*Scientific paper*

# The Students' Perceptions Using *3DChemMol* Molecular Editor for Construction and Editing of Molecular Models

**Danica Dolničar,[1,*] Bojana Boh Podgornik[1] and Vesna Ferk Savec[2]**

[1] *Faculty of Natural Sciences and Engineering, University of Ljubljana, Snežniška 5, 1000 Ljubljana, Slovenia*

[2] *Faculty of Education, University of Ljubljana, Kardeljeva ploščad 16, 1000 Ljubljana, Slovenia*

* *Corresponding author: E-mail: danica.dolnicar@ntf.uni-lj.si*

*Received: 09-30-2021*

## Abstract

The paper presents a study in which 54 university students were introduced to a newly developed, free, web-based *3DChemMol* molecular editor with a toolbar, which they then evaluated. The tool aims to increase representational competence related to submicroscopic representations. Students who used the software for the first time, were instructed to create molecular models using the model building/editing tools in three activities with varying levels of difficulty: 1) building a simple model (butanoic acid), 2) converting one model (hexane) into two models, 3) converting from a non-cyclic to a cyclic structure (glucose). It took students from two up to 15 minutes to accomplish each of the activities. Several types of help were available in the *3DChemMol* molecular editor toolbar to assist students during their activities, including a video tutorial, button hovering, action status display, and a help menu. Undo/redo and restart options were also available. Students' completion level, difficulties, and use of the help features were investigated using student self-evaluation questionnaires. The *3DChemMol* molecular editor proved to be a useful support for students in completing simple chemistry activities. Students were successful in model building, although they encountered some specific difficulties, especially in steps that involved spatial operations, such as rotating the selected part of molecule around the bond. In students' perception, the video tutorials were the preferred and most frequently used type of help, and the undo function was considered essential. The results suggest that the *3DChemMol* molecular editor can be used effectively in introductory chemistry courses at the tertiary level, whether for direct instruction, self-study, or other forms of support in the pedagogical process. The results and new findings of this study will be used to further optimize the interface in future versions of the evaluated tool.

**Keywords:** Representational competence; submicroscopic representations; learning chemistry; 3D model building; model editing tool

## 1. Introduction

### 1. 1. Visualization and Molecular Models in Chemistry Education

The concept of visualization can be understood in three ways:[1] visualization of objects (physical or graphic representations, static or dynamic, analog or digital, can be accompanied by sensory data), introspective visualization (mental models), and interpretive visualization (making meaning from the previous two forms). Vekiri[2] states that graphical representations allow for more efficient processing of information compared to verbal representations, which reduces working memory load. The adoption of visualization is not automatic but a function of prior knowledge.[3]

Understanding the core ideas introduced in chemistry education involves engagement with their representations and the associated phenomena.[4] Johnstone[5,6] was the first to propose three levels of representation of scientific concepts and processes: (1) macroscopic (e.g., chemistry experiments), (2) submicroscopic (e.g., molecular models) and (3) symbolic (e.g., chemical formulae). The three types of representations relate to phenomena perceived through our senses and support explanations at qualitative and quantitative levels.[4] Students often struggle with understanding and using the triplet concept. 3D models of molecules represent the submicroscopic representation,

the use of which is important to bridge the gap between the macroscopic and symbolic levels.[7]

Kozma and Russell[8] defined representational competence in science education as a set of five distinct abilities of students: to analyze the features of representations, transform between representations, create new representations, explain the usefulness of representations, and explain the advantages of representations. Activities aimed at improving representational competence support spatial thinking[9] which is critical for understanding 3D spatial concepts in STEM (science, technology, engineering and mathematics) disciplines.[10]

The use of physical and virtual molecular models promotes representational competence[11–13] and fosters spatial understanding,[14] although the impact of spatial ability on success is influenced by learning strategy and task demands.[15] Students who used models were more likely to implement new concepts, transform from 2D to 3D representations, and answer visual-spatial tasks. In the past, physical modeling kits with balls and sticks or magnets were used to construct 3D analog models of chemical compounds.[16–18] Later, molecular modeling software brought chemical visualizations into the digital virtual realm.[19–21] Since then, numerous stand-alone and web-based applications for viewing and manipulating chemical structures have become available, such as, ArgusLab, Avogadro, BALLView, Biovia discovery studio visualizer, Chime, Chimera, JME molecular editor, Jmol/JSmol, Oscail X, Pymol, RasMol, Spartan, SwissPDB Viewer, Tinker, Chemis 3D Molecular Viewer Applet, VMD, Yasara, and others.[20,22–26]

Some reported course activities and research involved the construction or use of physical models by students.[27–32] Thayban et al.[33] found that virtual models were more effective than physical model in learning symmetry. On the other hand, the use of physical or virtual molecular models was found to assist students in solving chemistry problems that require spatial thinking.[34]

Studies at all levels of chemistry education indicate that in order to construct correct mental models of chemical compounds, students should be engaged in constructing and manipulating three-dimensional (3D) visualizations.[35,36] The construction of submicroscopic models is part of representational competencies.

Kelly and Akaygun[37] suggested that visualizations are too often used only as a method of direct instruction. Instead of being passive observers students should become interactive participants and critical thinkers. In a survey[38] that was part of the workshop for molecular visualization in science education researchers, educators, and software developers discussed the role of molecular modeling in college chemistry and were asked about the features of molecular representation and the types of interactions with molecular visualization that most help students. The responses suggested that students should be able to create their own visualizations and interact with existing ones.

In some reported course activities, students were using molecular modeling software. Some of the advantages over physical modeling are flexibility in model building, switching between different representations, and accuracy of structural representations.[39] According to Kozma,[8] the construction, calculations and manipulation of molecular models support the laboratory practice of synthesis by looking at reaction sites and speculating on reaction mechanisms. Clauss and Nelsen[40] used WebMo and Gaussian to teach students the fundamentals of computational chemistry by performing *ab initio* and DFT (density functional theory) calculations in an undergraduate laboratory course with the goal of gaining a deeper understanding of their experimental work. Linenberger et al.[41] conducted a guided experiment using the student version of Spartan to discover the relationship between structure and molecular properties, e.g., through measurements, calculating dipole moments, and studying electron density potential maps and molecular shapes. Raiyn and Rayan[42] reported on the impact of a workshop using ChemDraw in a college chemistry course that significantly improved students' understanding of 3D structure and polarity, boiling point, and isomerism. Rothe & Zygmunt[43] used Gauss View 5 and Gaussian in an undergraduate chemical reaction engineering course to promote understanding of the relationship between molecular properties and macroscopic concepts such as internal energy, enthalpy, rate constants, and activation energies. In a web-based chemistry course, Dori et al.[44] gave first-year students the task of using Weblab and IsisDraw to create molecular models, calculate molecular weight, and construct the hybridization and electric charge distribution of carbon atoms. On the posttest, which required higher-order thinking skills, the experimental students showed better reasoning skills and a better ability to transfer between levels of representation than the control group. Ealy[45] introduced molecular modeling using Spartan Pro to a general chemistry laboratory. Students performed measurements and investigated properties such as symmetry, electrostatic potential, and dipole. The experimental group performed significantly better than the control group, and the test results at the end of the semester also showed that a transfer of knowledge had occurred. In an ethnographic study by Kozma,[46] students who first conducted experiments in the laboratory and then constructed molecular models using Spartan. When using the computer modeling software, students referred to chemical concepts (e.g., atoms, bonds, electronegativity, dipole moment) more frequently than in the laboratory session. Yet, they did not relate the models to the materials they synthesized. Molecular modeling was used by pre-service teachers in combination with classroom materials and mind map tools to learn hydrogen bond.[47] Kolar et al.[48] suggested the didactic use of computational chemistry to create models of amides to illustrate acid-base properties. Winfield et al.[49] have developed activities that incorporate model building in the iSpartan

tool to teach conformations of alkanes. Similarly, Johnson et al.[50] reported integrating of iSpartan into the classical organic chemistry laboratory experiment to help students learn about the stability of alkenes. Conformational analysis of small molecules using Vega ZZ software was used by Soulère[51] in an undergraduate chemistry course.

User-friendliness of graphical interfaces to optimize small and medium sized molecules has enabled the possibility to introduce computational chemistry tools to the undergraduate level.[52] Rodriguez-Becerra et al.[53] described the use of educational computational tools on pre-service chemistry teachers, with Avogadro used for model building.

Due to the identified deficiency in educational use of molecular modeling in chemistry classes by teachers and/or students,[54] molecular modeling was introduced into chemistry education by Aksela et al.,[55] developing pedagogical solutions, training mentors, creating teaching materials and investigating their effectiveness. The modeling approach was adopted by schools and the experiences were shared in a book.[56] The Edumol.fi web application was used.[57]

## 1. 2. Tools for Building Molecular Models in Teaching Organic Chemistry

At the beginning of this study, we analyzed existing molecular modeling tools for teaching organic chemistry at the university undergraduate level in order to select the most appropriate tool to serve as the basis for the development of a new tool, *3DChemMol* molecular editor.[58] Its editing functionality and help tools are described and evaluated in this article.

Some of the external factors influencing the potential for wider adoption of molecular visualization tools for teaching and active learning could be their suitability for a particular level of education (primary/secondary and college), their focus (small molecules, macromolecules, crystal structures), the presence of editing feature (molecular modeling), functionalities (display of properties), and their cost and convenience. The degree of complexity and the usability of the user interface could also play a role. With the advent of web-based technologies (HTML5, CSS, WebGL, canvases, and the use of JavaScript), there has been a shift from standalone applications and web applications requiring plug-ins to readily available web-based tools.[59] In terms of availability, molecular modeling tools have been developed that are open source.[60] In this study we focus on the software that is suitable for education, focuses on small molecules, allows molecular modeling and is freely available. Some of the tools are compared in Table 1. Due to immediate availability, we limited our choice to web-based applications that do not require installation. These criteria exclude tools such as *Spartan*[20] (proprietary, standalone), *Web Doodle Web Components*[61] (proprietary, web-based), *Avogadro*[62] and *Jmol*[63] (free, standalone), leaving us with mainly web-based tools. We also excluded web tools that are viewers only (e.g. *3dmol.js*[64]) or those that involve creating a 3D model by drawing a 2D structure (e.g. *MolView*[65]). The remaining web-based interfaces were based on *JSmol*,[66] a web version of *Jmol*. They included interfaces for the creation of 3D models: *CheMagic*,[67] *MolCalc*[68] and *3DChemMol*.[58] The latter was developed by the first author of this study. The original *JSmol* editing module is menu-based, cumbersome to use, and lacks a functional undo and help function. *CheMagic* has implemented both, but the functionalities of the tool (as in *JSmol*) are all visible at once, which can be distracting if you are only focused on editing. *MolCalc's* editing feature creates the input for the computational software. It is simple and efficient but uses only basic editing functions. *3DChemMol* was designed to structure the *JSmol* functionalities into multiple toolbars accessible from the main menu, including editing, with additional interactive functions with toolbars for model exploration (e.g., electronegativity, measurement, symmetry, creating conformations and isomers, model comparison, and exercises). It was chosen for our study because the new editing interface is intended to resemble that of familiar 2D editing tools.

## 1. 3. Motivation and Aims of the Study

The aim of this study was to evaluate the newly developed *3DChemMol* molecular editor tool and to investigate university students' first encounter with a 3D structure editing tool while performing three specific activities

**Table 1:** Characteristics of selected freely available user interfaces for 3D model building

| Tool name | Type | Technology | GUI elements | Characteristics |
|---|---|---|---|---|
| *Avogadro* | S | C++, Qt | Menus, toolbars, dialogs | Editing dialog, mode switching for rotation |
| *Jmol* | S | Java | Menus, toolbar, dialogs | Editing menu on right click |
| *JSmol* (original) | W | JavaScript, JQuery | Menus (right click) | Editing menu on right click |
| *CheMagic* (JSmol) | W | JavaScript, JQuery | Dashboard buttons | All tool functionalities at once, editing buttons, undo, help |
| *MolCalc* (JSmol) | W | JavaScript, JQuery | Buttons | Basic editing (adding, deleting), input for computational software |
| *3DChemMol* (JSmol) | W | JavaScript, JQuery | Menus, toolbars | Editing toolbar, undo, help |

Types: S = standalone, W = web-based

for creating and editing molecular models. The research questions were as follows:

- RQ1: How successful were students in performing simple chemistry activities using the *3DChemMol* molecular editor, and how was their success related to the time required and the perceived difficulty of the activity?
- RQ2: What types of difficulties did students encounter when performing activities with *3DChemMol* molecular editor? What was the cause and a possible remedy?
- RQ3: How did students use the different types of help available in *3DChemMol* molecular editor and additional support when they encountered problems?

# 2. Methods

## 2. 1. Participants

A total of 54 students of the University of Ljubljana participated in the study. They were enrolled in the second year of study (aged 20 to 21) at the Faculty of Education (17 students, 31.5%) or the Faculty of Health (37 students, 68.5%) in the study year 2020/21. They had already taken basic chemistry courses in general and inorganic chemistry; therefore, basic knowledge and understanding of chemistry principles and basic ICT skills were assumed. Introduction to building 3D models of chemical compounds was designed as a foundation for organic chemistry and other higher level chemistry courses that follow in their program of study. Apart from the field of study, there were no additional differences between the groups, important for the purpose of this research.

## 2. 2. Materials

### 2. 2. 1. Model Building Tool

The editing module of the web-based tool *3DChemMol* molecular editor (http://www2.arnes.si/~supddoln/3dchemmol), previously created by the author of this study,[58] was used to construct the molecular models. The tool is based on *JSmol* software for visualization and editing of 3D molecular models. Model creation is performed in 3D using a graphical user interface consisting of the model window and toolbar (Figure 1). The tool contains basic model building functionalities, but also some advanced features that allow the creation of different conformations and isomers.

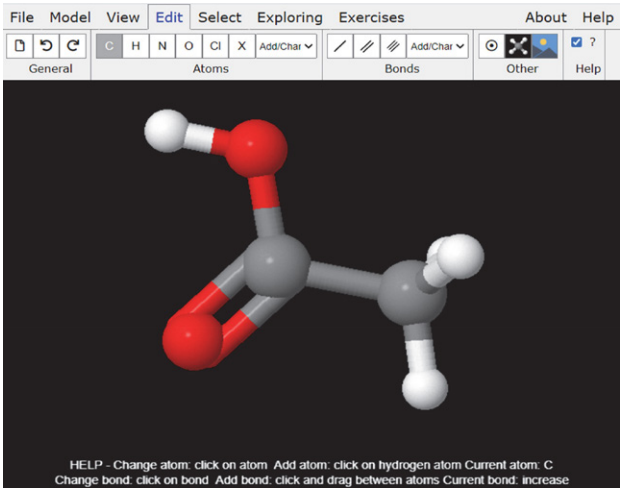


**Figure 1:** User interface of the *3DChemMol* molecular editor

The available model interactions (e.g., clicking or dragging on atoms/bonds) depend on the current action mode. There are four atom action modes (add/edit, delete, move, invert-substitute switch) and three bond action modes (add/edit, delete, rotate around bond). Switching between action modes is done by selecting a mode from the list.

One of the additional elements implemented in the tool is the Undo/Redo function, which did not work in the original *JSmol* application.

Four types of help are integrated and available at all times: a) status indicator of the currently available action mode, displayed at the bottom of the model window (optional), b) explanations of button actions when hovering the mouse over them, c) help menu with image and text explanations of the toolbar, d) video tutorial with examples of structure building, also available from the help menu.

One of the standard functions of model building is geometry optimization. The tool also allows to quickly create an image from the model window.

### 2. 2. 2. Problem Set

Three simple activities were designed to guide students in building and editing models using our tool. Each activity required students to create or edit a specific molecule with a limited number of actions.

- Activity 1: Build a simple model of the molecule – butanoic acid (new model, add/change atoms, change bond type). This activity did not require any change in action mode – all the functions needed to build a model were already present.
- Activity 2: Convert from one to two models of the molecules – hexane to ethene and butane (delete bonds, delete atoms, manually add hydrogen atoms, change bond type).
- Activity 3: Convert from a non-cyclic to a cyclic model of the molecule – glucose (add bonds, rotate branches around a bond, change bond type).

The full list of steps for each activity can be found in Table 2. All activities included common features such as changing the bond type (with some differences) and automatic geometry optimization. At the end of each activity, students had to create an image of the final model of the molecule. Time for each activity was not limited.

Some steps required a simple click on a toolbar button, while others required direct interaction with the model or a combination of both (Table 2). The model interactions available depended on the current action modes.

**Table 2:** Steps for each activity with the required interaction with the toolbar and the 3D model

| | | Interaction with the toolbar | | | Interaction with the 3D model | | |
|---|---|---|---|---|---|---|---|
| **Step #** | **Step content** | **Button click** | **Type change** | **Mode change** | **Atom click** | **Atom drag** | **Bond click** |
| **Activity 1: Building a simple model of the molecule** | | | | | | | |
| 1 | New model | x | | | | | |
| 2 | Adding C atoms | | | | x | | |
| 3 | Adding heteroatoms | | x | | x | | |
| 4 | Changing the bond type | | | | | | x |
| 5 | Model centering | x | | | | | |
| 6 | Geometry optimization | x | | | | | |
| 7 | Creating an image | x | | | | | |
| **Activity 2: Converting one model into two models of the molecules** | | | | | | | |
| 1 | Deleting bonds | | | x | | | x |
| 2 | Changing the bond type | | x | | | | x |
| 3 | Deleting atoms | | | x | x | | |
| 4 | Adding hydrogen (manually) | | x | x | | x | |
| 5 | Geometry optimization | x | | | | | |
| 6 | Creating an image | x | | | | | |
| **Activity 3: Converting from a non-cyclic to a cyclic form of the molecule** | | | | | | | |
| 1 | Adding a bond | | | | | x | |
| 2 | Changing the bond type | | | | | | x |
| 3 | Geometry optimization | x | | | | | |
| 4 | Rotating a branch around the bond | | | x | | | x |
| 5 | Geometry optimization | x | | | | | |
| 6 | Creating an image | x | | | | | |

For each activity, students were provided with the editing tool interface, which contained the initial model on the left half of the screen and activity instructions in Google Forms on the right half (Figure 2). The activity instructions consisted of a) general information about the availability of free model rotation, undo/redo functions, and various types of help; b) an image of the 3D output model (which was also displayed in the interface); c) a

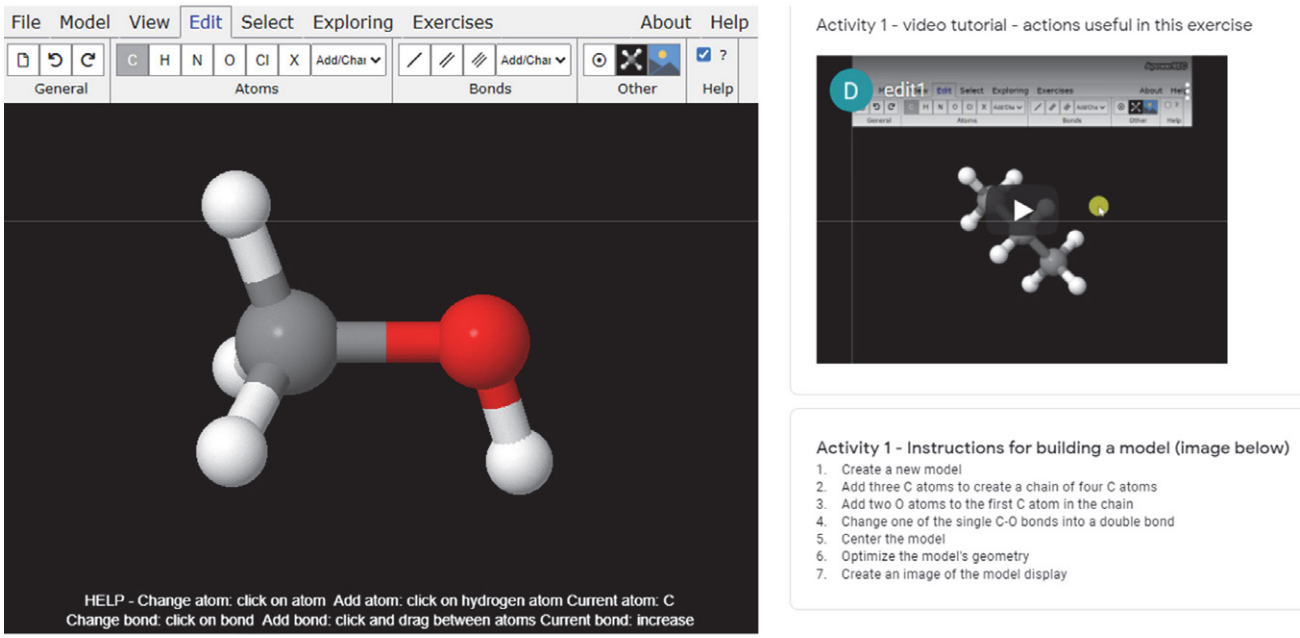


**Figure 2:** Activity display for the first activity (left: interface for model building, right: activity instructions)

short, annotated video tutorial explaining relevant actions on another example model; d) step-by-step instructions on how to build the target model, which referred to individual actions rather than elements of the interface; e) an image of the 3D target model. Students could scroll up and down through the instructions.

### 2. 2. 3. Students' Self-evaluation Questionnaires

For each activity, a self-evaluation questionnaire was included at the end of the activity instructions (Google Forms) with the following items/questions:

- degree of activity completion – completion level (Likert scale 1–5: 1 = started, 5 = fully completed);
- time spent on the activity (in minutes, as reported by students);
- perception of activity difficulty – perceived difficulty level (Likert scale 1–5: 1 = easy, 5 = difficult);
- type(s) of help used (multiple choice: a) video tutorial (single view), b) video tutorial (multiple views), c) hover on toolbar, d) current action status, e) help menu);
- other actions used (multiple choice: a) free view rotation, b) undo, c) redo, d) restart activity);
- severity of difficulties encountered for each step of the activity – step difficulty level (Likert scale 1–5: 1 = no difficulties, 5 = severe difficulties);
- difficulty description (text).

Prior to the study, two researchers (the co-authors of the study) optimized the instrument by performing a face validity[69] check. They completed the suggested activities and reviewed the questionnaires and then suggested changes and adjustments.

## 2. 3. Data Collection

The testing was conducted in May 2021 and was supervised by the authors in an online format. The Zoom videoconferencing tool and a web browser were used to display the tool and instructions with the questionnaires. Students consented to data analysis.

Prior to testing, a standardized introductory protocol was used that included clarification of purpose, instructions, voluntary participation, and acknowledgement of participation. The research was approved by the competent authorities of University of Ljubljana. None of the students had any prior experience with the tool. The teacher first gave a general introduction/demonstration of the entire *3DChemMol* molecular editor. Students had access to the interface. Students were then given links to the activities. After completing each activity, they completed the questionnaire and moved on to the next activity.

## 2. 4. Data Analysis

Data from the students' self-evaluation questionnaires were collected in Google Spreadsheets and transferred to Excel and Statistical Package for the Social Sciences (SPSS), version 26 for analysis, which was performed for each of the three activities.

- Mean scores were calculated for continuous and ordinal questionnaire items, including completion level, time spent, perceived activity difficulty level, and step difficulty levels. Step difficulty mean was also calculated for each activity. The two multiple-choice questions (type of help used, other items used) were transformed into multiple dichotomous variables, one for each response (1 if the response was selected and 0 if it was not). Means were calculated for each response.
- The distributions of the variables were examined using the frequency of the results expressed as a percentage of students. This was done for ordinal items and multiple-choice responses, and also for time spent on activity, where scores were first divided into five groups.
- Correlations between parameters were calculated using Spearman correlation coefficient ($r_s$).
- The open-ended questions from the student self-evaluation questionnaires were also recorded in Google Spreadsheets and transferred to Excel. The students' responses were coded using a coding table. The coding table was derived from a qualitative analysis of 20% of the questionnaires (n = 11 participants); the reliability of the coding was ensured by independent coding by two researchers (the authors of this article). Finally, both evaluations were contrasted at the points where differences occurred and, after consideration, the more appropriate one was selected. Altogether, 99% reliability was achieved.

# 3. Results and Discussion

## 3. 1. Completion Level of the Activities

Completion level of the activities was measured by the self-evaluation questionnaire. For each activity, the time spent on the activity and the perceived level of difficulty were also reported.

### 3. 1. 1. Means and Distributions

Students were relatively successful in completing the simple chemistry activities, as measured on a Likert scale of 1 to 5. The average score was above 4 for all 3 activities (Figure 3). For the first two activities, the completion level was very high with 91 and 96% of students reporting that they completed the activity, compared to only 53% for the third activity (Figure 4).

The completion time, measured in minutes, showed that the majority of students took between 3 and 5 minutes for each of the first two activities, while most students took 6–10 minutes for the last activity (Figure 5), with a significantly higher mean (Figure 3).

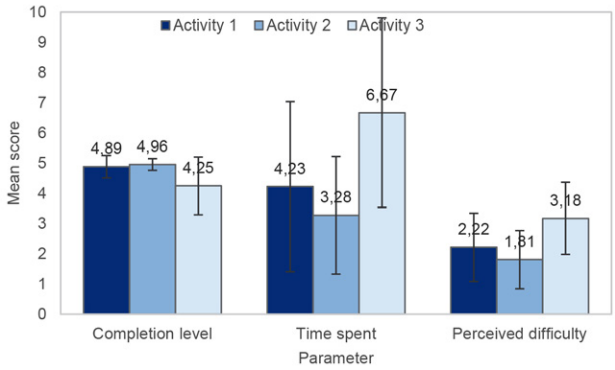


**Figure 3:** Mean scores with SD (whiskers) by activity for activity completion level (1–5), time spent on activity (min), and perceived activity difficulty (1–5)

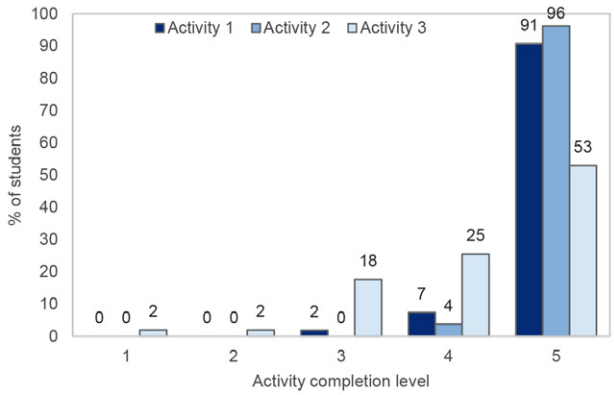


**Figure 4:** Distribution of activity completion levels by activity (5 = fully completed)

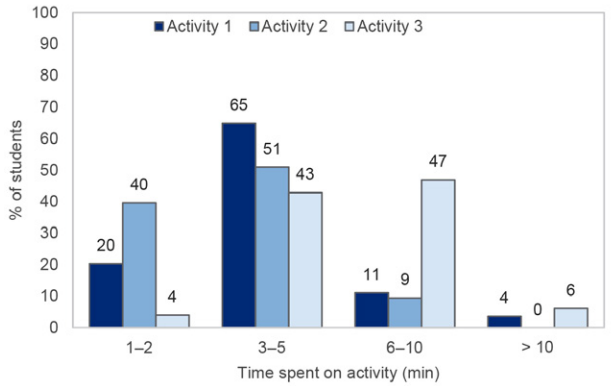


**Figure 5:** Distribution of time spent on activity by activity

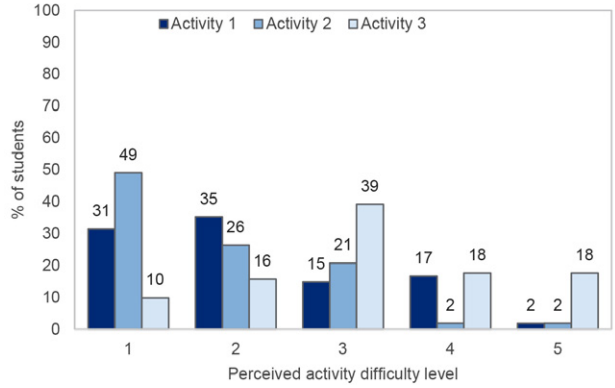


**Figure 6:** Distribution of perceived activity difficulty by activity (5 = difficult)

Perceived difficulty, expressed on a Likert scale of 1–5 (5 being difficult), showed that the second activity was considered the easiest with a mean of 1.81, and the third activity was considered the most difficult, with a mean of 3.18 (Figure 3). The most common response for activity 1 was difficulty level 2, for activity 2 was difficulty level 1, and for activity 3 was difficulty level 3 (Figure 6).

### 3. 1. 2. Correlations

No significant correlation was found between time spent and activity completion (Table 3). Some students took more time, but still completed the activity. An example is a comment on activity 1: "I had trouble adding atoms at first but figured it out after a few minutes." As expected, time spent correlated positively with perceived difficulty (most strongly for the second – overall easiest activity). Students who spent more time on the activity perceived it to be more difficult. The negative correlation between completion and perceived difficulty was significant for the third – the hardest overall activity – suggesting that students who did not complete the activity perceived it to be more difficult. For example, a student's comment was: "It is difficult to have spatial orientation." The lower correlation between perceived difficulty and completion level for the first two activities was due to the high completion levels for these activities. Similar correlations between perceived difficulty as a determinant of Web search performance and time have been found in a study by Kim.[70]

**Table 3:** Spearman correlations between completion level (Compl.), time spent (Time) and perceived difficulty of activities (Perc. diff.)

| Param. | Compl. | Time | Perc. diff. |
|---|---|---|---|
| **Activity 1: Building a simple model of the molecule** | | | |
| Compl. | 1.000 | | |
| Time | –0.069 | 1.000 | |
| Perc. diff. | –0.239 | 0.404[b] | 1.000 |
| **Activity 2: Converting one model into two models of the molecules** | | | |
| Compl. | 1.000 | | |
| Time | –0.081 | 1.000 | |
| Perc. diff. | –0.266 | 0.584[b] | 1.000 |
| **Activity 3: Converting from a non-cyclic to a cyclic form of the molecule** | | | |
| Compl. | 1.000 | | |
| Time | –0.158 | 1.000 | |
| Perc. diff. | –0.469[b] | 0.435[b] | 1.000 |

[b] $p < 0.01$

## 3. 2. Difficulties During the Activities

### 3. 2. 1. Mean Scores by Activity

The step difficulty mean for each activity reflects the average amount of difficulties students encountered during steps of an activity. The scores (Figure 7) show the same trend as the time spent and perceived difficulty of the activities (Figure 3). Students reported the greatest step difficulty mean on the third activity and the smallest on the second activity. Means ranged from 1.62 to 1.91, which is relatively low given the Likert scale of 1 and 5. For all activities, some students specifically stated: "No problems," and several others made no comment. Mean scores are low due to the proportion of steps that are not problematic and those that are less problematic. Examples of repeated comments in all activities related to some technical difficulties were: "I can't save the image."

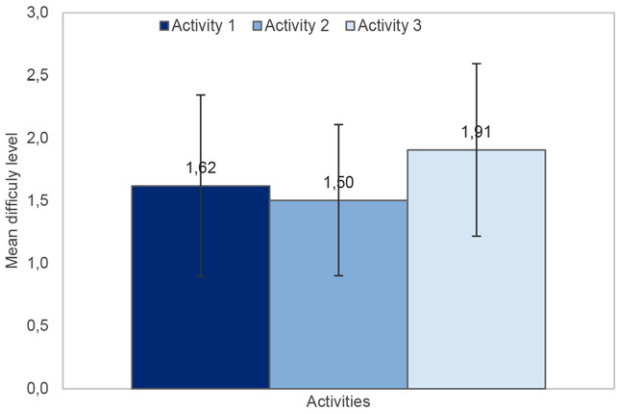


**Figure 7**: Step difficulty mean with SD (whiskers) by activity (1 = no difficulties, 5 = severe difficulties)

### 3. 2. 2. Mean Scores by Interaction Type

In the previous section the steps were grouped by activities. Here we grouped steps in multiple ways and calculated step difficulty mean for each group. The grouping in Table 4 by type of interaction shows that bond interactions caused more difficulties than atom interactions. Toolbar interactions with button click were the least problematic.

**Table 4:** Step difficulty mean by interaction type

| Interaction type | Step diff. mean |
|---|---|
| Toolbar button click | 1.48 |
| Atom interaction | 1.76 |
| Bond interaction | 1.86 |

Steps with atom and bond interactions were also classified into four groups (Table 5). Actions that required selection of the atom or bond type on a toolbar button prior to direct interaction with the model caused fewer difficulties than those that did not require a preceding action on the toolbar. On average, the most difficult actions were those that required a change of action mode (selection on the toolbar from a list of modes, e.g., add/change, delete). The action requiring a combination of type and mode change was also deemed more difficult.

**Table 5:** Step difficulty means for direct interaction with the model, depending on the preceding action

| Preceding action | Step diff. mean |
|---|---|
| Button type change | 1.54 |
| No action | 1.80 |
| Button mode change | 1.95 |
| Button type + mode change | 1.98 |

Another classification of steps was applied to direct interactions with atoms and bonds: clicking, dragging and repeated actions (Table 6). Repeated mouse clicking caused the most difficulties, followed by mouse dragging. A single mouse click on a bond or on atom was the least problematic. Repeated clicking was related to geometry changes in our case.

**Table 6:** Step difficulty means in direct interaction with the model, depending on the type of mouse interaction and repetition

| Direct interaction type | Step diff. mean |
|---|---|
| Mouse click | 1.58 |
| Mouse drag | 2.07 |
| Mouse click + repetition | 2.90 |

The last grouping of atom and bond interactions concerned geometry change (Table 7). The fewest difficulties arose from automatic geometry optimization. No direct interaction with the model was required. Actions where no significant geometry change occurred (nothing added, no automatic hydrogen adjustment) were considered less problematic. The most difficulties occurred when the geometry was changed, highlighting the importance of spatial abilities.

**Table 7:** Step difficulty means when interacting directly with the model, depending on the type of geometry change

| Type of geometry change | Step diff. mean |
|---|---|
| Geometry optimization | 1.35 |
| Small geometry change | 1.59 |
| Significant geometry change | 1.96 |

### 3. 2. 3. Scores by Step

Step difficulty levels for each step of the three activities, presented in Table 8, were ranked from 1 (easiest) to 18 (most problematic). Scores for individual steps ranged between 1.21 and 2.90. Total step difficulty mean was 1.66.

*Activity 1: Building a model of butanoic acid.* The easiest steps involved two actions available through a simple button click: creating a new structure (ranked 4 out of 18) and geometry optimization (ranked 5). Moderate difficulties were encountered in adding C atoms (rank 9) to build the main skeleton of the structure. This step is crucial. Some of the students reported difficulties, such as: "When clicking with the mouse, an atom was deleted instead of added." This was because the mouse was moved when clicking on a hydrogen atom. Instead, the "drag" event was registered, which in *Jmol* is associated with deleting an atom when applied to a hydrogen atom. Comments also related to adding heteroatoms (rank 13): "I can't position the chain as it is shown in the result." and "Sometimes atoms are added in strange ways." Another comment: "In the beginning, I had a lot of problems with adding atoms unevenly." Students were paying attention to structure but not configuration. Adding and replacing atoms only required clicking on existing atoms. There was not much chance for error, so "strange ways" and "unevenly" likely refers to configurations that result in isomers of the target structure. In this first activity, students have not yet learned how to make configuration changes. Adding atoms correctly required good spatial orientation. There were some difficulties with centering the model (ranked 12). Comment: "I had trouble centering the model until I found the centering button. It would be beneficial if centering was automatic because centering has to be applied repeatedly when building larger structures." This difficulty could have to do with familiarity with the center button, but students also forgot that they could not only rotate the model during model construction but also zoom it out. The zoom button was not part of the editing toolbar, but was an available mouse shortcut (mouse wheel). Surprisingly, most of the difficulties with this activity occurred when it came to changing the bond type (ranked 15), which should be quite simple by just clicking on a bond to increase its order. Increasing the bond order was not included as a toolbar button but was part of the default add/delete action mode. There was no need to change the action mode. The comment "The number of hydrogens doesn't automatically adjust." suggests that students tried to use a different method where they selected the bond type and clicked on a bond. This process does not currently adjust the hydrogens. Students did not know the shortcut even though it was shown in the introductory video. The two methods should be made compatible. Creating an image (ranked 14) also caused difficulties for some students, as expressed in a comment: "I can't convert to an image. Numbers appear instead." The reason here was that some system configurations automatically generated a text file with the structure in mol format

**Table 8:** Steps for each activity with interaction types, step difficulty levels and ranks

| Step # | Step content | Button, atom, bond | Type, mode chg . | Mouse click, drag, rep. | Geom. chg. | Inter. type* | Step diff. level | Step diff. rank |
|---|---|---|---|---|---|---|---|---|
| **Activity 1: Building a simple model of the molecule** | | | | | | | | |
| 1 | New model | c | | | | c | 1.44 | 4 |
| 2 | Adding C atoms | a | – | k | y | a | 1.52 | 9 |
| 3 | Adding heteroatoms | a | t | k | y | t+a | 1.67 | 13 |
| 4 | Changing the bond type | b | – | k | y | b | 1.93 | 15 |
| 5 | Model centering | c | | | | c | 1.63 | 12 |
| 6 | Geometry optimization | c | | | g | c | 1.46 | 5 |
| 7 | Creating an image | c | | | | c | 1.69 | 14 |
| **Activity 2: Converting one model into two models of the molecules** | | | | | | | | |
| 1 | Deleting bonds | b | m | k | n | m+b | 1.49 | 8 |
| 2 | Changing the bond type | b | t | k | n | t+b | 1.40 | 3 |
| 3 | Deleting atoms | a | m | k | n | m+a | 1.47 | 6 |
| 4 | Adding hydrogen | a | tm | d | n | tm+ad | 1.98 | 16 |
| 5 | Geometry optimization | c | | | g | c | 1.21 | 1 |
| 6 | Creating an image | c | | | | c | 1.47 | 7 |
| **Activity 3: Converting from a non-cyclic to a cyclic form of the molecule** | | | | | | | | |
| 1 | Adding a bond | a | – | d | y | ad | 2.16 | 17 |
| 2 | Changing the bond type | b | – | k | y | b | 1.57 | 11 |
| 4 | Rotating a branch | b | m | kr | y | m+br | 2.90 | 18 |
| 3&5 | Geometry optimization | c | | | g | c | 1.37 | 2 |
| 6 | Creating an image | c | | | | c | 1.53 | 10 |

* Key to interaction types: c – toolbar button click, a – atom interaction, b – bond interaction, t – button type change, m – button mode change, k – mouse click, d – mouse drag, r – repetition, g – geometry optimization, n – small geometry change, y – significant geometry change

instead of the image file. This technical issue needs to be addressed and fixed in the future. The issue mentioned in a comment: "I had no particular problems constructing the model, but the angles between atoms aren't the same." was either related to configuration or the student did not optimize the model geometry correctly. A comment from a student who reported no individual difficulties was: "The correct tool is not visible." In this case, the comment could refer to shortcuts built into the editor that are not explicitly visible in the toolbar (e.g., changing the bond type in general mode). This activity did not require any action mode changes but some students had expected them.

*Activity 2: Splitting the model of hexane into models of butane and ethene (cracking).* In this assignment, several students reported, "I had no problems." Geometry optimization and bond change were considered the easiest steps by students (ranked 1 and 3, respectively). Here, bond change was performed by first selecting the bond type from the toolbar (no shortcut used). This method did not automatically adjust the number of hydrogen atoms, but unlike the first activity, the subsequent steps were designed to solve this problem. Deleting atoms and bonds did not cause too many difficulties (rank 6 and 8), however, a student commented: "Problems switching between adding and deleting atoms." The reason is that the delete function is not immediately visible but is in a list of action modes in the toolbar. The most problematic part of the activity was the manual hydrogen addition (ranked 16). It consists of selecting the hydrogen atom type in the toolbar and then dragging out an existing atom with the mouse. A typical comment was: "Problems with adding the single H atom due to the fact that addition and modification appear together." As with the first activity, more than one action is available in Add/Change mode, depending on the type of interaction (click, drag), the object of interaction (atom, bond), and sometimes the type of atom (hydrogen, non-hydrogen). There is no separate button or selection on the toolbar for this action. As with the first activity, students may have been looking for a separate mode and could not find the button. Adding the H atoms by dragging was otherwise covered in the tutorial video and also shown in the action mode text help at the bottom of the screen. Interestingly, some of the difficulties were related to a functionality not being available. A student commented: "The button to move one of the models did not work, so I could only rotate the left model." The reason is that moving and rotating individual models is not possible in edit mode. Only the entire view can be rotated. This functionality could be incorporated in the future, as it is already present in other toolbars of this software. Image creation difficulties were not rated as severe (rank 7) for this activity, although the same technical obstacles were encountered. Comment: "I could not save the image, so I took a screenshot instead." Perhaps the severity changed or there were other novice difficulties saving the file in the first activity.

*Activity 3: Converting the noncyclic form to a cyclic form of glucose.* The only unproblematic action in this activity was geometry optimization (rank 2). Changing the bond type from double to single bond was perceived moderately difficult (rank 11). Some students remembered the shortcut from the first activity, others did not. A typical comment was: "I had a problem changing the bond." Creating an image was also still an issue (ranked

**Table 9:** Summary of the most frequent difficulties with example student comments

| Act. # | Step # | Theme / Step | Category* | Possible issue | Step diff. rank** | Example student comment |
|---|---|---|---|---|---|---|
| 1 | 2 | Ading C atoms | a | Interface | 9 | "When clicking with the mouse, an atom was deleted instead of added." |
| | 3 | Adding heteroatoms | a | Spatial ability | 13 | "I can't position the chain as it is shown in the result." |
| | 4 | Changing the bond | b | Interface | 15 | "The number of hydrogens doesn't automatically adjust." |
| | 5 | Model centering | c | Interface | 12 | "I had trouble centering the model until I found the centering button." |
| | 7 | Creating an image | c | Technical | 14 | "I can't convert to an image. Numbers appear instead." |
| 2 | 4 | Adding hydrogen | a | Interface | 16 | „Problems with adding the single H atom due to the fact that addition and modification appear together." |
| 3 | 1 | Adding a bond | b | Interface | 17 | „I didn't know how to connect the O atom to the other side..." |
| | 4 | Rotating a branch | b | Spatial ability | 18 | "One of the groups was always oriented in the wrong direction." „It is difficult to have spatial orientation." |

* Key to categories – interaction types: a – atom interaction, b – bond interaction, c – toolbar interaction

** Key to step difficulty rank: 1 = easiest, 18 = most difficult among all steps

10) to some, with a comment: "I couldn't save the image." Adding a bond between two existing atoms and especially rotating a branch around a bond were the two most problematic steps overall (ranked 17 and 18). The latter step had a difficulty of 2.9, which is one grade above the former step at 2.16. Some students did not know how to connect two atoms, as evident in a comment: "I didn't know how to connect the O atom to the other side and what the correct rotation was." or a comment: "Having trouble connecting the structure properly." Dragging was required in Add/Modify mode, so no mode change was required in this step and no toolbar button was available. The appropriate action was demonstrated in the tutorial video and shown in the action status help at the bottom of the screen. Perhaps the model itself was part of the problem. It needed to be properly oriented so that the atoms could be reached with the mouse. Good spatial orientation could be related to this action. This was even more evident when the branch was rotated, as a student wrote in a comment: "I couldn't get the model aligned the way it was in the picture. One of the groups was always oriented in the wrong direction." or another student "I couldn't place the atoms in the position shown in the resulting image." The branch rotations around the bond were done in 60-degree increments. Students had to determine the correct degree of rotation by applying (repeating) the action the appropriate number of times. Another comment "It is difficult to have spatial orientation." suggested that this activity required more spatial orientation than the first two activities. Comment, "It was difficult to begin the activity. Watching the tutorial video was crucial. Still, I had trouble rotating the bonds." The first sentence (beginning of the activity) refers to the bond addition. Although this activity proved to be the most difficult overall, four students indicated, "No problems." This is consistent with the research of Harle and Towns who noted that rotational transformations were among the tasks that students had particular difficulty with.[71]

The most typical themes and categories of students' difficulties that emerged from the above analysis are listed in Table 9. Of the eight themes, three each related to atom and bond manipulations and the remaining two to toolbar interaction. Two of the issues are probably related to the students' lack of spatial orientation, which could be improved through training. Another requires solving a technical issue. The rest could be possibly avoided/fixed by redesigning parts of the user interface (e.g. even more visible action status, separation of actions that are too similar, separate buttons instead of mode selection).

### 3. 2. 4. Correlations

There are significant correlations between most steps within an activity in terms of difficulties (Tables 10–12). Mean of step difficulties is included as step mean. In the

**Table 10:** Spearman correlations between step difficulty levels within Activity 1

| Step | Description | Step 1 | 2 | 3 | 4 | 5 | 6 | 7 | Step mean |
|---|---|---|---|---|---|---|---|---|---|
| 1 | New model | 1.000 | | | | | | | |
| 2 | Adding C atoms | 0.620[b] | 1.000 | | | | | | |
| 3 | Adding heteroatoms | 0.479[b] | 0.646[b] | 1.000 | | | | | |
| 4 | Changing the bond type | 0.441[b] | 0.508[b] | 0.482[b] | 1.000 | | | | |
| 5 | Model centering | 0.408[b] | 0.473[b] | 0.414[b] | 0.505[b] | 1.000 | | | |
| 6 | Geometry optimization | 0.426[b] | 0.587[b] | 0.392[b] | 0.343[a] | 0.718[b] | 1.000 | | |
| 7 | Creating an image | 0.272[a] | 0.408[b] | 0.255 | 0.238 | 0.281[a] | 0.506[b] | 1.000 | |
| | Step mean | 0.629[b] | 0.690[b] | 0.625[b] | 0.752[b] | 0.690[b] | 0.631[b] | 0.568[b] | 1.000 |

[a] $p < 0.05$, [b] $p < 0.01$

**Table 11:** Spearman correlations between step difficulty levels within Activity 2

| Step | Description | Step 1 | 2 | 3 | 4 | 5 | 6 | Step mean |
|---|---|---|---|---|---|---|---|---|
| 1 | Deleting bonds | 1.000 | | | | | | |
| 2 | Changing the bond type | 0.562[b] | 1.000 | | | | | |
| 3 | Deleting atoms | 0.687[b] | 0.740[b] | 1.000 | | | | |
| 4 | Adding hydrogen | 0.401[b] | 0.283[a] | 0.332[a] | 1.000 | | | |
| 5 | Geometry optimization | 0.423[b] | 0.672[b] | 0.439[b] | 0.351[a] | 1.000 | | |
| 6 | Creating an image | 0.185 | 0.313[a] | 0.254 | 0.119 | 0.357[b] | 1.000 | |
| | Step mean | 0.675[b] | 0.657[b] | 0.698[b] | 0.765[b] | 0.537[b] | 0.474[b] | 1.000 |

[a] $p < 0.05$, [b] $p < 0.01$

**Table 12:** Spearman correlations between step difficulty levels within Activity 3

| Step | Description | Step 1 | 2 | 4 | 3 and 5 | 6 | Step mean |
|---|---|---|---|---|---|---|---|
| 1 | Adding a bond | 1.000 | | | | | |
| 2 | Changing the bond type | 0.350[a] | 1.000 | | | | |
| 4 | Rotating a branch | 0.276[a] | 0.270 | 1.000 | | | |
| 3 and 5 | Geometry optimization | 0.285[a] | 0.326[a] | 0.086 | 1.000 | | |
| 6 | Creating an image | 0.365[b] | 0.169 | 0.037 | 0.331[a] | 1.000 | |
| Step mean | | 0.777[b] | 0.579[b] | 0.630[b] | 0.501[b] | 0.516[b] | 1.000 |

[a]$p < 0.05$, [b]$p < 0.01$

final step – saving the image of the result – the correlations are not as strong, as the difficulties with image creation were largely a technical issue. Difficulties with rotating a branch around a bound (third activity) also do not correlate with all other steps of the activity, as many students had difficulties in this step.

### 3. 2. 5. Correlations with Completion Level of the Activities

The step difficulty mean for each activity correlated positively with time spent and perceived activity difficulty and negatively with activity completion (Table 13). The completion level for the second activity was very high, so the correlation with step difficulty mean was not significant.

## 3. 3. Help Tools Used During Activities

The forms of help available included the tutorial video, the help menu, the description of the toolbar button when the user hovers over it, and the description of the actions currently available on the structure (atom and bond actions). If students made mistakes, they could undo and

**Table 13:** Spearman correlations of step difficulty mean with completion level (Comp.), time spent (Time) and perceived activity difficulty (Perc. diff.)

| Step | Description | Comp. | Time | Perc. diff. |
|---|---|---|---|---|
| Activity 1: Building a simple model of the molecule | | | | |
| 1 | New model | –0.419[b] | 0.421[b] | 0.522[b] |
| 2 | Adding C atoms | –0.421[b] | 0.422[b] | 0.503[b] |
| 3 | Adding heteroatoms | –0.235 | 0.512[b] | 0.553[b] |
| 4 | Changing the bond type | –0.135 | 0.503[b] | 0.290[a] |
| 5 | Model centering | –0.231 | 0.585[b] | 0.353[b] |
| 6 | Geometry optimization | –0.290[a] | 0.458[b] | 0.356[b] |
| 7 | Creating an image | –0.121 | 0.224 | 0.292[a] |
| Mean | | –0.334[a] | 0.620[b] | 0.539[b] |
| Activity 2: Converting one model into two models of the molecules | | | | |
| 1 | Deleting bonds | –0.305[a] | 0.410[b] | 0.307[a] |
| 2 | Changing the bond type | –0.341[a] | 0.488[b] | 0.518[b] |
| 3 | Deleting atoms | –0.296[a] | 0.494[b] | 0.492[b] |
| 4 | Adding hydrogen (manually) | –0.041 | 0.467[b] | 0.496[b] |
| 5 | Geometry optimization | 0.083 | 0.506[b] | 0.428[b] |
| 6 | Creating an image | –0.152 | 0.205 | 0.276[a] |
| Mean | | –0.215 | 0.558[b] | 0.599[b] |
| Activity 3: Converting from a non-cyclic to a cyclic form of the molecule | | | | |
| 1 | Adding a bond | –0.104 | 0.305[a] | 0.280[a] |
| 2 | Changing the bond type | –0.333[a] | 0.298[a] | 0.344[a] |
| 4 | Rotating a branch | –0.445[b] | 0.409[b] | 0.468[b] |
| 3 and 5 | Geometry optimization | –0.115 | 0.203 | 0.236 |
| 6 | Creating an image | –0.211 | 0.063 | 0.179 |
| Mean | | –0.424[b] | 0.493[b] | 0.508[b] |

[a]$p < 0.05$, [b]$p < 0.01$

redo previous actions. They were free to rotate the models during the construction process. If none of the previous actions helped, they could restart the activity.

### 3. 3. 1. Distributions

Of the above actions with help tools, free rotation and the undo button were used by most students (70–94%) (Figure 8). The frequency of free rotation was lowest in the second activity because fewer configuration changes (deleting atoms and bonds as opposed to adding them) were made than in the other two activities. Nevertheless, 14% of students reported not rotating the model in the third activity, which involved a larger configuration change when adding a bond to form a ring, as well as rotating a branch around a bond. The number of students who used the undo feature increased by 20% in the third activity, as only 6% of students did without it. This indicates the importance of the undo function, which did not work in the original *JSmol* interface. Redo function was not used as frequently, although its use increased with each activity and one in four students used it by the third activity.

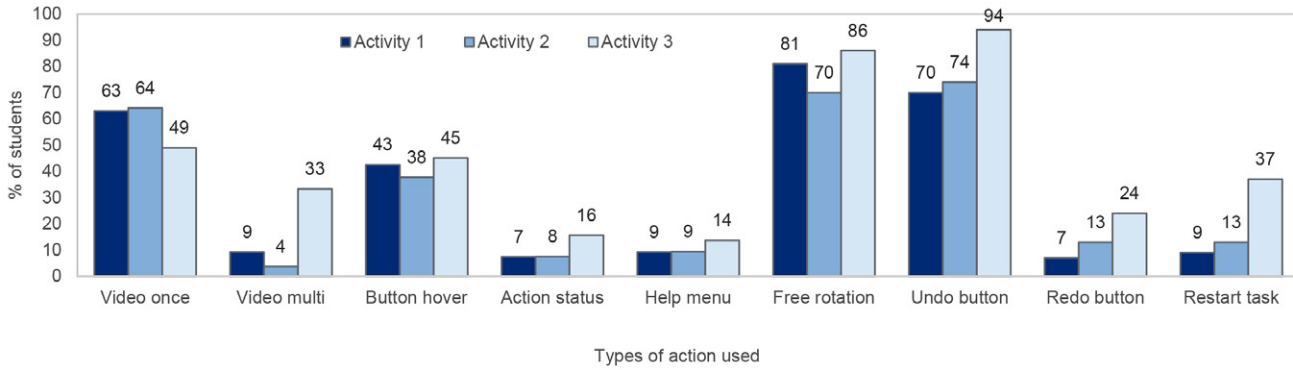


**Figure 8:** Distribution of actions with help tools by activity

The most commonly used type of help was watching the tutorial video once, followed by the mouse-over button action. About 30% of students reported not watching the video in the first two activities, but in the third activity, the number of multiple video viewings increased significantly: One in three students watched the video more than once, compared to 4–9% in the previous activities. An example of a student comment on this activity is: "Watching the tutorial video was crucial." The use of the mouse-over action was comparable in all three activities and was used by less than half of the students. The last two help options (action status and help menu) were used less frequently, increasing from less than 10% in the first two activities to about 15% in the last activity. This could mean that students were not confused about the current action status (work mode) or that they missed the textual status display at the bottom of the screen. Interestingly, they also made little use of the help menu, which could indicate that they found the video tutorials largely sufficient. This is consistent with the conclusion of a study by Van Der Meij,[72] in which video tutorials that previewed the training activities were the most effective for learning software. The help menu provided similar information to hovering over the buttons. Finally, the level of activity restarting was low (9%) for the first activity, indicating that building a new structure by adding atoms and changing bonds was not a problem, especially because the undo function was available. This value increased slightly in the second activity and significantly in the third activity. Nearly two out of five students estimated that they were too far off course compared to the target model or did not get close enough, so they started over. They were not discouraged and there was no time limit on the activity. In this activity, the importance of good spatial ability was probably most pronounced. Starting over was the chosen strategy.

### 3. 3. 2. Correlations

Interestingly, for all three activities, there was a significant negative correlation between using the video (once) and hovering buttons, suggesting that students who did not watch the video relied on hovering buttons in the toolbar (Table 14). No significant correlation with the four types of help was found for free rotation or the use of the undo button in any of the activities. This could mean that these two functionalities were used by all. In the first activity, the negative correlation with button hovering was also observed for multiple video views. There, the use of redo was positively associated with the help menu and negatively associated with watching the video once. In the second activity, use of the help menu was negatively correlated with viewing the video once, indicating that students for whom viewing the video once was sufficient did not use it. With the fewest geometry changes in this activity, students who used free rotation were less likely to use the undo button. In this way, the rotation helped. It is surprising that this was not the case in the third activity, where students could benefit from free rotation even more. There, use of the help menu correlated significantly with other types of help, aside from watching the video once. Students who

**Table 14:** Spearman correlations between actions with help tools

| | Video once | Video multi | Button hover | Action status | Help menu | Free rotat. | Undo button | Redo button | Restart activity |
|---|---|---|---|---|---|---|---|---|---|
| Activity 1: Building a simple model of the molecule | | | | | | | | | |
| Video once | 1.000 | | | | | | | | |
| Video multi | –0.416[b] | 1.000 | | | | | | | |
| Button hover | –0.270[a] | –0.275[a] | 1.000 | | | | | | |
| Action status | 0.071 | –0.090 | 0.185 | 1.000 | | | | | |
| Help menu | –0.152 | –0.102 | –0.017 | –0.090 | 1.000 | | | | |
| Free rotat. | –0.168 | 0.152 | 0.218 | 0.135 | –0.177 | 1.000 | | | |
| Undo button | 0.006 | 0.067 | 0.067 | 0.184 | 0.067 | –0.205 | 1.000 | | |
| Redo button | –0.369[b] | –0.090 | 0.042 | 0.190 | 0.398[b] | 0.135 | 0.029 | 1.000 | |
| Restart activity | –0.020 | 0.118 | 0.242 | 0.154 | 0.118 | 0.152 | 0.207 | –0.090 | 1.000 |
| Activity 2: Transformation of one into two models of the molecules | | | | | | | | | |
| Video once | 1.000 | | | | | | | | |
| Video multi | –0.058 | 1.000 | | | | | | | |
| Button hover | –0.554[b] | –0.154 | 1.000 | | | | | | |
| Action status | –0.084 | –0.057 | 0.072 | 1.000 | | | | | |
| Help menu | –0.297[a] | –0.064 | 0.015 | 0.152 | 1.000 | | | | |
| Free rotat. | –0.149 | 0.130 | 0.258 | 0.188 | –0.069 | 1.000 | | | |
| Undo button | –0.002 | –0.106 | 0.113 | 0.009 | 0.193 | –0.301[a] | 1.000 | | |
| Redo button | –0.057 | –0.077 | 0.271[a] | 0.100 | 0.255 | 0.135 | 0.234 | 1.000 | |
| Restart activity | –0.057 | –0.077 | 0.156 | –0.111 | 0.065 | 0.014 | 0.107 | 0.012 | 1.000 |
| Activity 3: Transformation from noncyclical to cyclical form of the molecule | | | | | | | | | |
| Video once | 1.000 | | | | | | | | |
| Video multi | –0.610[b] | 1.000 | | | | | | | |
| Button hover | –0.337[a] | –0.139 | 1.000 | | | | | | |
| Action status | –0.099 | 0.038 | 0.259 | 1.000 | | | | | |
| Help menu | –0.163 | 0.322[a] | 0.326[a] | 0.298[a] | 1.000 | | | | |
| Free rotat. | –0.179 | 0.161 | 0.132 | 0.015 | –0.006 | 1.000 | | | |
| Undo button | 0.078 | 0.177 | –0.108 | 0.108 | 0.100 | 0.142 | 1.000 | | |
| Redo button | –0.174 | 0.098 | 0.333[a] | 0.269 | 0.047 | 0.087 | 0.139 | 1.000 | |
| Restart activity | –0.107 | 0.315[a] | 0.198 | 0.002 | 0.282[a] | –0.164 | 0.020 | 0.146 | 1.000 |

[a]$p < 0.05$, [b]$p < 0.01$

needed help used all available types of help. Students who restarted the activity were also more likely to consult the help menu and watch the video multiple times.

### 3. 3. 3. Correlations with Completion Level of the Activities

For the first two activities, activity completion correlated negatively, and perceived difficulty correlated positively with help menu use (Table 15). Students who did not need to consult the help menu were more likely to complete the activity. Those who did consult the help menu perceived the activity to be more difficult. On the third activity, students who did not have to watch the instructional video multiple times were more likely to complete the activity. Multiple video viewings also correlated positively with perceived activity difficulty. It seems that consulting the static help menu did not help solve the easier activities and that the tutorial videos were not sufficient to solve the more difficult activities. One of the possible remedies would be to create help tutorials/videos for individual actions that students found particularly difficult, covering multiple examples. The use of undo correlated with time spent on the first two activities and redo did on the last two activities. Both also correlated positively with perceived difficulty – students who used them found the activities more difficult. With the third activity, the amount of time spent restarting was significantly higher, and these students were less likely to complete the activity they also perceived as more difficult. Starting over did not help enough.

### 3. 3. 4. Correlations with Difficulties by Activity

The difficulty level referenced is the average step difficulty for each activity (step difficulty mean). In the first activity, one video view seemed sufficient for students who reported fewer difficulties overall (Table 16). In the second

**Table 15:** Spearman correlations between actions with help tools and completion level (Comp.), time spent (Time) and perceived difficulty (Perc. diff.)

| | Video once | Video multi | Button hover | Action status | Help menu | Free rotat. | Undo button | Redo button | Restart activity |
|---|---|---|---|---|---|---|---|---|---|
| Activity 1: Building a simple model of the molecule | | | | | | | | | |
| Comp. | 0.286[a] | –0.114 | 0.022 | 0.090 | –0.351[b] | 0.024 | –0.070 | –0.149 | –0.330[a] |
| Time | –0.114 | 0.079 | 0.062 | –0.207 | 0.252 | 0.034 | 0.286[a] | 0.078 | 0.033 |
| Perc. diff. | –0.108 | 0.028 | 0.088 | –0.161 | 0.293[a] | –0.008 | 0.205 | 0.033 | 0.101 |
| Activity 2: Transformation of one into two models of the molecules | | | | | | | | | |
| Comp. | 0.0584 | 0.039 | –0.050 | 0.057 | –0.275[a] | 0.085 | –0.119 | –0.508[b] | –0.215 |
| Time | –0.164 | 0.235 | 0.059 | 0.010 | 0.420[b] | –0.068 | 0.371[b] | 0.336[a] | 0.185 |
| Perc. diff. | –0.106 | 0.266 | 0.122 | 0.129 | 0.351[b] | 0.090 | 0.353[b] | 0.502[b] | 0.219 |
| Activity 3: Transformation from noncyclical to cyclical form of the molecule | | | | | | | | | |
| Comp. | 0.138 | –0.419[b] | 0.050 | –0.084 | –0.187 | –0.187 | –0.224 | –0.228 | –0.315[a] |
| Time | –0.185 | 0.165 | 0.308[a] | –0.006 | 0.371[b] | 0.130 | 0.147 | 0.435[b] | 0.349[a] |
| Perc. diff. | –0.195 | 0.391[b] | 0.106 | 0.086 | 0.177 | 0.181 | 0.330[a] | 0.379[b] | 0.297[a] |

[a]$p < 0.05$, [b]$p < 0.01$

activity, more difficulties likely resulted in multiple video views. On the third activity, no correlation was found between difficulty and video views. Difficulty level correlated positively with help menu use on the first two activities. This means that students who had difficulties were more likely to consult the help menu. In both activities where the action mode was changed (activities two and three), the difficulty level correlated with the use of the action status help. Students who had difficulties consulted this help. Hovering over buttons, free rotation, and restarting the activity did not significantly correlate with difficulty levels. For all activities, using the undo button, as well as the redo button, were positively correlated with problems.

was visible in the action mode description. Those who had difficulties changing the bond type also used the undo and redo buttons. Difficulties with centering the model correlated with the use of button hover, indicating difficulty in visually identifying the correct button. Students who used free rotation were less likely to have difficulties with geometry optimization.

*Activity 2.* The use of the help menu, as well as the use of the redo button, correlated with difficulty levels in this activity. The exception was manually adding hydrogen, the step that was perceived as the most difficult and, like the shortcut for changing the bond, was not explicitly shown in the toolbar. Undo was used most frequently with the

**Table 16:** Spearman correlations between actions with help tools and step difficulty mean

| Activity no. | Video once | Video multi | Button hover | Action status | Help menu | Free rotat. | Undo button | Redo button | Restart activity |
|---|---|---|---|---|---|---|---|---|---|
| 1 | –0.278[a] | –0.012 | 0.238 | 0.117 | 0.313[a] | –0.068 | 0.336[a] | 0.243 | 0.187 |
| 2 | –0.186 | 0.287[a] | 0.110 | 0.305[a] | 0.357[b] | –0.191 | 0.331[a] | 0.325[a] | 0.151 |
| 3 | –0.0724 | 0.169 | 0.026 | 0.299[a] | 0.169 | 0.021 | 0.296[a] | 0.313[a] | 0.176 |

[a]$p < 0.05$, [b]$p < 0.01$

### 3. 3. 5. Correlations with Difficulties by Step

*Activity 1.* Consultation of the help menu correlated with step difficulty levels in almost all individual steps (Table 17). In general, students who had difficulties consulted the help menu. The exception was changing the bond type, where difficulties were inversely correlated with watching the video multiple times. Students who watched the video multiple times had fewer difficulties with this step. The shortcut for this step was not available in the toolbar but

manual hydrogen addition. In this activity, multiple video views correlated with difficulties changing bond type and deleting atoms. Students used multiple videos when they encountered these difficulties.

*Activity 3.* In contrast to the previous two activities, correlations between difficulty and help menu use were absent or low (not significant). For the two most difficult steps, bond addition and branch rotation, there was a low correlation with the use of action status and undo. Two problems were possibly associated with these steps:

**Table 17:** Spearman correlations between use of help tools and step difficulty level

| Step | Video once | Video multi | Button hover | Action status | Help menu | Free rotat. | Undo button | Redo button | Restart activity |
|---|---|---|---|---|---|---|---|---|---|
| Activity 1: Building a simple model of the molecule | | | | | | | | | |
| 1 New model | –0.005 | –0.178 | 0.125 | 0.015 | 0.416[b] | 0.014 | 0.090 | 0.294[a] | 0.290[a] |
| 2 Adding C atoms | –0.219 | –0.047 | 0.040 | –0.043 | 0.440[b] | –0.149 | 0.215 | 0.308[a] | 0.122 |
| 3 Adding heteroat. | –0.298[a] | 0.176 | 0.119 | –0.065 | 0.303[a] | 0.088 | 0.269 | 0.145 | 0.090 |
| 4 Chg. bond type | –0.196 | –0.272[a] | 0.237 | 0.158 | 0.247 | –0.014 | 0.314[a] | 0.334[a] | 0.050 |
| 5 Model centering | –0.385[b] | –0.023 | 0.300[a] | –0.173 | 0.351[b] | –0.017 | 0.129 | 0.227 | 0.135 |
| 6 Geometry optim. | –0.192 | –0.022 | 0.117 | –0.158 | 0.520[b] | –0.292[a] | 0.280[a] | 0.158 | 0.129 |
| 7 Creating image | –0.048 | –0.075 | 0.170 | 0.168 | 0.080 | –0.310[a] | 0.139 | –0.018 | 0.115 |
| Mean | –0.278[a] | –0.012 | 0.238 | 0.117 | 0.313[a] | –0.068 | 0.336[a] | 0.243 | 0.187 |
| Activity 2: Converting one model into two models of the molecules | | | | | | | | | |
| 1 Deleting bonds | –0.132 | 0.120 | 0.181 | 0.140 | 0.272[a] | –0.203 | 0.158 | 0.433[b] | 0.119 |
| 2 Chg. bond type | –0.151 | 0.390[b] | 0.124 | 0.204 | 0.442[b] | –0.039 | 0.214 | 0.453[b] | 0.127 |
| 3 Deleting atoms | –0.078 | 0.408[b] | 0.120 | 0.121 | 0.381[b] | –0.203 | 0.192 | 0.329[a] | 0.162 |
| 4 Adding hydrogen | –0.238 | 0.137 | 0.096 | 0.218 | 0.2548 | –0.097 | 0.450[b] | 0.118 | 0.046 |
| 5 Geometry optim. | –0.356[b] | 0.218 | 0.098 | 0.098 | 0.427[b] | 0.043 | 0.121 | 0.299[a] | 0.129 |
| 6 Creating image | –0.2206 | 0.185 | –0.104 | 0.243 | 0.328[a] | –0.122 | –0.144 | 0.214 | –0.187 |
| Mean | –0.186 | 0.287[a] | 0.110 | 0.305[a] | 0.357[b] | –0.191 | 0.331[a] | 0.325[a] | 0.151 |
| Activity 3: Converting from a non-cyclic to a cyclic form of the molecule | | | | | | | | | |
| 1 Adding a bond | 0.032 | 0.015 | 0.079 | 0.203 | 0.241 | –0.096 | 0.259 | 0.106 | 0.059 |
| 2 Chg. bond type | –0.034 | 0.069 | 0.115 | 0.261 | 0.162 | 0.046 | 0.031 | 0.408[b] | 0.130 |
| 4 Rotating a branch | 0.015 | 0.198 | –0.029 | 0.267 | –0.022 | 0.152 | 0.228 | 0.293[a] | 0.250 |
| 3,5 Geom. optim. | –0.394[b] | 0.061 | 0.180 | 0.198 | –0.034 | 0.070 | 0.123 | 0.315[a] | –0.185 |
| 6 Creating image | 0.012 | 0.071 | –0.350[a] | 0.066 | –0.196 | –0.084 | 0.123 | –0.050 | –0.058 |
| Mean | –0.0724 | 0.169 | 0.026 | 0.299[a] | 0.169 | 0.021 | 0.296[a] | 0.313[a] | 0.176 |

[a]$p < 0.05$, [b]$p < 0.01$

recognizing the correct action and performing the action correctly. Action status could help with the first part. The tutorial video could help with the second part. Only for branch rotation difficulties was there a low correlation with multiple video views.

## 4. Conclusions and Implications for Teaching

The experience of undergraduate students in construction and editing of molecular models of small organic compounds aimed to equip them with the knowledge and ability to create their own presentations and to proceed with further exploration and analysis of model properties in chemistry courses beyond introductory chemistry. The success of the course also depends on the design of the course and the teacher, which would be worth of further study.

Manipulation of 3D molecular models has been associated with the development of representational skills, particularly when used to support learning.[12,13] Students of all ages encounter problems and misunderstandings when asked to explain chemical phenomena at the submicroscopic level.[73] Molecular modeling has long been used to support experimental work, and to teach fundamental concepts.[39] Previous studies have also shown that software usability, expressed as perceived meaningfulness and ease of use, has an impact on learning.[74] Spatial ability is another factor involved in learning science.[75] Its active promotion in college-level chemistry and biochemistry has increased, but not to the same extent as other cognitive skills.[76]

The *3DChemMol* molecular editor for building/editing 3D molecular models was used in the study. Features implemented in the user interface allowed for ease of use: a toolbar; separation of the editing function from other functions; the ability to undo and redo changes for multiple steps; various types of help, including video tutorials, button hovering, action status display, and help menu.

The *3DChemMol* molecular editor incorporating an editing toolbar was tested in a group of 54 university students using three model building/editing activities of varying difficulty: 1) building a simple model, 2) splitting a model into two, 3) creating a cyclic from a non-cyclic structure.

In relation with **first research question (RQ1)**, it was found that students were successful overall in using the tool and graphical interface and in completing the activities. They were excellent on the first two activities and good on the third activity. As expected, the more time they spent on an activity, the more difficult it appeared to them. When they were unable to complete the activity, they perceived it to be more difficult. No relationship was found between time spent and success rate.

As expected, the average step difficulty of the activity correlated inversely with activity completion and directly with perceived activity difficulty. The more difficulties students encountered, the more difficult the activity seemed to them; more difficulties also meant more time spent on the activity.

When it comes to the **second research question (RQ2)**, it was found that actions for direct model manipulation (atoms, bonds) caused more difficulties than using the toolbar buttons. There were more difficulties interacting with the model by dragging than by clicking. Steps that involved changing the model configuration or required changing the working mode of the interface were more problematic. It was also found that actions were perceived as easier if they were preceded by a clear mode change. This means that a lot of emphasis needs to be placed on displaying the state of the system so that the user is immediately aware of the actions available.

The most difficult individual actions reported were 1) rotating a branch around a bond, 2) adding a bond between two existing atoms, and 3) manually adding a hydrogen atom, but also 4) changing a bond type, 5) creating an image, and 6) adding heteroatoms. Issue #5 was technical in nature. Actions 2 and 3 involved dragging the mouse on or between model atoms. Issues 2–4 had a common denominator: the actions were not implicitly given in the toolbar but were available as part of the default add/change action mode, so students could not discover them without either watching the video tutorial or reading the available actions displayed at the bottom of the screen. Correct addition of bonds and heteroatoms probably requires good spatial orientation, which could be especially true for branch rotation. Action 1 required repeated clicking on a bond until a satisfactory configuration was achieved. The latter was done in 60-degree increments.

Difficulties related to the user interface will be addressed in future improvements of the tool, such as highlighting the action state or even separating actions. Difficulties related to spatial abilities could be mitigated by simple video tutorials and exercises focusing on a single issue.

Related to the **third research question (RQ3)**, the study indicated that among the four types of help provided, and regardless of reported difficulties, students most frequently watched video tutorials once or used hovering over buttons to indicate button meanings. Use of other forms of help increased only on the third activity, which was perceived as most difficult. Use of the multiple undo feature was high, indicating that it was absolutely necessary, and increased with activity difficulty. Similarly, free rotation compensated for the use of the undo function on the second activity. The most difficult and complex activity was found to have a relatively high rate of restarting the activity and re-watching the learning video.

When difficulties occurred, students most often used the help menu and the undo/redo actions. Use of the undo function increased for the most difficult steps. For activities/steps that required a mode change, more students consulted the action state that contained the correct answer. Individual activities were associated with multiple video views, with video views generally increasing on the most difficult activity. Mouse hovering over the toolbar was used more often when students could not visually identify the correct button. Sometimes the wrong type of help was consulted, such as button hovering (looking for an appropriate action) when no toolbar interaction was required. Reading the action status would have helped there. In other cases, consulting the action status did not contain the answer and the tutorial video should be watched. Negative correlations between difficulties and single video views may indicate that the video was a sufficient aid in activity completion for many students.

Despite using all the help available (multiple tutorial video views and restarting the activity), some students were not able to complete the most difficult activity. This could be related to the difficulty of the activity and the need for good spatial orientation and/or mean that the help menus and system status were not fully utilized.

Some of the lessons learned in this work, particularly the shortcomings of the user interface for editing, have already been implemented and further improvements are planned. Video tutorials became an important part of the help menu. Bond change methods will be unified so that they always include hydrogen adjustment. The toolbar will be upgraded with additional buttons, e.g., for actions that were part of the working modes but were not explicitly present. The action status display will be improved, and video tutorials for individual actions that proved most difficult will be added and immediately available. Alternative help display could be considered, e.g., when you hover over the model parts.

The **implications for teaching** of this study are multifaceted. Using the new tool, students successfully created 3D models with the help of video tutorials and various types of help. In general, the availability of tools is not yet sufficient for students to use them for learning. Their use must to be encouraged through pedagogical approaches. We suggest that the tool is suitable for direct instruction or self-study. Students can easily use this tool to visualize the structure of chemical compounds during their studies and create images of 3D models to include in their own products, such as seminar works, reports, and theses.

*3DChemMol* could also be used to improve students' development of chemistry knowledge and representation-

al skills. Some students may be afraid of special chemistry visualization software because they think it requires special skills. Because of its simplicity, even students who were not previously familiar with molecular modeling tools and may not have had experience drawing 3D representations or molecules can use it after studying short tutorials. Using *3DChemMol* allows students to construct molecular models to visualize the structure of compounds and understand their properties, rather than memorizing facts and writing about them.

The accessibility of the *3DChemMol* tool makes it easy to incorporate into various educational settings. The models created form the basis for further investigation and study of chemistry concepts through display of chemical properties. Teachers can use the tool directly in the classroom during lectures or prepare study materials for students in electronic or printed form. For example, visualizations created in *3DchemMol* can be part of lectures on various topics. Moreover, it can be used in students' individual work when they can check their understanding on new examples. Different levels of task difficulty can be accommodated in the tool by the teacher.

We are aware that our observational study has some limitations. One of them is the self-reporting nature of the questionnaires. Further insight into students' behavior and efficiency in building molecular models could be gained by using additional recording and analysis methods, such as eye-tracking, video recording during activity performance, and structured interviews afterwards. Another limitation was that the study was focused only on the editing feature of the tool. Future research could include experimental studies such as comparing the usability and effectiveness of other features of the tool (e.g. molecular property display and exploration), comparing it with other 2D and 3D model editing tools, and with building physical models, investigating correlations with other internal or external factors such as students' spatial skills, representational competence, chemistry knowledge and teaching methods. However, this is already beyond the scope of this study.

In further development of *3DChemMol* more interactive online tutorials and exercises tailored to specific chemistry courses could be prepared.

### Acknowledgements

This study was co-financed by University of Ljubljana (grant no. 704-8/2016-229). The authors would like to thank all of the students who participated in the survey.

## 5. References

1. K. L. Vavra, V. Janjic-Watrich, K. Loerke, L. M. Phillips, S. P. Norris, J. Macnab, *Alta. Sci. Educ. J.* **2011**, *41*, 22–30.
2. I. Vekiri, *Educ. Psychol. Rev.* **2002**, *14*, 261–312. **DOI:**10.1023/A:1016064429161
3. S. R. Hinze, D. N. Rapp, V. M. Williamson, M. J. Shultz, G. Deslongchamps, K. C. Williamson, *Learn. Instr.* **2013**, *26*, 12–21. **DOI:**10.1016/j.learninstruc.2012.12.002
4. J. K. Gilbert, D. F. Treagust, in: J. K. Gilbert and D. Treagust (Eds.): Multiple Representations in Chemical Education, Springer Netherlands, **2009**, pp. 1–8. **DOI:**10.1007/978-1-4020-8872-8_1
5. A. H. Johnstone, *Sch. Sci. Rev.* **1982**, *64*, 377–379. **DOI:**10.1017/S0035336100178700
6. A. H. Johnstone, *J. Comput. Assist. Learn.* **1991**, *7*, 75–83. **DOI:**10.1111/j.1365-2729.1991.tb00230.x
7. V. Ferk Savec, I. Sajovic, K. S. W. Grm, in: Multiple representations in chemical education, Springer Netherlands, **2009**, pp. 309–331. **DOI:**10.1007/978-1-4020-8872-8_14
8. R. Kozma, J. Russell, in: J. K. Gilbert (Ed.): Visualization in Science Education, Springer Netherlands, **2005**, pp. 121–145. **DOI:**10.1007/1-4020-3613-2_8
9. M. Stieff, A. Origenes, D. DeSutter, M. Lira, L. Banevicius, D. Tabang, G. Cabel, *J. Educ. Psychol.* **2018**, *110*, 1160–1174. **DOI:**10.1037/edu0000258
10. N. A. Kiernan, A. Manches, M. K. Seery, *Chem. Educ. Res. Pract.* **2021**, *22*, 626–639. **DOI:**10.1039/D0RP00354A
11. M. Stieff, S. Scopelitis, M. E. Lira, D. Desutter, *Sci. Educ.* **2016**, *100*, 344–363. **DOI:**10.1002/sce.21203
12. A. T. Stull, M. Gainer, S. Padalkar, M. Hegarty, *J. Chem. Educ.* **2016**, *93*, 994–1001. **DOI:**10.1021/acs.jchemed.6b00194
13. A. T. Stull, M. Hegarty, *J. Educ. Psychol.* US, **2016**, *108*, 509–527. **DOI:**10.1037/edu0000077
14. Y. J. Dori, M. Barak, *J. Educ. Technol. Soc.* **2001**, *4*, 61–74.
15. S. R. Hinze, V. M. Williamson, M. J. Shultz, K. C. Williamson, G. Deslongchamps, D. N. Rapp, *Cogn. Process.* **2013**, *14*, 129–142. **DOI:**10.1007/s10339-013-0539-3
16. E. Francoeur, *Soc. Stud. Sci.* **1997**, *27*, 7–40. **DOI:**10.1177/030631297027001002
17. D. Gabel, D. Briner, D. Haines, *Sci. Teach.* **1992**, *59*, 58–63. **DOI:**10.1038/s41578-019-0146-8
18. A. M. Ingham, J. K. Gilbert, *Int. J. Sci. Educ.* **1991**, *13*, 193–202. **DOI:**10.1080/0950069910130206
19. N. Barnea, in: J. K. Gilbert and C. J. Boulter (Eds.): Developing Models in Science Education, Springer Netherlands, Dordrecht, **2000**, pp. 307–323. **DOI:**10.1007/978-94-010-0876-1_16
20. H. Hugel, *Chem. Aust.* **2005**, *72*, 31.
21. H.-K. Wu, J. S. Krajcik, E. Soloway, *J. Res. Sci. Teach.* **2001**, *38*, 821–842. **DOI:**10.1002/tea.1033
22. W. L. DeLano, *CCP4 Newsl. Protein Crystallogr.* **2002**, *40*, 82–92.
23. Free Molecular Modeling Software, **1999**, https://www.edinformatics.com/mathmol/free-molecular-modeling-software.html, (accessed: December 20, 2021)
24. A. Moll, A. Hildebrandt, H.-P. Lenhof, O. Kohlbacher, *Bioinformatics* **2006**, *22*, 365–366. **DOI:**10.1093/bioinformatics/bti818
25. E. F. Pettersen, T. D. Goddard, C. C. Huang, G. S. Couch, D. M. Greenblatt, E. C. Meng, T. E. Ferrin, *J. Comput. Chem.*

**2004**, *25*, 1605–1612. **DOI:**10.1002/jcc.20084
26. R. A. Sayle, E. J. Milner-White, *Trends Biochem. Sci.* **1995**, *20*, 374–376. **DOI:**10.1016/S0968-0004(00)89080-5
27. M. D. Casselman, J. F. Eichler, K. Atit, *Sci. Educ.* **2021**, 1–30. **DOI:**10.1002/sce.21675
28. Erlina, C. Cane, D. P. Williams, *J. Chem. Educ.* **2018**, *95*, 991–995. **DOI:**10.1021/acs.jchemed.7b00687
29. B. Mohamed-Salah, D. Alain, *Chem. Educ. Res. Pract.* **2016**, *17*, 862–877. **DOI:**10.1039/C5RP00180C
30. A. T. Stull, M. J. Gainer, M. Hegarty, *Learn. Instr.* **2018**, *55*, 80–92. **DOI:**10.1016/j.learninstruc.2017.09.008
31. A. Taly, F. Nitti, M. Baaden, S. Pasquali, *Interface Focus* **2019**, *9*, 1–11. **DOI:**10.1098/rsfs.2018.0065
32. C. A. Terrell, M. A. Franzen, T. Herman, S. Malapati, D. L. Newman, L. K. Wright, in: T. J. Bussey, K. Linenberger Cortes and R. C. Austin (Eds.): Biochemistry education : from theory to practice, American Chemical Society, Washington, DC, **2019**, pp. 43–62. (ACS Symposium Series; vol. 1337). **DOI:**10.1021/bk-2019-1337.ch003
33. T. Thayban, H. Habiddin, Y. Utomo, M. Muarifin, *Acta Chim. Slov.* **2021**, *68*, 736–743. **DOI:**10.17344/acsi.2021.6836
34. V. Ferk Savec, M. Vrtacnik, J. K. Gilbert, in: J. K. Gilbert (Ed.): Visualization in Science Education, Springer Netherlands, **2005**, pp. 269–297. **DOI:**10.1007/1-4020-3613-2_14
35. M. Barak, in: J. P. Suits and M. J. Sanger (Eds.): Pedagogic Roles of Animations and Simulations in Chemistry Courses, Amer Chemical Soc, Washington, **2013**, pp. 273–291. **DOI:**10.1021/bk-2013-1142.ch011
36. M. T. Springer, *J. Chem. Educ.* **2014**, *91*, 1162–1168. **DOI:**10.1021/ed400054a
37. R. Kelly, S. Akaygun, *Chem. Educ. Res. Pract.* **2019**, *20*, 657–658. **DOI:**10.1039/C9RP90009H
38. T. J. José, V. M. Williamson, *J. Chem. Educ.* **2005**, *82*, 937–943. **DOI:**10.1021/ed082p937
39. W. J. Hehre, A. J. Shusterman, J. E. Nelson, The molecular modeling workbook for organic chemistry, Wavefunction, Irvine, CA, **2004**.
40. A. D. Clauss, S. F. Nelsen, *J. Chem. Educ.* **2009**, *86*, 955–958. **DOI:**10.1021/ed086p955
41. K. J. Linenberger, R. S. Cole, S. Sarkar, *J. Chem. Educ.* **2011**, *88*, 962–965. **DOI:**10.1021/ed100727r
42. J. Raiyn, A. Rayan, *World J. Chem. Educ.* **2015**, *3*, 1–4. **DOI:**10.12691/wjce-3-1-1
43. E. Rothe, W. Zygmunt, *Chem. Eng. Educ.* **2016**, *50*, 125–129. **DOI:**10.1007/s10749-016-0672-0
44. Y. J. Dori, M. Barak, N. Adir, *J. Chem. Educ.* **2003**, *80*, 1084–1092. **DOI:**10.1021/ed080p1084
45. J. B. Ealy, *J. Sci. Educ. Technol.* **2004**, *13*, 461–471. **DOI:**10.1007/s10956-004-1467-x
46. R. Kozma, *Learn. Instr.* **2003**, *13*, 205–226. **DOI:**10.1016/S0959-4752(02)00021-X
47. J. Lundell, *Educ. Quím.* **2017**, 33–36. **DOI:**10.2436/20.2003.02.157
48. K. Kolar, R. Dolezal, N. Karaskova, N. Maltsevskaya, S. Krizkova, *Chem.-Didact.-Ecol.-Metrol.* Warsaw, **2019**, *24*, 45–51. **DOI:**10.2478/cdem-2019-0003
49. L. L. Winfield, K. McCormack, T. Shaw, *J. Chem. Educ.* Washington, **2019**, *96*, 89–92. **DOI:**10.1021/acs.jchemed.8b00145
50. S. S. Johnson, L. Winfield, S. H. Sung, *J. Chem. Educ.* **2021**, *98*, 982–985. **DOI:**10.1021/acs.jchemed.0c01134
51. L. Soulère, *J. Chem. Educ.* **2021**, *98*, 2709–2713. **DOI:**10.1021/acs.jchemed.1c00017
52. A. Grushow, M. S. Reeves, in: Using Computational Methods To Teach Chemical Principles, American Chemical Society, **2019**, pp. 1–10. (ACS Symposium Series; vol. 1312). **DOI:**10.1021/bk-2019-1312.ch00110.1021/bk-2019-1312.ch001
53. J. Rodríguez-Becerra, L. Cáceres-Jensen, T. Díaz, S. Druker, V. B. Padilla, J. Pernaa, M. Aksela, *Chem. Educ. Res. Pract.* **2020**, *21*, 638–654. **DOI:**10.1039/C9RP00273A
54. M. Aksela, J. Lundell, *Chem. Educ. Res. Pract.* **2008**, *9*, 301–308. **DOI:**10.1039/B818464J
55. M. Aksela, J. Pernaa, P. Blomgren, I. Rautiainen, Collaborative science education at the University of Helsinki: ChemistryLab Gadolin: a science lab as an inspiring environment for learning, development and research since 2008, Unigrafia Oy, Helsinki, **2018**.
56. J. Pernaa, M. Aksela, S. P. Ghulam, Introduction to Molecular Modeling in Chemistry Education, e-Oppi Ltd. & Edumendo Publishing, Jokioinen, **2017**.
57. J. Pernaa, *LUMAT Int. J. Math Sci. Technol. Educ.* **2015**, *3*, 960–975. **DOI:**10.31129/lumat.v3i7.977
58. D. Dolničar, B. Boh Podgornik, in: I. Devetak (Ed.): Eurovariety 2021: 9th European Variety in University Chemistry Education Conference: 7-9 July 2021, Ljubljana, Slovenia, online conference: book of abstracts, University of Ljubljana, Faculty of Education, **2021**, p. 74. http://pefprints.pef.uni-lj.si/id/eprint/6794
59. L. A. Abriata, *Inform.-Basel* **2017**, *4*, 1–18. **DOI:**10.3390/informatics4030028
60. S. Pirhadi, J. Sunseri, D. R. Koes, *J. Mol. Graph. Model.* **2016**, *69*, 127–143. **DOI:**10.1016/j.jmgm.2016.07.008
61. M. C. Burger, *J. Cheminformatics* **2015**, *7*, 1–7. **DOI:**10.1186/s13321-015-0085-3
62. B. Rayan, A. Rayan, *World J. Chem. Educ.* **2017**, *5*, 136–141. **DOI:**10.12691/wjce-5-4-4
63. R. M. Hanson, *J. Appl. Crystallogr.* **2010**, *43*, 1250–1260. **DOI:**10.1107/S0021889810030256
64. N. Rego, D. Koes, *Bioinformatics* **2015**, *31*, 1322–1324. **DOI:**10.1093/bioinformatics/btu829
65. H. Bergwerf, *ACS CHED CCCE Newsl.* **2015**, https://confchem.ccce.divched.org/2015FallCCCENLP9, (accessed: December 20, 2021)
66. R. M. Hanson, J. Prilusky, Z. Renjian, T. Nakane, J. L. Sussman, *Isr. J. Chem.* **2013**, *53*, 207–216. **DOI:**10.1002/ijch.201300024
67. O. Rothenberger, Virtual Molecular Model Kit, https://chemagic.org/molecules/amini.html, (accessed: December 20, 2021)
68. J. H. Jensen, J. C. Kromann, *J. Chem. Educ.* **2013**, *90*, 1093–1095. **DOI:**10.1021/ed400164n
69. B. Nevo, *J. Educ. Meas.* **1985**, *22*, 287–293. **DOI:**10.1111/j.1745-3984.1985.tb01065.x

70. J. Kim, *Inf. Res.* **2008**, *13*, 13–14. **DOI:**10.1111/j.1469-8749.1971.tb03071.x
71. M. Harle, M. Towns, *J. Chem. Educ.* **2011**, *88*, 351–360. **DOI:**10.1021/ed900003n
72. H. Van der Meij, J. Van Der Meij, *Comput. Educ.* **2014**, *78*, 150–159. **DOI:**10.1016/j.compedu.2014.06.003
73. M. Slapničar, V. Tompa, S. A. Glažar, I. Devetak, J. Pavlin, *Acta Chim. Slov.* **2020**, *67*, 904–915. **DOI:**10.17344/acsi.2020.5908
74. Z. Merchant, E. T. Goetz, W. Keeney-Kennicutt, O. Kwok, L. Cifuentes, T. J. Davis, *Comput. Educ.* **2012**, *59*, 551–568. **DOI:**10.1016/j.compedu.2012.02.004
75. M. Tanweer, *Eur. J. Phys. Educ. Sport Sci.* **2019**, *4*, 145–151. **DOI:**10.5281/zenodo.3407001
76. M. Oliver-Hoyo, M. A. Babilonia-Rosa, *J. Chem. Educ.* **2017**, *94*, 996–1006. **DOI:**10.1021/acs.jchemed.7b00094

## Povzetek

V članku je predstavljena študija, v kateri je 54 univerzitetnih študentov preizkusilo in ovrednotilo *3DChemMol* - novo razviti, brezplačni spletni urejevalnik modelov molekul z orodno vrstico. Namen orodja je povečanje reprezentacijske kompetence v povezavi s submikroskopskimi predstavitvami. Študenti so programsko opremo uporabili prvič. Z orodjem za gradnjo/urejanje modelov so izdelali modele molekul v naslednjih treh aktivnostih z različnimi stopnjami težavnosti: 1) gradnja preprostega modela (butanojska kislina), 2) pretvorba enega modela (heksan) v dva modela, 3) pretvorba iz neciklične v ciklično obliko (glukoza). Študenti so za izvedbo vsake od aktivnosti potrebovali od dveh do 15 minut. V orodni vrstici urejevalnika *3DChemMol* je bilo na voljo več vrst pomoči, ki so študentom olajšale izvajanje aktivnosti, vključno z video vodnikom, prikazom pomoči ob preletu gumbov orodne vrstice z miško, prikazom statusa/načina dela in menijem pomoči. Na voljo so bile tudi možnosti razveljavitve in ponovne uveljavitve posameznih korakov ter ponovnega začetka celotne aktivnosti. Stopnjo dokončanja aktivnosti, težave in uporabo pomoči smo preučevali s pomočjo vprašalnikov za samoocenjevanje študentov. Urejevalnik molekul *3DChemMol* se je izkazal kot koristna podpora študentom pri preprostih kemijskih aktivnostih. Študenti so bili pri gradnji modelov uspešni, čeprav so naleteli na nekatere specifične težave, zlasti pri korakih, ki so vključevali prostorske operacije, kot je vrtenje izbranega dela modela molekule okoli vezi. Po mnenju študentov so bila video navodila najprimernejša in najpogosteje uporabljena vrsta pomoči, funkcija razveljavitve pa je bila pri delu bistvenega pomena. Rezultati kažejo, da lahko urejevalnik modelov molekul *3DChemMol* učinkovito uporabljamo pri osnovnih predmetih kemije na terciarni ravni izobraževanja, bodisi za poučevanje, samostojno učenje študentov ali druge oblike podpore v pedagoškem procesu. Rezultati in ugotovitve študije bodo uporabljeni tudi za nadaljnjo optimizacijo uporabniškega vmesnika v prihodnjih različicah ovrednotenega orodja.