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Novel phosphate-containing imidazoles as potential green biologically active substrates

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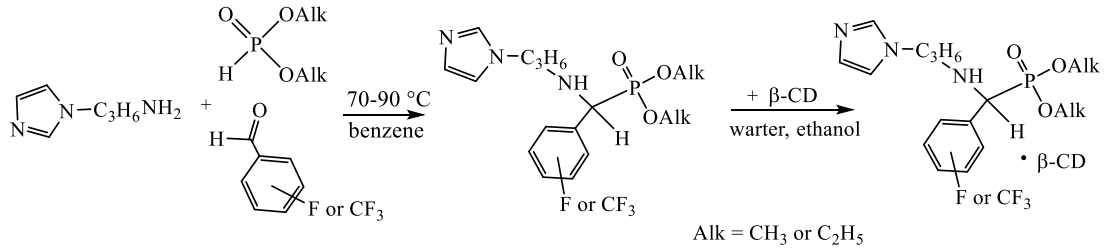
In crop production, the need for novel environmentally friendly fertilizers is due not only to the fact that when they are introduced, plant productivity increases, but their impact on the soil is accompanied by the reproduction of soil fertility, an increase in its main features (humus, nutrients, effective microorganisms). Ways to increase the efficiency of fertilizers include their modification with plant growth regulators. The problem of fertilizer modifiers, which not only stimulate the growth and development of plants, but enhance their protective functions to natural and technogenic stressful situations (adaptogens for plants), is multifaceted and its solution requires the efforts of many specialists. The chemical aspect of this problem involves the synthetic design of novel molecules with the above properties.

Several reasons served as the basis for realization the Research: in particular, the activity of the imidazole-containing bispidins synthesized by us [1]; biological potential of fluorimidazole derivatives [2]; the practical value of both biologically active substances and highly selective ligands in complexes with copper (II) and nickel (II) ions, structures containing fragments of imidazole and phosphonate [3].

In this work, in order to obtain green plant growth regulators - fertilizer modifiers, we carried out a synthetic design of new imidazole derivatives combined with phosphonate and fluorine fragments under the conditions of a three-component "one-pot" Kabachnik-Fields reaction.



The interaction of 1-(3-aminopropyl)imidazole with di(methyl- or ethyl-)phosphite and the carbonyl component – *o*-, *m*- or *p*-(fluoro- or trifluoromethyl-)benzaldehyde is carried out by boiling in benzene using a Dean-Stark nozzle to remove from the reaction zone of the obtained water as azeotrope with benzene. The yield of target α-aminophosphonates as viscous oils is 19-91%. In the IR spectra, the bands at 1047-1238 cm^{-1} are attributed to the absorption of P=O. In spectra 13C NMR the signal of the tertiary carbon atom (CHP) is observed in the region of 58.2-71.7 ppm. The signals of carbon atoms of the imidazole ring are observed in the region of 119.8-137.6 ppm.

To study the bioactivity, complexes of aminophosphonates with β-cyclodextrin (1:1) were obtained.

As expected, among the synthesized aminophosphonates, samples were identified that stimulate seed germination, growth and development of 3 Kazakhstan wheat varieties under normal and drought conditions. But, unexpectedly, it turned out that cyclodextrin complexes cause local pain relief on models of infiltration and conduction anesthesia at the level of used local anesthetics - lidocaine and trimecaine in terms of anesthesia index and duration of action. Acute toxicity (LD_{50} = 1125 mg/kg) was 3-5 times less than the used anesthetics.

Thus, the expediency of combining fragments of imidazole and phosphonate in one molecule, which has a pronounced biological effect with low toxicity, has been experimentally confirmed.

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