

UNIVERSITY OF LOUISIANA AT LAFAYETTE

STEP Committee

Technology Fee Application

Purchase of MicroLab Expert Software for an Infrared
Spectrometer in Chemistry

Title

August A. Gallo, Ryan Simon & Wu Xu

Name of Submitter
(Faculty or Staff Only)

Department of Chemistry

Organization

Title: Professor of Chemistry
Name (Contact Person): August Gallo

Date: 07/14/2021

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Department/College/Org: Chemistry/Sciences/UL Lafayette

ABSTRACT (250 words or less):

Funding is requested to purchase software for an infrared spectrometer funded by a STEP proposal in the Department of Chemistry. The acquisition of this software will be used by students as they learn the theory and application of IR spectroscopy in their teaching laboratories. The IR instrument did not come with a computer system nor any software to manipulate its data or any functional platforms to use in its spectral analysis. The proposed software, MicroLab Expert by Agilent, will teach the student to manipulate/process data, visualize at the 2D and 3D level, interpret and apply functional group analysis, perform basics kinetic analysis, and help determine a molecule's structure via a library search. In addition, all standard mathematical methods used in spectroscopy including normalization, derivatives, baseline correction, spectral arithmetic, smoothing and peak picking are parameters used by students and are possible with MicroLab Expert. This software package is a commonly used and essential learning tool for students in the field of spectroscopy.

Approximately, 450 students per year use IR spectroscopy and this software package will be used for the successful training and understanding of the principles that are taught in both lecture and the laboratory. Funding of this proposal will benefit not only chemistry students, but also all students majoring in the sciences and engineering disciplines.

3a. Purpose of grant and impact to student body as a whole

The purpose of this project is the acquisition of software for our newly purchased Fourier-Transform infrared spectrometer. A STEP proposal for the purchase of an IR spectrometer was funded in the fall of 2019 for chemistry. This instrument is a workhorse for our chemistry program as students in chemistry labs from the sophomore level to senior level use this instrument in teaching and undergraduate research. An IR spectrometer measures the vibrations of atoms and is used by chemists to help determine the structure of a molecule by what functional groups are present. The acquired instrument was in fact just the instrument itself. The

department of chemistry purchased a desktop computer, monitor and printer to complement the spectrometer. Installation of the instrument by the factory engineer provided only software that allows one to operate the instrument and visualize the IR spectrum, nothing more. The proposed software, MicroLab Expert by Agilent, will allow the student to manipulate/process data, visualize at the 2D and 3D level, interpret and apply functional group analysis, perform basic kinetic analysis, and help determine a molecule's structure via a library search. All of these are standard platforms used by students in the chemistry lab on our other spectrometers and more importantly, none of this is possible with the present "run and see" software on the instrument. All standard mathematical methods used in spectroscopy- including normalization, derivatives, baseline correction, spectral arithmetic, smoothing and peak picking are features used by students and are possible with MicroLab Expert. Moreover, the software uses a best fit to residual approach in matching spectra to a database as well as an intuitive approach for confirming molecular structures. These are all standard platforms we teach students to use in our chemistry laboratories.

The teaching of IR spectroscopy begins at the sophomore level when students enrolled in analytical, inorganic, and organic chemistry. The requested software will be heavily used by students in organic chemistry, analytical chemistry, biochemistry, inorganic chemistry and physical chemistry. Students in chemistry along with the disciplines of biology, engineering, environmental sciences and geosciences will be affected by this project. Students enrolled in Chemistry 233 (organic I lab) and Chemistry 234 (organic II lab) will be the major users of this software each semester. Student enrollments just in these two labs amount to over 380 students per year. Students enrolled in Chemistry 252,452 (inorganic chemistry), Chemistry 221 ,430 (analytical chemistry), Chemistry 319 (biochemistry), Chemistry 320 (macromolecular chemistry) and Chemistry 362,462 (undergraduate research) account for another 70 students per year. Students in organic, inorganic and polymer chemistry will use the software to follow the course of a chemical reaction and help characterize the chemical structure of known and unknown organic compounds. Students in biochemistry(319) will use the software to help identify lipids and carbohydrates and follow the kinetics of enzyme catalyzed reactions. Therefore, the number of students who will be impacted by the use of the requested software is appropriately 450 per year.

The project director, Dr. Gallo, has been a leader in implementing the teaching of spectroscopy including FT-IR, mass spectrometry, and FT-NMR spectroscopy after the acquisition of these instruments through grants. Students in organic, inorganic and biochemistry are presently using these combined methods of spectroscopic analysis and the software associated with running these instruments to characterize small and macromolecules. Experience in operating a FT-IR spectrometer and using the requested software in data manipulation and interpretation of the data benefits students with a wide range of majors, not just those in chemistry. The co- PI, Dr. Simon, has extensive IT skills- both software and hardware- and will help in the installation of the software and training of students. Dr. Xu is trained in biochemistry and kinetics and will teach pre-professional/allied health students how to use the software in biochemical transformations.

3b. Projected lifetime of enhancement

The average life expectancy for software is about 7-8 years, while the lifespan for an infrared spectrometer is 10 years. Typically, there will be an update to the software package, which means it will last as long as the instrument lasts.

3c. Person(s) responsible for:

I. Implementation

Dr. August Gallo will be responsible for ordering the software and receiving it.

ii. Installation

Dr. Simon will install the software and the tutorial of its use on the computer

iii. Maintenance

Typically, there is no maintenance for the software, only updates as they become available. Dr. Simon will be responsible for update installation.

iv. Operation

Students and faculty members will use the instrument and the requested software after they have been trained.

v. Training

Both Dr. Gallo, Dr. Simon and Dr. Xu will train students, faculty and walk up users on the operation of the instrument and the software requested in this proposal. Typically, the training is in the organic chemistry courses they teach- Chemistry 231,232,233 and 234. They will teach all faculty members of the department so that those faculty members can teach their students in the associated laboratories they teach. Dr. Gallo will teach other departments that frequently use the software/instrument, in many cases, engineering and biology. Dr. Simon will also assist with all undergraduate research students. Dr. Xu will train students how to use the kinetic and arithmetic platforms of the software.

Budget Proposal

| | | |
|----|--------------------|------------|
| 1. | Equipment | \$ |
| 2. | Software | \$ 3550.40 |
| 3. | Supplies | \$ |
| 4. | Maintenance | \$ |
| 5. | Personnel | \$ |
| 6. | Other | \$ |

TOTAL: \$ 3550.40

3d. Budget narrative:

The budget consists of the cost for the software, installation packet and familiarization at installation. Agilent has been gracious to apply a special discount of 30%, which drops the base cost of the software from \$5072 to \$3550.40 as shown in the attached price quote.

Previous funded STEP Projects

August Gallo has previously authored the following funded STEP proposals:

- Smart Classrooms in Chemistry, A. Gallo, W. Xu and D. Wellman, \$30,000, Awarded, 2013
- Smart Classrooms in Chemistry, T. Junk and A. Gallo, \$30,000, Awarded 2014.
- Purchase of an Attenuated Total Reflectance (ATR) Tool for Chemistry to Conduct Infrared Spectroscopy on Solids, T. Junk and A. Gallo, \$5,602.50, Awarded 2016.
- Organic Chemistry Laboratory Equipment Grant, R. Simon and A. Gallo, \$3666.50, Awarded in May 2016.
- Acquisition of a Polarimeter for Chemistry Laboratories, A. Gallo and W. Xu, \$540.00, Awarded January 2017.
- Digital Thermometers Grant Proposal, R. Simon and A. Gallo, \$1850.00, Awarded May 2018
- Purchase of an Infrared Spectrometer for Chemistry, T. Junk, A. Gallo & R. Simon, \$23,500, Awarded. 2019

Ryan Simon has previously authored the following funded STEP proposals:

- Organic Chemistry Laboratory Equipment Grant, R. Simon and A. Gallo, \$3666.50, awarded in May 2016.
- Demonstration Equipment Grant, R. Simon, \$501.64, awarded in January 2017.
- Maker Lab for Montgomery Hall, R. Simon and Y. Wang, \$3649.79, awarded in May 2017.
- Whiteboards for Montgomery Hall, R. Simon, \$6371.96, awarded January 2018.
- Chemical Reactions with Light: UV Lamps for Photochemical Experiments in Organic Chemistry Labs, T. Junk and R. Simon, \$2100.00, awarded January 2018.
- Electric Thermometers Grant Proposal, R. Simon and A. Gallo, \$1850.00, awarded May 2018
- Purchase of an Infrared Spectrometer for Chemistry, T. Junk, A. Gallo & R. Simon, \$23,500, Awarded. 2019



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| 1000 | G4997AA | 1.000 EA | 5,072.00 USD | 1,521.60- | 3,550.40 | |
| <p>MicroLab Expert Software for advanced data processing, interpretation, library searching, quantitative analysis, and data acquisition from legacy MicroLab products. Requires MicroLab PC 5.3 or greater for full data integration between the two platforms and appropriate driver installation. Win 7 (64 bit) or Win 10 (64 bit) OS Recommended</p> <p>With the following configuration: Enter Qty of Option 100 : 1 Ship-to Country : USA</p> <p>MicroLab Expert Base SW Installation (44K) Introduction (44L)</p> <p>Special discount of 30.00 % is applied.</p> | | | | | | |
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