Ecological Risk Assessment Workshop for Central America

Substantial amounts of pesticides are used in agriculture in Latin America, in both crops for local consumption and export crops such as bananas, plantains, and pineapples. It is important that the pesticides used do not pose a risk to human health and the environment.

Regarding the environment, it is proposed that an Ecological Risk Assessment Workshop for Central America be held in Costa Rica, in order to:

1. promote and transfer current scientific knowledge on ecological risk assessment
2. highlight the advantages and disadvantages of risk assessment procedures
3. provide a guidance document on the development of ecological risk assessment

This guidance document will give participants more detailed information on risk assessment. However, it is not intended to be a comprehensive handbook, but rather to enable participants to ask the right questions when risk assessments are required.

It is intended that the workshop in Costa Rica will form an integral part of the 6th Latin American Pesticide Residue Workshop (LAPRW 2017, 14-17 May, https://laprw2017.fundacionucr.ac.cr), a biennial forum for discussion in which different concepts and future developments are presented on pesticide residues in food and the environment. Key partners will be CropLife International and the Red Analitica de Latino América y el Caribe (RALACA).

For more information about this project contact the Task Group Chairs Elizabeth Carazo Rojas or John Unsworth <unsworjo@aol.com>

https://laprw2017.fundacionucr.ac.cr

www.iupac.org/project/2016-025-1-600

A Critical Review of Reporting and Storage of NMR Data for Spin-Half Nuclei in Small Molecules

The last IUPAC recommendations on nomenclature, nuclear spin properties and chemical shift conventions were published in 2001 [1], and followed by some additional recommendations in 2008 [2]. Recently, a publication by Pauli *et al.* [3] presented some arguments for the need for enhanced precision in ^{1}H NMR measurement and concluded by recommending the use of four decimal δ values in ppm and one to two decimal *J* values in Hz for interpretation and reporting; members of the organic chemistry ("small molecule") community routinely placing NMR data in the literature for characterization purposes would generally resist such a detailed approach.

RSC, ACS, Elsevier, and Wiley journals all use different conventions for reporting NMR data; some journals also use tabular formats, again with inconsistent presentation modes. Practicing organic chemists would prefer a single uniform approach for the routine characterization of small organic molecules, so as to avoid inconsistencies and/or the tedious process of editing data according to individual journal formats. However, conventions for reporting NMR data need to be agreed on together with the specialist spectroscopy and metabolomics communities. In principle, given the availability of NMR processing software, tabular presentation of NMR data could be supplemented and possibly even replaced by the provision of raw FID data.

In view of modern access to (very) high field NMR spectrometers, combined with the data storage capability provided by the internet, the task group aims to revisit the previous IUPAC recommendations (2001, 2008), to reconsider them in the light of access to very high field NMR spectrometers, and to provide a single agreed-upon format for the reporting and storage of (spin-half) NMR data for solution spectra of small molecules in the mainstream chemical literature.

File format specifications need to be assessed (*e.g.* JCAMP-DX) and explored (*e.g.*, NMRml) with all stakeholders, so as to inform practices for archiving and publication, and ultimately for chemists collecting and managing their raw NMR data. Ideally, consensus on specifications would be achievable as an outcome of TG deliberations, but the specific requirements of individual software manufacturers need to be respected. As the interpretation of the data is crucially important, metadata becomes more and more important for any data format. Thus, this topic is not just a topic for the

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

References

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2. 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
3. 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
4. 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