

APPLICATION OF ARTIFICIAL NEURAL NETWORKS FOR ORGANIC ACIDS PARTITION COEFFICIENTS PREDICTION

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Organic acids partitions coefficients prediction (on an example iodium benzoic acids) between water and organic phases with application of artificial neural networks algorithm was carried out. Partitions coefficients were established by extraction of acids from aqueous-salt solutions with hydrophilic solvents (butanol, isobutanol and tert. butanol). Application of artificial neural networks (nonlinear model) allows receiving the quantitative information on values of partition coefficients of organic acids.