

Public (Q)SAR Services, Integrated Modeling Environments, and Model Repositories on the Web: State of the Art and Perspectives for Future Development

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Abstract

© 2017 Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim Thousands of (Quantitative) Structure-Activity Relationships (Q)SAR models have been described in peer-reviewed publications; however, this way of sharing seldom makes models available for the use by the research community outside of the developer's laboratory. Conversely, on-line models allow broad dissemination and application representing the most effective way of sharing the scientific knowledge. Approaches for sharing and providing on-line access to models range from web services created by individual users and laboratories to integrated modeling environments and model repositories. This emerging transition from the descriptive and informative, but "static", and for the most part, non-executable print format to interactive, transparent and functional delivery of "living" models is expected to have a transformative effect on modern experimental research in areas of scientific and regulatory use of (Q)SAR models.

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Keywords

chemoinformatics, model repositories, on-line modeling environments, QSAR, QSPR, web-based models

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