New Route to Benzoxazoles Based on Annulation Induced Transformations of 1,2,3-triazoles

Moskalenko, Uliana

Benzoxazoles represent an important class of heterocyclic compounds, because this fragment is a well-known pharmacophore. A variety of natural and synthetic molecules containing benzoxazole moiety were shown to exhibit anticancer and antibacterial effects. Besides, benzoxazoles are used in agriculture and production of fluorescent dyes. I have developed a new synthetic approach to benzoxazoles based on intramolecular nucleophilic substitution reaction in 5-iodo-1,2,3-triazoles. Annulation of a new aromatic ring to 1,2,3-triazole induces tautomeric equilibrium between fused triazole and highly reactive diazobenzoxazole. I have investigated a possibility to trap the diazo tautomer by copper-catalyzed reaction with thiols or by using electrocyclic reaction. Cascade annulation/ring opening/diazo trapping was promoted by Cu(Ph3P)3Br and Et3N in dioxane at 100 °C. Using this method I have obtained 20 previously unknown benzoxazole derivatives in good yields (52–95 %). Structures of new compounds were confirmed by 1H and 13C NMR spectroscopy and their composition – by MALDI-TOF mass spectrometry and elemental analysis.

Awards Won: