Overview of PT-QSRR models for predicting yield of reaction

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Introduction

In organic chemistry the prediction of yield of reaction Yld(%) is very important. In almost all cases, organic chemists infer qualitatively the yield of a query reaction $Yld(\%)_{new}$ taking into consideration the experimental results for a previous reaction of reference $Yld(\%)_{ref}$. The PT-QSRR models are a quantitative expression of this idea because they applied Perturbation Theory (PT) to seek Quantitative Structure-Reactivity Relationship models. PT-QSRR predict the yield of some reactions comparing quantitatively the molecular properties of components such as catalyst, substrate, product, and nucleophile as well as controlled variables such as time, temperature and catalyst loading of both the new reaction and the reaction of reference. Other authors have previously developed a PT-QSPR approach, which combines perturbation theory (PT) and QSRR ideas, to correlate and predict different outputs (properties) in complex molecular systems (metabolic reactions) nanoparticles, and so forth (1). The method has also been extended to predict the enantioselectivity and/or yield of intramolecular carbolithiation and Heck–Heck cascade reactions (2). In some cases, the developed PT-QSRR models use trace operators, like spectral moments, or eigenvalues of chemical structure matrices, like bond adjacency matrix, as the inputs.

Methods

The molecular descriptors of type k, structural variables, $V_k(Mi)$ are calculated for each molecule Mi in both reactions. Next, the deviations $\Delta V_k(Mi) = V_k(Mi)_{new} - V_k(Mi)_{ref}$, can be used to quantify the structural perturbations or structural changes in the new molecules with respect to the query ones. In the same form deviation operators canc be used to measure perturbations on variables $V_k(cj)$ depending on the experimental conditions cj, $\Delta V_k(cj) = V_k(cj)_{new} - V_k(cj)_{ref}$.

Model

$$Yld(\%)new = Yld(\%)ref + \sum ak \cdot \Delta\mathrm{Vk(Mi)} + \sum ak \cdot \Delta\mathrm{Vk(Mi)} + e0$$

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