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# EXPLORATION OF CONFORMATIONS FOR AN IDP

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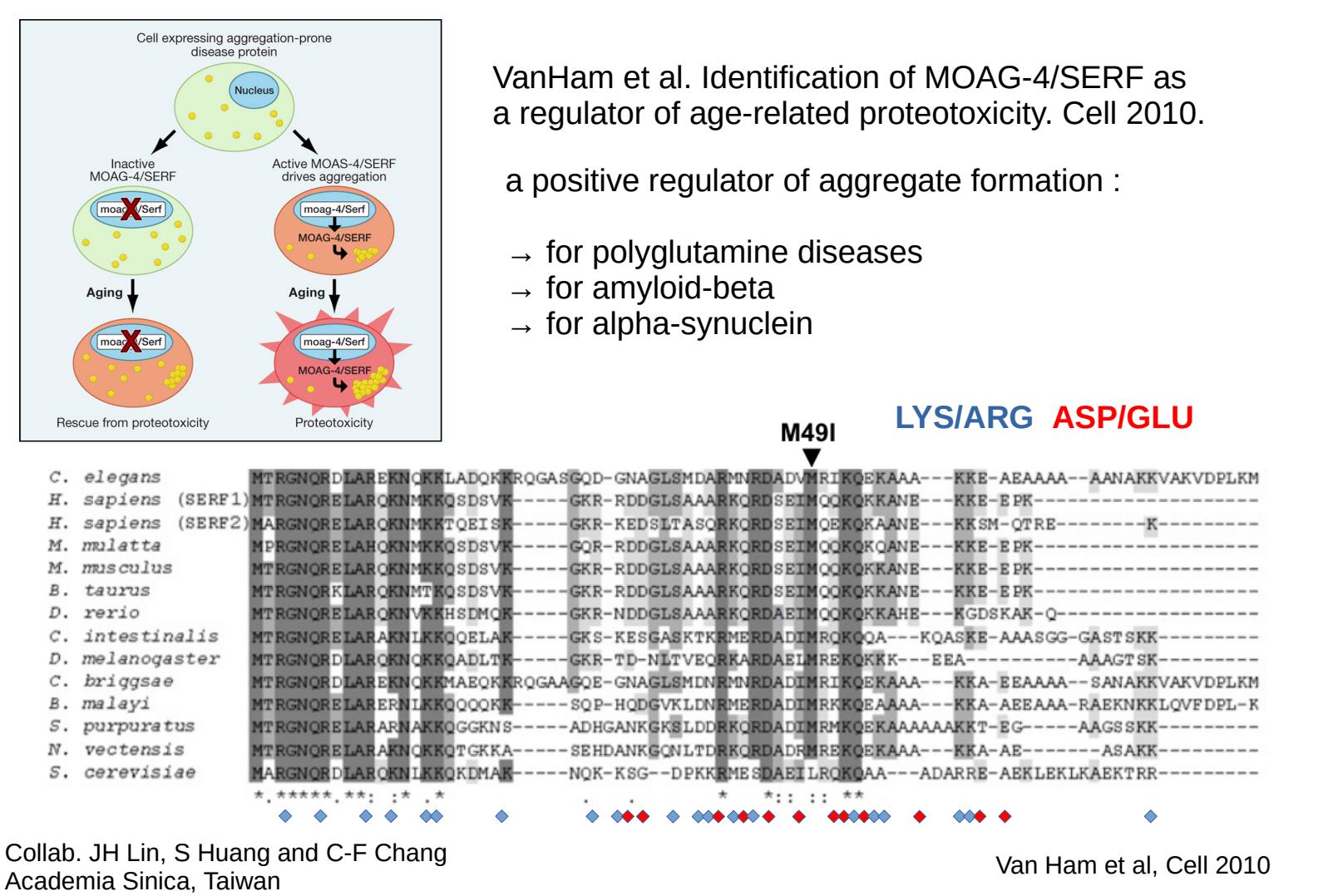
## Abstract

Intrinsically disordered proteins (IDP) are at the center of numerous biological processes, and attract consequently extreme interest in structural biology. A systematic enumeration of protein conformations, based on distance geometry, was performed on SERF1a, a 62-residue IDP involved in interactions with amyloid peptides. The results obtained with the threading-adapted interval Branch-and-Prune (TAiBP) approach have been analyzed using various input predictions for backbone torsion angles  $\phi$  and  $\psi$ , provided by TALOS and  $\delta$ 2D, as well as a NOE measurement. The fitting of SAXS data permitted to select various sets of conformations depending on the input predictions. The similarity between profiles of local gyration radii provides to a certain extent a converged view of the SERF1a. A better convergence of these profiles is observed when using the TALOS inputs than using the  $\delta$ 2D inputs. All sets of conformations point to the same locations for maxima of pocketedness along protein sequences.

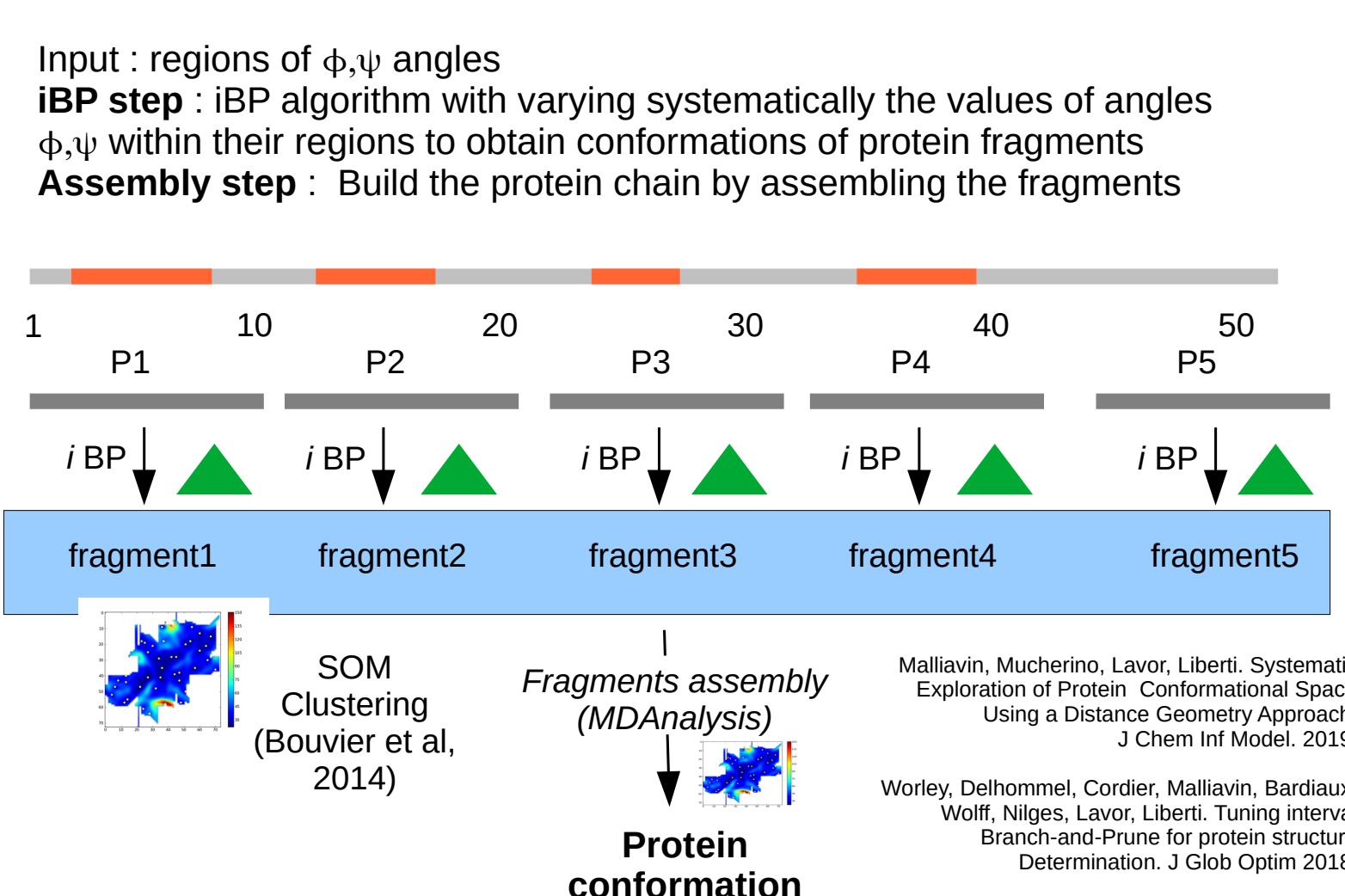
# Experimental measurements

NMR spectra were recorded at 298K on Bruker Avance 800MHz equipped with cryoprobe, using samples of 0.5mM  $^{13}\text{C}$ -  $^{15}\text{N}$ - labeled SERF1a in 20mM NaPi, and 20mM NaCl buffers. Spectra were processed with TopSpin 3.6.5 (Bruker) and peak picked with SPARKY. SAXS data were measured at NSRRC by Dr Orion Shih and Yi-Qi Yeh.

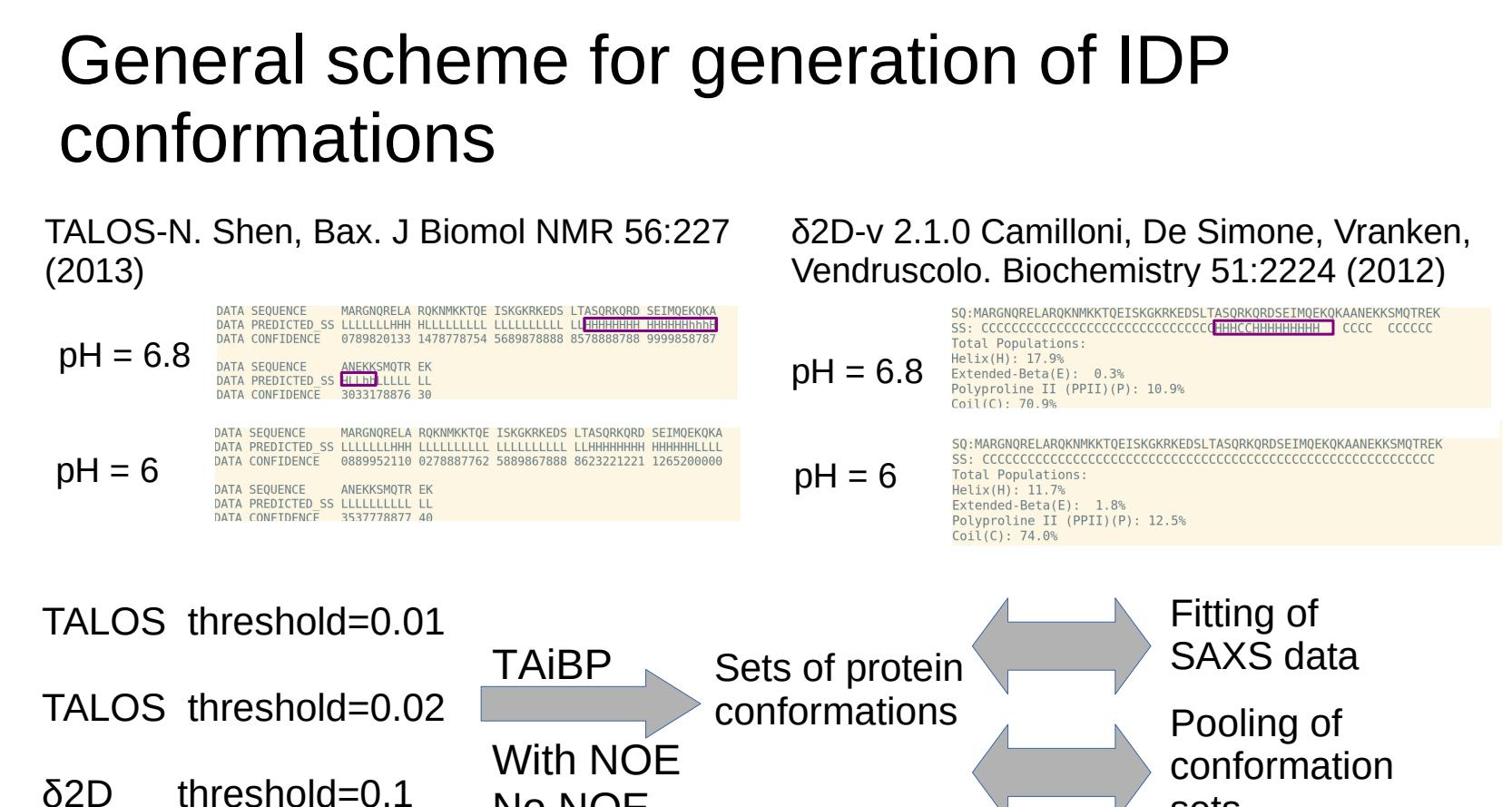
# Function of SERF1a



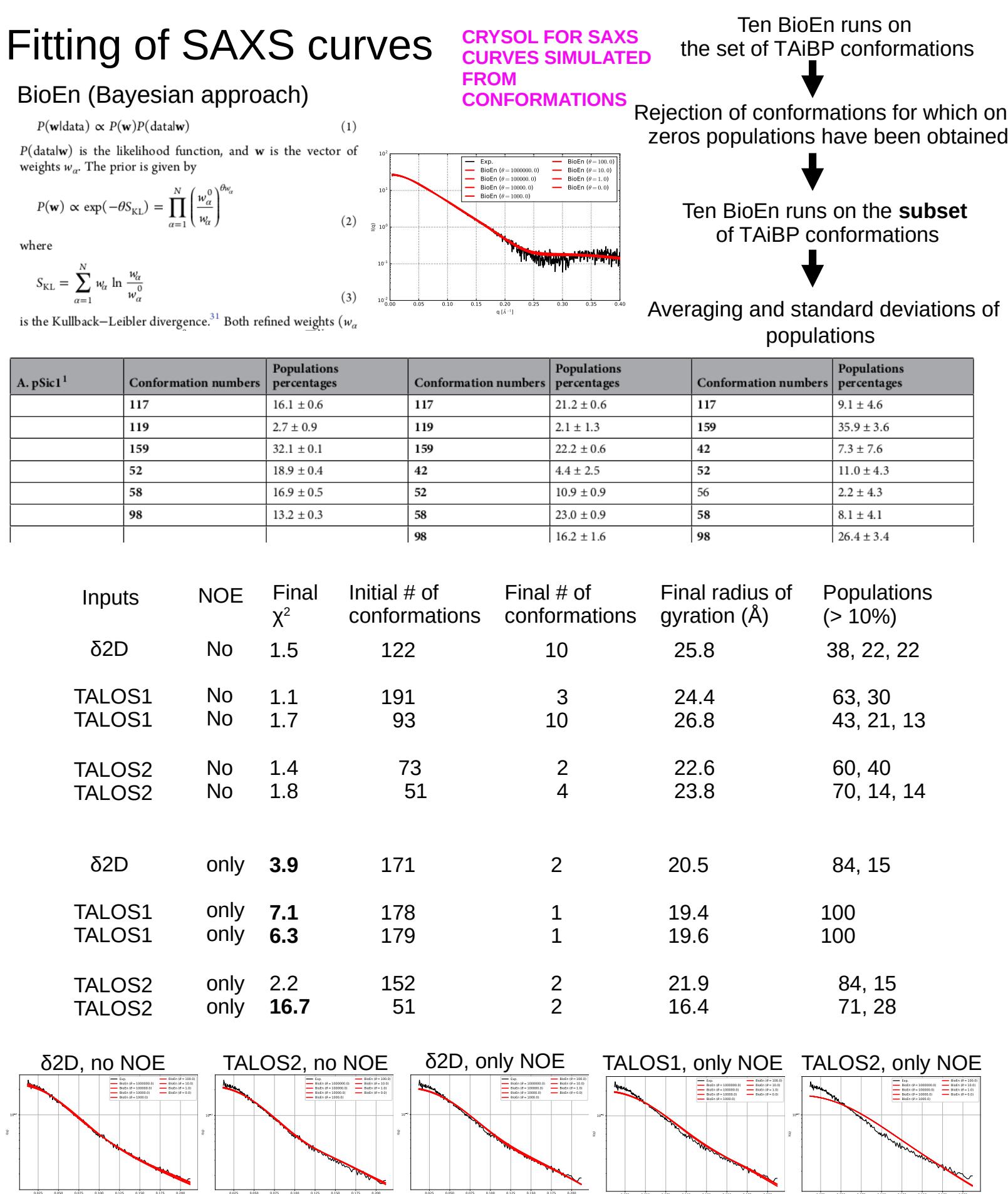
# TAiBP approach



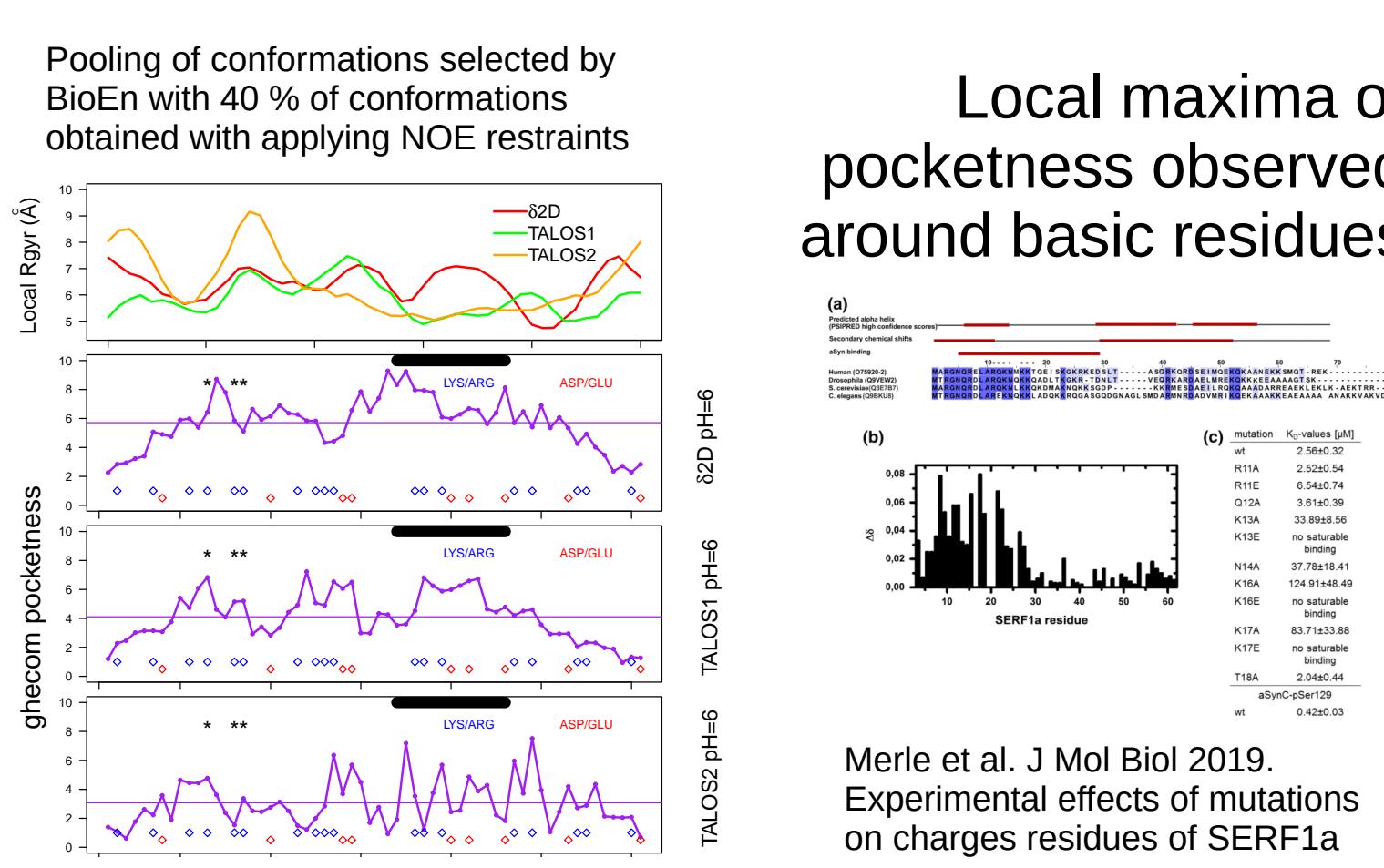
# Procedure of calculation



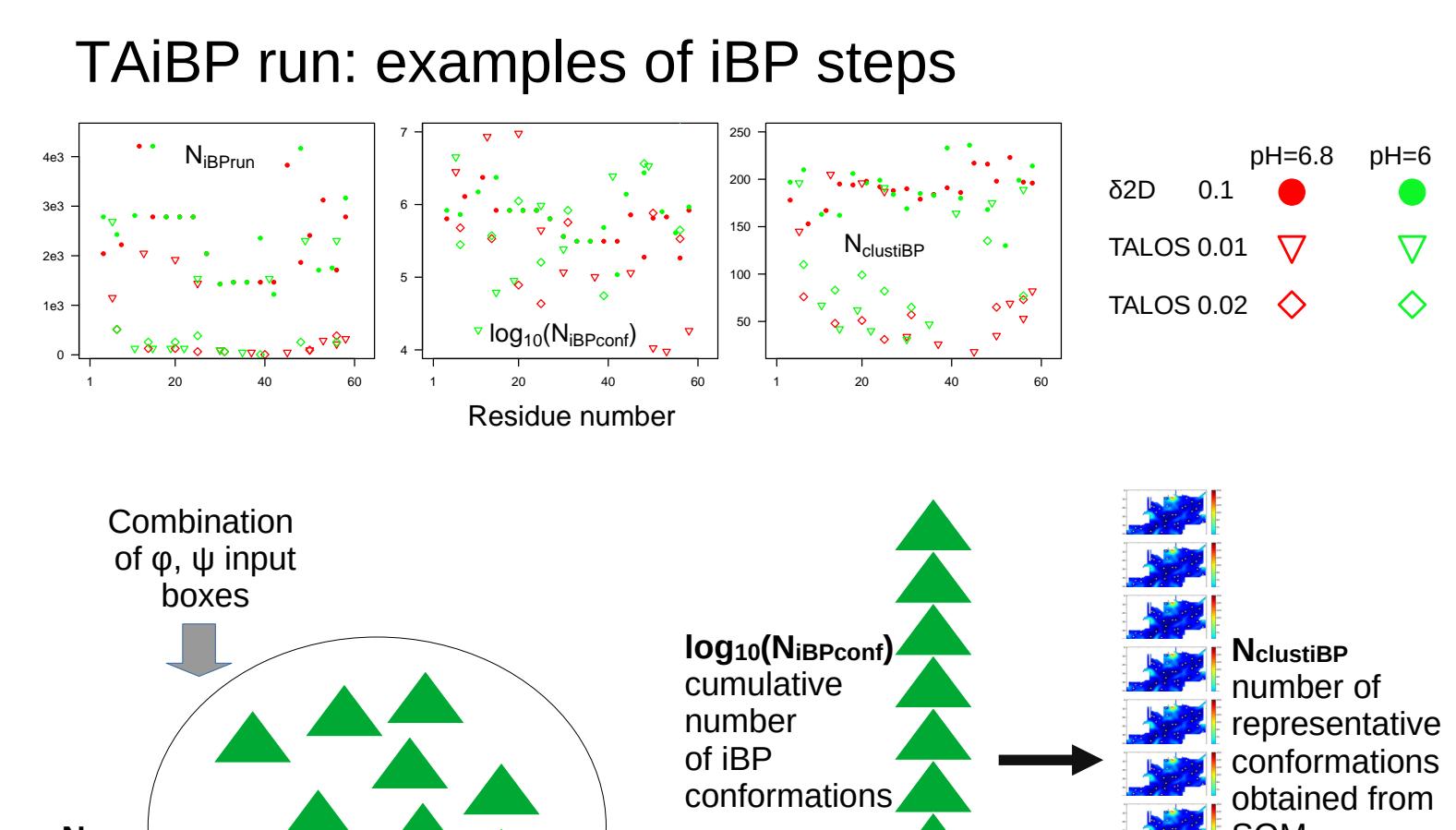
# Fitting SAXS data



# Pocket detection



# Calculation examples



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