Hop (*Humuluslupulus L.*) is a genus of flowering plants. The medicinal use of extracts prepared from the parts of the *Cannabaceae* genus dates back to ancient times. The female flowers, commonly called hops, are used as flavouring agents and stabilisers during beer brewing.

At the base of the hop scales there are two hard nuts covered in aromatic, yellow dust called lupulin. Lupulin contains from 5 to 30% bitter substances including acylphloro-glucides, humulones [1], lupulones; essential oil containing mono- and sesquiterpenes, aroma substances, flavonoids, xanthohumol and other chalcones [2,3]. Isolated prenylflavonoids show interesting biological activities witch may be used as cancer chemopreventive agents, anti-oxidative or as antiviral agents [3].

The purpose of this review is to show an overview of the anti-oxidative activities of prenylflavonoids from hops.

Prenylflavonoids were isolated from supercritical carbon dioxide extracted hops. The particular residues were extracted by solvent extraction. The fractions containing xanthohumol and isoxanthohumol were collected, evaporated in vacuo and purified by repeated column chromatography on silica gel. The structures were confirmed by spectroscopic methods: UV-VIS, IR, ^{1}H NMR.

Anti-oxidative property of xanthohumol and isoxanthohumol from hops were compared with other natural antioxidants extracted from the evening primrose (*Oenothera paradoxa* L.) and black chokeberry (*Aronia melanocarpa*).

The induction time and oxidative stability of prenylflavonoids from hops and natural extracts were determined by rancimat test. With the results presented in this study, we concluded that isoxanthohumol and xanthohumol had the highest oxidative stability. Both of those compounds indicate that they are two times stronger in antioxidative activity than the natural extracts from evening primrose and black chokeberry.

References:

1. M. Piastowska; *Panace:***2004**,2,7-9.

A. Rumuńska, A. Ożarowski; *Leksykon roślin leczniczych*: Warszawa **1990.**

2. J. F. Stevens, E. Pagaj; *Phytochemistry*: **2004,**65,1317-1330.

Q. Wang, Z.Ding, J. Liu, Y. Zheng; *Antiviral Research*: **2004**,64,189-194.

3. J. F. Stevens, A.W. Taylor, M. L. Deinzer; *Journal of Chro:***1999**, 832, 97-107.

M. Anioł, K. Szymańska, A. Żołnierczyk; *Tetrahedron*: **2008**, 64, 9544-9547.

17:00 Poster 66

Identification of Novel 5-HT$_7$R Ligands via Multistep Virtual Screening of Commercially Available Compounds Databases

Rafał J. Kurczab[1], Mari Gabrielsen[2], Zdzislaw Chilmonczyk[3], Ingebrigt Sylte[2], Andrzej J. Bojarski[1]

1. *Institute of Pharmacology Polish Academy of Sciences, Department of Medicinal Chemistry, Smętna 12, Kraków 31-343, Poland* **2.** *Research Group of Medical Pharmacology and Toxicology, Department of Medical Biology, Faculty of Health Science, University of Tromso, Tromso, Norway (UIT), Tromso N-9037, Norway* **3.** *Narodowy Instytut Lekow (NIL), Chełmska 30/34, Warszawa 00-725, Poland*

e-mail: rkurczab@gmail.com

In order to find potential new structures of 5-HT$_7$R ligands we used previously developed and tested hierarchical multistage strategy of virtual screening [1]. This workflow was based on two-dimensional (2D) pharmacophore similarity searching, physicochemical scalar descriptors, ADME/Tox filter, three-dimensional (3D) pharmacophore searches and docking protocol. Additionally, in order to increase chemotype's diversity of virtual hits, the chemical topology and pharmacophore topology fingerprints have been applied at the stage of similarity search. The six chemical classes of 5-HT$_7$R antagonists [2] were used as a query structures in double-path virtual screening scheme. The commercially available resources, offered by the ChemBridge [3] and ChemDiv [4] companies, have been adopted and used as a molecular screening space consisting of approximately 1 300 000 compounds. Finally, the best virtual hits were selected and acquired in order to determine their affinity for 5-HT$_7$ receptor. The binding mode of selected virtual hits are shown in comparison to those of known antagonists [2].

This study was partly supported by a grant PNRF-103-AI-1/07 from Norway through the Norwegian Financial Mechanism.

References:

[1] R. Kurczab, M. Nowak, Z. Chilmonczyk, I. Sylte, A. J. Bojarski, Bioorg. Med. Chem. Lett., doi:10.1016/j.bmcl.2010.03.012.

[2] M. Kołaczkowski, M. Nowak, M. Pawłowski, A. J. Bojarski J. Med. Chem. 2006, 49, 6732.

[3] http://www.chembridge.com/

[4] http://www.chemdiv.com/