Organic Process Research & Development

EDITORIAL

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Is Your Yield Truly Quantitative?

I am sure that all of us have experienced difficulty in obtaining the quoted yield in a paper describing an organic synthesis (*Org. Process Res. Dev.* (OPRD) excepted, of course, being often known as the Journal of Reproducible Results). A recent interesting report from Tomas Hudlicky, Brock University in Canada, in *Synlett* (**2010**, *18*, 2701−2707) helps to explain why. He noticed that when comparing papers from 1955 to 1980 with those from 1980 to 2005, there was a much greater preponderance in yields of >95% in the modern papers, yet such high yields are rarely found in *Organic Syntheses*, where experiments are checked and independently produced. Most experiments in OPRD, if carried out in industrial process chemistry laboratories and scaled up, will have been repeated many times by different experimenters and so, in contrast to results in many other journals, should be reproducible in the laboratory, and on larger scale, giving the reported yield. The yields reported will mostly be measured by quantitative methods, and most methods will have been calibrated by the time work is written up for publication.

Hudlicky examines in detail the practical limits for obtaining yield data (and other data such as ratios of isomers) and concludes that there are serious discrepancies in the reporting of values for yields and ratios in the current literature. The facilities and equipment available in a typical academic laboratory, he concludes, are not adequate to support the accuracy of claims frequently made, because calibrations and absolute standards are rarely used in the analysis.

Of course in industry, and especially in process chemistry, the accurate analysis of yield and selectivity is common, and procedures for ensuring the accuracy of data abound. Process chemists, even if they carry out the initial analysis such as HPLC themselves, are usually aware of the limitations of their methodology, and only when a QC department has performed a more rigorous quantitative analysis, is the accuracy of the data relied upon.

So I urge you to read Professor Hudlicky's interesting and controversial paper, and to be cautious of literature data claiming quantitative yield. In industry we know how easily final products can be contaminated with inorganic salts which do not show up in NMR or HPLC nonquantitative analysis, and this is why residue on ignition or sulphated ash tests are routine for final products in industry, but rarely carried out in academic laboratories.

Hudlicky suggests a number of remedies including providing evidence of calibration, reporting a range of yields whenever multiple experiments are carried out, and changing editorial policies of journals. He indicates that the current practice of reporting unrealistically high isolated product yields and isomer ratios creates serious problems in reproducibility and hence leads to diminished credibility of authors.

I wholeheartedly agree!

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Editor

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