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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 Model2.2.4 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
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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<br