



NMR Data Interpretation Explained: Understanding 1D and 2D NMR Spectra of Organic Compounds and Natural Products

By Neil E. Jacobsen

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Through numerous examples, the principles of the relationship between chemical structure and the NMR spectrum are developed in a logical, step-by-step fashion

- Includes examples and exercises based on real NMR data including full 600 MHz one- and two-dimensional datasets of sugars, peptides, steroids and natural products
- Includes detailed solutions and explanations in the text for the numerous examples and problems and also provides large, very detailed and annotated sets of NMR data for use in understanding the material
- Describes both simple aspects of solution-state NMR of small molecules as well as more complex topics not usually covered in NMR books such as complex splitting patterns, weak long-range couplings, spreadsheet analysis of strong coupling patterns and resonance structure analysis for prediction of chemical shifts
- Advanced topics include all of the common two-dimensional experiments (COSY, ROESY, NOESY, TOCSY, HSQC, HMBC) covered strictly from the point of view of data interpretation, along with tips for parameter settings

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Editorial Review

From the Back Cover

Teaches through detailed discussion of examples and exercises ranging from the simplest to very complex how to look at NMR spectra and translate this information into a chemical structure

NMR Data Interpretation Explained teaches how to get from an NMR spectrum to a chemical structure through numerous examples and exercises. Each topic is introduced with one or more examples of NMR data with detailed explanations of the interpretation of that data. Examples are then followed by a number of exercises using detailed images of NMR data, and these are followed by solutions, again with detailed explanation of the step-by-step reasoning used to solve the exercise.

Every detail and aspect of the NMR data is explained, not just the simple and beautiful spectra but also the complex and surprising spectra. At the end of each chapter there are a large number of additional exercises, nearly every one showing detailed graphics of NMR data. Solutions with detailed explanations are provided for half of the exercises, with the remaining solutions provided to instructors on a website.

All of the commonly used techniques of small molecule solution-state NMR are covered:

- Simple one-dimensional (¹H and ¹³C),
- Edited (DEPT) ¹³C,
- Selective one-dimensional ¹H (NOE, ROE and TOCSY)
- Two-dimensional (COSY, TOCSY, NOESY, ROESY, HSQC and HMBC)

The final chapter puts all of these techniques together to solve the structures of a number of complex natural products: sesquiterpenes, steroids, alkaloids, sugars and triterpenes. Many exercises are provided for each of these molecule types.

Another aspect of this book that is unique is that it does not attempt to explain the theory of NMR. Other books do an excellent job of explaining the theoretical basis of NMR and how the experiments actually work to give the NMR data, but this book focuses exclusively on the interpretation of NMR data.

Since NMR spectrometers are expensive (around \$800,000 for a 600 MHz instrument), and require specialized expertise and expensive cryogens (liquid nitrogen and liquid helium) to operate, many teaching and research institutions are unable to obtain a high-field NMR instrument. It is for industry researchers as well as undergraduates, graduate students and postdoctoral researchers in chemistry, biochemistry, medicinal chemistry and pharmacy, that this book was written.

Neil E. Jacobsen, PhD, has been Director of the NMR Facility in the Department of Chemistry and Biochemistry at the University of Arizona for the last 20 years. He teaches an undergraduate course in NMR Spectroscopy (Organic Qualitative Analysis) using a series of unknowns including monoterpenes and steroids, with students acquiring their own 400 MHz 1D and 2D NMR data. He also teaches a graduate course in Organic Synthesis and NMR Spectroscopy that is focused on using the spectrometers and interpreting complex NMR data. He has 30 years of experience working in the field of NMR spectroscopy, during that time he has authored 46 publications in peer-reviewed journals as well as the 2007 Wiley book *NMR Spectroscopy Explained*.

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Kathryn Glover:

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The book NMR Data Interpretation Explained: Understanding 1D and 2D NMR Spectra of Organic Compounds and Natural Products has a lot of knowledge on it. So when you read this book you can get a lot of profit. The book was written by the very famous author. Tom makes some research prior to write this book. This book very easy to read you can find the point easily after reading this book.

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