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iChem3d

Supporting lifelong learning: enhancing the value of interactive 3D chemistry

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Executive Summary

The iChem3D project set out to enhance the value of interactive 3D chemistry, by investigating the current use of ChemTube3D and also developing a number of transferable learning designs to encourage the effective use of the resource within undergraduate and postgraduate programmes. A number of methods were used to achieve this goal and we are now more aware of how people use the resource. Through the use of existing freeware produced by Half-Baked Software we have managed to produce a number of transferable learning designs, with the vast majority of students surveyed saying they liked the new assisted learning approaches that have been developed.

During the first few months of the iChem3D project we managed to establish that there are a number of Higher Education institutes using the resource effectively from different University groups within the UK. In addition to the use of ChemTube3D within the UK we managed to locate a few universities overseas that use the resource in their teaching. Schools and colleges also use ChemTube3D during A Level Chemistry lessons to provide a visual representation of the material they are teaching.

Research into a number of different learning designs incorporating interactive animations from ChemTube3D has been carried out using a program called Hot Potatoes, which is a piece of software published by Victoria University and Half-Baked Software "*enabling you to create interactive multiple-choice, short-answer, jumbled-sentence, crossword, matching/ordering and gap-fill exercises for the World Wide Web.*"¹ Hot Potatoes allows you to customise the layout of the exercises you make and input the information of your choosing, which was ideal for this project and can also be used across many disciplines. Using another program called Quandary, which is another piece of free software from Half-Baked Software, which allows the users to create an "*interactive case-study*"², we produced learning designs that guide users through material in a step-by-step manner.

Results indicate that the new learning approaches, created as part of the iChem3D project, are generally highly appreciated by academics and students. Out of a sample of 45 students the majority (93%) said they liked the new assisted approach created for ChemTube3D (Fig. 18).

Through the use of existing freeware produced by Half-Baked Software we have managed to develop a way of support lifelong learning by enhancing the value of interactive 3D chemistry, with the vast majority of students surveyed saying they liked the new assisted learning approach developed as part of this project. We hope that we have managed to make ChemTube3D even more beneficial for its users and that people will have the time to look at and explore these new learning designs effectively.

1. Background

Interactive simulations are becoming an increasingly important component for learning in the Physical Sciences. They can be used very effectively in traditional lecture demonstrations but are also invaluable for individual study in a personalised learning environment. Interactive computer generated simulations offer the opportunity for uniquely informative, enjoyable, and lasting learning. Until recently, they required specialised software but now a high quality experience is possible using only a web browser and the free open source molecular viewer applet Jmol <http://jmol.sourceforge.net/>. Jmol has recently undergone major development with the introduction of new features that are particularly powerful in a learning environment.

The addition of 3D simulations and animations is a burgeoning approach to the teaching of chemistry adding to existing metaphors and models used to describe chemical molecular structures, properties and their reactivity. Google Analytics shows 60,000 visits in the launch year from 155 countries to the website <http://www.chemtube3d.com>, "Stickability" is varied, with some users spending significant amounts of time in one place. Visitors are from HEIs, industrial organisations and individuals. Initial interrogation of this data reveals a wide variety of search strategies which are used to access the website. (Although the resources are linked to learning object repositories, e.g. Merlot these do not appear to be the main route).

We have sparse information on how Chemtube3D is being used. We do know, it is embedded in some academic programmes as part of a learning activity created by tutors, while some students are simply pointed to the resources for their own self-directed learning while for others it is more tightly integrated. We believe that in organisations such as Pfizer individuals are finding them through their own research, possibly for refreshment/revision purposes? We know very little about the effectiveness of these different approaches for different types of learners, at different levels and in different contexts.

2. Aims and Objectives

To investigate the uses being made of an interactive, freely available, resource providing 3D simulations and animations modelling the structure and reactivity of organic molecules (<http://www.chemtube3d.com>). Chemtube3D, created by the principal investigator at Liverpool using Jmol, is used by a diverse range of learners including undergraduates and professional industrial chemists. We will research its current use and investigate the development of a range of learning designs to support the effective integration of these resources for blended self-directed learning.

Problems to be addressed are therefore:

1. How and why are different people using the resource?
2. Can we identify examples of effective use of the resource?
3. Can additional learning designs be created to support different learners and/or tutors?
4. If so, are the principals of design transferable to other educational contexts?

Further questions arising include: Can this type of e-learning resource better support a diversity of users when some 'framing' is developed alongside the resource? If so, how can learners/users best be guided to the appropriate level of framing? How does this 'framing' of the resource impact on how students use them and in turn on the potential benefits to their learning?

If such framing benefits learners, can these be transferred across related educational contexts? Can effective combinations of these e-learning resources, learning activities and assessment tasks (related to module and programme learning outcomes) be created that can be re-used in different educational contexts? Can learning designs developed, for the effective use of 3D simulations and animations in this educational context, be transferred to different educational contexts? Are there any principles of using 3D simulations and animations resource that can be extracted and disseminated?

3. Investigation into the current use of the ChemTube3D learning resource

The iChem3D project was split into two major sections with the first half focusing on investigating the current use of the resource through Google Analytics and contacting users, followed by the second part (covered in section 4) which was the development and testing of new approaches to improve the existing resource and make it more beneficial to its users. Google Analytics allowed us to pull out information on who uses the resource and once this had been established contact could be made with individual universities and companies.

3.1 Google Analytics

Using Google Analytics we looked into how much use was being made of the resource in the following categories:

- Countries – to find out which countries use the resource the most
- Traffic Sources – to find out where visitors come from (i.e. direct, through a search engine or through a referring website)
- Top University Networks – to find out which universities use the resource both in and outside the UK
- University Groups – to find out which universities use the resource within the different UK university groupings.
- Colleges / Schools – to find out if any schools or colleges use the resource for either GCSE or A Level teaching
- Companies – to find out which professional companies use the resource

All of the reports associated with these categories include information about the number of visitors who used ChemTube3D and also the amount of time spent on the resource. When looking at the universities, information was gathered on which pages were used the most and also if the visitors were new or returning to the site. All this information allowed us to get a detailed visitor profile and discover who was using the resource the most.

Results from Google Analytics showed that the countries that use ChemTube3D the most are the United States of America (USA), the United Kingdom (UK) and India, over the period from September 1st 2008 to June 22nd 2009. Google Analytics calculated the total number of visits to ChemTube3D during this period at 90,096. Figures for the USA showed that nearly 40% of the total visits during this period were from this country/territory and the regions with the most visits were New York and California. The UK had the second highest number of visitors worldwide during the academic year studied, with London and Liverpool being the top two cities with the highest number of visitors. All of the top ten cities with the most visits have universities within them and the two cities with the highest amount of time spent on the resource are Liverpool and Birmingham. The use of ChemTube3D within India accounted for nearly 8% of the total visits over the period studied with the number of visits increasing towards the end of the covered academic year. Usage came from across the whole of India with the time spent on the resource being above the site average.

The main source of visitors to ChemTube3D was search engines, with Google being the most popular. Direct visits were also popular with 14% of the visitors accessing the resource via this route. This included people who were returning to the site and also others who had been directed to the site by colleagues or friends.

Leading on from the more general results on Google Analytics we were able to establish more detailed visitor profiles by using university, college and company searches. The detailed visitor profiles allowed us to establish which departments to contact to ask for information on how they use the resource. We initially contacted a number of universities, colleges and companies to try and gather information, which led us to find out information about how ChemTube3D is used. Encouraging responses were received from various HE institutions but trying to get staff and students to agree to take part in the testing and evaluation of the learning designs in the early stages proved difficult.

Initially we had the impression that it would be easier to gain support from other universities and that gaining support from industrial partners and colleges would be most difficult. However, an unexpected achievement was that we managed to build up good contact with a school, which uses the resource for teaching A Level chemistry. The members of staff that teach the A Level syllabus initially provided us with some encouraging feedback on how the resource is incorporated into lessons, followed by an agreement to become involved in the evaluation of the learning designs that are suitable for A Level study. As the year progressed we found that staff at this school were busy with teaching and exam periods, which led to a decrease in help on evaluating the new approaches.

In terms of HE institutes we managed to gain feedback from a number of academic staff at various universities about how they use the resource. Responses from companies were low due to the limited information we could find for contacts within large organisations. Of the companies we did manage to get in touch with they all had positive things to say about the resource and said that it would be very useful for their internship students, however, one made it clear that the level of detail was not suitable for leading researchers.

Using Google Analytics to gain data on who uses the resource was extremely valuable as it allowed us to build up an idea of who uses the resource and also after contacting certain individuals we managed to find out why they were using it. The next stage in finding out more information about how people use ChemTube3D was through users surveys, which are described in more detail below.

3.2 Surveys

A brief survey constructed using Survey Monkey was sent out to members of the ChemTube3D Facebook group (Appendix 1.1), which was set up as part of this project, followed by a revised survey being introduced to the ChemTube3D site, which was constructed using Kwik Surveys (Appendix 1.2). The reasoning behind the change in the survey host was the ability to receive the results of the survey more easily using Kwik Surveys and the added bonus that it was free for an unlimited amount of questions.

In order to try and understand the benefit of ChemTube3D to students at other HE institutes another survey was constructed with five questions to ask students if they find the resource useful and also to establish what they like/dislike about the resource (Appendix 1.3). This survey was first sent to a university in the United States of America, as ChemTube3D is one of the online resources that is recommended to their students studying organic chemistry who are non chemistry majors. Following on from this, the survey was sent to students at the UoL and three other UK universities including Loughborough.

Results from both the survey sent out through Facebook and the one added to the ChemTube3D website provided information on the aspects of the site that visitors use most and also provided an opportunity for respondents to express their opinion on what they like/dislike about the resource and also any ideas they may have to improve the site.

In total we received 15 responses to the survey sent out through Facebook to approximately 80-90 members. The results we received were very encouraging with many of the respondents liking the resource and also suggesting some helpful ways in which we can improve the site for them. A member of the Facebook group who answered our survey suggested using the combination of Jmol and Hot Potatoes for ChemTube3D and set the ball rolling for ways in which we could develop new learning approaches for the resource. The development of these new learning approaches is described in more detail later on in section 4.2.

The survey on the ChemTube3D website finished with 362 responses. From responses we received, the countries with the highest number of visits were India, the USA and the UK, which tallies up with the results provided by Google Analytics. The main source of visits to the site came through a Search Engine, with the majority of people initially wanting to look at the site for help learning chemistry. These people now say they use ChemTube3D to look at and learn new material. The features of the site that are most commonly used are the animated reaction mechanisms and the ability to rotate the models in 3D. In relation to the functionality of the site over 60% of the responses were either "Very Satisfied" or "Satisfied" with each of the aspects of the site, which included the Subjects Covered, the Search Box, the Site

Navigation and finally the Overall site. The final questions of the survey contained comment boxes for users to express their opinion on what they liked or dislike about the resource and also about what they would like to see improved. By the time these questions came nearly two thirds of the respondents had stopped answering the questions. Results showed (Fig. 2) that 22% of the respondents when asked what they would like improved said “nothing” indicating that the resource is useful as it is. Feedback received through both surveys was used to improve the resource in ways that users wanted, including the re-design of the website (which will be explained in more detail in section 4.1) in order to improve navigation as this was a common theme brought up in the surveys and focus groups.

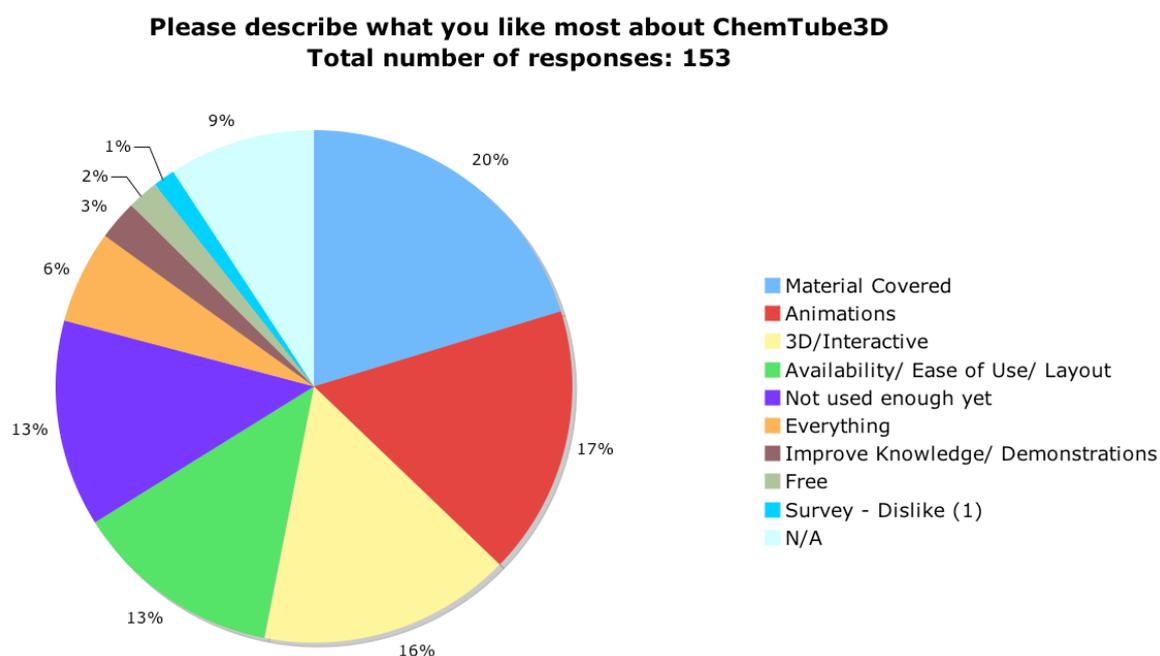


Fig. 1. Results from the ChemTube3D website survey indicating what users like most about the resource. “N/A” refers to inappropriate answers.

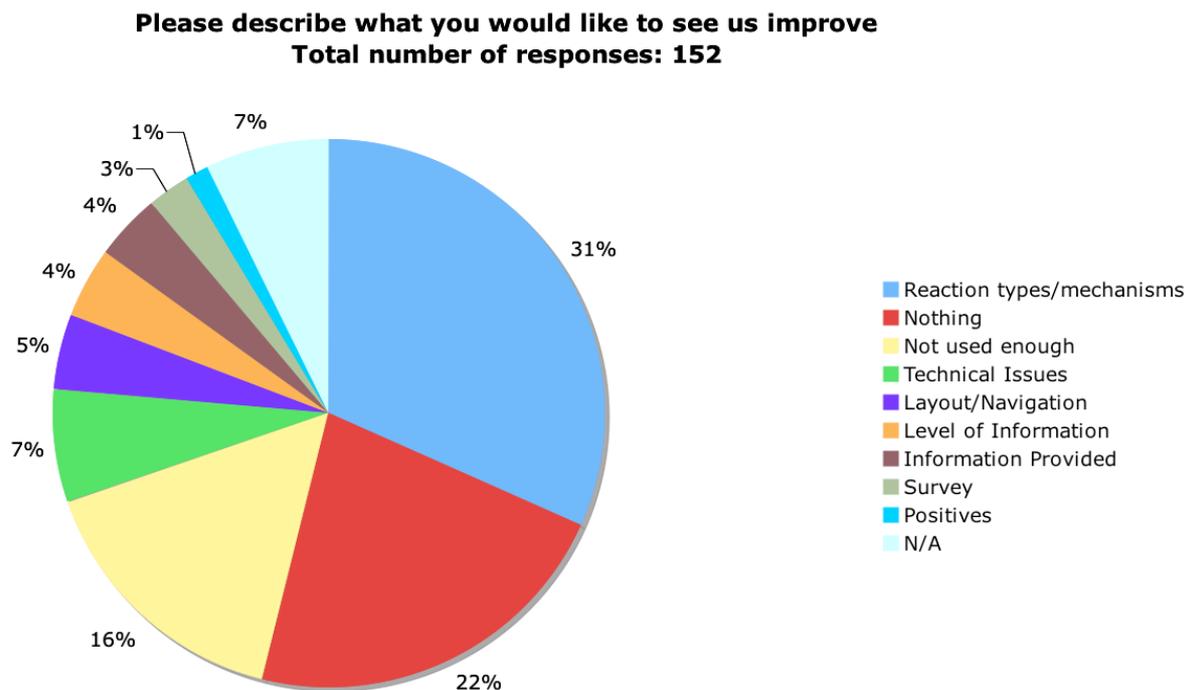


Fig. 2. Results from the ChemTube3D website survey indicating what users would like to be improved. "Positives" relates to one comment about quick accessibility and another, which says it is wonderful. "N/A" refers to inappropriate answers

The Facebook group set up for ChemTube3D is quite popular and now has over 400 members, however, participation in the discussions has been limited with only two members making comments. A few people have posted comments on the wall about how useful the resource is for undergraduates and also how they would like to use the resource to improve their knowledge in certain areas.

The numbers of results received from the survey sent to a university in America to find out the benefits of ChemTube3D, were a little disappointing as only 11 people responded out of a class of 700+. However, the results that we did receive were very encouraging and showed that the resource was beneficial to the students learning. Responses were again limited from Liverpool and no responses were received from any of the other three universities.

3.3 Student focus groups

Student focus groups were held for 1st and 2nd year Chemistry students at the University of Liverpool (UoL) to establish the benefits of the site and also to highlight any problems they have with the resource. The focus groups contained a short workshop asking students to look through some of the content they had met in their Organic Chemistry courses and also included a task in which the students were guided through a reaction mechanism in a step-by-step approach. Food incentives were offered to encourage students to attend. A total of 6 students were asked to comment on whether they found it easier to understand the material when they were led through it step-by-step.

A student focus group similar to the one held at the UoL was run for students at Loughborough University. The structure was mainly the same with a workshop based on using ChemTube3D and an opportunity for any feedback on the resource, followed by the students testing and evaluating the new learning designs.

Focusing on the initial aspects of the project (the investigation into the use of ChemTube3D) the feedback received from students during these focus groups was mostly positive with the 6 students that attended the focus groups at the UoL all saying they preferred a guided learning approach when given a set of instructions to follow on paper. The three students who attended the focus group at Loughborough University also said the same. In terms of improving ChemTube3D students expressed their thoughts on how to improve the navigation of the site and also how to improve simple features, for example changing buttons into check boxes to allow certain features of the site to be turned on and off as required.

All the feedback received from the focus groups was used to improve ChemTube3D. As a common suggestion for improvement from both the surveys and these focus groups was the re-design of the site, which we decided to carry this out at the same time as developing the new learning approaches.

4. Development of ChemTube3D and testing of new approaches to support learners/tutors

As a result of the feedback received whilst investigating the current use of ChemTube3D we decided that a re-design of the website would benefit our users. This was carried out as an addition to the project alongside the development of the new learning approaches. The development of these new learning approaches started with the investigation of using Hot Potatoes and Jmol as mentioned previously. After some research into Hot Potatoes we discovered that it is a piece of software published by Victoria University and Half-Baked Software "*enabling you to create interactive multiple-choice, short-answer, jumbled-sentence, crossword, matching/ordering and gap-fill exercises for the World Wide Web.*"¹ This sounded ideal for what we wanted to achieve through the iChem3D project and we managed to find another piece of freeware, also produced by Half-Baked Software, called Quandary which we thought would be useful for making explicit the activities currently used by the two lecturers most experienced in using the resource.

4.1 New site design

The re-design of the ChemTube3D website was important to many people, with the main focus being on the navigation of the site. Students found it hard to find what they were looking for when using the resource outside of lectures and they also said there was not enough guidance on the website as to how to use the resource to its full potential. The old layout of the homepage of ChemTube3D (Fig. 3) was quite hard to navigate and to get to sections of the site such as solid state chemistry or polymer chemistry it was quite difficult as you could only access them from the home page.

The screenshot shows the homepage of ChemTube3D. At the top, there is a banner with the University of Liverpool logo and the text 'ORGANIC CHEMISTRY'. Below this is a search bar and the text 'Welcome to the News Page'. The main content area is divided into several sections:

- Left-hand navigation menu:** Lists various chemical topics such as 'Stereochemistry', 'Conjugate addition', 'Diels-Alder reactions', 'Nucleophilic substitution', 'Elimination', 'Electrophilic aromatic substitution', 'Enols and Enolates as nucleophiles', 'Pericyclic reactions', 'Atomic and Molecular Orbitals', 'Molecular vibrations-IR', 'Dipoles and Electrostatic surfaces', 'UV - conjugation', 'Rearrangements', 'Fragmentations', 'Aromatic heterocycles', 'Carbene chemistry', 'Advanced Topics', and 'Feedback to Nick Greeves facebook group'.
- Central News Section:** A table of updates with the following entries:

Jan 2010	Major new section on stereochemistry including chirality, conformation, configuration, diastereoisomers, meso, Newman projections, cyclohexane and decalins
Sep 2009	Organopalladium catalytic cycles for Heck reaction and Stille coupling added
Jul 2009	Major new section on aromatic heterocyclic chemistry - pyridine, pyridine N-oxide, pyridone, pyrrole
Jan 2009	Press release: 64,000 visitors from 158 countries in first year of operation
Sep 2008	Major new sections on Rearrangements, Fragmentations, Carbenes, Baldwin's Rules, Alkene synthesis and reactions involving Silicon and Boron . Charges and lone pairs are now included in the animated sequences.
Jun 2008	Discussion forum opened and new logo designed by Lyndsey Vernon.
May 2008	Lecturers/Instructor's guide added
May 2008	Pericyclic reactions added based on Richard Windsor's project-1,3-dipolar cycloadditions, sigmatropic rearrangements, electrocyclic reactions
Feb 2008	Stereospecific E2 eliminations in acyclic and cyclic molecules added
Feb 2008	Molecular photo booth feature in resizable window view - works with IE
Feb 2008	UV spectroscopy and MOs added
Jan 2008	Atomic and bonding molecular orbitals for small molecules added
Jan 2008	Dipoles and electrostatic surfaces with HOMO and LUMO added
Dec 2007	Molecular vibrations - infra-red spectroscopy added
- Right-hand side:** A 3D molecular model of a complex organic structure, a text box stating 'iChem3D is a JISC funded project that sets out to investigate the use of ChemTube3D and develop a range of learning designs to be used in blended self-directed learning.', and a 'Solid State Structures' logo.
- Bottom:** A row of four molecular images (one with a 0.4 nm scale bar) and a link to the 'molecular photobooth gallery'.

At the bottom of the page, there is a footer with the text: 'These pages were developed by Nick Greeves, Alex Lawrenson, Kirsty Barnes and Neil Berry on Mac OS X using Spartan 04-08, GAMESS, MacMolPlt and visualised using Jmol. We gratefully acknowledge support from the UK Physical Sciences Centre, Faculty of Science TQEF and EPSRC. © 2007-10 The University of Liverpool'.

Fig. 3. Layout of original ChemTube3D homepage.

The new layout (Fig. 4) has all the content split into different topics across the top of the page with sections for organic chemistry, organic structure and bonding, polymers and solid state. When each of these topics are clicked there are guidelines describing how to use the ChemTube3D website, with a list of all the content available in a menu down the left hand side, for example the organic chemistry section is shown in Fig. 5.

UNIVERSITY OF LIVERPOOL

Google Custom Search Search Site

Organic Chemistry Organic Structure and Bonding Polymers Solid State

ChemTube3D

Information

ChemTube3D contains interactive 3D animations and structures, with supporting information for some of the most important topics covered during an undergraduate chemistry degree.

Explore the various sections using the menu bar above to find the content of interest to you.

Please send any [feedback to Nick Greeves](#)

Quick links

Jmol uses Java - if you would like to make sure that your machine is up to date check here

New facebook group started - join here

iChem3D is a JISC funded project that aims to enhance the value of interactive 3D chemistry

Molecular photobooth gallery

ChemTube3D news

Major new section on [stereochemistry](#) added

Organopalladium catalytic cycles for [Heck reaction](#) and [Stille coupling](#) added

Major new section on [aromatic heterocyclic chemistry](#)

Press release: 64,000 visitors from 158 countries in first year of operation

[Visit the ChemTube3D news page>](#)

These pages were developed by [Nick Greeves](#), Alex Lawrenson, Kirsty Barnes and Neil Berry on Mac OS X using [Spartan 04-08](#), [GAMESS](#), [MacMolPlt](#) and visualised using [Jmol](#).

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Fig. 4. Image showing the homepage of ChemTube3D after the re-design of the website.
(<http://www.chemtube3d.com>)

On the old design all of the organic chemistry sections were presented in a long list down the left hand side of the page. The list started off being in a similar order to how the material is covered in an undergraduate degree, but as the website become more developed the new sections were added onto the end of the list. This made it difficult for students to find reactions and led to the restructuring of the content to follow the order in which topics are taught. During the re-design of the ChemTube3D website, some additional features were added into the Jmol window. These included optional buttons to switch the colour of the window background between black and white and also the ability to resize the Jmol window within the webpage to three different sizes, in addition to the larger view already available. The reasoning behind these changes was to firstly allow anyone who doesn't like the dark background to be able to change to a light one at the click of a button (instead of using the longer method in the Jmol menu). And secondly, the ability to resize the Jmol window within a page means that the user can use the interactive 2D mechanism to click through the different stages within the same window as the enlarged view. This was not possible before as when using the 'larger view' mode, only the currently selected model becomes enlarged, therefore meaning that you would have to have a new window for each stage in the mechanism.

The screenshot shows the 'Organic Chemistry Animations' page on ChemTube3D. It includes a navigation bar, a sidebar with a list of topics, and a main content area with text and interactive chemical diagrams. The 2D diagram shows the Diels-Alder reaction with arrows indicating electron flow and labels for reactants, mechanism, and products. Below it is a 3D ball-and-stick model of the same reaction.

Fig. 5. Image showing the Organic Chemistry section of ChemTube3D, with added guidelines (<http://www.chemtube3d.com/Main%20Page.html>).

Since the redeployment of the site under a new image (March 2010) we have received numerous responses to the message we put on the Facebook group indicating that ChemTube3D has a new layout/design including that it *“really looks pretty good and it is so easy to go to any section now rather than before...that is really a perfect work...many thanks for that...that is a very useful website...”* and *“I love it!!! Sooo much easier to find what i'm looking for :) A little button to change the text background colour n size would be nice- i find the white background is rather difficult to read from...Keep up the good work!!!”*⁵. In response to the second comment, we are looking to change the background colour to be permanently pale blue, as we believe this will make it easier for everyone to read text on the pages.

4.2 Development and testing of new learning approaches

The developments of new transferable learning designs to support different levels of users were produced using freeware provided by Half-Baked Software. Quandary is the program used to produce learning sequences to guide users through material on ChemTube3D, whilst two programs from Hot Potatoes (JQuiz and JMatch) were investigated to produce self-assessment activities related to the material on the resource. All outputs from the Half-Baked Software are in standard HTML and use JavaScript.

Quandary allows the creator to develop a sequence of steps, which are interlinked, based on any topic from any discipline. This is the good thing about the software, the only thing that you may see as a downside is you have to come up with all the information yourself! JQuiz allows the creator to produce a number of multiple choice self-assessment activities with the option of having text or images for the answers. Whilst JMatch allows the creator to input up to four starting images/text followed by up to four answers for the user (in this case the students) to match up. Combinations, say for example, of two starting images and four answers can be used with two right and two wrong answers as the number of each does not have to be equal.

The initial designs for the new step-by-step guide/learning sequence started off based on the Quandary style with a reading column on the left hand side and a sequence on the right. As ChemTube3D is based on Jmol and includes interactive animations these were to be included in the new learning designs and the reading column was the ideal place (Fig. 6). As shown in Fig. 6 the step-by-step guide initially started with the text split into three stages with instructions on the layout of the rest of the learning sequence and also information on how to start using the help guide. A background colour of blue was chosen to make the new material accessible to most students including those with dyslexia. Group meetings were held regularly during the design process to ensure that the designs were suitable for all learners. Feedback from team members involved in educational development indicated that text should be left aligned to make it more accessible and this was implemented in the second design (Fig. 7) along with a slight variation in the text used.

Cyanohydrin Formation

[Bookmark](#) [Restart](#)

Instructions for each stage are shown in blue at the top of each page

Followed by

A response question given in black

To begin the Step by Step help for the Formation of Cyanohydrin please click the Start button below

[Start](#)

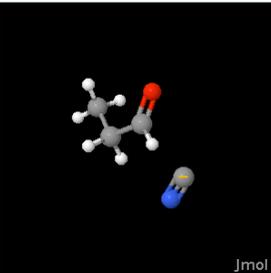


Fig. 6. Initial layout for learning sequence

Cyanohydrin Formation

[Bookmark](#) [Restart](#)

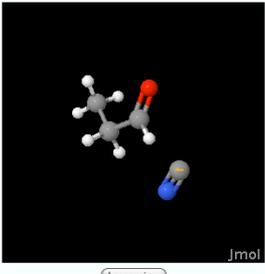
What you should do for each stage is shown in blue at the top of each page

Followed by

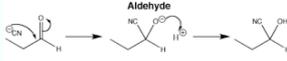
A question given in black

To begin the Step by Step help for the Formation of Cyanohydrin please click the Start button below

[Start](#)



Aldehyde



Ketone

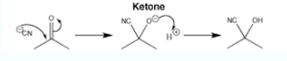


Fig. 7. Changes to initial design including the left alignment of the text

After consulting on the layout of the starting screen for new learning sequence, it was suggested that we move the Jmol applet over to the right hand side of the screen (Fig. 8). This was made possible by the fact the Quandary is fully customisable in relation to the layout and presentation of the outputs by altering the Cascading Style Sheets (CSS) using a web design program such as Dreamweaver CS3 or even a text editor such as Notepad (Windows) or TextWrangler (Macintosh).

The screenshot shows a web page titled "Cyanohydrin Formation". At the top, there are "Bookmark" and "Restart" buttons. Below them, a blue instruction reads: "What you should do for each stage is shown in blue at the top of each page". This is followed by the text "Followed by" and "A question given in black". A paragraph states: "To begin the Step by Step help for the Formation of Cyanohydrin please click the Start button below". A "Start" button is located below this text. On the right side of the page, there is a Jmol applet window displaying a 3D ball-and-stick model of a cyanohydrin molecule. Below the Jmol window is a "larger view" button. At the bottom of the page, there are two chemical reaction schemes: one for an aldehyde and one for a ketone, both showing the reaction with cyanide ion and water to form a cyanohydrin.

Fig. 8. Jmol window moved to the right hand side of the screen

One thing led to another and after a few minor adjustments, including the addition of a border around the text (Fig. 9) and a change of the text we eventually ended up with the layout shown in Fig. 10. This layout also includes an "AddThis" bookmark button, instead of the inbuilt one provided by Half-Baked Software, to allow users to bookmark and share the page using the likes of Delicious, Twitter and Facebook.

This screenshot is similar to Fig. 8 but with a blue border around the text area. The text "What you should do for each stage is shown in blue at the top of each page" is now enclosed in a blue-bordered box. The "Start" button is also within this box. Below the box, there are "Bookmark", "Restart", and "Go Back" buttons. The Jmol applet and the chemical reaction schemes remain in the same positions as in Fig. 8.

Fig. 9. Border added around the text.

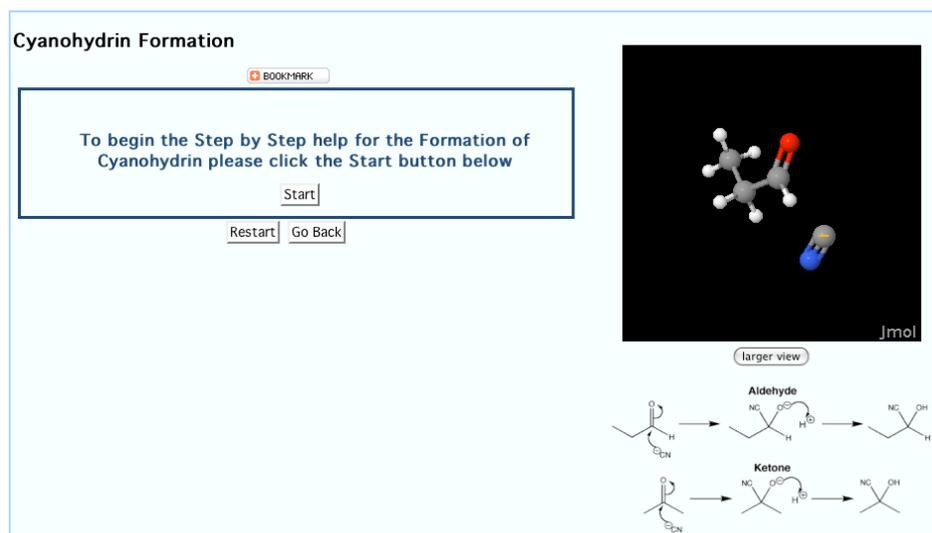


Fig. 10. Change of text on starting screen and addition of “AddThis” bookmark button.

The text inside the learning sequence was originally laid out to coincide with the text on the initial layout for the starting screen (Fig. 11), but after the changes were made to the text on the starting screen the text for each step had to be changed. In the penultimate design three different font styles were used to distinguish between the different stages of each step (Fig. 12). Bold font style stands out more and was therefore used for the first stage, telling the user what to do initially, followed by regular text indicating any important aspects to note. Questions, shown in italics, are used to see if the user understands a particular step, this method has been used to try and encourage students to go and look up an answer if they have difficulty with it and the questions asked are based on the important steps in the mechanism.

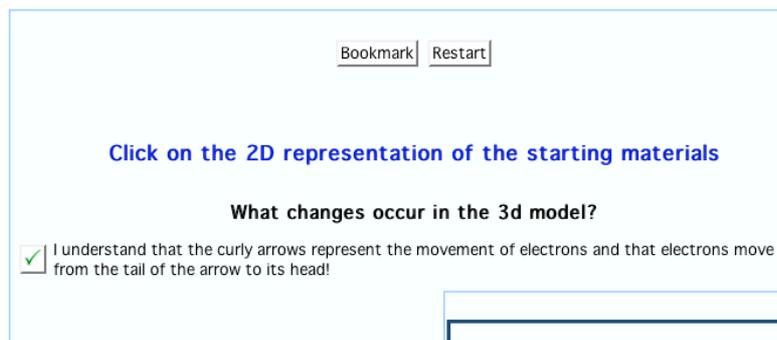


Fig. 11. Layout of text for third stage to coincide with initial layout for starting

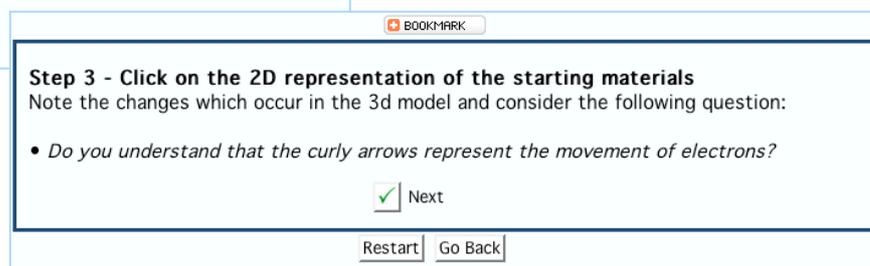


Fig. 12. Layout of text for third stage coincides with the new layout

Each learning sequence is linked to an optional multiple choice self-assessment activity via the final stage, which indicates that the step-by-step guide is complete. The self-assessment activities were constructed using JQuiz (part of the Hot Potatoes package) and were based on the same colour scheme/layout as the learning sequences (Fig. 13). The multiple choice questions used in these activities

are made up from two sources, some questions were produced by the project team and others were taken from the work done in the "Testing Your Organic Chemistry Knowledge to Reinforce Comprehension and Understanding using Web-Based Multiple Choice Questions"³ project funded by the HEA.

Cyanohydrin Formation

Choose the correct answer for each question. Once you have completed a question, click next to move on.

[Index](#)
1 / 4 [Next](#)

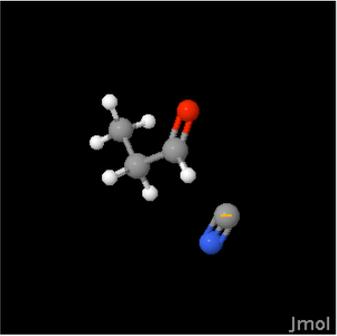
What type of reaction occurs during the formation of cyanohydrin?

A. Nucleophilic Substitution

B. Electrophilic Addition

C. Nucleophilic Addition

D. Electrophilic Substitution



[larger view](#)

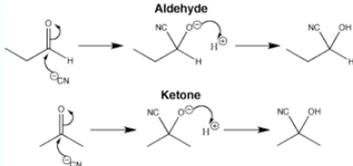


Fig. 13. Layout and content of self-assessment activity

Some of the new changes that were made to the Jmol window in the main site were also included in the new learning designs. The addition of the optional window size was included and we also added a refresh button in the final designs to allow users to reload the molecules to their original starting positions (Fig. 14).

Cyanohydrin Formation

Choose the correct answer for each question. Once you have completed a question, click next to move onto the next one.

What type of reaction occurs during the formation of cyanohydrin?

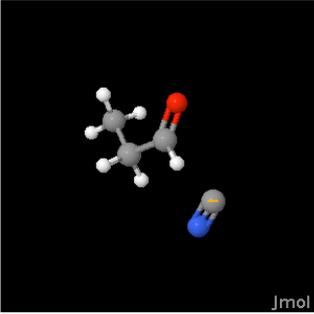
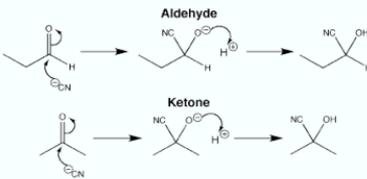
A. Nucleophilic Substitution

B. Electrophilic Addition

C. Nucleophilic Addition

D. Electrophilic Substitution

1 / 3 [Next](#)



[Small \(300 px\)](#) [more controls](#) [refresh model](#)

Fig. 14. Final layout of self-assessment activity including new Jmol features

In order to test the effectiveness of the new learning designs we set up several different approaches to try and gain feedback on them. This included contacting academic staff at various universities and asking for their opinion, holding student focus groups, showing students at the UoL the designs in lectures and emailing them with links to the designs whilst offering a reward for the best feedback. Finally we held a lecture at Loughborough in which students were shown the new designs and asked to provide instant feedback using the individual personal response system TurningPoint.⁴

We had hoped to encourage contributing organisations by showing them some of the draft learning designs and encouraging them to take part in the testing and evaluation of them. This worked well in terms of getting feedback on the designs from academic staff, but when we asked if it would be possible to hold student focus groups to get a students perspective we only received a yes from Loughborough University, who had already agreed to be involved in the project from the very beginning.

A number of learning designs have been produced to support various types of material on the ChemTube3D website, including the addition of new learning sequences covering organic chemistry structures and reactions from within 8 of the 19 topics currently available and also a new A Level section. Self-assessment activities have also been produced for 5 of these 8 topics. The topics covered include examples from across different years of an undergraduate degree and they are:

- Nucleophilic addition at the carbonyl group*,
- Nucleophilic substitution at the carbonyl group*,
- C=O addition - loss of carbonyl oxygen*,
- Electrophilic addition to alkenes,
- Electrophilic aromatic substitution,
- Enols and Enolates as nucleophiles*,
- Aromatic heterocycles and
- Fragmentations*

The first five topics listed above are all covered during the first year of an undergraduate degree in chemistry and examples from within each of these sections are available for students. The Aldol reaction, covered in the 'Enols and Enolates as nucleophiles' section is taught during second year, whilst aromatic heterocycles are covered in both the second and the third year. Fragmentation reactions are more complex and are therefore studied during the third year of an undergraduate degree. The topics with self-assessment activities are indicated with an asterisk (*).

When asked to evaluate the new learning designs, academics have said that they like the step-by-step approach for beginners and that the graphics are very useful for students. The first group of students to test and evaluate the new designs were the 3 that attended the focus group at Loughborough University. When asked if they preferred the instructions to be on screen or downloadable as a PDF, all three said they liked the on screen version better as each step was separated and there was no possibility of skim reading through the content like there is with a PDF.

Testing the designs with a larger audience was possible at the lecture in Loughborough University. The results from using the electronic individual response systems showed that out of the 46 students who attended the majority of students answered questions related to ChemTube3D and the new learning designs (Figures 15-19). A very positive result is that when asked "Do you like the new assisted learning approach for ChemTube3D presented today?" 93% of the 45 students who replied said yes (Fig. 18).

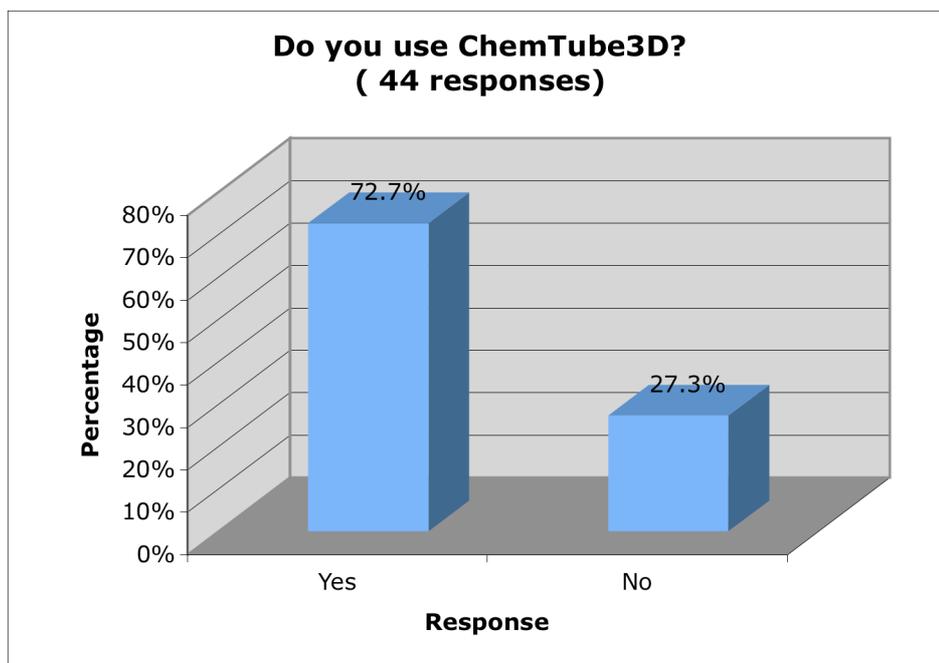


Fig. 15. Indicates if students have accessed ChemTube3D before. Yes indicates one or more visits to the site.

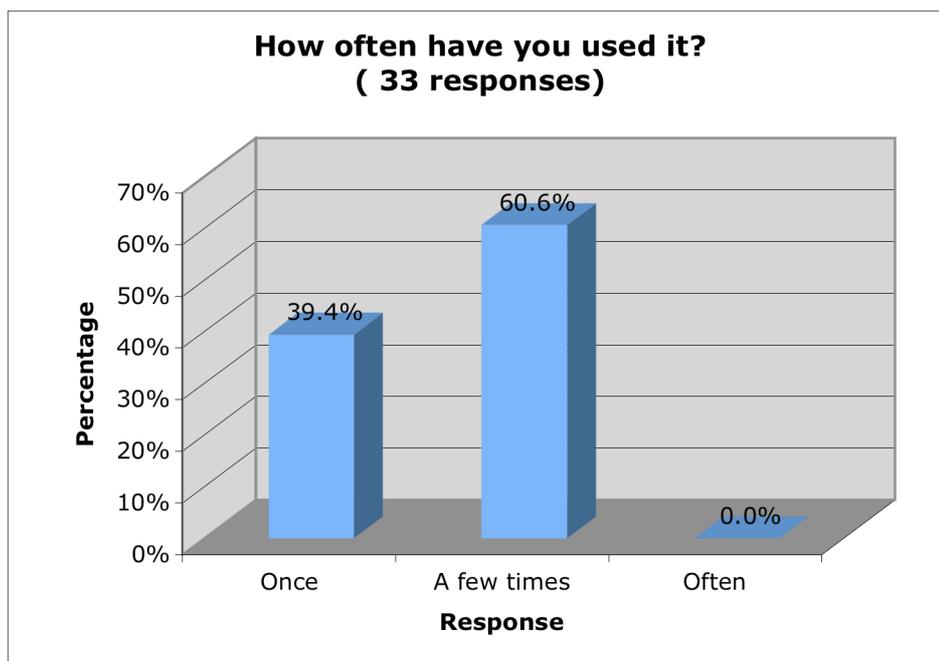


Fig. 16. Indicates how often the students use the resource. This includes the 32 students who answered yes in Fig. 15 and also an extra student who said they had used it once.

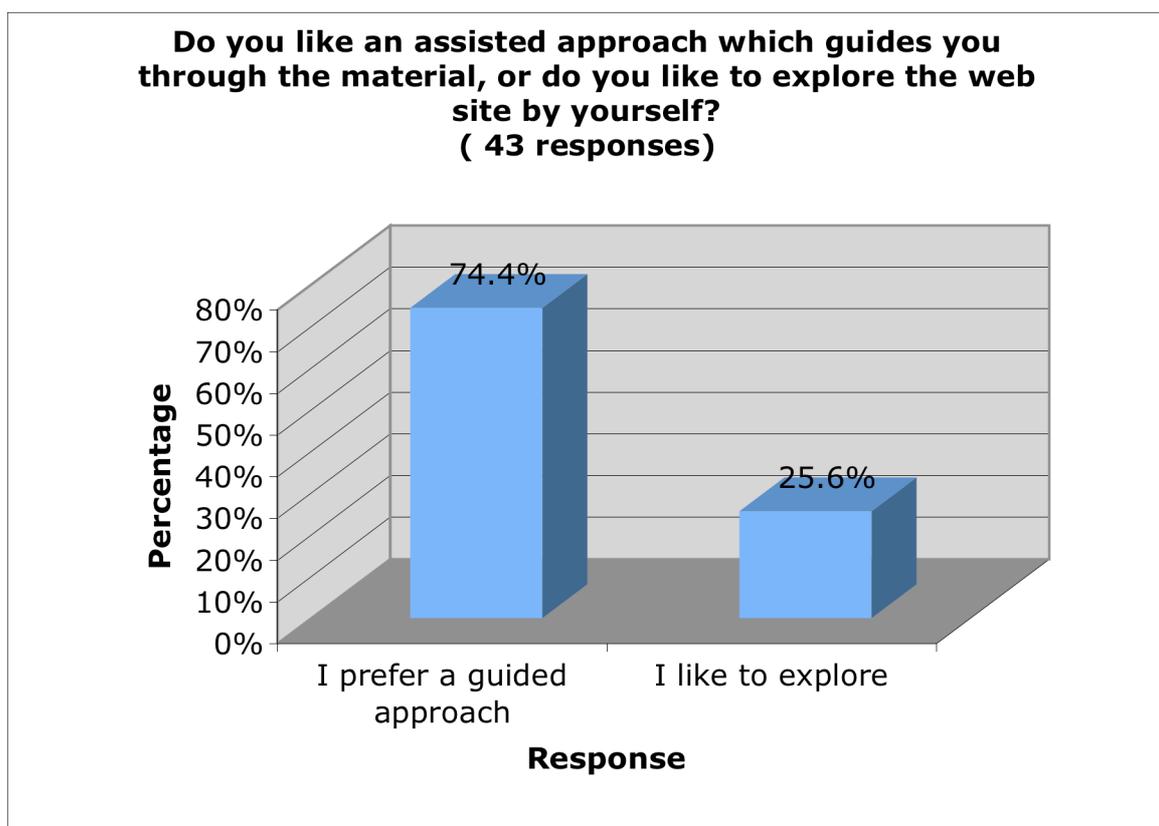


Fig. 17. Indicates whether the students prefer to be guided when using ChemTube3D or whether they like to find things out by themselves.

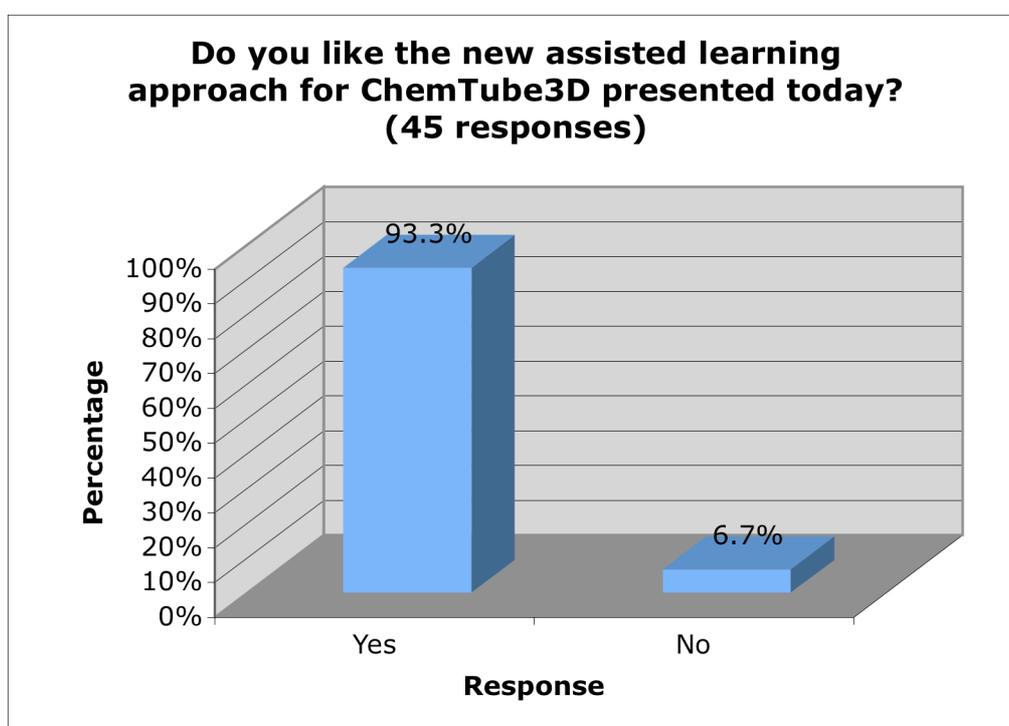


Fig. 18. Indicates whether or not the students like the new step-by-step learning sequence presented to them during the lecture

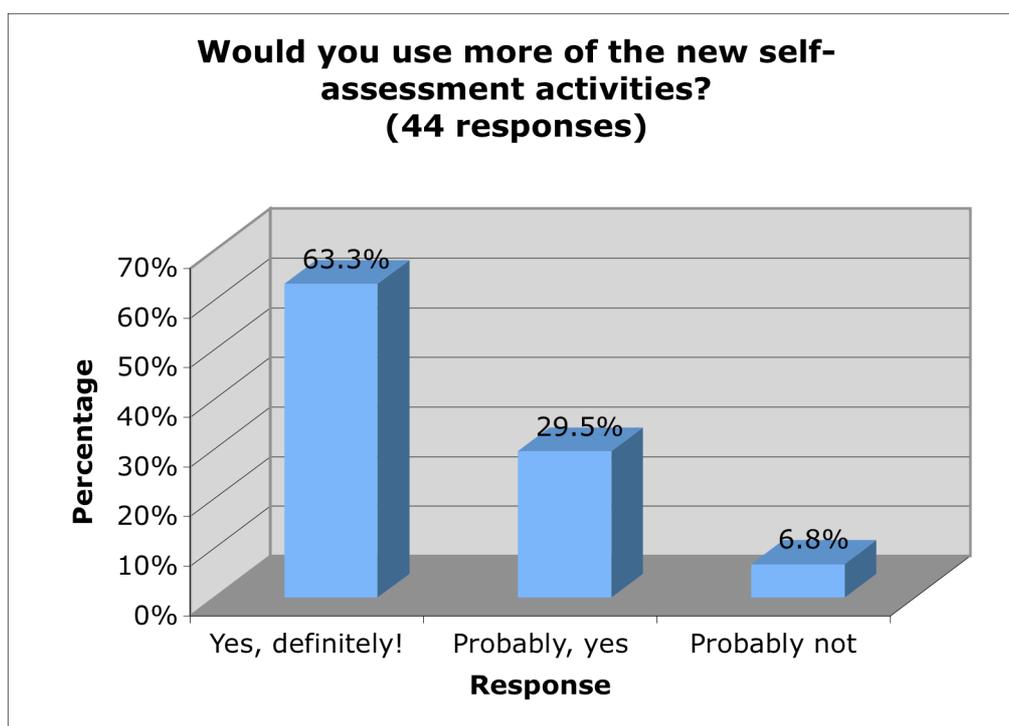


Fig. 19. Indicates whether or not the students will use the new self-assessment activities in the future

When the first year students from the UoL were asked to look at new designs in their own time and provide feedback with the chance to win a reward for the best feedback, we received some very encouraging remarks from two of the students. One student said that they liked the simple way that everything was laid out and gave a list of some improvements that could be made including making the 2D reaction mechanism bigger so that it is clearer to see and also annotating the 3D animation with text. Both of these refinements were made within the final designs and now when an animation is played the name of the reaction is included along with the important change, which is occurring during the step. Another student said they like the self-assessment activity and the ability to go back to the reaction mechanism if the chosen answer is wrong.

5. Implementation

Investigation into the current use of ChemTube3D was carried out using Google Analytics as mentioned previously. This information gave us a strong basis for the project and allowed us to identify HE institutions, companies and colleges to contact with regards to finding out information and also testing and evaluating the new learning approaches developed as part of the project. Surveys were sent out to earlier members of the Facebook group (Appendix 1.1) and then a similar survey was implemented more widely on the ChemTube3D website (Appendix 1.2). The approach to adding the survey to the website was to add a drop down box on the home page with basic information on the project and the survey, followed by a banner at the top of each page asking for users to help us improve ChemTube3D for them by completing our online survey.

A member of the Facebook group who answered our survey suggested using a combination of Jmol and Hot Potatoes for ChemTube3D. After some research into Hot Potatoes we discovered that it is a piece of software published by Victoria University and Half-Baked Software “*enabling you to create interactive multiple-choice, short-answer, jumbled-sentence, crossword, matching/ordering and gap-fill exercises for the World Wide Web.*”¹ First impressions of this software were that it could prove very useful in creating a number of learning designs. The background information and examples definitely showed how useful the resource could be, so we planned to explore it further and see how useful it could be to the project development.

After getting used to the different types of exercises that can be produced using Hot Potatoes we found it to be a valuable resource. Using prior knowledge of CSS style sheets, original source codes could be edited, using Dreamweaver and TextWrangler, in order to display the pages in an appropriate way/colour scheme. Even if you are not familiar with CSS style sheets or HTML code the colour scheme of the exercises can easily be manipulated using the configurations box within each application. The only downside is that you have to make these changes for each of the six applications otherwise the resulting pages will look different (that’s why the main source code was changed to make life a little easier). The main exercises that we thought could be useful for ChemTube3D were:

- JQuiz - used to make multiple choice exercises
- JMatch - for matching/ordering exercises and
- JMix - to create jumbled up exercises

By adapting the main source code it was possible to include the Jmol window in the Hot Potatoes exercises. The Jmol window sits nicely along side the questions in the JQuiz exercises and this development allowed us to make the self-assessment activities more interactive by providing the option to use the 3D animated models in the Jmol window. The basic Jmol window was included into the main source code for each page, so the only thing that needed to be added to each new page was the code for the relevant 3D animation and this was already available from the existing pages on ChemTube3D.

The general layout of the pages produced by Quandary was again changed to include the Jmol window. Quandary allowed the production of a learning sequence to guide the user through a set of tasks. These tasks were designed to help users understand the 3D reaction that they are looking at.

In order to find out whether or not students find ChemTube3D helpful in their learning a number of focus groups were set up for 1st, 2nd and 3rd year chemistry students at the UoL. To try and get students involved in these focus groups we offered food incentives to all attending and numbers were limited at 10 students per session. Participation was limited with a total of six students attending from years 1 and 2 and none from year 3, however, the feedback received was very beneficial to the project development.

Testing and evaluating the new learning approaches was carried out via a few different routes. Initially when the first draft designs of the learning sequences were complete for the heterocyclic chemistry section we sent them to a member of academic staff at the UoL to evaluate the designs based on content, layout etc. with the view of holding a workshop for 3rd year students at the UoL for them to use, test and evaluate the designs further. These designs were developed first as a first semester module based on this material was at the time being taught. The impression we had was that if students were currently being taught the material then they would be willing to use these new designs to help them understand further what they were covering in lectures. This however, was not the case, as students were not prepared to come to the workshop and look at the new designs even with the offer of muffins and donuts for those attending.

The next strategy was to develop some designs based on A Level material and send these to a member of staff who uses ChemTube3D in their A Level teaching. Feedback from staff at the school was encouraging, however, when the links for the new learning designs were sent to the A Level students this resulted in no further feedback being obtained.

In order to obtain feedback on the new learning designs based on undergraduate level material we sent links to academics at a number of universities both in the UK and the USA and asked them to provide feedback.

Whilst holding a student focus group at Loughborough University we managed to gain feedback on some of the designs created for first year organic chemistry material. Students who attended the focus group were from both the first and second year and provided feedback on the new approaches developed during the project. Whilst at Loughborough University we decided to try and organise a session to get feedback from a larger audience using the TurningPoint⁴ individual response system that they have available. The session was organized to take place in the last lecture slot for the 1st year organic chemistry students and out of approximately 100 students 46 turned up. This session gave us the opportunity to use the new learning designs in a lecture environment and also get instant feedback from the students via pre-developed multiple-choice questions.

6. Outcomes and Limitations

The main problems/aims to be addressed during the iChem3D project were:

1. How and why are different people using the resource?
2. Can we identify examples of effective use of the resource?
3. Can additional learning designs be created to support different learners and/or tutors?
4. If so, are the principals of design transferable to other educational contexts?

All of the above aims were successfully completed during the project, as we now have a better understanding of our users and are more aware as to how ChemTube3D is being used in different environments. Lecturers from different HEI's are using ChemTube3D to reinforce lecture material, with the hope that when

students see a 3D visualisation it will increase their understanding. Students are also using the resource effectively in their own time as they use it to try and understand more about how certain molecules react. Additional learning designs have been created to support different learners and as the new learning approaches are optional, users who wish to use the resource as they were doing beforehand still have that option and those who would like some more guidance can use the new approach. The new designs are based on available freeware, which can be used by anyone as long as it is not for commercial purposes and can therefore be used in any educational context. Hot Potatoes and Quandary can both be customised to include any information and due to this they can be used across many disciplines with just the underlying principals being the same.

The work carried out during this project will hopefully have immense value to the students/tutors who use it over the coming years. Early feedback on the new learning approaches suggests that students like the new step-by-step sequence and also the self-assessment activities. Self-assessment activities could also be used during lectures to test students understanding on particular topics and this would lead to a more active learning environment.

Guides on how we manipulated the HTML and CSS to create the layout and designs shown will be available on request after the project has ended.

The main limitation that has arisen from the project is that Quandary is only available for Windows, which is a slight problem for any Mac users. However, once the HTML page has the basic structure it can easily be transferred and then manipulated further using Dreamweaver. Hot Potatoes is available to download for both Windows and Mac so the self-assessment activities can be created by most people.

Another factor that we see as a limitation was the problem of trying to involve other HEIs in the project. We managed to find out information about how the resource was being used at various institutions but trying to involve staff and students in the testing and evaluation of the new learning approaches proved difficult. Even with the offer of food incentives and reward vouchers students were not keen to get involved with the testing of the new learning designs. We tried numerous methods to get academics and students involved, but participation was very limited. Perhaps a way around this would be to get partner institutions involved from the start, as our contact with Steven Christie at Loughborough proved to be the most beneficial in collecting results.

7. Dissemination

As part of the dissemination of the iChem3D project a number of proposals have been submitted a variety of conferences. Listed below are the conferences we have sent proposals too and also the outcomes of the decisions:

- **Presented** at University of Liverpool Learning and Teaching Conference June 2010. Showing how the development of ChemTube3D can be used to improve teaching and learning within the university.
- **Presenting** a demonstration and a poster at ALT-C 2010: *“Into something rich and strange”* – making sense of the sea change. Based on the new learning designs and how they can be transferable across a range of disciplines
- Variety in Chemistry Education Conference 2010
 - 2 hour workshop proposal **submitted** based on ChemTube3D in general, showing how lecturers and students can use all aspects of the resource including the new learning designs

The learning designs produced, as part of the iChem3D project, will also be added to ChemTube3D and will be freely available to use or modify under the Creative Commons Attribution-Noncommercial-Share Alike 2.0 UK: England and Wales Licence.⁶

8. Conclusions

The iChem3D project set out to enhance the value of interactive 3D chemistry, by investigating its current use and also developing a number of transferable learning designs to encourage the effective use of the resource within undergraduate and postgraduate programmes. A number of methods were used to achieve this goal and we are now more aware of how people use the resource. Through the use of existing freeware produced by Half-Baked Software we have managed to produce a number of transferable learning designs, with the vast majority of students surveyed saying they liked the new assisted learning approaches that have been developed. Guidelines have been produced to allow users to understand how to use the resource more effectively as both academics and students did not know how to use ChemTube3D to its full potential.

Students at both the UoL and Loughborough University have expressed an interest in lecturers holding a workshop to teach them how to use the resource at the beginning of first year. As a result of this additional information in PDF format will be available on the ChemTube3D website to support any academics who would like to run such a session for their students.

We have managed to make ChemTube3D even more interactive for its users and hope that people will have the time to look at and explore these new learning designs effectively.

9. Implications

Future implications of the work developed during the iChem3D project include the use by learners across the world and also lecturers/tutors. The new learning designs, which have been created as an addition to the material already available on ChemTube3D, will be of help to anyone studying chemistry from A Level up until Masters level work. In the future work could be carried out using new approaches currently being developed by the creators of Jmol. These include the ability to draw molecules in 2D and then converting the structures into 3D via the simple click of a button.

We hope that academics will use the support we have provided during this project to hold workshops for students and teach them how to use the most important aspects of ChemTube3D, either at A Level or at the start of their undergraduate degree.

Academics from any discipline can build on the work we have carried out by making step-by-step sequences and self-assessment activities related to their modules and programmes using Quandary and Hot Potatoes.

References

- ¹ Hot Potatoes, Victoria University and Half-Baked Software - <http://hotpot.uvic.ca/>
- ² Quandary, Half-Baked Software - <http://www.halfbakedsoftware.com/quandary.php>
- ³ Testing Your Organic Chemistry Knowledge to Reinforce Comprehension and Understanding using Web-Based Multiple Choice Questions, A. Boa and J. Eames - http://www.heacademy.ac.uk/assets/ps/HEAPS_Eames_653_MCQs_with_Feedback.pdf
- ⁴ TurningPoint, Turning Technologies - <http://www.turningtechnologies.co.uk/>
- ⁵ ChemTube3D Facebook group - <http://www.facebook.com/group.php?gid=104293140871&ref=mf>
- ⁶ Creative Commons Attribution-Noncommercial-Share Alike 2.0 UK: England and Wales Licence - <http://creativecommons.org/licenses/by-nc-sa/2.0/uk/>

Appendixes

1. Survey Questionnaire

The questions listed below were included in the surveys sent out through each medium:

1.1 Facebook Survey

This survey was constructed using the free basic package from Survey Monkey. A limit of 10 questions per survey and a maximum of 100 responses applied. Options include in the drop down menu's in question 10 are included in the callouts.

The screenshot shows a SurveyMonkey questionnaire titled "ChemTube3D" with the section "1. Background Information". A progress bar at the top right indicates 33% completion. The questionnaire contains three questions:

1. What country do you live in?
A dropdown menu is shown with a small blue arrow on the right, and a text input field is provided below it.

2. What is your highest level of study?
Radio button options: School, A Level, Undergraduate, Postgraduate, Professional, Other (please specify). A text input field is provided below the "Other" option.

3. How did you initially find out about ChemTube3D?
Radio button options: Search Engine, Friend's Recommendation, Lecturer's Recommendation, Other (please specify). A text input field is provided below the "Other" option.

A "Next" button is located at the bottom right of the questionnaire area.

ChemTube3D

2. Using ChemTube3D

67%

4. Why did you initially want to look at ChemTube3D? (Please select all that apply)

As part of a course
 Seeking help on chemistry learning
 Seeking "Refresher" information
 Other (please specify)

5. What do you now use ChemTube3D for? (Please select all that apply)

Learning New Material
 Revision
 Lecture Demonstrations
 Other (please specify)

6. Which features of the site do you use? (Please select all that apply)

Animated Reactions
 Atomic and Molecular Orbitals
 Molecular Vibrations - IR
 Dipoles and Electrostatic surfaces
 Rotating the Models in 3D
 Measuring Bond Lengths
 Measuring Angles
 Enlarging and Shrinking the Models
 Resizable Window
 Molecular Photo Booth
 Additional options (right mouse click or CTRL-Click for MacOS)
 Other (please specify)

7. Website functionality - please rate your level of satisfaction with the following:

	Very Satisfied	Satisfied	Neutral	Unsatisfied	Very Unsatisfied	No Opinion
Available Resources	<input type="radio"/>					
Search Box	<input type="radio"/>					
Site Navigation	<input type="radio"/>					
Overall Site	<input type="radio"/>					

Do you have any suggestions or comments that will help us improve the ChemTube3D website?

Prev Next

ChemTube3D

3. Your Views of ChemTube3D

100%

8. Please describe what you like most about ChemTube3D.

9. Please describe what you do not like about ChemTube3D and what you would like to see us improve.

10. How often do/will you return to Chemtube3D?

To Date In the Future

Frequency

If you would be prepared to partake in further discussion please enter your Name and Email address below:

Prev Finished

First Visit, Daily, Weekly, Monthly, Quarterly, Yearly

Daily, Weekly, Monthly, Quarterly, Yearly, Never

1.2 ChemTube3D website survey

This survey for the ChemTube3D website was constructed using KwikSurveys as it is free to use and there are no limits on how many questions or responses you can have.

* 1. What country do you live in?
< Select >
Other (please specify)

* 2. What is your highest level of study?
 School
 A Level
 Undergraduate
 Postgraduate
 Professional
[Reset](#)
Other (please specify)

* 3. How did you initially find out about ChemTube3D?
 Search Engine
 Friend's Recommendation
 Lecturer's Recommendation
[Reset](#)
Other (please specify)

Next >>

* 4. Why did you initially want to look at ChemTube3D? (Please select all that apply)
 As part of a course
 Seeking help learning chemistry
 Seeking "Refresher" information
[Reset](#)
Other (please specify)

* 5. What do you now use ChemTube3D for? (Please select all that apply)
 Learning New Material
 Revision
 Lecture Demonstrations
[Reset](#)
Other (please specify)

* 6. Which features of the site do you use? (Please select all that apply)
 Enlarging and Shrinking the Models
 Measuring Angles
 Molecular Vibrations - IR
 Jmol Menu (right mouse click or CTRL-Click for MacOS)
 Molecular Photo Booth
 Measuring Bond Lengths
 Rotating the Models in 3D
 Resizable Window
 Dipoles and Electrostatic surfaces
 Atomic and Molecular Orbitals
 Animated Reactions
[Reset](#)
Other (please specify)

* 7. Website functionality - please rate your level of satisfaction with the following:

	Very Satisfied	Satisfied	Neutral	Dissatisfied	Very Dissatisfied	No Opinion
Subjects Covered	<input type="radio"/>					
Search Box	<input type="radio"/>					
Site Navigation	<input type="radio"/>					
Overall Site	<input type="radio"/>					

[Reset](#)

<< Back Next >>

* 8. Please describe what you like most about ChemTube3D.

* 9. Please describe what you do not like about ChemTube3D.

* 10. Please describe what you would like to see us improve.

<< Back Next >>

* 11. How often do/will you return to Chemtube3D?

	First Visit	Daily	Weekly	Monthly	Quarterly	Yearly
To Date	<input type="radio"/>					
In the future	<input type="radio"/>					

[Reset](#)

12. If you would be prepared to participate in further discussion please enter your Name and Email address below:

Name:

Email Address:

Affiliation (school/university/professional)

<< Back < Finish Survey >

1.3 Universities survey

This survey sent out to students at universities both in the UK and the USA was also constructed using KwikSurveys.

1. Do you find ChemTube3D a useful learning aid for you?

- Yes
 No

[Reset](#)

Comment

2. Which features of the site do you use? (Please select all that apply)

- Rotating the Models in 3D
 Enlarging and Shrinking the Models
 Jmol Menu (right mouse click or CTRL-Click for MacOS)
 Molecular Photo Booth
 Animated Reactions
 Resizable Window
 Measuring Bond Lengths
 Atomic and Molecular Orbitals
 Molecular Vibrations – IR
 Dipoles and Electrostatic Surfaces
 Measuring Angles

[Reset](#)

Other (please specify)

3. Please describe what you like about ChemTube3D.

4. Please describe what you do not like about ChemTube3D and what you would like to see us improve.

5. If you would be prepared to participate in further discussion please enter your Name and Email address below:

Name:

Email Address:

< Finish Survey >

2. Glossary of Acronyms

3D – 3 dimensional

ALT – The Association for Learning Technology

CSS – Cascading style sheet

GCSE – General Certificate for Secondary Education

HE – Higher Education

HEA – Higher Education Academy

HEIs – Higher Education Institutions

HTML – HyperText Markup Language

JISC – Joint Information Systems Committee

PDF – Portable document format

UK – United Kingdom

UoL – University of Liverpool

USA – United States of America