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Research Article

Quantitative structure-property relationship modelling for predicting retention indices of essential oils based on an improved horse herd optimization algorithm

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ABSTRACT

The horse herd optimization algorithm (HOA), one of the more contemporary metaheuristic algorithms, has demonstrated superior performance in a number of challenging optimization tasks. In the present work, the descriptor selection issue is resolved by classifying different essential oil retention indices using the binary form, BHOA. Based on internal and external prediction criteria, Z-shape transfer functions (ZTF) were tested to verify their efficiency in improving BHOA performance in QSPR modelling for predicting retention indices of essential oils. The evaluation criteria involved the mean-squared error of the training and testing datasets (MSE), and leave-one-out internal and external validation (Q^2). The degree of convergence of the proposed Z-shaped transfer functions was compared. In addition, K-fold cross validation with $k=5$ was applied. The results show that ZTF, especially ZTF1, greatly improves the performance of the original BHOA. Comparatively speaking, ZTF, especially ZTF1, exhibits the fastest convergence behaviour of the binary algorithms. It chooses the fewest descriptors and requires the fewest iterations to achieve excellent prediction performance.

KEYWORDS: QSPR modelling, horse herd optimization algorithm, transfer function, descriptor selection, retention indices

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