

Chemistry Department

Organic Synthesis & Chemical Biology

Research Team:

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Maria Manuel Marques

2001 PhD (FCT-UNL)

2001-2003

Postdoc at the Mulzer group (Austria)

2003-present

Assistant Research fellow
REQUIMTE, FCT-UNL.

Objectives

The main research topics encompass:

- 1) synthesis of complex glycoconjugates involved in cellular recognition processes (**Figure 1**).
- 2) cyclooxygenase (COX) inhibitors design and synthesis (**Figure 2 and 3**).

Methodology

1) A one-pot procedure has been established to assemble glucosamine building blocks crucial for Peptidoglycan synthesis (**Scheme 1**).

(M. M. B. Marques *et al.* *Synlett* **2010**, *18*, 2711-2716; *Arkivoc* **2012**, *iv*, 90-100; *Chem. Asian J.* **2012**, *7*, 2482-2501).

A glycopeptide was prepared by solid-phase synthesis, and monitored by HR-MAS NMR. (M. M. B. Marques *et al.* *Magn. Reson. Chem.* **2010**, *48*, 323-330).

2) A rational drug design approach was developed towards novel compounds to elucidate the mechanism of COX inhibition: Synthesis, molecular modelling and biological and NMR screening (**Figure 2 and 3**). (M. M. B. Marques *et al.* *Eur. J. Med. Chem.* **2012**, *54*, 823-833).

Expected Results

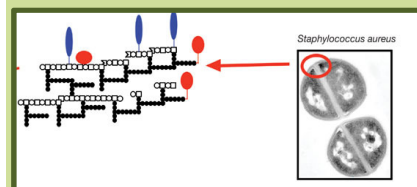
It is expected to:

- develop novel synthetic methodologies towards complex glycopeptides;
- identify the molecular interactions between the synthesized ligands and key biological targets to understand how the peptidoglycan (bacterial cell wall) is recognized by the host;
- identify novel COX-2 selective inhibitors and elucidate the COX inhibition mechanism.

Funding:

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Figure 1



Scheme 1

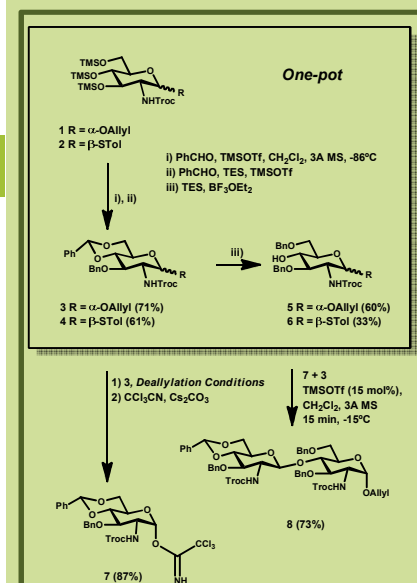


Figure 2

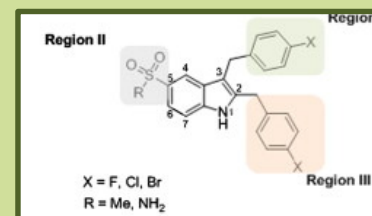


Figure 3

