ESTIMASI HUBUNGAN KUANTITATIF STRUKTUR-AKTIVITAS (HKSA) MENGGUNAKAN ARTIFICIAL NEURAL NETWORKS (ANN)

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Abstract	The Quantitative structure-Activity Relationship (QSAR) study has been performed on pattern of structure-molecule relationship. Artificial Neural Network (ANN) model used to estimate pattern of enzyme activity structure-molecule and atomic location in three-dimension for compound of flavonoid as the predictors. Value of determination coefficient used to compare between actual value and value of estimating by ANN models based on enzymeÃ¢Â€Â™s wavelength, so resulting cross validating is obtained. We use Quasy-Newton algorithm with Broyden-Fletcher-Goldfarb-Shanno (BFGS) procedure.
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Author	SUPRIYANTO, S.Si, M.Si