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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)

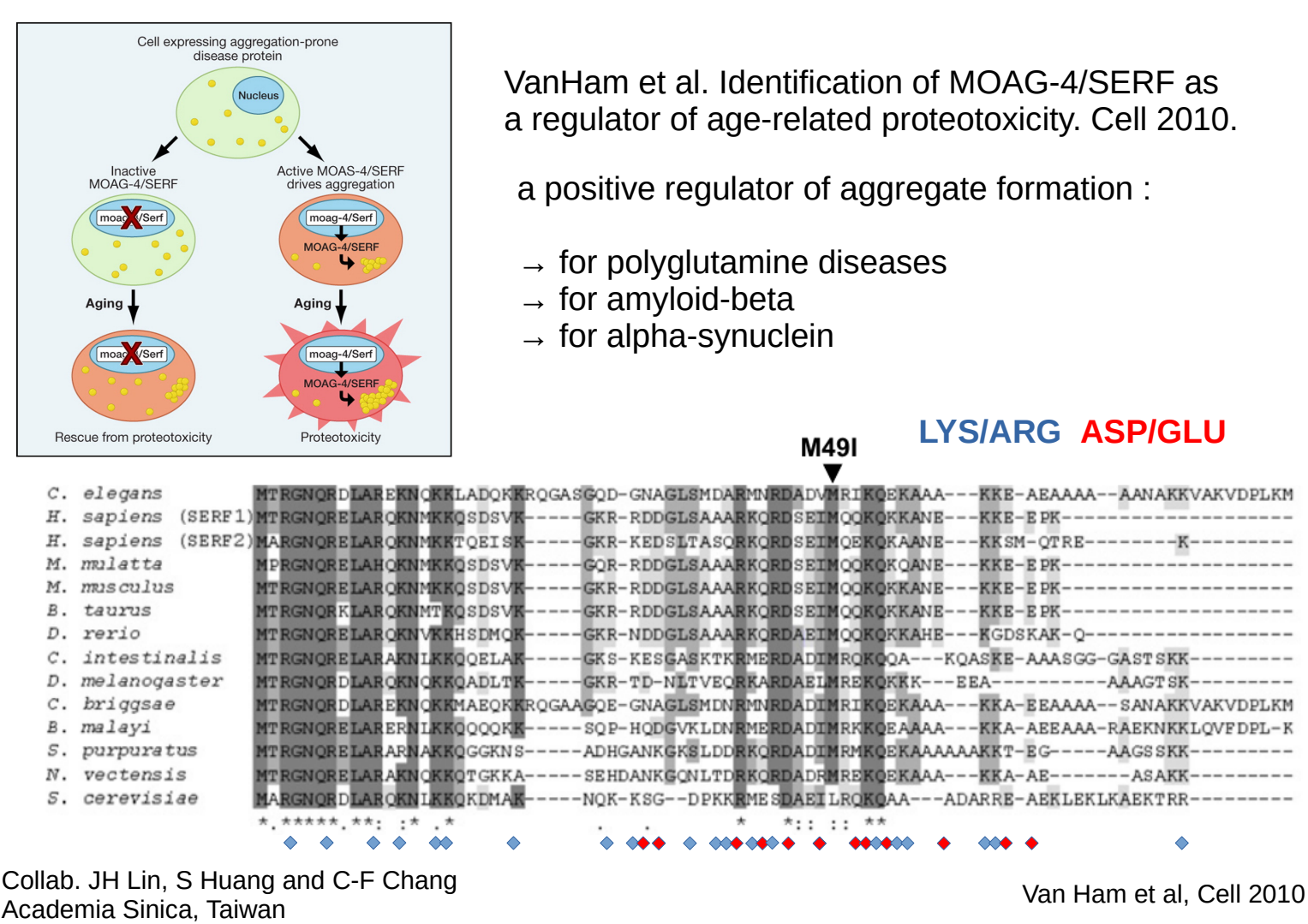
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NMR for Life Science, October 10-12, 2023



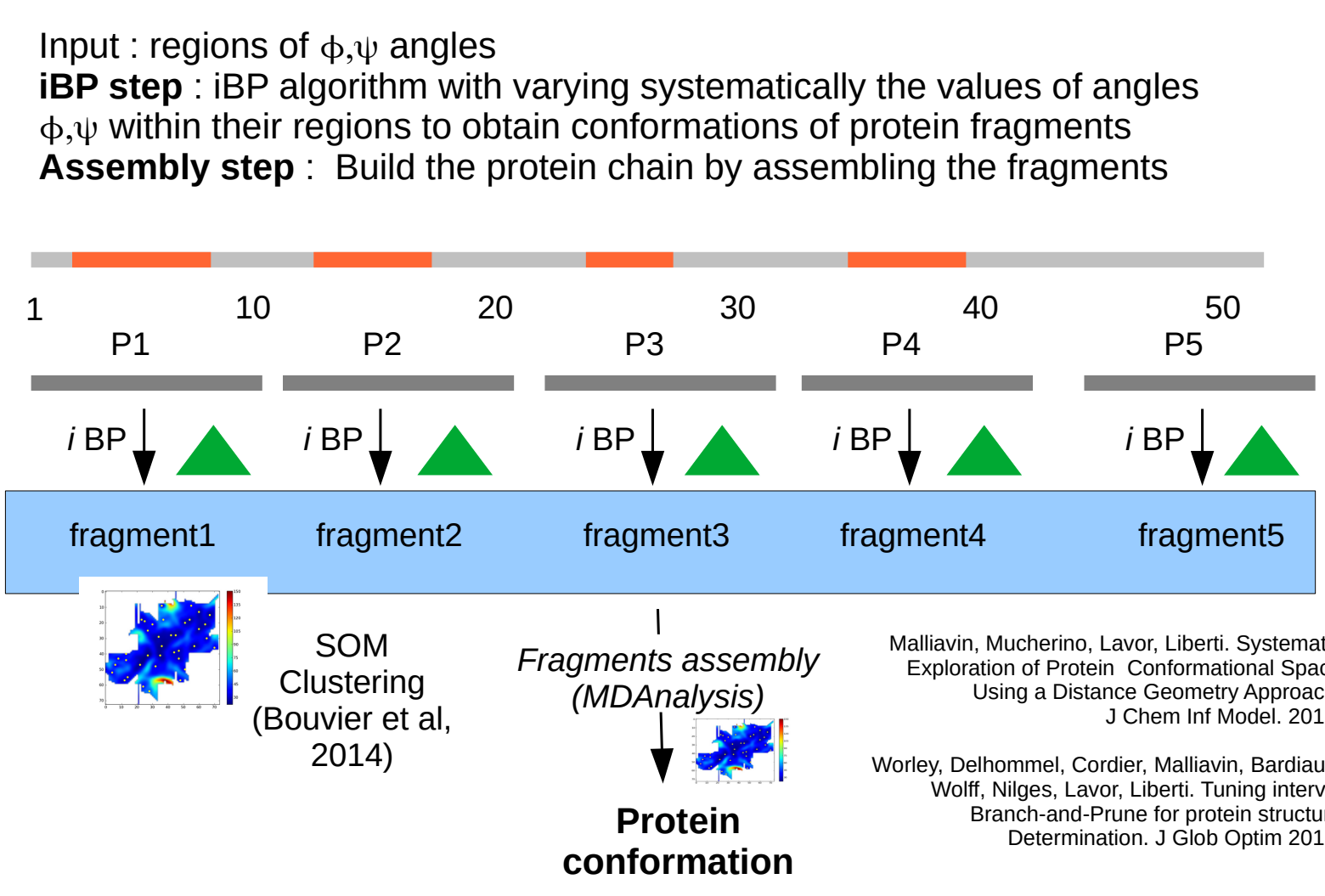
## Experimental measurements

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

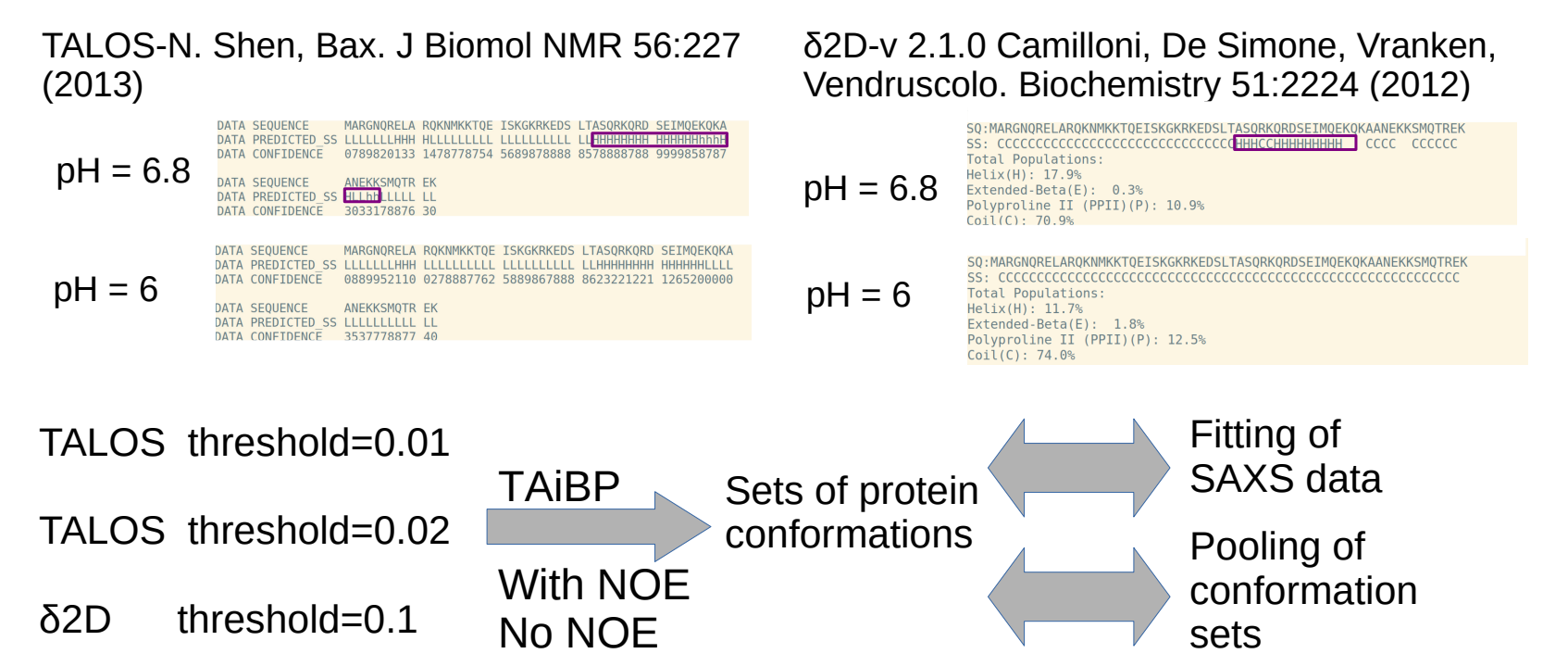


### TAiBP approach

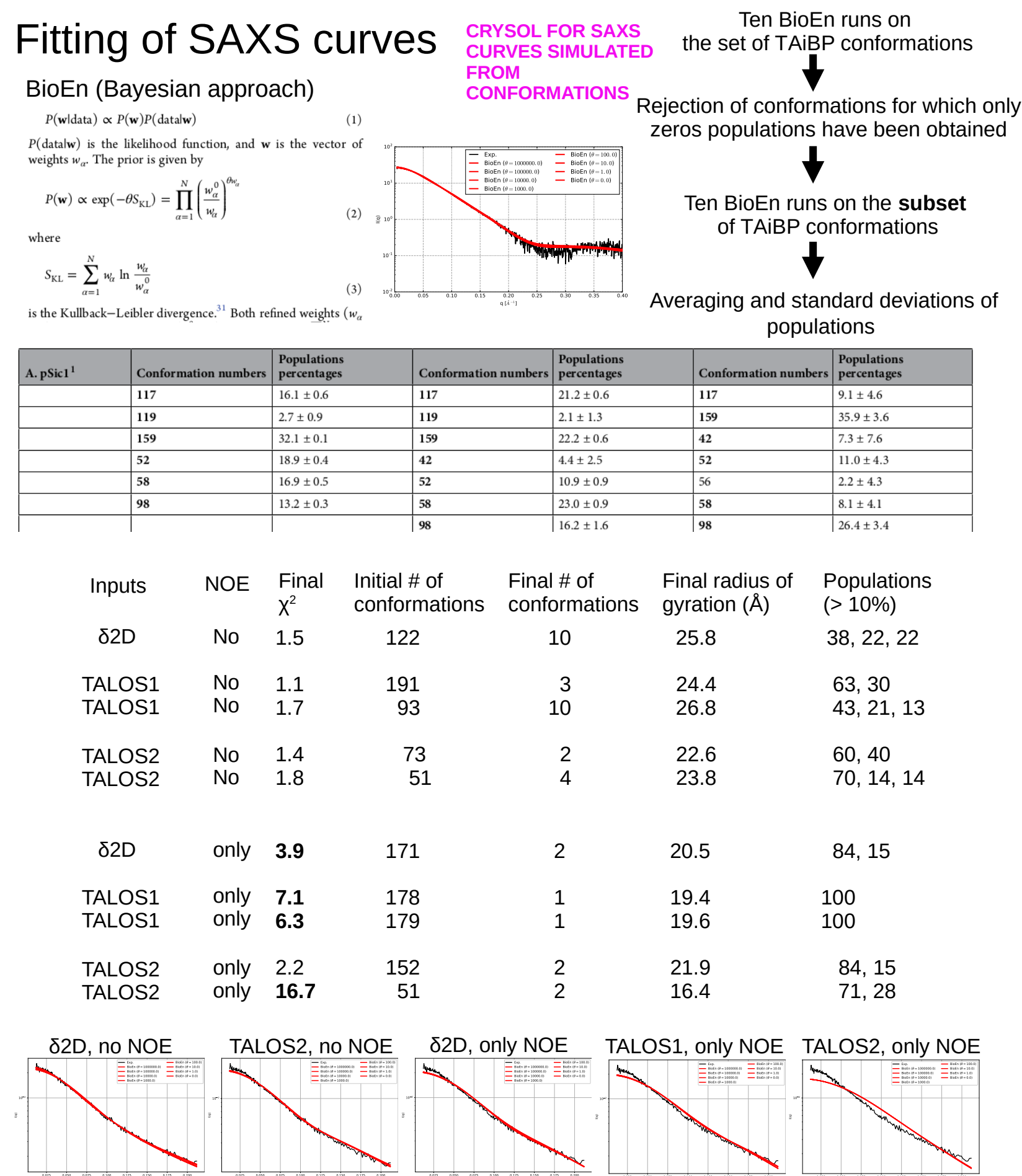


### Procedure of calculation

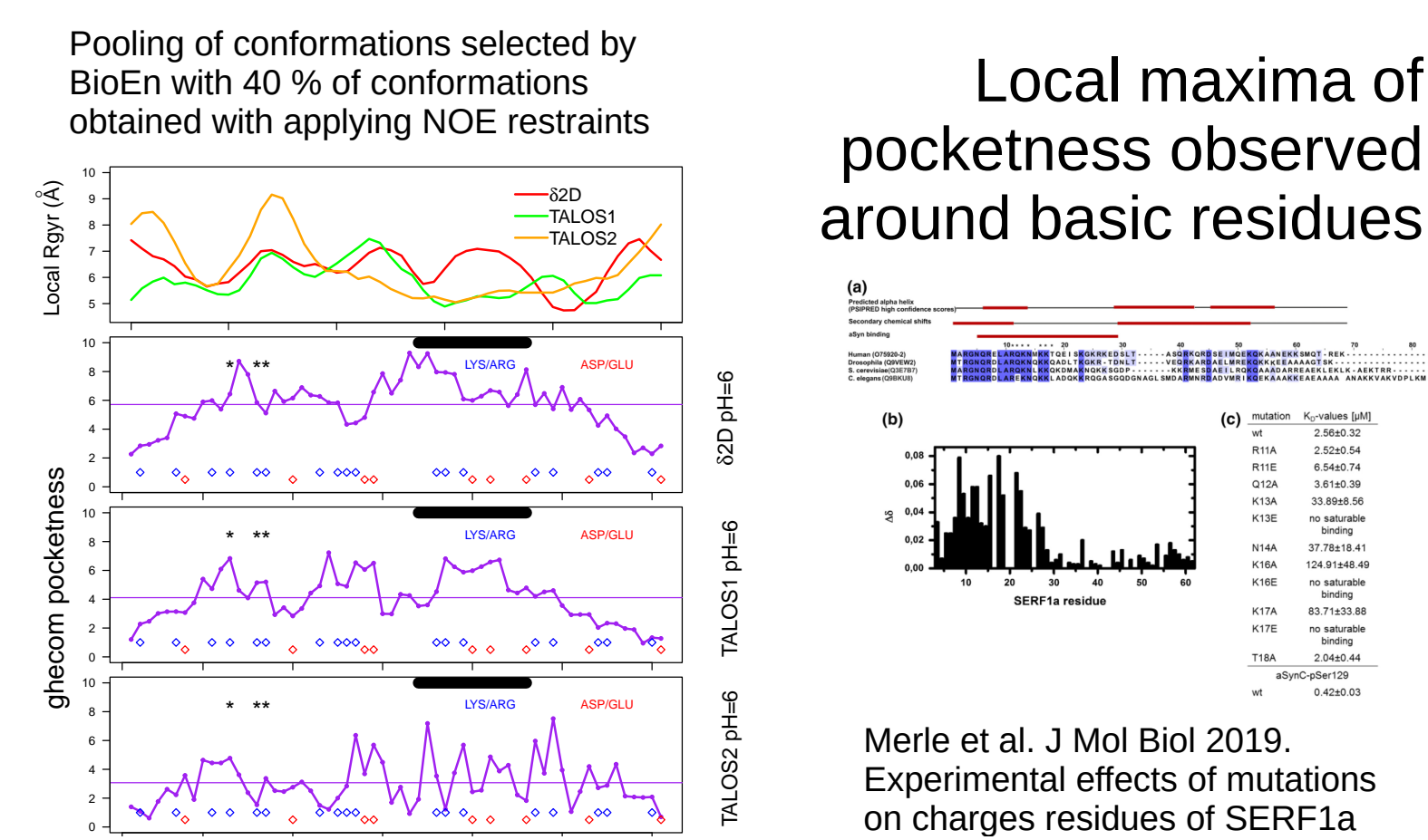
#### General scheme for generation of IDP conformations



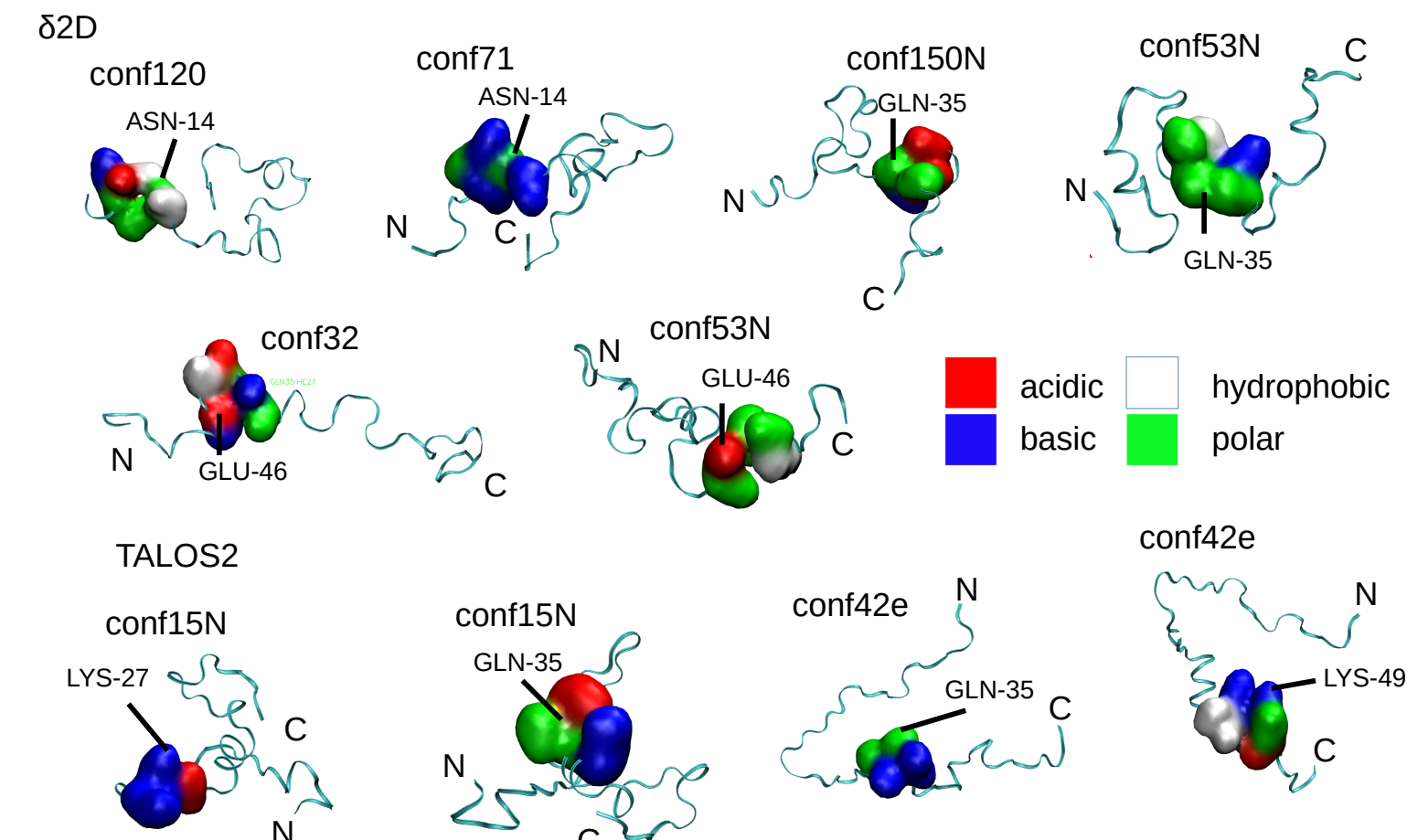
### Fitting SAXS data



### Pocket detection

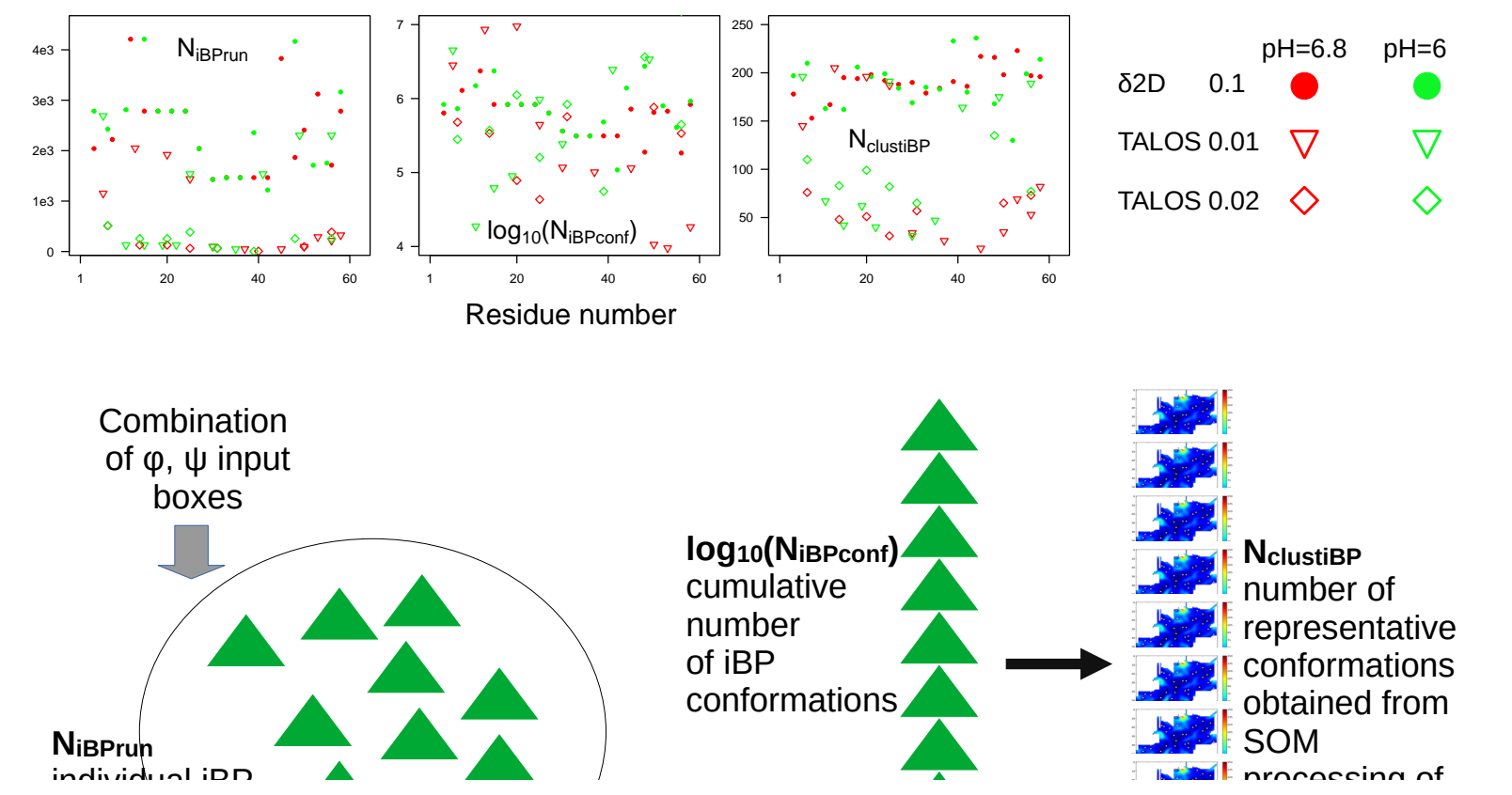


#### Examples of possible binding pockets sampled in conformations of SERF1a

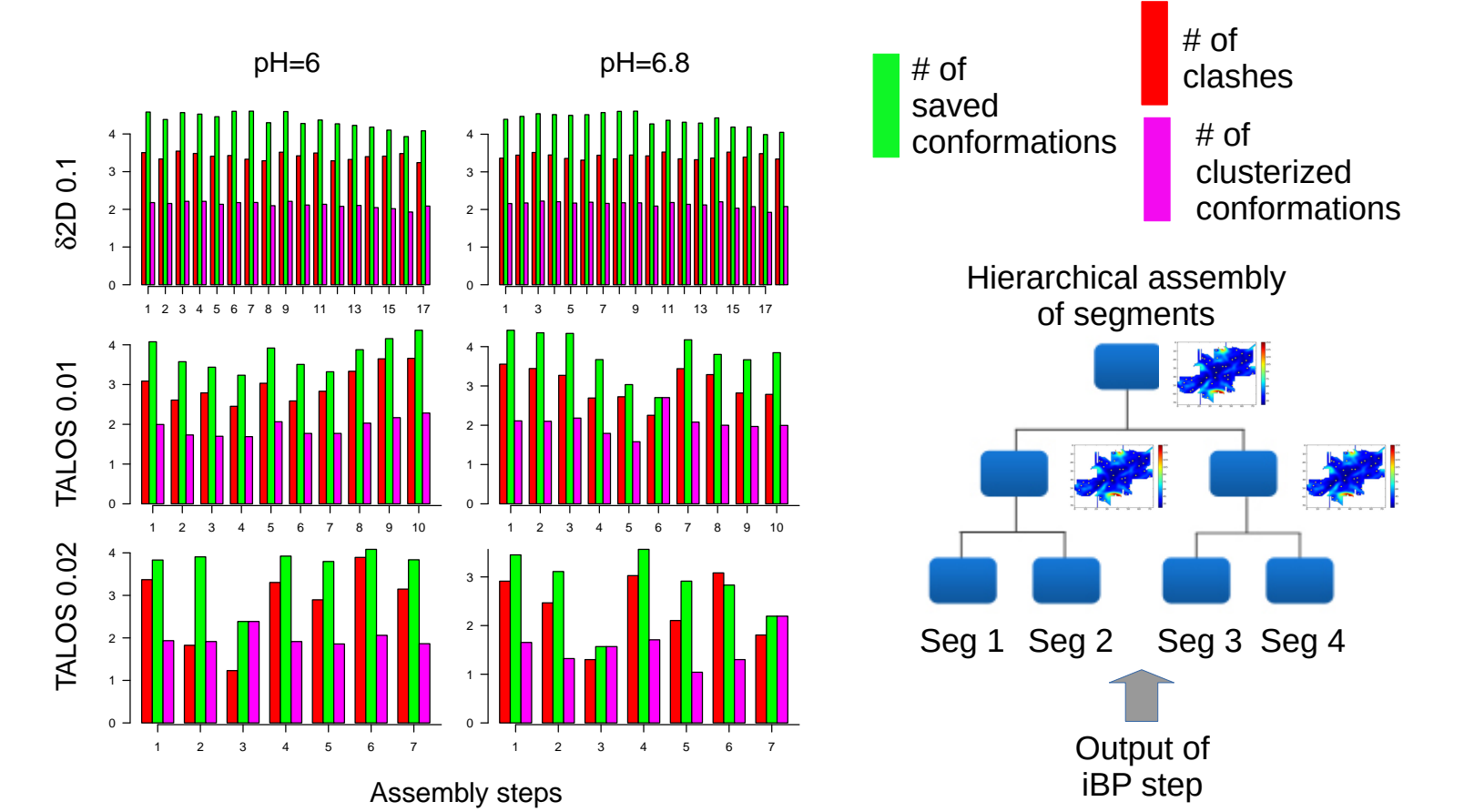


### Calculation examples

#### TAiBP run: examples of iBP steps



#### TAiBP run: examples of assembly steps



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