

Article

Supplementary materials to: Application of recurrence plot analysis to examine dynamics of biological molecules on the example of aggregation of seed mucilage components.

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In the supplementary materials, we present additional results from computer experiments, specifically focusing on the number of intermolecular interactions (Figures 1 and 2) and recurrence plots (Figure 3) from the second experiment iteration of aggregation process in the model mucus. These data are akin to those shown in Figure 5 of the main body of the article but are derived from a distinct series of simulations initiated with a different seed for the random number generator.

Referring to Figure 3, we can observe similar locations of crosses detected for the case of HBo than in the other series of data discussed in the main body of the article. This is the argument for the robustness of the method. For PW HBo and HP cases, we observe random locations of crosses, which coincides again with the data series analyzed in the main body of the article. Finally, as for the case of HP, fewer white regions are observed than in the main body of the article. However in analyses here series, we observe (especially for 310K) many randomly located crosses, what is the other (than white regions observed in the main body of the article) evidence of oscillations. (White regions separated by dark regions are the full evidence of oscillations).

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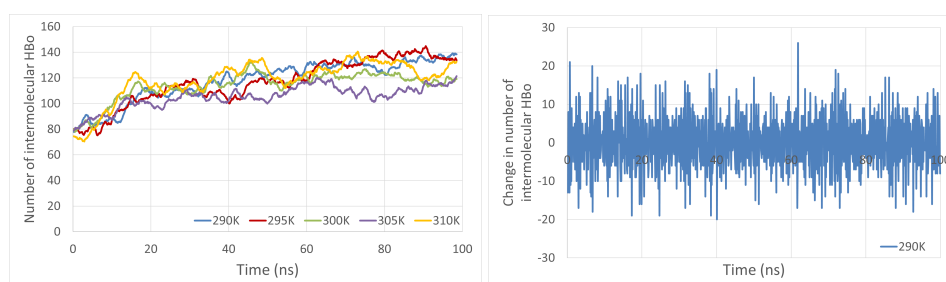


Figure 1. Number of all intermolecular HBo as a function of simulation time in five temperatures (a). Example of analyzed time series (b). The time series consists of increments in the number of intermolecular HBo at temperature 290K (computed from the blue line from picture (a)).

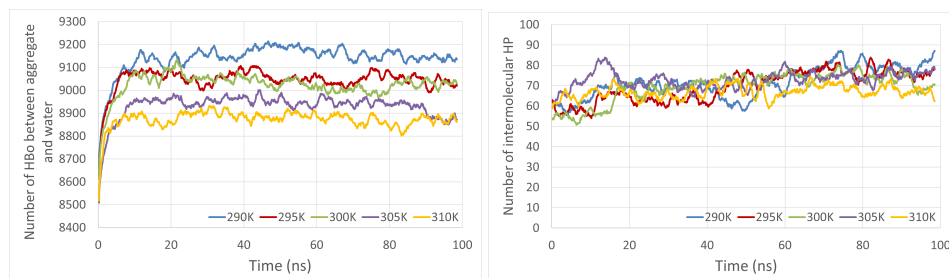


Figure 2. Number of all HBo between model polysaccharides and water molecules (PW HBo) as a function of simulation time in five temperatures (a). Number of all intermolecular HP interactions as a function of simulation time in five temperatures (b).

Recurrence Plots, seed 2

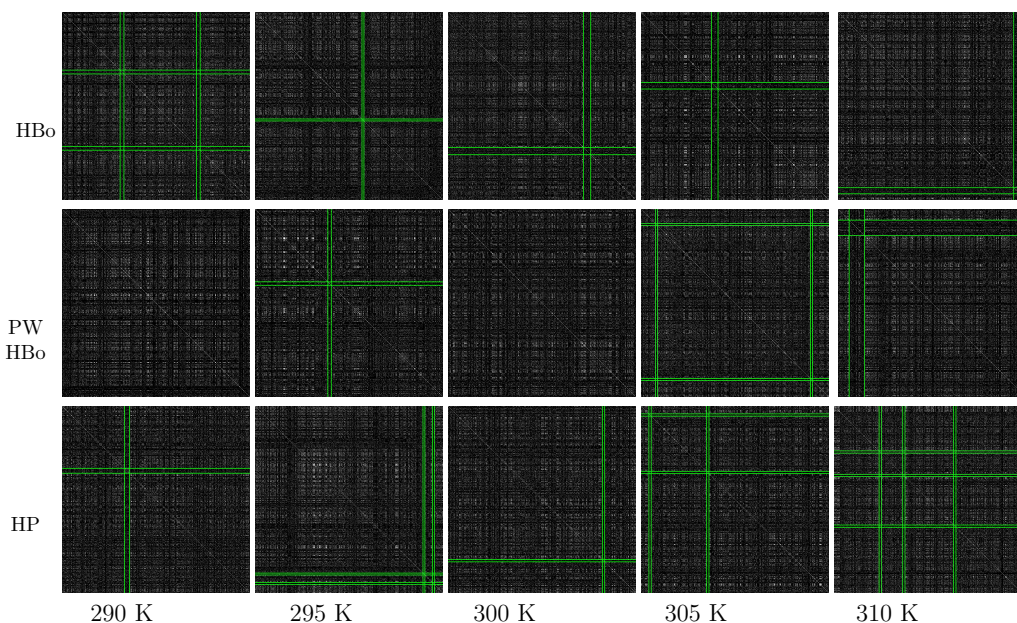


Figure 3. Recurrence plots for data with other initial seed, cross detection: intermolecular HBo (upper panel), PW HBo (middle panel), and intermolecular HP (lower panel). Temperatures from left (290K, 295K, 300K, 305K, 310K). By majority voting among the whole data set, we used constant $\tau = 2$ and $d = 1$ and $RR = 9\%$. The cross was detected with the threshold standard score equal to 2.5σ (standard deviations).