

# Investigation Report on Research Misconduct Occurred at Hokkaido University

## I. Background and outline of the investigation

### A. Process from receiving allegation to accepting it

April 1, 2022	The University received the allegation.
April 5	The University acknowledged the allegation after it determined that the allegation of misconduct regarding the articles in question was based on science and other reasonable matters (Article 8 of the Hokkaido University Regulations on Research Misconduct, “the Regulations”).

### B. Outline of the allegation

Nature of the allegation	Fabrication and falsification of data in journal articles	
Respondent	Ronald Lazo Reyes, a former ICRéDD Specially Appointed Assistant Professor *After resigned from the University on May 13, 2022, he was appointed as Associate Professor, Sciences and Mathematics Department, College of Education, Arts and Sciences, National University, Philippines from August 1, 2022.	
Accused articles		
Article 1	Title	Enantioselective Rh- or Ir-catalyzed Directed C(sp <sup>3</sup> )-H Borylation with Phosphoramidite Chiral Ligands
	Published by	Chemistry Letters
	Published on	September 23, 2017
Article 2	Title	Iridium-Catalyzed Asymmetric Borylation of Unactivated Methylene C(sp <sup>3</sup> )-H Bonds
	Published by	Journal of the American Chemical Society
	Published on	April 15, 2019
Article 3	Title	Asymmetric Synthesis of α-Aminoboronates via Rhodium-Catalyzed Enantioselective C(sp <sup>3</sup> )-H Borylation
	Published by	Journal of the American Chemical Society
	Published on	December 10, 2019
Article 4	Title	Asymmetric remote C-H borylation of aliphatic amides and esters with a modular iridium catalyst
	Published by	Science
	Published on	August 21, 2020

### C. Background to the investigation

April 5, 2022	Establishment of the Preliminary Investigation Committee (Article 14 of the Regulations), 1st meeting of the Preliminary Investigation Committee (start of the preliminary investigation)
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April 20	Preliminary investigation results compiled
May 12	Having confirmed the reasonable basis for the allegation and the possibility of misconduct through the preliminary investigation, a decision was made to conduct an investigation (“the Investigation”) to determine whether misconduct had occurred (Article 15 of the Regulations).
May 18	Establishment of the Research Misconduct Investigation Committee (Article 15 of the Regulations), and the provision of notification of implementation of the Investigation and the names of the Research Misconduct Investigation Committee members to the Complainant and the Respondent (Article 17 of the Regulations) *After the Complainant and the Respondent were notified, there were no objections from either concerning the committee members. The opportunity to file an objection was also given to the additional individuals who were subject to investigation, and they filed no objections.
June 17	The 1st meeting of the Research Misconduct Investigation Committee (start of the Investigation)

## II. Investigation

### A. Investigation scheme

The Investigation was conducted by the Research Misconduct Investigation Committee (“the Committee”), which consisted of the following members.

Junji Yamaguchi, Chairperson	Executive Director and Vice President, Hokkaido University	Internal member
Takeshi Aoki	Lawyer, Aoki Law Office	External member
Nobuharu Iwasawa	Professor Emeritus, Tokyo Institute of Technology	External member
Hiroaki Sasai	Professor Emeritus, Osaka University	External member
Kazuki Sada	Dean, Graduate School of Chemical Sciences and Engineering, Hokkaido University	Internal member
Hiroshi Shinokubo	Professor, Graduate School of Engineering, Nagoya University	Internal member *

\*Prof. Shinokubo worked as a part-time lecturer under an employment contract with the Hokkaido University on October 6 and 7, 2022; therefore, he served as an external committee member until October 5 and as an internal committee member from October 6 onward.

### B. Details of the investigation

#### 1. Investigation period

June 17, 2022 to June 9, 2023

#### 2. Targets of the investigation

##### a. Articles investigated

Article 1	Title (Research article)	Enantioselective Rh- or Ir-catalyzed Directed C(sp <sup>3</sup> )-H Borylation with Phosphoramidite Chiral Ligands
	Published by	Chemistry Letters
	Published on	September 23, 2017
Article 2	Title (Research article)	Iridium-Catalyzed Asymmetric Borylation of Unactivated Methylene C(sp <sup>3</sup> )-H Bonds

	Published by	Journal of the American Chemical Society
	Published on	April 15, 2019
Article 3	Title (Research article)	Asymmetric Synthesis of $\alpha$ -Aminoboronates via Rhodium-Catalyzed Enantioselective C(sp <sup>3</sup> )-H Borylation
	Published by	Journal of the American Chemical Society
	Published on	December 10, 2019
Article 4	Title (Research article)	Asymmetric remote C-H borylation of aliphatic amides and esters with a modular iridium catalyst
	Published by	Science
	Published on	August 21, 2020
Article 5	Title (Review article)	An Introductory Overview of C-H Bond Activation/Functionalization Chemistry with Focus on Catalytic C(sp <sup>3</sup> )-H Bond Borylation
	Published by	KIMIKA
	Published on	May 13, 2021
	Remarks	*This article was targeted for the investigation because it is a review article that summarizes the findings of previous studies in the field, including research articles 1 through 4.

b. Individuals investigated, and reasons for their inclusion in the investigation

Names of individuals investigated and affiliations (At the start of the investigation)	Reasons for inclusion in the investigation
Ronald Lazo Reyes, former Specially Appointed Assistant Professor, ICRReDD, Hokkaido University	He was the first author on all articles in question and is the Respondent. He admitted in the preliminary investigation that he had manipulated data in some of the articles.
Masaya Sawamura, Professor, Faculty of Science; principal investigator, ICRReDD, Hokkaido University	He was the corresponding author on all articles in question.
X, Professor, Faculty of Science; Director, ICRReDD, Hokkaido University	X was the corresponding author of article 2 in question.
Y, Lecturer, Graduate School of Arts and Sciences, the University of Tokyo* *Assistant Professor, Faculty of Science, Hokkaido University until October 2020	Y was the co-author on all articles in question and was judged to be the author most familiar with the conditions when the experiments were conducted and the articles were written in a closer position to the Respondent compared to the corresponding authors.
Z, Doctoral student, Hokkaido University	Z was the co-author of articles 3 and 4 in question and had conducted the experiments together with the Respondent.

None of them above has ever been subject to any debarment from competitive research funding from the government for involvement in misconduct.

### 3. Investigative methods/procedures and committee meetings held

• The 1 <sup>st</sup> committee meeting (June 17, 2022, 14:00-16:00)	Confirmation of the nature of the allegation and the results of the preliminary investigation, and determination of the method of the Investigation
• The 2 <sup>nd</sup> committee meeting (August 2, 14:00-16:20)	Determination of the guidelines for conducting a hearing, confirmation of expenditures directly related to the articles, and determination of the methods for scrutinizing the articles
• Implementation of document investigations on corresponding authors and a co-author	
• Implementation of close examination on the articles	
• The 3 <sup>rd</sup> committee meeting (August 24, 13:30-17:00)	Implementation of hearings with corresponding authors and a co-author
• The 4 <sup>th</sup> committee meeting (October 3, 14:30-16:30)	Authorization of expenditures directly related to the articles, and confirmation of the results of close examination on the articles
• The 5 <sup>th</sup> committee meeting (email-based) (October 28 - November 2)	Deliberation regarding the need for further implementation of hearings with corresponding authors and co-authors
• Implementation of document investigation on the Respondent	
• The 6 <sup>th</sup> committee meeting (November 21, 13:30-15:30)	Implementation of a hearing with the Respondent, deliberation on the necessity of conducting another round of hearings with co-authors
• Implementation of document investigations on a corresponding author and co-authors	
• The 7 <sup>th</sup> committee meeting (December 21, 13:30-17:30)	Implementation of hearings with a corresponding author and co-authors, deliberation on changes to the approved details of expenditures directly related to the articles, finalization of the judgment regarding each of the articles, and identification of research misconduct and management responsibility
• The 8 <sup>th</sup> committee meeting (email-based) (January 11 - 16, 2023)	Deliberation on changes to the approved details of expenditures directly related to the articles
• The 9 <sup>th</sup> committee meeting (email-based) (May 31 - June 9)	Deliberation and decision on an investigation report

#### \*Appeal Procedures

After the committee's judgement, the Individuals investigated appealed in accordance with formal procedures. The committee examined the contents of appeals at the 10th committee meeting held on August 3, 2023 and the 11th committee meeting held on August 24 - 30, 2023 by email, and decided to partially revise the statements to the extent that it does not affect the degree of the judgement on research misconduct or the conclusions, although no need for a re-investigation was approved.

### III. Results of the investigation

#### A. Definitions at the University

The University defines research misconduct, fabrication, and falsification as follows (Article 2 of the Regulations).

- Research misconduct is defined as any act in research committed by executives and staffers affiliated with the University and others engaged in research at the University with intention or who seriously fail to use reasonable care as a researcher.
- Fabrication means the making up of data or research results that do not exist.
- Falsification means the manipulation of research materials, equipment or processes or changing data or results such that the research is not accurately represented in the research record.

#### B. Types of misconduct identified

With regard to the data in the main text of articles 1 through 4 and the figures and data in each supporting information (SI) that were related to Mr. Reyes, two committee members for each article based on their expertise examined the raw data in the lab notebooks and research reports of Mr. Reyes and Z that were submitted by Mr. Sawamura, as well as examining the raw experimental data, such as high-performance liquid chromatography (HPLC) charts, various nuclear magnetic resonance (NMR) charts, and their FID files, that was submitted by Mr. Sawamura after he had checked that data at his own lab. Then the Committee came to the consensus that misconduct of fabrication and/or falsification had occurred.

The committee also identified as fabrication a case in which the lab notebooks describe that some experiments were conducted but the results were not recorded, while the main text of the article or its SI describes experimental results whose basis cannot be verified.

Meanwhile, article 5 was not subject to close examination because it was a review article that summarized the findings of previous research in the field, including research articles 1 through 4, and it did not report original or unpublished research results as a research article; however, fabrication and/or falsification were identified for the article as well in accordance with the above-mentioned identification.

The misconduct identified above is defined by the MEXT as specific misconduct of fabrication and/or falsification. It is important to note that there were no other acts that should be identified as misconduct (e.g., plagiarism, duplicate submission, and inappropriate authorship) for articles 1 through 5.

- Number of figures identified as misconduct\*

	Article 1	Article 2	Article 3	Article 4
Fabrication	55	54	209	201
Falsification	27	85	95	110

\*The total number of figures identified as misconduct exceeds the total number of figures in the article and its SI because the figures were subdivided according to the type of data in the scrutiny of the figures.

\*The number of figures identified as misconduct for Article 5 is not shown because it is duplicated in articles 1 through 4.

- Number and percentage of figures where the misconduct was identified

	Article 1	Article 2	Article 3	Article 4
Number of figures identified as fabricated (A percentage of (a) below)	15 (26.8%)	17 (18.1%)	81 (40.7%)	79 (35.9%)
Number of figures identified as falsified (A percentage of (a) below)	14 (25.0%)	44 (46.8%)	69 (34.7%)	98 (44.5%)
(Ref.) (a): Number of figures in the article and its SI	56	94	199	220

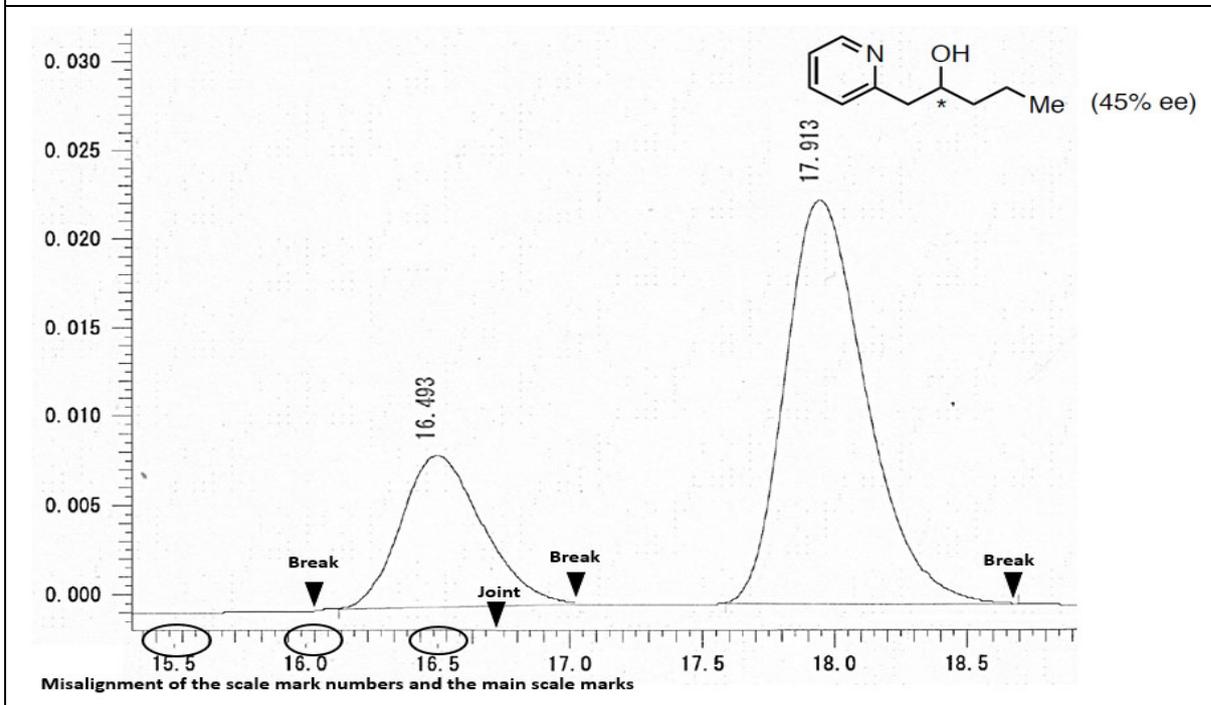
The following are sections that would not have been included in the articles if the experimental and other data had been properly verified prior to submission for publication.

	Examples of data deficiencies/error or fraud determined to have been overlooked due to inadequate pre-publication check
Article 1	<ul style="list-style-type: none"> <li>• The spectra of some compounds cannot be identified as alcohols are presented.</li> </ul>
Article 2	<ul style="list-style-type: none"> <li>• Some NMR charts of apparently different compounds are shown in its SI.</li> <li>• Some of the data are unnatural because a J-coupling analysis tool was used.</li> <li>• Some of the data counted noise associated with the singlet.</li> <li>• Some data are processed such that signals and peak values in the chart do not match, retention time or scale is skipped, or there are unnatural intervals or joints.</li> </ul>
Article 3	<ul style="list-style-type: none"> <li>• There are many peaks that are difficult to attribute in the synthesis of racemic compounds.</li> <li>• Some of the NMR data are not properly read in the aromatic region.</li> <li>• Some of the chemical shifts of the proton at the root of the boron and the piperidine ring moiety are unnatural.</li> <li>• The starting points of integrations are partially misaligned.</li> <li>• The spectra of some compounds have unnatural breaks or seams, and there are traces of processing on the integration lines.</li> </ul>
Article 4	<ul style="list-style-type: none"> <li>• Spectra with insufficient identification of compounds are presented.</li> <li>• Some spectra were processed and spliced, and some of the peak shapes and baselines are unnatural.</li> </ul>

- Examples of apparent misconduct
  - Article 1

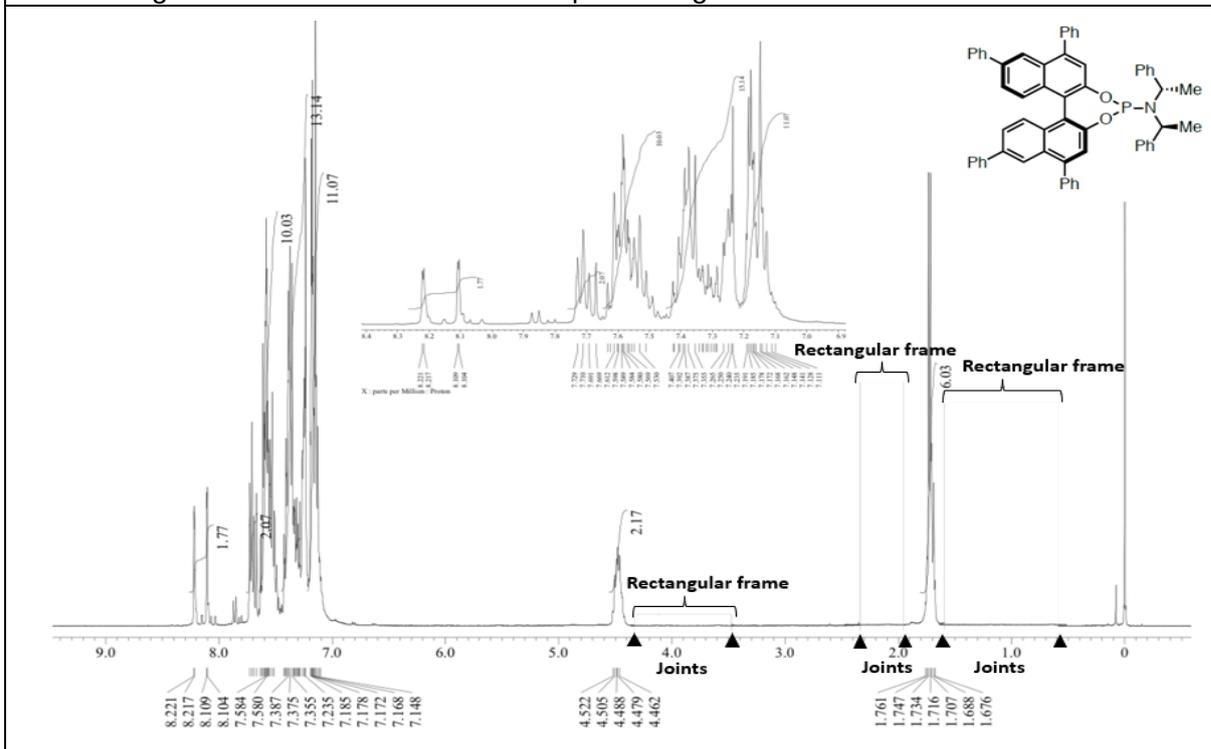
Example 1: Supporting Information S20 Enantioenriched 6a

On the chart, which should be plotted as a single line, there are blanks that are evidence of processing, as well as misalignment of the major scale marks and main axis numbers that would not be seen if it were a measurement file.



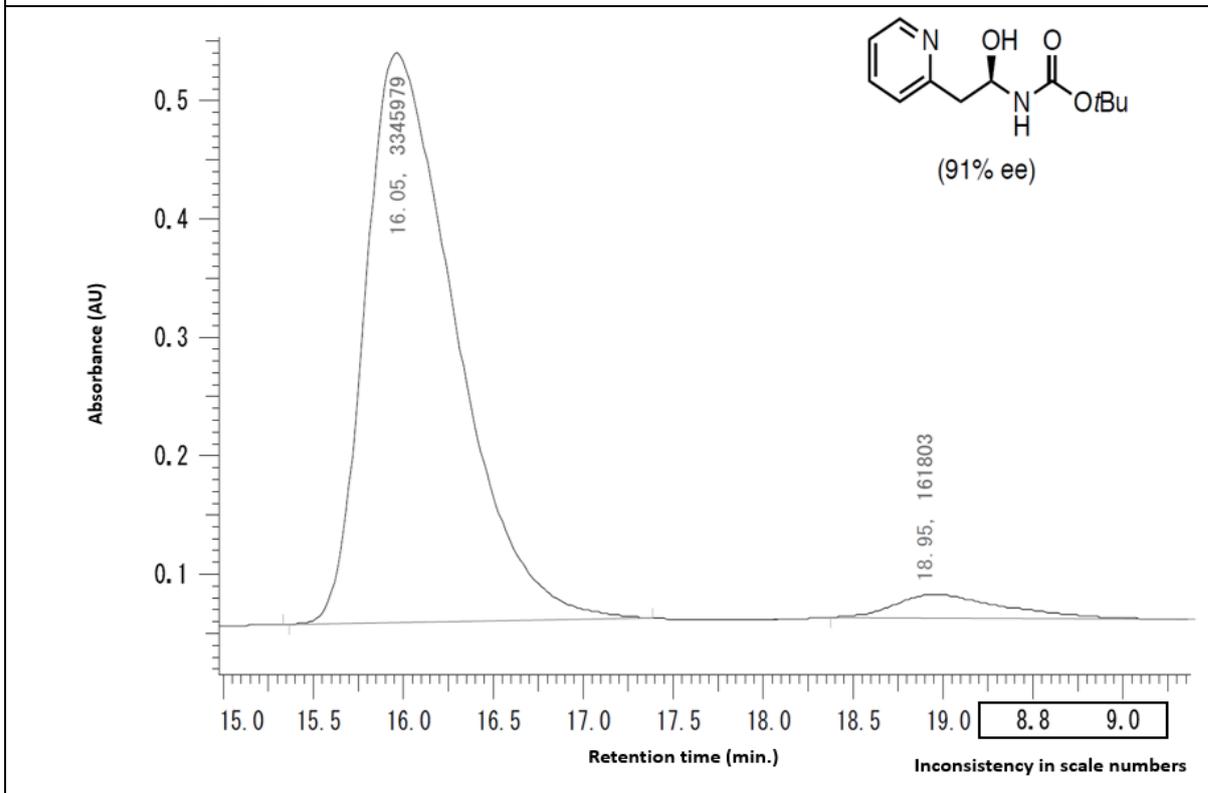
Example 2: Supporting Information S23 <sup>1</sup>H NMR spectrum of (S,S,S)-L11 in CDCl<sub>3</sub>

On the chart, which should be plotted as a single line, there are joints of two overlapping lines and rectangular frames that are evidence of processing.



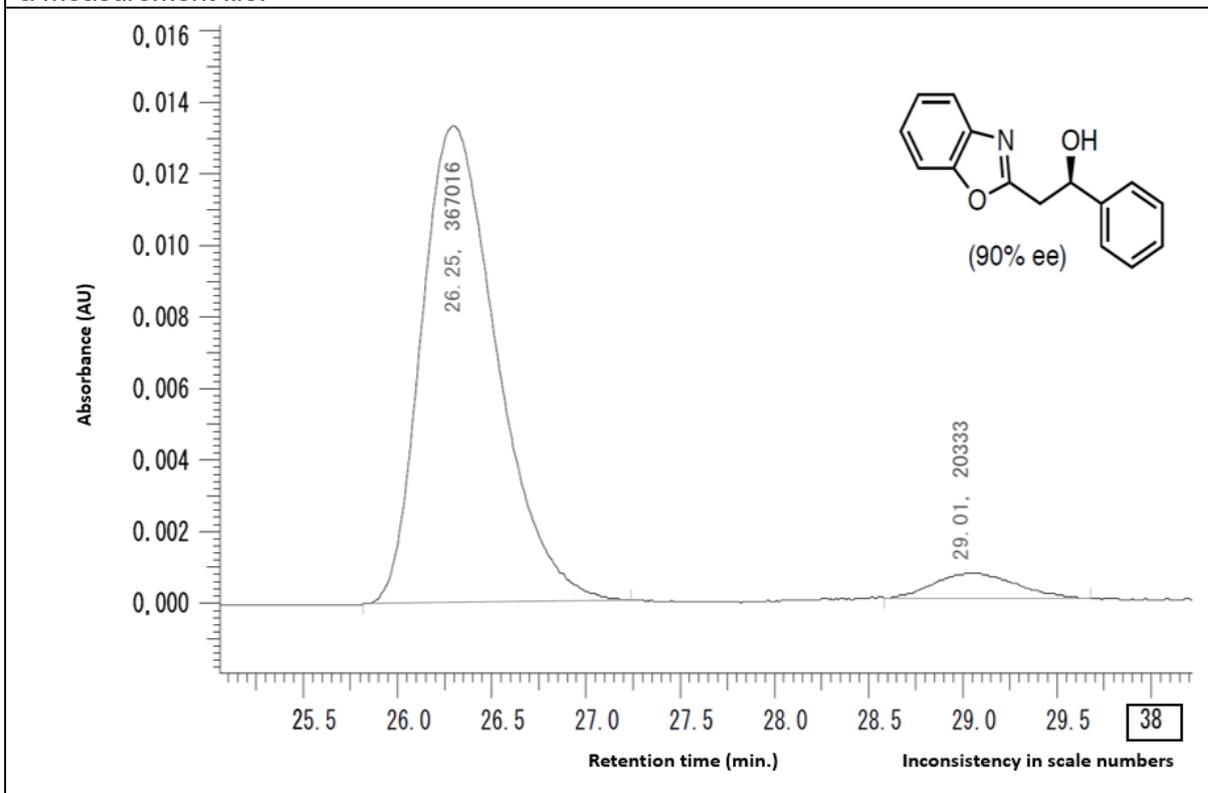
Example 1: Supporting Information S48 (S)-4f

There is a row of unnatural numbers on the main scale marks that would not be seen if this were a measurement file.



Example 2: Supporting Information S58 (R)-4p

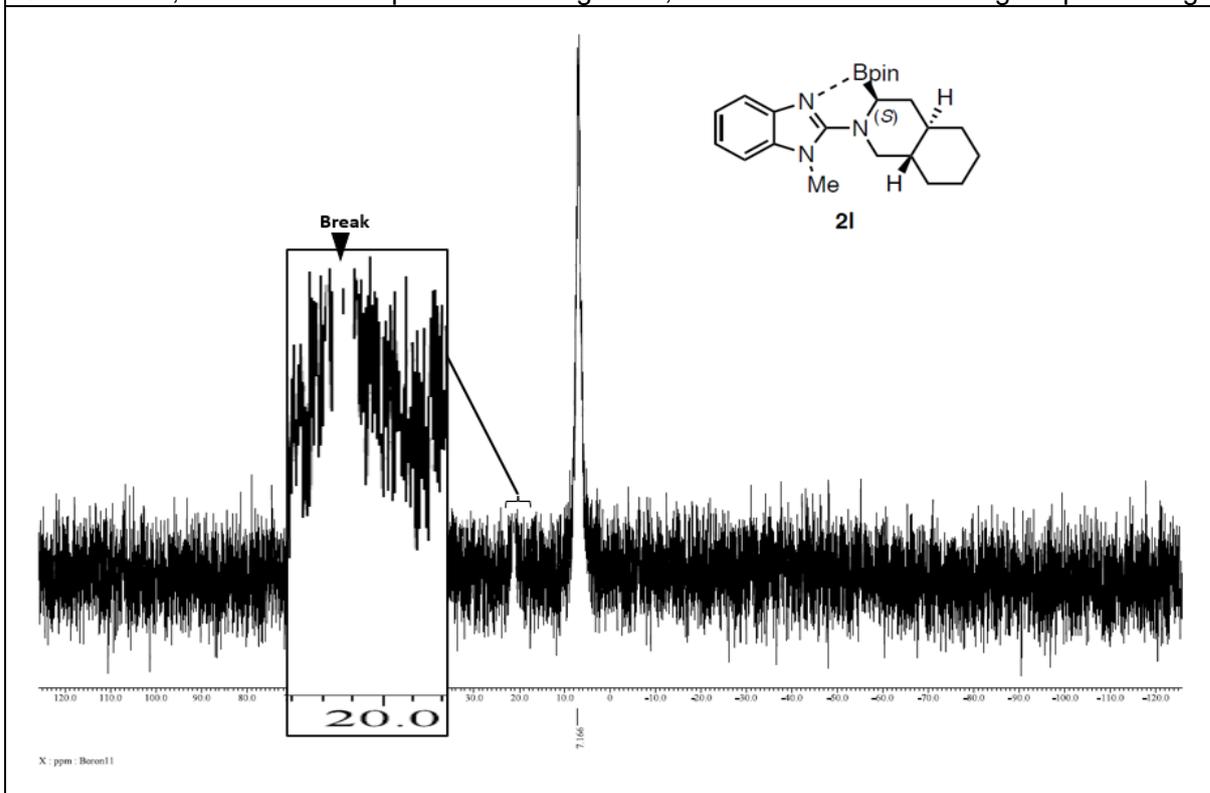
There is a row of unnatural numbers on the main scale marks that would not be seen if this were a measurement file.



· Article 3

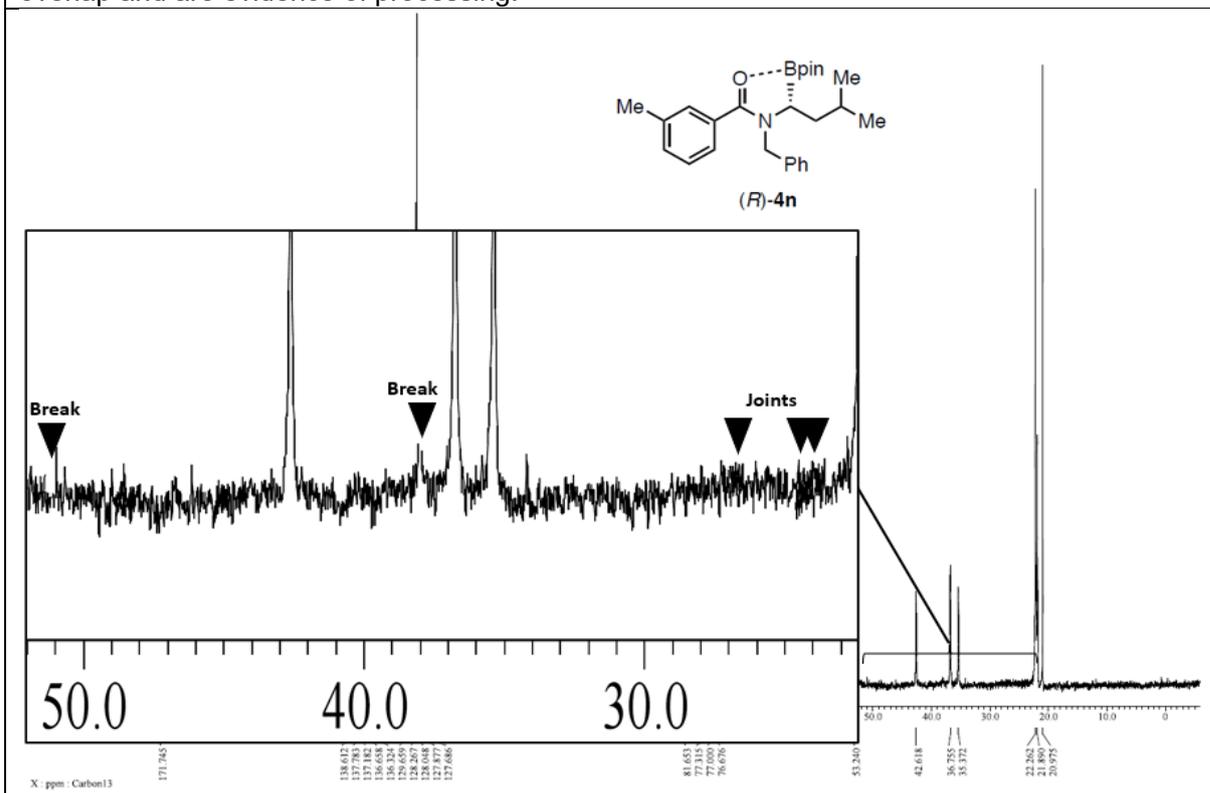
Example 1: Supporting Information S115  $^{11}\text{B}$  NMR spectrum of 2l in  $\text{CDCl}_3$

On the chart, which should be plotted as a single line, there is a blank that is a sign of processing.



Example 2: Supporting Information S135  $^{13}\text{C}$  NMR spectrum of (R)-4n in  $\text{CDCl}_3$

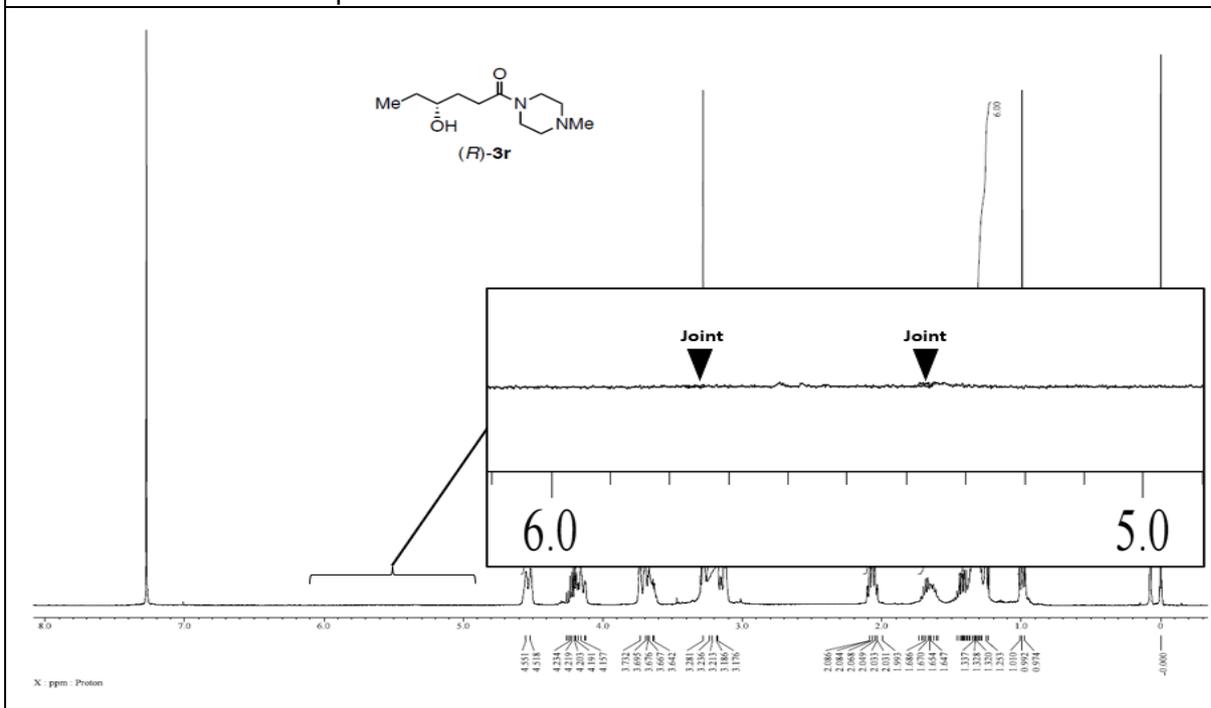
On the chart, which should be plotted as a single line, there are blanks and joints where two lines overlap and are evidence of processing.



· Article 4

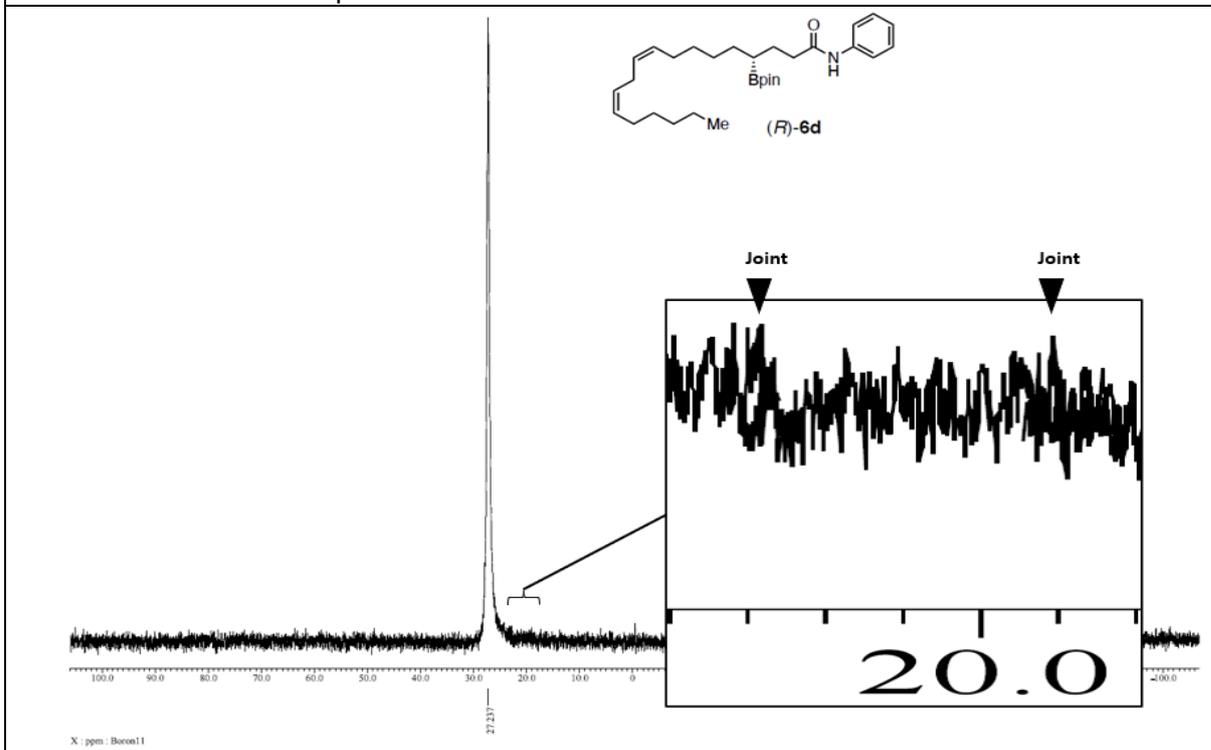
Example 1: Supporting Information S170  $^1\text{H}$  NMR spectrum of (R)-3r in  $\text{CDCl}_3$

On the chart, which should be plotted as a single line, there are joints where two lines overlap that are evidence of manipulation.



Example 2: Supporting Information S196  $^{11}\text{B}$  NMR spectrum of (R)-6d in  $\text{CDCl}_3$

On the chart, which should be plotted as a single line, there are joints where two lines overlap that are evidence of manipulation.



C. Articles in which misconduct was found

Articles 1 – 5 listed in II. B. 2. a. were identified as the articles emanating from the research where the misconduct was found.

D. Identification of the individual engaged in the misconduct, and the grounds for the decision

1. Individual identified as engaged in the misconduct:

- Ronald Lazo Reyes (Researcher No. 30845475), a former Specially Appointed Assistant Professor, ICRReDD, Hokkaido University

General grounds and background for the decision

- Mr. Reyes was responsible for the overall research and the preparation of the first draft of article 1 and for the overall research and the finishing touches from the first draft to the final draft of articles 2 through 4. He played the following roles in preparing the articles.

Article 1:

- The experiment started in October 2015, and he conducted the overall experiments under the guidance of Y. He had discussions with Y on a daily basis and with Mr. Sawamura every couple of weeks.
- The first draft of the article and its SI were prepared in August 2017. After confirmation and revision by Y, the article was revised by Mr. Sawamura. It was submitted to *Chemistry Letters* in September and was published in that journal on the 23rd of that month.

Article 2

- The experiment started in October 2015. He played the same role as in article 1, together with Mr. Sawamura and Y.
- The first draft of the article and its SI were prepared in May 2018, and these were reviewed and revised by Y, followed by revisions by Mr. Sawamura.
- The article was submitted to *Journal of the American Chemical Society* in February 2019 and was published in that journal on April 15, 2019.

Article 3

- Since the experiment started in October 2015, he played the same role as in article 1, together with Mr. Sawamura and Y.
- The first draft of the article was prepared in April 2019. After confirmation and revision by Y, it was revised by Mr. Sawamura. Its SI was prepared in September. After confirmation and revision by Y, it was revised by Mr. Sawamura. The article was submitted to *Journal of the American Chemical Society* in November and was published in that journal on December 10, 2019.

Article 4

- Since the experiment started in February 2019, he played the same role as in article 1, together with Mr. Sawamura and Y. While Y was on a two-month leave of absence beginning February 1, 2020, the confirmation and revising work was done online and by email, which relatively increased the weight of guidance by Mr. Sawamura.

- The first draft of the article was prepared in March 2020, and it was checked and revised mainly by Mr. Sawamura. Its SI was prepared in the same month. After confirmation and revision by Y, it was revised by Mr. Sawamura. The article was submitted to *Science* in May, and it was published in that journal on August 21, 2020.

As a result of comparing and verifying the experimental results described in each article with the lab notebooks of Mr. Reyes, who was the first author, numerous cases were identified in which the experimental results were not recorded in the lab notebooks, or the numerical values of the experimental results were falsified.

Mr. Reyes and other members of the Sawamura lab were instructed to record and manage the results of their experiments in their own lab notebooks, and Mr. Reyes was exclusively responsible for preparing his lab notebooks. The individuals under investigation other than Mr. Reyes unanimously stated that they did not check every single experimental result and raw data, such as NMR charts, described in Mr. Reyes' lab notebooks. Meanwhile, Mr. Reyes himself admitted that in some cases he did not record the results of the experiments in his lab notebooks, or that in some cases he gave different values. The fact that all individuals under investigation except Mr. Reyes stated that they were unaware of any fabrication or falsification committed by him also led to the conclusion that Mr. Reyes was solely responsible for the process of creating meeting materials based on values that were not based on experimental results or were not included in the lab notebooks and then presenting them as experimental results in the manuscript of the articles.

It was also confirmed that Z, the co-author, had frequent discussions and joint experiments with Mr. Reyes on parts of articles 3 and 4. Z, who was then a student at the University (article 3) or was a master's student at the University (article 4), testified that (1) Z was in a position to receive guidance from Mr. Reyes, (2) Mr. Reyes was given raw data such as NMR charts by Z and had free access to such data, (3) Mr. Reyes was also in charge of storing experimental results, (4) Mr. Reyes was in charge of preparing all data sheets (in the Sawamura lab format that organizes synthetic methods, physical property data, and other information for each compound), and (5) Z did not check the content before submitting the articles. Meanwhile, Mr. Reyes stated that he checked the experimental results given to him by Z, and if they differed from his own "experimental results," he obtained Z's approval and adopted his own "experimental results." In light of this testimony, it can be determined that the parts of the results of the experiments conducted by Z with Mr. Reyes in articles 3 and 4 that are not authentic were also prepared solely by Mr. Reyes.

Based on the above, it was determined that the circumstances under which the experimental results described in articles 1 through 4 were not recorded in his lab notebooks or were processed improperly resulted solely from the act of Mr. Reyes himself.

- Regarding the results of the experiments described in the articles, Mr. Reyes reiterated his assertion that although he noted in his lab notebooks that he had conducted the experiments,

he often recorded the results on different paper media than the lab notebooks. However, since none of the paper media were submitted, it was not possible to find any basis for Mr. Reyes' assertion.

Furthermore, Mr. Reyes finally stated that he was unable to submit those other paper media because he had accidentally discarded them himself, but he gave only a very vague defense as to when and how he did so. The period that Mr. Reyes claimed to have recorded on separate paper media covers the period from October 2015 to March 2020, when articles 1 to 4 were prepared, and the instances of misconduct have been identified as numbering 836: 519 fabrications and 317 falsifications. The amount of materials involved is presumably enormous. The excuse that Mr. Reyes, who should have been fully aware of the necessity of preserving materials based on the rules of the lab, mistakenly destroyed all those separate paper media was peculiar and not credible.

- While Mr. Reyes stated in his defense that there were cases where he accidentally rewrote the scales of figures on the scanned files to the incorrect ones for better visibility or he tried to remove some peaks due to possible contamination and some unwanted minor peaks in spectrum by placing annotations, he was not aware of any wrongdoing in a series of alleged acts. He also stated that it was partly due to his own carelessness, and he repeatedly denied allegations of misconduct. However, active intent to fabricate or falsify is not necessary to constitute misconduct. In the case of fabrication, a researcher who recognizes that he/she has described in the article experimental results that do not exist, or in the case of falsification, a researcher who recognizes that he/she has altered the experimental results and described in the article something that is not authentic will be held liable for intentional misconduct. Furthermore, as stipulated in Article 2 of the Regulations, if fabrication or falsification results from a significant failure to exercise one's basic duty of care as a researcher, then the researcher shall also be held liable for intentional misconduct.

Mr. Reyes himself admitted that he had heard about how to make lab notebooks and manage experimental data at the beginning of each semester, when he was briefed by Mr. Sawamura on the lab and related matters in a group meeting format. Y also stated that he/she instructed Mr. Reyes by providing copies of his/her own lab notebooks as samples. Mr. Sawamura stated that lab-designated notebooks were used by all lab members and remained as the property of the lab. He also noted that he had instructed all lab members to record all matters related to experiments, including experimental results, in their lab notebooks, and to never allow any data other than raw data from measurement instruments, such as NMR charts, to be left on any other media.

Based on the situation of guidance on research in the lab described by Mr. Sawamura and Y and based on the fact that Mr. Reyes himself stated that the results of any experiment must be recorded in a lab notebook, otherwise suspicion of misconduct would arise, it can be determined that Mr. Reyes was aware that the results of his experiments needed to have been based on the original experimental results recorded in the lab notebooks when he

wrote the results in articles 1 through 4.

As mentioned above, since Mr. Reyes gave the defense that he left some experimental results on different paper media than the lab notebooks and he admitted that these results differed from what he wrote in the lab notebooks, he was fully aware that he included “experimental results” in each article that were not present in the lab notebooks or that differed from those in the lab notebooks. Therefore, it was determined that Mr. Reyes is liable for willful misconduct regarding the fabrications and falsifications identified in articles 1 through 4.

- Even if Mr. Reyes mistakenly believed that recording the experimental results on separate paper media would serve as a substitute for the lab’s prescribed experimental notebooks, there is no compelling reason to believe that such an alternative method of recording would be acceptable in the preparation of the four articles over a long period of time, in light of the instructional situation in the lab. Therefore, he cannot be absolved of responsibility for willful misconduct.

Recording in a lab notebook is a rule of the lab. If he violated this rule and chose a preservation method with a risk of loss, failed to record in the lab notebooks, and discarded all paper media as replacements, it must be said that he seriously neglected his basic duty of care as a researcher, which resulted in fabrication and falsification. From this point, it can be concluded that he committed willful misconduct.

- Mr. Reyes also claimed that the physical and mental strain of working long hours on his research at the time, the pressure he put on himself to finish the articles before the lab closure due to the COVID-19 pandemic, and his personal issues were all factors in the misconduct that he is accused of. However, none of these can be said to be unavoidable circumstances under which misconduct can be tolerated. In particular, the WHO announced the pandemic on March 11, 2020, which was when the first draft of article 4 was submitted and did not coincide with the preparation of articles 1 through 3. It thus was not considered a circumstance to be taken into account in recognizing responsibility for misconduct.
- Article 5 is a review article that summarizes the findings of previous studies in the field concerned. Mr. Reyes took the role of writing texts and drawing pictures as its first author, and he cited articles 1 through 4 as examples of previous studies. Since he was found liable for willful misconduct with regard to the content of each article identified as fabrication or falsification as described above, Mr. Reyes cannot be exempted from liability for willful misconduct concerning article 5.

Severity of the specific misconduct: ‘Critical’ **Severe** ‘Moderate’ ‘Low’

Grounds for the decision:

Articles 1 and 2 were written when Mr. Reyes was a doctoral student at the University, article 3 when he was a doctoral student and then a postdoctoral fellow, and article 4 when he was a

postdoctoral fellow and then a specially appointed assistant professor, under the guidance of Mr. Sawamura and Y. Therefore, it cannot be recognized that the corresponding author in a leadership position committed the misconduct.

In the case of article 1, Mr. Reyes took over research that had been conducted by another student, and he conducted the experiments himself. As such, it cannot be said that Mr. Reyes intended to commit misconduct from the very beginning of the research. However, the data and figures in the final article were written by Mr. Reyes. Since there are parts of the article that were identified as fabricated or falsified, it was determined that Mr. Reyes committed misconduct in the process of writing the article.

He was the first author of the subsequent articles 2 through 4 and was responsible for the overall research and completion from the first draft to the final draft. Accordingly, it was likewise determined that Mr. Reyes was the author responsible for the content of the articles.

Numerous instances that reflect misconduct can be seen in all articles 1 through 4 over multiple years, and as indicated before, the scale of the misconduct is not small, so it cannot be said that it was not a significant part of each article, and it must be said that it affects the conclusion of the articles. It is noted above that this misconduct was intentionally committed by Mr. Reyes.

Based on the above, the degree of severity of the specific misconduct by Mr. Reyes was judged to be 'severe' in the Guidelines for Appropriate Execution of Competitive Research Funds provided by the Inter-Ministry/Agency Liaison Group Regarding Competitive Research Funds (all judgment results below are based on the same guidelines).

Impact of the misconduct on the progress of research in the same field and society:

'Severe' 'Moderate' 'Low'

Grounds for the decision:

As mentioned above, the experimental results identified as reflecting misconduct in articles 1 through 4 are numerous, and many of them are apparently important parts of the articles and affect their conclusions. If they were authentic, they would have been of high academic value. Accordingly, it was determined that their impact on the progress of research in the same field addressed by the articles is severe. In particular, the results of article 4 were widely publicized by Mr. Sawamura, who sent out a press release through the University's Public Relations Office at the time the article was published in *Science*, because of the expected contribution to a sustainable society through the conversion of biomass to useful chemical materials. If the content had been authentic, its academic value would have been high. Mr. Sawamura testified that the article advocated research results with a high degree of academic novelty, and Y testified that the research viewpoints and ideas in the article were novel, although they were no longer novel as research results due to the withdrawal of the article.

The impact factor (IF) of a journal does not always accurately reflect the actual number of citations of an article itself; therefore, it is not necessarily an indicator for evaluating an article

or its author. The latest data show that the number of citations of the articles ranges from a low of 42 (article 1) to a high of 74 (article 2) and that the IF of the journals ranges from a low of 1.715 (article 1) to a high of 63.832 (article 4) while each journal's distribution range differs; but overall, it was concluded that the social impact of the misconduct is also severe.

Based on the above, it was judged that the degree of impact of the specific misconduct on the progress of research in the said field and society is 'severe'.

2. Individual identified as not engaged in the misconduct but as being responsible for the content of the articles emanating from the research where the misconduct was found:

- Masaya Sawamura (Researcher No. 40202105), Professor, Faculty of Science, Hokkaido University; Principal Investigator, ICR/DD

Management responsibility as the author responsible for the content of the article:  
'Severe' 'Moderate' 'Low' 'None'

Grounds for the decision:

- Mr. Sawamura, who was the corresponding author of articles 1 through 4, stated that Mr. Reyes was exclusively responsible for the experiments and the draft preparation and he left the direct supervision of Mr. Reyes to Y while he himself had discussions with Mr. Reyes and others every two to three weeks. He also noted that he first became aware of the possibility of misconduct by Mr. Reyes on March 26, 2022, when a member of his lab who was not the author of any article in question pointed out that Mr. Reyes stated that he just manipulated data and did not explicitly admit to any misconduct, but he also noted that his co-authors were not aware of any data that was not recorded in his lab notebooks nor were they aware of some sections containing data that differed from the data in his lab notebooks. Accordingly, it was determined that Mr. Sawamura was not involved in the misconduct.
- As the corresponding author, Mr. Sawamura was obligated to verify the scientific validity and reproducibility of the raw data of measurements and other experimental results by the first author and other co-authors, and to take care to ensure that there was no research misconduct. In addition, as the principal investigator (PI) of the lab to which Mr. Reyes belonged, he is in a position to supervise the students in the lab and has supervisory responsibility for preventing misconduct.
- Mr. Sawamura provides instructions at meetings on how to conduct research, prepare lab notebooks, collect, and organize experimental data, and write articles. For experimental results, he explained that a data sheet in the lab's own format is prepared, in which synthetic methods, various spectral data, and physical property data are organized for each compound with the corresponding experiment number, and the symbols corresponding to the file names of the measured data are written in the experimental notebook. In this way, a system is established to link data sheets → experimental notes → spectral and physical property data, and the data sheets must be used to prepare an article and its SI, and each data entry must be handwritten.

Despite these rules, Mr. Sawamura only confirmed the figures in the documents Mr. Reyes

submitted at the meetings. Since there are many discrepancies between the numerical values in the lab notebooks and the experimental results or data not recorded in the lab notebooks in article 1 through 4, it was determined that he little followed the above process to check the lab notebooks, spectra, and other data, nor did he perform a final check before submitting the articles. Mr. Sawamura entrusted Y to check each data sheet of the article, trusted that his/her checking was sufficient, and did not check the data sheets himself. He assumed that others were confirming whether the data sheets were submitted. Later, with regard to article 4, he partially revised his defense by saying that he remembered that he had carefully checked the regioselectivity of the borylation reaction, a new reaction, based on spectral and other data.

In this case, as mentioned above, extremely large numbers of fabrications and falsifications were made over a long period of time. It is inconceivable that such misconduct could not have been noticed if the confirmation work to trace the raw data had been properly conducted at each stage of article preparation. Mr. Sawamura explained that he did not notice anything suspicious because of the clever fabrication and falsification committed by Mr. Reyes, but the fact that the data itself, which is the basis of the articles, was riddled with problems, regardless of whether it had been manipulated, clearly shows that the data confirmation was inadequate. Among other things, it has been confirmed that in articles 1 and 2, there are cases where NMR charts of apparently different compounds are shown in their SIs. Since these are presumably the raw materials for the reactions, it can be considered that Mr. Sawamura did not conduct the necessary verification of the scientific validity of the experimental results, which is his responsibility as a PI and a corresponding author.

Mr. Reyes' lab notebooks contain numerous sections without entry dates or experiment numbers, as well as numerous blank pages with no descriptions of the experiments. Thus, the beginning of the misconduct could be easily realized as a formal violation of the rules without the need for elaborate confirmation. Since misconduct of this magnitude can be confirmed in the four articles over a long period of time, it must be said that the obligation to confirm has been neglected.

Mr. Sawamura stated that he entrusted Y and other co-authors as well as members of his lab with the checking of the article data, and that he relied on their confirmation as sufficient. However, a corresponding author and a PI for an article are those who are in a position to bear the ultimate responsibility after they have confirmed the authenticity of the entire article prepared by the co-authors based on their experiences, abilities, positions, and authority as researchers; entrusting the confirmation work to co-authors or lab members does not reduce their own responsibility or relieve them of their obligation to confirm the work. If, in their own judgement, they entrusted the performance of the confirmation work to another person, then the corresponding author and the PI must naturally be held responsible for that person's failure to perform the work.

Mr. Sawamura only explained that he thought that Y and others were checking the articles, but it was not confirmed that he gave instructions for confirmation work, received regular reports on the results, or performed final confirmation before submitting the articles for publication. Since Mr. Sawamura was not deemed to have exercised due care with regard to the work performed by them, no reason was found to exempt him from liability.

- The misconduct by Mr. Reyes can be seen in all articles 1 through 4. In other words, there was a long period of continued wrongdoing by Mr. Reyes, from October 2015 to May 2020, from article preparation to submission for publication. As a result, it has created a situation that can be called “routinized success in misconduct.” This is consistent with Mr. Sawamura’s statement that he gradually stopped pointing out issues with the content of the experimental data and other content of articles or instructing Mr. Reyes, as Mr. Reyes progress in his career from a student to a postdoctoral fellow to a specially appointed assistant professor.

When Mr. Sawamura recognized that there were experimental results that could not be reproduced by Z or other students after the articles 3 and 4 were published, before he knew of the possibility of misconduct, he considered that the results would be obtained if the experiment was reproduced correctly. He stated that difficult-to-reproduce cases often arise in other studies as well. Accordingly, it can be said that he did not take appropriate measures, such as performing his own checks.

Mr. Sawamura was also the corresponding author of article 5, which cited articles 1 through 4 and summarized the findings of previous studies in the same field as a review article. When doing so, he was required to confirm each article’s content; however, as mentioned above, he neglected his duty to check it. As such, it was determined that Mr. Sawamura also failed in his duty regarding article 5.

In light of this, it must be concluded that he was grossly negligent in his duty of care as a corresponding author and a PI who should have prevented the misconduct.

Even considering that Mr. Sawamura requested each journal to withdraw each article and that he cooperated with the Investigation, his breach of duty of care as a corresponding author and a PI was still serious. Therefore, it was determined that his management responsibility as an author responsible for the content of the articles was ‘severe’.

3. Individuals identified as not engaged in the misconduct nor as being responsible for the content of the articles emanating from the research where the misconduct was found:

- a. X, Professor, Faculty of Science, Hokkaido University; Director, ICReDD

Management responsibility as the author responsible for the content of the articles:

‘Severe’ ‘Moderate’ ‘Low’  ‘None’

Grounds for the decision:

- X was responsible for the part of articles 2 and 4 that described theoretical calculations. However, the misconduct by Mr. Reyes was related to the presence/absence or the modification of experimental results in the experimental science part of the articles, which

differs from the computational science part involving X. Mr. Reyes stated that he just manipulated data and did not explicitly admit to any misconduct, but he also noted that his co-authors were not aware of any data that was not recorded in his lab notebooks nor were they aware of some sections containing data that differed from the data in his lab notebooks. Accordingly, it was determined that X was not engaged in the misconduct.

- X initiated a joint research project with Mr. Sawamura, in which roles are shared between the experimental science group and the computational science group. Since he/she was responsible for the latter, X had no knowledge of the portions of the articles written by the former, based on the understanding that Mr. Sawamura responsible for the former would naturally judge the appropriateness of the content and results of the experiments conducted by the former. Theoretical calculations are not completely accurate, as approximations come into play. In articles 2 and 4, the discrepancies were not that large at the level of approximation. When experimental and calculated results do not match, researchers move toward the idea that there may be some deficiency on the part of the calculations. Thus, X did not suspect any misconduct regarding the experimental results until there was clear evidence pointing to it. X stated that he/she did not examine the results of individual experiments in assuming that the experimental results did not include data involving misconduct. X also mentioned that he/she had no expertise to verify the results.

Considering X's position in this joint research, it is difficult to hold him/her accountable for directly suspecting the existence of misconduct involving the results of the experiment and confirming whether such misconduct existed. It is not reasonable to assume that X, who oversaw the theoretical calculation part of the experiment, had the responsibility to confirm whether there was any misconduct regarding the results of experiments for which no suspicion of misconduct was pointed out in meetings in the Sawamura Lab. Accordingly, X was not identified as an individual with management responsibility as the author of articles 2 and 4.

b. Y, Lecturer, Graduate School of Arts and Sciences, the University of Tokyo

Management responsibility as the author responsible for the content of the articles:  
'Severe' 'Moderate' 'Low'  'None'

Grounds for the decision:

- Y stated that although he/she was a co-author of articles 1 through 4, Mr. Reyes was exclusively responsible for conducting the experiments and preparing the articles, and that he/she only became aware of the alleged misconduct by Mr. Reyes when he/she was contacted by Mr. Sawamura on March 30, 2022. Mr. Reyes stated that he just manipulated data and did not explicitly admit to any misconduct, but he also noted that his co-authors were not aware of any data that was not recorded in his lab notebooks nor were they aware of some sections containing data that differed from the data in his lab notebooks. Accordingly, it was determined that Y was not engaged in the misconduct.
- Y was a co-author of articles 1 and 2 when Mr. Reyes was a doctoral student. During a period of preparing article 3, Y as a co-author was the closest supervisor to Mr. Reyes, a doctoral student, and he/she was familiar with the situation at the time of writing each article. However,

he/she was not the corresponding author, but was responsible for checking and revising the overall structure of each article and its SI. His/Her role in article 4, which was written during Mr. Reyes' tenure as a postdoctoral fellow and then as a specially appointed assistant professor, relatively declined, especially after Mr. Reyes became independent when he was employed by the University. Accordingly, Y should not be considered an author with a duty to guide and supervise Mr. Reyes to prevent misconduct.

- As to whether Y, who was the closest one to Mr. Reyes, could have failed to detect his misconduct and he/she failed to check that he/she should have performed as a co-author, the co-author's obligation is limited to confirming misconduct based on materials used for articles and drafts presented at meetings by Mr. Reyes. The obligation to trace back raw data to confirm the truth or falsity of the experimental results on the articles is not considered to be part of the confirmation obligation that a co-author is supposed to perform.

Co-authors work together to complete an article using authentic data and materials based on a relationship of trust. If co-authors are obliged to trace the raw data of each other's experimental results to confirm whether there is any misconduct, it may cause unnecessary feelings of doubt and suspicion among them and undermine mutual trust, thereby impeding smooth research and the completion of the article. Thus, it is considered sufficient for the corresponding author to be responsible for such confirmation work.

In this case, it was confirmed that many of the lab notebooks submitted by Mr. Reyes included manipulated data. Y said he/she had no suspicion and could not have been aware of the misconduct. Other co-authors, including Mr. Sawamura, only became aware of it when others pointed it out to them. Under these circumstances, it is considered difficult to notice the beginning of the misconduct from the drafts of the articles that Mr. Reyes had presented at the preparation stage, and it is not found that Y neglected to check that he/she should have performed as a co-author.

- Y was entrusted by Mr. Sawamura, the corresponding author, to provide direct guidance to Mr. Reyes in preparing the articles. The following is a description on whether Y was negligent in the performance of his/her duties as an employee.

Y recognized that his/her role was to check the overall structure of each article and its SI, make corrections, and provide advice as necessary. According to Y, in article 1, which was published when Mr. Reyes was a doctoral student, his/her role was to review the entire article. In articles 2 through 4, as Mr. Reyes obtained his doctoral degree, became a postdoctoral fellow, and assumed an independent position as a specially appointed assistant professor, his/her role in writing the articles declined, and particularly in Article 4, Mr. Sawamura's intention in line with the theme of the article was reflected. During the two months that Y was on leave, he/she only provided advises to Mr. Reyes online.

Mr. Sawamura only stated that he trusted and relied on Y, and his instructions to him/her were extremely vague. Considering the fact that Mr. Sawamura was rarely conscious of

checking to prevent misconduct in his own lab, it must be said that it was extremely vague as to whether Y was instructed to trace lab notebooks and other materials and to check for misconduct in the preparation of the articles.

It is also unclear whether Y was given clear supervisory authority and whether Mr. Reyes was aware of this. It can be inferred that Mr. Reyes' status as a specially appointed assistant professor would have made Y hesitant to provide guidance and supervision, such as checking lab notebooks in his/her position as an assistant professor, regardless of whether Mr. Reyes was specially appointed or not. In other words, there were unavoidable circumstances in which confirmation was insufficient.

In his/her defense, Y mentioned that he/she could not have become aware of the misconduct due to his/her poor ability as a researcher and that he/she could have recognized the misconduct when Mr. Reyes told him/her about the unreproducible experimental results prior to submission of article 4, but that he/she could not recognize it at the time. It is sufficient to probe whether any misconduct occurs based on his/her ability at the time, and he/she should not be charged with breach of duty of care due to his/her lack of ability. While Y was told by Mr. Reyes that he could not reproduce the results, he/she was also told that Mr. Reyes had obtained appropriate values after conducting experiments multiple times. It can be inferred that there was no need to reproduce the experiment because Mr. Sawamura, the corresponding author, trusted Mr. Reyes. Accordingly, even though Y did not conduct a replication study himself/herself or suggest Mr. Sawamura to do so, he/she was not immediately found to have violated his/her duty of care as an employee. Therefore, Y should not be held responsible for the performance of his/her duties as Mr. Sawamura's employee.

Based on the above, it was concluded that Y was not negligent in his/her management responsibility as the author responsible for the content of the articles.

c. Z, Doctoral student, Hokkaido University

Management responsibility as the author responsible for the content of the articles:  
'Severe' 'Moderate' 'Low' **None**

Grounds for the decision:

- Z conducted experiments with Mr. Reyes and submitted the results to him. The Committee found in articles 3 and 4 there were some instances in which "experimental results" different from those submitted by Z were adopted or altered by Mr. Reyes. Z also stated that there were "experimental results" that could not be reproduced in the preparation of both articles. As mentioned earlier, Mr. Reyes noted that a series of alleged acts was solely his own, and that he handled the experimental results he received from Z. If the results of Z had differed from those of Mr. Reyes, he explained that he had used his own "experimental results" with the consent of Z. Accordingly, it was determined that Z was not involved in the misconduct.
- At the time of preparation of articles 3 and 4, Z, an undergraduate or Master's student, was in a position to receive guidance from specially appointed assistant professor Reyes, and he was free to use the experimental results of Z. Furthermore, Mr. Reyes was the sole judge

when the experimental results of the two parties differed. It can be said that Z was in a difficult situation to oppose Mr. Reyes' ideas or methods, and that he/she did not have sufficient expertise to do so.

Based on the above, it was determined that Z was not negligent in his/her management responsibility as an author regarding the misconduct in articles 3 and 4.

#### E. Expenses and research projects related to the misconduct

The Committee examined as to whether any expenditure which is directly, scientifically, and academically related to the articles exists by asking authors concerned and looking through documents submitted in the process of accounting procedures within the University. The targets of the examination were the competitive research funds described in the articles' acknowledgements and research findings mentioned in final reports of the same article's author-related research projects which were funded by competitive research funds other than the said funds.

It was concluded that the costs of reprints of articles emanating from the research where the misconduct was found and participation and travel expenses for conferences attended solely for the purpose of presenting the findings of the articles 1 through 4 were identified as expenses with a direct scientific and academic relevance with the said articles in the following three competitive research funds.

The Committee also found that the following research projects had a scientific and academic relevance with research themes covered by the articles 1 through 5.

1	<p>Grantor agency Japan Science and Technology Agency            Program Strategic Basic Research Program (ACT-C)            Project title Development of Asymmetric C-H Activated Catalysts Based on Quantum Simulation            Research period FY 2012 - 2017            PI Masaya Sawamura, Professor, Faculty of Science, Hokkaido University (Researcher No. 40202105)</p> <p>Articles whose acknowledgements cite the grant: 1, 2, 3, 5            Articles scientifically and academically related to the grant: 1, 2, 3, 5</p> <p>Identified expenditures FY 2017            &lt;Related articles&gt;</p> <table style="width: 100%; border-collapse: collapse;"> <tbody> <tr> <td style="padding-left: 20px;">• Reprints of articles</td> <td style="text-align: right;">40,000 yen</td> <td style="text-align: right;">&lt;1&gt;</td> </tr> <tr> <td style="padding-left: 20px;">• Travel expenses for conference</td> <td style="text-align: right;">78,870 yen</td> <td style="text-align: right;">&lt;1, 2&gt;</td> </tr> <tr> <td style="text-align: right; border-top: 1px solid black;">Total</td> <td style="text-align: right; border-top: 1px solid black;">118,870 yen</td> <td></td> </tr> </tbody> </table>	• Reprints of articles	40,000 yen	<1>	• Travel expenses for conference	78,870 yen	<1, 2>	Total	118,870 yen	
• Reprints of articles	40,000 yen	<1>								
• Travel expenses for conference	78,870 yen	<1, 2>								
Total	118,870 yen									
2	<p>Grantor agency Japan Society for the Promotion of Science            Program Grant-in-Aid for Scientific Research (A)            Project title Development of C-H Bond Asymmetric Conversion Based on Ligand Design            Research period FY 2018 – 2020            PI Masaya Sawamura, Professor, Faculty of Science, Hokkaido University (Researcher No. 40202105)</p> <p>Articles whose acknowledgements cite the grant: 2, 3, 4, 5            Articles scientifically and academically related to the grant: 2, 3, 4, 5</p>									

	Identified expenditures <Related articles>	FY 2018	
		• Conference participation fees	72,974 yen <2>
		• Travel expenses for conference	642,755 yen <2>
		Subtotal	715,729 yen
		FY 2019	
		• Reprints of articles	146,051 yen <2, 3>
		• Article illustration production	108,000 yen <2>
		• Conference participation fees	18,200 yen <3>
		• Travel expenses for conference	76,320 yen <3>
		Subtotal	348,571 yen
		FY 2020	
		• Reprints of articles	461,234 yen <4>
		• English proofreading for articles	72,238 yen <4>
		Subtotal	533,472 yen
		Total	1,597,772 yen
3	Grantor agency Program Project title  Research period PI  Articles whose acknowledgements cite the grant: 4, 5 Articles scientifically and academically related to the grant: 2, 3, 4, 5 Identified expenditures <Related articles>	Japan Society for the Promotion of Science Grant-in-Aid for Early-Career Scientists Asymmetric Borylation of Remote C(sp <sup>3</sup> )-H Bonds for the Construction of Compounds with Three-Dimensional Structural Diversity  FY 2020 – 2022 Ronald Lazo Reyes, ICR <sub>e</sub> DD Specially Appointed Assistant Professor (Researcher No. 30845475)	
		• Conference participation fees	10,203 yen <2>
		Total	10,203 yen

#### IV. Measures taken or to be taken by the University

##### A. Withdrawal of articles

Each of the journals retracted the articles related to the research in which misconduct was found to have occurred upon receiving a request from the authors to withdraw the articles. For articles 1 through 4, a statement regarding the retractions was released to society at large on the website of Mr. Sawamura's lab.

The withdrawal of these articles was the responsibility of the authors. Since the University had already acknowledged the allegation and initiated the procedures for investigation, no recommendation or other action was taken against the authors to withdraw the articles in question.

April 29, 2022	<ul style="list-style-type: none"> <li>• The journal in which article 4 was published announced the retraction of the article.</li> <li>• The University sent out a press release.</li> <li>• Mr. Sawamura posted a statement on his lab's website.</li> </ul>
June 7	<ul style="list-style-type: none"> <li>• The journal in which articles 2 and 3 were published announced the retraction of the articles.</li> <li>• Mr. Sawamura posted a statement on his lab's website.</li> </ul>
July 5	<ul style="list-style-type: none"> <li>• The journal in which article 1 was published announced the retraction of the article.</li> <li>• Mr. Sawamura posted a statement on his lab's website.</li> </ul>
August 15	<ul style="list-style-type: none"> <li>• The journal in which article 5 was published announced the retraction of the article.</li> </ul>

#### B. Suspension of research funds

Regarding the Grant-in-Aid for Early-Career Scientists for which Mr. Reyes, who was found to be involved in misconduct, was the grantee, the University applied for approval to discontinue the grant project because he will no longer be eligible to receive the funds due to his resignation from the University, and the Japan Society for the Promotion of Science approved that discontinuance.

#### C. Disciplinary sanctions

Since Mr. Reyes resigned from the University on May 13, 2022, the University's working regulations do not apply to him; therefore, he is not subject to any disciplinary sanctions.

Meanwhile, Mr. Sawamura, who was not involved in the misconduct but was found to be responsible for the content of the articles describing the misconduct-related research, will be dealt with appropriately in accordance with the University's employment regulations.

#### D. Dissertation

The document investigation and hearings regarding Mr. Reyes and the individuals subject to the Investigation indicate that article 1 is the research paper on which the dissertation submitted by Mr. Reyes to the University in 2018 was based and that article 2 is listed with article 1 in that thesis as being in the pre-publication stage at the time of its review. Thus, the dissertation will be dealt with appropriately in the future in accordance with the University's Regulations on Academic Degrees.

### V. Causes of misconduct and measures to prevent recurrence

#### A. Causes

##### 1. Inadequate documentation and verification system required for article submission

In this case, numerous traces of fabrication and falsification committed by the individual who received the University's Research Misconduct Prevention Training and research ethics education were found, such as the absence of experimental results in the lab notebooks that should have been the basis for the experimental results described in the articles and the alteration of the numerical values of the results. Many of them could have easily been detected if the articles had been cross-checked with the lab notebooks before submission.

However, as described above, the data sheets → lab notebooks → spectral and physical property data were not properly checked in this order prior to submission, and these were not finally checked by the corresponding author. As a result, the articles were submitted for publication while the misconduct remained unnoticed.

## 2. Lack of awareness of the need to check for misconduct

In this case, although the corresponding author had the duty to finally confirm that the research had been conducted correctly and that the results were compiled in the articles, the performance of that duty was inadequate. In addition, the corresponding author did not give specific instructions to the other authors, such as to check for misconduct or trace lab notebooks, judged that these were done by said authors, and failed to check whether they had checked the results.

As a result of a lack of awareness that everyone, including the corresponding author, had to confirm the existence or absence of misconduct due to a preconceived notion that such things could not happen, the articles were published in the journals without proper confirmation.

## 3. Failure to make confirmations by replication studies or other means prior to submission for publication

If the earliest article, article 1, had been verified by replication studies before submission, it would not have been published, at least in its current form, and the misconduct in the subsequent articles could have been prevented, or further articles could not have been prepared.

## 4. Failure to corroborate meeting materials and lab notebooks

It is considered that the results of experiments in accordance with the article's theme should be verified at meetings and that the culmination of that verification should be summarized in the article. However, it is difficult to recognize that Mr. Reyes submitted the experimental results "as is" in lab notebooks at every meeting. The articles were published without sufficient confirmation of the final experimental results and without confirmation of any misconduct in the process of article preparation.

## 5. Insufficient confirmation of lab notebooks

In this case, there are pages in Mr. Reyes' lab notebooks in which the results of experiments are not described at all, and there are numerous sections in which the experiment numbers and dates of experiments, which are required to be described, are not written down. This alone clearly shows that the lab notebooks were sloppily prepared and could have been enough to lead to the discovery of the misconduct. The fact that the lab notebooks were not properly verified over a long period of time became a "success" for Mr. Reyes, and article 1 and subsequent articles were published with completely fictitious or unrelated experimental results to those described in the lab notebooks as authentic.

## 6. Mr. Reyes' personal issues, growing impatience and a lack of recognition from others

Mr. Reyes' defense showed that he was caught up in his personal issues, and that his employment as a specially appointed assistant professor at ICRéDD gave him a strong sense of urgency to achieve successful results and to publish high-impact articles in journals as soon as possible. As a result, he seems to have repeatedly fabricated and falsified experimental results that were convenient for him to

include in his articles. It can be inferred that the successful experience of not being found guilty of misconduct in article 1 led to the escalation of misconduct in articles 2, 3, 4, and 5.

In addition, the possible background of this misconduct and Mr. Reyes' state of mind were not recognized by his peers inside or outside the lab. Especially after the COVID-19 pandemic began, he was unable to release his stress. It appears that he lost the opportunity to stop his misconduct.

#### B. Measures to prevent recurrence

The University has established regulations and systems concerning misconduct in research activities based on national guidelines and has made efforts to raise awareness concerning research ethics to date, recognizing the importance of achieving fair research by preventing misconduct in research activities.

ICReDD, to which Mr. Reyes, who was found to be involved in the misconduct, belonged, has the advantage of an excellent research environment and extremely high research standards, with leading researchers gathering from around the world at a research area that integrates computational science, information science, and experimental science. It is a unique institute in that it is a center consisting of researchers, many of whom, including Mr. Sawamura, originate from different departments. Based on the above, X, as the director of the institute, is instructed to examine the points to be recognized as issues related to this case with the relevant departments and to steadily take necessary measures to prevent recurrence of research misconduct, such as by centrally managing data obtained through experiments and data described in articles as well as assigning a specialist to cross-check that data from an objective standpoint.

In response to this incident, university-wide efforts will be strengthened to ensure thorough compliance with the Code of Conduct for Scientists, which was established based on the basic philosophy of education and research that is the founding spirit of the university, and to inform and alert researchers within the University about the importance of research data and the role required of the corresponding author of an article by adding this case to past examples within and beyond the University in Research Misconduct Prevention Training, which is conducted every fiscal year for each member of the University in Japanese and English, and to the Research Handbook, which is updated annually.

The University will continue to provide research ethics education through faculty development (FD; organized training and other efforts by universities).

Future efforts will also include enhancing compliance education and research misconduct prevention education from an earlier stage by making research integrity a theme in inter-graduate school classes for first-year master's and doctoral students in all graduate schools, and encouraging the individuals in charge of departments and organizations that deal with research misconduct within the University to take the necessary actions to confirm the corroboration of publication data and to understand the management status of experimental data through training courses to strengthen the system for the appropriate storage of research data.

The University will continue its efforts to ensure that the authors of the research articles associated with this misconduct and all members of the University have a keen awareness of their responsibility to live up to the trust and confidence that society places on research and have a keen awareness of their responsibility to reaffirm the importance of fulfilling their responsibilities commensurate with their authorship, including those of the corresponding author, and commensurate with the recognition they will gain when they publish their findings in articles.