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Of Special Interest

Report On "Generate and Select: An Expert-System-Derived, Active-Learning Approach for Teaching Organic Chemistry"

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"The medium is the message…implies that the critical content of any learning experience is the method or process through which the learning occurs."

The faculty in a small, progressive chemistry department have joined to revise and redefine its undergraduate program. In this session, Dr. Scudder examined the consequences of these changes in the context of organic chemistry instruction as well as the nature of the change.

Introduction

Creating a Map of Alternatives

The focus of Dr. Scudder's "Day 2-to-40" seminar was teaching science as a process, not science as a result. Dr.

"Generate and Select: An Expert-System-Derived, Active-Learning Approach for Teaching Organic Chemistry" by P. H. Scudder was presented at the "Day 2 to 40" workshop symposium held May 10–11, 1997. The two-day event was held in the Willard H. Dow Chemical Sciences laboratory building on the central campus of The University of Michigan in Ann Arbor, Michigan. Each of the articles that comprise this issue was written by one of the group of reporters whom I asked to attend each session to take field notes and then follow up with the session leader and participants afterwards.

—Brian P. Coppola, Proceedings Editor

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Scudder refers to Postman and Weingartner's (1969) analysis of Marshall McLuhan, "The medium is the message…implies that the critical content of any learning experience is the method or process through which the learning occurs." Using this as a framework, he built his New College Organic Chemistry course to teach students critical thinking and outcome analysis rather than rote memorization. Students are taught to create a map of alternative solutions called "problem space" and then use a rational process to decide the feasibility of each pathway.

Sorting and Classifying as an Evaluative Activity

The steps in examining the problem space for a particular concept are: rank, web, weave, map, branch or generate, and best first search. In this system students sort the ideas into general categories and then add layers of detail onto the developing framework. The process of organizing their thoughts into a concept map for a problem teaches students science by having their minds go through the steps of the science. As students evaluate the branches they have created, they use their knowledge to make judgments of the most likely possibility in problem space. This process sets up a framework that also allows them to evaluate new data by themselves, rather than by memorizing the way someone classifies it. It also allows for student questioning, skepticism, and a Socratic teaching style that produces independent thinkers who are empowered by this system of classification and evaluation.

The Session

Dr. Scudder began his presentation with a brief overview of the context of this curriculum reform at New College. (See Figure 1.) He went on to indicate two decisions that were made at New College. First, organic chemistry needed to change. The "passive" method of a strictly lecture-based course that is based on "memorization-oriented acquisition of factual knowledge" was thrown out. The database approach was also discarded as a valid teaching method due in part to the "tyranny of content." (See Figure 2.)

The second decision was that the general chemistry curriculum also needed to be fixed. On the surface, the problem was identified as twofold. First, the curriculum lost the weaker students due to its mathematics content and bored the better students due to the other content. Only now has New College moved to a split course for the different levels of students.

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- Located on the Florida Gulf Coast (Sarasota)
- Small Size: 650 Students, 55 Faculty (3 chemists)
- 4-1-4 Calendar (January Independent Study Period)
- Narrative Evaluations instead of Grades
- Advanced Work in Small-Group Tutorial Format
- Senior Thesis (and its Defense) is a
- Graduation Requirement
- 3–4 Chemistry majors per year

FIGURE 1. NEW COLLEGE OF THE UNIVERSITY OF SOUTH FLORIDA.

- Organic chemistry has a well-deserved reputation for difficulty, memorization, and information overload. Most textbooks are well over 1000 pages, and the instructor feels the pressure to fit in as much as possible. This “tyranny of content” discourages novel approaches to teaching.
- Too often such a course is an exercise in trivia collection rather than one in reasoning. The very thing that makes science interesting can be left out of the introductory courses in the time pressure to cover all the material.

FIGURE 2. THE DATABASE TEACHING MODEL, TYRANNY OF CONTENT.

Change was then implemented as follows. A one-semester introductory chemistry course was created as a “general-interest, concepts-based course for the poorly prepared and for general-interest students.” As such, organic chemistry was moved to become the first course in the chemistry sequence. It was set up as a “high-interest, low-quantitative, integrative course that is based on first-principles.” Among other things, this has allowed the first-year calculus sequence at New College to “repair the mathematics background” of incoming students to give them the tools they need to succeed in general chemistry. Then, in the second year, math-based chemistry principles are introduced as a precursor to inorganic chemistry and physical chemistry. (See Figure 3.)

Dr. Scudder went on to indicate the kinetics of this change. This “gradual change” has been put to the test by bringing more and more first-year students into organic

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- Entering students had a wide range of backgrounds in chemistry.
    1. The weaker students were lost (calculation intensive course).
    2. The better students were bored (not up to placing into Organic directly).
- Placed a modified Organic Chemistry as the first course.

  This is a high-interest, low-math, integrative course, first-principles-based, with direct impact on their life and possible major.
- Decided recently to split the General Chemistry course.
    1. One-semester Introductory Chemistry begun as general interest concepts-based course for the poorly prepared and for general-interest students.
    2. Allow first-year calculus sequence to repair students' mathematics background.
    3. In the second year, a one-semester Chemical Principles will be a calculation-intensive precursor to Inorganic Chemistry and Physical Chemistry
    4. Our changes were similar to that at the University of Michigan and elsewhere, thus allowing us to feel we were not alone in our curricular experiment.
    5. Strategy for Conducting Gradual Change

    a) Organic Chemistry became more first-principles-based.

    b) Gradually tested in more first-year students into Organic.

    c) Phase out the year-long General Chemistry and replace with Introductory Chemistry and Chemical Principles.

FIGURE 3. CHANGES TO GENERAL CHEMISTRY.

TABLE 1. 1997/1998 Chemistry Program at New College.

	First Semester	Second Semester
	Introductory Chemistry (some students start here)	Introductory Chemistry Laboratory
First-Year	Structure & Reactive I (Lecture/Laboratory) (many students start here)	Structure & Reactivity II (Lecture/Laboratory)
Second-Year	Chemical Principles (Lecture/Laboratory)	Inorganic Chemistry (Lecture/Laboratory)
Third-Year	Physical Chemistry I and Instrumental Methods	Physical Chemistry II (Lecture/Laboratory)
Fourth-Year	Thesis and Advanced Course	Thesis and Advanced Course

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TABLE 2. Sorting the Common Electron Sources into Eight Generic Types [1].

Generic Source Class	Examples
Organometallics	alkyllithiums
Group 1 Metal Hydrides	sodium hydride
Complex Metal Hydrides	sodium borohydride
Active Metals	lithium metal
Lone-Pair Nucleophiles/Bases	alcohols, amines
Allylic sources	enolates, enamines
Simple Pi Bonds	alkenes, alkynes, dienes
Aromatic Rings	benzene

chemistry and by phasing out the general chemistry class to be replaced by the introductory chemistry and chemical principles class.

Above and beyond a simple curricular reform, Dr. Scudder has implemented new teaching methods into the chemistry sequence. Based strongly on the idea of "expert systems block diagonals," this system is well summarized in the following statement by Dr. Scudder:

> To teach students to think like experienced chemists, one must focus on the problem-solving process, similar to what is done in expert system design. The essence of the field must be extracted: the conceptual tools, the general rules, the trends, the modes of analysis—everything used to construct an expert system.

The "inference engine" that drives this system is the search process. The notion that "postulating a reasonable hypothesis can be taught" was discussed and examined by grouping the eight common electron sources and sinks into generic types. (See Tables 2 and 3.) Also, Dr. Scudder's example of viewing a mechanism as an "assembly of recognizable mechanistic units, which takes energetics into consideration" is another example of this system. (See Figure 4.)

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TABLE 3. Sorting the Common Electron Sinks into Eight Generic Types [2].

Generic Sink Class	Examples
Electron-Deficient Species	carbocations, boron trifluoride
Acids	hydrogen chloride
Single Bonds between Heteroatoms	bromine
Leaving Groups on sp^3 Carbons	methyl iodide
Carboxyl Derivatives (sp^2-bound L)	Acyl halides, anhydrides, esters
Heteroatom-Carbon Multiple bonds	Aldehydes, ketones, nitriles, carbon dioxide
Conjugate Acceptors	enones, acrylates
Redox-Active Metals	chromium trioxide

A proper sentence uses known words within a grammatical framework. Likewise a reasonable reaction mechanism is an assembly of recognizable mechanistic units that takes energetics into consideration.

The Twelve Common Mechanistic Units are [2]:

- Proton transfer to and from an anion or lone pair
- Ionization of a leaving group
- Trapping of an electron-deficient species by a nucleophile
- Electrophile addition to a multiple bond
- Electrophile loss from a cation to form a pi bond
- 1,2 rearrangement of a carbocation
- The S_N2 substitution
- The E2 elimination
- The AdE3 addition
- Nucleophilic addition to a polarized multiple bond
- Beta elimination from an anion or lone pair
- Concerted six-electron pericyclic

FIGURE 4. ELEMENTAL MECHANISTIC PROCESSES.

The process of using tree searches in order to trace a thought process was then discussed (See Figure 5.) Of the three methods of searching discussed, the “best-first-search” model was “what we want to instill,” as Dr. Scudder indicated.

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The Combinatorial Explosion

A binary tree with *n* levels has 2^n possible final states. If our mechanistic tree were to consider twelve elemental processes at each level, three levels would produce 123 or 1,728 states to consider.

Common Methods of Searching

A Depth-First Search dives into the search tree ignoring the other alternatives at each node and keeps going. If a dead end is reached, then it backs up to the nearest node and makes another choice. This is a classic bad habit, which we wish to avoid, of running with the first idea that pops into our mind.

A Breadth-First Search explores all possible alternatives from each node, then proceeds to the next level and repeats. It guarantees that all alternatives are checked and can find the shortest route to the goal. This is good for a computer but not for us.

A Best-First Search is a breadth-first search in which only the best nodes are explored at each level. Good alternative nodes are retained in case a dead end is reached. Control knowledge is required to determine which nodes are best.

It is this best-first search strategy that the students must master, if they learn to perform a deliberate best-first search, it will become internalized with practice.

FIGURE 5. TREE SEARCHES.

Build Control Knowledge from First Principles
Bonding theory: what makes a strong or weak bond?
VSEPR: the shapes of molecules, balloon demo
Electronegativity and dipoles: polar covalent bonds
Lewis structures: find all valence electrons
Formal charges & resonance delocalization: locate all partial charges
Acids, bases: introduce structural effects on reactivity
Equilibrium and proton transfer: K_{eq}—first major cross check
Direction of electron flow: understanding the language of arrows
Thermodynamics: position of equilibrium
Kinetics: rates of reaction and energy barriers
Hard-soft acid-base theory: Coulomb's law, polarizability
Hybridization and pi bonding: polarized multiple bonds
Stabilization of charges: solvation, pi donors, and pi acceptors
Molecular orbital theory: spring standing-wave demonstration
Trends Are Critical Control Knowledge

An experienced chemist, after learning several thousand reactions, internalizes whatever trends are associated with the aggregate. However, by teaching those trends directly we can reduce the volume of material taught, and at the same time provide our students with a set of important tools. Using these trends, they can recognize reactive sites on a molecule and decide between mechanistic alternatives. Ranking the reactivity of groups allows the student to focus on the most reactive partners in the reaction mixture and not be distracted by others. For example, in electrophilic additions to alkenes, the cation-stability trend is the basis for Markovnikov's rule.

FIGURE 6. RELEVANT FIRST PRINCIPLES.

Next, Dr. Scudder began to discuss the technique that an instructor must use to introduce tree searches and the expert-system method to students. This can be thought of as teaching "control knowledge to guide the search." The method starts with bringing in relevant first principles (See Figure 6). Next, students are encouraged to

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pK_a *rule*: The leaving group or anion produced in a reaction should be no more than ten pK_a units more basic than the incoming nucleophile or base.

Coulomb's Law: Anions are electrostatically attracted to cations and vice versa; furthermore, cations do not attack cations nor anions attack anions. Dications or dianions are rare.

Electron Flow Check: In each step, the electron flow indicated by the arrows should start with a good electron source, end at a good electron sink, and proceed by a known elemental mechanistic process (electron flow path).

Proton transfer K_{eq} calculation: Proton transfers tend to form the weaker base. A proton transfer K_{eq} less than 10 is not useful, which can be considered just a subset of the pK_a rule.

Stability Trends: The stability of intermediates such as carbocations, carbanions, and radicals can be used to select between reasonable alternatives (e.g., Markovnikov's rule).

Reactivity Trends: Identifying of the most reactive nucleophile and electrophile in the reaction mixture is essential to finding the most probable reaction partners. The student should be able to rank the relative reactivity of lone pair nucleophiles, acids, bases, organometallics, leaving groups, carboxyl derivatives, electron donating groups, and electron withdrawing groups.

pK_a *span*: No medium can possibly be both strongly acidic and strongly basic. A pK_a span of 8 units between species in equilibrium is acceptable, but a span of 14 pK_a units or more is probably not useful.

Media p*H*: The route proposed must be consistent with the pH of the medium; acidic media contain powerful electrophiles and rather weak nucleophiles, whereas basic media contain excellent nucleophiles and weak electrophiles.

ΔH of reaction calculation: "Bonds broken minus bonds made" gives a crude approximation for comparing the relative stabilities of neutrals with neutrals and can be used to select between competing products in reversible systems.

HSAB principle: "Hard with hard and soft with soft" can help explain the dual reactivity of many systems under irreversible conditions (large drops in pK_a), such as ambident electrophiles (e.g., organometallic addition to enones) or ambident nucleophiles (e.g., enolate alkylation).

Access and alignment: Steric hindrance can drastically limit some reaction paths, such as the S_N2. The E2 requires the carbon-hydrogen and carbon-leaving group bonds involved to be nearly coplanar.

Kinetics: The search tree can be trimmed by determining what processes are expected to be the fastest. For example, proton transfers are usually exceptionally fast and often comprise the first step in many reactions. This rule must be tempered with the fact that proton transfers between carbon acids and carbon bases are slow enough to allow nucleophilic additions to compete.

Typo check: Check Lewis structures, formal charges, charge balance, etc., for any errors and omissions.

FIGURE 7. CROSS CHECKS FOR MECHANISMS [1].

cross check their first-principle thoughts (See Figure 7). Finally, students should consider common errors to make sure they are not falling into a trap (See Figure 8).

The presentation then turned to an analysis of this active-learning system and its recent addition to New College's curriculum. As an instructor, there are three key components to implementing this system. First, the instructor must overcome the students' 12 years of "sit-down-and-shut-up" instruction. Second, lecture must be

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- Lewis structure errors
- Charge-balance errors
- Multiple-charge errors
- Media pH incompatibilities
- pK_a-rule errors
- Wide pK_a spans
- Kicking-out of poor leaving groups
- S_N2 of hindered centers
- S_N2 of sp^2-bound leaving groups
- Unstable anions
- Unstable cations
- Electron-flow errors
- Impossible proton transfers
- Ignoring the polarization of a bond
- Orbital-alignment errors
- Line-structure errors—vaporization of hydrogens

FIGURE 8. COMMON ERRORS HELP IDENTIFY CONTROL KNOWLEDGE.

Sort: Classify into Generic Types.

The ability to generalize and conceptualize is essential to manage the intimidating volume of an ever-expanding field. Elementary processes help our students see the similarities in all reactions, as well as how to classify reactants into a limited number of common generic types of electron sources and electron sinks. New examples become variations on a theme rather than new special cases.

Rank: Identify Trends.

An experienced chemist, after learning several thousand reactions, internalizes whatever trends are associated with the aggregate. By teaching those trends directly, we reduce the volume of material taught and provide our students with a set of important tools. Using these trends, they can recognize the reactive sites on a molecule.

Web: Build Concept Maps.

Concept maps are valuable for working out the relationships between ideas, reactions, and functional groups. They are useful in class as a brainstorming device to pull in all ideas on a certain topic.

Weave: Create Correlation Matrices.

Correlation matrices allow for easy comparison of two or more items. They are the best way to make sure all the possible interactions are considered.

Map: Interrelate Processes with an Energy Surface.

Energy surfaces are often confined to graduate-level texts; however, surfaces are not only easily understood by undergraduates, but they also provide them with a powerful tool to interrelate competing mechanisms.

Branch: Generate a Tree.

The problem space of any decision process can be viewed as a tree graph. From the starting point at the first decision level, branches fan out to two or more alternatives, leading to other decisions on the next level.

FIGURE 9. SIX CRITICAL ORGANIZERS FOR COMPLEX SYSTEMS [3].

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- The exams are the syllabus.
    1. Test for decisions and judgment. Present puzzles that seem relevant.
    2. Keep recall questions to the bare essentials; test for higher level skills.
- Students must be actively and frequently confronted in class and on exams with problems that require them to make decisions using the control knowledge.
- Quality time in the classroom means doing something students can't get from reading the text. It is easy to back-slide and just lecture.
- It is hard to watch mistakes made. Encourage the generation step. Resist the temptation to jump in with the "right answer;" allow for reasonable alternatives within available information.
- Errors abound in texts; teach students to read critically. Activate and arm their "crap detectors." Question authority.
- Be satisfied with a limited number of examples—have students understand archetypes well and learn to classify into those archetypes.

FIGURE 10. IMPLEMENTING CHANGE AS FORMING NEW HABITS.

broken up with activities in order to ease the approach into a curriculum. Last, group work is essential for students to discuss alternate routes and follow the active-learning pathway. Next, the organization of the complex systems approach was discussed. This is based on six critical organizers. (See Figure 9.)

Dr. Scudder then turned to a reflection on implementing these changes and following them in a "Day 2-to-40" context. He identified six critical points for successful implementation (See Figure 10).

Conclusions

The draw of the sciences is the mystery of a good puzzle; few students enter the field because they love to memorize.

Students have much less tendency to write nonsense with arrows because they are assembling proven mechanistic units.

Students gain confidence as they discover that even unfamiliar, more complex mechanisms yield to their methods of analysis.

The students feel empowered by cross checks that allow them to judge whether a mechanistic hypothesis is reasonable—regardless of source.

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Finally, students develop methods of analyzing complex systems that extrapolate well into other fields.

Take Home Messages

If the inference engine and control knowledge are up and running well, the knowledge base can be incomplete.

The student will know to go to a reference text.

In reality, the knowledge base is always incomplete.

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