2-BENZOPYRYLIUM DERIVATIVES CONTAINING PYRAZOLE, BENZIMIDAZOLE, AND BENZOTHIAZOLE RESIDUES

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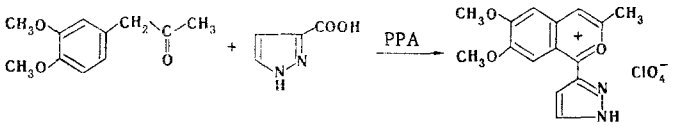
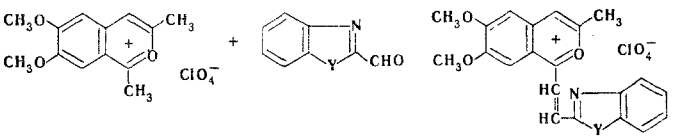
Considering the high biological activity of pyrylium salts and the heterocyclic nitrogen bases that are readily obtained from them, we made an attempt to synthesize the practically unknown 2-benzopyrylium derivatives that contain azole substituents.

By acylation of 3,4-dimethoxyphenylacetone with pyrazole-3-carboxylic acid in the presence of polyphosphoric acid (PPA) by the method in [1] we obtained 1-(3-pyrazolyl)-3-methyl-6,7-dimethoxy-2-benzopyrylium perchlorate in 12% yield as light-brown crystals with mp > 355° (dec., reprecipitation from acetone by the addition of ether). IR spectrum: 1100, 1370, 1520, 1580, 1620 cm^{-1}. Found: C 48.8; H 4.8; Cl 9.4; N 7.8%. $C_{15}H_{15}ClN_2O_7$. Calculated: C 48.6; H 4.5; Cl 9.6; N 7.6%.



The condensation of 1,3-dimethyl-6,7-dimethoxy-2-benzopyrylium perchlorate with 2-formylbenzimidazole, 2-formylbenzothiazole, and 1-methyl-4-formylpyrazole gives better results.



Y = NH, S

The reaction was carried out by brief (1-2 h) refluxing of equimolecular amounts of the components in glacial acetic acid by the method in [2].

This method was used to synthesize 1-[2-(2-benzimidazolyl)vinyl]-3-methyl-6,7-dimethoxy-2-benzopyrylium perchlorate [in 56% yield as light-yellow crystals with mp > 355° (dec., reprecipitation from acetone by the addition of ether). IR spectrum: 1100, 1380, 1520, 1570, 1600, and 1630 cm^{-1}. Found: C 56.1; H 4.5; Cl 7.4; N 6.5%. $C_{21}H_{19}ClN_2O_7$. Calculated: C 56.4; H 4.3; Cl 7.9; N 6.3%]. 1-[2-(2-benzothiazolyl)-vinyl]-3-methyl-6,7-dimethoxy-2-benzopyrylium perchlorate [in 57% yield as brown crystals with mp >350° (dec., from glacial acetic acid). IR spectrum: 1100, 1380, 1470, 1520, and 1610 cm^{-1}. Found: C 54.7; H 4.1; Cl 7.7; S 6.4%. $C_{21}H_{18}ClNO_7S$. Calculated: C 54.4; H 3.9; Cl 7.6; S 6.9%]; and 1-[2-(1-methyl-4-pyrazolyl)vinyl]-3-methyl-6,7-dimethoxy-2-benzopyrylium perchlorate [in 44% yield as dark-green crystals with red fluorescence (in solution) and mp 245° (from glacial acetic acid). IR spectrum: 1100, 1470, 1520, 1610, 1660 cm^{-1}. Found: C 52.9; H 4.6; Cl 8.3; N 6.5%. $C_{18}H_{19}ClN_2O_7$. Calculated: C 52.6; H 4.6; Cl 8.6; N 6.8%].

When the synthesized compounds were treated with ammonium hydroxide they were converted in almost quantitative yield to the corresponding azolylvinylisoquinolines.

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2. G. N. Dorofeenko, E. I. Sadekova, and V. M. Goncharova, Khim. Geterotsikl. Soedin., 1308 (1970).