Interdisciplinary Science

PA2013

Molecules by Design

University of Leicester

Contents

Welcome

Organic chemistry is important in many areas of industry and in the field of pharmaceuticals. In this module you will explore some of the key aspects of organic chemistry in the context of the design and delivery of drugs. This brings together issues of fundamental research, industrial scaling up of processes, environmental impact and patent law.

Module Authors

Dr. Derek Raine	Physics
Dr. Paul Jenkins	Chemistry (synthesis and mechanisms).
Dr Dylan Williams	Chemistry
Dr. Mark Lowe	Chemistry (scale up)
Prof. Clive Bagshaw	Biochemistry (enzyme kinetics and dynamics).
Prof. Paul Cullis	Chemistry (NMR characterisation).
Dr. Anton Hutter	Patents

Cover image: The Atomium by O Palsson CC-BY

http://www.flickr.com/photos/opalsson/3773629074/

The Centre for Interdisciplinary Science would like to thank Mrs Rebecca Cowling for her input into this module.

Problem Statement

It should be noted that the treatment, drugs and enzymes used in this module are fictitious. We will be exploring the process of design and delivery of drugs, rather than the actual drugs themselves.

Biosoftware Solutions Ltd.

Driving Innovation Forward

Internal MEMO

I want you to take a look at this. A full scale implementation is too ambitious for our company, but we should look at a range of simplified steps we'd need to implement to follow the drug delivery process. I think we should base our initial exploration on the BeDa case.

Simon MacIntyre

Simon MacIntyre
CEO Biosoftware Solution Ltd.

PRESS RELEASE

GE To Develop Biotic Man To Help Accelerate Drug Development

New study in partnership with D.O.D. aimed at addressing biological threats

Last update: 9:11 a.m. EST Nov. 20, 2008

NISKAYUNA, N.Y., Nov 20, 2008 (BUSINESS WIRE) -- GE Global Research, the technology development arm for the General Electric Company

GE announced today a two-year, $1.1 million collaboration with the Transformational Medical Technologies Initiative (TMTI) to develop a physiologically based "virtual human." This collaboration is supported by a contract awarded by the Defence Threat Reduction Agency (DTRA), a division of the U.S. Department of Defence.

The so-called Biotic Man project will involve the design of a computer model that could dramatically speed drug design in response to the threat of biological attacks on the battlefield or in domestic situations. The project will advance a software program originally developed by GE Global Research. This Physiologically Based Pharmacokinetic (PBPK) software tool uses computational models to measure a drug's response in the body long before clinical trials.

GE researchers will adapt the PBPK tool to computationally model the impact of bacterial, viral and other infectious agents on the human body. The modified tool will simulate the response of new antibiotic or antiviral drug therapies to a specific threat. In addition, the tool will be designed to accurately represent the physiological changes in a critically ill patient suffering from burns, trauma, or recent surgery to help evaluate the effectiveness of the drug therapy under the various conditions it might be administered.

"GE's Biotic Man project is all about speed. The goal is to enable faster development of drugs to respond to new biological threats," said John Graf, Principal Investigator on the project for GE Global Research. "This new software tool also could have broad impact across the pharmaceutical industry, helping to accelerate efforts to develop new drug remedies at substantially reduced costs."

"This new, enhanced software tool will enable researchers to test and develop new drug therapies in a virtual, safer environment with better quantitative information," Graf added.

The main obstacles to faster, more efficient drug development today are challenges with safety and the inability to predict drug failures earlier, before human testing or even in initial stage clinical trials. These limitations also can lead to dramatically higher testing costs. Gains in productivity and potential cost savings may be achieved from better decisions based on quantitative information, identification of lead compounds, and more effective trials.

http://www.marketwatch.com/news/story/GE-To-Develop-Biotic-Man/story.aspx?guid=%7B7F1C72B4-C28E-42BA-BDCB-292589C5D510%7D

Numerate Completes $4 Million Financing

SAN BRUNO, Calif.--(BUSINESS WIRE)--Numerate, Inc., a biotechnology company leveraging a novel drug engineering process to design lead-stage drug compounds, announced today that it has completed a $4 million Series A financing. Investors included Foundation Capital, Lanza techVentures and various individuals. Concurrent with the financing, Adam Grosser, a general partner with Foundation Capital, has joined Numerate's Board of Directors.

"We are confident that Numerate's computationally-based drug design process can help fill the critical gap that currently exists between basic research and the development of high-potential clinical candidates," stated Mr. Grosser. "This novel capability has the potential to serve as an alternative to the in-licensing of preclinical drug candidates, at a fraction of the cost and in less time than the in-licensing process."

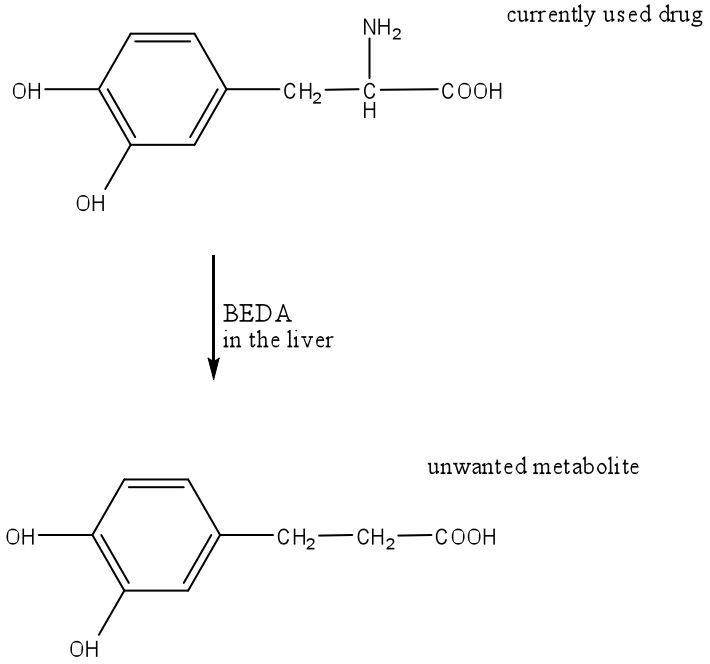
According to Guido Lanza, Numerate's president and chief executive officer, "This investment will help Numerate to pursue a broad range of partnering opportunities. Our plan is to deliver robust lead-stage programs in return for significant milestone and royalty payments that are linked to success in the lab, the clinic and the marketplace. In this way, we mitigate the chemical design risk for our partners. Adam Grosser's extensive experience in launching innovative start-ups will be invaluable as we implement this strategy."

Numerate's drug engineering process combines advances in computer science, statistics, and molecular modeling to address, in parallel, the key objectives of safety, efficacy and novelty at design-time. The result is active, selective, synthesizable, and patentable drug leads.

http://www.businesswire.com/portal/site/google/?ndmViewId=news_view&newsId=20081118005497&newsLang=en

The BeDa story

The molecule shown in the scheme below was once used as a treatment for depression under the trade name *Infra*↑ ™. Unfortunately, after a limited time, it fails due to the presence of an enzyme in the liver called BeDa. This enzyme metabolises the drug according to the scheme shown, meaning there is limited availability of the drug by the time it gets to the brain where it is required.



The solution was to produce a drug to be used in combination with *Infra*↑ in sufficiently high purity that would inhibit the action of BeDa, and hence allow the anti-depressant, now called *Infra*$^{+}$↑, to continue working for longer. Environmental concerns meant that it took a number of years to scale-up the process for industrial production. By this time there were a number of competitors on the market which did not have the side-effects of *Infra*$^{+}$↑. This sent the company back to the drawing board to take a closer look at how enzyme action could be inhibited. But too late for the investors!

Staff

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Prof. Clive Bagshaw	Biochemistry (enzyme kinetics and dynamics).
Prof. Paul Cullis	Chemistry (NMR characterisation).
Dr. Anton Hutter	Patents

Learning Objectives

Organic chemistry

To be able to:

- Name simple organic compounds (including haloalkanes, alcohols, ketones, amines, carboxylic acids and esters) and their associated functional groups.
- Describe the mechanism and conditions necessary for an esterification reaction.
- Interpret a range of reaction mechanisms, including synthesis.
- Describe the difference between a transition state and a reaction intermediate, and show these on an energy profile diagram.
- Determine a possible reaction pathway for the synthesis of a compound using retrosynthetic analysis given some known functional group transformations.
- Calculate the yield of a reaction.
- Give the meanings of the labels (L) and (D).

Theoretical background to laboratory techniques

To be able to:

- Describe how to carry out reflux, distillation, liquid-liquid extraction and rotary evaporation experiments.
- Describe some purification methods used in organic chemistry, especially recrystallisation.

Enzyme and dynamics

To be able to:

- Draw and explain an energy profile diagram with and without a catalyst.
- Explain why the transition state is important when considering enzymes.
- Understand the importance of binding coefficients.
- Describe how pH, temperature and the presence of an inhibitor can affect enzyme function.
- Describe how Michaelis-Menten kinetic data may be obtained by use of a Lineweaver-Burke Double Reciprocal plot.
- Describe the assumptions underlying the Michaelis-Menten data, and the significance of the results to determining enzyme characteristics.
- Recognise the three modes of inhibition, competitive, uncompetitive and non-competitive from appropriate Michaelis Menten kinetic data.
- Describe some ways in which an inhibitor for an enzyme might be found.

Industrial chemistry

To be able to:

- Discuss problems which may occur when scaling up a reaction to an industrial context.
- Be able to discuss the use of the properties of azeotropes in industrial organic synthesis.
- Describe the stages of commercialisation necessary to bring a new drug to the market.

- Describe the importance of purification in drug design.
- Describe ways potential drug candidates may be found, and give examples.
- Describe the nature and importance of clinical trials.
- Briefly describe the type of intellectual property protected by trademarks, copyright and design.
- Describe the process of obtaining a patent for a new invention, and the parts of a patent.
- Describe the measures chemical firms put in place in order to minimise their effect on the environment.

Chemical information skills

Green chemistry

- Be able to describe the measures chemical firms put in place in order to minimise their effect on the environment.

Spectroscopy characterisations

To be able to:

- Describe the physical basis for the technique of NMR.
- Analyse simple NMR spectra, given tabulated data.
- Analyse the main bands for an IR spectrum of a simple compound.
- Analyse mass spectroscopy data.

Reading List

Books

Brown, LeMay & Bursten, (2006) *Chemistry, The Central Science, 10th Edition*.

- Section 19.7: Looks at the relationship between Gibbs Free Energy and the equilibrium constant.
- Chapter 25: This chapter revises some of the prerequisite knowledge you will need for this module, most of which was covered in Science of the Invisible.

McMurry, (1998 / 2003) *Fundamentals of Organic Chemistry, 4th (1998) or 5th (2003) Edition.*

- Chapter 3: This chapter gives a general introduction to organic chemistry, including an introduction to the types of organic reaction, reaction mechanisms, intermediates and transition states, and energy profile diagrams.
- Chapter 6: This chapter looks at stereochemistry, racemic mixtures, and the resolution of enantiomers. It is strongly recommended that you read this with a chemical modelling set to hand.
- Fourth Edition, section 7.5 – 7.8 or Fifth Edition, section 7.4 – 7.6: Nucleophilic substitution reactions and their stereochemistry. Note: this is the general mechanism for the conversion of an acid into an ester.
- Fourth Edition, section 10.6 or Fifth Edition, section 10.5: Reactions of carboxylic acids, including that required to form an ester from a carboxylic acid and an alcohol.
- Chapter 13: This chapter is on structure determination, and includes IR, NMR, and UV-visible spectroscopy.

Berg, M., Tymoczko, J. L., & Stryer, L. (2007) *Biochemistry, 6th Edition*.

- Chapter 8: Enzymes: basic concepts and kinetics
- Chapter 35: Drug development – an overview of the process.

Patrick, G. L. (2005) *An introduction to Medicinal Chemistry, 3rd Edition.*

- Part B, Chapters 9 -12; Gives a lot more detail on Drug discovery, design and development.

Williams, D.H. (1996) *Spectroscopic methods in organic chemistry, 5th Ed*. McGraw-Hill.

Papers

Anastas, P.T. & Kirchoff, M.M. 2002. *Origins, Current Status, and Future Challenges of Green Chemistry*. Acc. Chem. Res., 35, 686-694

Kirchoff, M.M. 2005. *Promoting sustainability through green chemistry – Resources, Conservation and Recycling*., 44, 237-243

Poliakoff, M., Fitzpatrick, J.M., Farren, T.R. & Anastas, P.T. 2002. *Green Chemistry: Science and Politics of Change.* Science., 297, 807-810

Fiorino, T. 2007. *Industry, Clinical Trails, and the Cost of Cancer Drugs: An Investor's Perspective.* Journal of Clinical Oncology., 25, no. 19, e21-e23

Mestres, R. 2004. *A brief structured view of green chemistry issues.* Royal Society of Chemistry., G10-G12

Clark, J.H. 2006. *Green Chemistry: today (and tomorrow)*. Green Chem., 8, 17-21

Websites

http://orgchem.colorado.edu/hndbksupport/cryst/cryst.html
This website gives you information about how to carry out a recrystallisation, including a 'recrystallisation movie' which should answer any questions.

http://www.whfreeman.com/stryer4/
This gives online access to the fourth edition of a key biochemistry textbook. It should be noted however, that the current edition of this book is the sixth edition, available from the i-Science Library, and it contains a full chapter on drug design and delivery, so you are encouraged to borrow this text also.

http://www.cis.rit.edu/htbooks/nmr/inside.htm
Practically a textbook on NMR

http://vam.anest.ufl.edu/forensic/nmr.html
For a great animation of how NMR signals arise

http://spectraschool.org
Gives you several different types of spectra including IR, nmr, which you can carry out integrations, expand, zoom yourself. Due to go live in January!

http://gb.espacenet.com
Free searchable online database of patents, hosted by the European Patent Office

A Guide to Module Pacing

Session	Preparation	Learning Outcomes
FS01	• If you did A-level Biology or Chemistry review your notes on catalysts and enzymes. • Fundamentals of Chemistry (4th/5th Ed.): Chapter 3. • Chemistry, The Central Source: Chapter 25. • Biochemistry: Chapter 8.	Catalysts Enzymes Energy profile diagrams
FS02	• Review functional groups from the Science of the Invisible module. • Chemistry, The Central Source: Chapter 25. • Fundamentals of Organic Chemistry: Section 7.5-7.8, 10.6 (4th Ed.) or section 7.4-7.6, 10.5 (5th Ed.).	Functional groups; transformations Reaction yields
ES01		Esterification
FS03	• Review material covered in ES01. • Chemistry, The Central Source: section 19.7. • Fundamentals of Organic Chemistry: Chapter 3, 6 (both editions). • Fundamentals of Organic Chemistry: Section 7.5-7.8, 10.6 (4th Ed.) or section 7.4-7.6, 10.5 (5th Ed.).	Esterification Reaction Mechanisms
LS01		Preparation of methyl pentanoate
LS02		Recrystallisation of Benzoic Acid
FS04	• Laboratory notes from LS01 & LS02 • Research separation and purification techniques • http://orgchem.colorado.edu/hndbksupport/cryst/cryst.html	Methods of separation and purification Physical basis for these techniques
ES02		Industrial Scale Up
FS05	• Re-read notes from ES02 • Biochemistry, 6th Ed.: chapter 35. • An introduction to Medicinal Chemistry: Part B, chapters 9-12.	Industrial Scale Up Stages of Commercialisation
FS06	• Basic Guide to SciFinder Scholar. Papers: • *Origins, Current Status, and Future Challenges of Green Chemistry*. Acc. Chem. Res., 35, 686-694 • *Promoting sustainability through green chemistry – Resources, Conservation and Recycling*., 44, 237-243	SciFinder Scholar, Google Scholar, Web of Knowledge, SDBS Green Chemistry

	• *Green Chemistry: Science and Politics of Change.* Science., 297, 807-810 • *Industry, Clinical Trails, and the Cost of Cancer Drugs: An Investor's Perspective.* Journal of Clinical Oncology., 25, no. 19, e21-e23 • *A brief structured view of green chemistry issues.* Royal Society of Chemistry., G10-G12 • *Green Chemistry: today (and tomorrow)*. Green Chem., 8, 17-21	
FS07	• Basic Guide to SciFinder Scholar Papers: • *Origins, Current Status, and Future Challenges of Green Chemistry*. Acc. Chem. Res., 35, 686-694 • *Promoting sustainability through green chemistry – Resources, Conservation and Recycling*., 44, 237-243 • *Green Chemistry: Science and Politics of Change.* Science., 297, 807-810 • *Industry, Clinical Trails, and the Cost of Cancer Drugs: An Investor's Perspective.* Journal of Clinical Oncology., 25, no. 19, e21-e23 • *A brief structured view of green chemistry issues.* Royal Society of Chemistry., G10-G12 *Green Chemistry: today (and tomorrow)*. Green Chem., 8, 17-21	SciFinder Scholar, Google Scholar, Web of Knowledge, SDBS Green Chemistry
FS08	• Biochemistry: chapter 8. • http://www.whfreeman.com/stryer4/	Enzyme inhibition Lock and Key Mechanism
FS09	• Read the laboratory script for the Enzyme Kinematics (laccase) experiment. • Biochemistry: chapter 8. • http://www.whfreeman.com/stryer4/	Enzyme kinematics
ES03		Enzyme kinetics and dynamics
LS03		Enzyme kinetics (laccase)
FS10	Background reading.	Enzyme Kinetics and dynamics
FS11	Background reading.	Methods of finding inhibitors
FS12	Review course material so far.	Assessing purity
ES04		Physical basis of NMR
FS13	• Re-read notes from ES04 • http://www.cis.rit.edu/htbooks/nmr/inside.htm • http://vam.anest.ufl.edu/forensic/nmr.html	Physical basis of NMR Introduction to Patent Law

ES05		Patent Law
FS14	• Re-read notes from ES05. • Fundamentals of Organic Chemistry: chapter 13. • http://spectraschool.org • Spectroscopic methods in organic chemistry, 5th Ed.	Patent Law NMR spectra
ES06		Assigning NMR spectra
FS15	• Re-read notes from ES06 • Fundamentals of Organic Chemistry: chapter 13. • http://spectraschool.org	Assigning NMR spectra
ES07		Spectroscopy Workshop
FS16	There is no FS16	---

Facilitation Sessions

Facilitation Session 01

Pre Session Preparation

- If you did A-level Biology or Chemistry review your notes on catalysts and enzymes.
- Fundamentals of Chemistry (4^{th}/5^{th} Ed.): Chapter 3.
- Chemistry, The Central Source: Chapter 25.
- Biochemistry: Chapter 8.

Introduction to Module

Introduction to the module as a whole, including a brief overview of the documentation (highlighting the CLEs/Deliverables). Introduction to the Problem Statement.

Introduction to Catalysts and Enzymes

Initiate a class discussion on catalysts and enzymes;

What do the students know from their previous studies?

Do they know anything about the kinetics and thermodynamics of chemical reactions?

Energy Profile Diagrams

Ensure that students are able to draw and describe in detail an energy profile diagram for a reaction with and without the presence of a catalyst.

Facilitation Session 02

Pre Session Preparation

- Review functional groups from Science of the Invisible.
- Chemistry, The Central Source: Chapter 25.
- Fundamentals of Organic Chemistry: Section 7.5-7.8, 10.6 (4th Ed.) or section 7.4-7.6, 10.5 (5th Ed.).

Review of Functional Groups

Review functional groups covered in the Science of the Invisible module. Types of molecules/functional groups to cover:

- Alcohol
- Carboxylic acid
- Aldehyde
- Haloalkane
- Ester
- Amine
- Ketones

Determine which functional groups are present in the anti-depressant drug.

As a class determine some ways in which we might try to prevent BEDA from binding to the anti-depressant by looking at some chemical reactions that might be carried out in order to achieve this. Discuss relevant functional group transformations.

Reaction Yields

Discuss the method used to calculate the yield of the reactions discussed above.

Prepare for the Expert Session

Prepare a list of questions to ask the Expert in ES01 “Esterification”.

Facilitation Session 03

Pre Session Preparation

- Review material covered in ES01.
- Chemistry, The Central Source: section 19.7.
- Fundamentals of Organic Chemistry: Chapter 3, 6 (both editions).
- Fundamentals of Organic Chemistry: Section 7.5-7.8, 10.6 (4^{th} Ed.) or section 7.4-7.6, 10.5 (5^{th} Ed.).

Discussion of Esterification

Class discussion about the material covered in the previous Expert session. Following the Expert Session are the students able to interpret reaction mechanisms?

Use the mechanism to determine the eventual fate of the oxygen atom from the alcohol. Discuss retrosynthetic analysis; how would we create a scented coating for the drug?

As a class determine a possible reaction pathway for the synthesis of a compound given some known functional group transformations.

Further Reaction Mechanisms

Further discussion of relevant reaction mechanisms.

Facilitation Session 04

Pre Session Preparation

- Re-read laboratory notes for LS01 and LS02.
- Research separation and purification techniques.
- http://orgchem.colorado.edu/hndbksupport/cryst/cryst.html

Laboratory session feedback

Discussion of the "Preparation of methyl pentanoate" and "Recrystallisation of Benzoic Acid" experiments. How did the students do and what did they find out?

Methods of Separation and Purification

As a class make a list of the various separation and purification techniques used and/or encountered so far in the module.

- What techniques are used in industry?
- What is the physical basis for each method?
- Why is purification so important in chemistry?

Facilitation Session 05

Pre Session Preparation

- Re-read notes from ES02.
- Biochemistry, 6th Ed.: chapter 35.
- An introduction to Medicinal Chemistry: Part B, chapters 9-12.

Discussion of Scaling up Chemical Processes

Class discussion about the material covered in the previous Expert session.

Following the preliminary discussion of FS 04 and ES02 discuss the following:

- How would you scale up the experiments you have conducted with methyl pentanoate (LS01) and Benzoic acid (LS02)?

Stages of Commercialisation

We will consider how the stages of commercialisation undergone in conventional medicine safeguard us against ineffectual and dangerous medicines making it onto the market.

Have a look at the 'stages of commercialisation' from yesterday's Expert Session. Consider that you are an alternative therapist, wanting to introduce sound therapy, whereby you make sounds of different frequencies in crystal bowls, and these sounds are supposed to resonate the healing points inside your body to make you well. Use this premise to write a mock 'stages of commercialisation' for your alternative therapy, detailing how you are going to make money from your therapy.

Facilitation Session 06

Pre Session Preparation

- Basic Guide to SciFinder Scholar (Supplementary Material).

Papers:

- *Origins, Current Status, and Future Challenges of Green Chemistry*. Acc. Chem. Res., 35, 686-694
- *Promoting sustainability through green chemistry – Resources, Conservation and Recycling*., 44, 237-243
- *Green Chemistry: Science and Politics of Change.* Science., 297, 807-810
- *Industry, Clinical Trails, and the Cost of Cancer Drugs: An Investor's Perspective.* Journal of Clinical Oncology., 25, no. 19, e21-e23
- *A brief structured view of green chemistry issues.* Royal Society of Chemistry., G10-G12

Green Chemistry: today (and tomorrow). Green Chem., 8, 17-21

SciFinder Scholar

The number of licenses available at any one time for SciFinder Scholar is limited. Therefore the facilitator will guide you through the Supplementary Material contained in this document whilst providing a real-time 'walk through' of the key features of this application on the SMARTboard.

You will then be expected to try this application out yourselves in groups. Both sessions 6 and 7 have been scheduled for this to give you ample time, whilst a facilitator is available, to explore this application.

Other methods of locating materials

Whilst waiting for a SciFinder license to become available you should investigate the following sources of information:

- Google scholar,
- Web of knowledge,
- Spectral Data Base System (SDBS) for organic compounds.

Continue work on Deliverables

Whilst waiting for a SciFinder license to become available you should continue to work on your Deliverables.

Green Chemistry

A discussion of the Green Chemistry within your group.

Facilitation Session 07

Pre Session Preparation

- Basic Guide to SciFinder Scholar (Supplementary Material).

Papers:

- *Origins, Current Status, and Future Challenges of Green Chemistry*. Acc. Chem. Res., 35, 686-694
- *Promoting sustainability through green chemistry – Resources, Conservation and Recycling*., 44, 237-243
- *Green Chemistry: Science and Politics of Change.* Science., 297, 807-810
- *Industry, Clinical Trails, and the Cost of Cancer Drugs: An Investor's Perspective.* Journal of Clinical Oncology., 25, no. 19, e21-e23
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- Google scholar,
- Web of knowledge,
- Spectral Data Base System (SDBS) for organic compounds.

Continue work on Deliverables

Whilst waiting for a SciFinder license to become available you should continue to work on your Deliverables.

Green Chemistry

A discussion of the Green Chemistry within your group.

Facilitation Session 08

Pre Session Preparation

- Biochemistry: chapter 8.
- http://www.whfreeman.com/stryer4/

Enzyme Inhibition

Students should come to the session prepared to discuss the factors affecting enzyme function and the three ways in which enzymes can be inhibited.

Lock and Key Mechanism

Students should draw a 'comic strip' (i.e. a simple sequence of pictures) showing the lock and key model of enzyme function. Make sure each picture has a caption explaining what is happening.

Facilitation Session 09

Pre Session Preparation

- Read the laboratory script for Enzyme Kinematics.
- Biochemistry: chapter 8.
- http://www.whfreeman.com/stryer4/

Enzyme Kinematics

Read the script associated with the Enzyme Kinematics experiment. Use this session to construct a plan for this laboratory session.

Facilitation Session 10

Pre Session Preparation

Background reading.

Discussion of Enzyme Kinematics and Dynamics

Class discussion about the material covered in the previous Expert session.

Facilitation Session 11

Pre Session Preparation

Background reading.

Brainstorming Exercise

Knowing what you now know about enzymes as a class conduct a brainstorming exercise about how you think inhibitors might be found. Discuss methods of finding inhibitors.

Facilitation Session 12

Pre Session Preparation

Review course material so far.

Assessing purity

Class discussion on the various techniques that you have come across so far in the course of your studies for assessing purity (rather than purifying) and determining aspects of structure. What do these techniques tell us?

Facilitation Session 13

Pre Session Preparation

- Re-read notes from ES04.
- http://www.cis.rit.edu/htbooks/nmr/inside.htm
- http://vam.anest.ufl.edu/forensic/nmr.html

Discussion of the physical principles behind *NMR*

Class discussion of the material covered in the previous Expert session.

Introduction to Patent Laws

In your group generate a series of questions for the Expert Session on Patent Law.

Facilitation Session 14

Pre Session Preparation

- Re-read notes from ES05.
- Fundamentals of Organic Chemistry: chapter 13.
- http://spectraschool.org
- Spectroscopic methods in organic chemistry, 5th Ed.

Discussion of Patent Law

Class discussion of the material covered in the previous Expert session.

NMR spectra

Download the IR and MS for the inhibitor being studied from SDBS.

Facilitation Session 15

Pre Session Preparation

- Re-read notes from ES06.
- Fundamentals of Organic Chemistry: chapter 13.
- http://spectraschool.org

Discussion of assigning NMR spectra

Class discussion of the material covered in the previous Expert session.

Deliverables

Please name your deliverables in accordance with the standard naming convention (see the handbook for details). A sample filename is provided for you to cut and paste - please complete with submission date and username/group letter as appropriate.

All deliverables to be submitted to the subject centre.

Please note that although deliverable deadlines (except for CLEs) are at the end of the module, you are strongly urged not to leave all work on the deliverables until the final weekend! In particular, if you would like formative feedback on your works-in-progress from your facilitator and/or experts, please provide them with draft copies in good time.

DELIVERABLES	TYPE	FILENAME	DUE	WEIGHTING
CLE01:	I	PA1012_I_CLE01_*username_date*.pdf	Week 2, Day 1	30%
CLE02:	I	PA1012_I_CLE02_*username_date*.pdf	Week 3, Day 1	
CLE03:	I	PA1012_I_CLE03_*username_date*.pdf	Week 4, Day 1	
CLE04:	I	PA1012_I_CLE04_*username_date*.pdf	Week 5, Day 1	
D01: Report	G	PA2013_G_D01_Report_*groupletter_date*.pdf	Week 5, Day 1	50%
D02: Funding Proposal	I	PA2013_I_D02_FundingProposal_*groupletter_date*.pdf	Week 5, Day 1	10%
D03: Funding Proposal Interview	I		Week 5, Day 2	10%

Core Learning Exercise 01

1. Define the term ‘catalyst’. [2]

2. Explain how a catalyst alters the rate of a chemical reaction, using an energy profile diagram as part of your answer. [3]

3. Complete the following table: [9]

Scent	**Alcohol name**	**Alcohol structure**	**Carboxylic acid name**	**Carboxylic acid structure**	**Ester name**	**Ester structure**
Nail polish remover	Ethanol		Ethanoic acid		Ethyl ethano-ate	$CH_3C(O)O-CH_2CH_3$
Pine-apple	Butanol		Butanoic acid		Butyl butan-oate	
Pear		$CH_3CH_2-CH_2OH$		$CH_3CH2C(O)OH$	Propyl ethan-oate	$CH_3C(O)O-(CH_2)_2CH_3$
Flowers		CH_3OH		$CH_3(CH_2)_3C-(O)OH$		$CH_3(CH_2)_3C(O)OCH_3$
Jasmine	Benzyl alcohol	$Ph*CH_2-OH$			Benzyl ethan-oate	
Pepper-mint					Methyl ethan-oate	

*Ph = a benzene ring.

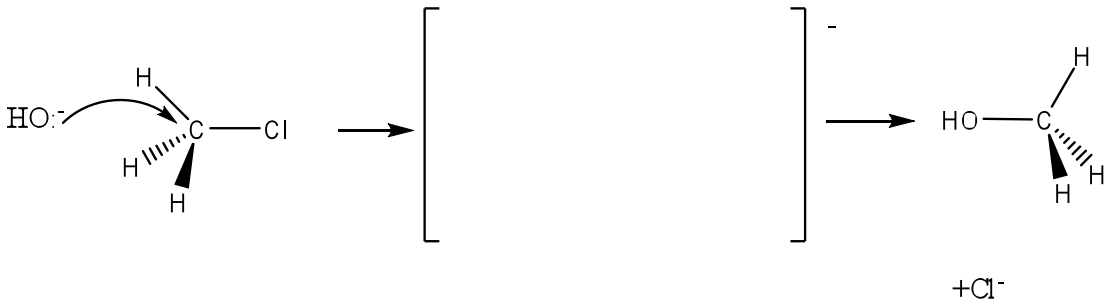
4. Identify the limiting reagent and then use this to determine the theoretical mass and the percentage yield of the following esterification reaction.

In the synthesis of ethyl ethanoate, 21.00 g of ethanoic acid and 63.00 g of ethanol were used. To this was added a catalytic amount of concentrated sulphuric acid. The final product was obtained as a clear liquid with mass 24.85 g.

5. In a reaction mechanism, what does the ‘curly arrow’ represent? [2]

6. (a) Give the reaction mechanism for the synthesis of ethyl ethanoate, stating any other reagents/conditions required. (You may wish to use the programme ‘chemdraw’ for this but it is not compulsory) [5]
   (b) Explain how sulphuric acid acts as a catalyst in this case. [2]
   (c) What is the fate of the oxygen atom from the hydroxyl group of the ethanoic acid? [2]
   (d) On your reaction mechanism, clearly label two reaction intermediates. [2]

7. In the following single step reaction, the chloro leaving group leaves at the same time as the hydroxy group enters from the opposite side of the molecule.



(a) Draw the transition state for the reaction in the square brackets provided. [2]

(b) Draw an energy profile diagram for the reaction, labelling the transition state. [2]

(c) Describe the difference between a transition state and a reaction intermediate. [2]

8. Compound X is slightly soluble in water, but more soluble in the organic solvent isopropanol. Describe how you would extract it from an aqueous solution into a solution of isopropanol, naming any equipment you would use. [5]

9. Describe the purpose of:
(a) A reflux [2]
(b) A distillation [2]

10. It is known that primary alcohols can be converted into carboxylic acids by refluxing with acidified dichromate. Describe how you might produce ethyl ethanoate using ethanol as your only organic reagent. [2]

Core Learning Exercise 02

1. Your fifteen year old cousin wants you to help her win her school's 'Best Crystals' competition, in which students are required to use only copper sulphate, water and general laboratory apparatus.

(a) Describe what you would tell her to do in order to obtain the best possible crystals, giving reasons why the method should work. [5]
(b) Describe the properties of a good solvent for recrystallisation. [2]
(c) If there were no suitable single solvent for recrystallisation, explain how you might go about finding a good two-solvent system. [3]

2. All types of chromatography, whether column chromatography, thin-layer chromatography, high performance liquid chromatography or gas chromatography, rely on separation of the compounds occurring. On the basis of which physical properties does this separation occur? [4]

3. Solutions of two forms of the same compound labelled (L) and (D) get placed in unlabelled flasks.

(a) Describe how the labels (L) and (D) relate to the rotation of plane polarised light in the molecule glyceraldehyde. [2]
(b) Describe how you would assign a molecule as (L) or (D) giving an example. [2]

4. Describe the problems that you might encounter if you were to scale-up an undergraduate laboratory based esterification reaction to an industrial scale. [8]

5. Put the following stages of commercialisation of a drug molecule into the correct order, writing a sentence describing each. [14]

- small scale 'academic' testing
- feasibility studies
- synthesis in academic lab
- industry synthesis to confirm properties
- Full-scale production
- production for safety testing
- pilot plant

6. Aspartame, a compound widely used as an artificial sweetener, is reputed to have been discovered when a researcher working on an unrelated subject, accidentally tasted a small amount of substance.
(a) Whilst aspartame is not a 'drug' as such, this story broadly fits into which of the three main routes to drug discovery? [2]
(b) Give an example of another method of drug discovery. [4]

7. Describe the advantages of 'double blind' testing of the efficiency of new drugs. [4]

Core Learning Exercise 03

1. Haemoglobin is an important biological transporter of oxygen. It is a protein consisting of four subunits, which alters its conformation slightly depending on the partial pressure of oxygen, and in so doing, allows the reversible bonding of oxygen to it. By reference to the molecule haemoglobin, describe the primary, secondary, tertiary and quaternary structure of proteins. [4]

2. Enzymes are organic catalysts. Define the term ‘catalyst’ and state what properties a catalyst must have. [2]

3. Why must a cell have thousands of different kinds of enzymes? [2]

4. PKU or phenylketonuria is a disease tested for in almost all babies in the UK. Explain the cause of the disease at the enzymatic level, and explain why it is so important to catch this disease early on. [4]

5. Whilst enzymes generally have only a small temperature range within which they operate productively, they can be stored quite readily at low temperatures for later use. However, if enzymes are heated and then later cooled, they are denatured and no longer work. Explain why this is so at the molecular level. [4]

6. Enzymes usually have a very specific pH range within which they work optimally. Explain what happens at the molecular level which alters their function outside of this optimal range. [4]

7. The transition state of a reaction is the point at which the molecule is halfway between its shape as a reactant and its shape as a product. Explain why it is necessary for enzymes to have a high affinity for the transition state, rather than for the reactant or the product. [4]

8. What is an enzyme cofactor? Give an example. [4]

9. Two variables which can give us a lot of information about enzymes are the Michaelis Constant, KM, and the maximal velocity, Vmax.

(a) Give a description of each variable in words. [4]
(b) Give a mathematical definition of each, defining all terms. [4]
(c) A Lineweaver-Burke double reciprocal plot can be used to find these values. Explain how you would go about achieving this. [4]

10. There are three modes of inhibition of enzymes.

(a) Describe each of these, using diagrams where appropriate. [6]
(b) Explain how you would use KM and Vmax to distinguish between the two forms of reversible inhibition. [4]

Core Learning Exercise 04

1. Outline the type of information that can be obtained from the following techniques:

(a) Microanalysis [2]
(b) Infrared Spectroscopy [2]
(c) Mass spectrometry [2]
(d) ^{1}H NMR Spectroscopy [2]
(e) Melting point analysis [2]

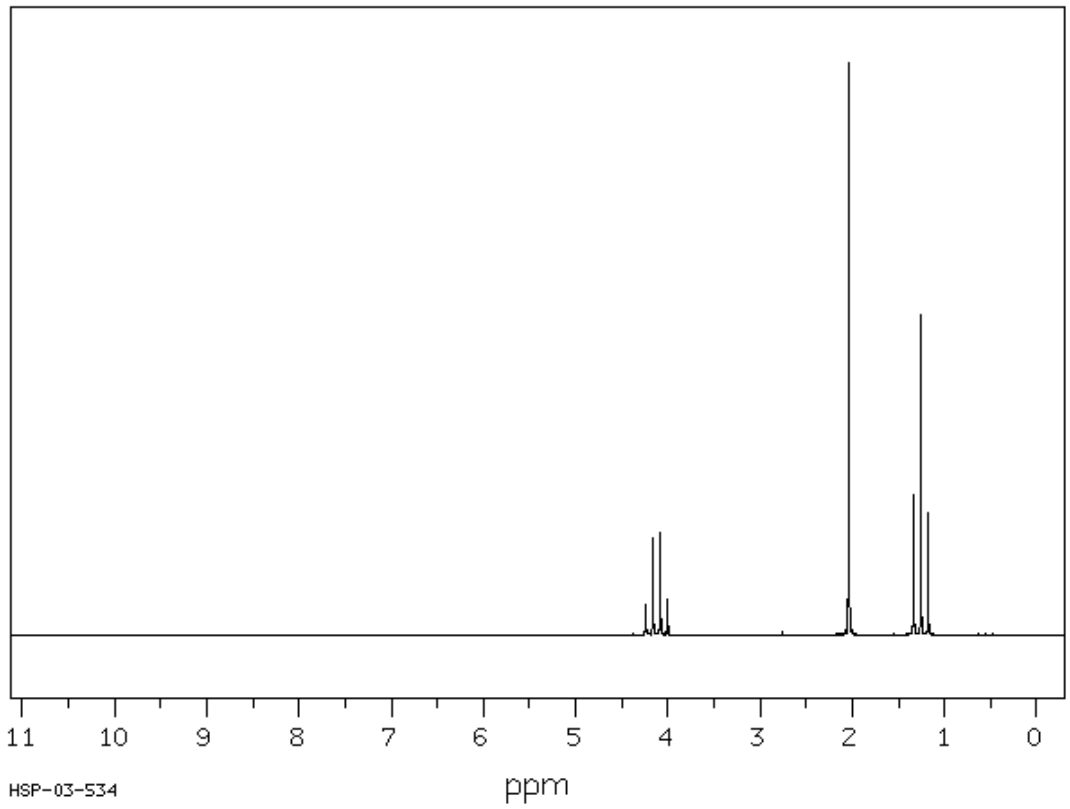
2. Below are the microanalysis results of a compound showing a parent ion peak in its mass spectrum at 122.

Microanalysis;

Element	Composition
C	68.8 %
H	5.0 %
O	26.2 %

(a) Give the empirical formula of the compound. [3]
(b) Give the molecular formula, stating your reason. [2]
(c) Give a possible structure for the compound. [2]

3. Given below is the H^{1} NMR spectrum of an ester product synthesised from ethanol and ethanoic acid. By drawing the structure of the compound and labelling it appropriately, assign the peaks on the spectrum to your compound, stating the reasons for your assignments. [6]



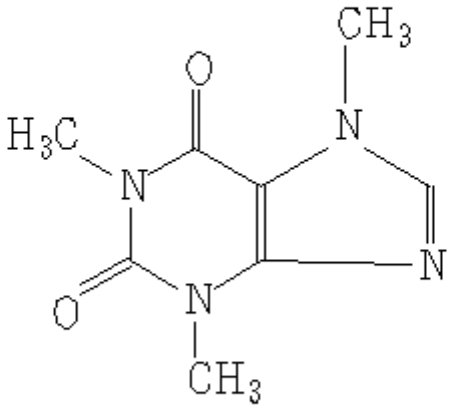
Assign. Shift (ppm)

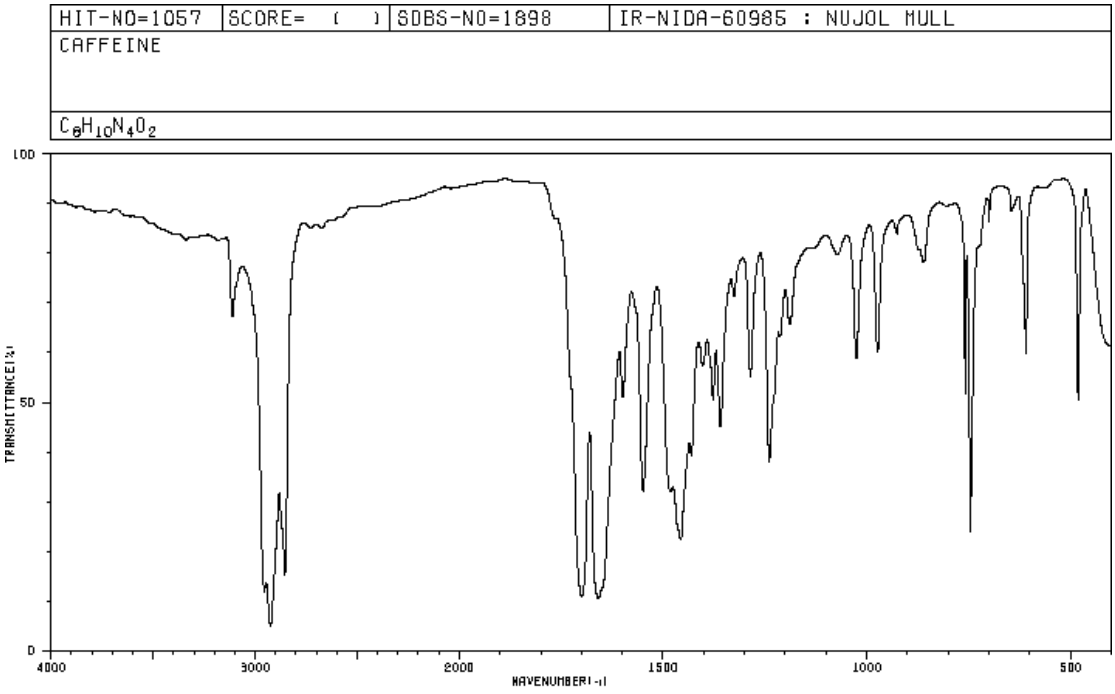
A 4.119
B 2.038
C 1.260

4. Shown below is the structure of caffeine with its infrared spectrum taken as a nujol mull. Using the appendix from your first organic synthesis lab (or other sources):

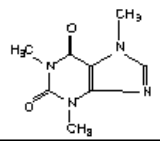
(a) Assign the bands that have come from the nujol [2]
(b) Give possible assignments for at least three other bands in the infrared spectrum. [3]

SDBS-NO= 1898
CAFFEINE





3110	64	1549	31	1286	53	927	81	638	86
2954	11	1457	21	1240	36	873	77	610	57
2925	4	1431	37	1213	60	861	74	482	49
2854	14	1404	56	1189	62	769	60		
1699	10	1378	49	1072	77	746	23		
1659	10	1360	45	1026	57	700	64		
1599	49	1326	68	974	68	645	84		

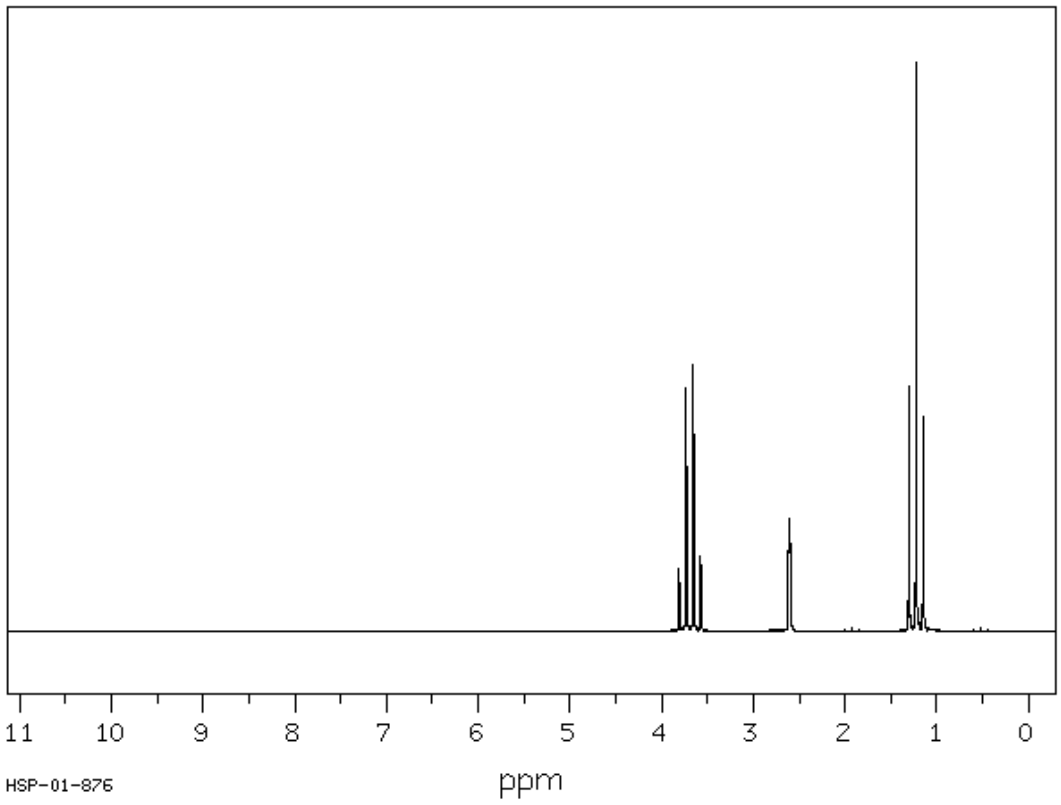


5. Below are some spectra from a small organic molecule. Use the information provided to ascertain the structure of the molecule, assigning all the spectra as fully as possible, and explaining all of the data. [15]

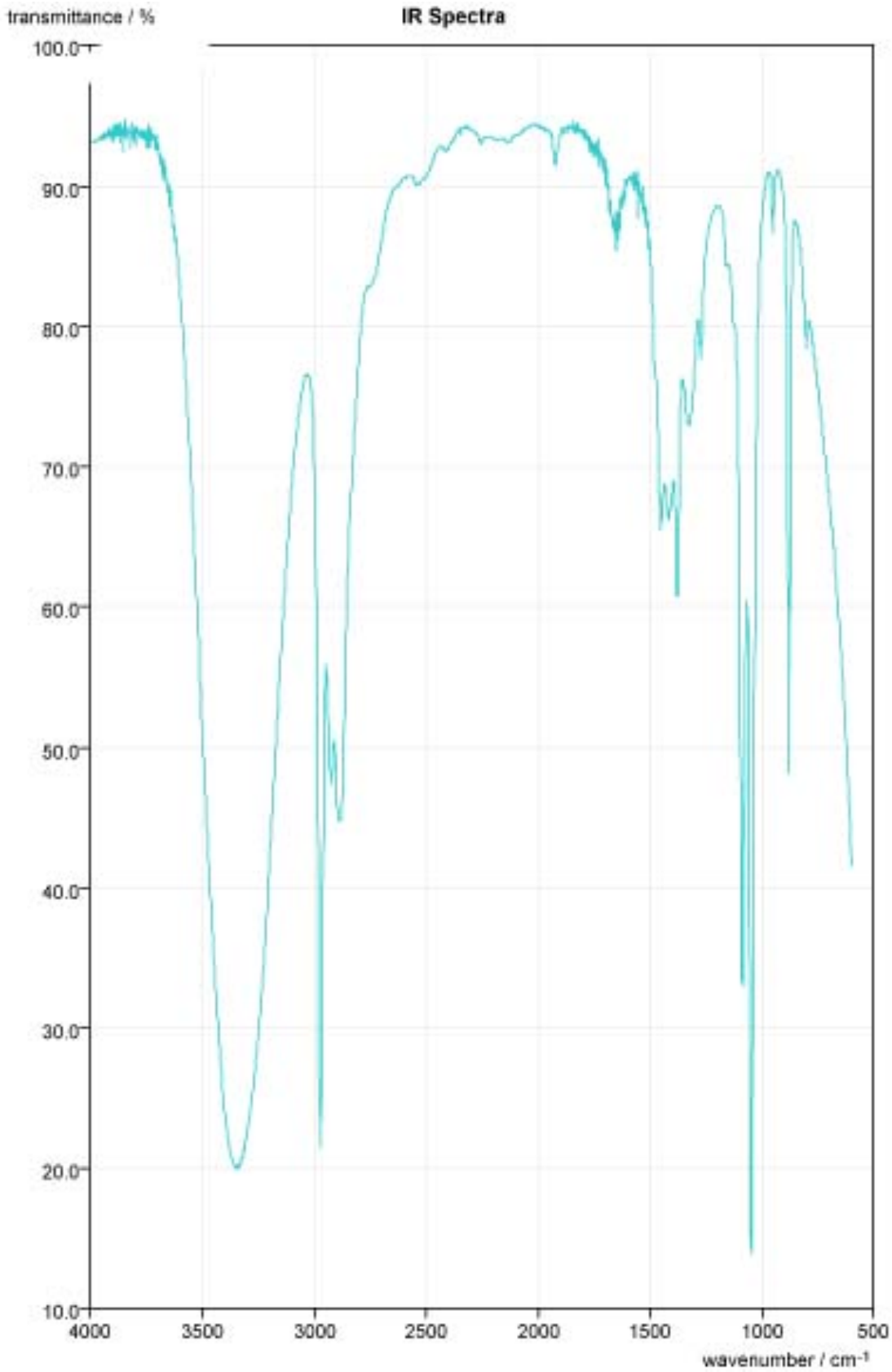
Composition:

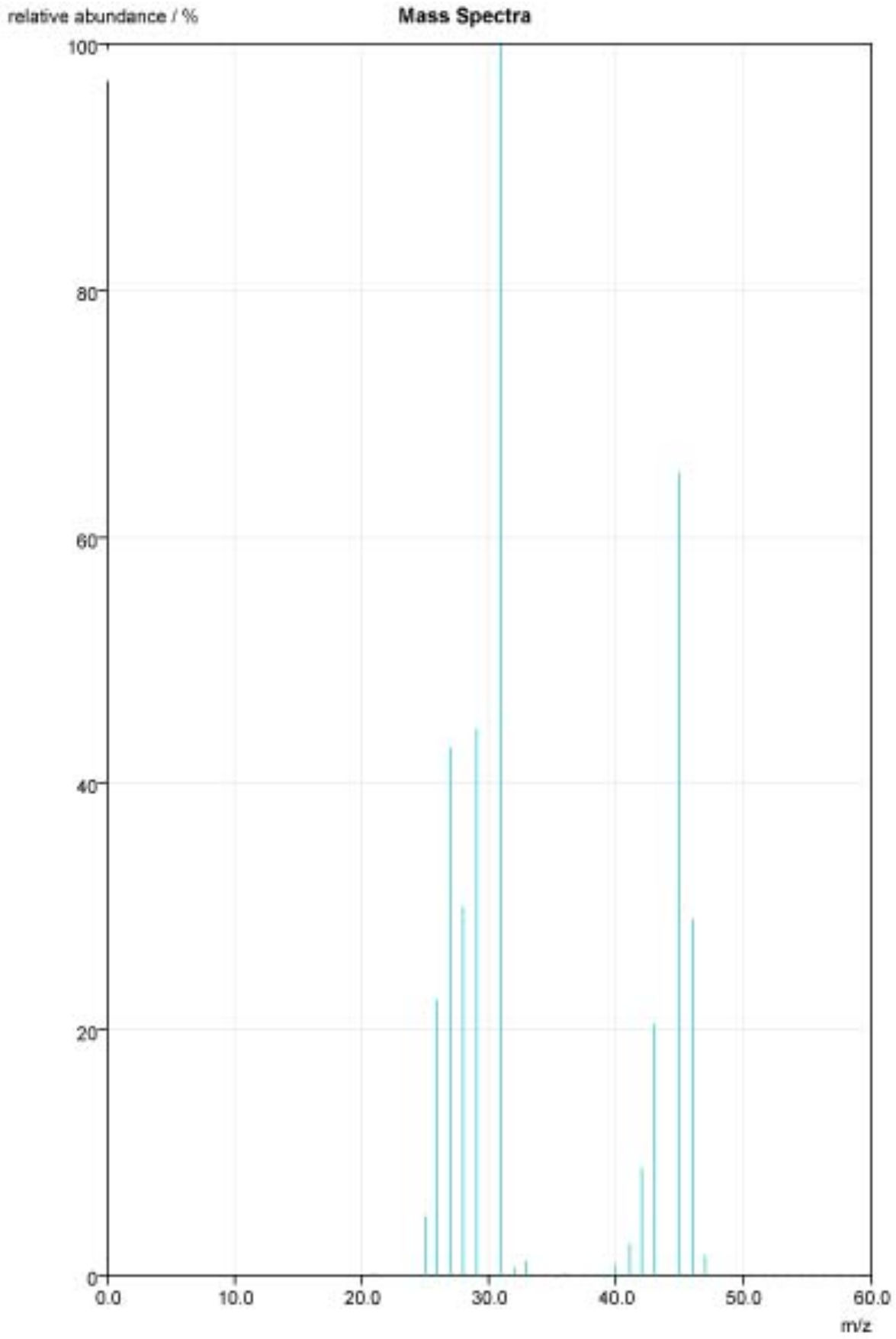
C	52.17 %
H	13.04 %
O	34.78 %

^{1}H NMR spectrum:



Hz	ppm	Int.
341.25	3.811	109
334.00	3.730	427
327.00	3.652	469
320.19	3.576	132
233.44	2.607	199
232.69	2.599	168
116.63	1.303	430
115.13	1.286	23
109.75	1.226	1000
108.06	1.207	36
107.38	1.199	25
102.63	1.146	376


IR Spectra
transmittance / %
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
4000
3500
3000
2500
2000
1500
1000
500
wavenumber / cm-1



6. (a) What is intellectual property? [2]

(b) Name 4 different types of intellectual property. [1]

7. What are the criteria for determining whether a patent can be granted for an invention? [4]

Deliverable 01: Report

As a group you should write a report responding to Simon MacIntyre's memo (given in the Problem Statement) at an appropriate scientific level. The report should be ~4000 words.

Deliverable 02: Funding Proposal

As part of your academic career you want to develop the process described in deliverable 01 further. As such you must convince an appropriate University funding body to support your research.

Individually write a funding proposal to be submitted to the University funding body; this should be approximately 2 sides of A4 (~500-1000 words).

Deliverable 03: Funding Proposal Interview

As part of your academic career you want to develop the process described in deliverable 01 further. As such you must convince an appropriate University funding body to support your research.

You will be interviewed on the scientific content of the proposal you submit. The interview will last ~10 minutes; you will not need to prepare additional materials or slides for this deliverable.

Supplementary Material

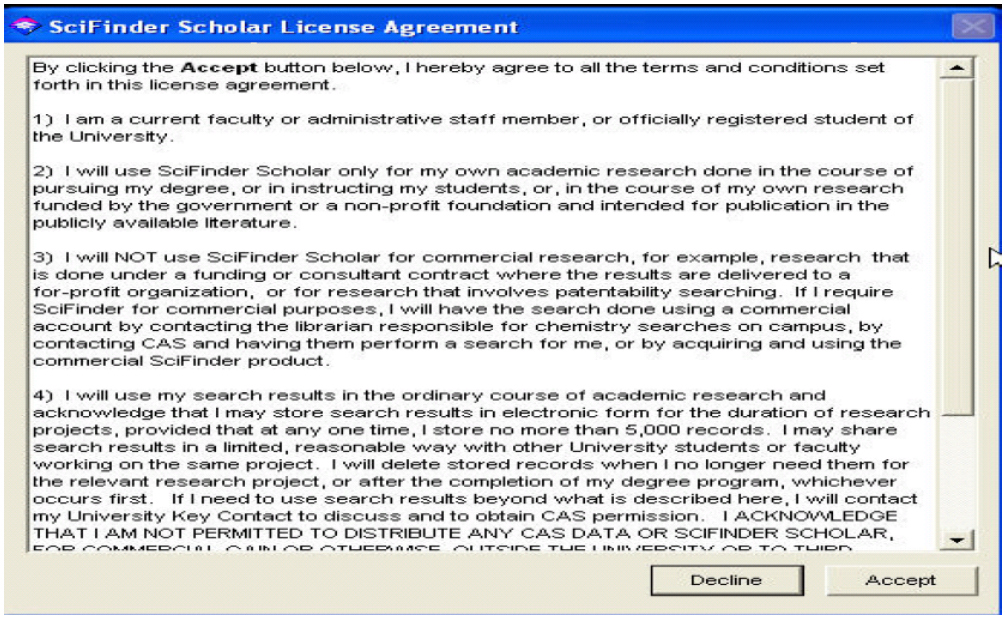
Basic Guide to SciFinder Scholar

What is SciFinder Scholar?

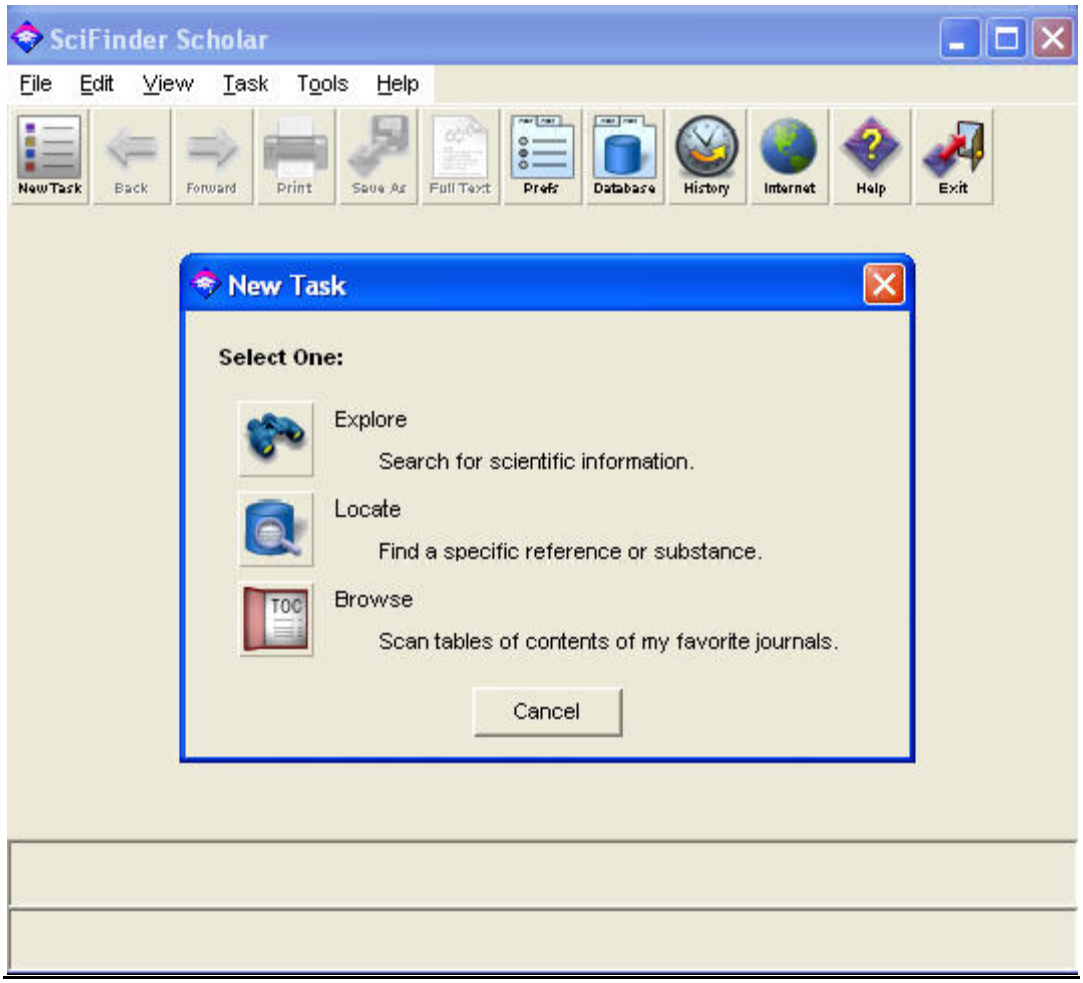
A desktop software package available in CFS allowing staff and students to search databases produced by the Chemical Abstracts Service and the National Library of Medicine.

You may need to try several attempts to log into SciFinder Scholar, as the University of Leicester only have a **two user concurrent licence**.

Once logged in you will need to click 'accept' on the SciFinder Scholar licence agreement each time you use the database.



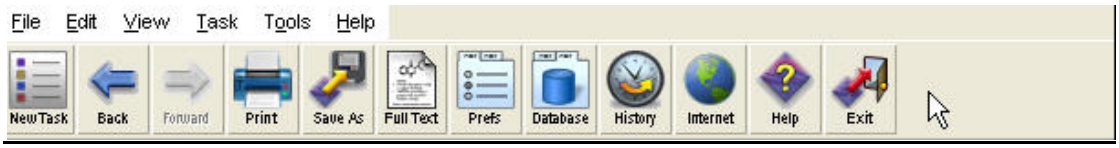
Main Menu



Click on ‘explore’, ‘locate’ or ‘browse’ to search.

Toolbar

The toolbar allows you to navigate around the site, and to print or save information. It also allows you to refine your searches, or access the internet:



New Task: Return to the main menu. Begin a new search Load "Explore" menu.

Back: Move backwards in current search history.

Forward: Move forwards in current search history.

Print: Prints the displayed window according to setup in Print setup some configuration options available Compact = Titles only Standard= Compact plus bibliography Summary= Standard plus abstract & patent family (where available) Full=Summary plus indexing, controlled terms & citations (CA only).

Save As: Answer sets can be saved in several formats

- Rich Text Format (.rtf,) (NB can only save reactions as RTF) Plain ASCII (.txt)
- Quoted format (.txt) (Use for import into Access, Excel, Lotus)
- Tagged format (.txt) (Use for import into Endnote, ProCite, RefMan)
- Answer keys (.txt)

Full Text: Access full text of documents via ChemPort (where available)

Database: Select databases to be searched. Can only be changed at the **start** of a task. Default setting searches all databases at once i.e.: CAPLUS, REGISTRY, CASREACT, MEDLINE.

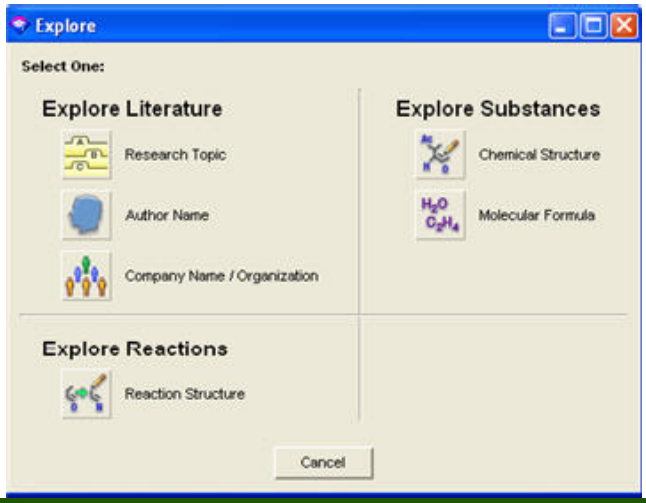
History: Details of all actions performed in current session.

Internet: Launches web browser. Connects to ACS Chem Centre, ACS Publications Chemical Abstracts Service, Scifinder Scholar Web site.

Explore menu

Take the case that we want to find out about any articles published concerning pesticide residues in milk. We don't know the names of any potential researchers, nor any details about the relevant structures.

Click on 'new task' on the tool bar, and then the most appropriate of the three choices is 'Explore'. Click on it, and the following menu will appear:



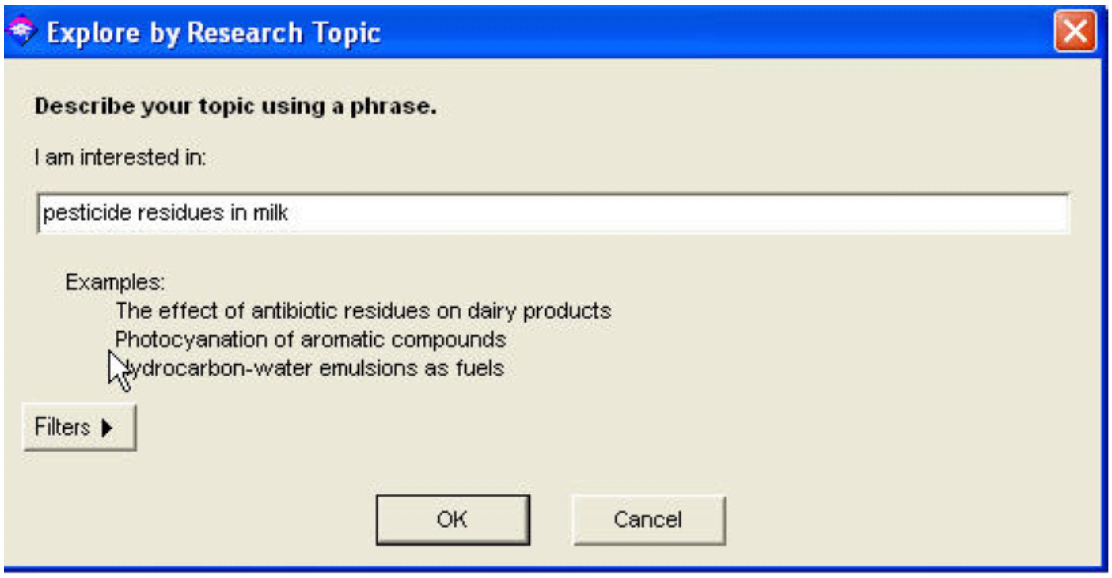
Have a look at all the choices on offer. Clearly again, as we do not know structure or author details, the most appropriate choice of those on offer is 'Research Topic'.

Tasks:

Explore Research Topic: How to search by subject…

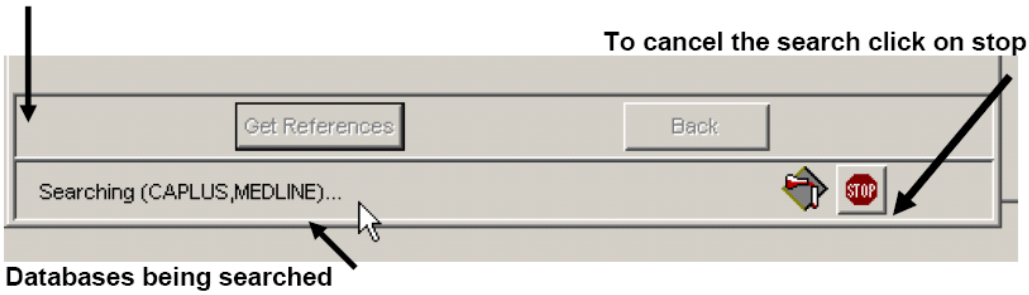
1. Select Research Topic from the 'Explore' menu.
2. Enter the phrase as you would normally complete the sentence,*" I am interested in…"* in addition to this type 'and review' at the end of the sentence, as review papers normally give good summaries of your research topic of interest.
3. **Synonyms** are automatically searched e.g. enter cancer, SFS searches cancer, neoplasm, carcinoma etc.
4. **American and British Spellings** automatically mapped & searched
5. Not case sensitive
6. The phrase can be any length (the dialogue box scrolls on)

Copy the following example:



Filters limit search by: author, year, company name, language, document type.

To cancel the search click on stop.
While the Scifinder is searching the following will appear at the bottom of the screen:

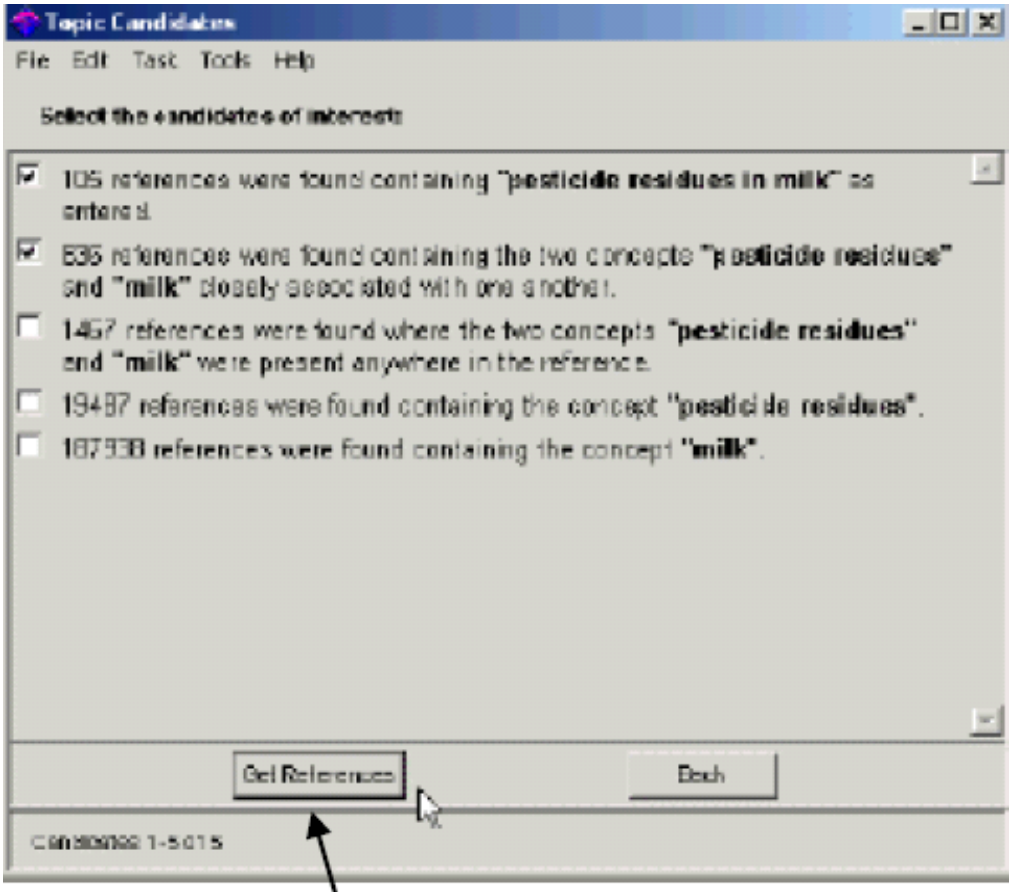


Displaying Results:

A list of relevance ranked candidates containing the concepts in your chosen search will be presented as follows:

1. Phrase as entered (exact order)
2. Closely associated (all concepts identified in same sentence)
3. Anywhere in record (same record)
4. Combinations of concepts (More than one per record – where you have searched for three or more)
5. Single concepts in records
6. The number of references is given for all candidates
7. To view records: Select the appropriate boxes: First 10,000 can be viewed, printed or saved.
8. Complete set may be analysed.

Tick the top 2 boxes of the options listed.


Topic Candidates
File Edit Task Tools Help
Select the candidates of interest:
105 references were found containing "pesticide residues in milk" as entered.
836 references were found containing the two concepts "pesticide residues" and "milk" closely associated with one another.
1467 references were found where the two concepts "pesticide residues" and "milk" were present anywhere in the reference.
19487 references were found containing the concept "pesticide residues".
187938 references were found containing the concept "milk".
Get References
Back

Click on 
Get References

1. References in default format & order
Standard format
accession # order

To change defaults select Prefs from the toolbar

3. Search terms are highlighted

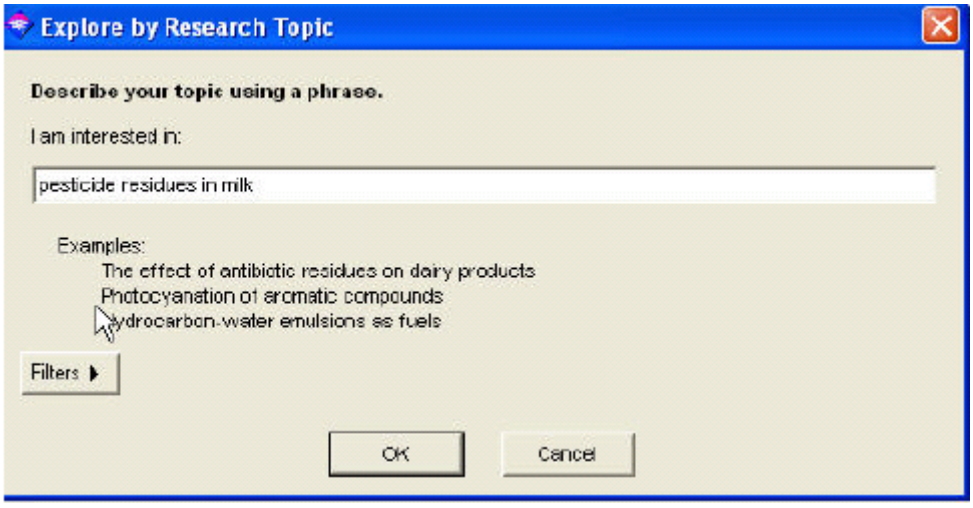
4. Titles in bold

5. Click on  to view details of reference (abstracts, index hypertext links)

6. Click on  to find document details or full text (where available)

To modify the search click on 

you will then return to the original screen.



Take the case that you found a paper that was really interesting, and you want to know what other papers that same author has published.

Click on 'New Task' on the toolbar. Then click 'Explore' again.

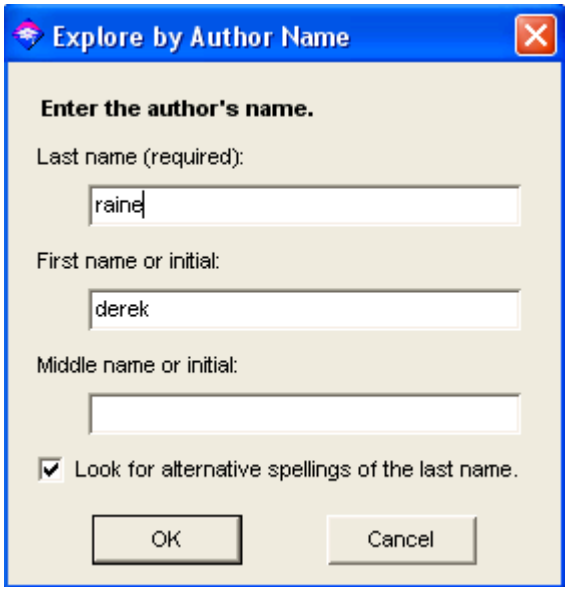
This time, click on 'Author Name'.

Explore author name

Enter as much of the author's name as you know:
Scifinder will search for:

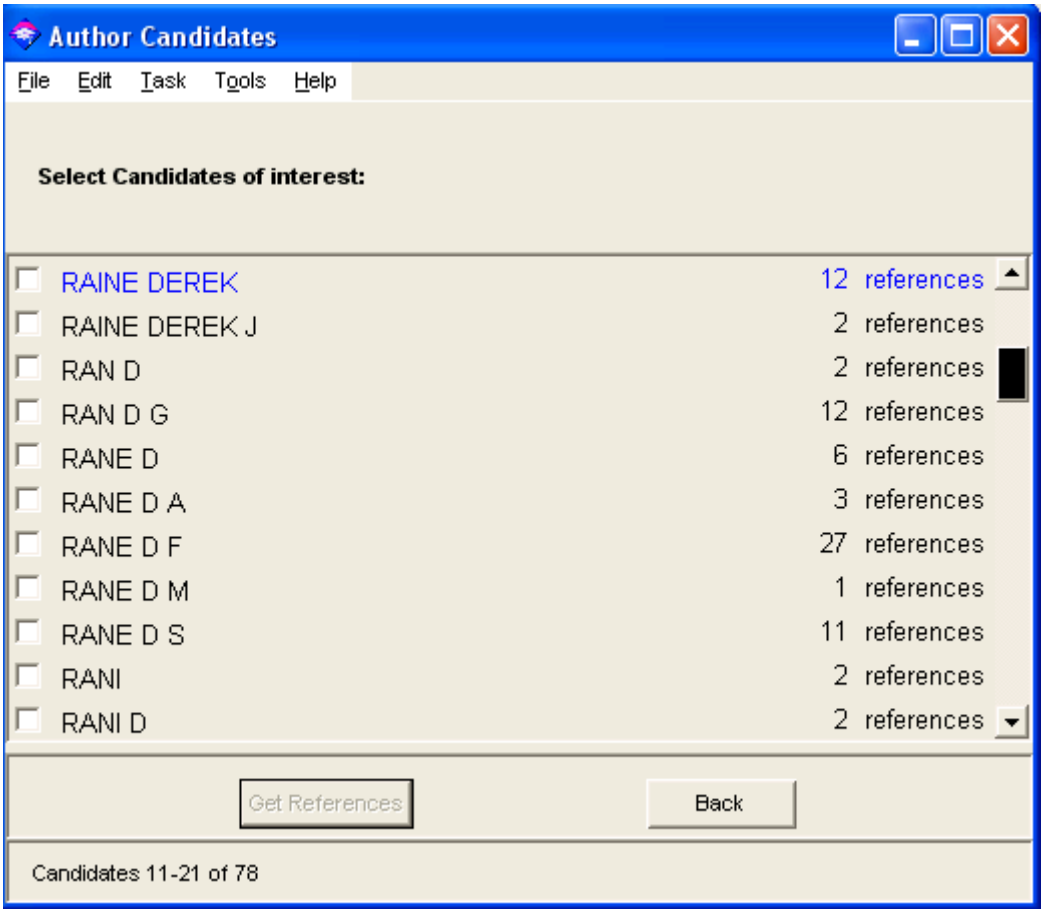
- Exact name as entered
- Common variants of the name
- Similar sounding last names
- Nicknames

Follow this example:



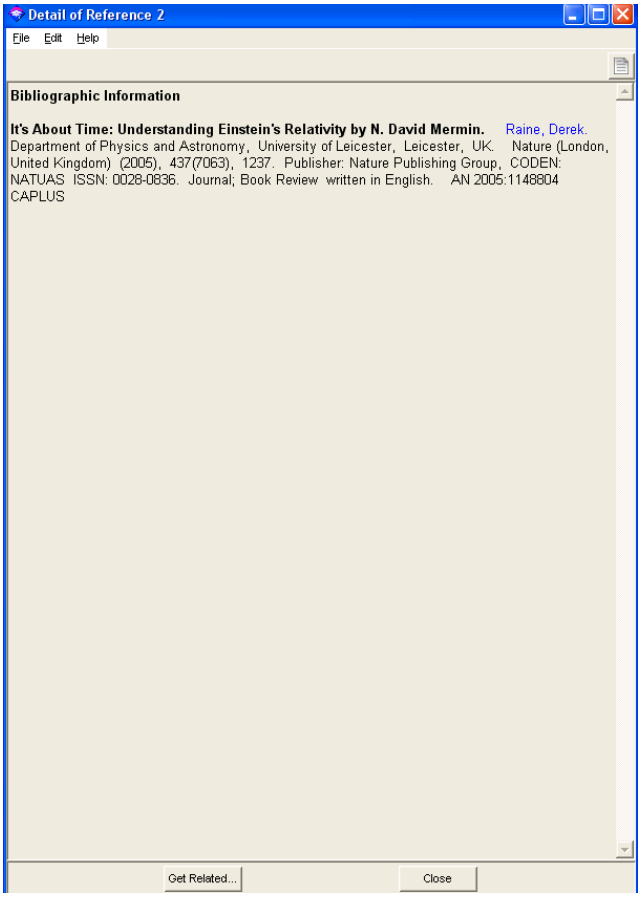
An author candidate list appears

- Includes all variants of the search term entered
- The original name entered is highlighted in blue
- Numbers of references for each author-candidate are given
- *Select variants and click on get references to view records*
- Select back to modify search



1. Search terms are highlighted in blue
2. Titles in bold
3. Click on to  view details
4. Click on  for full text

Try getting the bibliographic information for Dr. Raines 'It's about time' article by clicking on the microscope next to it.

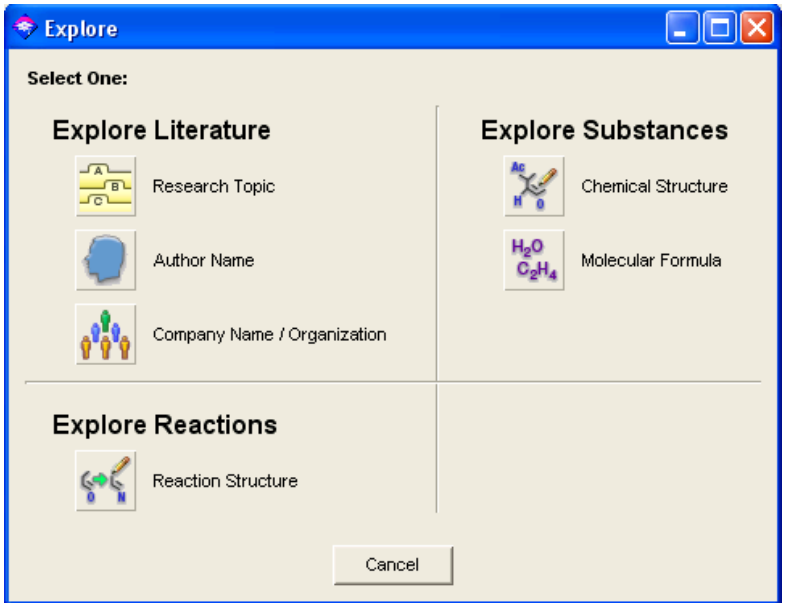


Search by a chemical substance or reaction

Search by:

- Chemical structure (Uses internal drawing package)
- Reaction Structure
- Molecular formula

Click on 'New Task', select 'Explore' and click on 'Molecular Formula'.



Molecular formula

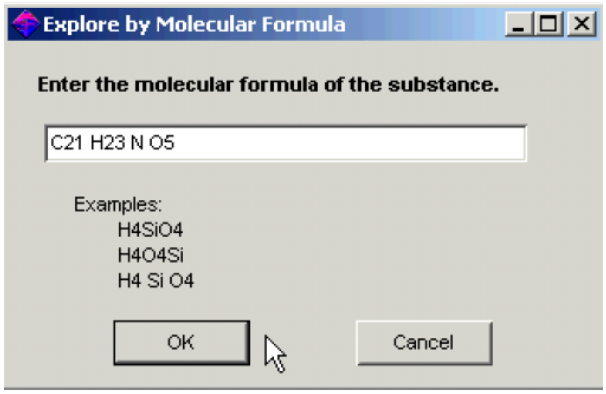
Molecular Formulas may used to find:

- CAS Registry Numbers
- Chemical Names
- Commercial Sources for Chemicals
- Regulatory Compliance Data
- References

Enter molecular formulas with atoms arranged in any order: Scifinder rearranges the molecular formula you entered: Atoms are rearranged in Hill System order.

Hill System Order: C Carbon first (if present), H Hydrogen next (if present) Then all other elements in alphabetical order. Not the preferred method searching, however, because many compounds have the same molecular formula when expressed in this way (Because atoms are summed).

Enter the following example then click ‘OK’;



Searching in this way, you will then be given a choice of structures, from which you can choose the one you are interested in. You can then either get more details about it, by clicking on the microscope, or search for any references relating to it, by clicking on the book icon as before.

Chemical structure search

Click on ‘New Task’, then ‘Explore’ then ‘Chemical Substance’

This allows you to search by drawing chemical structures – structure candidates include:

- Exact structure (as drawn)
- Stereoisomers
- Tautomers
- Co-ordination Compounds
- Radicals of radical ions
- Isotopes
- Polymers

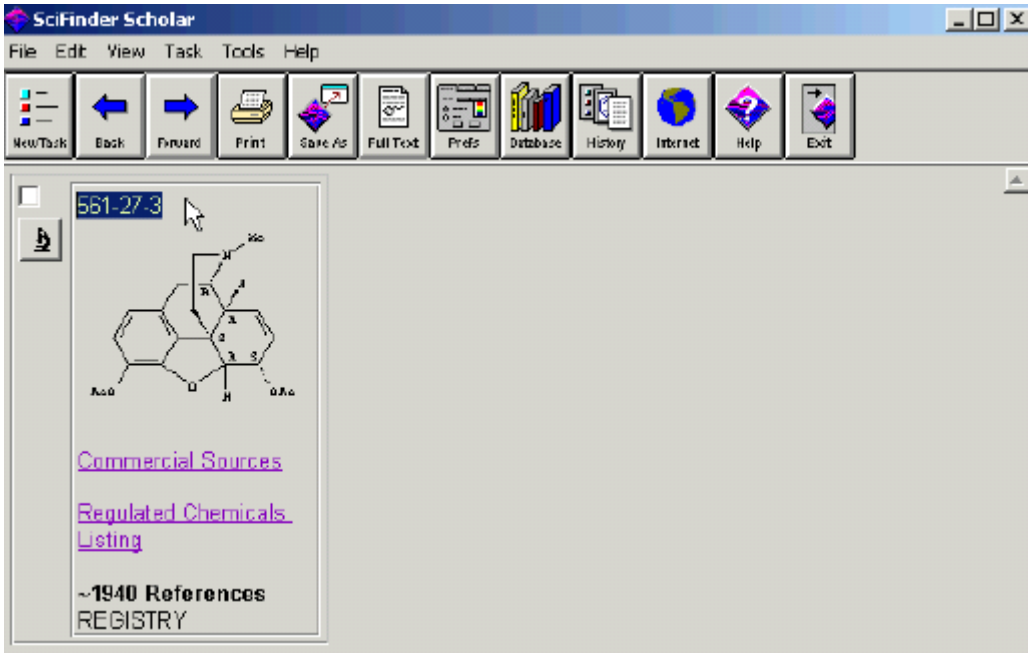
Structures may be:

- Drawn via the Structure Drawing Menu
- Imported from other drawing packages
- Cut and pasted from substance records in the Registry file

Substance Record from Registry

To cut and paste structures from the registry (you’ve already done this in the previous section)

- Highlight registry number in registry results screen from your previous search under molecular formula
- Ctrl C (or Edit/Copy)
- CAS Registry Number is pasted to the clipboard



Chemical Structure Drawing Module

- Open Chemical Structure Drawing Module
- Ctrl V (or Edit/Paste)
- Structure is pasted from the clipboard
- Modify structure
- Search reactions or substances

This allows you to search for similar substances without having to redraw them completely every time.

Reaction structure search

Allows you to retrieve reactions by drawing a participating chemical structure or structures, and / or one or more functional groups.
You may retrieve reactions based on the role played by the structure you have drawn**:**

- Product
- Reactant
- Reagent
- Reactant or Reagent
- Any role (present anywhere in the reaction)
- (Functional groups only) Non-reacting

Reactions may be:

- Drawn via the Reactions Drawing Menu
- Imported from other drawing packages i.e. chemdraw
- Cut and pasted from substance records in the Registry file

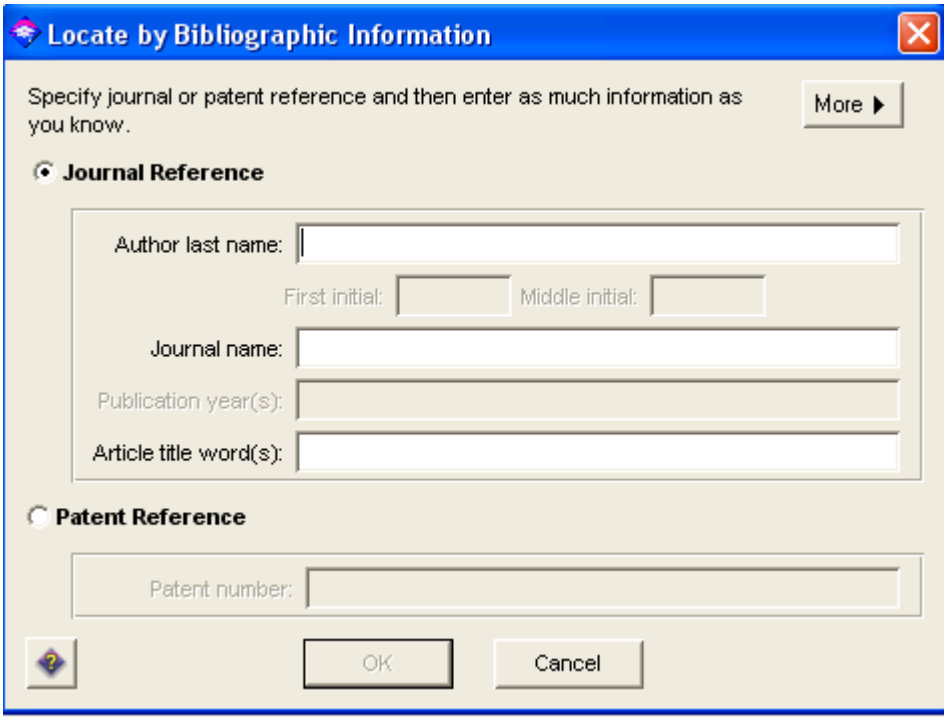
This is all done in a similar manner to the chemical structure search section above.

Locate Literature

Bibliographic information

If you know something about the paper you want to read, i.e. you have some bibliographic information already, but want the paper, then doing the following will bring up the full bibliographic information.

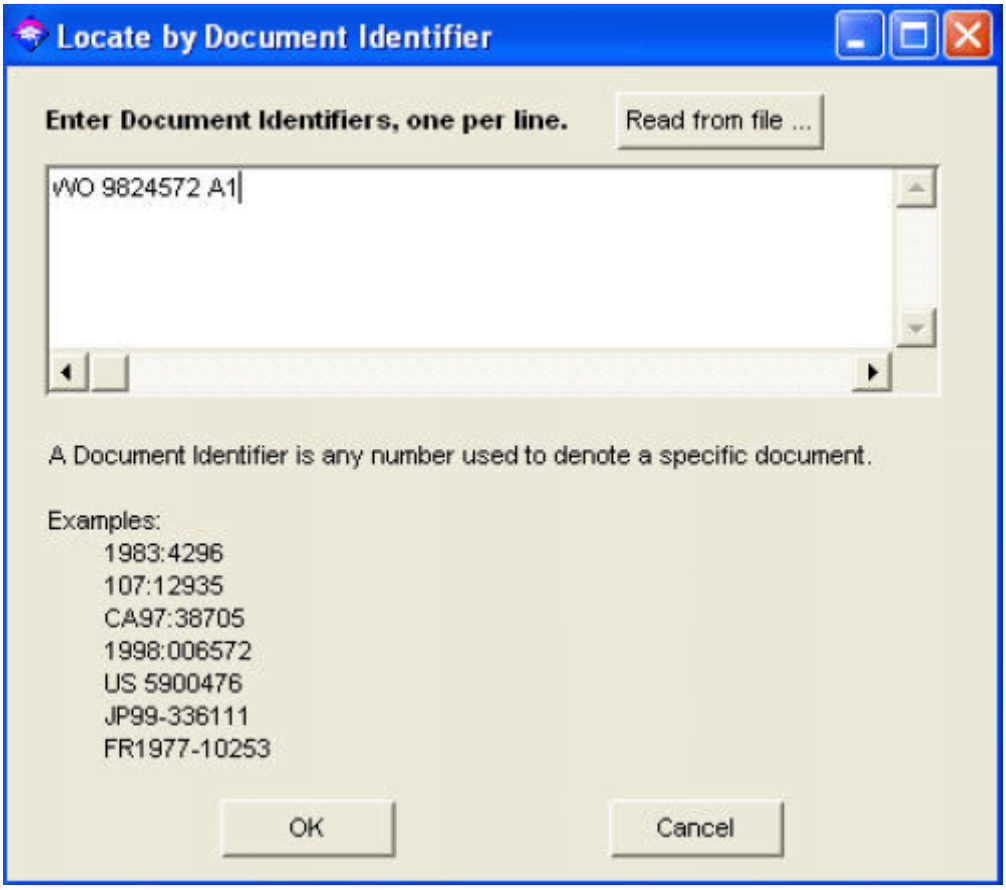
Click on ‘New Task’ then ‘Locate’ then ‘Bibliographic Information’ to bring up the following screen:



Select journal or patent reference via radio buttons, after this, enter information fields. Try entering ‘Raine’ again, and click ‘OK’

Document identifier

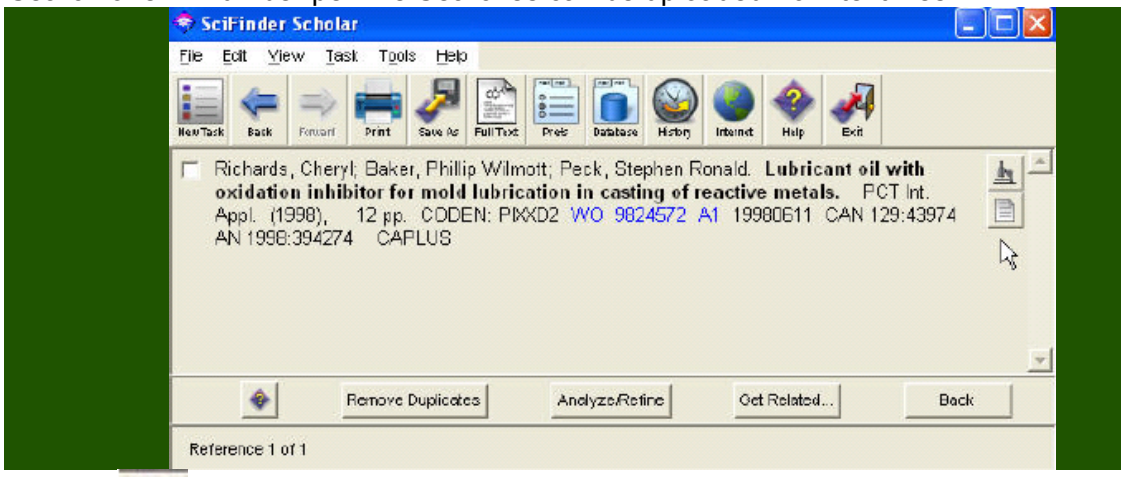
If you have a CAS number or a patent number which you want more information about, then from ‘New Task’, choose ‘Locate’ and then ‘document identifier’. Try the following example:



Any number used to denote a specific document can be searched.

- Patents 3.7 million searchable 1982- 38 countries Many full text WO 9824572 A1
- Patent application & priority numbers
- Chemical Abstracts accession numbers (Follow printed volumes) 1998:394274

Search one ID number per line Searches can be uploaded from text files.



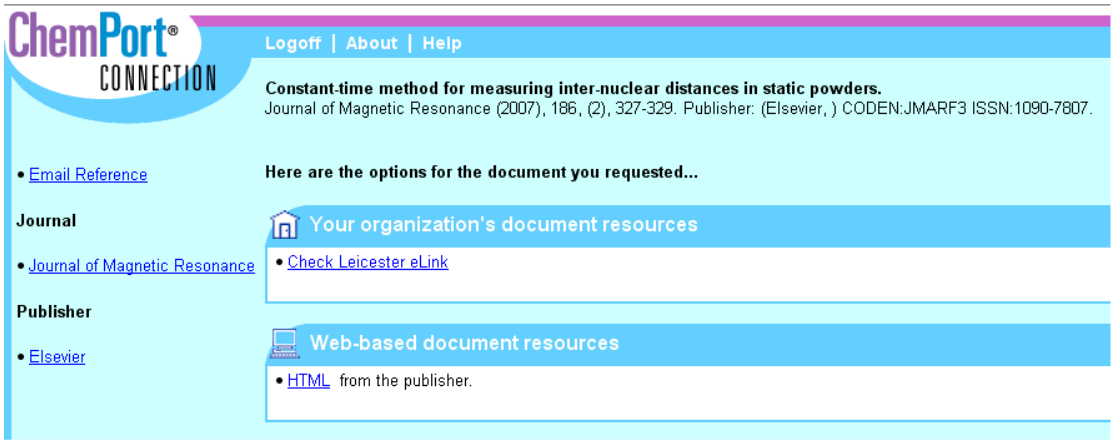
Click on  for full text.
ChemPort is launched through your web browser.

Retrieving full text patents/journals via ChemPort connection.

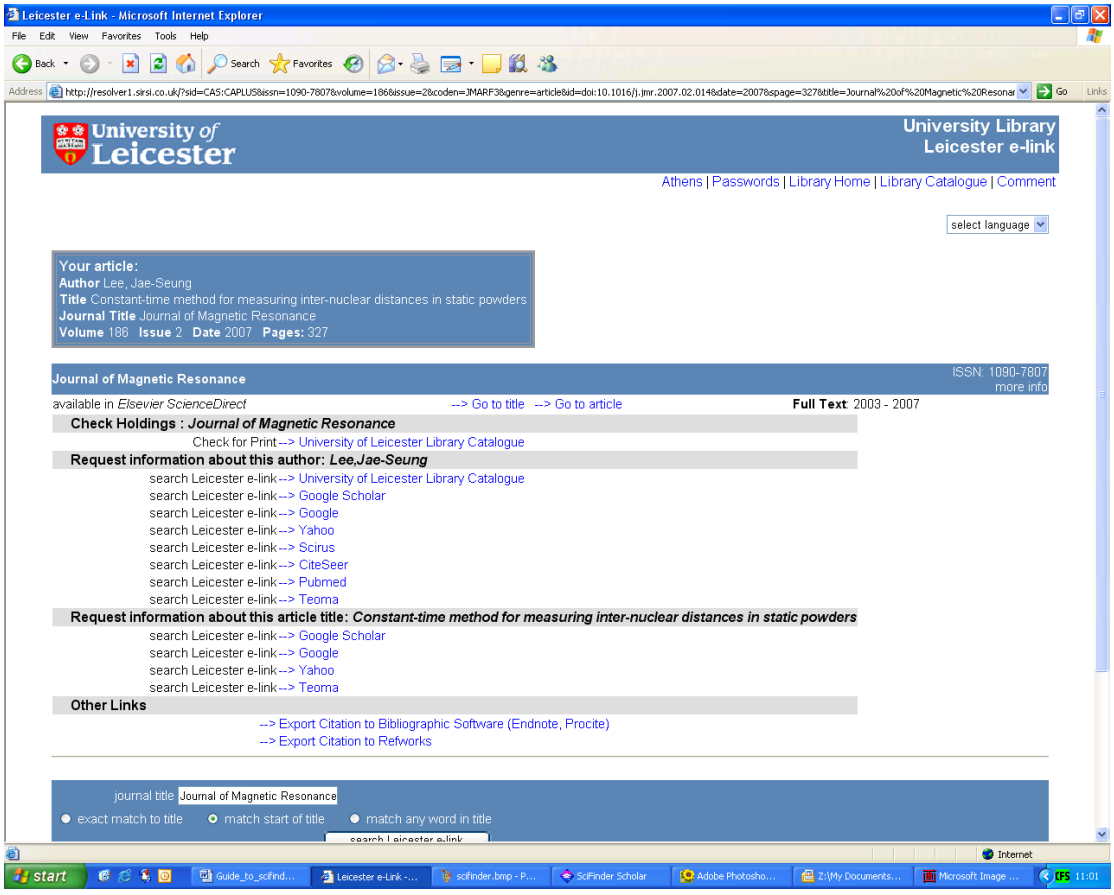
When you have found a journal article or patent you are interested in, you can look at the whole article or patent as follows:

Click on ‘New Task’ and ‘Explore’, then ‘Research Topic’ and type in ‘Measuring inter-nuclear distances, and then click ‘OK’. Tick the first box and then click ‘Get References’. Select the article ‘Constant time method for measuring inter-nuclear distances’

Click on  in document lists for access to full text
ChemPort is launched through your web browser and a screen similar to the following will appear (but with the polarimetry article).



In order to upload the patent/journal click on ‘check Leicester eLink’ which will give you access to all of the electronic materials that Leicester University is subscribed to.

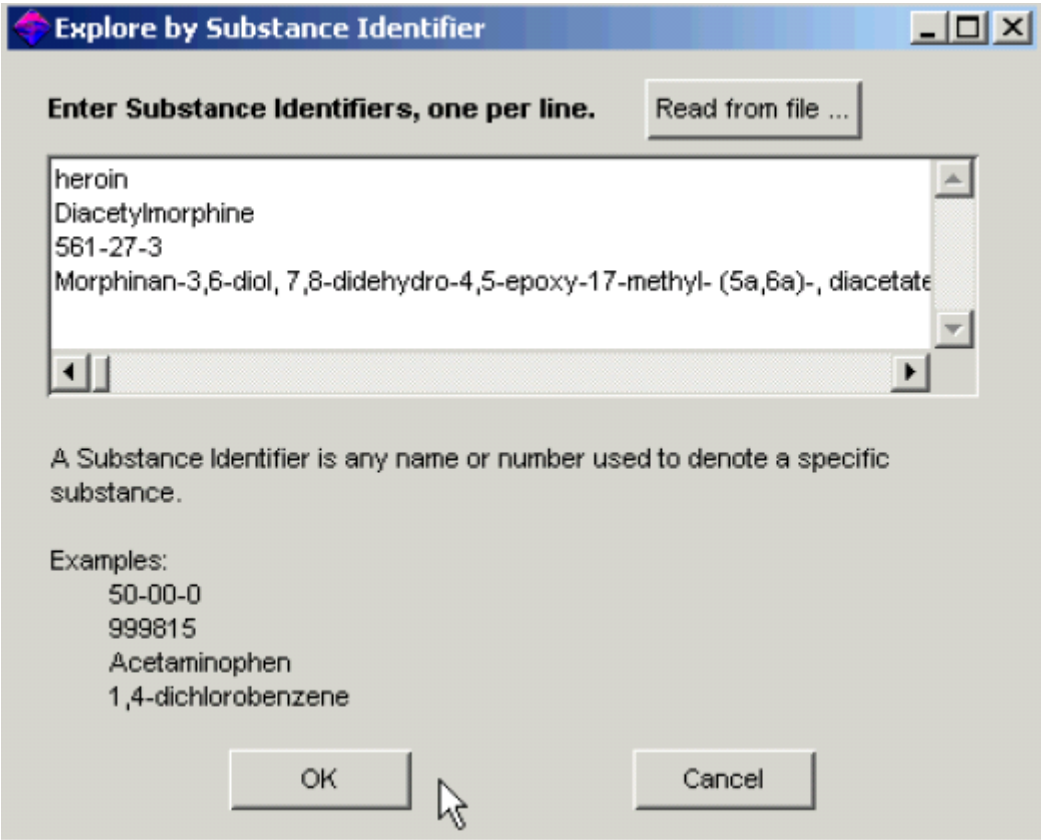


Once you have reached this web page the location of the journal can be found, in this case it is available in the Elsevier ScienceDirect database. (Please note that in some cases not all journals can be found electronically). Click on 'Go to article' to retrieve your chosen article. (If the article appears as an html document, simply scroll down the screen and click on pdf in order to access the pdf version of this article).

Locate substances

If you want to find out more about a particular chemical, of which you have either the name or number to identify it, then you can search for references about it in the following way:

Click on 'New Task', then click 'Locate', and 'Locate Substances'. Enter 'heroin' in the box which appears.

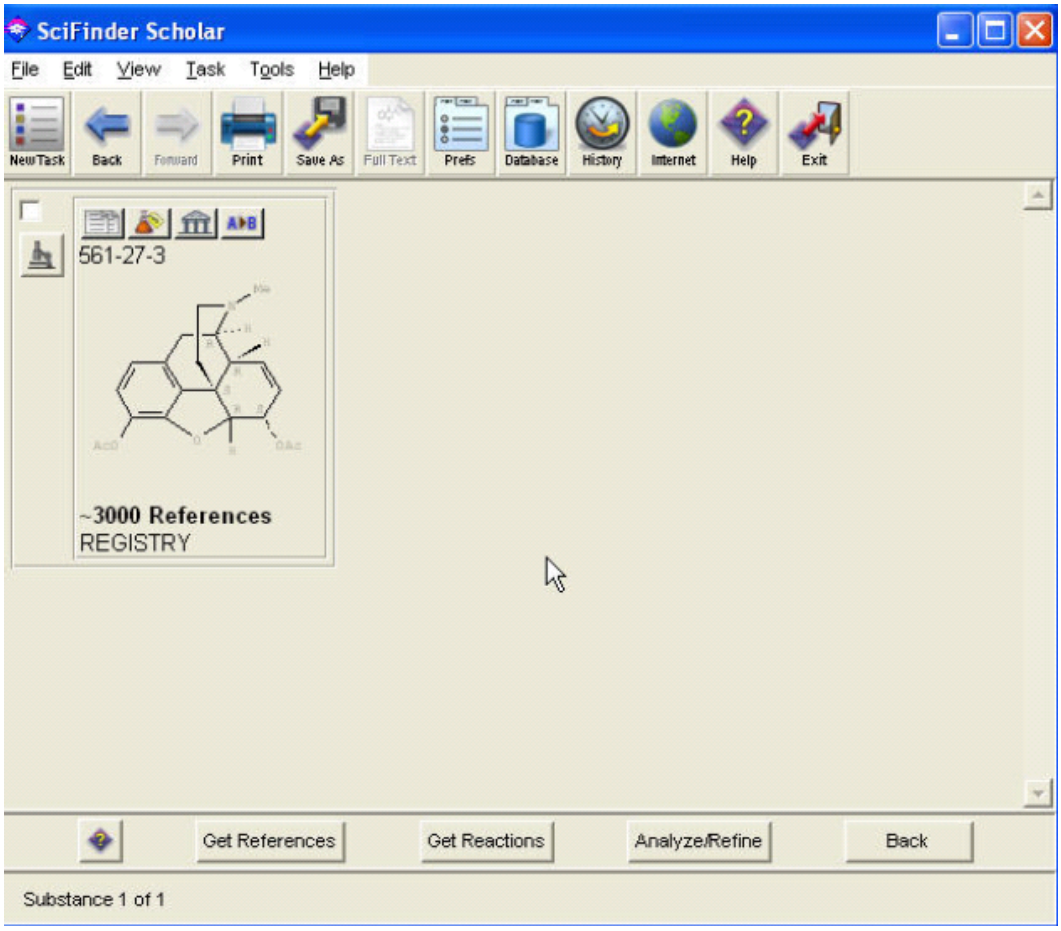


Search substances by:

- CAS Registry Number
- Chemical Name
- Common Name
- Trade Name
- Acronym

Also note,

- Enter one substance per line
- Punctuation & spaces may be used



Substance Identifier Results

- SciFinder searches the registry file and displays matching records
- Details of the substance can be viewed via the microscope icon 
- References may be analysed or refined, and then retrieved by clicking on 

A number of retrieval options are available for each substance by using the radio buttons, for example

- Get all references
- Get references associated with your topics of interest only.

For example

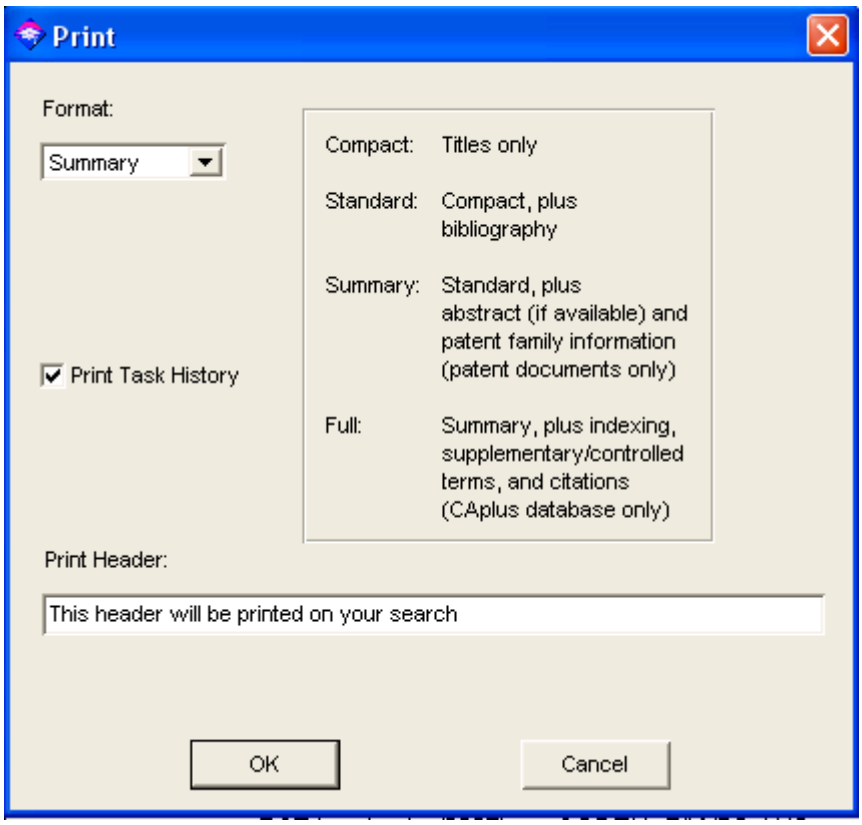
- Adverse effect
- Analytical Study
- Biological Study
- Combinatorial Study
- Crystal Structure
- Formation
- Miscellaneous
- Occurrence
- Preparation

- Properties
- Process
- Reactant
- Spectral Properties
- Uses

Printing and Saving Records

Once you have a list of references you are interested in, and have selected them using the tick boxes next to them, click the 'Print' button on the toolbar 

, and the following screen will appear:



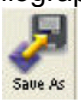
The print options will appear as a menu, similar to the above screen.

The print options available are;

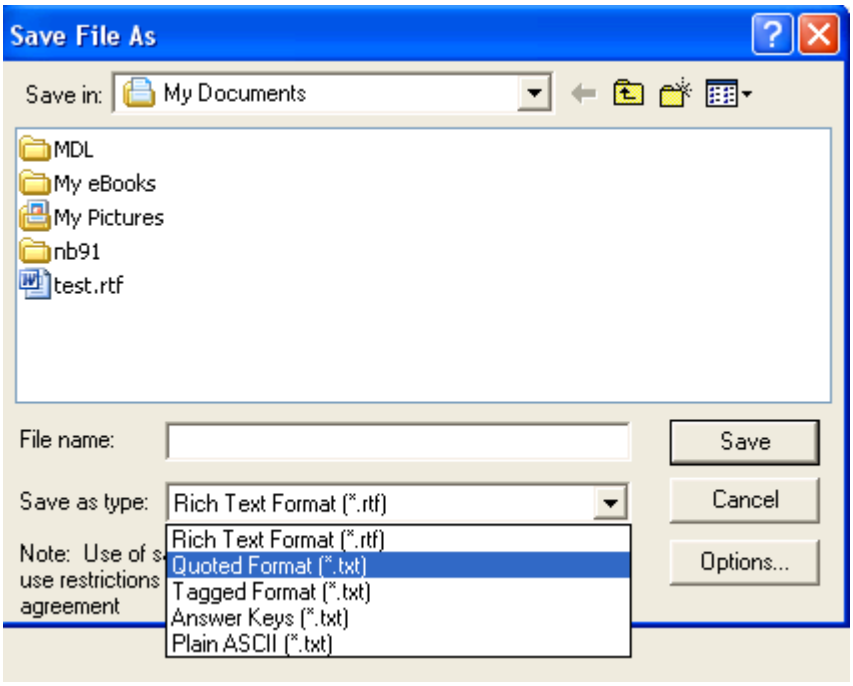
- Compact
- Standard
- Summary
- Full
- Print header – to describe your search

Use the drop down menu under the heading format to select your print option, fill in the print header with a description of your search and click 'OK'. Choose the correct printer and click 'Print'.

Saving Records

If you wish to save the bibliographic information you have selected, then click on the 'save as' icon 

in the main toolbar, this action will open the save file as menu, (see below).



References must be saved as:

- Rich Text Format .rtf
- Quoted Format .txt (Access, Lotus, Excel)
- Tagged Format .txt (EndNote. ProCite, RefMan)
- Answer Keys .txt
- Plain ASCII .txt

Finally, further help is available by clicking on 

icon. Or alternatively, by searching on **http://www.cas.org/SCIFINDER/**

Patent Specification

Espacenet is a freely available searchable online patent database put together by the European Patent Office. You may wish to access this to have a look at some actual examples of patent specifications.

Bibliographic data

The bibliographic data should contain the following:

- The date the application was filed
- The filing language
- The publication language
- The name of the applicant (company)
- The name of the inventor (person)
- The name of the agent (patent attorneys)
- The geographical area to which the patent applies
- References to cited documents
- The abstract (as for any scientific paper)
- A drawing of the structure of the drug

Description

This should tell the reader about the area of technology to which the invention relates, and the advantages the invention offers. There should be a description of at least one way of implementing the invention, and an explanation of its commercial use.

You should include in the description the following:

- A statement outlining any prior patents which you wish to claim the benefit of.
- A statement about 'prior art' in relation to the intended use of the invention.
- A detailed description of the invention, including any background science necessary for an understanding of the invention, and the specifics of the science relating to this particular invention. Any kinetic data which you can produce to support the effectiveness of the invention should be included here, along with an explanation of the meaning of such data. (you can find this data in problem statement 4 at the beginning of the fourth week of the module document). Any data showing the purity of the inhibitor, fully assigned, should also be included.
- Any tables and graphs which are relevant to this section should be included in the 'mosaics' section, and referred to here.

Claims

This section normally gives a detailed legal description of all of the uses to which your patent applies, including any variations to the structure, solution concentrations, and modes of delivery.

Mosaics

Any relevant pictures or graphs from earlier should be included in this section.

Legal Status

This should tell the reader at what stage of the process this patent application is currently. It should tell the reader if the patent has been granted, or has expired.

Meta tags

Author: Bagshaw, C.; Cullis, P.; Hutter, A.;Jenkins, P.; Lowe, M.; Raine, D.; Williams, D.

Owner: University of Leicester

Title: Interdisciplinary Science Molecules by Design Student Document

Classification: PA2013 / Molecules by Design

Keywords: Biology; Biochemistry; Chemistry; Pharmacology; Patents; Problem-Based Learning; Systems; sfsoer; ukoer

Description: Organic chemistry is important in many areas of industry and in the field of pharmaceuticals. In this module you will explore some of the key aspects of organic chemistry in the context of the design and delivery of drugs. This brings together issues of fundamental research, industrial scaling up of processes, environmental impact and patent law.

Language: English

File Size: 4.7*MB*

File Format: PDF

Version: 1.0

Additional Information

This module pack is the open student version of the teaching material. An expanded module pack for facilitators and additional information can be obtained by contacting the Centre for Interdisciplinary Science at the University of Leicester. http://www.le.ac.uk/iscience

This pack is the Version 1.0 release of the module.