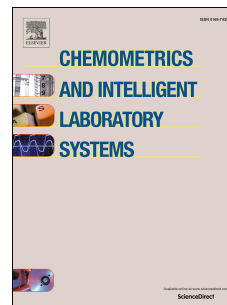


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# A strategy on the definition of applicability domain of model based on population analysis

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## Abstract

In recent years, there have been growing concerns about quality evaluation of predictions of developed quantitative structure-activity relationship (QSAR) models. Well-defined applicability domain (AD) is very crucial in the validation of QSAR models as stated in the third principle of Organization for Economic Co-operation and Development (OECD). In this study, a new perspective on defining AD of model based on population analysis (PA) strategy, including model population analysis (MPA) and approach population analysis (APA), was proposed. MPA employed classical AD approaches to define AD with a vast amount of sub-datasets derived from training set. On the basis of MPA, the classical AD approaches could distinguish part of the samples that cannot be distinguished by full training samples. APA was then used to get a union of all results generated by the used AD approaches to give a

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