

Processing and analysis of SEC-SAXS data

Alejandro Panjkovich

EMBL Hamburg

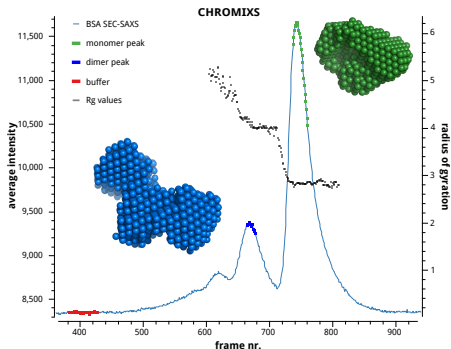
11.12.2017

Outline

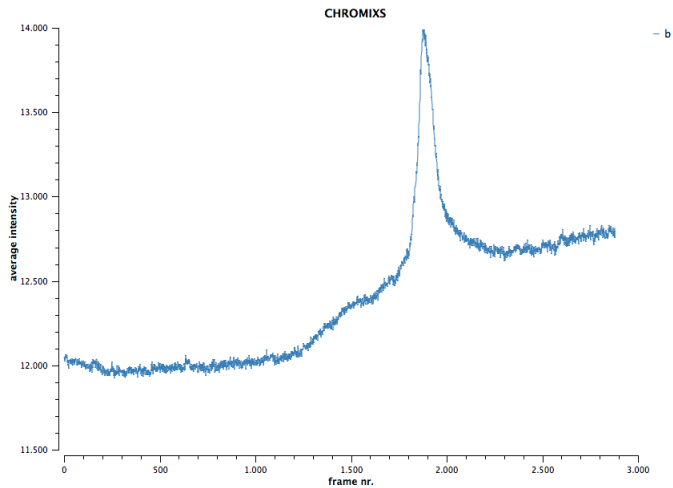
- Visualize elution profile in term of scattering
- Common issues
- Identify sample and buffer region
- Evaluate sample behaviour (R_g and MW)
- Align with additional data

CHROMIXS: CHROMatography Inline X-ray Scattering

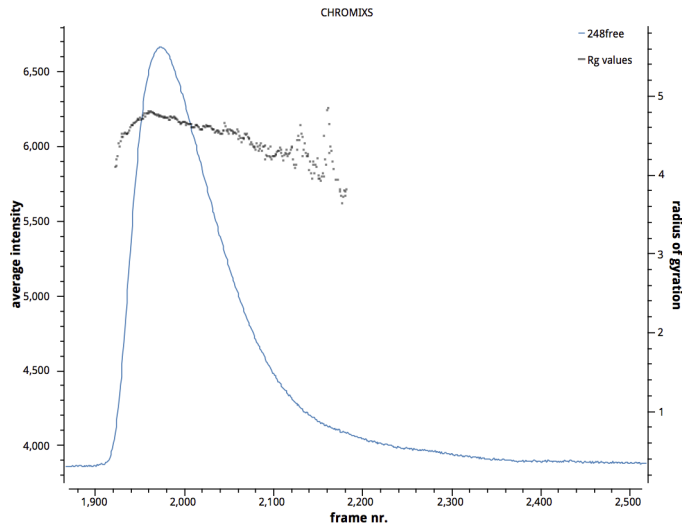
- Visualize SEC-SAXS run
- Manually or automatic region selection
- Compare additional parameters and data
- Export data and figures
- Complete automatic processing



Experimental issues



Experimental issues



Reference and other programs for further analysis

- **CHROMIXS** (part of ATSAS package) Panjkovich and Svergun (2017)
CHROMIXS: automatic and interactive analysis of chromatography-coupled small angle X-ray scattering data. *Submitted*
- **US SOMO** Brookes et al. (2016) "US-SOMO HPLC-SAXS Module: Dealing with Capillary Fouling, and Extraction of Pure Component Patterns from Poorly Resolved SEC-SAXS Data", J. Appl. Cryst. 49.
- **BioXTAS RAW** Hopkins, J. B., Gillilan, R. E., and Skou, S. (2017).
Bioxtas raw: improvements to a free open-source program for small-angle x-ray scattering data reduction and analysis. Journal of applied crystallography, 50, 15451553.
- **Scatter** <http://www.esrf.eu/UsersAndScience/Experiments/CRG/BM26/SaxsWaxs/DataAnalysis/Scatter>

Summary

- Visualize elution profile in term of scattering
- Common issues
- Identify sample and buffer region
- Evaluate sample behaviour (R_g and MW)
- Combine with additional data