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Partition coefficient prediction of Baker's yeast invertase in Aqueous Two Phase Systems using Hybrid Group Method Data Handling Neural Network

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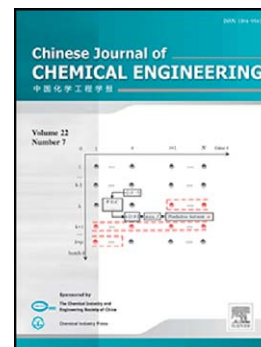
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## Partition coefficient prediction of Baker's yeast invertase in Aqueous Two Phase Systems using Hybrid Group Method Data Handling Neural Network

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### Abstract

A hybrid GMDH neural network model has been developed in order to predict the partition coefficients of invertase from Baker's yeast. ATPS experiments were carried out changing the molar average mass of PEG (1500-6000 Da), pH (4.0-7.0), percentage of PEG (10.0-20.0 w/w), percentage of  $MgSO_4$  (8.0-16.0 w/w), percentage of the cell homogenate (10.0-20.0 w/w) and the percentage of  $MnSO_4$  (0-5.0 w/w) added as co-solute. The network evaluation was carried out comparing the partition coefficients obtained from the hybrid GMDH neural network with the experimental data using different statistical metrics. The hybrid GMDH neural network model showed better fitting (% AARD = 32.752) of the partition coefficients of the ATPS than the original GMDH network approach and a BPANN model as well as showed good generalization capacity. Therefore hybrid GMDH neural network model appears as a powerful tool for predicting partition coefficients during downstream processing of biomolecules.

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