

Mississippi EPSCoR Program Research Activities Annual Reporting (REVISED 2/17/03 FORM)

Each investigator in the Mississippi EPSCoR Program should complete this form for activities from **Jan. 1, 2003 through October 31, 2004**. No activities occurring outside that time frame should be reported. The completed form is due to your **Cluster Technical Director** and to **this office (barbara@research.msstate.edu)** by **May 1**. Each lettered item below is a tally of the corresponding letters on succeeding pages. Please be complete. Co-authors and co-investigators should coordinate reports before submitting them.

NOTE: Except for Section I, Nos. 1 & 2, the material you report does not need to be related directly to the EPSCoR project. The EPSCoR program is concerned with competitiveness of researchers, so tracks all professional activity. Section I, No. 3 may include findings from the previous EPSCoR funding.

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University **Mississippi College**
Primary Discipline **Theoretical Chemistry**
Department **Department of Chemistry**
Project Cluster **Computational Chemistry Cluster - Computation of Conventional Strain Energy in Small Heterocycles**

Activity Report for Period Jan 1, 2003 to Oct. 31, 2004

- A. Number of Refereed Journal Articles 1
- B. Number of Invited Presentations 2
- C. Number of Theses/Dissertations Completed under Your Direction 4
- D. Number of Books 0
- E. Other developments/products 0
- F. Number of Patents 0
- G. Number of Proposals Submitted 3
- H. Number of Awards Received 2
(Do not include EPSCoR awards or any on-campus awards)
- I. Project Activities/Accomplishments
(do not tally on this page; just include in section I)

Additional Information: For each item enumerated on the preceding page, please provide the requested information in the following data base format. Copy/paste the requested info under each letter as many times as there are items to report.

A. Refereed Publications

Title Conventional Strain Energy in the Oxadiazetidines
Year 2004
Author(s) Christopher W. Benton and David H. Magers
Journal name *International Journal of Quantum Chemistry*
Volume number in press
Page numbers
Results of EPSCoR Yes No
In NSF support formally acknowledged? Yes No

B. Invited Presentations

Title Computation of Ring Strain in Small Cyclic Compounds
Organization Department of Chemistry, Samford University
Location Birmingham, Alabama
Date October 2, 2003

Title What Is Science and What Is Not
Organization College of Arts and Sciences Distinguished Lecture Series,
Mississippi College
Location Clinton, Mississippi
Date October 23, 2003

C. Theses/Dissertations Completed Under Your Direction

Title *Computational Studies of 2,4,6-trinitrotoluene and Its Anionic Complexes*
Degree B.S., Senior Honors Thesis
Author Laura Jamison Lewis
Month/Year. May, 2004

Title *Conformational Energetics of Naphthylquinoline Derivatives*
Degree B.S., Senior Honors Thesis
Author Margie Jeanann Lovell
Month/Year. May, 2004

Title *Conventional Strain Energy in the Diazetidines, Diphosphetanes, Thiaphosphetanes, & Thiadiphosphetanes*
Degree B.S., Senior Honors Thesis
Author Patricia Leigh Honea
Month/Year. May, 2004

H. Awards

Investigator(s) David H. Magers and G. Reid Bishop
Title "An MRI/RUI proposal for a 32-processor Beowulf cluster for the calculation of molecular properties: Application of *ab initio* and density functional methods to quantitative structure thermodynamic relationships"

Funding Source National Science Foundation

Amount [No university match]

1. Full Multi-year Amount \$73,825

2. Current Year Amount Awarded \$73,825

Dates of project

1. Multi-year Beginning Date (09/01/03) and Ending Date (08/31/05)

2. Current year Beginning Date (09/01/03) and Ending Date (08/31/04)

Funding Source Award No. DBI-0321397

Investigator(s) G. Reid Bishop, David H. Magers, and Edward J. Valente

Title "Folding and binding energetics of DNA aptamers"

Funding Source The Mississippi Functional Genomics Network from the National Institutes of Health

Amount [No university match]

1. Full Multi-year Amount \$29,997

2. Current Year Amount Awarded \$29,997

Dates of project

1. Multi-year Beginning Date (07/01/03) and Ending Date (04/30/04)

2. Current year Beginning Date (07/01/03) and Ending Date (04/30/04)

I. Project Activities/Accomplishments

1. Equipment purchased (list with \$ value) - *list for your cluster director=s report, especially if you are on a different campus or in a different department from your cluster director*

One Dual Opteron Workstation from Microway comprising \$4813.00
two AMD Opteron 244 cpus with 1 MB L2 Cache each,
1 GB RAM, and 146 GB SCSI hard drive

Three Optiplex 3.20 GHz Pentium4 personal computers \$4066.44
From Dell (an additional \$983.22 paid by another grant)

2. New courses as a result of the cluster emphasis NA

3*. Science nuggets

My six undergraduate research students have attended 13 conferences and made 57 presentations since January 1, 2003. In addition, four Senior Honors Theses were completed this semester. At the conferences attended, my two students who were considering attending graduate school both made contacts and were offered top fellowships at several graduate schools. My student Ashley Ringer who has been paid by NSF EPSCoR funds for two summers will be attending Georgia Institute of Technology in the fall where she has accepted one of their top, school-wide graduate fellowships.