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DIRECTIONS OF HETEROCYCLIZATION IN REACTIONS OF 4,6-DIMETHYL-2-PYRIMIDINESULFENYL CHLORIDE WITH 2-ALLYLPHENOL

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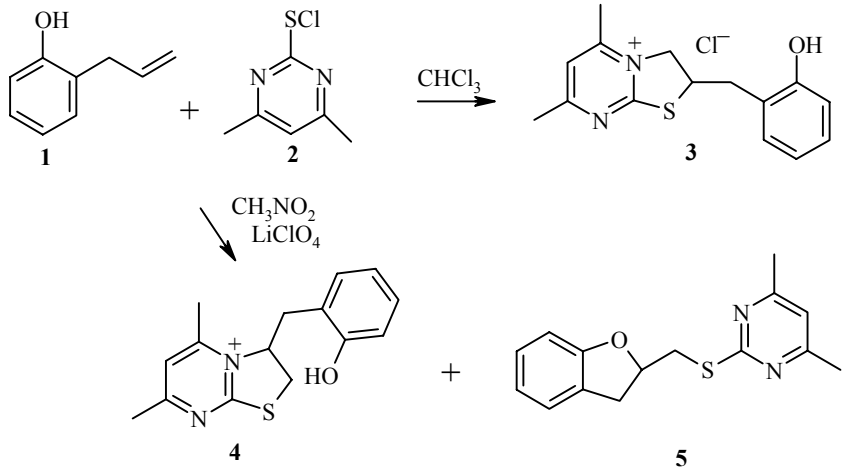
When 2-allylphenol (**1**) is reacted with electrophilic reagents, including sulfur-containing reagents, typically intramolecular cyclization products are formed as a result of closure of the ring by the oxygen atom of the phenol moiety [1, 2].



We have shown that in the reaction of alkene **1** with 4,6-dimethyl-2-pyrimidinesulfenyl chloride (**2**) in chloroform, the ring is closed by the pyrimidine nitrogen atom, and the thiazolo[3,2-*a*]pyrimidine derivative (**3**) is formed in 72% yield. In nitromethane in the presence of a two-fold excess of lithium perchlorate, the condensed S,N-heterocycle (**4**) and 2,3-dihydrobenzofuran (**5**) are obtained in 47% and 43% yields, respectively.

By ^{1}H NMR spectroscopy, we have established that in the first reaction, the intermediate products are regioisomeric β-chlorosulfides. In the second case, formation of heterocyclic systems occurs directly in an Ad_E process.

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2,3-Dihydro-2-(*o*-hydroxybenzyl)-5,7-dimethylthiazolo[3,2-*a*]pyrimidinium Chloride (3); mp 141°C (decomp.). IR spectrum (KBr), ν, cm^{-1}: 3270-3540 (OH), 1610, 1539, 1457, 1380, 770 (Het). ^1H NMR spectrum (DMSO-d_6, 300 MHz), δ, ppm, *J*, Hz: 9.88 (1H, br. s, OH); 7.64 (1H, s, Het); 7.15-6.75 (4H, m, Ar); 5.02 and 4.84 (2H, dd and dd, ^3J = 8.0, 5.4, ^2J = 12.8, CH_2N^+); 4.70 (1H, m, CHS); 3.15 (2H, t, ^3J = 6.5, CH_2Ar); 2.68 and 2.58 (6H, s and s, $2CH_3$). Found, %: C 58.25; H 5.43; N 9.01, S 10.27. $C_{15}H_{17}ClN_2OS$. Calculated, %: C 58.34; H 5.55; N 9.07, S 10.38.

2,3-Dihydro-3-(*o*-hydroxybenzyl)-5,7-dimethylthiazolo[3,2-*a*]pyrimidinium Perchlorate (4); mp 175-177°C. IR spectrum (KBr), ν, cm^{-1}: 3280-3570 (OH), 1608, 1535, 1460, 1387, 775 (Het), 1112 (ClO_4). ^1H NMR spectrum (DMSO-d_6, 300 MHz), δ, ppm, *J*, Hz: 9.66 (1H, br. s, OH); 7.60 (1H, s, Het); 7.20-6.77 (4H, m, Ar); 5.69 (1H, m, CHN^+); 3.96 and 3.56 (2H, dd and dd, ^3J = 7.5, 5.2, ^2J = 11.8, CH_2S); 3.12 (2H, ddd, ^3J = 8.0, 5.9, ^2J = 13.9, CH_2Ar); 2.60 and 2.59 (6H, s and s, $2CH_3$). Found, %: C 48.21; H 4.52; N 7.43, S 8.52. $C_{15}H_{17}ClN_2O_5S$. Calculated, %: C 48.32; H 4.60; N 7.51, S 8.60.

2-(4,6-Dimethylpyrimidylthiomethyl)-2,3-dihydrobenzofuran (5). Oil. IR spectrum (film), ν, cm^{-1}: 3040, 1582, 1527, 1478, 1432, 1335, 1250, 759, 677. ^1H NMR spectrum (DMSO-d_6, 300 MHz), δ, ppm, *J*, Hz: 7.23-6.72 (4H, m, Ar); 6.89 (1H, s, Het); 5.01 (1H, m, CHO); 3.58 and 3.43 (2H, dd and dd, ^3J = 5.9, 5.9, ^2J = 13.8, CH_2S); 3.35 and 3.02 (2H, dd and dd, ^3J = 9.2, 7.2, ^2J = 16.4, CH_2Ar); 2.35 (6H, s, $2CH_3$). Found, %: C 66.02; H 5.83; N 10.18; S 11.62. $C_{15}H_{16}N_2OS$. Calculated, %: C 66.15; H 5.92; N 10.29, S 11.77.

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