

ChemMark-WWW: Chemical Structure Drawing and Marking on the Web

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Current tutorial programs in web-based teaching and learning are limited to text inputs. Thus, in the field of chemistry, while questions may be asked in text or graphic formats, answers may be text only. This has severe limitations in tutorials (particularly in organic chemistry) where the only effective way to teach and to learn is through chemical structure diagrams.

As there are many ways in which a single chemical structure may be correctly drawn, it would be totally impractical to create a library of correct structures against which student structures are to be matched. Accordingly, *ChemMark-WWW*, a chemical structure drawing and recognition web interface which enables chemical structures to be drawn and marked, has been developed. The program automatically creates a structure connection table for the answer given by the student and matches it against the structure connection table for the answer provided by the instructor. Answers can be post-processed so that the student gets immediate feedback, and the lecturer can immediately see what marks have been awarded – and can also see exactly what the students did!

While it is a simple matter for teachers to insert their own questions into the program, the first release of *ChemMark-WWW* will have a number of already prepared tutorial questions. The questions cover the usual materials presented in First Year Organic Chemistry courses.

ChemMark-WWW currently is restricted to structure input only, but stereochemical issues and reactive intermediates can be accommodated. For example, it is possible to ask a question: “Draw the structure of the intermediate formed when propene is treated with HCl”. Here the carbocation required is easily recognised by the program.

ChemMark-WWW allows for multiple answers to be drawn on the one page. Thus, in answer to a question: “Draw the structure(s) of the products formed when toluene is treated with a mixture of nitric and sulfuric acids”, the *ortho*- and *para*- products can be drawn in the one diagram. *ChemMark-WWW* also allows for alternative answers. For example, in answer to a question: “Draw the structure of the alkyl iodide and the carbonyl compound that could be used for the preparation of methylenecyclohexane”, either of the alternatives (formaldehyde/cyclohexyl iodide or cyclohexanone/methyl iodide) are accepted.

On the other hand, *ChemMark-WWW* does not handle the “arrow notation”, where in any case organic chemists have slightly different interpretations of what is “correct”.

While a number of questions are available in the first release of *ChemMark-WWW*, it is a relatively easy task for the teacher to present specific tutorials. Text is entered into a simple word-processor program (for example, *Notepad*), and questions and answers which involve structures are prepared with the same structure drawing program used within *ChemMark-WWW*. *ChemMark-WWW* may be used at all levels in the teaching of organic chemistry and, where mechanistic aspects are required it is a simple matter to present questions that address the structures of the key intermediates.

ChemMark-WWW was alpha tested with a group of students in Chemistry 1 from The University of Sydney in September/October. Students learnt the structure drawing program in about 20 minutes.

They found the program provided a very exciting and informative way of learning organic chemistry. They liked the immediate feedback on their own answers, and the general comments.

ChemMark-WWW is produced by Hampden Data Services, UK, in conjunction with the School of Chemistry at The University of Sydney.

Flexible Learning and Assessment Package for Teaching Data Analysis and Chemometrics in Analytical Chemistry

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Instrumentation for analytical chemistry has become enormously productive and convenient to use in recent times. However, despite successes in automation and computer software, the person driving the instrument is still of prime importance. In the wrong hands, even the very best computer controlled instrumentation will only produce more meaningless data faster. In analytical chemistry it is the quality of the data produced that is of the utmost importance. A related issue is the spread of chemometrics into the workplace for solving routine analytical chemistry problems in areas, which include everything from the petroleum industry to the environment to foodstuffs to forensic science.

Students do learn about quality and data analysis principles in a statistics unit that they undertake but usually they are unable to make the connection between what they learn in statistics and what they learn in analytical chemistry. In any case, generalist statistics units don't go far enough to prepare students for using chemometrics software packages in professional life.

In order to cater for student needs in these areas a package of flexible learning modules has been developed and used with 2nd and 3rd level students in analytical chemistry. These modules are web-based and include the following features:

- students can use them in an on-line mode using an Internet connection;
- students can obtain an installer program on a floppy disk which installs the system onto a home or work computer for off-line use;
- in off-line mode students can do everything except submit answers for on-line checking and connect to the discussion forum;
- the package is integrated with discussion forum software which allows students to keep in close contact with staff and to cooperate more effectively with each other;
- each module contains a set of "real life" analytical data for the students to analyze and interpret;
- students can use a variety of software tools for data analysis and visualization, including *Microsoft Excel*, *Statlets* and *Matlab*;
- once the students have finished the analysis they are required to answer a series of questions, some of these questions are multiple choice or tick the box and these are automatically computer checked for rapid feedback;
- for convenience of teaching staff the web software writes student results directly to an *Excel* spreadsheet; and
- other questions require students to display deeper reasoning skills and are marked manually.

These modules are set in the early part of the semester before laboratory classes start. Where possible the laboratory program has been designed to link in with the data analysis modules. The skills developed with *Microsoft Excel* (and other software) greatly assist students with general laboratory report writing in the later part of the semester.