PROCEEDINGS OF THE BIOCHEMICAL SOCIETY

The 500th Meeting of the Society was held at University College London on Monday, Tuesday and Wednesday, 15, 16 and 17 December 1969, when the following papers were presented:

COMPUTER AND INSTRUMENTATION GROUP COLLOQUIUM ON 'THE FUTURE IN COMPUTING'

Information Retrieval in Chemistry and Allied Sciences

BY A. K. KENT. (*U.K. Chemical Information Service, University of Nottingham, Nottingham, U.K.*)

The 'information explosion' is almost matched by the increase in both conventional and non-conventional information retrieval services. Computer-based services, both experimental and operational, have mushroomed during the past 5 years. The majority of these, however, are of limited significance to biochemists.

Essentially three major computer-based systems are likely to be of interest and value to them. The *Chemical Abstracts Service* (CAS) system, operated in this country by the U.K. Chemical Information Service at Nottingham, provides a service in chemistry that substantially covers biochemical interests. Current-awareness searches can be made on four 'free-text' data bases: *Chemical Titles* (CT), *Chemical-Biological Activities* (CBAC), *CA Condensates* and *Polymer Science and Technology* (POST). The first three of these cover biochemical areas, and CBAC is specifically biochemical in scope. The Institute for Science Information at Philadelphia (ISI) offers a current-awareness service *Automatic Subject Citation Alert*, which is unique in its ability to retrieve information by citation linkage and is particularly valuable in fringe areas of science, and are now making available *Index Chemicus* on magnetic tape. The *Index Chemicus* service is being investigated by the Oxford Experimental Information Unit in collaboration with the U.K. Chemical Information Service and has the important characteristic that it permits substructure search by way of Wiswesser Line Notations of all novel compounds reported. The MEDLARS (Medical Literature Analysis and Retrieval Service) system, which originates from the National Library of Medicine in Washington, is operated in the U.K. through the National Lending Library at Boston Spa. It differs from the CAS and ISI systems in being a 'controlled-language' data base and consequently requires a rather different approach to search strategy.

All these systems require the preparation by the user of a 'search profile', which is a set of search terms linked in some logical way. They are all current-awareness systems with the exception of MEDLARS, which may also be, and is normally, used for retrospective search.

In this paper we shall review the main characteristics of these data bases, the problems of their use, the cost of using them and the advantages that may be gained by their use.

Computer-Aided Approaches to Biochemical Reaction Mechanisms

BY B. CHANCE. (*Johnson Research Foundation, University of Pennsylvania, Philadelphia, Pa. 19104, U.S.A.*)

The Computer-Aided Determination of Peptide Sequences

BY R. A. UPHAM. (*Department of Organic Chemistry, University of Liverpool, Liverpool L69 3BX, U.K.*)

The mass spectra of acylated peptide esters and, in particular, their permethylated derivatives (Lederer & Das, 1967) show a regular fragmentation pattern corresponding to cleavages of the amide bonds. Other peaks arising by loss of CO from the acyl ion and by fragmentations in the side chains are also observed. The regularity of these fragmentation patterns and the ease of acquisition of accurate mass data in digital form make peptide spectra ideally suited to computer-aided interpretation.

Computer programmes have been devised (Biemann, Cone & Webster, 1966; Senn, Venkataraghavan & McLafferty, 1966) that recognize the first *N*-acyl-amino acid and then reconstruct the sequence by successive additions of amino acid units to give in turn other recognizable sequence ions. An alternative programme (Barber, Powers, Wallington & Wolstenholme, 1966) deduces the molecular ion from the atomic composition. The sequence is determined by comparison of the