

# SASSIE: A BioSAS Experiment Planning and Data Analysis Tool

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Biomolecules often contain flexible, structurally disordered regions that make possible a wide range of conformations. While enabling a wider range of functionality, this flexibility makes structural studies by x-ray crystallography and cryo-electron microscopy challenging. Small-angle scattering (SAS) provides complementary lower resolution information to study flexible biomolecules and their complexes with binding partners in solution. SASSIE [1] is a suite of program modules to perform Monte Carlo (MC) and molecular dynamics (MD) simulations of biomolecules, calculate experimental SAS data and compare results to experiment. Structures can be sampled rapidly for a variety of protein, nucleic acid and carbohydrate systems, facilitating the generation of simulation trajectories. SAS model data are generated using an all-atom SAS calculator. Contrast variation small-angle neutron scattering (SANS) experiments are supported. Software development is guided by the scientific needs of the bioSAS user community. An overview of SASSIE-web [2], the web version of SASSIE, will be presented along with examples that illustrate the use of the MC/MD modules for various types of biomolecules, including how they are used in a workflow that enables SAS experiment planning and data analysis.

## References

- {1} J.E. Curtis, S. Raghunandan, H. Nanda and S. Krueger, *Computer Physics Communications* **183** 382 (2012).  
{2} S.J. Perkins, D.W. Wright, H. Zhang, E.H. Brookes, J.Chen, T.C. Irving, S. Krueger, D.J. Barlow, K.J. Edler, D.J. Scott, N.J. Terrill, S.M. King, P.D. Butler and J.E. Curtis, *J. Appl. Cryst.* **49** 1861 (2016).