

Physical, Chemical, and Technological Property Correlation with Chemical Structure: The Potential of QSPR*

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Z. Naturforsch. **61b**, 373 – 384 (2006); received January 4, 2006

Correlations of simple and complex physical, and chemical, biological and technological properties with chemical structure are reviewed. When an adequate training set of structures and experimentally determined property values are available, the equations produced enable the prediction of these properties of molecules as yet synthesized or indeed as yet unknown. Frequently they also offer considerable insights into the manner in which the structure controls the property. Many further applications of this methodology can be anticipated.

Key words: QSPR, QSAR, CODESSA PRO, Multilinear Regression, Molecular Descriptors