<table>
<thead>
<tr>
<th>Title</th>
<th>Elemental Analysis Workstation</th>
<th>Request Date</th>
<th>12/13/2011</th>
</tr>
</thead>
<tbody>
<tr>
<td>Department</td>
<td>Chemistry and Biochemistry</td>
<td>Email</td>
<td><a href="mailto:livinghouse@chemistry.montana.edu">livinghouse@chemistry.montana.edu</a></td>
</tr>
<tr>
<td>Requestor</td>
<td>Professor Thomas Livinghouse</td>
<td>Phone</td>
<td>994-5408</td>
</tr>
</tbody>
</table>

### STRATEGIC ALIGNMENT

### Core Themes and Objectives
(check all that apply)

#### Educate Students
- [ ] Our graduates will have achieved mastery in their major disciplines
- [ ] Our graduates will become active citizens and leaders
- [ ] Our graduates will have a multicultural and global perspective
- [ ] Our graduates will understand the ways that knowledge & art are created and applied in a variety of disciplines
- [x] Our graduates are prepared for careers in their field
- [ ] We will provide increased access to our educational programs
- [x] Communities and external stake holders benefit from broadly defined education partnerships with MSU

#### Create Knowledge and Art
- [x] Students, faculty, and staff will create knowledge and art that is communicated widely

#### Serve Communities
- [x] We help meet a fundamental need of the citizens of Montana by providing degree programs for our students
- [ ] We help meet the educational needs of the citizens of Montana by providing a wide range of educational opportunities to a variety of students
- [x] Our students, faculty, staff, and administrators reach out to engage and serve communities
- [ ] Our students, faculty, staff, and administrator reach in to build the university community

#### Integrate Learning, Discovery, and Engagement
- [x] Each graduate will have had experiences that integrate learning, discovery and engagement
- [x] Outreach activities will educate students and address the needs of the communities we serve
- [x] Students, faculty, and staff will create knowledge and art that addresses societal needs
- [ ] MSU is a community that will be characterized by synergy within and across disciplines, roles and functions.

#### Stewardship
- [ ] The public trusts the institution to operate openly and use resources wisely
- [ ] The faculty and staff are well-qualified and supported
- [x] MSU will support Native American students, programs, and communities
- [x] MSU will be an inclusive community, supporting and encouraging diversity
- [ ] Our publicly provided resources are used efficiently and effectively
- [ ] Natural resources are used efficiently and sustainably
- [ ] MSU nurtures a culture of resource conservation and ecological literacy among students, faculty and staff
- [x] Our physical infrastructure (e.g., building, equipment, open spaces) will be well-maintained and useful
INSITUTIONAL BENEFIT

<table>
<thead>
<tr>
<th>Campuses</th>
<th>Bozeman</th>
<th>☑</th>
<th>Billings</th>
<th>☑</th>
<th>Havre</th>
<th>☑</th>
<th>Great Falls</th>
<th>☑</th>
<th>FSTS</th>
<th>☑</th>
<th>Extension</th>
<th>☑</th>
<th>MAES</th>
</tr>
</thead>
</table>

Cross Depts

Please List: ______________________________________  ______________________________________

TIMEFRAME

<table>
<thead>
<tr>
<th>Proposed Dates</th>
<th>Start: 4/1/2012</th>
<th>End: N.A.</th>
</tr>
</thead>
</table>

COST AND REQUIREMENTS

<table>
<thead>
<tr>
<th>Funding Type</th>
<th>One-Time ($)</th>
<th>Multi-Year ($)</th>
<th>Base ($)</th>
<th>FTE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Personnel (w/benefits)</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Materials &amp; Supplies</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Travel</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Contracted Services</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Capital</td>
<td>$ 45,000.00</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Other Operations</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>TOTAL</td>
<td>$ 45,000.00</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

This is a request for a much needed piece of capital equipment. Specifically, $45,000.00 is requested for a FLASH 2000 Series Carbon/Hydrogen/Nitrogen/Sulfur/Oxygen Analyzer. Elemental analysis is a critical technique for the characterization of organic and inorganic compounds of the type synthesized by several research groups in the Department of Chemistry and Biochemistry. The department currently has no in-house means for performing this important procedure. We currently also lack the ability to reliably perform High Resolution mass spectra on small molecules. These services currently must be performed externally at a high cost and with reduced efficiency.
PROPOSAL SCOPE
Describe the Proposal

The specifications for this scientific instrument are as follows:

- Conceived as a flexible platform; designed as a reliable 24/7 solution
- Simple, precise and cost-effective tool offers accurate, simultaneous CHNS determination as well as versatile, precise oxygen determination
- Combustion reactor reaches 1800 degrees Celsius, at which temperature both organic and inorganic substances are converted into elemental gases which, after further reduction, are separated in a chromatographic column and delivered to thermal conductivity detector
- Oxygen determination is achieved by pyrolysis reactor; sulfur determinations are made possible by flame photometric detector (FPD)
- Features improved speed of analysis and ease of use, with highest sample throughput for either solid and liquid samples; analysis time: CHN 8 min.; CHNS, 10 min.; Oxygen, 5 min.
- Highest degree of accuracy is ensured by complete conversion of sample to elemental gases without dilution or splitting
- Requires minimal maintenance downtime
- Boasts powerful, fully digital instrument control and data handling software
- Dedicated Eager Xperience software is able to satisfy virtually every analytical request (i.e. evaluate and present the data, and provide personalized reporting dedicated features for QC labs)
- Local Area Network connection

The research groups of Professors Mary Cloninger (bioorganic chemistry), Robert Szilagyi (inorganic and physical chemistry), Tom Livinghouse (organometallic chemistry), Trevor Rainey (organic synthesis), Paul Grieco (organic synthesis), Trevor Douglas (bioinspired materials chemistry), and others will benefit greatly from the acquisition of this analytical instrument. Two excerpts of the research component and impact of this proposal follow:

- Dr. Robert Szilagyi: The availability of a CHNS/O Analyzer, such as a fully automated Flash 2000 Series from Thermo Scientific would be a long desired instrument for my research group. Currently, we send our samples to Columbia Analytical Services, Inc. in Tucson, Arizona for similar analysis to be done for about $500 each sample. For transition metal content, we built collaboration with Prof. Robin Gerlach’s research group from the Chemical and Biological Engineering Department. The proposed instrument would be essential for complementary low-Z element analysis. Quite often we deal with chemical compounds that are difficult to crystallize or oily compounds. However, most often the crystallinity is not needed at all for spectroscopic characterization, but we must know the exact composition in order to correct for contamination of excess starting material or potential side products that could contribute to spectral features and thus hinder the quantitative analysis. Specifically, the exact knowledge of sulfur and nitrogen content is essential in characterizing nickel coordination complexes with N- and S-ligands. We study these compounds to understand the atomic scale mechanism of sunlight responsive windows by characterizing the chromophore with UV-vis electronic absorption and X-ray electron core excitation techniques. Furthermore, the sulfur content is also needed for characterizing the chemical composition of Fe-S molecules, particles, and minerals. The atomic absorption and inductive coupled plasma-based Fe content would be well supplemented with the proposed S analyzer. By knowing the concentrations, we can further develop the multi-edge X-ray absorption spectroscopic technique from an electronic structural tool to a powerful analytical technique to study homogeneous and heterogeneous catalytic systems based on Fe-S composition.
• Dr. Mary Cloninger: Although the macromolecules that are a primary focus of interest in the Cloninger research group can be characterized using matrix-assisted laser desorption ionization time of flight (MALDI-TOF) mass spectrometry, the component smaller molecules that are used to synthesize our macromolecules require characterization using mass spectrometry techniques which are not currently available at Montana State University. We routinely synthesize carbohydrate derivatives, and acquisition of mass spectral data for these compounds is of necessity out-sourced. For one project this semester, we synthesized six carbohydrate derivatives in the span of two weeks that could not be characterized using existing instrumentation at MSU. In the future, all of these small molecules will be characterized using elemental analysis with the proposed instrument at MSU. Leading journals require such characterization prior to publication. The Journal of Organic Chemistry, for example, states "For most new compounds, the data should include HRMS or elemental analysis data, and copies of proton and carbon NMR spectra in the supporting information."
This elemental analysis instrumentation will be used for summer training of MAP (Montana’s Apprenticeship Program) students. Students will bring in "smell samples" - flowers, perfume, plants - to analyze using the new equipment. Each summer, the MAP program brings 20-30 high school students to the MSU-Bozeman campus for a six-week enrichment experience. MAP students are primarily from high schools on Montana’s Native American Indian Reservations. In addition, eighth graders at the local middle schools will be able to use the new instrumentation. We will create a unit for economically underprivileged 8th graders from Livingston using elemental analysis to practice fractions while also learning about molecules. Mrs. Wendy Dlakic, an 8th grade science teacher at Sleeping Giant Middle School in Livingston, brings students to campus four times per year for enrichment activities. Finally, the new instrumentation will be used in training workshops with REU (Research Experience for Undergraduates) students. These students are primarily from small colleges that have no (or very minimal) research opportunities and are located in the upper Northwest region of the United States. Priority admission is given to Native American and Tribal College students. Workshops to teach the REU students how to use instrumentation including NMR, MALDI, EPR, and X-ray crystallography are provided weekly. The REU program is a 10-week summer research program that has been offered since 2000 in the Department of Chemistry and Biochemistry, reaching 138 students including 33 Native American students.

The proposed instrumentation will also be incorporated into the curriculum for undergraduate laboratory experiments. In Honors Organic Chemistry I, the students learn about purification techniques including recrystallization, distillation, and chromatography. They learn about characterization techniques including infrared spectroscopy, nuclear magnetic resonance spectroscopy, gas chromatography, melting point determination, and mass spectrometry. However, we do not currently have any way to teach the students about elemental analysis, and the mass spectroscopy instrumentation that is appropriate for use in the teaching labs is limited to one GC-MS instrument that must be run by a technician rather than by the students. The class would be dramatically improved if students could perform elemental analyses on their recrystallization products. In Honors Organic Chemistry II, the students perform many reactions. This class would be dramatically improved if students could perform routine elemental analysis characterization of the molecules that they synthesize.

We will start integrating the instruments into teaching labs by incorporating them into the Honors Organic series. Then, we will include these instruments in upper level undergraduate instrumentation/analytical courses and (as needed) also in the physical chemistry laboratory class. This will allow students who will graduate with a chemistry or biochemistry undergraduate degree to obtain first-hand knowledge of how to use state-of-the-art instrumentation, improving their preparation for graduate school and for the workforce.
### ADDITIONAL INFORMATION

#### Implementation Plan (Please describe with timelines)

The instrument will be ordered and installed upon successful procurement of funding. Upon installation, all of the faculty whose research will most directly benefit from the availability of elemental analysis will be trained in the use of the instrument. Graduate students will also be trained on the use of the instrument immediately; undergraduates and middle school students will begin using the instrument during the first semester after the instrument has been installed. Summer MAP and REU (high school and small college) students will use the instrument each summer.

#### Assessment Plan (Please describe with indicators)

REU and MAP students fill out anonymous questionnaires about the instrument training workshops at the conclusion of each summer. Undergraduate students fill out course evaluations at the end of each semester. Middle school students fill out evaluations at the end of each field trip to MSU. These assessments will be used to refine the training workshops and protocols that are available to the users. In addition, use by graduate students for research projects will be monitored to ensure that appropriate training and technical advice is provided as needed by faculty.

#### If assessed objectives are not met in the timeframe outlined, what is the plan to sunset this proposal?

This instrument is definitely needed by members of the Department of Chemistry and Biochemistry and by the constituent groups that we serve. Because the objective of the proposal is to provide access to faculty, graduate students, undergraduate students, summer students, and local K-12 students, we cannot envision any circumstances for which “sunsetting” this program would be appropriate.
<table>
<thead>
<tr>
<th><strong>SIGNATURES</strong></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Department Head (please print)</strong></td>
<td><strong>Signature (required)</strong></td>
<td><strong>Date</strong></td>
</tr>
<tr>
<td>Bern Kohler</td>
<td>[Signature]</td>
<td>12-21-2011</td>
</tr>
<tr>
<td><strong>Dept Head Priority (please circle one):</strong></td>
<td>Very High</td>
<td>High</td>
</tr>
<tr>
<td><strong>Dean/Director (please print)</strong></td>
<td><strong>Signature (required)</strong></td>
<td><strong>Date</strong></td>
</tr>
<tr>
<td>Paula Lutz</td>
<td>[Signature]</td>
<td>1-3-12</td>
</tr>
<tr>
<td><strong>Dean/Director Priority (please circle one):</strong></td>
<td>Very High</td>
<td>High</td>
</tr>
<tr>
<td><strong>Executive/VP (please print)</strong></td>
<td><strong>Signatures (required)</strong></td>
<td><strong>Date</strong></td>
</tr>
<tr>
<td><strong>Executive/VP Priority (please circle one):</strong></td>
<td>Very High</td>
<td>High</td>
</tr>
</tbody>
</table>