BOTTOM-UP CHARACTERIZATION OF SYNTHETIC AND NATURAL MACROMOLECULES BY HYPHENATED CHROMATOGRAPHIC TECHNIQUES

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ABSTRACT

The classical workflow in applied chemical research is the top-down, starting with intended end-use properties and looking for potential candidates, which may exhibit such behavior. Then application tests are performed, potential candidates screened and in the final stage of the development different characterization techniques are employed to understand structure-property relationship which allow to optimized product synthesis, processing and formulation. Obviously, this can be a time-consuming process.

Alternatively, bottom-up concepts rely on molecular properties macromolecules to predict macroscopic properties and application behavior. Theoretical concepts allow to scale molecular behavior to concentrated solutions and melts. Recent advances in the understanding of molecular self-organization, self-assembly and/or supramolecular chemistry support bottom-up workflows. Benefits include less strain on research resources, faster time-to-market and recovering R&D cost in shorter time.

This contribution will present examples of synthetic and natural macromolecular products in which bottom-up characterization approaches were successfully applied in developing various types of products.

Figure 1 shows the molar mass distribution of a heparin products which are used in clinical applications to suppress blood clogging after surgery. The effectiveness of Heparin molecules in anti-thrombotic applications is closely related to their chemistry (chemical composition), to its molecular weight and architecture. In order to achieve optimized product performance and prevent failure in the human body, bottom-up allows to minimize expensive clinical studies and support earlier treatment of diseases with less side effects.



Fig. 1: Overlay of heparin samples which meet (green) or fail (red) the molecular weight test for anti-thrombotic effectiveness