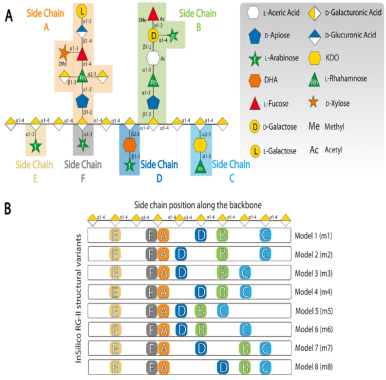
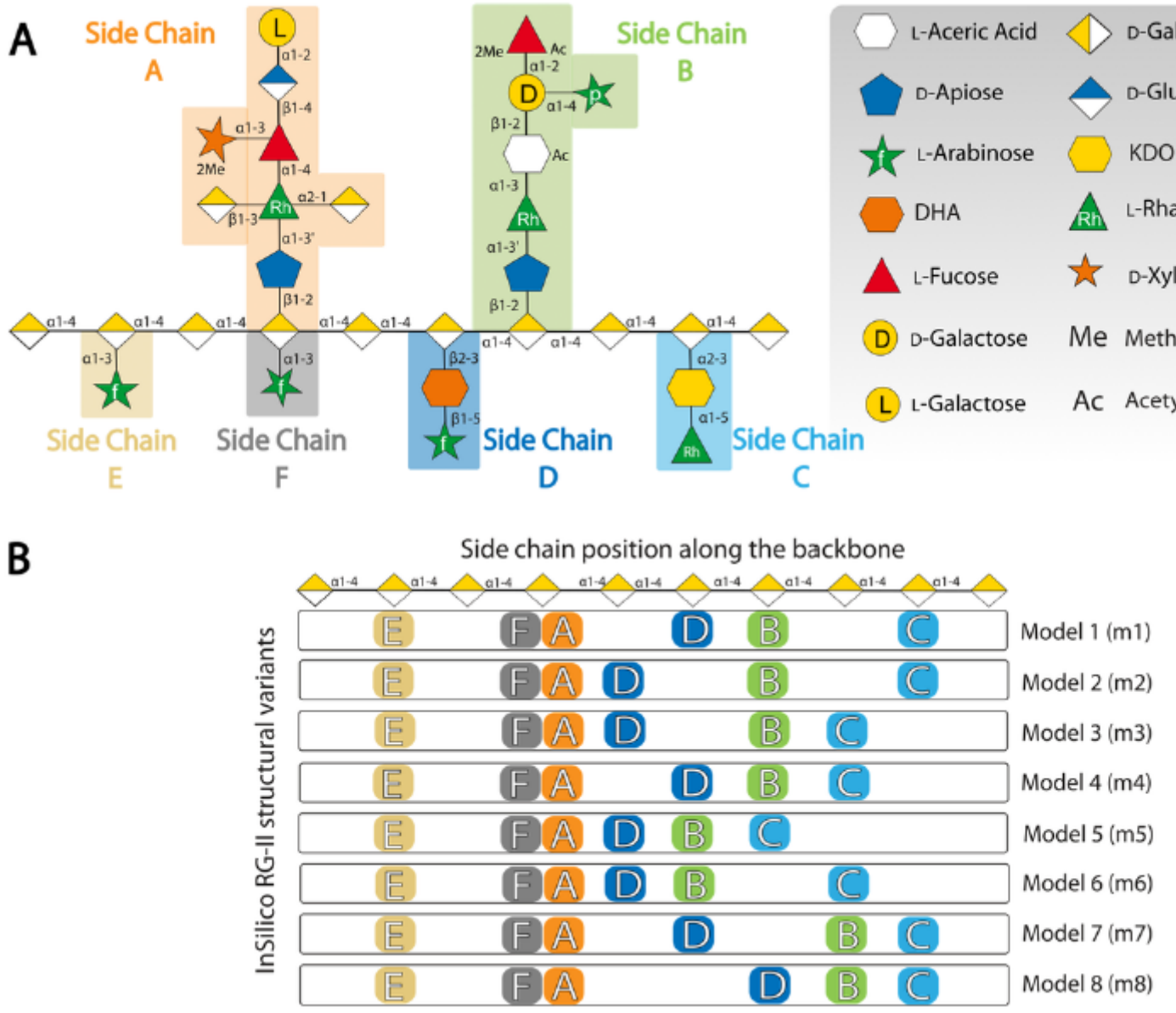


Probing Sequence-Structure Paradigms in Complex Carbohydrates – A Case Study on Rhamnogalacturonan-II

Description

Rhamnogalacturonan-II (RG-II) is the most complex polysaccharide known in Nature and plays an indispensable role in the growth and development of all vascular plants. RG-II is characterized by 12 different monosaccharides connected via a multiplicity of glycosidic linkages. The constituent monosaccharide units are arranged into six different sidechains along a polygalacturonic-acid backbone connected by ?-1-4 linkages. While the side-chain constituent residues are known, their relative locations along the backbone have not yet been resolved. In this study, we grow, isolate, and characterize RG-II from celery cells and use solution-based NMR in concert with molecular dynamics simulations on 8 distinct structural variants to identify and propose the first atomistic 3-D structure of RG-II that best represents the experimental NOE data. The authors parameterize the forcefields for unique sugars and linkages and employ replica-exchange molecular dynamics to sample the complex conformational landscape for RG-II adequately. The present biophysical approach provides a foundation for establishing sequence-structure relationships for RG-II and enabling the tools and metrics to relate its structure to its function.



The glycosyl sequence of Celery RG-II. (A) 2-D representation of the glycosyl RG-II monomer structure. (B) The eight variants of RG-II monomer with different sidechain positions along the galacturonic acid backbone explored in silico in this study.

Category

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