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Book Review

NMR Spectroscopy: Processing Strategies

P. Bigler; Wiley-VCH, Weinheim, 2000, xviii + 253 pages, ISBN 3-527-29990-4, £85.00

High-resolution NMR techniques provide excellent information with respect to molecular structure. Nowadays, it is common practice for NMR data to be acquired by automated instrumentation, with remote processing of the data being performed by non-experts. The aim of the first edition of this book was to introduce newcomers to the field of NMR to the important step of data processing. This second edition also takes into account the newest versions of the powerful BRUKER data processing software 1D WINNMR, 2D WIN-NMR and GETFILE, providing an interactive tutorial via the accompanying CD-ROM, which provides the necessary software tools and data.

This volume is divided into six chapters, the first providing a general introduction to the content of the book. The second chapter details your personal 'NMR Processing Station', and discusses how to install and use the software and NMR database provided on the CD-ROM. Topics such as importing data from remote computers, and the different types of data format and format conversion are also discussed. The third chapter gives an overview of modern homo- and hetero-nuclear 1D- and 2D-NMR spectra, as applied to the analysis of peracetylated β-D-glucose. This chapter begins with a general description of 1D and 2D experiments, briefly describes a number of pulse experiments, and the kind of structural information that can be obtained. The fourth chapter shows how 1D WIN-NMR and 2D WIN-NMR software are used to process, display and plot spectra.

The penultimate chapter is the most important part of the book, since it deals with all aspects of modern NMR data

processing. In the first section, the general scheme for processing 1D- and 2D-NMR data are outlined. The theoretical background and reasons for applying a particular processing option are discussed. Practical advice is given on how to use the option together with examples demonstrating its effect on the final spectrum. Later sections of this chapter deal with more advanced and specialised processing options such as zero filling, linear prediction, deconvolution and the manipulation of 2D data sets. The final chapter deals exclusively with the determination of the structure of an unknown oligosaccharide and is designed to test the skill and understanding of data processing of the reader. The chapter starts with a discussion of the different types of strategies that may be used in structural determination. The last section discusses what kind of information can be extracted from the processed spectra and how it can be combined to elucidate the structure of the unknown carbohydrate.

This informative volume forms part of the Wiley-VCH 'Spectroscopic Techniques: An Interactive Course' series. Other volumes in the series include 'Spectra Interpretation of Organic Compounds', 'NMR Spectroscopy: Modern Spectral Analysis', 'NMR Spectroscopy: Data Acquisition' and 'NMR Spectroscopy: Intelligent Data Management'. It is highly recommended for all researchers whose interests involve the elucidation of chemical structure using NMR techniques.

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