Guest Editorial Preface

Special Issue on Predictive Capabilities of QSAR and QSPR Models

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Nowadays there is a plethora of methods available to derive quantitative structure-property relationship (QSPR) models. In the literature, many related aspects are being covered in order to establish the basis of a good modeling practice, and the statement of the predictive capabilities constitutes one of the main cornerstones. In fact, despite the construction of a robust and reliable model is a must, it is not a neat or independent aspect. The achievement of a good predictor inherently drags other issues to be well combined and controlled (source of descriptors and their selection, mathematical nature of the model, applicability domain analysis, validation procedures, and so on). In this special issue, the concept of prediction is always underlying along the contributions and is being covered from distinct points of view when applying quantitative structure-property relationship (QSPR) methodology in diverse areas.

For instance, Gozalbes and De Julián-Ortiz focus on the REACH regulation, showing how this legislation justifies the need to develop good SAR methods and models and, in particular, how the concept of reliable predictions in toxicology is always present in the scientific forum. On the other side, in the contribution of Roy and collaborators linear and non-linear methods are being combined. The authors are able to reproduce *in silico* the *in vivo* vero cell cytotoxicity of antitubercular compounds. They propose to check the predictive power of the models by means of several validation strategies. Similarly, the team of Nandi applies the methodology in the field of anticancer drug design, in particular to avoid the collateral effects of the actual drug therapy treatments. The authors show how the modeling of Aryl pyrido[2,3-d]pyrimidin-7(8H)-ones asks for a proper descriptor selection. They arrived at this conclusion precisely at the stage of validation, after testing the predictability of the QSAR models. Finally, Torrens and Castellano present a QSPR application in the physicochemical field: the prediction of retention times of several compounds by means of use of a particular descriptor. As expected, the descriptor validation encompasses the test of predictability.

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