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Book Review

Gas-chromatographic retention indices of toxicologically relevant substances on SE-30 or OV-1 (Report II of the Deutsche Forschungsgemeinschaft Commission for Clinical-Toxicological Analysis; special issue of The International Association of Forensic Toxicologists Bulletin), VCH Verlagsgesellschaft, Weinheim, Deerfield Beach, Basle, 2nd ed., 1985, 176 pp., price DM 68.00, ISBN 3-527-27335-2.

The book lists the gas chromatographic (GC) retention indices (RI values) of about 1400 toxicologically relevant substances; it will doubtless be of great help to toxicologists or forensic chemists confronted with the demanding task of rapidly identifying a life-threatening xenobiotic in a case of acute poisoning. Gas chromatography clearly is one of the most general and powerful methods for the rapid tentative identification and quantitative determination of many drugs, pesticides, metabolites and other common constituents of biological samples. Although RI values of relevant substances can be found in various publications, some of them are not easily accessible. Therefore, a well ordered compilation of RI values is necessary to keep the time required for diagnosis to the minimum and to ensure a rapid initiation of effective therapy. The book is meant to serve this purpose.

In the first ten pages the gas chromatographic technique and the concept of the retention index are introduced. This is followed by a table of compounds in alphabetical order of International Nonproprietary Names (INNs), a list of compounds according to their RI values, a concordance list of CAS Registry Numbers and INNs and finally an alphabetical order of the corresponding CAS index names. The compilation is based on 42 references, 12 of which are "personal communications".

In spite of its undisputed practical usefulness, the book has a considerable number of flaws, some of which are mentioned below. It seems that not all data extracted from the literature were critically examined; it immediately springs to the eye that the two enantiomers (D and L) of N-acetyltryptophan are listed with two different RI values; this is impossible on a non-chiral stationary phase. The way in which metabolites are designated is confusing; the name of the parent drug followed by an M is meant to indicate that the peak listed with its RI value represents a metabolite, and when its identity is known the name of the metabolite is also given; but this is not always so as sometimes the name listed in alphabetical order and followed by M is just a metabolite itself, and a number of compounds that are clearly metabolites are not designated as such.

There are also problems with nomenclature; the use of INNs and trivial names entails some risks, but a more meticulous examination could have eliminated a number of inconsistencies. Parathion is entered as such, whereas the related paraoxon is referred to as diethyl-*p*-nitrophenyl phosphate, without any indication that the latter is also a metabolite of the former. Another example is clofenotane; this is the proposed term for a well known insecticide, but chlorophenotane is also very often used; the name adopted by the International Standards Organization, DDT, does not appear at all, but is by far the most common; it is used, for instance, in the Merck Index. On the other hand, the metabolites of DDT are listed as DDE and TDE (why not DDD?), but not identified as metabolites. One table (5.2.1) contains hyoscyamine without any reference to atropine, in another table (5.2.3) it is the reverse; the α -, β - and δ -isomers of the hexachlorocyclohexanes are entered as "benzenehexachloride, alpha-", "beta-" and "delta-", whereas the γ -isomer is referred to only as lindane. In all these cases multiple entries with cross-references would have been helpful. Another example of cursory terminology is acetamido-clonazepam; in spite of its use in the literature, this is wrong; a prefix such as "acetamido" means that the residue replaces a hydrogen atom; in this case, however, the acetamido group substitutes a nitro group. Such lapses might be acceptable for laboratory jargon but not in a scientific publication. Taking clonazepam as a structural entity, an acceptable term would have been 7-acetamido-7-denitroclonazepam.

The indiscriminate listing of two or more RI values for one compound is peculiar. It should have been mentioned at least in the introductory text that these cases represent either mixtures of isomers or homologues or decomposition products that may arise during GC. For benzyl butyl sebacate, for instance, three RI values are given; it is not mentioned that they represent dibutyl sebacate, benzyl butyl sebacate and dibenzyl sebacate; the knowledgeable reader may assume this. Linoleic acid is listed with two very different RI values, while linolenic acid has one. Besides wondering about their toxicological relevance one tends to ask, "why then is palmitic, oleic or arachidonic acid not included?". Lecithin is given, although it is not one but a class of related compounds, which are not amenable to gas chromatography. More than 50 compounds are listed with an RI value of 9999, which is meant to indicate that no peak is observed; it would add clarity to the tables if this were indicated by a dash instead of a fake RI value, even for a toxicologically irrelevant compound (urea). Several others are included that are unimportant, but some relevant poisons are not given, such as various phosphoric and phosphonic acid esters and other pesticides.

Capillary gas chromatography is not mentioned at all; this misses the state of the art, which is in almost all respects superior to packed-column GC [cf., W.H. Anderson and D.T. Stafford, *J. High Resolut. Chromatogr. Chromatogr. Commun.*, 6 (1983) 247]. A cautionary note in the introduction about the reproducibility of RI values would have been appropriate; it is certainly true that in most instances the reproducibility is high, but comparison with other sources shows that there are notable exceptions with differences of more than 100 units, as in the case of acepromazine, acetylsalicylic acid and benzocaine — to name only a few.

The issue of a readily accessible compilation of retention indices is a very worthwhile undertaking. The book is meant for the practitioner, but scientific precision and critical evaluation of methodology should not be left aside completely. It is to be hoped that these shortcomings will be eliminated in a more carefully edited version of this book. Considering its great usefulness for every laboratory and institute of clinical toxicology or forensic chemistry and the relatively low price, the book is still recommended.

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