Talanta 82 (2010) 864–865

Contents lists available at ScienceDirect

Talanta

journal homepage: www.elsevier.com/locate/talanta

Letter to the Editor

Significant Figures: Comments on "Process sampling module coupled with purge and trap–GC–FID for in situ auto-monitoring of volatile organic compounds in wastewater" by Hsin-Wang Liu et al. [Talanta 80 (2) (2009) 903–908]

The aim of this letter is to comment on the handling of Significant Figures in the above mentioned article [1]. Significant Figures is a basic concept that must be mastered in order to deal properly with the analysis and presentation of laboratory data. Thus, the classic textbook "Analytical Chemistry" (1963) by Brown and Sallee [2] begins chapter V "Theory of Error and Presentation of Experimental Data" with a first section entitled "V-1. Significant Figures". Similarly, the applied Analytical Chemistry handbook entitled "Standard Methods for the Examination of Water and Wastewater" [3], devotes an entire section, section 1050 B, to dealing with Significant Figures. Even though the "Guidelines for Authors" in analytical chemistry journals (Talanta included) do not contain specific instructions on how Significant Figures are to be used in the presentation of data (it is understood that manuscript authors are able to use them correctly), journals have, in general, always shown an interest in the matter. In 1948, The Analyst published the article "Significant Figures in Analytical Chemistry" [4]. In the seventies, Talanta published a series of four articles by Wilson [5–8] entitled "The performance–characteristics of Analytical methods" where the author reviewed the concepts of errors, precision, sensitivity and bias. Recently, there have been numerous publications in the analytical chemistry literature dealing with statistical concepts and techniques developed for handling and analysing experimental data. All these concepts are part of a new discipline called Chemometrics. But we should not forget the first lesson in Chemometrics: making correct use of standard deviation, precision and Significant Figures to properly present experimental data.

A Significant Figure is a digit which denotes the amount of the quantity in the position which it occupies in a number. A number should never contain more than one doubtful digit. This basic rule is not followed consistently in [1] as there are some mistakes in Tables 1 and 2 of the paper. First of all, the columns with headings precision, accuracy and MDL have not been rounded off to the correct number of Significant Figures, which as mentioned above, is a key and basic aspect of Analytical Chemistry [2,3]. If precision, accuracy and MDL are determined correctly, it is not reasonable to round off to four digits (two integers and two decimal figures). Those are too many Significant Figures which incorrectly overstate the precision of these measurements. For instance, the precision of the 1,1-dichlorethylene measurement in Table 1 should be reported as 13% and not 13.35%. Second, it is also not reasonable, based on the precision of measurements in Table 1, to give that many Significant Figures in Table 2. For example, if acetone is measured to within a precision of 5% (according to Table 1 in [1]), the value of the first column in Table 2 (523.26 ppb) has an uncertainty of at least 25 ppb and therefore the last three digits cannot be significant. Apart from that, Table 2 shows a certain lack of care for the data presented there since two of the eight values shown in the last row, with heading total VOCS (ppb), are, surprisingly, smaller than one of their components, acetone, shown in the first row (see columns 1 and 7 in Table 2).

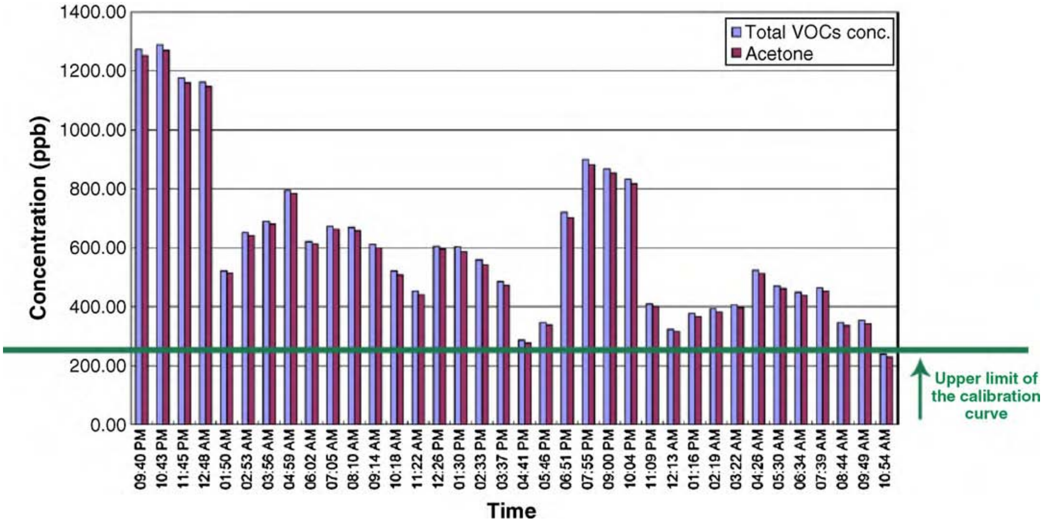

Fig. 1. Copy of Fig. 7 from [1]. A green line has been drawn to show the upper limit of acetone calibration curve used in [1]. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

DOI of original article: 10.1016/j.talanta.2009.08.011.

doi:10.1016/j.talanta.2010.04.022

Another common aspect of analytical chemistry that was neglected in [1] is that the extrapolation of calibration curves to quantitatively determine concentrations is not good practice. In [1], the calibration curves of acetone (Section 2.3 in the paper) are obtained from 6 standards ranging from 60 to 240 μg L^{-1}. Nevertheless, acetone values beyond the 240 μg L^{-1} upper limit of the calibration curve (namely 523.26, 543.71, 609.06, 620.98, 472.7, 483.23, 248.94 and 254.14 ppb) have been reported in Table 2. The same bad practice is also evident in Figs. 7 and 8. See for instance Fig. 1 below, which is a copy of Fig. 7 from [1], to which we have added a green line to indicate the 240 μg L^{-1} upper limit of the calibration curve for acetone. Fig. 8 of the paper is very similar to Fig. 7.

All these errors make the data presented in this publication highly questionable. We suggest, therefore, that both the Guides for Authors and the Guides for Reviewers in analytical chemistry journals should contain clear guidelines regarding Significant Figures and their correct use in the presentation of data so that this concept will not be forgotten from now onwards.

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