

1. Record Nr.	UNINA9910298582103321
Autore	Hoeck Casper Rønn
Titolo	Solving a 3D Structural Puzzle // by Casper Rønn Hoeck
Pubbl/distr/stampa	Cham : , : Springer International Publishing : , : Imprint : Springer, , 2018
ISBN	3-319-96172-1
Edizione	[1st ed. 2018.]
Descrizione fisica	1 online resource (xli, 238 pages) : illustrations
Collana	Springer Theses, Recognizing Outstanding Ph.D. Research, , 2190-5053
Disciplina	543.0877
Soggetti	Spectroscopy Microscopy Chemistry, Physical and theoretical Medicinal chemistry Spectroscopy/Spectrometry Spectroscopy and Microscopy Theoretical and Computational Chemistry Medicinal Chemistry
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di bibliografia	Includes bibliographical references.
Nota di contenuto	NMR spectroscopy: Past to present -- Theory – 3D structural information from NMR, part 1 -- Application of NOEs and 3JHH-couplings in 3D structure determination -- Development of NMR experiments for determination of long-range J-coupling constants -- Theory – 3D structural information from NMR, part 2 -- Determination of long-range residual dipolar coupling constants -- Chiral alignment media for enantiodiscrimination -- Tensor free RDC calculations -- Overall perspective and conclusions.
Sommario/riassunto	This book explores how nuclear magnetic resonance (NMR) spectroscopy may be used for spatial structural elucidation of novel compounds from fungal and synthetic sources. Readers will discover the exciting world of NOE (nuclear Overhauser effect), RDC (residual dipolar coupling) and J-coupling constants, both short- and long range. With emphasis on obtaining structural knowledge from these NMR observables, focus is moved from solving a static 3D structure to

solving the structural space inhabited by small organic molecules. The book outlines the development and implementation of two Heteronuclear Multiple Bond Correlation-type NMR experiments, and the 3D structural elucidation of multiple known and novel compounds. In addition, a new method of back-calculating RDCs (allowing for more flexible structures to be investigated), and the synthesis and evaluation of novel chiral alignment media for ab initio determination of absolute stereochemistry of small molecules using RDCs are also included. Challenges that 3D structural generation of small compounds face are also covered in this work.
