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## Lipophilicity assessment and chromatographic characterization of new spirohydantoin derivatives potential anticonvulsant agents

Tatjana Djaković Sekulić<sup>1</sup>, A. Smolinski<sup>2</sup>, K. Tot<sup>1</sup>, A. Lazić<sup>3</sup>

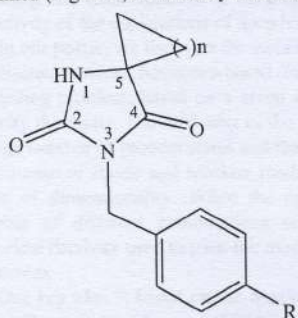
<sup>1</sup> Department of Chemistry, Biochemistry and Environmental Protection,  
Faculty of Sciences, Novi Sad, Republic of Serbia,  
E-mail: tatjana.djakovic-sekulic@dh.uns.ac.rs;

<sup>2</sup> Department of Energy Saving and Air Protection, Central Mining Institute,  
Katowice, Poland

<sup>3</sup> Faculty of Technology and Metallurgy, Belgrade, Republic of Serbia

Spirohydantoin and their derivatives represent a pharmacologically important class of heterocycles. For example, hydantoin derivatives are important anticonvulsant drugs which are employed for the treatment of neurological disorders such as epilepsy and trigeminal neuralgia. Anticonvulsant activity of hydantoin is mediated by their interaction and inhibition of the voltage-gated sodium channels in the brain.

In this poster presentation the retention data of new cycloalkane-5-spirohydantoin bearing a substituted benzyl group in position 3 of the heterocyclic ring have been examined (Figure 1). Previously the intermolecular interactions of the crystal structures of cycloalkane-5-spirohydantoin with halogeno substituted benzyl group (R = Cl and Br) in position 3 had been studied [1]. Besides, the effect of R substituent on the absorption UV-Vis spectra of cyclopentanespiro-5-hydantoin [2] had been studied, too.



**Figure 1.** General formula of investigated cycloalkylspiro-5-hydantoin ( $n=3-5$ ; R=H, CH<sub>3</sub>, OCH<sub>3</sub>, Cl, Br, CN and NO<sub>2</sub>).

Since the investigated derivatives contain a low number of the rotatable bonds and thus moderate conformational changes due to binding to a receptor are possible. From that viewpoint the polarity of the substituent "R", particularly the presence of electron donating groups like methoxy in the *para*-position of the phenyl ring may be of significance for the activity.

### References

- [1] A. Lazić, N. Trišović, L. Radovanović, J. Rogan, D. Poletić, Ž. Vitnik, V. Vitnik, G. Ušćumlić, *CrystEngComm.*, **19** (2017) 469-483.
- [2] A. Lazić, B. Božić, V. Vitnik, Ž. Vitnik, J. Rogan, L. Radovanović, N. Valentić, G. Ušćumlić, *J. Mol. Struct.*, **1127** (2017) 88-98.