OPTIMIZATION OF THE REACTION PATHWAY FOR THE SYNTHESIS OF SUBSTITUTED 1,3-BIS(CARBAZOLYL)UREA ANION RECEPTORS

Alo Rüütel[1], Mihkel Ilisson

[1] *Institute of Chemistry, University of Tartu, Ravila 14a, Tartu, Estonia*

e-mail of presenting author: alo.ruutel@ut.ee

Carbazole has been used as a backbone for developing several receptor molecules, which have been investigated as ionophores for anion-selective electrodes.[1] The development of these sensor systems has prompted for an effective synthetic approach.

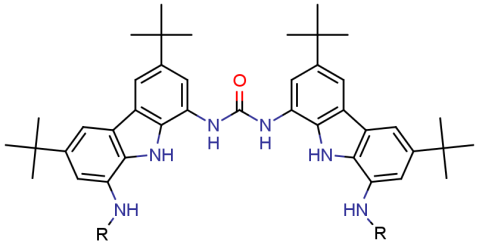

Figure 1. Structure of 1,3-bis(carbazolyl)urea type anion receptors.

Currently, the main synthetic route for 1,3-bis(carbazolyl)urea receptors has been the protection of 3 and 6 positions in the carbazole structure, followed by subsequent nitration and reduction of the 1 and 8 positions.[3] However, in our experience, this method is accompanied by the loss of one tert-butyl protective group due to the highly acidic reaction environment as shown in figure 2. The resulting mixture of compounds is challenging to purify due to structural similarities.

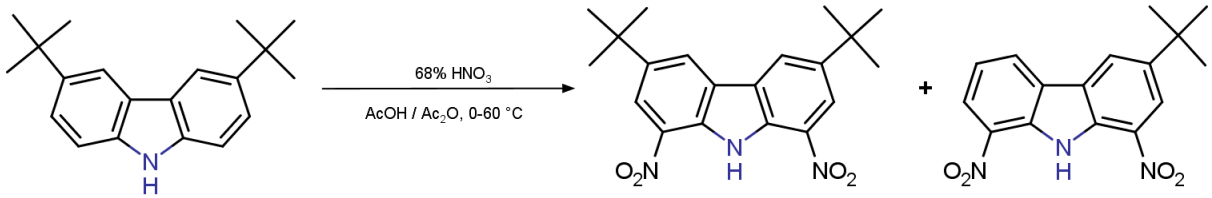

Figure 2. The cleavage of one tert-butyl protective group during nitration.

Several approaches give low overall yields in the synthetic pathway or are time consuming. We present a new synthetic pathway that, instead of nitrating the compound, uses bromination of the 1 and 8 positions. The product is aminated in the next phase, improving product purity and yield.

References:

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2. G. Sanchez, A. Espinosa, D. Curiel, A. Tarraga, P. Molina, *J. Org. Chem.* **2013**, *78*, 9725–9737.

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