

Title: BioXTAS RAW: a free open-source program for small-angle X-ray scattering data reduction and analysis

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Abstract:

BioXTAS RAW is a graphical-user-interface-based free open-source Python program for reduction and analysis of small-angle X-ray solution scattering (SAXS) data. The software is designed for biological SAXS data and enables creation and plotting of one-dimensional scattering profiles from two-dimensional detector images, standard data operations such as averaging and subtraction and analysis of radius of gyration and molecular weight, and advanced analysis such as calculation of inverse Fourier transforms and 3D reconstructions. It also allows easy processing of inline size-exclusion chromatography coupled SAXS data and data deconvolution using the evolving factor analysis method. It provides an alternative to closed-source programs such as *Primus* and *ScÅtter* for primary data analysis. Because it can calibrate, mask and integrate images it also provides an alternative to synchrotron beamline pipelines that scientists can install on their own computers and use both at home and at the beamline. *RAW* is currently used by at least four SAXS beamlines worldwide, including two in North America (the MacCHESS BioSAXS beamline at CHESS and BioCAT at the APS). It is also used at numerous home source SAXS instruments worldwide and is distributed by SAXSLAB/Xenocs with some of their SAXS instruments.