NATIONAL SCIENCE FOUNDATION
OFFICE OF INSPECTOR GENERAL
OFFICE OF INVESTIGATIONS

CLOSEOUT MEMORANDUM

Case Number: A11040023

We received an allegation of data fabrication and falsification involving a student's research advisor[1] and an NSF proposal.[2] When we contacted the university[3] for additional information, we learned that the original allegations were against the student,[4] and that the university was already conducting an inquiry with both the student and the advisor as subjects. Subsequently, the university concluded that an investigation was warranted only with respect to the student. We concurred and referred the investigation to the university.

The university completed its investigation, during which the student was non-responsive to requests for information. The university concluded that the student had committed intentional research misconduct and that he was solely responsible for it. The university formally expelled the student who was believed to have already left the U.S.

We reviewed the university report and concurred that the evidence supported a finding of intentional research misconduct. We prepared a report of investigation (attached) for NSF, recommending: a letter of reprimand with a findings of research misconduct; responsible conduct of research training; and a 5-year debarment, followed by a 5-year ban from serving NSF as a reviewer, advisor or consultant and 5 years of certifications and assurances. NSF accepted our recommendations (attached).

Accordingly, this case is ***closed***.

1 [redacted]
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3
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NATIONAL SCIENCE FOUNDATION
4201 WILSON BOULEVARD
ARLINGTON, VIRGINIA 22230

OFFICE OF THE
DEPUTY DIRECTOR

[redacted]

VIA CERTIFIED MAIL/RETURN RECEIPT REQUESTED

[redacted]

Re: Notice of Debarment

Dear [redacted]:

On [redacted], 2013, the National Science Foundation ("NSF") issued to you a Notice of Proposed Debarment and Notice of Research Misconduct Determination ("Notice"), in which NSF proposed to debar you from directly or indirectly obtaining the benefits of Federal grants for a period of five years. As reflected in the Notice, NSF proposed your debarment because, as a student at the [redacted], you falsified and fabricated data and results that were incorporated with your knowledge into a proposal that was submitted to NSF. In that Notice, NSF provided you with thirty days to respond to the proposed debarment.

Over thirty days have elapsed and NSF has not received a response. Accordingly, you are debarred until [redacted], 2018.

Debarment precludes you from receiving Federal financial and non-financial assistance and benefits under non-procurement Federal programs and activities unless an agency head or authorized designee makes a determination to grant an exception in accordance with 2 CFR 180.135. Non-procurement transactions include grants, cooperative agreements, scholarships, fellowships, contracts of assistance, loans, loan guarantees, subsidies, insurance, payments for specified use, and donation agreements.

In addition, you are prohibited from receiving Federal contracts or approved subcontracts under the Federal Acquisition Regulations at 48 CFR Subpart 9.4 for the period of this debarment. 2 CFR 180.925. During the debarment period, you may not have supervisory responsibility, primary management, substantive control over, or critical influence on, a grant, contract, or cooperative agreement with any agency of the Executive Branch of the Federal Government.

Lastly, please note that, in the Notice, NSF also took the following actions against you, which continue to remain in effect:

- From the end of your debarment period through [redacted], 2023, you are required to submit certifications to NSF's Office of Inspector General that any proposals or reports you submit to NSF do not contain plagiarized, falsified, or fabricated material.

- From the end of your debarment period through [redacted], 2023, you are required to submit assurances by a responsible official of your employer that any proposals or reports you submit to NSF do not contain plagiarized, falsified, or fabricated material. These assurances must be submitted to NSF's Office of Inspector General.

- You are prohibited from serving as an NSF reviewer, advisor, or consultant through [redacted], 2018; and

- You are required to complete a comprehensive responsible conduct of research training course by [redacted], 2014, and provide documentation of the program's content to the OIG. The instruction should be in an interactive format (e.g., an instructor-led course, workshop, etc.) and should include a discussion of *data fabrication and falsification.* [Please note that the [redacted], 2013, Notice erroneously indicated that you were required to complete a course covering plagiarism and proper citation practices].

All certifications, assurances, and training documentation should be submitted in writing to NSF's OIG, Associate Inspector General for Investigations, 4201 Wilson Boulevard, Arlington, VA 22230.

Should you have any questions regarding the foregoing, please contact [redacted], Assistant General Counsel, at (703) 292-8060.

Sincerely,

Fae Korsmo
Senior Advisor

NATIONAL SCIENCE FOUNDATION
4201 WILSON BOULEVARD
ARLINGTON, VIRGINIA 22230

OFFICE OF THE
DEPUTY DIRECTOR

[redacted]

[redacted]

Re: Notice of Proposed Debarment and Notice of Research Misconduct Determination

Dear [redacted]:

As a student at the [redacted] ("University"), you falsified and fabricated data and results that were incorporated with your knowledge into a proposal that was submitted to NSF. In light of your misconduct, this letter serves as formal notice that NSF is proposing to debar you from directly or indirectly obtaining the benefits of Federal grants for five years. During your period of debarment, you will be precluded from receiving Federal financial and non-financial assistance and benefits under non-procurement Federal programs and activities. In addition, you will be prohibited from receiving any Federal contracts or approved subcontracts under the Federal Acquisition Regulations ("FAR"). During your debarment period, you will be barred from having supervisory responsibility, primary management, substantive control over, or critical influence on, a grant, contract, or cooperative agreement with any agency of the Executive Branch of the Federal Government.

In addition to proposing your debarment, I am prohibiting you from serving as an NSF reviewer, advisor or consultant to NSF until [redacted], 2018. Furthermore, for five years from the expiration of your debarment period, I am requiring that you submit certifications, and that a responsible official of your employer submit assurances, that any proposals or reports you submit to NSF do not contain plagiarized, falsified, or fabricated material. Lastly, you must complete a comprehensive responsible conduct of research training course by [redacted], 2014, and provide documentation of the program's content to the OIG. The instruction should be in an interactive format (e.g., an instructor-led course, workshop, etc.) and should include a discussion of plagiarism and proper citation practices.

Research Misconduct and Administrative Actions other than Debarment

Under NSF's regulations, "research misconduct" is defined as "fabrication, falsification, or plagiarism in proposing or performing research funded by NSF ..." 45 CFR § 689.1(a). NSF defines "plagiarism" as "the appropriation of another person's ideas, processes, results or words without giving appropriate credit." 45 CFR § 689.1(a)(3). A finding of research misconduct requires that:

(1) There be a significant departure from accepted practices of the relevant research community; and

(2) The research misconduct be committed intentionally, or knowingly, or recklessly; and

(3) The allegation be proven by a preponderance of evidence.

45 CFR § 689.2(c).

You falsified and fabricated data and results using cut-and-paste and white-out manipulations related to the NMR spectrum and HPLC chromatograms for individual compounds. Your conduct unquestionably constitutes falsification and fabrication. I therefore conclude that your actions meet the applicable definition of "research misconduct" set forth in NSF's regulations.

Pursuant to NSF's regulations, the Foundation must also determine whether to make a *finding* of misconduct based on a preponderance of the evidence. 45 CFR § 689.2(c). After reviewing the Investigative Report, NSF has determined that, based on a preponderance of the evidence, your falsification and fabrication was committed intentionally and constituted a significant departure from accepted practices of the relevant research community. I am, therefore, issuing a finding of research misconduct against you.

NSF's regulations establish three categories of actions (Group I, II, and III) that can be taken in response to a finding of misconduct. 45 CFR § 689.3(a). Group I actions include issuing a letter of reprimand; conditioning awards on prior approval of particular activities from NSF; requiring that an institution or individual obtain special prior approval of particular activities from NSF; and requiring that an institutional representative certify as to the accuracy of reports or certifications of compliance with particular requirements. 45 CFR §689.3(a)(1). Group II actions include award suspension or restrictions on designated activities or expenditures; requiring special reviews of requests for funding; and requiring correction to the research record. 45 CFR §689.3(a)(2). Group III actions include suspension or termination of awards; prohibitions on participation as NSF reviewers, advisors or consultants; and debarment or suspension from participation in NSF programs. 45 CFR § 689.3(a)(3).

In determining the severity of the sanction to impose for research misconduct, I have considered the seriousness of the misconduct; our determination that it was committed intentionally; the fact that your actions were part of a pattern of misconduct and the impact of your actions tainted both

the reputations of your former advisor as well as your former institution; and that you engaged in this misconduct despite having taken departmentally required responsible conduct or research training, been party to informal discussions among your research group regarding publicized cases of research misconduct and served as a teaching assistant in a course that covered responsible conduct of research material. Based on the foregoing, I am imposing the following actions on you:

- For five years from the end of your debarment period, you are required to submit certifications that any proposals or reports you submit to NSF do not contain plagiarized, falsified, or fabricated material.

- For five years from the end of your debarment period, you are required to submit assurances by a responsible official of your employer that any proposals or reports you submit to NSF do not contain plagiarized, falsified, or fabricated material.

- From the date of this letter through [redacted], 2018, you are prohibited from serving as an NSF reviewer, advisor, or consultant.

- You are required to complete a comprehensive responsible conduct of research training course by [redacted], 2014, and provide documentation of the program's content to the OIG. The instruction should be in an interactive format (e.g., an instructor-led course, workshop, etc.) and should include a discussion of plagiarism and proper citation practices.

All certifications, assurances, and training documentation should be submitted in writing to NSF's Office of Inspector General, Associate Inspector General for Investigations, 4201 Wilson Boulevard, Arlington, Virginia 22230.

Debarment

Regulatory Basis for Debarment

Pursuant to 2 CFR 180.800, debarment may be imposed for:

> (b) Violation of the terms of a public agreement or transaction so serous as to affect the integrity of an agency program, such as –
>
> (1) A willful failure to perform in accordance with the terms of one or more public agreements or transactions;
>
> ...
>
> (3) A willful violation of a statutory or regulatory provision or requirement applicable to a public agreement or transaction; or

(d) Any other cause of so serious or compelling a nature that it affects your present responsibility.

In any debarment action, the government must establish the cause for debarment by a preponderance of the evidence. 2 CFR 180.850. In this case, you intentionally falsified data and fabricated results that appeared in publications that were integral to the proposal's scientific merit. Thus, your action supports a cause for debarment under 2 CFR 180.800(b) and (d).

Length of Debarment

Debarment must be for a period commensurate with the seriousness of the causes upon which an individual's debarment is based. 2 CFR 180.865. Generally, a period of debarment should not exceed three years but, where circumstances warrant, a longer period may be imposed. 2 CFR 180.865. Having considered the seriousness of your actions, as well as the relevant aggravating and mitigating factors set forth in 2 CFR 180.860, we are proposing your debarment for five years.

Appeal Procedures for Finding of Research Misconduct and Procedures Governing Proposed Debarment

Appeal Procedures for Finding of Research Misconduct

Under NSF's regulations, you have 30 days after receipt of this letter to submit an appeal of this finding, in writing, to the Director of the Foundation. 45 CFR 689.10(a). Any appeal should be addressed to the Director at the National Science Foundation, 4201 Wilson Boulevard, Arlington, Virginia 22230. If we do not receive your appeal within the 30-day period, the decision on the finding of research misconduct will become final. For your information, we are attaching a copy of the applicable regulations.

Procedures Governing Proposed Debarment

The provisions of 2 CFR Sections 180.800 through 180.885 govern debarment procedures and decision-making. Under our regulations, you have 30 days after receipt of this notice to submit, in person or in writing, or through a representative, information and argument in opposition to this debarment. 2 CFR 180.820. Comments submitted within the 30-day period will receive full consideration and may lead to a revision of the recommended disposition. If NSF does not receive a response to this notice within the 30-day period, this debarment will become final. Any response should be addressed to Lawrence Rudolph, General Counsel, National Science Foundation, Office of the General Counsel, 4201 Wilson Boulevard, Room 1265, Arlington, Virginia 22230. For your information, we are attaching a copy of the Foundation's regulations on non-procurement debarment and FAR Subpart 9.4.

Should you have any questions about the foregoing, please contact [redacted] Assistant General Counsel, at (703) 292-[redacted].

Sincerely,

Fae Korsmo
Senior Advisor

Enclosures:
Investigative Report
Nonprocurement Debarment Regulations
FAR Regulations
45 CFR Part 689

National Science Foundation
Office of Inspector General

Report of Investigation
Case Number A11040023
March 29, 2013

This Report of Investigation is provided to you
FOR OFFICIAL USE ONLY.

It contains protected personal information, the unauthorized disclosure of which may result in personal criminal liability under the Privacy Act, 5 U.S.C. § 552a. This report may be further disclosed within NSF *only* to individuals who *must* have knowledge of its contents to facilitate NSF's assessment and resolution of this matter. This report may be disclosed outside NSF only under the Freedom of Information and Privacy Acts, 5 U.S.C. §§ 552 & 552a. Please take appropriate precautions handling this report of investigation.

Executive Summary

Allegation: Falsification and fabrication of data submitted in an NSF proposal.

Inquiry: The University inquiry found sufficient evidence to warrant a detailed investigation of falsification and fabrication of data by a student (Subject). The Subject had provided data to his advisor who included it in an NSF proposal, an NIH proposal, and two publications. The Subject made a counter-allegation against his advisor (Advisor). The University inquiry found no evidence to support an allegation of research misconduct against the Advisor. We concurred with the University and referred the allegations against the Subject for a detailed investigation.

University Investigation and Action: At the time the University conducted an investigation, the Subject had left the University and did not respond to attempts to obtain his comments or testimony. The University concluded that the Subject intentionally falsified and fabricated data in 2 papers, 2 proposals, and presentations. Specifically, the Subject provided the data to his advisor for the NSF proposal with the knowledge that it was important to obtaining funding for the Subject's salary.

OIG's Assessment:

- **The Act**: The Subject falsified and fabricated data and results with the knowledge that the data would be submitted by his advisor in a NSF proposal to secure funding for the Subject's continued work.
- **Significant Departure:** The falsification was a significant departure from the accepted practices of the relevant research community.
- **Intent:** The Subject acted intentionally (*i.e.*, purposefully).
- **Standard of Proof:** The preponderance of evidence supports a finding of research misconduct.
- **Pattern:** The Subject's actions constitute a pattern of misconduct.

OIG Recommendation:

- A finding of research misconduct.
- A letter of reprimand.
- Require ethics training within 1 year of the finding.
- Debar the Subject for 5 years.
- For 5 year after the debarment period:
  - Bar from participating as a reviewer, advisor, or consultant.
  - Require certifications.
  - Require assurances.

OIG's Inquiry

We received from several sources forwarded copies of an email[1] that a graduate student at a university (University)[2] had distributed to numerous individuals. In the email the graduate student alleged that his advisor (Advisor)[3] committed research misconduct in proposals by knowingly using fabricated and falsified data in a NSF proposal (NSF Proposal)[4] and a NIH proposal (NIH Proposal).[5]

Subsequently, we learned from the University research integrity officer (RIO)[6] that the student's email was a counter-allegation to allegations against the student (Subject)[7] involving falsification and fabrication of data published in two articles (Paper 1[8] and Paper 2[9]). These articles were reported as preliminary results in the two proposals. Because the University was already conducting an inquiry, we referred the matter to the University to assess the allegations against both the Subject and the Advisor.[10]

The University's Inquiry[11]

The RIO conducted an inquiry under the University's academic misconduct policy and procedures.[12] The allegations included falsification and fabrication of nuclear magnetic resonance (NMR) spectra and high pressure liquid chromatography (HPLC) data in a synthesis project. The Advisor and the Subject published the data in two articles and presented them at multiple venues. The Advisor also submitted the data in the NSF Proposal (withdrawn) and the NIH Proposal.

The RIO interviewed four individuals, including the Advisor; however, the Subject was non-responsive to requests for an interview. The Subject's only response to the allegations against him consisted of three emails submitted during the RIO's initial assessment of the allegation.[13] The Subject did not deny the allegation but alleged misconduct by the Advisor. The RIO concluded there was sufficient evidence to warrant a detailed investigation only with

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[1] Tab 6 at 146. Throughout this report we refer to the OIG generated page numbers, which are in the lower right corner of the document preceded by the case number. The page numbering is sequential from Tab 1 through Tab 20.

[2] [redacted]

[3] [redacted]

[4] Tab 8, [redacted]

[5] Tab 8, [redacted]

[6] [redacted]

[7] [redacted]

[8] [redacted]

[9] [redacted]

[10] Tab 1, OIG Inquiry Referral Letter.

[11] Tab 2, University Inquiry Report.

[12] Tab 4, Academic Misconduct Policy.

[13] Tab 6 at 112 – 211. One of these emails was the initial email we received containing the allegation against the Advisor.

respect to the Subject.[14] The deciding official (DO)[15] concurred and the University investigation commenced.[16]

The inquiry report noted that the Advisor had discussed the allegations with his group members at his Friday group meeting before the formal University procedure commenced. He solicited their assistance in reviewing the Subject's data files and printouts. Earlier that day, the Advisor met with the Subject, another student (Student),[17] and the departmental graduate program director (Director).[18] During this meeting the Advisor confronted the Subject with an explicit allegation of research misconduct corroborated by the Student. The Subject admitted to the misconduct, and the Director indicated that the Subject could leave the program voluntarily or be expelled. The Subject turned in his key to the lab and had supervised access the following Monday to retrieve personal items. Although the Director was aware of the allegation, there was no formal allegation made until the department chairman (Chair)[19] independently learned of the situation from another student in the Advisor's lab and initiated the University process.

The Advisor's subsequent review of the Subject's papers revealed an employment offer letter to the subject and "the discovery of photocopied printouts in [the Subject's] desk of data that had been cut and pasted."[20] The Advisor's retention and review of the data raises some concerns with respect to the appropriate and timely sequestration of evidence, in part because the Advisor was the subject of a counter-allegation.

Despite our concerns, we found sufficient substance to warrant an investigation of the Subject's actions and referred an investigation to the University.[21] Our referral did not preclude the University from considering additional individuals, including the Advisor, as potential subjects if the evidence warranted their inclusion.

The University's Investigation[22]

The University appointed an ad hoc investigation committee (IC) and conducted an investigation under its policies and procedures.[23] The IC reviewed and considered: hard-copy and electronic records of the data; the Subject's laboratory notebooks; email correspondence; the affected journal articles and proposals; and testimony of four witnesses interviewed during the inquiry phase, two of whom were interviewed again during the investigation. The Subject did not respond to the IC's requests for an interview and was non-responsive throughout the investigation process.

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[14] Tab 6 at 96 – 97.
[15] [redacted]
[16] Tab 6 at 98 – 99.
[17] [redacted]
[18] [redacted]
[19] [redacted]
[20] Inquiry report, page 4
[21] Tab 3, OIG Investigation Referral Letter.
[22] Tab 5, The University's Investigation Report and Appendixes.
[23] Tab 4.

Background[24]

Through interviews, the Committee learned that the Subject "is a talented chemist who is a source of knowledge for others in the laboratory."[25] The Subject significantly contributed to earlier publications, which after review by the Advisor's group showed no indication of misconduct. They determined the Subject received training in the responsible conduct of research through a course in his department. The Advisor used lab group meetings that both the Subject and Student attended to discuss research misconduct cases in the news. The Subject was also a teaching assistant in the Advisor's class in which data falsification and fabrication were discussed.

The Committee found that the Subject had the "talent to complete the synthesis in a legitimate fashion" but chose to take actions which would help him graduate more quickly.[26] The Advisor and the Student surmised that the Subject faced financial and familial pressures to graduate and move to a waiting industrial position. A letter from an industrial firm found by the Advisor's group after the Subject left the lab confirms that the Subject had an offer with an expected start-date of 30 May 2011.[27] The offer was contingent upon the Subject's completing his degree program and maintaining his GPA. The Subject's signature appears on the acceptance form with a date of 2 February 2011.[28]

The allegations involve two types of data, NMR spectra and HPLC chromatograms, the Subject reported as experimental confirmation of the chemical structures he claimed to have made. The Subject's work focused on developing synthetic procedures intended to favor formation of one enantiomer over another. Enantiomers are compounds which have the same atoms linked in the same way but in differing three-dimensional orientations, often referred to as non-super-imposable mirror images (Figure 1). In general, the NMR spectra primarily confirmed the atom linkages, and the HPLC chromatograms differentiated between the three-dimensional orientations.

[24] Generally, Tab 5 at 57 – 58.
[25] Tab 5 at 64.
[26] Tab 5 at 64 – 65.
[27] Tab 20 at 2118.
[28] Tab 20 at 2121.

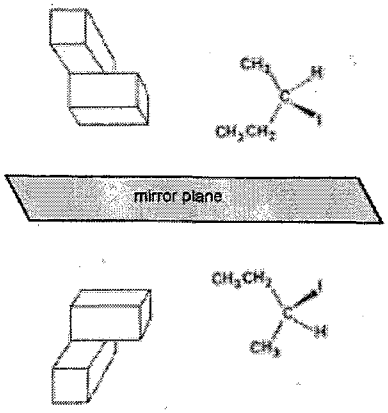

Figure 1. Enantiomers: Three-dimensional orientations reflected through a mirror that cannot be superimposed when rotated around an axis.[29]

Natural processes in plants and other biological systems often favor production of one enantiomer over another, whereas laboratory preparations typically result in racemic (50:50) mixtures of enantiomers. It is a goal of many research efforts, such as the Advisor's and Subject's, to develop conditions which selectively produce high yields of a single enantiomer, measured as the enantiomeric excess (ee). These efforts can have significant importance in fields, such as pharmaceutical development, because different enantiomers often have different biologicial effects. Where one enantiomer may be an effective antibiotic, the other may have no effect at all.

Discovery of the Misconduct[30]

In their respective interviews, the Advisor and Student described a series of events beginning in June 2010 during which the Subject admitted that he fabricated data because he did not have enough time to complete the project.[31] Subsequently, the Advisor gave the Subject a second chance to complete the project.[32] Sometime in the following two months the Subject reported a good result on the project but declined to present his findings at a large national professional meeting. The Advisor and the Student planned to attend the meeting, and it was decided that the Advisor would present the Subject's new results.

The Advisor directed the Student to replicate the Subject's new result before the national meeting. However, the Student was unable to do so, because one of the reagents for the procedure was missing. The Student ultimately located it outside of the refrigerator where it should have been stored to prevent decomposition. The Student attempted the synthesis with the reagent anyway, but the procedure failed. The Subject also repeated the synthesis side-by-side with the Student without success. Therefore, the Advisor chose not to present the Subject's new

[29] Adapted from A. Streitwieser, Jr. and C.H. Heathcock, *Introduction to Organic Chemistry*, Macmillan, 1976, New York, page 105-106.
[30] Generally, Tab 5 at 57 – 58; and Tab 15.
[31] Tab 5 at 58.
[32] Tab 5 at 66, Tab 15 at 1872 and 1928.

result at the meeting. When the Advisor and Student returned from the meeting, the Subject showed the Advisor an NMR spectrum showing that the reagent had decomposed. The Subject continued the project using a new reagent suggested by the Advisor.

In October 2010 the Subject reported new successful results. This coincided with the preparation of the NSF Proposal and the NIH Proposal. The Advisor asked the Student to repeat the Subject's results. The Student obtained a product according to the Subject's procedure which was confirmed by NMR to have the desired atom linkages. However, the Student had to rely on the Subject's assistance with the HPLC because he was the only group member with experience in running it. When the HPLC chromatogram indicated the run conditions for the ee determination for a standard sample were incorrect, the Subject worked alone to correct the conditions. Ultimately the Subject produced a chromatogram that he presented to the Advisor and Student demonstrating a 99% ee for the desired enantiomer. The Advisor and Student both agreed that they supported the 99% ee result. The Advisor then incorporated the data into the proposals for submission in November.

The Student provided the Subject with four other samples for the HPLC for which the Subject returned results that were "too good to be true."[33] The Student decided to repeat the work independently, including the HPLC which he had by that time learned to run. When he told the Subject about his intentions, the Subject suggested that the Student use alternate methods which would preclude using the standard HPLC method for determining the ee. The Student rejected these approaches.

When the Student set out to do the synthesis, he found the stock supply of a necessary reagent was depleted. It was a reagent that the Subject used frequently and typically reordered before the supply was exhausted. The Subject placed an order for the reagent at the Student's request causing a delay such that the Student was not able to begin the synthesis until two days before the Subject presented "outstanding" results at a lab group meeting.[34] The Subject presented a high ee value (99%) to the group. Approximately one week later, the Student reported his result (24% ee) to the Advisor. The Advisor and Student met with the Subject to ask why there was such a large difference in ee (24% versus 99%). After initially offering possible scenarios, the Subject admitted to fabrication. The next day the Advisor, Student, and Subject met with the Director as described above.

[33] Tab 15 at 1876.
[34] Tab 15 at 1877.

Findings

The IC addressed the Subject's conduct under five categories based on the where the alleged falsified and fabricated data were used: 1) in Paper 1; 2) in Paper 2; 3) in the NIH Proposal; 4) in the NSF Proposal; and 5) at conferences. The allegations involved data originally published in Paper 1 and Paper 2 and subsequently used as preliminary results in the NSF and NIH proposals as well as the conference presentations. The IC's analysis follows this chronology. Although neither publication was a result of federally-funded research, the publications, the NIH Proposal, and the presentations are relevant to our assessment of pattern. Under each of the categories the IC addressed the NMR spectra and HPLC data separately.

Paper 1.[35] The Committee determined that the Subject was the primary person who conducted the study reported in 2010 in Paper 1. A competing research group had published a less efficient process with only a moderate ee, and the Advisor recommended broadening the range of compounds in the Subject's study to increase the likelihood of publication. As a result, the Subject conducted additional work which led to Table 2 in the paper, where much of the affected data are summarized. The Supplemental Information referenced in the paper and available online included copies of the supporting spectra and chromatograms.

The Subject prepared all of the spectra, chromatograms, and quantification tables in the Supporting Information for the paper. He provided these in electronic form to the Advisor who did not review the original paper copies. Publication of this paper was based on the purported "streamlined method, the high overall yield (up to 88%), and the high ee."[36]

Although 14 separate examples of fabrication and falsification were alleged, the IC focused on 2 of these allegations in depth. In the first, the IC found that the Subject falsified the hardcopy of a NMR spectrum for compound 5 in Table 2 by pasting a resonance in one location and removing another by "painting with white-out solution." The IC noted that the identification block on the spectrum had been pasted over with a new block identifying it as compound 5 with the unique spectrum number of the original (compound 7) still showing. The NMR facility director obtained the original data files corresponding to the identification numbers; the data retrieved for compound 5 did not match the spectrum reported in the Paper 1. The IC identified "at least 11 cases" of similar cut-and-paste and white-out manipulations of NMR spectra in Paper 1,[37] evidenced by several "doctored printouts" corresponding to these spectra found in the Subject's desk.[38]

The second allegation involved the falsification of the HPLC data supporting the claimed high selectivity for one enantiomer (*i.e.*, a high ee). The Committee relied substantially on the testimony of the Advisor and the Student in concluding "that most of the ee values" the Subject reported in Paper 1 are "suspect."[39] The Advisor and the Student each stated their "belief" that

[35] Generally, Tab 5 at 59 – 60.
[36] Tab 5 at 59.
[37] Tab 5 at 59.
[38] Tab 5 at 60.
[39] Tab 5 at 60.

the Subject altered the conditions for the experimental separation.[40] The Committee identified a specific example to corroborate the Advisor's and Student's beliefs. The Committee found evidence of cut-and-paste manipulations on the chromatograph for one of the title compounds, in part supported by the original hard-copy with the cut-and-paste manipulations found in the Subject's desk.

The Committee did not make an explicit finding of falsification or fabrication regarding the HPLC data. For Paper 1, the Committee noted the goals of the research were to find a "more efficient route" to the products with "a remarkably high ee."[41] However, it found generally that "falsification and fabrication of the data by [the Subject] subverted both of these goals, because it is unlikely that the desired products were made and that the ee values were incorrectly assessed for some and perhaps most of the reactions."[42] The Committee found that these actions were a significant departure from the accepted practices of the relevant research community and that the Subject acted intentionally (purposefully).

Paper 2.[43] The Committee described Paper 2 as a continuation of the work reported in Paper 1 with "more experimental detail and a broader range of reactions."[44] Again the Committee found that the Subject was the primary person who conducted the experiments and assembled the data for publication. The Committee specifically described the NMR spectra (proton and carbon-13) and HPLC chromatogram for compound 27b as an example of the data falsification and fabrication in Paper 2. The Committee did not produce a comprehensive list of all the affected data. Instead it found "the identity of the data falsification methods used [in both papers] demonstrates a pattern of purposeful deception. It brings into question the large amount of data presented in both publications."[45] As with Paper 1 the Committee found the Subject's actions to be a significant departure from the accepted practices of the relevant research community.

NIH Proposal.[46] The Committee described the NIH Proposal as focused on the use of the synthetic route reported in Paper 1 and Paper 2 for the development of new molecules of therapeutic value. In addition to the specific examples of falsification and fabrication the Committee described for those papers and the NSF Proposal (below), the Committee identified an example specific to the NIH Proposal that was integral to a "key proof-of-principle synthesis" and based on the procedures reported in Paper 1 and Paper 2.[47] The Committee found that the Subject intentionally falsified the supporting NMR spectra for compound 22 using the same cut-and-paste methods described above. The Committee concluded that the Subject was aware that the NIH Proposal, if successful, would have provided salary funds for him. In addition, the Subject "would have had ample opportunity to review the grant proposal before it was submitted to correct errors or recommend removal of questionable data."[48] The Committee found that the

[40] Tab 5 at 60.
[41] Tab 5 at 60.
[42] Tab 5 at 60.
[43] Generally, Tab 5 at 60 – 61.
[44] Tab 5 at 61.
[45] Tab 5 at 61.
[46] Generally, Tab 5 at 61 – 62.
[47] Tab 5 at 59.
[48] Tab 5 at 62.

Subject's actions were a significant departure from the accepted practices of the relevant research community and that the Subject acted intentionally (purposefully).

NSF Proposal.[49] The Committee described the NSF Proposal as focused on a general understanding of "the underlying basis for the reactivity" in contrast to the application of the approach in the NIH Proposal.[50] The role of the Lewis acid and the influence of the catalyst's geometry were of specific interest in the proposed work. In the preliminary work it was the choice of Lewis acid that had been attributed as the factor increasing efficiency over other published procedures. The Committee noted again that the proposal relied on Paper 1 and Paper 2 as justification for the work.

As an example the Committee selected compounds 30 and 31 for closer examination. The Committee found that the NMR spectra supporting the successful synthesis of both compounds suffered from the same cut-and-paste falsification as described in each of the examples above. The Committee relied on the physically altered hardcopies of the spectra found in the Subject's desk. The Committee found that the Subject's actions were "deliberate" and with the knowledge that the NSF Proposal, if successful, would provide salary funding for his continued work.[51] The Committee found that the Subject's actions were a significant departure from the accepted practices of the relevant research community and that the Subject acted intentionally (purposefully).

Presentations.[52] The Committee identified several presentations given by either the Advisor or the Subject that included the falsified and fabricated data. The Subject presented the data at the University Graduate Research Symposium in 2010. The Advisor presented the data in a poster at a Gordon Research Conference and in an oral presentation at the American Chemical Society National meeting in that same year. The Advisor also presented the work in a regional meeting from which the University recruits graduate students for the department. The Committee found that the retractions of the two papers upon which these presentations were based "tarnished" the reputation of the Advisor and the University.[53]

In summary, the Committee concluded that the Subject's actions over the two years constituted a pattern of serious, knowing and intentional research misconduct. The Committee concurred with the conclusion in the inquiry that there was no support for the allegations against the Advisor and therefore no support for the defense the Subject offered in his initial emails to the RIO. The Committee noted that the Subject never denied the allegations of fabrication and falsification in these emails.

The University's Actions

The University made a finding of academic misconduct with respect to both papers, both proposals, and the presentations. It recommended that the actions be taken to formally dismiss

[49] Generally, Tab 5 at 62.
[50] Tab 5 at 62.
[51] Tab 5 at 62.
[52] Generally, Tab 5 at 62 – 63.
[53] Tab 5 at 62.

the Subject from the University.[54] Because the Subject had already left the University, no further actions were taken.

OIG's Investigation and Assessment

A finding of research misconduct requires that: (1) there be a significant departure from accepted practices of the relevant research community, (2) the research misconduct be committed intentionally, or knowingly, or recklessly, and (3) the allegation be proven by a preponderance of the evidence.[55]

As noted above, we had general concerns about the integrity of the evidence because it was not secured in a timely manner. The Advisor and Director both failed to follow the formal University process for allegations of misconduct when confronted with the Subject's admissions. With respect to the Advisor, the Committee noted the Advisor's inexperience as an Assistant Professor as an explanation.[56] After the Advisor announced the allegation to his research group, a group member informed the Chair, and the Chair initiated the formal process. Despite the delay in securing the evidence and the lack of confidentiality regarding the allegation, we conclude there is sufficient corroboration among documentary and testimonial evidence to support the University's conclusions. The Committee made numerous attempts to communicate with the Subject and received no responses. Accordingly, we conclude that the University investigation was accurate, complete, and followed reasonable procedures.

The Act

We concur with the University that the evidence, including the Subject's admissions, supports finding falsification and fabrication in the NSF proposal, which appears as unpublished data as well as data and results incorporated from Paper 1 and Paper 2. Specifically, the Subject falsified NMR spectra using manual cut-and-paste and white-out techniques to support the synthesis of compounds. The falsified spectra support his fabricated reports that he prepared those compounds. Although the Student subsequently prepared those compounds by the Subject's methods, there is no evidence to support finding that the Subject synthesized them himself. The HPLC chromatograms on which the Subject used the same manual cut-and-paste and white-out techniques are falsified data that support the high ee claimed for the desired enantiomer. It is the high ee relative to that previously published by another research group that increased the value of the resulting publications and scientific merit of the proposals. The Subject had a reasonable expectation that the results would be incorporated into the proposals and that if awarded funding for his salary would be available.

We concur with the University that it is a significant departure from the accepted practices of any research community to fabricate and falsify experimental data and results for use in a proposal for NSF funding. It is also a significant departure to participate actively in the further use of the published falsified and fabricated data and results as prior work in any NSF proposal.

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[54] Tab 5 at 47.
[55] 45 C.F.R. 689.2(c).
[56] Tab 5 at 66.

Intent

We concur with the University that the evidence supports finding that the Subject's falsification and fabrication were intentional (purposeful). The literal cutting with scissors and pasting of resonances on NMR spectra along with whiting out resonances by painting on liquid correction fluid followed by scanning into a digital format are in the aggregate intentional deceptive actions. Regardless of the underlying motivation, the Subject accepted an offer for employment that necessitated his completing his degree by the end of the 2011 academic year. In doing so he imposed his own deadline for completing his degree when the Advisor had submitted both the NSF Proposal and the NIH Proposal, both of which requested salary support for the Subject. The facts support the University's conclusion that the Subject had all the requisite skills and abilities to have completed the work but chose instead to falsify and fabricate data and results. Therefore, the evidence supports finding that the Subject acted intentionally (purposefully).

Standard of Proof

The preponderance of the evidence demonstrates that the Subject falsified and fabricated NMR spectra and HPLC chromatograms to support his reported synthetic approach for obtaining high selectivity among enantiomers. The Subject's lack of participation in the investigation process following his admissions necessitates reliance almost exclusively on the testimony of the Advisor and the Student. Their testimony is corroborated to a large extent by the documentary evidence and the testimony of the Director and Chair.

OIG's Recommended Disposition

When deciding what appropriate action to take upon a finding of misconduct, NSF must consider:

> (1) How serious the misconduct was; (2) The degree to which the misconduct was knowing, intentional, or reckless; (3) Whether it was an isolated event or part of a pattern; (4) Whether it had a significant impact on the research record, research subjects, other researchers, institutions or the public welfare; and (5) Other relevant circumstances.[57]

Seriousness

The Subject's falsification and fabrication are not only misconduct in his local academic community related to completing his Ph.D. but also misconduct in the broader scientific community. Although a competing group had published a similar synthetic approach before the Subject and the Advisor published Paper 1, the falsified and fabricated work represented a significant advance over their competitor's method. The advances included a more efficient synthetic approach and a higher degree of enantio-selectivity, both highly valued characteristics in industrial processes. Although the Student later validated the synthetic approach with a lower

[57] 45 C.F.R. 689.3(b).

but significant selectivity, the Subject's falsification and fabrication required the investment of additional time and resources to repeating the work. Furthermore the reputational damages associated with his actions extend not only to the Advisor who is nearing his tenure review, but to the research group and University as well.

Degree to which the Act was Intentional (Purposeful)

The Subject's limited participation in the investigation consists of emails the RIO received during her initial assessment of the allegations. The Subject did not deny the allegations against him and instead counter-alleged misconduct by the Advisor for knowingly or intentionally using the data. The facts available not only support dismissing the counter-allegations but also demonstrate the Subject's failure to accept responsibility for his own actions and admitted conduct.

Pattern of Behavior

The Subject's research misconduct occurred months after a previous incident of similar falsification that, when confronted, he admitted to the Advisor. The Advisor chose to give the Subject a second chance to do the work correctly.[58] The Subject's conduct not only continued but also took on an additional element of deceptiveness in frustrating the Student's attempts to replicate the results.

Impact on the Research Record

The Subject's falsified and fabricated data appeared in two publications (Paper 1 and Paper 2) which the Advisor later retracted. Both papers appear in the online journals with markings to indicate that they have been retracted and provide reference to the retraction notices. The Supporting Information is still available online for Paper 1 but not Paper 2, reflecting a difference in approach between the respective journals. Although the Subject's presentation of the work was limited to a research group meeting, the Advisor, in reliance on the Subject's work, presented the results at two large meetings and as part of departmental recruitment activities. Retraction or correction of oral presentations of falsified and fabricated materials is a more difficult proposition. We have not identified any associated conference proceedings that require retraction.

Other Relevant Circumstances

The Subject received training in the responsible conduct of research (RCR) while at the University; it was a departmental requirement. The Advisor supplemented this training with group discussions of publicized cases of research misconduct, and the Subject served as the Advisor's teaching assistant in a course that covered RCR elements. Therefore, the Subject had sufficient instruction and exposure to the research community's expectations for handling data.

[58] Tab 5 at 66, Tab 15 at 1872 and 1928.

Recommendations[59]

Based on the evidence, OIG recommends that NSF:

- Send the Subject a letter of reprimand notifying him that NSF has made a finding of research misconduct.[60]
- Require the Subject to certify to the Assistant Inspector General for Investigations (AIGI) his completion of a responsible conduct of research training program and provide documentation of the program's content within 1 year of NSF's finding.[61] The instruction should be in an interactive format (*e.g.*, an instructor-led course) and specifically include data falsification and fabrication.
- Debar the Subject for 5 years.[62]

For a period of 5 years immediately following the debarment period:

- Bar the Subject from participating as a peer reviewer, advisor, or consultant for NSF.[63]
- Require for each document (proposal, report, etc.) to which the Subject contributes for submission to NSF (directly or through his institution),
  - the Subject to submit a contemporaneous certification to the AIGI that the document does not contain plagiarism, falsification, or fabrication.[64]
  - the Subject to submit contemporaneous assurances from a responsible official of his employer to the AIGI that the document does not contain plagiarism, falsification, or fabrication.[65]

The Subject's Response to OIG's Draft Investigation Report

We made several attempts to contact the Subject through his last known addresses to obtain his comments on our draft investigation report.[66] We sent emails to both his last known personal and school email accounts and received delivery confirmations. We confirmed that his last known phone number is no longer active. We have received no response from the Subject.

At our request, the University provided the Subject's last known address in his home country from the Subject's admission records. We attempted to deliver a copy of our draft report to the Subject, however the courier service has reported the letter we sent was undeliverable.

[59] 45 C.F.R. 689.6(f) and 689.9(c)(2)(ii).
[60] A Group I action 45 C.F.R. 689.3(a)(1)(i).
[61] This action is similar to Group I actions 45 C.F.R. 689.3(a)(1).
[62] A Group III action 45 C.F.R. 689.3(a)(3)(iii).
[63] A Group III action 45 C.F.R. 689.3(a)(3)(ii).
[64] This action is similar to 45 C.F.R. 689.3(a)(1)(iii).
[65] A Group I action 45 C.F.R. 689.3(a)(1)(iii).
[66] Tab 21.