

COMPUTER TECHNIQUES: IDENTIFYING SIMILARITIES BETWEEN SMALL MOLECULES

PETER MEEK, GUILLERMO MOYNA, AND RANDY ZAUHAR

University of the Sciences in Philadelphia, Philadelphia, Pennsylvania

Contents

- 1 Introduction
- 2 Computer-Aided Drug Design (CADD)
- 3 Harvesting Data from Small Molecules
- 4 Representing Molecules for Interpretation by Computers
 - 4.1 Importance of Continuity Within Molecular Representations
- 5 Defining Similarity
 - 5.1 Why Do We Wish to Compare Molecules?
 - 5.2 Utilizing External Sources of Information
- 6 Detecting Similarity with *in silico* Techniques
 - 6.1 HQSAR
 - 6.2 QSAR
 - 6.3 Superimposition
 - 6.4 Program Suites
 - 6.5 Comparative Molecular Field Analysis (CoMFA) and Related Approaches
 - 6.6 Shape Signatures
- 7 Conclusion
 - Acknowledgments
 - References