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Why Integrity? Why Now?

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Abstract: This article introduces scientific and research integrity, with a particular emphasis on its implications for the active chemical community in Switzerland. It attempts to equate research integrity to good scientific practice and presents this as benefiting the researcher, the institution, and the discipline. The concepts are developed, and current and future challenges are identified.

Keywords: Good scientific practice · Research ethics · Research integrity

Ed Constable studied chemistry at the University of Oxford, then moved to Cambridge, where he remained until 1993, when he was appointed Professor of Chemistry in Basel. Recently retired, he has over 700 publications in all areas of chemistry. He chaired the group responsible for the 2021 Swiss Academies of Arts and Sciences publication *Code of Conduct for Scientific Integrity*. He is currently Vice-President of Division VIII of IUPAC and President of the Committee for Research Integrity of the Swiss Academies of Arts and Sciences.

1. Introduction

Law-makers, regulatory bodies and the popular press are increasingly becoming engaged in the debate about 'scientific integrity'. The concept is at least two centuries old but has come under increasing scrutiny in a world battling climate change and global pandemics. Scientific integrity is based on fundamental principles established to aid scientists in addressing the practical, ethical, and intellectual challenges they encounter in their work. At their simplest, these principles can be referred to as good scientific practice and are often discipline-specific. The principles that should be applied to all scientific research are *reliability*, *honesty*, *respect* and *accountability*.

What this means in practice is discussed in Section 5, but it is appropriate to state from the beginning that the public acceptance of science and its results is fundamentally anchored in the assumption that these standards will be maintained. If this is not the case, the value and reputation of entire disciplines can be jeopardised. Inherent in this view of scientific integrity is that any standards and rules adopted are intended not to impose additional burdens on the academic freedom of scientists but rather to provide a framework to validate their work and protect the reputation of individuals, institutions and disciplines.

Like all other disciplines, chemistry has its own standards of good scientific practice. Many chemists react negatively to the concept of scientific integrity without realising that these standards have been established to protect them. This article aims to explore scientific integrity, particularly its meaning for chemistry.

2. Ethics and Integrity

The words ethics and integrity are widely used and abused. They are often incorrectly viewed as interchangeable. Without entering into the debate, a good working definition of ethics is the science and understanding of values, morality and correct conduct. Similarly, integrity may be defined as the adherence to moral values and principles, particularly on an individual or corporate basis.[1] In a naive way, integrity can be seen as implementing ethics.

Medical sciences have operated under the oversight of ethical approval committees for many years. The extension of oversight to other disciplines is a significant change to the working practices of many scientists. Applicants for European Commission Horizon Europe funding must complete an ethics self-assessment document, regardless of discipline. It is no longer acceptable to tick the compliance box and assume that 'this does not apply to me; I am not a medic.' The need for a 50-page guide, 'How to complete your ethics self-assessment',[2] gives some measure of how unprepared the broader scientific community was for these innovations. Compliance with requirements for personal data protection has an immediate impact on the practice of research in the social sciences. For chemists, there is a potential time-bomb in the statements: 'The precautionary principle requires that where there is plausible scientific evidence for serious risks, you must prove that a new technology will not harm the environment'[2] and 'If new substances and/or formulations (*e.g.* nanomaterials) are developed, you must provide adequate risk assessments'.[2]

3. Codes of Conduct – Why now? Why at all?

It seems as if the scientific community is swimming in codes of conduct and documents addressing scientific and research integrity and ethics. While preparing the new *Swiss Code of Conduct for Scientific Integrity* which was launched in 2021,[3] we were often asked why it was necessary when other guides, such as *The European Code of Conduct for Research Integrity, Revised Edition 2023*, existed.[4] The answer to this is multifold. Firstly, the research environment within Switzerland and, in particular, the independence of the academic institutions, is different to other European nations, and guidelines appropriate to this unique constellation were needed. Secondly, the overall environment had changed beyond recognition since the earlier Swiss 2008 *Integrity in scientific research – Principles and procedures* (https://api.swiss-academies.ch/site/assets/files/25571/richtlinien_integrita_t_en.pdf). Social media, unmoderated oversight of science, Open Access, Open Science, Data Management and Curatorship and Citizen Science all bring their own challenges to scientific behaviour and research integrity and were either unheard of or in their infancy in 2008.

At the same time, high-profile cases such as that of Paolo Macchiarini,[5] who was found criminally responsible for unethical medical research practices, resonated throughout Europe. The fall-out from these cases seriously affected the reputation of institutions involved and had a negative impact on the

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trust in ethical behaviour in the medical sciences. These impacts were beginning to be felt throughout science as a whole, and there was a need to ensure that Switzerland had robust guidelines for 'correct' scientific and research behaviour.

The third imperative for the new Code of Conduct was to dispel the false paradigm that guidelines for research integrity were to limit academic freedom and restrict the choice of scientific fields and research methods. The aim was to develop a set of guidelines that the community would embrace as a spreadsheet for successful and world-leading science rather than a set of restrictions to be superficially obeyed.

4. Science, Society and Public Perception

Today, science's conduct and accountability are subject to public, political, and regulatory scrutiny not seen since the European Dark Ages and the Renaissance. Open Science and greater oversight are changes to be welcomed but present new challenges to scientists, both in their acceptance and implementation. Scientists need to be able to justify their research in multiple ways – value for money, benefit to society and, of greatest importance to this article, transparency and reliability.

Recent debates on scientific issues of societal importance, such as the global pandemic or climate change, have been characterised by a distinctly non-scientific rhetoric. Increasingly, there is a tendency within the body politic and broader society to dismiss unwanted or unpalatable scientific results with comments such as 'I don't believe that' or 'That is only one individual's opinion'.

In one sense, scientists themselves are responsible for this. We are very poor at communicating the nature of scientific progress, the debate over interpretation of results and the difference between proven interpretation and uncorroborated raw data. However, research integrity lies at the core of this issue. When scientific results are communicated, the research must conform to the highest standards of good scientific practice. In an ideal world, it should not be possible to dismiss scientific results with 'I don't believe that'.

Every scientific publication that is withdrawn and every scientist shown to have acted outside the standards of good scientific practice and research integrity damages the reputation of science as a whole and further validates society's rejection of scientific results. If the public faith in science is destroyed, the search for knowledge is futile.

Unfortunately, that faith in science is being severely tested. Retraction Watch has identified 422 publications on COVID-19 that have been retracted, undoubtedly only the tip of the iceberg.[6] As early as 2016, *Nature* raised concerns about reproducibility in science, claiming 70% of researchers had tried and failed to reproduce published experiments and citing reproducibility rates of 40% and 10% in psychology and cancer biology, respectively.[7] Very recently, an analysis of biomedical publications from European Institutions retracted based on research misconduct in the period 2000–2021 revealed disturbing trends.[8] The highest retraction rates involved authors from Germany, the United Kingdom, Italy and Spain, with a total of 2069 publications being withdrawn. Most concerning was the number withdrawn based on falsification and fabrication of results and the quadrupling of the retraction rate over the time period (normalised to the number withdrawn *per* 100,000 publications). Although there are multiple reasons why a paper might be retracted, ranging from genuine error to research misconduct, it is concerning that over 10,000 papers were retracted in 2023, the bulk from a subsidiary of the publisher Wiley. Research misconduct is real and increasing!

Unfortunately, chemistry is not exempt from these general observations and trends, and some 1,300 papers have been retracted in the past 20 years, with almost two-thirds of these being on the basis of misconduct.[9]

5. The Basics of Scientific Integrity – Best Practice in the Discipline

As mentioned in Section 1, scientific integrity is based on four principles. If we examine these, it is clear that these are simply the basics of good scientific practice and not some obscure and abstruse set of rules imposed on the community.

Reliability ensures the highest quality of research and increases trust in scientific results. It dictates the design and analysis of research and involves transparent communication of results. This implies using FAIR (Findable, Accessible, Interoperable, and Reusable) publishing principles for making primary data available to the broad community.

The second principle is *honesty* in all aspects of scientific activity. This includes transparent development, design, and reporting of scientific results and impartiality in the scientific review and assessment process.

The third principle is *respect* for all individuals involved in research, considering life experience, cultural heritage, and diversity. The principle of respect also extends to the impact of research on ecosystems and the environment.

The final principle is *accountability* for all aspects of research, including valorisation and transfer, as well as training, supervision, and mentoring activities. This last aspect has broad-ranging consequences. In principle, all publication authors should hold equal responsibility for the validity of its content. The concept of ownership should be communal, rather than the commonly encountered 'Oh, (s)he is the lead author, and it is her or his problem'. COPE, The Committee on Publication Ethics is quite clear on the criteria for authorship, 'Two minimum requirements define authorship across all definitions – making a substantial contribution to the work and *being accountable for the work and its published form*.'[10]

Translating these principles into good scientific practice in chemistry is simple. Experiments should be well-planned and not wasteful of resources, co-workers' contributions should be respected and reflected in the eventual dissemination of results, and scientific results should be critically examined to ensure that there is no misconduct or bias in their acquisition or analysis.

It is appropriate to mention one facet of the principle of respect. Probably 90% of scientific integrity cases dealt with by institutions relate to authorship. These cases involve claims that individuals have been excluded from authorship or that others have been included without contributing to the research results. They also involve claims that the sequence of authors on a publication is incorrect or misleading. On the one hand, journals and codes of conduct provide clear and rigorous criteria for authorship, but on the other hand, these are emotive and highly personalised issues. Many can be avoided by using the principle of respect and inclusiveness in preparing publications. On a purely legalistic note, in the majority of cases, the act of submitting a publication to a journal explicitly commits the lead author(s) and all authors to a statement that the authorship is correct and accords with the standards and criteria of the publisher. This, on the one hand, ensures a communal responsibility if the authorship is subsequently shown to be incorrect and, on the other, should preclude subsequent changes to the list of authors.

6. What are the Common Infringements – FFP?

Inevitably, we need to consider activities that are considered prime examples of scientific misconduct. These are usually called FFP – *falsification*, *fabrication*, and *plagiarism*. In this section, these will be presented together with modern examples of what constitutes unacceptable practice.

6.1 *Falsification*

Falsification is manipulating research data to favour a particular interpretation, including the alteration, over-emphasis, omis-

sion or deletion of results. Even if data are not modified or omitted, misrepresenting research results is also seen as falsification.

At first glance, these are things that one should obviously not do! However, it is often a little less clear-cut. Imagine that you have a data set of values: 2.1, 2.8, 3.1, 1.9, 2.6, and 7.8. Most of us would recognise the value of 7.8 as an outlier – but what is an outlier, and how should it be treated in the data set? Firstly, it is absolutely unacceptable to simply omit the data without comment from published data sets and analysis. *This constitutes falsification and is scientific misconduct*. If the reason for the outlier is known, for example, a power spike, it should be stated. Otherwise, excluding outliers may be explicitly justified based on statistical analyses such as Dixon's Q-test or the Grubbs test. In all cases, the full data set, including all outliers, should be deposited as supplementary material or in an appropriate repository.

A second way in which data may be passively falsified is in the omission or incorrect inclusion of errors. I return to the data set 2.1, 2.8, 3.1, 1.9, 2.6, and 7.8. In the preceding paragraph, we identified the value of 7.8 as an outlier. This is actually far from obvious on the data presented, If the estimated standard deviation (esd) on each data point were 5 – 2.1(5), 2.8(5), 3.1(5), 1.9(5), 2.6(5), and 7.8(5) – then identification as an outlier may be justified. However, if the data set were 2.1(50), 2.8(50), 3.1(50), 1.9(50), 2.6(50), and 7.8(50), *i.e* an error of ±5, then it would be scientifically incorrect to exclude any point – indeed, arguably all points have the same value.

Physical and analytical chemistry have well-established traditions and best practices of including estimates of errors in data sets, but in synthetic chemistry, it is still common to find raw data sets without statistical justification or validation. If we compare with known reproducibility issues in the biological sciences, it is relevant to ask how often has an individual synthetic step been repeated. How often is the yield the same? How often have you obtained the same yield as reported in a published procedure? When a step has been repeated multiple times on multiple scales, what have you reported as the yield? If you quote the best yield obtained (91%) rather than a range (0-91%), or that 91% was obtained on a scale-up from the reported reaction, *then there is a good case for scientific misconduct*.

One final issue related to falsification is the nature of deposited data sets. Very often, the primary data obtained from measurements are obtained in proprietary formats (NMR spectroscopic data, for instance) or in user-unfriendly formats such as ASCII. If the data are in a proprietary format, there is a tendency to deposit processed data, for example spectra, according to the approved data management strategy. It is arguable that the spectra are insufficient, and that the primary raw data should be deposited. This raises a secondary issue concerning FAIR access – to what extent are proprietary data interoperable and reusable? Similar questions arise when ASCII data are imported into open-source or proprietary spreadsheet software. Should the processed spreadsheets or the ASCII files be deposited? In this case, best practice would advocate depositing both. However, as all sciences are increasingly entering the era of 'big data', questions arise as to what should and what can reasonably be deposited or curated.

So falsification is often a sin of omission rather than commission, but all scientists should be alert to the possibility of introducing bias into their data sets.

6.2 *Fabrication*

If falsification can result from ignorance or imprecision and lack of rigour, fabrication is a different matter. Fabrication is presenting non-existent data, principles, or results in scientific communications. This includes not only the full or partial fabrication of data sets or experiments but also citing non-existent work or incorrectly citing works by third parties.

There is generally less ambiguity about the fabrication of results. It is wrong and a clear breach of scientific integrity standards. However, one aspect is generally misunderstood in the community. On numerous occasions, I have heard supervisors stating that they accepted data presented to them by a co-worker in good faith, although those data were subsequently proved to be fabricated. Within the research integrity community, these 'good faith' arguments are increasingly unlikely to be accepted as an excuse for the abrogation of responsibility. The COPE criteria for authorship presented in Section 5 clearly identify that all authors, especially the lead author(s), are responsible for the entire content of the publication. There is clearly a need for greater awareness of the responsibility to examine primary research data used in publications. This is an aspect of good supervision and good stewardship.

Independent oversight organs such as PubPeer and Retraction Watch detect many cases of data falsification or fabrication, leading to the question, 'If the research community can so rapidly and conclusively identify these issues in the publication, why did the senior author(s) not do so?' I also raise this question.

6.3 *Plagiarism*

I now come to the contentious topic of plagiarism. It is appropriate to quote the definition from the Swiss Code of Conduct for Scientific Integrity,[3] which provides a modern and robust definition: "Plagiarism refers to situations in which a person's own work cannot be sufficiently distinguished from his or her previous work or the work of another person."

It is clearly inappropriate behaviour and misconduct to take another publication, in part or *in toto*, and to republish it as one's own work without due acknowledgement. In the case of publication *in toto*, with the obvious exception of editions and edited commentaries, even publication with acknowledgement is likely to be seen as misconduct. In chemistry, it is simply unacceptable to republish another person's work under your own name.

Identifying plagiarism is often difficult. Many publishers rely on textual analysis tools such as Turnitin. These tools regularly give very high plagiarism counts for publications in the experimental sciences, where there are only a limited number of ways of stating the instrumentation used. Similarly, there are only limited ways to describe experimental procedures ('was heated to reflux', 'was purified by chromatography', 'was recrystallised', *etc.*). Such automated analyses are only of real benefit when considering the body of the text rather than experimental sections. Automatic analysis may also not detect material that has been translated from one language to another.

However, the *Code of Conduct's* definition also covers a number of types of plagiarism that are often not recognised by the community. The first explicitly recognises that reusing unpublished material without acknowledgement also constitutes plagiarism. This is less likely to concern the chemical community, but it should be noted that this would apply to material presented in research colloquia and lectures.

Another behaviour identified as plagiarism is slightly adapting or translating material without acknowledging the source. Naturally, in these cases, an infinite number of devils lie in the details – what is a 'slight adaptation'?

The aspect most likely to raise concern in the chemical community relates to the issue of self-plagiarism, defined as 'reusing substantial parts of one's own work from scientific publications and research proposals as well as from non-published sources without correct indication of the sources or indication of the participation of third parties in one's own proposals and work.' How often are the introductory paragraphs to your publications very similar? Are you aware that you could be accused of scientific misconduct on this basis?

The issue of self-plagiarism is actually much broader. Extending to unpublished sources means that text used in a re-

search proposal can neither be sourced from a previous publication nor re-used in a subsequent publication without appropriate citation. Similarly, research proposals to the same or different funders must include explicit citations to earlier or concurrent proposals if there is significant text overlap.

7. New Times, New Challenges

In Section 3, I indicated that new factors in the scientific landscape had contributed to the need for a new code of conduct in Switzerland. In this Section, I will briefly describe these and why they are likely to have a far-reaching and somewhat unpredictable impact on the scientific community.

One development is the increase in external oversight of scientific output by web-based organs such as Retraction Watch and PubPeer. In effect, these provide a robust post-publication peer review process. Although there are criticisms of a lack of transparency through anonymous reporting, it must be said that in most cases, the pre-publication peer review process equally lacks transparency. In general, I welcome the involvement of such sites, although others may differ! One unexpected consequence is that university management teams often hear of suspected misconduct from external and public rather than internal and private sources.

A second new factor is the upswing in social media and its use for the dissemination, discussion, and critique of scientific results. This is a more complex issue as the uptake and usage of social media are more encompassing than the oversight websites. In turn, this means that comments on social media may be less well-informed. Transparency at the expense of validity? Another concern is losing priority and intellectual property protection if results are communicated early using social media. To the best of my knowledge, there has not been a case of results disclosed on social media being published by a third party. But I am certain that there will be, and I look forward to the ensuing debate!

A final aspect that has emerged and is relevant to research integrity is the 'Open Revolution'. Funding agencies are increasingly requiring publications to be Open Access and research data to be made available using FAIR, Open Data and Open Science principles, in addition to prescribing data management and curatorship plans. In parallel, and especially in the medical and biological sciences, there is a recognition that negative results should be published if this is an efficient use of resources or necessary for ethical reasons.

Open Access publishers have been accused of lacking robust reviewing structures and quality control. If this is the case, the funding agencies' requirements might result in a flood of poorly refereed and low-quality publications which could have integrity implications.

Open Data is another concept that can have consequences misunderstood by the research community. In chemistry, once a substance or modified biomolecule has been published, the data are in the public domain and can be reused by any other scientist. The original author(s) do not generally expect co-authorship in subsequent publications from external research groups. This is not the case in some related disciplines, in particular clinical medicine, where there is an expectation of authorship on subsequent research publications involving the same strains or organisms. There is some concern for violating established integrity norms in such cases as the criteria for authorship might not have been fulfilled.

Of more concern to the chemical community is the concept of 'data ownership'. Who actually 'owns' and has the right to utilise data and experimental results? The first principle to stress is that once research has been published and data deposited, those data are available for any other researcher to utilise under FAIR principles. It is worth noting that there have been examples of publishers flagrantly disregarding these requirements to provide deposited data to third-party researchers. More complex is the issue of unpublished data. The international opinion suggests that, in the absence of contractual restrictions, the primary collectors of the data (researcher, doctoral candidate, supervisor) have the right to reuse data, although legal ownership is often unclear.

8. Issues on the Edge of Scientific Integrity

There are a number of emerging 'hot topics' that codes of conduct often ignore or sidestep, either because they are too recent or too difficult to codify within the conventional integrity landscape. I will identify three of these here and explain how the chemical community could be impacted.

8.1 *Dual-Use Research of Concern*

All European Academies (ALLEA) defines dual-use research of concern as that which can be reasonably anticipated to provide knowledge, information, products, or technologies that could be directly misapplied to pose a significant threat with broad potential consequences to public health and safety, agricultural crops and other plants, animals, the environment, materials, or national security. What has this to do with scientific integrity? Research performed in good faith could be misapplied for other purposes, contradicting the integrity principles of respect and accountability. In addition to conforming to institutional, national, and international norms and regulatory control, individual researchers should be educated to ask themselves if a particular line of research or funding for a particular project could lead to potential misapplication. Just because 'you can do it' does not mean that 'you should do it'. A typical example might include developing facial recognition algorithms within an app for personalising cosmetics when those same algorithms could also be utilised in drones targeting individuals. For the chemical community, questions abound. Is publishing a new and facile synthesis of lysergic acid derivatives appropriate? Or describing simple routes to high-energy materials utilising readily available consumer products? These are questions that must be asked but which have no simple answers.

8.2 *Whistleblowing*

Whistleblowing is when a person, often but not necessarily an employee, reveals information concerning illegal, immoral, illicit, unsafe, or fraudulent activity within an organisation. In the research environment this typically involves fabrication or manipulation of data, improper publication practices or inappropriate management behaviour, all of which comprise integrity transgressions. Whilst the principles are clear, the practice of reporting is often complex, and in Switzerland, individuals making such allegations outside their organisation have little protection in employment law. Similarly, although whistle-blowers might make anonymous claims for good reasons, for example, a doctoral candidate accusing a research supervisor, it is very often difficult to retain that anonymity as the case is investigated. This creates problems both in implementing codes of conduct and in the wider legal implications of related investigations. Institutions have to deal with these complex issues within their internal legislation.

8.3 *Artificial Intelligence (AI)*

It is almost impossible to open a scientific journal or newspaper without being confronted with articles on the benefits, sins, or existential threats of generative artificial intelligence. There is little doubt that AI will change the research landscape in the forthcoming years. Equally, there is little point in wringing hands and wailing – AI is a reality and is here to stay. Undoubtedly the increasing use of AI will result in new challenges and conundrums for research integrity.

Generative AI is being used in the preparation of research publications today. This ranges from the (acceptable) use to improve grammar, spelling, and comprehensibility or to design a synthesis or write code to the (unacceptable) preparation of entirely spuri-

ous manuscripts with no underlying experimental data. Publishers are converging on a position that if AI is used in the preparation of a manuscript, its use should be clearly identified. The generation of spurious manuscripts is, of course, major scientific misconduct. Equally clear is the position of publishers and funding agencies that using generative AI for reviewing proposals or manuscripts or even improving the text of reviews is unacceptable and a breach of confidentiality. This also constitutes research misconduct.

9. Final Thoughts and the Future in Switzerland

In Switzerland, there is a legal requirement for research to fulfil the requirements of good research practice: 'Research funding institutions shall ensure that the rules of scientific integrity and good scientific practice are observed in the research they fund' (Federal Act on the Promotion of Research and Innovation (RIPA) Research and Innovation (RIPA) Art. 12). The Swiss Academies of Arts and Sciences document *Code of Conduct for Scientific Integrity* provides guidelines for institutions and individuals to fulfil their individual and collective responsibilities to the legal requirement.

It is, unfortunately, a fact that today (June 2024), we have no idea how many cases of scientific misconduct occur in Switzerland, the degree of severity or how they are investigated and sanctioned. Hopefully this situation will be redressed in the course of 2025 with the establishment of a Swiss Centre for Scientific Integrity.[11]

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