Estimation of Physical Properties of Amino Acids by Group-Contribution Method

In this paper, we present group-contribution (GC) based property models for estimation of physical properties of amino acids using their molecular structural information. The physical properties modelled in this work are normal melting point ($T_m$), aqueous solubility ($W_s$), and octanol/water partition coefficient ($K_{ow}$) of amino acids. The developed GC-models are based on the published GC-method by Marrero and Gani (J. Marrero, R. Gani, Fluid Phase Equilib. 2001, 183-184, 183-208) with inclusion of new structural parameters (groups and molecular weight of compounds). The main objective of introducing these new structural parameters in the GC-model is to provide additional structural information for amino acids having large and complex structures and thereby improve predictions of physical properties of amino acids. The group-contribution values were calculated by regression analysis using a data-set of 239 values for $T_m$, 211 values for $W_s$, and 335 values for $K_{ow}$. Compared to other currently used GC-models, the developed models make significant improvements in accuracy with average absolute error of 10.8 K for $T_m$ and logarithm-unit average absolute errors of 0.16 for $K_{ow}$ and 0.19 for $W_s$.

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Corresponding author: Gani, R.
Contributors: Jhamb, S. V., Liang, X., Gani, R., Hukkerikar, A. S.
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