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PREFACE

Complex natural product structures not closely related to known natural products are usually characterized by X-ray diffraction if a good single crystal is available. Higher-intensity X-ray sources with rotating anodes and more sensitive detectors have recently cut the data-collection time by a factor of ten and permit the use of a smaller crystal. The first paper in this symposium includes four crystal structure determinations performed in an effort to understand the nature of several forms observed for a complex natural antibiotic.

As more powerful NMR methods arrive, higher percentages of natural product structures are being determined by various combinations of non-X-ray methods, many of which are employed in the symposium papers. 1-D NMR correlation methods such as selective INEPT can be very helpful in answering particular questions, especially with small samples, as is illustrated in the second and third papers.

In the rapidly evolving 2-D NMR area, the most important new method is long-range (2- and 3-bond) $^{1}H-^{13}C$ heteronuclear correlations. If done at carbon sensitivity as in the next four papers, the method is usually called long-range HETCOR or COLOC. If an inverse probe is available to greatly cut the instrument time needed via polarization transfer from carbons to the much more sensitive protons, the technique is generally called HMBC as illustrated in the next four papers. These methods provide connectivity information (importantly, even across quaternary carbons and heteroatoms) beyond that available from ordinary ^{1}H-^{1}H COSY (2- and 3-bond) and $^{1}H-^{1}H$ NOESY (through space).

2-D INADEQUATE can be used to establish carbon-carbon connectivities between directly bonded carbons. This method, at present rarely used due to its high cost, is illustrated in the next paper.

The next to last paper shows how molecular mechanics calculations are being used to learn conformational preferences and other structural points.

Structure determination may eventually be largely automated, and one of the attempts in this direction based on HBMC and HMQC data is described in the last paper.

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