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Chemoinformatics methods in the thermodynamics of equilibrium. The dissociation of acetic acid.

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Abstract

Methods of Chemical Informatics (Chemoinformatics) - multiple linear regression and neural network modeling-were used to analyze the dependence of Gibbs energy of the dissociation (the dissociation constant) of acetic acid on the properties of water and organic solvents. The significant factors were identified which affect the acid dissociation equilibrium. The neural network model (three-layer perceptron) was constructed and the perspective of application of neural networks in prediction of dissociation constants (strength) of acetic acid in water and organic solvents was shown.