DEPARTMENT OF HEALTH & HUMAN SERVICES

Office of Public Health and Science
Office of Research Integrity
1101 Wootton Parkway, Suite, 750
Rockville MD 20852
Phone: 240-453-8200
FAX: 301-594-0043

NOV 18 2010

VIA ELECTRONIC MAIL TRANSMISSION TO: (b)(6) and (b)(7)(C)

Bengu Sezen, Ph.D.

Re: Notice of Administrative Actions -- ORI 2006-15

Dear Dr. Sezen:

By letter dated October 4, 2010, the Office of Research Integrity (ORI), Department of Health and Human Services (HHS), notified you that based on the findings of an investigation by Columbia University (CU) and additional analysis conducted by ORI during its oversight review of the CU investigation report, ORI had made findings of misconduct in science against you.

In its notification letter, ORI advised you of proposed administrative actions and gave you an opportunity to request a hearing on the findings and proposed administrative actions before an Administrative Law Judge with the HHS Departmental Appeals Board. As you have not requested a hearing within the required 30-day period, the following administrative actions have been implemented for a period of five (5) years, beginning on November 4, 2010:

- You are debarred from eligibility for any contracting or subcontracting with any agency of the United States Government and from eligibility or involvement in nonprocurement programs of the United States Government, referred to as "covered transactions," pursuant to HHS' Implementation of OMB Guidelines to Agencies on Governmentwide Debarment and Suspension (2 C.F.R. § 376 *et seq.*).

- You are prohibited from serving in any advisory capacity to U.S. Public Health Service (PHS), including but not limited to service on any PHS advisory committee, board, and/or peer review committee, or as a consultant.

In accordance with PHS policy, your name also has been entered in the PHS ALERT system. Your name will remain in the system for a period of five (5) years beginning on November 4, 2010, and ending on November 3, 2015.

Pursuant to ORI procedures, a brief summary of the misconduct finding and administrative actions will be placed in the *Federal Register*, the *NIH Guide for Grants and Contracts*, and the *ORI Newsletter*.

Sincerely,

Donald Wright MD MPH

Donald Wright, M.D., M.P.H.
Acting Director
Office of Research Integrity

cc: Ms. Naomi J. Schrag, Director of Research Compliance and Training, Office of the Executive Vice President for Research, CU
Dr. Lawrence Tabak, ARILO, NIH
Dr. Sally Rockey, AERIO, NIH

DEPARTMENT OF HEALTH & HUMAN SERVICES Public Health Service

Office of the Assistant Secretary for Health
Office of Research Integrity
1101 Wootton Parkway, Room 750
Rockville, Maryland 20852
mailto:sflemingr@osophs.dhhs.gov Phone: 240-453-8800
FAX: 301-594-0043

DEC 9 2010

TO: Nancy Gunderson
Acting Deputy Assistant Secretary
Office of Grants and Acquisition Policy and Accountability

FROM: Acting Director
Office of Research Integrity

SUBJECT: Debarment ORI Case No. 2006-15 – Final Notice

Please be advised that the Respondent, Bengu Sezen, Ph.D., failed to request a hearing in accordance with 42 C.F.R. Part 93, Subpart E. Accordingly, please issue a final notice of debarment in this matter. Enclosed please find a proposed final notice of debarment for your review and approval.

Should you have any questions about this matter, please feel free to contact me or Christian Mahler, legal counsel, at (301) 443-2212.

Donald Wright MD MPH

Donald Wright, M.D., M.P.H.

Enclosures
Tab A: Final Notice of Debarment

cc: Chris Mahler
Office of the General Counsel

DEPARTMENT OF HEALTH & HUMAN SERVICES

Office of the Secretary

Washington, D.C. 20201

Via Electronic Mail Transmission Only To: bengusez@hotmail.com

Bengu Sezen, Ph.D.

DEC 13 2010

Re: Final Notice of Debarment
ORI Case No. 2006-15

Dear Dr. Sezen:

By letter dated October 4, 2010, the Department of Health and Human Services notified you of findings of misconduct in science made by the Office of the Research Integrity (ORI) and the Department's intent to debar you for a period of five (5) years pursuant to the Public Health Service Policies on Research Misconduct, 42 C.F.R. Parts 50 and 93, and HHS's Implementation (2 C.F.R. Part 376) of the Office and Management and Budget (OMB) Guidelines to Agencies on Governmentwide Debarment and Suspension (2 C.F.R. Part 180).

In accordance with Part 93, Subpart E, you were afforded 30 days within which to request a hearing in this matter. As of November 4, 2010, this period of time to request a hearing expired.

Please be advised that you are hereby debarred for a period of five (5) years from eligibility for contracting or subcontracting with any agency of the United States Government and from eligibility or involvement in nonprocurement programs of the United States Government pursuant to HHS's Implementation (2 C.F.R. Part 376) of the Office and Management and Budget (OMB) Guidelines to Agencies on Governmentwide Debarment and Suspension (2 C.F.R. Part 180). Your debarment is effective December 13, 2010 and runs through December 12, 2015.

This constitutes my final decision as the HHS Debarring Official on behalf of the Secretary of Health and Human Services. In accordance with applicable regulations, your name will be entered into the General Services Administration's "Excluded Parties List System."

Sincerely,

Nancy J. Gunderson
Deputy Assistant Secretary
for Acquisition Management and Policy

cc: Donald Wright, Acting Director

2006-15
DEB-6

Item No.	Bureau	Subject
4	CONSUMER AND GOVERNMENTAL AFFAIRS.	The Bureau will present an overview of the Twenty-First Century Communications and Video Accessibility Act, Public Law 111–260, the Commission's implementation plans, and demonstrate accessibility technologies.

The meeting site is fully accessible to people using wheelchairs or other mobility aids. Sign language interpreters, open captioning, and assistive listening devices will be provided on site. Other reasonable accommodations for people with disabilities are available upon request. In your request, include a description of the accommodation you will need and a way we can contact you if we need more information. Last minute requests will be accepted, but may be impossible to fill. Send an e-mail to: *fcc504@fcc.gov* or call the Consumer & Governmental Affairs Bureau at 202–418–0530 (voice), 202–418–0432 (tty).

Additional information concerning this meeting may be obtained from Audrey Spivack or David Fiske, Office of Media Relations, (202) 418–0500; TTY 1–888–835–5322. Audio/Video coverage of the meeting will be broadcast live with open captioning over the Internet from the FCC Live Web page at *http://www.fcc.gov/live.*

For a fee this meeting can be viewed live over George Mason University's Capitol Connection. The Capitol Connection also will carry the meeting live via the Internet. To purchase these services call (703) 993–3100 or go to *http://www.capitolconnection.gmu.edu.*

Copies of materials adopted at this meeting can be purchased from the FCC's duplicating contractor, Best Copy and Printing, Inc. (202) 488–5300; Fax (202) 488–5563; TTY (202) 488–5562. These copies are available in paper format and alternative media, including large print/type; digital disk; and audio and video tape. Best Copy and Printing, Inc. may be reached by e-mail at *FCC@BCPIWEB.com.*

Marlene H. Dortch,

Secretary, Federal Communications Commission.

[FR Doc. 2010–30169 Filed 11–24–10; 4:15 pm]

BILLING CODE P

FEDERAL RESERVE SYSTEM

Formations of, Acquisitions by, and Mergers of Bank Holding Companies

The companies listed in this notice have applied to the Board for approval, pursuant to the Bank Holding Company Act of 1956 (12 U.S.C. 1841 *et seq.*) (BHC Act), Regulation Y (12 CFR part 225), and all other applicable statutes and regulations to become a bank holding company and/or to acquire the assets or the ownership of, control of, or the power to vote shares of a bank or bank holding company and all of the banks and nonbanking companies owned by the bank holding company, including the companies listed below.

The applications listed below, as well as other related filings required by the Board, are available for immediate inspection at the Federal Reserve Bank indicated. The application also will be available for inspection at the offices of the Board of Governors. Interested persons may express their views in writing on the standards enumerated in the BHC Act (12 U.S.C. 1842(c)). If the proposal also involves the acquisition of a nonbanking company, the review also includes whether the acquisition of the nonbanking company complies with the standards in section 4 of the BHC Act (12 U.S.C. 1843). Unless otherwise noted, nonbanking activities will be conducted throughout the United States.

Unless otherwise noted, comments regarding each of these applications must be received at the Reserve Bank indicated or the offices of the Board of Governors not later than December 9, 2010.

A. Federal Reserve Bank of San Francisco (Kenneth Binning, Vice President, Applications and Enforcement) 101 Market Street, San Francisco, California 94105–1579:

1. Franklin Resources, Inc., San Mateo, California; to acquire additional voting shares of First Chicago Bancorp, and thereby indirectly acquire voting shares of First Chicago Bank & Trust, both of Chicago, Illinois.

Board of Governors of the Federal Reserve System, November 24, 2010.

Robert deV. Frierson,

Deputy Secretary of the Board.

[FR Doc. 2010–30050 Filed 11–26–10; 8:45 am]

BILLING CODE 6210–01–P

DEPARTMENT OF HEALTH AND HUMAN SERVICES

Office of the Secretary

Findings of Misconduct in Science

AGENCY: Office of the Secretary, HHS.

ACTION: Notice.

SUMMARY: Notice is hereby given that the Office of Research Integrity (ORI) has taken final action in the following case:

Bengu Sezen, Ph.D., Columbia University: Based on the findings of an investigation by Columbia University (CU) and additional analysis conducted by the Office of Research Integrity (ORI) during its oversight review, ORI found that Bengu Sezen, former graduate student, Department of Chemistry, CU, engaged in misconduct in science in research funded by National Institute of General Medical Sciences (NIGMS), National Institutes of Health (NIH), grant R01 GM60326.

Specifically, ORI made twenty-one (21) findings of scientific misconduct against Dr. Sezen based on evidence that she knowingly and intentionally falsified and fabricated, and in one instance plagiarized, data reported in three (3) papers [1] and her doctoral thesis.

The following administrative actions have been implemented for a period of five (5) years, beginning on November 4, 2010:

(1) Dr. Sezen is debarred from eligibility for any contracting or subcontracting with any agency of the United States Government and from eligibility or involvement in nonprocurement programs of the United States Government, referred to as "covered transactions," pursuant to HHS' Implementation of OMB Guidelines to Agencies on Governmentwide Debarment and Suspension (2 CFR 376 *et seq.*); and

(2) Dr. Sezen is prohibited from serving in any advisory capacity to the U.S. Public Health Service (PHS), including but not limited to service on any PHS advisory committee, board, and/or peer review committee, or as a consultant.

[1] Sezen, B., Franz, R., & Sames, D. "C–C bond formation via C–H bond activations: Catalytic arylation and alkenation of alkane segments." *J. Am. Chem. Soc.* 124:13372–13373, 2002. Retracted in *J. Am. Chem. Soc.* 128:8364, 2006.

Sezen, B. & Sames, D. "Oxidative C-arylation of free (NH)—heterocycles via direct (sp^3) C–H bond functionalization." *J. Am. Chem. Soc.* 126:13244–13246, 2004. Retracted in *J. Am. Chem. Soc.* 128:3102, 2006.

Sezen, B. & Sames, D. "Selective and catalytic arylation of N-phenylpryrrolidine: sp^3 C–H bond functionalization in the absence of a directing group." *J. Am. Chem. Soc.* 127:5284–5285, 2005. Retracted in *J. Am. Chem Soc.* 128:3102, 2006.

FOR FURTHER INFORMATION CONTACT: Director, Division of Investigative Oversight, Office of Research Integrity, 1101 Wootton Parkway, Suite 750, Rockville, MD 20852, (240) 453–8800.

John Dahlberg,

Director, Division of Investigative Oversight, Office of Research Integrity.

[FR Doc. 2010–29867 Filed 11–26–10; 8:45 am]

BILLING CODE 4150–31–P

DEPARTMENT OF HEALTH AND HUMAN SERVICES

National Toxicology Program (NTP): Office of Liaison, Policy, and Review; Availability of Draft NTP Technical Reports; Request for Comments; Announcement of a Panel Meeting to Peer Review Draft NTP Technical Reports

AGENCY: National Institute of Environmental Health Sciences (NIEHS); National Institutes of Health (NIH).

ACTION: Availability of Draft Reports; Request for Comments; and Announcement of a Meeting.

SUMMARY: The NTP announces the availability of draft NTP Technical Reports (TRs; available at *http://ntp.niehs.nih.gov/go/36051*) that will be peer-reviewed by an NTP Technical Reports Peer Review Panel at a meeting on January 26, 2011. The meeting is open to the public with time scheduled for oral public comment. The NTP also invites written comments on the draft reports (*see* "Request for Comments" below). Summary minutes from the peer review will be posted on the NTP Web site following the meeting.

DATES: The meeting to review the draft NTP TRs will be held on January 26, 2011. The draft NTP TRs will be available for public comment by December 8, 2010. The deadline to submit written comments is January 12, 2011, and the deadline for pre-registration to attend the meeting and/or provide oral comments at the meeting is January 19, 2011.

ADDRESSES: The meeting will be held at the Rodbell Auditorium, Rall Building, NIEHS, 111 T. W. Alexander Drive, Research Triangle Park, NC 27709. Public comments and any other correspondence on the draft TRs should be sent to Dr. Lori White, NIEHS, P.O. Box 12233, MD K2–03, Research Triangle Park, NC 27709, *FAX:* (919) 541–0295, or *whiteld@niehs.nih.gov.* Courier address: 530 Davis Drive, Room 2136, Morrisville, NC 27560. Persons needing interpreting services in order to attend should contact (301) 402–8180 (voice) or (301) 435–1908 (TTY). Requests should be made at least seven business days in advance of the meeting.

FOR FURTHER INFORMATION CONTACT: Dr. Lori White, NTP Designated Federal Officer, (919) 541–9834, *whiteld@niehs.nih.gov.*

SUPPLEMENTARY INFORMATION:

Preliminary Agenda Topics and Availability of Meeting Materials

The agenda topic is the peer review of the findings and conclusions of draft NTP TRs of toxicology and carcinogenicity studies. The preliminary agenda listing the draft reports and electronic files (PDF) of the draft reports should be posted on the NTP Web site by December 8, 2010. Any additional information, when available, will be posted on the NTP Web site (*http://ntp.niehs.nih.gov/go/36051*) or may be requested in hardcopy from the Designated Federal Officer (*see* **ADDRESSES** above). Following the meeting, summary minutes will be prepared and made available on the NTP Web site. Information about the NTP testing program is found at *http://ntp.niehs.nih.gov/go/test.*

Attendance and Registration

The meeting is scheduled for January 26, 2011, from 8:30 a.m. EST to adjournment and is open to the public with attendance limited only by the space available. Individuals who plan to attend are encouraged to register online at the NTP Web site (*http://ntp.niehs.nih.gov/go/36051*) by January 19, 2011, to facilitate access to the NIEHS campus. A photo ID is required to access the NIEHS campus. The NTP is making plans to videocast the meeting through the Internet at *http://www.niehs.nih.gov/news/video/live.* Registered attendees are encouraged to access the meeting page to stay abreast of the most current information regarding the meeting.

Request for Comments

The NTP invites written comments on the draft reports, which should be received by January 12, 2011, to enable review by the panel and NTP staff prior to the meeting. Persons submitting written comments should include their name, affiliation, mailing address, phone, e-mail, and sponsoring organization (if any) with the document. Written comments received in response to this notice will be posted on the NTP Web site, and the submitter will be identified by name, affiliation, and/or sponsoring organization.

Public input at this meeting is also invited, and time is set aside for the presentation of oral comments on the draft reports. In addition to in-person oral comments at the meeting at the NIEHS, public comments can be presented by teleconference line. There will be 50 lines for this call; availability will be on a first-come, first-served basis. The available lines will be open from 8:00 AM until adjournment on January 26, although public comments will be received only during the formal public comment periods indicated on the preliminary agenda. Each organization is allowed one time slot per draft report. At least 7 minutes will be allotted to each speaker, and if time permits, may be extended to 10 minutes at the discretion of the chair. Persons wishing to make an oral presentation are asked to notify Dr. Lori White via online registration at *http://ntp.niehs.nih.gov/go/166,* phone, or e-mail (*see* **ADDRESSES** above) by January 19, 2011, and if possible, to send a copy of the statement or talking points at that time. Written statements can supplement and may expand the oral presentation. Registration for oral comments will also be available at the meeting, although time allowed for presentation by on-site registrants may be less than that for pre-registered speakers and will be determined by the number of persons who register on-site.

Background Information on NTP Peer Review Panels

NTP panels are technical, scientific advisory bodies established on an "as needed" basis to provide independent scientific peer review and advise the NTP on agents of public health concern, new/revised toxicological test methods, or other issues. Previously, a subcommittee of the NTP Board of Scientific Counselors provided peer review of draft NTP Technical Reports. The subcommittee has been discontinued and peer review of the draft reports will now be conducted by peer review panels. These panels help ensure transparent, unbiased, and scientifically rigorous input to the program for its use in making credible decisions about human hazard, setting research and testing priorities, and providing information to regulatory agencies about alternative methods for toxicity screening. The NTP welcomes nominations of scientific experts for upcoming panels. Scientists interested in serving on an NTP panel should provide a current *curriculum vita* to Dr. Lori White (*see* **ADDRESSES**). The authority for NTP panels is provided by 42 U.S.C. 217a; section 222 of the Public Health Service (PHS) Act, as amended.

DEPARTMENT OF HEALTH & HUMAN SERVICES

Public Health Service

Office of Public Health and Science
Office of Research Integrity
1101 Wootton Parkway, Room 750
Rockville, Maryland 20852
Phone: 240-453-8800
FAX: 301-594-0043

OCT 4 - 2010

CONFIDENTIAL/SENSITIVE

VIA ELECTRONIC MAIL TRANSMISSION TO: (b)(6) and (b)(7)(C)

Bengu Sezen, Ph.D.

Re: ORI Case No. 2006-15

Dear Dr. Sezen:

This is to notify you that the Office of Research Integrity (ORI),Department of Health and Human Services (HHS), is making findings of misconduct in science under 42 C.F.R. Part 50, Subpart A against you based upon the findings of an investigation report by Columbia University ("CU") transmitted to ORI on October 3, 2007, and additional analysis conducted by ORI in its oversight review of the CU investigation report.[1]

The following sets forth a summary of ORI's findings of scientific misconduct and HHS' proposed administrative actions. This notice also provides information about your opportunity to contest these actions. Enclosed please find a charging document setting forth the basis for ORI's findings of misconduct in science and the HHS administrative actions. A copy of the CU investigation report (without attachments) is appended as ORI Ex. 1 to the enclosed charging document.

I. Summary of the ORI's Findings of Research Misconduct

As set forth more fully in the attached charging document, ORI has made twenty one (21)

[1]This is transmitted to you at the aforementioned electronic mail account address pursuant to your request to ORI dated August 10, 2010.

findings of scientific misconduct, based on evidence that you knowingly and intentionally fabricated and falsified and, in one instance, plagiarized, data reported in three (3) papers and your doctoral thesis.[2] ORI has concluded that these acts seriously deviated from those that are commonly accepted within the scientific community for proposing, conducting, and/or reporting research.

At the time you falsified, fabricated and plagiarized research results in the papers described above, HHS defined "Misconduct in Science" as "fabrication, falsification, plagiarism, or other practices that seriously deviate from those that are commonly accepted within the scientific community for proposing, conducting, or reporting research." 42 C.F.R. § 50.102. 42 C.F.R. Part 50, Subpart A has been replaced by the final rule, "Public Health Service Policies on Research Misconduct," codified at 42 C.F.R. Part 93, which became effective on June 16, 2005. For purposes of defining misconduct in science,[3] HHS shall use the definition applicable at the time the misconduct occurred. *See* 70 Fed. Reg. 28370, 28380. However, the procedures set forth in the final rule (Part 93) for requesting and conducting a hearing on these ORI findings apply to this case. *Id.*

II. Proposed HHS Administrative Actions

The Deputy Assistant Secretary for Grants and Acquisition Policy and Accountability (Debarring Official), the HHS official who is authorized to impose debarment, has reviewed these findings and finds that the scientific misconduct involved in this case is a cause for debarment under 2 C.F.R. § 376 *et seq.*

A. Debarment

The Debarring Official proposes to debar you for a period of five (5) years from eligibility for any contracting or subcontracting with any agency of the United States Government and from eligibility for, or involvement in, nonprocurement programs of the United States Government referred to as "covered transactions," pursuant to HHS' Implementation of OMB Guidelines to Agencies on Governmentwide Debarment and Suspension. 2 C.F.R. § 376 *et seq.*

Some of the significant consequences of debarment are:

- You will be ineligible to receive or participate in nonprocurement transactions, such as grants and cooperative agreements, of the Federal Government, except as

(b)(6) and (b)(7)(c)

[3] Misconduct in science is also commonly referred to as scientific misconduct, and will be referred to as such throughout this document.

provided in 2 C.F.R § 180.135.

- Bids and proposals will not be solicited from, contracts will not be awarded to, subcontracts will not be approved with, and existing contracts or subcontracts, if any, will not be renewed or approved for you by any Federal department or agency, except as provided in 2 C.F.R. Part 376 *et seq.*

- Your name will be placed on the "List of Parties Excluded from Federal Procurement and Nonprocurement Programs," which is maintained by the General Services Administration.

B. Additional Administrative Actions

It is also proposed that you be prohibited from serving in any advisory capacity to the Public Health Service including but not limited to service on any Public Health Service advisory committee, board, and/or peer review committee, or as a consultant for a period of five (5) years.

III. Opportunity to Contest ORI's Findings of Scientific Misconduct

In accordance with the PHS Policies on Research Misconduct, Subpart E, you may contest the ORI findings of misconduct in science and HHS administrative actions by requesting an administrative hearing before an administrative law judge with the HHS Departmental Appeals Board (DAB).

This request must be made within 30 days of receipt of this letter by writing to:

Chief Administrative Law Judge
Departmental Appeals Board
Department of Health and Human Services
MS6132
330 Independence Ave., S.W.,
Cohen Building, Room 6-G-644, Washington, DC 20201

The PHS Policies on Research Misconduct, 42 C.F.R. Part 93, can be found on the ORI website at:

http://ori.dhhs.gov/policies/regulations.shtml

Additional details may be provided to you by the DAB if and when you make a hearing request.

Please be advised that the PHS Policies on Research Misconduct, Subpart E, provide for a hearing only to address "a dispute over facts material to the findings of research misconduct or proposed administrative action." 42 C.F.R. § 93.503(a). Thus, any request for a hearing should identify the specific material facts in the ORI findings of misconduct in science that you dispute, including a statement of the reason(s) for disputing the finding(s).

A copy of your written request to the DAB must also be sent to:

Donald Wright, M.D., M.P.H.
Acting Director
Office of Research Integrity
1101 Wootton Parkway, Suite 750
Rockville, MD 20852-5003

If you do not request a hearing, the scientific misconduct findings and administrative actions set forth above will become effective 30 days from the date of receipt of this letter.

Sincerely,

Donald Wright MD MPH

Donald Wright, M.D., M.P.H.
Acting Director
Office of Research Integrity

Nancy Gunderson
Acting Deputy Assistant Secretary for
Acquisition Management and Policy

Enclosures

cc: Agency Research Integrity Liaison Officer, NIH, w/o Exhibits
Chief ALJ, HHS Departmental Appeals Board, w/o Exhibits
Columbia University

THE OFFICE OF RESEARCH INTEGRITY FINDINGS OF MISCONDUCT IN SCIENCE AGAINST BENGU SEZEN

The Office of Research Integrity (ORI) makes Findings of Misconduct in Science against Bengu Sezen (Respondent).[1] The Findings of Misconduct in Science are based on evidence and findings of an investigation conducted by Columbia University (CU), ORI's review of CU's findings, and additional evidence gathered by ORI in its oversight review. CU submitted an Investigation Committee Report to ORI on October 3, 2007 (CU Report), attached as Attachment 1.

I. JURISDICTION

A. ORI's Statutory and Regulatory Authority

ORI has the statutory and regulatory authority to make findings of scientific misconduct[2] and propose administrative actions. *See* 42 U.S.C. § 289b; 42 C.F.R. § 93.404.

B. Public Health Service Financial Support

The questioned research was supported in part by National Institutes of Health grant R01 GM060326 (b)(6) and (b)(7)(C)

C. "Misconduct in Science" Defined

At the time the events in this case occurred, the United States Department of Health and Human Services (HHS) defined "Misconduct in Science" as "fabrication, falsification, plagiarism, or other practices that seriously deviate from those that are commonly accepted within the scientific community for proposing, conducting, or reporting research. It does not include honest error or honest differences in interpretations or judgments of data." 42 C.F.R. § 50.102. 42 C.F.R. Part 50, Subpart A has been replaced by the final rule, "Public Health Service Policies on Research Misconduct," codified at 42 C.F.R. Part 93, which became effective on June 16, 2005. For purposes of defining scientific misconduct,[3] HHS will use the definition applicable at the time the misconduct occurred. *See* 70 Fed. Reg. 28370, 28380. However, for

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[1] The information contained in this charge letter and its attachments are maintained in the ORI Privacy Act exempt system of records pursuant to 09-37-0021, "HHS Records Related to Research Misconduct Proceedings" and is being provided as a Privacy Act release pursuant to Routine Use 12. 74 *Fed. Reg.* 44847 (Aug. 31, 2009). The Privacy Act requires that the enclosed information be maintained in a secure manner and not be further released. Should you receive a request for this charge letter and/or its attachments, please refer the requester to the U.S. Public Health Service Freedom of Information Act Office for a release determination.

[2] *See infra* section 1.C concerning the applicable terminology and definition of misconduct in science.

[3] Misconduct in science is also commonly referred to as scientific misconduct, and will be referred to as such throughout this document.

purposes of requesting a hearing on these ORI findings, the hearing will be conducted in accordance with the procedures promulgated by the final rule. *Id.*

II. SUMMARY OF ORI FINDINGS AND HHS ADMINISTRATIVE ACTIONS

ORI has made twenty one (21) findings of scientific misconduct, based on evidence that Respondent knowingly and intentionally fabricated and falsified, and, in one instance, plagiarized, data reported in three (3) publications and her doctoral thesis. In particular, Respondent fabricated and falsified numerous Nuclear Magnetic Resonance (NMR) spectra, each claimed to be the spectrum of a specific chemical species, by using standard software programs available on NMR spectrometers to transform an existing authentic spectrum into a spectrum of the desired complexity. Respondent also fabricated and falsified combustion analysis data that she reported in her publications and thesis. ORI has concluded that these acts seriously deviated from those that are commonly accepted within the scientific community for proposing, conducting, and/or reporting research.

ORI finds that Respondent's knowing and intentional falsification and fabrication of data constitutes "misconduct in science" within the meaning of 42 C.F.R. § 50.102. Additionally, ORI finds that Respondent's pattern of dishonest conduct and other intentionally deceptive conduct, including Respondent's assertions that other individuals were responsible for the falsified data, establish her lack of trustworthiness and present responsibility to be a steward of Federal funds. 2 C.F.R. § 376 *et seq.*

In accordance with this finding, the HHS Deputy Assistant Secretary for Grants and Acquisition Policy and Accountability (Debarring Official) proposes that for a period of five (5) years Respondent be debarred from any contracting or subcontracting with any agency of the United States Government and from eligibility for, or involvement in, nonprocurement programs of the United States Government referred to as "covered transactions" as defined in 2 C.F.R. §§ 180 and 376. HHS also proposes that, for a period of five (5) years, Respondent be prohibited from serving in any advisory capacity to the Public Health Service (PHS), including but not limited to service on any PHS advisory committee, board, and/or peer review committee, or as a consultant.

III. FACTUAL BACKGROUND

Respondent

1. Respondent entered the graduate program at the CU Department of Chemistry in August, 2000.

2. (b)(6) and (b)(7)(C)

3. Respondent's scientific misconduct occurred while Respondent was a member of (b)(6) and (b)(7)(c)

4. Respondent defended her dissertation on July 1, 2005, and received her doctoral degree from CU, with distinction, on October 19, 2005.

5. In February, 2006, Respondent enrolled as a graduate student in molecular biology at the University of Heidelberg, in the laboratory of (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C)

Respondent's Publications

6. While a member of the (b)(6) and (b)(7)(C) Respondent co-authored eight (8) papers and was the first author of six (6) of those papers.

7. Each of the papers for which Respondent was the first author has been retracted or corrected by (b)(6) and (b)(7)(C) also corrected one of the other papers that Respondent coauthored, as well as another paper, not co-authored by Respondent, that had incorporated a revised protocol for one of Respondent's chemical reactions.

8. The three papers that are the subject of the allegations of scientific misconduct herein, all of which have been retracted, are:

(b)(6) and (b)(7)(c)

9. The research contained in the papers for which Respondent was the first author was also incorporated into Respondent's doctoral dissertation (also referred to herein as Respondent's thesis). For the purposes of the scientific misconduct described herein, the fabricated and falsified data in the JACS 2002 paper is also found in Chapter 1 of Respondent's thesis, the fabricated and falsified data in the JACS 2004 paper is also found in Chapter 5 of Respondent's thesis, and the fabricated and falsified data in the JACS 2005 paper is also found in Chapter 6 of the Respondent's thesis. In addition, Chapter 7 of Respondent's thesis contained additional research that was not published, some of which was fabricated.

Description of Respondent's Research

10. Respondent's field of study at CU was organometallic chemistry, which is the study of chemical compounds that have one or more carbon atoms bonded to one or more metal atoms.

11. Some organometallic compounds act as catalysts, which are substances that promote chemical reactions, transforming one set of molecules into another, without themselves being consumed.

12. Respondent's papers and thesis describe the discovery of new chemical reactions by which, under the influence of small quantities of organometallic catalysts, simple organic molecules, called substrates, are linked together through new chemical bonds to form more complex structures, called products.

13. Respondent's research concentrated on the catalytic activation of carbon-hydrogen chemical bonds, which normally are highly unreactive. In particular, Respondent's research involved the use of catalysts to target a specific carbon-hydrogen bond in a molecule, which would allow chemical syntheses to be conducted more quickly, inexpensively, and with higher yields of the desired product. The ability to create reactions targeted at particular carbon-hydrogen bonds would have practical applications, e.g., in industrial processes to make pharmaceuticals. Respondent's research in this area was regarded as important within the organic chemistry community.

14. The molecular structure of each of the materials used in experiments such as Respondent's, including the substrates, catalysts, reaction mixtures, and products, is identified and characterized using various techniques, two of which are relevant to this matter: Nuclear Magnetic Resonance (NMR) Spectroscopy and combustion or elemental analysis (combustion analysis).

15. The result of an NMR analysis, referred to as an NMR spectrum, shows how the atoms of molecules are linked together and whether all the molecules in a sample are the same.

16. Combustion analysis is used to determine the composition of a sample, i.e., how much of the mass of a sample is contributed by each constituent chemical element. The results of the analysis are expressed as percentages of each element, and the elements usually analyzed include hydrogen, carbon and nitrogen.

17. The CU Department of Chemistry uses the services of commercial laboratories to obtain combustion analyses.

Use of NMR Spectrometers at CU

18. At all times relevant to this matter the CU Department of Chemistry maintained a facility that housed four (4) NMR spectrometers. A wide-bore 300 MHz NMR spectrometer, a narrow-bore 400 MHz NMR spectrometer, and a narrow-bore 500 MHz spectrometer are located on the second floor of a CU building. A narrow-bore 300 MHz spectrometer is located on the first floor of the same building. There is no indication that Respondent used the 500 MHz spectrometer.

19. The manager of the NMR facility at all times relevant to this matter was (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C)

20. The spectrometers incorporate UNIX workstations that control spectrometer operations.

21. The NMR facility is accessible to authorized users at all times. Users can reserve time to use the 400 MHz and wide-bore 300 MHz spectrometers using sign up sheets. These instruments can also be used on a walk-up basis when no other user has reserved them. Reservations are not taken for the narrow-bore 300 MHz spectrometer.

22. To be authorized to use the NMR facility, all users must obtain training and pass a test in the operation of the NMR instruments.

23. Once a researcher passes the test, (b)(6) and (b)(7)(C) assigns the user a unique UNIX login account number. These accounts are password-protected.

24. Members of a research group (b)(6) and (b)(7)(C) can read the data belonging to members of the group, but only the user can create or modify data in his or her account.

25. Because NMR spectrometry is a central analytic tool in organic chemistry, new graduate students normally are trained to use the instruments and receive a user login account soon after they join a research group.

26. There have been instances where researchers have used the accounts and passwords of other group members in order to use the spectrometers prior to completing training.

Events Leading Up to the Allegation of Scientific Misconduct

27. Beginning in 2002, concerns about the reproducibility of Respondent's research were raised both by members of the (b)(6) and (b)(7)(C) and by scientists outside CU.

28. Members of the (b)(6) and (b)(7)(C) reported that they were able to reproduce reactions described by Respondent successfully only when Respondent was in the laboratory and was aware that the experiments were being performed.

29. In July 2005, (b)(6) and (b)(7)(C) who had been unable to reproduce Respondent's results for a particular experiment over the course of several months, noted that the reaction had worked on a day in which Respondent was in the laboratory. (b)(6) and (b)(7)(C) suspected that Respondent had added the expected product to his reaction mixtures.

30. (b)(6) and (b)(7)(C) tested his suspicions by preparing two reactions at a time when Respondent was present in the laboratory. One of the reactions used the starting material required by Respondent's procedures and one used a different starting material. He reported that both reactions appeared to have produced the same product, which was surprising because this product would only have been expected to be produced from the starting materials required by Respondent's procedures.

31. On the following day, (b)(6) and (b)(7)(C) then repeated the reactions in the laboratory of (b)(6) and (b)(7)(C) and tried to ensure that he, (b)(6) and (b)(7)(C) labmate was present throughout the experiments. These experiments yielded no trace of the product produced in (b)(6) and (b)(7)(C) experiments during the previous day.

32. After (b)(6) and (b)(7)(C) presented these results to (b)(6) and (b)(7)(C) arranged for (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) to review Respondent's research.

33. At the time this review was taking place, Respondent, who had finished defending her dissertation, was not present at CU. Prior to leaving CU, Respondent had packed up her research records and other materials and left them in the (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) because the (b)(6) and (b)(7)(C) was preparing for a move from the (b)(6) and (b)(7)(c) of the Chemistry building.

34. As part of the review, members of the (b)(6) and (b)(7)(C) reviewed Respondent's research records.

35. (b)(6) and (b)(7)(C) who was assisting in the review of Respondent's records, discovered, among Respondent's records, a composite figure composed of four (4) phosphorus-31 (^{31}P) NMR spectra, in which certain peaks had been removed from the spectrum using white-out or a similar product ("White-Out Spectrum").

36. The White-Out Spectrum matched, in peak positions, peak heights, and background noise, a spectrum that was published in the JACS 2004 paper and in Respondent's thesis.

37. After the discovery of the White-Out Spectrum, (b)(6) and (b)(7)(C) searched for Respondent's NMR data on the computers at the NMR facility (see paragraph 24, *supra*).

38. In consultation with (b)(6) and (b)(7)(C) learned that no NMR account had ever been assigned to Respondent.

39. (b)(6) and (b)(7)(C) then discovered spectra on the 400 MHz and narrow-bore 300 MHz spectrometers that appeared relevant to Respondent's research in the account of (b)(6) and (b)(7)(C), a former member of the (b)(6) and (b)(7)(C) These spectra were recorded after (b)(6) and (b)(7)(C) had left CU and were unrelated to (b)(6) and (b)(7)(C) research.

40. In particular, (b)(6) and (b)(7)(C) found, on the narrow-bore 300 MHz spectrometer, four (4) ^{31}P NMR spectra that he identified as the individual spectra that comprised the White-Out Spectrum. He also located a series of processed data files that demonstrated that each spectrum had been constructed by manipulating the single peak that constitutes the ^{31}P NMR spectrum of triphenylphosphine (PPh_3), a readily available compound.

41. An NMR spectrum can be fabricated and falsified by using standard software programs available on NMR spectrometers to duplicate an authentic spectrum containing a single resonance line, rescale the intensity of the duplicated spectrum, shift the duplicated spectrum right or left to shift the apparent resonance frequency, and add the duplicated spectrum to the original. Using this method, a spectrum consisting of a single line can be transformed into one with two resonance lines with apparently different frequencies and intensities. When repeated, this process of duplication and manipulation can generate a spectrum of any complexity.

42. The ^{31}P NMR spectra that comprise the White-Out Spectrum were identical to the ^{31}P NMR spectra found in the rayane account, except for the peaks that were removed with White-Out. It appeared that the sample of PPh_3 that was used to create the original, authentic spectrum was contaminated with a small amount of Ph_3PO, and the small peaks generated by this contaminant were those removed with White-Out.

43. (b)(6) and (b)(7)(C) also discovered, in the rayane account on the 400 MHz spectrometer, a data set consisting of 63 processed data files that had been sequentially generated using the process described in paragraph 41, *supra*, to create a final spectrum. In other words, rather than being an analysis of a product of a reaction, the final spectrum, like the spectra described in paragraph 40, had been fabricated and falsified.

44. The final spectrum contained in the sixty-third processed data file is identical in all material respects to the spectrum identified as that of compound 21 in the JACS 2004 paper and in Respondent's dissertation.

45. NMR spectra contain very small satellite peaks, frequently overlooked, that reflect the coupling of ^{13}C and ^{1}H nuclei. The distance in Hertz (Hz) between the

pair constituting a satellite is called the $^{1}J_{CH}$ coupling constant. (b)(6) and (b)(7)(c) examined the $^{1}J_{CH}$ coupling constants associated with each peak in the final (63rd) spectrum discovered on the 400 MHz spectrometer.

46. (b)(6) and (b)(7)(C) found that the spectrum exhibited $^{1}J_{CH}$ coupling constants of 177.6 Hz. This is the $^{1}J_{CH}$ coupling constant expected for the common chemical methylene chloride and is significantly different from the $^{1}J_{CH}$ coupling constant that would be expected for each of the peaks in a spectrum of the compound reported by Respondent in the JACS 2004 paper and her dissertation.

47. (b)(6) and (b)(7)(C) prepared an analysis in which he described the findings concerning the White-Out Spectrum and the spectrum constructed in 63 processes from the spectrum of methylene chloride. (b)(6) and (b)(7)(C) also concluded that four (4) other spectra from the JACS 2004 paper (identified as compounds 1, 7, 9 and 10) had been fabricated from the spectrum of methylene chloride and that another spectrum from the JACS 2004 paper (compound 12) had been fabricated from the spectra of two (2) known compounds, 3-bromo-1-TIPS-indole and pyrroline.

Investigation by the CU Inquiry Committee

48. In a memorandum dated November 7, 2005, and sent to the (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) that Respondent had fabricated certain research results. (b)(6) and (b)(7)(C) attached to that memorandum the analysis by (b)(6) and (b)(7)(C) describing the fabrication of data in the JACS 2004 paper.

49. In response to the memorandum, the Dean of the CU Graduate School of Arts and Sciences appointed a three-person Inquiry Committee to conduct an inquiry into the allegations. *See* 42 C.F.R. § 93.307.

50. After interviewing witnesses and reviewing the White-Out Spectrum and the spectra on the NMR spectrometers that had been discussed in (b)(6) and (b)(7)(C) analysis, the Inquiry Committee concluded that there was clear evidence of misconduct and fraud by Respondent and that a more detailed investigation was warranted. The Inquiry Committee submitted a report documenting its findings on February 16, 2006, to the Dean of the CU Graduate School of Arts and Sciences.

51. The Chair of the CU Department of Chemistry and Department of Chemistry staff made numerous attempts to notify Respondent of the allegations and inquiry, including sending electronic mail to her Columbia account and her account at the University of Heidelberg.

52. The emails to the University of Heidelberg account were not replied to, and until March 2006 the emails to the CU account were replied to with responses stating that the account was no longer being used.

53. The CU Department of Chemistry also sent a letter to Respondent via FedEx at (b)(6) and (b)(7)(C) (listed in CU records as Respondent's home address), advising her that the inquiry had commenced.

54. A program coordinator in the CU Department of Chemistry subsequently received an email from a person at the (b)(6) and (b)(7)(C) to which the FedEx letter had been sent indicating that the letter could not be delivered because Respondent was no longer at that address. In response to a reply from the CU program coordinator that she would try to locate Respondents' parents, the person from the apartment building stated that Respondents' parents were no longer in that apartment complex.

55. On March 23, 2006, shortly after learning that the CU Office of Public Affairs had received an email from Respondent using her CU account, the Chair of the Department of Chemistry forwarded to Respondent, at her CU email account, the Inquiry Committee's report and copies of previous messages he had attempted to send her.

56. On March 27, 2006, Respondent acknowledged receipt of the Inquiry Report.

57. Subsequently, CU provided Respondent with documents and additional information that she had requested, and Respondent provided comments on the report on May 19, 2006.

58. Respondent's comments included allegations that (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) had committed scientific misconduct by fraudulently claiming that Respondent's work could not be reproduced (counter-allegations). The counter-allegations were forwarded to a separate inquiry committee.

59. Respondent's comments were provided to the Inquiry Committee, which reviewed them and issued its own final comments.

Procedural History of the Investigation by the CU Ad Hoc Committee

60. CU's Standing Committee on the Conduct of Research accepted the recommendation of the Inquiry Committee that a full investigation was warranted, and an Ad Hoc Committee was appointed.

61. The Ad Hoc Committee interviewed eighteen (18) witnesses and reviewed over 10,000 pages of documents.

62. Between June, 2006, and August, 2006, CU made numerous unsuccessful attempts to schedule a teleconference with Respondent concerning both the allegations against her and her counter-allegations.

63. On August 16, 2006, Respondent indicated by email that she would be available for an in-person interview but declined to make arrangements for the interview until she received documents she had requested pertaining to the (b)(6) and (b)(7)(C) attempts to reproduce her work.

64. From August 16, 2006, to August 29, 2006, Respondent sent emails complaining about CU's handling of her counter-allegations to CU officials, reporters from Science, Nature, and the New York Times, and the chemistry faculties of numerous universities.

65. CU and Respondent had numerous communications via email regarding Respondent's requests to review records, including records related to Respondent's counter-allegations. Respondent replied to CU on several occasions by indicating that the records provided by CU were insufficient.

66. During one such email exchange, on August 31, 2006, Respondent indicated that she only used her own NMR account and that she was staying at a (b)(6) and (b)(7)(c) (b)(6) and (b)(7)(c) on the date that one of the spectra at issue in this matter was created.

67. Respondent also indicated in her August 31, 2006, email that she would be available for a telephone interview on October 6, 2006.

68. CU and Respondent had further email correspondence regarding CU's preference that the interview take place in person at CU. Respondent advised CU that she was unable to satisfy the visa requirements necessary for her to travel to the United States and that previous visa applications she had submitted had been denied.

69. Thereafter, CU retained White and Case, a law firm with an office in Ankara, Turkey. CU sent approximately 6,000 pages of documents related to the case to White and Case's Ankara office so that Respondent would have the opportunity to review the documents.

70. Respondent did not review the documents sent to White and Case, nor did she accept an offer to have White and Case deliver the documents to Respondent for the interview.

71. On October 5, 2006, after having received a letter from the Committee Chair, Respondent emailed the Committee Chair a response that included her purported NMR account name and an electronic copy of a (b)(6) and (b)(7)(c) which allegedly contained information relevant to (b)(6) and (b)(7)(c) referenced in paragraph 66, *supra*.

72. On October 6, 2006, the Committee called Respondent at the number she had provided and conducted a telephone interview with her.

73. Thereafter, Respondent requested from CU, and received, photocopies of her eleven (11) laboratory notebooks. CU sent the copies to Respondent at an (b)(6) and (b)(7)(C) address that Respondent provided.

74. The findings and recommendations in the Final Report of the Ad Hoc Committee were accepted by the Standing Committee on April 18, 2007 and by the CU Executive Vice President for Research on May 17, 2007.

75. CU notified Respondent of the final adjudication of scientific misconduct against her by letter dated May 18, 2007.

76. Respondent sent a letter, dated June 5, 2007, to several CU officials. CU construed this letter as an appeal from the findings of scientific misconduct.

77. Respondent's letter, along with the Ad Hoc Committee's Final Report, were reviewed by the CU Provost, who denied Respondent's appeal.

78. CU made a supplemental adjudication of scientific misconduct against Respondent on May 9, 2008. This supplemental adjudication involved scientific misconduct described in detail in the section entitled ORI Issue #11, *infra*. Respondent did not submit comments on or appeal this supplemental adjudication to CU.

CU Findings of Fact

79. The Committee found that Respondent never had an authorized user account at the CU NMR facility.

80. The finding that Respondent never had an authorized user account at the CU NMR facility was based on (b)(6) and (b)(7)(C) testimony that he had (1) no record of an account issued to Respondent in the logbook he keeps of all NMR accounts issued and (2) no record in the NMR Facility's computer files of an account belonging to Respondent (including no record of a login ID of "bengu," which Respondent identified as her login ID in her October 5, 2006, letter to the Committee Chair).

81. In addition, the monthly usage reports created by (b)(6) and (b)(7)(C) for the Department of Chemistry Business Office contained no reference to charges for any account belonging to Respondent.

82 The Committee found the failure to obtain an authorized account to be a major departure from standard practice.

83. The (b)(6) and (b)(7)(C) was repeatedly used after (b)(6) and (b)(7)(C) departure from the (b)(6) and (b)(7)(C) closed her account in September, 2004.

84. The Committee found that the Respondent used the accounts of other members of (b)(6) and (b)(7)(C)

85. Spectra found in Respondent's thesis and publications were found in the (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C)

86. The Committee compared the signup sheets for the 400 MHz NMR spectrometer to the accounting system logs. Approximately three-quarters of the logins to the (b)(6) and (b)(7)(C) occurred at times when Respondent had signed up for access.

87. Many of the data sets in the rayane account on the 400 MHz spectrometer and the narrow-bore 300 MHz spectrometer that were created after (b)(6) and (b)(7)(C) left the (b)(6) and (b)(7)(C) have names of chemical compounds that Respondent used in her research.

88. Spectra found in Respondent's thesis and publications were also found in the account belonging to (b)(6) and (b)(7)(C)

89. (b)(6) and (b)(7)(C) testified that he had shared the password for his NMR account with Respondent.

90. The Committee compared the signup sheets for the 400 MHz NMR spectrometer to the accounting system logs. Approximately 35% of the logins to (b)(6) and (b)(7)(C) account after he left the (b)(6) and (b)(7)(C) (in December 2002) occurred at times when Respondent had signed up for access.

91. (b)(6) and (b)(7)(C) testified that he shared the password for his NMR account with Respondent and (b)(6) and (b)(7)(C) both of whom used his account until he asked them to delete their files from the account. A Zip disk found among Respondent's records contained NMR data sets (b)(6) and (b)(7)(C) the user.

92. The Committee made findings regarding the research records kept by Respondent, specifically her laboratory notebooks, archival NMR spectra, electronic research records, and records regarding combustion analyses.

93. Respondent's research records were sequestered by CU as part of its investigation in April, 2006.

94. The Committee found that the maintenance of accurate records of procedures and results is a standard principle of research in organometallic chemistry.

95. The Committee examined eleven (11) laboratory notebooks belonging to Respondent and labeled BS-I to BS-XI and found those notebooks to be all the laboratory notebooks relevant to Respondent's research.

96. Respondent's notebooks contained few detailed experimental procedures for novel reactions performed by Respondent.

97. Respondent claimed to have had four (4) additional notebooks that contained her experimental procedures.

98. The Committee did not credit Respondent's claim because (1) neither (b)(6) and (b)(7)(C) who reviewed Respondent's work, nor other members of the (b)(6) and (b)(7)(C) recalled seeing such notebooks and (2) none of the laboratory notebooks examined by the Committee refer to the existence of any experimental procedure notebooks, as would be expected if such notebooks existed and contained experimental protocols related to the research documented in the numbered laboratory notebooks.

99. The Committee found that six (6) binders containing NMR spectra and one Zip disk, see paragraph 91, *supra*, that were sequestered constitute the entire record of original NMR spectra relevant to Respondent's research.

100. Although most of the reactions in Respondent's laboratory notebooks include a code for NMR spectra, the spectra in the NMR binders are not labeled with a corresponding code. Therefore, the spectra in the binders cannot be linked to any specific reaction described in the notebooks.

101. The Committee did not credit Respondent's claim that she had eight (8) to twelve (12) additional NMR binders, the spectra in which were properly labeled. No member of the (b)(6) and (b)(7)(C) interviewed by the Committee remembered seeing fourteen (14) to eighteen (18) binders belonging to Respondent.

102. Despite the absence of proper labeling, in some cases, the Committee was able to match spectra in Respondent's binders to spectra published in Respondent's thesis and publications. Resonance frequencies and peak integrals are printed on the spectra and are reported to a very high precision. Therefore, a spectrum in the binder and a spectrum in a publication can be matched by finding an exact equivalence between the frequencies and integrals.

103. No supporting NMR data were located in Respondent's NMR binders for many products described in her publications.

104. The Committee found that the 29 zip disks, 22 floppy disks, and 4 CD ROMs sequestered in this case constitute the entirety of Respondent's electronic research records.

105. One zip disk includes six (6) data sets that originated in the NMR account of (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) Other than this data, no other raw NMR data sets were found in Respondent's electronic materials.

106. The Committee found that, like most other members of the (b)(6) and (b)(7)(C) at that time, Respondent did not back up her electronic data sets.

107. The Committee did not credit Respondent's claim that other electronic records pertaining to her research exist, including eighteen (18) disks containing NMR spectra, because (1) no one else recalled seeing such items and (2) Respondent apparently kept no copies of these additional electronic records.

108. Respondent's thesis states that all combustion analyses for her thesis were conducted by the (b)(6) and (b)(7)(C)

109. A search of Respondent's records yielded documentation for two (2) combustion analyses by (b)(6) and (b)(7)(C) and no documentation of combustion analyses conducted by any other laboratory.

110. According to the CU Department of Chemistry Business Office, four (4) laboratories provide combustion analysis services to CU, one of which is (b)(6) and (b)(7)(C)

111. The Committee examined invoices for combustion analyses that were charged to the (b)(6) and (b)(7)(C)

112. Five (5) invoices addressed to Respondent from (b)(6) and (b)(7)(C) were located. No invoices from other laboratories to Respondent were located.

113. In January, 2006, (b)(6) and (b)(7)(C) and requested copies of data previously reported to the (b)(6) and (b)(7)(C)

114. These reports correspond to the purchase order numbers in the CU financial office records. In other words, for each transaction with (b)(6) and (b)(7)(C) recorded by CU's financial offices, the corresponding documentation and data provided by (b)(6) and (b)(7)(C) group was identified.

115. The Committee found that the records provided by (b)(6) and (b)(7)(C) reflect all of (b)(6) and (b)(7)(C) records of combustion analyses conducted at the (b)(6) and (b)(7)(C) request while Respondent was at CU.

116. The Committee did not credit Respondent's claim that she had an entire binder of combustion analysis reports. Although Respondent claimed that some of her samples were submitted under another student's name, the documentation received from (b)(6) and (b)(7)(C) for other (b)(6) and (b)(7)(C) members did not include data for Respondent's experiments.

117. The Committee also did not credit Respondent's claims to have obtained analyses through free trials from up to 25 vendors because (1) she produced no records

supporting this claim; (2) CU contacted some of the companies named by Respondent as having provided free trials and was told they had no records of combustion analyses done for CU and did not provide free trials in any event; (3) there would be little incentive for a student to obtain free trials; and (4) Respondent's thesis states that analyses were conducted by (b)(6) and (b)(7)(C)

CU Findings Concerning the Allegation that Respondent Fabricated and Falsified NMR Spectra in Her Thesis and Publications

118. The Committee found by a preponderance of the evidence that Respondent intentionally fabricated and falsified NMR spectra reported in at least Chapters 1, 5 and 6 of her thesis and in JACS 2002, JACS 2004, and JACS 2005.

119. The basis for these findings is set forth in detail in the ORI Findings, *infra*.

120. The NMR spectra identified as fraudulent by the Committee in JACS 2002 (Chapter 1 of the thesis) and JACS 2005 (Chapter 6 of the thesis) had not previously been identified as fraudulent by either members of the Sames Group or the initial Inquiry Committee.

121. In the case of the spectrum for 1,2-diphenylpyrrolidine, contained in JACS 2005 and Chapter 6 of Respondent's thesis, CU found evidence of plagiarism as well as fabrication and falsification.

122. The Committee was also unable to find data that supported the results of many other reactions that Respondent reported in her notebooks, publications and thesis.

123. The Committee found that this absence of documentary evidence concerning NMR spectra was further evidence of Respondent's scientific misconduct.

CU Findings Concerning the Allegation that Respondent Fabricated and Falsified Combustion Analysis Data Reported in Her Thesis and Publications

124. The Committee found by a preponderance of the evidence that Respondent intentionally fabricated and falsified combustion analysis data in JACS 2004 and JACS 2005 and in Chapters 5, 6 and 7 of her thesis.

125. The basis for these findings is set forth in detail in the ORI Findings, *infra*.

CU Findings Concerning the Allegation that Respondent Fabricated and Falsified Experimental Procedures Reported in her Thesis and Publications

126. The Committee found by a preponderance of the evidence that Respondent's research record did not meet the standards of the scientific research community and did not adequately document the procedures and results reported in her thesis and publications.

127. In addition, the Committee found so little evidence in the research record to support Respondent's published description of results and procedures that it concluded that substantial numbers of the experiments reported in the thesis and in the six (6) publications where Respondent was the first author were never successfully performed as described.

128. The Committee found by a preponderance of the evidence that Respondent fabricated and falsified her experimental procedures.

Respondent's Defenses and Credibility

129. Pursuant to 42 C.F.R. § 93.106(b)(2), Respondent had the burden of proving, by a preponderance of the evidence, any and all affirmative defenses to a finding of scientific misconduct.

130. CU found that Respondent failed to meet that burden.

131. Respondent claimed that she could not have fabricated and falsified spectra in the (b)(6) and (b)(7)(C) that were modified on June 11 and 12, 2004, because she was on vacation in (b)(6) and (b)(7)(C) on those dates. Respondent provided a copy of a credit card statement purporting to show (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C)

132. CU did not credit this claim because Respondent's signature appeared on the signup sheets for the 400 MHz spectrometer for June 11, 2004, and because other fraudulent data was created during the period from June 23, 2004 to June 26, 2004, at times when Respondent's signature also appears on the spectrometer sign-up sheets.

133. CU noted that the copy of the credit card statement provided by Respondent contained irregularities and did not prove in any event that Respondent was in (b)(6) and (b)(7)(C) on the dates the charges accrued.

134. Respondent also claimed that the ^{31}P spectrum found in JACS 2004 and at page 333 of her thesis was not identical to the White-Out spectrum.

135. CU found that the spectra were materially identical and that differences noted by Respondent were irrelevant (in the case of different labeling) or due to the lower resolution of the spectrum published in the thesis.

136. Respondent also claimed that other members of the (b)(6) and (b)(7)(C) – particularly (b)(6) and (b)(7)(C) - framed her by planting NMR spectra in her binders, which she then unwittingly included in her thesis and publications. Respondent suggested that (b)(6) and (b)(7)(C) framed her in order to later publish a paper based on her ideas without giving her credit.

137. CU found that the first fraudulent spectra were produced long before the chemistry in the paper published by (b)(6) and (b)(7)(C) (in 2006) was developed.

138. CU found no credible evidence that any individual other than Respondent fabricated and falsified the NMR spectra in Respondent's thesis and publications.

139. CU also determined that the review of Respondent's work was triggered by (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) who joined the (b)(6) and (b)(7)(C) in February 2005, that it was (b)(6) and (b)(7)(C) who discovered the White-Out Spectrum, and that some of the fabricated and falsified spectra (included those found in JACS 2002) were discovered by the Committee, not by members of the (b)(6) and (b)(7)(C)

140. CU also found that, given that fabricated and falsified spectra appeared in Respondent's publications as early as 2002, it was unlikely that a member of the (b)(6) and (b)(7)(C) would plant fraudulent spectra in Respondent's binders in 2002 and then wait three (3) years before exposing Respondent.

141. Respondent also claimed as a defense that others had independently reproduced her experiments, in particular (b)(6) and (b)(7)(C), a company called (b)(6) and (b)(7)(C) and (b)(6) and (b)(7)(C)

142. CU concluded both that reproducibility does not directly bear on whether Respondent fabricated and falsified her results and that, by a preponderance of the evidence, none of the individuals or companies cited by Respondent independently reproduced her results.

143. The two CU students referred to by Respondent testified that they were unable to reproduce Respondent's reactions except when she was present.

144. The chief technical officer of (b)(6) and (b)(7)(C) informed CU that (b)(6) and (b)(7)(C) never attempted to reproduce Respondent's work.

145. CU found that (b)(6) and (b)(7)(c) Ralf Decter, and the purported company she worked for, Duha Chemisches Katalyse-Labor (Duha), were all fictional beings or entities and claims that (b)(6) and (b)(7)(c) reproduced Respondent's reactions should be accorded no weight.

146. Electronic mail correspondence received by CU in connection with its investigation purportedly from (b)(6) and (b)(7)(c) and Mr. Decter were in fact sent from computers in (b)(6) and (b)(7)(c) and at the University of Heidelberg, and at least one email purportedly from Mr. Decter to CU originated from the same IP address as electronic mail sent to CU by Respondent.

147. A letter purportedly from (b)(6) and (b)(7)(C) sent to CU by Respondent was sent on Duha letterhead. CU obtained written testimony from Dr. Bernard Hollborn, the managing director of (b)(6) and (b)(7)(c) which is the business located at the address on the Duha letterhead. Dr. Bernard Hollborn explained that no business by the name Duha exists at that address, that the (b)(6) and (b)(7)(C) in his business' name refers (b)(6) and (b)(7)(C) and that no living person named (b)(6) and (b)(7)(C) is known to him.

148. CU conducted a telephone interview with a person who identified (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) on September 18, 2006. This person claimed to be employed at (b)(6) and (b)(7)(C) at the address given on the letterhead and indicated that the head of the company was Ralf Decter, who supposedly could be reached at the same phone number as (b)(6) and (b)(7)(C)

149. CU identified several examples of Respondent damaging her credibility by misleading the Committee, specifically by (1) claiming to have had an NMR account with the login ID of "bengu," (2) denying during her interview with the Committee that she was enrolled at the University of Heidelberg (a statement she subsequently corrected two days after the Committee interviewed (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) in whose laboratory Respondent (b)(6) and (b)(7)(C) and (3) presenting an expert witness (b)(6) and (b)(7)(C) who was not genuine.

CU Findings Regarding the Impact of Respondent's Actions

150. CU found that researchers inside and outside CU made substantial and futile efforts to reproduce and extend Respondent's research results.

151. Members of the (b)(6) and (b)(7)(C) expended considerable time attempting to reproduce Respondent's results. The Committee found that the wasted time and effort, and the onus of not being able to reproduce the work, had a severe negative impact on the graduate careers of three (3) of those students, two of whom (b)(6) and (b)(7)(C) were asked to leave the (b)(6) and (b)(7)(C) and one of whom decided to leave after her second year.

IV. ORI'S OVERSIGHT REVIEW AND ORI FINDINGS OF SCIENTIFIC MISCONDUCT

152. ORI received and accepted the CU Report in fulfillment of CU's obligations to submit a final investigation report in compliance with the PHS policies. 42 C.F.R. § 93.313.

153. ORI's Division of Investigative Oversight (DIO) conducted an independent and objective oversight review of the CU Report in accordance with the authority conferred on ORI by statute, 42 U.S.C. § 289b(d), and through the promulgation of the Public Health Service Policies on Research Misconduct, 42 C.F.R. § 93.403.

154. The ORI oversight review determines that ORI findings of misconduct in science against Respondent are warranted, and charges Respondent with having engaged in scientific misconduct as set forth herein below.

The following are the twenty one (21) Office of Research Integrity findings of scientific misconduct against Respondent.

ORI ISSUE #1: That Respondent knowingly and intentionally fabricated and falsified the ^{1}H NMR spectrum of compound 21 in JACS 2004 and in her thesis.

155. Page S34 of JACS 2004 and Chapter 5, page 347, of Respondent's thesis include an NMR spectrum identified as the ^{1}H spectrum of compound 21. Tabular data referencing the NMR spectrum of compound 21 is found at page S16 of JACS 2004 and Chapter 5, page 327, of Respondent's thesis.

156. A data set located in the rayane account of the 400 MHz NMR spectrometer includes a spectrum with peak resonance frequencies and peak integrals identical to those identified in the spectrum of compound 21 in the JACS 2004 article and Respondent's thesis.

157. This data set includes individually processed data files that were generated and sequentially added together to generate the final spectrum, which is materially identical to that of compound 21, demonstrating that the spectrum was fabricated and falsified through progressive construction.

158. The satellite resonance peaks in this spectrum have a coupling constant of 177.6 Hz, which is the expected value of methylene chloride, a common solvent.

159. The existence of resonance peaks with a coupling constant of 177.6 Hz demonstrates that the NMR spectrum of methylene chloride was used to construct the fabricated and falsified spectrum.

160. ^{1}H NMR data for compound 21 was also found in Respondent's binders.

161. The fabricated and falsified spectrum for compound 21 was created on June 11, 2004.

162. User logs for the 400 MHz spectrometer indicate that the rayane account was used from 9:52 am to 10:12 am on June 11, 2004, and the 400 MHz sign up sheet indicates that Respondent was signed up to use the spectrometer at that time.

ORI FINDING #1: Respondent knowingly and intentionally committed scientific misconduct by fabricating and falsifying the ^{1}H NMR spectrum of compound 21 in JACS 2004 and in her thesis.

ORI ISSUE #2: That Respondent knowingly and intentionally fabricated and falsified the ^{1}H NMR spectrum of compound 1 in JACS 2004 and in her thesis.

163. Page S29 of JACS 2004 and Chapter 5, page 342, of Respondent's thesis include an NMR spectrum identified as the ^{1}H NMR spectrum of compound 1. Tabular data referencing the NMR spectrum of compound 1 is found at page S6 of JACS 2004 and Chapter 5, page 311, of Respondent's thesis.

164. A data set located in the rayane account of the 400 MHz NMR spectrometer includes a spectrum with peak resonance frequencies and peak integrals identical to those identified in the spectrum of compound 1 in the JACS 2004 article and Respondent's thesis.

165. This data set includes individually processed data files that were generated and sequentially added together to generate the final spectrum, which is materially identical to that of compound 1, demonstrating that the spectrum was fabricated and falsified through progressive construction.

166. The satellite resonance peaks in this spectrum have a coupling constant of 177.6 Hz, which is the expected value of methylene chloride.

167. The existence of resonance peaks with a coupling constant of 177.6 Hz demonstrates that the NMR spectrum of methylene chloride was used to construct the fabricated and falsified spectrum.

168. ^{1}H NMR data for compound 1 was also found in Respondent's binders.

169. The fabricated and falsified spectrum for compound 1 was created on June 11, 2004.

170. User logs for the 400 MHz spectrometer indicate that the rayane account was used from 9:52 am to 10:12 am on June 11, 2004 , and the 400 MHz sign up sheet indicates that Respondent was signed up to use the spectrometer at that time.

ORI FINDING #2: Respondent knowingly and intentionally committed scientific misconduct by fabricating and falsifying the ^{1}H NMR spectrum of compound 1 in JACS 2004 and in her thesis.

ORI ISSUE #3: That Respondent knowingly and intentionally fabricated and falsified the ^{1}H NMR spectrum of compound 7 in JACS 2004 and in her thesis.

171. Page S31 of JACS 2004 and Chapter 5, page 344, of Respondent's thesis include an NMR spectrum identified as the ^{1}H NMR spectrum of compound 7. Tabular data referencing the NMR spectrum of compound 7 is found at page S8 of JACS 2004 and Chapter 5, page 314, of Respondent's thesis.

172. A data set located in the (b)(6) and (b)(7)(c) of the 400 MHz NMR spectrometer includes a spectrum with peak resonance frequencies and peak integrals identical to those identified in the spectrum of compound 7 in the JACS 2004 article and Respondent's thesis.

173. This data set includes individually processed data files that were generated and sequentially added together to generate the final spectrum, which is materially identical to that of compound 7, demonstrating that the spectrum was fabricated and falsified through progressive construction.

174. The satellite resonance peaks in this spectrum have a coupling constant of 177.6 Hz, which is the expected value of methylene chloride.

175. The existence of resonance peaks with a coupling constant of 177.6 Hz demonstrates that the NMR spectrum of methylene chloride was used to construct the fabricated and falsified spectrum.

176. ^{1}H NMR data for compound 7 was also found in Respondent's binders.

177. The fabricated and falsified spectrum for compound 7 was created on June 11, 2004.

178. User logs for the 400 MHz spectrometer indicate that the (b)(6) and (b)(7)(C) was used from 9:52 am to 10:12 am on June 11, 2004 , and the 400 MHz sign up sheet indicates that Respondent was signed up to use the spectrometer at that time.

ORI FINDING #3: Respondent knowingly and intentionally committed scientific misconduct by fabricating and falsifying the ^{1}H NMR spectrum of compound 7 in JACS 2004 and in her thesis.

ORI ISSUE #4: That Respondent knowingly and intentionally fabricated and falsified the ^{1}H NMR spectrum of compound 9 in JACS 2004 and in her thesis.

179. Page S30 of JACS 2004 and Chapter 5, page 343, of Respondent's thesis includes an NMR spectrum identified as the ^{1}H NMR spectrum of compound 9. Tabular data referencing the NMR spectrum of compound 9 is found at page S8 of JACS 2004 and Chapter 5, page 315, of Respondent's thesis.

180. A data set located in the (b)(6) and (b)(7)(c) of the 400 MHz NMR spectrometer includes a spectrum with peak resonance frequencies and peak integrals identical to those identified in the spectrum of compound 9 in the JACS 2004 article and Respondent's thesis.

181. This data set includes individually processed data files that were generated and sequentially added together to generate the final spectrum, which is materially

identical to that of compound 9, demonstrating that the spectrum was fabricated and falsified through progressive construction.

182. The satellite resonance peaks in this spectrum have a coupling constant of 177.6 Hz, which is the expected value of methylene chloride.

183. The existence of resonance peaks with a coupling constant of 177.6 Hz demonstrates that the NMR spectrum of methylene chloride was used to construct the fabricated and falsified spectrum.

184. ^{1}H NMR data for compound 9 was also found in Respondent's binders.

185. The fabricated and falsified spectrum for compound 9 was created on June 11, 2004.

186. User logs for the 400 MHz spectrometer indicate that the (b)(6) and (b)(7)(C) was used from 9:52 am to 10:12 am on June 11, 2004 , and the 400 MHz sign up sheet indicates that Respondent was signed up to use the spectrometer at that time.

ORI FINDING #4: Respondent knowingly and intentionally committed scientific misconduct by fabricating and falsifying the ^{1}H NMR spectrum of compound 9 in JACS 2004 and in her thesis.

ORI ISSUE #5: That Respondent knowingly and intentionally fabricated and falsified the NMR spectrum of compound 10 in JACS 2004 and in her thesis.

187. Page S32 of JACS 2004 and Chapter 5, page 345, of Respondent's thesis include an NMR spectrum identified as the ^{1}H spectrum of compound 10. Tabular data referencing the NMR spectrum of compound 10 is found at page S9 of JACS 2004 and Chapter 5, page 316, of Respondent's thesis.

188. A data set located in the (b)(6) and (b)(7)(c) of the 400 MHz NMR spectrometer includes a spectrum with peak resonance frequencies and peak integrals identical to those identified in the spectrum of compound 10 in the JACS 2004 article and Respondent's thesis.

189. This data set includes individually processed data files that were generated and sequentially added together to generate the final spectrum, which is materially identical to that of compound 10, demonstrating that the spectrum was fabricated and falsified through progressive construction.

190. The satellite resonance peaks in this spectrum have a coupling constant of 177.6 Hz, which is the expected value of methylene chloride.

191. The existence of resonance peaks with a coupling constant of 177.6 Hz demonstrates that the NMR spectrum of methylene chloride was used to construct the fabricated and falsified spectrum.

192. ^{1}H NMR data for compound 10 was also found in Respondent's binders.

193. The fabricated spectrum for compound 10 was created on June 11, 2004.

194. User logs for the 400 MHz spectrometer indicate that the (b)(6) and (b)(7)(c) was used from 9:52 am to 10:12 am on June 11, 2004 , and the 400 MHz sign up sheet indicates that Respondent was signed up to use the spectrometer at that time.

ORI FINDING #5: Respondent knowingly and intentionally committed scientific misconduct by fabricating and falsifying the ^{1}H NMR spectrum of compound 10 in JACS 2004 and in her thesis.

ORI ISSUE #6: That Respondent knowingly and intentionally fabricated and falsified the ^{1}H NMR spectrum of compound 12 in JACS 2004 and in her thesis.

195. Page S33 of JACS 2004 and Chapter 5, page 346, of Respondent's thesis include an NMR spectrum identified as the ^{1}H NMR spectrum of compound 12. Tabular data referencing the NMR spectrum of compound 12 is found at page S10 of JACS 2004 and Chapter 5, page 318, of Respondent's thesis.

196. A data set located in the (b)(6) and (b)(7)(c) of the 400 MHz NMR spectrometer includes a spectrum with peak resonance frequencies and peak integrals identical to those identified in the spectrum of compound 12 in the JACS 2004 article and Respondent's thesis.

197. This data set includes individually processed data files that were generated and sequentially added together to generate the final spectrum, which is materially identical to that of compound 12, demonstrating that the spectrum was fabricated and falsified through progressive construction.

198. The spectrum was fabricated and falsified in four steps from the spectra of two known compounds, 3-bromo-1-TIPS-indole and pyrroline.

199. ^{1}H NMR data for compound 12 was also found in Respondent's binders.

200. The fabricated and falsified spectrum for compound 12 was created on June 23, 2004.

201. User logs for the 400 MHz spectrometer indicate that the (b)(6) and (b)(7)(C) was used from 8:50 a.m. to 9:09 a.m. on June 23, 2004, and the 400 MHz sign-up sheet indicates that Respondent was signed up to use the spectrometer at that time.

ORI FINDING #6: Respondent knowingly and intentionally committed scientific misconduct by fabricating and falsifying the ^{1}H NMR spectrum of compound 12 in JACS 2004 and in her thesis.

ORI ISSUE #7: That Respondent knowingly and intentionally fabricated and falsified a figure comprised of four (4) ^{31}P NMR spectra in JACS 2004 and in her thesis.

202. Page S21 of JACS 2004 and Chapter 5, page 333, of Respondent's thesis include a figure consisting of four (4) ^{31}P NMR spectra, which were purportedly the ^{31}P NMR spectra of a crude catalytic reaction mixture.

203. The spectra in this figure are identical, except for the labeling of the spectra, to the White-Out Spectrum found in Respondent's NMR binders, see paragraph 35, *supra*.

204. The spectra in this figure and the White-Out Spectrum are identical to spectra located in the (b)(6) and (b)(7)(c) of the narrow bore 300 MHz NMR spectrometer, except that the spectra found in the rayane account contain certain small peaks, discussed at paragraph 206, *infra*.

205. Each of the four spectra located in the rayane account of the narrow bore 300 MHz spectrometer was fabricated by manipulating the single peak that constitutes the ^{31}P NMR spectrum of triphenylphosphine (PPh_3).

206. The small peaks that appear in the spectra in the (b)(6) and (b)(7)(c) were removed from the White-Out Spectrum using White-Out. These peaks were the result of contamination of the sample of PPh3 with PH_3PO, an oxidation product of PPh_3.

207. The fabricated and falsified ^{31}P spectra were produced on June 25, 2004. No sign-up sheets for the narrow bore 300 MHz spectrometer exist because no reservations are taken for that spectrometer, see paragraph 21, *supra*.

ORI FINDING #7: Respondent knowingly and intentionally committed scientific misconduct by fabricating and falsifying a figure comprised of four (4) ^{31}P NMR spectra in JACS 2004 and in her thesis.

ORI ISSUE #8: That Respondent plagiarized data and used the plagiarized data to fabricate and falsify the ^{1}H NMR spectrum of 1,2-diphenylpyrrolidine in JACS 2005 and in her thesis.

208. Page S7 of JACS 2005 and Chapter 6, page 399, of Respondent's thesis contain a table setting forth the ^{1}H and ^{13}C NMR resonance frequencies of 1,2-diphenylpyrrolidine.

209. The resonance frequencies reported in this table are identical to values reported in an article by Lewis *et al.* (Lewis, F.D., Wagner-Brennan, J.M., and Miller, A.M., Formation and behavior of intramolecular N-(styrlalkyl)aniline exciplexes, Can. J. Chem. 77:595-604, 1999).

210. However, the resonance frequencies in Respondent's table should not be identical to those reported in Lewis *et al.* because Lewis recorded the spectrum using a 300 MHz NMR spectrometer, whereas Respondent stated she used a 400 MHz spectrometer. A 400 MHz instrument would show couplings, when measured in ppm, that are three-quarters of those recorded on a 300 MHz instrument.

211. Page S30 of JACS 2005 and Chapter 6, page 433, of Respondent's thesis include an NMR spectrum identified as the ^{1}H NMR spectrum of 1, 2-diphenylpyrrolidine.

212. A data set with an unusual number of processed subdirectories located in the account of (b)(6) and (b)(7)(C) of the 400 MHz NMR spectrometer and found in a directory named "CM-9-27-03" contains a processed data set with a spectrum materially identical to that identified in JACS 2005 and Respondent's thesis as the spectrum of 1,2-diphenylpyrrolidine. This spectrum was created on September 13, 2004.

213. The satellite resonance peaks in this spectrum each have a coupling constant of 177.6 Hz, which is the expected value of methylene chloride, a common solvent.

214. The ^{1}H NMR spectrum of 1, 2-diphenylpyrrolidine was fabricated and falsified on the spectrometer from the NMR spectrum of methylene chloride, using the plagiarized ^{1}H resonance frequencies.

ORI FINDING #8: Respondent knowingly and intentionally committed scientific misconduct by plagiarizing data and using plagiarized data to fabricate and falsify the ^{1}H NMR spectrum of 1, 2-diphenylpyrrolidine in JACS 2005 and in her thesis.

ORI Issue #9: That Respondent knowingly and intentionally fabricated and falsified the ^{1}H NMR spectrum of a deuterated analog of 1,2-diphenylpyrrolidine in JACS 2005 and in her thesis.

215. Page S31 of JACS 2005 and Chapter 6, page 434, of Respondent's thesis report an NMR spectrum identified as the ^{1}H NMR spectrum of a deuterated analog of 1, 2 – diphenylpyrrolidine (N, 2 – diphenyl – 3,3,4,4,-d4-pyrrolidine).

216. A data set with an unusual number of processed subdirectories located in the (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) of the 400 MHz NMR spectrometer and found in a directory named "CM-9-27-03" contains a processed data set with a spectrum nearly identical to the spectrum found at Page S31 of JACS 2005 and Chapter 6, page 434, of Respondent's thesis. This spectrum was created on October 23, 2004.

217. The satellite resonance peaks in this spectrum each have a coupling constant of 177.6 Hz, which is the expected value of methylene chloride.

218. The existence of resonance peaks with a coupling constant of 177.6 Hz demonstrates that the NMR spectrum of methylene chloride was used to construct the fabricated and falsified spectrum.

219. The spectrum located in the (b)(6) and (b)(7)(C) contains peak positions and intensities that are identical to those found in the spectra on Page S31 of JACS 2005 and Chapter 6, page 434, of Respondent's thesis. The only material differences between the spectrum in the (b)(6) and (b)(7)(c) and the spectra in JACS 2005 and Respondent's thesis is that the latter (1) excludes a portion of the spectrum, thereby omitting a peak that is visible in the (b)(6) and (b)(7)(C) and (2) does not include another peak that is visible on the spectrum in the (b)(6) and (b)(7)(C) This missing peak could have been removed via White-Out or electronic processing.

ORI FINDING #9: Respondent knowingly and intentionally committed scientific misconduct by fabricating and falsifying the ^{1}H NMR spectrum of a deuterated analog of 1,2-diphenylpyrrolidine in JACS 2005 and in her thesis.

ORI Issue #10: That Respondent knowingly and intentionally fabricated and falsified the ^{1}H NMR spectrum of another deuterated analog of 1,2-diphenylpyrrolidine in JACS 2005 and in her thesis.

220. Page S32 of JACS 2005 and Chapter 6, page 435, of Respondent's thesis include an NMR spectrum identified as the ^{1}H NMR spectrum of a deuterated analog of 1, 2 – diphenylpyrrolidine (N, 2 – diphenyl – 2,5,5,-d3-pyrrolidine).

221. A data set with an unusual number of processed subdirectories located in the (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) of the 400 MHz NMR spectrometer and found in a directory named "CM-9-27-03" contains a processed data set with a spectrum nearly identical to the spectrum found at Page S32 of JACS 2005 and Chapter 6, page 435, of Respondent's thesis. This spectrum was created on October 23, 2004.

222. The satellite resonance peaks in this spectrum each have a coupling constant of 177.6 Hz, which is the expected value of methylene chloride.

223. The existence of resonance peaks with a coupling constant of 177.6 Hz demonstrates that the NMR spectrum of methylene chloride was used to construct the fabricated and falsified spectrum.

224. The spectrum located in the (b)(6) and (b)(7)(C) contains peak positions and intensities that are identical to those found in the spectra on Page S32 of JACS 2005 and Chapter 6, page 435, of Respondent's thesis. The only material differences between the spectrum in the (b)(6) and (b)(7)(C) and the spectra in JACS 2005 and

Respondent's thesis are that the latter (1) excludes a portion of the spectrum, thereby omitting a peak that is visible in the (b)(6) and (b)(7)(C) and (2) does not include another peak that is visible on the spectrum in the (b)(6) and (b)(7)(C). This missing peak could have been removed via White-Out or electronic processing.

ORI FINDING #10: Respondent knowingly and intentionally committed scientific misconduct by fabricating and falsifying the ^{1}H NMR spectrum of another deuterated analog of 1,2-diphenylpyrrolidine in JACS 2005 and in her thesis.

ORI ISSUE #11: That Respondent knowingly and intentionally fabricated and falsified the ^{31}P NMR spectrum of a reaction mixture in JACS 2005 and in her thesis.

225. Page S20 of JACS 2005 and Chapter 6, page 420, of Respondent's thesis include an NMR spectrum identified as the ^{31}P NMR spectrum of a reaction mixture.

226. A data set located in the (b)(6) and (b)(7)(C) of the narrow-bore 300 MHz NMR spectrometer includes a spectrum (the H-encarbamate 03/3/12 spectrum) nearly identical to the spectrum found at Page S20 of JACS 2005 and Chapter 6, page 420, of Respondent's thesis.

227. This data set includes individually processed data files that were generated and sequentially added together to generate the H-encarbamate 03/3/12 spectrum, demonstrating that the spectrum was fabricated and falsified through progressive construction.

228. The H-encarbamate 03/3/12 spectrum was also located in Respondent's NMR binders, with annotations that appear to be in Respondent's handwriting.

229. With one exception, the peaks in the H-encarbamate 03/3/12 spectrum are identical in frequency and amplitude to the peaks in the published spectra. In addition, the baseline noise of the H-encarbamate 03/3/12 spectra is identical to that visible in the published spectra, demonstrating that the published spectra were fabricated and falsified from the H-encarbamate 03/3/12 spectrum. The sole difference between the fabricated and falsified H-encarbamate 03/3/12 spectra and the published spectra is that the amplitude of one of the peaks in the published spectra was enhanced, constituting a further falsification of the fabricated spectrum.

ORI FINDING #11: Respondent knowingly and intentionally committed scientific misconduct by fabricating and falsifying the ^{31}P NMR spectrum of a reaction mixture in JACS 2005 and in her thesis.

ORI ISSUE #12: That Respondent knowingly and intentionally fabricated and falsified the ^{1}H NMR spectrum identified as the spectrum of compound 4 in JACS 2002 and of compound 11 in Chapter 1 of Respondent's thesis.

230. Page S25 of JACS 2002 includes a ^{1}H NMR spectrum identified as the spectrum of compound 4 (the product compound). The same spectrum is identified in Chapter 1, page 67, of Respondent's thesis as the spectrum of compound 11. Tabular data referencing these spectra is found at page S12 of JACS 2002 and Chapter 1, page 44, of Respondent's thesis.

231. The spectrum for the starting compound used in Respondent's experiment contains $^1J_{CH}$ coupling constants that vary with the ^{1}H chemical shift as expected in accordance with chemical principles, demonstrating that the spectrum of the starting compound is authentic.

232. However, each resonance peak in the spectrum of the product compound has a $^1J_{CH}$ coupling constant of ~ 177 Hz, demonstrating that the NMR spectrum of methylene chloride, which has a coupling constant value of 177.6 Hz, was used to construct the fabricated and falsified spectrum of the product compound.

233. An original ^{1}H NMR spectrum identical to the published spectra was located in Respondent's NMR binders.

234. Software, such as ChemDraw, can be used to predict NMR spectrum resonance frequencies for compounds. Respondent's NMR binders also included ChemDraw predictions for the product compound and the starting compound.

ORI FINDING #12: Respondent knowingly and intentionally committed scientific misconduct by fabricating and falsifying the ^{1}H NMR spectrum identified as the spectrum of compound 4 in JACS 2002 and of compound 11 in Chapter 1 of Respondent's thesis.

ORI ISSUE # 13: That Respondent knowingly and intentionally fabricated and falsified the ^{1}H NMR spectrum identified as the spectrum of compound 6 in JACS 2002 and of compound 16 in Chapter 1 of Respondent's thesis.

235. Page S26 of JACS 2002 includes a ^{1}H NMR spectrum identified as the spectrum of compound 6 (the product compound). The same spectrum is identified in Chapter 1, page 68, of Respondent's thesis as the ^{1}H NMR spectrum of compound 16. Tabular data referencing this spectrum is found at page 59 of JACS 2002 and Chapter 1, page 40, of Respondent's thesis.

236. Respondent fabricated and falsified this spectrum in the same manner as set forth in paragraphs 231 through 234, *supra*.

ORI FINDING # 13: Respondent knowingly and intentionally committed scientific misconduct by fabricating and falsifying the ^{1}H NMR spectrum identified as the spectrum of compound 6 in JACS 2002 and of compound 16 in Chapter 1 of Respondent's thesis.

ORI ISSUE # 14: That Respondent knowingly and intentionally fabricated and falsified the ^{1}H NMR spectrum identified as the spectrum of compound 7 in JACS 2002 and of compound 21 in Chapter 1 of Respondent's thesis.

237. Page S27 of JACS 2002 includes a ^{1}H NMR spectrum identified as the spectrum of compound 7 (the product compound). The same spectrum is identified in Chapter 1, page 69, of Respondent's thesis as the ^{1}H NMR spectrum of compound 21. Tabular data referencing this spectrum is found at page S10 of JACS 2002 and Chapter 1, page 42, of Respondent's thesis.

238. Respondent fabricated and falsified this spectrum in the same manner as set forth in paragraphs 231 through 233, *supra*.

ORI FINDING # 14: Respondent knowingly and intentionally committed scientific misconduct by fabricating and falsifying the ^{1}H NMR spectrum identified as the spectrum of compound 7 in JACS 2002 and of compound 21 in Chapter 1 of Respondent's thesis.

ORI ISSUE # 15: That Respondent knowingly and intentionally fabricated and falsified the ^{1}H NMR spectrum identified as the spectrum of compound 10 in JACS 2002 and of compound 22 in Chapter 1 of Respondent's thesis.

239. Page S29 of JACS 2002 includes a ^{1}H NMR spectrum identified as the spectrum of compound 10 (the product compound). The same spectrum is identified in Chapter 1, page 71, of Respondent's thesis as the ^{1}H NMR spectrum of compound 22. Tabular data referencing this spectrum is found at page S14 of JACS 2002 and Chapter 1, page 47, of Respondent's thesis.

240. Respondent fabricated and falsified this spectrum in the same manner as set forth in paragraphs 231 through 233, *supra*.

ORI FINDING # 15: Respondent knowingly and intentionally committed scientific misconduct by fabricating and falsifying the ^{1}H NMR spectrum identified as the spectrum of compound 10 in JACS 2002 and of compound 22 in Chapter 1 of Respondent's thesis.

ORI ISSUE # 16: That Respondent knowingly and intentionally fabricated and falsified the ^{1}H NMR spectrum identified as the spectrum of compound 12 in JACS 2002 and of compound 24 in Chapter 1 of Respondent's thesis.

241. Page S30 of JACS 2002 includes a ^{1}H NMR spectrum identified as the spectrum of compound 12 (the product compound). The same spectrum is identified in Chapter 1, page 72, of Respondent's thesis as the ^{1}H NMR spectrum of compound 24. Tabular data referencing this spectrum is found at page S20 of JACS 2002 and Chapter 1, page 55, of Respondent's thesis.

242. Respondent fabricated and falsified this spectrum in the same manner as set forth in paragraphs 231 through 233, *supra*.

ORI FINDING # 16: Respondent knowingly and intentionally committed scientific misconduct by fabricating and falsifying the ^{1}H NMR spectrum identified as the spectrum of compound 12 in JACS 2002 and of compound 24 in Chapter 1 of Respondent's thesis.

ORI ISSUE # 17: That Respondent knowingly and intentionally fabricated and falsified the ^{1}H NMR spectrum identified as the spectrum of compound 13 in JACS 2002 and of compound 25 in Chapter 1 of Respondent's thesis.

243. Page S31 of JACS 2002 includes a ^{1}H NMR spectrum identified as the spectrum of compound 13 (the product compound). The same spectrum is identified in Chapter 1, page 73, of Respondent's thesis as the ^{1}H NMR spectrum of compound 25. Tabular data referencing this spectrum is found at page S21 of JACS 2002 and Chapter 1, page 57, of Respondent's thesis.

244. Respondent fabricated and falsified this spectrum in the same manner as set forth in paragraphs 231 through 233, *supra*.

ORI FINDING # 17: Respondent knowingly and intentionally committed scientific misconduct by fabricating and falsifying the ^{1}H NMR spectrum identified as the spectrum of compound 13 in JACS 2002 and of compound 25 in Chapter 1 of Respondent's thesis.

ORI ISSUE # 18: That Respondent knowingly and intentionally fabricated and falsified the ^{1}H NMR spectrum identified as the spectrum of compound 14 in JACS 2002 and of compound 26 in Chapter 1 of Respondent's thesis.

245. Page S32 of JACS 2002 includes a ^{1}H NMR spectrum identified as the spectrum of compound 14 (the product compound). The same spectrum is identified in Chapter 1, page 74, of Respondent's thesis as the ^{1}H NMR spectrum of compound 26. Tabular data referencing this spectrum is found at page S23 of JACS 2002 and Chapter 1, page 59, of Respondent's thesis.

246. Respondent fabricated and falsified this spectrum in the same manner as set forth in paragraphs 231 through 233, *supra*.

ORI FINDING # 18: Respondent knowingly and intentionally committed scientific misconduct by fabricating and falsifying the ^{1}H NMR spectrum identified as the spectrum of compound 14 in JACS 2002 and of compound 26 in Chapter 1 of Respondent's thesis.

ORI ISSUE #19: That Respondent knowingly and intentionally fabricated and falsified combustion analysis data reported in JACS 2004 and in Chapter 5 of her thesis.

247. Respondent's thesis states that all combustion analyses were conducted by (b)(6) and (b)(7)(C)

248. Respondent's research records contain documentation for only two (2) combustion analyses conducted by (b)(6) and (b)(7)(C) and no documentation of combustion analyses conducted by any other companies.

249. Through a search conducted by the CU Department of Chemistry Business Office and the CU Accounts Payable Department, and a request to (b)(6) and (b)(7)(C) for copies of data previously reported to the (b)(6) and (b)(7)(C) reports sent to Respondent were identified. These records demonstrate that these (b)(6) and (b)(7)(C) reports were the only combustion analysis reports sent to Respondent by any company.

250. Certain of the companies identified by Respondent as having provided free combustion analyses were contacted and advised CU that they had not done combustion analyses for CU and did not provide free services.

251. With the exception of two (2) combustion analyses of commercially available compounds, the combustion analysis data reported in JACS 2004, JACS 2005, and Chapters 5, 6 and 7 of Respondent's thesis does not match reports provided by (b)(6) and (b)(7)(C) either because no (b)(6) and (b)(7)(C) reports contain results for the compound or because the (b)(6) and (b)(7)(C) reports disagree with the data reported by Respondent.

252. In particular, the combustion analysis data for four (4) compounds in JACS 2004 and Chapter 5 of Respondent's thesis differs from the (b)(6) and (b)(7)(C) reports, demonstrating that the combustion analysis data in Respondent's publications and thesis for these compounds was falsified. The compounds are $RhH(CO)(PPh_3)_3$, $RhH(CO)(PFur_3)_3$, $RHCl(I)(Ph)(CO)(PFur_3)_2$, and $Rh(Pyrr)(CO)(PFur_3)_2$.

253. No (b)(6) and (b)(7)(C) reports exist for two (2) compounds in Chapter 5 of Respondent's thesis, one of which also appeared in JACS 2004, demonstrating that the combustion analysis data in Respondent's publication and thesis for these compounds was fabricated. The compounds are $RhCl(CO)(PFur_3)_2$ and $Rh(Ph)(CO)(PFur_3)_2$ (the latter reported in Respondent's thesis only).

ORI FINDING #19: Respondent knowingly and intentionally committed scientific misconduct by fabricating and falsifying combustion analysis data reported in JACS 2004 and in Chapter 5 of her thesis.

ORI ISSUE #20: That Respondent knowingly and intentionally fabricated and falsified combustion analysis data reported in JACS 2005 and in Chapter 6 of her thesis.

254. The combustion analysis data for two (2) compounds in JACS 2005 and Chapter 6 of Respondent's thesis differs from the (b)(6) and (b)(7)(C) reports, demonstrating that the combustion analysis data in Respondent's publication and thesis for those compounds was falsified. The compounds are $RuH_2(CO)(PCyPh_2)_3$ and $RuH_2(CO)(PCy_3)_3$.

255. No (b)(6) and (b)(7)(C) reports exist for three (3) compounds in JACS 2005 and Chapter 6 of Respondent's thesis, demonstrating that the combustion analysis data in Respondent's publication and thesis was fabricated. The compounds are $RuH_2(CO)(PCy_2Ph)_3$, $RuCl(Ph)(CO)(PCy_3)_2$, and $Ru(I)(Ph)(CO)(PCy_3)_2$.

256. The basis for the conclusion that Respondent fabricated and falsified combustion analysis data reported in JACS 2005 and in Chapter 6 of her thesis is further set forth in paragraphs 247 to 251, *supra*.

ORI FINDING #20: Respondent knowingly and intentionally committed scientific misconduct by fabricating and falsifying combustion analysis data reported in JACS 2005 and in Chapter 6 of her thesis.

ORI ISSUE #21: That Respondent knowingly and intentionally fabricated combustion analysis data reported in Chapter 7 of her thesis.

257. No (b)(6) and (b)(7)(C) reports exist for two (2) compounds in Chapter 7 of Respondent's thesis, demonstrating that the combustion analysis data in Respondent's thesis was fabricated. The compounds are identified in the thesis as Complex 5 and Complex 6.

258. The basis for the conclusion that Respondent fabricated combustion analysis data reported in Chapter 7 of her thesis is further set forth in paragraphs 247 to 251, *supra*.

ORI FINDING #21: Respondent knowingly and intentionally committed scientific misconduct by fabricating combustion analysis data reported in Chapter 7 of her thesis.

V. RESPONDENT ENGAGED IN A PATTERN OF SERIOUS MISCONDUCT AND HAS FAILED TO ACCEPT RESPONSIBILITY FOR HER MISCONDUCT; RESPONDENT'S MISCONDUCT IS A CAUSE FOR DEBARMENT.

259. The purpose of debarment is to protect the federal government from an individual who has proven to be untrustworthy. Kimon J. Angelides, DAB No. 1677, at 163, 168 (1999).

260. Moreover, the policy underlying debarment is that the government should only conduct business with responsible contractors and grantees. *See* Dr. Paul F. Langlois, DAB No. 1409 (1993), 1993 WL 742594 (H.H.S.).

261. The Departmental Appeals Board has also held that "[t]he scientific community functions on trust and openness; once that trust is breached, the harm from incidents of fabrication and falsification of data is far greater than simply discrediting the work known to be false or fabricated." *Id.*

262. Respondent's deliberate and elaborate fabrication and falsification of data central to her publications establishes a lack of trustworthiness.

263. Respondent pursued a widespread course of dishonest and deceptive conduct by committing numerous acts of data fabrication and falsification over at least a three year period of time.

264. Respondent's actions seriously deviated from those that are commonly accepted within the scientific community for proposing, conducting, and/or reporting research.

265. Respondent's scientific misconduct necessitated the retraction of JACS 2002, JACS 2004, and JACS 2005, as well as the retraction or correction of other papers. These papers had been regarded as important contributions to the field of organic chemistry.

266. The (b)(6) and (b)(7)(C) who attempted unsuccessfully to reproduce Respondent's results were negatively affected by Respondent's scientific misconduct.

267. Respondent did not take responsibility for her misconduct and instead claimed that she was framed by other (b)(6) and (b)(7)(C)

268. Respondent attempted to mislead the Committee in a number of ways, including falsely claiming to have had an NMR account, denying that she was enrolled in the University of Heidelberg, and presenting an expert witness who was not genuine.

269. For the foregoing reasons, the scope of Respondent's conduct is so serious and compelling in nature that it demonstrates her lack of present responsibility to be a steward of federal funds.

270. Accordingly, Respondent's knowing and intentional fabrication, falsification, and plagiarism of data included in her papers and thesis constitutes scientific misconduct under the applicable regulation, 42 C.F.R. § 50.102. HHS also determines that Respondent's pattern of dishonest conduct through the commission of scientific misconduct establishes her lack of present responsibility to be a steward of federal funds. 2 C.F.R. § 376 *et seq*.

HHS ADMINISTRATIVE ACTIONS AGAINST RESPONDENT

Based on the preponderance of the evidence supporting the ORI findings of scientific misconduct stated herein *supra*, the HHS Debarring Official proposes that for a period of five (5) years Respondent be debarred from any contracting or subcontracting with any agency of the United States Government and from eligibility for, or involvement in, nonprocurement programs of the United States Government referred to as "covered transactions" pursuant to the Department of Health and Human Services Implementation of OMB Guidelines to Agencies on Governmentwide Debarment and Suspension. 2 C.F.R. § 376 *et seq*. HHS also proposes that for a period of five (5) years that Respondent be prohibited from serving in any advisory capacity to the PHS including but not limited to service on any PHS advisory committee, board, and/or peer review committee, or as a consultant.

CONFIDENTIAL

Final Report of the Ad Hoc Committee to the Standing Committee on the Conduct of Research of Columbia University

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PRELIMINARY STATEMENT

The Ad Hoc Committee (the "Committee") appointed by Columbia University's Standing Committee on the Conduct of Research (the "Standing Committee") submits this Investigative Report as to whether or not a finding of research misconduct should be upheld against Dr. Bengü Sezen and, if so, what corrective actions are appropriate. Copies of the evidence upon which this Report is based are available upon request as a separate Appendix of Exhibits.

The members of the Committee are:

(b)(6) and (b)(7)(C)

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This investigation was conducted between August 2006 and February 2007.[1] The Committee interviewed 18 individuals, including the Complainant and Respondent. One member of the Committee was absent for two of these interviews; another, very brief interview was conducted by (b)(6) and (b)(7)(C) Otherwise, all members of the Committee were present for the remaining interviews. All of the interviews were transcribed by a court reporter. The Committee convened 13 times; each meeting lasted between ca. two and five hours. Over 10,000 pages of documents were sequestered and reviewed.

The Complainant and Respondent were each provided a copy of a draft of this Report ("Draft Report") and each provided comments to it, which have been separately circulated to the Standing Committee. After receiving these comments, the Committee finalized the Report. Any changes from the Draft Report are documented in an attachment at the end of this Report.

This Report documenting the Committee's findings is being submitted to the Standing Committee. If the Standing Committee accepts this Committee's findings and recommendations, (b)(6) and (b)(7)(C) will, after consulting with (b)(6) and (b)(7)(C), accept, reject, or modify the recommendations of the Standing Committee. An appeal of (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) decision may be made to Provost Alan Brinkley.

Columbia University adopted its new Institutional Policy on Misconduct in Research ("Misconduct Policy") in February, 2006. The Misconduct Policy closely

(b)(6) and (b)(7)(C)

tracks the Federal Policy on Research Misconduct of the Office of Science and Technology Policy. Because the alleged misconduct occurred before the effective date of the new Misconduct Policy, the Committee applied the definition of research misconduct that was in effect when the alleged misconduct occurred: "gross lack of integrity in conducting basic or clinical investigations involving dishonesty, knowing misrepresentations of data, and/or violation of accepted standards." (Faculty Handbook, Appendix E (2003)) (Attachment 1 at 2). The Committee interpreted this definition to encompass fabrication, falsification, and plagiarism, and focused on those issues in particular. To the extent possible, the Committee applied the procedures of the new Misconduct Policy to this Investigation.

This Report begins with an overview of the allegations of research misconduct; a summary of federal grant support that was involved in the contested research; background information on the field of organometallic chemistry, the Complainant, and the Respondent; and a description of issues of reproducibility that arose before the Complaint was filed. Next, the Report reviews the procedural history of this case, including the preliminary Inquiry, the decision to pursue a full Investigation, and an overview of the Investigative process. Thereafter, the Report documents the Committee's Findings of Fact, including Findings concerning the Research Record, each of the Allegations, and the Respondent's credibility. Finally, the Report closes with a summary of the Committee's conclusions and recommendations for corrective action.

THE ALLEGATIONS

In November 2005, (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) allegations that Dr. Bengü Sezen (the "Respondent") fabricated scientific data while she was a graduate student conducting doctoral research in the (b)(6) and (b)(7)(C) These allegations were referred to an Inquiry Committee, which focused on issues of fabrication and irreproducibility in Dr. Sezen's doctoral research. The Inquiry Committee recommended, and the Standing Committee initiated, a full investigation of the allegations.

Although the initial allegations considered by the Inquiry Committee focused on one instance of fabrication in one of Dr. Sezen's research publications, the Ad Hoc Committee uncovered other instances of fabrication and other forms of scientific misconduct during the subsequent full investigation. Accordingly, the Ad Hoc Committee refined the allegations as follows:

1. Whether Dr. Sezen fabricated NMR spectra in her thesis and publications;
2. Whether Dr. Sezen falsified data supporting combustion analyses reported in her thesis and publications; and
3. Whether Dr. Sezen fabricated experimental procedures reported in her thesis and publications.

FEDERAL RESEARCH SUPPORT

The research that is the subject of this investigation received support from several private sources, from the National Institutes of Health (NIH) Grant R01 GM060326 ("NIH Grant"), and from the National Science Foundation (NSF) Grant CHE-0301092 ("NSF Grant"). This research was described in one of the Specific Aims of the NIH Grant proposal as:

> **Project 4. Development of Catalytic Systems for Directed C-H Activation of Complex Substrates.** Based on recent disclosures from the PI and other laboratories, the development of catalytic systems for directed C-H activation will be pursued. In this project, a monodentate heteroatom ligand will be used to activate and direct the metal complex. The chelation process will be reversible and will thus allow for potential turnover of the metal catalyst. Judiciously selected low valent complexes, in combination with several atom donor types and additional ligands, will be explored.

(Exh. L11 at 013473).[3]

1. Federal Support Provided for Dr. Sezen's Research

From September 2002 through May 2003, Dr. Sezen received graduate student stipend support from the NIH Grant in the amount of $16,050 (direct costs). From 2001 to 2004, an additional $45,000 (direct costs) was spent on supplies for Dr. Sezen's research. According to (b)(6) and (b)(7)(C) in total, $61,050, or approximately 8% of the NIH Grant, was expended directly on Dr. Sezen's work. In addition, (b)(6) and (b)(7)(C) reported that the NSF Grant was charged $10,000 for supplies used by Dr. Sezen to conduct the research at issue, or approximately 3% of the total direct funding awarded.

[3] The NSF Grant application did not include a separate list of Specific Aims.

2. Publications Acknowledging Federal Support

The following publications concern research that is the subject of this Investigation and acknowledge partial support by the NIH Grant:

(b)(6) and (b)(7)(c)

The following publication concerns research that is the subject of this Investigation and acknowledges partial support by the NSF Grant:

7. Godula K., Sezen B., Sames D. (2005) Site-Specific Phenylation of Pyridine Catalyzed by Phosphido-Bridged Ruthenium Dimer Complexes: A Prototype for C-H Arylation of Electron-Deficient Heteroarenes, *J. Am. Chem. Soc.* **127**, 3648-3649 (Exhs. K20-K22).

All of the above publications have been either retracted in full or corrected in part. (b)(6) and (b)(7)(c)

(b)(6) and (b)(7)(c)

(b)(6) and (b)(7)(c)

BACKGROUND FACTS

1. Introduction to Organometallic Chemistry

Organometallic chemistry, which combines aspects of both inorganic and organic chemistry, is the study of chemical compounds that have one or more carbon atoms bonded to one or more metal atoms. Some organometallic compounds act as catalysts. Catalysts are substances that, without being consumed themselves, promote chemical reactions, transforming one set of molecules into another. For this reason, organometallic chemistry has important industrial applications in enabling the production of novel materials, improving the efficiency by which known chemicals are produced, and lowering the costs of chemical production.

Dr. Sezen's publications and dissertation describe the discovery of a number of new chemical reactions by which, under the influence of small quantities of organometallic catalysts, simple organic molecules, called substrates, are linked together through new chemical bonds to form more complex structures, called products. Dr. Sezen's research concentrated on the catalytic activation of C-H chemical bonds, which normally are highly unreactive. At least some of the reactions investigated by Dr. Sezen had stoichiometric, non-catalytic, analogues leading to the same products.

[4] All of the retractions and corrections were handled directly (b)(6) and (b)(7)(C) without input from the Inquiry Committee or the Ad Hoc Committee.

The success of a reaction procedure is measured by the *yield*, which is defined as the amount of the desired product obtained relative to the theoretical maximum that could be obtained if all of the substrate were converted to product, and by the *selectivity*, which is defined as the amount of the desired product obtained relative to the total of all products generated in the reaction. Both yield and selectivity usually are expressed as percentages. The molecular structures of the materials used in the experiments (the substrates, catalysts, products) are defined by means of various analytical chemical techniques. The techniques of elemental analysis, gas chromatography-mass spectrometry (GC-MS), and nuclear magnetic resonance (NMR) spectroscopy are pertinent to this Investigation. These three methods are described briefly below.

Elemental analysis, also called combustion analysis, determines how much of the mass of a sample is contributed by each constituent chemical element. The results of the analysis are expressed as percentages of each element, and the elements usually analyzed include hydrogen, carbon, and nitrogen. The results of elemental analysis are easily predicted for pure molecular substances of known composition. Empirical results may deviate from theoretical values for two reasons: (*i*) the sample is pure, but the chemical species does not have the expected composition and thus does not have the anticipated identity; or (*ii*) the sample contains some of the expected chemical species, but it is mixed with other materials, called impurities. Both the empirical and theoretical results of an elemental analysis are reported in scientific publications to demonstrate congruence between the two sets of numbers and thereby to validate the compositions and purities of materials. The Columbia University Department of Chemistry uses the services of commercial analytical laboratories to obtain elemental analyses.

Gas chromatography (GC) separates mixtures into constituent molecules and determines how much each molecule contributes to the total mass of the mixture. Mass spectrometry measures the molecular mass of chemical compounds that have been converted to ionized gases. The numbers and kinds of atoms constituting the individual molecules define the molecular masses of these molecules. Thus, mass spectrometry provides an alternative to elemental analysis for establishing the atomic composition of a given molecular species. (b)(6) and (b)(7)(C) laboratory has a combined gas chromatograph-mass spectrometer (GC-MS) instrument that not only effects the separation of mixtures but also analyzes the masses of the individual molecules comprising each constituent.[5]

Nuclear magnetic resonance spectroscopy (NMR) provides the most conclusive information about the identity of a chemical species. The result of an NMR analysis, usually referred to as the NMR spectrum, shows how the atoms of molecules are linked together and whether all the molecules in a sample are the same ("purity"). NMR spectroscopy is sensitive to so-called "NMR-active" atoms, including most commonly, but not exclusively, the atomic isotopes ^{1}H, ^{13}C and ^{31}P. The Columbia University Department of Chemistry has a shared instrument facility that houses four NMR spectrometers. Research students who need to perform NMR analyses do so routinely by using the instruments within the facility.

[5] Although not discussed directly in this Report, numerous interviewees mentioned GC-MS analysis, so an explanation is included here as background.

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2. The Complainant

(b)(6) and (b)(7)(C)

3. The Respondent

Dr. Bengü Sezen entered the graduate program of the Department of Chemistry in August 2000 and joined the (b)(6) and (b)(7)(c) in December 2000. While a member of the Group, Dr. Sezen co-authored eight published papers, the seven redacted or corrected papers mentioned above plus one published earlier (No. 8, below):

(b)(6) and (b)(7)(c)

(b)(6) and (b)(7)(c)

Dr. Sezen is the first author of papers 1 through 6. The research published in these six papers was incorporated by Dr. Sezen into her doctoral dissertation, entitled *Development of Selective Catalytic Arylation Methods for sp^2 and sp^3 C-H Bonds in Complex Organic Molecules*. (Exh. K1). Additional research described in Chapter 7 of the thesis has not been published. Dr. Sezen defended her dissertation on July 1, 2005. Her degree was formally conferred, with distinction (an honor reserved for the upper 10% of doctorates), on October 19, 2005.

In February 2006, Dr. Sezen enrolled as a graduate student in molecular biology at the University of Heidelberg, in the laboratory of (b)(6) and (b)(7)(C) Tr. at 6 (transcripts of all interviews are available in Exhibit OO); Exhs. P; J34 at 012153-012154).

A copy of Dr. Sezen's *curriculum vitae* is attached as Exh. AA6.

4. The Department of Chemistry NMR Facility

The Department of Chemistry has a facility for NMR spectroscopy ("NMR Facility"), with instruments located on the first and second floors of the Havemeyer building. The second-floor location houses three Bruker NMR spectrometers: a wide-bore 300 MHz NMR spectrometer, a narrow-bore 400 MHz NMR spectrometer, and a narrow-bore 500 MHz NMR spectrometer.[6] One computer data station for off-line data analysis is available at the second-floor location. The first-floor location contains a narrow-bore 300 MHz Bruker NMR spectrometer. The NMR spectrometers incorporate industry-standard UNIX workstations that control spectrometer operations using proprietary software provided by Bruker Bio Spin Corp. The data station also is a UNIX workstation that runs the same proprietary software.

The (b)(6) and (b)(7)(C) holds a doctorate in Chemistry from the (b)(6) and (b)(7)(c) and (b)(6) and (b)(7)(C) Facility since 1994. A copy of (b)(6) and (b)(7)(C) is attached as Exh. AA1. (b)(6) and (b)(7)(C) explained the NMR Facility's management and operations in the course of two interviews with the Committee. (b)(6) and (b)(7)(C) testimony is summarized below.

The NMR Facility is accessible to authorized users 24 hours a day, seven days a week (b)(6) and (b)(7)(C) Each instrument has its own rules for usage. For example, users can sign up to use the 400 MHz and wide-bore 300 MHz instruments for 20-minute time slots from 10:00 a.m. to 8:00 p.m.; for two-hour time slots from 8:00 a.m. to 10:00 a.m. and from 8:00 p.m. to 12:00 a.m.; and for unlimited time periods

[6] "Bore" refers to the diameter of the opening in the NMR magnet, into which samples are inserted. Until 2002, the Department of Chemistry also had a Varian narrow-bore 200 MHz NMR spectrometer, located on the 6th floor of (b)(6) and (b)(7)(C) This instrument could be used without an account or password. (b)(6) and (b)(7)(C).

overnight.[7] (b)(6) and (b)(7)(C) These instruments also can be used on a walk-up basis when no other user has reserved them. Reservations are not taken for the narrow-bore 300 MHz NMR spectrometer. It operates as a walk-up instrument and can be used to analyze a maximum of two samples during the hours of 10 a.m. to 8 p.m. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) The 500 MHz instrument has special access restrictions; the Committee is not aware of any NMR spectra reported in Dr. Sezen's thesis or publications that were recorded using the 500 MHz NMR spectrometer.

To be authorized to use the NMR Facility, all researchers must obtain basic training and pass a test in the operation of the NMR instruments. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) Training is conducted by (b)(6) and (b)(7)(C) Once a researcher passes the test, (b)(6) and (b)(7)(C) a unique UNIX login account to the researcher that allows access to the NMR instruments and data station. (b)(6) and (b)(7)(C) records in a logbook the user name (chosen by the researcher), user number (the UNIX operating system user number), and the user group (the UNIX user group is defined by the principal investigator of the research group to which the researcher belongs). (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) If a researcher changes research groups, the user name and user number are preserved, but the group affiliation is changed by (b)(6) and (b)(7)(C) (Exh. N20). Each research group is allotted a block of consecutive user numbers and these are assigned to individual group members in numerical order as researchers join the group. (b)(6) and (b)(7)(C)

User accounts are password protected, and the UNIX system allows only the user to create or modify NMR data in his or her account. However, members of a research

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(b)(6) and (b)(7)(C) retained the Facility's sign-up sheets, approximately 2500 pages, for the use of the wide-bore 300 MHz, the 400 MHz, and the 500 MHz NMR spectrometers during the years 2000-2005. All of these documents were sequestered for this Investigation; excerpts are in Exh. N1 at 004152-004153.

group can read the NMR data belonging to other members of the group. Users outside the group can neither read nor write (i.e., create or modify) NMR data belonging to group members. (b)(6) and (b)(7)(C) Because NMR spectroscopy is a central analytical tool in organic chemistry, new graduate students (and other researchers) normally are trained to use the instruments and receive a user login account soon after they join a research group.

(b)(6) and (b)(7)(C) and other witnesses explained that new researchers might use the accounts and passwords of other group members in order to use the NMR spectrometers prior to completing their NMR training. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) discourages this practice. (b)(6) and (b)(7)(C). However, (b)(6) and (b)(7)(C) and several other witnesses stated that, even if researchers initially used someone else's account and password, they cease to do so after they obtain their own accounts and passwords. (b)(6) and (b)(7)(C)

The Department of Chemistry charges its faculty an hourly fee for NMR usage. During the years that Dr. Sezen worked in the (b)(6) and (b)(7)(C) the fee ranged from $10 to $15 per hour. (Exhs. DD2-DD7). (b)(6) and (b)(7)(C) maintains an accounting system on the NMR spectrometers (and data station) that records each login and logout to the NMR software (as distinct from logins to the UNIX operating system). The accounting software records the user name, date, and time of each login to and each logout from the NMR software. (b)(6) and (b)(7)(C) This accounting system is used to generate usage records for each research group. (b)(6) and (b)(7)(C) provides the manager of the (b)(6) and (b)(7)(C) a monthly itemized report showing the usage charged to each user account within the individual research groups.

(b)(6) and (b)(7)(C) then provides each faculty member a monthly summary report showing the total NMR usage charges for the faculty member's group; however, the monthly report provided to faculty is not broken down by individual usage. (*E.g.*, Exh. DD1).

5. Background on Reproducibility

The reproducibility of Dr. Sezen's research results was one of the two primary foci of the preliminary Inquiry report. This issue is not central to the present Investigation, during which the Committee has focused on allegations of fabrication and falsification. However, the history of attempts by researchers to reproduce Dr. Sezen's work is summarized below to document the following issues:

1. Although the formal allegation of research misconduct giving rise to this proceeding was not made against Dr. Sezen until the fall of 2005, concerns about the reproducibility of her research were raised as early as the summer of 2002.
2. At least five other members of the (b)(6) and (b)(7)(C) including both new graduate students and experienced post-doctoral scientists, encountered difficulties when they attempted to confirm or extend Dr. Sezen's results.
3. As accounts of Dr. Sezen's research were published, scientists outside Columbia University also reported to (b)(6) and (b)(7)(C) that they were experiencing difficulties in reproducing the work.
4. Researchers within the (b)(6) and (b)(7)(C) were able to successfully complete the reactions only when Dr. Sezen was present in the laboratory

[8] Copies of (b)(6) and (b)(7)(C) NMR charge documentation for the years 2000-2005 were sequestered as part of this Investigation. *See* Master Index, Exhs. DD2-DD7.

and either directly participated in setting up the reactions or was aware that the experiments were being performed.

5. (b)(6) and (b)(7)(C) initiated an investigation of Dr. Sezen's work in July 2005 after receiving a report that reactions conducted by a member of his laboratory might have been tampered with by the addition of exogenous product.

(b)(6) and (b)(7)(C)

(b)(6) and (b)(7)(C) began studying the mechanism of Dr. Sezen's arylation chemistry and attempted, also without success, to isolate the reaction intermediate. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) In the meantime, (b)(6) and (b)(7)(C) and Dr. Sezen prepared a manuscript reporting Dr. Sezen's novel chemistry. (b)(6) and (b)(7)(C) After the paper was submitted to the *Journal of the American Chemical Society* ("JACS") (on July 28, 2002), but before it was published, (b)(6) and (b)(7)(C) to reproduce Dr. Sezen's reaction and to assist (b)(6) and (b)(7)(C) in his efforts. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C)

(b)(6) and (b)(7)(C) stated that for several months they tried, without success, to reproduce the reaction for the catalytic arylation of a tert-butyl group (the reaction of compound 5 to produce product 6 in the paper published at *JACS* (2002) **124**, 13372-13373). (b)(6) and (b)(7)(C) Despite their efforts, neither (b)(6) and (b)(7)(C) on their own, ever obtained yields greater than 5%. (*Id.* at 18:14-15). They successfully reproduced the arylation reaction only once and then only when Dr. Sezen prepared the starting material herself and, according to (b)(6) and (b)(7)(C) was present while the experiment was being performed.[1] (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) However, even in this case, the yield was lower than expected. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) hen tried again to reproduce the reaction with his own starting material, but he failed.[12] (b)(6) and (b)(7)(C)

(b)(6) and (b)(7)(C) retained printed NMR spectra documenting the results of the one time that the reaction had worked. (Exhs. GG2B (crude reaction mixture) and GG2A (purified product)).

[12]When asked whether there was another method, in addition to Dr. Sezen's catalytic reaction, to prepare the desired product, (b)(6) and (b)(7)(C) answered affirmatively. (b)(6) and (b)(7)(C). A stoichiometric reaction appears to be documented in Dr. Sezen's notebooks at page BS-IV-16; however, whether this reaction actually works as indicated has not been checked by the Committee or members of the (b)(6) and (b)(7)(C)

(b)(6) and (b)(7)(C) asked both (b)(6) and (b)(7)(C) at the beginning of their third year of graduate study and (b)(6) and (b)(7)(C) made further attempts to extend or reproduce these reactions. (b)(6) and (b)(7)(C) was included as a co-author on the publication *JACS* (2002) 124, 13372-13373, because (b)(6) and (b)(7)(C) believed that (b)(6) and (b)(7)(C) had made an intellectual contribution to the paper that merited co-authorship. (b)(6) and (b)(7)(C)

(b)(6) and (b)(7)(C)

(b)(6) and (b)(7)(C) joined the (b)(6) and (b)(7)(C) in January 2003. Initially she worked with Dr. Sezen and planned to develop an offshoot of Dr. Sezen's research. (b)(6) and (b)(7)(C) The new reactions that (b)(6) and (b)(7)(C) was attempting to perform worked at first, but later the yields decreased to almost zero. (b)(6) and (b)(7)(C) At this point, (b)(6) and (b)(7)(C) suggested that, as a control, (b)(6) and (b)(7)(C) try to replicate the parent reaction, developed by Dr. Sezen. (b)(6) and (b)(7)(C) tried to do so unsuccessfully during the summer of 2003, while Dr. Sezen was on vacation. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) When Dr. Sezen returned, (b)(6) and (b)(7)(C) asked for her guidance. (b)(6) and (b)(7)(C) said that although in the spring of 2003 Dr. Sezen had stated that she ran her reactions without purifying the reagents, at the end of the summer Dr. Sezen gave contrary

(b)(6) and (b)(7)(C)

instructions, stating that she had recrystallized the reagents and dried and distilled all her solvents. (b)(6) and (b)(7)(C) thereupon followed Dr. Sezen's instructions and tried various procedures to purify the reagents, but yields continued to be erratic. (b)(6) and (b)(7)(C) said that Dr. Sezen finally came into (b)(6) and (b)(7)(C) laboratory and set up the reaction herself. In that instance, the reaction worked satisfactorily. (b)(6) and (b)(7)(C)

(b)(6) and (b)(7)(C) said that she met with (b)(6) and (b)(7)(C) in about December 2003 and raised several specific concerns that related to issues beyond her inability to reproduce Dr. Sezen's work consistently, including that Dr. Sezen kept changing her instructions to (b)(6) and (b)(7)(C) about how reactions were to be performed.[14] (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) said that, for the next several months, she attempted unsuccessfully to develop more robust methods for Dr. Sezen's reactions. (b)(6) and (b)(7)(C)

(b)(6) and (b)(7)(C) documented her work in her second-year graduate student report, presented this work in a (b)(6) and (b)(7)(C) meeting, and passed her second-year defense.

(b)(6) and (b)(7)(C)

[14] The Inquiry Report cited a seeming anomaly in one of Dr. Sezen's reaction procedures that was noticed (b)(6) and (b)(7)(C) believed that the procedure for preparing indolylmagnesium bromide was impossible because the reaction was to be conducted in dioxane cooled to 0 °C, whereas dioxane freezes at 12 °C. (b)(6) and (b)(7)(C) asked Dr. Sezen about this seeming inconsistency. Dr. Sezen instructed her to allow the reaction to warm up to room temperature. (*Id.* at 17:12-14). (b)(6) and (b)(7)(c) believed that this instruction deviated from Dr. Sezen's Supporting Information. When asked about this, Dr. Sezen referred the Committee to page 136 of her thesis, which states, "…the mixture was allowed to warm to room temperature under argon…." (Exh. K1 at 06031; Sezen Tr. at 75:19-77:9). The Supporting Information for her paper corresponding to this page of the thesis (page S21 of the Supporting Information for *J. Am. Chem. Soc.* (2003) **125**, 5274, Exh. K18 at 05759) contains this same instruction. Although unusual, this procedure is consistent with Dr. Sezen's instructions to (b)(6) and (b)(7)(C)

(b)(6) and (b)(7)(C) transferred from the (b)(6) and (b)(7)(C) she was contacted by Dr. (b)(6) and (b)(7)(C) who said he wanted to include (b)(6) and (b)(7)(C) as a co-author on a paper he was writing. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) This paper was later published as *JACS* (2005) **127**, 8050-8057 (Exhs. K25; K27) and is discussed in additional detail below.[15]

B. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) also described difficulties in reproducing Dr. Sezen's work. (b)(6) and (b)(7)(C) is currently a process (b)(6) and (b)(7)(C)

(b)(6) and (b)(7)(C) stated that when he was drafting a paper concerning arylation of indoles, ultimately published in *JACS* (2005) **127**, 8050-8057, (b)(6) and (b)(7)(C) wanted to refer to Dr. Sezen's previously published work, and to include an updated experimental procedure. (b)(6) and (b)(7)(C) wished to include the modified procedure only if he himself was able to repeat Dr. Sezen's reactions.[16] (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) explained that he "tried and tried [to reproduce Dr. Sezen's experiments] … without much success." (b)(6) and (b)(7)(C) said that he found this process difficult because Dr. Sezen repeatedly changed her verbal descriptions of the procedures. (b)(6) and (b)(7)(C) said that, in the end, Dr. Sezen worked together with him and "we got the procedure to work while she was there."

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[15] The Committee asked (b)(6) and (b)(7)(C) about the article's Supporting Information, which reported an 84% yield for the arylation of indole. (b)(6) and (b)(7)(C) said she did not see the Supporting Information before the paper was published. The Committee reviewed (b)(6) and (b)(7)(C) notebook for the reaction of indole with halogenated phenyl rings. Her yields ranged from 0% to 84%; the highest yield was obtained on October 30, 2003. (Exh. PP).

[16] (b)(6) and (b)(7)(C) said that he told (b)(6) and (b)(7)(C) that he believed Dr. Sezen's revised procedure should be published as an addition or correction to the original paper and not be included in (b)(6) and (b)(7)(C) paper. However, (b)(6) and (b)(7)(C) said that (b)(6) and (b)(7)(C) responded that Dr. Sezen's revised procedure should be included so that all the related procedures would be reported in one place. (b)(6) and (b)(7)(C)

(b)(6) and (b)(7)(C) Nonetheless, because of the difficulty he had in obtaining the results, (b)(6) and (b)(7)(C) insisted on including in the paper a statement highlighting the reaction's variability. (b)(6) and (b)(7)(C) stated that Dr. Sezen provided him with the section of the Supporting Information of his paper that updated her reaction procedure, as well as the table documenting the results. (Exh. K25 at S-17; (b)(6) and (b)(7)(C) However, the publication does not state that this section was provided by someone other than the authors.

In July 2005, just after Dr. Sezen had defended her thesis, (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(c) advised (b)(6) and (b)(7)(C) that he had concerns about Dr. Sezen's research results. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) explained to the Committee that he had been attempting to reproduce Dr. Sezen's results for the arylation of imidazole. (b)(6) and (b)(7)(C) For several months, he had obtained inconsistent results, including yields ranging from as low as 0% to as high as approximately 40%. (*Id.* at 16:13-23). (b)(6) and (b)(7)(C) said that the reaction he was studying suddenly worked on a day in which Dr. Sezen was in the laboratory, even though he had made only minor changes to the procedure on that day. Consequently, he became suspicious that Dr. Sezen was adding the expected product to his reaction mixtures. (*Id.* at 16:25-18:14).

[17] The Committee asked (b)(6) and (b)(7)(C) about a statement in Dr. Sezen's section of the Supporting Information stating that for her reaction, the yield was increased over the original publication. (b)(6) and (b)(7)(C) disagreed with that statement. (b)(6) and (b)(7)(C) pointed to Dr. Sezen's original paper (Exh. K17), which reported an initial yield of 53% that was later optimized to 84%. (Exh. K17 at 05720; K18 at 05739). The highest yield reported in the Supporting Information for (b)(6) and (b)(7)(C) paper was 86%. (Exh. K25 at S17). (b)(6) and (b)(7)(C) said that the difference between 86% and 84% was negligible. (b)(6) and (b)(7)(C)

C. Reports from Outside Columbia University

(b)(6) and (b)(7)(C) stated that he received several emails from researchers from industry who tried to reproduce the indole arylation reaction (b)(6) and (b)(7)(C) reported in *JACS* (2003) **125**, 5274-5275. (b)(6) and (b)(7)(C) said that he asked Dr. Sezen to help these individuals "as much as possible." (*Id.* at 56:24). (b)(6) and (b)(7)(C) recalled specifically asking these individuals to indicate whether the reactions ultimately were successful (b)(6) and (b)(7)(C), however he never received replies. (*Id.* at 57:17-20).

After his initial interview, (b)(6) and (b)(7)(C) provided copies of several emails he had received from individuals outside Columbia concerning reproducibility.[18] (Exh. J21). These emails were from (*Id.*)[19]:

- (b)(6) and (b)(7)(C)
-
-

(b)(6) and (b)(7)(C) recalled that, in the fall of 2003, (b)(6) and (b)(7)(C) told her that he and Dr. Sezen had received emails from scientists outside Columbia seeking help in reproducing Dr. Sezen's reactions. (b)(6) and (b)(7)(C) One of these emails, dated November 23, 2003, from (b)(6) and (b)(7)(C) who at the time was a (b)(6) and (b)(7)(C) the laboratory of (b)(6) and (b)(7)(C), was forwarded to (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) so that she could respond to the inquiry. (b)(6) and (b)(7)(C) After her

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(b)(6) and (b)(7)(C) stated that his computer did not contain any received email from before 2004, nor any sent mail from before 2005. Columbia's information technology department does not retain back-up tapes for more than 8 weeks at a time.

[19] This exhibit is referred to incorrectly in the (b)(6) and (b)(7)(C)

interview, (b)(6) and (b)(7)(C) provided the Committee copies of the forwarded email and the researcher's response. (Exhs. J7; J9).

Although these issues of reproducibility had been raised both inside and outside of Columbia, (b)(6) and (b)(7)(C) believed at the time that his group had identified the source of the sensitivity of these reactions and that the inquiries from researchers outside of Columbia University had all been addressed. (b)(6) and (b)(7)(C)

D. (b)(6) and (b)(7)(C) Effort to Determine Whether Dr. Sezen Was Adding Product to His Reactions

Because of his suspicions, (b)(6) and (b)(7)(C) said he decided to attempt to test whether Dr. Sezen was tampering with his reactions. He said that the only person he told about this plan was (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) set up two reactions in his own chemical fume hood. For one, he used imidazole, the starting material required by Dr. Sezen's procedures, but for the other, he used *N*-methylimidazole, a derivative of the usual starting material. He reported that, to his surprise, both reactions produced phenylimidazole, the product expected from the usual starting material (imidazole). (b)(6) and (b)(7)(C) analyzed the samples using HPLC, GC-MS and NMR techniques. (*Id.* at 20:17-21; Exhs. R1-R9).

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[20] The Committee attempted to contact each of these three individuals to find out whether they were ever able to reproduce Dr. Sezen's reactions. However, the Committee was only able to communicate with (b)(6) and (b)(7)(C) who stated that his "coworker could not reproduce the results" even after receiving the expanded procedure from (b)(6) and (b)(7)(C) (Exh. J36). One other instance of irreproducibility was reported in a 2006 publication (F. Bellina, S. Cauteruccio, R. Rossi, Palladium- and Copper-Mediated Direct C-2 Arylation of Azoles - Including Free (NH)-Imidazole, -Benzimidazole and -Indole -- Under Base-Free and Ligandless Conditions, *Eur. J. Org. Chem.* (2006) 6, 1379-1382 at 1380 (Exh. K26)). These researchers stated that they were unable to reproduce Dr. Sezen's reaction for arylation in imidazole using the original procedure reported in Sezen and (b)(6) and (b)(7)(C) *JACS* (2003) 125, 5274 (Exh. K17 at 05720), or the revised procedure included in the Supporting Information of (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(c)

[21] Dr. Sezen has disputed this point, stating that she did know about this so-called "trapping reaction." (Exh. T at 012354).

(b)(6) and (b)(7)(C) explained that on the next day and using the correct starting material he repeated the reactions in the laboratory of (b)(6) and (b)(7)(C) ran the experiments during the day rather than overnight, and tried to ensure that he, Dr. (b)(6) and (b)(7)(C) were continuously present throughout. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) said that these experiments yielded no trace of product. (b)(6) and (b)(7)(C), the apparati used for the experiments conducted in his hood and in (b)(6) and (b)(7)(C) were identical. (*Id.* at 21:11-16).

After (b)(6) and (b)(7)(C) collected these data, he reported the results to (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) (*Id.* at 21:17-20). (b)(6) and (b)(7)(C) results suggested an alternative explanation for the difficulties others had in reproducing Dr. Sezen's reactions: the reactions were not "sensitive" as had been thought, but were being manipulated by the addition of product by some individual.

6. (b)(6) and (b)(7)(C) Review of Dr. Sezen's Research Records

In response to (b)(6) and (b)(7)(C) arranged for members of his laboratory to investigate Dr. Sezen's research.[22] (b)(6) and (b)(7)(C) Four researchers primarily were involved: (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C). These researchers produced a series of reports documenting their efforts to validate Dr. Sezen's results. These reports are

(b)(6) and (b)(7)(C)

provided as Exhibits I4-I16; as discussed below, an early report by (b)(6) and (b)(7)(C) was provided to and relied upon by the Inquiry Committee. (Exh. I4A).

At the time that the (b)(6) and (b)(7)(C) began reviewing Dr. Sezen's work, Dr. Sezen was not present at Columbia University. In late July 2005, Dr. Sezen attended a conference at Stanford University. Thereafter, she went to her home (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) (Sezen Tr. at 40:5-9).

In her absence, members of the (b)(6) and (b)(7)(C) reviewed Dr. Sezen's Research Records.[24] In mid-August 2005, (b)(6) and (b)(7)(C) was helping (b)(6) and (b)(7)(C) to review Dr. Sezen's NMR spectra and discovered a composite figure of a series of phosphorus-31 (^{31}P) NMR spectra in which certain peaks had been removed from the spectra by obscuring them with "White-out" or another similar product (the "White-out Spectrum"). (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) *see also* Exhs. W1-W5, digital photographs of the White-out Spectrum). The White-out Spectrum was comprised of four ^{31}P NMR spectra that had been taped onto a backing sheet of paper that on the reverse side displayed a spectrum that had belonged to a former (b)(6) and (b)(7)(C) Exh. H8). As discussed in more detail below, the composite matched, in peak positions, peak heights, and background noise, a spectrum that was published in the Supporting Information for a paper Dr. Sezen co-authored (*JACS* (2004) **126**, 13244-13246 (2004)

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[23] (b)(6) and (b)(7)(C) 13).

[24] As discussed in greater detail at pp. 57-58 below, before she left Columbia, Dr. Sezen had packed her laboratory notebooks, NMR binders, CD Roms, and other materials, in boxes, so that these materials could be moved with the rest of the (b)(6) and (b)(7)(C) (Sezen Tr. at 38:8-13).

(Exh. K8); Exh. I4A at 2) and that was incorporated into Sezen's dissertation on page 333.

After (b)(6) and (b)(7)(C) discovered the White-out Spectrum, (b)(6) and (b)(7)(C) began searching for Dr. Sezen's original NMR data on the computers in the NMR Facility. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) After conferring with (b)(6) and (b)(7)(C) learned that no NMR account had been assigned to Dr. Sezen. (b)(6) and (b)(7)(C) He then began looking for spectra relevant to Dr. Sezen's work in accounts of other (b)(6) and (b)(7)(C) members.[25] (*Id.* at 22:10-15). (b)(6) and (b)(7)(C) said that he looked in all the accounts belonging to members of the (b)(6) and (b)(7)(C) In the course of this review, he discovered spectra on the 400 MHz and narrow-bore 300 MHz NMR spectrometers that appeared relevant to Dr. Sezen's research, but were in the accounts, with user name (b)(6) and (b)(7)(C) of a former (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C). These spectra had no relation to (b)(6) and (b)(7)(C) work and were recorded long after (b)(6) and (b)(7)(C) had left Columbia. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C)

In particular, and as discussed more fully below, (b)(6) and (b)(7)(C) found four individual ^{31}P NMR spectra that he identified as the individual spectra shown in the composite White-out Spectrum. Inspection of a series of intermediate processed data files stored in the "pdata" processed data directory (these are the standard data directory structures on a Bruker NMR spectrometer) showed that each spectrum had been produced by manipulating the single peak that constitutes the ^{31}P NMR spectrum of the readily available compound triphenylphosphine. (b)(6) and (b)(7)(C)

[25] Users of the NMR Facility have read-only access to all other accounts within the same research group. (b)(6) and (b)(7)(C)

(b)(6) and (b)(7)(C) then looked for additional data files that had large numbers of processed data files stored as subdirectories in the "pdata" directory (these are discussed below on pages 71-76) and in this way discovered, on the 400 MHz NMR spectrometer, the ^{1}H NMR spectrum stored that was the subject of (b)(6) and (b)(7)(C) report of November 8, 2005 and additional spectra discussed below. The evidence found by (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) showed that the NMR spectrum of compound 21 that was published in the Supporting Information to *JACS* (2004) **126**, 13244-13246 and reproduced on page 347 of the thesis was produced in 63 processes from the single peak of the common chemical methylene chloride. (Exh. I4A at 2). (b)(6) and (b)(7)(C) to review the spectra. (b)(6) and (b)(7)(C) suggested examining the C-H coupling constants associated with each peak in the spectrum. (b)(6) and (b)(7)(C). The small satellite peaks resulting from the presence of the rare ^{13}C isotope, present at a level of 1.1% in natural carbon, are commonly overlooked. (b)(6) and (b)(7)(C) found that the coupling constants for every peak for which the satellites could be discerned in the spectrum were exactly those characteristic of methylene chloride (177.6 Hz) and very different from those expected for the peaks in the spectrum of the professed product. (b)(6) and (b)(7)(C) 18; 43:12-22).

In August 2005, (b)(6) and (b)(7)(C) submitted draft reports to (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) concerning the findings of their initial investigation.[26] (Exs. I1-I3A). (b)(6) and (b)(7)(c) (b)(6) and (b)(7)(c) told the Committee that, in September and October 2005, in light of the information he had learned about Dr. Sezen's work, he revised a competitive renewal

[26] From that time through approximately June 2006, members of the (b)(6) and (b)(7)(C) continued reviewing Dr. Sezen's work in efforts to determine its reproducibility. (*See* Exhs. I4-I16). Ultimately, the results of their efforts, documented in their reports, became the basis for (b)(6) and (b)(7)(C) retractions and corrections of the papers Dr. Sezen co-authored.

application he was submitting to NIH. (b)(6) and (b)(7)(C) told the Committee that also in September 2005, he contacted (b)(6) and (b)(7)(C) who had offered Dr. Sezen a post-doctoral position. (b)(6) and (b)(7)(C) that he had concerns about Dr. Sezen's research; as a result, according to (b)(6) and (b)(7)(C) the (b)(6) and (b)(7)(C) was "put on hold." (b)(6) and (b)(7)(C) In November 2005, (b)(6) and (b)(7)(C) competitive renewal was re-submitted. (Exh. L8 at (b)(6) and (b)(7)(C) s Comments on Draft Inquiry Report dated March 4, 2007). (b)(6) and (b)(7)(C) later obtained a supplement award in July 2006. (Exh. L8 at 011474-011480).

PROCEDURAL HISTORY

1. The Initial Allegation

On November 7, 2005, (b)(6) and (b)(7)(C) sent a memorandum to Professor (b)(6) and (b)(7)(c) alleging that Dr. Sezen had fabricated some of her research results (the "November Allegation") (Attachment 2). (b)(6) and (b)(7)(C) attached to his memo the report by (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) described the apparent fabrication of data that were published in an article co-authored by Dr. Sezen and (b)(6) and (b)(7)(C) entitled Oxidative C-Arylation of Free (NH)-Heterocycles via Direct (sp^3) C-H Bond Functionalization, *JACS* (2004) **126**, 13244-13246. Specifically, the (b)(6) and (b)(7)(C) described the apparently fabricated NMR spectra found in the (b)(6) and (b)(7)(c) hat matched spectra published in this paper. Wang also

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(b)(6) and (b)(7)(C)

described the White-out Spectrum that appeared to match in essential respects a composite figure published in the same paper.

2. The Inquiry

At the time that (b)(6) and (b)(7)(C) submitted the November Allegation, Columbia's research misconduct policy required that the Dean of the Graduate School of Arts and Sciences ("GSAS") convene an Inquiry Committee to conduct a preliminary review of the allegation. (Attachment 1 is a copy of the Policy in effect in the fall of 2005). Accordingly, (b)(6) and (b)(7)(C) forwarded the memorandum he received from (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) GSAS Dean Henry Pinkham. In early December 2005, Dean Pinkham appointed the following Inquiry Committee:

(b)(6) and (b)(7)(C)

The Inquiry Committee met several times and interviewed the following witnesses:

(b)(6) and (b)(7)(C)

The Committee also reviewed the White-out Spectrum and viewed the allegedly fabricated spectra found in (b)(6) and (b)(7)(C) NMR account.

The Inquiry Committee concluded that a full investigation into the allegation against Dr. Sezen was warranted. The Inquiry Committee documented its findings in an Inquiry Report. On February 16, 2006, the Inquiry Committee submitted the Report to Dean Pinkham. (Attachment 3).

3. Notice to Dr. Sezen

In December 2005, after the Inquiry Committee was appointed, (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) made several attempts to notify Dr. Sezen by email that Allegations of Research Misconduct had been made against her and that an Inquiry Committee had been appointed. (Exh. J2 at 05598, 05595). A few days after sending these emails, he received emails in response stating, "Please do not send any further correspondence to this e-mail account. It is no longer actively used." (*Id.* at 05597).

Thereafter, (b)(6) and (b)(7)(C) telephoned Dr. Sezen's (b)(6) and (b)(7)(C) and was told Dr. Sezen would be home later. (Exh. J29A at 012038). On January 4, 2006, (b)(6) and (b)(7)(C) sent a letter by FedEx to Dr. Sezen's (b)(6) and (b)(7)(C) (also the home address recorded in Dr. Sezen's student file in the Department of Chemistry) notifying her that the Inquiry had commenced (Exh. J2 at 05592; *see also* Exh. J29).[28]

On January 6, 2006, (b)(6) and (b)(7)(C) received an apparently hand-delivered letter from Dr. Sezen expressing concern about (b)(6) and (b)(7)(C) investigation into her

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(b)(6) and (b)(7)(C)

work (Exh. J1A).[29] On January 11, 2006, (b)(6) and (b)(7)(C) forwarded this letter to the Inquiry Committee.[30] (Exh. J2 at 05577).

On January 18, 2006, (b)(6) and (b)(7)(C) received an email from (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) listed as Dr. Sezen's home address). (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) explained that she had obtained (b)(6) and (b)(7)(C) address from Columbia's webpage and that although the Department of Chemistry's FedEx package had been accepted by the (b)(6) and (b)(7)(C) it could not be delivered to Dr. Sezen "[b]ecause she does not stay in our buildings anymore." (Exh. J27). The email further explained that Dr. Sezen "is currently in US but we do not have her forwarding address." (*Id.*). In response, (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) wrote that she would try to find Dr. Sezen's parents. (*Id.*). (b)(6) and (b)(7)(C) answered, "According to our files (b)(6) and (b)(7)(C) and moved to (b)(6) and (b)(7)(C) We will ask them to contact you if they contact us." (*Id.*).

Shortly thereafter, (b)(6) and (b)(7)(C) sent Dr. Sezen an email to her Columbia email account, requesting a forwarding address and explaining that she needed to send a package to Dr. Sezen. (Exh. J29A at 012038). On January 22, 2006, (b)(6) and (b)(7)(C) received an email in response stating "To whom this may correspond to: Please do not send any further correspondence to this e-mail account. It is no longer actively used. Bengu Sezen." (*Id.*).

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[29] The envelope was not postmarked and contained no return address. (Exh. J2 at 05578-91).

[30] Dr. Sezen's letter referred to an "M. Atkas," whom she stated was her lawyer. On February 27, 2006, members of the (b)(6) and (b)(7)(C) received a memo from "M. Atkas," purporting to be an attorney at Barrington Law Firm, 387 Madison Avenue, New York, New York, requesting any reports they had written concerning their investigation into Dr. Sezen's work. Jane E. Booth, Esq., of Columbia's Office of the General Counsel, wrote back to M. Atkas, requesting verification that M. Atkas was licensed to practice in New York and had been retained by Dr. Sezen. The letter was returned unopened and stamped, "attempted – not known unable to forward." (Exh. J38). Searches of "Barrington Law Firm" and "M. Atkas" in the law firm database, Martindale Hubble, did not produce any results.

After he received the Inquiry Committee's report, Dean Pinkham learned from a World Wide Web search that Dr. Sezen appeared to be enrolled in a graduate program at the University of Heidelberg, in the laboratory of (b)(6) and (b)(7)(C) (Exh. P). Dean Pinkham attempted to contact Dr. Sezen at her Heidelberg email address but received no response. (Exh. J2 at 05553). On March 21, 2006, he sent a copy of the Inquiry Report and Columbia's Policy to Dr. Sezen's Heidelberg email account. (Exh. J2 at 05556-76).

On March 23, 2006, using her Columbia email account, Dr. Sezen emailed members of Columbia's Office of Public Affairs inquiring about retractions of papers she co-authored.[31] (Exh. J35). Later that same day, after being advised of this email, Dean Pinkham forwarded his March 21 email and the Inquiry Report and Policy, along with copies of the messages he had previously attempted to send to her, to Dr. Sezen's Columbia email address. (Exh. J2 at 05552-5554).[32]

On March 27, 2006, Dr. Sezen responded to Dean Pinkham's email, stating she had received and examined the Inquiry Report. (Exh. J2 at 05552).

In her March 27, 2006 email, Dr. Sezen stated that she would provide a written response within one month of receiving certain materials. (*Id.*). Over the next month, Columbia provided numerous documents and additional information that Dr. Sezen requested, to the extent the material was available.[33] (Exh. J2 at 05534, 05530-05531,

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[31] Three retractions or corrections of articles co-authored by Dr. Sezen were initially published in March 2006. *See* Exhibit K10. Four additional articles were retracted or corrected in June 2006. *See* Exhs. K7; K16.

[32] On March 26, 2006, (b)(6) and (b)(7)(C) notified Dr. Sezen by email that he had retracted two papers on which Dr. Sezen was a co-author, and corrected a third. (Exh. J2 at 05549-05550).

[33] One document that Dr. Sezen requested – a copy of the White-out Spectrum – was available only in hard copy, so the University requested a mailing address for Dr. Sezen. In response, Dr. Sezen provided the same mailing address to which the Department of Chemistry attempted to send notice in January 2006:

(b)(6) and (b)(7)(C)

05514-05529, 05502-05503). Dr. Sezen requested additional time to respond to the Inquiry Report and the University agreed. (Exh. J2 at 05492).

On May 19, 2006, Dr. Sezen provided her comments in response to the Inquiry Report. Dr. Sezen's comments were provided to the Inquiry Committee, which reviewed them and submitted its own final comments.[34] (Exh. T). The Inquiry Committee's final report was also provided to Dr. Sezen. (Exh. J2 at 05447-05450).

4. Transition to a New Institutional Policy

As discussed above, on February 3, 2006, the University's Faculty Senate approved a new Institutional Policy on Misconduct in Research. (Attachment 4). The new Misconduct Policy outlined new procedures and protections for allegations of research misconduct. After the Misconduct Policy was approved, the University began to implement the Misconduct Policy and its procedures, as recommended in the comments to revised 42 CFR Parts 50 and 93.

The prior policy on research misconduct was silent on the University's obligation to sequester research records. (Attachment 1). In accordance with the new Misconduct Policy, in the first week of April 2006, Columbia's Director of Research Compliance and Training and (b)(6) and (b)(7)(c) collected from the (b)(6) and (b)(7)(c) (b)(6) and (b)(7)(c) four boxes of materials that had belonged to Dr. Sezen.[35] These materials

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(b)(6) and (b)(7)(C)

On April 4, 2006, Columbia sent by FedEx to Dr. Sezen the hard copy of the White-out Spectrum. (Exh. J2 at 05530-05531). This package was received by Dr. Sezen: in an April 24, 2006 email, Dr. Sezen queried whether the two-page photocopy she had received was two sides of the same document or two separate documents. (Exh. J2 at 05495).

[34] Dr. Sezen's comments included allegations that (b)(6) and (b)(7)(C) had themselves committed research misconduct by fraudulently claiming her work could not be reproduced. These allegations (the "Counter-Allegations") were forwarded to a second Inquiry Committee pursuant to Columbia's Policy. (Exh. T2 at 05458-05489).

[35] On October 25, 2006, (b)(6) and (b)(7)(C) collected a fifth box from (b)(6) and (b)(7)(C) laboratory that contains fourteen blue three-ring binders of published literature, and one laboratory notebook with flyers,

included 11 laboratory notebooks, six large binders containing NMR spectra, various computer disks and CD-Roms, and various personal effects. Attachment 5 is the initial index reflecting the contents of these boxes.[36]

In addition, in the first week of April and thereafter, (b)(6) and (b)(7)(C) took the following steps to collect and sequester relevant documents:

- Requested that (b)(6) and (b)(7)(C) "freeze" the (b)(6) and (b)(7)(c) NMR account containing the spectra referenced in the Inquiry Report, so that the account could be accessed only by (b)(6) and (b)(7)(C)
- Obtained a CD-ROM of the NMR spectra referenced in the Inquiry Report;
- Collected four laboratory notebooks of (b)(6) and (b)(7)(c) that included documentation of his investigation into Dr. Sezen's work;
- Obtained excerpts of laboratory notebooks of other members of the (b)(6) and (b)(7)(c) (b)(6) and (b)(7)(c) concerning their investigations into Dr. Sezen's work (the notebooks were in current use, but are hard-bound with pre-printed numbered pages);
- Obtained CD-ROMs of NMR spectra and other electronic data corresponding to the (b)(6) and (b)(7)(C) laboratory records;
- Obtained copies of reports produced by the (b)(6) and (b)(7)(C) concerning their investigations into Dr. Sezen's work;
- Obtained copies of correspondence between (b)(6) and (b)(7)(C) and Dr. Sezen dating from the summer and fall, 2005;
- Obtained a copy of Dr. Sezen's thesis;
- Obtained the hard copy White-out Spectrum referenced in the Inquiry Report;
- Obtained copies of the progress reports and other grant materials submitted to NIH and NSF in connection with the NIH Grant and the NSF Grant;
- Obtained electronic copies of other relevant data;

Department of Chemistry schedules, and speakers' announcements as well as some personal notes. (Section CC on the Master Index). (b)(6) and (b)(7)(C) did not initially collect this box with the others because of its irrelevance to the investigation.

[36] This index was compiled by the Office of the General Counsel shortly after the documents were gathered. It was later reconfigured and expanded into the Master Index, at Attachment 6.

- Obtained from Dr. Sezen a CD-Rom described as a copy of her computer desktop at Columbia;
- Obtained copies of relevant business records from the Department of Chemistry's business office;
- Obtained copies of relevant business and other records from the Department of Chemistry's NMR Facility.

Finally, throughout the course of the investigation, the Committee requested and received additional documents from witnesses who appeared before it. Attached as Attachment 6 is the final Master Index listing the documents collected in the course of this Investigation.

The Misconduct Policy required the appointment of a new University-wide Standing Committee on the Conduct of Research ("Standing Committee") to implement the Misconduct Policy. The Standing Committee appointments were completed by May 2006. The Committee is chaired by (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) As required by the Misconduct Policy, the Committee's 19 members represent the biomedical and non-biomedical campuses and include a graduate student, an Officer of the Libraries, and representatives of other key areas in the University. The members are listed in Attachment 7.

5. The Standing Committee Decides that an Investigation is Warranted

On May 31, the Standing Committee met and discussed the Sezen case. After discussion, the Standing Committee accepted the Inquiry Committee's recommendation that a full Investigation as defined in the Misconduct Policy was warranted. (*See* Attachment 8). The Committee also approved the appointment of four proposed members of an Ad Hoc Committee charged to investigate the Allegation of Research

Misconduct, and granted (b)(6) and (b)(7)(C) the authority to appoint additional members as needed. (*Id.*). The Committee emphasized the need to include scientists from outside Columbia University on the Committee, the need to include a graduate student not affiliated with the Department of Chemistry, and the need for gender diversity. (*Id.* at 2). Thereafter (b)(6) and (b)(7)(c) appointed three additional members to the Committee.[37] *Curricula vitae* for the members of the Ad Hoc Committee are attached as Attachment 9. On June 27, 2006, (b)(6) and (b)(7)(C) sent the members of the Ad Hoc Committee a charge letter.[38] A copy of the Charge Letter is attached as Attachment 10.

6. The Investigation

The Committee held planning meetings on August 16 and September 6, 2006. Thereafter, the Committee held ten additional meetings to interview persons with relevant information and prepare this Report. Each session lasted between two and five hours.

A. Interviews

Pursuant to the Policy, both (b)(6) and (b)(7)(C) and Dr. Sezen were invited to identify persons with relevant information to be interviewed for this Investigation (Exh. J2 at 05199; J39). (b)(6) and (b)(7)(C) (Exh. J41). Dr. Sezen identified (b)(6) and (b)(7)(C) the (b)(6) and (b)(7)(c)

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[37] (b)(6) and (b)(7)(C) of the Columbia University Department of Chemistry, was approved by the Standing Committee but declined to participate. (b)(6) and (b)(7)(C), also of the Columbia University Department of Chemistry, was selected in (b)(6) and (b)(7)(C) place. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) laboratory was on the same floor as (b)(6) and (b)(7)(C). As a result, he was acquainted with many current and former students in the (b)(6) and (b)(7)(C) However, (b)(6) and (b)(7)(C) did not collaborate with (b)(6) and (b)(7)(C) on any research, papers or grants. The University considered these facts and determined that they did not give rise to any apparent or actual conflict of interest for (b)(6) and (b)(7)(C) service on the Committee. Dr. Sezen requested a formal statement on this issue, which the University provided. (Exh. J34 at 012140-012141).

[38] After receiving the Charge Letter, one member declined to participate because of other commitments. A replacement member was appointed on July 20, 2006.

(b)(6) and (b)(7)(C) (Exh. J2 at 05181). The Committee identified additional individuals with relevant information.[39] In total, the Committee interviewed 18 individuals, some on more than one occasion, as follows:

(b)(6) and (b)(7)(C)

(b)(6) and (b)(7)(c)

(b)(6) and (b)(7)(C)

Curricula vitae for these individuals, where available, are attached as Exhs. AA1-AA12 and Exh. X. Except for the interviews of (b)(6) and (b)(7)(C) for which one member of the Committee was absent, and for the interview of (b)(6) and (b)(7)(C) conducted (b)(6) and (b)(7)(C) all members of the Ad Hoc Committee were present at every interview. The interviews were transcribed by a court reporter. Initial drafts were sent to each interviewee, who then had the opportunity to provide necessary corrections. Transcripts of the interviews are attached in Exhibit OO.

B. Document Review

In the course of the Investigation, over 10,000 pages of documents were sequestered and reviewed, including Dr. Sezen's research records and publications, Department of Chemistry business records, (b)(6) and (b)(7)(C) reports, and computer records from the NMR Facility. In addition (b)(6) and (b)(7)(C) reviewed all of the electronic research records (Exhs. B13-B56; H9; H10A; H10B).

C. The University's Efforts to Obtain Information and Testimony from Dr. Sezen

Between late June and mid-August, 2006, the University attempted to communicate with Dr. Sezen concerning both this Investigation and her Counter-

Allegations. (Exh. J2 at 05348-05403).[40] In late June, (b)(6) and (b)(7)(C) advised Dr. Sezen that the Inquiry Committee reviewing her Counter-Allegations wanted to speak with her. (Exh. J2 at 05438). In response, on June 28 and June 30, Dr. Sezen promised to contact (b)(6) and (b)(7)(C) schedule an interview.[41] (Exh. J2 at 05437 and 05435).

Thereafter, the University repeatedly tried to convene a teleconference with Dr. Sezen. Dr. Sezen provided a telephone number (b)(6) and (b)(7)(C) and stated that she would be available at a certain time. (*Id.* at 05431). However, the University's call could not be completed. (Exh. J34 at 012831-012832). After this, Dr. Sezen repeatedly stated her availability was restricted. (*E.g.*, Exh. J2 at 05412, 05406, ; Exh. J34 at 012836). In her email of July 12, 2006, Dr. Sezen stated, "Thus I can only ask you for e [sic] new schedule after July 25." (Exh. J34 at 012830).

On July 17, 2006, Dr. Sezen forwarded a letter from (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) concerning the reproducibility of Dr. Sezen's work.[42] (Exh. J2 at 05404-05405). In response (b)(6) and (b)(7)(C) again sought to reschedule Dr. Sezen's telephone interview for July 26 at 12:30 p.m. and provided her own telephone number for Dr. Sezen to call in case the University could not reach Dr. Sezen. (*Id.* at 05403). Dr. Sezen did not respond to this email. After this, Dr. Sezen responded to several emails sent by (b)(6) and (b)(7)(C) by stating that she could not read the messages.[43] (*Id.* at 05401; 05400; 05392; 05390).

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[40] Due to a technical error, documents 05166-06359 were incorrectly numbered, omitting a 0. The numbering for these documents should include an additional 0 prefix: 005166-006359.

[41] In one of these instances, Dr. Sezen stated she needed to consult with an attorney concerning scheduling. (Exh. J2 at 05437). However, no attorney has ever appeared on Dr. Sezen's behalf in this case.

[42] (b)(6) and (b)(7)(C)

[43] (b)(6) and (b)(7)(C) learned that, in accord with standard University practice, Dr. Sezen's Columbia email account had been closed because Dr. Sezen was no longer enrolled as a Columbia student. (b)(6) and (b)(7)(C) immediately instructed Columbia University Information Technology ("CUIT") to reactivate Dr. Sezen's

Eventually, on August 10, 2006 (b)(6) and (b)(7)(C) successfully faxed and emailed a letter to Dr. Sezen seeking to schedule an in-person interview.[44] (*Id.* at 05337-05347). The letter also requested Dr. Sezen's laptop computer or an image of the computer's hard disk; a print-out of Dr. Sezen's current directories; and a list of all NMR user accounts accessed by Dr. Sezen at Columbia. The letter asked Dr. Sezen to respond by August 24, 2006, and also sought updated contact information including a mailing address, telephone and fax numbers, and email addresses. (*Id.* at 05338-05339).

On August 16, 2006, Dr. Sezen responded by email that she would be available for an in-person interview. However, she refused to make any arrangements or provide any of the requested information until the University provided her documents she had requested in June concerning the (b)(6) and (b)(7)(C) efforts to reproduce her work. (*Id.* at 05314). Starting on August 16, 2006, Dr. Sezen also sent emails to the President of the University and other University officials, as well as reporters from *Science*, *Nature*, and the *New York Times*, complaining about the way the University was handling her Counter-Allegations. (Exh. J2 at 05310). On August 17, she forwarded this same email to the entire membership of the Department of Chemistry at Harvard University. (Exh. J2B at 05306). Between August 18 and August 29, Dr. Sezen forwarded the same email to the chemistry faculties of MIT; the University of California, Berkeley; Stanford University; Princeton University; Yale University; Scripps Research Institute; California Institute of Technology; the University of Illinois at Champaign-Urbana; Penn State University; Cornell University; and Georgia Institute of Technology. (Exh. J2B).

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account. She confirmed to Dr. Sezen that as of July 27, 2006, the account was active again and functioning appropriately (Exh. J2 at 05393).

(b)(6) and (b)(7)(c)

On August 18 (b)(6) and (b)(7)(C) sent ten reports to Dr. Sezen, in response to her requests. These reports were drafted by members of the (b)(6) and (b)(7)(C) and documented their attempts to validate Dr. Sezen's work. (Exh. J2 at 05301; 05240-05296). On August 21, 2006, Dr. Sezen acknowledged their receipt but stated that they were insufficient to fulfill her request, and she submitted a detailed list of documents she sought concerning the (b)(6) and (b)(7)(C) efforts to reproduce her work. She also continued to refuse to schedule an interview or answer any of the Committee's questions until her requests were satisfied. (Exh. J2 at 05227).

In subsequent emails, (b)(6) and (b)(7)(C) reiterated the Committee's requests for information; proposed October 6, 2006 for Dr. Sezen's interview; and invited Dr. Sezen to come to Columbia at the University's expense to review the relevant Research Records in advance of the interview. (*Id.* at 05211). In addition, (b)(6) and (b)(7)(C) invited Dr. Sezen to provide any relevant documents in her possession (*Id.*) and to identify any other persons who had information relevant to the Investigation. (*Id.* at 05199). On August 29, (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) reiterated these points and also forwarded to Dr. Sezen additional documents responsive to her request. (Exh. J34 at 012732-012829).

On August 31, 2006, Dr. Sezen stated that the documents she had received also were insufficient. (Exh. J2 at 05179). She also responded in some detail to the Committee's earlier queries, including statements that she used only her own NMR account and that she could not have fabricated the spectrum identified in the (b)(6) and (b)(7)(c) Report because she was staying in (b)(6) and (b)(7)(C) on the date the spectrum was fabricated. (*Id.* at 05181). Dr. Sezen stated that she would be available for an interview on the proposed date, October 6, 2006, at an office she had arranged to use

(b)(6) and (b)(7)(C) (*Id.* at 05181). Finally, Dr. Sezen advised that she would be "away from [her] e-mail between dates 1-18th September 2006," and thus unable to respond to any e-mails between those dates. (*Id.* at 05178).

Upon receipt of Dr. Sezen's August 31, 2006 email, (b)(6) and (b)(7)(C) responded that Dr. Sezen's interview would take place at Columbia, and reiterated the University's earlier offer to pay for Dr. Sezen's travel expenses. (Exh. J2 at 05175). (b)(6) and (b)(7)(C) also requested that Dr. Sezen provide: (1) the account name she used to access Columbia's NMR spectrometers; and (2) any documentation of her stay at the (b)(6) and (b)(7)(C) (Exh. J2 at 05171). On September 1, 2006, (b)(6) and (b)(7)(C) received an email with the heading, "Auto-reply," stating "I will be away from my email until Sep 18th. I will respond to your e-mail after that date." (*Id.* at 05170). Still later on September 1, (b)(6) and (b)(7)(C) received another response from Dr. Sezen stating that she had arranged to conduct her interview in (b)(6) and (b)(7)(C) because her visa for the United States had expired and she was not able to renew it. (*Id.* at 05166).

The Committee continued to plan to interview Dr. Sezen in person at Columbia University. On September 18, 2006, (b)(6) and (b)(7)(C) sent Dr. Sezen an email with additional information about the visa application process and attaching a letter of support for Dr. Sezen's application. (Exh. J34 at 012728-012729). (b)(6) and (b)(7)(C) further explained that if Dr. Sezen did not come to Columbia for the interview, the interview would occur by telephone at a conference room (b)(6) and (b)(7)(C) that Columbia would arrange. (*Id.*). Dr. Sezen responded that she was unable to satisfy visitor visa requirements and that "all [her] previous applications were denied …." (Exh. J34 at 012724-012725).

D. The University Arranges for Dr. Sezen's Telephone Interview

After Dr. Sezen advised the Committee that her visa application had been rejected, the University retained White & Case LLP, a United States law firm with offices in (b)(6) and (b)(7)(C) so that Dr. Sezen could have access to the Research Records and conduct the interview from a location with sufficient telecommunications capability. (b)(6) and (b)(7)(C) sent to White & Case in (b)(6) and (b)(7)(C) approximately six thousand pages of documents. (b)(6) and (b)(7)(C) advised Dr. Sezen that these documents were available for her to review at White & Case, and also emailed Dr. Sezen copies of the index of evidence that had been sequestered. (Exh. J34 at 012464-012477; 012478; 012443).

On September 23, the Committee's Chair, Prof. (b)(6) and (b)(7)(C) sent Dr. Sezen a letter outlining key points about the upcoming interview. (*Id.* at 012487-012491). (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) reiterated the Committee's request for Dr. Sezen's login for the NMR Facility and queried her about her research records and data management processes. (*Id.* at 012484-012486). Finally, (b)(6) and (b)(7)(C) also provided the Index of Documents and directories of four CD-Roms apparently containing Dr. Sezen's computer files. (*Id.* at 012492-01720). He invited Dr. Sezen to identify any documents or information she wished the Committee to review or wished to review herself. (*Id.* at 012485).

On September 28, 2006, Dr. Sezen responded that the most important document she wanted to review before the interview was the final Inquiry report concerning her Counter-Allegations. She added:

> I would like to emphasize that I will not be able to respond to any questions in (b)(6) and (b)(7)(C) letter or any other questions during the phone conference if I will not receive this highly necessary document for my interview.

(*Id.* at 012461; 012442).

Thereafter, Dr. Sezen sent a number of emails with queries about the interview and Investigation, to which (b)(6) and (b)(7)(C) responded. (*Id.* at 012438-012441). She also expressed concern about potential bias in the Investigation.[45] (*Id.* at 012437). Dr. Sezen also asked that the documents at White & Case be given to her so she could bring them to the place where she had her computer and her own records. (*Id.* at 012431). (b)(6) and (b)(7)(C) suggested instead that Dr. Sezen bring her materials and computer to White & Case's office, which agreed to provide Dr. Sezen work space during the week before the interview. (*Id.* at 012429). Dr. Sezen stated that this would not be possible. (*Id.* at 012426). Finally, Dr. Sezen stated that on September 1, she had sent by regular mail to (b)(6) and (b)(7)(C) information concerning her account name for the Columbia NMR facility and a copy of her (b)(6) and (b)(7)(C) She stated that as these items were not listed in the Index of Evidence, she had sent another copy by regular mail the day before.[46] (*Id.*).

On October 4, (b)(6) and (b)(7)(C) asked Dr. Sezen to email her NMR account information immediately and reminded Dr. Sezen that the Committee continued to await her responses to the questions in (b)(6) and (b)(7)(C) September 23 letter. (*Id.* at 012423). (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) provided Dr. Sezen a fax number so she could fax the (b)(6) and (b)(7)(C) and any other documents, and stated that if Dr. Sezen did not have access to a fax machine, she could bring the documents to White & Case's office for assistance in faxing. (*Id.*). (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) again invited Dr. Sezen to review the documents that had been sent to White & Case. (*Id.*). She also offered that, for the interview, White & Case could bring the

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[45] Dr. Sezen expressed concern that (b)(6) and (b)(7)(C) might be biased because of his proximity to the (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) and resulting acquaintance with many Group members. The University provided Dr. Sezen with a formal response to this concern. *See* footnote 37.

[46] (b)(6) and (b)(7)(C) never received these mailings.

documents to Dr. Sezen at a location she designated. (*Id.*). Dr. Sezen did not respond to this offer.

On October 5, 2006, Dr. Sezen emailed a response to (b)(6) and (b)(7)(C) September 23 letter, including her NMR account name and an electronic copy of a (b)(6) and (b)(7)(C) (Exh. J15).

On October 6, at the appointed hour, the Committee called Dr. Sezen at the number she provided (011-90-312-240-7148.). The Committee offered to delay the interview so that White & Case could deliver documents to Dr. Sezen, but Dr. Sezen refused to give her address and declined to receive the documents.[47] (Sezen Tr. at 8:12-9:25).

7. **Dr. Sezen's Access to the Research Record**

Columbia's Policy provides that, "During an Inquiry, the Respondent shall have the right … to have reasonable access to the data and other evidence supporting the Allegation…." (Attachment 4 at K(4)(c)(ii)). The Policy further provides that, "Upon Completion of the Investigation, the Ad Hoc Committee shall provide the Respondent with (a) a draft written report … and (b) a copy of, or supervised access to, the evidence on which the Investigation Report is based." (Attachment 4 at H(5)). In this case, Columbia went beyond the requirements of its own Policy.

First, as discussed above, during the Inquiry phase of this case, Dr. Sezen requested numerous additional documents (including information that was not part of the Research Record when the Inquiry Committee drafted its report, *see* Attachment 3). To

[47] Although she had been provided with White & Case's address and the name of a contact person in the office, Dr. Sezen claimed that she could not find White & Case's telephone number. (Sezen Tr. at 8:4-7; Exh. J34 at 012401). However, the phone number is readily available on the White & Case website. *See* Exh. KK at 013457.

the extent that these materials were available, they were provided to Dr. Sezen. (*See* pp. 31-34 above).

Second, after the Inquiry phase was complete, Dr. Sezen requested additional materials concerning the (b)(6) and (b)(7)(C) efforts to reproduce her work. (Exh. J2 at 05443). On June 27, 2006, (b)(6) and (b)(7)(C) explained that to the extent Dr. Sezen sought additional materials in connection with her allegations of research misconduct against (b)(6) and (b)(7)(C) Columbia's Policy did not afford her, as the Complainant, access to evidence concerning her allegation. (*Id.* at 05437).

However, (b)(6) and (b)(7)(C) further explained that to the extent Dr. Sezen sought information in connection with the allegations of research misconduct against her, Columbia's Policy provided that after the draft investigative report was completed, Dr. Sezen would be entitled to a copy of, or supervised access to, the evidence upon which the report was based. (*Id.*).

As discussed above, in August 2006 Dr. Sezen renewed her request for documents. Although still not obligated to provide any documents under the University's Policy, the University provided the materials she requested to the extent they were available. As discussed above, the Committee also repeatedly invited Dr. Sezen to come to Columbia to review the Research Records, and offered to pay her travel and visa-related expenses. (Exh. J2 at 05211, 05175; Exh. J34 at 012728-012729).

Third, after Dr. Sezen advised the Committee that she was unable to obtain a visa to come to Columbia and wished to conduct the interview in (b)(6) and (b)(7)(c) the Committee sent approximately six thousand pages of documents to White & Case's (b)(6) and (b)(7)(C) office and arranged to have work space provided to Dr. Sezen so she would be able to review these

Research Records. But Dr. Sezen never went to White & Case's office to review these documents. The Committee also repeatedly sent Dr. Sezen the Index of Evidence and invited her to identify documents she wished the Committee to review and to identify documents she wanted sent to her. (Exh. J34 at 012490, 012464-012478).

Fourth, after Dr. Sezen's interview, the University asked White & Case to retain the Research Records in case Dr. Sezen wished to review them; (b)(6) and (b)(7)(C) also offered to send additional copies to Dr. Sezen. (Exh. J34 at 012228; *see also* 012163, 012171-012193). However, Dr. Sezen did not request any additional materials except for copies of her 11 laboratory notebooks. The Committee had these notebooks photocopied. On November 6, 2006, it sent their photocopies – ca. 3500 pages – to Dr. Sezen at an (b)(6) and (b)(7)(C) address she provided. (Exh. J34 at 012148).

Fifth, in accordance with Columbia's Policy, this Report has also been provided to Dr. Sezen for comment along with a copy of the Master Index. (Exh. J34 at 013585). Dr. Sezen was also told that the 4,000 pages of supporting evidence would be sent to her once she provided a mailing address. (Exh. J34 at 013574-013584). Dr. Sezen never indicated that she wanted the supporting evidence and did not provide a mailing address.

FINDINGS OF FACT

1. Dr. Sezen Never Had a User Account in the NMR Facility

The Committee finds that, although her research depended heavily on NMR spectroscopy, Dr. Sezen never had an authorized computer account for access to NMR spectrometers and data stations in the NMR Facility.

(b)(6) and (b)(7)(C) facility since 1994, issues all computer accounts for the NMR facility. (b)(6) and (b)(7)(C) records every account issued in a single logbook. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(c) He organizes the records in this logbook by research group. In his interview, (b)(6) and (b)(7)(C) confirmed that page 129 of his logbook contains all of the records for the (b)(6) and (b)(7)(C) explained that each research group has a unique UNIX group number and that he assigns the UNIX user numbers consecutively for individuals within the group.

Until 2005, the UNIX group number for the (b)(6) and (b)(7)(C) was 108.[48] (Exh. N19). (b)(6) and (b)(7)(C) was the first member of his group to receive a login; he was assigned the user number 2700. (b)(6) and (b)(7)(C) further explained that he assigns all numbers chronologically in the order that researchers complete their training in the use of the NMR spectrometers. (*Id.* at 15:19-25). Dr. Sezen entered the Columbia University graduate program in the fall semester of 2000 and joined the (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) in December 2000, along with (b)(6) and (b)(7)(C) Thus, if Dr. Sezen had completed NMR training as usual, she would have been assigned a user number near the user numbers of these other students. Although the logbook identifies

[48] In 2005, the UNIX group number was changed to 1108. (Exh. N16 at 013450).

accounts assigned to every other member of the (b)(6) and (b)(7)(C) who used the NMR spectrometers as part of their research, the logbook contains no record of any account assigned to Dr. Sezen and no gaps occur in the numerical listing of user numbers.[49] (*See* Exh. N2A)

In August 2005, after making this discovery, (b)(6) and (b)(7)(C) searched the NMR Facility's computer files for any record of an account belonging to Dr. Sezen. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C). The UNIX operating system records the user number and group identification for any user who creates or modifies any file stored on the hard drive of the NMR spectrometer computers. (*Id.* at 25:6-18; 81:9-82:17). (b)(6) and (b)(7)(C) explained that to find an account, he needed to know the user name for the account, which usually is some form of the user's name. In August 2005, (b)(6) and (b)(7)(C) searched his computer files for "bengu" and "sezen" and variations thereon, but found no record of any account. (b)(6) and (b)(7)(C).

On August 10, 2006, the Committee asked Dr. Sezen to provide the Committee a list of all NMR accounts she had used at Columbia. On August 31, 2006, Dr. Sezen responded by email that, "I HAVE NEVER USED ANYONE ELSE'S NMR ACCOUNT. I HAVE NEVER USED (b)(6) and (b)(7)(C) NMR ACCOUNT; I DID NOT KNOW HER PASSWORD, I DID NOT HAVE ACCESS TO HER ACCOUNT." (Exh. J2 at 05177, emphasis in original). However, she did not provide the user name for her own account. As discussed above, on August 31, 2006 and September 22, 2006, the Committee asked Dr. Sezen to provide her account name for her NMR account at Columbia, but she did not respond until October 5, 2006, the day before

[49] The fact that Dr. Sezen did not have an NMR account was first reported by (b)(6) and (b)(7)(C) in his November 8, 2005 report. *See* Exh. I4A at 2.

her interview with the Committee. In her letter of that date, Dr. Sezen stated that her login ID was "bengu." She further stated that she obtained this login ID during a course she took entitled "Chemistry G4145 NMR Spectroscopy," taught by (b)(6) and (b)(7)(C) (Exh. J15 at 012413) Dr. Sezen confirmed these statements in her testimony to the Committee. (Sezen Tr. at 18:6-16; 19:11-23).[50]

The Committee then asked (b)(6) and (b)(7)(C) to search for any record of any account with the name "bengu." (b)(6) and (b)(7)(C). The UNIX operating system maintains a record of all user accounts in a file named "passwd" that is modifiable only by the system administrator (b)(6) and (b)(7)(C) (*Id.* at 72:6-9). At his September 22, 2006, interview, (b)(6) and (b)(7)(C) explained that approximately two years earlier he had transferred all his passwd files from one computer system to another. (*Id.* at 28:18-21). At the Committee's request, (b)(6) and (b)(7)(C) searched his current passwd files and the hard disks belonging to the old system for any record of the user name "bengu." (*Id.* at 70:3-23). After searching all current and outdated passwd files on every computer in the NMR Facility, (b)(6) and (b)(7)(C) found no record of any user account named "bengu." (b)(6) and (b)(7)(c) at 70:3-72:23; Exh. N11).[51]

(b)(6) and (b)(7)(C) maintains an accounting system on the NMR spectrometers that records each login and logout to the NMR software (as distinct from login to the UNIX operating system). This accounting system is used to generate billing records for each research group. The accounting software records in a log file the user name, date, and

[50] In his interview, (b)(6) and (b)(7)(C) stated that the course did not require an NMR login account, and that the process for obtaining an NMR login account was separate from his course. (b)(6) and (b)(7)(C)).
[51] In addition, because in her laboratory notebooks, Dr. Sezen referred to her NMR spectra with the prefix "BS," the Committee also asked (b)(6) and (b)(7)(C) to search all NMR accounts for any files with the fragment "bs" in their file names. (b)(6) and (b)(7)(C) found no such files attributable to Dr. Sezen. (b)(6) and (b)(7)(C) 28:17).

time of each login to and each logout from the NMR software. (b)(6) and (b)(7)(C) has searched these log files for the username "bengu" and "sezen"; no matches were found. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C)

In addition, the Committee obtained from the Department of Chemistry's Business Office monthly reports created by (b)(6) and (b)(7)(C) to document NMR usage charges. As discussed above, the NMR Facility charges for each hour of usage of NMR spectrometers. These charges ranged from $10 to $15 per hour over the years of Dr. Sezen's work in the (b)(6) and (b)(7)(C). (Exhs. DD2-DD7). Each month, (b)(6) and (b)(7)(C) provides the Business Office with data showing the time accrued by each professor's group and, within that group, by each individual user. (b)(6) and (b)(7)(C) The Committee obtained copies of all of the Business Office's NMR usage records for the years 2000-2005. (Exhs. DD2-DD7). Although these records document charges for other (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) members, they make no reference to any charges to any account for Dr. Sezen. The account names do not include "bengu," "sezen," or a combination of the two. In addition, the financial records do not list any login names that are not linked to known members of the (b)(6) and (b)(7)(C) as recorded in (b)(6) and (b)(7)(C) logbook.

(b)(6) and (b)(7)(C) knows of no other student who, at least since 1997, has completed a doctorate in a field of chemistry that requires acquisition of NMR spectra but has not had an authorized account to use the NMR facility.[52] (b)(6) and (b)(7)(C) The failure to obtain an authorized account is a major departure from standard practice.

[52] Before 1997, students did not need logins and passwords to access the computers in the NMR facility. Students thus performed NMR spectroscopy and graduated without having accounts. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C)

2. Dr. Sezen Used the Accounts of Other Members of the (b)(6) and (b)(7)(C)

The Committee finds that Dr. Bengü Sezen accessed the NMR spectrometers by using the accounts of at least (b)(6) and (b)(7)(C). The following testimony and evidence are relevant to this question:

1. Spectra published in Dr. Sezen's thesis and publications were found in the (b)(6) and (b)(7)(C) accounts, belonging to (b)(6) and (b)(7)(C) respectively.

2. (b)(6) and (b)(7)(C) left the (b)(6) and (b)(7)(C) in August 2002 and went to MIT as a (b)(6) and (b)(7)(C) in Fall 2002; (b)(6) and (b)(7)(C) has testified that she did not use her account after her departure. (b)(6) and (b)(7)(C) Nonetheless, the accounting software shows that (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) account was repeatedly used from that time until (b)(6) and (b)(7)(C) closed the account in September 2004. (Exh. N12 at 007155). In addition, the Department of Chemistry's records reflect that the (b)(6) and (b)(7)(C) was charged for NMR usage attributed to (b)(6) and (b)(7)(C) account between Fall 2002 when (b)(6) and (b)(7)(C) left Columbia and September 2004 when the account was closed. (*See, e.g.*, DD6, DD7, 006998, 007046, 007060, 007076, 007078, 007081).

3. The sign-up sheets for the 400 MHz NMR spectrometer have been compared with the accounting system logs. Approximately three quarters of the logins to (b)(6) and (b)(7)(C) account recorded by the accounting system after (b)(6) and (b)(7)(C) left Columbia University occur at times when Dr. Sezen signed up for access on the sign-up sheets. (Exh. NN2).

4. The data directories in the (b)(6) and (b)(7)(C) accounts on the 400 MHz spectrometer and the narrow-bore 300 MHz spectrometer (Exh. N18) contain numerous data sets acquired after (b)(6) and (b)(7)(C) left the (b)(6) and (b)(7)(C). The names of many of these data sets are those of chemical compounds used by Dr. Sezen in her research.

5. (b)(6) and (b)(7)(C) testified that Dr. Sezen knew his password and that of (b)(6) and (b)(7)(C) 21).

6. The sign-up sheets for the 400 MHz spectrometer have been compared with the accounting system logs showing usage of (b)(6) and (b)(7)(C) account. The comparison shows that after December 2002 (when (b)(6) and (b)(7)(C) left the (b)(6) and (b)(7)(C) account was used roughly 35% of the times that Dr. Sezen had signed up for access on the sign up sheets. (Exh. NN1).

7. (b)(6) and (b)(7)(C) testified that Dr. Sezen and (b)(6) and (b)(7)(C) both knew his password and used his account until he asked them to cease because so many files were accumulating in his data directory. In support of his testimony, the Committee identified a Zip disk among Dr. Sezen's research records (Exh. B39), which contains six original NMR data sets named using Dr. Sezen's convention for NMR data set names (*see* below at p. 62). In each data set directory, the NMR spectrometer software records the user name and file directories under which the spectrum was acquired in a file named *acqus*. In all six cases, this file identifies (b)(6) and (b)(7)(c) as the user and the "300nb," the narrow-bore 300 MHz spectrometer, as the NMR instrument. A comparison of the sign-up sheets for the wide-bore 300 MHz spectrometer and the accounting system logs shows that on 17 occasions, the (b)(6) and (b)(7)(c) was accessed when Dr. Sezen signed up to use the spectrometer. (Exh. NN3)

This evidence strongly suggests that Dr. Sezen knew the passwords to the NMR accounts belonging to (b)(6) and (b)(7)(C) and used these accounts to access the 400, narrow-bore 300, and wide-bore 300 NMR instruments[53] How Dr. Sezen learned the password to (b)(6) and (b)(7)(C) account has not been established. In her testimony, (b)(6) and (b)(7)(C) does not recall sharing her password with Dr. Sezen (although (b)(6) and (b)(7)(C) knew it). (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) testified that (b)(6) and (b)(7)(C) login name and password were posted on a

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(b)(6) and (b)(7)(C) testified that he did not believe that Dr. Sezen used his account after he transferred to the (b)(6) and (b)(7)(C) group, because (b)(6) and (b)(7)(C) only observed his own NMR spectra displayed when he logged into the NMR instrument. (b)(6) and (b)(7)(C) When a user starts the NMR spectrometer software, the program displays the NMR spectrum that was being displayed when the user last terminated the program. However, this feature of the software is easily circumvented by recording the name of the NMR data set that is displayed at login and then re-opening this data set prior to terminating the program.

wall in the (b)(6) and (b)(7)(c) however, (b)(6) and (b)(7)(C) and other group members could not verify this statement.

3. The Research Record

A. Standards of the Relevant Research Community

The Committee finds that the maintenance of accurate records of procedures and results is, as in other scientific disciplines, a standard principle of research in organometallic chemistry. Members of the (b)(6) and (b)(7)(C) stated that they understood that this principle governs their work in the (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C). A monograph on scientific notekeeping published by the American Chemical Society succinctly states, "The guiding principle for notekeeping is to write with enough detail and clarity that another scientist could pick up the notebook at some time in the future, repeat the work based on the written descriptions, and make the same observations that were originally recorded." (Kanare HM, *Writing the Laboratory Notebook*, American Chemical Society, 1985, p. 1).

(b)(6) and (b)(7)(C) explained that standard practice in his laboratory is to retain printouts of NMR spectra. He said that students also are encouraged to back up their data in electronic format. When members leave the group, they provide (b)(6) and (b)(7)(C) with hard copies of NMR data and, more recently, electronic copies of NMR data. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) Some members of the (b)(6) and (b)(7)(C) group, who joined as beginning graduate students, said that (b)(6) and (b)(7)(C) instructed them explicitly to keep a laboratory notebook and archival NMR spectra. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C). Other researchers, such as post-doctoral

scientists, who have had more experience, were assumed to already know these standard practices. (b)(6) and (b)(7)(C). Some individuals also described the importance of having a system to correlate NMR spectra and other data with laboratory notebook entries. (b)(6) and (b)(7)(C). Based on this testimony and its own expertise in good scientific practice, the Committee finds that an accepted practice of the relevant research community is to maintain research records, including detailed experimental procedures that correlate to archived raw data (*e.g.*, NMR spectra).

B. Dr. Sezen's Research Records

The Committee finds that Dr. Sezen did not meet the relevant research community's standards for maintaining research records. In support of this finding, the Committee has determined that Dr. Sezen's Research Record comprises NMR binders, laboratory notebooks, background research materials, CD-ROMs, and computer disks. (Sections A-D on the Master Index; Exhs. H9; H10A; H10B). As described below, these items comprise the entirety of Dr. Sezen's Research Record for her thesis and publications. The discrepancy between the results and procedures presented in the publications and thesis and the documentation in the Research Record is so large as to indicate that substantial numbers of the reported experiments were never performed as described in the publications and thesis.

In making this finding, the Committee recognizes that the sequestration of evidence in this case was difficult. As discussed above (b)(6) and (b)(7)(C) initiated the review of Dr. Sezen's research results by members of (b)(6) and (b)(7)(C) in July, 2005. The initial Allegation was made four months later, in November 2005, after (b)(6) and (b)(7)(C) with the aid of members of (b)(6) and (b)(7)(C) group, reviewed Dr. Sezen's Research Record in detail. The

Research Record was sequestered by Columbia's Director of Research Compliance and Training and Research Integrity Officer, (b)(6) and (b)(7)(C) during first week of April 2006. The Committee has taken these issues into consideration, as discussed below.

Dr. Sezen stated that, before she left Columbia in late July 2005, she packed all of her belongings in more than 20 boxes and left them in the (b)(6) and (b)(7)(C) on the second floor, so they could be moved with the rest of the Laboratory to (b)(6) and (b)(7)(c) Dr. Sezen stated that she did not have any inventory of these boxes or their contents. (Sezen Tr. at 38:4-39:15). After Dr. Sezen left Columbia, and in accordance with (b)(6) and (b)(7)(C) began investigating Dr. Sezen's work and reviewed Dr. Sezen's Research Records. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C). Dr. Sezen stated that when she briefly returned to the laboratory in late July 2005, during a layover between her trip to (b)(6) and (b)(7)(C), she saw that her boxes had been opened and her NMR binders and notebooks were dispersed around the laboratory. (Sezen Tr. at 40:5-18).

At the beginning of August 2005, the (b)(6) and (b)(7)(C) moved the laboratory from (b)(6) and (b)(7)(C) testified that employees of a professional moving company moved all of Dr. Sezen's boxes. (b)(6) and (b)(7)(C) He explained that in late August or early September, Dr. Sezen requested the return of some personal materials, including her computer and some books. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C); stated that, in response to Dr. Sezen's request, and with (b)(6) and (b)(7)(C) authorization, he, (b)(6) and (b)(7)(C) brought Dr. Sezen's personal items back to the second floor laboratory. That day, they advised Dr. Sezen that the materials were available in (b)(6) and (b)(7)(c) laboratory; by the next morning, all of

these materials had been removed. (b)(6) and (b)(7)(C) and (b)(6) and (b)(7)(C) testified that Dr. Sezen's research records and other materials were later repacked and delivered to (b)(6) and (b)(7)(C) The Committee believes with reasonable certainty that the University has sequestered all of the relevant Research Records.

1. **Laboratory Notebooks**

The Committee finds that Dr. Sezen's 11 laboratory notebooks labeled BS-I through BS-XI constitute the entire record of laboratory notebooks relevant to the research reported in Dr. Sezen's thesis and publications.

The laboratory notebooks are hard-bound notebooks with preprinted numbered pages. (Exhs. B1-B11). Although not every page is dated, BS-I begins with the date January 26, 2001. The last recorded date is June 9, 2003 and was found in BS-VIII. No dates are recorded in notebooks BS-IX to BS-XI. The notebooks contain few detailed experimental procedures for novel reactions performed by Dr. Sezen. The detailed procedures that are described in the notebooks most commonly are for reactions that were previously reported in the literature and used to prepare precursors or other reagents. Mainly, entries in the notebooks show a chemical equation, followed by a list of reagents and associated numbers that appear to be the theoretically calculated amounts of reagents, but not the amounts of the reagents actually used.[55] In large part, these entries do not show the sources of the reagents used or describe the experimental apparatus and how the experiments were conducted. They do not explain the steps by which reagents were

[54] As discussed above, this did not occur until the first week of April 2006, after Columbia's new Policy took effect.

(b)(6) and (b)(7)(C) disputed this characterization of the amounts of reagents, but the Committee was not convinced. (b)(6) and (b)(7)(C)

purified or characterized. They do not describe observations made during the course of reactions. They do not provide details about how products were separated from reaction mixtures and identified.

The absence of detailed procedures and records is especially unusual because, as (b)(6) and (b)(7)(C) explained in his interview (b)(6) and (b)(7)(C), reactions such as those studied by Sezen were thought to be especially sensitive to small changes in experimental protocol, such as exposure or lack of exposure to moisture and the exact method of purifying reagents. Members of the (b)(6) and (b)(7)(C) charged with reproducing Dr. Sezen's work testified that the notebooks provided little or no guidance for replicating Dr. Sezen's results, because they lacked detailed experimental procedures. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C). Several also stated that such limited information departed from standard data management practices. (*E.g.*, (b)(6) and (b)(7)(C)

In its September 23, 2006 letter to Dr. Sezen, the Committee noted that her notebooks did not document her experimental procedures, and asked Dr. Sezen whether these notebooks were the only ones that she used. In her October 5 response, Dr. Sezen stated that she had four additional notebooks, entitled BS-EXP-I – BS-EXP-IV, in which she recorded her experimental procedures. (Exh. J15; *see also* Sezen Tr., 21:19-25). Notebooks with these labels have not been located in Dr. Sezen's possessions or

[56] The reports prepared by members of the (b)(6) and (b)(7)(C) as part of their investigation also repeatedly discuss the absence of necessary documentation of reaction procedures and results in the notebooks. (Exhs. I1; I2; I5; I6; I7; I8; I10; I11; I13; I14).

elsewhere in the (b)(6) and (b)(7)(C) The Committee finds that Dr. Sezen's claim that she kept two sets of notebooks is not credible for the following reasons:

1. (b)(6) and (b)(7)(C) stated that although he reviewed Dr. Sezen's work, he never saw these additional notebooks. (b)(6) and (b)(7)(C)
2. When questioned, members of the (b)(6) and (b)(7)(C) did not recall ever seeing such notebooks. (*See, e.g.*, Exh. J19; Exh. J20; (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C)
3. None of the entries in the notebooks entitled BS-I – BS-XI refer to any other notebooks, as would be expected if such notebooks existed and contained detailed experimental protocols relevant to the research documented in BS-I – BS-XI. In her testimony, Dr. Sezen states that she kept the second set of notebooks so she did not need to write detailed experimental protocols each time she ran a particular reaction. (Sezen Tr. at 22:4-11). However, each successive iteration of a particular reaction procedure in notebooks BS-I to BS-XI refers to an earlier reaction within the same notebooks; BS-I – BS-XI contain no reference to another set of notebooks. If the other notebooks existed, a cross-reference to earlier reactions within the notebooks BS-I – BS-XI would be superfluous. Dr. Sezen's claim that she entered cross-references only into the allegedly missing notebooks BS-EXP-I to BS-EXP-IV is not plausible. (*Id.* 23:15-23).

Finally, some witnesses from (b)(6) and (b)(7)(C) group stated that separating the experimental procedures from the documentation of the reactions themselves, rather than following the usual practice of maintaining a single, linear record, would be illogical. (b)(6) and (b)(7)(C) (describing his notebook-keeping practice); (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) In light of the above evidence, the Committee does not credit Dr. Sezen's claim that she documented her experimental procedures in four additional notebooks.

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[57] After receiving Dr. Sezen's October 5 letter, (b)(6) and (b)(7)(C) went to the (b)(6) and (b)(7)(C) and searched all six laboratory rooms, the (b)(6) and (b)(7)(C) conference room, the Group's administrative assistant's office, and (b)(6) and (b)(7)(C) office. No research records belonging to Dr. Sezen were found.

2. Archival NMR Spectra

The Committee finds that Dr. Sezen's six NMR binders and one Zip disk sequestered in this case constitute the entire record of original NMR spectra relevant to Dr. Sezen's thesis and publications.

Until recently (and during the time period relevant here), NMR data sets were periodically erased from the NMR spectrometer disks because insufficient disk space was available for long-term archival storage. (b)(6) and (b)(7)(C) Over the years, an evolving set of backup mechanisms existed for NMR spectroscopic data, including tape drives, Zip disks, CD-ROMs, and DVDs. (*Id.* at 30:3-9). (b)(6) and (b)(7)(C) has testified that users were provided information about electronic backup during the training process, but that each user was responsible for backing up his or her data. (*Id.* at 29:22-25). Members of the (b)(6) and (b)(7)(c) more commonly printed the processed NMR spectrum on 11"x14" paper and stored these printed pages in large "NMR binders" as archival records. (b)(6) and (b)(7)(C) members have only recently begun extensively using electronic backups.

Dr. Sezen's six NMR binders consist of collections of printed NMR spectra bound in standard-issue, red, three-ring binders. (Exhs. A1-A6). In addition to the spectra, the binders contain copies of published articles and other relevant literature, predicted NMR spectra produced by a software package named ChemDraw, combustion analysis results, and Dr. Sezen's notes. These additional materials are inserted into the binders in clear plastic pouches.

In her October 5, 2006 letter, Dr. Sezen stated that she had 14 NMR binders in total; in her testimony, she stated that she had 18 binders in total. (Exh. J15 at 012414; Sezen Tr. at 35:19). Although those individuals interviewed by the Committee had

differing estimates of how many NMR binders Dr. Sezen possessed (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C), no individual recalled seeing as many as 14 to 18 NMR binders. Moreover, as one witness noted, so many NMR binders would have taken up a noticeable amount of shelf space in the (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) which no witness recalled. (b)(6) and (b)(7)(C)

Nearly all reactions described in Dr. Sezen's notebooks (Exhs. B1-B11) record a code for NMR spectra in the format BS-YY-ZZZ, in which YY refers to the number on the spine of the laboratory notebooks labeled BS-I to BS-XI, and ZZZ refers to a particular page number within the notebooks. However, the printed NMR spectra in the six NMR binders, as well as the spectra provided in her thesis, published papers, and Supporting Information to published papers, are labeled at most only with the chemical name of the compound whose NMR spectrum is shown. The spectra are not labeled with either a date or a code number in the above format. Thus, the spectra in the binders cannot be linked to any specific reaction described in Dr. Sezen's notebooks. For example, stoichiometric and catalytic reactions to produce phenyl pivaloyl pyridine are repeated numerous times in Dr. Sezen's notebooks. (*see* BS-III-230, BS-III-232, BS-III-234 for examples of stoichiometric reactions and BS-III-272 and BS-III-276 for examples of catalytic reactions. Many more instances are listed in notebooks BS-III and BS-IV). The NMR spectra of this product in her NMR binders (Exh. A2F at 0001532-0001539) contain no information that would indicate which of these many reactions produced the samples from which the NMR spectra were created.

Dr. Sezen states in her testimony that the spectra in the six binders that are in possession of the Committee do not contain her code numbers because these spectra were

intended to document the identities of purified samples for publication. (Sezen Tr. at 37:6-13). This statement is not supported by the evidence: the binders contain NMR spectra that are not of publication quality and are not identified in any specific manner, even with a compound name. Essentially, Dr. Sezen claims that all of the binders containing spectra that were properly labeled have disappeared. The Committee finds that Dr. Sezen's last-minute claim that she had eight to twelve additional NMR binders that contained all of her properly labeled spectra is not credible.

Even though Dr. Sezen's NMR spectra are not labeled with code numbers to match her notebook entries, in some cases, the Committee was still able to match spectra in Dr. Sezen's NMR binders to spectra published in Dr. Sezen's thesis and publications. NMR data are reported in Dr. Sezen's thesis and in the Supporting Information of her papers in two ways. First, ^{1}H and ^{13}C spectroscopic data for individual compounds are presented in tabular form. These tables list the resonance frequencies, multiplet patterns, and coupling constants observed in the ^{1}H NMR spectra and the resonance frequencies observed in the ^{13}C NMR spectra. Second, ^{1}H NMR spectra of individual compounds are reproduced by scanning and reducing the printed spectra stored in the NMR binders. Usually, ^{1}H spectra are provided for only a subset of the compounds whose spectroscopic data are reported in tables. Although the printed spectra stored in the NMR binders do not contain identification codes beyond the names of the compounds, resonance frequencies are printed across the top and peak integrals are printed across the bottom of the spectra for individual resonances. These frequencies and integrals are reported to very high precision (typically 0.01 and 0.001 respectively). Thus, in many cases, a spectrum reported in the thesis or publication can be matched to a spectrum in the NMR

binders or spectrometers by an exact equivalence between the frequencies and integrals reported on the spectra in each location. As discussed further below, however, no supporting NMR data have been located in Dr. Sezen's NMR binders for many products described in her publications.

3. Electronic Research Records

The Committee finds that the electronic research records sequestered in this case, including 29 zip disks, 22 floppy disks, and four CD-Roms (Exhs. B13-B56), constitute the entirety of Dr. Sezen's electronic research records.

The 29 zip disks and 22 floppy disks include both labeled and unlabeled disks; however, even the labeled disks contain only minimal, handwritten descriptions of the contents. Some descriptions, like "Bengu Supp. Info. JACS 2002" and "Ref. Spectra" suggest that the data included is related to Dr. Sezen's work, while other descriptions, like "Class 68148 Fall 2001," appear not to include research records. Some disks contain no description at all, or only numbers like "1" and "2." Two floppy disks (Exhs. B50 and B52) contain the scanned electronic versions of printed NMR spectra that were used for publication.

The four CD-Roms are labeled "Bengu's Laptop Backup," "Bengu's Desktop," "Bengu GC-MS Data," and "Bengu HPLC Data." (Exhs. B21-B23). According to (b)(6) and (b)(7)(C) these CD-Roms are the only CD-Roms Dr. Sezen provided him before she left the laboratory. (b)(6) and (b)(7)(C) stated that he believed that these CDs contained the relevant back-up data for Sezen's thesis and publications. (*Id.*, 50:25-51:6). The directories for these CDs are attached as Exh. J34 at 012492-012708. In addition, members of the (b)(6) and (b)(7)(C) downloaded to CD-ROM

data belonging to Dr. Sezen that they found on the (b)(6) and (b)(7)(C) computer GC and HPLC instruments. (Exh. H9; H10A; H10B). The Committee Chair Prof. (b)(6) and (b)(7)(C) reviewed these electronic materials. Most of the disks reviewed did not contain any data, or were unreadable on both Macintosh and PC computers.[58]

Finally, the Ad Hoc Committee has been able to locate only six electronic NMR data sets named with the coding scheme used in the laboratory notebooks. These data sets are stored on a Zip disk, entitled simply "3." (Exh. B39). Exhibit B39 includes six data sets that originated in the NMR account of (b)(6) and (b)(7)(C) These data sets are labeled: BS-IV-120, BS-IV-122, BS-IV-130, BS-IV-132, BS-IV-134, and BS-IV-136. (Exh. B39). Although the disk has the capacity to store 100 MB of data, these six data sets – about 10 MB of data – are the only data on the disk. These same data are the only NMR data sets that were found on the (b)(6) and (b)(7)(C) Computer that are attributable to Dr. Sezen. (Exh. H9). Other than these data, no other raw NMR data sets were found in Dr. Sezen's electronic materials.[59] The Committee finds that, like most other members of the (b)(6) and (b)(7)(c) (b)(6) and (b)(7)(c) at that time, Dr. Sezen did not back up her electronic data sets electronically (except for the data sets from (b)(6) and (b)(7)(C) directories backed up at (b)(6) and (b)(7)(C) request).

In her October 5 letter, Dr. Sezen claimed that several additional electronic records exist, including: (1) 18 disks containing NMR spectra; (2) 7 CD-Roms containing GC-MS spectra; and (3) 4 CD-Roms containing HPLC spectra. (Exh. J15 at 012415). However, no other individual recalled seeing any such items. (Exhs. J19-J20;

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[58] The CD-Roms prepared by the (b)(6) and (b)(7)(C) contained some additional GC and MS data that are coded consistently with entries in Dr. Sezen's notebooks. (Exh. H10A and H10B).

[59] The spectra in these electronic files have not been locatable in the NMR binders because the hardcopy printouts are not labeled with the identification codes, as noted above. The laboratory notebooks pages BS-IV-120, BS-IV-122, BS-IV-130, BS-IV-134 described reactions to produce phenyl pivaloyl pyridine. The spectra are not identical to the spectra of the reaction product phenyl pivaloyl pyridine located in the NMR binders (Exh. A2F at 001532-001539) and may be spectra of crude reaction mixtures.

(b)(6) and (b)(7)(C). Although Dr. Sezen preserved in her possession a substantial number of other documents related to her research – including hard copies of close to 1,000 pages of her manuscripts with handwritten comments by (b)(6) and (b)(7)(C) (Exh. J31) – she does not appear to have preserved any copies of the electronic materials she disclosed on October 5. In light of these facts, the Committee does not credit Dr. Sezen's claim to have created these electronic archives of her research records.

4. Combustion Analysis Records

According to the Experimental Sections in Dr. Sezen's thesis, all combustion analyses for her thesis were conducted by an outside analytical laboratory company, the (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) (Exh. K1 at pp. 35 (05931), 109 (06005), 307 (06202), 391 (06285) and 453 (06347). A search of Dr. Sezen's NMR binders turned up documentation for only two combustion analyses performed by (b)(6) and (b)(7)(C) (Exh. A3A at 001619-001620; Exh. A5A at 002448-002449) and no documentation for analyses performed by any other company. No other records of results of combustion analyses, by (b)(6) and (b)(7)(C) or by any other analytical laboratory, were found among Dr. Sezen's notebooks or files. No results of such analyses were found recorded in Dr. Sezen's eleven research notebooks.

The Committee asked the Department of Chemistry Business Office ("Business Office") to identify any laboratories that provided combustion analysis services to the Department of Chemistry. The Business Office identified four laboratories: (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) (Exh. O1). The Committee then asked the Business Office to search the University's computerized accounts payable system ("AP/CAR") for all invoices charged to the

(b)(6) and (b)(7)(C) by these four laboratories. (Exh. O1). This search located two invoices (b)(6) and (b)(7)(C), from 2003 and 2004, addressed to former (b)(6) and (b)(7)(C) member (b)(6) and (b)(7)(C) Exh. O2 at 000786, 000790), and 11 invoices from (b)(6) and (b)(7)(C)

Of the 11 invoices, three date from September 2005 through May 2006, after Dr. Sezen left the (b)(6) and (b)(7)(C) (Exh. O2 at 000817-000827). The remaining 8 invoices range in date from January 2004 through April 2005. (Exh. O2 at 000795-000815). Five were addressed to Dr. Sezen (Exh. O2 at 000802, 000805, 000808, 000810, 000812).[60] One was addressed to another (b)(6) and (b)(7)(C) member, (b)(6) and (b)(7)(C) (000815, in the amount of $104.00). Finally, one invoice was addressed to (b)(6) and (b)(7)(C) (Exh. O2 at 000796, for $156.00), and one to (b)(6) and (b)(7)(C) (*Id.* at 000799, for $188.00).[61] .

Because the AP/CAR system does not store records for more than two fiscal years, the Committee asked Columbia's central Accounts Payable Department to carry out a similar search for all earlier records of invoices charged to the (b)(6) and (b)(7)(C) by the same four companies. (Exh. O1). That Department provided data for the period 2001 through June 2004. During that period, the (b)(6) and (b)(7)(C) was charged for twelve transactions. As shown on the spreadsheet provided by Accounts Payable, two of these transactions were with (b)(6) and (b)(7)(C) and the remaining ten transactions were with (b)(6) and (b)(7)(C) (Exh. O10 at 013523)

Accounts Payable was able to locate invoices for eight of these twelve transactions, including the two (b)(6) and (b)(7)(C) transactions. These documents show that

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[60] Although invoice detail for one invoice, 000810, was not available from AP/CAR, the Committee was able to confirm through (b)(6) and (b)(7)(C) records that this invoice was addressed to Dr. Sezen.

[61] (b)(6) and (b)(7)(C) was a member of the (b)(6) and (b)(7)(C) this invoice appears to have been mistakenly charged to the (b)(6) and (b)(7)(C)

the two (b)(6) and (b)(7)(C) transactions are two of the same transactions that were identified by the AP/CAR search. (Exh. O4 at 010702, 010703). The six (b)(6) and (b)(7)(C) invoices list as "contacts," (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C)

In January 2006, as part of the (b)(6) and (b)(7)(C) investigation into the reproducibility of Dr. Sezen's results, (b)(6) and (b)(7)(C) and requested copies of data previously reported to the (b)(6) and (b)(7)(C) (Exh. O3 at 006370-006392).[62] These reports correspond to the purchase order numbers in the AP/CAR and Accounts Payable records. In other words, for each transaction with (b)(6) and (b)(7)(C) recorded by Columbia University's financial offices, the corresponding documentation and data provided by (b)(6) and (b)(7)(C) has been identified. Dr. Sezen confirmed that she requested two of these analyses. (Exh. J2 at 05512).

In her October 5, 2006 letter, Dr. Sezen claims to have had an entire binder of combustion analysis reports; in her interview, she stated that she obtained a "huge, huge number" of combustion analyses. (Sezen Tr., 62:7-10; Exh. J15 at 012416). However, Columbia's AP/CAR and Accounts Payable records show only a small number of requests for combustion analyses. Dr. Sezen claimed that in some instances, her samples were submitted to (b)(6) and (b)(7)(C) under another student's name. (Sezen Tr. at 61:22-62:6). In the documentation provided by (b)(6) and (b)(7)(C) however, results addressed to other students do not include data for Dr. Sezen's experiments.

Dr. Sezen further claims that she obtained many analyses as free trials from as many as 25 vendors. (Sezen Tr. at 62:18-63:13; Exh. J15 at 012416). She has produced no records corresponding to these analyses. Moreover, the Committee contacted some of

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(b)(6) and (b)(7)(C) later provided two additional reports (Exhs. O9 and O11).

the companies Dr. Sezen mentioned and was told that these companies had no record of any combustion analyses conducted for Columbia University, and that these companies did not provide free services. (Exh. J5). Also, the Committee considers it implausible that a busy student in the (b)(6) and (b)(7)(C) would expend significant time trying to obtain free combustion analyses because the cost of elemental analysis is relatively low, and (b)(6) and (b)(7)(C) was well-funded. Finally, even if these companies had provided the analyses, those analyses were not the basis for Dr. Sezen's published work: the Experimental Sections in Dr. Sezen's thesis repeatedly state that "combustion analyses were performed by (b)(6) and (b)(7)(C) (Exh. K1 at pp. 35 (05931), 109 (06005), 307 (06202), 391 (06285) and 453 (06347).[63]

Accordingly, the Committee finds that Exhibits O3, O9 and O11 reflect the totality of (b)(6) and (b)(7)(C) records of combustion analyses conducted at the (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) request during Dr. Sezen's tenure. The Committee does not credit Dr. Sezen's claim to have obtained other analyses from other laboratories. The evidence demonstrates that the binder containing a large number of reports of combustion analyses, described by Dr. Sezen in her October 5 letter, does not and never did exist.

The absence of substantial numbers of combustion analyses is particularly noteworthy because Dr. Sezen has repeatedly claimed, in her critiquing of efforts to reproduce her work by other members of the (b)(6) and (b)(7)(C) that combustion analyses need to be performed for each catalyst prepared for these reactions. (*See, e.g.*, Exh. T at 012345; Exh. J2 at 05179; *see also* Sezen Tr. at 59:14-19). Her notebooks and other Research Records record no such analyses. The absence of combustion analyses, beyond

[63] Dr. Sezen's published papers and Supporting Information that report elemental analyses are silent as to which company provided the reported combustion analysis results.

these few identified as described above, suggests that many of the reactions recorded in her laboratory notebooks were never performed.

4. The Committee's Findings Concerning Allegation No. 1: Whether Dr. Sezen fabricated NMR spectra in her thesis and publications

A. Identification of Fabricated Spectra

The Committee identified multiple NMR spectra in Dr. Sezen's thesis and publications as fabricated, including spectra in the Supporting Information for the publications:

1.

5.

(b)(6) and (b)(7)(c)

6.

and in the corresponding Chapters 1, 5 and 6, respectively, in the thesis of Dr. Bengü Sezen. (Exh. K1 at 05897-05971, 06090-06168, 06245-06330). These fabricated spectra are reported in papers that range from Dr. Sezen's initial first-author paper from the (b)(6) and (b)(7)(C) in 2002 to her final first-author paper in 2005. Notably, the spectra identified as fraudulent in Chapters 1 and 6 were not previously identified as fraudulent either by members of the (b)(6) and (b)(7)(C) or by the initial Inquiry Committee. Rather, these fraudulent spectra were identified by the present Committee in the course of its work.

Furthermore, the Committee cannot state with confidence that these are the only fabricated spectra in the thesis.[64]

B. Fabrication of NMR spectra

When (b)(6) and (b)(7)(C) learned, through conversations with (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) that Dr. Sezen did not have an NMR account, they, with (b)(6) and (b)(7)(C) assistance, searched the user accounts of other members of the (b)(6) and (b)(7)(C) to see whether data files in other accounts might contain Dr. Sezen's missing data. Their attention was drawn to data sets in the user account (b)(6) and (b)(7)(C) originally belonging to (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) because the account contained data sets that appeared unusual. First, the data sets were recorded after (b)(6) and (b)(7)(C) had left Columbia University. Second, some of the data sets were named according to chemical compounds used in Dr. Sezen's research. Third, some of the data sets contained an unusually large number of processed data files (*see* Exh. N18). The contents of data sets with large numbers of processed files suggested to them that these data sets recorded sequential steps in the construction of fraudulent NMR spectra.

Before considering evidence that these NMR spectra were fabricated, we briefly describe a method by which fabrication can be accomplished and a relevant feature of proton NMR (^{1}H NMR) spectra, *e.g.*, the coupling between carbon and hydrogen nuclei. To first approximation, a ^{1}H NMR spectrum consists of a series of resonances for groups of magnetically equivalent ^{1}H nuclei. A resonance may be split into additional lines ("a multiplet") because nearby ^{1}H nuclei interact (or are "coupled"). One approach to generating synthetic spectra begins with an authentic NMR peak or peaks and uses the

[64] In one report, (b)(6) and (b)(7)(C) identified other potentially fabricated spectra. (b)(6) and (b)(7)(C) Because Dr. Sezen's records did not include spectra for this compound, the Committee could not verify whether the results she reported were fraudulent.

standard software programs on NMR spectrometers to carry out such operations as the following:

1. duplicating a spectrum containing a single resonance line;
2. rescaling the intensity of the duplicated spectrum;
3. shifting the duplicated spectrum right or left to shift the apparent resonance frequency;
4. adding the duplicated spectrum to the original.

In this way, a spectrum consisting of only a single line can be transformed into one that has two resonance lines with apparently different frequencies and intensities. When iterated, this process can generate a spectrum of any complexity.

This procedure requires the user to know the locations of the resonance peaks. These locations can be estimated in a number of ways. One approach, mentioned above, is to use commonly available software programs, such as ChemDraw, to predict resonance frequency for any chemical structure. Dr. Sezen's NMR binders contain numerous examples of ChemDraw predicted NMR resonance frequencies for compounds appearing in her thesis. Another approach is to use lists of NMR resonance peak frequencies of previously synthesized compounds reported in publications in the chemical literature. A final approach uses recorded spectra of compounds that are related to the target compound, such as reaction precursors.

The resonances in ^{1}H NMR spectra are split into multiplets not only because ^{1}H nuclei couple with other ^{1}H nuclei, as noted above, but because ^{1}H nuclei also couple with ^{13}C (or other NMR-active) nuclei to which they are attached. The intensities of the multiplets (in this case doublets) resulting from C-H couplings are very small because ^{13}C constitutes only 1.1% of natural carbon. These small doublets are commonly called satellite peaks because they symmetrically straddle the large peaks produced by ^{1}H nuclei

attached to the more abundant ^{12}C nuclei. The distance in Hertz (Hz) between the pair constituting a satellite is called the C–H coupling constant and is designated $^{1}J_{CH}$.

The methods for fabricating synthetic ^{1}H NMR spectra described above can be used to include satellite peaks, but someone fabricating a spectra might not pay attention to the satellites for three reasons. First, the intensities of the satellites are very small, and the satellites are therefore easily overlooked. Second, non-specialist users of NMR spectroscopy may not know the proper magnitudes of C-H couplings. Third, great effort is required to place these many small peaks in the spectrum. Knowing this, (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) suggested to members of the (b)(6) and (b)(7)(C) that they inspect the satellite peaks in the NMR spectra in the (b)(6) and (b)(7)(C) The Committee adopted this approach and applied it to the NMR spectra shown in Dr. Sezen's thesis, NMR binders, and publications to determine whether they have the correct coupling constant magnitudes.

The Committee has established that Dr. Bengü Sezen's thesis and published papers contain a number of fraudulent NMR spectra. The bases for concluding that particular spectra are not authentic are described below.

(1) Chapter 5 and *JACS* 126, 13244 (2004)

As part of the initial investigation conducted by the (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) located in the directory belonging to the (b)(6) and (b)(7)(C) login account on the 400 MHz NMR spectrometer six NMR data sets that contained spectra found in the thesis of Dr. Sezen and in the Supporting Information for the paper *JACS* **126**, 13244 (2004). Another data set in the (b)(6) and (b)(7)(c) on the narrow bore 300 MHz NMR spectrometer, with name /300nb/data/rayane/nmr/PPh3, also contained spectra found in

the thesis and paper. The directory trees for the data found on the narrow-bore 300 MHz and 400 MHz NMR spectrometers are shown in Exh. N18.

These data sets evidence the progressive constructions of fabricated NMR spectra.[65] The final spectra were constructed by repeated application of the above procedure. Intermediate stages in the process were stored in different processed data directories (listed by number in the NMR spectrometer software). The progressive construction of the fabricated spectra is illustrated by Exh. N24, which shows data for (b)(6) and (b)(7)(c) Within this data set, 63 individual processed data sets are generated and sequentially added together to generate the final spectrum in process number 63. (Exh. K1 at 06241). Both methyl resonances in the final fabricated spectrum exhibit $^{1}J_{CH}$ scalar coupling constants of 177.6 Hz (measured using the NMR spectrometer software by (b)(6) and (b)(7)(C) These values of the coupling constants are those expected for methylene chloride and are not those expected for methyl groups chemically bonded to C, N, O, S, or Si atoms, which are known to have coupling constants <150 Hz. Notably, the file within this data set that contains the raw data acquired by the spectrometer prior to any Fourier transformation, when transformed, yields the NMR spectrum of methylene chloride, characterized by a singlet resonance at 5.3 ppm and ^{13}C satellites with a coupling constant of 177.6 Hz. These results demonstrate that the NMR spectrum of methylene chloride, a common solvent, was used to construct the fabricated spectrum. The final spectrum in process number 63 is identical, as judged by appearance, peak resonance frequencies and peak integrals, to the spectrum identified on page 347 of the thesis (*Id.*) and page S34 of the Supporting Information of the paper as that of

[65] Dr. Sezen does not dispute that these spectra are fabricated. (*E.g.*, Exh. T at 012340; Sezen Tr. at 51:7-18; 58:17-23). However, as discussed below, Dr. Sezen does deny that she produced fraudulent spectra and that they match spectra in her publications.

compound 21. (Exh. K9 at 05847). The UNIX software records the last modification date of the final spectrum file, (b)(6) and (b)(7)(c) to be June 12, 2004.

The ^{13}C satellite peaks of the methyl resonances of compound 21 (at 0.06 and 0.89 ppm) are easily seen on the spectra on page 347 of the thesis (Exh. K1 at 06241) and page S34 of the Supporting Information of the paper. (Exh. K9 at 05847). The frequencies of these satellite peaks are displayed above the spectrum. For the resonance centered at 0.06 ppm, the satellites have frequencies of 109.9 Hz and −67.70 Hz, giving by difference $^{1}J_{CH} = 177.6$ Hz. For the resonance centered at 0.89 ppm, the satellites have frequencies of 442.93 Hz and 265.33 Hz, giving by difference $^{1}J_{CH} = 177.6$ Hz.

(b)(6) and (b)(7)(C) as part of the initial investigation by the (b)(6) and (b)(7)(C) described in his report to the Inquiry Committee dated June 8, 2006, (Exh. I16), synthesized compound 21 by an independent procedure that had been published in *Synlett*. (2001) **11**, 1808-1810. The ^{1}H and ^{13}C one-dimensional and COSY and HSQC two-dimensional NMR spectra of the authentic compound 21 obtained by (b)(6) and (b)(7)(C) differ substantially from those reported by Dr. Sezen in the thesis and in the Supporting Information to the paper. Significant differences between the ^{1}H NMR spectrum of the authentic material and the spectrum reported by Sezen are the following:

1. The methyl resonances at 0.12 and 0.92 ppm in the authentic compound show $^{1}J_{CH}$ scalar coupling constants of 118.4 and 124.8 Hz, in accord with expected values and clearly not 177.6 Hz;

2. The resonances of the two H-3 nuclei are given in the table on page 327 of the thesis (Exh. K1 at 06221) and S16 of the Supporting Information (Exh. K9 at 05829) as multiplets with frequencies 2.06-2.19 and 2.27-2.39 ppm. In the authentic spectrum, these signals are doublets of doublets whose frequencies, 2.96-3.01 ppm, are nearly a part-per-million downfield from these positions;

3. The resonances of the H-1 and H-3 nuclei are extremely complex multiplets in the spectrum shown on page 347 of the thesis (Exh. K1 at 06241) but are the expected doublets of doublets in the spectrum of the authentic compound. The methylene

protons at both positions are coupled to each other, with a large $^2J_{HH}$ ca. 17 Hz, and to the H-2 nucleus, with a smaller $^3J_{HH} < 6$ Hz; these values of the coupling constants are consistent with expected chemical trends.

The NMR spectra for compounds 1, 7, 9, and 10 in the thesis and publication also appear to have been fabricated from the spectrum of methylene chloride by the same procedure as that used for compound 21. The ^{1}H NMR spectra of each of these compounds could be found on the (b)(6) and (b)(7)(C) account on the 400 MHz instrument, and (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) has determined that the satellite resonance peaks in these specta are separated by 177.6 Hz, the expected value for methylene chloride. ((b)(6) and (b)(7)(C)). The resonance frequencies and integrals of these spectra on the NMR instrument are identical to those of the spectra published in the thesis and paper. These identities establish that the spectra in the thesis and publication correspond to the fabricated spectra found on the NMR spectrometer.

The ^{1}H NMR spectrum of compound 12 also was fabricated on the NMR spectrometer by the procedure described above, but in this instance (b)(6) and (b)(7)(C) identified the spectrum as having been fabricated in four steps from the spectra of two known compounds, 3-bromo-1-TIPS-indole and pyrroline. (b)(6) and (b)(7)(C) (Exh. I4A)). The spectrum of 3-bromo-1-TIPS-indole was recorded on June 23, 2004 and the final spectrum was generated on June 26, 2004.

The Committee identified fabricated NMR spectra on the (b)(6) and (b)(7)(C) account on the 400 MHz spectrometer, and matched them to spectra presented by Dr. Sezen in her thesis and paper, as shown in Table 1. The spectra from the (b)(6) and (b)(7)(C) account are included as Exhs. N15 and N17.

Table 1. Fabricated spectra in Chapter 5 and *JACS* (2004) **126**, 13244

Compound Number		Page References to NMR Spectroscopic Data in Thesis (Exh. K1)		400 MHz NMR
Thesis, Chapter 5	JACS	Tabular data	^{1}H Spectrum	data set name
1	1	p. 311 (06206)	p. 342 (06236)	/1
7	7	p. 314 (06209)	p. 344 (06238)	/2
9	9	p. 315 (06210)	p. 343 (06237)	/3
10	10	p. 316 (06211)	p. 345 (06239)	/4 and /5
12	12	p. 318 (06213)	p. 346 (06240)	/Br-TIPS-indole
21	21	p. 327 (06221)	p. 347 (06241)	/6

Sezen's thesis and the publication in *JACS* (2004) **126**, 13244 do not show the NMR spectra of many of the products reported in the publication; only tabular data are presented. Critically, NMR spectra of compound 23 are not shown in the thesis or paper, and these spectra have not been located in Dr. Sezen's NMR binders. Absence of these data is particularly critical because the reaction to produce compound 23 was the one highlighted in the abstract that constitute the journal's table of contents, and it was cited by Dr. Sezen in her rebuttal to the preliminary Inquiry report. (Exh. T at 012350). She stated on page 11 of the rebuttal, "There is no other way to make the second product [compound 23] by known chemical methods than the currently discussed methodology." Dr. Sezen has not produced any evidence in her thesis, publication, or Research Record that documents her having synthesized this compound. In addition, in her response to the Inquiry Report, Dr. Sezen said that (b)(6) and (b)(7)(C) statement that they could not repeat this and related experiments is invalidated by their inability to prepare the catalyst she found to work the best, $RhCl(CO)(PFur_3)_2$. Dr. Sezen said that unless (b)(6) and (b)(7)(C) could provide the NMR spectra and elemental analysis of this and another catalyst, "[he] cannot claim that they had prepared these catalysts in pure form

and thus they cannot claim that they had performed the catalysis reactions," and maintained that "these analyses … must be performed routinely each time the catalyst is made." (Exh. T at 012345). However, no evidence supports that Dr. Sezen ever made the catalyst either (*see* pp. 102-105 and Table 7 below).[66]

Page 333 of the thesis (Exh. K1 at 06227) and page S21 of the Supporting Information (Exh. K9 at 05834) of the paper show a figure consisting of a composite of four ^{31}P NMR spectra. The spectra shown in this figure are identical to the spectra shown in the White-out Spectrum found in Dr. Sezen's NMR binders (discussed above) except for minor changes in the labels.[67] The Committee also found in Dr. Sezen's NMR binders (Exh. A3B at 001621-001622) additional versions of the figure with labels that have features of both the published spectra and the White-out Spectrum. These findings support the reasonable conclusion that multiple versions of the figure were prepared prior to the preparation of the version that was ultimately published.

In addition, the individual spectra that make up the composite figure are identical, except for the peaks that have been whited-out, to the spectra found in the (b)(6) and (b)(7)(C) account on the narrow-bore 300 MHz NMR spectrometer, /300nb/data/rayane/nmr/PPh_3, and to spectra found in Dr. Sezen's NMR binders (Exhs. A3C and A3D). The data on the spectrometer clearly show that these spectra also were fabricated by the procedure described above, in this case from the authentic spectrum of PPh_3. The sample of PPh_3 that was used for this purpose appears to have been contaminated with Ph_3PO, the oxidation product of PPh_3, and the small peaks generated from this contaminant are the

[66] Moreover, Dr. Sezen's objection that (b)(6) and (b)(7)(C) used the commercially available catalyst, $RhCl(CO)(PPh_3)_2$, is invalidated by her published claim that this catalyst is effective. (Exh. K8 at 05710).
[67] The labels also differ between the spectra published in the Supporting Information and in Dr. Sezen's thesis.

ones removed with White-out on the White-out Spectrum. The fabricated spectra were produced on June 25, 2004.

(2) **Chapter 6 and *JACS* 127, 5284 (2005)**

The principle reaction of interest in Chapter 6 and in *JACS* **127**, 5284 (2005) is the arylation of *N*-phenylpyrrolidine to produce 1,2-diphenylpyrrolidine, summarized in the dissertation in Tables 1 and 2 on pages 376 and 387 (Exh. K1 at 06270 and 06281) and in the publication in Tables 1 and 2 on page 5285. (Exh. K2 at 05709). The ^{1}H and ^{13}C NMR resonances of 1,2-diphenylpyrrolidine are summarized in a table on page 399 of the thesis (Exh. K1 at 06293) and on page S7 of the Supporting Information for the paper. (Exh. K3 at 05854). The ^{1}H NMR spectrum is displayed on page 433 of the thesis (Exh. K1 at 06327) and on page S30 of the Supporting Information. (Exh. K3 at 05877). Spectra for two deuterated analogues of 1,2-diphenylpyrrolidine are displayed on pages 434 (S31) (Exh. K1 at 06328; Exh. K3 at 05878) and 435 (S32) (Exh. K1 at 06329; Exh. K3 at 05879).

After the Committee received testimony that Dr. Sezen knew the password to (b)(6) and (b)(7)(C) computer account for the NMR facility, the Committee requested (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) to search the (b)(6) and (b)(7)(C) account on the NMR spectrometers for data sets with unusual numbers of processed subdirectories. (b)(6) and (b)(7)(C) located two such directories on the 400 MHz NMR spectrometer. One contains a fabricated ^{13}C NMR spectrum that does not appear in Dr. Sezen's thesis or publications. The other data set, named "CM-9-27-03," contains NMR spectra that have been identified as relevant to the present investigation. Three processed data sets within the CM-9-27-03 directory correspond to

the spectra shown in the thesis and Supporting Information of the paper and appear to have been fabricated.

The spectrum identified by process number 6 is identical to the spectrum on page 433 of the dissertation. (Exh. K1 at 06327). To six significant figures, peak positions are the same on the two spectra. Intensities of the peaks also are identical. (b)(6) and (b)(7)(C) reports that ^{13}C satellites of the peaks at ca. 0, 1.95, 4.7, 6.46, and 7.2 ppm have coupling constants of 177.6 Hz. The peak at 0 ppm, which should be that produced by the internal standard tetramethylsilane, not only shows an incorrect ^{13}C coupling constant (177.6 Hz rather than 118 Hz) but also fails to show satellite peaks, with a coupling constant of 6 Hz, that must be produced by the ^{29}Si isotope in tetramethylsilane. (Exh. N7).

The spectrum identified by process number 11 is nearly identical to the spectrum on page 434 of the dissertation. (Exh. K1 at 06328). To six significant figures, peak positions are the same on the two spectra. Intensities of the peaks also are identical. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) reports that ^{13}C satellites of the peaks at ca. 0, 3.4, 3.7, 4.7, and 6.45 all have coupling constants of 177.6 Hz. (Exh. N5 at 06555). The only significant differences between the spectra shown in the dissertation and Supporting Information and the spectrum in process 11 of the (b)(6) and (b)(7) account are that the former exclude the region beyond 8 ppm, and therefore do not show a peak at 13 ppm, and they do not show a peak at ca. 5.25, which is seen in the latter spectra.

The spectrum identified by process number 4 in the (b)(6) and (b)(7) account is nearly identical to the spectrum on page 435 of the dissertation. (Exh. K1 at 06329). To five or six significant figures, peak positions are the same on the two spectra. Intensities of the peaks also are identical. (b)(6) and (b)(7)(C) reports that ^{13}C satellites of the peaks at ca. 0, 1.96,

and 7.23 all have coupling constants of 177.6 Hz. The only significant differences between the spectra shown in the dissertation and Supporting Information and the one in process number 4 are that the former exclude the region beyond 8 ppm, and therefore do not show a peak at 13 ppm, and do not show a peak at ca. 5.7, which is seen in the latter spectrum.

The two missing peaks (at 5.25 and ca. 5.7) in the published spectra could easily have been removed either through electronic processing or by the use of White-out. Strong evidence that the spectra in the processed data sets and the thesis and publication are one and the same is provided by the equalities between the resonance frequencies and the intensities in the electronic files and in the published spectra.

Other evidence exists of fabrication, as well as plagiarism, in the generation of these NMR spectra. As shown in Tables 2 and 3, the resonance frequencies for 1,2-diphenylprrolidine reported in the table on page 399 of the dissertation (Exh. K1 at 06293) are identical to the figures recorded in a publication by Lewis *et al.* (*Can. J. Chem.* (1999) **77**: 595–604 (Exh. K30 at 013535)), a paper cited by Dr. Sezen in her thesis (p. 436, Exh. K1 at 06330) and publication (p. S29, Exh. K3 at 05876).

Table 2. NMR results from Dr. Sezen's thesis, page 399

^{1}H NMR data (400MHz, $CDCl_3$)		^{13}C NMR data (100MHz, $CDCl_3$)
H-1	3.38-3.46, 1H, m	23.1 (CH_2)
	3.69-3.74, 1H, m	36.1 (CH_2)
H-2 and H-3	1.92-2.04, 3H, m	49.1 (CH_2)
	2.36-2.43, 1H, m	62.9 (C-H)
H-4	4.72-4.76, 1H, d, J=8.7 Hz	112.3 (C-H)
H-5–H-7 and H-9		115.8 (2 C-H's)
	7.14-7.34, 7H, m	126.0 (C-H)
H-8	6.49-6.52, 2H, d, J=6.6 Hz	126.7 (2 C-H's)
H-10	6.63-6.67, 1H, t, J=7.3 Hz	128.5 (2 C-H's)
		129.0 (2 C-H's)
		144.6 (quat. C)
		147.2 (quat. C)

Table 3. NMR results from Lewis *et al.* (*Can. J. Chem.* (1999) 77, 595–604), page 603

N-*Phenyl-2-phenylpyrrolidine*
^{1}H NMR δ: 7.14–7.34 (m, 7H), 6.63–6.67 (dd, J = 7.3 Hz, 1H), 6.49–6.52 (d, J = 6.6 Hz, 2H), 4.72–4.76 (dd, J = 8.7 Hz, 1H), 3.69–3.74 (m, 1H), 3.38–3.46 (m, 1H), 2.36–2.43 (m, 1H), 1.92–2.04 (m, 3H).
^{13}C NMR δ: 147.2, 144.6, 129.0, 128.5, 126.7, 126.0, 115.8, 112.3, 62.9, 49.1, 36.1, 23.1.

However, the two lists of frequencies should not be identical because Lewis *et al.* recorded the NMR spectrum using a 300 MHz NMR spectrometer, whereas Sezen stated that she used a 400 MHz spectrometer. A 400 MHz instrument would show couplings, when measured in ppm, that are three-quarters of those recorded on a 300 MHz instrument, and the complex multiplet pattern in spectra measured on the two instruments should look very different. When asked about this issue, Dr. Sezen had no explanation. (Sezen Tr. at 55:22-23).

Furthermore, the coupling constants for the resonance peaks at ca. 6.64, 6.5, and 4.74 ppm reported by Dr. Sezen in the table on page 399 of the dissertation (Exh. K1 at 06293) should summarize the values found by analyzing the spectrum on page 433 of the dissertation. (*Id.* at 06327). However, the data in the table and in the spectrum are not consistent. For example, the table reports a coupling constant of 8.7 Hz for the doublet at ca. 4.47 ppm, whereas, the splitting in the NMR spectrum on page 433 is 1886.54 – 1875.28 = 11.3 Hz. The coupling constant (when measured in Hz) appears to be too large by a factor of 11.3/8.7 = 1.3, corresponding to the ratio of NMR instrument field strengths (400/300 = 1.33). Thus, the spectrum on page 433 of the thesis would appear to have been fabricated by matching the resonance frequencies that Lewis et al. reported in ppm. This would incorrectly scale the coupling constants, resulting in the observed mismatch between the values for these constants recorded in the table on page 399 and those measured from the spectrum on page 433. The table, although it purports to show data measured by Dr. Sezen, appears instead to have been copied from the paper by Lewis et al. [68]

Dr. Sezen discusses the compound *N*-phenyl-2-phenylpyrrolidine on page 13 of her rebuttal to the preliminary Inquiry Committee. She states, "The product of this reaction is not available by known chemical reactions," implying that she could not have fabricated results or tampered with others attempts to reproduce her results. Dr. Sezen's statement is inaccurate. More significantly, she plagiarized the ^{1}H and ^{13}C spectral data

[68] The Committee also noted an instance of apparent plagiarism in the Acknowledgments in Dr. Sezen's thesis. Her Acknowledgements duplicate almost exactly several sections of the Acknowledgements published in the dissertation of Dhiman Chakraborty (State University of New York at Stony Brook, September 1994). *See* Exh. K24A at 013542, 013544. The dissertation also is available online at http://lss.fnal.gov/archive/thesis/fermilab-thesis-1994-05.pdf.

and fabricated the ^{1}H NMR spectrum that she presents as proof that she made this compound.

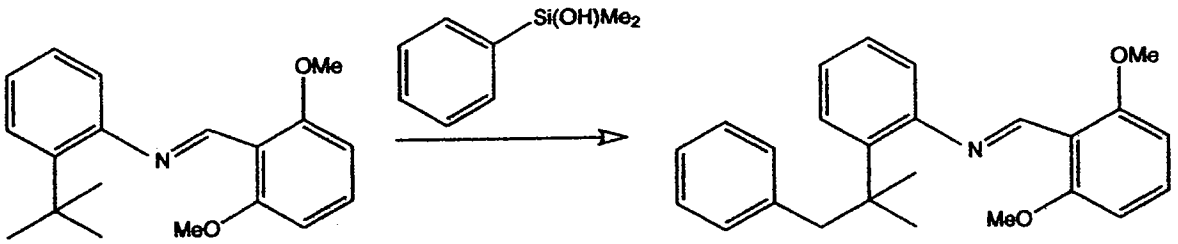
(3) Chapter 1 and *JACS* 124, 13372 (2002)

Additional fraudulent NMR spectra in the thesis and publications of Dr. Sezen were identified by the Committee during the course of its investigation, even though the electronic files associated with them could not be located. These fraudulent spectra were not identified in earlier investigations; in fact, when asked about them, (b)(6) and (b)(7)(C) who investigated this paper at Dr. Sezen's request, stated that he thought these spectra were accurate. (b)(6) and (b)(7)(C)

As described below, these spectra appear to have been fabricated by the same approaches described above, even though no corresponding data sets have been located on the NMR spectrometers. Chapter 1 of the thesis (Exh. K1 at 05897-05971) describes on pages 16 and 17 (*Id.*) the reactions of compound 9 to produce compound 11 and compound 15 to produce compound 16[69]:

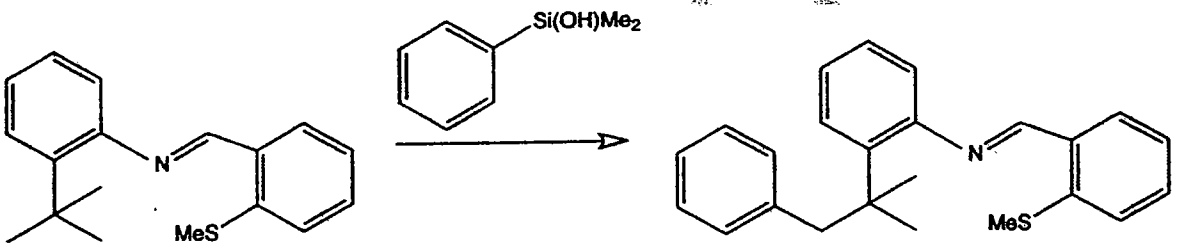
[69] The Committee produced Figures 1 and 2 based on figures in Dr. Sezen's thesis.

Figure 1. Reaction of compound 9 to produce compound 11.



Compound 9 Compound 11

Figure 2. Reaction of compound 15 to produce compound 16.



Compound 15 Compound 16

The Committee matched the data and spectra in the thesis to the data and spectra in Dr. Sezen's NMR binders. The thesis shows the ^{1}H NMR spectrum of compound 11 on page 67 (*Id.* at 05963); its parameters are summarized on page 44. (*Id.* at 05940). The original ^{1}H NMR spectrum is located in the NMR binders. (Exh. A2C at 001476). The ChemDraw prediction for this compound also appears in Dr. Sezen's NMR binders. (Exh. A2E at 001457). Similarly, the thesis summarizes the spectroscopic parameters of compound 9 on page 43. (Exh. K1 at 05939). Although the ^{1}H NMR spectrum of this compound is not displayed in the thesis, it is among the spectra in the NMR binders. (Exh. A2D at 001464). The ChemDraw predicted ^{1}H NMR resonance frequencies for this compound are also in the NMR binders (Exh. A2E at 001457). The ^{1}H NMR

spectrum of compound 16 is shown on page 68 of the thesis, and its parameters are summarized on page 40. (Exh. K1 at 05964 and 05936). The original ^{1}H NMR spectrum is located in the NMR binders (Exh. A2B at 001508). The ^{1}H NMR ChemDraw predicted resonance frequences are also in the NMR binders (Exh. A2 at 001480). Finally, the spectroscopic parameters for compound 15 are summarized on page 37 of the thesis. (Exh. K1 at 05933). Although the ^{1}H NMR spectrum of this compound is not displayed in the thesis, it is among the spectra in the NMR binders. (Exh. A2A at 001499). The ChemDraw predicted ^{1}H NMR resonance frequencies for this compound are also in the NMR binders. (Exh. A2A at 001482).

A comparison of the coupling constants for the starting materials and purported products reveals that the results of these experiments were fabricated. The ^{13}C satellites of a number of resonances are visible in these printed NMR spectra, which allowed the Committee to measure the $^{1}J_{CH}$ coupling constants with a ruler. (The estimated precision of the measurements is ~2 Hz). A graph of the results is shown in Figure 3:

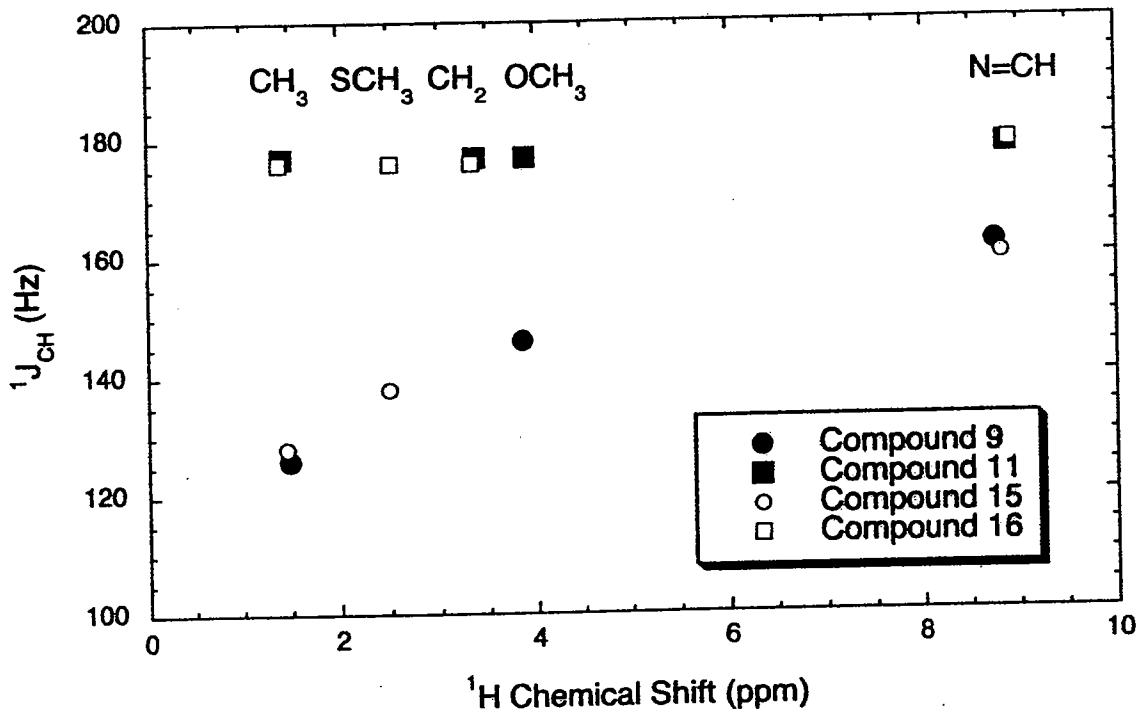


Figure 3. Correlation between $^1J_{CH}$ and ^{1}H chemical shift for compounds described in Chapter 1 of the thesis of Dr. Bengü Sezen (created by the Committee).

For the two starting compounds, 9 and 15, the graph shows, in accord with known chemical principles, that $^1J_{CH}$ varies with the ^{1}H chemical shift. The resonance of the methyl group attached to carbon (the resonance with smallest chemical shift parameter) has a scalar C-H coupling constant of ~127 Hz and the resonance of the imine group (the resonance with the largest chemical shift parameter) has a C-H coupling constant of ~161 Hz.

In contrast, for the two product compounds 11 and 16, $^1J_{CH}$ does not vary with the ^{1}H chemical shift. All the resonances have identical coupling constants, ~177 Hz. The pattern of coupling constants demonstrate that the NMR spectra of the starting compounds are authentic, while the spectra of the products have been constructed by the procedure described above from a ^{1}H resonance peak with a C-H coupling constant of

~177 Hz. Within the precision of these measurements, this coupling constant is identical to that of the common solvent methylene chloride ($^1J_{CH}$ = 177.6 Hz).[70]

The Committee was able to conduct the above analysis of the spectra of compounds 9, 11, 15, and 16 in the thesis because the ^{13}C satellites for 3-4 resonances were visible in the spectra. A smaller number of $^1J_{CH}$ coupling constants also could be measured for other compounds reported in Chapter 1 of the thesis and in the Supporting Information to the corresponding paper. The conclusions were the same: when identifiable, the $^1J_{CH}$ coupling constants for starting materials varied as expected with ^1H chemical shift, while for products the coupling constants were all ~177 Hz. The conclusion is that the ^1H NMR spectra for product compounds 11, 16, 21, 22, 24, 25, and 26 all appear to have been fabricated. The references for the fabricated spectra are summarized in Table 4:

Table 4. Fabricated NMR Spectra in Chapter 1 and *JACS* (2002) **124**, 13372

Compound Number		Page References to the NMR Spectroscopic Data in the Thesis (Exh. K1)		NMR binder (Exh. A2)
Thesis	JACS	Tabular data	^1H Spectrum	Bates stamp
11	4	p. 44 (05940)	p. 67 (05963)	001476
16	6	p. 40 (05936)	p. 68 (05964)	001508
21	7	p. 42 (05938)	p. 69 (05965)	001512
22	10	p. 47 (05943)	p. 71 (05967)	001540
24	12	p. 55 (05951)	p. 72 (05968)	001426
25	13	p. 57 (05953)	p. 73 (05969)	001443
26	14	p. 59 (05955)	p. 74 (05970)	001448

The Committee had to limit its analysis to these compounds because the sensitivity and resolution of most of the printed spectra was insufficient to show ^{13}C satellites.

[70] The reactions to produce compounds 11 and 16 are reported in the publication (b)(6) and (b)(7)(c) (b)(6) and (b)(7)(c) (Exhs. K14-K16). Compounds 9 and 11 in the thesis are referred to as compounds 1 and 4 in the paper. Compounds 15 and 16 in the thesis are referred to as compounds 5 and 6 in the paper. NMR spectroscopic data for compounds 1, 4, 5, and 6 are given on pages S11, S12, S6, and S9 of the Supporting Information of the paper. (Exh. K15). The NMR spectra of compounds 4 and 6 are given on pages S25 and S26. (*Id.*).

The reaction to produce compound 16 is the same reaction that (b)(6) and (b)(7)(C) attempted to reproduce (*see* pp. 17-18 above). The spectrum recorded by (b)(6) and (b)(7)(C) of the product on the one occasion the reaction worked for him (with Dr. Sezen's assistance) does not have sufficient sensitivity to allow ^{13}C satellites to be discerned, and was recorded on a 300 MHz, rather than a 400 MHz, NMR spectrometer. Nonetheless, the principal resonance signals of compound 11 have the same chemical shifts in the fabricated spectra in Dr. Sezen's thesis and in (b)(6) and (b)(7)(C) spectra. For example, the CH_2 group created as a result of the reaction resonates at 3.35 ppm in both spectra, and the distinctive imine resonance appears at 8.91 ppm in both spectra, 0.09 ppm downfield from the corresponding resonance for the starting material. These observations suggest that, as indicated by (b)(6) and (b)(7)(C) compound 16 could be synthesized by another route, which would have allowed Dr. Sezen to know the exact resonance frequencies. (b)(6) and (b)(7)(C)

(b)(6) and (b)(7)(C)

C. Absence of Dr. Sezen's Research Records

As discussed at pp. 61-66 above, the Committee found that Dr. Sezen's original NMR Research Records are limited to six NMR binders and six electronic data sets. In the following instances, the Committee was unable to find any data in Dr. Sezen's NMR Research Records to support the results of reactions she reported in her notebooks, publications, and thesis:

1. With the exception of six data sets, located on a Zip disk, that were acquired using the account of (b)(6) and (b)(7)(C) no electronic or hardcopy NMR spectra or data sets have been located labeled with NMR codes matching the identification names listed in Dr. Sezen's notebooks.

2. Printed NMR spectra in the NMR binders do not contain dates or labels, other than compound names, that would allow these NMR spectra to be linked to any specific reaction recorded in Dr. Sezen's laboratory notebooks.

3. Product compounds are reported in Dr. Sezen's thesis and publications for which no NMR spectra are reported in the thesis or publications and no NMR spectra can be located in the Research Record.

The Committee finds that this absence of documentary evidence is further evidence of Dr. Sezen's Research Misconduct.

PHS regulations provide that the destruction, absence of, or respondent's failure to provide research records adequately documenting the questioned research is evidence of research misconduct if a preponderance of the evidence establishes that the respondent had the opportunity to maintain the records but did not do so, or maintained the records and failed to produce them in a timely manner, and that the respondent's conduct constitutes a significant departure from accepted practices of the relevant research community. 42 C.F.R. § 93.106(b)(1).

The Committee finds that, like every other student in the (b)(6) and (b)(7)(C) Dr. Sezen had the opportunity to maintain relevant research records. The Committee finds, however, that the preponderance of the evidence shows she did not do so. The Committee further finds that Dr. Sezen's NMR spectra are insufficiently identified to permit correlation with Dr. Sezen's notebooks. Finally, the Committee also finds that although Dr. Sezen has known since August of 2005 that her work was the subject of investigation, she has failed to produce any additional relevant research records since that time. As discussed above, her last-minute claims that additional research records exist, when those records cannot be located and are recalled by no individual who worked with her, are not credible. The Committee finds that these deficiencies and absences in Dr.

Sezen's Research Record constitute significant departures from accepted practice in the relevant research community and are evidence of misconduct.

D. Dr. Sezen's Defenses

Although the Committee has the burden to determine whether a preponderance of evidence shows that Dr. Sezen committed research misconduct, Dr. Sezen bears the burden to prove her defenses. (50 C.F.R. § 93.106(2)). As discussed below, Dr. Sezen has offered a number of defenses to the Allegations against her. The Committee finds that Dr. Sezen has failed to prove these defenses.

1. The Spectra in the (b)(6) and (b)(7)(c)

Dr. Sezen claims that she could not have fabricated the spectra found in the (b)(6) and (b)(7)(c) belonging to former group member (b)(6) and (b)(7)(C) because she was on (b)(6) and (b)(7)(C) on the date the files were modified, June 11-12, 2004. (Sezen Tr. at 90:14-18; Exh. T at 012361). As discussed above, as evidence Dr. Sezen presented a copy of a page from a (b)(6) and (b)(7)(C) for June 10 and 12, 2004, in (b)(6) and (b)(7)(C) (Exh. J18; Sezen Tr. at 90:17-18).

The Committee finds that Dr. Sezen's claim is not credible. First, as discussed above, the sign-up sheets and computer log files show that Dr. Sezen reserved time on the 400 MHz NMR spectrometer the majority of occasions when the (b)(6) and (b)(7)(C) on that instrument was utilized, strongly suggesting that she was the individual who used this account. Second, Dr. Sezen's signature appears on the sign-up sheets as reserving the 400 MHz spectrometer on June 11, 2004, when the fraudulent raw data used to create the fraudulent spectum were recorded. (Exh. N1 at 04152). Third, and as discussed above, at pp. 74-75, other fraudulent data were created on other dates, within the period of June 23-26, 2004, and Dr. Sezen's signature also appears on the sign-up sheets during that

time period. (Exh. N1 at 04164). Finally, the Committee notes some irregularities in the (b)(6) and (b)(7)(C) statement and, moreover, even though the statement appears to reflect a charge to Dr. Sezen's (b)(6) and (b)(7)(C) card, it would not prove that she was actually in (b)(6) and (b)(7)(C) on the date the charge accrued.[71] In light of all of the evidence, the Committee does not credit Dr. Sezen's claim that, because she was on vacation at the time and did not know the account password, she could not have created the fraudulent spectra found in (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) account and the matching spectra published in her publications and thesis.

Dr. Sezen also contested evidence that particular fraudulent spectra were identical to the spectra in her thesis and papers. Both in her response to the Inquiry Committee (Exh. T at 012359-012360) and in her interview with the Committee, Dr. Sezen claimed that the ^{31}P spectrum on page 333 of her thesis (Exh. K1 at 06227) and the White-out Spectrum were not identical. (Sezen Tr. at 46:22-51:18). The main points she raises are discussed below:

1. The labeling of the two spectra is different.
2. The P-Rh scalar coupling constants reported in the text of the thesis differ from those in the White-out Spectrum.
3. The peak shapes and noise patterns of the two spectra differ.

[71] The Committee has never been provided the original of the (b)(6) and (b)(7)(C) statement. The Committee notes that the copy appears to have certain peculiarities. The statement does not include reference numbers for any of the transactions, does not refer to amounts in (b)(6) and (b)(7)(C) and does not include the charge, described in the Statement Messages, (b)(6) and (b)(7)(c) (Exh. J18). In addition, (b)(6) and (b)(7)(C) attempted to obtain corroborating records from the two hotels listed on the statement. The (b)(6) and (b)(7)(C) hotel did not keep records from before 2005 (Exh. J40), but the (b)(6) and (b)(7)(C) hotel chain did. Staff at the (b)(6) and (b)(7)(C) that they had no records of anyone named Sezen having stayed at their hotels in 2004. (Exh. J43).

The Committee has considered these points and has made the following findings:

a) Labeling

As discussed above, the differences in labeling are trivial and the labels could have been modified at any time prior to publication. The critical issue is whether the spectra themselves are identical. As noted above, the labeling of the figure is different in the thesis and publication; another version of the figure was found by the Committee in Dr. Sezen's NMR binders. (Exh. A3B at 001621-001622 and 002450-002451). These observations support the conclusion that multiple versions of the figure were prepared prior to the final published version.

b) Coupling Constants

The coupling constants Dr. Sezen claims to have obtained from Exhibit E1 are inaccurate. The Committee has examined the thesis and Exhibit E1 and found that the differences between the coupling constants in that exhibit and in Sezen's dissertation and publication (*JACS* (2004) **126**, 13244) are negligible. The data obtained by the Committee are compared to Dr.Sezen's testimony in Table 5.

Table 5. ^{31}P-Rh coupling constants

Compound	^{31}P Shift (ppm)	*J* in Exh. E1 (Hz)		*J* in Thesis (Hz)		Diff. (Hz)	Thesis (Page) (Exh. K1)
		Interview	Actual	Interview	Actual		
$RhCl(CO)(PFur_3)_3$	–16.4	146.77	148.1	148.2	148.2	**0.1**	304 (06199)
$Rh(Pyrr)(CO)(PFur_3)_2$	–20.2	147.26	147.9	148.9	148.0	**0.1**	331 (06225)
$Rh(Cl(I)(Ph)(CO)(PFur_3)_2$	–24.3	123.66	124.2	124.2	124.2	**0.0**	330 (06224)

The raw data for the subcolumn "Actual" under the heading "*J* in Exhibit E1 (Hz)" were obtained as shown in Table 6, using the resonance frequencies printed on the spectrum. The values of *J* in units of ppm are converted to Hz using the factor 121.497

Hz, which is the ^{31}P resonance frequency of the narrow-bore 300 MHz NMR spectrometer recorded in the "procs" files of the NMR data sets.

Table 6. ^{31}P spectrum analysis to determine *J*

Compound	^{31}P Shift (ppm)		*J* (ppm)	*J* (Hz)
	Downfield Component	Upfield Component		
$RhCl(CO)(PFur_3)_3$	–15.787	–17.006	1.219	148.1
$Rh(Pyrr)(CO)(PFur_3)_2$	–19.594	–20.811	1.217	147.9
$Rh(Cl(I)(Ph)(CO)(PFur_3)_2$	–23.790	–24.812	1.022	124.2

c) Peak Shapes and Noise Patterns

Although Dr. Sezen has claimed repeatedly that the White-out Spectrum has different peak positions, shapes and noise than the spectrum on p. 333 of her thesis (*e.g.*, Sezen Tr. at 51:7-18), these statements are erroneous and are based in part on failure to recognize the lower resolution of the spectrum reproduced in the thesis compared to the White-out Spectrum.

In order to clarify the issues, the Committee prepared Figure 4. The spectrum in the Supporting Information and the White-out Spectrum were scanned into TIFF format computer files. Photoshop was used to change the color of the published spectrum to green and the White-out Spectrum to red. Photoshop was used to scale and superpose the two spectra. To allow additional inspection, two portions of the spectra were expanded; these correspond to the regions called "Region A" (at ca. 6 ppm) and "Region B" (at ca. –20 ppm) by Dr. Sezen. As the figure makes clear, the peaks of the spectra overlap, not only in position, but in height; the vertical distances between the different spectra that constitute each composite are identical; and the background noise in the two copies are identical.

Confidential

Both in her response to the Inquiry Committee (Exh T at 012361) and in her interview with the Committee (Sezen Tr. at 89:10-92:5), Dr. Sezen claimed that the ^{1}H NMR spectrum on page 347 of her thesis (Exh. K1 at 06241) and the spectrum found in (b)(6) and (b)(7)(c) were not identical. Dr. Sezen stated that the coupling constants for the methyl resonances are not 177.6 Hz, but rather 188 Hz. (Exh. T at 012361). However, as discussed above, the coupling constants in question are clearly 177.6 Hz. Dr. Sezen's statements to the contrary are simply inaccurate.

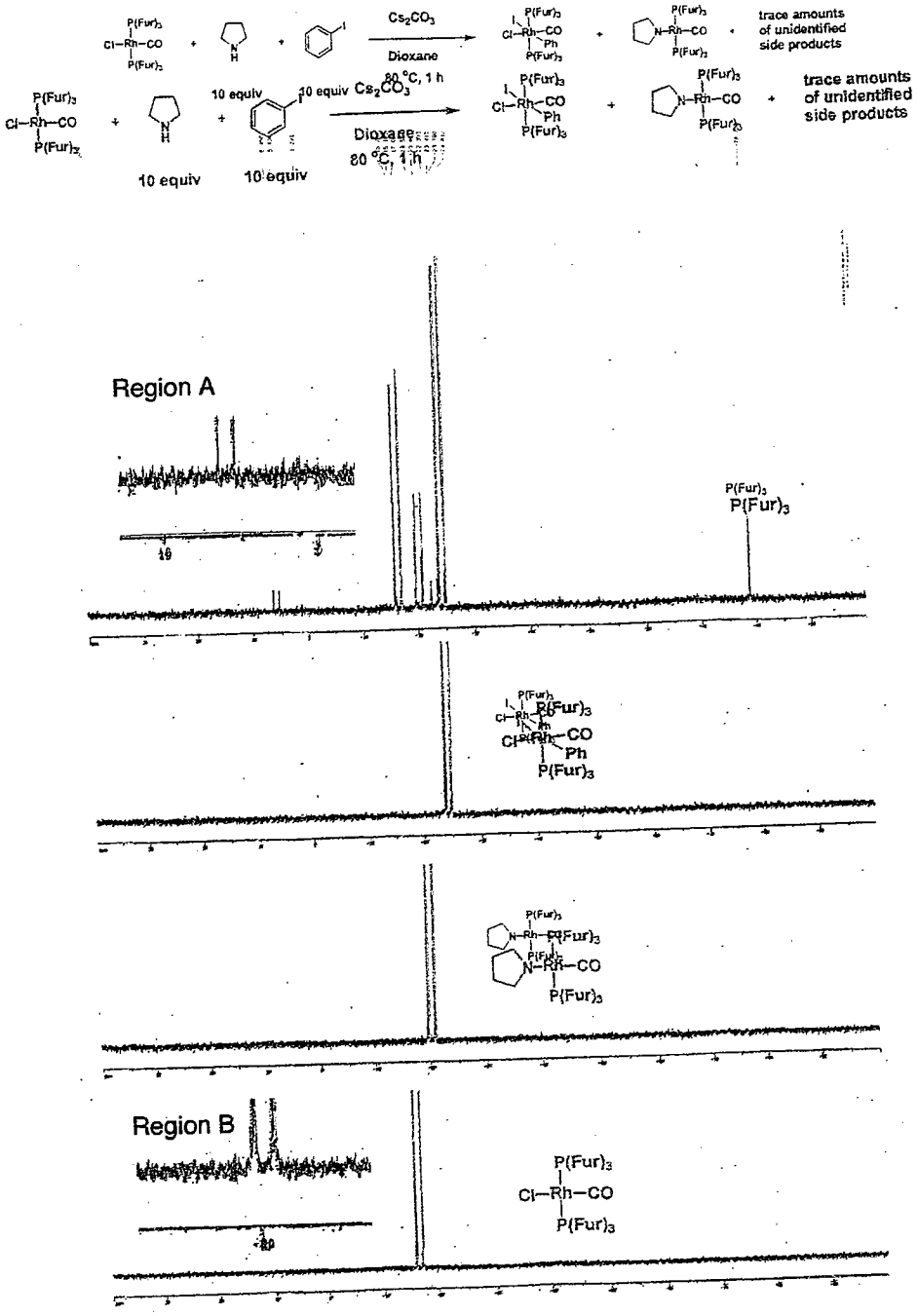


Figure 4. Superposition of spectra on page 333 of the thesis and the White-out Spectrum.

In sum, the Committee finds that the preponderance of the evidence does not support Dr. Sezen's defenses as to the spectra in the (b)(6) and (b)(7)(C) account. To the contrary, the Committee finds that the evidence shows, more likely than not, that Dr. Sezen was not in (b)(6) and (b)(7)(c) when some fabricated spectra were created, and that the identified spectra in the (b)(6) and (b)(7)(C) account are identical to spectra in Dr. Sezen's thesis and publications.

2. **Dr. Sezen's "Framing" Theory**

Dr. Sezen claims that others in the (b)(6) and (b)(7)(C) – particularly (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) "framed" her by planting fabricated spectra in her NMR binders, which she then scanned and unwittingly included in her thesis and papers. (Sezen Tr. at 82:8-11; 89:10). In October 2006, Dr. Sezen advised the Committee of a suggested motive for this conspiracy: (b)(6) and (b)(7)(C) framed her in order to be able to later publish a paper (*JACS* (2006) **128**, 14220-14221) based on her ideas without according her credit.[72] (Exh. J34 at 012195-012197).

The Committee finds no credible evidence that any individual other than Dr. Sezen fabricated the NMR spectra in her thesis and publications.

First, the first fraudulent spectra were produced long before the chemistry in the paper published by (b)(6) and (b)(7)(C) was developed. Although (b)(6) and (b)(7)(C) joined the (b)(6) and (b)(7)(C) in May 2001 (b)(6) and (b)(7)(C)), the documents Dr. Sezen provided to prove (b)(6) and (b)(7)(C) motive for framing her date from 2004 and 2005, well after much of the fabrication at issue occurred.[73] Similarly, (b)(6) and (b)(7)(C) only joined the

[72] Pursuant to the Policy, these specific allegations are the focus of another confidential Inquiry.
[73] Exhibit H13, a timeline showing (b)(6) and (b)(7)(C) membership, indicates that (b)(6) and (b)(7)(C) joined the (b)(6) and (b)(7)(C) in December 2001. However, in his interview, (b)(6) and (b)(7)(C) confirmed that (b)(6) and (b)(7)(C) also worked in the (b)(6) and (b)(7)(C) in the summer of 2001. (b)(6) and (b)(7)(C) also recalled that Dr.

(b)(6) and (b)(7)(C) in May 2004. Therefore, he could not have conspired to frame Dr. Sezen in 2002. (b)(6) and (b)(7)(C)

Second, neither (b)(6) and (b)(7)(C) prompted the (b)(6) and (b)(7)(C) investigation of Dr. Sezen's work. (b)(6) and (b)(7)(C) triggered the review, and he joined the Sames group only in February 2005. (b)(6) and (b)(7)(C) discovered the White-out Spectrum. (b)(6) and (b)(7)(C)[74] Moreover, although some fraudulent NMR spectra were identified by members of the (b)(6) and (b)(7)(C) other fraudulent spectra, including the earliest fabricated spectra, reported in *JACS* (2002) **124**, 13372-13373, were identified by the Committee in the course of its own investigation.

Third, fabricated spectra appeared in a paper published in 2002 (b)(6) and (b)(7)(c) (b)(6) and (b)(7)(c) According to Dr. Sezen's theory, the individual in question would have had to begin falsifying Dr. Sezen's data within the first year of Dr. Sezen's joining the (b)(6) and (b)(7)(C) If any person other than Dr. Sezen produced these initial fraudulent spectra, then that individual would have been unlikely to wait three years after planting the spectra before exposing Dr. Sezen. Such a lengthy delay potentially would have allowed Dr. Sezen to notice the disparities in the NMR spectra and to correct them on her own, foiling the scheme.

Finally, the Committee considers that framing Dr. Sezen with fabricated data would be contrary to the self-interest of any member of the (b)(6) and (b)(7)(C) because

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(b)(6) and (b)(7) worked on projects that were not related to Dr. Sezen's, did not share space with Dr. Sezen. and also stated that he was not aware of any conflicts or problems between them at that time. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) confirmed (b)(6) and (b)(7)(C) recollection (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C)

[74] The components of the White-out Spectrum were not taped to the back of one of (b)(6) and (b)(7)(C) spectra, as Dr. Sezen originally claimed; rather, the composite was taped to a spectrum belonging to (b)(6) and (b)(7)(C) (b)(6) and (b)(7) another former (b)(6) and (b)(7)(C) member. (Exh. H8).

significant stigma would result from association with a research director who issued multiple retractions of prominent publications.

In sum, the Committee finds that Dr. Sezen has failed to meet her burden of proof with respect to the "framing theory."

3. Dr. Sezen's Defense that Others Reproduced Her Work

As a third defense, Dr. Sezen has claimed that various individuals and one company independently reproduced her experiments, including (b)(6) and (b)(7)(C) and (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) The Committee notes that reproducibility or the lack thereof does not directly bear on whether Dr. Sezen fabricated or falsified her results. The Committee further finds that a preponderance of the evidence shows that none of the individuals or companies cited by Dr. Sezen independently reproduced her results.

a. (b)(6) and (b)(7)(C) The Indole Reaction

In her response to the Inquiry Committee report dated May 19, 2006, Dr. Sezen stated that (b)(6) and (b)(7)(C) reproduced her indole arylation reaction (published in JACS in 2003) "independently for numerous times." (Exh. T at 012347). Dr. Sezen further stated that (b)(6) and (b)(7)(C) "published an independent paper on [the indole] reaction where they reported that they obtained an increased 84 % yield. The original yield reported for this reaction was 53 % in our publication."[75] (Exh. T at 012347 (emphasis omitted)). She added that these data were cited at page 99 of her

[75] Dr. Sezen misstates her own results in her testimony. The initial yield was 53%, but the optimized yield was 84% in Dr. Sezen's publication.

thesis (Exh. K1 at 05995), and was thus accepted by (b)(6) and (b)(7)(C) and the other (b)(6) and (b)(7)(C). (*Id.*; *see also* Sezen Tr. at 87:24-88:2).[76]

Statements by (b)(6) and (b)(7)(C) contradict Dr. Sezen's view. First, as discussed above (b)(6) and (b)(7)(C) explained that, although he tried repeatedly, he was able to reproduce Dr. Sezen's indole reaction only when she was present. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) For this reason, (b)(6) and (b)(7)(C) said he insisted that Part B of the Supporting Information to his paper *JACS* (2005) 127, 8050-8057 (Exhs. K25, K27) explain that the yields were highly variable ("0% and up") for this procedure. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) further stated that even if the reaction had worked, it did not improve upon the prior reaction described by Dr. Sezen. He explained that his paper reported a yield of 86%, but that this did not differ significantly from the previous yield of 84%. (b)(6) and (b)(7)(C) 74:1). Furthermore, (b)(6) and (b)(7)(C) also stated that, aside from a "forward" explaining the variability in the yield, the section of the Supporting Information concerning her reactions was written by Dr. Sezen, who also provided (b)(6) and (b)(7)(C) with the table reporting the results. (b)(6) and (b)(7)(C)

Second, as also described above, (b)(6) and (b)(7)(C) stated that she had great difficulties reproducing Dr. Sezen's reactions, except when Dr. Sezen set the reaction up herself.

Third, (b)(6) and (b)(7)(C) s has concluded that the (b)(6) and (b)(7)(C) should be corrected to make clear that Dr. Sezen's arylation reaction was not reproducible. As (b)(6) and (b)(7)(C) explained to the Committee, he submitted a proposed correction to the (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) The Correction has now been published and reads:

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[76] Dr. Sezen also pointed to a quote attributed to (b)(6) and (b)(7)(C) that was published in an article in *Science*, stating that "some of Sezen's work has been replicated and has been used by chemists in the pharmaceutical industry." (Sezen Tr. at 88:15-89:3). Dr. Sezen suggested that this quote showed that (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) believed her reactions were reproducible. (*Id.*) (b)(6) and (b)(7)(C) said the *Science* reporter misquoted his comments. (b)(6) and (b)(7)(C)

> For comparison purposes, this article refers to a palladium catalyzed arylation of free azoles in the presence of magnesium oxide, published previously in a separate communication. Although the magnesium oxide procedure has recently been found irreproducible (J. Am. Chem. Soc. (2006) **128**, 8364), this fact does not affect the conclusions of this paper. Consequently, the magnesium oxide protocol has been removed from the Supporting Information. Also, Figures S5 and S8 have been replaced with corrected versions.

(Exh. K29).

In light of these facts, the Committee does not credit Dr. Sezen's defense that (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) independently reproduced the indole arylation reaction.

b. (b)(6) and (b)(7)(c)

In her interview, Dr. Sezen also mentioned that a company called (b)(6) and (b)(7)(c) had reproduced her work. (Sezen Tr., 74:4-25). She later emailed a print-out from a website called (b)(6) and (b)(7)(c) which referenced "the (b)(6) and (b)(7)(c) (Exh. J34 at 012387). However, the (b)(6) and (b)(7)(c) website no longer posts this information. (Exh. MM). Furthermore, (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) stated that after the (b)(6) and (b)(7)(C) were first published, (b)(6) and (b)(7)(c) included the (b)(6) and (b)(7)(C) on the (b)(6) and (b)(7)(c) website for informational purposes only. After the retractions (b)(6) and (b)(7)(c) removed the information. (b)(6) and (b)(7)(c) said that (b)(6) and (b)(7)(c) itself never attempted to reproduce the (b)(6) and (b)(7)(C) (Exh. J42).

c. (b)(6) and (b)(7)(C)

The only other person Dr. Sezen claims to have reproduced her reactions is (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C). As discussed at pages 107-113 below, the Committee has concluded that a preponderance of the evidence

shows that (b)(6) and (b)(7)(C) is not a credible witness, and, moreover, that documents purported to have been submitted to the Committee by (b)(6) and (b)(7)(C) and her supervisor, Ralf Decter were actually sent from Dr. Sezen's computer at the University of Heidelberg.

5. The Committee's Findings Concerning Allegation No. 2: Whether Dr. Sezen falsified data supporting combustion analyses reported in her thesis and publications

The Committee finds that in the instances described in the following tables, the majority of elemental (combustion) analysis data reported in Chapters 5, 6 and 7 of Dr. Sezen's thesis and the publications:

- (b)(6) and (b)(7)(c)
-

do not match any of the reports provided by (b)(6) and (b)(7)(C) Laboratory, either because no reports from (b)(6) and (b)(7)(C) contain results for the indicated compound or because the results reported by (b)(6) and (b)(7)(C) lisagree with the those reported in the thesis and publications.

Dr. Sezen reports 15 combustion analyses in her first-author papers and thesis. The Committee located reports of eight analyses by (b)(6) and (b)(7)(C) Of these, six have been altered in Sezen's publications. The other two analyses, which Sezen reported accurately, are of commercially available compounds. This highly skewed distribution of changes is strong evidence that the changes are not errors in transcription, but are

falsifications made to make the results appear closer to Dr. Sezen's theoretical calculations. The following tables summarize the discrepancies:[77]

Table 7. Elemental analyses reported in Chapter 5 of the thesis and in the publication *JACS* (2004) **126**, 2004, 13244-13246.

Compound **Molecular formula** **Calculated composition**	**Elemental Analysis (reported in thesis and publication) (Exhs. K1 and K9)**	**Elemental Analysis** (b)(6) and (b)(7)(C) **Laboratory) (Exh. O3 at 006376, 006378)**
$RhCl(CO)(PPh_3)_2$ **commercially available** $C_{37}H_{30}ClOP_2Rh$ C: 64.32; H: 4.38	Thesis page 303 (06198) Publication page S2 (05814) C: 64.44; H: 4.22	Date received: 5/13/04 Invoice#: P20388 (006376) Name: sample#2 C: 64.44; H: 4.22
$RhCl(CO)(PFur_3)_2$ $C_{25}H_{18}ClO_7P_2Rh$ C: 47.61; H: 2.88	Thesis page 304 (06199) Publication page S2 (05814) C: 47.72; H: 2.97	Not found
$RhH(CO)(PPh_3)_3$ **commercially available** $C_{55}H_{46}OP_3Rh$ C: 71.90; H: 5.05	Thesis page 305 (06200) Publication page S3 (05815) C: 71.82; H: 4.91	Date received: 5/13/04 Invoice#: P20388 (006376) Name: sample#3 C: 69.82; H: 4.91
$RhH(CO)(PFur_3)_3$ $C_{37}H_{28}O_{10}P_3Rh$ C: 53.64; H: 3.41	Thesis page 306 (06201) Publication page S3 (05815) C: 53.54; H: 3.47	Date received: 5/13/04 Invoice#: P20388 (006376) Name: sample#5 C: 55.14; H: 3.57
$RhCl(I)(Ph)(CO)(PFur_3)_2$ $C_{31}H_{23}ClIO_7P_2Rh$ C: 44.61; H: 2.78	Thesis page 330 (06224) Publication page S19 (05832) C: 44.97; H: 3.02	Date received: 7/2/04 Invoice#: P20624 (006378) Name: sample#1 C: 44.93; H: 3.94
$Rh(Pyrr)(CO)(PFur_3)_2$ $C_{29}H_{26}NO_7P_2Rh$ C: 52.35; H: 3.94; N: 2.11	Thesis page 330 (06224) Publication page S19 (05832) C: 51.72; H: 3.17; N: 2.29	Date received: 7/2/04 Invoice#: P20624 (006378) Name: sample#2 C: 50.93; H: 3.86; N: 1.06
$Rh(Ph)(CO)(PFur_3)_2$ $C_{31}H_{23}O_7P_2Rh$ C: 52.35; H: 3.94	Thesis page 331 (06225) Publication page: -- C: 55.77; H: 3.21	Not found

[77] These tables have been reformatted, corrected, and extended from the report provided by (b)(6) and (b)(7)(C) in Exh. I9 at 000753-000755.

Table 8. Elemental analyses reported in Chapter 6 of the thesis and in the publication *JACS* (2005) **127**, 5284-5285.

Compound **Molecular formula** **Calculated composition**	**Elemental Analysis (reported in thesis and publication) (Exhs. K1 and K3)**	**Elemental Analysis** (b)(6) and (b)(7)(C) **(Exh. O3 at 006382-006383)**
$RuH_2(CO)(PPh_3)_3$ **commercially available** $C_{55}H_{47}OP_3Ru$ C: 71.96; H: 5.16	Thesis page 392 (06286) Publication page S3 (05850) C: 71.65; H: 5.41	Date received: 9/23/04 Invoice#: P20950 (06382) Name: sample#1 C: 71.65; H: 5.41
$RuH_2(CO)(PCyPh_2)_3$ $C_{55}H_{65}OP_3Ru$ C: 70.57; H: 7.00	Thesis page 393 (06287) Publication page S3 (05850) C: 70.08; H: 7.09	Date received: 9/23/04 Invoice#: P20950 (06383) Name: sample#3 C: 70.08; H: 5.09
$RuH_2(CO)(PCy_2Ph)_3$ $C_{55}H_{83}OP_3Ru$ C: 69.23; H: 8.77	Thesis page 394 (06288) Publication page S4 (05851) C: 69.91; H: 9.09	Not Found
$RuH_2(CO)(PCy_3)_3$ $C_{55}H_{101}OP_3Ru$ C: 67.94; H: 10.47	Thesis page 395 (06289) Publication page S4 (05851) C: 67.57; H: 10.97	Date received: 9/23/04 Invoice#: P20950 (06383) Name: sample#2 C: 65.28; H: 8.91
$RuCl(Ph)(CO)(PCy_3)_2$ $C_{43}H_{71}ClOP_2Ru$ C: 64.36; H: 8.92	Thesis page 418 (06312) Publication page S19 (05866) C: 64.97; H: 9.24	Not Found
$Ru(I)(Ph)(CO)(PCy_3)_2$ $C_{43}H_{71}IOP_2Ru$ C: 57.77; H: 8.01	Thesis page 419 (06313) Publication page S19 (05866) C: 57.25; H: 8.28	Not Found

Table 9. Elemental analyses reported in Chapter 7 of the thesis.

Compound **Molecular formula** **Calculated composition**	**Elemental Analysis (reported in thesis) (Exh.K1)**	**Elemental Analysis** (b)(6) and (b)(7)(C)
Complex 5 C: 60.41; H: 7.41; N: 5.42	Thesis page 462 (06356) C: 60.97; H: 7.87; N: 5.20	Not found
Complex 6 C: 53.15; H: 5.95; N: 6.89	Thesis page 462 (06356) C: 52.78; H: 5.63; N: 6.20	Not found

In contrast, Godula et al., (*JACS* (2005) **127**, 3648-3649), reported combustion analyses for five compounds in the Supporting Information. Each of these combustion analyses

have been located in reports from (b)(6) and (b)(7)(C) and are accurately reported in the publication.[78]

Table 10. Elemental analyses in the publication *JACS* (2005) **127**, 3648-3649.

Compound **Molecular formula** **Calculated composition**	**Elemental Analysis (reported in publication) (Exhs. K20-K22)**	**Elemental Analysis** (b)(6) and (b)(7)(C) **(Exh. O3 at 006371-006383; Exh. O11 at 013571)**
$Ru_3(\mu\text{-}H)(\mu\text{-}NC_5H_4)(PPh_3)(CO)_9$ $C_{32}H_{20}NO_9PRu_3$ C, 42.86; H, 2.25; N, 1.56.	Publication page S3 (012852) C, 43.06; H, 2.43; N, 1.52	Date received: 7/2/04 Invoice#: P20624 (006378) Name: sample #3 C, 43.06; H, 2.43; N, 1.52
$Ru_3(\mu\text{-}H)(\mu\text{-}NC_5H_4)(PPh_3)_2(CO)_8$ $C_{49}H_{35}NO_8P_2Ru_3$ C, 52.04; H, 3.12; N, 1.24	Publication page S7 (012856) C, 52.06; H, 3.03; N, 1.16	Date received: Invoice#: P20796 (006371) Name: (b)(6) and (b)(7)(C) #3 C, 52.06; H, 3.03; N, 1.16
$Ru_2(\mu\text{-}PPh_2)(\mu\text{-}NC_5H_4)(PPh_3)(CO)_5$ $C_{40}H_{29}NO_5P_2Ru_2$ C, 55.36; H, 3.37; N, 1.61	Publication page S10 (012859) C, 55.50; H, 3.48; N, 1.59	Date received: 7/2/04 Invoice#: P20624 (006378) Name: Sample #4 C, 55.50; H, 3.48; N, 1.59
$Ru_3(\mu\text{-}H)_2(\mu\text{-}NC_5H_4)_2(PPh_3)_2(CO)_6$ $C_{52}H_{40}N_2O_6P_2Ru_3$ C, 54.12; H, 3.49; N, 2.43	Publication page S14 (012863) C, 53.85; H, 3.14; N, 2.38	Date received: Invoice#: P20796 (013571) Name: (b)(6) and (b)(7)(C) C, 53.85; H, 3.14; N, 2.38
$Ru_2(\mu\text{-}PPh_2)(\mu\text{-}NC_5H_4)(PPh_3)_2(CO)_4$ $C_{57}H_{44}NO_4P_3Ru_2$ C, 62.12; H, 4.02; N, 1.27	Publication page S17 (012866) C, 62.57; H, 4.25; N, 1.35	Date received: 9/23/04 Invoice#: P20950 (006382) Name: Sample #5 C, 62.57; H, 4.25; N, 1.35

The Committee finds that no other reports of combustion analysis exist in the Research Record that match the results published in Dr. Sezen's publications. The Committee finds that a preponderance of the evidence shows that Dr. Sezen fabricated or falsified these combustion analysis data.

[78] According to the Correction published for this paper, the primary reaction in the paper was not reproducible. The combustion analyses reported here relate not to the primary reaction product, but to purported catalysts of the reactions. Dr. Sezen has stated that she made only an intellectual contribution to this paper.

6. The Committee's Findings Concerning Allegation No. 3: Whether Dr. Sezen fabricated experimental procedures reported in her thesis and publications.

As discussed above, numerous witnesses commented that Dr. Sezen's laboratory notebooks did not adequately document her experimental procedures. In its own review of Dr. Sezen's laboratory notebooks, the Committee was unable to find documentation of the procedures Dr. Sezen reported in the Supporting Information for her first-author papers and thesis. As also discussed above, the Committee does not credit Dr. Sezen's claim that she had four additional notebooks in which she documented experimental procedures. The Committee finds that the records in Dr. Sezen's laboratory notebooks are insufficiently detailed to provide a basis for the experimental procedures that she published (*see* pp. 89-91 above). The Committee finds that these deficiencies and absences in Dr. Sezen's Research Record constitute significant departures from accepted practice in the relevant research community, provide strong evidence that the reported procedures were never performed as described, and are evidence of misconduct.

7. The Committee's Findings Concerning Dr. Sezen's Credibility

The Committee finds that on at least four occasions, Dr. Sezen deliberately misled the Committee, damaging her credibility. First, as discussed above, although Dr. Sezen claims that she had an NMR account with the login ID of "bengu," the Committee finds that no such account, or any variation thereof, existed. Second, during her interview, Dr. Sezen told the Committee that she was not enrolled at the University of Heidelberg:

Q: Since leaving Columbia, have you enrolled in another Ph.D. program?
A: No, I didn't.
Q: So you're not in a Ph.D. program at this point?
A: No, currently I am not.
Q: (b)(6) and (b)(7)(c) Were you ever enrolled at the University of Heidelberg?

A: No.

(Sezen Tr. at 14:15-23). Shortly after Dr. Sezen's interview, Committee staff contacted (b)(6) and (b)(7)(C) Dr. Sezen is listed as a member of (b)(6) and (b)(7)(c) (Exh. P) (b)(6) and (b)(7)(C) confirmed that Dr. Sezen is a current student in his laboratory at the University of Heidelberg. (b)(6) and (b)(7)(C). Two days after the (b)(6) and (b)(7)(C) Dr. Sezen sent an email "correcting" this portion of her transcript:

> As I mentioned in my previous e-mails I do have corrections to the transcript you provided. I realized that (perhaps due to the fact that the interview was held on the phone) I misunderstood many of the questions and answered them in totally unrelated manner, or my answers were themselves misunderstood.
>
> Just to give you an example: page 14 of the transcript states that I said I was not enrolled in a program in Heidelberg. This is obviously incorrect. I am enrolled in a PhD program at the Department of Molecular Biology of University Heidelberg. This fact is listed in the web page http://www.zmbh.uniheidelberg.de/Schiebel/members.shtml since February 2006, it appeared in print in many news articles of magazines and newspapers. The list of evidence also lists this information as Exhibit P even before our interview.

(Exh. J34 at 012153-012154).[79]

Third, as discussed below, the Committee finds that Dr. Sezen misled the Committee by presenting an expert witness who is not genuine. Dr. Sezen has presented several letters and a report from (b)(6) and (b)(7)(C) who claims to have reproduced four of Dr. Sezen's reactions (Exhs. J4, J13, J14 and J17). In July and August 2006, Dr. Sezen sent Columbia electronic copies of a letter from (b)(6) and (b)(7)(C) stating she had

[79] Dr. Sezen never submitted any other corrections to her transcript, although offered several opportunities to do so. (Exh. J34 at 012073, 012133, 012148, 012153, 012158, 012161, 012163, 012228).

successfully reproduced four of Dr. Sezen's reactions. The letters appeared on letterhead for a company called (b)(6) and (b)(7)(C) with an address of (b)(6) and (b)(7)(C) The letterhead also includes (b)(6) and (b)(7)(C) which can be downloaded from the (b)(6) and (b)(7)(C) company website. (Exh. J2 at 05404-05).

A. (b)(6) and (b)(7)(C)

In an effort to obtain background information on (b)(6) and (b)(7)(C) and her company, the Committee searched for her name and the company name on the World Wide Web. Although the searches revealed no references either to (b)(6) and (b)(7)(C) the Committee did find a website for a company called (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) located at the same address as appeared on the (b)(6) and (b)(7)(C) (Exh. LL at 013463).

The Committee then attempted to determine whether (b)(6) and (b)(7)(C) was affiliated with (b)(6) and (b)(7)(C). The University retained German counsel who spoke with the managing director of (b)(6) and (b)(7)(C) obtained written testimony from him. (Exh. BB).

In his affidavit, Dr. Bernd Hollborn explained that (b)(6) and (b)(7)(C) a "medium-sized family owned business, which engages in the production of reagents for medical and other science research purposes." (Exh. BB at ¶ 2). He further testified that (b)(6) and (b)(7)(C) "is one of two occupants of the building (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) and explained that "the second occupant of this building is (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) with its managing director (b)(6) and (b)(7)(C) business which engages in the sales and distribution of chemicals." (Exh. BB at ¶ 3). Finally, (b)(6) and (b)(7)(C) testified that (b)(6) and (b)(7)(C) in his company's name stands

for Dr. Karl Hollborn, who died in the 1940s and was Dr. Bernd Hollborn's grandfather. Dr. Bernd Hollborn concluded, "A living person with the name (b)(6) and (b)(7)(C) is not known to me and is not working at (b)(6) and (b)(7)(C) (*Id.* at ¶¶ 4-5).

B. Email from (b)(6) and (b)(7)(C)

On September 11, 2006, (b)(6) and (b)(7)(C) received an email from (b)(6) and (b)(7)(C) responding to an email from (b)(6) and (b)(7)(C) seeking to schedule a telephone interview. (Exh. HH11). The Committee asked (b)(6) and (b)(7)(C) Columbia University Information Technology ("CUIT"), to attempt to determine where this email originated. (b)(6) and (b)(7)(C) explained to the Committee that the internet headers for (b)(6) and (b)(7)(C) September 11 email show that the email originated from a computer with the IP address (b)(6) and (b)(7)(C). This IP address is owned by a company called (b)(6) and (b)(7)(C) (*Id.* at 23:16-22). (b)(6) and (b)(7)(C) concluded that (b)(6) and (b)(7)(C) September 11 email was sent from (b)(6) and (b)(7)(C)] (b)(6) and (b)(7)(C)

C. Interview with (b)(6) and (b)(7)(C)

On September 18, 2006, the Committee interviewed (b)(6) and (b)(7)(C) by telephone at a number she provided. (b)(6) and (b)(7)(C) stated that she was a research assistant in the (b)(6) and (b)(7)(C) had held that position for six months and had been with the firm for eight years. She stated that in 1995, she obtained a doctorate in catalysis from (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) She also stated that her research director for her

doctorate was (b)(6) and (b)(7)(C) stated that she had not published any papers in the field of catalysis. (*Id.* at 8:7-10). She said that she had not been in (b)(6) and (b)(7)(C) stated that she successfully conducted four experiments based on Dr. Sezen's publications at Dr. Sezen's request. (*Id.* at 8:11-9:2; 10:11-14; Exh. J17). (b)(6) and (b)(7)(C) stated that she conducted the experiments because Dr. Sezen contacted her directly and requested that she do so. (*Id.* at 11:15-21). She further explained that her company did not charge Dr. Sezen for conducting the experiments, but that Dr. Sezen paid for chemicals and an experimental device used. (*Id.* at 12:5-14). When asked for a copy of the invoice provided to Dr. Sezen, and the name of the person who handled the payment, (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) stated that she would "have to check." (*Id.* at 12:23-24). (b)(6) and (b)(7)(C) stated that Dr. Sezen told her that Dr. Sezen had contacted (b)(6) and (b)(7) after seeing an advertisement for the firm in a magazine. (b)(6) and (b)(7)(C) promised to provide a copy of the magazine to the Committee but has not done so. (*Id.* at 11:22-12:4; 13:4-9).

(b)(6) and (b)(7)(C) stated that (b)(6) and (b)(7)(C) was located in (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) (*Id.* at 13:19-23). When asked about (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) answered, "I'm not aware of that company; it's not in the technologic part." She denied that the two companies were at the same location. (*Id.* at 14:11-20). (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) stated that the name of the head of (b)(6) and (b)(7)(C) that he was not available to speak to the Committee at the time of her interview, and that he had the same phone number that the Committee had used to contact her. (*Id.* at 16:9-22). The Committee does not believe that at a German company with eleven employees, five of

[80] The Committee searched the (b)(6) and (b)(7)(C) website and did a basic Google search for any record of (b)(6) and (b)(7)(C) but found none. The Committee also searched the Chemical Abstracts data base, the most comprehensive index of the chemical literature, for any articles by (b)(6) and (b)(7)(C), but found none.

whom have doctorate degrees, the head of the firm and a recently promoted research assistant would share the same telephone line. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C)

D. Email from Ralf Decter

On September 21, 2006, (b)(6) and (b)(7)(C) received an email from Ralf Decter that included purported electronic images of an invoice (b)(6) and (b)(7) had sent to Dr. Sezen, a copy of a bank transfer statement recording payment of the invoice by Dr. Sezen.[81] Mr. Decter promised to send by regular mail hard copies of these documents and a copy of the catalog in which Dr. Sezen saw the (b)(6) and (b)(7)(C) advertisement. (Exh. HH2). Again, the Committee never received this catalog or the hard copies. The Committee asked (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) to review the internet headers for Mr. Decter's email. According to (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C), the IP address of the computer from which Mr. Decter's email originated, (b)(6) and (b)(7)(C) is that of a computer named (b)(6) and (b)(7)(C) (*Id.* at 15:14-15; 10:4-10). (b)(6) and (b)(7)(C) searched this computer name using the UNIX program "whois," and found that it was registered to The University of Heidelberg. (*Id.* at 14:7-9; Exh. HH3).

The Committee also asked (b)(6) and (b)(7)(C) to review internet header information for an email from Dr. Sezen to (b)(6) and (b)(7)(C) on October 9, 2006. (Exh. HH1). (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) explained that the IP address of the computer Dr. Sezen used to send the email was the same as the IP address of the computer used by Mr. Decter, 129.206.92.96. In

[81] The Committee noted that although the bank transfer statement identifies (b)(6) and (b)(7)(C) account as a (b)(6) and (b)(7)(C) account, the website of the (b)(6) and (b)(7)(C) branch of the (b)(6) and (b)(7)(C) which is the bank corresponding to the identification code on (b)(6) and (b)(7)(C) invoice (BLZ 84051010), does not appear to offer such an account. According to its website, the Heidelberg branch of the (b)(6) and (b)(7)(C) does offer such an account among its "personal," but not among its "business," accounts.

other words (b)(6) and (b)(7)(C) email and Dr. Sezen's email were both sent from the same computer, named (b)(6) and (b)(7)(C) (*Id.* at 16:18-24).[82]

Next, the Committee asked (b)(6) and (b)(7)(C) to review the header on an email sent by (b)(6) and (b)(7)(C) of The University of Heidelberg to (b)(6) and (b)(7)(C) on October 31, 2006. (Exh. HH13). The IP address contained in the internet header for that email is (b)(6) and (b)(7)(C), which corresponds to a computer with the name (b)(6) and (b)(7)(C) HH14).

In a follow-up telephone conversation (b)(6) and (b)(7)(C) stated that he did not know anyone named Ralf Decter, and has no knowledge of anyone named Decter either working in his laboratory or enrolled at The University of Heidelberg.[83] (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C)

Finally, (b)(6) and (b)(7)(C) also determined that other emails sent by Mr. Decter and (b)(6) and (b)(7)(C) originated from another University of Heidelberg IP address, (b)(6) and (b)(7)(C)

In light of the above facts, the Committee concludes that (b)(6) and (b)(7)(C) Decter, and Duha Chemisches Katalyse-Labor, are all fictional beings or entities and that the evidence presented by Dr. Sezen of (b)(6) and (b)(7)(C) successful reproduction of Sezen's work should be accorded no weight. The Committee finds that Dr. Sezen intentionally fabricated the (b)(6) and (b)(7)(C) and Decter documents in an effort to mislead the Committee. It

[82] As discussed above, Dr. Sezen is currently a graduate student in the laboratory of (b)(6) and (b)(7)(C) at the University of Heidelberg. Many, if not all of the other emails Columbia has received from Dr. Sezen originated from the same IP address (b)(6) and (b)(7)(C)

[83] The Committee searched on Google for both Ralf Decter and Ralph Decter but found no results.

concludes that the (b)(6) and (b)(7)(C) and Decter evidence significantly damages Dr. Sezen's credibility as to her defenses.

8. The Committee's Findings on the Impact of Dr. Sezen's Actions

The Committee finds that Dr. Sezen's actions had a significant impact on other researchers both within and outside Columbia University. As discussed above, researchers made substantial and futile efforts, with consequent loss of time and expenditure of resources, to reproduce and extend Dr. Sezen's research results.

Two graduate students, (b)(6) and (b)(7)(C) were asked by (b)(6) and (b)(7)(C) to leave his group at the beginning of the third year of their graduate study and one graduate student, (b)(6) and (b)(7)(C) decided to leave the (b)(6) and (b)(7)(C) after passing the second-year qualifying examination. Each of these students had spent much time unsuccessfully trying to reproduce and extend Dr. Sezen's work. (b)(6) and (b)(7)(C) and (b)(6) and (b)(7)(C) have differing recollections as to why the students were either asked to leave or voluntarily left his group. The students believe that their lack of success with Dr. Sezen's chemistry was a major factor, while (b)(6) and (b)(7)(C) says that other factors were determinative. The Committee is not charged to resolve these differing recollections and opinions, but it believes that the wasted time and effort, coupled with the onus of not being able to reproduce the work, had severe negative impacts on the graduate careers of these students.

In addition, other graduate students and post-doctoral fellows, including (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) also expended significant time and effort attempting to reproduce Dr. Sezen's reactions and develop them further. Later, after (b)(6) and (b)(7)(C) initiated his internal investigation into Dr. Sezen's work, (b)(6) and (b)(7)(C)

(b)(6) and (b)(7)(C) expended significant time and effort attempting to determine whether Dr. Sezen's work was valid. Another post-doctoral fellow in the (b)(6) and (b)(7)(C) also contributed to these efforts.

The email correspondence between (b)(6) and (b)(7)(C) and researchers outside Columbia also documents time and effort spent on fruitless attempts to reproduce Dr. Sezen's work. These efforts were made by scientists around the world, including students, faculty, and industry scientists.

CONCLUSION

Upon consideration of the evidence described above, the Committee has reached the following conclusions with regard to the Allegations of Research Misconduct by Dr. Bengü Sezen.

1. Whether Dr. Sezen fabricated NMR spectra in her thesis and publications.

The Committee finds that a preponderance of the evidence shows that Dr. Sezen intentionally fabricated NMR spectra reported in at least Chapters 1, 5, and 6 of the thesis and in the following publications:

1.

5.

(b)(6) and (b)(7)(c)

6.

These publications include the first and the last of Dr. Sezen's first-author papers with (b)(6) and (b)(7)(c) and represent work performed over at least three years of Dr. Sezen's

graduate work at Columbia University. This fabrication of data constitutes a significant departure from accepted practices in the relevant research community.

2. **Whether Dr. Sezen falsified data supporting combustion analyses reported in her thesis and publications.**

The Committee finds that a preponderance of the evidence shows that Dr. Sezen intentionally fabricated and falsified combustion analyses in Chapters 5, 6 and 7 of the thesis and in the following publications:

5.

(b)(6) and (b)(7)(c)

6.

The Committee finds that this falsification and fabrication of data constitutes a significant departure from accepted practices in the relevant research community.

3. **Whether Dr. Sezen fabricated experimental procedures reported in her thesis and publications.**

The Committee finds that a preponderance of the evidence shows that the Research Record maintained by Dr. Sezen does not meet the standards of the scientific research community and does not adequately document the procedures and results reported in her thesis and publications. The Committee could find so little evidence in the Research Record to support Dr. Sezen's published descriptions of results and procedures that it concludes that substantial numbers of the experiments reported in the

thesis and in Dr. Sezen's six first-author publications were never performed successfully as described.[84]

The Committee recognizes that while the first two allegations are based on fabricated or fraudulent reported results, the preponderance of the evidence for the third allegation is based on the absence of documentation in the Research Record. The main uncertainty the Committee faced in reaching its conclusion is the possibility that exculpatory evidence was lost prior to sequestration. However, the Committee finds the evidence for the nonexistence of the additional research materials claimed by Dr. Sezen is so strong that the preponderance of the evidence shows that Dr. Sezen fabricated her experimental procedures.

Recommended Corrective Action

The Committee makes the following recommendations for corrective action:

First, the Committee concludes that, in light of the falsification and fabrication described above, the following papers for which Dr. Sezen is the first author should be retracted or corrected by the authors:

1. (b)(6) and (b)(7)(c)

2. (b)(6) and (b)(7)(c)

3.

4.

(b)(6) and (b)(7)(c)

5.

6.

The Committee notes that (b)(6) and (b)(7)(C) has already taken steps to retract or correct the indicated papers.[85]

Second, the Committee recommends that, in light of the extensive fabrication and falsification described above, and the significant departure from established standards of the relevant research community, Columbia University should initiate a proceeding to revoke Dr. Sezen's Columbia degrees.

Third, as discussed above, the Committee recognizes that a number of researchers at Columbia University were adversely affected by Dr. Sezen's research misconduct, including those who expended substantial effort in attempting to reproduce and extend Dr. Sezen's work (b)(6) and (b)(7)(C) or who conducted the initial investigations of her work in the (b)(6) and (b)(7)(C) and tried to reproduce her results (b)(6) and (b)(7)(C). The Committee recommends, subject to the individual students' approval, that the Chair of the Department of Chemistry provide an addendum to any letters of recommendation written

(b)(6) and (b)(7)(c)

on behalf of these individuals that acknowledges their contributions to the resolution of this case.

The Conclusions and Recommendations of this Ad Hoc Committee do not preclude additional findings that may result from any other investigations of this matter by Columbia University, any agency, or other organization.

Respectfully submitted,

(b)(6) and (b)(7)(C)

Changes Made to the Draft Report

1. On page 3 of the final report, the following paragraph was inserted:
   "The Complainant and Respondent were each provided a copy of a draft of this Report ("Draft Report") and each provided comments to it, which have been separately circulated to the Standing Committee. After receiving these comments, the Committee finalized the Report. Any changes from the Draft Report are documented in an attachment at the end of this Report."

2. On page 25 of the final report, footnote 22 with the following text was added:
   "Also in response to (b)(6) and (b)(7)(C) report, (b)(6) and (b)(7)(C) withdrew a competitive renewal he had submitted to NIH. (b)(6) and (b)(7)(C) (b)(6) and (b)(7)(C) Comments on Draft Inquiry Report dated March 4, 2007)."

3. On page 29 of the final report, the following changes about (b)(6) and (b)(7)(C) grant applications were made to the text:
   "In November 2005, (b)(6) and (b)(7)(C)' competitive renewal was re-submitted. (Exh. L8 at 011464-011472; (b)(6) and (b)(7)(C) Comments on Draft Inquiry Report dated March 4, 2007). (b)(6) and (b)(7)(C) later obtained a supplement award in July 2006. (Exh. L8 at 011474-011480)."

4. On page 48 of the final report, the following language was inserted to reflect the fact that Dr. Sezen never requested the supporting evidence:
   "Fifth, in accordance with Columbia's Policy, this Report has also been provided to Dr. Sezen for comment along with a copy of the Master Index. (Exh. J34 at 013585). Dr. Sezen was also told that the 4,000 pages of supporting evidence would be sent to her once she provided a mailing address. (Exh. J34 at 013574-013584). Dr. Sezen never indicated that she wanted the supporting evidence and did not provide a mailing address."

5. On page 51 of the final report, the following sentence was inserted:
   "She further stated that she obtained the login ID during a course she took entitled 'Chemistry G4145 NMR Spectroscopy,' taught by (b)(6) and (b)(7)(C) (Exh. J15 at 012413)."

6. On page 51 of the final report, footnote 50 with the following text was added:
   "In his interview, (b)(6) and (b)(7)(C) stated that the course did not require an NMR login account, and that the process for obtaining an NMR login account was separate from his course. (b)(6) and (b)(7)(C)

COLUMBIA UNIVERSITY
IN THE CITY OF NEW YORK

OFFICE OF THE EXECUTIVE VICE PRESIDENT FOR RESEARCH
RESEARCH COMPLIANCE AND TRAINING

MEMORANDUM

TO: Sezen File
FROM: (b)(6) and (b)(7)(C)
CC:
RE: Transcript of Interview o (b)(6) and (b)(7)(c)
DATE: May 1, 2007

Through inadvertence, the six-page transcript of (b)(6) and (b)(7)(C) and my interview of (b)(6) and (b)(7)(C), dated Nov. 2, 2006, was not sent to (b)(6) and (b)(7)(C) for review.

(b)(6) and (b)(7)(C)

102 Low Library Mail Code 4312 535 West 116th Street New York, NY 10027 212-854-8123 Fax 212-854-1680 (b)(6) and (b)(7)(c)