

(Form 1-ENH, Rev. 20)

Name of Institution (Include Branch/Campus and School or Division)

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Address (Include Department)

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Title of Project:

Bridging Molecular Modeling and Chemical Synthesis to Enhance Inquiry-Based Learning

Abstract (DO NOT EXCEED 250 WORDS)*

The strength of our academic environment is increasingly dependent on our ability to provide interactive, inquiry-driven learning in the both the classroom and the laboratory. Students yearn to see the connection between the facts they learn in their courses and the significance of real-world applications. There is often gap that must be bridged between merely teaching a concept to students and being able to get their eyes to light up with excitement because they see why it is so important that they learn this. Although abstract concepts like chirality present educators with unique challenges, such concepts also provide us with opportunities to truly inspire our students. One area where we can inspire students to see the big picture is in the significance of the three-dimensional shapes of molecules. It is the goal of this proposal to bridge the gap between facts and applications by enhancing the learning process with new software and instrumentation tools.

We propose to address this situation in several chemistry courses by incorporating the following into both the classroom and laboratory environment: 1) Accelrys *DS Model* molecular modeling software, 2) CEM *Explorer S-Class* microwave-assisted chemical synthesis system. 3) Perkin Elmer *Model 343* Polarimeter. These additions will enhance the educational and research infrastructure at LSUS, and inspire creativity in our students. The students will also benefit and become more marketable in the job market from having had exposure to the graphical molecular modeling software and new chemical instrumentation. Ultimately, this will produce a greater number of higher quality graduates that meet the ever-increasing needs of graduate/ professional schools, as well as the chemical and biotechnology companies in Louisiana and the nation.

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NARRATIVE

A. THE CURRENT SITUATION

1. Institutional Description: Louisiana State University in Shreveport (LSUS) serves 4,200 full-time students (28% minority; 37% low income) per year, drawn largely from the Shreveport-Bossier City metropolitan area (population: 400,000). It is the only public, comprehensive, four-year institution of higher learning in this metro area, which is Louisiana's third largest urban area. Established in 1967 and awarding B.S. degrees since 1975, LSUS now has several graduate programs, three of which are in the College of Sciences: Master's in Biochemistry in cooperation with LSU Health Sciences Center (LSUHSC) in Shreveport; Master's in Environmental Science in cooperation with LSU-BR; and Master's in Systems Technology (offered in cooperation with Louisiana Tech University at Barksdale Air Force Base). In the last academic year, 1,800 students took chemistry courses, largely from these six B.S. curricula: Chemistry, Biochemical Science (Biochemistry), Biological Sciences, Environmental Science, Allied Health, and Science Education. LSUS is accredited by the *Southern Association of Colleges and Schools (SACS)*, and the LSUS Chemistry program is certified by the *American Chemical Society (ACS)*. The College of Sciences enrolls the largest number of student majors at LSUS. In responding to regional needs, the College stresses solid preparation for chemists, biochemists, biologists, and related scientists to support area industries, in particular the rapidly growing biomedical and environmental sectors.

In addition to the ACS-accredited B.S. program in chemistry, LSUS offers a B.S. in Biochemistry that is jointly operated by the Departments of Chemistry and Biological Sciences. These two departments also partner to offer a B.S. program in Environmental Science as well as the M.S. program in Biochemistry/Molecular Biology in cooperation with Louisiana State University Health Sciences Center (LSUHSC) in Shreveport and the M.S. program in Environmental Science in cooperation with Louisiana State University in Baton Rouge. A total of 20 full-time faculty members and several part-time faculty at LSUS are involved in these programs. In the Fall 2007 semester, the number of chemistry majors formally declared was 34, biochemical science, 60, environmental science, 14. A five-year average of five ACS-certified graduates/year places our Chemistry Dept. near the top of Louisiana universities in production, without considering the respective campus student populations. The introduction of our biochemistry program has drawn many majors, and we graduate, on average, 10 biochemistry students annually.

This proposed enhancement project will improve student training in chemistry and biochemistry. Students will observe demonstrations of this powerful instrumentation, and many will perform relevant hands-on experiments with materials prepared in their laboratory courses and in independent research projects. Students and faculty will also utilize the new instrumentation in research focusing on the Department's organic and polymer chemistry research emphases.

2. Rationale for Project:

We have a knowledge-based economy today, meaning that intellectual property and information have now become the most important assets. Gone are the days when our society could rely on the existence of a strong manufacturing base. Rather, we must rely mainly on the inventive spirit of our people as the driving force of our economy. This new reality provides educators with both challenges and opportunities. First, is important that we provide our students with a broad education that will prepare them for careers in a global economy, where science, medicine, and technology serve as the common currency. In chemistry, new specialties, such as nanotechnology and materials science, are opening up career opportunities for chemists that will allow students with training in these areas to make an impact on our lives in more ways than ever before. However, we must not only provide our students with scientific facts and procedures, but we must also stimulate them to be creative, so that they develop the capability to invent the new technologies for tomorrow.

Science has become far more interdisciplinary than most people could have anticipated, even just 20 years ago. New developments place challenges upon us as educators to shape our undergraduate curriculum to keep pace with new educational paradigms. Doing this successfully is one of our main goals as educators. The proposed acquisition of new molecular modeling software and laboratory instrumentation will enable us make great strides toward accomplishing these goals.

The current problems include : (1) a lack of any high-quality molecular visualization and modeling software in the Dept. of Chemistry, (2) difficulty uniting abstract concepts (like chirality and stereochemistry) between the organic chemistry lecture and laboratory courses, (3) difficulty in providing our students with the opportunity to truly experiment in the teaching laboratory (*i.e.*, “if I did this and then this, what would be the outcome”), (4) no means of assessing the optical activity of samples containing chiral molecules.

Molecular Display and Design Software-The newly released Accelrys *Discovery Studio Model (DS Model)* 2.0 represents an excellent molecular mechanics and visualization package that runs on a Windows or Linux PC. This software package serves a dual educational and research purpose. It is module-based, and each user is free to order the specific modules that suit their needs. It has a floating license, so that it can be used as a demonstration tool in the classroom, as well as by up to a maximum of five students at a time in the computer lab (note that the number of simultaneous students access nodes could be expanded for an additional cost of \$400 per node). The molecular mechanics and visualization tools will be most useful in our lectures and laboratory discussions, and the students will also be able to work on their own to discover and design new molecules that meet specific requirements. This software package will help to revolutionize the way we teach chemistry at LSUS, starting with sophomore-level organic chemistry.

There is no substitute for building models of molecules to view them as they look in three dimensions. Hand-held models, though useful for some in-class exercises and exams, cannot touch the potential of this modern computer-based modeling system.

Microwave-Assisted Organic Synthesis-The ability to go into the laboratory and readily achieve a particular goal (*i.e.*, a specific chemical transformation) quickly and efficiently is contingent upon the safety, versatility, and convenience of the reaction apparatus and procedure. Conventional heating (by convection) has its drawbacks, namely slow heat transfer to the molecules in the reaction mixture, long reaction times, and the need to remain at or close to ambient pressure. Glassware connected with ground glass joints has its drawbacks, in that it is not safe to work above atmospheric pressure. Microwave-assisted organic synthesis presents several advantages, particularly by saving time and improving the reaction yield.

Microwave-induced heating is believed to produce local “hot-spots” in a reaction mixture. This is responsible for broadening the energy distribution of the molecules; thereby causing tremendous rate accelerations and improved reaction yields. Also it is also much safer to run some reactions (e.g., catalytic transfer hydrogenation) under the sealed pressure tube configuration provided in a microwave reactor than in a conventional laboratory apparatus. These safety features are particularly important in the teaching laboratories. Using this apparatus with the automated sample tube changer, our students will be able to conduct experiments in a few minutes each that would require several hours under conventional heating methods.

A “mono-mode” microwave instrument, such as CEM’s *Discover S-Class* reactor, uses microwave radiation that has been polarized, allowing the concentrated and focused delivery of microwave energy to the reaction vessel. By contrast, conventional kitchen-style microwave ovens work in “multi-mode”, delivering microwave that bounces randomly around the oven cavity and thus is not focused on any particular spot. Note that “kitchen-style” microwave ovens, although reportedly used in the past in some large scale chemical synthesis applications, are wholly inadequate for our purposes. Such conventional kitchen microwave ovens operate in “multi-mode” and thus have insufficient focus of microwave energy. They also present severe safety issues due to a lack of feedback power control and unregulated vapor pressure in the reaction vessels.

Digital Polarimeter--The measurement of the specific rotation of optically active substances is of prime importance in the real world. Once students first learn about chirality during organic chemistry lecture, many are anxious to see applications of the fascinating phenomenon optical activity. Unfortunately, however, we are currently unable to give them the opportunity to apply their knowledge in this area, since our department does not have a polarimeter. Upper-level laboratory courses in structural identification and synthesis also generally require students to measure the specific rotation of their compounds as a characterization tool. We have had to forego that important characterization tool due to a lack of a polarimeter.

A Perkin-Elmer *Model 343* digital polarimeter represents the ideal choice for our undergraduate teaching and research laboratories. This instrument provides the best optics and electronic stability of the ones we have investigated. The configuration and operation of this instrument is straightforward, and students are able to obtain results quickly. The polarimeter provides “unity of purpose” to the sequence of ideas in this proposal by providing key characterization data for optically active samples.

Table 1. Molecular Modeling/Chemical Synthesis/Polarimetry Analysis

Course	<i>DS Model 2.0</i> Software Package	CEM Explorer S- Class Microwave- Assisted Synthesizer	Perkin-Elmer Model 343 Polarimeter
CHEM 265/265L Organic Chem-I (lecture and lab) 90 students per year	1) 3-D visualization of organic molecules/ stereochemistry /superposition of structures. 2) Energy minimization of cycloalkane conformations. 3) Visualization of chiral molecules that lack stereogenic centers (e.g. chiral biphenyls)	Introduction to microwave assisted organic synthesis (rate accelerations in the S_N2 reaction)	Measurement of optical activity / determination of %ee of unknowns and chemical reaction products.
CHEM 266/266L Organic Chem.-II (lecture and lab) 70 students per year	1) Visualization of chiral catalysts to explain how optically active reaction products are synthesized. 2) Visualization of the building blocks of biomolecules: peptides, peptides, and nucleic acids.	Synthesis of optically active hydrogenation products, using any one of several chiral catalysts--a true “chemistry experiment” without a pre-determined outcome.	Analysis of the specific rotation of optically active reaction products
CHEM 366 Structural Elucidation of Organic Compounds (lecture and lab) 18 students per year	Molecular modeling is an important tool in predicting certain properties, such as NMR coupling constants in conformationally rigid molecules. This provides information that is useful in the identification of unknowns.	1) Rapid preparation of chemical derivatives for unknown identification. 2) Peptide digestion for sequence determination of an unknown.	Measurement of the specific rotation of the purified components of an unknown.
CHEM 467/667 Advanced Chem. Synthesis (lecture and lab) 8 students per year	Modeling is a useful tool in predicting the product(s) of stereocontrolled reactions. Thus, it is an important tool in this advanced synthesis course.	Used as an optional tool at the student’s discretion in carrying out the assigned multi-step synthesis	Measurement of the optical purity of the various reaction intermediates and final product.
CHEM 490 Medicinal Chemistry (lecture only) 20 students per year	1) Visualization of protein / small molecule complexes and the design of competitive inhibitors. 2) Lead optimization in drug design. 3) Pharmacophore searching with the <i>Catalyst</i> modules		

3. Impact on Existing Resources.

The requested software and instrumentation will enhance our ability to teach and inspire our students in a variety of courses. Each item requested in this proposal serves a role in the progression of the scientific inquiry process, which proceeds from the visualization of chemical structures to the conception of ideas with the modeling software, followed by laboratory applications in chemical synthesis, and, lastly by analysis of optically active products with a digital polarimeter. The state-of-the art software and equipment will revolutionize the way we can teach abstract concepts like chirality and drug design at LSUS. This inquiry-driven approach will be exciting for the students, particularly when ideas are carried into applications and results. Each selected component of this grant is chosen to streamline the progression of inquiry-driven learning. This new approach will also allow us to do some "true experiments" in the sophomore-level teaching laboratories. These will be experiments that do not necessarily have a pre-determined outcome in the laboratory, where students can select from a variety of substrates and chiral catalysts and report their results to one another at the end of the experiment. The 48-vessel automated sample changer on the microwave synthesizer makes this possible in the teaching lab. The requested equipment will also facilitate the LSUS undergraduate research program. The students' research experiences will be aided by access to advanced software and equipment, which will increase the motivation for students to spend more time on their independent research and be more productive in their efforts.

B. THE ENHANCEMENT PLAN

1. Project Goals and Objectives:

This proposal is a request for funds to support the purchase of software, microwave-assisted synthesizer, and digital polarimeter necessary to improve student's practical and advanced chemistry laboratory learning. The primary objective of this project is to enhance specific chemistry lecture course and laboratories. The new instruments will allow students to perform inquiry-driven experiments and to become familiar in using technologically advanced instrumentation. These technical skills will greatly serve students as they explore various chemical related avenues either graduate schools, professional schools, or employments in chemical companies/industries. We are requesting the purchase of three major items: 1) *Accelrys' DS Model 2.0* molecular visualization and modeling software package; 2) *CEM-Explorer S-Class Microwave-Assisted Synthesizer*; 3) *Perkin-Elmer 343 Digital Polarimeter*. The direct beneficiaries of this project will be approximately 150 students per year at LSUS, which includes 60 biochemistry, 35 chemistry, and at least 20% of our 500 biological science majors (according to the Fall 2007 statistics).

We will evaluate the impact of this project on our students and our department through a combination of measurable outcomes. First of all, over the next three years, we will compare the overall performance of our students on the ACS standardized exams in both Organic Chemistry and Biochemistry to their performance over the prior three-year period. We will specifically monitor if our students demonstrate a stronger performance on those test questions related to chirality, molecular shape, and the higher order structure of biomolecules, since those concepts are emphasized in this particular enhancement. We will also examine the results of our *SIR-II* course evaluations and compare student satisfaction with those specific courses before and after the enhancement. Thirdly, we will monitor the total number of Chemistry majors and Biochemistry majors, because it is a significant goal of this project to increase those numbers, particularly chemistry majors. Lastly, during the Chair's exit interview with each of our Chemistry and Biochemistry graduates, we will conduct a short survey asking the students to address the strengths and weaknesses of this enhancement and what impact they felt it had on their education.

2. Work Plan of Proposed Project:

Instructional Utilization: Chemistry is filled with concepts of an abstract nature. It is our ability to convey the significance of the facts and information we deliver that is the best gauge of our effectiveness as educators. Abstract concepts can be explained carefully, but oftentimes the significance of these concepts goes unappreciated by the students when we do not convincingly show them the big picture about why those concepts are so important. One example is the importance of appreciating molecules as three-dimensional objects and addressing the questions about why that 3-D shape of chiral molecules is so important in the real world. We need to convince the students that stereoisomerism is not simply a concept that they need to dig up from their notes only when they have a quiz or exam in this area. Rather, it forms the basis for the variety of biological effects for the majority of natural substances and pharmaceuticals.

Table 1 provides an overview of how the requested software and equipment can be used in a variety of lecture and laboratory courses at LSUS. A few more detailed examples are provided below:

CHEM 265 and 265L Organic Chemistry Laboratory I: 90 students/year. These courses are required for chemistry, biochemistry, environmental science, and biological science majors. The current lab experiment that covers stereochemistry will be revised and expanded. The large handheld models we currently use will be supplemented and gradually supplanted with graphical modules involving the molecular visualization software. This will have important benefits, in that we will no longer be limited to the type and number of models we can build. The students will more quickly and effectively be able to build a pair of stereoisomers, overlay them on a computer screen, measure dihedral angles, etc. than they can with the floppy, hand-held models. The students will also be motivated and excited to learn how to draw and manipulate molecules as 3-D objects on a computer screen. This state-of-the-art technology will have important consequences in overall student outcomes in these courses.

Another advantage will be obtained in how we evaluate the energy of different conformations in the lecture course. The energy minimization routines of the *DS Model* software will be able to do this for us, using constraints that we specify. This often cannot be done with handheld molecular models, as the tabular values needed to perform these calculations are often limited in scope. Such applications involving conformational energy will solidify the understanding that our students have of free energy.

In both the lecture and lab, we will introduce a brief unit on microwave-assisted organic synthesis and why it is so useful. This is important, as many employers today look very favorably upon applicants who have had some experience with microwave-assisted chemical synthesis. A simple demonstration of the operation of the instrument will be conducted and the results/rates will be compared with reactions run with traditional convection heating. This demo will be done with a familiar organic chemistry reaction (e.g., Williamson ether synthesis).

The availability of a digital polarimeter will be of tremendous benefit in the Organic-I Lab course. It will enable us to introduce a new lab experiment on polarimetry, where the students are provided with an enantiomeric mixture that has an unknown composition and must determine its enantiomeric % enantiomeric excess. The students will also be expected to prove whether specific chemical reactions (S_N1 and S_N2) proceed with inversion, retention, or racemization, based on the optical activity measurements that they make. This type of experiment would allow students to associate the nature of a specific chemical reaction mechanisms with the ultimate three-dimensional shape of their product.

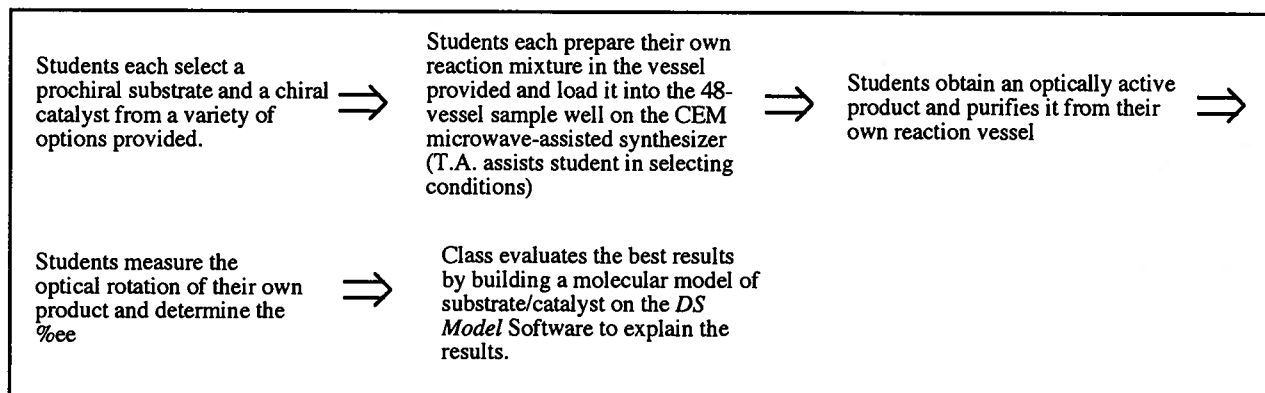
CHEM 266 and 266L Organic Chemistry Laboratory-I I: 70 students/year

These courses are required for our chemistry, biochemistry, and environmental science majors, and are often taken as electives by biological science majors. We will employ the *DS Model* software and equipment in a variety of useful ways. First of all, the Biopolymer module within *DS Model 2.0* provides the user with the opportunity to quickly and seamlessly assemble protein structures, polysaccharides, and nucleic acids from their fundamental building blocks. This will be of value for both classroom demonstrations and for student exercises outside of class. The software will enhance the preparation of these organic chemistry students for the subsequent course in Biochemistry.

Furthermore DS Model has the ability to display images of molecules in 3-D. We can accomplish this with two digital projectors, a pair of optical polarizers, and a pair of polarized glasses for each student. A recent demonstration of this setup by faculty in our *Bioinformatics* group at LSUS provided convincing evidence that this would be highly beneficial to use in our chemistry courses. It would represent a tremendous enhancement of our capabilities at a minimal additional cost (*ca.* \$4,000). The dual projectors/polarizers may either be ceiling-mounted or cart-mounted for wider access to other classrooms.

A second application of the software and equipment in these courses involves an inquiry-driven experiment into the role of chiral catalysts in chemistry. Our students have never seen a reaction that produces anything other than a racemic mixture of products. A new lab experiment could be implemented that employs some chiral catalysts to produce an optically active chiral product. The outline of this idea shows the type of sophisticated new experiments that would become possible in the organic laboratory:

Figure 1: Example of a Proposed New Inquiry-Driven Experiment for the CHEM266 Organic Lab



Although chiral catalysts are generally rather expensive (*ca.* \$200 per gram), only very small amounts (15 mg per student) would be needed to carry out a transfer hydrogenation reaction in the CEM microwave-assisted synthesizer. Students would be allowed to select from a small variety of prochiral substrates and chiral catalysts to customize their own experiment and determine the stereochemical outcome by analyzing their purified product on the digital polarimeter. The 48-well automated sample changer on the *Explorer* unit would make the set-up process for this reaction “painless” for all involved, and the students could work with the T.A. to program the conditions for their reactions, as well as get the opportunity to select their own substrate and catalyst. It is this type of experiment that would help to change the way our students currently view organic chemistry labs.

Of course, it is important that the students also develop proper lab technique and a strong knowledge about setting up traditional microscale reactions, so no more than one or two experiments would be devoted to working with the microwave synthesizer in this 200-level course. Nevertheless, the exposure that our students would receive to experiments of this nature would serve as enough of an “eye opener” to make them want to take more chemistry courses and perform their independent research in our department.

CHEM 490 Medicinal Chemistry: 20 students/year

A popular new upper level course in our department is *Medicinal Chemistry*, which is taught by Dr. Salvatore. This course delineates the drug discovery process and gives both historical and modern perspectives of how drugs are designed, synthesized, and used. The inclusion of the *DS Model* software in our curriculum will prove very advantageous for this course. In particular, the Quantitative Structure Activity Relationship (QSAR) modules (*DS Model Catalyst* and *Ligand Fit*) will provide students with new insights about how drugs work. The three-dimensional display capabilities of *DS Model* will be particularly useful. This would be accomplished by using dual projector equipped with polarizing filters, and the students would each wear a pair of glasses. It will enable us to provide new

insights like never before. For example, the HIV protease protein is an important drug target in the treatment of AIDS. With this new software, students will be able to see how protease inhibitors work to inhibit this enzyme and disable the AIDS virus. They will virtually feel as if they were “walking into” the enzyme. The students will also be able to design potential new protease inhibitors based on existing ones. Instilling creativity in our students is important, particularly in upper level courses, and this new software would enable us to do that. In short, the acquisition of this software would significantly enhance our ability to teach this course and many others (see Table 1), and this will greatly increase the marketability of our students, both in the job market and in their graduate/professional school endeavors.

Research Utilization: In addition to the use of the requested software and instrumentation in chemistry laboratory courses, the faculty and some students will employ the proposed instrumentation in their research. Drs. Mahdavian and Salvatore and their collaborators at *LSUHSC-S* are involved in a number of research projects in the field of medicinal chemistry, with an emphasis on the design and synthesis of new cancer therapeutic agents. The goals of this research include the development of new mitochondrially-targeted compounds, anti-angiogenic agents, and substances that block the cell-signaling processes associated with cancer metastases. The microwave-assisted synthesizer is well suited for applications in drug discovery synthesis. It will greatly accelerate the reaction times for a variety of chemical transformations that we carry out and is amenable to scale-up to 120 mL vessels. Dr. Salvatore recently visited CEM to explore the advantages of this apparatus. In one case, a reaction that required 48 hours to complete with conventional heating in our research lab was completed within 1 hour on the microwave synthesizer. This would be a great addition to the research infrastructure of our core chemistry research laboratories at LSUS.

The *DS Model* software will also be very important in research applications. In particular the *Catalyst Hypothesis*, *Catalyst Score*, and *LUDI* modules are useful in drug design. These programs have algorithms that perform quantitative 3D-quantitative structure-activity relationships (3D-QSAR) and pharmacophore searching. In modern computational chemistry, *pharmacophores* are used to define the essential features of one or more molecules with the same biological activity. Using the pharmacophore search tools, we will be able to search databases of molecules to identify others, which share the same features (e.g., dipoles located a similar distance apart from each other). This is particularly important for the design of new mitochondrially-targeted compounds, because we have new information from a collaborator that several of our synthetic compounds are binding at the ubiquinone binding site within mitochondrially redox complex-II. The *Catalyst* modules are able to examine a variety of conformations and propose new active structural fragments based on the 3-D steric and electrostatic demands of groups within a given molecule. The use of this software will provide us with new insights and insure that our research hypothesis are based on the most modern drug design principles.

Roles/Responsibilities: Dr. Salvatore's (P.I.) primary responsibility will involve purchasing, general oversight, upkeep of the software and instrumentation. Together, Drs. Salvatore and Mahdavian will oversee the use of the new software and instrumentation in most instructional coursework in the chemistry/biochemistry curricula. They will also be responsible for training their colleagues and in coordinating student and faculty use of these items in both teaching and research. In all cases, each faculty member associated with a particular demonstration or new experiment will test them in the laboratory and revise them as necessary.

Schedule: This is a 1-year grant program request (6-1-08 to 6-30-09). If fully funded, the three major items will be purchased and installed as quickly as possible. The equipment will be used in the courses as they are scheduled during their normal rotation through the 2008-2009 academic years, and it would begin to be used in research at the same time. The timeline will run as follows:

June 1, 2008 -- All of the funded software and equipment will be ordered, and the

installation will be scheduled.

August 10, 2008 -- Preliminary instructional experiments will be completed and testing of the experiments underway.

October 1, 2008 -- Faculty will be trained by the P.I. and Co-PI on the use of the new software and instrumentation. All new and revised laboratory experiments will be tested by faculty and selected teaching assistants. Faculty and student research using the new instrumentation will also be underway.

June 30, 2009 -- All experiments will have been performed in appropriate courses and revised as needed. More faculty and student research will be in progress. Project evaluation reports will be completed for *Board of Regents*.

3. Evidence of Potential to Achieve Recognized Eminence. The proposed chemical instrumentation facility enhancement will help to increase LSUS's level of regional eminence, commensurate with our status as a primarily undergraduate institution. Faculty members involved in the interdisciplinary efforts of the Department of Chemistry and Physics (including the biochemistry subdivision) are already active in scholarly activity, participation, and publication. The proposed project will support increased educational quality and eminence in LSUS's tri-fold mission of Education, Research, and Community Service/Outreach:

Educational Eminence: Undergraduate Education: LSUS's College of Sciences has taken the lead in applying innovations in science education reform to its degree programs and to teacher training programs, both on and off campus. Guided inquiry-driven laboratory work is now a major part of all lower and upper level science courses. Our Chemistry Dept. has adopted the spiral learning approach recommended by the *Council on Undergraduate Research* and the *Journal of Chemical Education*. This approach builds student interest with relevant, real-world examples to introduce concepts and experiments in lecture, laboratory, and research experiences. The final report of the review of Louisiana chemistry programs by the Louisiana Board of Regents states "The (LSUS) department maintains a quality undergraduate program," and that the "Faculty are dedicated and competent." A five-year average of ACS-certified graduates/year places LSUS second only to LSU-BR among Louisiana universities in the annual production of ACS-certified chemistry graduates. LSUS ranks first in the state in the percentage of chemistry graduates certified by the American Chemical Society.

We have high expectations from our chemistry and biochemistry graduates, and student success provides a good measure of eminence for a primarily undergraduate program. In the past eight years, LSUS chemistry graduates have sought advanced education and have been accepted into graduate programs at the LSUHSC and at other institutions: LSU-BR, University of New Orleans, Mississippi State University, Arizona State University, University of Colorado, University of Arkansas (2 students), University of Idaho, and the University of South Carolina.

During the current decade, our faculty members have received awards for instructional laboratory improvement from the NSF for integration of UV-visible spectrometry, liquid chromatography, and NMR technology in undergraduate chemistry education. Our chemistry faculty has received over 20 campus research and development grants, which has helped the faculty publish over 20 papers. The undergraduate chemistry program at LSUS has made the transition from the original, strictly teaching mission of this institution to a more balanced blend of instruction and research. In recognition of the early phase of this transition in the late 1990's, the National Science Foundation awarded the College of Sciences an Academic Research Infrastructure (ARI) grant of \$1.47 million (largest NSF-ARI award ever given in LA) to renovate the Science Building. This award supplemented \$3.5 million in state funds for the renovation, which was completed seven years ago. Most chemistry faculty members are active in research and seriously involve their students in research. The Departments of Chemistry and Biological Sciences have formed major cooperative interdisciplinary efforts in biochemistry, biotechnology, and environmental science.

During the current decade, 120 chemistry, biochemistry, and environmental science undergraduate majors have participated in faculty-led research projects, and LSUS has been officially recognized by the Board of Regents for excellence in involving undergraduates in research.

Research Eminence: New opportunities for LSUS to gain greater research eminence will be enhanced via utilization of the proposed software and instrumentation. The P.I., co-P.I. and their students are actively involved in several exciting research projects, and it is their goal to attract significant state and federal funding within the next 18 months. These investigators all have consistent publication track records, demonstrating that they are serious about research. Over the past two years, Dr. Salvatore has been invited to attend and give lectures at two separate meetings of the *Society for Free Radical Research*, which were held in Brisbane and Perth, Australia. Earlier this year, Jacob Lowring, one of Dr. Salvatore's current research students was awarded a prestigious *ACS Undergraduate Student Travel Award* to present the results of his research at the *National Organic Symposium* in Durham, NC, among other awardees from U of California (Berkeley), U of Michigan, U of Illinois, Harvard, Brown, and CalTech. The LSUS College of Science has several established collaborations and partnerships with major area universities, industries, federal and state agencies, and local governments. These include: LSU-HSC-S, Feist-Weiller Cancer Center, BASF Pharmaceuticals, International Paper, Penzoil/Calumet, UOP, Olin, Calloway Chemicals, LSU Health Sciences Center, Willis Knighton Health Care System, Christus Schumpert Health System, National Wetlands Research Center, EPA, USDA, Barksdale AFB, LDEQ, LSU Agricultural Center, Shreveport Wastewater Treatment Division.

Our current science students will likely go on to work in exciting new fields like nanotechnology, rational drug design, and "smart polymer" chemistry, and companies are seeking students who not only have very strong fundamental classroom and practical laboratory knowledge, but also interdisciplinary research experience. The new software and instrumentation will enable us to continue meeting the new research demands placed upon it by our faculty and students.

Community Service/Outreach Eminence: LSUS College of Science faculty are very active in community service and outreach programs designed to foster science-related activities for the public and improve science instruction at the pre-college level. Dr. Salvatore is currently the Chairman of the *NW Section of the American Society*. During his year as Chair, he has attracted over \$3,000 in private donations from companies and organizations in Shreveport to sponsor student meals at the meetings. As a result, student participation in our local ACS section has increased by over 200%. The companies have been grateful to sponsor the professional development of these students, because they recognize that these young people represent the future of this community and state.

LaPrep, a summer science enrichment program for minority and women middle school students has won national acclaim from the U.S. Department of Education Minority Science Improvement Program and the U.S. Department of Energy. The College of Sciences has hosted the *NSF Young Scholars Program*, in which promising high school students participated in faculty research projects. LSUS annually hosts the Northern Louisiana Regional Science Olympiad for regional school students. LSUS Science faculty members also assisted in the establishment of *SciPort*, a "hands-on" science museum, and several College of Science faculty continue to serve on the *SciPort* board of directors.

LSUS Sciences faculty members have also provided leadership in applying the concepts of science education reform to primary and secondary education teacher training. Teacher preparation has been the focus of *LaSIP* (*Louisiana Systemic Initiative Program*) and *LaCEPT* (*The Louisiana Collaborative for Excellence in the Preparation of Teachers*) grants to science faculty who have conducted annual summer workshops to train almost 600 teachers in the guided inquiry approach to science teaching. *LaSIP* programs held on the LSUS campus are part of a statewide effort designed to bring about systemic change in the way science is taught. The Chemistry faculty has also developed a three-course sequence of integrated science lecture and laboratory courses that are based solely on inquiry pedagogy; these courses serve as the science foundation sequence for all LSUS elementary

teacher education majors. (LSUS offers the only NCATE-accredited Education programs in Shreveport, Louisiana's third largest metro area. An average of 98% of our Education graduates pass the national teacher exam for certification on the first try.

4. Impact on Curriculum and Instruction: The new software and instrumentation will have a significant impact on our curriculum and instructional opportunities. It will create greater "unity of purpose" between several co-requisite lecture and laboratory courses, and it will strongly support our College of Science's efforts to emphasize laboratory experiences as a source of learning concepts in chemistry. Students will regularly use the software and equipment to engage in self-guided exercises and assignments, and experiments. This will not only be fun but it will also enhance learning and the development of greater problem-solving skills. The fact that *Accelrys* is now offering a specially designated 5-year "teaching licenses" on their software is unprecedented in their corporate history, and it represents a tremendous opportunity for us to now provide our students with access to professional-grade molecular modeling software. Our request for the inclusion of five student access nodes (in addition to the research node) is something that can be increased for ca. \$400 per student node. Science education students in these courses will obtain additional experience in inquiry-driven learning pedagogy and interdisciplinary concepts, important components of science reform. Expanded opportunities for student research will offer experience in a greater range of research methods and projects. This in turn will enhance curricular interest and retention in chemistry, biochemistry, and related fields.

5. Impact on Quality of Students. The Louisiana community college system has significantly expanded statewide over the past several years. Therefore, we need to increase our competitive advantage in attracting those students who want more than just a textbook education. Enhanced inquiry-driven learning and research opportunities in the sciences are two big advantages that LSUS has over community colleges. By supporting instrumentation enhancement for both education and research, this grant will increase our ability to attract a greater percentage of the best and brightest students from area high schools. About 150 students per year at LSUS will be exposed to the new software and instrumentation requested in this proposal. This enhancement will dramatically improve the way our students learn, with hands-on access to the new software and instrumentation. The impact vs. cost ratio of this enhancement is very high. In fact, assuming that the requested instrumentation and software is used for at least the next 10 years, the overall cost of this enhancement amounts to less than \$65 per student per year. Thus the proposed enhancement represents a tremendous investment in our current and future students.

This grant project will also help address the problem of too few students, especially women and minorities, entering science related careers. Access to modern technology can attract first year students who are undecided about a curriculum. High quality educational and research projects will also attract high quality students. These students will gain valuable training in interdisciplinary technology utilization, as well as application of the scientific approach to research. According to the Report of the NSF Disciplinary Workshops on Undergraduate Education, involvement in research is one of the best ways to recruit and retain good science students. Over the past 8 years, 300 undergraduates have participated in LSUS College of Science research projects, but the majority of these have been biology majors. The enhanced software and instrumentation will help to increase faculty-led research opportunities for students in our department. The final result will be the production of a greater number of better-trained chemistry and biochemistry graduates who go on to success in their careers and/or advanced academic endeavors.

6. Impact on Faculty Development. Our motto at LSUS is "Expect Excellence", and we as faculty members try to adhere to this in every aspect of our profession. We expect it from ourselves and from our students. We also believe that the excellence of our facilities and our instrumentation is very important, as it helps set the standard for how we convey knowledge to our students, and how they acquire a practical understanding of the things we teach them. The fact that we lack the

requested software and instrumentation is a deficiency that we must remedy if we are to truly be excellent. Also, this year we are again hiring a new young faculty member in our department, and the availability of these items will make our department a more desirable place for that individual to teach and conduct research.

We, as faculty with Ph.D. degrees (and in some cases postdoctoral training) are obliged to keep abreast of powerful new experimental techniques and to convey those new techniques to our students. This is particularly true for things that are difficult to teach with a textbook alone such as modern biochemical techniques. Since the P.I. and co-P.I. use this instrument in our research, we can bring this knowledge directly to our students, regardless of how it is described in the textbook. We will be able to devise new lessons and experiments that would use the more advanced capabilities of the new software and instrumentation in order to teach the upper level laboratory courses as well as in research.

In a recent evaluation of the Science faculty at LSUS, the Louisiana Board of Regents stated, "The caliber of faculty at LSU-Shreveport is very high". It went on to say that the Science faculty, as a whole, are "meeting the triad of teaching, research, and service in various ways." It is apparent that the investigator of this project could improve further in their profession as educators if this request is fully funded. We need the requested experimentations to provide effective practical experience to our students in teaching laboratories as well as in our own research. . Excellent facilities and up-to-date instrumentation are the catalysts that will allow us to maintain this philosophy in our pursuit of excellence.

7. Performance Measures: Quantitative and qualitative measures will be used to document progress toward meeting objectives, with specific benchmarks to be achieved by the end of the grant funding. These short-term benchmarks include: **1.** At least 150 students from the courses listed in Table 1 will have performed one or more experiments with the new software and instrumentation. **2.** At least four faculty and 7 students will have used the new equipment in independent research projects that produce both publications and research presentations. **3.** At least two new research grants will be submitted by July 1, 2009, describing key experiments that take advantage of the enhanced capability of the new software and instrumentation.

For assessing longer-term effectiveness, several types of information will be collected. Records of usage of the equipment and the nature of that usage will be maintained. Students will evaluate courses through SIR-II surveys, and faculty will evaluate the competence of students in the courses and in research work, using ACS standardized exams in Chemistry and Biochemistry as benchmarks for comparison. Student enrollment, retention, completion, grades and other records will also be analyzed, and the students in each of the courses using the new items will be surveyed concerning the value of the enhanced practical training in the course and their intent to take additional related courses.

Faculty and students will be surveyed concerning how the new software and instrumentation has affected their teaching and research activities. Over the longer term, faculty and student research production can be assessed from publications, presentations, successful grant applications, etc. The Department of Chemistry and Physics maintains accurate records of the post-graduate activities of its alumni. Graduates will be surveyed to determine the value of the skills learned in their careers.

C. EQUIPMENT

1. Equipment Request (See details in Budget Narrative section)

2. Equipment on Hand for Project

There is no closely related equipment on hand for this project. Thus this grant award would greatly expand our capabilities in all of these areas. We do have access to *RasMol*, a public-domain molecular visualization computer program that we use in our biochemistry lab courses. The *DS Model 2.0* software is far more capable and versatile program. It would make the use of *RasMol* redundant and unnecessary.

3. Equipment Housing and Maintenance

The molecular modeling software equipment will be based on a computer that will be located in Room 308 of the Science Bldg. This is a room that lies between Dr. Salvatore's office and the organic teaching laboratories. The installed software will have a "floating license", meaning that the executable modules can be downloaded by any computer on campus. Regular maintenance and network access will also be funded via the *LSUS College of Science's* budget.

The microwave synthesizer and polarimeter will be housed in the organic chemistry teaching lab, and a computer to operate the synthesizer will be provided by the College of Science.

D. FACULTY AND STAFF EXPERTISE

Brian A. Salvatore, Associate Professor of Chemistry, teaches organic chemistry courses including CHEM 265, 265L, 266, 366, 467 as well as electives, CHEM 464 (Intermediate Organic Chemistry), CHEM 490 (Medicinal Chemistry) and CHEM 301 (Chemical Literature). Dr. Salvatore is a synthetic organic chemist with additional specialized training in biophysical NMR techniques. Dr. Salvatore came to LSUS from the University of South Carolina in 2003 and has 14 years of professional experience beyond his Ph.D. degree, working as both an educator and research scholar. Dr. Salvatore was awarded an NIH postdoctoral fellowship at Yale University in the laboratory of Professor James H. Prestegard, a renowned biophysical NMR spectroscopist. During his own academic career, Dr. Salvatore has trained and supervised 25 research students at the undergraduate, masters, and Ph.D., levels. He is knowledgeable about molecular modeling and chemical synthesis, as well as the associated instrumentation.

A significant part of Dr. Salvatore's departmental service work at LSUS includes oversight and maintenance of the instrumentation (NMR, GC-MS, IR, etc). Recently, he visited CEM in Charlotte, NC to gain familiarity with the operation of the new *Explorer S-Class* microwave - assisted synthesis unit. He also attended a 3-day short course on the use of *DS Model* and is thus well qualified to execute the goals of this project. It is his sincere goal to keep the new instrumentation requested in this enhancement grant performing to its utmost capabilities, and this grant will help to ensure that students and faculty at LSUS benefit from the ever-increasing capabilities of its instrumentation. His current research interests are in the synthesis of mitochondrially-targeted anti-cancer agents and new compounds that block the cell signaling processes that lead to cancer metastases. In 2006, Dr. Salvatore was selected as the *Outstanding Scholar* in the LSUS College of Science and currently serves as the chairman of the *Northwest Region of the American Chemical Society*.

Elahe Mahdavian, Assistant Professor of Chemistry. Dr. Mahdavian teaches organic chemistry courses including CHEM 265, 265L, physical chemistry CHEM 304, 304L, 306, 306L, and Biochemistry labs, BCHM 410L and 412L. She joined the LSUS faculty in Fall 2003, after having served on the faculty of South Carolina State University for four years. She has a Ph.D. from the Department of Chemistry and Biochemistry at the University of South Carolina (Columbia, SC) with Professor R. Bruce Dunlap. Through her graduate training, she has obtained extensive experience in several areas of biophysical chemistry, organic chemistry, and biochemistry. She is knowledgeable in qualitative and quantitative analytical characterization methods, such as PCR, DNA/Protein electrophoresis, enzyme kinetics, protein purification, UV-VIS, IR, ^1H - and ^{13}C -NMR, mass spectrometry. Although teaching constitutes the major part of her job, she also conducts research with LSUS students. She will employ the new software and instrumentation in both teaching and research. Her current research interests involve medicinal chemistry and bioorganic chemistry, with an emphasis on the synthesis and development of anti-angiogenic compounds as new anticancer agents.

E. ECONOMIC AND/OR CULTURAL DEVELOPMENT AND IMPACT

1. Relationships With Industrial/Institutional Sponsors: The LSUS College of Science has numerous industrial/institutional collaborations, and the enhancement of the biochemical/biomedical instrumentation facilities at LSUS is important to several of these partners as well. The *Biomedical Research Foundation (BRF) of Northwest Louisiana*, which established the \$50 million Biomedical Research Institute adjacent to the LSUHSC, has provided instrumentation grants to LSUS faculty. The *BRF Positron Emission Tomography Imaging Center* and CTI Cyclotron Systems, Inc. also partnered in a three-year *BORSF Industrial Ties* research grant with faculty in the department of chemistry. The *BRF* was also instrumental in recruiting Drs. Salvatore and Mahdavian to LSUS, and it paid for some of the instrumentation in their research laboratories at LSUS.

Students are also an important part of these research partnerships. Our students often develop relationships with new local companies and then go on to work for them after graduation. Red River Pharma, L.L.C., for example, is a brand new company in Shreveport's *InterTech Science Park* (described more in Section E2). After being heavily recruited, three of our department's May 2004 graduates accepted jobs in research and development at Red River Pharma, and we anticipate maintaining close ties with these students and this company. Clearly, local partnerships between industry, the BRF, and LSUS are paying off, as more of our top chemistry graduates take jobs in the Shreveport area. We believe that our highly technological instrumentations can serve as an important analytical tool to the scientists at Red River Pharma and other companies throughout the Shreveport metropolitan area.

In the regional Industrial/Manufacturing field, our chemistry program is well respected by firms who have hired our graduates. The first students graduated from our B.S. chemistry program in 1975, and many have been placed in regional positions in industry. For example, our graduates have earned managerial laboratory positions in the regional facilities of BASF Pharmaceuticals, International Paper, Pennzoil/Calumet, UOP, Union Carbide, Vista Chemical, Olin, Calloway Chemicals, and Texas Instruments. Several area laboratories of major industrial firms and commercial analytical laboratories partner with us on opportunities for mutual benefit, such as the internship program with several area firms (BASF Pharmaceuticals, UOP, NORAM, a natural gas utility; SWEPCO, an electrical, City of Shreveport Wastewater Treatment Division). This internship program benefits both LSUS science students and the sponsors. Many of our graduates find

employment in regional laboratories and in government agencies, such as EPA, USDA, National Wetlands Research Center, Barksdale AFB, US Army Corps of Engineers, Louisiana Department of Natural Resources, Louisiana Department of Environmental Quality, City of Shreveport, Caddo and Bossier Parish (county) agencies, Northwest LA Crime Laboratory, Southwest Laboratories, ArkLaTex Environmental Lab, Region 7 Public Health Lab (state designated regional bioterrorism lab), etc.

2. Promotion of Economic Development and/or Cultural Resources: The Chemical & Allied Products (incl. Pharmaceuticals) sector is the largest manufacturing employment sector in Louisiana, employing more than 30,000 workers with average annual earnings of \$50,688 per worker (highest of any manufacturing sector), thus totaling more than \$1.52 billion in payroll per year. Other major Louisiana economic sectors employing scientists, technicians, and related workers include: health care services, environmental services, paper and forest products, food manufacturing, petroleum refining, oil and gas production, and government agencies. Production of better-trained chemists, biochemists, and related scientists has a direct impact on economic development in this State. Major **existing firms** already established in Louisiana with manufacturing, research and distribution facilities that employ chemists and biochemists include: Abbott Laboratories International Div., Akorn Inc., American Biomedical, BASF, Betz labs, Ciba-Geigy, Cytec, Dow, DuPont, ICI, LaRoche, Medco Pharmaceuticals, Monsanto, Nalco, Rhone-Poulenc, Sage Pharmaceuticals, Sherman Pharmaceuticals, and Witco. Major petrochemical firms include Exxon, Chevron/Texaco, Mobil, Marathon, BP, Shell, OxyChem, Olin, Citgo, etc.

In addition to existing firms utilizing graduates trained in chemical/biochemical analysis technology, **new companies** in North Louisiana are also seeking trained scientists. Kinzie & Payne Biomedical Corp., a biotechnology firm with a focus on water treatment with enzymes and microbial agents, has recently located in Shreveport. The Biomedical Research Foundation of Northwest Louisiana has established InterTech Science Park in Shreveport (about 8 miles from the LSUHSC campus), which is projected to add at least 6,000 technology jobs with a \$225 million annual payroll over the next 25 years. Besides Red River Pharma, another new chemistry-related company in the Park is SteriFx, Inc., a specialty chemical company specializing in antimicrobial solutions for industrial, consumer, healthcare, and defense markets. Their patented technology is a low pH (<1) bleach-free aqueous solution that is highly effective in controlling pathogens (microorganisms/bacteria) with exceptionally low toxicity to humans or animals. It has no deleterious effects on processing equipment or work surfaces. SteriFx is proving to be a local success story, with one of its products, *FreshFx*, already approved by the USDA's Food Safety and Inspection Service (FSIS) for use as a shelf life extender (food additive) and a processing aid.

In 2001, the Louisiana Department of Economic Development restructured to focus on **"Industry Clusters"** as key to the State's **Vision 2020** long-term plan to improve the economy. Five of the nine major clusters offer opportunities for chemists/biochemists: Biotechnology/Biomedical; Petrochemical/Environmental; Ag/Forest/Food Products; Advanced Materials; and Oil & Gas.

Our relationships with the Biomedical Research Foundation (BRF) described in the preceding section emphasize projects that have high potential to become technology for the regional and national biomedical industry. Several of our biochemistry graduates are now Research Associates at LSUHSC and the BRF. **More and better chemistry, biochemistry, biology graduates will partially address the shortage of professionals needed by the year 2010.** LSUHSC sociologist, Dr. Kenneth Hinze, has projected a large increase in Shreveport area needs for natural and other scientists (1,940 net new jobs; > 100% increase) and biomedical professions (2,740 net new jobs; 54% increase). One response to this need has been the establishment of industrial internships for students. Several chemistry students have received excellent on-site training with internships at several local firms (See previous section) and an optional professional project is now part of our B.S. in chemistry. More and better-prepared professional chemists/biochemists in our region will also assist the regional industry, biomedical/health care and government sectors to

improve regional environmental quality and overall quality of life for residents, thus providing additional support for economic expansion.

F. ADDITIONAL FUNDING SOURCES

No external organizations are funding this enhancement project. However, LSUS will contribute \$34,679 in the form of cash and in-kind matching funds.

5. PREVIOUS BORSF AWARDS:

1) LEQSF (2003-04)-- "*Enhancement of the 300 MHz NMR Instrument at LSUS*", Drs. Brian Salvatore, Elizabeth Zippi, and Elahe Mahdavian, \$ 76,600. The primary objective of this project was to enhance the nuclear magnetic resonance (*NMR*) instrumentation at *LSUS*. It involved both the hardware upgrade and the acquisition of new software that increased the capabilities of our facility and enabled us to place more practical emphasis on *NMR* in a variety of chemistry courses as well as research.

2) BORSF-RCS (2005-08) -- "*Synthesis of Novel Vitamin E Analogs with Potent Anti-Cancer Activity*", Drs. Elahe Mahdavian, and Brian Salvatore, \$66,542. The objective of this project was to synthesize a broad spectrum of novel *vitamin E* amide and ester derivatives of tocopheryl succinate. We are currently in the last year of the grant. Thus far, we have synthesized and determined biological activities of a number of the synthetic analogs. We have established the *structure-activity* relationships of these molecules and have demonstrated the important structural features for the observed potency and anti-cancer activity. We have also gathered further evidences that derivatives of *vitamin E* succinate exhibit selective toxicity toward cancer cells, with virtually no toxicity exhibited against normal cells. This is a promising therapeutic advantage of these molecules over most other currently established anti-cancer drugs which are either non-selective, causing considerable systemic toxicity, or they lose of efficacy, due to constant mutations of malignant cells.

**BOARD OF REGENTS SUPPORT FUND
TRADITIONAL AND UNDERGRADUATE ENHANCEMENT, FY 2008-2009**

6. Budget and Budget Justification Pages

Directions: Each line item under the columns "Support Fund Money Requested," "Institutional Match," and "Private Sector/Other Match" must be itemized, fully explained, and justified on a separate budget justification page(s). Attach additional justification pages as needed.

Title of Proposal: **Bridging Molecular Modeling and Chemical Synthesis to Enhance Inquiry-Based Learning**

Project Director(s): **Brian A. Salvatore (P.I.) and Elahe Mahdavian (co-P.I.)**

Institution(s) of Higher Education: **Louisiana State University in Shreveport (LSUS)**

PROPOSED BUDGET:

	Support Fund Money Requested	Institutional Match ¹	Private/Other Match ²
A. Equipment ³	\$71,268	\$2,000 (cash)	None
B. Software	\$24,982	\$6,542 (cash)	
C. Supplies	\$1,000	\$2,000 (cash)	
D. Shipping/handling	\$250		
E. Installation		\$1,200 (in kind)	
F. Personnel training	\$1,000	\$2,000 (cash)	
G. Other			
1. Faculty time		\$10,000 (in kind)	
2. Fringe benefits		\$2,500 (in kind)	
3. (etc.)			
H. Indirect costs	Not allowed	\$6,437 (in kind)	
I. Maintenance	Strongly discouraged	\$2,000 (in kind)	
J. Total costs (A-I)	\$98,500	\$34,679	

¹ Stipulate whether in-cash or in-kind. The Board strongly encourages the sharing of costs for proposed projects. Applicants and institutional officials should note, however, that the employing institution will be required to honor the commitments made in the original proposal before any awards are made. Discounts for equipment purchases are not allowable as institutional match.

² The budget page(s) must reflect and the budget justification pages must explain any external funds that are claimed in the proposal. External funds and their expenditure must be accounted for in the same manner as Support Fund money and institutional match.

³ Equipment. If applicable, itemize and describe briefly the proposed equipment and its intended use in the project. Include the name, model number, and manufacturer(s).

(TR and UG Enhancement Program Budget and Budget Justification, Rev. 8/2007)

BUDGET NARRATIVE

The necessary equipment for this enhancement grant is itemized as follows, with a brief explanation following each item, below. Written documentation of the actual price quotes is provided in Appendix A (*Equipment Manufacturer's Price Quotes*).

A. Equipment

Explorer Discover S-Class Microwave-Assisted Chemical Synthesizer \$44,784

This 300-watt monomode automated microwave synthesizer package includes a 48-vessel sample changer with infrared temperature sensing an internal camera that gives the user visual access to the reaction mixture. Synergy software included.

Dual Digital Projectors (NEC Model LT380)

When equipped with differentially polarized filters, two digital projectors will provide stereo imagery, providing the molecular visualization software with 3-D display capability in the classroom. Each projector delivers a powerful 3000 *ANSI* lumens. \$3,200

Perkin-Elmer Model 343 Digital Polarimeter \$20,112

This significant hardware addition includes a pneumatic unit for magic angle spinning, as well as a new $^1\text{H}/^{13}\text{C}$ inverse solids probe with deuterium lock capabilities. It also includes a deuterium *TX* board for the console that provides enhanced deuterium acquisition and gradient shimming capabilities.

Dell Precision Computer Workstation \$3,172

This workstation will be equipped with *Windows Vista* and will operate the *DS Model 2.0* software. It will be equipped with a 250 GB hard-drive, a 256 MB graphics card, and a 30-inch flat panel display.

B. Software

Discovery Studio Model 2.0 \$24,982

This is the latest version of Accelrys' molecular visualization and modeling software for educational and research applications

C. Supplies \$1,000

These funds (matched 2:1 by LSUS) will cover the purchase of projector mounts, polarization filters for the projects, visualization glasses for the students, and chiral catalysts and reagents for the new organic laboratory experiments

D. Freight Charges (shipping charges for polarimeter and microwave synthesizer) \$250

F. Personnel Training \$1,000

These funds (matched 2:1 by the LSUS, College of Science) will allow Dr. Salvatore to attend a course on the Catalyst Pharmacophore Searching features of *DS Model* at Accelrys' headquarters

Total Funding Request **\$98,500**

INSTITUTIONAL MATCH:

- A. Equipment: LSUS will provide \$2,000 (cash) to purchase a computer to operate the microwave synthesizer.
- B. The LSUS College of Science will provide \$6,542 (cash) to pay for one year's to Chemical Abstracts Services' *Sci-Finder Scholar* database, a very useful web-based database that is used by students and faculty to survey the chemical literature for education and research.
- C. Supplies: LSUS will provide \$2,000 (cash) in to purchase additional reagents and chiral catalysts for the new experiments proposed.
- D. Additional funds will be provided as needed.
- E. Installation: \$40/hr X 20 hrs = \$1,200 (in kind).
- F. Additional funds provided for attending software training classes at Accelrys, \$2,000 (cash).
- G1. Faculty time: \$40 X 250 hrs. = \$10,000 (in kind).
- G2. Fringe benefits: @ 25% of G1= \$2,500 (in kind).
- H. Indirect costs: 41% of E, G1, G2, and I = \$6,437 (in kind)
- I. Maintenance: \$25/hr X 80 hrs = \$2,000 (in kind)

TOTAL LSUS MATCHING FUNDS: \$34,679

B. PROJECT ACTIVATION DATE AND ANTICIPATED DATE OF COMPLETION

Activation Date: June 1, 2008

Completion Date: June 30, 2009.

BIOGRAPHICAL SKETCH			
Name Brian A. Salvatore		Position Title Associate Professor	
EDUCATION			
INSTITUTION AND LOCATION	DEGREE	YEAR CONFERRED	FIELD OF STUDY
University of Michigan (Ann Arbor)	B.S. (Magna Cum Laude)	1987	Chemistry
Univ. of Pennsylvania (Philadelphia)	Ph.D.	1993	Organic Chemistry
Yale University (New Haven, CT)	NIH Postdoctoral Fellowship	1993-1996	Organic/Biophysical Chemistry

Current Position

Associate Professor, Department of Chemistry and Physics, Louisiana State University-Shreveport, One University Place, Shreveport, LA 71115 (primary appointment commenced August 20, 2003). and Adjunct Associate Professor in the Department of Biochemistry and Molecular Biology, LSUHSC-Shreveport.

Other (Past) Work Experience

Assistant Professor, Department of Chemistry and Biochemistry, University of South Carolina, Columbia, SC 29208. Aug. 1996-May 2003.

Research Assistant (Summer 1986)

The University of Utah, Department of Chemistry with Professor C. Dale Poulter

Research dealt with the immobilization of farnesyl pyrophosphatase, an enzyme involved in cholesterol biosynthesis, onto an inert acrylic support for potential *in vitro* synthetic applications.

Research Assistant (Summer 1985)

General Motors Biomedical Research Laboratories (Warren, MI) with Dr. Tai Chan

Research project involved determining the size of spray paint particles using fluid dynamics (inertial impaction techniques). This research addressed important environmental concerns raised by the federal government regarding automobile plant paint particle emissions.

Recent Awards and Distinctions

Awarded *Outstanding Faculty Scholarship Award*, LSUS, College of Sciences, (June 2006).

Elected chairman of the *Northwest Louisiana Section of the American Chemical Society* (2007).

Selected Peer-Reviewed Publications

1. Vitamin E analogs as selective anti-cancer agents with multiple mode of action: The necessity of being redox-silent, Jiri Neuzil*, M. Tomasetti, Y. Zhao, L.-F. Dong, X.-F. Fang Wang, M. Birringer, P. Low, M.W. Fariss, M.P. Malafa, S.J. Ralph, K. Wu, B.A. Salvatore, *Molec. Pharmacol.* (submitted June 2006), *Molec. Pharmacol.*, **71**, 1185-1199 (2007).
2. "Vitamin E amides, a new class of vitamin E analogues with enhanced proapoptotic activity" Tomic-Vatic, A.; EyTina, J.; Chapman, J.; Mahdavian E.; Neuzil, J.; Salvatore. B.A., *Int. J. Cancer*; **117**, 188-193 (2005).
3. "a-Tocopheryl Succinate Selectively Induces Apoptosis in Neuroblastoma Cells: Potential Therapy of Malignancies of the Nervous System?", Swettenham, E.; Witting, P.K.; Salvatore, B.A.; Neuzil, J., *J. Neurochem.*, **94**, 1448-1456 (2005).
4. "Vitamin E analogues: A New Class of Inducers of Apoptosis with Selective Anti-Cancer Effects", Neuzil, J.; Tomasetti, M.; Mellick, A.S.; Alleva, R.; Salvatore, B.A.; Birringer, M.; Fariss, M.W., *Current Cancer Drug Targets* 267-283 (2004).
5. "Origin of Avian Epidermal Appendages: The Bristles of the Wild Turkey Beard Express Feather-Type B Keratins", Sawyer, R.H.; Washington L.D.; Salvatore, B.A.; Glenn, T.C.; Knapp, L.W. *J. Exp. Zoology (Mol. and Dev. Evol)*, **297**, (2003).
6. Vitamin E analogs as Inducers of Apoptosis: Structure-Function Relationship", Birringer, M.; EyTina, H.J.; Salvatore, B.A.; Neuzil, J. *British J. Cancer*, **88**, 1948, (2003).
7. "Origin of Feathers: Feather Beta (b) Keratins Are Expressed in Discrete Epidermal Cell Populations of Embryonic Scutate Scales", Sawyer, R.H.; Salvatore, B.A.; Potylicki, T.-T.F.; French, J.O.; Glenn, T.C.; Knapp, L. *J. Exp. Zoology (Mol. Dev. Evol)*, **295B**, 12, (2003).
8. "NMR Spectroscopy-II", Salvatore, B.A. *Annual Reports on the Progress of Chemistry, Royal Society of Chemistry*, **95**, 395, (1999).
9. Total Synthesis of (+)-Calyculin A and (-)-Calyculin B: Cyanotetraene Construction, Asymmetric Synthesis of the C(26-37) Oxazole, Fragment Assembly, and Final Elaboration", Smith, A.B., III; Friestad, G.K.; Barbosa, J.; Bertounesque, E.; Duan, J.J.W.; Hull, K.G.; Iwashima, M.; Qiu, Y.P.; Spoors, P.G.; Salvatore, B.A. *J. Am. Chem. Soc.*, **121**, 10478, (1999).
10. "NMR Spectroscopy", Salvatore, B.A. *Annual Reports on the Progress of Chemistry, Royal Society of Chemistry*, **94**, 361, (1998).
11. Total Synthesis of (+)-Calyculin A and (-)-Calyculin B: Asymmetric Synthesis of the C(9-25) Spiroketal Dipropionate Subunit, Smith, A.B., III; Friestad, G.K.; Barbosa, J.; Bertounesque, E.; Hull, K.G.; Iwashima, M.; Qiu, Y.P.; Salvatore, B.A.; Spoors, P.G.; Duan J.J.W. *J. Am. Chem. Soc.*, **121**, 10468, (1999).
12. "Synthesis of a ¹⁵N, ¹³C-Labeled Lactam Analog of a G_M4-Lactone Cell-Surface Glycolipid", Salvatore, B.A.; Prestegard, J.H. *Tetrahedron Lett.*, **39**, 9319, (1998).
13. "Total Synthesis of (+)-Calyculin A and (-)-Calyculin B", Smith, A.B., III; Friestad, G.K.; Duan, J.J.W.; Barbosa, J.; Hull, K.G.; Iwashima, M.; Qiu, Y.; Spoors, P.G.; Bertounesque, E.; Salvatore, B.A. *J. Org. Chem.*, **63**, 7596, (1998).
14. "Total Synthesis of (+)-Acutiphycin and (+)-trans-20, 21-Didehydroacutiphycin", Smith, A.B., III; Chen, S.S.Y.; Nelson, F.C.; Reichert, J.M.; Salvatore, B.A. *J. Am. Chem. Soc.* **119**, 10935, (1997).
15. NMR Studies of a ¹³C, ¹⁵N-Labeled G_M4-Lactam Glycolipid at an Oriented Model-Membrane Interface", Salvatore, B.A.; Ghose, R.; Prestegard, J.H. *J. Am. Chem. Soc.*, **118**, 4001, (1996).
16. "Total Synthesis of (+)-Acutiphycin and (+)-trans-20, 21-Didehydroacutiphycin", Smith, A.B., III; Chen, S.S.-Y.; Nelson, F.C.; Reichert, J.M.; Salvatore, B.A. *J. Am. Chem. Soc.*, **117**, 12013, (1995).
17. "Calyculin Synthetic Studies. 3. Enantiomeric Purity Determination for the C(26)-C(32) Oxazole Segment via the Silks-Odom ⁷⁷Se NMR Method", Salvatore, B.A.; Smith, A.B., III *Tetrahedron Lett.*, **35**, 1329, (1994).
18. "Calyculin Synthetic Studies. 2. Stereocontrolled Assembly of the C(9)-C(13) Dithiane and C(26)-C(37) Oxazole Intermediates", Smith, A.B., III; Salvatore, B.A.; Hull, K.G.; Duan, J.J.W. *Tetrahedron Lett.*, **32**, 4859, (1991).

BIOGRAPHICAL SKETCH

Provide the following information for the key personnel and other significant contributors in the order listed on Form Page 2.
Follow this format for each person. DO NOT EXCEED FOUR PAGES.

NAME Elahe Mahdavian		POSITION TITLE Assistant Professor of Chemistry	
eRA COMMONS USER NAME			
EDUCATION/TRAINING (Begin with baccalaureate or other initial professional education, such as nursing, and include postdoctoral training.)			
INSTITUTION AND LOCATION	DEGREE (if applicable)	YEAR(s)	FIELD OF STUDY
Tabriz University, Tabriz, IRAN	<i>B.S.</i>	1987	<u>Chemistry</u>
Sharif University of Technology, Tehran, IRAN	<i>M.S.</i>	1991	<u>Organic Chemistry</u>
University of South Carolina, Columbia, SC	<i>Ph.D.</i>	1998	<u>Biochemistry</u>

RESEARCH/PROFESSIONAL EXPERIENCE

2003-present Assistant Professor of Chemistry, Louisiana State University, Shreveport, LA
 1999-2003 Assistant Professor of Chemistry, South Carolina State University, Orangeburg, SC
 1993-1998 Research & Teaching Assistant, University of South Carolina, Columbia, SC
 1991-1993 Chemistry Lecturer, Sharif University of Technology, Tehran, IRAN

Publications

1. **Elahe Mahdavian**, Trent Spencer, and Bruce Dunlap, "Kinetic Studies on Drug Resistant Variants of *Escherichia coli* Thymidylate Synthase: Functional Effects of Amino Acid Substitutions at Residue 4", Archives of Biochemistry and Biophysics, 368: 257-264, **1999**.
2. Jason Phan, **Elahe Mahdavian**, W. Minor, Sandra Berger, Trent Spencer, Bruce Dunlap, and Lucas Lebioda, "Catalytic Cysteine of Thymidylate Synthase is Activated Upon Substrate Binding", *Biochemistry*, 39: 6969-6978, **2000**.
3. Adisa Tomic-Vatic, H. John EyTina, James M. Chapmann, **Elahe Mahdavian**, Jiri Neuzil, and Brian Salvatore, "Vitamin E Amides, A New Class of Vitamin E analogs with Enhanced Pro-Apoptotic Activity, *International Journal of Cancer*, 117 (2), 188-193, **2005**.
4. Fan Wu, **Elahe Mahdavian**, and Brian A. Salvatore, "Total Synthesis of *Fusarochromanone* and its Novel Analogs", *J. Org. Chem*, **2007**, Manuscript In Preparation.

CURRENT AND PENDING SUPPORT

The following information MUST be provided for each investigator and other senior personnel.

NAME OF INVESTIGATOR: **Brian Salvatore**

Status of Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future

Contract Number/Proposal Title: **LEQSF (2005-08)-RD-A-15, "Synthesis of Novel Vitamin E Analogs with Potent Anti-Cancer Activity"**

Source of Support: **BORSF-RCS**

Award Amount (or Annual Rate): **\$ 66,542** Period Covered: **7/2005-6/2008**

Location of Activity: **LSUS**

Person-Months or % of Effort Committed to the Project: ☐ Cal Yr ☐ Acad ☒ 12.0% Summ

Status of Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future

Contract Number/Proposal Title: **Enhancement of the Chemistry Laboratory Courses at LSUS**

Source of Support: **BORSF - Traditional Enhancement Program**

Award Amount (or Annual Rate): **\$ 122,590** Period Covered: **7/2008- 6/2009**

Location of Activity: **LSUS**

Person-Months or % of Effort Committed to the Project: ☐ Cal Yr ☒ 5% Acad ☒ 5% Summ

Status of Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future

Contract Number/Proposal Title: **Bridging Molecular Modeling and Chemical Synthesis to Enhance Inquiry-Based Learning**

Source of Support: **BORSF - Traditional Enhancement Program**

Award Amount (or Annual Rate): **\$ 98,500** Period Covered: **7/2008- 6/2009**

Location of Activity: **LSUS**

Person-Months or % of Effort Committed to the Project: ☐ Cal Yr ☒ 5% Acad ☒ 5% Summ

Status of Support: ☐ Current ☐ Pending ☐ Submission Planned in Near Future

Contract Number/Proposal Title:

Source of Support:

Award Amount (or Annual Rate): \$ _____ Period Covered: _____

Location of Activity:

Person-Months or % of Effort Committed to the Project: ☐ Cal Yr ☐ Acad ☐ Summ

(Form 3, rev.2007)

CURRENT AND PENDING SUPPORT

The following information MUST be provided for each investigator and other senior personnel.

NAME OF INVESTIGATOR: **Elahe Mahdavian**

Status of Support: ☒ Current ☐ Pending ☐ Submission Planned in Near Future

Contract Number/Proposal Title: **LEQSF (2005-08)-RD-A-15, "Synthesis of Novel Vitamin E Analogs with Potent Anti-Cancer Activity"**

Source of Support: **BORSF-RCS**

Award Amount (or Annual Rate): **\$ 66,542** Period Covered: **7/2005-6/2008**

Location of Activity: **LSUS**

Person-Months or % of Effort Committed to the Project: ☐ Cal Yr ☐ Acad **12.0%** ☐ Summ

Status of Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future

Contract Number/Proposal Title: **Enhancement of the Chemistry Laboratory Courses at LSUS**

Source of Support: **BORSF - Traditional Enhancement Program**

Award Amount (or Annual Rate): **\$ 122,590** Period Covered: **7/2008- 6/2009**

Location of Activity: **LSUS**

Person-Months or % of Effort Committed to the Project: ☐ Cal Yr **5%** Acad **5%** ☐ Summ

Status of Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future

Contract Number/Proposal Title: **Bridging Molecular Modeling and Chemical Synthesis to Enhance Inquiry-Based Learning**

Source of Support: **BORSF - Traditional Enhancement Program**

Award Amount (or Annual Rate): **\$ 98,500** Period Covered: **7/2008- 6/2009**

Location of Activity: **LSUS**

Person-Months or % of Effort Committed to the Project: ☐ Cal Yr **5%** Acad **5%** ☐ Summ

Status of Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future

Contract Number/Proposal Title: **Enhancement of the Biochemistry Laboratory Courses at LSUS**

Source of Support: **BORSF - Traditional Enhancement Program**

Award Amount (or Annual Rate): **\$ 72,432** Period Covered: **8/2008- 7/2009**

Location of Activity: **LSUS**

Person-Months or % of Effort Committed to the Project: ☐ Cal Yr **5%** Acad **5%** ☐ Summ

Status of Support: ☐ Current ☒ Pending ☐ Submission Planned in Near Future

Contract Number/Proposal Title: **Enhancement of Spectrophotometry in Biochemistry Laboratory**

Source of Support: **BORSF - Undergraduate Enhancement Program**

Award Amount (or Annual Rate): **\$ 58,200** Period Covered: **7/2008- 6/2009**

Location of Activity: **LSUS**

Person-Months or % of Effort Committed to the Project: ☐ Cal Yr **5%** Acad **5%** ☐ Summ

(Form 3, rev.2007)

***Appendix A -- Equipment Manufacturer's
Price Quotes***



Attachment A to License/Service Agreement
Louisiana State University

Quote ID		Quote Start Date		Quote Expiration Date	
SAN-NDE-400304		17-Oct-2007		30-Apr-2008	
Qty	Product Name	Description	Unit Price	Total	
1	PR3016 DS STANDALONE	The visual framework (core) to the DS client-server environment. Provides tools for sequence and 3D structure characterization, visualization, analysis, PERL scripting, charting, job monitoring, file access, and modeling of molecular systems, all integrated through an easy-to-use environment, giving you seamless flow of information between all DS products. Includes the local Pipeline Pilot Server. Required for all DS server modules. Formerly DS Visualizer Pro Enterprise. Duration: Perpetual Maintenance: Annual	2,142.90	2,142.90	
1	PR11785 DS CATALYST SCORE	Performs fitting and scoring of conformations to a particular hypothesis or pharmacophore. Provides various possible model permutations, mappings and conformations. Duration: Perpetual Maintenance: Annual	4,464.30	4,464.30	
1	PR11787 DS CATALYST HYPOTHESIS	Automated pharmacophore model generations to include HypoGen (3D-QSAR Quantitative Pharmacophore), HipHop (Common Feature Pharmacophore), and HypoRefine (Excluded Volume from Inactives). Duration: Perpetual Maintenance: Annual	8,571.45	8,571.45	
1	PR11786 DS CATALYST CONFORMATION	Diverse conformational generator algorithms for coverage of chemical space. Duration: Perpetual Maintenance: Annual	3,750.00	3,750.00	
1	PR1517 DS LUDI	Used for Receptor-based de novo searching of fragments (Receptor mode) and for building on an existing ligand scaffold (Link mode). Ludi score functionality is also available in DS LigandScore to Ludi users. Duration: Perpetual Maintenance: Annual	3,571.50	3,571.50	
1	PR1515 DS LIGANDFIT	Provides docking capabilities previously available in C2.LigandFit. Additional functionality includes full parallelization on all platforms and option to concatenate experiments automatically with in situ ligand minimization using DS CHARMM Lite and scoring using DS LigandScore. Duration: Perpetual Maintenance: Annual	3,035.70	3,035.70	

Quote ID		Quote Start Date		Quote Expiration Date	
SAN-NDE-400304		17-Oct-2007		30-Apr-2008	
Qty	Product Name	Description	Unit Price	Total	
1	PR1516 DS LIGANDSCORE	DS LigandScore enables the user to objectively evaluate ligand-protein interactions with scoring functions and their individual descriptors. The scoring functions include LigScore2, PLP1, PLP2, Jain, PMF, and Ludi energy estimates (Ludi energy estimates require a DS Ludi license). Also, a Consensus Score can be calculated from scoring results to rank ligands in virtual screening studies. Duration: Perpetual Maintenance: Annual	1,607.10	1,607.10	
1	PR2444 DS BIOPOLYMER	For building and modifying peptides, proteins, DNA and RNA. Perform DelPhi electrostatics and solvation calculations. Includes X-BUILD and X-LIGAND basic x-ray crystallography functionality. Duration: Perpetual Maintenance: Annual	5,357.10	5,357.10	
1	PR2463 DS CFF	A Class II force field derived within a consistent quantum mechanical framework, including anharmonicity and cross terms. Optimized to describe common organic and biomolecular chemical functional groups. Duration: Perpetual Maintenance: Annual	2,857.20	2,857.20	

Quote ID		Quote Start Date	Quote Expiration Date	
SAN-NDE-400304		17-Oct-2007	30-Apr-2008	
Qty	Product Name	Description	Unit Price	Total

1	PR3276 TEACHING LICENSE	Teaching License. The Software subject to this teaching license may be used solely for teaching purposes. "Teaching purposes" means use of the Software for course instruction, course homework and student research required as part of a course, even if such student research may result in publication by the student of the paper submitted for course credit (Customer agrees to use reasonable efforts to provide Accelrys with copies of any such papers that reference use of the Software). For purposes of this Agreement, "course" means a University offered course or seminar with a specific course description and number and a reasonable classroom instruction component (i.e. not an "independent study" course or seminar). "Teaching purposes" does not include other research (independent or sponsored), even if such research would result in credit toward a degree. Customer agrees that its points of contact for Accelrys maintenance and support of the Software subject to this teaching license will be limited to one designated employee of Customer at any one time, who will act as the support liaison between Accelrys and Customer, and that hotline support services for the Software subject to this teaching license will be available to Customer only via electronic mail communication. The following Software is included in this license: Duration: 60 months Maintenance: Annual	2,000.00	2,000.00
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Quote ID	Quote Start Date	Quote Expiration Date
SAN-NDE-400304	17-Oct-2007	30-Apr-2008

TOTALS:	
Sub Total	37,357.25
Total Discount	12,375.03
Total	24,982.22
Prices are Quoted in US DOLLARS	

Accepted By

S I G N H E R E	Customer		Accelrys Software Inc. (For itself and its affiliates)	
	Signature		Signature	
	Name (Please Print)		Name (Please Print)	
	Title		Title	
	Date	PO#	Date	



CEM Corporation

3100 Smith Farm Rd. - Matthews, NC 28104 -
Phone: 800-726-3331 - Fax: 704-821-5185 - Email: sales@cem.com

QUOTE

	Quote #
10/22/07	CEMQ3367

LOUISIANA STATE UNIVERSITY

Brian Salvatore

One College Place
Dept of Chemistry & Physics
SC 308
Shreveport, LA 71115

Phone: 318-797-5224

Fax: 318-797-5090

Please Provide Billing Information If Different Than Quote

Contact _____

Address _____

City _____ State _____

Zip _____

Phone _____ Fax _____

<u>Ln #</u>	<u>Part #</u>	<u>Description</u>	<u>Qty.</u>	<u>List Price</u>	<u>Unit Price</u>	<u>Ext. Price</u>
1	925461	Explorer 48-position Automation System Discover S-class unit and Explorer 48 automation deck. Package supports automated handling capability for both 10- and 35-mL elevated pressure vials with IntelliVent snap-on caps and septa, as well as the capability for atmospheric pressure reactions. The package also includes an accessory kit containing: (1) 10mL pressure vial attenuator adapter, (1) 35mL pressure attenuator, (1) atmospheric pressure attenuator, (4) vial racks that accommodate both 10- and 35-mL vials, (1) starter set of 10mL pressure vials with caps and septa (100 each), (1) starter set of 35mL pressure vials with caps and septa (25 each), (1) pack of 50- 3mm stir bars, (5) egg-shaped 19mm X9.5mm stir bars (non rare earth), (1) pressure regulator, (1) 6 ft. length of 1/4 in. cooling tubing, (1) microwave synthesis textbook on CD-ROM, (1) calibration tool, (1) operation manual and (1) external controller with Synergy control software.	1	\$39,000.00	\$39,000.00	\$39,000.00

<u>Ln #</u>	<u>Part #</u>	<u>Description</u>	<u>Qty.</u>	<u>List Price</u>	<u>Unit Price</u>	<u>Ext. Price</u>
2	909020	Camera Option The Camera Option provides the ability to view reactions during microwave irradiation.	1	\$7,650.00	\$7,650.00	\$7,650.00
3	921220	Installation and Training, 1/2 Day (Life Sciences) This service provides for a one-half day training session for users on operation, routine maintenance, and basic applications for the instrumentation platform.	1	\$970.00	\$0.00	\$0.00
4	*99	ACADEMIC DISCOUNT	1	-\$1,866.00	-\$1,866.00	-\$1,866.00
Total						\$44,784.00

Comments

Sales Rep	Terms	P.O. Number	Ship Via
Greg Barlow	Net 30 Days		

Please sign here

Note: This quote can be used as a purchase order by entering purchase order number and signing

Date

Delivery is **28** days ARO

Quote expiration date: **12/21/2007**

**For information on leasing CEM products, contact Tammy Grimshaw at
CEM Financial Services Phone 973-292-0025 X14**

Terms

1. Payment - Make all checks payable to CEM Corporation and mail to Accounts Receivable at the address given below.
2. General - Net 30 Days FOB Matthews, NC. Freight is prepaid and added to invoice. Clerical errors are subject to corrections.
3. All orders subject to shipping and handling charges.
4. Taxes - All prices are quoted exclusive of any sales, excise, use or similar tax. The amount of tax applicable is the buyers responsibility.
5. Renters Casualty - Renter shall bear the risk of loss or damage to the equipment from delivery to customer site until it is returned to CEM.
6. Warranty - All instruments are warranted against defects in workmanship or material for one (1) year from the date of shipment.
7. Returns - All returns must be authorized with an RMA# by the CEM customer Service Department. Call (800) 726-3331 for authorization.
8. Quantity - Any changes to quantities other than complete instruments will not effect the validity of this quote.



Dr. Brian Salvatore
Louisiana State University
10013 Commander Drive
Shreveport, LA, 71106
USA
318 797 5224
318 797 5090
brian.salvatore@lsus.edu

► **PerkinElmer Instruments**

710 Bridgeport Avenue
Shelton

CT 06484-4794

Phone: 800.762.4000

Fax: 203.944.4914

Website: <http://perkinelmer.com>

Preliminary Quotation

JLMUSD0547

Prepared By: JERRY MAINE

Quotation Date: 10/22/2007

Valid Until Date: 12/21/2007

Your ref:

LSUS Polarimeter

Part Number	Qty	Description	Unit	Value
L3000014	1	MODEL 343 POLARIMETER - PC READY (60Hz)^	21,600.00	21,600.00
09991420	1	MAINS LEAD USA 2M 125V 16A	38.00	38.00
B0041693	1	STANDARD CELL 10CM/6.2ML	634.00	634.00
Sub Total				22,272.00
discount				2,160.00
Total				20,112.00

Notes:

This is a preliminary quotation and is issued for budgetary purposes only. Prices and terms may differ from those appearing on this form. Any orders resulting from this preliminary quotation are subject to acceptance by PerkinElmer in Shelton, CT, USA.