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Modeling PPARα Activation of Benzoxazole-Phenoxyalkyl-Phenoxybutyric Acids Using Diverse Descriptors

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***SUMMARY*. A quantitative structure activity relationship (QSAR) analysis was performed on two series of benzoxazole-phenoxyalkyl-phenoxybutyric acids with potent PPARα activation activity using diverse descriptors. The 31 compounds were divided into a training set and a test set based on Euclidean distance. The model was derived through multiple linear stepwise regression method and the predictive ability of the best model was validated by leave-one-out cross-validation and external validation on the test set. The best generated QSAR model explained good fits to the experimental data with approximate 80 % of the variance in the biological activity. Also, the important cross-validated squared correlation coefficient (r^2 = 0.697) and the accuracy of 90 % correct predictions for the test set further confirmed that the model exhibited reliable predictive power ability. The generated QSAR model revealed that PPARα activation activity of benzoxazole-phenoxyalkyl-phenoxybutyric acids was influenced by the presence of chiral centers and hydrogen bonding donor groups and the number of positive charges and positive polar charges in the molecule, which might help in developing new PPARα agonists with better activity.**

KEY WORDS: Benzoxazole-phenoxyalkyl-phenoxybutyric acids, PPARα, QSAR.

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