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EXPLORATION OF THE CONFORMATIONAL SPACE OF SERF1A

Shu-Yu Huang(1), Chi-Fon Chang(2), Jung-Hsin Lin(1)
and Thérèse E Malliavin(3)

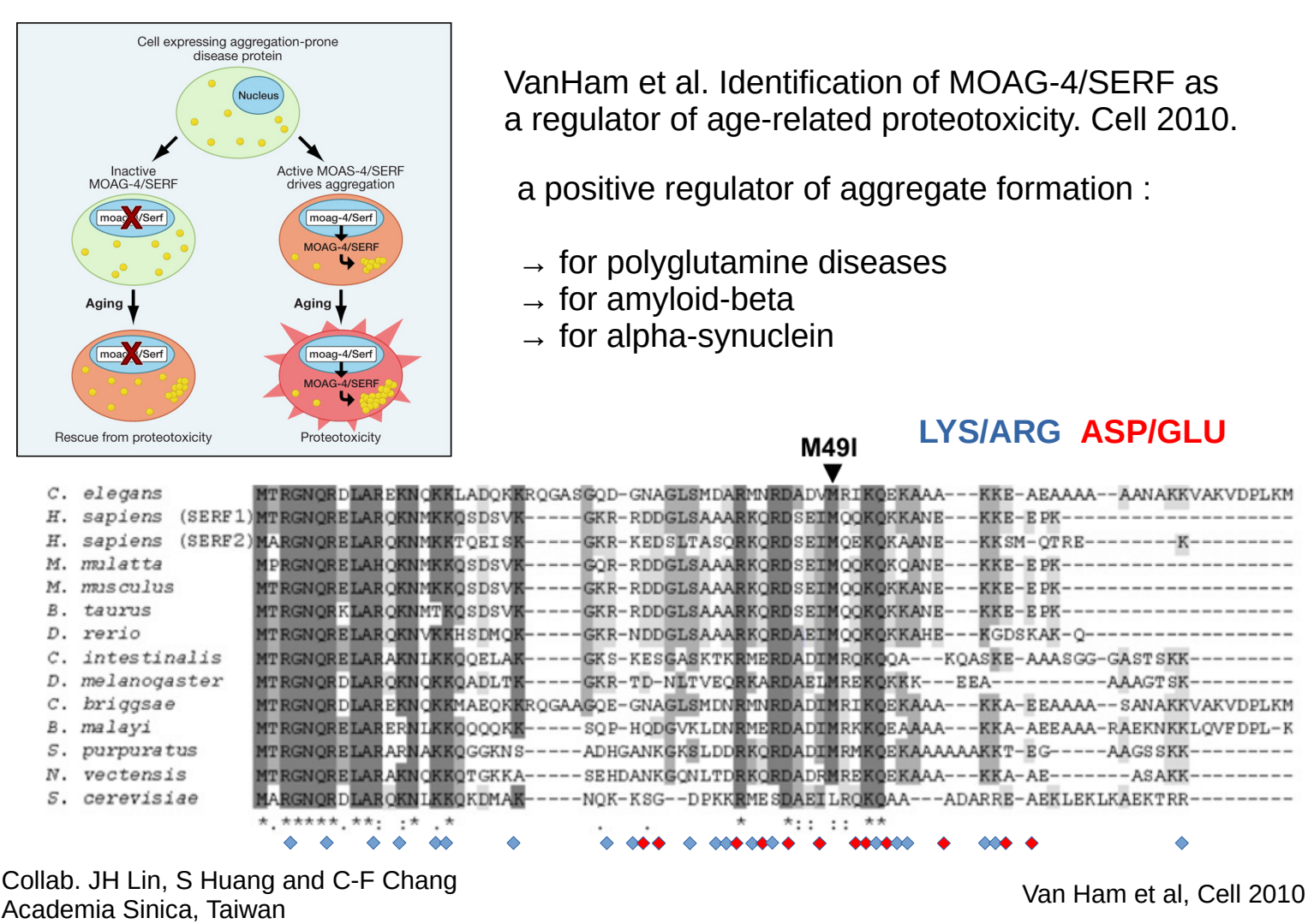
(1) Research Center for Applied Sciences, Academia Sinica, Taipei, Taiwan, (2) Genomics Research Center, Academia Sinica, Taipei, Taiwan, (3) Laboratoire de Physique et Chimie Théoriques (LPCT), University of Lorraine, Vandoeuvre-lès-Nancy, France
NMR for Life Science, October 10-12, 2023



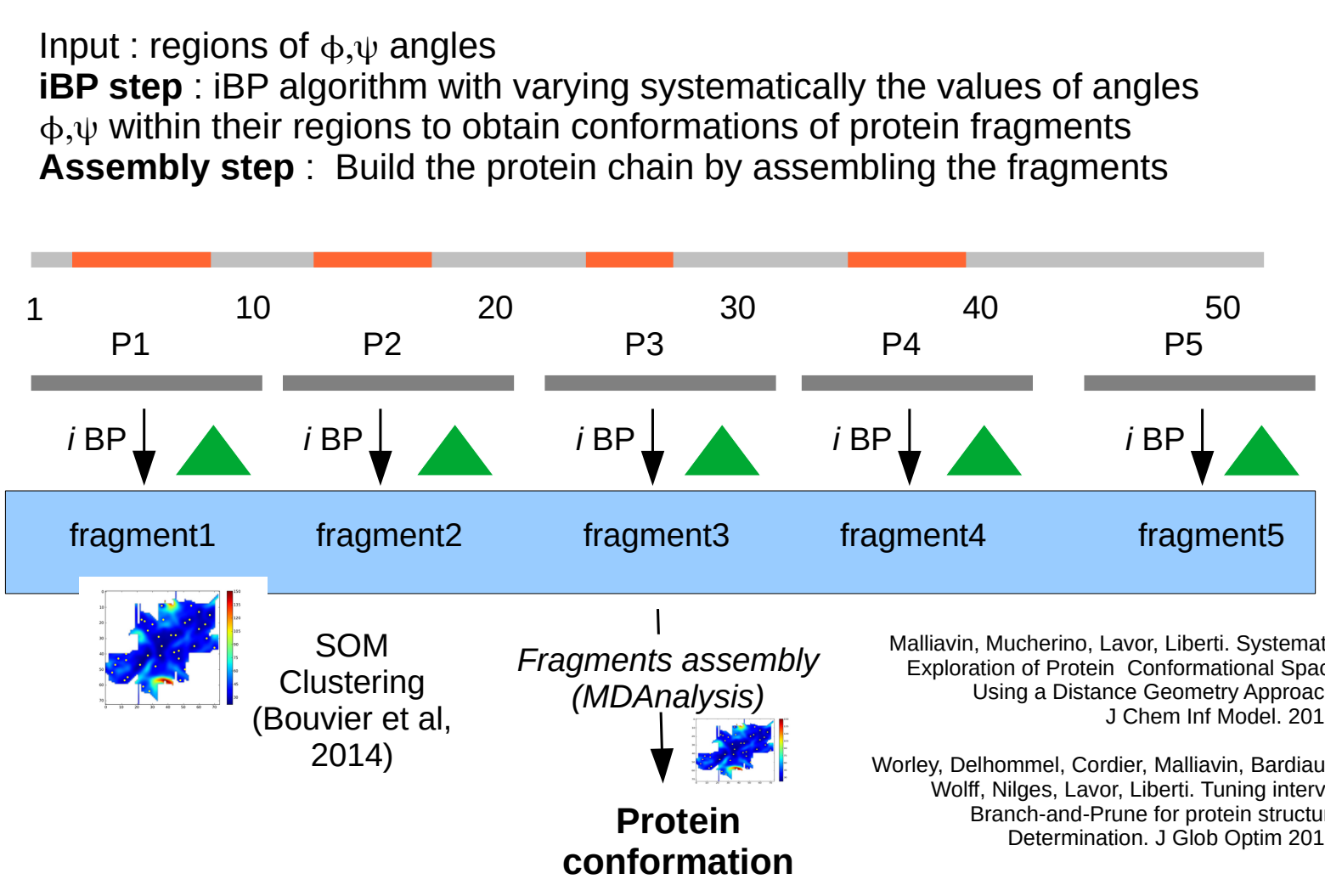
Experimental measurements

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

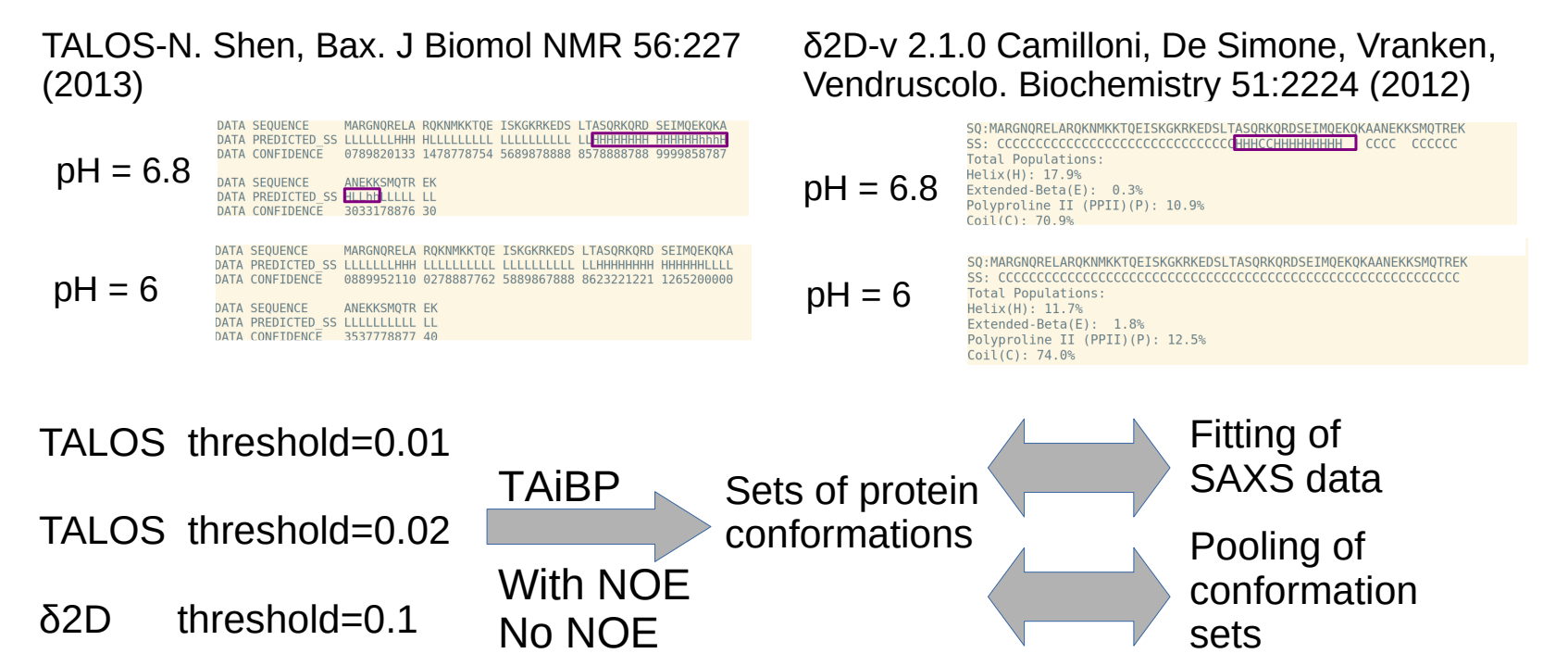


TAiBP approach

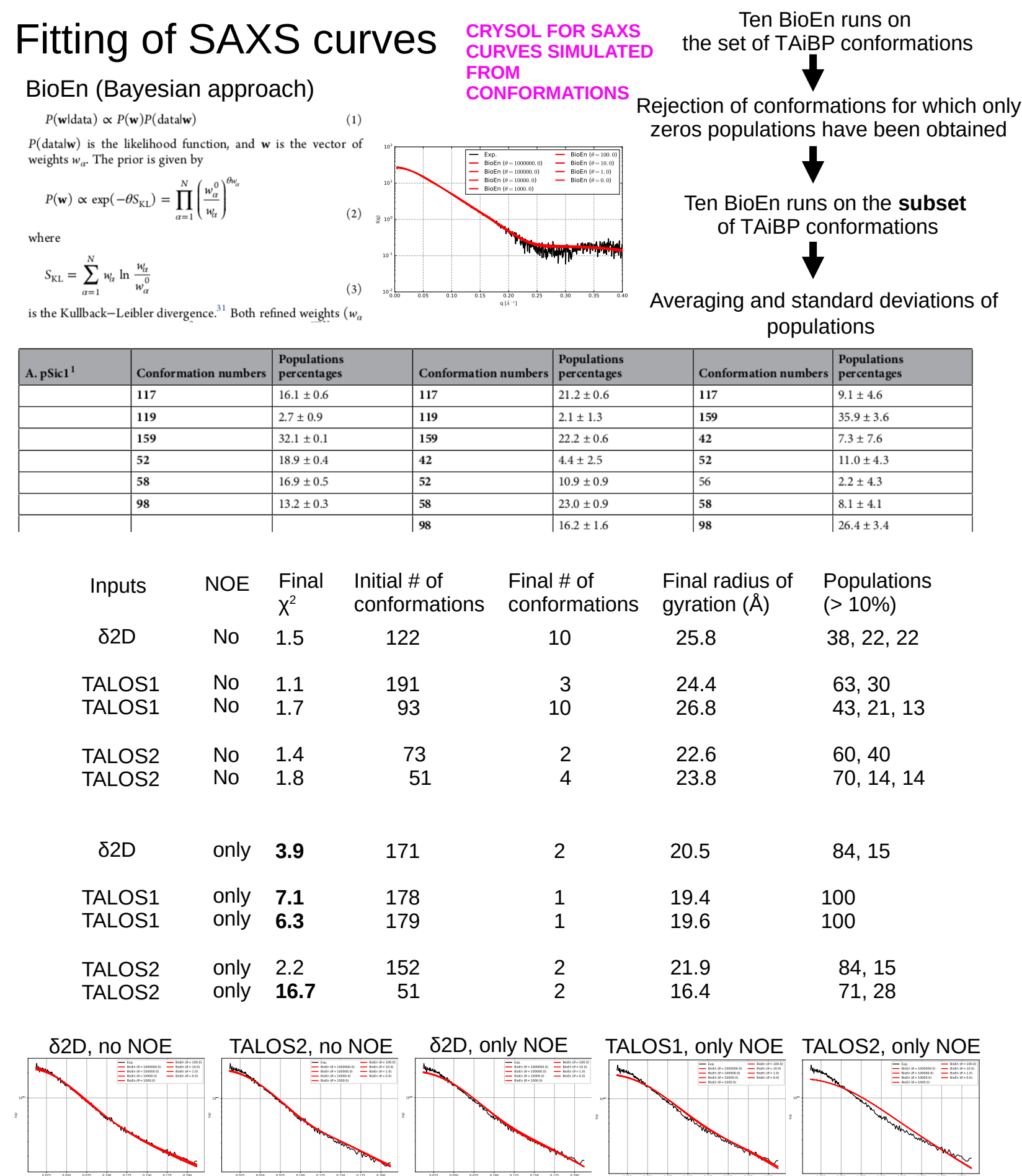


Procedure of calculation

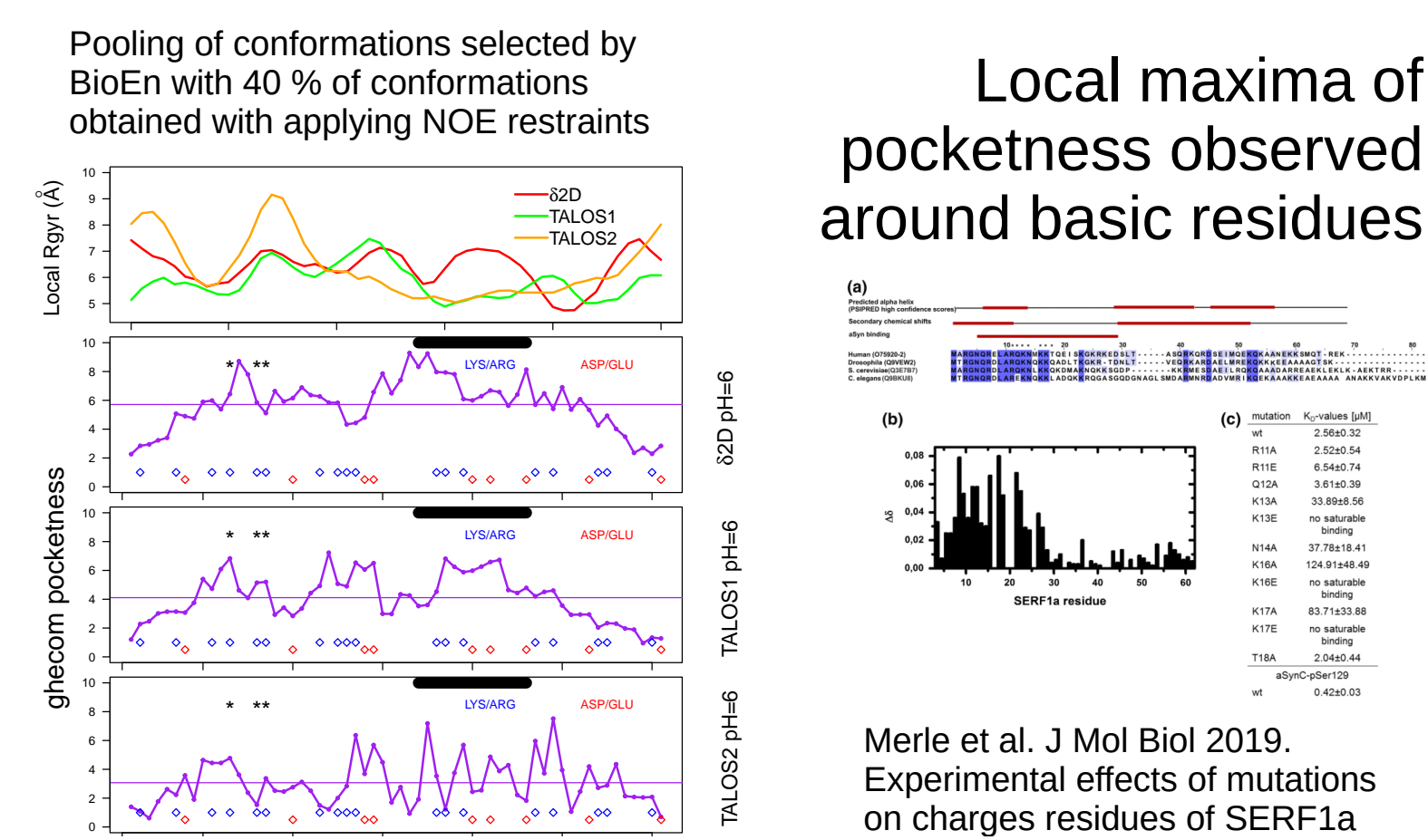
General scheme for generation of IDP conformations



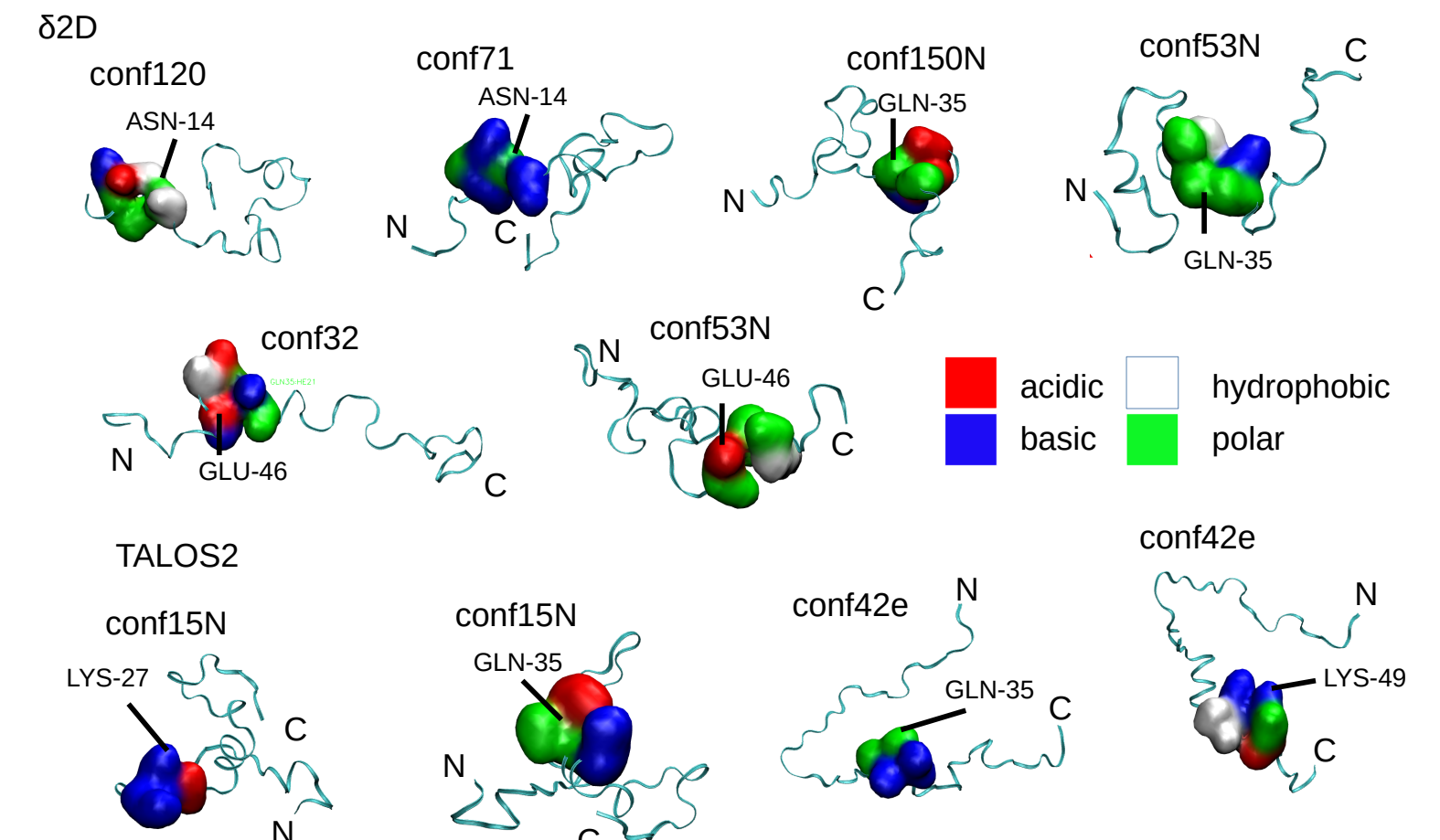
Fitting SAXS data



Pocket detection

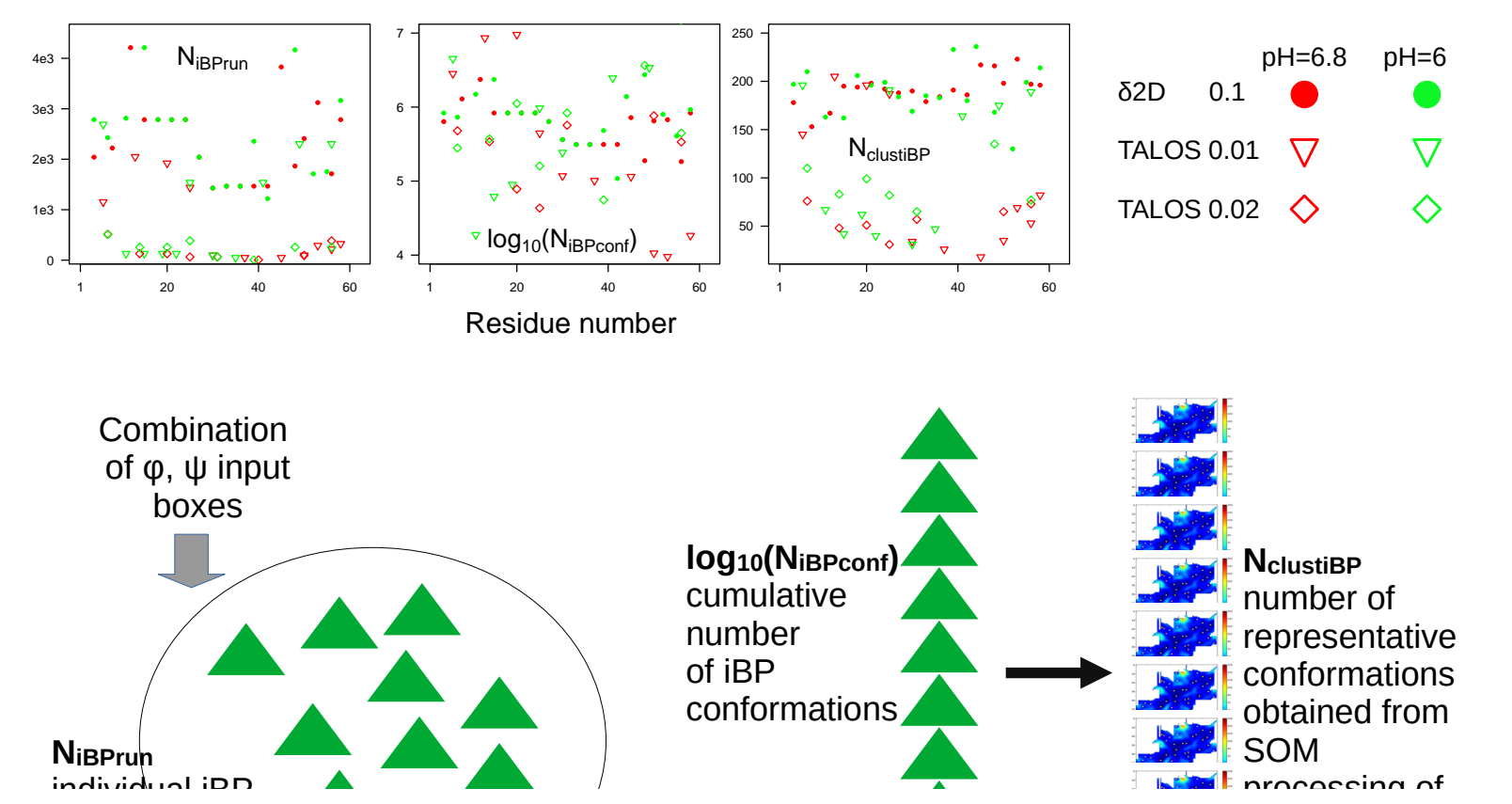


Examples of possible binding pockets sampled in conformations of SERF1a

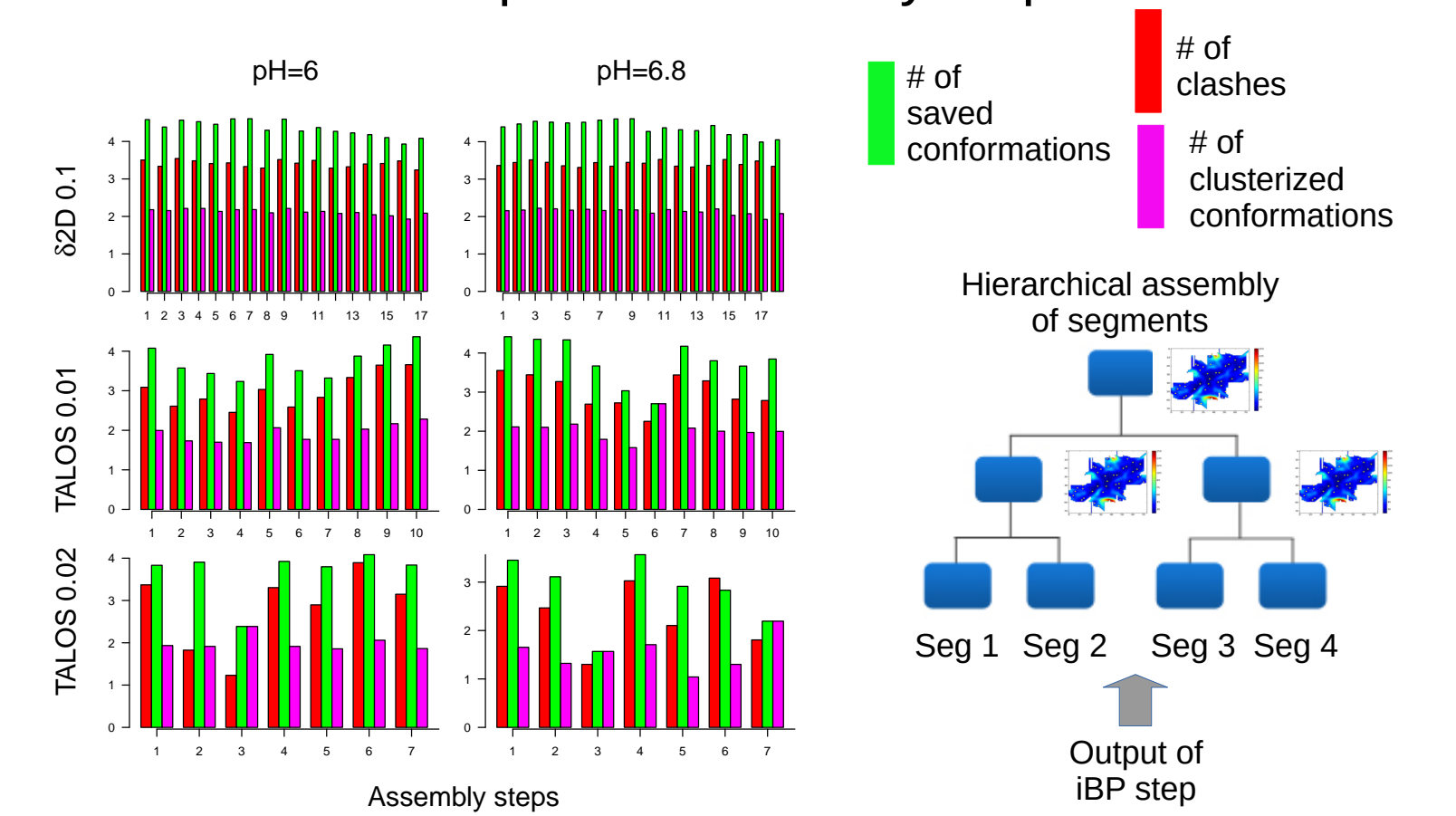


Calculation examples

TAiBP run: examples of iBP steps



TAiBP run: examples of assembly steps



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