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2.2.2.1 Molecular Alignment; 2.2.2.2 Charges; 2.2.2.3 Generating 3D Fields; 2.2.2.4 Compilation of GRID Maps; 2.2.2.5 Inclusion of Macroscopic Descriptors with 3D Field Data; 2.2.3 Statistical Analysis; 2.2.3.1 Results of the Analysis; 2.2.3.2 Testing the Model; 2.2.4 Conclusions; References; 2.3 GOLPE Philosophy and Applications in 3D QSAR; 2.3.1 Introduction; 2.3.1.1 3D Molecular Descriptors and Chemometric Tools; 2.3.1.2 Unfolding Three-way Matrices; 2.3.2 The GOLPE Philosophy; 2.3.2.1 Variable Selection; 2.3.3 Applications; 2.3.3.1 PCA on the Target Matrix; 2.3.3.2 PCA on the Probe Matrix; 2.3.3.3 PLS Analysis on the Target Matrix; 2.3.3.4 PLS on Target Matrix as a Strategy to Ascertain the Active Conformation; 2.3.3.5 GOLPE with Different 3D Descriptors; 2.3.4 Conclusions and Perspectives; References

3 Rational Use of Chemical and Sequence Databases

3.1 Molecular Similarity Analysis: Applications in Drug Discovery; 3.1.1 Introduction; 3.1.2 Similarity-Based Compound Selection; 3.1.2.1 Similarity Measures and Neighborhoods; 3.1.2.2 Application of 2D and 3D Similarity Measures; 3.1.2.3 Application of Dissimilarity-Based Compound Selection for Broad Screening; 3.1.3 Structure-Activity Maps (SAMs); 3.1.3.1 A Visual Analogy; 3.1.3.2 Representing Inter-Structure Distances; 3.1.3.3 Structure Maps; 3.1.3.4 Coloring a Structure Map; 3.1.4 Field-Based Similarity Methods

3.1.4.1 Field-Based Similarity Measures; 3.1.4.2 Field-Based Molecular Superpositions; 3.1.4.3 An Example of Field-Based Fitting: Morphine and Clonidine; 3.1.5 Conclusions; References; 3.2 Clustering of Chemical Structure Databases for Compound Selection; 3.2.1 Introduction; 3.2.2 Review of Clustering Methods; 3.2.2.1 Hierarchical Clustering Methods; 3.2.2.2 Non-Hierarchical Clustering Methods; 3.2.3 Choice of Clustering Method; 3.2.3.1 Computational Requirements; 3.2.3.2 Cluster Shapes; 3.2.3.3 Comparative Studies; 3.2.4 Examples of the Selection of Compounds from Databases by Clustering Techniques

Sommario/riassunto

The use of powerful computers has revolutionized molecular design and drug discovery. Thoroughly researched and well-structured, this comprehensive handbook covers highly effective and efficient techniques in 3D-QSAR and advanced statistical analysis. The emphasis is on showing users how to apply these methods and avoid costly and time-consuming methodical errors. Topics covered include*

- combination of statistical methods and molecular modeling tools*
- rational use of databases*
- advanced statistical techniques*
- neural networks and expert systems in molecular design