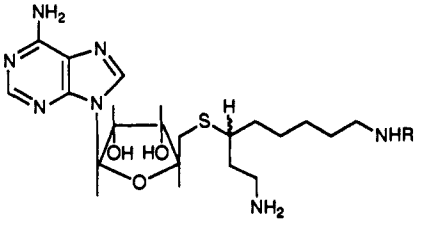
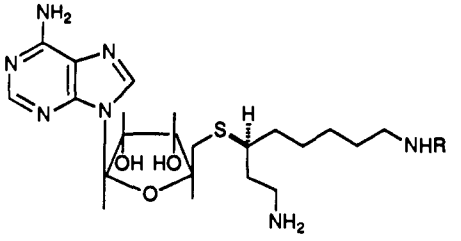
**Chin Liu and James K. Coward***: Stereospecific Synthesis of (*R*)- and (*S*)-S-Adenosyl-1,8-diamino-3-thiooctane, a Potent Inhibitor of Polyamide Biosynthesis. Comparison of Asymmetric Induction vs Enantiomeric Synthesis.

Pages 2095–2099. Clearer representations of the stereochemistry of the compounds are given below.

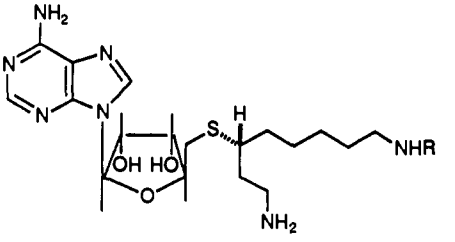


1

a, R = H
b, R = $CH_2CH_2CH_2NH_2$



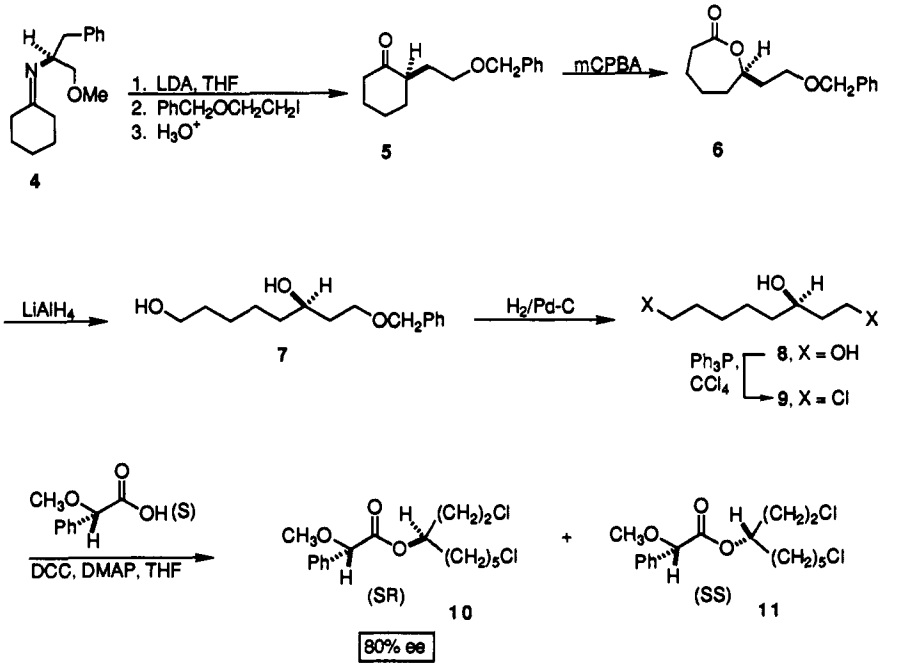
2



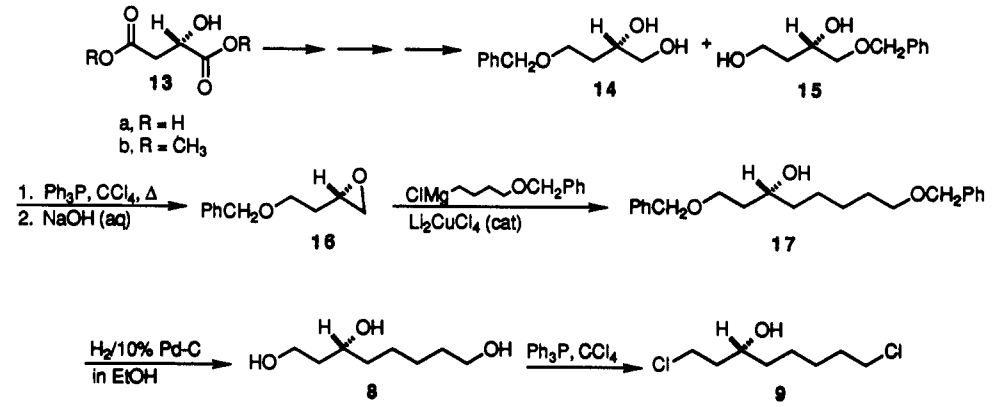
3

a, R = H
b, R = $CH_2CH_2CH_2NH_2$

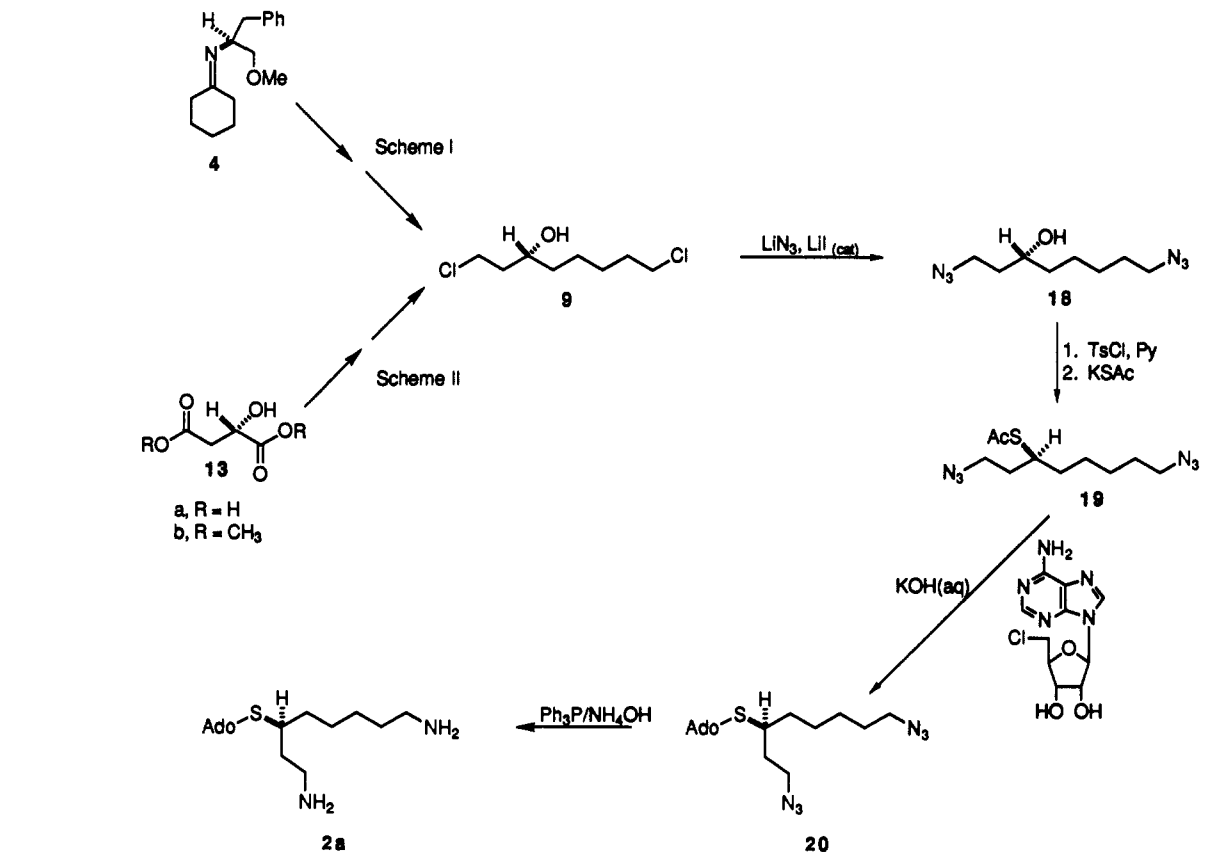
**Scheme I**

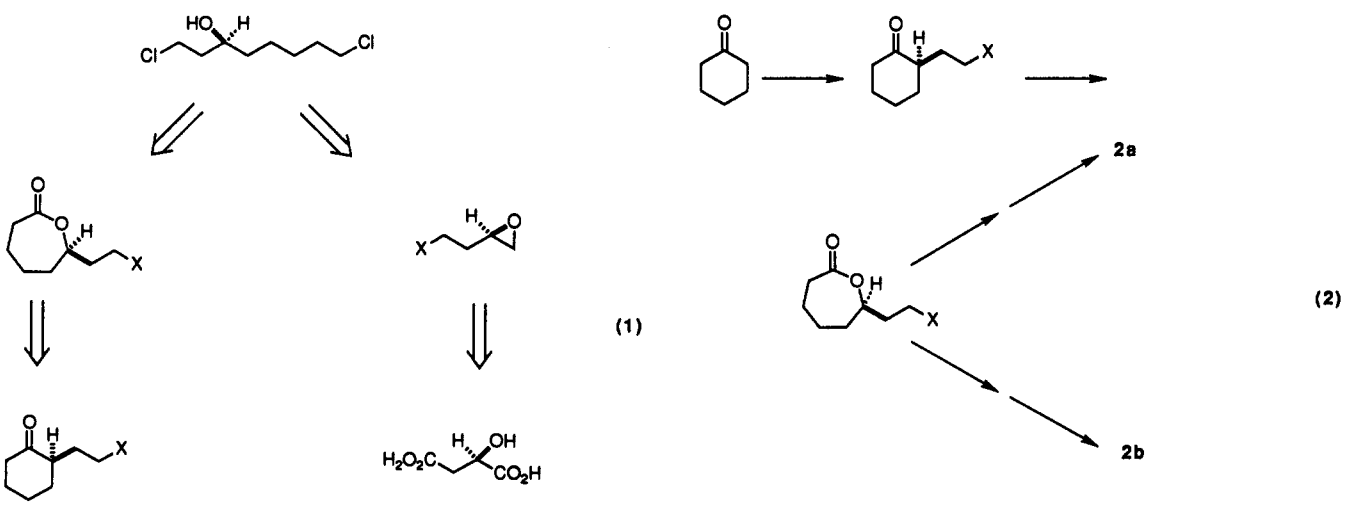


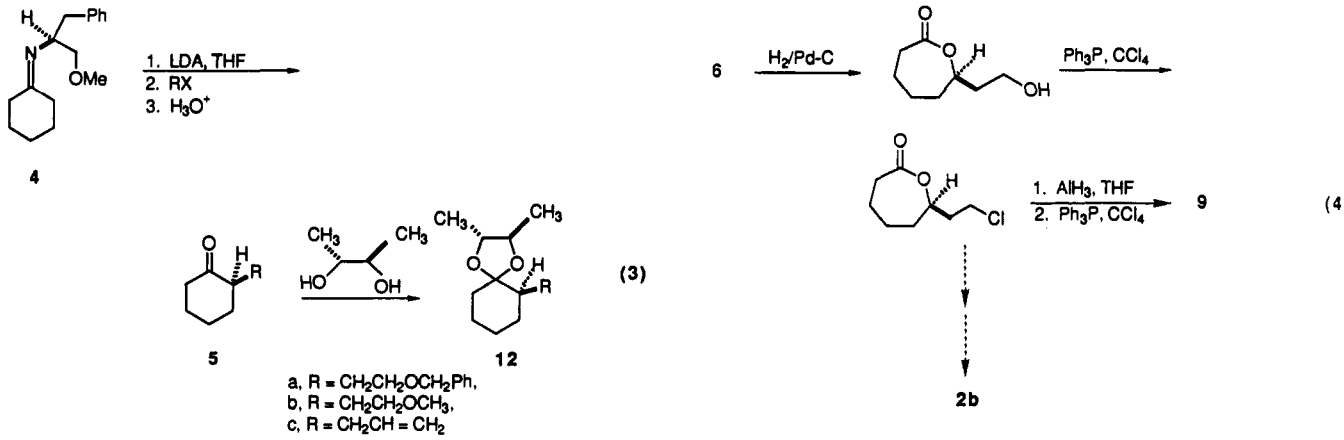
**Scheme II**




**Scheme III**






# Book Reviews

**Concepts and Applications of Molecular Similarity.** Edited by M. A. Johnson and G. M. Maggiora. Wiley-Interscience, New York, 1990. xix + 393 pp. 16.5 × 25 cm. ISBN 0-471-62175-7. $65.00.

What could be as subjective as the notion of similarity, depending as it does on personal experience? Yet, as this volume makes clear, no concept is more fundamental to the scientific method, nor to our assimilating the overwhelming amount of data we must process. Indeed, as indicated in the scholarly chapter by Dennis Rouvray, the advancement of science, from taxonomic classification in biology to the periodic table of the chemical elements and the structural theory of matter, can be read as progress in developing objective criteria of similarity. Fortunately, *molecular* similarity lends itself to expression by mathematical methods which are objective and quantitative. An introductory chapter by the editors defines the current mathematical representations of molecules in terms of descriptors, and introduces mathematical operations on the descriptors as unifying themes for the following chapters.

Based on a symposium on computer-based methods of molecular similarity at the fall 1988 American Chemical Society National Meeting in Los Angeles, this book aims (according to the preface) to provide "definitive overviews" of topics related to the definition, computation, and application of molecular similarity and to promote and focus research efforts in this area. It succeeds admirably in these aims.

A major focus of the book is the development of molecular descriptors from topological (graph–theoretic, fragment-based) to topographical (shape and surface-based). From chapters 3 (by Peter Willett) and 4 (by David Bawden), describing methods for searching large databases of 2-D and 3-D molecular structures by similarity, to chapter 7 (by A. J. Hopfinger and B. J. Burke) on molecular shape analysis to quantitatively establish spatial molecular similarity, to chapter 8 (by Philip Dean) on molecular similarity in ligand–receptor interaction, to chapter 11 (by Paul Mezey) on similarity of molecular shapes and molecular surfaces, there is a progression in complexity and sophistication of concepts. Other topics covered include an extensive review of topological measures of similarity in chapter 5 (by Milan Randic) including an interesting attempt to extend these concepts to a 3-dimensional connectivity index, quantum mechanics derived measures of molecular similarity in chapter 6 (by R. Carbo and B. Calabuig), application of graph theoretic and matrix methods to description of chemical reaction similarity and stereochemical similarity in chapter 9 (by Ivar Ugi and co-workers), a formalism for modeling similarity in chemical transformation pathways in chapter 10 (by Mark Johnson, Eric Gifford, and C.-c. Tsai), and finally, the foundations of a mathematical theory of molecular similarity in chapter 12 (by Robert Rosen).

The book is heavy on definitions of molecular descriptors to be compared, as is appropriate for one oriented toward computer implementation of the concepts; it is somewhat light on presentation of significant chemical applications of the approaches, although there are plenty of such examples cited. There are a number of current research frontiers covered, with many 1989 references, and several chapters give proposals for future research. Particularly interesting research directions, to this reviewer's mind, include the concept of "self-similarity" (chapter 2), searching for critical fragments and for the optimal structure (chapter 5), determining "optimal similarity" and similarity of part structures (chapter 7), "blind searching" for common motifs and automatic creation of novel ligands containing these motifs (chapter 8), and treatment of molecular electrostatic, accessibility, and dynamic shape similarity (chapter 11). The book is oriented to small molecules; thus, similarity of peptide sequences is only obliquely addressed in chapters 5 and 12, and similarity of macromolecular structures does not appear to be addressed at all.

In summary, this volume constitutes an admirable review and synthesis of concepts and accomplishments in this fast-moving field of research and points directions for future progress. Several of the chapters can be read with profit by practicing medicinal chemists wishing to improve their understanding of molecular similarity concepts. For practitioners of computational chemistry, this volume is a must.

There is a detailed table of contents and a good subject index. There is no author index.

*Merck Sharp & Dohme Research Laboratories*
*Rahway, New Jersey 07065*
**Peter Gund**

**Reductions by the Alumino- and Borohydrides in Organic Synthesis.** By J. Seyden-Penne. VCH Publishers, New York. 1991. xiii + 193 pp. 16 × 24 cm. ISBN 1-56081-099-8. $65.00.

Since the earliest days of organic chemistry, functional-group reduction has constituted one of the most useful and frequently used tools in the synthetic chemist's armamentarium. The development of hydrides of aluminum and boron, beginning in the late 1930s and continuing unabated through the present day, has revolutionized the field, greatly expanding the number of functional groups which may be conveniently reduced and introducing an extraordinary degree of chemo-, regio-, and stereoselectivity. Unfortunately, the very profusion of these reagents, and the lack