

## Supporting Information

**Molecular simulation and experimental study of the oligopeptide-mediated fouling mechanisms of polyamide reverse-osmosis membranes**

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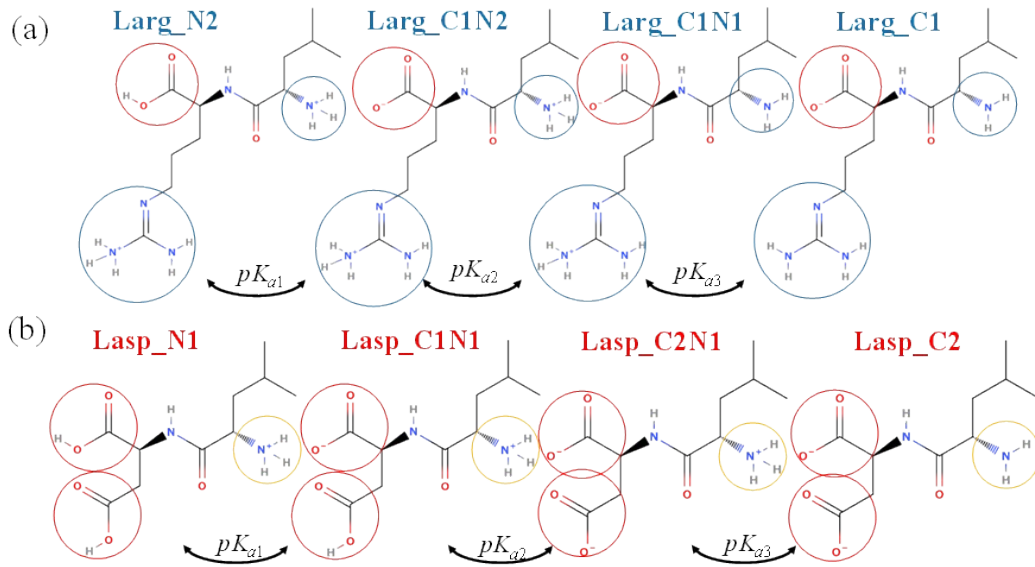
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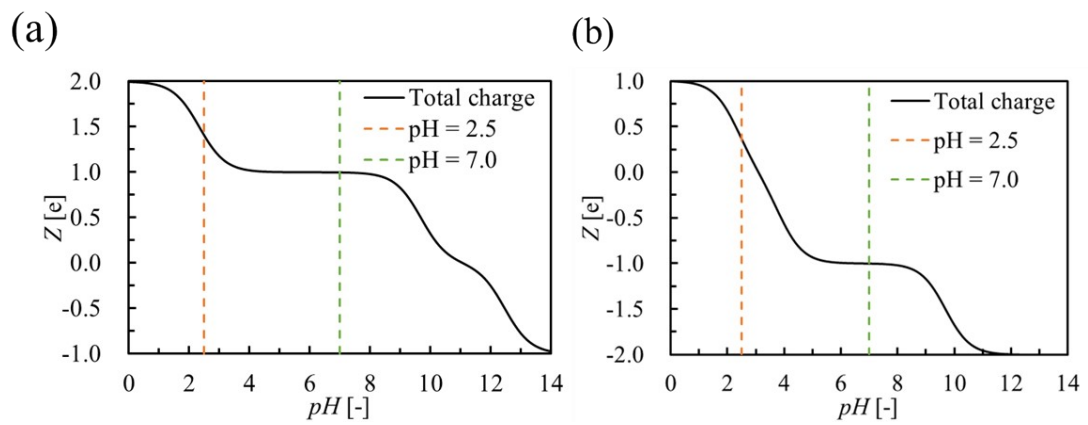
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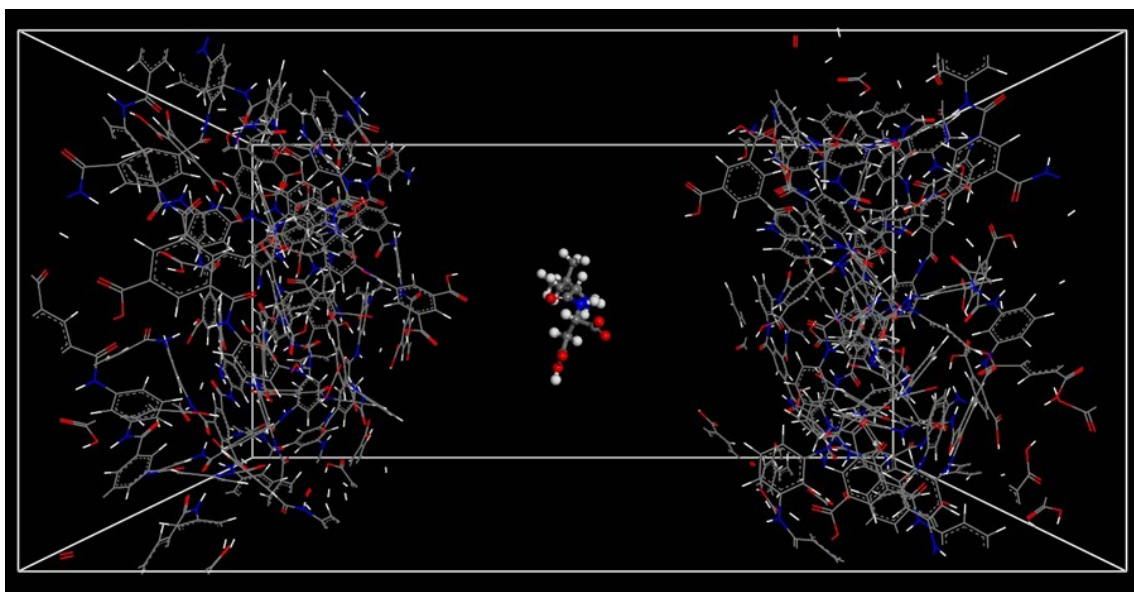
## 1. Simulation model



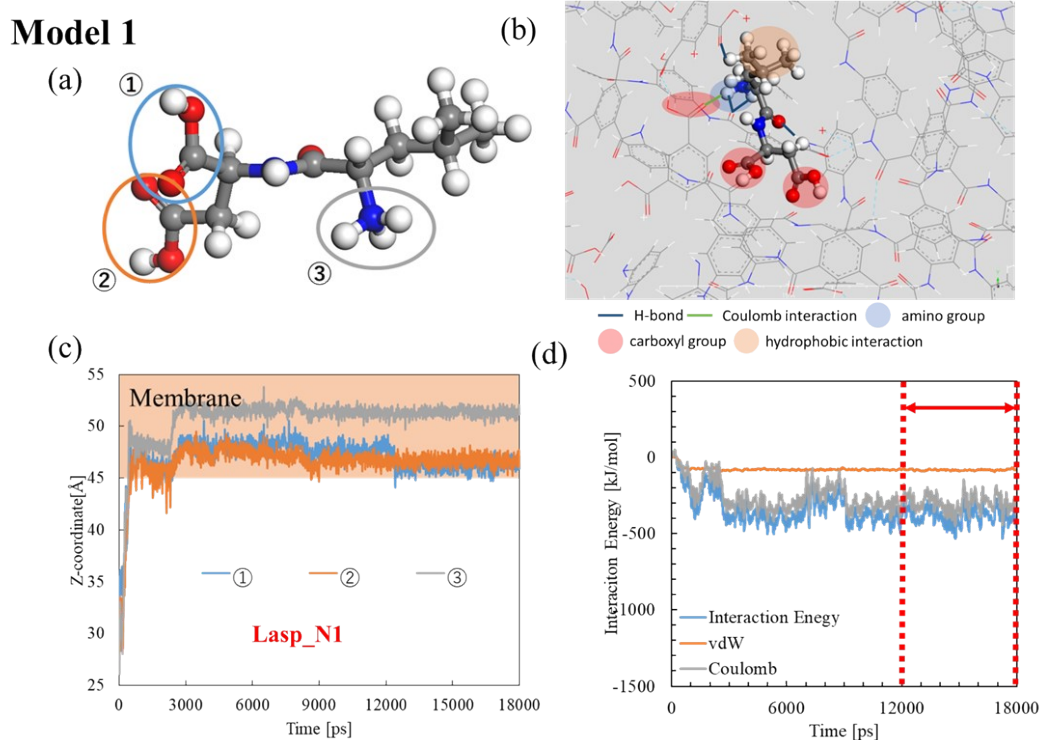
**Figure S1.** Foulant dissociation changes: (a) Larg and (b) Lasp.



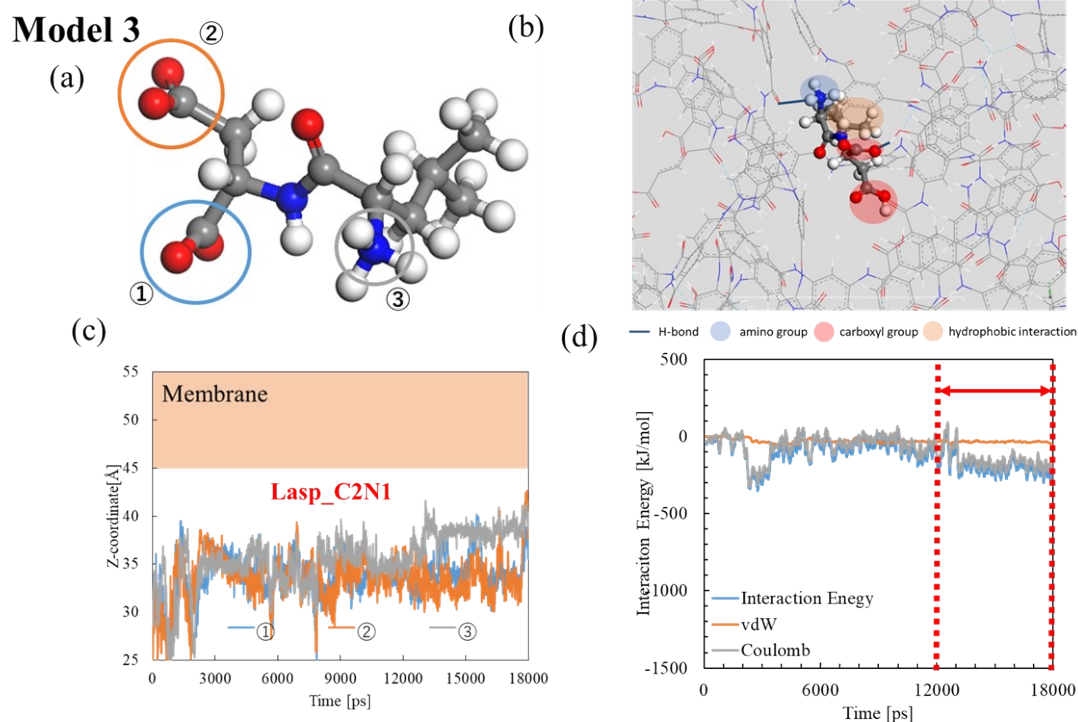
**Figure S2.** Net charges of the foulants according to pH : (a) Larg and (b) Lasp.



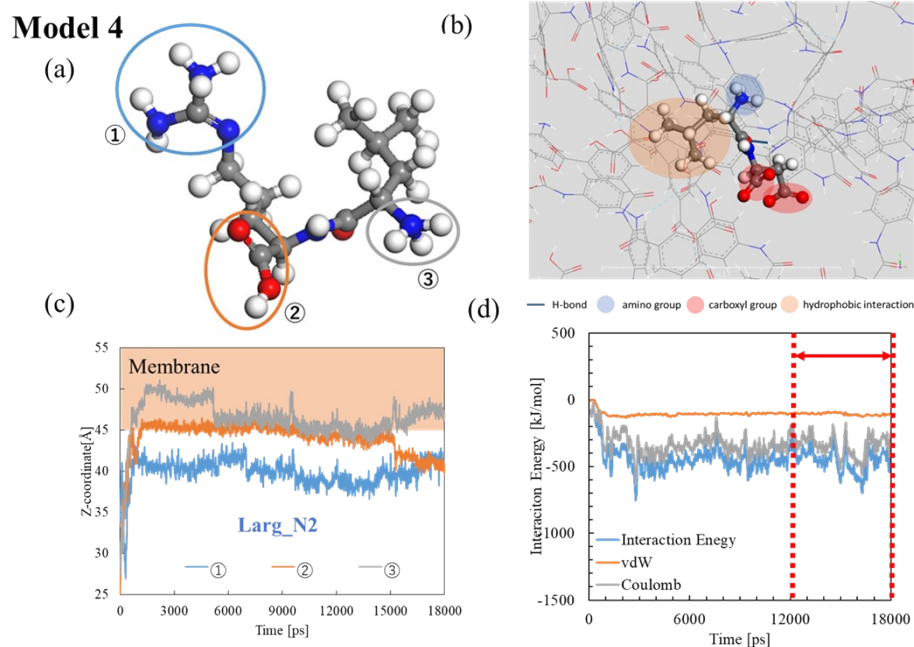
**Figure S3.** Behavior of the adsorption simulation of Model 2 (Lasp\_C1N1/C0).



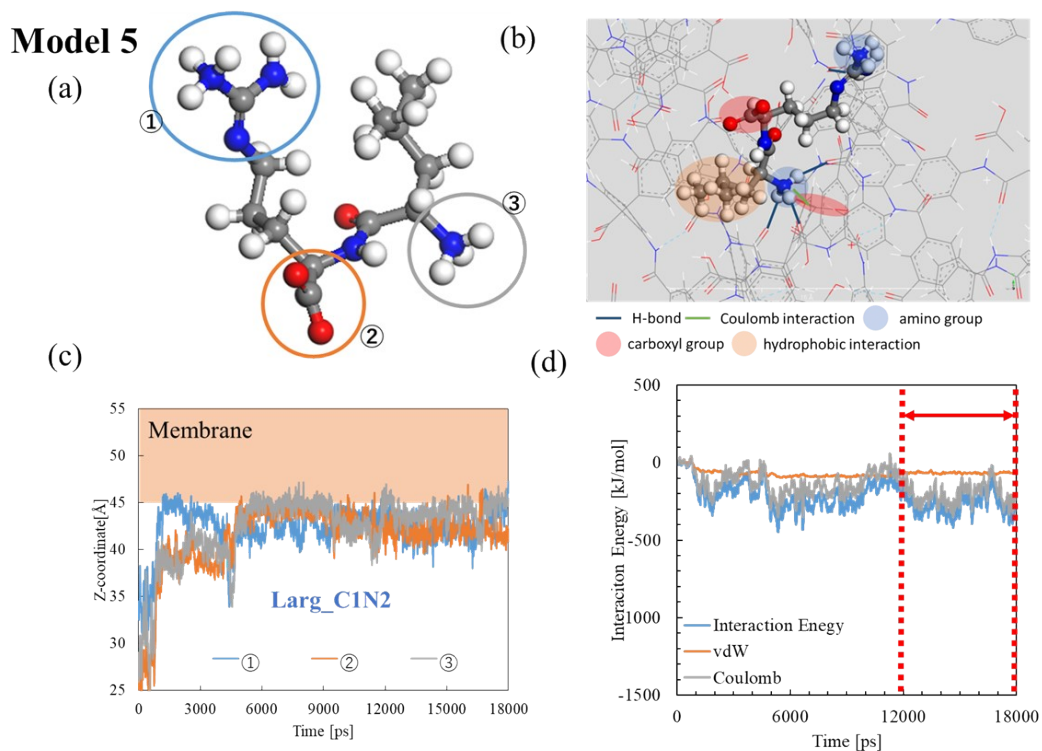
**Figure S4.** Model 1: (a) Lasp\_N1 foulant model, (b) Snapshot of the foulant in the neighbourhood of PA membrane, (c) Z-coordinate change of the foulant along with time, and (d) Interaction energy between the PA membrane and the foulant. The dashed range was used to calculate the average value.



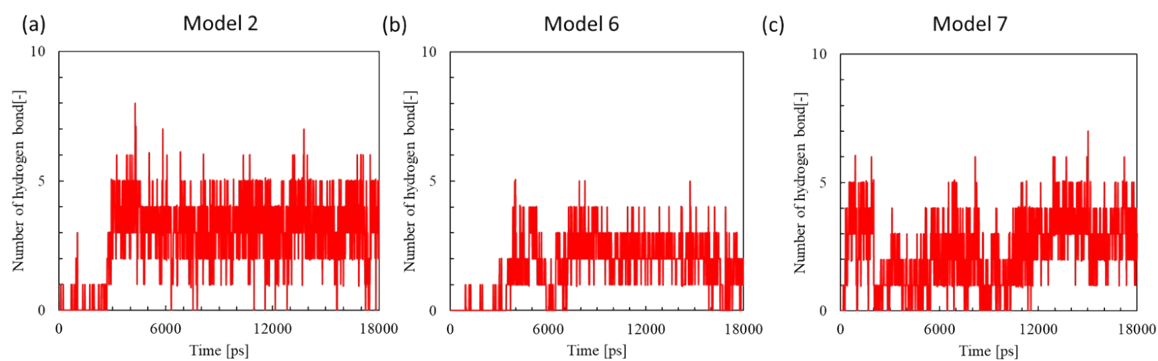
**Figure S5.** Model 3: (a) Lasp\_C2N1 foulant model, (b) Snapshot of the foulant in the neighbourhood of PA membrane, (c) Z-coordinate change of the foulant along with time, and (d) Interaction energy between the PA membrane and the foulant. The dashed range was used to calculate the average value.



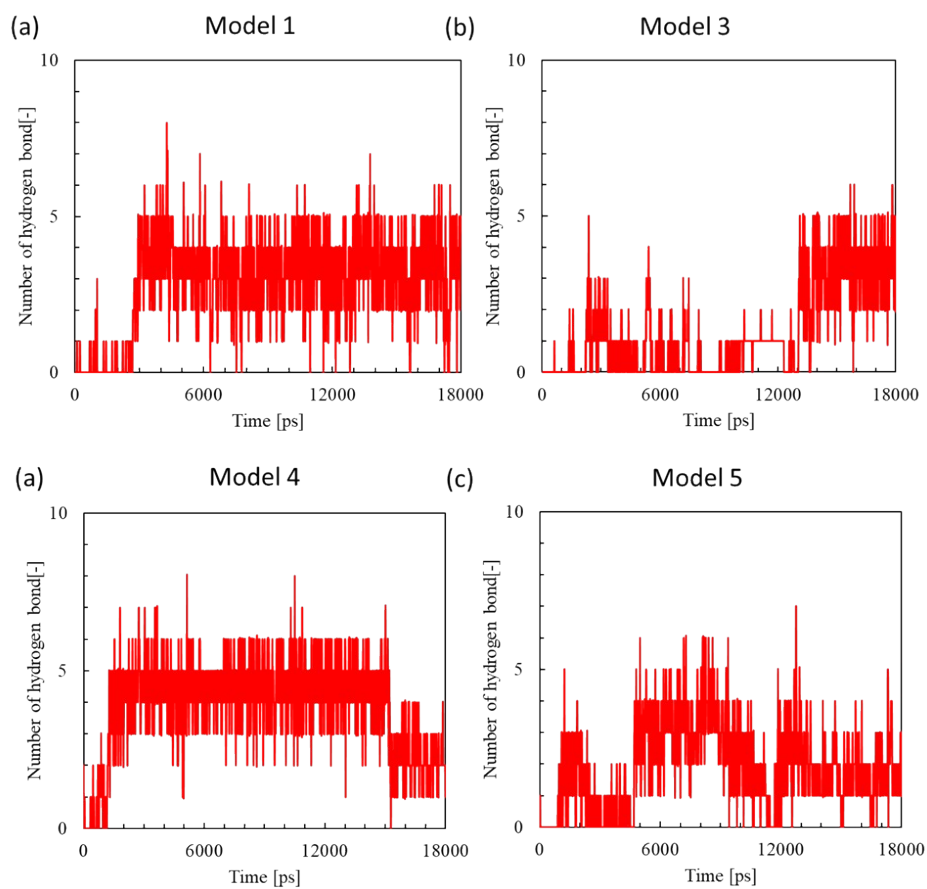
**Figure S6.** Model 4: (a) Larg\_N2 foulant model, (b) Snapshot of the foulant in the neighbourhood of PA membrane, (c) Z-coordinate change of the foulant along with time, and (d) Interaction energy between the PA membrane and the foulant. The dashed range was used to calculate the average value.



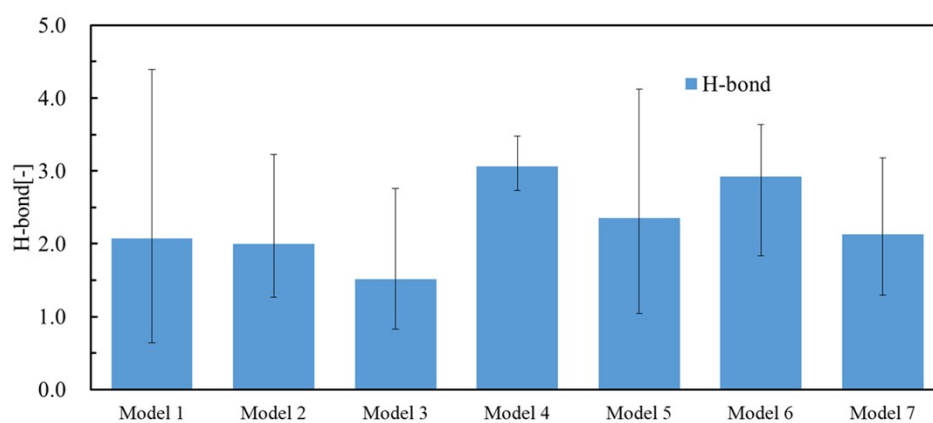
**Figure S7.** Model 5: (a) Larg\_C1N2 foulant model, (b) Snapshot of the foulant in the neighbourhood of PA membrane, (c) Z-coordinate change of the foulant along with time, and (d) Interaction energy between the PA membrane and the foulant. The dashed range was used to calculate the average value.



**Figure S8.** The relationship between time and the number of hydrogen bond between the membrane and the foulant (a) Model 2, (b) Model 6, (c) Model 7.



**Figure S9.** The relationship between time and the number of hydrogen bond between the membrane and the foulant (a) Model 1, (b) Model 3, (c) Model 4, (d) Model 5.



**Figure S10.** The average number of hydrogen bond for each model.

## 2. Membrane properties and performance

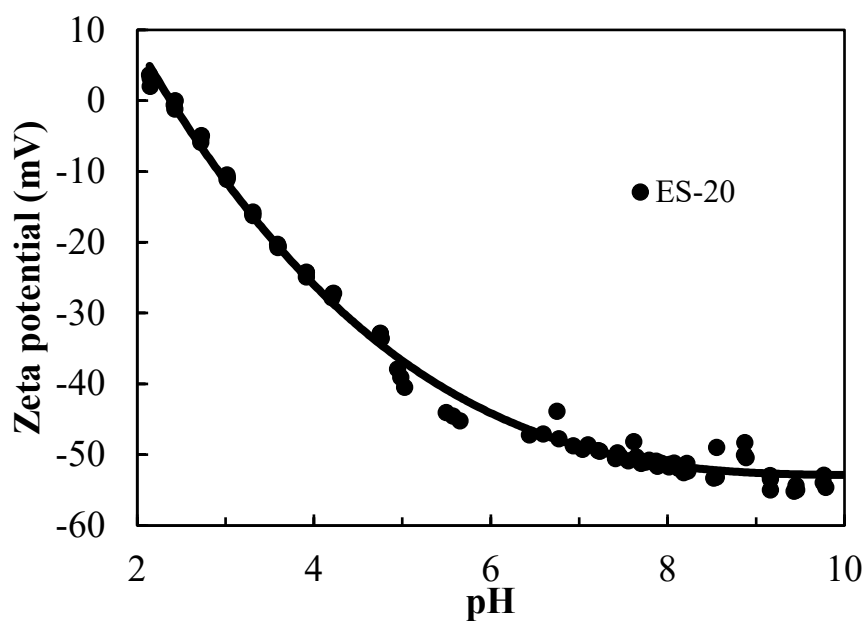


Figure S11. pH dependence of zeta potential of ES-20.

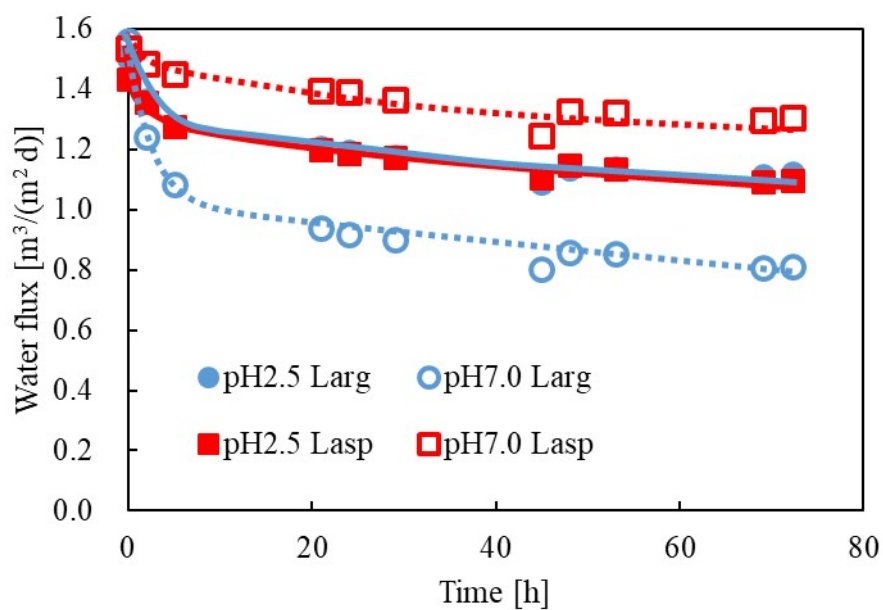


Figure S12. Changes in water flux for Larg and Lasp in ES-20 membranes with time.