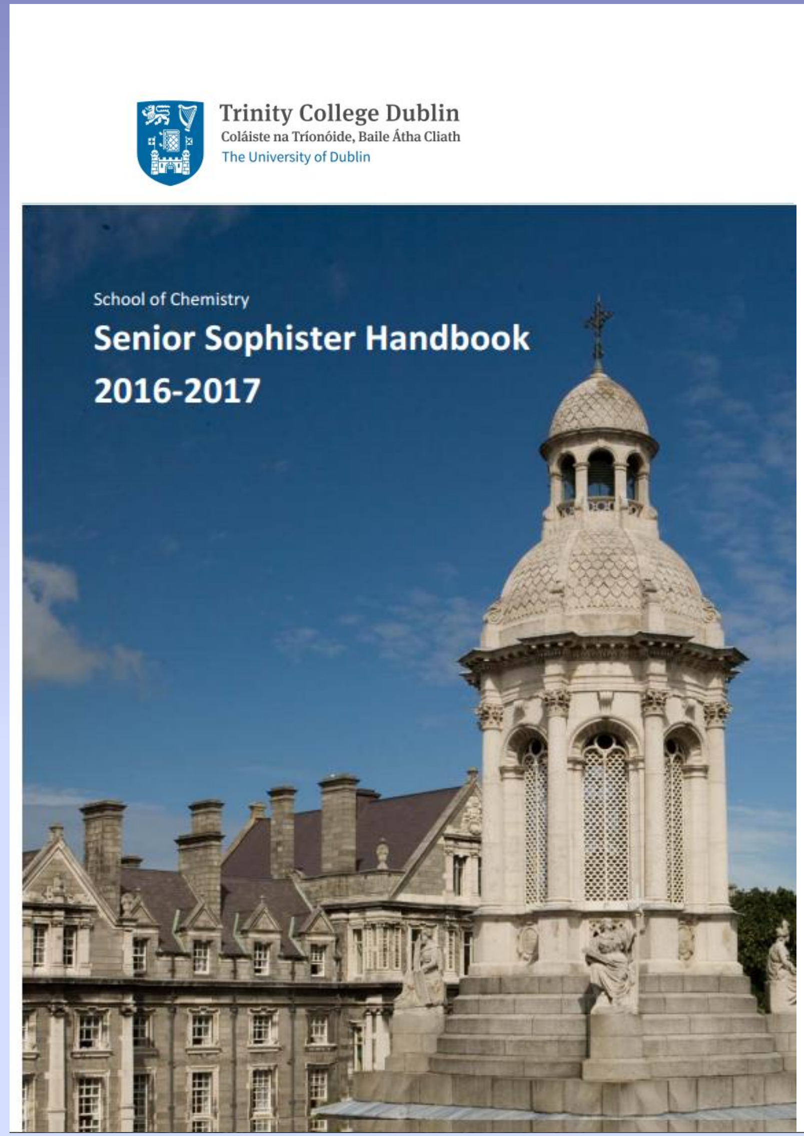
Trinity College Dublin
School of Chemistry
Presentation

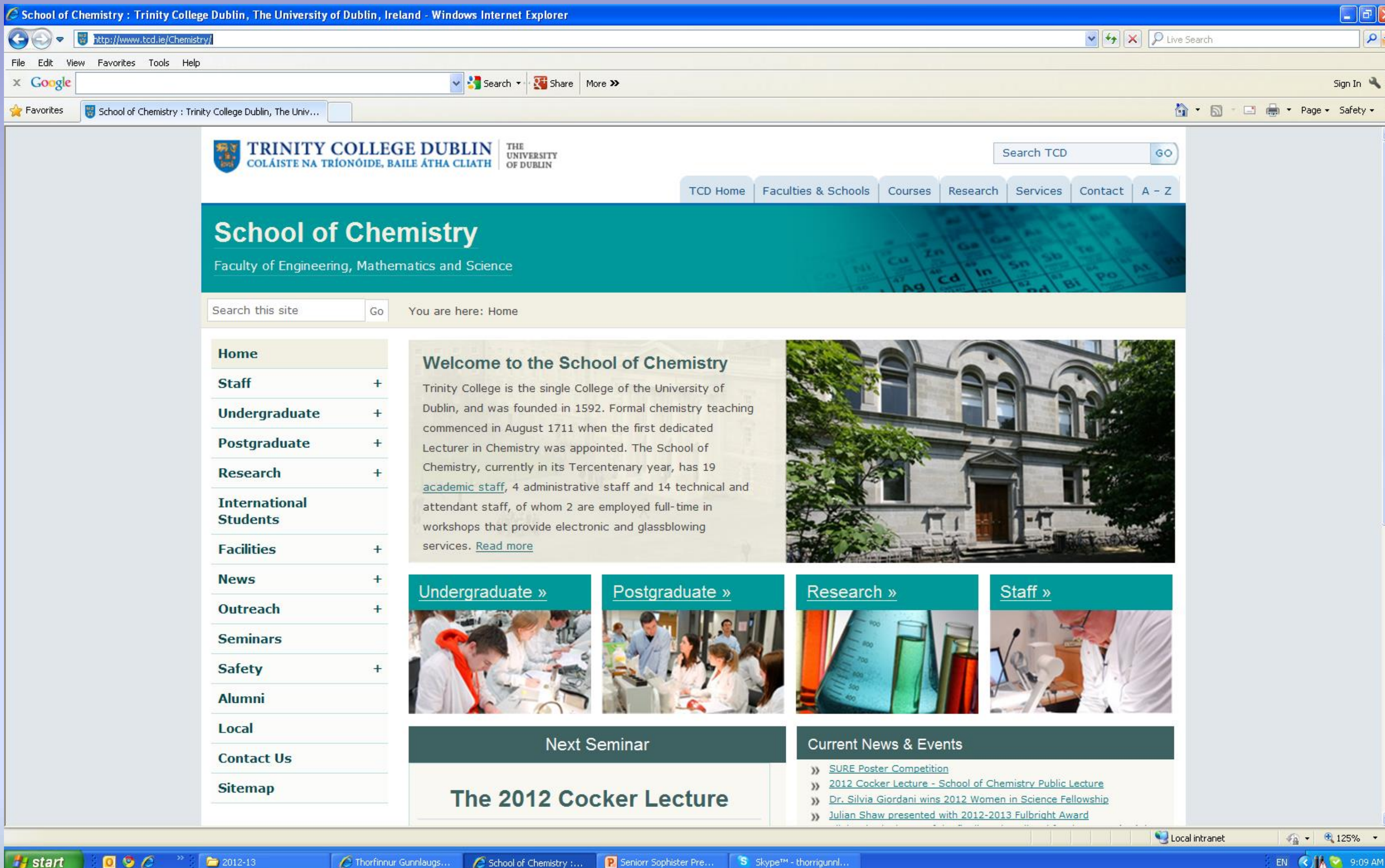


Senior Sophister 2016-2017



A link to the updated 2016-2017 handbook is: https://chemistry.tcd.ie/assets/pdf/Course%20Booklets/SS%20course%20booklet%202016-17_v1.pdf

Trinity College Dublin – School of Chemistry



Trinity College Dublin – School of Chemistry




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

Research Project (20 credits) – Important Dates

Start of the Project: **September 12th 2016**

Duration: 12 weeks (teaching week 8)
Safety workshop 20th of September

Electronic Submission of Report: **16.30 on 2nd December 2016**

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 5th December 2016.**

Make sure you have shown your supervisor your 'final copy' by 18th of November

Examination: **The week of 12-16th of December 2016**

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 18th 2016 (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 2 December 2016. Two hard copies of the identical report should be handed in to the School Office by no later than 16:30 on Monday 5 December 2016.

20th 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 12th December and Friday 16th December 2016.** 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….

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

SCHOOL OF CHEMISTRY
REPORT ON FINAL YEAR PROJECT
SENIOR SOPHISTER 2016-2017
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 and abstract – originality and appropriateness of references and setting the project in context. Does the abstract accurately and concisely summarise the work and results? - *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/abstract– 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): ……………………………………

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):

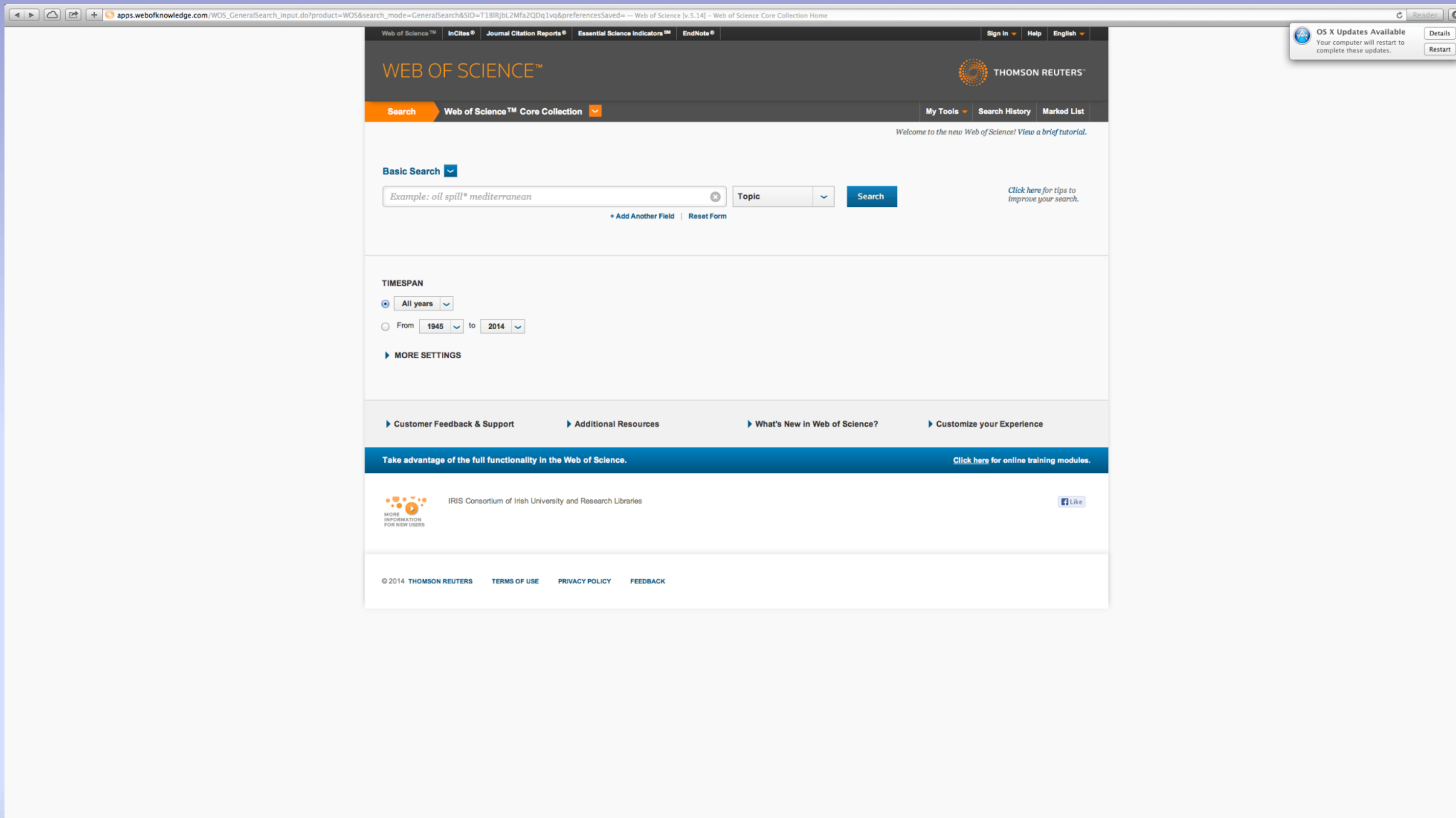
***N*-[1-Methyl-pyprazino-ethyl]-4-nitro-1,8-naphthalimide,** (8)
Compound **8** was synthesised by reacting 1-(2-aminoethyl)-4-methylpiperazine (2.47 g, 2.58 mL, 17.2 mmol, 1.4 eq.) with 4-nitro-1,8-naphthalic anhydride (3.0 g, 12.3 mmol, 1 eq.) and Et_3N (2.5 g, 3.56 mL, 24.6 mmol, 2 eq.) in anhydrous 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.

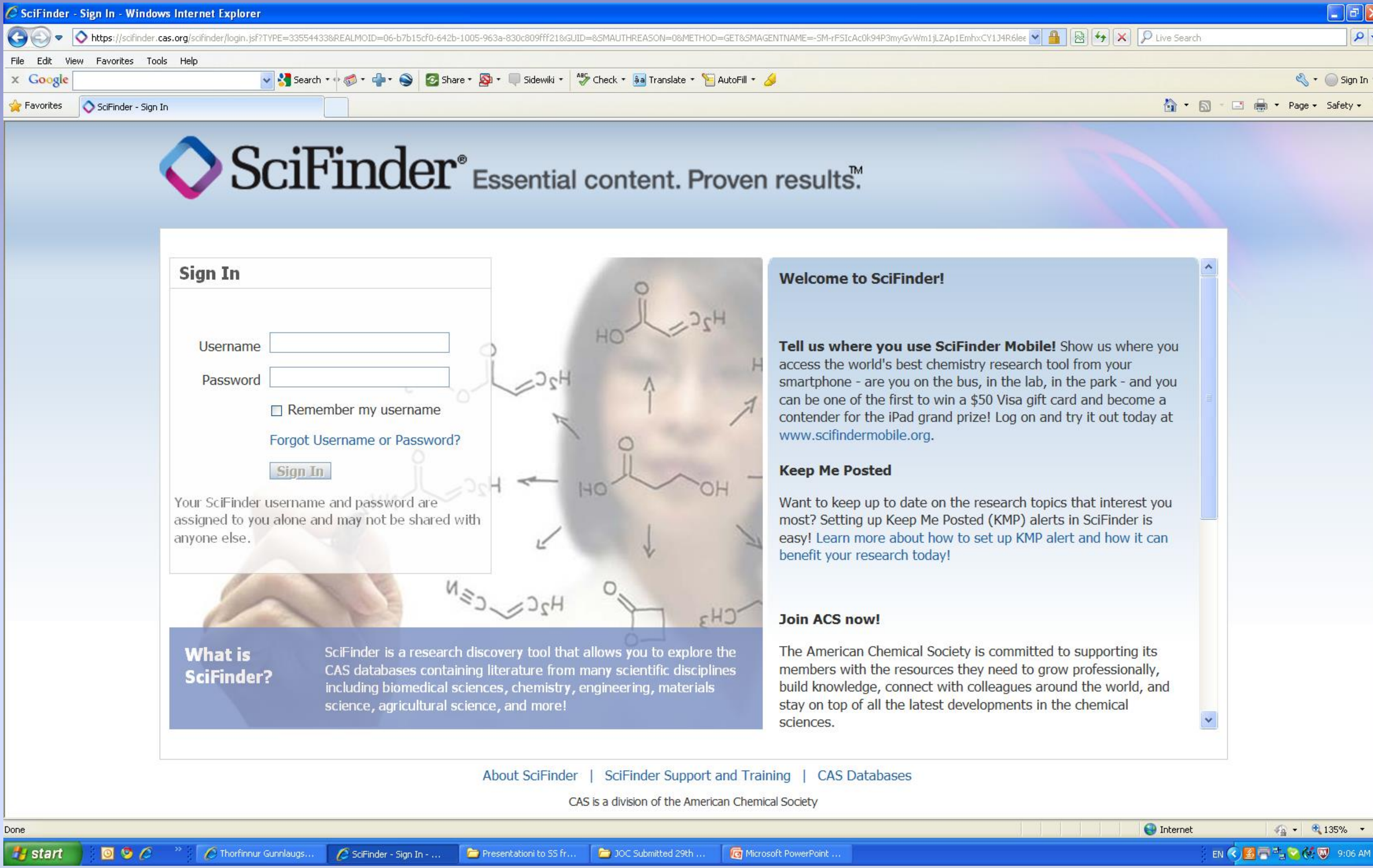
Project - Safety

- 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
20^{th} of September 2016

Project – the use of electronic databases




SciFinder - Sign In - Windows Internet Explorer
SciFinder® Essential content. Proven results.™
Sign In
Username
Password
Remember my username
Forgot Username or Password?
Sign In
Your SciFinder username and password are assigned to you alone and may not be shared with anyone else.
What is SciFinder?
SciFinder is a research discovery tool that allows you to explore the CAS databases containing literature from many scientific disciplines including biomedical sciences, chemistry, engineering, materials science, agricultural science, and more!
Welcome to SciFinder!
Tell us where you use SciFinder Mobile! Show us where you access the world's best chemistry research tool from your smartphone - are you on the bus, in the lab, in the park - and you can be one of the first to win a $50 Visa gift card and become a contender for the iPad grand prize! Log on and try it out today at www.scifindermobile.org.
Keep Me Posted
Want to keep up to date on the research topics that interest you most? Setting up Keep Me Posted (KMP) alerts in SciFinder is easy! Learn more about how to set up KMP alert and how it can benefit your research today!
Join ACS now!
The American Chemical Society is committed to supporting its members with the resources they need to grow professionally, build knowledge, connect with colleagues around the world, and stay on top of all the latest developments in the chemical sciences.
About SciFinder | SciFinder Support and Training | CAS Databases
CAS is a division of the American Chemical Society

SciFinder - Explore References - Windows Internet Explorer

https://scifinder.cas.org/scifinder/view/scifinder/scifinderExplore.jsf

File Edit View Favorites Tools Help

SciFinder®

Explore References | Explore Substances | Explore Reactions

Saved Answer Sets | Help
KMP Alert Results | History
SciPlanner | Preferences

Welcome Thorfinnur Gunnlaugsson | Sign Out

Explore References

- Research Topic
- Author Name
- Company Name
- Document Identifier
- Journal
- Patent
- Tags

Research Topic

Examples:
The effect of antibiotic residues on dairy products
Photocyanation of aromatic compounds

Search

Publication Year(s)

Examples: *1995, 1995-1999, 1995-, -1995*

Document Type(s)

Biography	Dissertation	Patent
Book	Editorial	Preprint
Clinical Trial	Historical	Report
Commentary	Journal	Review
Conference	Letter	

Language(s)

Chinese	German	Polish
English	Italian	Russian
French	Japanese	Spanish

Author Name

Last * | First | Middle

Company Name

Examples:
Minnesota Mining and Manufacturing
DuPont

Saved Answer Sets

reaction for christoph
Autosaved Substance Set

View All

Import

Keep Me Posted Results

No profiles exist

Contact Us | Copyrights and Trademarks

Scopus

Scopus SciVal Register Login Help

Search Alerts My list My Scopus

Chrome 45 cease support of Scopus Document Download Manager

Document search Author search Affiliation search Advanced search Browse Sources Compare journals

Search for... *Eg., "heart attack" AND stress* | Article Title, Abstract, Keywords

Add search field

Limit to:

Date Range (inclusive)

- Published All years to Present
- Added to Scopus in the last 7 days

Document Type

ALL

Subject Areas

- ☑ Life Sciences (> 4,300 titles .)
- ☑ Health Sciences (> 6,800 titles . 100% Medline coverage)
- ☑ Physical Sciences (> 7,200 titles .)
- ☑ Social Sciences & Humanities (> 5,300 titles .)

Learn more about how to Improve Scopus

Stay up-to-date on Scopus. Follow @Scopus on Twitter

Watch tutorials and learn how to make Scopus work for you

Get citation alerts pushed straight to your inbox

Get started with Scopus APIs

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 ***Tuesday*** **6th December 2016.**

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:**

There is a change to previous years hence, exact dates will be confirmed later in the academic year.

We expect it to be held in the first two week of the examination period.

- **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 2-3rd THIS IS TO BE CONFIRMED) and they may request a viva voce with any candidate.

IRISH RESEARCH COUNCIL
An Chomhairle um Thaighde in Éirinn

http://www.research.ie/funding/postgraduate-funding

Important dates

Call open	7 September 2016
FAQ deadline	16:00 (Irish time) 26 October 2016
Applicant deadline	16:00 (Irish time) 2 November 2016
Supervisor and referee deadline	16:00 (Irish time) 9 November 2016
Research office endorsement Deadline:	16:00 (Irish time) 16 November 2016
Scheme outcome	March 2017
Scholarship start date	1 October 2017

Please note that the timings provided here are indicative and may be subject to change by the Council.

Contacts:

Prof. Thorri Gunnlaugsson
SS Year Co-ordinator
Room 712
TBSI
gunnlaut@tcd.ie

Prof. Paula Colavita
Associate Director of Teaching & Learning (UG)
Room 1.5, Chemistry Extension
colavitp@tcd.ie

Prof. Mike Bridge
Director of Teaching & Learning (UG)
Room 2.5, Chemistry Building
mbridge@tcd.ie

Prof. Eoin Scanlan
Director of Medicinal Chemistry
Room 7.11, TBSI
Eoin.scanlan@tcd.ie

Prof. Graeme Watson
Director of Chemistry with Molecular Modelling
Room 2.13, Lloyd Building
watsong@tcd.ie