

## A Spin-Trapping Database Implemented on the IBM PC/AT

ANSON S. W. LI,\*† KIRAN B. CUMMINGS,† H. PETER ROETHLING,†  
GARRY R. BUETTNER,‡ AND COLIN F. CHIGNELL†

†Laboratory of Molecular Biophysics, National Institute of Environmental Health Sciences, P.O. Box 12233, Research Triangle Park, North Carolina 27709; and ‡GSF Forschungszentrum, Institut für Strahlenbiologie, D-8042 Neuherberg, Federal Republic of Germany

Received October 27, 1987; revised December 14, 1987

Spin trapping is a technique in which highly reactive free radicals are detected by reaction with a diamagnetic molecule (usually a nitron or nitroso compound) to form more stable free radicals (spin adducts) that can be observed by conventional electron spin resonance spectroscopy (1). Since its inception in 1969, spin trapping has gained wide acceptance in the study of short-lived reactive free radical species generated in chemical reactions, as well as in biochemical and biological systems (2-6). More recently, the technique has been employed to detect free radicals in isolated organs and intact animals (7, 8). The breadth of spin-trapping applications ranges from the undergraduate physical chemistry laboratory (9) to high-energy physics (10). The number of useful spin traps has also increased and now includes compounds such as unsaturated substituted alkanes (10) and quinones (11).

At present, *Chemical Abstracts* lists nearly 1000 references that contain the key word "spin trap(ping)." Unfortunately, abstracts often do not contain the ESR parameters of the spin adducts and other such useful information. Even if these data are present, it is usually necessary to consult the full publication for the experimental conditions, since ESR parameters are known to be system dependent (12). Buettner (2) has recently published a list of spin adducts derived from DMPO,<sup>1</sup> PBN, MNP, and other popular spin traps. Each entry contains the type of adduct(s), the solvent system, the ESR parameters, experimental information, and reference. This compilation is very useful for finding the range of hyperfine parameters for a known adduct. However, in order to search for spin adducts with a given set of hyperfine parameters, obtained under defined experimental conditions, it is necessary to peruse the entire list. This approach is similar to trying to find an address in a telephone book using only a telephone number. The chore of manually searching a vast amount of printed information, plus the inflexibility in arranging such information, warrants the use of a computer. For information retrieval purposes a computer system is much less tedious, less time consuming, and less error prone than a paper-based system.

\* To whom correspondence should be addressed.

<sup>1</sup> Abbreviations used: DMPO, 5,5-dimethyl-pyrroline-*N*-oxide; MNP, 2-methyl-2-nitrosopropane; ND, nitrosodurene or 2,3,5,6-tetramethylnitroso-benzene; PBN,  $\alpha$ -phenyl-*tert*-butylnitron; POBN,  $\alpha$ (4-pyridyl-1-oxide)-*N*-*tert*-butylnitron.

In order to make full use of all the available spin-trapping information, a database has been designed and implemented on an IBM PC/AT. A customized menu-driven program, STDB II, has been written to provide various functions. This report describes the implementation of the database and its potential use.

The database files, STDB, and the accompanying program, STDB II, can be stored on two 360K floppy diskettes. The hardware requirements are an IBM PC/AT (or 100% compatible) running DOS 3.xx, at least one floppy drive with 512K RAM or a hard disk with 384K RAM. A RAM drive of 2 Mbyte (Lotus-Intel-Microsoft specification) is highly recommended.

The database currently spans from 1967 to 1987 (*Chemical Abstracts*). Most of the references found in the recent review by Buettner (2) have been incorporated into the present database, which will be updated on a regular basis. At present, data on the following most popular spin traps have been compiled: DMPO, MNP, ND, PBN, and POBN. Expansion to include additional spin traps is planned when warranted.

From the initial menu of STDB II, it is possible to choose a particular spin trap for searching. Then follows a main menu for either SEARCH, REPORT, or CHOOSE (spin traps). SEARCH allows the unlimited search for almost any kind of information contained in the database file. This includes searches against one or more of the following:

- (1) spin adduct(s);
- (2) ranges of the nitrogen hyperfine splittings (N);
- (3) ranges of the hydrogen hyperfine splittings (H);
- (4) solvent systems;
- (5) conditions or methods of generating adducts;
- (6) author or year of publication;
- (7) title and complete reference of the publication.

In addition, it is possible to carry out a nine-nested cross search as demonstrated in the following example: "reports of  $\cdot\text{OH}$  generated by UV-irradiation and trapped by DMPO to yield adducts with N in the range 14 to 16 G and H in the range 14.5 to 16.5 G, published in 1980 by a particular author as part of a study on photosensitization. . . ."

Using the present database and the powerful and flexible STDB II program, a search can usually be completed within a few minutes. The information may be either displayed on screen or sent to a printer. From each search output STDB II can generate the currently accepted range of ESR parameters for a given adduct and can calculate the mean value of each hyperfine splitting constant. This feature is particularly useful when it is necessary to rely upon the ESR parameters of adducts generated *in vitro* to identify adducts observed *in vivo*. The availability of an acceptable range of ESR parameters for a given adduct also makes it possible to identify possible misassignments or errors in published data. The STDB II program is, however, capable of listing experiments that were reported by the authors to contain artifacts or misinterpretations.

The program also provides a more flexible way of grouping the information. For example, in addition to listing the database files according to the type of spin

adducts, it is possible to select other arrangements. One which has been found to be very helpful involves the grouping of a given adduct with increasing nitrogen hyperfine splittings, followed by increasing hydrogen hyperfine splittings. This type of listing was found to be very useful for detecting trends in ESR parameters, particularly when a large number of citations were present, e.g., superoxide or hydroxyl adducts of DMPO.

In summary, the present database system using a personal computer is far superior for retrieving and grouping spin-trapping data than any other means of information handling. In addition, the files and the accompanying program STDB II operate as a stand-alone package that does not require any extra "add-ons." This database system should be a useful tool especially in situations where fingerprint identification of spin adducts is limited to their ESR parameters. The database is available upon request.

#### ACKNOWLEDGMENTS

The authors are indebted to Drs. C. M. Dubose, D. Rehorek, and U. M. Oehler and Professor E. G. Janzen for communications on their aminoxyl computer database that is being prepared.

#### REFERENCES

1. E. G. JANZEN, H. J. STRONKS, C. M. DUBOSE, J. L. POYER, AND P. B. MCCAY, *Environ. Health Perspect.* **64**, 151 (1985).
2. G. R. BUETTNER, *Free Radicals Biol. Med.* **3**, 259 (1987).
3. A. S. W. LI AND C. F. CHIGNELL, *Photochem. Photobiol.* **45**, 565 (1987).
4. P. J. THORNALLEY, *Life Chem. Rep.* **4**, 57 (1986).
5. C. F. CHIGNELL, A. G. MOTTEN, AND G. R. BUETTNER, *Environ. Health Perspect.* **64**, 103 (1985).
6. A. SAMUNI, A. J. CARMICHAEL, A. RUSSO, J. B. MITCHELL, AND P. RIESZ, *Proc. Natl. Acad. Sci. USA* **83**, 7593 (1986).
7. H. D. CONNOR, R. G. THURMAN, M. D. GALIZI, AND R. P. MASON, *J. Biol. Chem.* **261**, 4542 (1986).
8. S. KUBOW, E. G. JANZEN, AND T. M. BRAY, *J. Biol. Chem.* **259**, 4447 (1984).
9. S. R. HOMER, S. J. MCKINNON, AND S. L. WHITTENBURG, *J. Chem. Educ.* **63**, 1103 (1986).
10. E. RODUNER, *Hyperfine Interact.* **32**, 741 (1986).
11. K. A. M. CREBER, T.-I. HO, M. C. DEPEW, D. WEIR, AND J. K. S. WAN, *Can. J. Chem.* **60**, 1504 (1982).
12. E. G. JANZEN, G. A. COULTER, U. M. OEHLER, AND J. P. BERGSMAN, *Can. J. Chem.* **60**, 2725 (1982).