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(54) Title: METHOD FOR PREDICTING CHEMICAL OR PHYSICAL PROPERTIES OF COMPLEX MIXTURES

(57) Abstract

A method for predicting the propreties of a complex hydrocarbon mixture which comprises selecting one or more known chemical, perceptual, physical or performance properties of the complex mixture and creating a training set from reference samples which contain characteristic molecular species present in the mixture. The reference samples are subjected to GC/MS analysis wherein the often collinear data generated are treated by multivariate correlation methods. The training set produces coefficients which are multiplied by the matrix generated from a GC/MS analysis of an unknown mixture to produce a predicted value for the chemical, performance or physical property or groups of properties selected.