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AZIDE-TETRAZOLE EQUILIBRIUM IN PYRIDO[3,2-d]PYRIMIDINES

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Heterocycles with an azido-azomethine structural entity are interesting due to their intrinsic dynamic azide-tetrazole tautomeric equilibrium in the solution phase [1] alongside rich azide functional group chemistry [2]. Herein, a method for the synthesis of 5-substituted tetrazolo[1,5-a]pyrido[2,3 e] pyrimidines from 2,4-diazidopyrido[3,2-d]pyrimidine in SNAr reactions with N-, O-, and S nucleophiles is presented [3]. The tetrazolo[1,5-a]pyrimidine derivatives can be regarded as 2 azidopyrimidines due to present azide-tetrazole valance tautomerism and functionalized in copper(I)-catalyzed azide-alkyne dipolar cycloaddition (CuAAC) and Staudinger reactions. Equilibrium constants and thermodynamic values were determined using variable temperature 1H NMR and were found to be $\Delta G298 = -3.33$ to -7.52 (kJ/mol), $\Delta H = -19.92$ to -48.02 (kJ/mol) and $\Delta S = -43.74$ to -143.27 (J/mol·K). The negative Gibbs free energy values assert tetrazole as the major tautomeric form in solutions. Furthermore, the key starting material 2,4-diazidopyrido[3,2-d]pyrimidine shows a high degree of tautomerization in different solvents presenting up to 7 tautomeric forms.

Primary authors: LEŠKOVSKIS, Kristaps (Riga Technical University); Dr NOVOSJOLOVA, Irina; Prof. TURKS, Māris

Presenter: LEŠKOVSKIS, Kristaps (Riga Technical University)

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