Book Reviews

NMR Data Processing. By Jeffrey C. Hoch and Alan S. Stern (Rowland Institute of Science). Wiley: New York. 1996. xi + 196 pp. $69.95 ISBN 0-471-03900-4.

There have been times when NMR spectroscopy used to be critically dependent on data processing by computers. Richard Ernst had to answer skeptical questions about the new approach using pulsed irradiation in combination with Fourier transform for simple 1D applications (ref 1 in the book); however, at that time available computers offered less than a digitized toy does today. Since then there is an ongoing race between capabilities and capacity of computers and NMR applications. Multidimensional NMR represents a special subset, due to the large size and relative complexity of the data. Recently NMR data processing has lost its attraction as a marketable product, in part because many applications became routine and hidden behind buttons and "user-friendly" automated macros. Also, we could witness a strong concentration of the market in the hands of only a few manufacturers for whom this segment of the software brings in little profit. As an overall result, data processing is truly understood by less and less users, and the lack of competition leaves most major commercial processing engines behind increasingly popular academic developments of few laboratories and individuals.

In this era the book of Jeffrey Hoch and Alan Stern, which fills big holes in common understanding of signal processing for NMR spectroscopy and opens "black boxes" of the data processing protocol, cannot be welcomed enthusiastically enough. The Hoch group at Rowland Institute developed their own noncommercial data processing engine (Toolkit) which is perfectly open and highly powerful in their own hands, and which is used for all illustrations in the book (except the inviting still-life in "Le Jardin à Akron" and a couple of other photos).

The book extends to a modest size of 196 pages, and consists of seven chapters. One can immediately feel the pleasant flavor of the casual, yet highly professional style in the Introduction, which highlights some anchor points in the history of NMR data processing and gives essential definitions for the most important terms. Chapter two summarizes the fundamentals of discrete Fourier transform (DFT) which keeps playing an essential role in NMR data processing, while the next chapter goes through major application steps in the processing protocol using DFT. There are many books and publications out there which present similar information, but either they offer too much for an NMR user, or they are not nearly as clear and as concentrated and focused on the basic steps as this one.

Chapters four and five, applications of linear prediction (LP) and maximum entropy reconstruction (MaxEnt) in NMR, respectively, take us to the home ground of Hoch and his teammates. These chapters might seem to be oversized in this book and peppered with a bit much of heavy duty mathematics for an everyday user, but certainly this is the area of computer applications in NMR data processing which is most challenging and promises further expansion of capabilities. One can find perhaps the most clear assessment of various LP approaches so far, as well as that of the maximum entropy reconstruction (MaxEnt) method, which is a must when nonlinear sampling, a promising novel experimental enhancement in multidimensional NMR spectroscopy, is concerned. It seems to be a paradox that in the summary the authors can give only largely qualitative advise on how to optimize parameters, but let us keep in mind that it stems from the nature of nonlinear methods and professional judgment relies on careful error analysis.

It was a great idea to present some "emerging methods", such as wavelets and Bayesian techniques in Chapter six, even in the case that we do not know yet which of these (or others) will become truly involved in NMR processing for general use. However, error analysis could have deserved some more discussion than only a few pages in the final chapter given its essential role and frequent neglect in publications.

The virtue of this book being intentionally focused and concentrated comes with some limitations too. If one goes by the title which offers something very broad and general, he/she could miss some more discussion of experimental aspects which have strong influence on the processing protocol required. Data format, data layout—a common headache for most software developers—or some critical overview of major software packages could be examples of this. Some data processing approaches which are perhaps not part of the home protocol, but may be found useful by many users, are not discussed, such as reference deconvolution. Also, simultaneous visualization, assignment, and data analysis of multiple correlated nD experiments are not subjects of this book. It is arguably over the limit of direct signal processing in NMR, however. The reference list is reasonably up to date and is elegantly short and focused, and "further reading" guides interested readers to appropriate additional sources at the end of individual chapters. Some summary of those few additional reviews and book chapters which did discuss data processing aspects before could be presented here, however. The color figures in the book make it even more inviting, although likely with the price of some elevation in the cost of the volume.

This is a book which can be strongly recommended to all, graduate students, professionals, practitioners, and teachers, who want to be familiar with the most important signal processing aspects of NMR and future perspectives, and is a must to those who want to take on the adventure of developing their own tools, or contribute to software development in the field.

István Pelczer, *Princeton University*

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