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Artificial Intelligence-2 Tools in Modelling Chemical Response[#]: Part III. Neural Network Modelling and Prediction of ^{13}C NMR Response of Halomethanes

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(Dedicated to I. Suryanarayana, IICT, Hyderabad during his 70th birth anniversary)

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ABSTRACT

Neural networks (NNs), a data driven second generation artificial intelligence technology is employed to model and predict ^{13}C NMR chemical shifts of 23 halomethanes with charge and functions of polarizability (α and α^2). Optimum single layer perceptron (SLP), 4-layer multi layer perceptron (MLP), radial basis function (RBF) and generalized regression (GR) neural network (NN) models (i.e. architectures, transfer function) are reported using the commercial software package TRAJAN 5.0. The analysis of data sets with (NP = 23) and without outliers (NP=18) using explanatory (causative) variables (α, C and α^2, C) was performed with IPS (Intelligent Problem Solver), a fast solution provider of TRAJAN and designed experimental runs for the task. The optimum set of models adequately explaining and predicting ^{13}C NMR response are SLP 2-9-1, 2-5-1; MLP 2-6-2-1, 2-5-5-1; RBF 2-16-1 and GRNN 2-23-2-1 (with smoothing factor in the range of 0.01 to 0.02). The best models of the best set based on the principle of parsimony are SLP 2-9-1 for full data set and SLP 2-5-1 for a subset of 18 compounds. The results of test data sets ensure the single and two compound predictions are within tolerable error limits. Multiple linear regression (MLR), a hard regression model, least median squares (LMS) and partial least squares regression (PLSR) (soft) models are inadequate even in explaining the variance in response, leaving the only alternative of non-linear input-to-output (I/O) mapping. The simulated and ^{13}C response data sets belong to function approximation task and the imbibing NN paradigm is not an alternate but indispensable tool for the current endeavour.

Keywords: ^{13}C NMR, Halomethanes, Neural Networks, PLSR, Artificial intelligence, Function approximation.

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