

We've Added a Weekly *Substructure Index* to *Current Abstracts of Chemistry* and *Index Chemicus*

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In its first issue for 1975, we added a new *Substructure Index* to *Current Abstracts of Chemistry and Index Chemicus*® (*CAC/IC*®). The index employs the Wiswesser Line Notation (WLN). Each weekly issue of *CAC/IC* covers about 3000 new compounds. Readers who are familiar with WLN can use the new index to discover (or recover) any new compounds or any compound containing a particular substructural feature. Those who are not familiar with WLN may be stimulated to learn something about it. We do not wish to hide the fact that we hope, in either case, that readers of *CAC*® will want to use the cumulated and rotated version of the weekly index that is already available in ISI's® *Chemical Substructure Index*® (*CSI*®).

I have written about ISI's use of WLN before.^{1,2} WLN is probably the easiest chemical notation to learn. Wiswesser's original concept was eminently sound. Further, he has sought and acted on feedback from a large and growing number of users. Many of these belong to the Chemical Notation Association (CNA). CNA has not been hesitant to scrap, change or add to rules of the notation as dictated by actual use. WLN devotees are an unusually enthusiastic group. Some would call them fanatics. But fanaticism is sometimes required to sell an idea. Dr. Wiswesser has had to buck a very well-entrenched establishment.

The basic simplicity of Wiswesser's concept makes WLN easy to *learn*. I can say with justifiable pride that ISI has made WLN easy to *use*, in several ways.

In the first place, we've used WLN to encode and make retrievable almost 1.5 million compounds. In its next weekly issue (No. 585, 12 February 1975) *CAC* will publish abstract No. 226525, dealing with new benzotriazepinones.³ One of them will be

CAC's two-millionth compound. All two million, and more, will ultimately be encoded with WLN. It's remarkable how easy something new is to learn when there is adequate incentive. I should think access to a file of two million compounds would be adequate incentive for any serious chemist.

Nevertheless, we've accepted reality and recognized that many chemists won't bother to learn WLN. For them, we've published a two-part dictionary that translates familiar names of chemical structures and substructures into WLN and *vice versa*.⁴ Thus, any chemist can use the new weekly *Substructure Index* of *CAC* without mastering the notation—just as anyone can more easily learn to read a language than to write it. Actually, one of the simplest ways to learn the notation will be by using the new *Substructure Index*. Incidentally, copies of the dictionary are available on request.

In addition to substructure searching, the new index can be used to find information on particular compounds. Each notation is unique and unambiguous. It follows that you can easily spot compounds related to the one or to the type that interests you.

The new *Substructure Index* supplements the other weekly sections of *Index Chemicus*® (*IC*®), the index portion of *CAC*. With WLN experience, some readers may find that the *Substructure Index* can be used instead of the molecular formula and subject indexes in many instances. We will continue the other sections of *IC*, including the subject index (chemical-name and biological-action word index); the molecular formula index; the author index; and the corporate index of authors' affiliations. The corporate index was added in 1974.

As before, these other indexes will be cumulated quarterly and annually. However, the weekly *Substructure Index* is cumulated monthly and annually in our *Chemical Substructure Index*.^{5,6} In *CSI* moreover, all the notations are rotated to make each substructure of any compound a main entry. Readers who would like more information about the *Chemical Substructure Index* and/or sample issues should let me know.

The new *Substructure Index* can do a unique job for you. There is extensive literature available on the subject. If the thought of another pack of reprints deters you, then we'll be glad to make the contact more personal. ISI can provide a seminar or course on WLN at your own laboratory, office or library. You have only to write or to call.

1. Garfield, E. The retrieval and dissemination of chemical information. II. The Wiswesser Line Notation. *Current Contents (CC)* No. 29, 22 July 1970, p. M1-2.
2. ----- Are you ready for chemical linguistics? chemical semantics? chemical semiotics? *CC* No. 50, 13 December 1972, p. 5-7.
3. Takahashi, M. *et al.* The synthesis of 1,3,4,-benzotriazepin-5-one derivatives from isatoic anhydrides. *Bull. Chem. Soc. Japan* 47(11):2724-26, 1974.
4. *ISI Chemical Substructure Dictionary (CSD)*. (Philadelphia: Institute for Scientific Information, 1974), 72 pp.
5. Garfield, E. New *Chemical Substructure Index* is creative theoretical tool for molecule manipulators as well as practical system for retrieval. *CC* No. 24, 16 June 1971, p. 5-6.
6. ----- ISI's *Chemical Substructure Index*—research resource and invaluable tool for health and environmental sciences. *CC* No. 20, 17 May 1972, p. 3-4.