

MEMORANDUM

07 April 2004

To: MPS Advisory Committee

From: Michael S. Turner, AD/MPS

Subject: Response to the Division of Chemistry Committee of
Visitors Report

Please find attached the MPS response to the Committee of Visitors (COV) report from the 3-5 February 2004 COV review of the Division of Chemistry. The review was thorough and insightful, and the findings will be very helpful to me and to the Division of Chemistry in fulfilling our responsibilities to the scientific community and to the nation.

The Division of Chemistry drafted the attached response, and I concur with its substance. I therefore adopt it as the official response of the MPS Directorate. I hope the full MPS Advisory Committee finds this COV review and the MPS response useful and acceptable.

Division of Chemistry Response to Findings and Recommendations of the Committee of Visitors

February 3-5, 2004

The Committee of Visitors (COV) met February 3-5, 2004, at the National Science Foundation to review:

- The integrity and efficiency of the processes used to solicit, review, recommend and document proposal actions, and the technical management of awards made by programs;
- The relationships between award decisions, program goals, and Foundation-wide programs and goals;
- Results, in the form of outputs and outcomes of NSF investments for the relevant fiscal years, as they relate to the Foundation's current strategic goals and annual performance goals;
- The significant impacts and advances that have developed since the previous COV review and their link to NSF investment, regardless of when these investments were made; and
- Response of the programs under review to recommendations of the previous COV review.

The Division is pleased that the COV feels that the Division is "operating extremely well" and that it "was impressed with the quality and effectiveness of the Program Officers, Executive Officer and Division Director in managing a large portfolio of tasks." We are gratified that the COV found that the balance across the Division's investments was appropriate, including the high level of support for core, individual investigator awards and for undergraduate research, and that the Division had effectively integrated research and education. In connecting the Division's performance to the NSF Strategic Plan, the COV observed that "The Chemistry Division is a success story: it supports a diverse, internationally competitive workforce of scientists, engineers, and well-prepared citizens." The COV identified a number of areas in which the Division could improve its internal processes, better communicate with the community, and work with the community to address challenges and opportunities in basic research and education. Comments on the major recommendations of the COV are given below.

Internal processes

The COV reiterated an observation made by the last COV: "The workload of the Division is huge." A number of suggestions to address this issue were made by the COV.

1. Increase the number of program officers and perhaps alter the balance of permanent to rotator program officers.

Response and Action. The Division will explore these and other options for addressing the workload issue in the context of a new strategic goal for NSF, called “organizational excellence”. The Division has been at the forefront of testing new technologies like eJacket that are part of a move to all-electronic processing of proposals. Implementation of eJacket has significant human resource implications for the Division. We will be evaluating its impact with respect to the number and type of staff needed.

January 1, 2005 Update. The Division has advertised nationally for permanent staff members in its Experimental Physical Chemistry and Theoretical and Computational Chemistry programs. We hope to fill these positions soon. We have introduced the position of Senior Science Advisor to the Division, initially on a part-time basis. A Science Assistant added by the Division has been extremely effective in addressing a variety of workload issues, and the Division is planning to add a second Science Assistant soon. Other personnel changes will reflect further developments in eJacket and the nature of the Division’s workload.

2. Add a second deadline for the submission of proposals, increase grant duration and the number of creativity renewals.

Response. Adding a second window should spread the workload over a longer timeframe, but would then reduce the number of proposals that can be compared directly when funding recommendations are made. The Division will consider this possibility. The suggestion of making longer grants is consistent with NSF’s plans to expand the length and size of awards. The Division has begun to move in this direction with increased use of four-year awards based on peer review and creativity extensions, but the extent to which this can be done depends on the Division’s resources. The number of creativity extensions is limited by NSF policy.

January 1, 2005 Update. The Division is continuing to explore alternative models for receiving unsolicited proposals, such as a second window. We will likely not make any changes before FY2007, as some time is needed to assess the impact of new tools like intelligent databases (see below) on workload. The Division has continued to make a limited number of four-year awards based on merit review, and is awarding nearly the maximum allowable number of creativity extensions.

3. Use tools like intelligent databases and SciFinder.

Response and Action. We agree that the Division could benefit substantially by using intelligent databases that facilitate reviewer selection and identify conflicts

of interest. The Division will investigate whether this is feasible and, if so, how it is most easily and economically accomplished.

January 1, 2005 Update. The Division has contracted to establish an intelligent reviewer database and has collected information on areas of expertise from its community electronically. Reviewer-identified expertise areas will be used to facilitate identification of suitable reviewers. The system is being implemented at the start of 2005. The NSF's library is currently exploring adding SciFinder to the Foundation's resources.

Communication with the community

Several issues were raised by the COV that call for enhanced communication with the community.

4. The Division was pleased to learn that the Dear Colleague letter of 2002 addressing the broader impacts review criterion has "decreased the anxiety" in the community. The COV notes, however, that "more needs to be done to educate the community" and suggests the use of additional instructions.

Response. The Division will explore possible mechanisms for helping reviewers better integrate this criterion into their reviews, but does not want to be overly prescriptive in what it requests or how to weight this criterion. We recognize that educating the community is a process that takes some time, and we will work with the community to achieve better consistency.

January 1, 2005 Update. The Division has published a second Dear Colleague letter, 04-045 (<http://www.nsf.gov/pubsys/ods/getpub.cfm?nsf04045>). This letter invites PIs to submit nuggets that illustrate the broader impacts of their work. Chemists on the Mathematical and Physical Sciences Advisory Committee (MPSAC) have selected a set of illustrative nuggets from among the submissions. PIs who submitted the selected nuggets will be invited to present their work at a Division-sponsored poster session at the 2005 Fall ACS National Meeting in Washington, D.C. We intend to publicize this session extensively and use it as an opportunity to continue discussions with the community on the broader impacts of Division-supported awards.

5. The COV considered mechanisms for providing feedback to PIs on proposals, such as sending a redacted, written version of the review analyses prepared by Program Officers, and expressed concern over panel summary reviews, which were felt to be uneven.

Response and Action. In providing feedback to PIs on their proposals, the Division's staff prefers to speak with PIs after they have read the reviews and

believes this to be the most effective way to describe the decision made on a proposal. It also enables staff members to mentor unsuccessful PIs so that they can craft stronger proposals. For proposals reviewed by panels, the Division agrees that summaries have been uneven and will identify and implement mechanisms to ensure that PIs receive adequate information about the decisions. A suggestion was made about communicating the planned use of panel reviews to PIs, but this is not always feasible because of timing issues, nor does the Division have evidence to indicate that it affects the outcome of the review.

January 1, 2005 Update. The Division has formed a committee that is developing guidelines for ensuring that panel summaries are consistently prepared in a manner that will provide adequate information to PIs regarding decisions on their proposals. We expect to implement their recommendations early in 2005.

6. The COV discussed the removal of the cost-sharing requirement for individual instrumentation requests that has occurred since the last COV report and noted that the impact needs to be assessed, as it could result in significantly fewer awards.

Response and Action. The Division will indeed track the impact of this change and report back to the community. An associated issue that was raised was whether the Division should provide support for technical personnel to operate and maintain the instruments. The community seems comfortable with the PI's institution rather than the Division bearing this cost, and the Division has no immediate plans to change this practice.

January 1, 2005 Update. Results from FY2004 data indicate that in this first year during which no cost sharing was required on individual instrumentation requests, there was little effect: instrumentation accounted for about 10% of individual investigator awards, as it has the past few years. However, there may be a lag in community awareness of this change in practice, and the Division will continue to monitor the situation.

Challenges and opportunities

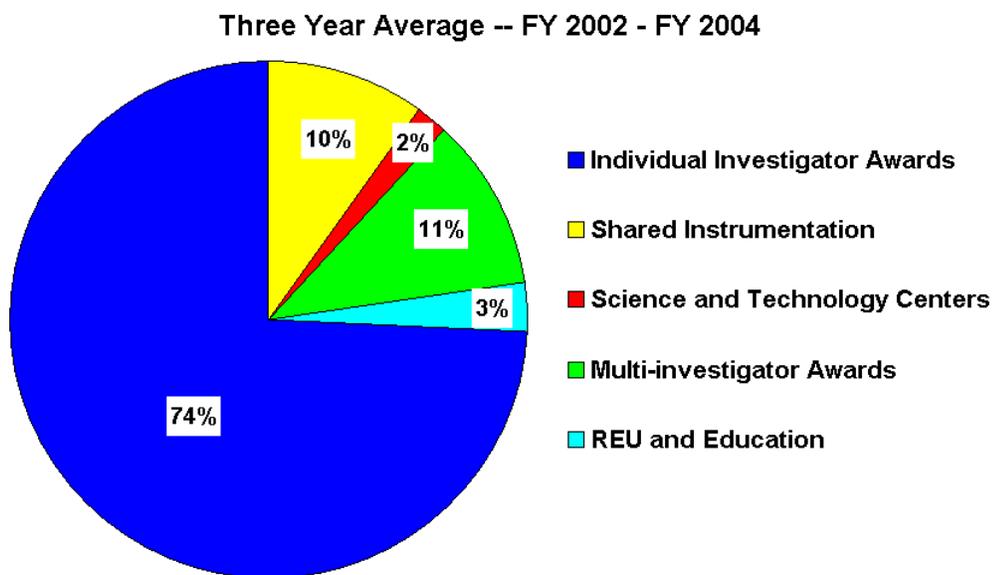
The COV addressed a number of challenges related to management of the Division's current portfolio. Exciting opportunities were also identified for which the Division is urged to provide leadership.

7. The COV affirmed the critical importance of individual investigator awards, noting, for example, some of the many Nobelists who have been supported by the Division and the significance of their contributions. The COV notes that advances supported by the Division through the core

programs have had an enormous economic impact through the chemical, electronic and pharmaceutical industries. The key role of the Division in supporting the training of the workforce in the chemical sciences was discussed by the COV, which noted “strong demand is expected for chemists with a master’s or Ph.D. degree”. Given the importance of the individual investigator awards, the COV expressed concern over the significant budgetary pressure on the Division’s core programs: the buying power of individual investigator awards has been relatively stagnant over the past half-dozen years and “many excellent proposals were unable to be funded due to budgetary constraints.” The COV believes the present mix of individual investigator awards (approximately 70% of the budget) is optimal.

Response. The Division reaffirms its commitment to a strong core of individual investigator awards. The Division recognizes the importance of these awards in producing breakthroughs in basic research, strengthening the economy, and developing workforce. As resources permit, the Division will support additional awards and increase grant size and duration. Support for individual awards needs to be balanced with multi-investigator projects that the COV also described as worthwhile. The Division will do its best to find the right balance across its funding portfolio.

January 1, 2005 Update. The FY2004 budget was nearly the same as the FY2003 budget, and the Division made a similar distribution in its investments. The individual investigator awards continue to comprise nearly three-fourths of the budget, representing an investment on the order of \$130M. A breakdown in the form of a pie chart for FY2002-2004 is shown below.



8. The COV expressed support for continued use and perhaps expansion of the high-risk, high-payoff Small Grants for Exploratory Research (SGER).

Response. The Division has increased the number of these awards in the past year and views them as an important part of our portfolio. We have been advertising them more aggressively and will continue to do so.

January 1, 2005 Update. The number of SGER awards in FY2004 was 11, nearly the same as the 12 awarded in FY2003. The dollar value of these awards decreased slightly to \$0.8M from \$1.0M.

9. The COV suggested that CAREER applicants would benefit from additional mentoring if they are to craft persuasive education sections to their proposals.

Response and Action. The Division will work with the community to develop effective mechanisms that will provide guidance to young investigators regarding the development of plans for integrating research and education in their CAREER proposals.

January 1, 2005 Update. The Division supported a workshop at Oak Ridge National Laboratory (ORNL) of CAREER awardees working at the chemistry/life science interface and asked them for guidance on this issue. Their recommendations are included in the workshop report, which is available at http://www.chem.ucdavis.edu/groups/gervay-hague/MBLP_Final_Report.pdf. Recommendations include workshops for CAREER applicants, improving efforts for mentoring young investigators, and strengthening efforts to “re-educate reviewers who evaluate CAREER grant proposals, with an emphasis on those reviewers dealing more responsibly with teaching and ‘broader impact’ components.”

10. Of particular concern to the COV is “the increasing disparity between the average size and duration of individual investigator awards from the NIH and NSF.” The COV notes that “not only is this disparity driving excellent science out of the NSF portfolio, federally funded chemists are increasingly redirecting their research towards medically-related areas. If this trend continues, critical areas of national need (e.g., chemical and biological sensors, instrumentation), scientific infrastructure and workforce training will be underserved.”

Response and Action. The Division concurs with this alarming assessment. We will gather information on the nature and extent of the problem and work toward a solution. As noted below, the issue is particularly timely, since we have opportunities to engage the life science community on initiatives involving the

NIH/NSF life science/physical science interface and a new MPS emphasis area in the President's fiscal year 2005 budget: the molecular basis of life processes.

January 1, 2005 Update. The Division is exploring the use of sophisticated knowledge mapping tools to track the direction and rate of movement of the chemistry/life science interface and has had several meetings with colleagues at NIH/NIGMS to discuss aspects of this complex issue. To better understand the research opportunities at this interface, the Division supported two workshops to identify the science drivers for the molecular basis of life processes (MBLP). MBLP is an emphasis area within the Mathematical and Physical Sciences directorate that is being coordinated by the Division of Chemistry. The first workshop was organized by the ACS and involved senior investigators. The second workshop was held at ORNL for CAREER awardees (see above), and the report is available at http://www.chem.ucdavis.edu/groups/gervay-hague/MBLP_Final_Report.pdf. The two workshops were complemented by a workshop organized jointly by NSF and NIH in November, 2004. Collectively, these inputs will be used to identify a path forward on MBLP, although the Division is clearly constrained by the current relatively flat budgetary situation. In related developments, the Division is co-funding with DOE a NRC study on chemical imaging that will be initiated in early 2005. Several workshops are also providing input for this area:

Opportunities in Terahertz Science (joint with DOE and NIH), report at <http://www.sc.doe.gov/bes/reports/list.html>; and

Models of Thought Processes (joint with three other NSF directorates), report at <http://hopf.chem.brandeis.edu/thoughtworkshop.html>. At the MPSAC meeting in November, 2004, there was considerable enthusiasm for an emphasis area in sustainability, which would embrace many non-biomedical research areas. The Division is already supporting a considerable number of sustainability-related research projects and will be working with the MPS Directorate to discuss the feasibility of a directorate-wide investment strategy.

11. With respect to broadening participation, the COV observes that "diversity is still problematic for chemistry as for many of the sciences." Even though "the Chemistry Division supports underrepresented faculty well," the COV notes that increasing representation of underrepresented groups at research universities is a particular challenge for the entire community.

Response and Action. Based on a variety of studies, the Division believes that the limited diversity of its community is a systemic problem that needs to be addressed by a concerted community-based effort. We will work to make progress on this problem with the ACS and through awards made through the Foundation's ADVANCE program and the Division's Special Projects Office. The Division welcomes and will support innovative approaches that can make the basic research and education it supports far more inclusive and will keep the community informed of progress.

January 1, 2005 Update. The Division has been using a multi-faceted strategy to broaden participation. At the undergraduate level the Division has encouraged its community to engage first- and second-year college students from the full spectrum of postsecondary institutions in cutting-edge research. A Joint Subcommittee comprising members of the MPS Advisory Committee and the Advisory Committee of the Education and Human Resources Directorate endorsed the idea of engaging students in MPS research areas within the first two years of college and of reaching out to two-year institutions as an important element of such an effort. The Undergraduate Research Center (URC) program's first awards were made in FY2004, comprising both planning and full grants through a partnership with the Office of Multidisciplinary Research (OMR) and the EHR directorate. Nearly 700 institutions responded to the program announcement. Twenty planning grants were awarded and one full URC was funded. There are many two-year institutions and minority-serving institutions among the awardees. To involve its community in an ongoing discussion about the URC program, a second URC workshop was held in FY2004 and a report posted on the web at

<http://www.scu.edu/cas/research/upload/revisedURCreportdraftJan2005.doc>.

A second URC competition is being held in FY2005 and the announcement may be found at <http://www.nsf.gov/pubsys/ods/getpub.cfm?nsf05539>. The Division maintained its strong investment in the Research Experiences for Undergraduates (REU) program. Through an award to an REU Leadership Group, REU site directors and site directors for the Louis Stokes Alliances for Minority Participation (LSAMP) program have begun to coordinate their efforts. This partnership will help REU site directors recruit students more broadly and is enabling LSAMP students to attend national ACS meetings.

At the postdoctoral and senior levels, new models for professional development are being supported. In partnership with OMA and the EHR directorate, the first Discovery Corps Fellowships were awarded in FY2004 to provide opportunities for postdoctoral and mid-career chemical scientists to combine their research expertise with professional service to address such national needs as linkages between chemistry and other fields, job creation, workforce development, and enhancement of research infrastructure, both nationally and internationally. This pilot program is focused in the chemical sciences and in interdisciplinary areas supported by the chemical sciences. A second set of awards will be made in FY2005.

A two-year award was made to the ACS to conduct an experiment designed to make faculty recruiting more inclusive and efficient: the ACS held a poster session at its Fall, 2004 meeting in which some 120 prospective faculty members presented their work. ACS will track the presenters and the faculty search committee members who came to meet them to assess the impact of this experiment.

12. The COV states, "We urge the chemistry division to energize the community to take part in the nascent NSF programs in cyber-technology." Moreover, the COV notes that "the strength of the community in the

visualization of science” can be leveraged through cyber technology as well. “The Division could act as a catalyst for innovative advances in this area.”

Response and Action. The COV recognizes the unique strengths of the chemistry community in molecular-level computation and envisions use of the grid to make these tools available everywhere for use in basic research and education. The Division agrees with this assessment and, as suggested, will provide leadership by obtaining community input and developing strategic partnerships that will define “cyber-enabled chemistry.” We believe that the broadly distributed nature of the grid will allow the highly dispersed chemistry community to create extraordinary new paradigms for basic chemical research and education, as envisioned by the COV. In planning, we will work with the MPS Advisory Committee (MPSAC) and the ACS to ensure community participation.

January 1, 2005 Update. Opportunities in cyberinfrastructure are summarized in “Revolutionizing Science and Engineering through Cyberinfrastructure: Report of the National Science Foundation Advisory Panel on Cyberinfrastructure.” The report may be accessed at http://www.communitytechnology.org/nsf_ci_report/. The Division actively participated in a MPS-wide workshop on cyberinfrastructure and then supported a workshop on cyber-enabled chemistry; the report is available at http://bioeng.berkeley.edu/faculty/cyber_workshop/. The Division plans to make funding opportunities available for development of cyber-enabled chemistry in FY2005 and FY2006.

13. Large instrumentation was addressed by the COV: “The new mid-range instrumentation initiative...is an opportunity for the chemistry community. The NSF Chemistry Division should take a lead in organizing workshops and the like to encourage this.” “...The hope is that the Division will provide a process by which the community can define future instrumentation needs.”

Response and Action. The Division will begin planning this process in collaboration with the MPSAC and the ACS. We anticipate that cyber-enabled projects and next-generation instruments will be enabled by the mid-range instrumentation initiative, and we look forward to working with the community on this important venture.

January 1, 2005 Update. The aforementioned workshop for CAREER awardees was held at ORNL so as to acquaint this group of young investigators with the Spallation Neutron Source that is expected to be on-line in 2006. In a related strategy, through a Dear Colleague letter, 04-025, the Division and Pacific Northwest National Laboratory (PNNL) established a program like one

available with NIST that allows NSF PIs in a number of NSF directorates to apply for supplements to their grants to permit themselves and their co-workers to travel to PNNL and make use of PNNL facilities and expertise. The NSF-DOE/PNNL Interaction in Environmental Molecular Sciences Supplement Opportunity can be found at

<http://www.nsf.gov/pubs/2004/nsf04025/nsf04025.htm>.

Division staff members are planning a town meeting for the Fall, 2005 ACS National Meeting in Washington, D.C. to discuss mid-range instrumentation opportunities with the community.

14. The COV recognizes the considerable opportunity that exists in “the emerging area of the basic molecular understanding of living processes,” identifying this as “another place where chemistry and other divisions can partner, and provide a launching pad for the community.” The COV notes that objectives of the NIH roadmap include new tools and that many of the developments upon which the roadmap rests are the result of advances in chemistry: “If our national science and technology strategy is to support the goal of such revolutionary advances, it must be fed by accelerating advances in chemistry, and NSF is the logical home of such activities.”

Response and Action. The Division is strongly committed to providing leadership for the MPS emphasis area of the molecular basis of life processes. We intend to work with the MPSAC, with other NSF divisions, and with NIH and other agencies to develop an appropriate strategy. The initiative is also in accord with Congressional interest in strengthening NSF/NIH interactions across the physical science/life science interface.

January 1, 2005 Update. Developments here are covered in the answer to point number 10 above.

15. The COV notes at the conclusion of its report that “there is a concern that the essential and enabling role that chemistry plays in related fields and in meeting public needs often goes unnoticed. The community as a whole needs to do a better job in selling chemistry both to attract the next generation of chemists and to reinforce the fact that an increased investment in basic research in chemistry is in the public interest.”

Response and Action. The Division is committed to helping with this important objective in several ways. First, we have been aggressively collecting and distributing “nuggets” from PIs that describe advances in their research and will continue to do so. Second, the Division has launched new programs that can raise consciousness about chemistry. The Chemical Bonding Centers (CBCs) are large projects that must be able to engage the public in “big ideas” centered in chemistry. Undergraduate Research Centers (URCs) are expected to make far larger numbers of entering college students aware of opportunities in the

chemical sciences by exposing them to research. Finally, we will continue to encourage submission of proposals for projects that will enable the public to better understand the research that we are supporting.

January 1, 2005 Update. The Division launched its new *Chemical Bonding Centers (CBCs)* program in FY2004, a program with the potential to raise the profile of the discipline. This program is meant to support large, high-risk, long-term projects centered in the chemical sciences that would have substantial intellectual and societal impact. In partnership with OMA, the first set of three awards was made in the areas of Darwinian chemical systems, multifunctional materials, and activation of strong chemical bonds. A second solicitation for proposals was released in FY04 with awards to be made in FY2005. Another new program –Discovery Corps Postdoctoral and Senior Fellowships – is also attracting public interest. With the leadership of a group of Research Experiences for Undergraduates (REU) PIs, the Division is planning to support a national on-line poster session of undergraduate research. We hope that the broadly distributed nature of this effort will attract considerable positive media attention as it highlights the creation of new knowledge and the training of our future workforce. The Division will work with its Office of Legislative and Public Affairs (OLPA) to publicize the event. The Division worked with OLPA to organize an event featuring developments related to sensors that was presented to Congressional staffers, the media, and to the public in a “science café” format.

16. It was noted in several of the program reviews that incomplete 2001 COV reports had been provided to the 2004 COV members in advance of the 2004 COV meeting.

Response. The Division discovered shortly before mailing out background materials to the 2004 COV members that some inappropriate information had inadvertently been included in a few of the 2001 COV program reports. Rather than delay sending out the materials, only the summary of the 2001 COV report was sent. However, the full 2001 COV report, with inappropriate text deleted, was available at the meeting to all 2004 COV members.

We are extremely grateful to the COV members and to the chair of the COV, Robert Silbey, for their dedication, hard work, and thoughtful analysis. We believe that their report will enable the Division to better serve its community.

Arthur B. Ellis
Division Director
Division of Chemistry