

# A Brief Survey of State-of-the-Art BioSAXS

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# Overview

Review of SAXS

Data Analysis using BioSAXS

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Advancements in BioSAXS

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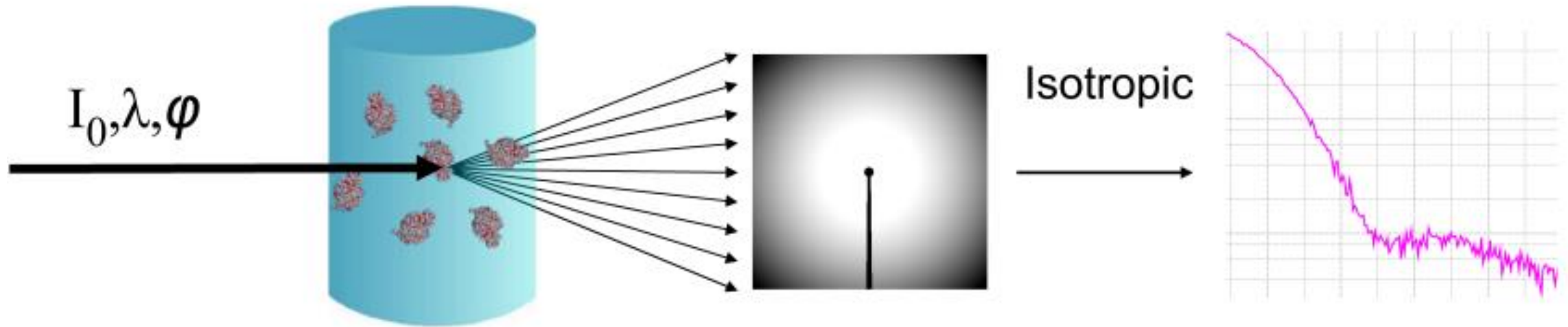
Applications of BioSAXS

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Future Directions of BioSAXS

# Review of SAXS

SAXS, a tool for characterizing the structural properties of a wide range of materials at the nanoscale, helping better understand their properties and behavior.



(Brookes, 2024)

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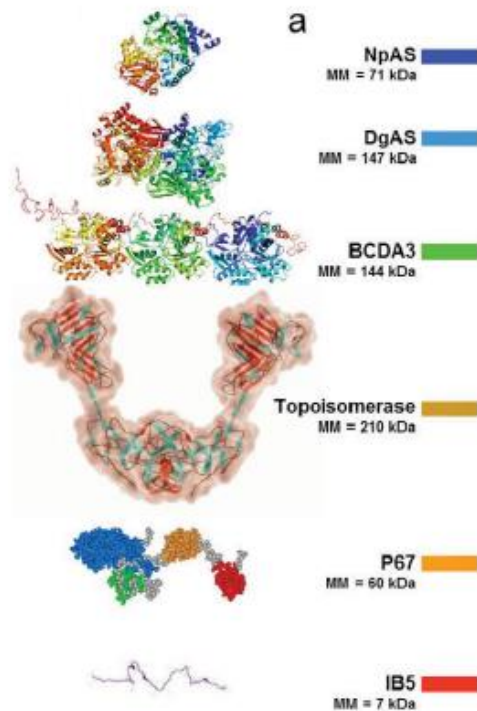
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Future Directions of BioSAXS

# Data Analysis in SAXS

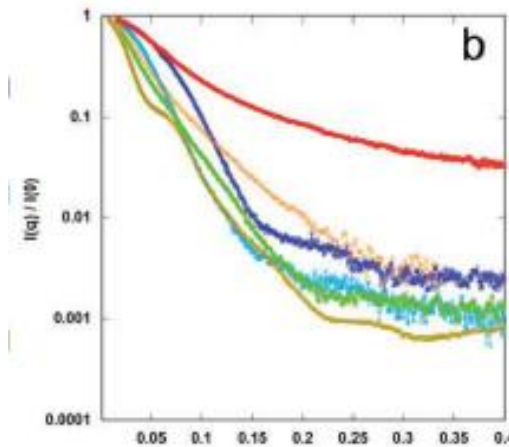
## Guinier Analysis

- Can be plotted with  $I(q)$  vs  $q$ , where  $I(q)$  is the intensity for a given scattering angle ( $q$ ).
- Can be converted to the Guinier plot, in which the slope can provide useful information on the Radius of Gyration or  $R_g$  of the sample.



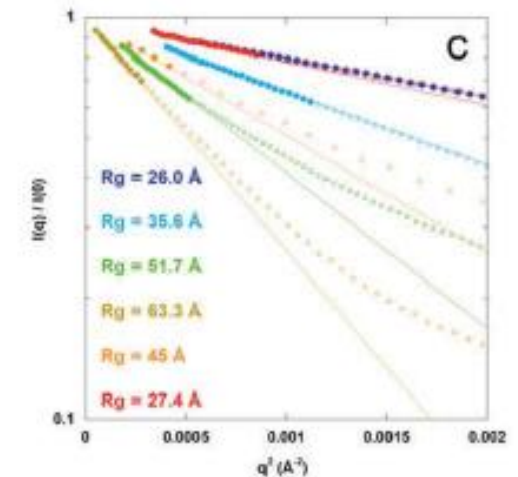
**Figure 1a:** A 3D representation of the selected proteins, whose structures fit the BioSAXS data

$$I(q) = I(0) e^{-\frac{q^2 R_g^2}{3}}$$



**Figure 1b:** The usual representation of a SAXS pattern,  $I(q)$  vs  $q$  in log scale, normalized to 1 at  $q=0$ .

$$\ln[I(q)] = \ln[I(0)] - \frac{q^2 R_g^2}{3}$$



**Figure 1c:** The Guinier Plot,  $I(q)$  vs  $q^2$  in log scale, displays a negative linear slope at small  $q$  values directly proportional to  $R_g^2$

# Data Analysis in SAXS Kratky Analysis

- When  $qRg^2 I(q)$  is plotted against  $qRg$  it can tell us about the compactness of a protein. It can tell us if it is globular or unfolded based on the shape of the curve.

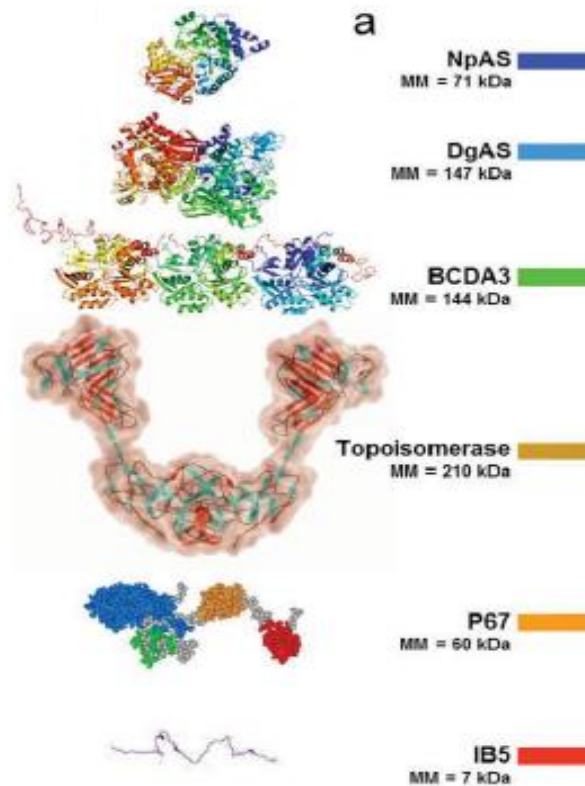


Figure 1a: A 3D representation of the selected proteins, whose structures fit the BioSAXS data

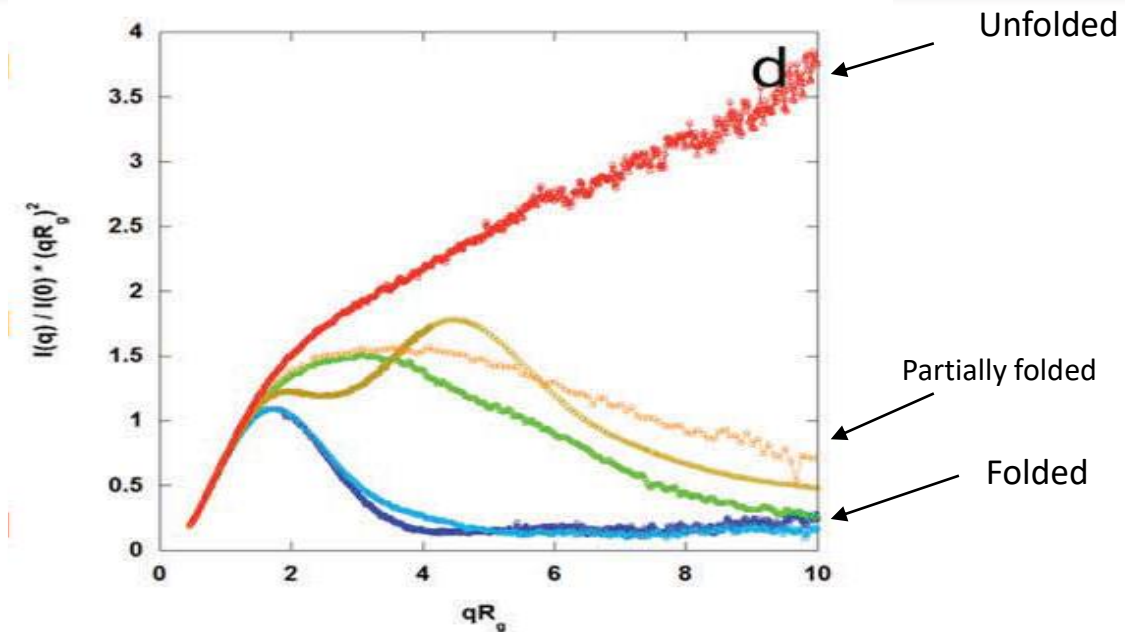
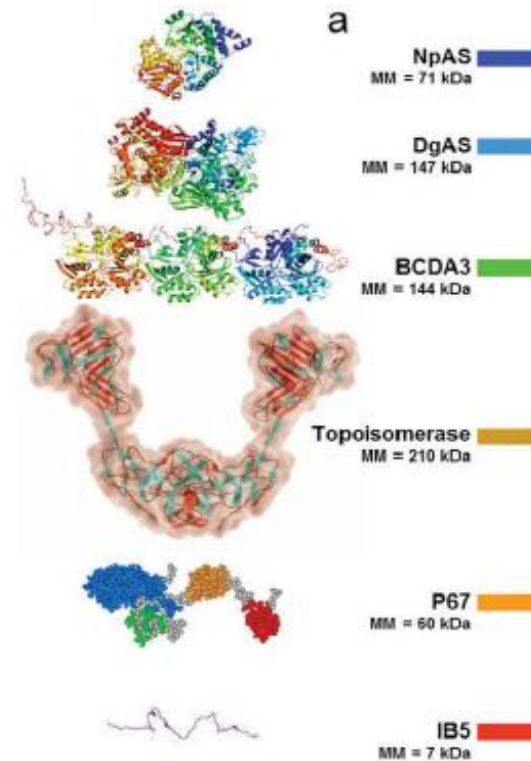


Figure 1d: The dimensionless Kratky Plot,  $I(q)/I(0)(qRg)^2$  vs  $qRg$ , is extremely useful to distinguish between different degrees of folding. Proteins containing folded domains display a bell shaped curve, which has a maximum of about 1.1 at around  $qRg=1.75$ . With increasing elongation and degree of unfolding, the curve maximum shifts to the upper right and the slope of the right side of the curve increases.

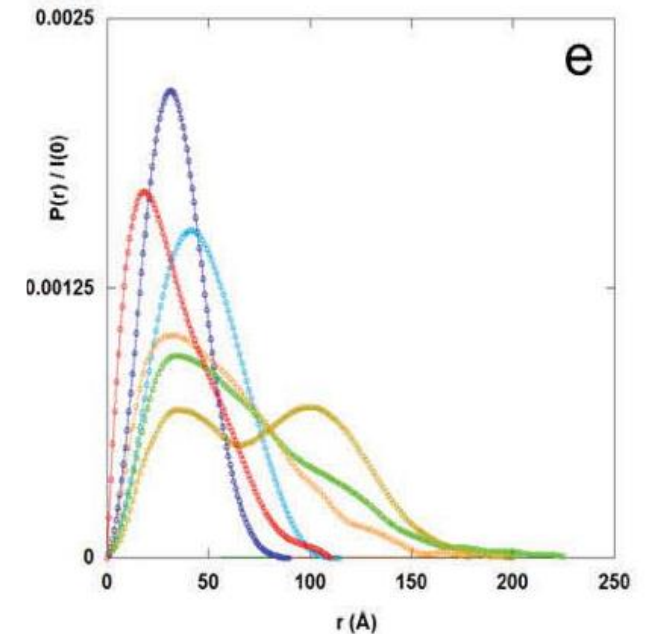
# Data Analysis in SAXS

## Distance Distribution Analysis

This plot provides insight into the geometry of the sample. It can tell us if it is a more elongated or spherical shape, as well as if there are large separate domains in the protein.



**Figure 1a:** A 3D representation of the selected proteins, whose structures fit the BioSAXS data



**Figure 1e:** The distance distribution function,  $P(r)$ , directly derived from the previous curves using programs such as Gnom, and normalized to  $I(0)$ . The maximum extension,  $D_{max}$ , of the  $P(r)$  corresponds to the maximum spatial extension of the protein.

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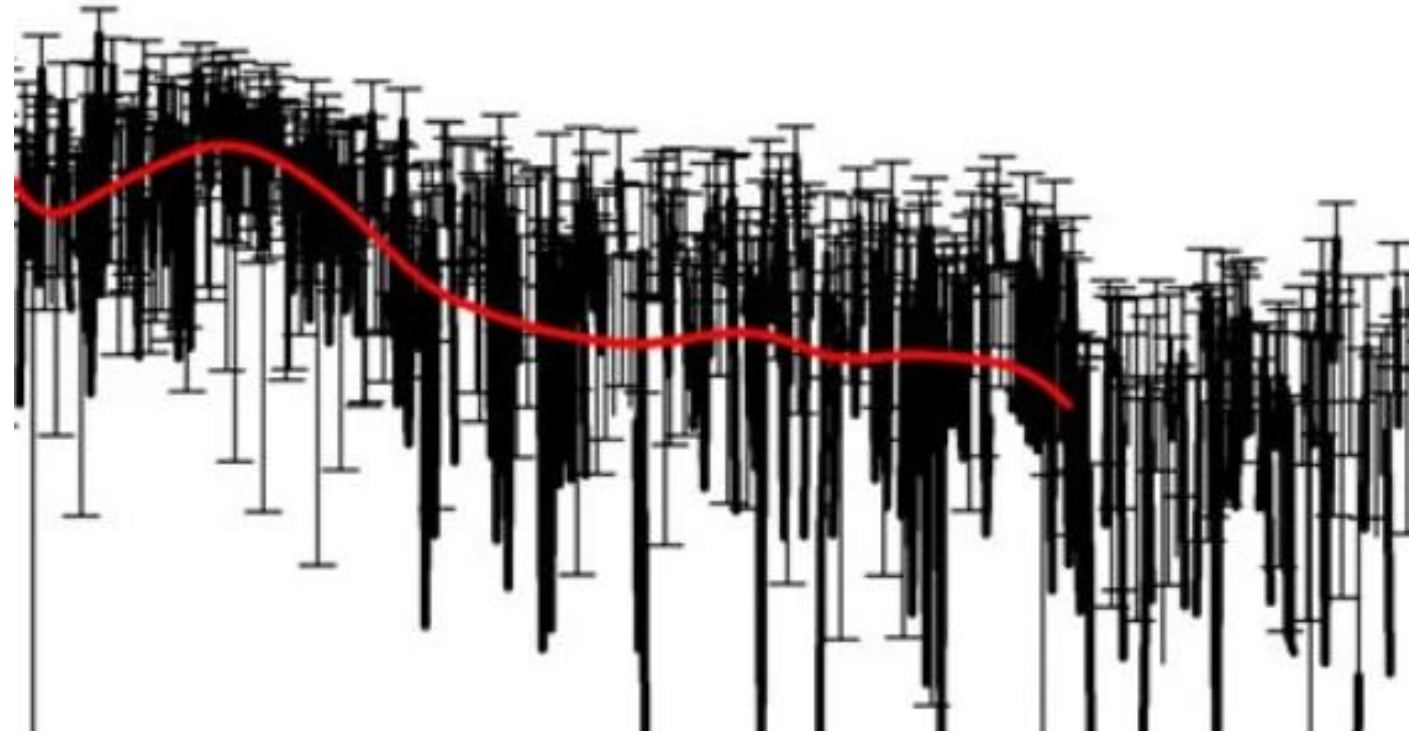
Future Directions of BioSAXS



## Recent Advances and Applications in BioSAXS Hybrid Methods

- The introduction of hybrid pixel X-ray detectors has dramatically improved the signal-to-noise ratio in SAXS.
- Enables data collection at lower concentrations and enhancing the quality of results.
- Measurement cells have been designed to operate in vacuum to reduce parasitic scattering from the air.

— original data  
— denoised data

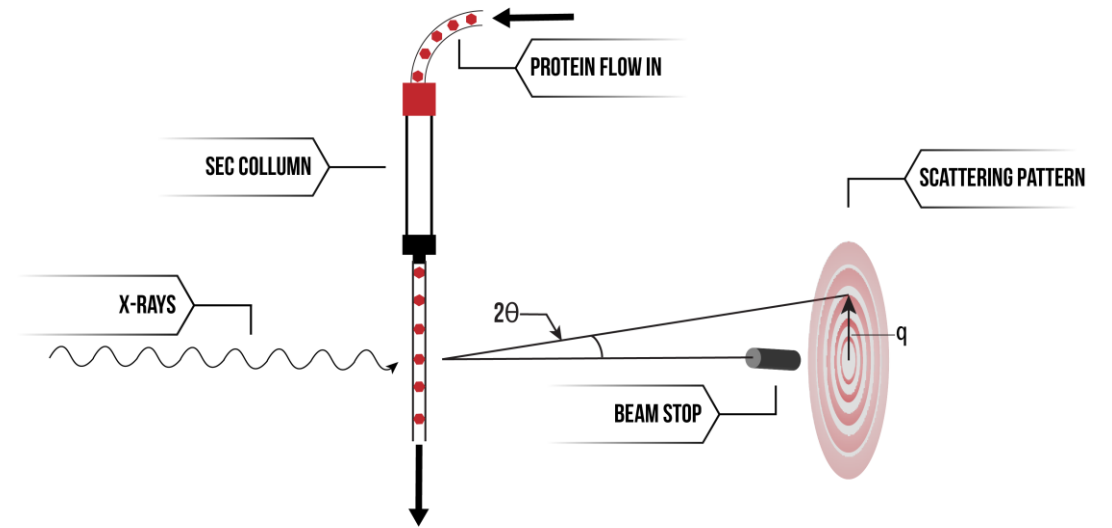


# Recent Advances and Applications in BioSAXS

## SEC-SAXC

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- One major issue with SAXS is the formation of aggregates
- To counteract that SAXS has been used in relation with Size Exclusion Chromatography (SEC), to separate aggregated molecules.



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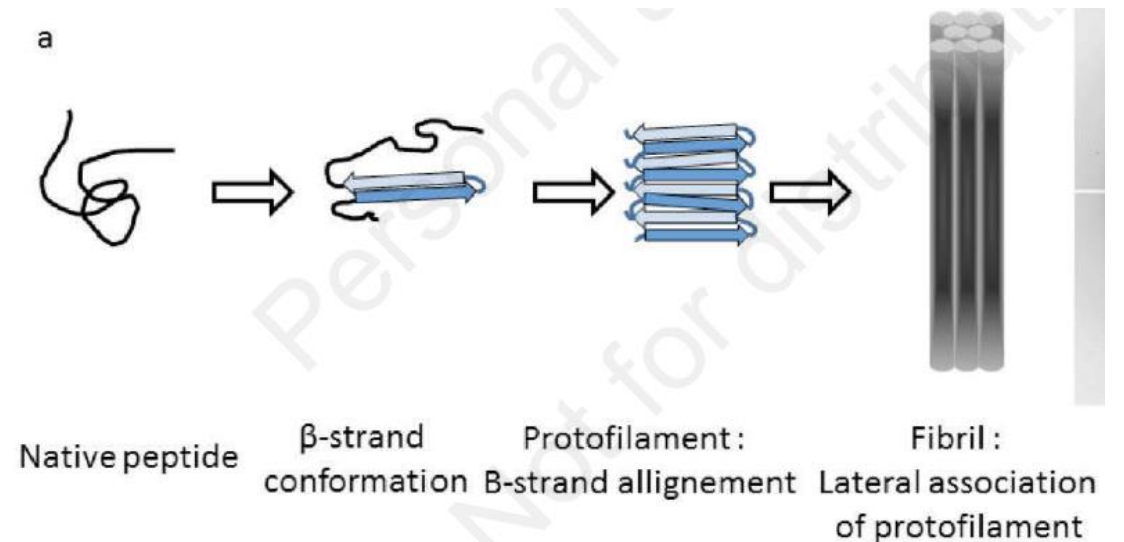
Future Directions of BioSAXS

# Applications of SAXS

## Fiber Growth Analysis

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- SAXS is used to investigate the process of fiber growth, where such as peptides or proteins, form organized structures through intrinsic interactions without external stimuli.
- By analyzing the scattering patterns generated by SAXS, information on the structural characteristics and organization of the fibers formed during the self-assembly process can be determined.



**Figure 2a:** Amyloids hierarchical formation sketch. Peptides or protein unfold and acquire a  $\beta$ -strand secondary structure. These  $\beta$ -strands then assemble into protofibrils. The  $\beta$ -strands are perpendicular to the protofibrils main axis. The protofibrils then assemble into fibrils by lateral association.

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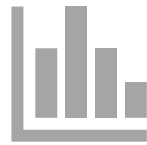
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Future Directions of BioSAXS

# Future Directions With SAXS



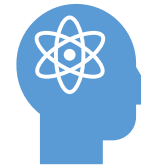
Improved Resolution and  
Complementary  
Techniques



Enhanced Data  
Interpretation and  
Modeling



Integration of Advanced  
Detectors



Exploration of Novel  
Applications

# References

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Questions