

Processing and analysis of SEC-SAXS data

Alejandro 'Sasha' Panjkovich

Celgene Corporation

2019.10.19

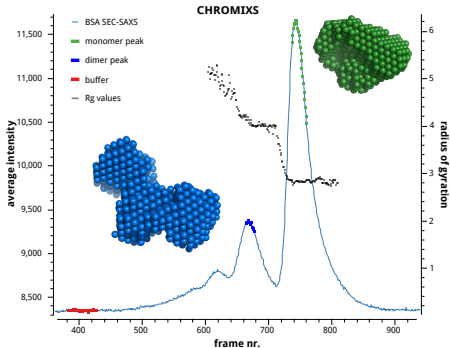
Outline

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

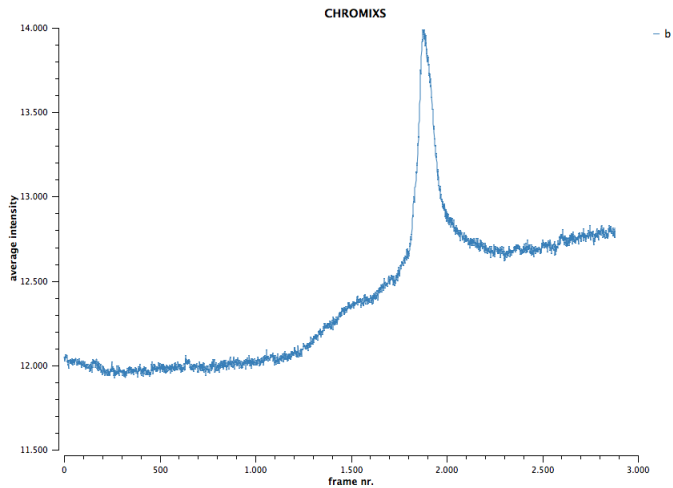


CHROMIXS: CHROMatography Inline X-ray Scattering

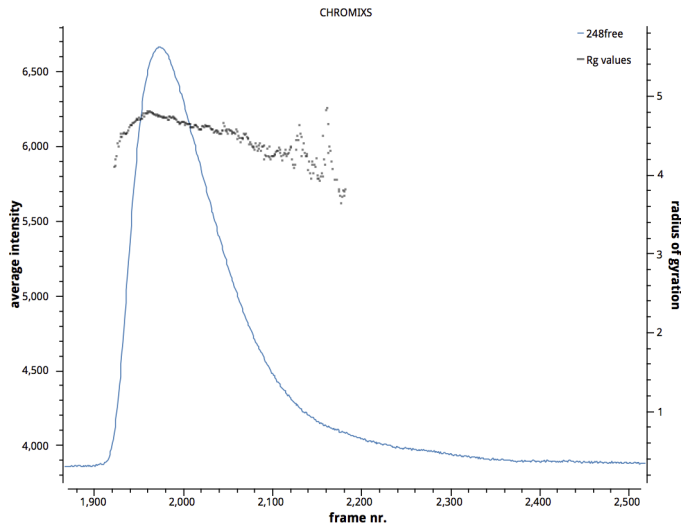
- Visualize SEC-SAXS run
- Manual or automatic region selection
- Compare additional parameters and data
- Export data and figures
- Complete automatic processing



Experimental issues



Experimental issues



Reference and other programs for further analysis

- **CHROMIXS** (part of ATSAS package) Panjkovich and Svergun (2018) CHROMIXS: automatic and interactive analysis of chromatography-coupled small angle X-ray scattering data. *Bioinformatics* 34:1944-46
- **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, 1545–1553.
- **Scatter** <http://www.esrf.eu/UsersAndScience/Experiments/CRG/BM26/SaxsWaxs/DataAnalysis/Scatter>

Summary

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



Structural and biophysical methods for biological macromolecules in solution

14 – 20 October 2019 | Santiago, Chile



PONTIFICIA
UNIVERSIDAD
CATÓLICA
DE CHILE



Anton Paar

DECTRIS
detecting the future

THE
EMBO
JOURNAL



EMBOpress

BI((O))SAXS

Xxenocs
Exploring the very small