Xavier Prat-Resina¹

Using data-driven activities with *ChemEd X Data* to practice structure-property relationships in General Chemistry

¹ Center for Learning Innovation, University of Minnesota Rochester, Rochester, MN 55902, USA, E-mail: pratr001@r.umn.edu.
<https://orcid.org/0000-0002-1380-6025>.

Abstract:

General Chemistry covers a wide variety of structure-property relationships that rely upon electronic, atomic, crystal or molecular factors. Giving students experimental data will allow them to identify the structure-property patterns as well as identify the limit of predictability of such patterns. “*ChemEd X Data*” is a web interface designed by the author that facilitates the navigation, filtering and graphical representation of chemical and physical data. It can assist students at identifying trends in structure-property relationships, they can create controlled experiments to test a relationship as well as investigating how different molecular factors may affect a single macroscopic property. In particular, since the site offers unstructured but dynamically searchable data, it is designed to have students learn control of variable strategies (CVS). This paper describes the implementation of a five-step sequence of activities related to structure-property relationships in a General Chemistry semester. *ChemEd X Data* is used for the open-ended or data-driven steps of this sequence. Student performance is analyzed with the objective of understanding which activities require a higher cognitive skill, as well as identify student previous performances that correlate with success in the activities and in the course in general.

Keywords: structure-property relationships, general chemistry, web resources, data-driven learning

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Introduction

There is a significant agreement among science faculty about the positive impact that the implementation of evidence-based pedagogical approaches and supportive learning environments have on student learning. Many science faculty have already adopted different forms of active learning in the class in order to increase student success, engagement, and retention. On the other hand, the content for science courses has not yet changed at the same rate. In other words, we changed “how to teach”, but we have not significantly changed “what to teach”. In order to revisit and improve what science students should learn, the President’s Council of Advisors on Science and Technology (PCAST)(Executive Office of the President Council of Economic Advisers, n.d) and the National Research Council (NRC) (*A Framework for K-12 Science Education*, 2012) called instructors during the first 2 years of college to focus on deeper and transferable knowledge.

As a response to this call to action, the Next Generation for Science Standards (NGSS) has provided a very detailed framework and assessment tools for such implementation in K-12, which they can be easily applied to introductory science courses in college (National Research Council, 2013). Following the standards provided by the NGSS, instructors should focus on core ideas, crosscutting concepts and science practices. Activities that include these three aspects aim at what it is has been called the three-dimensional learning (Lavery et al., 2016).

The *science practices*, as they are listed by the NRC, are:

1. Asking Questions
2. Developing and Using Models
3. Planning and Carrying Out Investigations
4. Analyzing and Interpreting Data

Xavier Prat-Resina is the corresponding author.

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5. Using Mathematics and Computational Thinking
6. Constructing Explanations
7. Engaging in Argument from Evidence
8. Obtaining, Evaluating, and Communicating Information

The aim of this paper is to shed some light on how instructors may successfully address several science practices in an introductory Chemistry course. In particular, it focuses on one of the most prevalent Chemistry's core concepts identified by the NRC, the "Atomic/Molecular Structure and Properties" or what is commonly known as structure-property relationships. This study will investigate how can the *ChemEd X Data* website best help in some of the most open-ended or data-driven types of science practices. The several student activities presented and analyzed here pertain to different topics and they are spread throughout a typical first semester of General Chemistry, and should not require any major curriculum redesign.

The tool: *ChemEd X Data* website

ChemEd X Data (Eklund & Prat-Resina, 2014; Prat-Resina, 2016) (<http://chemdata.r.umn.edu/chemedXdata/>) was created for learning activities that address scientific practices during introductory courses of chemistry. More specifically, *ChemEd X Data* was designed for chemistry students to navigate, filter and graphically represent chemical and physical data. The kind of activities that *ChemEd X Data* offers to students must be placed within the data-first or data-driven learning approach (Grubbs, 2007; Nichol, Szymczyk, & Hutchinson, 2014). Even though data-first activities, data-driven activities and problem-based learning can sometimes be used interchangeably, there is some variability in terms of how data are made available to students. On one end, the data may be a table of already pre-selected values. In many of these cases the activity will be more focused on interpreting and manipulating the given data rather than navigating, plotting and choosing them. Therefore, it may exclude the possibility for open-endedness. On the other end of the spectrum, the student could be offered an unstructured spreadsheet of data or access to a database or a web portal such as Pubchem or Wikipedia (Pence & Williams, 2016; Walker & Li, 2016). In the latter case, the "open-endedness" may overwhelm students, or their performance may rely too much on their information literacy skills. The *ChemEd X Data* website tries to find a balance between the two extremes, where a large quantity of unstructured data is available while still trying to lower the technical barrier by making it easy to navigate, sort, rank and instantly plot different types of physical and chemical data.

Implementation

The results presented in this paper were collected during the fall semester of a "General Chemistry 1" course at the University of Minnesota Rochester (UMR). A total of 61 students were enrolled in the class, and 59 students were involved in all the activities presented here. The course was structured as a "flipped classroom" (Pienta, 2016). In this type of delivery, students were assigned to watch three or four videos (with a length of approximately 5–10 min each) and turn in the answers to a series of pre-class questions. However, the days when students were asked questions related to creation of knowledge no videos nor any pre-class questions were assigned in regards to the knowledge they were going to create in class. The majority of students were in their sophomore year. UMR only offers two Bachelor of Sciences, both in the field of Health Sciences, and students must take at least one semester of introduction to Organic structure during their first year before enrolling in General Chemistry. This curriculum approach is called "organic first" (Muthyala & Wei, 2013) and it is intended, in part, to improve their quantitative skills during their first year of college before enrolling in General Chemistry (Dame, Aryal, Huq, & Prat-Resina, 2018). This approach also means that students are already very familiar with organic functional groups and organic molecular structures, which allowed the design of activities involving a wider range of organic compounds. Instructors at other institutions without an organic-first approach, should reformulate the activities that match students' previous knowledge of molecular structure.

All the activities were delivered using the Moodle Learning Management System and students completed them individually either during class time or as homework outside of class. Some of the exercises required the use of *ChemEd X Data* but not all. Thanks to the laptop program, all students had a laptop during class time.

A common five-step sequence for several topics

During this implementation students completed three sets of activities that pertain to three different topics within structure-property relationships, namely, periodic table trends, effect of size and charge on ionic bond strength, and factors affecting the boiling point of molecular liquids. In all of these three topics, the exercise can be scaffolded using the following five-step sequence or progression:

1. Identify molecular factors
2. Connect structure and property by investigating data
3. Predict and apply relationship
4. Explain observations
5. Identify conflicting factors and limit of predictability

While one can find many examples of steps one, three, and four in any textbook at this level, steps two and five are not as common, and they may deserve further explanation.

Step 2. Investigating data and control of variable strategy

Step 2 consists of being able to select experimental data to show evidence of a specific trend or law, or what is commonly known as designing a controlled experiment or control of variable strategies (CVS) (Schwchow, Zimmerman, Croker, & Härtig, 2016). See the work by Schwchow et al. (2016) for an excellent overview on the pedagogical background in control of variable strategies. This activity represents one step further from what is commonly known as data-first problems (Nichol et al., 2014). In data-driven activities students are typically shown a specific arrangement of data. In the CVS case, however, students select the substances they want to represent, they must build a controlled experiment by keeping the rest of variables constant and varying the only one being tested. Therefore, if the given dataset is large enough, there is not a unique valid answer and the problem becomes open-ended. In particular, the science practices listed by the NRC that CVS-type exercises may help achieve are “Planning and Carrying Out Investigations” and “Analyzing and Interpreting Data”. As it has been previously described (Eklund & Prat-Resina, 2014), *ChemEd X Data* was specifically designed to practice CVS activities. Table 1 shows an example from students of a correct and incorrect selection of molecules to show evidence of the effect of linear/branching on the boiling point of organic molecules.

Table 1: An example of a correct (first row) and an incorrect (second row) selection could be when students are presented with the question “Select 4 compounds to show evidence of how the linear/branched chain may affect boiling points”.

Correct selection for CVS				
Boiling Point (K)	273	262	309	301
Incorrect selection for CVS				
Boiling Point (K)	273	355	309	341

Step 5. Conflicting factors and limit of predictability

In General Chemistry, there are several curricular examples where there is typically more than one factor deciding an outcome. In introductory levels, the instructor may decide to either avoid examples with conflicting factors or have students learn to recognize the limit of predictability at a given level of theory. For example, students may learn that hydrogen bonds are stronger than London forces, but that is only true if other factors such as mass and shape are kept constant. Several works have been published on how to better understand and teach this topic (Beauchamp 2005; 2008; Glazier, Marano, & Eisen, 2010; Peckham & McNaught, 2012). If students are asked to predict whether methanol or hexane have the highest boiling point, they should first recognize that mass and intermolecular forces (IMF) are in conflict and that, at this level of theory, they do not

have enough tools to predict an outcome. Alternatively, one can also reverse the question; if students are told that hexane has a higher boiling point than methanol they should be able to recognize that the mass is playing a larger role than the strength of intermolecular forces. This pedagogical route may be the recommended one. This type of activity is a good opportunity to address some of the science practices listed above, such as “Analyzing and interpreting data” as well as “Constructing Explanations and Engaging in Argument from Evidence” (National Research Council, 2013). Addressing these problems may potentially eliminate any misconceptions or frustration that some students may feel when they realize that they are not being told “the total truth” or that chemistry has too many exceptions (Carter & Brickhouse, 1989; Scerri, 2013). Table 2 lists the different cases in a typical “General Chemistry 1” semester where this conflict among factors may appear.

Table 2: Topics typically present in a first semester of a college General Chemistry course where more than one structural or energetic factor may affect the property.

Property to be predicted	Several factors that may come into conflict	Examples where content in introductory courses does not predict an outcome
Melting point or heat of fusion of molecular solids Periodic table trends: atom size and ionization energy of elements.	Intermolecular forces, molecular shape and mass Nuclear charge, electronic shielding and orbital size.	Highest boiling point? Methanol vs. Hexane What element has a larger radius among diagonal elements? (Li is bigger than Mg but O is smaller than Cl)
Ionic lattice energy of a crystalline solid Electronic configuration of elements (ground state)	Cation and anion size and their ionic charge Hund’s rule and Aufbau principle	What compound has a higher ionic lattice energy, KF or NaCl? For chromium and molybdenum, the ground state is “s ¹ d ⁵ ”, but for tungsten is “s ² d ⁴ ” and carbon is “s ² p ² ”
VSEPR theory: molecular angle	Lone pairs and double bonds affecting the regular angle	Molecules where lone pairs and double bonds are present in the central atom: SO ₂ , O ₃ , NOCl
Heat capacity of molecules	Molecular mass, number of covalent bonds and intermolecular forces.	Highest heat capacity? propanol (more mass) vs. butane (more bonds)
Miscibility of two liquid substances	Intermolecular forces and molecular shape	What is more soluble in water, butanol or dichloromethane?

The different factors may potentially be in conflict with each other.

Results and discussion

The analysis of student performance in the structure-property relationship activities may be enriched if it is compared with students’ performance at the end of the course as well as in previous college courses.

As Figure 1 below shows, three very distinct groups of students can be identified when representing “final course grade” vs. “College GPA held at the beginning of the semester”. These three groups labeled as low performers (LP, black squares), intermediate performers (IP, green circles), and high performers (HP, red triangles) are the three clusters obtained using the k-means clustering analysis as it is implemented in the R package. All the points in the graph correlate fairly well to a linear behavior, with a Pearson’s product-moment correlation coefficient of 0.807 (“n.d.”). As it has been noted elsewhere (Noble & Sawyer, 2002), albeit not being very informative in regards to students profile, the current students’ GPA is a good predictor for future course performances. These three groups of students, LP, IP and HP, will be used throughout the analysis of activities presented below.

Figure 1: The clustering of “students’ GPA at the beginning of the course” vs. “course final grade” at the end of the course gives three groups of students labeled as Low Performers (LP, black squares), Intermediate Performers (IP, green circles), and High Performers (HP, red triangles).

The next three subsections present the graphical analysis of students answers to the sequence of the five questions in three General Chemistry topics: Periodic Table Trends, Ionic Lattice Energy of Crystalline Solids, and Boiling Point of Molecular Liquids. As it is indicated in the example questions, students had to use *ChemEd X Data* in some parts of the activity, but not all.

Periodic table trends

In this first activity, students investigate the periodic table trends, and answered a set of questions that follow the common progression indicated above. For space reasons the entire questions are not shown verbatim.

1. Identify Atomic factors: Identify Z , shielding and orbital size.

Example: The charge of oxygen’s nucleus is ____, and the charge of carbon’s nucleus is ____, the number of electrons of neutral oxygen is ____, oxygen valence electrons are in $n =$ ____.

2. Connect Structure and Property.

Example: Use *ChemEd X Data* and choose a series of elements that show how the atomic radius is affected by the nuclear charge.

3. Predict and Apply Relationship: Explain factors for regular PT trend

Example: Explain what factors make oxygen smaller than carbon.

4. Explain Observations: Explain factors for diagonal elements

Example: Use *ChemEd X Data* to explain that Oxygen is *smaller/bigger* than Chlorine because Oxygen has *higher Z/lower shielding/smaller valence orbitals* (choose the correct answer).

5. Identify limit of predictability

Example: Which pair of elements present a conflict of factors that does not allow you to predict what atom is bigger: Choose one or more. “Li vs. O”, “O vs. Mg”, “Li vs. Mg”, “O vs. Cl”

Figure 2 is a Sankey diagram which is a specific kind of flow chart. All Sankey diagrams were built using the RawGraphs software (DensityDesign Lab | RAWGraphs). Each column represents a question in the activity. The horizontal stripes connecting the columns indicate the fraction of students who answered that specific question correctly (green) or incorrectly (red). For example, in the first question labeled as “Identify molecular factors”, the vertical line tells us that about 70 % of students answered it correctly. Moving to the next question, labeled as “Connect structure and property”, that initial 70 % of correct answers increases to 85 %. One of the main advantages of this diagram is that it shows the flow of students’ answers among adjacent questions.

Figure 2: Sankey diagram showing the flow of students' answers to a series of questions related to periodic table trends. The last column labeled "College performance" shows the fraction of students belonging to High Performers (HP), Intermediate Performers (IP), and Low Performers (LP) that answered correctly or incorrectly the last question on "identifying the limit of predictability".

The last column in Figure 2 is not a question in this activity, it is a first attempt at understanding how performance in higher-level activities may relate to course performance and college GPA. In this case, because of the limitations of the Sankey diagram, we can only see what portion of students who correctly answered the last question "Identify limit of predictability" belonged to each of the three college performance levels, LP, IP, and HP. A trend that we will see throughout the different exercises presented here is that while the group of students who perform well in these specific higher-skill activities is composed largely by High Performers (HP), there will typically be a significant portion of Intermediate Performers (IP), and in a much smaller fraction Low Performers (LP).

Ionic lattice energy of crystalline solids

This second activity is related to how the charge and size of ions affect the energy of the ionic lattice. Figure 3 shows students answers in form of another Sankey diagram. Students answered a set of questions that follow the common progression indicated above. As in the previous case, for space reasons the entire questions are not shown verbatim.

Figure 3: Sankey diagram showing the flow of students' answers to a series of questions related to the ionic bond. The last column labeled "College performance" shows the fraction of students belonging to High Performers (HP), Intermediate Performers (IP), and Low Performers (LP) that answered correctly or incorrectly the last question on "identifying the limit of predictability".

1. Identify molecular factors: ion charge and trends in size

Example: The size of Na is *smaller/larger* than the size of Cs. The charge of ion Na is *smaller/larger/equal* than ion Cs... (circle the correct option)

2. Connect structure and property: identify the role of size and charge in ionic lattice energy.

Example: Based on your observations in *ChemEd X Data*, the smaller the ion the *stronger/weaker* the ionic lattice is (circle the correct option)

3. Predict and apply.

Example: When comparing NaF and CsI, what compound will have a stronger ionic lattice?

4. Explain observations.

Example: The energy of the ionic lattice for KF is larger than for LiF. Can this observation be explained by this theory?

5. Limit of predictability.

Example: In what cases the theory cannot clearly predict an outcome?

1) Comparing LiF and NaCl 2) Comparing KCl NaBr 3) Comparing KF and LiF

Boiling point of molecular liquids

The last of the activities, the boiling point of molecular liquids, is probably the topic where *ChemEd X Data* can be more useful. In the two cases above, periodic table trends and energy of the ionic lattice, there is a more limited dataset that students can explore, just few elements and few periods of columns. Therefore, it is not until this present topic when some of the exercises are truly open-ended and each student uses a completely different dataset to justify a trend or an exception. Figure 4 shows the corresponding Sankey diagram for this activity. A sample of the sequence of questions is the following

Figure 4: Sankey diagram showing the flow of students' answers to a series of questions related to the boiling point of molecular liquids.

The last column labeled "College performance" shows the fraction of students belonging to High Performers (HP), Intermediate Performers (IP), and Low Performers (LP) that answered correctly or incorrectly the last question on "identifying the limit of predictability".

1. Identify molecular factors: Connect functional groups and IMF

Example: Identify each of the following functional groups with the intermolecular forces they present (H-bond, dipole-dipole or London forces)

2. Connect structure and property. Create relationship: building CVS

Example: Use *ChemEd X Data* to select a set of compounds that show evidence of how mass affects the boiling point of molecular liquids.

(see next section for a more detailed description of these activities)

3. Predict and apply relationship. Rank functional groups by boiling point.

Example: Based on your investigations, rank the strength of intermolecular forces as they affect the boiling point of their compounds: H-bonds, London forces, dipole-dipole interactions.

4. Explain observations: mass or dipole: CH_xCl_y vs. CH_xF_y

Example: The link below plots the boiling point of CH_3Cl , CH_2Cl_2 , CHCl_3 , CCl_4 .

<http://chemdata.r.umn.edu/chemedXdata/#stamp=1414679798226>

In this series, what is the property that prevails over the others. Is it the dipole? That is, the most polar has the highest boiling point? Is it the mass? That is, the most massive has the highest boiling point?

5. Limit of predictability: Alkanes vs. alcohols

Example: Alkanes only present London/dispersion forces, which are much weaker than hydrogen bonds. Does it mean that an alcohol because it presents hydrogen bond will always have a higher boiling point than an alkane? Investigate if a heavy alkane has a lower boiling point than a light alcohol. Explain and submit the URL with the selection of molecules.

Student performance in controlled variable strategies (CVS)

Step number two in any of the sequence of questions above is the ideal opportunity when students can build knowledge by investigating trends and creating controlled experiments in truly open-ended data-driven exercises. This is particularly pertinent when investigating the different factors affecting the boiling point of molecular liquids and it may justify a more detailed analysis.

ChemEd X Data offers a wide set of compounds and many ways to sort them. In this specific case, students were asked three different questions:

1. Select a set of molecules on *ChemEd X Data* in order to run a controlled experiment to investigate the effect of shape (linear or branched) on boiling points. Explain what you found out.
2. Select a set of molecules on *ChemEd X Data* in order to run a controlled experiment to investigate the effect of mass on boiling points. Explain what you found out.
3. Select a set of molecules on *ChemEd X Data* in order to run a controlled experiment to investigate what intermolecular forces are stronger (H-bonds, dipole-dipole or London forces) and therefore have a higher boiling point. Remember that in a controlled experiment the different molecules must keep shape and mass as constant as possible so that you are only assessing the effect of the intermolecular force.

As Table 3 shows, students perform very differently in CVS questions depending on what molecular property they are trying to investigate. When assessing the branch effect (first row), the majority of students are able to select a correct set of molecules in which the mass and IMF are kept constant while the level of branching of the alkyl chain is different and therefore being tested. While twice as many high performing students can answer that question correctly than low performing ones (81.3 % vs. 46.2 %) there is no significant difference in the final course grade between students who can answer this question successfully and those who cannot ($p = 0.12$). The results are different when students try to build a controlled experiment to test the effect of intermolecular forces (last row). A much lower fraction of students in all three categories can correctly answer this question. The fraction of high performers who can do it well more than triples the fraction of low performers who can (31.3 % vs. 7.7 %). Also, the average final grade between students answering correctly and student who did not is statistically significant ($p = 0.016$).

Table 3: Percent of students who answered correctly the three CVS questions investigating the effect of branch/linear chains (row 1), mass (row 2) and intermolecular forces (IMF, row 3) on the boiling point of molecular liquids.

	% of all students	% of HP students	% of IP students	% of LP students	Final % course grade; p-value
Branch effect	72.4 %	81.3 %	74.2 %	46.2 %	83.1/79.2; $p = 0.12$
Mass effect	46.6 %	50.0 %	48.4 %	30.8 %	83.1/81.1; $p = 0.37$
IMF effect	27.6 %	31.3 %	32.3 %	7.7 %	85.8/80.6; $p = 0.016$

Students are divided in three groups as defined above HP: high performing; IP: Intermediate performing, and LP: low performing. The last column gives the average final % course grade for students answering that CVS question correctly and incorrectly and p-value between the two groups.

The results in this table seem to indicate that students are not necessarily challenged by the open-endedness of the question, nor navigating the website, but, rather, by the fact that some molecular and atomic factors are more difficult to identify, select and keep constant in a controlled experiment than others. In this case, when testing IMF, it is difficult to keep the mass approximately constant while changing the functional group.

Conclusions

This paper presents the implementation and analysis of a five-step sequence of exercises to practice several instances of structure-property relationships in a first General Chemistry semester. The five-step sequence allows instructors to address some of the science practices as they have been identified by the NRC. In particular, by means of data-first activities, the *ChemEd X Data* website facilitated the “Planning and Carrying Out Investigations” and “Analyzing and Interpreting Data”. Students’ results were visually presented with Sankey diagrams showing how students answers flow through the sequence of steps. By classifying the group of students as high, intermediate, and lower performers, the analysis permitted to see what group of students performed better in the different activities. During step 2 of the sequence, students were asked to build the connection between structure and property and develop a “Control of Variable Strategy” or CVS. When analyzing the responses to the CVS activity where students investigate the molecular factors affecting the boiling point of molecular liquids, it was observed that student performance depended on the type of molecular factor being tested. In other words, students did significantly better when controlling for molecular factors that are easier to interpret in a molecule, such as mass or shape, than when controlling for electronic molecular factors such as intermolecular forces.

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