QSAR study of diarylalkylimidazole and diarylalkyltriazole aromatase inhibitors

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Abstract

A QSAR analysis was conducted on a series of long-chained diarylalkylimidazole and diarylalkyltriazole derivatives as potent aromatase inhibitors. To obtain more appropriate QSAR models from a source of very large number of descriptors, a two-step stepwise variable selection strategy was performed. Firstly, from each group of the calculated descriptors, separate QSAR models were obtained. Then, the descriptors appeared in all of the generated models were subjected to another variable selection method and the obtained models were subjected to cross-validation. Finally, an external test set was used to access the ultimate performance of the models. The selected descriptors were analyzed for their influence on aromatase inhibition. The effects of hydration energy, position of H-bond acceptor, presence of cyano group, and shape of HOMO orbital on aromatase inhibition were successfully described, and they were consistent with the previous reports. © 2016 Springer Science+Business Media New York.