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*Conformational Analysis
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The most concise and streamlined
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chemistry for the pharmacy student
Organic Chemistry for Pharmacy is
a textbook written specifically for
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Using a building-block approach,
the book delivers a basic, yet
thorough discussion of the mode of

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action, therapeutic applications, and limitations of various pharmaceutical agents. Organic Chemistry for Pharmacy is especially written for students who have a limited background in chemistry. In order to make the learning/teaching experience as

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efficient as possible, Organic Chemistry for Pharmacy includes outstanding pedagogical features such as chapter outlines, chapter summaries, boxed "take away points", quick-reference tables, and problems within each chapter. The focus and presentation of this text

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is particularly suited for Organic/Medical Pharmacy courses which are weighted heavily towards Organic, rather than Medical Pharmacy.

From the beginnings of modern chemistry, molecular structure has been a lively area of research and

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speculation. For more than half a century spectroscopy and other methods have been available to characterize the structures and shapes of molecules, particularly those that are rigid. However, most molecules are at least to some degree non-rigid and this non-

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rigidity plays an important role in such diverse areas as biological activity, energy transfer, and chemical reactivity. In addition, the large-amplitude vibrations present in non-rigid molecules give rise to unusual low-energy vibrational level patterns which have a dramatic

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effect on the thermodynamic properties of these systems. Only in recent years has a coherent picture of the energetics and dynamics of the conformational changes inherent in non-rigid (and semi-rigid) molecules begun to emerge. Advances have been made in a

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number of different experimental areas: vibrational (infrared and Raman) spectroscopy, rotational (microwave) spectroscopy, electron diffraction, and, most recently, laser techniques probing both the ground and excited electronic states.

Theoretically, the proliferation of

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powerful computers coupled with scientific insight has allowed both empirical and ab initio methods to increase our understanding of the forces responsible for the structures and energies of non-rigid systems. The development of theory (group theoretical methods

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and potential energy surfaces) to understand the unique characteristics of the spectra of these floppy molecules has also been necessary to reach our present level of understanding. The thirty chapters in this volume contributed by the key speakers at

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the Workshop are divided over the various areas. Both vibrational and rotational spectroscopy have been effective at determining the potential energy surfaces for non-rigid molecules, often in a complementary manner. Recent laser fluorescence work has

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extended these types of studies to electronic excited states. Electronic diffraction methods provide radial distribution functions from which both molecular structures and compositions of conformational mixtures can be found. Ab initio calculations have progressed

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substantially over the past few years, and, when carried out at a sufficiently high level, can accurately reproduce (or predict ahead of time) experimental findings. Much of the controversy of the ARW related to the question of when an ab initio is reliable.

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Since the computer programs are readily available, many poor calculations have been carried out. However, excellent results can be obtained from computations when properly done. A similar situation exists for experimental analyses. The complexities of non-rigid

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molecules are many, but major strides have been taken to understand their structures and conformational processes.

Introduction what is organic chemistry all about?; Structural organic chemistry the shapes of molecules functional groups;

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Organic nomenclature; Alkanes;
Stereoisomerism of organic
molecules; Bonding in organic
molecules atomic-orbital models;
More on nomenclature compounds
other than hydrocarbons;
Nucleophilic substitution and
elimination reactions; Separation

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and purification identification of organic compounds by spectroscopic techniques; Alkenes and alkynes. Ionic and radical addition reactions; Alkenes and alkynes; Oxidation and reduction reactions; Acidity or alkynes. This text will give the reader a firm

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understanding of all aspects of carbohydrate conformation by describing and explaining the importance of interactions between carbohydrates and interactions of carbohydrates with proteins, nucleic acids or any other macromolecule., The authors have

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gathered a wealth of information on carbohydrate structures, different methods of conformational analysis, the role of carbohydrates as recognition molecules in biological systems and their industrial applications., Whether you are a student, teacher or a

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basic researcher, this text book is a 'one-stop' source of current information on carbohydrate conformation and the potential use of conformational properties in industry and also of their crucial role in important biological events such as cell-cell interaction, cell

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adhesion, cellular signaling
mechanism.

"Excellent and very timely....It will undoubtedly become a standard reference for the application of circular dichroism (CD) to biomolecules." --- Quarterly Review of Biology, March 1997

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"[T]estament to the book's utility is the fact that during the course of my review I had to 'rescue' it from the desks of graduate students on an almost daily basis. In summary, this is a great book." --- American Scientist "Well documented chapters provide a very good

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insight into the problems surrounding the conformation of biomacromolecules...An indispensable source of information." --- Nahrung, 42(2), 1998 Renowned experts present the first state-of-the-art description of circular dichroism spectroscopy

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(CD). Chapters present in-depth discussions of the history of the field, the theory of CD for application to globular proteins, membrane proteins, peptides, nucleic acids and their interactions, carbohydrates, and instrumentation. Discussions also

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feature new techniques using synchrotron radiation, vibrational Raman optical activity, and vibrational CD. More than 250 illustrations supplement the text.

[The Conformational Analysis of Cyclic Molecules by NMR Spectroscopy](#)

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Sciences

Methodology, Concepts, and Mode-
of-Action

*The Peptides: Analysis,
Synthesis, Biology,
Volume 7: Conformation
in Biology and Drug*

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Design focuses on the analysis of peptides, emphasizing the use of physical methods in peptide conformational analysis and the relationship of

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*conformational
properties of peptides
to biological
properties. This book
consists of nine
chapters. Chapter 1
provides a brief*

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*overview of the
perspective on the
application of physical
methods to peptide
conformational analysis.
The use of circular
dichroism (CD)*

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*spectroscopy to examine
the conformational
properties of peptides
in solution is
elaborated in Chapter 2,
while the use of
fluorescence*

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*spectroscopy to examine
the special
relationships of
aromatic side-chain
groups to one another is
discussed in Chapter 3.
In Chapter 4, the use of*

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*various theoretical
methods to calculate the
conformations of
peptides is described.
The methods used to
stimulate peptide
conformations and*

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dynamics are outlined in Chapter 5. The last four chapters examine various aspects of the use of nuclear magnetic resonance (NMR) in peptide conformational

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*analysis. This volume is
suitable for biologists,
specialists, and
researchers interested
in peptides and
proteins.*

This book seeks to

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*introduce the reader to
current methodologies in
analytical calibration
and validation. This
collection of
contributed research
articles and reviews*

Where To Download Conformational Analysis Of Molecules In Excited States

addresses current

developments in the

calibration of

analytical methods and

techniques and their

subsequent validation.

Section 1,

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*"Introduction," contains
the Introductory
Chapter, a broad
overview of analytical
calibration and
validation, and a brief
synopsis of the*

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following chapters.

*Section 2 "Calibration
Approaches" presents
five chapters covering
calibration schemes for
some modern analytical
methods and techniques.*

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The last chapter in this section provides a segue into Section 3, "Validation Approaches," which contains two chapters on validation procedures and

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*parameters. This book is
a valuable source of
scientific information
for anyone interested in
analytical calibration
and validation.*

The goal of these two

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*volumes is to help fill
the gap between theory
and experiment in
membrane science. This
is the only work
available today which
covers the domain of*

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computer-aided

*conformational analyses
of membranes. Written in
a detailed, yet
comprehensive manner,
this book uses the semi-
empirical approach as a*

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*way to give a molecular
description of the
membrane structure in
organized systems. This
interesting work
establishes the validity
and quality of the*

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prediction by making a permanent comparison with the experimental data. This reference aims to use this comparison to open a new avenue in the molecular

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*description of the
biological membrane.
Those involved with
biochemistry,
biophysics,
pharmacology, and
biology will find these*

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*volumes interesting and
informative.*

*A series of one hundred
and nine rigid and
flexible molecules
(dibenzofurans,
biphenyls, fluorenes,*

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fluorenones and diphenyl ethers) with a range of substituents have been studied with a view to obtaining conformational data from vicinal ^{13}C - ^{13}C coupling

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constants. The molecules were characterized primarily by nuclear magnetic resonance spectroscopy (proton, carbon-13, fluorine-19, nitrogen-15,

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heteronuclear

(¹³C-¹H) correlation

spectroscopy,

DEPT-90/DEPT-135, NOE

spectroscopy). Finally,

the INADEQUATE

experiment was used to

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obtain ^{13}C - ^{13}C coupling constants. Twelve novel crystal structures were obtained from the study, and conformations obtained for biphenyls and diphenyl ethers

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*compared with
conformational studies
by other methods,
indicating that the
lowest energy
conformations can be
retained in both solid*

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*and solution states,
provided that other
factors, (e.g. crystal
packing forces) are not
dominant. Comparison of
our data, using state-of-
the-art techniques for*

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*assignments, with
previous theoretical
predictions of
conformations from
carbon chemical shifts
proved unsatisfactory.
Attempts to use vicinal*

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carbon coupling

constants to obtain a

dihedral angle

dependence were

unsuccessful. For rigid

molecules, vicinal

coupling constants could

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*not be assigned with
confidence and the
dihedral angle dependent
contribution could not
be quantified because of
the multifactorial
nature of these*

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couplings. Previous literature strongly suggests that these coupling constants do not exhibit a dihedral angle dependence. Previous literature has

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*also shown that the
vicinal coupling
constants required in
the present study for
the conformational
analysis of biphenyls do
not exhibit a dihedral*

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*angle dependence. The
dihedral angle dependent
contributions from
vicinal coupling
constants in certain
diphenyl ethers were
completely eclipsed by*

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additional "through-space" coupling. The results of a molecular mechanics study showed that it was not possible to obtain conformer distributions for

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*biphenyls or diphenyl
ethers. Therefore,
Karplus-type equations
for these molecules
could not be formulated.
This work represents one
of the most*

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*comprehensive and
diverse NMR analyses of
dibenzofurans, diphenyl
ethers and biphenyls,
and makes a significant
contribution to the
carbon coupling constant*

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*data currently
available.*

*The activity of many
biopharmaceutical
polymers is dependent on
conformation, and the
next several years will*

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*see increased interest
in the conformational
analysis of these
polymers resulting from
the development of
biosimilar or "follow-
on" biological products.*

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While a wide variety of approaches to analysis exists, finding the most viable ones would be much easier with a consolidated reference that details the

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*benefits and cost of
each approach, with an
emphasis on real results
and real products.*

*Explores the Growing
Role of Conformational
Analysis in Comparing*

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Generic

Biopharmaceuticals

Approaches to the

Conformational Analysis

of Biopharmaceuticals

gathers the most useful

techniques and methods

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*into a single volume,
putting the greatest
emphasis on those
approaches that have
proven the most
fruitful. Rather than
cover specific uses of*

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*techniques in detail,
this book provides
commercial
biotechnologists and
researchers with the
information and
references they need to*

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*make good choices about
the technology they
choose to use. With a
large number of
references that direct
readers to primary
source material, it*

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*includes studies drawn
from the gamut of
current literature,
covering physical
methods, such as
differential scanning
calorimetry, light*

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*scanning, and analytical
ultracentrifugation. It
also addresses chemical
methods, such as
hydrogen-deuterium
exchange and trace
labeling, along with*

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*infrared, ultraviolet,
and Raman spectroscopy.*

Written by Roger

*Lundblad, a true pioneer
in protein science, this
volume supplies the
necessary information*

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*researchers need to
access when deciding on
the most cost-effective
approach, including:
Comparability of
biopharmaceuticals
Characterization of*

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focus on relevant

commercial

biotechnology, this book

belongs on the shelves

of those serious

researchers who are

paving the way for the

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*next generation of
biopharmaceutical
polymers.*

*The Synthesis and
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Analysis of Small

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*The Nuclear Overhauser
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Method
Vibrational and
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of Some Molecules by
Infrared and Raman

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A unique guide to variable temperature CD spectroscopy and its application in organic chemistry This timely, original, thought-provoking work looks at organic stereochemistry from the perspective of circular dichroism (CD), using variable temperature CD

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spectroscopy to determine the conformation or absolute configuration of chiral molecules. With an emphasis on the analysis of optically active ketones and the carbonyl chromophore, the authors demonstrate the advantages of this highly sensitive spectroscopic tool for

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obtaining stereochemical information in diverse areas of organic chemistry, biochemistry, and medicinal/pharmaceutical chemistry. They combine detailed examples of stereochemical analysis with clear, thorough presentations, correlating chiroptical data with molecular

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mechanics calculations as well as data from NMR spectroscopy and other spectroscopic techniques. In addition, they provide a systematic survey of the professional literature, featuring an extraordinary collection of original CD spectra run at varying temperatures. Coverage includes: * Chiroptical

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measurements: CD and ORD (Optical Rotatory Dispersion) * Conformational analysis of compounds ranging from simple cyclic ketones to polycyclics * Conjugated and homoconjugated systems * Stereochemistry of the carbon-carbon double bond * Stereochemistry from exciton coupling

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of two or more chromophores * An interesting historical account of the development of stereochemical concepts

A unique look at some of the hottest topics in photophysics and photochemistry today The study of molecules in excited states has

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exploded over the past decade, providing new insights into conformational changes in organic molecules and opening up research opportunities for scientists and professionals in chemistry, physics, biology, medicine, and materials engineering. Using conformational

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analysis as a unifying concept, this important new work provides readers with a cohesive and cutting-edge overview of this fascinating and challenging field. From conformational changes accompanying photoinduced electron transfer to elementary photophysical and photochemical

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processes in living systems, the most representative and challenging topics are carefully gleaned from the vast literature, highlighting major conceptual problems along with the relevant experimental techniques. Authoritative, detailed contributions from both experimentalists and

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- Conformational changes in intramolecular excited state electron transfer
- Conformational aspects of excited state proton transfer
- The novel topic of solute-solvent friction in chemical reactions
- Mechanisms and structural aspects of exciplex

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formations * Conformational aspects of organic photochemistry * Calculations of excited state conformational properties

An authoritative review of the state of the art in the Nuclear Overhauser Effect-essential information for organic chemists, biochemists, biophysicists,

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and NMR spectroscopists The field of NMR spectroscopy has seen tremendous growth in the last twenty years, particularly advances relating to Nuclear Overhauser Effect (NOE) spectroscopy-the most powerful technique for obtaining structural information on molecules in solution.

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Extensive and engaging, the Second Edition of the leading reference on the NOE is significantly updated to reflect the latest changes and new approaches in the field. Neuhaus and Williamson provide an essential guide to the complexities and use of the NOE in a readily accessible,

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straightforward manner. Their practical handbook features a new chapter addressing the use of NOE data to calculate biomolecular structures. Chapters dealing with the kinetics of the NOE, the effects of exchange and internal motion, and applications of the NOE, are also extensively revised.

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Cross-referenced in remarkable depth,
The Nuclear Overhauser Effect is
organized into three main parts: * Part
I describes the theory of the Nuclear
Overhauser Effect in a clear,
comprehensive fashion * Part II
discusses the considerations involved
in implementing NOE experiments,

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including full coverage of all necessary details for both new and established techniques * Part III offers examples of how the NOE is used, including applications to defining molecular geometry, stereochemistry, conformation, and biomolecular structure and interactions The Nuclear

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Overhauser Effect in Structural and Conformational Analysis, Second Edition, uniquely explains the NOE in detail, making it an indispensable resource for the novice as well as the experienced NMR researcher.

This text describes the importance of molecular organization in organic

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chemical and biological systems, the quantum foundations of molecular spatial structure, molecular symmetry, chirality and physical methods for studying molecular geometry.

Unique work on structure-based drug design, covering multiple aspects of drug discovery and development. Fully

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colored, many images, computer animations of 3D structures (these only in electronic form). Makes the spatial aspects of interacting molecules clear to the reader, covers multiple applications and methods in drug design. Structures by mode of action, no therapeutic areas. Of high

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relevance for academia and industrial research. Focus on gene technology in drug design, omics-technologies computational methods experimental techniques of structure determination multiple examples on mode of action of current drugs, ADME-tox properties in drug development, QSAR methods,

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combinatorial chemistry, biologicals,
ribosome, targeting protein-protein
interfaces.

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All these results
demonstrate that our
conformational analysis
approach can provide

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reliable drug-target
structural information for
future use in ligand and
structure based drug
discovery applications.
Stereochemistry of Organic
Compounds The first fully
referenced, comprehensive

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book on this subject in more than thirty years, Stereochemistry of Organic Compounds contains up-to-date coverage and insightful exposition of all important new concepts, developments, and tools in the rapidly

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advancing field of
stereochemistry, including:
* Asymmetric and
diastereoselective synthesis
* Conformational analysis *
Properties of enantiomers
and racemates * Separation
and analysis of enantiomers

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and diastereoisomers *

Developments in spectroscopy
(including NMR),

chromatography, and

molecular mechanics as

applied to stereochemistry *

Prostereoisomerism *

Conceptual foundations of

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stereochemistry, including terminology and symmetry concepts * Chiroptical properties Written by the leading authorities in the field, the text includes more than 4,000 references, 1,000 illustrations, and a

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glossary of stereochemical terms.

The goal of this book is to present an overview of applications of molecular spectroscopy to investigations in organic and inorganic materials,

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foodstuffs, biosamples and
biomedicine, and novel
characterization and
quantitation methods. This
text is a compilation of
selected research articles
and reviews covering current
efforts in various

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applications of molecular spectroscopy. Sections 1 and 2 deal, respectively, with spectroscopic studies of inorganic and organic materials. Section 3 provides applications of molecular spectroscopy to

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biosamples and biomedicine.
Section 4 explores
spectroscopic
characterization and
quantitation of foods and
beverages. Lastly, Section 5
presents research on novel
spectroscopic methodologies.

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Overall, this book should be a great source of scientific information for anyone involved in characterization, quantitation, and method development.

This book leaves the

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conventional view of
chemical structures far
behind: it demonstrates how
a wealth of valuable, but
hitherto unused information
can be extracted from
available structural data.
For example, a single

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structure determination does not reveal much about a reaction pathway, but a sufficiently large number of comparable structures does. Finding the 'right' question is as important as is the intelligent use of

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crystallographic databases.
Contributions by F.H. Allen,
T.L. Blundell, I.D. Brown,
H.B. Bürgi, J.D. Dunitz, L.
Leiserowitz and others,
authoritatively discuss the
structure correlation method
as well as illustrative

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results in detail, covering
such apparently unrelated
subjects as * Bond strength
relations in solids *
Crystal structure prediction
* Reaction pathways of
organic molecules *
Ligand/receptor interactions

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and enzyme mechanisms This book will be useful to the academic and industrial reader alike. It offers both fundamental aspects and diverse applications of what will surely become a powerful branch of

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This textbook covers the most important aspects of what remains an actively changing area of knowledge. Topics include chirality, the determination of absolute configurations,

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stereochemical descriptors,
chiroptic properties,
asymmetric synthesis, and
the resolution of racemates.

[Circular Dichroism and the
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Molecules by NMR

Spectroscopy Using Vicinal
13C-13C Coupling Constants
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Some Halo Or Pseudohalo
Substituted Small Organic
Molecules by Spectroscopic
and Theoretical Methods

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Chemistry
Stereochemistry of Organic
Compounds

Conformational Analysis: Scope

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and Present Limitations contains the proceedings of the Brussels International Symposium on Conformational Analysis held in Brussels, Belgium, in September 1969. The papers focus on the theoretical aspects and applications of conformational analysis, such as

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those concerning the aliphatic and especially the cyclic series. Topics covered include the geometry of five-membered rings; conformational transmission in steroids; conformational aspects of N-quaternization; and applications of nuclear magnetic resonance

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spectrometry in conformational studies of cyclohexane derivatives. This book is comprised of 20 chapters and begins with a discussion on the conformational aspects of some five-membered ring compounds based mainly on observed (diffraction methods) and

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calculated torsional angles. The reader is then introduced to nuclear magnetic resonance studies of the conformations and conformational barriers in cyclic molecules; conformational studies of six-membered heterocycles; conformational transmission in

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steroids; and solvolytic cyclizations involving double bonds. The remaining chapters explore the conformational analysis of methylcyclohexane, cyclohexane systems, and carbonium ions; conformations of membrane-active cyclodepsipeptides; energetics of

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isomeric transition states and competitive reaction pathways in conformational analysis; and conformational aspects of the reaction of the 1-methylcyclodecane-1,6-diols with acid. This monograph will be of interest to organic chemists.

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This first work to be devoted entirely to this increasingly important field, the "Textbook" provides both an in-depth and comprehensive overview of this exciting new area. Edited by Johann Gasteiger and Thomas Engel, the book provides an introduction to

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the representation of molecular structures and reactions, data types and databases/data sources, search methods, methods for data analysis as well as such applications as structure elucidation, reaction simulation, synthesis planning and drug design. A "hands-on"

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approach with step-by-step tutorials and detailed descriptions of software tools and Internet resources allows easy access for newcomers, advanced users and lecturers alike. For a more detailed presentation, users are referred to the "Handbook of

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Chemoinformatics", which will be published separately. Johann Gasteiger is the recipient of the 1991 Gmelin-Beilstein Medal of the German Chemical Society for Achievements in Computer Chemistry, and the Herman Skolnik Award of the Division of Chemical

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*Information of the American
Chemical Society (ACS) in 1997.
Thomas Engel joined the research
group headed by Johann Gasteiger
at the University of Erlangen-
Nuremberg and is a specialist in
chemoinformatics.
This book reviews the advances*

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and challenges of structure-based drug design in the preclinical drug discovery process, addressing various diseases, including malaria, tuberculosis and cancer. Written by internationally recognized researchers, this edited book discusses how the application of

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the various in-silico techniques, such as molecular docking, virtual screening, pharmacophore modeling, molecular dynamics simulations, and residue interaction networks offers insights into pharmacologically active novel molecular entities. It presents a

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clear concept of the molecular mechanism of different drug targets and explores methods to help understand drug resistance. In addition, it includes chapters dedicated to natural-product-derived medicines, combinatorial drug discovery, the CryoEM

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technique for structure-based drug design and big data in drug discovery. The book offers an invaluable resource for graduate and postgraduate students, as well as for researchers in academic and industrial laboratories working in the areas of chemoinformatics,

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