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hard- and software part of the community, but really for everybody.

References

- R.K. Harris, et al., NMR nomenclature. Nuclear spin properties and conventions for chemical shifts (IUPAC Recommendations 2001) Pure Appl. Chem. 2001, 73, 1795-1818; http://dx.doi. org/10.1351/pac200173111795
- R.K. Harris, et al., Further conventions for NMR shielding and chemical shifts (IUPAC Recommendations 2008), Pure Appl. Chem. 2008, 80, 59-84; http://dx.doi.org/10.1351/ pac200880010059
- G.F. Pauli et al., Essential parameters for structural analysis and dereplication by 1H NMR spectroscopy, J. Nat. Prod., 2014, 77, 1473-1487; http:// dx.doi.org/10.1021/np5002384
- A.N. Davies and P. Lampen, JCAMP-DX for NMR, Appl. Spectrosc. 1993, 47, 1093-1099.

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Guides in Metrology

by Juris Meija and Stephen Ellison

The Joint Committee for Guides in Metrology (JCGM) is tasked with maintaining and promoting the use of the "Guide to the Expression of Uncertainty in Measurement" (known as the GUM) and the "International Vocabulary of Metrology" (known as the VIM). The JCGM operates through two working groups: JCGM-WG1, with responsibility for the GUM, and JCGM-WG2, with responsibility for the VIM. JCGM has eight member organizations, which include IUPAC. IUPAC is currently represented in the JCGM-WG1 by Stephen Ellison (LGC, UK) and Juris Meija (NRC, Canada).

The June 2016 meeting of WG1 focused primarily on two items of business: actions following member and National Metrology Institute (NMI) comments on the 2015 Committee Draft of a revision of the GUM [1], and steps towards a further JCGM Supplement covering the construction of a 'measurement model' suitable for the evaluation of measurement uncertainty.

The draft revision of the GUM (sometimes referred to as "GUM2") followed from a desire to improve the internal consistency of the GUM and its consistency with later Supplements ,and to improve its applicability

across measurement sectors; a summary of the rationale was given by Bich. [2] An on-line survey in 2012 gave further support to some of these objectives, particularly the need to address a wider range of measurement problems. To improve consistency, the JCGM decided to adopt a consistent Bayesian approach. This offers a more general framework, naturally incorporating non-normal distributions and non-linearity. It also provides for more consistent treatment of Type A and Type B evaluations of uncertainty and in many simple cases it avoids the need for a calculation of effective degrees of freedom. In December 2014, a Committee Draft [1] was produced and circulated among the eight Member Organizations, including IUPAC, as well as National Metrology Institutes of the States that have ratified the Metre Convention.

By June 2015, JCGM-WG1 had received a considerable body of feedback on the proposed Committee Draft. IUPAC provided an opinion similar to those given by other member organizations, such as ISO, and by leading National Metrology Institutes, such as NIST (USA), PTB (Germany), NRC (Canada), and LNE (France). Though there was some recognition that the new approach helped in some areas, the great majority of comments strongly opposed replacement of the existing document with the proposed revision. Many did not see sufficient justification for replacement, and it was clear that many felt that the costs associated with changes in procedure in calibration and testing laboratories would be disproportionate where the existing Guide had been found sufficient. [3] Some responses also identified technical issues that would hamper the new version's application in particular fields; for example, the proposed treatment could become problematic if some uncertainties are unavoidably associated with very small degrees of freedom.

JCGM-WG1 has now given careful consideration to all of the comments received. A detailed response to the comments has been prepared and will be made available to member bodies in due course. In general, however, the working group acknowledges that the proposed GUM2 has failed to adequately communicate the rationale for revision of the GUM. The working group has also taken note of concerns relating to the cost of change in laboratories that find the present Guide sufficient. As a result, JCGM-WG1 is considering a wider range of options for moving forward in the light of the feedback received. Replacement of the existing Guide is not envisaged in the short term. One option under active consideration is a "new paradigm" whereby the GUM becomes a multi-part guide, in which different parts differ in scope, complexity, and field of application.

Meanwhile, the working group is moving forward on other guidance. The majority of the JCGM-WG1 June

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2016 meeting time, together with a subsequent drafting group meeting in July, was spent on JCGM 103: Supplement 3 to the Guide to the Expression of Uncertainty in Measurement. This new guidance document deals with the development and use of measurement models. In addition to setting out the general structure of possible measurement models, the supplement covers a variety of mathematical aspects that are useful in metrology. Example topics include model choice for numerical stability, model parametrization, dealing with implicit measurement models (in which the result cannot be simply written as a function of input variables), and the use of transformations to simplify models or improve the accuracy of computation. A draft of this new Guide is in the late stage of completion and anticipated in early 2017.

References

- 1. JCGM 100:201X Committee Draft-Evaluation of measurement data—Guide to uncertainty in measurement, Issued to member bodies December 2014
- 2. W. Bich, Revision of the 'Guide to the Expression of Uncertainty in Measurement'. Why and how. *Metrologia* **51**:S155-S158 (2014)
- 3. W. Bich et al. Towards a new GUM—an update. Metrologia **53**:S149-S159 (2016)

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Books and publications hot off the press. See also www.iupac.org/what-we-do

Bookworm

Successful Drug Discovery

János Fischer and Wayne E. Childers (Eds) Wiley-VCH, 2016, ISBN: 978-3-527-34115-3

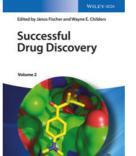
The goal of this book series is to help experts in drug research and development, both in academia and industry, with case histories described by their key inventors or by recognized experts whose contributions can also serve as teaching examples.

Published in December 2016, Volume 2 retains the successful approach found in the previous volume: inventors and primary developers of drugs that made it to market tell the story of the drug's discovery and development and relate the often

twisted route from the first candidate molecule to the final marketed drug. Eleven selected case studies describe recently introduced drugs that have not been previously covered in textbooks or general references. These range across six different therapeutic fields and provide a representative cross-section of current drug development efforts. Sections include:

- I. HDAC Inhibitor Anticancer Drug Discovery
- II. Steroidal CYP17 Inhibitor Anticancer Drug Discovery
- III. Anti-infective Drug Discoveries
- IV. Central nervous system (CNS) Drug Discovery

V. Antiulcer Drug Discovery VI. Cross Therapeutic Drug Discovery (Respiratory Diseases/Anticancer)



2016 marked the 10th anniversary of the approval of vorinostat, the first marketed histone deacetylase (HDCA) inhibitor. This event inaugurated a stream of HDAC inhibitor approvals and confirmed the validity of this drug target and of epigenetic modulation as a viable therapeutic mechanism. To celebrate this important milestone. Successful Drug Discovery presents a number of HDAC inhibitor drug discovery stories.

Backed by copious data and chemical information, the insight and experience of

the contributors makes this volume one of the most useful training manuals that a junior medicinal chemist can hope to find. The book is the outcome of an IUPAC project.

See detailed Table of Contents on wiley.com.

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