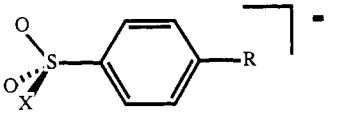
Additions and Corrections

Inhibition of Carbonic Anhydrase [*J. Am. Chem. Soc.* **1991**, *113*, 4484–4490]. KENNETH M. MERZ, JR.,* MARK A. MURCKO, and PETER A. KOLLMAN

The I_{50} for benzenesulfonic acid was reported to be 4.9 μM; however, we have become aware that this value is incorrect and that more representative I_{50} values are 34 mM[1] and 19.4 mM.[2] Using eq 6 (note that the K_a'' for benzenesulfonic acid should be 2.8×10^{-3} and not $3.16 \times 10^{+6}$) and the approximations given in the original manuscript we determine that the new estimates for the experimental $\Delta\Delta G_{bind}$ for **1** → **3** are 10.3 (using 34 mM) and 9.95 (using 19.4 mM) kcal/mol. Our original estimate was 5.0 kcal/mol. Using our new estimate for the $\Delta\Delta G_{bind}$ of **1** → **3** we find that our free energy perturbation results (4.7 kcal/mol) are in much poorer agreement with the experimental I_{50} than originally indicated. Finally, the structure on p 4484 should be replaced by the following:



1: X = NH, R = hexyl
2: X = NH, R = H
3: X= O, R = hexyl

(1) Maren, T. H. Personal communication.
(2) Schwam, H.; Sondey, J. M. Unpublished results.

Computer Software Reviews

MINSQ. Version 4.02. MicroMath Scientific Software: P.O. Box 21550, Salt Lake City, Utah 84121. List price $249.00.

MINSQ is a nonlinear curve-fitting package for IBM and compatible systems. A previous version (2.1) has been reviewed (*J. Am. Chem. Soc.* **1988**, *110*, 2693–2694) and only significant changes are addressed here. The new version addresses most of the limitations of the earlier version:

(i) Upon execution of the main program the user is provided with configuration data, including the number of data pairs that can be used with the available memory.

(ii) The graphics and hardcopy options have been expanded and allow the user many interactive tools to aid in the generation of graphical output. Residual plots are also available in this version.

(iii) The manual has been expanded to include descriptions of the analysis methods and limitations.

The reviewer still encountered system errors (infrequent) that resulted in odd displays or required a system reset. As a whole, the package has improved with minimal price increase. It is easy to use and contains most of the features needed for data analysis.

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NCSS STATISTICAL SOFTWARE: NCSS 5.03—Base Package and NCSS 5.1—Graphics Package. Pacific Ease Company: 601 Pacific Street, Santa Monica, CA 90405. List Price: Base Package $125.00, Graphics Package $79.00. No educational discount. Student/classroom, quantity, and network discounts are available.

Requires an IBM compatible XT, AT or 386, graphics card (Hercules, CGA, EGA or VGA), with 256K of memory for the base package, 512K or more of memory for Graphics, and DOS 2.1 or above and supports a variety of graphics printers (laser or dot matrix).

NCSS is a comprehensive statistical package geared (and priced) for the individual academic research group. The software is purchased in easy-to-add modules. The Base Package and Graphics Package were reviewed here and have not been significantly changed from an earlier review (*J. Am. Chem. Soc.* **1988**, *110*, 8572). The various statistical parameters available are too numerous to list, but include all basic calculations, such as t-tests, Analysis of Variance and Covariance, Univariate Statistics, Nonparametric Tests, Factor Analysis, Cluster Analysis, Multiple Regressions, etc. Also offered within the NCSS packages are the Power Pack (an advanced statistics package), Advanced Tables, and Curve Fitter, which should be of special interest to chemists. The Graphics Package has a variety of plots available, running from standard Least Squares Contour plots, Realtime Point Cloud rotations, Regression Planes, and "Sunflower" plots. One of the real advantages of the NCSS system is that more specialized areas, such as Experimental Design/Quality Control, Survival Analysis, Time Series Analysis, and Process Control, are addressed by the purchase of these specific modules. The modules are economically priced, generally costing about $50.00 or less each.

It is likely that the basic package, plus the graphics module, will contain much of the statistics that will be needed by the majority of scientists. Installation of the program(s) is easy, involving merely the creation of a subdirectory and copying of the disks into it. The program is not copy protected, so no "key disks" or other paraphernalia are required. The manual is clearly written and consists of an Installation/Quick Start Manual, a Reference Manual, and a Graphics Reference Manual (for the graphics package). The installation manual has a test data set and a good tutorial to work through the various aspects of the package. Data are entered into the data base as a matrix of columns (variables) and rows (data entries). Entering and editing data is very easy and intuitive after spending even a short time with the tutorial. All operations on the data are performed by transferring through a "Transfer Panel", which offers a menu of available operations, including program exit. Working through individual processes, for example, performing a regression, is straightforward, but you will need to keep the manual handy until you memorize some commands. A menu for most operations is always present at the bottom of the screen however. In general, the average user will quickly become comfortable with the overall user interface and become productive fairly quickly.

The graphics are easy to use, often merely a keystroke away. However, one should be warned that this is not really a publication-quality