MS37-P134 LATE | CONFIGURATION CONTROLLED CRYSTAL AND/OR GEL FORMATION OF FULLY PROTECTED D-GLUCOSAMINES

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Gel formation is widely spread in nature, essential for living organisms. Gels of natural and synthetic sources are also used in various fields of industry (e.g. pharmateuticals, food science, cosmetics, nano materials). Low molecular weight gelators (LMWGs) are of particular interest, having advantageous physico-chemical properties. For understanding and designing their characteristics, efforts are made to establish the molecular level criteria of gelation, including key interactions governing gel formation.

Carbohydrate derivatives having versatile configuration, molecular folds and self-assembly behaviours, are promising candidates of designing biocompatible LMWGs. Interactions stabilizing the gel structure were proposed for N-Fmoc-glucosamines, establishing a model for a group of free hydroxyl-containing hydrogels.

Here we present a comparative study of alpha and beta anomers of fully O-acetylated derivative of N-Fmoc-glucosamine. The beta anomer readily forms gels from different solvent mixtures, presenting solution-gel-crystalline transformation pathway. Interestingly the alpha anomer crystallizes from solution skipping the gel formation. This molecule pair makes a unique system to understand details of gelation, as they differ only in their anomeric configuration. We applied a combination of various methods for characterizing phase transformation processes of both anomers. Crystal structures along with results of NMR and ECD studies as well as in silico conformational analysis are presented. Key conformers as well as intra- and intermolecular interactions were identified proposing a possible explanation of the configuration dependent gelation ability of the protected D-glucosamines.

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