Computers in Chemistry

The Stereochem Game: Making Chemistry More Fun

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...developed a tutorial that tests students on stereochemical concepts presented in a two-dimensional format. n interactive stereochemistry tutorial has been made available on the World Wide Web for student use as a self-test. This tutorial is presented as The Stereochem Game, a game that maintains a running score and sells hints. Multiple versions of each question are available; one is randomly selected each time the tutorial is used. This allows use of the tutorial, as both a pre- and post-test exercise, to help students guide their study efforts and to evaluate their own progress.

INTRODUCTION

Although stereochemistry is a subject consisting of three-

dimensional concepts, examinations on the subject are often conducted on twodimensional paper. Recently, we developed a series of interactive, discovery-based stereochemistry tutorials [1, 2] that incorporate two-dimensional representations of molecules, with links to three-dimensional coordinates of the molecules that can be viewed using RasMol [3] or Chemscape Chime [4]. The availability of multiple representations of a given molecule helps students to build a mental correlation between various representations of chemical structures; however, it may also increase their reliance on the availability of three-dimensional physical models in order to demonstrate their understanding of stereochemical principles. To address this issue we developed a tutorial that tests students on stereochemical concepts presented in a two-dimensional format [2]. The tutorial consists of twenty questions, gradually increasing in difficulty, about stereochemical properties and relationships of a molecule or collection of molecules. The tutorial is presented in the form of a game with a high-score objective and is called The Stereochem Game. Students are allowed to fall back on "hints" in the forms of definitions and three-dimensional computer models, but receive fewer points for correct answers after receiving hints. Each of the questions can be asked in reference to any one of four molecules or sets of molecules, one of which is randomly chosen for the student; thus, each time the student plays the game a different "exam" will be given. This allows effective use of the tutorial as both a pre-test exercise, allowing students to discover their weaknesses (and focus their further study), and as a post-test exercise, where students can confirm that they are well-prepared for the examination. The Stereochem Game is available on the World Wide Web at http://www.chem.arizona. edu/courses /chem242/ by selecting "Tutorials" and then "The Stereochem Game" from the underlined links, taking advantage of the ability to provide chemical information in the form of hyperactive molecules [5, 6].

Web pages were implemented using HyperText Markup Language (HTML) with links to various MIME (Multipurpose Internet Mail Extension) types. The common MIME types video/quicktime,¹ image/gif, and chemical/x-pdb were used. Hyperactive molecules are typically Brookhaven Protein Data Bank atomic coordinate entry (PDB) files [7], which may be viewed with a helper application or plug-in. A web page describing how to download and properly configure a copy of RasMol [3] for use as a helper application or Chime [4] for use as a plug-in is available through the introductory

¹ QuickTime is a registered trademark of Apple Computer Corporation.

page. Interactive student responses to questions posed by the tutorial are submitted to, and evaluated by, a common gateway interface (CGI) script written in the Perl programming language.

RESULTS AND DISCUSSION

The Stereochem Game provides a series of twenty stereochemistry questions ranging in complexity from, "Does the molecule shown have a chiral center?" to, "Which of the following pairs of structures are atropisomers?". Each question used in the game has four possible molecules or molecule sets of which one is randomly chosen for each student. This variation in the game allows a single student to effectively use the tutorial during several stages of study without worry that the answers are derived from memory rather than conceptual understanding.

Three representative examples of the twenty questions asked during the course of the game follow (*vide infra*). The four random selections of structure or structure set to which the each question refers are shown in Figures 1-3. Hints available for each question are also described.

Example 1: What is the absolute configuration of the stereogenic center in the following molecule? (Figure 1)

The hint (available upon request) includes a link to the PDB file for the structure used in the question, and a reminder that stereogenic centers are assigned either R or S designations.

Example 2: What is the absolute configuration of the stereogenic center in the following molecule? (Figure 2)

The hint (available upon request) includes a link to the PDB file for the structure used in the question, and a reminder that the convention for assigning the R/S descriptor assumes that the lowest priority substituent is directed away from the viewer.

Example 3: Choose the enantiomer of Structure 1. (Figure 3)

The hint (available upon request) includes links to the atomic coordinate files for all structures used in the question, and a reminder that rotation around single bonds is a conformational change, rather than a configurational change.

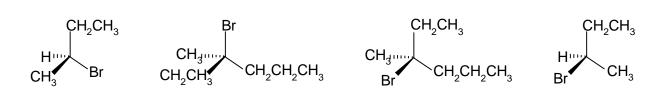


FIGURE 1. FOUR STRUCTURE SELECTIONS USED IN EXAMPLE 1.

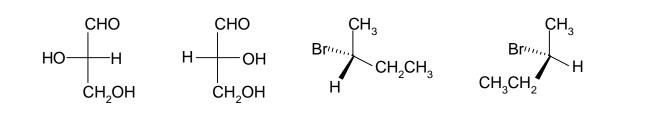


FIGURE 2. FOUR STRUCTURE SELECTIONS USED IN EXAMPLE 2.

At first glance, Examples 1 and 2 appear to be redundant. Nevertheless, they address different concepts and common problem areas for students. The molecules used in Example 1 have the lowest priority substituent directed away from the viewer whereas those in Example 2 do not. Example 2 requires students to either mentally rotate the molecule provided, or to exercise the common two-dimensional paper trick of switching an even number of substituent pairs until the lowest priority substituent is oriented away from the viewer. Students who do not recognize that they have these options can buy a hint in the form of the PDB file and rotate the molecule on the screen.

Additional questions test the ability of students to identify diastereomers, meso compounds, compounds expected to show optical rotation, E/Z configuration, atropisomers, and other important stereochemical concepts. These twenty questions offer a comprehensive stereochemistry study tool and self-evaluation for sophomore organic chemistry students. The questions cover identification and nomenclature of chiral centers, stereoisomeric relationships, meso compounds and a wide variety of structural representations used to represent stereochemistry. This tutorial is meant for use by students who have learned, or are in the process of learning, stereochemistry either through use of the discovery-based stereochemistry tutorials [1] or through lectures and assigned problems on the material.

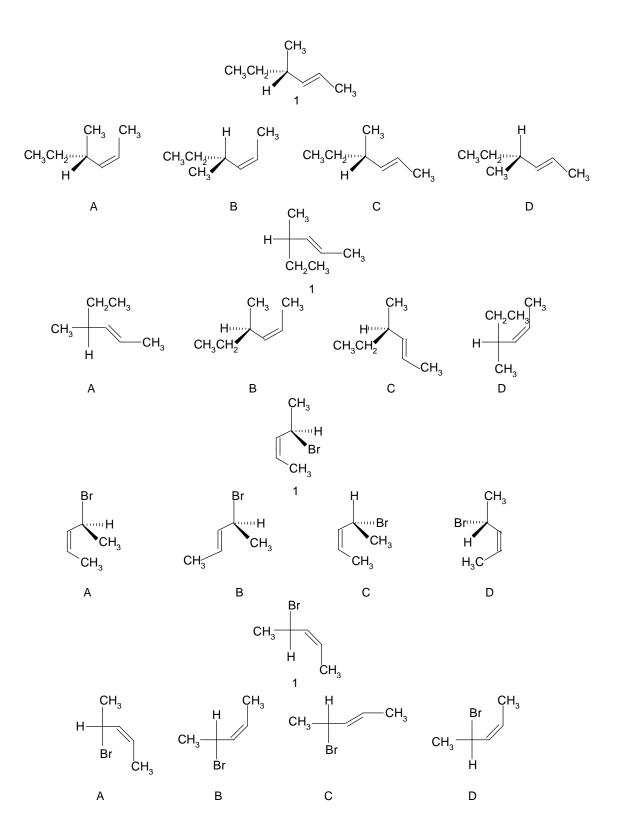


FIGURE 3. STRUCTURE SETS USED IN EXAMPLE 3.

EVALUATION

The Stereochem Game was evaluated by a volunteer group of students who learned stereochemistry without the aid of hypermedia tutorials. Response to this tutorial was enthusiastic with several strong points noted. One student said that having hints with an associated point penalty would have decreased her dependency on the book. She indicated that when performing problems from the book, she had often resorted to using the problem solution as a hint. Another student stated that the number of choices provided as solutions for each problem would discourage guessing. Many students cited the visual aspects of hypermedia available in the hints as strong points.

A more quantitative evaluation of this tutorial is planned for future semesters. One possible design of such an evaluation is to have students fill out a brief survey. This survey would include questions on time investment with various learning materials, student perceptions of the quality of such materials, student perceptions regarding their optimal learning style (auditory, kinesthetic, visual, etc.), and student indications of the learning style involved when using various learning materials. Statistical analysis of student responses to questions concerning time investments with study materials such as the tutorial, the assigned reading, the assigned problems, and regarding lecture attendance, correlated with exam scores should provide some quantitative assessment about the relative learning impact of each type of material. Such an analysis will be complicated by the lack of a true control group and possible bias due to student selfselection as tutorial users and nonusers. Our suspicion is that those students spending the most overall time will perform well, regardless of the type of learning material. Analysis of questions regarding student perceptions of the quality, ease of use, and interest generated during use of the materials is expected to provide us with more quantitative information about the impact of interactive materials on student study habits.

FINAL REMARKS

The Stereochem Game provides students with an interactive and challenging environment in which to practice their understanding of stereochemical concepts. Students have the option of buying a hint for certain questions, which provides a more "tutor-like" interaction than a solutions manual. No solution explanations are available, and a running score is maintained. Random guessing will result in scores of approximately twenty-five percent. An evaluation indicated that students will enjoy working with this interactive tutorial and possibly spend more time studying; therefore, they should retain more of what they learn.

ACKNOWLEDGEMENT

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REFERENCES

- 1. Parrill, A. L.; Gervay, J. "Discovery-Based Stereochemistry Tutorials Available on the World Wide Web" *J. Chem. Educ.*, in press.
- 2. Parrill, A. L. M.S. Thesis, The University of Arizona, 1996.
- 3. Available by anonymous ftp from ftp.dcs.ed.ac.uk/pub/rasmol/; Roger Sayle, BioMolecular Structures Group, Glaxo Research & Development, Greenford, Middlesex, UK.
- 4. Chemscape Chime is available from; http://www.mdli.com; MDL Information Systems Headquarters, 14600 Catalina Street ,San Leandro, CA 94577, (510) 895-1313, FAX: (510) 614-3608.
- 5. Casher, O.; Chandramohan, G. K.; Hargreaves, M. J.; Leach, C.; Murray-Rust, P.; Rzepa, H. S.; Sayle, R., Whitaker, B. J. "Hyperactive Molecules and the World-Wide-Web Information System" *J. Chem. Soc., Perkin Trans.* 2 **1995**, 7.
- 6. Rzepa, H. S.; Whitaker, B. J., Winter, M. J. "Chemical Applications of the World-Wide-Web System" *J. Chem. Soc., Chem. Commun.* **1994**, 1907.
- 7. Protein Data Bank, Brookhaven National Laboratory, Upton, NY.