

Small-Angle Scattering of Flexible Biopolymers

J. E. Curtis and S. Krueger

NIST Center for Neutron Research, NIST, 100 Bureau Drive, Gaithersburg, Maryland 20899, USA

Contact: joseph.curtis@nist.gov

We are developing a suite of computational methods to aide in the design and analysis of small angle scattering data with applications to macromolecular systems. This is achieved by generating an ensemble of macromolecular structures by varying sets of backbone dihedral angles and using mathematical methods to determine structures that have small angle scattering spectra that are consistent with experiment. We have used these tools to predict structures for the HIV-1 Gag protein under high salt conditions. The methods are applicable to the analysis of small-angle scattering spectra (X-ray or neutron) and can be applied to study intrinsically disordered proteins and other biopolymers in solution.