

Comparative analysis of fungicidal activity 2-methyl-5-nitrobenzoxazole and its derivatives

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Abstract

One of the trends in the development of modern chemistry is the synthesis and use of organic substances of various classes, as the basis for multifunctional preparations for agricultural production. The use of certain reagents with high fungicidal activity may lead to inhibition of growth processes in plants. This will not only prevent high yields, but also damage agriculture and human health. On the basis of the Department of Chemistry, research is being carried out, the task of which is to select substances that possess both high fungicidal and biological activity. This article is devoted to one of the stages of research - the study of the fungicidal activity of compounds of the nitrobenzoxazole group.

For the experiment, 2-methyl-5-nitrobenzoxazole, 2-methyl-5,7-dinitrobenzoxazole, 2-phenyl-5,7-dinitrobenzoxazole were chosen. Thus, the effect of nitro groups, methyl- and phenyl-substituents on fungicidal activity of benzoxazole was analyzed. For the initial assessment of the biological activity of the compounds studied, computer simulations were carried out using the PASS (Prediction of Activity Spectra for Substances) system.

Further, the analytes were tested for fungicidal activity *in vitro* on six fungi-phytopathogens from various taxonomic groups, which are among the most common pathogens of agricultural plants in the Central region of Russia. For the experiment, fungi were used: *V. inaequalis* – apple scab, *R. solani* – causative agent of rhizoctonia, *F. oxysporum*, *F. moniliforme* – causative agents of fusariosis of cereal crops, *B. sorokiniana* – causative agent of root rot and *S. sclerotiorum* – causative agent of white rot.

The radial growth of the mycelium was determined according to the procedure developed by NIITEKHIM, according to which the culture of fungal cultures in nutrient media with the addition of test substances was carried out. At the same time, control was conducted in the aquatic environment. The growth of mycelium was monitored by measurements on days 3, 6 and 9. The percentage inhibition of fungal growth was calculated using the Abbott formula.

For comparison, the activity of reference preparations from the list of permitted and the use of fungicides was studied.

Analysis of the data obtained in the experiment demonstrates the greatest fungicidal activity of 2-methyl-5-nitrobenzoxazole for all types of fungal cultures used in the study. The second nitro group, the introduced molecule of 2-methyl-5-nitrobenzoxazole, reduces the fungitoxicity by 1.5-2 times. Replacement of the methyl group by phenyl significantly reduces the fungicidal activity.

References

- [1] M.B. Nikishina, O.S. Polovetskaya, E.V. Ivanova, T.A. Zavershneva, S.O. Bondar, A.N. Novikova. The effect of organic acids on the accumulation of nitrate ions and heavy metals soil. *International electronic scientific and practical journal "Modern scientific researches and development" 2415-8402 literature*. 2017. Vol.4. No.12. P.204-209. (russian)

- Full Paper** __ L.G. Mukhtorov, G.V. Pestsov, M.B. Nikishina, E.V. Ivanova, Yu.M. Atroshchenko, and K.I. Kobrakov
- [2] M.B. Nikishina, O.S. Polovetskaya, E.V. Ivanova, T.A. Zavershneva, S.O. Bondar. The influence of oxalic, malonic and succinic acids on the growth and characteristics of tomato cultivar "Cranberry in sugar". *International electronic scientific and practical journal "Modern scientific researches and development" 2415-8402 literature*. **2017**. Vol.4. No.12. P.199-204. (russian)
- [3] S.O. Bondar, M.B. Nikishina, O.I. Boykova, E.V. Ivanova, O.S. Polovetskaya, Yu.M. Atroshchenko, L.L. Kirillova, K.I. Kobrakov. The effect of organic acids on growth characteristics and accumulation of nitrate ions by plants of lettuce. *Butlerov Communications*. **2017**. Vol.51. No.8. P.33-38. ROI: jbc-02/17-51-8-33
- [4] T.A. Zavershneva, M.B. Nikishina, O.I. Boykova, E.V. Ivanova, O.S. Polovetskaya, Yu.M. Atroshchenko, L.L. Kirillova, K.I. Kobrakov. Study of the effect of organic dicarboxylic acids on biometric indicators and accumulation of nitrate ions in cucumber fruits. *Butlerov Communications*. **2017**. Vol.51. No.9. P.76-82. ROI: jbc-02/17-51-9-76
- [5] I.I. Surova, E.V. Ivanova, Yu.M. Atroshchenko, G.V. Pestsov, K.I. Kobrakov. Synthesis and fungicidal activity of 2-methoxy-7-R-1,5-dinitro-3,7-diazabicyclo[3.3.1]non-2-ene. *Butlerov Communications*. **2017**. Vol.51. No.8. P.65-70. ROI: jbc-02/17-51-8-65
- [6] System fungicides. Edited by Melnikov N.N. Moscow: *Mir*. **1975**. 304p. (russian)
- [7] Methodological recommendations for determining fungicidal activity of new compounds. *Cherkasy: NIITEKHIM*. **1984**. 34p. (russian)
- [8] State catalog of pesticides and agrochemicals allowed for use in the territory of the Russian Federation. Part 1. *Moscow: Agrorus*. **2017**. 941p. (russian)
- [9] D.A. Filimonov, V.V. Poryokov. Prediction spectrum of biological activity of organic compounds. *Ros. Chem. J*. **2006**. Vol.L. No.2. P.66-75. (russian)