CS2-3 Role of Molecular Size in Determining Pharmaceutically Relevant Properties: Linear and Bilinear Models

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Molecular size is an easily available descriptor that is frequently overlooked by medicinal chemists and pharmaceutical scientists focused on substituent effects and on fragment-based contributions. Since it is closely related to the strength of general, nonspecific interactions, it is a major determinant of many pharmaceutically relevant properties, and it should not be omitted from any structure-property or structure-activity relationship study. Various data from boiling point through solubility and lipophilicity (log P) to receptor binding affinity will be reviewed to support this argument. A biphasic (bilinear) dependence may often confuse those interested in a simple trendline only; the utility of a recently introduced LinBiExp model in overcoming such problems will be discussed.