Resolution

of the Palacký University's Ethics Commission meeting on May 9, 2019 and May 30, 2019

Regarding the submission from Assoc. Prof. Martin Kubala, the Dean of the Faculty of Science (from March 18, 2019, case number UPOL-57650/3900S-2019) on the subject of data manipulation in the article in JACS 129, 10929 (2007) figure 2A of the authors: Martin Heřmánek, Radek Zbořil, Ivo Medřík, Jiří Pechoušek and Čeněk Gregor, the Ethics Commission UP (EC UP) came to the following conclusion:

Prof. RNDr. Radek Zbořil, Ph.D. violated the Ethical Code UP under part III: Principles for Creative Activity: Article 3: Researcher is aware of the responsibility for objectivity, reliability and accuracy of his/her research and respects the limits of the methods applied. Article 4: In the publication of his/her findings and results the researcher ensures their completeness, verifiability and objective interpretation. Article 13: If the researcher finds a mistake in his/her publications, he/she shall take all necessary and possible steps to correct it, he/she does not try to conceal or mask it. Namely by:

- 1. **Initiating the modification of a figure in publication** JACS 129, 10929 (2007), figure 2A, of the authors: Martin Heřmánek, Radek Zbořil, Ivo Medřík, Jiří Pechoušek a Čeněk Gregor.
- 2. Inaction since 2012, when he was demonstrably informed about the data manipulation by RNDr. Č. Gregor during his 1st and 2nd dissertation defense. Dr. Gregor also informed Prof. RNDr. J. Ševčík, CSc., at that time the Dean of FoS UP, about it. However, Prof. RNDr. Radek Zbořil, Ph.D. as the supervisor of a doctoral candidate, university professor, corresponding author of the article, in which he claimed 50% of the work, and the head of the department did not respond in any way until the submission from RNDr. Č. Gregor to the Dean of FoS, Assoc. Prof. Martin Kubala, Ph.D. on December 9, 2018, in which RNDr. Č. Gregor informed the dean about the data manipulation in the publication in JACS, and until the meeting of the Scientific Council of FoS UP on March 13, 2019, which ordered Prof. RNDr. Radek Zbořil, Ph.D. to inform the JACS Editorial Board about this fact and proposed a solution.

Mgr. Martin Heřmánek, Ph.D. violated the Ethical Code UP under part III: Principles for creative activity: Article 3: Researcher is aware of the responsibility for objectivity, reliability and accuracy of his/her research and respects the limits of the methods applied. Article 4: In the publication of his/her findings and results the researcher ensures their completeness, verifiability and objective interpretation. Namely:

Mgr. Martin Heřmánek, Ph.D. knew about the data manipulation, but he did not report it. Even the fear of possible consequences from the authority, Prof. RNDr. R. Zbořil, Ph.D., does not change the fact that it was a violation of the Ethical Code UP.

Justification:

- 1. The curve in the publication JACS 129, 10929 (2007) was clearly manipulated see the expert report by Ing. Antonín Korynta on this case, which was accepted by all people involved.
- 2. Prof. R. Zbořil submitted to the EC UP an expert report prepared by Mgr. Ludma, which declares that the manipulated curve presented in JACS is identical with the curve in the presentation "Synthetic methods in solid phase. Iron oxide" of which Dr. Heřmánek is the sole author. Prof. Zbořil deduces from it that Dr. Heřmánek is therefore the undisputed author of the manipulation. The supplement to this expert report prepared again by Mgr. M.

Ludma as Supplement No. 1 to expert report No 209/2019 of May 3, 2019, states that the figure in the slide 49 of Dr. Heřmánek's authorial work "Synthetic methods in solid phase. Iron oxide" is not identical to figure 2A of Heřmánek et al., JACS 129, 10929 (2007) and could not be created as a simple copy of it (without making any further adjustments). From that Prof. Zbořil deduces that: "Data manipulation in the JACS paper occurred at the level of X-ray diffraction record. The manipulation is based on the figure in the dissertation thesis of Dr. Heřmánek, who was also responsible for the measurement, processing and interpretation of X-ray diffraction records in the paper Heřmánek et al. JACS 2007. Dr. Heřmánek is therefore the only person who had to be (demonstrably) aware of the manipulation in 2007." According to the expert report, Dr. Heřmánek has demonstrably manipulated the data in another of his exclusively authorial works - in a scientific presentation entitled "Synthetic methods in solid phase. Iron oxide", which he delivered in 2008 in the presence of a number of former CVN employees and external partners. Dr. Heřmánek admitted the authorship of this presentation in his letter to the EC from May 6, 2019. According to the expert report, the data in Dr. Heřmánek's presentation (his exclusive authorial work) show analogous elements of manipulation as in the JACS 2007 paper.

- 3. All members of the authorship team, with the exception of Prof. Zbořil, confirmed that during the work on the article, there was a common access to the computers on which the data was stored. This unequivocally refutes Prof. Zbořil's assertion that Dr. Heřmánek was the only one who has access to the graph. Therefore, Prof. Zbořil's claim can be considered false and purpose-built.
- 4. Likewise, Prof. Zbořil's assertion that after the second defense of RNDr. Gregor's dissertation (i.e. after RNDr. Gregor drew attention to the manipulation of the data in the graph) he did not know that this claim was related to the graph used in the JACS article, turned out to be false. Given the dissertation topic and the fact that Prof. Zbořil was RNDr. Gregor's supervisor, it is absolutely inconceivable that Prof. Zbořil did not know what the manipulation, which RNDr. Gregor mentioned during his defense, was about. This was also confirmed by the statement of Dr. Heřmánek, of whom Prof. Zbořil was a consultant for the chemical part of his dissertation, so it was impossible for him to overlook the missing part of the graph in the JACS article.
- 5. According to Dr. Heřmánek's statement from May 30, 2019, his thesis contained the original data, including the actual phase composition of sample B, which was listed as sample A in JACS. Dr. Heřmánek is a physicist. Prof. Zbořil was a co-author of the presentation entitled "Effects of the precursor layer on properties of nanoscopic powders formed by thermally included solid-state reactions" given in Kočovice on June 11 – 15, 2006 and, though he denies it, he very well knew the original non-manipulated data. According to Dr. Hermánek, the data manipulation occurred between May 4, 2006 and April 2007, on the basis of an authoritative decision of Prof. Zbořil, who was the head of the "chemical part" of the department. Dr. Heřmánek says that at the ICAME conference on October 14-19, 2007 Prof. Zbořil gave an invited talk, which referred to the work cited in JACS. However, the data presented were untrue in several respects and, according to Dr. Heřmánek, in the next presentation Prof. Zbořil went even further in data manipulation to support his idea. According to Dr. Heřmánek, the character of these manipulations is the same as in the XRD record in JACS. To support his statements, Dr. Heřmánek supplied the electronic documentation, including the presentation "ICAME07 new", which was created by Prof. Zbořil on August 16, 2003 and last modified on October 10, 2007. This presentation was handed over for further analysis to Prof. Miloslav Dušek, the chairman of the expert committee of FoS. (Supplement 1)

- 6. After an oral hearing at the meeting of EC UP on May 9, 2019, as a response to the request of the EC chairman made in accordance with his competences, Assoc. Prof. Pechoušek sent his statement in writing by a letter dated May 20, 2019, enclosing not only additional information on the publication in JACS 2007, but also information on the publication in Nature Communications, the HRTEM image and information about the publication of interim results in Acc. Chem. Res. February 10, 2015. These findings support information on data manipulation provided by Dr. Heřmánek. (Supplement 2)
- 7. Based on the information in the article JACS 129, 10929 (2007), figure 2A, of the authors: Martin Heřmánek, Radek Zbořil, Ivo Medřík, Jiří Pechoušek and Čeněk Gregor, and the information gathered during oral hearings and supported by the written statement and other specific examples from Dr. Heřmánek and Assoc. Prof. Pechoušek with co-authors, the EC UP is inclined to the view that Prof. RNDr. Radek Zbořil, Ph.D. was the initiator of the modification of the figure in the publication JACS 129, 10929 (2007). However, the EC failed to clarify who specifically manipulated the data. Some of the circumstantial evidence, provided to the EC by Assoc. Prof. Pechoušek and Dr. Heřmánek as well as resulting from the interviews with RNDr. Gregor, suggest that there may have been more of that similar adjustments in scientific publications or communications and authoritative decisions of Prof. RNDr. R. Zbořil, Ph.D. in the workplace under his direction. However, a comprehensive examination of these contexts goes beyond the competence, expertise and capabilities of the EC UP.
- 8. In view of the above, Prof. Zbořil's claims appear to be purpose-built, cited in attempt to justify his mistake. On the other hand, the statements of other co-authors appear to be credible. That includes the one from Dr. Heřmánek, in which he states that he explicitly drew attention of Prof. Zbořil to the missing peaks and that he was rejected with the fact that the editor could have a problem with the original results. The statement of Prof. Ševčík, in which he explicitly said that he was talking to Prof. Zbořil about the data manipulation, cannot be overlooked either.
- 9. The EC UP has a strong impression (Supplement 3) that a "significant wave of displeasure" caused by his data manipulation statement may have contributed significantly to RNDr. Č. Gregor's dissertation defense failure. His statement was, however, in fact a fulfilment of the Ethical Code UP under part III: Principles for Creative Activity: Article 13: "If the researcher finds a mistake in his/her publications, he/she shall take all necessary and possible steps to correct it, he/she does not try to conceal or mask it". EC UP therefore recommends the Dean of the FoS UP to verify the conclusions of the second dissertation defense of RNDr. Č. Gregor.

EC UP acted in the following composition:

Assoc. Prof. Tomáš Bubík, Ph.D.; Prof. MUDr. Karel Indrák, DrSc.; Prof. Ing. Aleš Lebeda, DrSc.; JUDr. Zdenka Nováková, Ph.D.; Prof. MUDr. Martin Procházka, Ph.D.; Doc JUDr. Filip Ščerba, Ph.D. and MUDr. Renata Vařeková, Ph.D.,

and agreed on this Resolution in a ratio: 7 for

0 against

Prof. MUDr. Karel Indrák, DrSc., chairman of the EC UP in Olomouc