QSAR STUDY OF FLAVONOID–METAL COMPLEXES AND THEIR ANTICANCER ACTIVITIES

J.-Z. Qian[1,2], B.-C. Wang[1], Y. Fan[3], J. Tan[4], and X. Yang[5]

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Flavonoid-metal complexes have anticancer activities. However, the quantitative structure-activity relationship (QSAR) of flavonoid–metal complexes and their anticancer activities has not been known so far. Based on the 14 structures of flavonoid–metal complexes and their anticancer activities for HepG2 from the references, we optimised their structures using the density functional theory (DFT) method, and subsequently calculated 19 quantum chemical descriptors, such as dipole, charge, and energy. Then, we chose several quantum chemical descriptors that are very important for IC_{50} which represents the anticancer activities of flavornoid–metal complexes for HepG2 through the stepwise linear regression method. Meanwhile, we obtained six new variables through the principal component analysis. Finally, we built QSAR models based on those important quantum chemical descriptors, six new variables as independent variables, and IC_{50} as a dependent variable using an artificial neural network (ANN). At last, we validated the models using the experimental data from the references. The results show that models presented in this paper are accurate and predictive.

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