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Quantitative structure – fungicide activity relationship for 1,2,3-thiadiazoles and 1,2,3-triazoles

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Abstract

One of the worldwide problems is the trends of crop product losses increase as plant diseases spreading. The mail task of contemporary technologies for development of methods both for medicine and agrochemistry is reliable biological activity prediction for different organic compound. On the base synthesized library of 1,2,3-thiadiazoles and 1,2,3-triazoles and their fungicide activities against the representative typical fungi such as: *Verticilium dahlia, Fusarium oxysporum cucumerinum, Gibberella zeae* the quantitative structure – activity relationships were determined. The cross-validation method was used for QSAR modeling. According to this method the 38 available data of thiadiazoles were divided into two sets "training", contain N = 26 compounds, and "test" containing 12 compounds. As for 1,2,3-triazole data of 21 compound were also divided in "training" and "test" sets with 15 and 6 compounds respectively. 5-Amino-1,2,3-thiadiazoles and 5-mercapto-1,2,3-triazoles possess the same atom sequence, these compounds do not belong to the same scaffold. It was found that topological descriptors were significant for the fungicide activity of 1,2,3-thiadiazoles. However electronic descriptors influenced on the fungicide activity of 1,2,3-triazoles. 1,2,3-thiadiazoles possessing activity against *Fusarium oxysporum cucumerinum* (C), values were closely connected with such descriptors as average molecular weight AMV, mean atomic van der Waals volume (scaled on Carbon atom) Mv, mean atomic polarizability (scaled on Carbon atom) Mp, mean atomic Sanderson electronegativity (scaled on Carbon atom) Me. Absolutely different set of descriptors influenced on activity C among 1,2,3-triazoles: heat of formation H, HOMO energy EHOMO, ionization potential μ, number of Oxygen atoms nO.