

Correlation of blood-brain penetration and human serum albumin binding with theoretical descriptors

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Estimating the toxicities of organic chemicals in activated sludge process

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Fragment-based development of HCV protease inhibitors for the treatment of hepatitis C

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Prediction of cell-penetrating peptides using artificial neural networks

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QSAR prediction of HIV-1 non-nucleoside inhibitor activity based on 3D-molecular descriptors

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QSAR study of pharmacological permeabilities

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Quantitative structure-activity relationship modeling of bioconcentration factors of polychlorinated biphenyls

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Subchronic oral and inhalation toxicities : a challenging attempt for modeling and prediction

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