

Marseille, France - July 7 - 12, 2013
Esoc 2013

18th European Symposium on Organic Chemistry

POSTERS – SESSION 2





Synthesis and spectroscopic studies of novel carbopeptoids

Vitālijs Rjabovs[a], Diāna Zeļencova[b], Alison A. Edwards[c], Edvards Liepinsh[b], Māris Turks[a]

[a]Faculty of Material Science and Applied Chemistry, Riga Technical University, 14/24 Azenes Str., Riga, LV-1007, LATVIA

[b]Latvian Institute of Organic Synthesis, 21 Aizkraukles Str., Riga, LV-1006, LATVIA

[c] Medway School of Pharmacy, The Universities of Kent and Greenwich at Medway, Central Avenue, Chatham Maritime, Kent, ME4 4TB, UK

Email: maris_turks@ktf.rtu.lv

Oligopeptides arising from synthetic sugar amino acids exhibit interesting self-assembling structures in solution, and were intensively studied as peptidomimetics.¹ After the discovery of click synthesis of 1,2,3-triazoles,² the latter were studied as amide bond isosteres as they exhibit similar spatial arrangement and geometry.³

Using readily available D-glucose as starting material we have synthesized oligosaccharides with different linkers. By combination of two easily modifiable building blocks **1** and **2** (figure 1) we can synthesize oligomers with different ratio of amide and triazole linkers. Using amides as linkers adds more flexibility while 1,2,3-triazoles act as more rigid isosteres.

oligomers with triazole linkers between sugar residues and mixed "amide-triazole oligomers" such as **3** (figure 1) were synthesized in our laboratory and studied extensively by NMR and CD. Using ROESY spectra of compounds in chloroform distances between adjacent protons were calculated and used as the constraints for the molecular dynamics studies. They showed that the rotation of triazole-linked fragments is restricted and thus no regular secondary structure is formed. Conformation of **3** after the MD calculations is shown in figure 2.

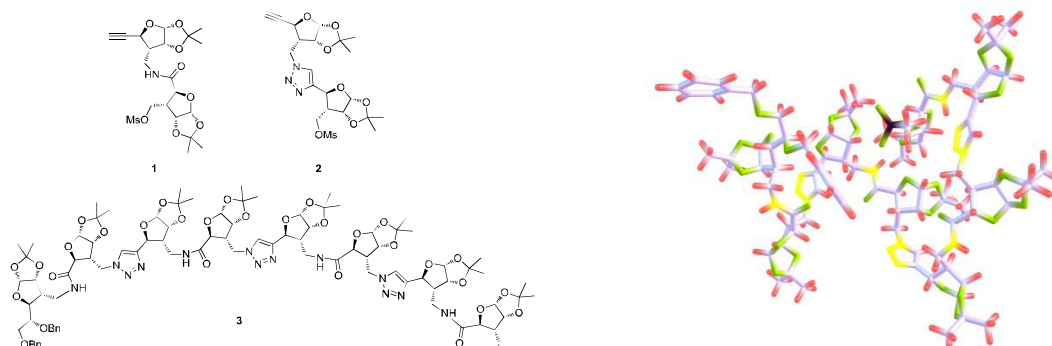


Figure 1. Hybrid building blocks **1** and **2** and mixed octamer **3**. Figure 2. Conformation of **3** after MD calculations.

Comparison of CD spectra of **3** in MeCN and TFE suggests that although there is no regular secondary structure evident, a significant change in conformational preference between these solvents exists.

Acknowledgements: This work has been supported by the European Social Fund within the project «Support for the implementation of doctoral studies at Riga Technical University».

Travel costs and participation fee for this conference are financially supported by ERDF project „The development of international cooperation, projects and capacities in science and technology at Riga Technical University” Nr.2DP/2.1.1.2.0/10/APIA/VIAA/003.

¹ Claridge, T. D. W.; Long, D. D.; Baker, C. M.; Odell, B.; Grant, G. H.; Edwards, A. A.; Tranter, G. E.; Fleet, O. W. J.; Smith, M. D. *J. Org. Chem.* **2005**, *70*, 2082-2090.

² Rostovtsev, V. V.; Green, L. G.; Fokin, V. V.; Sharpless, K. B. *Angew. Chem. Int. Ed.* **2002**, *41*, 2596-2599.

³ Angell, Y.; Chen, D.; Brahimi, F.; Saragovi, H. U.; Burgess, K. *J. Am. Chem. Soc.* **2008**, *130*, 556-565.