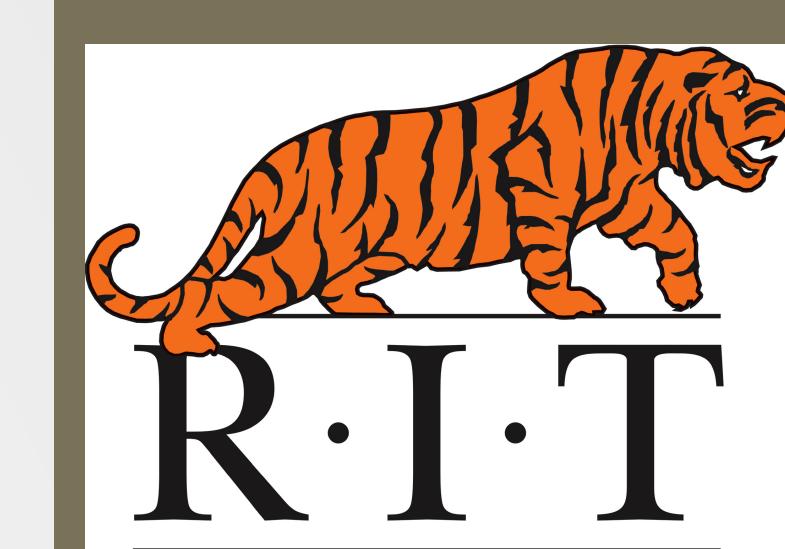


# Abstract #1425

# A 2DE-Tandem MS Simulation with a Structural Interface



Emily R. Sekera , Aidan Sawyer, Paul A. Craig Chemistry. College of Science Rochester Institute of Technology, Rochester,

2DE-Tandem MS is a computer program designed for use in the biochemistry, proteomics, or bioinformatics classroom. The program currently contains two simulations - 2D Electrophoresis and Tandem Mass Spectrometry. These integrated simulations are designed to teach the concept of proteome analysis of simple organisms. 2DE-Tandem MS can be used as a freestanding simulation or in conjunction with a wet lab, to introduce proteomics in the undergraduate classroom, and is freely available at <https://sourceforge.net/projects/jbf/>. 2DE-Tandem MS functions in Mac OSX, Windows, and Linux, ensuring that every student sees a consistent and informative GUI no matter the computer platform they choose. Peptide sequences from the Mass Spectrometer can now be displayed in a familiar structural format through the popular freeware program, MarvinSketch (<http://www.chemaxon.com/products/marvin/marvinsketch/>). Planned future applications include Ion Exchange and Reversed Phase Chromatography.

## Introduction

### What is JBioFramework (JBF)?

- JBF is a platform independent program.
- It contains simulations of 2D Electrophoresis, Tandem Mass Spectrometry and chemical structure information from the Mass Spectrometer.
- It is integrated with other chemistry resources such as SwissProt, BLAST, and Marvin Sketch.

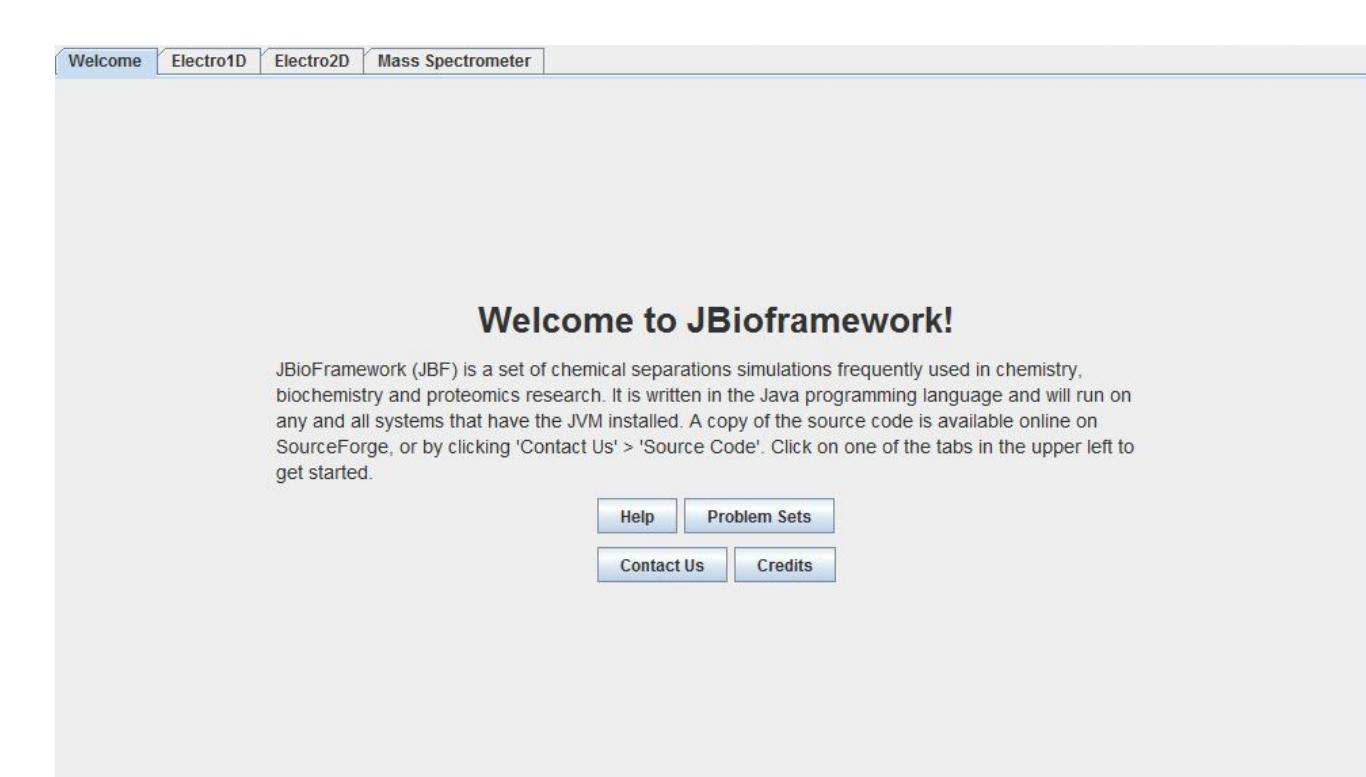


Figure 1: Welcome screen of JBF

### What's New with JBF?

- Our development team at RIT is focused on two aspects of JBF in parallel - *technical development* and *educational impact*. On the technical front, we are introducing new features to expand the suite. New code in the Tandem MS simulation enables users to see the peptide fragments that are generated during peptide sequencing in the MS. Users can generate a text output of the sequence for a specific fragment. Marvin, a chemical drawing program that is also platform-independent was then used for displaying the fragments (Marvin 5.11.1, 2012, ChemAxon (<http://www.chemaxon.com>)).
- We have just begun evaluating what students learn with the simulations to inform improvements in our basic design. We created a series of exercises for students to complete on a computer equipped with Camtasia software (TechSmith, Okemos, Michigan), which enables us to capture their screen activity, facial expressions and voice as they complete the exercises. Here we report some of our early findings from the students.

## Hypothesis

Students can be introduced to advanced instrumental methods in proteomics using computer simulations.

## Methods

### 2DE-Tandem Mass Spectrometry

- A bacterial proteome is separated by 2D electrophoresis in the first stage of the simulation.
- Individual proteins can then be fragmented and sequenced in the Tandem MS simulation.

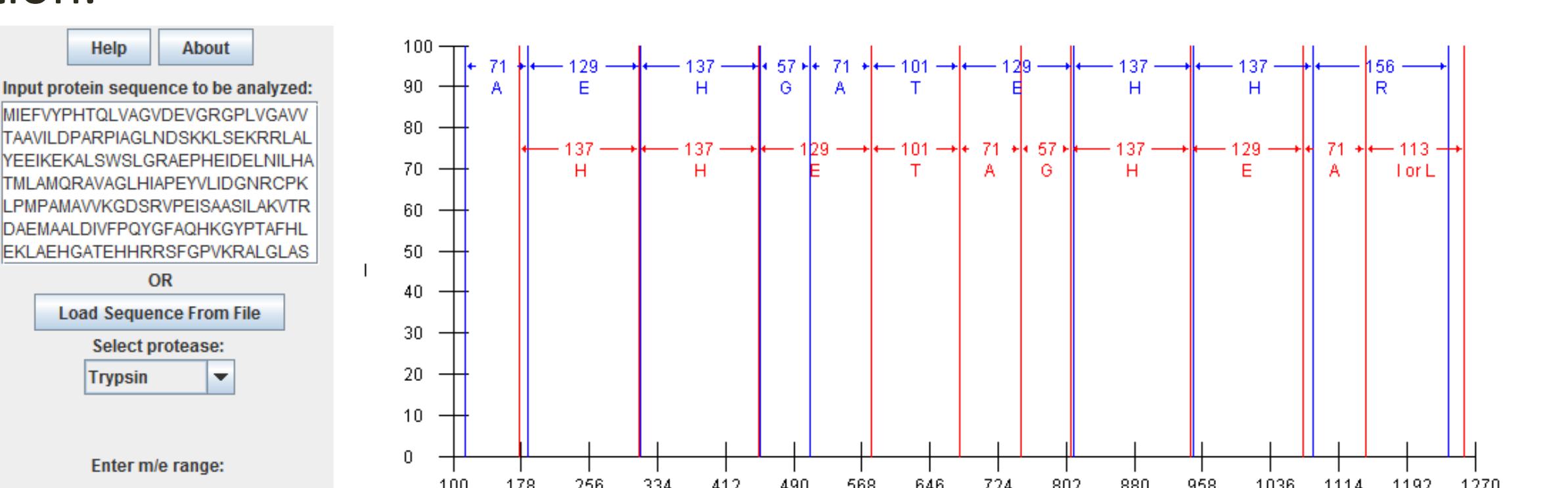


Figure 2: The output from the Tandem Mass Spectrometer simulation. A fragment with m/e 1257.31 yielded these B- and Y-fragments.

### Chemical Structures

- Clicking on an individual fragment it will display the sequence in a pop-up dialog box.
- The sequences can then be displayed in MarvinSketch.

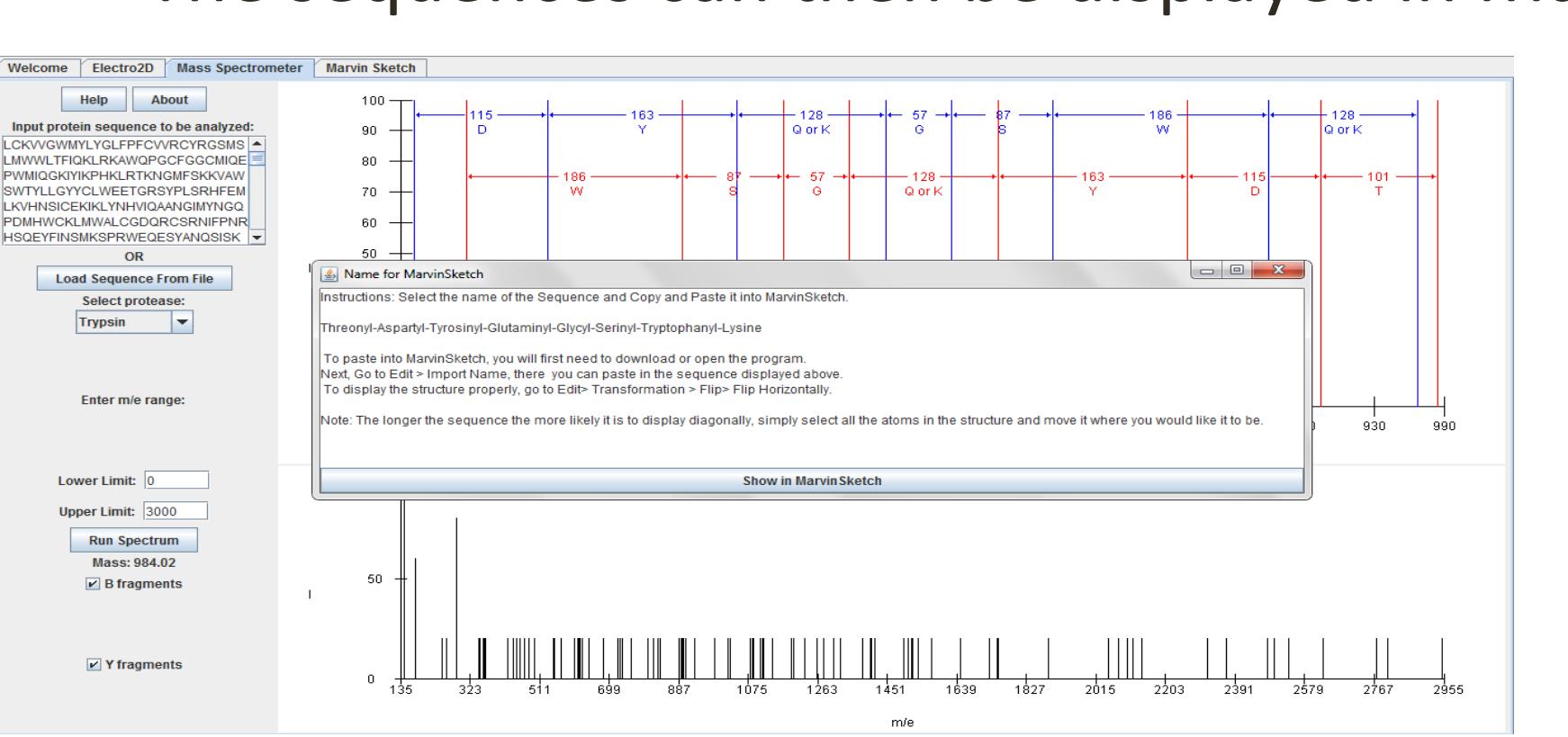


Figure 3: The output giving a chemical structure name from a Mass Spec. peak linking to MarvinSketch.

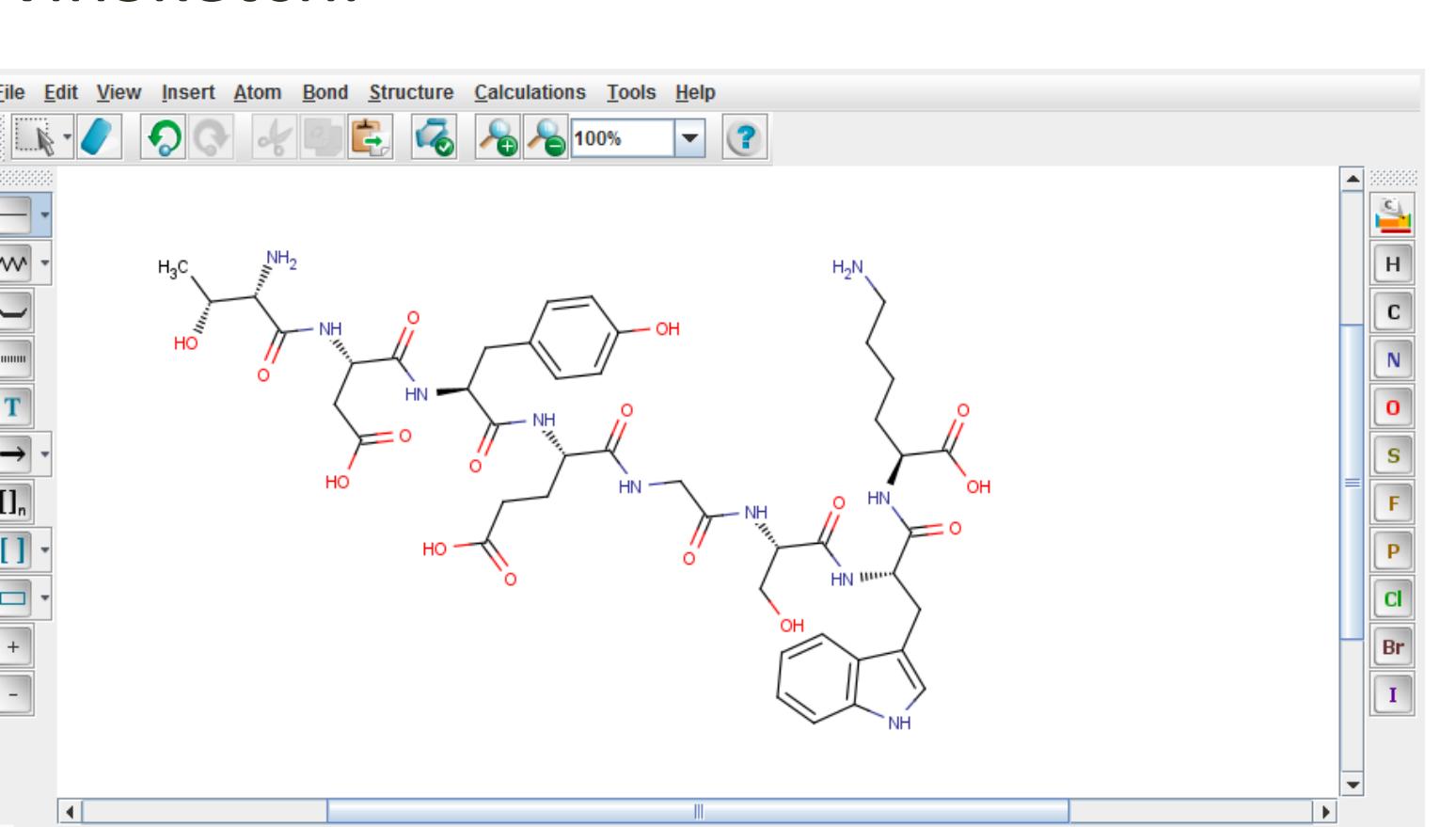


Figure 4. Display of the selected peptide in MarvinSketch

### How are the Sequences Generated

- The sequence from the given protein is analyzed by the Tandem MS and from there it generates the one letter codes. These codes are then transferred into a translator and converted to the full names which can be used in MarvinSketch.

### Software Testing Procedure with Students

- We created problem sets that followed the different levels of Bloom's Taxonomy.
- Students of different disciplines were given an hour to complete the first set of lower level questions .
- The students completed the exercises in the presence of two student members of the research team who were available and answered any questions the students had.
- Students were recorded with Camtasia that captured their screen activity, facial expressions, and their voice.
- Students filled out a post-exercise questionnaire about using the simulation and also gave constructive criticism.

## Student Interaction

Three students were recorded as they spent one hour solving problems using the JBF. The following are responses from the students .

### Chemistry Students

- "I didn't find it very useful. I think if I had more of a biochemistry background it would have made sense."
- "I understood the mass spec a lot more due to taking an instrumental analysis course."
- "Being able to separate the peaks further was also interesting."

### Biotechnology Student

- "I really like the design and ease of running the program."
- "The built in links to the major database sites was VERY NICE [sic]"
- "I took BAM [Bionformatic Analysis of Macromolecules] last quarter so a lot of this was nice to see like the correlation to function right away."

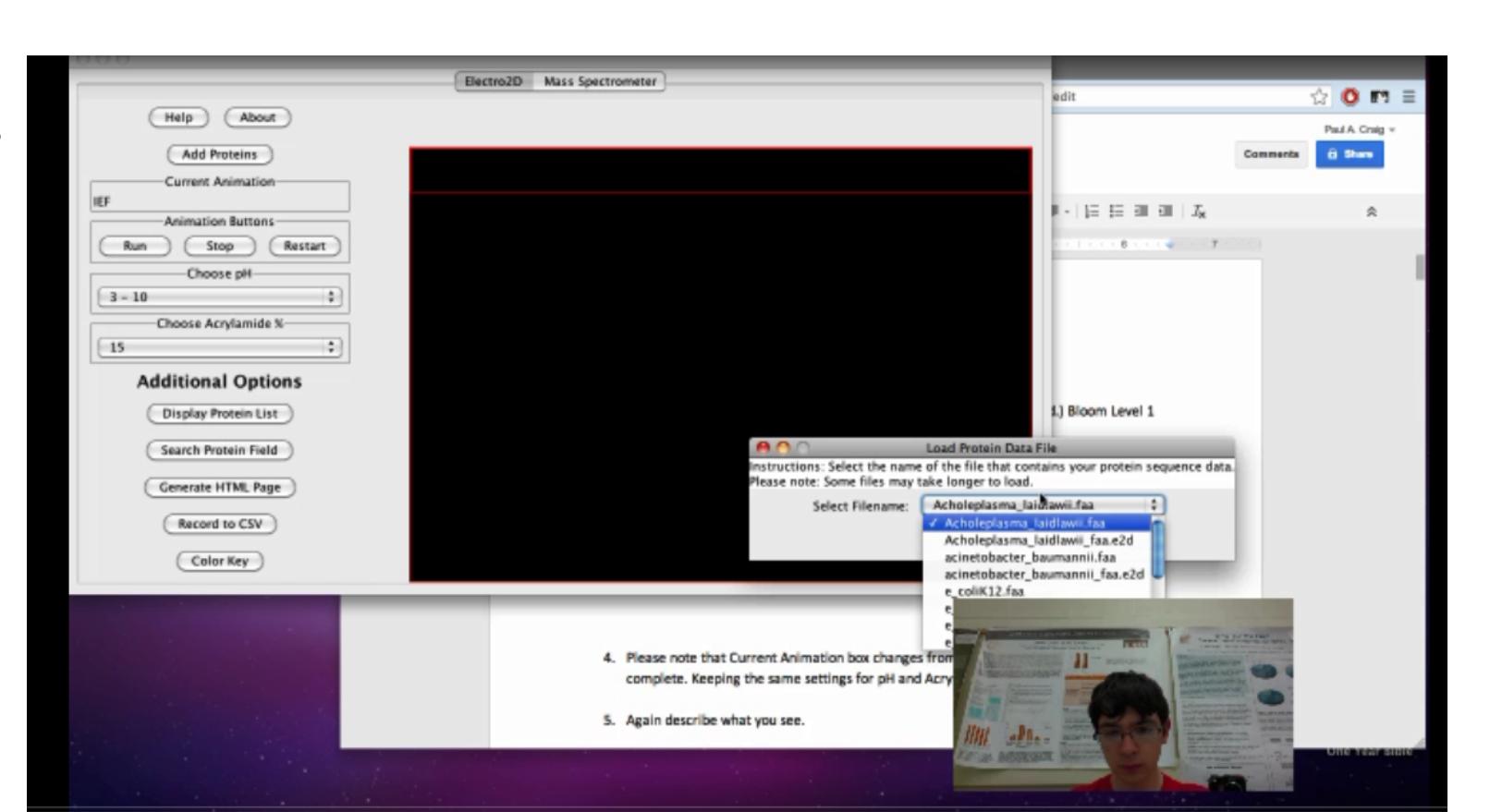


Figure 5: Camtasia recording a student's work.

## Student Data

Here are some data from the preliminary testing of three students. The students were asked to rate statements on a scale of 1-5, 1 being that they strongly disagreed, and 5 being that they strongly agreed.

"I understood the questions."

- Chemistry Student 1: 4
- Chemistry Student 2: 2
- Biotechnology Student: 4.5

"The simulation was stimulating."

- Chemistry Student 1: 3
- Chemistry Student 2: 2
- Biotechnology Student: 4.5

"I learned a lot about mass spectrometry by completing these exercises"

- Chemistry Student 1: 3
- Chemistry Student 2: 2
- Biotechnology Student : 5

"I learned a lot about 2-dimensional electrophoresis by completing these exercises"

- Chemistry Student 1: 1
- Chemistry Student 2: 2
- Biotechnology Student : 3

## Conclusions & Future Plans

### JBF Educational Impact

Our preliminary observations of students using the software will be followed by more detailed testing with assistance from the discipline based educational research collaboration at RIT. We plan to refine our problem sets and surveys, then use them with a larger audience of students from a variety of backgrounds. We hope to develop JBF as an effective means to help students learn the relationship between foundational principles (charge, pH and pKa, for example) and analytical methods they encounter in the lab.

### JBF Technical Development

Our coding team is working on several new features for JBF.

- Adding a tab that contains MarvinSketch functionality so that B- and Y-fragments can be displayed within JBF without the need for additional software.
- 1D electrophoresis – to update and incorporate our 1DE simulation in JBF (very close to completion)
- Ionex – to update and incorporate our ion exchange simulation in JBF
- Reversed Phase HPLC – this method is frequently coupled to Tandem MS in advanced analytical fields such as proteomics and metabolomics. It also presents a further opportunity to explore fundamental principles in a simulated instrumental setting: polarity, hydrogen bonding and buffers.

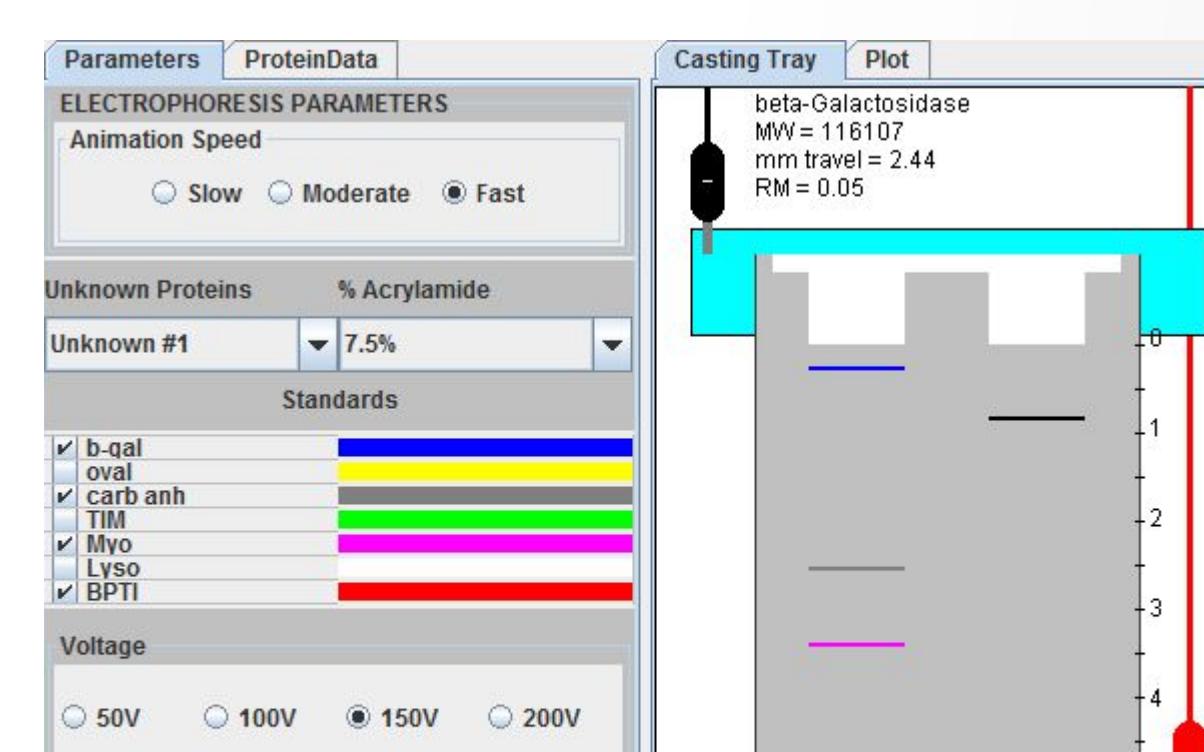


Figure 6: The newest version of the 1DE soon to be implemented.

## Acknowledgements

- RIT College of Science, GCCIS at RIT, Office of the Vice President for Research at RIT
- Merck/AAAS Undergraduate Science Research Program
- Sheneka Linton, Bader AlHarbi, Benjamin Russell, and Amanda Fisher
- Dr. Thomas Kim and Dr. Scott Franklin

Contact Us:  
Dr. Paul Craig, RIT  
paul.craig@rit.edu  
(585)475-6145

Emily Sekera  
ers3358@rit.edu  
(716) 474-3224