



Exploration of the conformational space of SERF1a

Shu-Yu Huang, Chi-Fon Chang, Jung-Hsin Lin, Thérèse Malliavin

► To cite this version:

Shu-Yu Huang, Chi-Fon Chang, Jung-Hsin Lin, Thérèse Malliavin. Exploration of the conformational space of SERF1a. NMR for Life Science, Oct 2023, Virtual Event, France. hal-04545876

HAL Id: hal-04545876

<https://cnrs.hal.science/hal-04545876>

Submitted on 14 Apr 2024

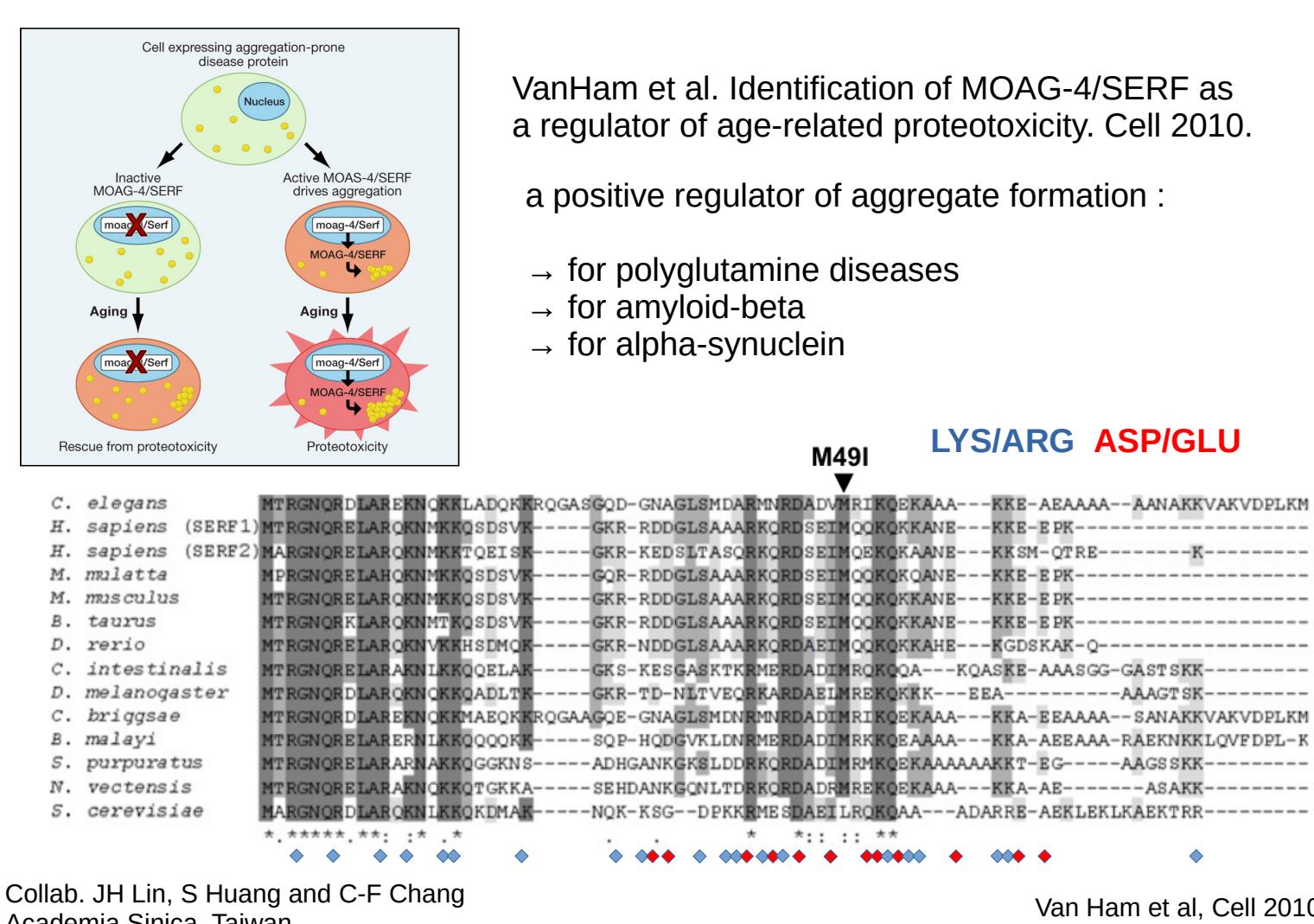
HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

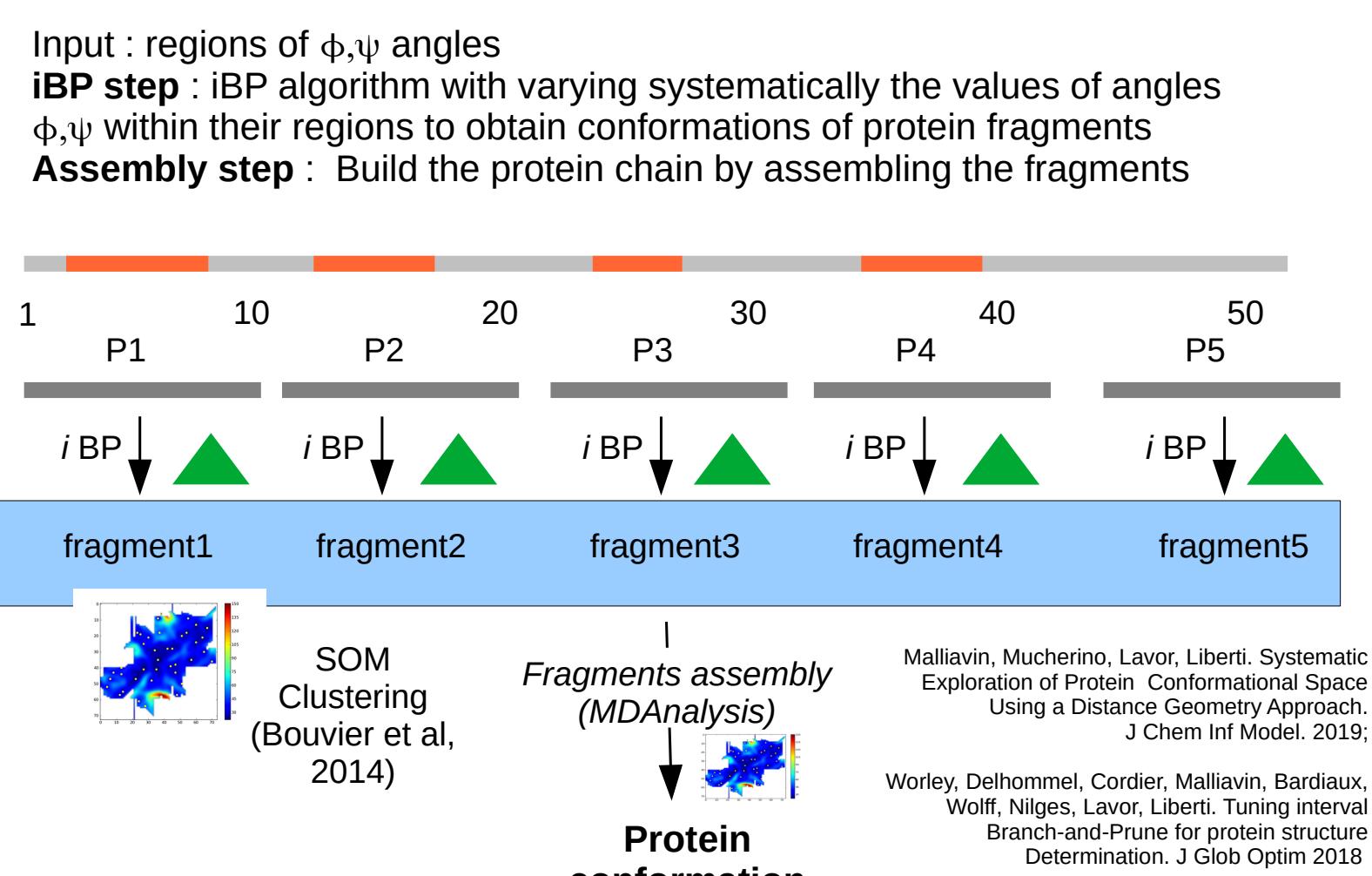
Experimental measurements

NMR spectra were recorded at 298K on Bruker Avance 800MHz equipped with cryoprobe, using samples of 0.5mM ^{13}C - ^{15}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.

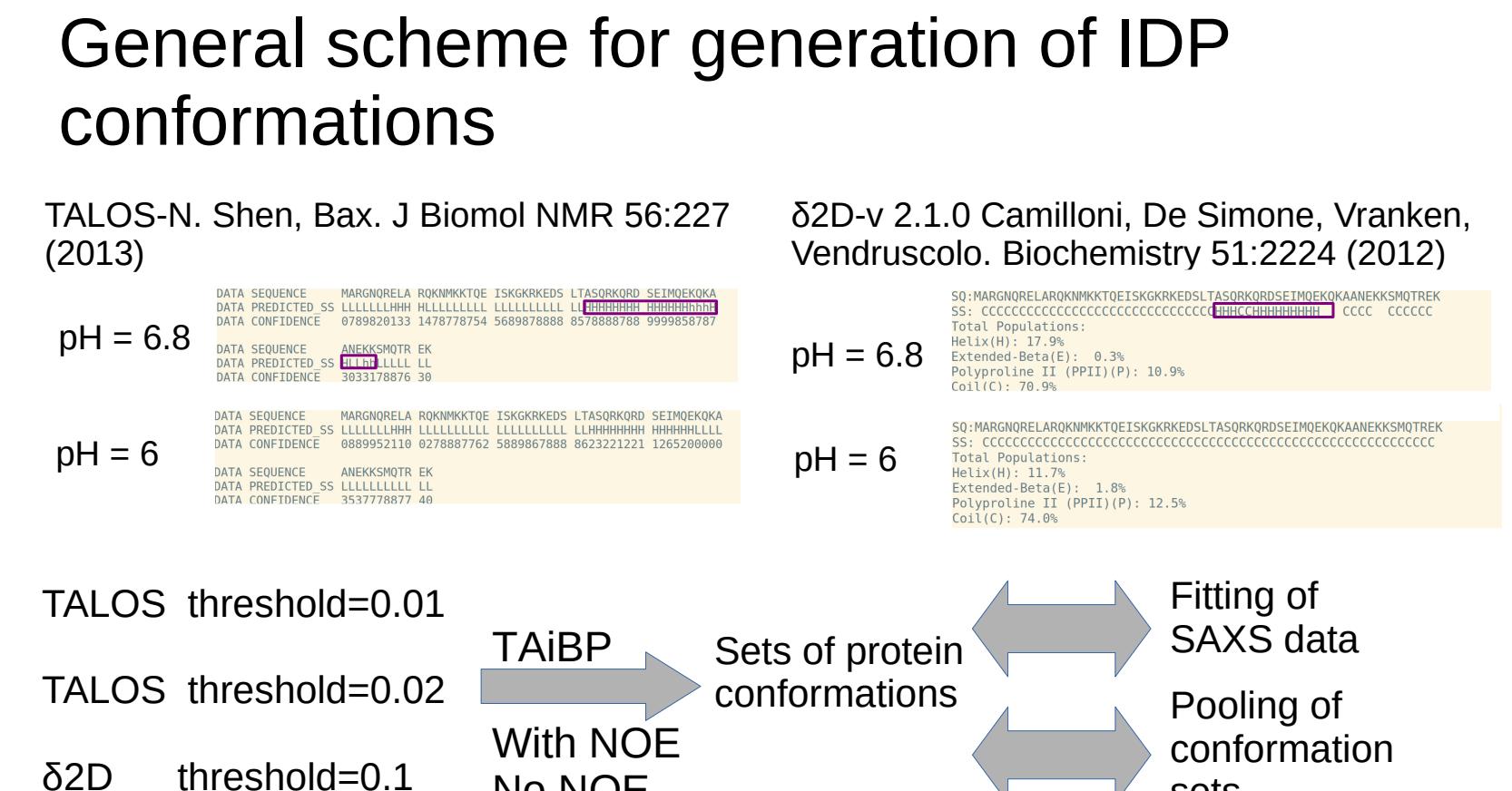
Function of SERF1a



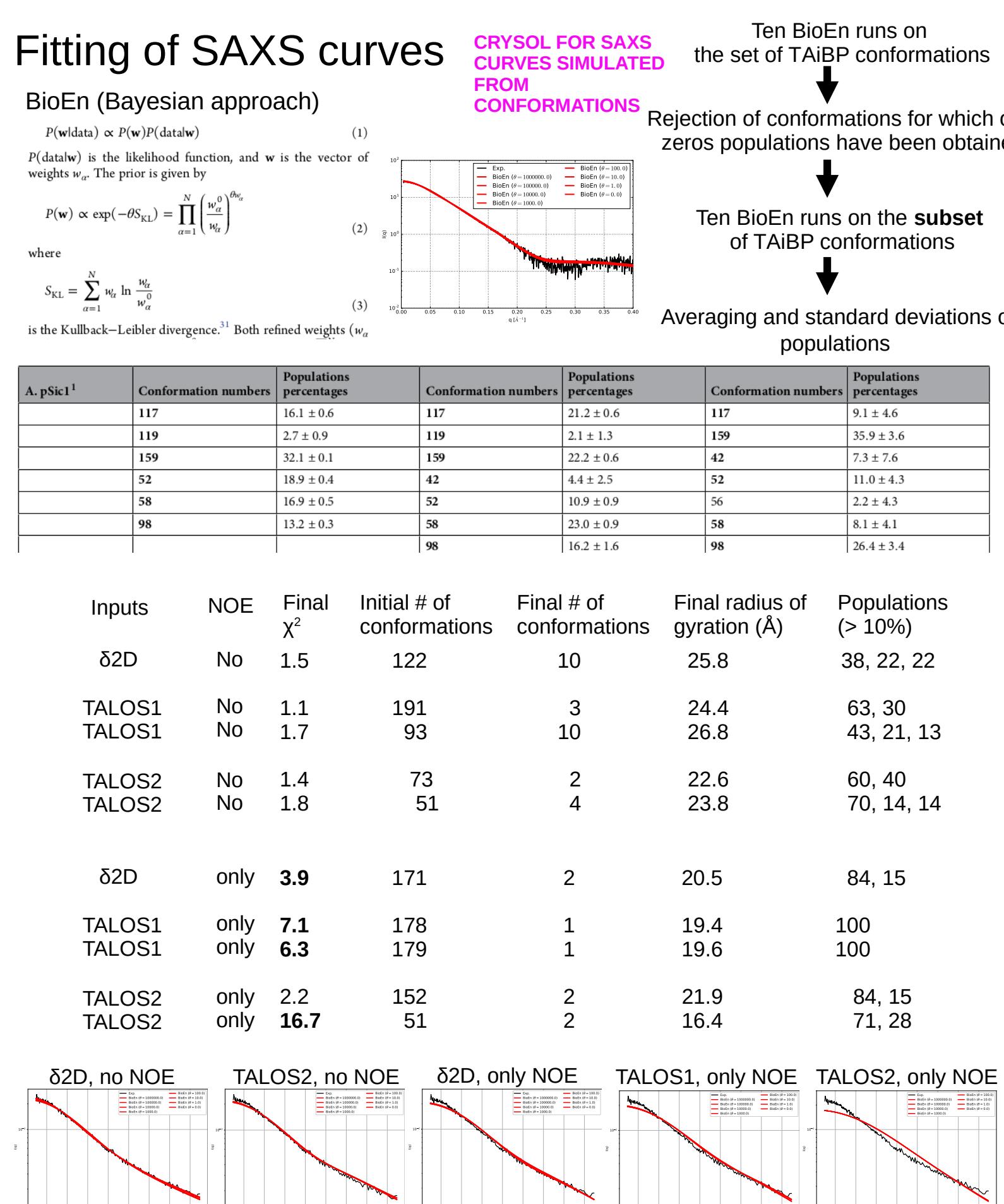
TAiBP approach



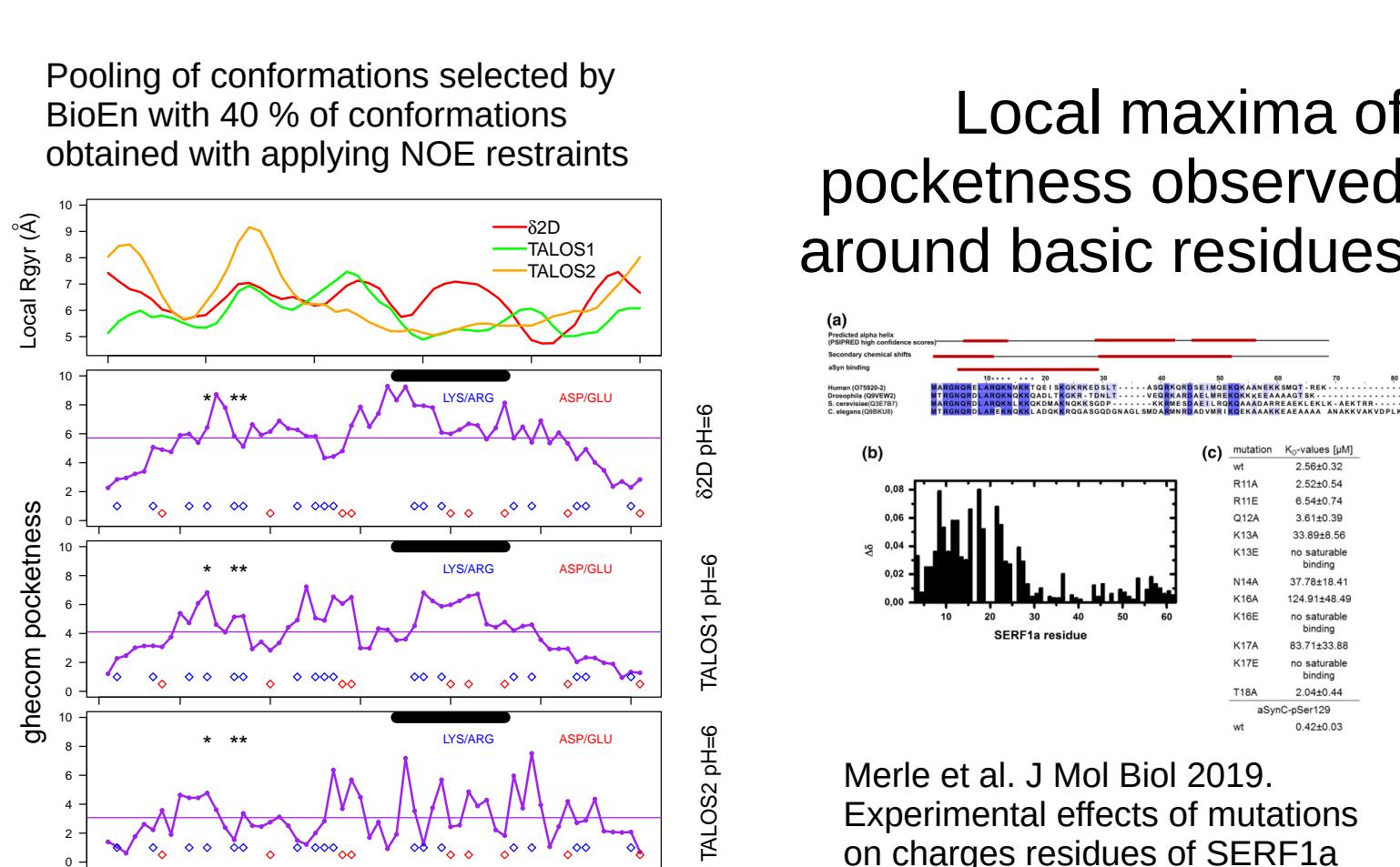
Procedure of calculation



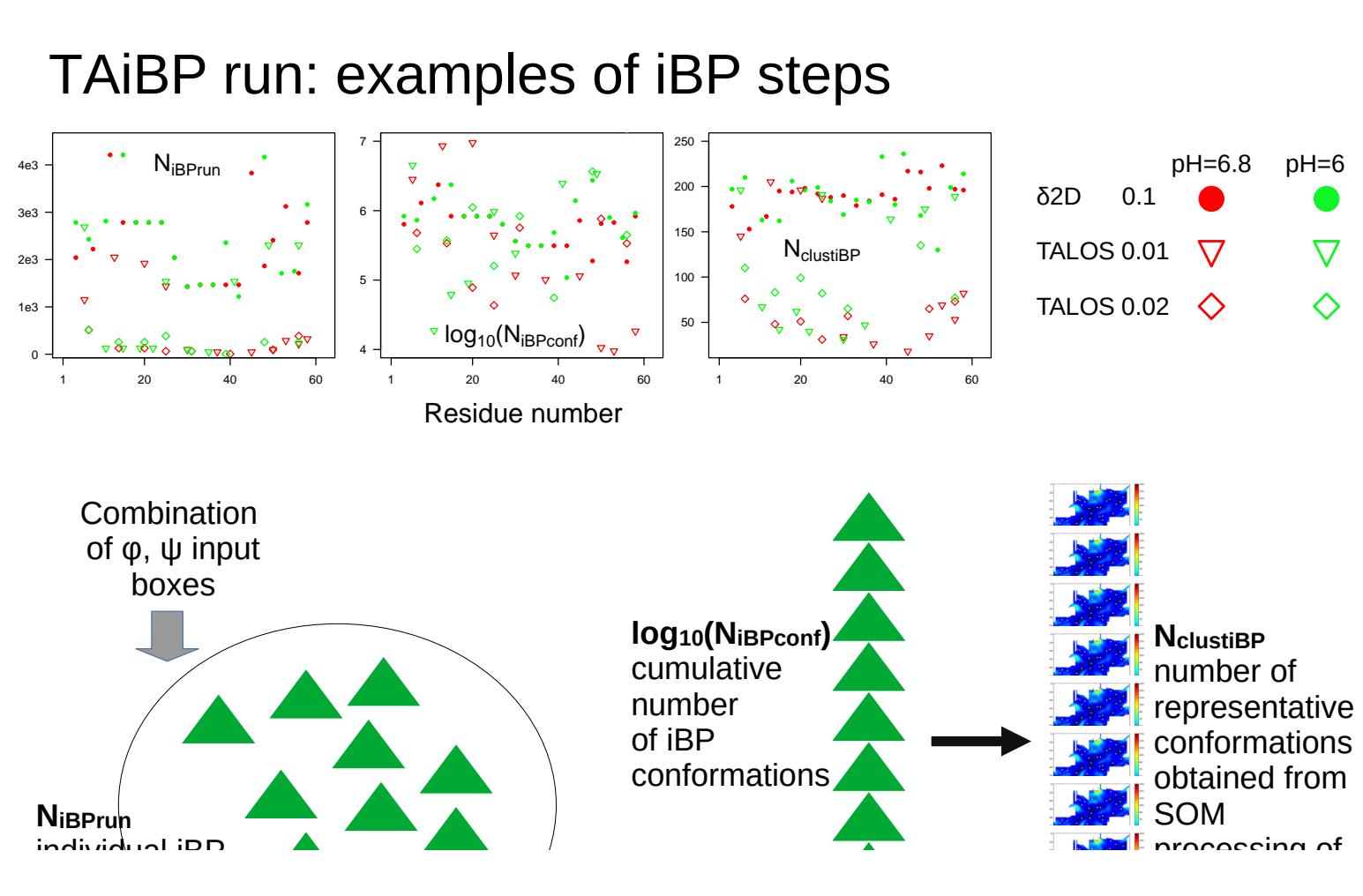
Fitting SAXS data



Pocket detection



Calculation examples



References

- [1] A. Pras et al. “The cellular modifier MOAG-4/SERF drives amyloid formation through charge complementation”. In: *EMBO J* 40 (2021), e107568.
 - [2] S. F. Falsone et al. “SERF protein is a direct modifier of amyloid fiber assembly”. In: *Cell Rep* 2 (2012), pp. 358–371.
 - [3] D. Förster et al. “Low-resolution description of the conformational space for intrinsically disordered proteins”. In: *Sci Rep* 12 (2022), p. 19057.
 - [4] T. E. Malliauin. “Tandem domain structure determination based on a systematic enumeration of conformations”. In: *Sci Rep* 11 (2021), p. 16925.
 - [5] T. E. Malliauin et al. “Systematic Exploration of Protein Conformational Space Using a Distance Geometry Approach”. In: *J Chem Inf Model* 59 (2019), pp. 4486–4503.
 - [6] Y. Shen and A. Bax. “Protein structural information derived from NMR chemical shift with the neural network program TALOS-N”. In: *Methods Mol Biol* 1260 (2015), pp. 17–32.
 - [7] C. Camilloni et al. “Determination of secondary structure populations in disordered states of proteins using nuclear magnetic resonance chemical shifts”. In: *Biochemistry* 51 (2012), pp. 2224–2231.
 - [8] D. I. Svergun, C. Barberato, and M.H.J. Koch. “CRYSTOL - a Program to Evaluate X-ray Solution Scattering of Biological Macromolecules from Atomic Coordinates”. In: *J. Appl. Cryst.* 28 (1995), pp. 768–773.
 - [9] J. Köfinger et al. “Efficient Ensemble Refinement by Reweighting”. In: *J Chem Theory Comput* 15 (2019), pp. 3390–3401.