Applicability of ASCA to the Literature Requirements of the Chemist

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A service is now available through which an individual may submit a wide variety of questions in the form of an ASCA profile and be alerted on \bullet current and personal basis to the most recent literature related to his interests (Figure 1). The ASCA computer system utilizes unique methods of phrasing the inquiries. In this paper we shall give some examples illustrating, in particular, the use of citation indexing in ASCA.

We shall first phrase some typical questions that chemists might ask of a literature-searching and alerting system and show for each question how it might be entered in an ASCA profile and produce appropriate answers.

Additional Works on a New Compound

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Let's assume a chemist is interested in publications that might describe additional work on a new compound of which the chemist is aware. For our illustration, let's assume the chemist has read <u>Index Chemicus</u> abstract No. 50851 (Figure 2).⁽¹⁾ In reading this article he learns of the identification of the structure and the testing of biological activity of the material. He desire to learn of further work on this compound is translated with the ASCA system, simply into the citation identifying the article by Arroyo, namely, "Arroyo E.R., Chem. & Ind., pp. 350-351, 1965.⁽²⁾ In the bibliography of the Arroyo paper, the user would also have been made aware of additional earlier works that studied the structure of this compound (Figure 3). Any of these also may be entered as questions in the ASCA profile. Reference 3 to the Hecker article would, for example, seem particularly appropriate as shown in the commentary by Arroyo about this reference, namely, "More recently an amorphous active fraction from croton oil was isolated, and some structural conclusions were given for a cocarcinogen (Al).³ However, these workers failed in their attempts to obtain a crystalline compound." The chemist would then receive in his weekly ASCA computer printouts a complete description of all the current works which cite any of these references indicated in the profile. For example, soon after its original publication, this chemist would have been informed by ASCA that the Arroyo paper was cited by Hecker's group in an article appearing in Tetrahedron Letters (Figure 4). (4) If he had entered reference 3 from the Arroyo paper as a question it would have served the same purpose. If he had entered both the Arroyo and the third reference as questions, the ASCA printout would have indicated that both were cited by themnew Hecker

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paper in <u>Tetrahedron Letters</u>. This more recent work provides, among other things, new additional information on the physical properties of the new compound.

Other varieties of ASCA questions could have also retrieved this new paper, but we shall confine ourselves here to discussion of citation questions only.

New Method of Synthesis

As our second example, let's assume the chémist is interested in synthetic methods for desacetylamino-colchiceine. This compound is of biological interest and is being employed by chemists, pharmacologists, and physicians in experimental biology and therapeutic research. The chemist's interest in the synthesis of this compound would have been expressed, for his ASCA profile, in terms of citations identifying the earlier known works on the subject. He might have entered questions, for instance, for "Van Tamelen E.E., Tetrahedron 14, 8 (1961)"(5) and for "Martel J., C.R. Acad Sci, 258, 243 (1964)."(6) Either of these questions would have resulted in notification of the current appearance of a paper by Martel J. et al in J. Org. Chem. 30(6). 1752, June 1965 entitled "A New Synthesis of Desacetamidocolchiceine and of natural colchicine. This example also illustrates the manner in which an ASCA citation question completely bypasses

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the nomenclature problems and even the variant spellings of the name of a specific compound in different languages. The Martel paper in <u>C.R. Acad Sci</u> names the compound "desace<u>tylamino</u>colchiceine" while in the 1965 paper (in <u>J. Org. Chem.</u>) it is spelled "desac<u>etamid</u>ocolchiceine." Citation indexing associates these two papers in spite of this difference and, in fact, would have done so even if the compound were not named in the title or even in the article itself.

Investigation of Biological Activity of a Compound

In the third example, let us illustrate how the chemist interested in following the biological development of a compound would be served by ASCA. Knowledge of the work by McCarthy and $Chen^{(8)}$ might be the starting point. In this paper the anesthetic action of CI-581 was demonstrated in monkeys. The McCarthy article, entered as a question in ASCA, would result in an alert describing the more recent paper by Domino, Chodoff, and Corssen⁽⁹⁾ in which the drug was tested in 20 prison volunteers. In this first human trial the drug was confirmed as an effective analgesic and anesthetic agent.

New Applications of a Type of Reaction

Extensions of work utilizing a type of reaction can be difficult or impossible to uncover by classical indexing techniques.

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The citation indexing principle in ASCA, however, quite readily leads from the papers reporting a type of reaction to the papers which apply or extend this reaction. This ASCA selectivity functions unimpaired even though the reaction may have no identifying name or eponym and even though the starting materials and/or end products may vary greatly.

The paper by Parham⁽¹⁰⁾ describes the preparation of tetrahydropyranyl derivatives of alcohols and phenols. ASCA would alert the chemist interested in extensions of this work to the paper by Garegg(11) summarizing several of his own studies, including the report wherein Garegg succeeded in separating the optical isomers resulting from the addition of a hydroxyl compound to dihydropyran in acid media. Another unique advantage of citation indexing can be illustrated with this case. The user asks a question phrased as "Parham W.E., J. Am. Chem. Soc., 70, 4187, (1948)" and is alerted to the article by Garegg which starts on page 28 and ends on page 50. The Garegg article lists 123 references in the bibliography. These references are the indexing terms used in citation indexing. Yet even though the Garegg article is indexed in such tremendous depth by ASCA (123 index terms), the chemist can quickly pinpoint the specific relationship of the Garegg paper to his own interests. The user

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merely observes that the Parham article is, in this case, Ref. 113 and readily locates the specific point in the text (in the middle of page 45) where Garegg cites Ref. 113 and describes the relationship between that reference and the newer work.

New Syntheses in a Family of Compounds

As our fifth example let us assume the chemist knows of the fundamental work by Brockman and Muxfeldt⁽¹²⁾ on the synthesis of the actinomycin chromophore. The Brockman article might be entered as part of a profile used to alert chemists to any new compound synthesized in this family. The ASCA notifications would later include the paper by Mauger⁽¹³⁾ on the synthesis of the 3-benzyloxy-4-methyl-2-nitrobenzoyl-L-threonine analog and related compounds. This newer work (one of several methods) describes a new purely chemical (not semibiological) synthesis. <u>Correction of Errors in the Published Literature</u>

In the sixth example we illustrate how ASCA even provides alerts for the corrections that may appear to an erroneous article. Corrections may, of course, be trivial or involve vital data from the original paper. A specific ASCA question for the article by Betina⁽¹⁴⁾ (Systematic Analysis of Antibiotics Using Paper Chromatography, <u>J. Chromatog.</u> 15, 379-392, 1964) would have alerted the ASCA user to the correction published the following year in <u>J. Chromatog.</u> 17, 204 (1965) in which the

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subclass to which <u>puromycin</u> was assigned, based on its R_F values in the principal solvent systems, was corrected.

Modification of Analytical Procedures

Modifications in analytical procedures can be followed by entering ASCA questions to the existing literature on the procedures involved. Thus, knowledge of any of several assemblies for continuous flow thin-layer chromatography⁽¹⁵⁻²⁰⁾ would have alerted the user to the paper "Continuous Flow Thin-Layer Chromatography" by T.M. Lees, M.J. Lynch and F.R. Mosher, <u>J.</u> <u>Chromatog 18</u>, 595 (1965)⁽²¹⁾ wherein two additional variations of thin-layer chromatography are described and illustrated. <u>New Methodology</u>

New chemical methodology can be called to the user's attention with ASCA as illustrated by the following. If the chemist were to enter ASCA questions which identify any of four of the early methods for testing for sulfoxides, (22-25) he would receive notification of the recent paper by L. Suchomelova (26) which describes the use of the Dragendorff reagent in the detection of sulfoxides.

A variety of additional methods of entering questions in the ASCA system are available. These include, in addition to the specific citation questions illustrated above, (1) reference

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author question by means of which the user can be alerted to all current items which cite any work by a given first author, (2) source author question by means of which the user can be alerted to all the current journal and patent publications of a given author no matter where his name appears in the authorship, (3) patent assignee question, by means of which the user is alerted to all current U.S. Patents assigned to a given organization, (4) patent classification question which will alert the user to the appearance of patents assigned to any given patent classification number by the U.S. Patent Office, (5) organizational question which will notify the user of all the journal publications attributed to a given corporation, institution, or other organization. These special indexing approaches to the literature, coupled with the broad (multidisciplinary) and comprehensive (all journals covered are processed in their entirety as well as all U.S. Patents issued) coverage of the weekly ASCA reports, can provide a significant service for chemists and associated users of the literature of science and technology.

SUMMARY

ASCA (Automatic Subject Citation Alert) is an information retrieval system designed to serve as an individualized current

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alerting service. Computer printouts are used to notify each client, at weekly intervals, of the current article and patents which cite any item in his interest profile. The references in the bibliographies of current works become the indexing terms used. The conceptual links established by these bibliographic citations provide the means of selecting appropriate items from a wide variety of publications including peripheral journals which might only publish occasional items of interest to a particular user. At present more than 1,080 journals and all U.S. Patents issued are indexed on a very current basis for ASCA. A variety of types of questions may be entered in an ASCA profile. The ASCA system allows the user to add new questions at any time, as additional pertinent works are discovered. Several ways in which the users of the chemical literature can utilize ASCA will be described, including: (1) alerting the user to additional works on a new compound; (2) new methods of synthesis of a known compound; (3) investigation of biological activity of a compound; (4) new applications of a type of reaction; (5) new syntheses in a family of compounds; (6) correction of errors in the published literature; (7) modification of analytical procedures; and (8) new methodology.

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