

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 Analítica de Latinoamérica y el Caribe (RALACA).

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



<https://laprw2017.fundacionucr.ac.cr>

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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 ^1H 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