

Dynamic footprint of sequestration in the molecular fluctuations of Osteopontin

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SUPPORTING INFORMATION

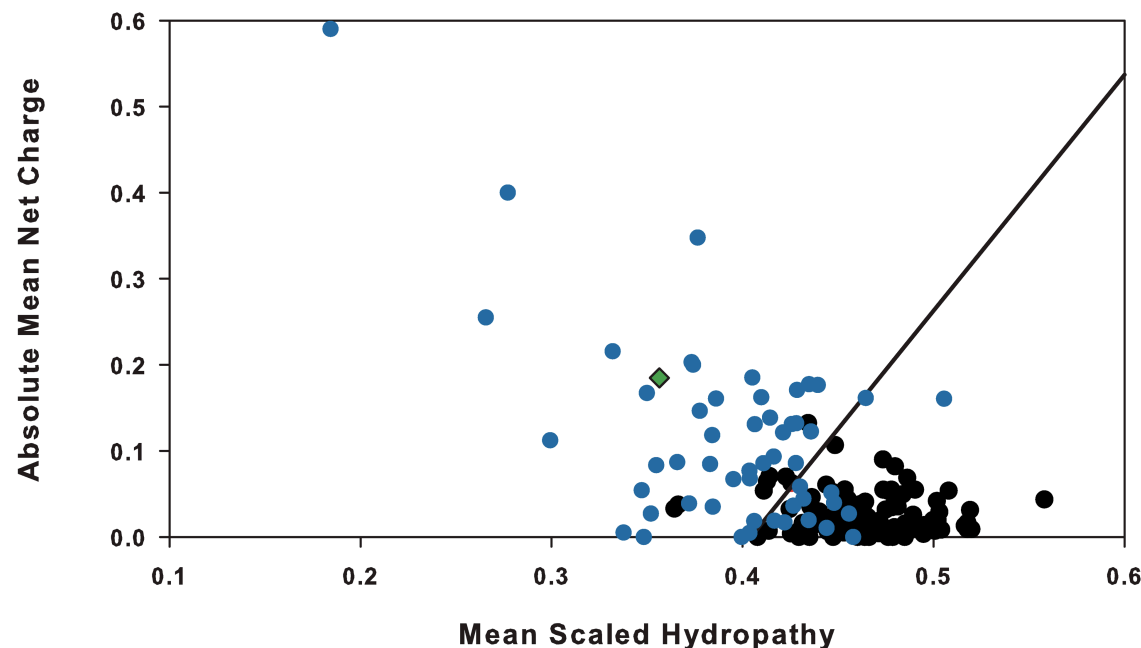


Figure 1: Charge-hydropathy plot showing positions of experimentally determined ordered (black dots) and disordered proteins, adapted from Uversky *et al.*¹, with the boundary between the ordered and disordered region indicated by the black line. The charge-hydropathy properties of the OPN1-149 peptide are indicated by the diamond mark, which lies well within the disordered region.

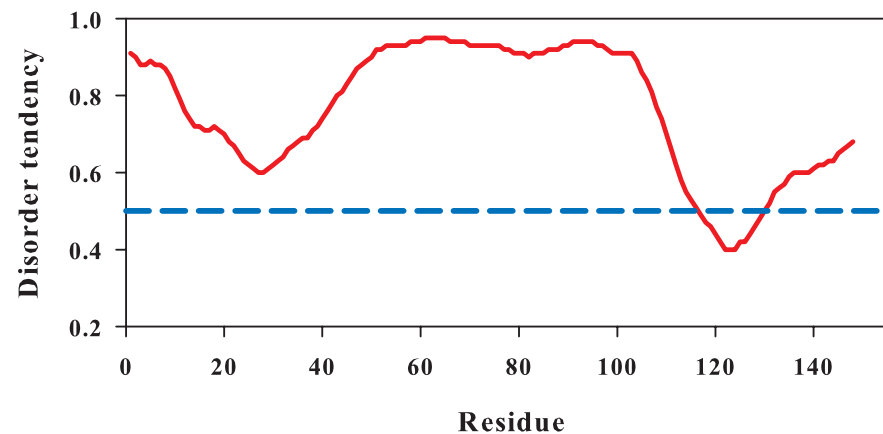


Figure 2: Prediction of disorder within the OPN1-149 amino acid sequence by the IUpred method². Regions with a disorder tendency above 0.5 are predicted to be highly disordered, which is the case for most of the aminoacid sequence of OPN1-149.

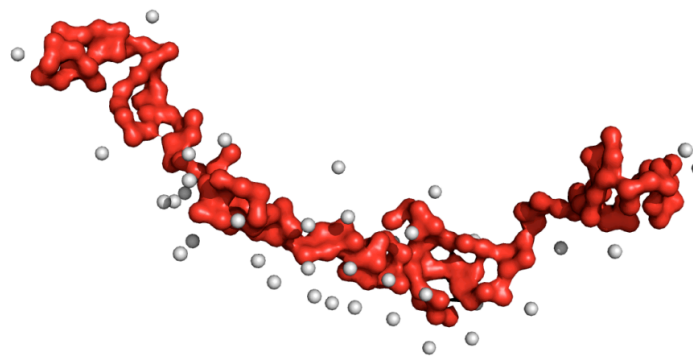


Figure 3: Scattering envelope of OPN1-149 calculated from the experimental SAXS data by the GASBOR software. The model indicates an elongated structure typical of the structures produced for intrinsically disordered proteins. Furthermore the structure is highly similar to the model produced by DAMMIF. The white spheres shown correspond to solvent molecules that contribute to the envelope scattering.

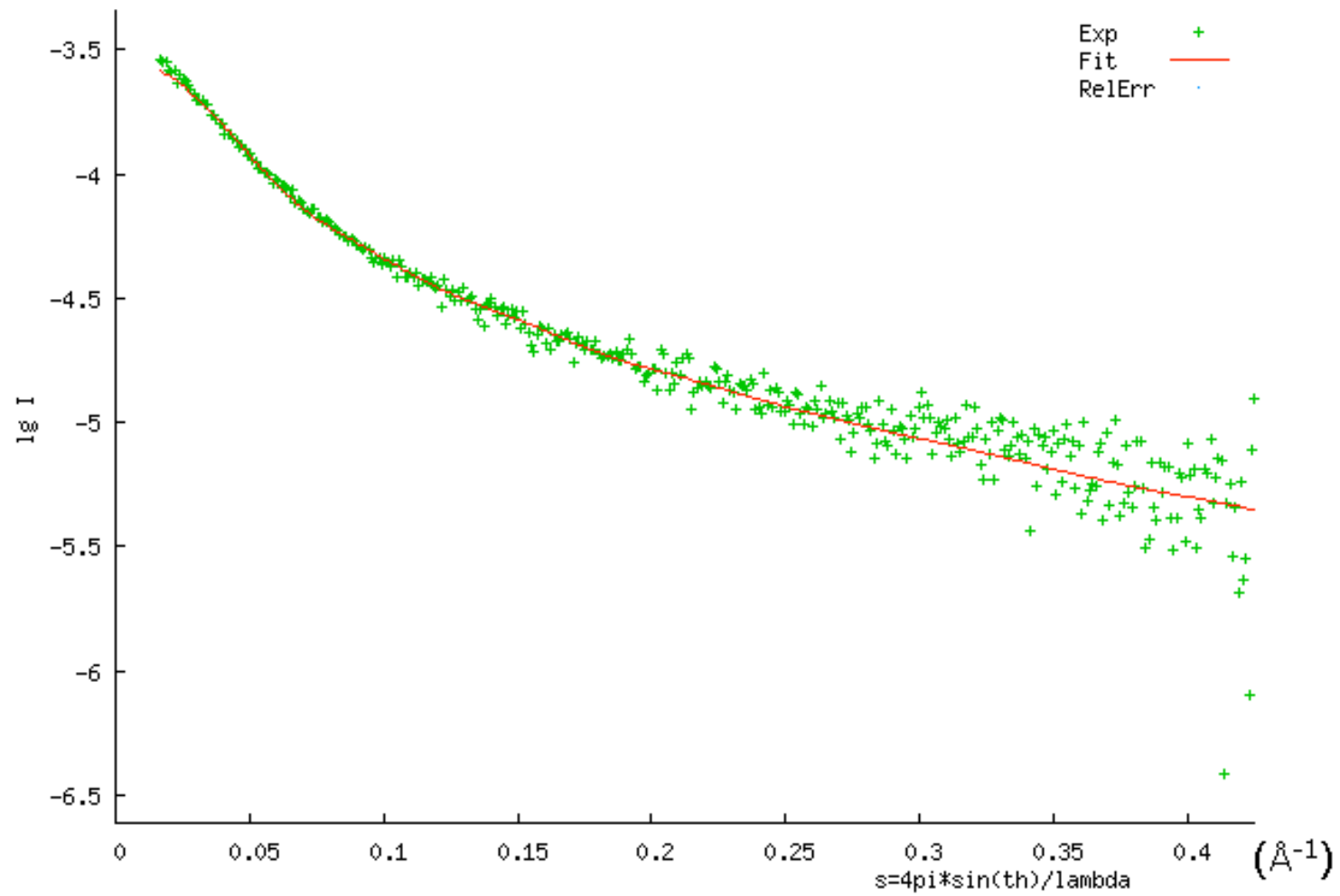


Figure 4: Fit of the scattering envelope (line) produced by GASBOR to the experimental SAXS curve (dots).

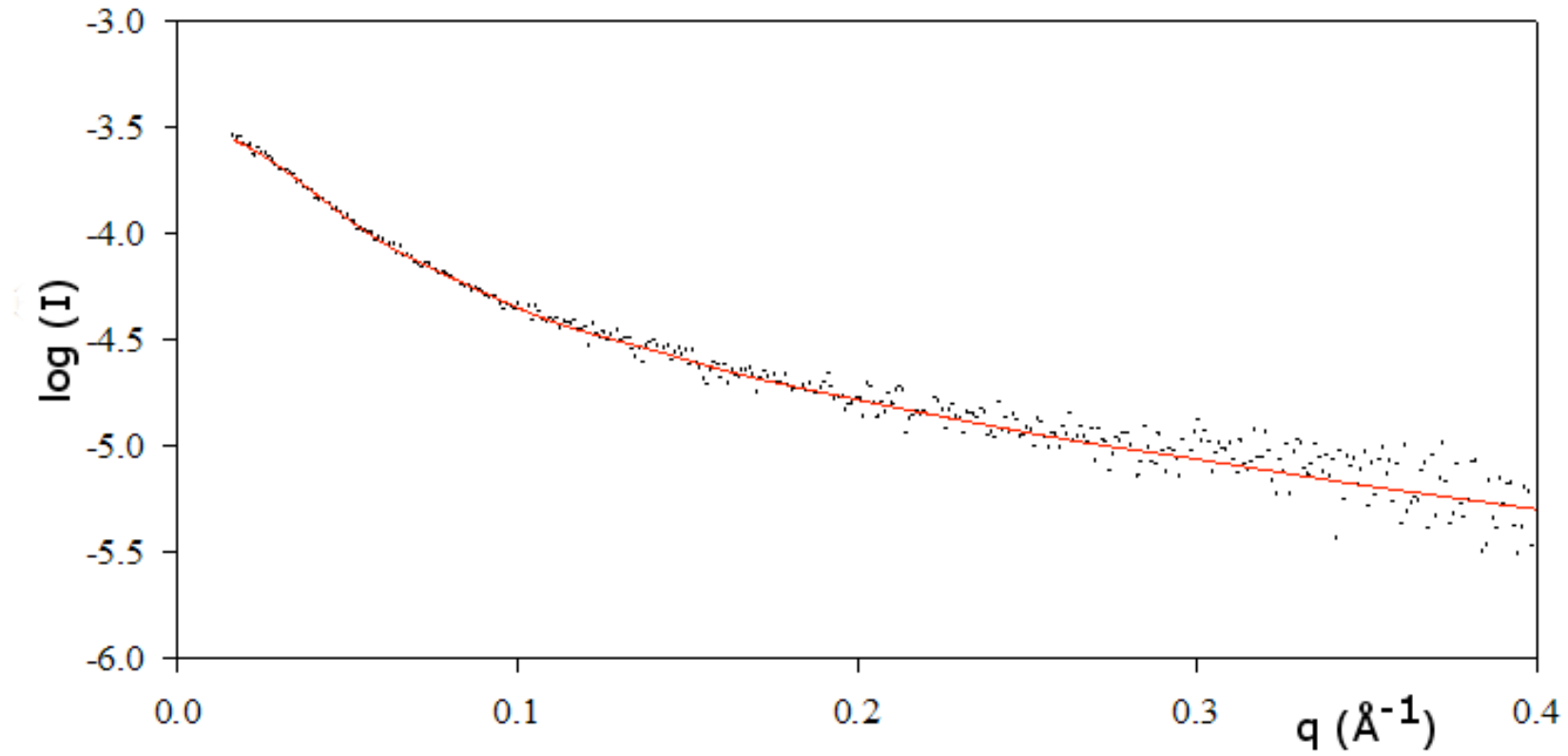


Figure 5: Fit of the scattering envelope produced by DAMMIF (line) to the experimentally collected OPN1-149 SAXS data (dots).

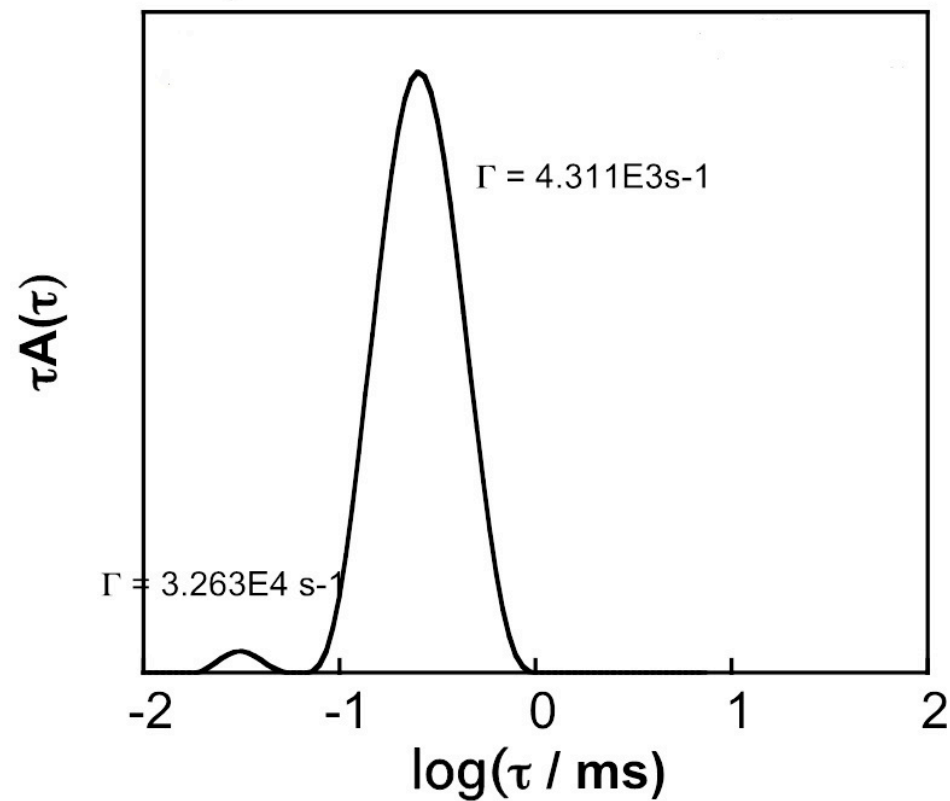


Figure 6: Dynamic light scattering experiments of the formed OPN1-149 CPN shown as a volume distribution, where Viscosity = 0.8904 cP, Temperature = 298 K, and the relaxation time is shown for each species. The peak with the lowest intensity corresponds to the excess free peptide (< 5% V/V) in the sample (R_h of 1.9 nm). The highest peak corresponds to an R_h of 23.1nm for the formed OPN CPN.

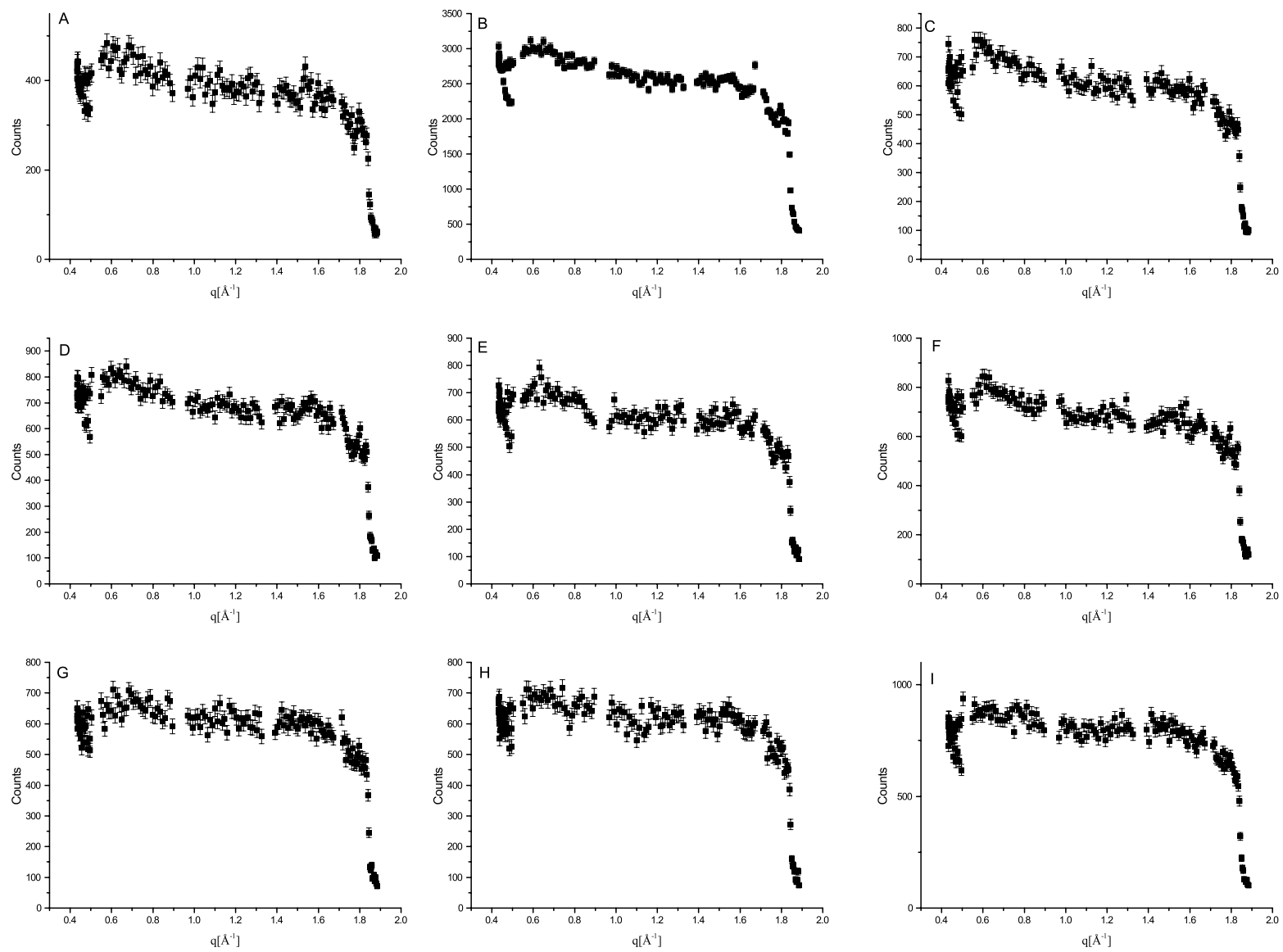


Figure 7: *In situ* diffraction measurements of the OPN1-149 sample summed for different temperature ranges: A 10-20K, B 20-30K, C 30-40K, D 40-50K, E 50-60K, F 250-260K, G 260-270K, H 270-280K and I 280-290K.

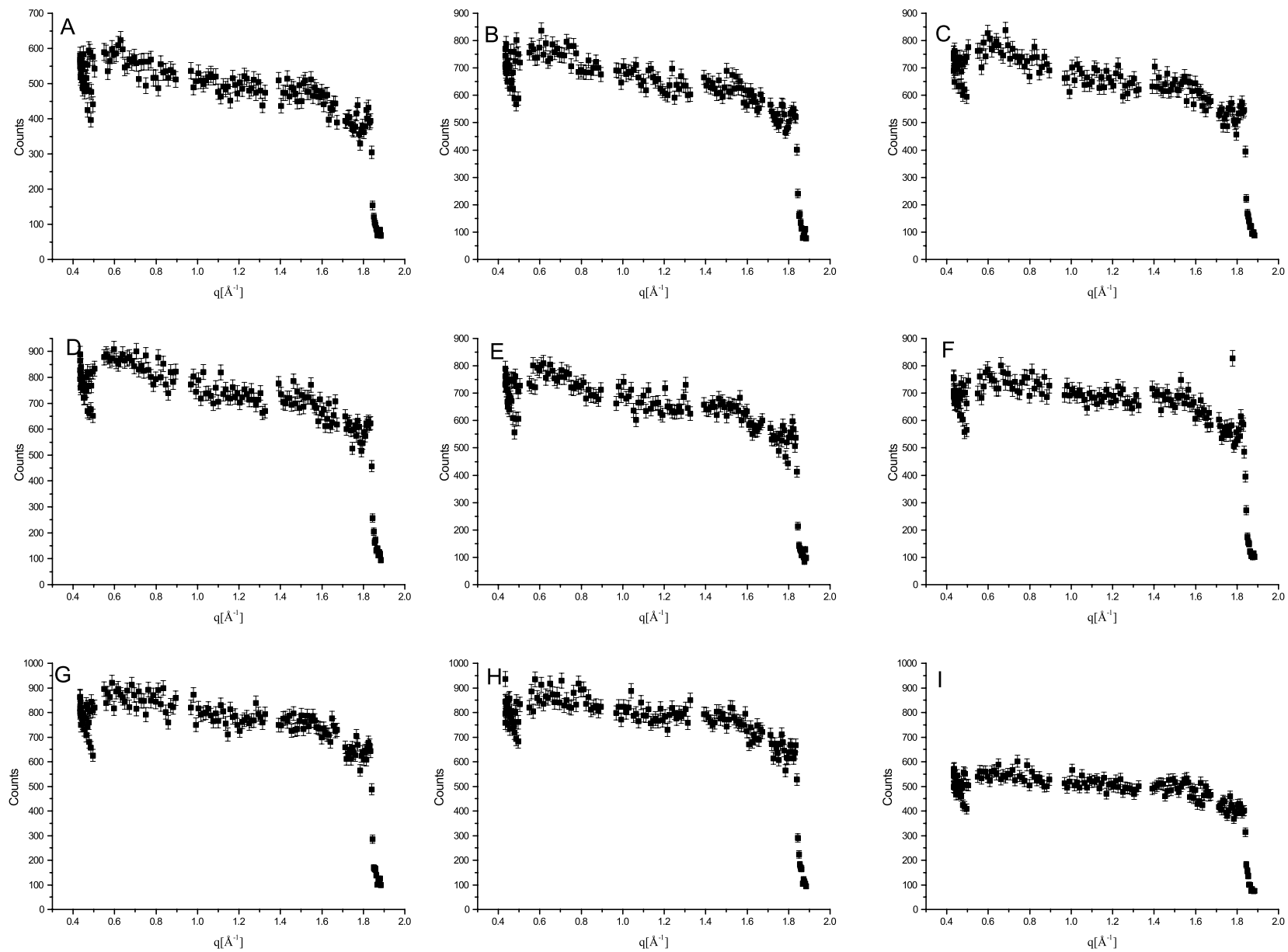


Figure 8: *In situ* diffraction measurements of the OPN CPN sample summed for different temperature ranges: A 10-20K, B 20-30K, C 30-40K, D 40-50K, E 50-60K, F 250-260K, G 260-270K, H 270-280K and I 280-290K.

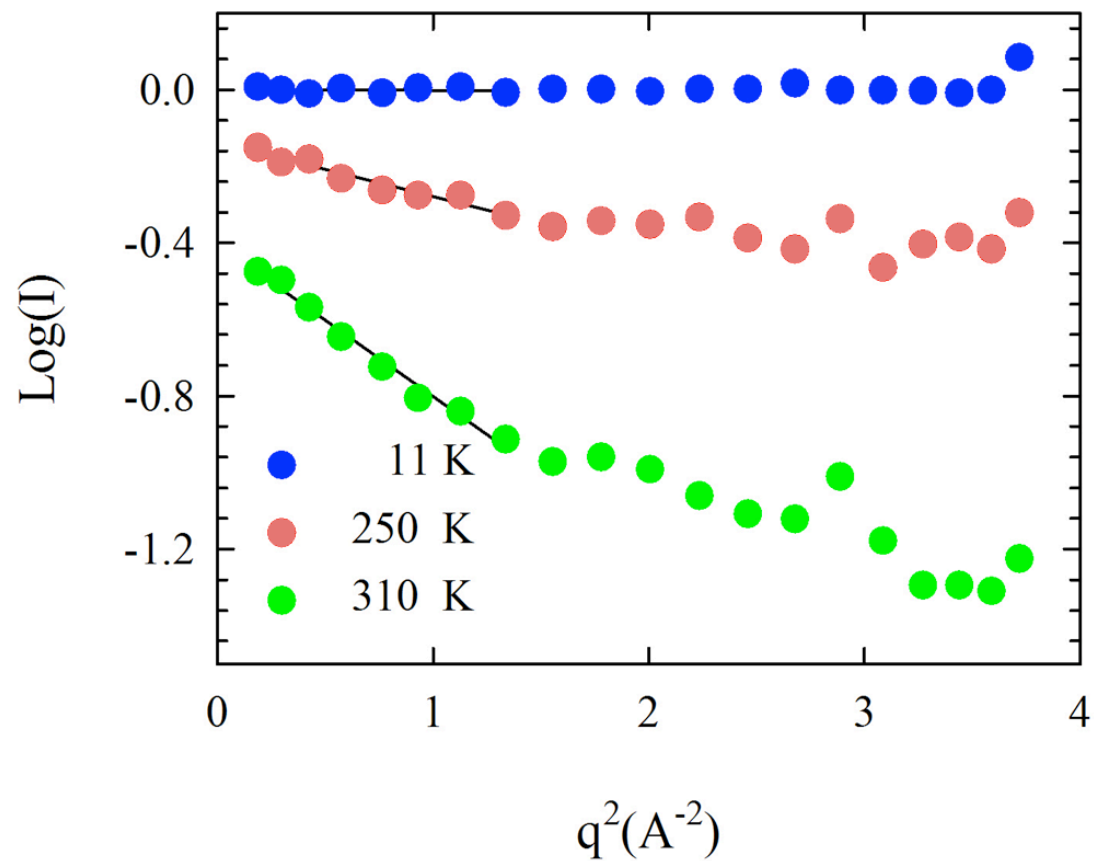


Figure 9: Representation of the logarithmic intensities as a function of q^2 observed for the OPN1-149 EINS temperature scan, performed on IN16. The figure highlights the q -region from which the Gaussian was applied and shows the fit of the straight line to the data.

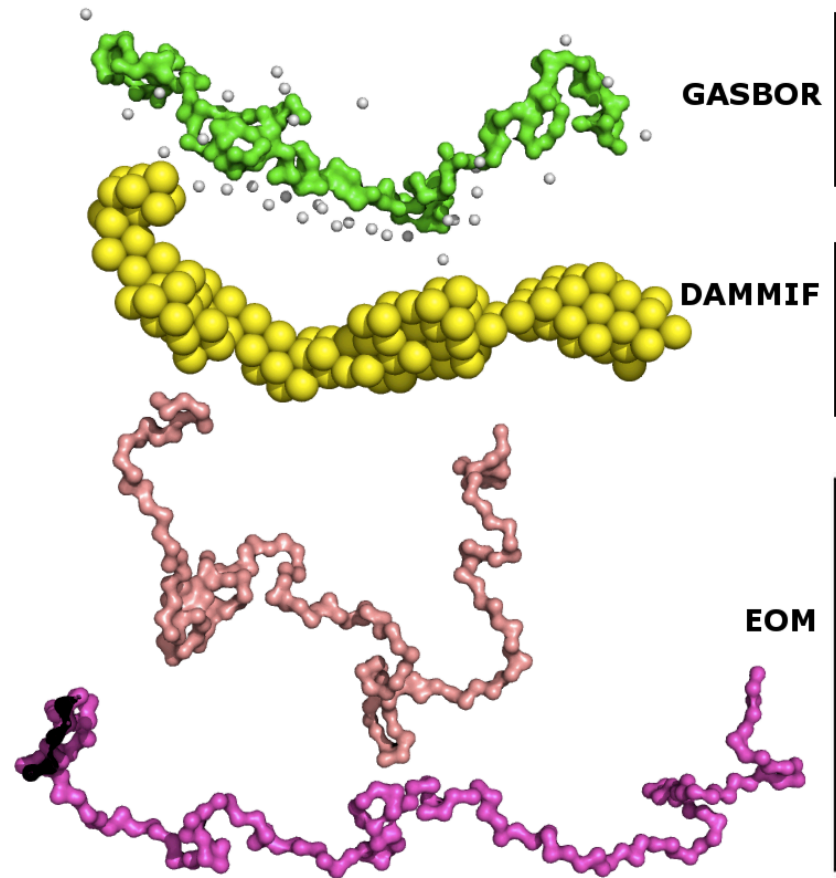


Figure 10: Comparison between scattering envelopes obtained by analysis of the OPN1-149 SAXS data by GASBOR, DAMMIF, and the extended and compact conformations of OPN1-149 obtained by the EOM method.

REFERENCES

- (1) Uversky, V. N.; Gillespie, J. R.; Fink, A. L. *Proteins* **2000**, 41, 415-27.
- (2) Dosztányi, Z.; Csizmók, V.; Tompa, P. and Simon, I. *J. Mol. Biol.* **2005**, 347, 827-839.