# SYNTHESIS AND CHARACTERIZATION OF CHIRAL TRIAZOLE-BASED HALOGEN BOND DONORS

Mikk Kaasik[1], Sandra Kaabel,[1] Kadri Kriis,[1] Ivar Järving,[1] Riina Aav,[1] Kari Rissanen,[2] Tõnis Kanger[1]

[1]*School of Science, Tallinn University of Technology, Akadeemia tee 15, 12618 Tallinn, Estonia*
[2]*Department of Chemistry, University of Jyvaskula, Nanoscience Center, P.O. Box 35, FI-40014 Jyvaskyla, Finland*
e-mail: Mikk.Kaasik@ttu.ee

A halogen bond (XB) is a noncovalent interaction between an electrophilic halogen atom and some nucleophilic counterpart of the same or another molecule.[1] It has been widely exploited in crystal engineering and the number of applications on the use of XBs in solution is also growing.[1] Similarities between the XB and the hydrogen bond make XB donors potential organocatalysts. To move towards asymmetric XB catalysis, information on how structural modifications influence the strength of XBs is needed.

Various chiral halotriazole and halotriazolium XB donors that differ from each other in terms of the main entities that define the XB donor properties have been synthesised via a cycloaddition reaction as a key transformation (Fig. 1).

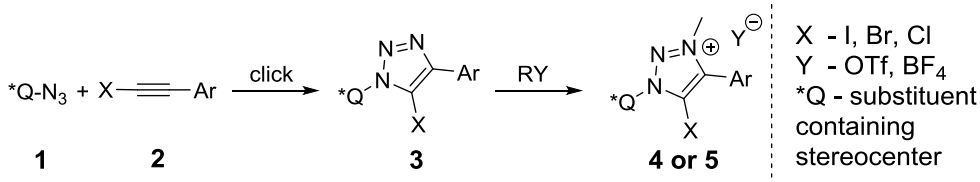


*Fig. 1. The click approach to halotriazole-based halogen bond donors.*

The XB donor abilities of these compounds were assessed by X-ray crystallography and solution NMR studies. The first example of XB between iodotriazoles and thioureas is presented. In addition, the enantiodiscrimination of acceptors in solution via halogen bond participation is described.

References

1. A. V. Jentzsch, *Pure Appl. Chem*. **2015**, *87*, 15–41.

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