Assessing the educational effectiveness of a CAL tutorial. 
Structure and molecular dynamics in biology; 
Part 1: water and molecular interactions

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Abstract: The educational use of an interactive tutorial illustrating and exploring core chemistry-biochemistry concepts in depth was evaluated with first year university students. The investigation tools were constructed by a multidisciplinary staff and included knowledge evaluation, student appreciation and silent observations of the students. The results show that the tutorial was appreciated by the students and that they were able to work at their own rhythm. We measured the learning outcomes resulting from the use of the tutorial and observed that the students’ knowledge on the topics covered was significantly improved. The behaviour of the students using this tutorial and some unexpected answers led us to propose a new version of the tutorial and a utilization procedure better adapted to the students’ skills as well as other possible uses are proposed. [Chem. Educ. Res. Pract., 2006, 7 (4), 248-265]

Keywords: Tutorial, CAL, molecular visualization, biochemistry, molecular dynamics, intramolecular forces, intermolecular forces, evaluation.

Introduction

Biology studies bear the brunt of the increasing mass of data and results; thus the basic concepts of chemistry and biochemistry tend to be swamped in an ocean of ‘facts’, which inhibits understanding for the students and reduces training efficiency. Therefore, reflecting on the fundamentals of the teaching contents (Taber, 2001; Nelson, 2003; Atkins, 2005) becomes a necessity. Pruning the chemistry and biochemistry curriculum to emphasise the core concepts is a first step to be taken in order to renovate the teaching. To do this, the Atelier de Recherche Pedagogique (ARPE) has explored means that are likely to help that renewal as well as to improve the understanding of complex chemistry and biochemistry concepts that students need (O’Leary, 2001). The implementation of new teaching tools may require a reorganization of the subject matters taught through effective educational practices (Brassard and Daele, 2003). De Jong (2000), Kempa (2002) and Gilbert et al. (2005) have argued for bridging the traditional gap between research and practice in science education by the collaboration between researchers and practitioners to the benefit of both.
We decided to adopt an interactive mode of teaching by using computer-aided visualization and modelling methods. ‘Structure and molecular dynamics in biology; Part 1: water and molecular interactions’ is an interactive tutorial relevant to the chemistry-biochemistry field. It represents a new approach for the study of basic concepts of molecular interactions according to the nature of molecules and to their physicochemical properties aimed at enhancing the understanding of the structure of biological molecules and of their functions through showing the biology students the relationships between chemistry and biology. It offers a consistent range of chapters dealing with basic chemistry concepts that allow the understanding of water interaction with biological molecules. It provides explanatory texts, as well as observations and activities, such as the possibility of manipulating molecular models with the ‘chime’ plug-in whose advantage is that hands-on learning occurs in a short time; this is the subject of the first section of the tutorial. The work reported here concerns the evaluation of the educational use of this application.

There have been few studies about the use of computers in the biochemistry area at University level. Bouvier (1999) used multimedia to teach molecular structures; Cognet et al. (1994) used software for mathematics teaching; and others used more specialized modelling software (Canning and Cox, 2001; Peterson and Cox, 2001; Honey and Cox, 2003). Parslow (2002) commented on the relevance of such approaches. The available assessment procedures are more often qualitative than quantitative (Wu et al., 2000; Canning and Cox, 2001; White et al., 2002; Honey and Cox, 2003).

Our tutorial underwent several pedagogical tests. It was used at University level for three years as a free-access revision application for 2nd year biology students after they had attended a lab session on the same themes in the teacher’s presence, using the molecular visualization software Rasmol (Bouvier and Leseney, in preparation). A survey showed a favourable student reaction to it. In Colmar this tutorial was put into use with first year students for three years to illustrate and explore core biochemistry concepts in depth. There soon appeared an evident need to assess the pedagogical impact of that tool and of its use both for the teacher and for its designers. The former wanted to use it for teaching rather than for revision, while the latter wanted to evaluate it with the intent of improving it. The evaluation became possible thanks to diverse trials that allowed the refinement of the evaluation procedure set in 2003.

Material and methods

The evaluating team

This team comprised a biochemistry teacher-researcher (the user) whose task was to put the tutorial into pedagogical use for her students (ascertaining the level of their knowledge and of the local context), designers whose goal is to improve their product and who need a reliable experimental procedure for that purpose, and evaluation and education science specialists to collect and interpret the outcome of the students’ use of the tutorial.

The tested tutorial

‘Structure and molecular dynamics in biology, Part 1: water and molecular interactions V.01’ is a tutorial concerned with the structures of biomolecules and their interactions with water. It addresses cellular biology notions in a very descriptive way, and has been devised for use as a revision application for young biology undergraduates. Its precise description and the educational motives underlying it will be discussed elsewhere (Bouvier and Leseney, in preparation).

In brief, starting from the example of the water molecule, basic chemistry concepts are dealt with a static and dynamic conception of the molecule. Interactivity is brought in by
the ‘Chime’ plug-in (http://www.mdl.com) and dynamics by animations achieved under Flash Macromedia (http://www.macromedia.com). After a learning session about the use of the tutorial and of Chime, the student is required to do a search on molecular models, on the geometry of the molecule (covalent bond, inter-atomic distance, bond angles) on electronic density and on isodensity surface of a molecule. The water molecules are then used for describing the hydrogen bond and its characteristics. A second part deals with the application of these ideas to biological molecules. The major types of biological monomers are described (carbohydrates, amino-acids, fatty acids). Their various parts and functions are highlighted; the notions of polarity, electrostatic potential and hydrophobicity typical of each of these major groups of molecules are illustrated. Finally, in the third part, these notions are investigated in the case of two macromolecular examples: cell membranes and DNA. The tutorial provides explanatory texts on the right side of the screen where buttons are to be found for calling or modifying the left side illustrations (see Figure 1). The illustrations can be static or animated images created with the help of molecular modelling software packages (Spartan: http://www.wavefunction.com) and/or of animation (Flash). The author programmed three-dimensional representations of molecules specifically emphasising the concepts being studied (highlighting of the different parts of a molecule, polarity, etc.). Each three-dimensional molecule representation can be manipulated by the student at will. He/she is not only able to observe it from all angles (360° rotation possible in all directions, zoom...) but to modify its representation by using the Chime menu (MDL) (representation mode, coloration mode...). The tutorial was designed so as to take into account the linear progression of the content; however, students can easily go from one page to the other thanks to access buttons enabling movement forward and backward and to a summary on every page.

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Figure 1. A screen copy of the tutorial

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The student population

All quoted Annexes can be consulted in their entirety on the reference site: http://wwwarpe.snv.jussieu.fr/colmar/article_colmar/index.html.

The student population was composed of 52 first-year students belonging to the Genie Biologique Department of the Colmar University Institute of Technology and attending a course of a conventional type. For the present experiment, the student population was randomly divided into four groups of thirteen students each.

At the time of the experiment those students were quite well equipped with computers; 94% of them had a computer available at home and 78% had an internet connection (as compared to 42% and 28% respectively in the case of the French population at large, http://www.internet.gouv.fr then ‘rubrique chiffres clé’). Yet they have relatively little use of informatics applications (Annex 3bis, Signalétique). As regards their work at University, they considered the use of a computer as totally normal (70%) and fruitful (62%). They use the computer and internet above all with the purpose of searching for the information required for individual assignments. The computer is not considered as a tool for inter-personal or collective exchange. Though the students do not use the computer for investigations in order to complete the course (Annex 3bis, Q1), they would like to find on-line their teachers’ course, exercises and corrections (Annex 3bis, Q2). There were no noticeable differences between the groups as regard their computer skills.

Tools made available to the students

Each student was provided with the following items: a local network computer with the necessary plugs-in installed, access to the tutorial on the local server and a ‘guide’, that is a typed document written by the teacher so as to give some instructions, further information and questions that should focus the student’s attention and bring him/her to reflecting on the topics suggested by the application. It invited them to engage in activities (drawing a molecule, taking advantage of interactivity); such guide highlighted the part to be studied: the whole tutorial apart from the ‘electrostatic potential’ part that is regarded as too complex at the students’ level, and from the DNA part that has not been approached at that time. The ‘guide’ is available on the reference site (Annex 1).

The experimental procedure

This tutorial allows in-depth searching and revision of the principles already dealt with in the chemistry or the biochemistry course. It was used independently by students during a 90 minute hands-on session in the presence of the teacher. The instructor’s involvement was limited to presenting the lab session and helping the students in need of technical support in the computer use. All through the experiment the students’ work was monitored by the silent observers. The four subgroups (13 students each) performed one or the other of the two experimental procedures described in Table 1. No response other than the questionnaire answers was required.

<table>
<thead>
<tr>
<th>Table 1. Experimental procedure</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Group 1</strong> (groups A and C)</td>
</tr>
<tr>
<td>Presentation of the experiment by the instructor: 15 min</td>
</tr>
<tr>
<td>Knowledge evaluation: 30 min</td>
</tr>
<tr>
<td>Coffee break</td>
</tr>
<tr>
<td>Distribution of the guide</td>
</tr>
<tr>
<td>Work on the tutorial: 90 min</td>
</tr>
<tr>
<td>Appreciation survey: 15 min</td>
</tr>
</tbody>
</table>

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Evaluation tools

A knowledge evaluation questionnaire (Annex 2)

The questionnaire was concerned with assessing the students’ knowledge about curriculum items handled in the tutorial either pre- or post-use.

An appreciation survey (Annex 3)

It comprised 36 questions, mainly multiple-choice questions and some open-ended ones so as to discover: 1. how familiar the students were with the computerized tools and what role they ascribed to it in their conceptual attitude towards their University work, 2. their perception of the tutorial and how they used it, 3. their recourse to interactivity, 4. the accessibility of the ideas involved for that audience, and 5. the students’ appreciation of the Chime application and its use.

Silent observations (Annex 4)

The three silent observers were biologists or education science specialists. Their status had been explained to the students in general terms during the introduction to the lab session. Each observer stood behind the students’ group and observed the behaviour of two students per lab session, without the knowledge of the students concerned.

Silent observers had been given clear instructions and a record sheet to note down their observations. They had to make systematic notes of the students’ actions and interactions, of the time spent and of their ways of proceeding at each step of the application. 12 reports describing the students’ approaches were collected.

Results

Knowledge evaluation

The knowledge evaluation questionnaire was filled in by a group of students pre-use of the tutorial (group 1), and by the other group post-use (group 2). The 14 single questions and the 13 multi-part questions were subdivided to provide 43 pieces of information for analysis. Overall 57 Items were identified, 7 of these, requiring either a comment or a drawing, were judged according to an established set of criteria (detailed Items: Annex 2bis). The students’ responses to the Items were scored as ‘correct answers’ (one point), ‘incorrect answers’ or ‘none’ (no points for either).

While going through the examination of the questionnaires and after debating with the teachers of chemistry and biochemistry, it seemed that the three items 7c, 9c and 9d might be ambiguous. The correct answer to Item 7c was considered by us as ‘Wrong’ because the statement: “a polar molecule includes electronegative and electropositive parts” was not sufficient to define a polar molecule. However we could not consider the answer ‘Right’ given by the majority of the students as incorrect, because indeed polar molecules do have electropositive and electronegative parts. Item 9d was an open-ended question asking the student to justify the answer given to item 9c. We could not accept an answer to item 9c as correct if the reasons given for it were wrong. These three ambiguous items were not taken into account when analysing the data.

Statistical results

Global analysis of the results

We first compared the distribution of responses (correct, incorrect or non existent) in the two groups (Figure 2)
Figure 2. Improvement in the average number of answers

Improvement in the average number of answers (correct, incorrect or none) per student of group 1 (tested before the tutorial, shown in grey) or group 2 (tested after the tutorial, shown in black).

An overall positive effect of the tutorial could be observed; there was a 25% increase in the correct answers and the number of incorrect and non existent responses decreased.

Analysis of results per item

When one compares the two groups of students, statistical analysis displays a significant improvement for 15 items and some deterioration for three items out of the 53 items analyzed (Table 2).

Table 2. Items whose evolution is statistically significant

<table>
<thead>
<tr>
<th>Items</th>
<th>Chi² result</th>
</tr>
</thead>
<tbody>
<tr>
<td>2a, 7d, 8a, 9b, 10, 12b, 16a, 16d, 19b, 22b, 22c, 8b, 22a, 26d</td>
<td>increase</td>
</tr>
<tr>
<td>2b, 26b, 27</td>
<td>decrease</td>
</tr>
</tbody>
</table>

For the remaining 35 items, there is no statistically significant improvement, yet a detailed examination of the results rather displays a trend towards progression for 33 of them while for the two last items the position was more ambiguous.

Those 15 items where significant improvement was seen address ideas scattered through the whole tutorial; 11 of these relate to ideas covered in a single chapter of the tutorial and the 4 remaining ones involve understanding ideas dealt with in several chapters. For 13 items a decrease in incorrect responses can be seen; yet for two items, the number of incorrect answers is unchanged since the improvement actually corresponds to a shift of the undecided students (‘no answers’) towards correct answers.

Analysis of the results per theme

The items were grouped in 8 categories according to various themes: Molecular geometry (8 Items), Notions about electrons (8), Molecular polarity (7), Hydrogen bond (12), Hydrophilicity (8), Hydrophobicity (16), Membranes (11), General knowledge (7). Some items have been attributed to more than one theme (detailed Items per theme: Annex 2bis).

For each student the average of points obtained was calculated. For each theme and for a group of students as a whole a qualitative analysis (number of correct, incorrect answers or none) has been drawn up and a score per theme calculated. The two students’ populations were then compared.
A gap between the 2 groups has been verified by applying a Chi-squared test with a 5% tolerance (Statbox) for the qualitative variables (correct, incorrect or non existent response), and an ANOVA test with 5% tolerance for the quantitative variables.

So as to avoid any bias resulting from the different number of items per theme, the score obtained for each theme by a given student was weighed and brought back to a maximum of one. The average weighed scores (AWS) of the students of groups 1 and 2 were compared (Table 3).

Table 3. Average weighed scores (AWS) of the students pre- and post-use of the tutorial and comparison of both groups by ANOVA statistical analysis

<table>
<thead>
<tr>
<th>Themes</th>
<th>geometry</th>
<th>electron</th>
<th>polarity</th>
<th>H. bonding</th>
<th>Hydrophilicity</th>
<th>Hydrophobicity</th>
<th>membrane</th>
<th>General knowledge</th>
</tr>
</thead>
<tbody>
<tr>
<td>AWS Pre-use</td>
<td>0.544</td>
<td>0.906</td>
<td>0.613</td>
<td>0.599</td>
<td>0.409</td>
<td>0.494</td>
<td>0.538</td>
<td>0.666</td>
</tr>
<tr>
<td>AWS Post-use</td>
<td>0.669</td>
<td>0.897</td>
<td>0.799</td>
<td>0.753</td>
<td>0.610</td>
<td>0.675</td>
<td>0.727</td>
<td>0.615</td>
</tr>
<tr>
<td>Probability*</td>
<td>0.033</td>
<td>0.79</td>
<td>0.0004</td>
<td>0.0009</td>
<td>0.001</td>
<td>0.0004</td>
<td>0.0007</td>
<td>0.47</td>
</tr>
</tbody>
</table>

* The two groups are significantly different when probability is under 0.05

One can observe a significant improvement for all themes except for those about electrons and general knowledge where the change was not statistically significant. These themes will not be considered further.

In the next analysis (Figure 3), for each theme, the average percentages of correct, incorrect or non-existent answers have been calculated for each group of students as well as the ratio between the obtained values (group 2/group 1).

Figure 3. Improvement of responses per theme linked to tutorial utilization

Ratio of the group 2 values versus those of group 1 concerning the correct (black), incorrect (grey) and non existent (white) answers according to the various themes studied. The red line indicates the absence of difference between the two groups.

In those themes where change had occurred, the ratio between average values obtained for group 2/group 1, varied from 1.25 to 1.49 as regards the correct answers, which points to an increase of 25 to 49 % of these. For the incorrect responses, the ratio varies from 0.98 to
0.46, which means a decrease ranging from 2 to 54%; and a decrease from 50 to 96% can be seen concerning the undecided students. The decrease in incorrect responses is less and less as the students proceed through the tutorial while the number of uncertain students decreases quite significantly towards the end of the tutorial. For the two last chapters the increase of the correct answers observed in group 2 (ratio group 2 / group 1 >1) is due fewer students being undecided rather than to the decrease of the number of incorrect answers.

**Validation of the method used**
We wanted to assess whether the questioning mode had an impact on the response given by the students. We chose two validation criteria: the influence of the type of expected answer for an item (C for correct, I for incorrect) and the independence of the response to the different items composing a question. Results indicate a little impact caused by the form of the question and an independent development of the answers to the different items within the same question. For more details see Annex 5.

**Search for possible causes of deterioration**
Surprisingly, we observed deterioration in the score of some Items, linked to the tutorial, so we tried to identify the reasons for it.

Question 2 was about the Brownian motion affecting molecules in solution (item 2a) and in cells (item 2b). Following the tutorial the 2a item responses greatly improved and those of item 2b greatly deteriorated (Figure 4).

**Figure 4.** Improvement of the answers to items 2a and 2b linked to the tutorial

In question 15, items 15a and 15b required identifying a sugar in two schematic forms: the Fischer linear representation (Figure 5b) and the cyclic Haworth representation (Figure 5c). In the former, one can see a decrease in incorrect answers that shift towards the ‘no answer’ category; however the change is not significant. On the other hand with the cyclic representation there is a clear decrease in correct answers that go equally to the ‘incorrect’ and to the ‘none’ category (Figure 5a). Let us note that the tutorial presented the same three-
dimensional molecule on one side and on the other, the cyclical form did not clearly show all OH groups.

**Figure 5.** Improvement of the answers to items 15a and 15b linked to the tutorial

![Graph showing improvement of answers to items 15a and 15b](image)

Percentages of answers (correct, incorrect and none) given to items 15a and 15b pre- (grey) or post- (black) tutorial use (5a) related to the Fischer (5b) or Haworth (5c) representations of sugars.

As regards the four items 26a to 26d that address the same concept, hydrophobicity, results differ. The change is positive for items 26a, 26c and 26d, which proves that the students grasped the ideas, but there was a substantial increase of incorrect answers to item 26b (Figure 6).

**Figure 6.** Improvement of the answers to item 26b linked to the tutorial

![Graph showing improvement of answers to item 26b](image)

Percentages of answers (correct, incorrect and none) given to item 26b pre- (grey) or post- (black) tutorial use

After careful examination and re-reading of the tutorial we decided that item 26b was ambiguous, as the question was formulated in terms of consequence instead of cause, and could thus be misunderstood by the students, so in this case it was not the tutorial that led to confusion but the questionnaire itself.

Answers to question 21 about the ions solubility demonstrate a deterioration of correct answers to the benefit of the ‘None’ category. The text of the tutorial does not tackle specifically that notion.

**Students’ attitudes towards the tool**

Complete answers given by the students to the appreciation survey can be found in Annex 3bis. The number corresponding to the question is given between brackets.
General appraisal of the tutorial and of its use by students

78% of the students perceived the tutorial as a training or revision tool and were rather satisfied; 84% wished to use the tutorial again. By a great majority they considered it to be easy of access, of manipulation and of quick navigation (Q5 and Q25).

More than 80% considered that the tutorial helped them to grasp the ideas presented (Q22).

The great majority of students appreciated that visualization of a molecule brought about a better understanding of its geometry (Q15) and that dynamic representation of water vibratory states favoured a better memorization of the idea (Q16).

Yet the proposed use did not seem adequate in their eyes. Most of them indeed considered that the best way of using such tutorial was to use it as supporting revision outside lectures and tutorial classes (Q26).

When asked about means of improving the tutorial, half the students made suggestions; the most frequent was to integrate exercises or multiple-choice questions (Q29).

Diagnostic elements

To identify the elements likely to promote or hinder the transmission of knowledge, we sought to analyze the attitude of students at work.

How the students work

To evaluate the way the students worked we have two types of information available: the students’ answers to the appreciation survey and the silent observations.

Concerning the supports they used, the great majority of students stated they used on line Chapter I dedicated to Chime hands-on work while only 68% turned to the guide provided by the teacher (Q6). The observers note: chapter I (Hands-on Chime) learning time is short (6 min. on average) and effective for eleven students out of twelve; only one student skimmed over the chapter and had to turn back to the explanations later. The guide handed out by the teacher was used at the very beginning of the work but only six students out of twelve used it more than five times during the session. The teacher was only asked to intervene twice; four students out of twelve attempted to work with their neighbours.

Concerning the way they read, the students declared they had read rather attentively (Q27). The majority mentioned that they had gone back to an earlier chapter in order to revise an idea. The observers had, in fact, noted periods of attentive reading of the text interspersed with phases of inattention. Note taking did not generally occur very often but this varied according to the students. Going backward in the page and/or in the chapters was observed for six students out of twelve.

Concerning their use of the buttons, the majority of students asserted they had always clicked on the buttons for illustrations, though 16% of them did not do it systematically. More than half the students said they read the text before clicking (Q27). The observers note that the time spent by the students for discovering the interactive buttons varied a lot (from 6 to 34 min.). Counting the exact number of uses of the buttons and evaluating the molecular manipulation time are hard tasks, yet the observations allow one to say that, as soon as they were found, the buttons were used very frequently.

Concerning the manipulation of 3D-models, two options were available: either observing the molecule by rotating or translating it or by zooming with the mouse, or modifying its representation modes, its colours and its status (static or rotating) through the MDL Chime menu. Two thirds of the students stated they had used the direct interaction possibilities (Q11); but apart from two of them, all returned to the MDL Chime menu more or less often (Q7). Two thirds used a form other than that first proposed by the computer; some of them (1/3) systematically tested the four possible modes of molecular representation whereas the
others occasionally tested several modes. The majority of students claimed they had adapted the representation mode to what they wanted to visualize (Q13). They mostly preferred the ball and stick representation (Q12). The observers noted that molecules were often manipulated for long periods of time. All students acted upon the status of the proposed molecule and they sometimes investigated well the different possibilities provided by the LDL menu to the point of getting unexpected images.

Evaluating the working sequences on the tutorial
12 observations were collected by the silent observers corresponding to 23% of the tested student population. Among these observations, 3 were only partly dealt with because of disruptive factors due to the computerized material and independently of the experimenters’ and students’ will. For each observed student the following data were analysed: total working time on the tutorial, time spent on each chapter. The observers evaluated the following in relation to the time spent: use of the tools (the teacher’s guide, online guide) and the frequency of use, the student’s behaviour while working (note taking, going back), the interactivity use (frequency and duration of use of the buttons and of molecular manipulation) as well as indicators of tiredness or inattention (yawning, chatter, stretching out). We define a working period as the time between two obvious signs of tiredness or inattention.

The observers noted that the time the students devoted to the study of the tutorial varied from 60 to 100 minutes for a nominal 90-minute session. They also noted a variation in the working time, which was one hour for the group C, whereas the groups A, B and D worked for a period of between 90 and 100 min. Each observed student showed at least one long working period (more than half an hour) and two students did not display any sign of tiredness after one hour and a half. The rest of the time was used for shorter working periods punctuated with signs of inattention. Such signs may reflect tiredness, saturation or the need for a break before concentrating anew. Silent observations also revealed the time spent on each chapter of the tutorial by the observed students (Figure 7).

Figure 7. Maximum, minimum and average time dedicated to each chapter by the students

<table>
<thead>
<tr>
<th>chapter</th>
<th>time spent</th>
</tr>
</thead>
<tbody>
<tr>
<td>Start</td>
<td>0,0</td>
</tr>
<tr>
<td>I</td>
<td>5,0</td>
</tr>
<tr>
<td>II</td>
<td>10,0</td>
</tr>
<tr>
<td>III</td>
<td>15,0</td>
</tr>
<tr>
<td>IV</td>
<td>20,0</td>
</tr>
<tr>
<td>V</td>
<td>25,0</td>
</tr>
</tbody>
</table>

Time (in minutes) spent on each chapter as recorded during the silent observations: maximum (top arrow), minimum (small bar) and average (diamond). ‘Start’ is time before work beginning, numbers refer to the chapters of the tutorial (I, Hands-on; II, molecular models; III, Molecular geometry; IV, Electron density models; V, Molecular polarity; VI, Hydrogen bonds; VII, Electrostatic potential models; VIII, lipophilicity profiles; IX, Hydrophobic effect and interactions; X, from lipids to membranes; XI: DNA structure).

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The time dedicated to each chapter study varied from 1 to 20 min. with average times varying from 3 to 11 minutes (Figure 7). On several occasions the observed students spent as few as 1 or 2 minutes on a whole chapter of the tutorial. This observation raises doubt about the 78% of the students who asserted they had worked on all the chapters (Annex 3bis, Q9). The observers also recorded working times ranging from 3 to more than 15 minutes for the study of DNA that had been suggested as an option in the teacher’s guide. Finally, the very variable time spent on the various chapters of the tutorial by different students, especially adjacent ones, indicated that each student was able to work at his own pace.

**Difficulties perceived**

Several questions aimed at identifying which notions had been perceived as difficult by the students. The notions perceived as easy to grasp were molecular geometry and molecular polarity as well as the hydrogen bond. The difficulty level of hydrophilicity/hydrophobicity and membrane structure notions was considered medium. Lastly, the notions perceived as being the most difficult ones were electron density and hydrophobic interactions.

**Discussion**

The tutorial ‘Structure and molecular dynamics in biology; Part 1: water and molecular interactions’ seeks to improve the understanding of core chemistry concepts as applied to biochemistry through providing an abundance of images, animations, 3D-molecular models as well as possibilities of interactivity. Thanks to modern modelling methods, we now have the chance of approaching interaction and reactivity notions in an original and realistic way (Bouvier and Leseney, in preparation). The theoretical content and the tutorial sequence offer a pedagogically constructed sequence (instructivist inspiration, Russell et al., 2004) to young undergraduates. The choice of water, a simple molecule, stood out as imperative since it allowed the introduction of shape and reactivity characteristics, all the more so as water is an essential molecule for understanding life. Hence, it logically follows to present the different interaction forces of the biological molecules and to provide clear examples. However we found it vital to enable students to take the initiative in learning structure and movement notions (constructivist inspiration, Russell et al., 2004). We think that, even if the use of analogies may be useful sometimes (Sarantopoulos and Tsaparlis, 2004), the teachers’ role at University level is rather to pass on to the students an approach of core concepts in as realistic and scientific a way as possible.

Experimenting with this tutorial requires a limited and relatively homogeneous student population; we chose to work with first-year undergraduates engaged in vocational training (Colmar IUT, University Institute of Technology); such students have seldom if ever used a computer as a learning aid. We analyzed their behaviour when using this tutorial in relatively autonomous conditions. We sought too to evaluate the impact of such use on the students’ knowledge. We have examined the possibilities provided by that tutorial without trying to establish a comparison of its ‘pedagogical effectiveness’ with that of a conventional type of tutorial class.

The experiment described here was carried out in October 2003 and concerned fifty-two students divided up into two groups. Three methods of analysis were devised: an appreciation survey for collecting the students’ context and their opinions, a knowledge questionnaire aiming at detecting possible improvements post-use, and a procedure of silent observing so as to relate the questionnaire results to the students’ behaviour.

The students showed contradictory wishes and practices. When they were given the chance of an interactive tutorial class, they wanted to have other tutorials of that type available, while they agreed that they had made little use of the internet in order to learn and
communicate. Most (90%) of them wished to find on line documents produced or recommended by their teachers, yet they did not consider turning to the wide range of complementary information provided by the internet on their own initiative. The apparent contradiction in this state of affairs can be ascribed to several factors.

First, these students have little time available since much of their working time is shared between conventional courses, conventional lab work and tutorial classes. On the Net available documents are most often on-line courses corresponding to those of their teachers, and they see no point in multiplying information sources; they ‘trust’ their teacher who is often also their examiner.

Second, because of the scant number of interactive documents, their difficulty of access and the students’ limited capacity for judging their relevance, guidance from a teaching instructor is required. Another possibility could be the use of dedicated Net Gates helping students and teachers to find relevant documents. For the moment, the few Net gates specifically devoted to help finding pedagogical tutorials at a Higher Education level indicate resource addresses but with little or no comment. In this respect let us mention the Deambulum on the Infobiogen site (http://www.infobiogen.fr/deambulum/); la Pitié Salpêtrière Hospital site (Paris): (http://www.chups.jussieu.fr/en-ligne/index.html); The Biology Project : Biochemistry (http://www.biology.arizona.edu/biochemistry/biochemistry.html). MERLOT: (Multimedia Educational Resources for Learning and On Line Teaching, http://merlot.org) ask for peer reviewing (Cooper, 2005).

The students’ work on the tutorial

The paper instruction guide distributed by the teacher was used at the beginning of the session, but the students generally dropped it quickly and very rarely went back to it while working. They made the effort to learn how to use the molecular visualization software suggested as an interactive manipulation in the tutorial (Chapter 1) before going any further (only one out of the twelve students observed skimmed through that first chapter and had to go back to it during the process). The progression of the students in using the tutorial shows that each student had been able to work at his/her own rhythm, as is testified by the variable values of the ‘time spent’ on the various chapters. Yet, in spite of the 90 min. given time, there can be seen a noticeable group effect: students belonging to the same group tended to synchronize the development of the sequences, which led to a total time spent on the tutorial quite similar among the students within a given group. The time that every student devoted to investigating the DNA molecule (in Chapter XI), an option suggested in the paper guide, varied greatly and was on average greater than the time they spent on the membrane paragraph that was part of the program. In our opinion investigation on the glamorous DNA macromolecule, abundance of interactivity and the beauty of the DNA representation focussed the students’ attention by the end of the session better than did the membrane paragraph which was poorly interactive and probably harder.

On the whole the students’ attention was sustained. We observed that for a majority of the students, attention reached its maximum during a limited period of 30 minutes; however, some of them had an apparent capacity for concentration beyond an hour. Attentive reading and in-depth searching were sometimes differently evaluated by the observers and by the students. A large majority of students claimed that they had worked through all sections of the tutorial, however the time dedicated to certain chapters was obviously too short for allowing in-depth work, especially in the group of students whose global working time had been around 60 minutes. Moreover a little more than half the students declared they had read the text carefully and indicated that they had sometimes gone back to the preceding chapter and indeed the observers witnessed little going back among half the students observed.
Critical analysis of the knowledge evaluation

We first searched for what could have been wrongly introduced because of the form and the orientation of the questions. What we can state is that order and meaning (C or I) of the correct and incorrect answer and the fact that the required answer was either exclusive or multiple had no bearing on the results.

The questions regarding knowledge evaluation addressed complex notions that often covered several themes taken up in the tutorial. Subdividing certain questions into items and regrouping items into themes proved to be a powerful analysis tool and provided information on the understanding of those different themes, highlighting the global improvement obtained. This allowed us also to bring to light a deficiency in the tutorial; it dealt with water and its interactions with biological molecules, and was not clear about ions and their solubility. Such a gap in the text might have been disconcerting for a certain number of students and could have introduced some doubt in their ways of answering. This has been taken into account in the new tutorial version presented on the reference site (Bouvier and Leseney, in preparation).

Analysis of the tutorial contribution

The experimentation allows defining the advantages, difficulties and deficiencies with regard to the conception and content of the tutorial and to its adequacy to the purpose of the authors.

The tutorial was judged by the students as being of easy access and handling with a well done navigation. Observers noticed few returning to the summary, which implies that the students had gone through the tutorial in the suggested direction. Silent observations attest the long attention periods bestowed on the tutorial by the students, and in particular, with regards to the handling of the molecules. The students applied interactivity to the representation of molecules well, and frequently beyond what had been suggested to them. Such interest in interactions might lead to real improvements in the pattern adopted and in the use of the tutorial.

As reported in previous studies (Wu et al., 2000; Dori and Barak, 2001), many other students besides ours preferred the ‘ball and stick’ representations where covalent bonds show up well. This representation is most like what they had previously seen when manipulating 3D physical models. In the case of the ‘compact’ representation the hydrogen bonds appear better, but visualization is more difficult as it is at a far more complex level, that of distance interactions.

The great majority of the students valued the help that the tutorial provides for understanding the concepts studied. This opinion is confirmed by the results obtained in the knowledge evaluation the statistics of which display a progression of the global score and of the scores per themes post-use. Use of the tutorial leads to a substantial decrease of ‘no responses’ to the knowledge evaluation questionnaire; this suggest that the students felt more confident in answering the questions (even though the given answer was sometimes incorrect).

One can infer from the results lesser effectiveness of the last chapters, which leads one to consider that the length of the tutorial and the amount and complexity of its content may cause saturation and both may need to be reconsidered bearing in mind the concentration capacity of the students on a given task.

The students suggested that the document would be improved if exercises and multiple-choice questionnaires were added, which would amount to lengthening the sessions or the time available for each tutorial sequence. During the discussion with the teachers some students said they had been disturbed because they felt ‘they had done nothing’. The fact of having nothing to hand in prevented them from checking whether they had achieved the assigned work; they seemed to consider that attentive reading and interactive use, seen by the
teachers as activities enabling further understanding and deepening, did not mean real work. In our opinion such demand highlights the need for a more precise pedagogical framework and probably emphasizes how interesting it would be to present the students concerned with the results of our experimentation. The students also suggested working in pairs, and even a closer relationship with the teacher, although they didn’t take up those two possibilities during the session. We believe that the facilities at their disposal (one computer per student) led them to think that we were asking for individual work, though no such instruction had been given.

**Contribution of animation, images and text to the comprehension**

When implementing the tutorial, priority has been given to the quality of the explanation and of the illustrations of the concepts dealt with, as well as the pedagogical fluidity of the sequence. Further requirements follow from the training objective and from the chosen media:

1. the tutorial was devised as a tool for revision and/or self-training, which requires adequate explanations so as not to need further information or explanations from the teacher;
2. to have readable texts on the computer screen demands very rigorous writing: the text must be concise, clear and with no redundancy.

Our results show that the animations constitute an element that fosters learning and they captured the students’ imagination: such is the case, for example, of the Brownian motion and of the vibratory state of water. They help the students memorize those notions. Yet the same notion of Brownian motion applied to the membranes was illustrated by a static image, which may have caused the confusion observed among the students. One may suppose that the students have new requirements because of the opportunities offered by new media and expect to see moving what moves. We think that, if visualization allows a more intuitive approach of theoretical notions, it is imperative that the authors of the tutorial provide scientifically valid illustrations, taking into account the present state of knowledge. At the present time constructing an animation about the movement of molecules within a membrane is hard; hence the global approach of that notion should be modified in the tutorial.

The poor score recorded for item 15b after use of the tutorial revealed that the students could not connect the 3D computer model of glucose and its conventional 2D Haworth representation. Thanks to the paper guide provided by the teacher, they got to know the ‘2D rendering’ Chime function which shows the relationship between the 2D schematic structure and the 3D structure of aspirin, and the majority of the observed students had tried it; yet they did not use it for other molecules. A specific working session devoted to the relation between 3D models and 2D representations would probably be useful before working on the tutorial. The authors of the tutorial have constructed convenient tools such as ‘virtual glucose’ (Bouvier et al., 1999; http://wwwarpe.snv.jussieu.fr, then ‘glucose virtuel’) and a course about sugars in the University on line (see http://wwwarpe.snv.jussieu.fr, ‘Université en ligne’ then ‘Biochimie’ then ‘glucides’, then ‘apprendre’ and Chapter 1-C3) where comparative learning of the different representations was offered in the form of an animation. These tools were drawn to the students’ attention, and indeed some of them were curious enough to take a look at them at the end of the session. In the evaluation questionnaire given to the students knowledge of the schematic structure of a carbohydrate (or sugar) had been wrongly assumed to be a pre-requisite.

The format of the written texts aroused few questions in the appreciation survey; however, one may note that the students did not always identify the texts printed in bold as drawing their attention onto a key notion. The necessary conciseness of the text and the absence of redundancy imply that very careful reading is needed to understand the texts fully. Such a task seems to be difficult for first year students. Introducing appropriate questions may deal with that problem to some extent.
Development of the tutorial and of its use

An examination of the various pieces of information derived from the three types of analysis reinforces the conclusions obtained with them and enables us to suggest further developments both in the tutorial itself and in its use.

In the new version of the tutorial (reference site; Bouvier and Leseney, in preparation) defects or difficulties have been corrected by introducing, for example, a section about ions and by modifying the approach concerning membrane mobility. The new version of the tutorial also includes contextual questions which encourage the students to pause and ponder more over the content.

To overcome the problem of length and complexity for first year students, the tutorial can be split into themes, each one being considered as an elementary module usable at different teaching times and referring to the other chapters whenever necessary. Each teaching sequence would be shorter, which could eliminate the drawbacks due to computer work lasting too long. Such a division could focus the students’ attention and keep them from investigating all the accessible sections thoroughly, even when it was recommended to drop certain parts. It is worth noting that we are confronted here with a contradiction: on one hand we had to let the students have a multi-use tool and encourage them to explore such possibilities; and on the other hand we had to seek a way for them to take a moderate line in exploring the different parts. The tutorial used as such without any subdivision is desirable only as a revision tool, and using it for learning should be conditional on an appropriate division of the work into phases to allow for shorter sequences.

The experiment described here demonstrates that it is possible to enhance the use of the tutorial. We note that the great majority of students wished to use the tutorial as a revision tool outside the course and the tutorial classes. And yet observations, as well as certain remarks from the students, suggest another way of using the tutorial. Students could be encouraged to work in pairs or even in groups in the tutorial class through arranging times for individual reading and for discussion supported by questions. Encouraging the students to keep personal written notes seems to us to be of importance. Another possibility would consist in giving the students a paper guide able to play a greater part as a support for thinking and learning by including questions they would have to answer. This was implemented when using the tutorial in 2004; the students’ attention was better captured and the tutorial working time showed less variation in getting closer to the allocated 90-minutes.

During one of the preliminary experiences (2002) there was another interesting attempt: suggesting a questionnaire at the end of the session that would be worked on with the tutorial; under such conditions the student did check his/her understanding and needed his/her ‘visual’ memory in order to identify the tutorial elements linked to the content of the question. It might be interesting to envisage a tutorial version with a multiple-choice questionnaire ‘on line’ at the end of every chapter. This would allow for immediate evaluation and correction, together with the possibility for the student of going back to the chapter concerned.

Enjoying the manipulation of molecules and the construction of representations, verifying the understanding through questions to be solved, and the possible return to texts at any time certainly contribute to make learning effective.

Conclusion

In our practice as teachers and researchers, the evolution of the teaching contents resulting from the progression of scientific knowledge and the heterogeneity of the student population are issues we have to address. The help provided by numerical tools and the new communication media foster new scientific and pedagogical approaches (Brassard and Duele, 2003). Our option has been to take advantage of the opportunity offered by utilization of new
media in order to construct innovative tutorials. Numerous authors point out the absence of impact of science education research in subject matter on the practice of education in that field (De Jong, 2000; Kempa, 2002; Tsaparlis, 2004; Gilbert et al., 2004). Yet Russell et al. (2004) observed that teachers enthusiastically set about creating tutorials, but their interest soon flags to such an extent that they give up because of too many discouraging difficulties arising from the implementation. In our conception of pedagogical networks, conception and use of such tools can be separated tasks. We have set up a laboratory, the ARPE (Atelier de Recherche Pédagogique), whose purpose is to establish connections between educational and scientific research and teaching practice by developing new educational tools, and improving and validating them through pedagogical experimentation. We hope these tools, together with recommendations about their use and documented evaluation about their efficiency would be widely distributed among the teaching community. These Net Gates fully annotated would encourage teachers to change their practice and adopt these new tools.

The tutorial evaluated in this article takes advantage of recent methods of modelling to bring out a new approach of biochemical molecules and of their reactivity, in a more intuitive way that is still correct from a scientific point of view (Bouvier and Leseney, in preparation). Testing of this tutorial both with statistical and behavioural indicators proved it to be a valuable pedagogical tool, accessible and easy to use. The students appreciated this tutorial and asked for more of this type; their knowledge on the topics covered improved significantly after using the tutorial. As expected, the students were able to work at their own pace, but we could identify difficulties linked to the tutorial and further, to Computer Assisted Learning. The new version of the tutorial (Bouvier et al., in preparation) addresses these difficulties. Moreover, utilisation procedures better adapted to the abilities of the students are proposed.

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References

Atkins P., (2005), Skeletal chemistry, Education in Chemistry, 42, 20, 25; see also: http://www.rsc.org/Education/EiC/issues/2005_Jan/skeletal.asp
Brassard C. and Daele A., (2003), Un outil réflexif pour concevoir un scénario pédagogique intégrant les TICE, Colloque Environnement informatiques pour l'apprentissage humain, 15-17 April 2003, Strasbourg.
De Jong O., (2000), Crossing the borders: chemical education research and teaching practices, University Chemistry Education, 4, 31-34.
Parslow G.R. (2002), Commentary: molecular visualisation tools are good teaching aids when used appropriately, Biochemistry and Molecular Biology Education, 30, 128-29.
Taber K.S., (2001), Building the structural concepts of chemistry – some considerations from educational research, Chemistry Education Research and Practice, 2, 123-58.
Tsaparlis G., (2004), Has educational research made any difference in chemistry teaching? Chemistry Education Research and Practice, 5, 3-4.


Tutorial V.01 ‘Structure et dynamique moléculaire en biologie; part 1: eau et interactions moléculaires’ as used for the experiment. (French).

Tutorial V.02 ‘Structure and molecular dynamics in biology; part 1: water and molecular interactions’ as modified after the experiment (English / French).

Annex 1: Guide written by the teacher.

Annex 2: Knowledge evaluation questionnaire

Annex 2bis: Items of the knowledge evaluation questionnaire

Annex 3: Appreciation survey

Annex 3bis: answers to the appreciation survey

Annex 4: Silent observation (an example)

Annex 5: Validation of the method used