

## Supporting Information

# Conformational Behavior of Genetically-Engineered Dodecapeptides as a Determinant of Binding Affinity for Gold.

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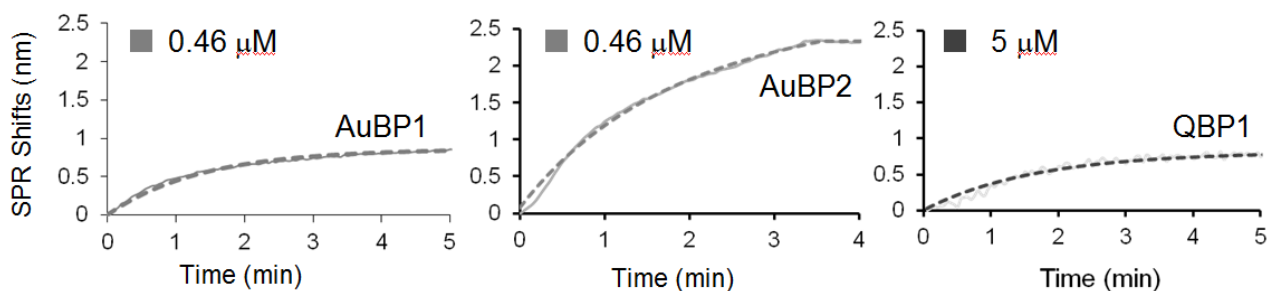


Figure S1. Raw SPR kinetic data for the binding of AuBP1, AuBP2 and QBP1 on gold substrate. For experimental details, see the main text. Note that the SPR shift of QBP1 is measured for a concentration approx. 10 times more than those of AuBPs.

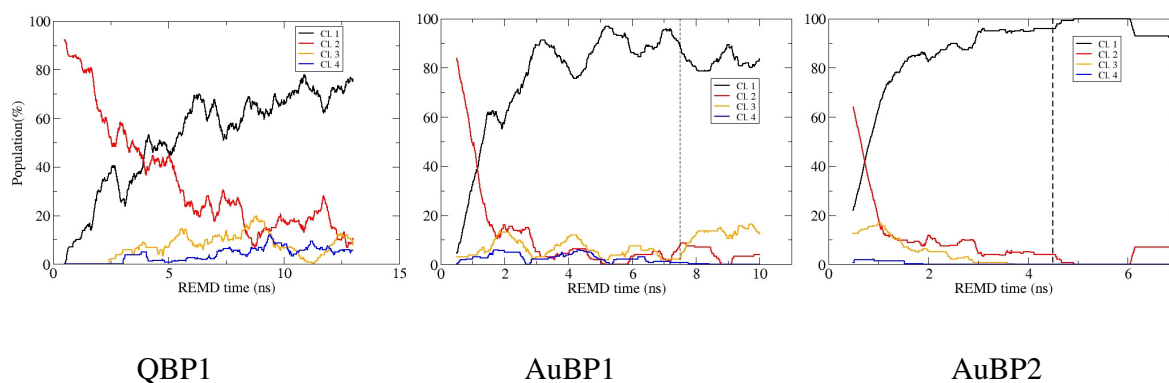
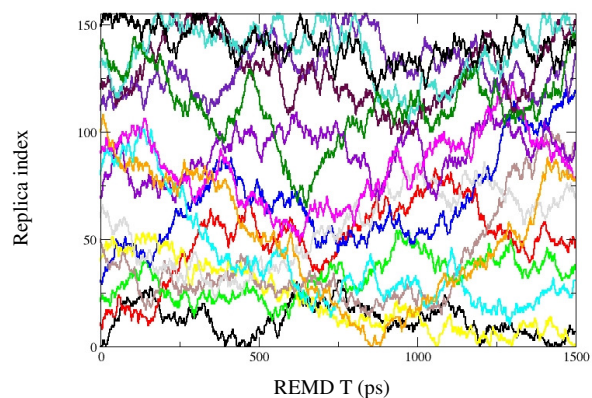
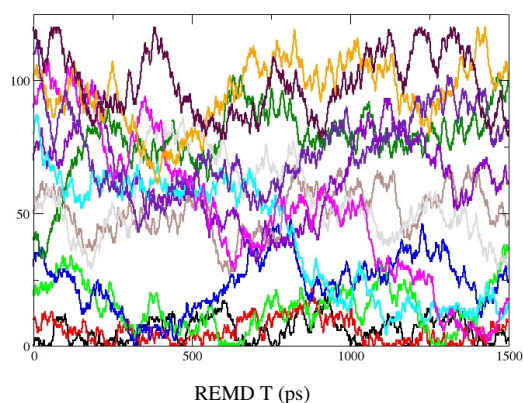


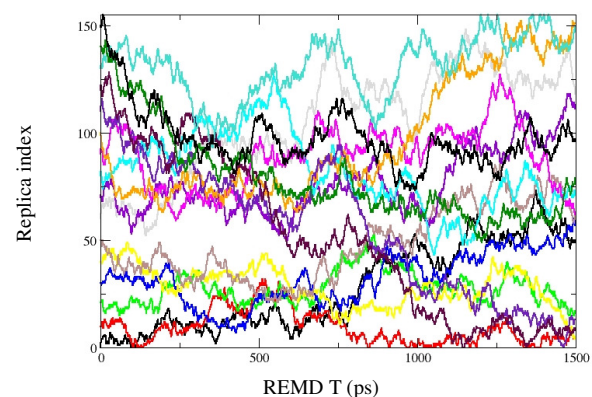
Fig. S2. Evolution of cluster population during REMD for the peptides on Au(111) in water. For all the peptides, the starting conformation at all temperature is the representative of the dominant cluster in solution. The dashed lines of the graphs for AuBP1 and AuBP2 indicate the time at which the cell lateral size has been enlarged, from  $4.06 \times 4.1 \text{ nm}^2$  to  $5.08 \times 4.98 \text{ nm}^2$ , to probe possible effects of the interaction between replicas. This was not needed for QBP1 since its structure remains less extended than those of AuBP1 and AuBP2.



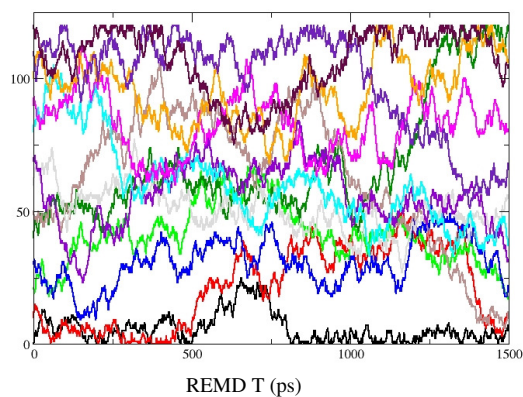
QBP1 in water.  $P_{\max}=0.69$ ,  $P_{\min}=0.39$



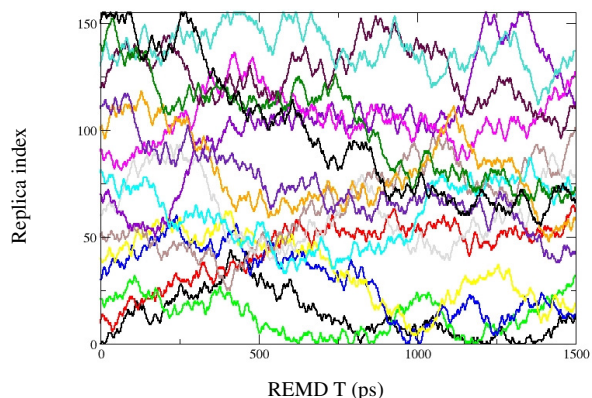
QBP1 in water on gold.  $P_{\max}=0.71$ ,  $P_{\min}=0.40$



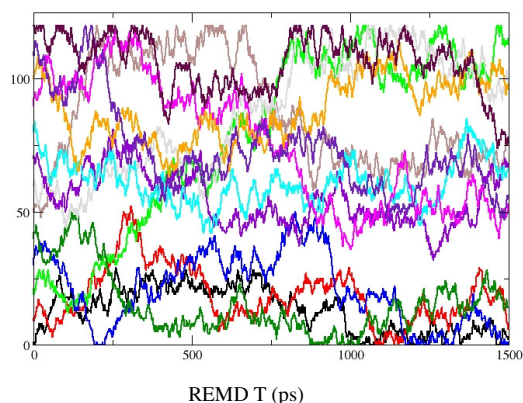
AuBP1 in water.  $P_{\max}=0.69$ ,  $P_{\min}=0.37$



AuBP1 in water on gold.  $P_{\max}=0.68$ ,  $P_{\min}=0.32$



AuBP2 in water.  $P_{\max}=0.8$ ,  $P_{\min}=0.51$



AuBP2 in water on gold.  $P_{\max}=0.67$ ,  $P_{\min}=0.31$

Fig. S3. Trajectory of a subset of replicas in the temperature space for all the performed REMD. The monitored replicas are initially chosen one every 10 replica, starting from the lowest in temperature (i.e., their indexes are 1, 11, 21, etc.) and are followed during the last 1.5ns of the REMD. As it can be seen, replicas span a large portion of the temperature space, and no segregation of replicas in T subdomains takes place. The minimum and maximum acceptance ratios for the replica swap (calculated over the last 1.5ns) are given in each panel as  $P_{\max}$  and  $P_{\min}$ , respectively.

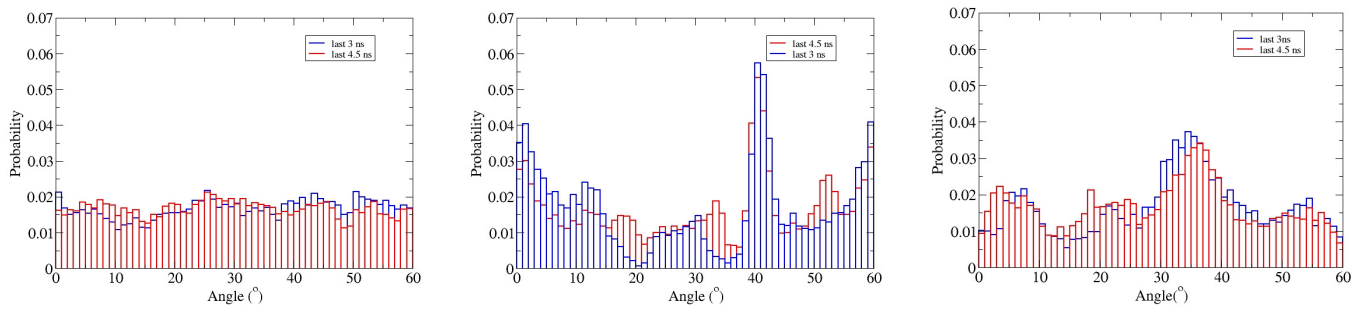


Fig. S4. Probability of backbone orientations on Au(111) for the various peptides under study during the last 3ns (blue) or 4.5 ns (red) of the REMD dynamics. The angle is defined as in Fig. 6 in the main text. Note that the main features of the distributions are not sensitive on the time interval used to calculate the average.