Tautomeric transformations N- and C-acyl derivatives of tetrahydro-1,4-diazepines

N.A. Anisimova[1,2], D.A. Melkova[1]
[1]*The Herzen State Pedagogical University of Russia, St. Petersburg, Russia*
[2]*Saint-Petersburg State University of Industrial Technologies and Design, St. Petersburg, Russia*
E-mail: mall30@mail.ru

It is well known that diazepines are structural fragments of biologically active natural (streptocarbazoles A and B1) and synthetic compounds. Based on diazepines, a wide range of drugs have been already obtained. For example, diazepines are used as effective tranquilizers (diazepam, lorazepam), hypnotics (bromazepam, phenazepam), and CNS depressants [1].

The interaction of 14-membered azamacrocycle (**1**) with chloroacetic acid chloride was used to obtain representatives of N-(**2**) and C-(**3a, b**) acyl derivatives of tetrahydro-1,4-diazepines according to the procedure we previously described [2]. Separation of N- and C-acyl diazepines was carried out by column chromatography.

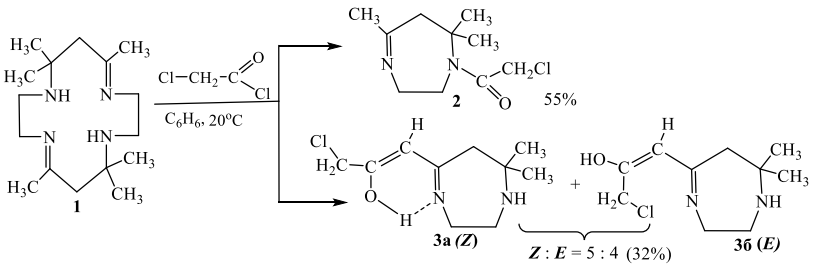

Figure 1. Interaction of 14-membered azamacrocycle (1) with chloroacetic acid chloride

Using ^{1}H, ^{13}C NMR, HMQC, HMBC, COZY spectroscopy, we studied the tautomeric transformations of the obtained N-(**2**) and C-(**3a,b**) acyl derivatives of tetrahydro-1,4-diazepines. It was shown that N-acyldiazepine (**2**) exists in the CD_3OD solution in the keto-imine form, while C-acyldiazepines (**3a,b**) exist in the enol-imine form. In a DMSO solution, both types of acyldiazepines (**2, 3 a,b**) acquire the corresponding keto- and enol-enamine forms.

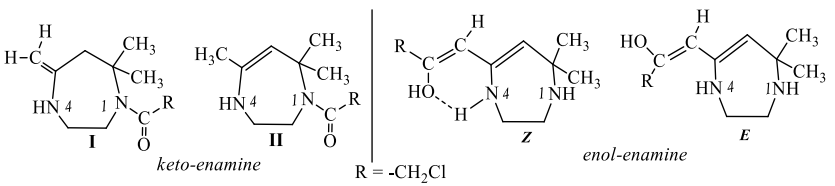

Figure 2. Keto and enol-enamine forms of diazepines (2,3 a,b) in DMSO solution

References

1. N. A. Meanwell, M.A. Walker. – *Comprehensive Heterocyclic Chemistry III*, 13, 183-235 (2008).
2. N. A. Anisimova, D. A. Melkova. – *Russian Journal of General Chemistry,* 12, 2809-2815 (2022).