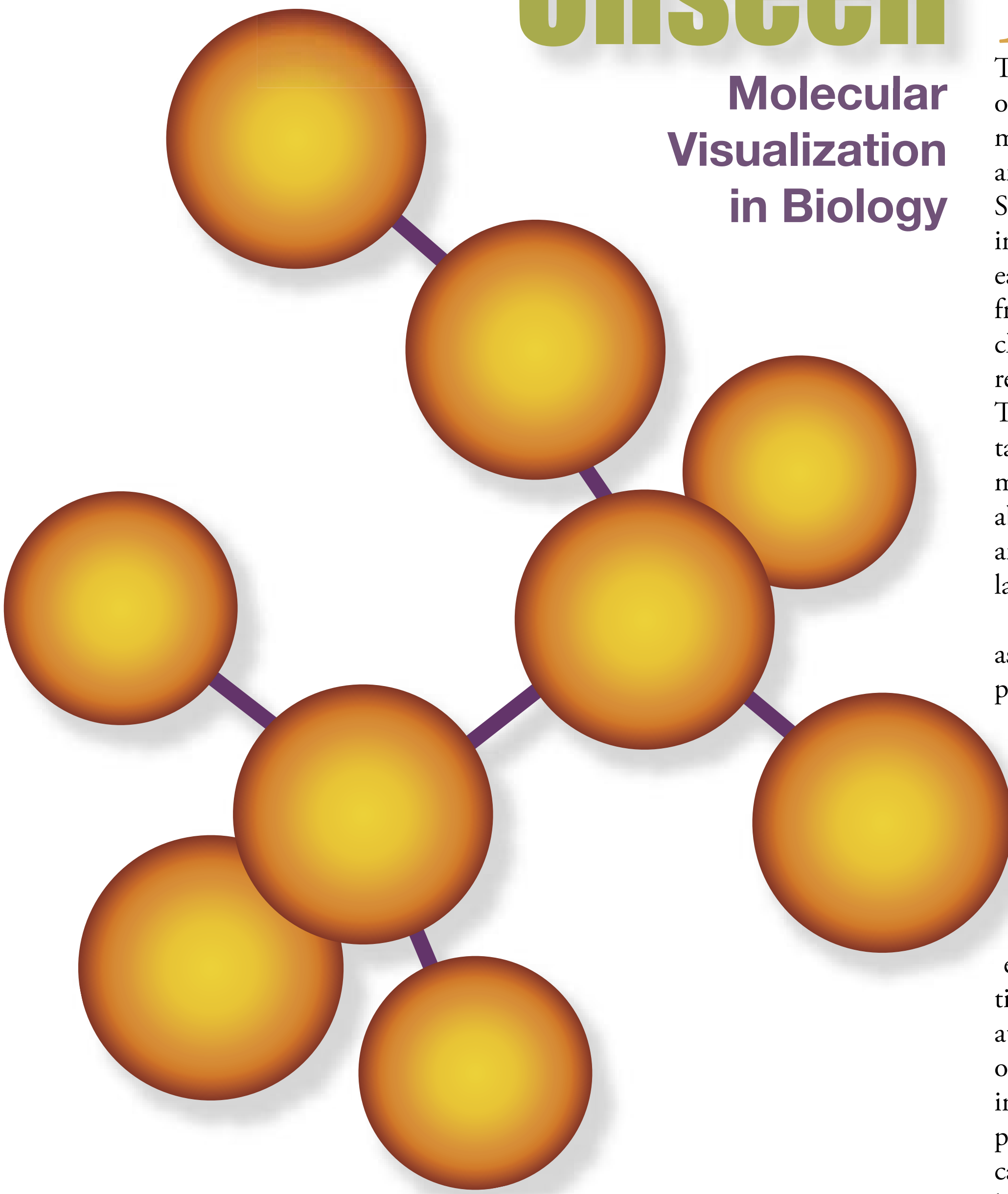
Seeing the Unseen

Molecular Visualization in Biology



By Jeff Finnan, Kim Taylor-Papp, and Mesut Duran

Subject: Biology, chemistry

Grades: 10–12 (Ages 15–18)

Standards: *NETS•S* 2–5; *NETS•T* II, III (http://www.iste.org/standards/)

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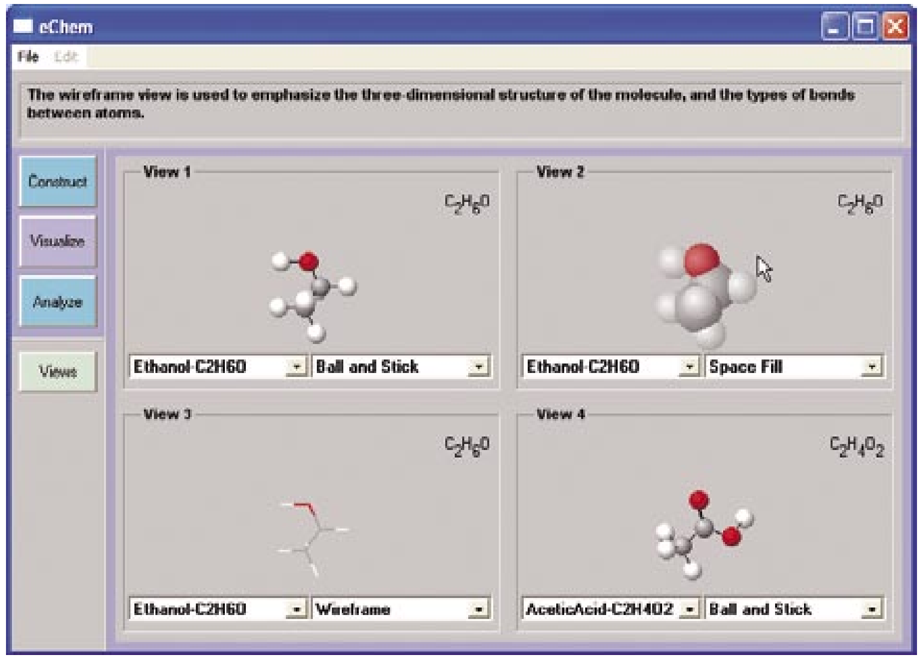
In high school biology, students are challenged by many molecular concepts and structures. They meander through a number of molecular structures, some in macromolecular form: carbohydrates, amino acids, fatty acids, nucleotides. Student difficulties arise in part from inability to visualize what they can't easily see. Students struggle moving from chemical name to symbolic chemical formula and from symbolic representation to the physical one. The problem with physical representation resides at opposite ends: the macroscopic level of directly observable physical and chemical properties and the microscopic level of molecular form and dimensions.

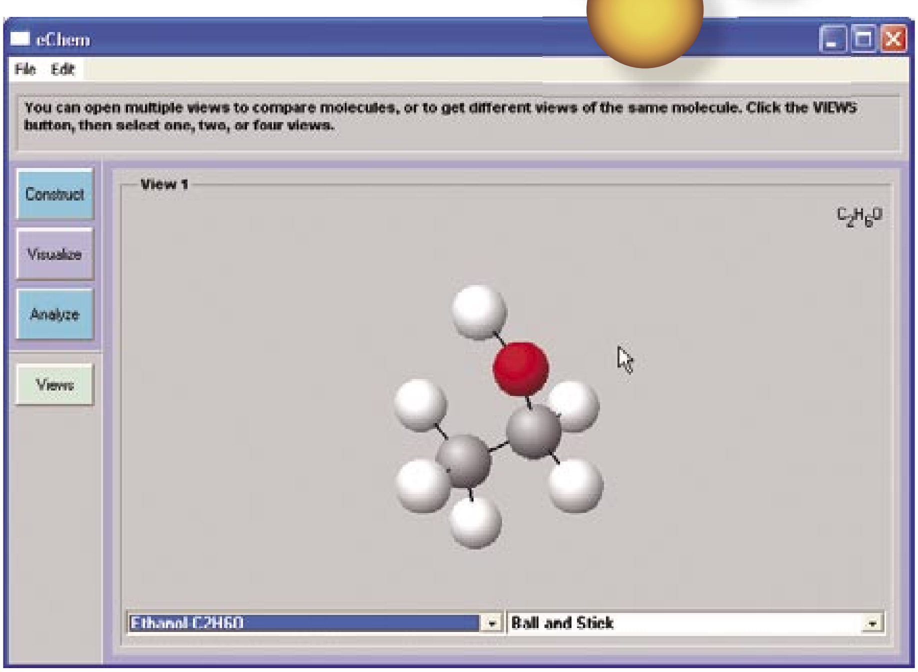
We addressed these challenges as participants in a federal research project known as Michigan Teachers' Technology Education Network (MITTEN), a component of the Preparing Tomorrow's Teachers to use Technology (PT³) initiative. A MITTEN project calls for the engagement, interaction, and collaboration of student teachers, cooperating teachers, and education faculty to develop and field-test authentic projects in which technology enhances teaching and learning in specific subjects. Our project incorporated several free technology applications into our a biology class taught by Jeff as part of his student teaching experience at Redford Union High School in Redford, Michigan. He worked in concert with his cooperating teacher Kim along with input by his educational technology professor Mesut during the design and implementation. We discovered that this alternative learning environment enhanced the understanding of abstract concepts covered in our biology curriculum.

Building One Atom at a Time

Students, on individual computers, started the project using eChem, a stand alone Java-based program that allows construction of simple compounds. Although it is a limited program, eChem allows the formation of some fairly sophisticated molecules. Students were already knowledgeable about atomic planetary models and bond formation through electron sharing. They introduced themselves to eChem with an extensive tutorial. A quick review of this tutorial assisted the transition to other ways of characterizing bonds and molecular shapes. Beginning with methane, students explored some simple molecules that we had constructed for them. The students stepped through



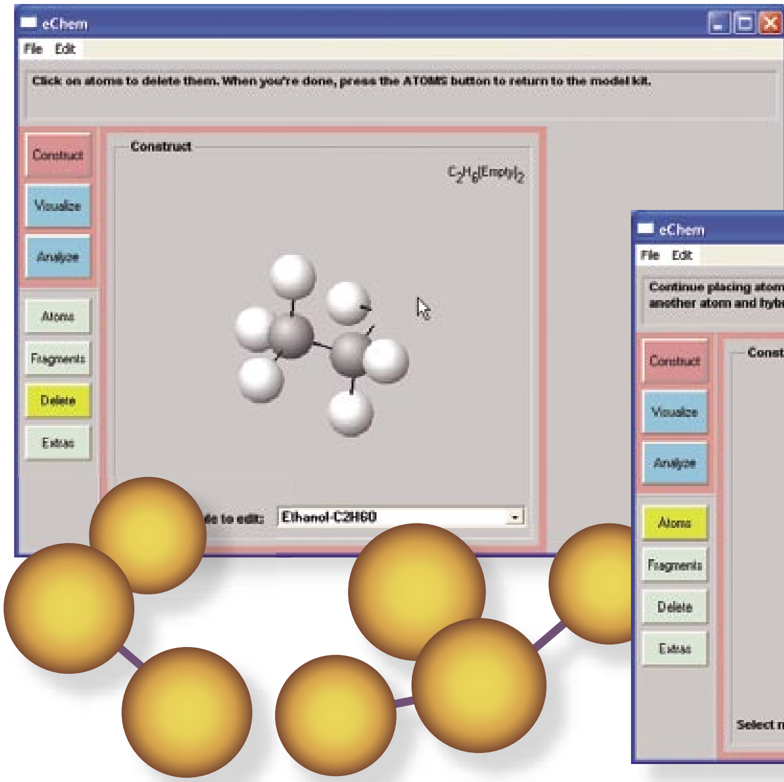
Students can view the same molecule in the three possible display modes and rotate them simultaneously while maintaining the same aspect view. They can be compared with other molecules in any mode if desired.

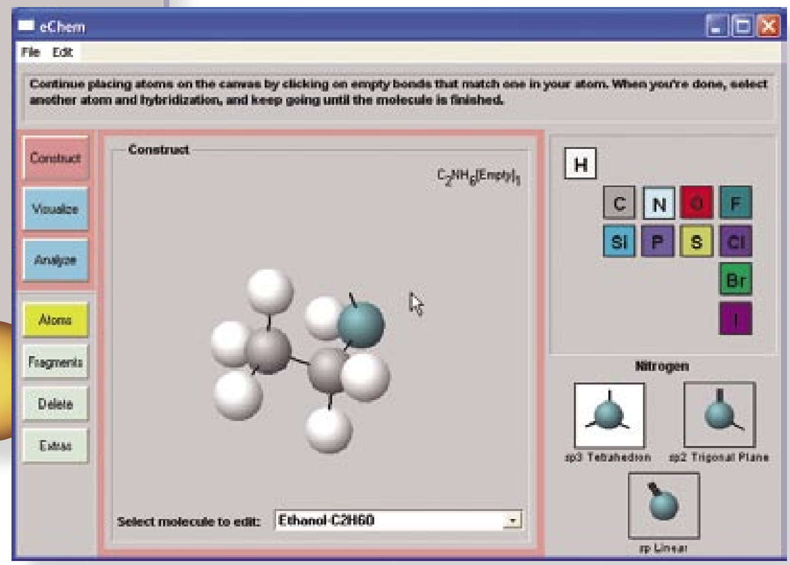


When students open up ethanol, they are presented with the ball-and-stick display, which can be freely rotated with the mouse. In all displays, the molecular formula appears in the upper right.

alternative display modes. They could opt for multiple views to compare the same or other molecules simultaneously. (***Editor's note:*** Find the URL for eChem and other Resources mentioned in this article on p. 29.)

Before building molecules from scratch, students transformed some of the premade molecules into others. The tutorial then guided the students through the construction of ethanol from its formula in straight-line notation, where straight lines represent bonds between element symbols. As the students constructed other simple molecules from straight-line formulas, they progressed rapidly through the tutorial. After teacher review of the student-built molecules, a few students had to correct errors. But most students were able to construct cyclohexane from its straight-line notation without direction on how to assemble cyclical molecules.





To convert ethanol to ethylamine, students can delete the oxygen atom of ethanol (left) and insert a nitrogen atom with three single bonds followed by adding another hydrogen to complete the [Empty] bond (right). eChem does not require the user to be knowledgeable of molecular orbitals. When selecting a particular element, icons offer the bonding options (single, double, triple, or combinations) unique to that element.

Connecting Structures to Properties

Students explored these molecules further on Chemfinder. This Web site is a depository of thousands of molecules with physical properties and structures. In Chemfinder, molecular structures are often shown as bond-line formulas, in which implicit carbon and hydrogen atoms often are not shown. Students retrieved some physical data for these molecules and compared the formula notation. They obtained additional information from The Merck Index using a paid link in Chemfinder.

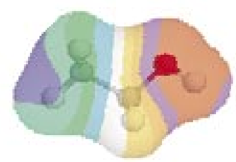
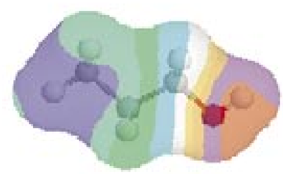
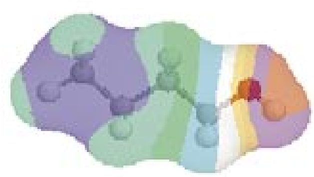
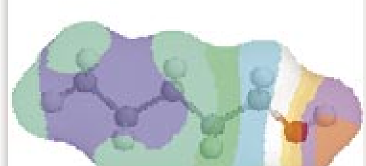
Extending the Range of Vision

Although eChem allows students to create molecules whose spatial relationships can be explored, detail and molecular complexity is limited. The Chime Web browser plug-in offers more robust microscopic information of unlimited molecular complexity. However, the instructor has to build Web pages incorporating desired molecules. You can find some links to tutorials that will help you code these pages in Jeff's online portfolio.

Although students cannot construct their own molecules in Chime, they can rapidly click through more display combinations than in eChem. Chime offers an additional stick presentation and a zoom feature. Students can render a view at any time to its bond-line structure, and two- and three-dimensional representations can be directly bridged. You can create molecular surfaces that can be color-coded to show the structures' comparative water and fat solubility. You can script Web pages to feature specific molecular aspects or to show animation. Chime can include and is particularly suited for visualizing macromolecules, such as protein and DNA. You can also turn on hydrogen bonds or simplify helical regions as strands or ribbons.

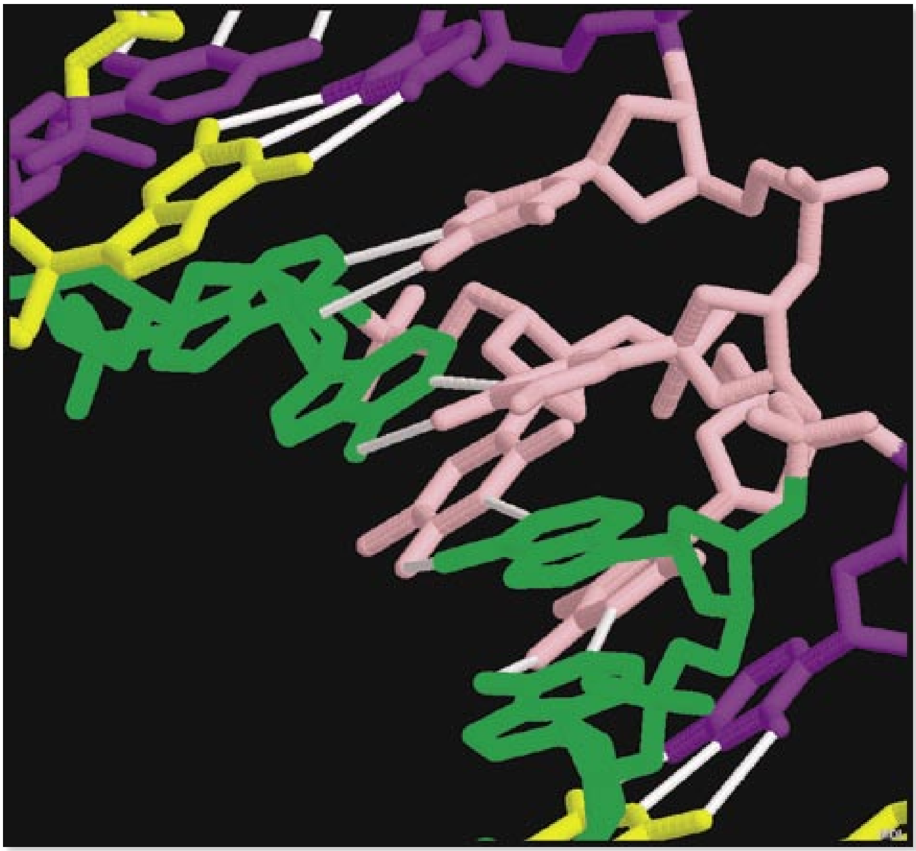
After introducing themselves to Chime with a Web page Jeff created to show how the Chime representations were different than those in eChem, students followed a tutorial illustrating how to generate molecular surfaces. Making surfaces transparent in some display modes (e.g., Ball & Stick) offers a great way to present the volume occupied by atoms with informative visual cues about the structural backbone. Students chose their own path. They viewed other pages incorporating various molecules of biological interest: fatty acids, carbohydrates, even a lipid bilayer. Chime views of starch and cellulose offered students insight into the chemical and physical differences between these two compounds. (***Editor's note:*** Find the Web pages Jeff created in his online portfolio in the Resources section on p. 29.)

In class, we demonstrated the dependency of water solubility of alcohols on the hydrocarbon chain length. In a Chime Web page, students examined these alcohols as transparent surfaces, color-coded to show relative fat solubility. Students correctly identified that as hydrocarbon chain length increased, the molecules had a greater proportion of lipophilic colors (fat soluble) relative to hydrophilic ones (water soluble). That is, they became less water soluble.

Miscibility (solubility) in water	Chemfinder	Chime red = hydrophilic blue =hydrophobic
Ethanol C_2H_6O miscible		
Propanol C_3H_8O miscible		
Butanol $C_4H_{10}O$ partially soluble 6.32 g butanol in 100 mL water		
Pentanol $C_5H_{12}O$ almost insoluble 1 g pentanol in 100 mL water		

Scripting the Chime plug-in allows the student to correlate the relative proportions of color and atoms types to water solubility.

During their introduction to the genetic basis of life, students built a paper replica of the insulin gene. They used Chime to explore a short segment of helical DNA. The Web page allowed students to color-code the nucleotides to match the colors they used in their paper gene. Chime's different display modes allowed them to appreciate the backbone and the stacking of the base pairs. The students could explore the hydrogen bonding between the base pairs.



Students color-coded nucleotides to match the colors in the paper gene exercise. They could show hydrogen bonds in white.

Taking Ownership

The opportunity for reflection came as soon as the students, now familiar with eChem and Chemfinder, learned to navigate with Chime. They undertook their My Molecule project. Students chose a molecule of biological significance to build with eChem, found physical and biological data, and incorporated this information into PowerPoint, which most students were familiar with from their required computer literacy course. A list of suggested molecules included alcohols, amino acids, fatty acids, small carbohydrates, and two dipeptides. Besides minimal requirements, students could garner more points based on the complexity of the molecules chosen, additional screenshots, Chemfinder structure, and a link to a simple Web page we supplied with a Chime presentation of their specific molecule.

Seeing the Unseen

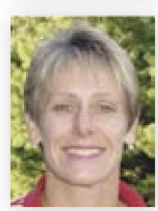
The day the students fired up eChem for the first time, we worried that our curriculum would exceed the students' capabilities. Would their comprehension improve through these largely inquiry-based technologies? But our apprehension was misplaced. Students quickly mastered building and controlling their own molecules. They moved so quickly through the eChem tutorial we had to throw in the challenge of making a cyclical molecule to slow them down. Students figured out, on their own, how to use [Empty] in the eChem formula to guide them while building molecules. The students precisely correlated solubility with structure.

As we reflected on the entire project, we found the new learning environment fostered a level of understanding of the abstract concepts beyond the traditional classroom experience. Students, however, did have some difficulty understanding the two-dimensional bond-line notations with some elements not shown. We had to draw many in straight-line notation to help them understand. In the future, we will address this issue from the beginning to make it easier for students to read those simplified formulas.

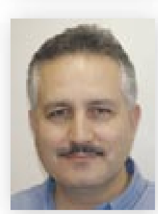
Resources

Chemfinder: http://chemfinder.cambridgesoft.com/
Chime: http://www.mdlchime.com/products/framework/chime/
eChem: http://www.hi-ce.org/soft_echem.html
Jeff Finnan's portfolio: http://www.umd.umich.edu/mitten/jfinnan/. Here you will find exhibits and annotated resource links. These links show how to script Web pages to incorporate Chime molecules and where to get or generate suitable molecules.
Jeff Finnan's Molecular Visualization site: http://expedioscientiam.net/molvis/
MITTEN Project: http://umd.umich.edu/mitten

Jeff Finnan, PhD, spent 20 years in corporate research and development as a chemist. Then he embarked on a second career in teaching. He is currently pursuing opportunities in secondary science education.



Kim Taylor-Papp teaches biology, molecular biology, forensics, and earth science at Redford Union High School. She has been there for 16 years and is currently the science chairperson.



Mesut Duran is an assistant professor of technology at the University of Michigan-Dearborn and is director of the MITTEN Project.