Application of Computer in Chemistry SSC 3533

INTRODUCTION

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Outline

- Fields of application
- Examples
- Types of computer
- Programming languages

Introduction

Computer plays a very important role in every aspects of our lives, including chemistry

Two types of applications:

- Interfacing: A computer is connected to an instrument for data collection
- Software applications: Data analysis, simulation, structural searching, modelling, drug design, etc.

Fields of Application

- Computational Chemistry
- Chemometrics
- Chemoinformatics

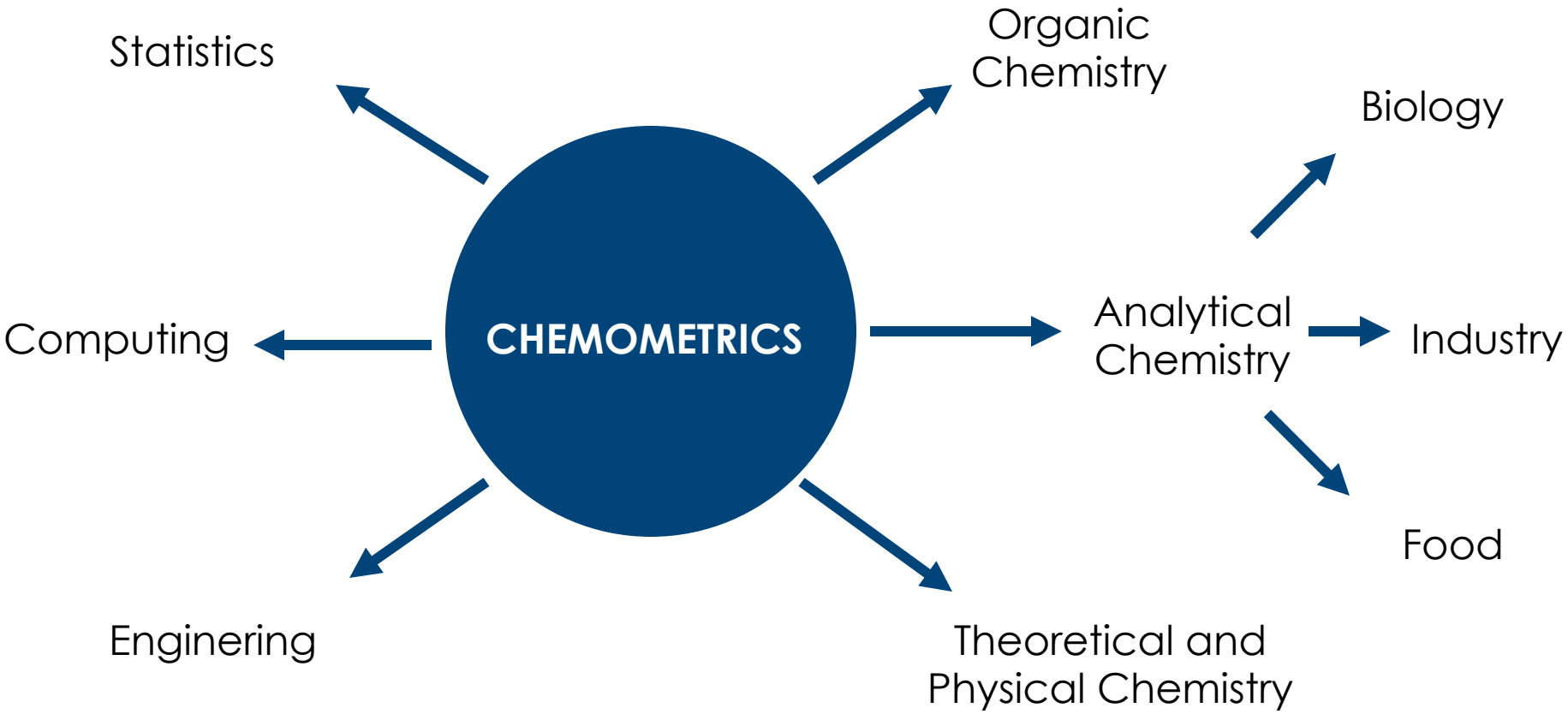
Computational Chemistry

- A branch of chemistry that uses the results of theoretical chemistry incorporated into efficient computer programs to calculate the structures and properties of molecules and solids, applying these programs to real chemical problems.
- Computational chemistry - when a mathematical method is well developed and can be implemented on a computer
- Examples: quantum mechanics, molecular mechanics, simulation, minimisation, conformational analysis.

Chemometrics

- The science of relating measurements made on a chemical system or process to the state of the system via application of mathematical or statistical methods.
- The chemical discipline that uses mathematical and statistical methods to design or select optimal measurement procedures and experiments, and to provide maximum relevant chemical information by analyzing chemical data
- Examples: experimental design, calibration, signal processing, pattern recognition.

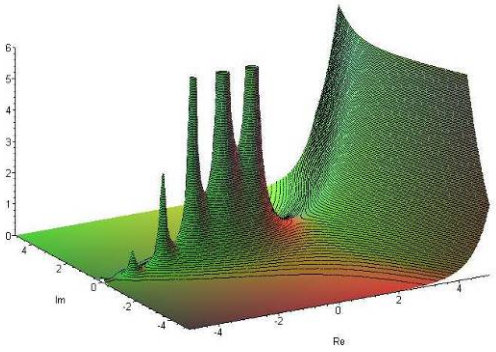
Chemometrics and other diciplines



Chemoinformatics

- The application of informatics methods to solve chemical problems
- The application of informatics to the management and processing of data, information and knowledge in chemistry
- Examples: Storage and searching of chemical structures, Quantitative Structure-Activity Relationships (QSAR), Structure elucidation, Drug design

What is ChemInformatics?

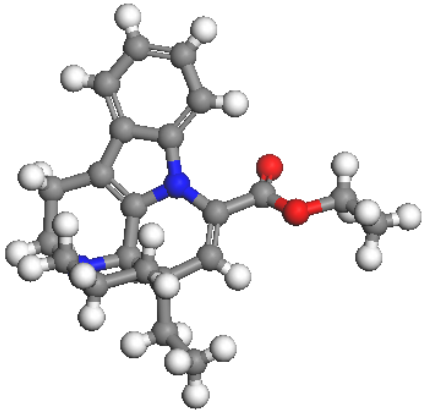


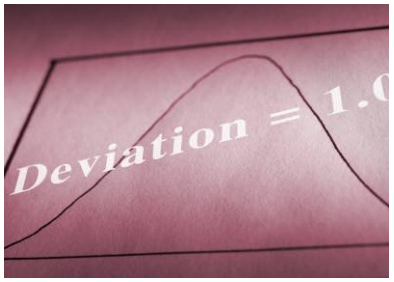
Mathematics

Chemistry

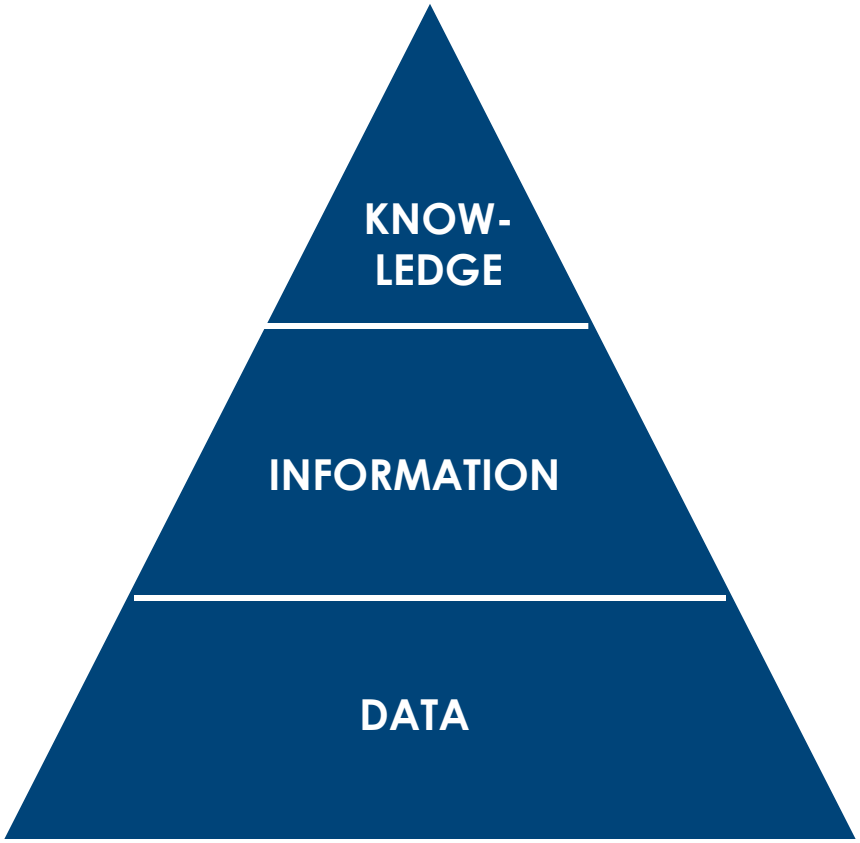
Informatics

Statistics





From Data to Knowledge



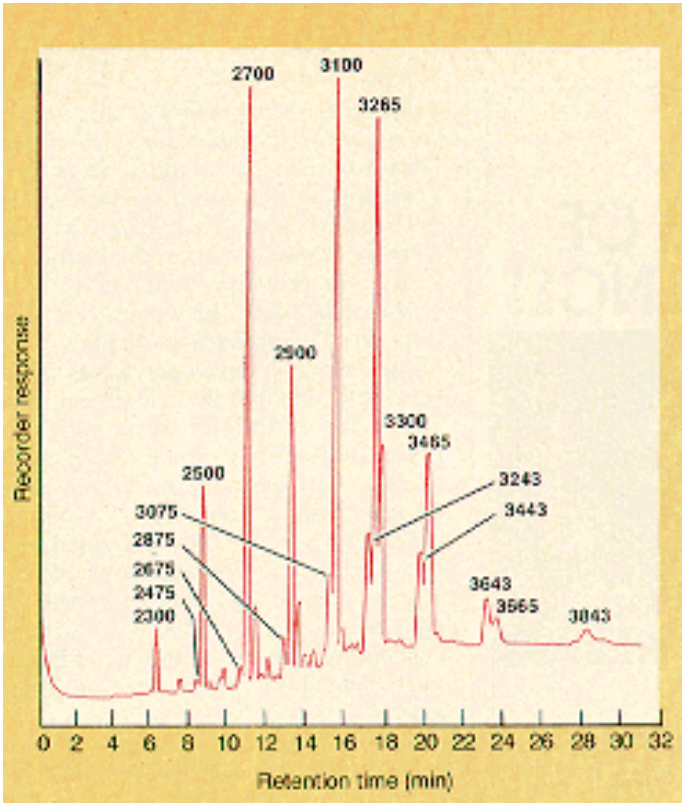
Abstraction

Context

Measurements

Calculations

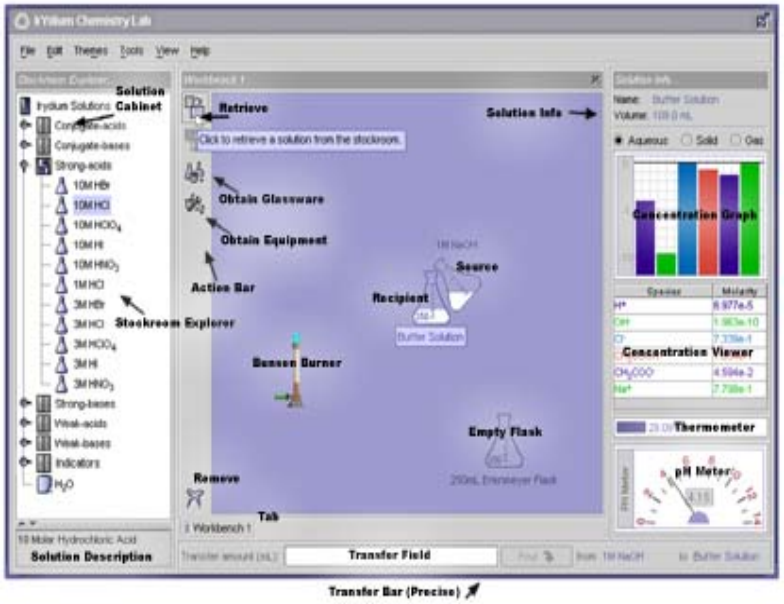
Data Processing



Signals received from an instrument or experiment are processed to become data and information

- Noise reduction
- Calibration
- Display

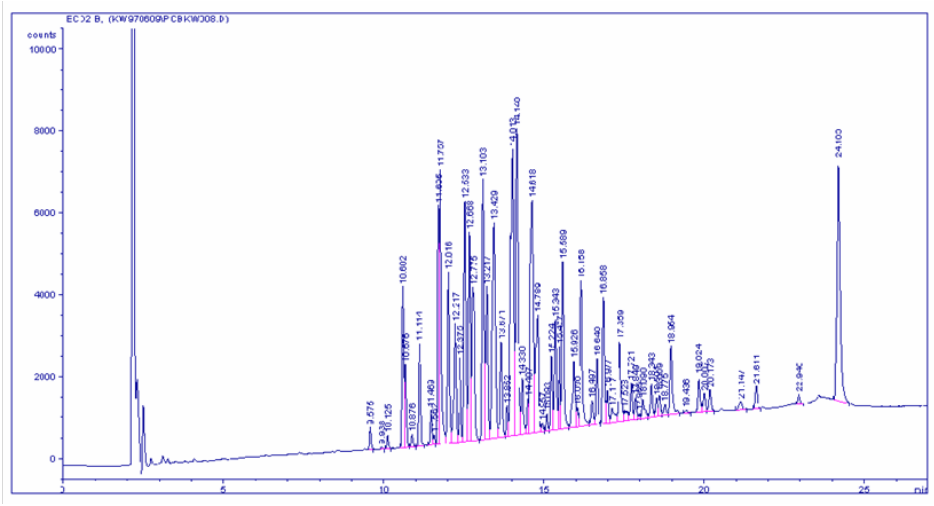
Simulation



Caption of Virtual Chemistry Lab software

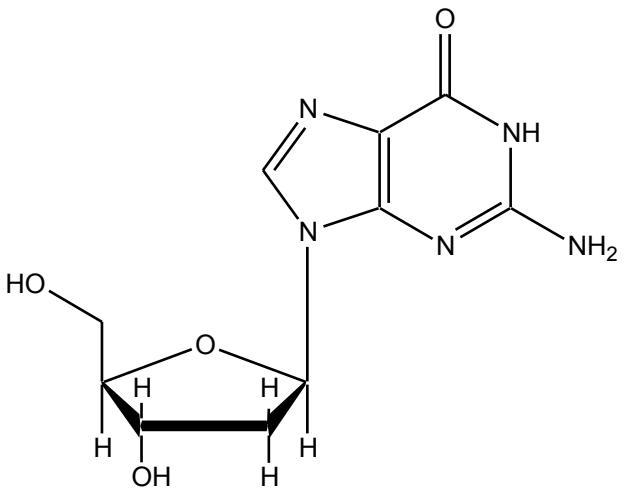
- Simulation of chemical processes
- Study factors affecting processes
- Determine important factors

Optimization of Experiments



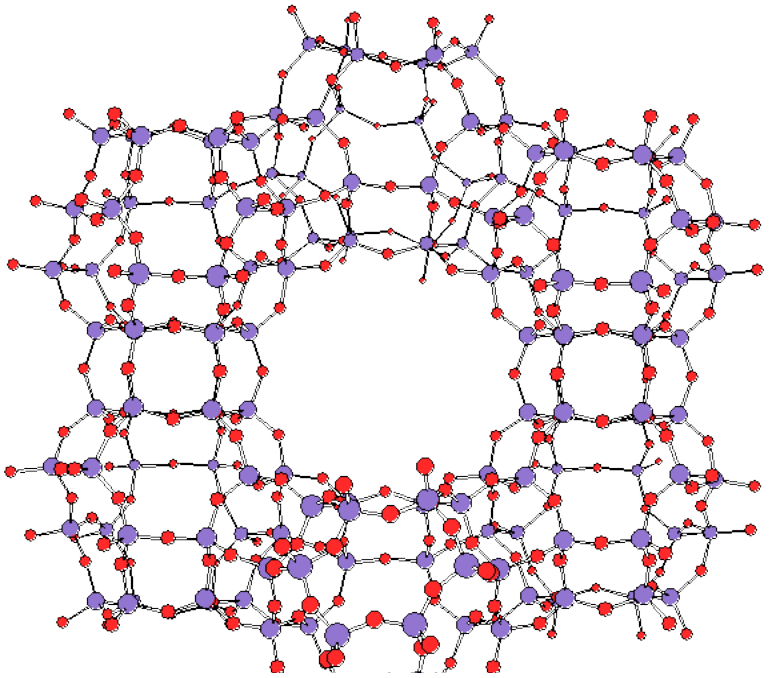
- Design of experiments
- Study factors affecting the experiments
- Establish optimum conditions

Handling of chemical Structures



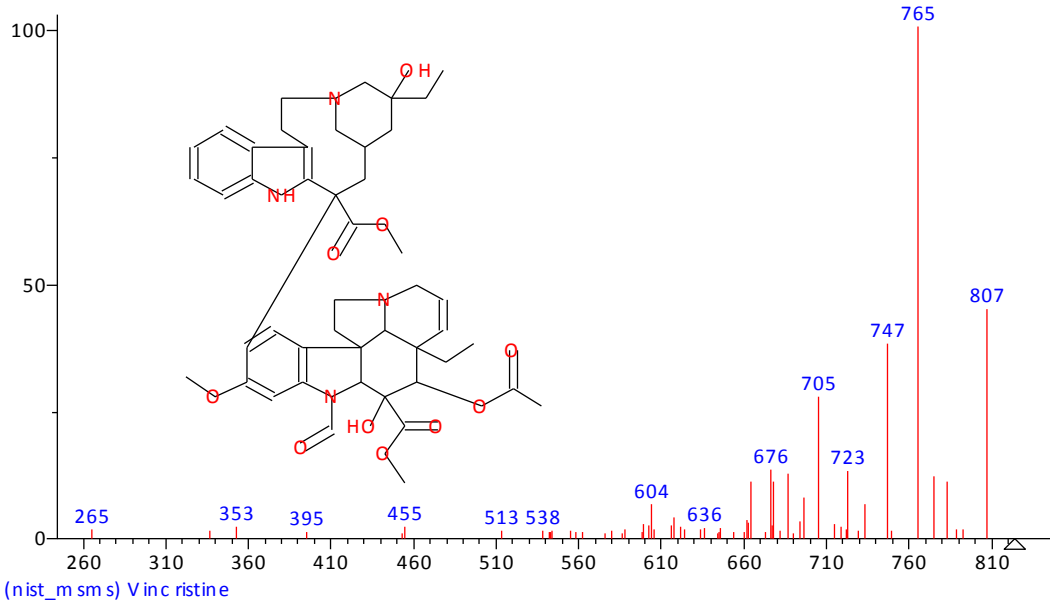
- Represent chemical structures with computer
- Establish database for searching of structures
- Use linear notation, fragment code, connection table.

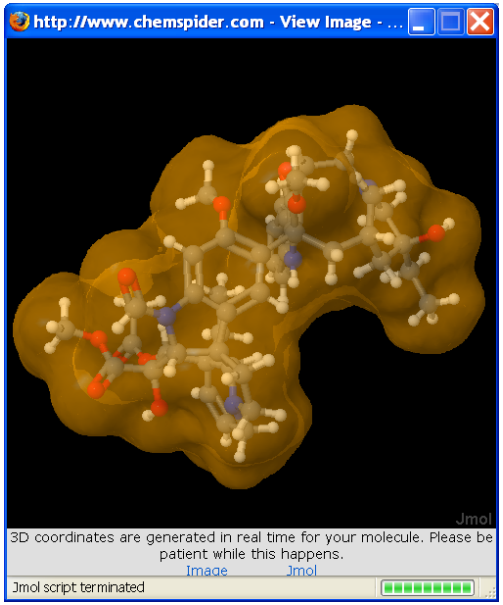
Molecular Modeling



- Develop 3-D model of structures
- Optimize structures
- Study reactions through simulations
- Calculate physical properties

Structure Elucidation

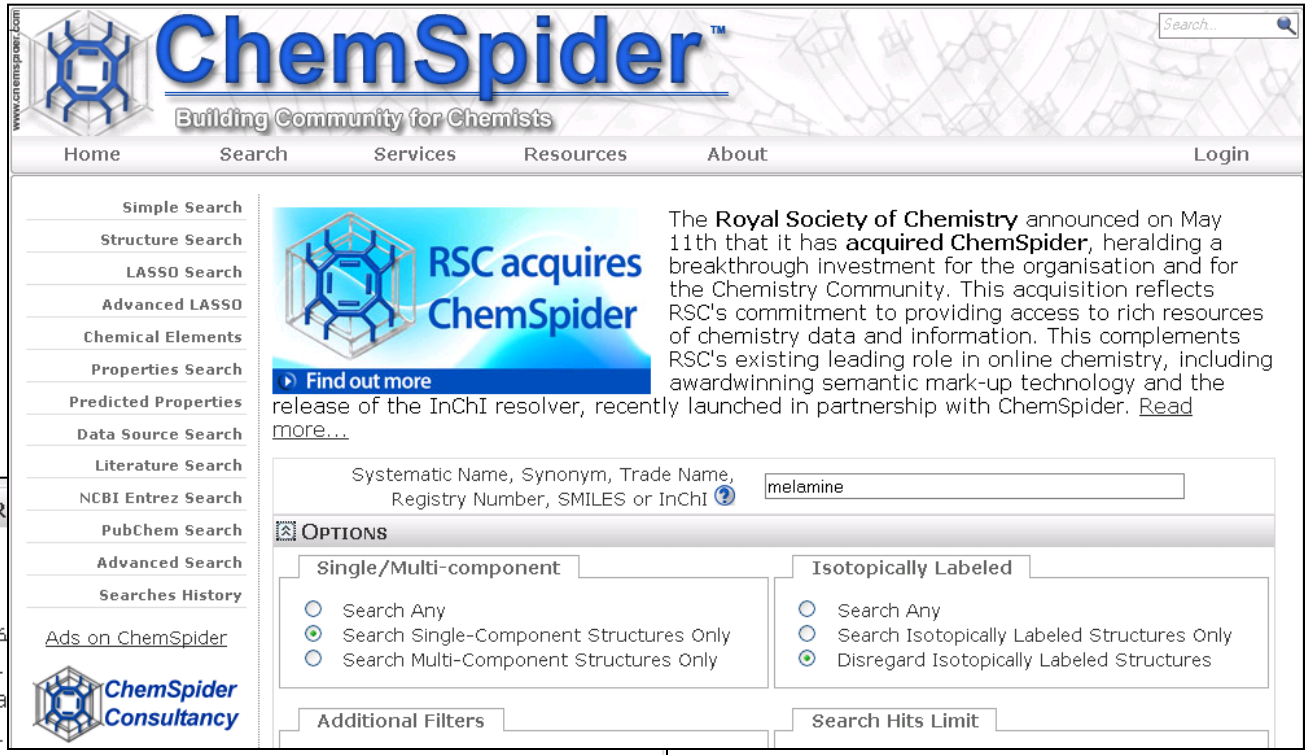


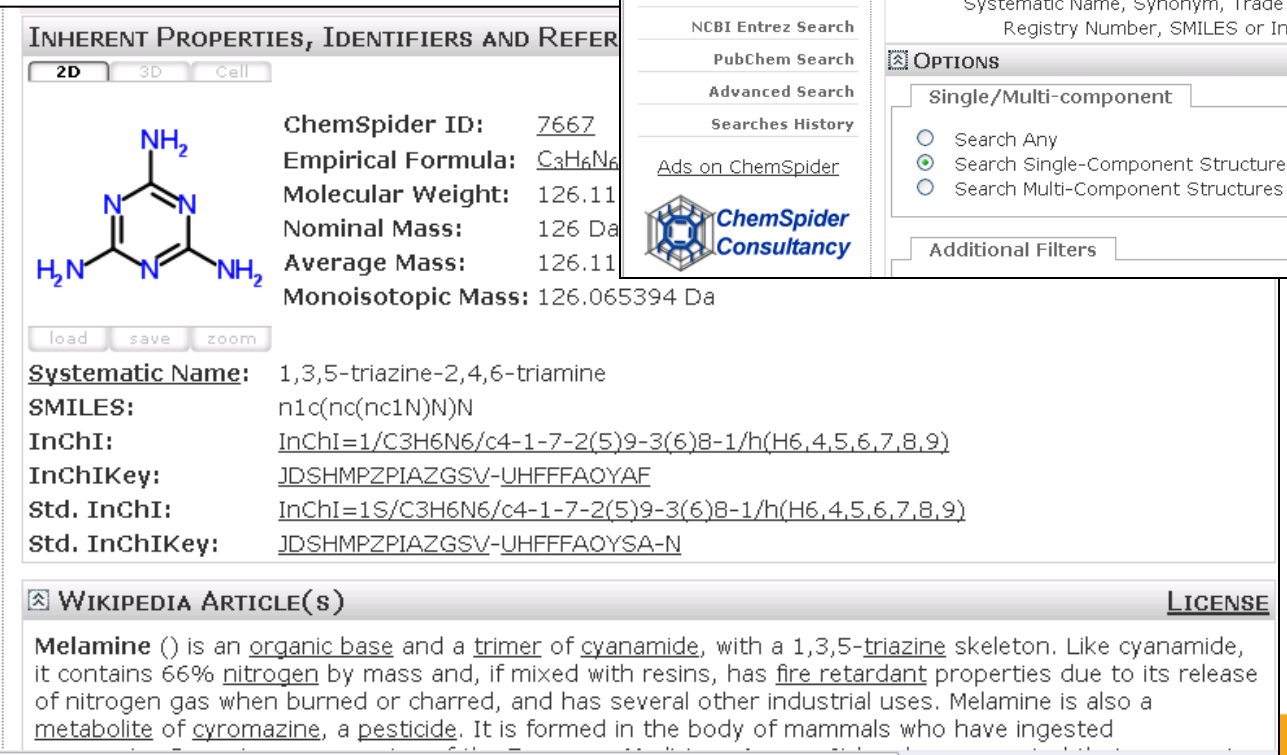


Caption from Chemspider

→ Complex MS data interpretations only possible with software
→ MS data obtained by hyphenated techniques (GC-MS, LC-MS)
→ Mass spectral database search and structure search routinely are used
→ Mass spectrometers deliver multidimensional data

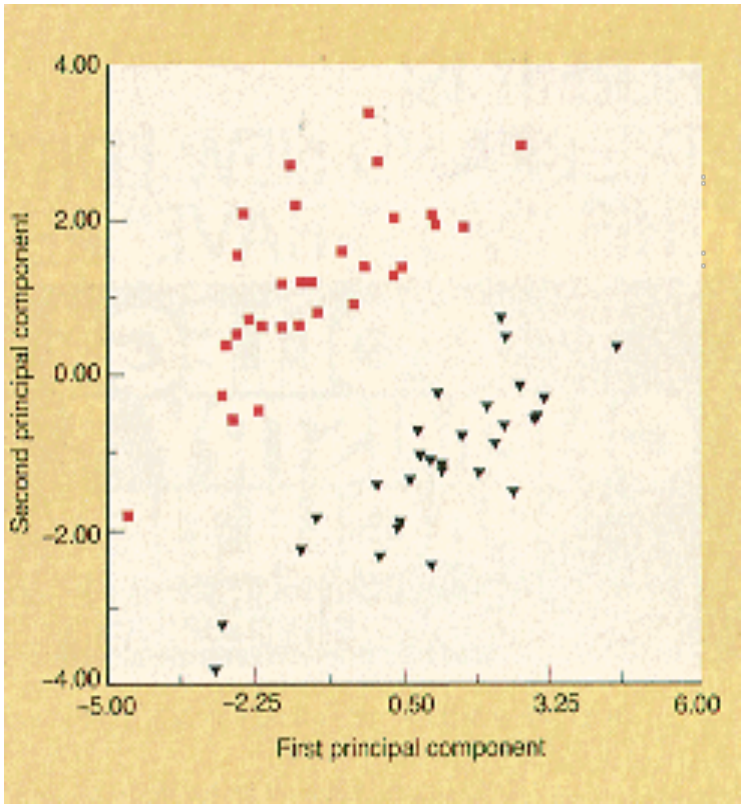
Structure search





http://chemspider.com

Pattern Recognition



- Identify pattern in complex chemical data
- Make classification based on information
- Examples:
  - Identify source of pollution
  - Classification of chemical substances according to biological activities

General Features of Computer

- Able to perform operations very fast
- Very low error rate
- Ability to process various types of information – not only numerical quantities
- Ability to store programs and data

Types of Computer

- Personal Computer (PC)
- Macintosh
- Workstation
- Mini Computer
- Mainframe
- Supercomputer
- Cluster

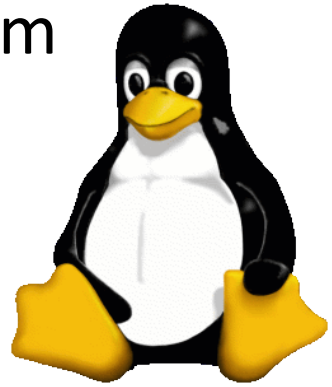
Operating System

- Windows

  - Operating system based on graphical user interface GUI on PC
  - Windows 95, Win 98, Win 2000, Windows XP, Vista, Windows 7
  - http://windows.microsoft.com

Operating System

- Unix
  - A multi-user, multitasking operating system
  - Developed in Bell Labs in early 1970s
  - Used in workstations, eg Solaris, AIX
  - Can also be used in PC



Operating System

- Linux
  - Free unix
  - Originally developed by Linus Torvalds, 1991
  - Red Hat, Fedora, Slackware, Debian, Ubuntu
  - http://www.linux.org

Operating System

- Mac-OS
  - Operating system on a macintosh
  - Easy to use, very user friendly
  - (http://www.apple.com/macosx/)

Programming Language

- Allows a user to communicate (give instructions) to the computer
- A person who wants to develop a computer application must know at least one programming language
- Example programming languages: BASIC, Visual Basic, Fortran, Pascal, C, C#, Java, PHP, Python