Analytical Sciences
The Japan Society for Analytical Chemistry

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A QSAR Study for Modeling of 8-Azaadenine Analogues Proposed as A1 Adenosine Receptor Antagonists Using Genetic Algorithm Coupling Adaptive Neuro-Fuzzy Inference System (ANFIS)

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A quantitative structure activity relationship (QSAR) study of 8-azaadenine, as antagonists for the A1 receptor, is described. A genetic algorithm (GA) method was used as the feature selection tool, and an adaptive neuro-fuzzy inference system (ANFIS) was employed for feature mapping. The best descriptors (GATS4v and BELv7) were applied to train the ANFIS model. The optimum number and shape of related functions were obtained through a subtractive clustering algorithm. The ability and robustness of the GA-ANFIS model in predicting the affinity of 8-azaadenine derivatives (pK_i) are illustrated by validation techniques of Leave One Out, heuristic and randomized methods. The results have indicated that the proposed model of ANFIS in this work is superior over two other methods, radial basis function (RBF) and multiple linear regression (MLR).

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To cite this article:

Somaieh AFIUNI-ZADEH and Gholamhassan AZIMI, *Anal. Sci.*, Vol. *26*, p.897, (2010) .

Japan Science and Technology Information Aggregator, Electronic