

P106

## Halogen bonding in serotonin transporter ligand-receptor complexes

Jakub Staroń,<sup>a</sup> Ryszard Bugno,<sup>a</sup> Dawid Warszycki,<sup>a</sup> Grzegorz Satała,<sup>a</sup>  
Rafał Kurczab,<sup>a</sup> Anna Wantuch,<sup>b</sup> Andrzej J. Bojarski<sup>a</sup>

<sup>a</sup>*Institute of Pharmacology, Polish Academy of Sciences, 31-343 Kraków, 12 Smętna Street, Poland*

<sup>b</sup>*State Higher Vocational School, 33-100 Tarnów, 8 Mickiewicza Street, Poland*

*e-mail: staron@if-pan.krakow.pl*

Halogen bonds (XB) are specialized non-covalent interactions known to chemists since XIX century, but only recently they were recognized as important in biological molecules. According to the IUPAC definition, halogen bond is “a net attractive interaction between an electrophilic region associated with a halogen atom in a molecular entity and a nucleophilic region in another, or the same, molecular entity”.<sup>1</sup> Docking of a recently obtained polypharmacological compounds<sup>2</sup> to a crystal structure of SERT, revealed their possible affinity towards this target. Because five out of six FDA approved SSRIs possess halogens in their structure, which suggests important role of halogen bonds in interaction between ligand and SERT, a halogen-enriched combinatorial library was prepared which was further analysed using the docking protocol. Obtained database contained a ranking list of structures with increasing potential affinity towards SERT. Subsequently, a group of compounds was selected and synthesized, and their affinity towards SERT was measured. The poster presents obtained results.

1. Desiraju, G. R. *et al.* Definition of the halogen bond (IUPAC Recommendations 2013). *Pure Appl. Chem.* 85, 1711-1713 (2013)
2. Staroń, J. *et al.* Halogen bonding enhances activity in a series of dual 5-HT 6 /D 2 ligands designed in a hybrid biosostere generation/virtual screening protocol. *RSC Adv.* 6, 54918–54925 (2016)

Acknowledgements: The research was supported from the grant SONATA UMO-2016/21/D/NZ7/00620 financed by National Science Centre.