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Editorial

QSAR/QSPR and Proprietary Data

The field of QSAR/QSPR analysis has undergone considerable evolution and expansion. Correspondingly, this Journal must also evolve its view of QSAR/QSPR manuscripts to reflect and incorporate these changes. In concert with the *Journal of Chemical Information and Modeling*, the *Journal of Medicinal Chemistry* now institutes the following general requirements for manuscripts reporting work done in this area.

(1) Authors should explicitly state in the Abstract, Introduction, and/or Results sections of the paper what is novel about the QSAR/QSPR study being reported.

(2) "Novel" must be presented with respect to methodology/theory and/or to the findings from the system(s) studied.

(3) If a new method/theory is being reported in the paper, it should be compared and "validated" against at least one other common data set for which a published study exists using at least one other method/approach and preferably a method/approach that has been widely used in the field. The data set should not be small.

(4) All data and molecular structures used to carry out a QSAR/QSPR study are to be reported in the paper and/or in its Supporting Information or be readily available without infringements or restrictions. The use of proprietary data is generally not acceptable because it is inconsistent with the ACS Ethical Guidelines for publications: "A primary research report should contain sufficient detail and reference to public sources of information to permit the author's peers to repeat the work." This is fundamental, although possible exceptions can be discussed with the Editor in the unusual circumstance that a convincing case could be made that the data are somehow a secondary issue.

Some guidelines to assist prospective Journal authors of manuscripts in the field of QSAR/QSPR analysis are as follows:

(1) Evidence that any reported QSAR/QSPR model has been properly validated using data not in the training set must be provided.

(2) 3D-QSAR studies that overlap with, and enhance, structure-based design (SBD) methods are encouraged. QSAR models that lead to subsequently validated experimental findings are encouraged.

(3) Papers reporting new and novel QSAR/QSPR methods and approaches for facilitating a mechanistic understanding of ADMET properties, and/or for reliable ADMET screening, are welcomed.

(4) New QSAR/QSPR methods that interface with chem- and bioinformatics methods and/or with data-mining techniques are encouraged.

(5) Only QSAR/QSPR analyses that bring new insights on the mechanism of activity are encouraged. QSAR/QSPR approaches for virtual high-throughput screening (VHTS) must demonstrate distinct advantages, or advances, over current VHTS schemes.

(6) QSAR/QSPR studies for new, novel endpoints, both biological and physical, are encouraged. Manuscripts that report new experimental data along with corresponding QSAR/QSPR models are encouraged.

(7) Specifically discouraged are (a) QSAR and QSPR modeling for data sets that have already been extensively modeled, (b) model development featuring high ratios of descriptors to data points, and (c) reports of new descriptors without clear evidence for their superiority in QSAR/QSPR modeling to existing, commonly used alternatives.

The Editors will periodically revisit the requirements and guidelines for QSAR/QSPR analysis and continue to make updates commensurate with the evolution of this important field.

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