

Glossary and tutorial of xenobiotic metabolism terms used during small molecule drug discovery and development (IUPAC Technical Report)

Paul Erhardt, Kenneth Bachmann, *et al.*

Pure and Applied Chemistry, 2021

Volume 93, Issue 3, pp. 273-403

<https://doi.org/10.1515/pac-2018-0208>

This project originated more than 15 years ago with the intent to produce a glossary of drug metabolism terms having definitions especially applicable for use by practicing medicinal chemists. A first-draft version underwent extensive beta-testing that, fortuitously, engaged international audiences in a wide range of disciplines involved in drug discovery and development. It became clear that the inclusion of information to enhance discussions among this mix of participants would be even more valuable. The present version retains a chemical structure theme while expanding tutorial comments that aim to bridge the various perspectives that may arise during interdisciplinary communications about a given term. This glossary is intended to be educational for early stage researchers, as well as useful for investigators at various levels who participate on today's highly multidisciplinary, collaborative small molecule drug discovery teams.

<https://iupac.org/project/2000-009-1-700>

Interpretation and use of standard atomic weights (IUPAC Technical Report)

Adriann M.H. van der Veen, Juris Meija, Antonio Possolo, and David Brynn Hibbert

Pure and Applied Chemistry, 2021

Volume 93, Issue 5, pp. 629-646

<https://doi.org/10.1515/pac-2017-1002>

Many calculations for science or trade require the evaluation and propagation of measurement uncertainty. Although relative atomic masses (standard atomic weights) of elements in normal terrestrial materials and chemicals are widely used in science, the uncertainties associated with these values are not well understood. In this technical report, guidelines for the use of standard atomic weights are given. This use involves the derivation of a value and a standard uncertainty from a standard atomic weight, which is explained in accordance with the requirements of the Guide to the Expression of Uncertainty in Measurement. Both the

use of standard atomic weights with the law of propagation of uncertainty and the Monte Carlo method are described. Furthermore, methods are provided for calculating uncertainties of relative molecular masses of substances and their mixtures. Methods are also outlined to compute material-specific atomic weights whose associated uncertainty may be smaller than the uncertainty associated with the standard atomic weights.

<https://iupac.org/project/2013-032-1-200>

Glossary of methods and terms used in analytical spectroscopy (IUPAC Recommendations 2019)

Heidi Goenaga Infante, John Warren, *et al.*

Pure and Applied Chemistry, 2021

Volume 93, Issue 6, pp. 647-776

<https://doi.org/10.1515/pac-2019-0203>

Recommendations are given concerning the terminology of concepts and methods used in spectroscopy in analytical chemistry, covering nuclear magnetic resonance spectroscopy, atomic spectroscopy, and vibrational spectroscopy.

<https://iupac.org/project/2017-027-1-500>

The Gender Gap in Science: PAC Special Topics Issue

Mark Cesa and Mei-Hung Chiu, co-editors

Pure and Applied Chemistry, 2021

Volume 93, Issue 8, pp. 829-961

In a recent article in *Chemistry International* (Chiu and Cesa, *Chem. Int.* 2020, 42(3), 16-21; <https://doi.org/10.1515/ci-2020-0306>) we reported on the results of the Gender Gap Project. The project, entitled, "A Global Approach to the Gender Gap in Mathematical, Computing, and Natural Sciences: How to Measure It, How to Reduce It?" (<https://gender-gap-in-science.org/>), was funded by the International Science Council (ISC, formerly ICSU) and was co-led by IUPAC and the International Mathematical Union, IMU. The results of the project clearly showed that women continue to have less positive experiences than men in education and employment across scientific disciplines, geographic regions, and levels of economic development