

Chapter 36

QSPR/QSAR Analyses by Means of the CORAL Software: Results, Challenges, Perspectives

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ABSTRACT

In this chapter, the methodology of building up quantitative structure—property/activity relationships (QSPRs/QSARs)—by means of the CORAL software is described. The Monte Carlo method is the basis of this approach. Simplified Molecular Input-Line Entry System (SMILES) is used as the representation of the molecular structure. The conversion of SMILES into the molecular graph is available for QSPR/QSAR analysis using the CORAL software. The model for an endpoint is a mathematical function of

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the correlation weights for various features of the molecular structure. Hybrid models that are based on features extracted from both SMILES and a graph also can be built up by the CORAL software. The conceptually new ideas collected and revealed through the CORAL software are: (1) any QSPR/QSAR model is a random event; and (2) optimal descriptor can be a translator of eclectic information into an endpoint prediction.

INTRODUCTION

Almost seventy years ago one of the areas of theoretical chemistry named the quantitative structure – property / activity relationships (QSPRs/QSARs) was established (Wiener, 1947, pp. 17-20; Wiener, 1948, pp. 425-430). However, if one considers the publication of Hammett's Free-energy relationship (Hammett, 1935, pp. 125–136) as the first exercise in the QSPR/QSAR analyses, then the introduction of this area of theoretical chemistry should be moved back by eighty years. This is obviously an evidence of the long lasting importance of the QSAR approaches. Such significance is due to their wide applications. The main target of QSPR/QSAR analyses is the prediction of the numerical data related to various endpoints (physicochemical in the case of QSPR; and biochemical, ecological, medicinal, etc., in the case of QSAR).

One can consider three periods of evolution in this field.

1. The first period can be defined as the construction of molecular descriptors and establishing of their correlation with various endpoints (Bonchev & Trinajstić, 1977; Balaban, 1982, pp. 399-404; Bonchev, 1995, pp. 137- 156; Diudea & Gutman, 1998; Ivanciuc, Ivanciuc, & Balaban, 1998; Randić, DeAlba, & Harris, 1998; Castro, Tueros, & Toropov, 2000; Randić & Basak, 2001; Nicolici, Kovacevic, Milicevic, & Trinajstić, 2003; Ren, 2003, pp. 29-39; González, Terán, Teijeira, & González-Moa, 2005; Melagraki, Afantitis, Sarimveis, Igglessi-Markopoulou, & Supuran, 2006).
2. The second period can be defined as the construction of molecular descriptors, establishing of their correlation with an endpoint for the compounds of “visible” training set with the further testing of the predictive potential of this correlation with “invisible” compounds (i.e. compounds which are not involved in building up of the model) involved in the test set (Cronin et al., 2002; Golbraikh & Tropsha, 2002; Taskinen & Yliruusi, 2003; Hemmateenejad, 2004, pp. 475–485; Duchowicz, Castro, Fernandez, & Gonzalez, 2005; Oberg, 2005, pp. 2189–2200; Afantitis et al., 2006; Coi et al., 2006; Leonard & Roy, 2006; Pan, Jiang, & Wang, 2007; Roy & Roy, 2008; Porto, Souza, Junkes, Yunes, & Heinzen, 2008; Toropova, Toropov, Benfenati, Leszczynska, & Leszczynski, 2010; Toropov et al., 2012a; Toropov, Toropova, Raska Jr, Benfenati, & Gini, 2012b; Nesmerak, Toropov, Toropova, & Kohoutova, 2013; Papa, van derWal, Arnot, & Gramatica, 2014).
3. The third period can be defined as building up of the QSPR/QSAR models according to OECD principles (Kruhlak, Contrera, Daniel Benz, & Matthews, 2007; Kar & Roy, 2010, 2012; Putz, Ionascu, Putz, & Ostafe, 2011; de Melo, 2012, pp. 213–222; Sahigara et al., 2012; Toropova & Toropov, 2014).

According to the OECD principles, the QSPR/QSAR model should be characterized by:

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