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Validation of macromolecular flexibility in solution by small-angle X-ray scattering (SAXS)

Authors	Authors and affiliatio
Michal Hammel 🖂	
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The dynamics of macromolecular conformations are critical to the action of cellular networks. Solution X-ray scattering studies, in combination with macromolecular X-ray crystallography (MX) and nuclear magnetic resonance (NMR), strive to determine complete and accurate states of macromolecules, providing novel insights describing allosteric mechanisms, supramolecular complexes, and dynamic molecular machines. This review addresses theoretical and practical concepts, concerns, and considerations for using these techniques in conjunction with computational methods to productively combine solution-scattering data with high-resolution structures. I discuss the principal means of direct identification of macromolecular flexibility from SAXS data followed by critical concerns about the methods used to calculate theoretical SAXS profiles from high-resolution structures. The SAXS profile is a direct interrogation of the thermodynamic ensemble and techniques such as, for example, minimal ensemble search (MES), enhance interpretation of SAXS experiments by describing the SAXS profiles as population-weighted thermodynamic ensembles. I discuss recent developments in computational techniques used for conformational sampling, and how these techniques provide a basis for assessing the level of the flexibility within a sample. Although these approaches sacrifice atomic detail, the knowledge gained from ensemble analysis is often appropriate for developing hypotheses and guiding biochemical experiments. Examples of the use of SAXS and combined approaches with X-ray crystallography, NMR, and computational methods to characterize dynamic assemblies are presented.

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Abstract

Nodal root angle in sorghum influences vertical and horizontal root distribution in the soil profile and is thus relevant to drought adaptation. In this study, we report for the first time on the mapping of four QTL for nodal root angle (qRA) in sorghum, in addition to three QTL for root dry weight, two for shoot dry weight, and three for plant leaf area. Phenotyping was done

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Authors Authors and affiliations

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Abstract

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(2) Keywords

Biofuels Climate change Conservation Forest Resources Forestry Forests Sustainable development

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Trevor Fenning 1

Forest Research, Northern Research Station, UK Forestry Commission, Edinburgh, United Kingdom

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3)Authors Michael G. Zeidler, Thomas L. Saunders 🖂

(4) Protocol First Online: 24 October 2018 ⁶⁴ (5)

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