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# Electronic Supplementary Information

# Molecular basis of substrate translocation through outer membrane channel OprD of Pseudomonas aeruginosa

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**Figure S1:** The location of the mutations used in the simulations.

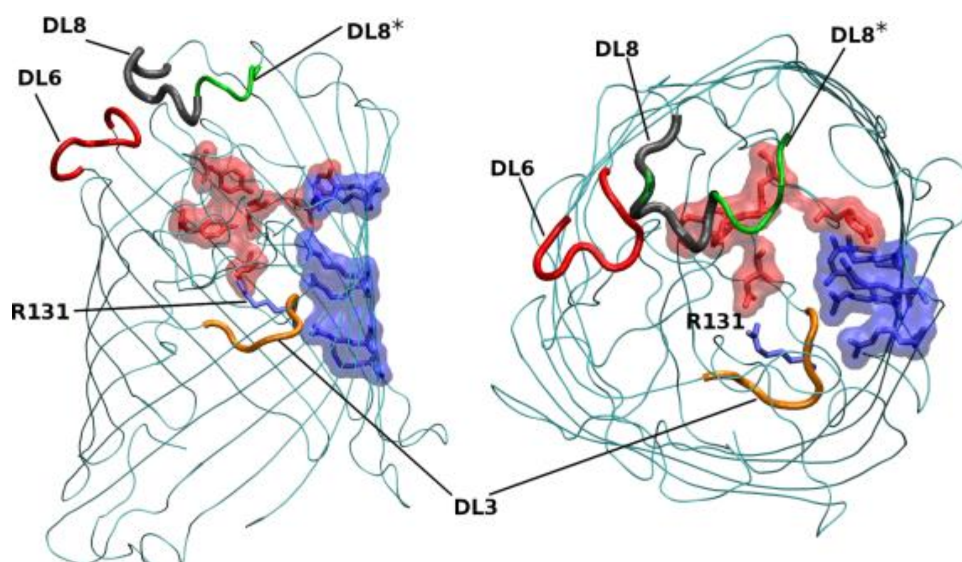
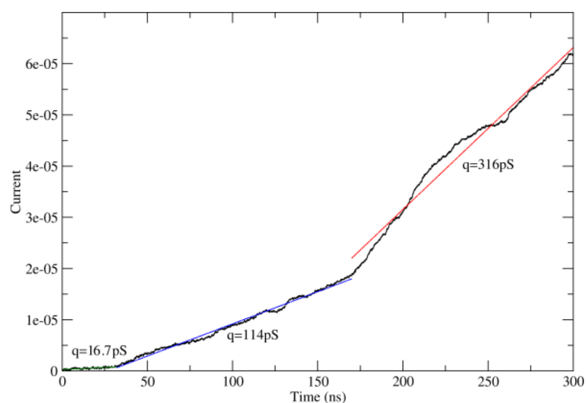
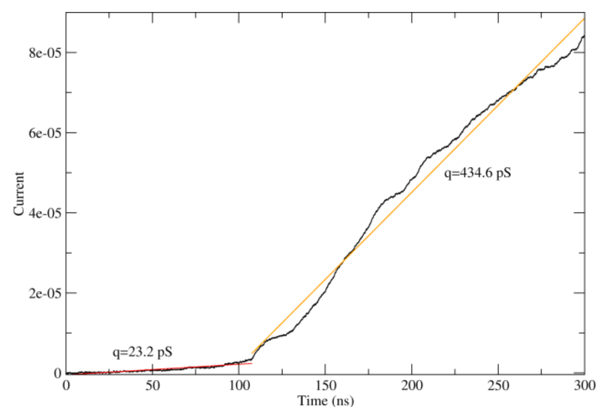



**Figure S2:** IV curves for the systems simulated.

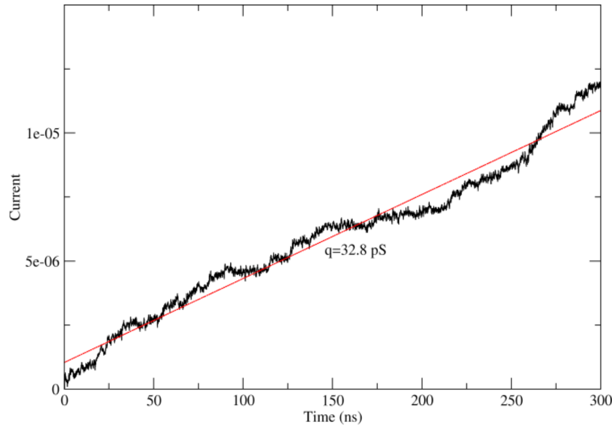
WT – pH7 - 0.3M KCl →



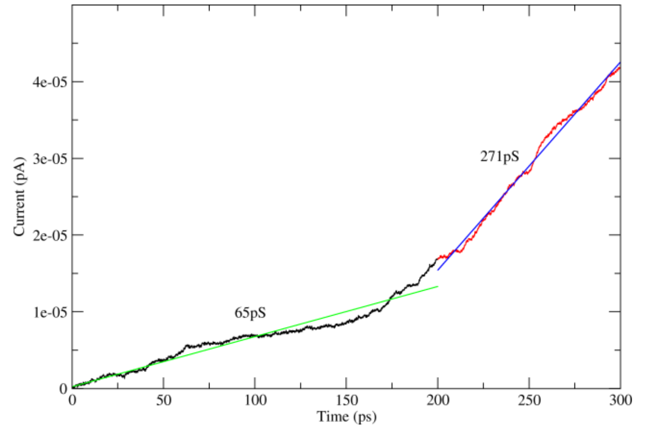

WT – pH5 - 0.3M KCl →



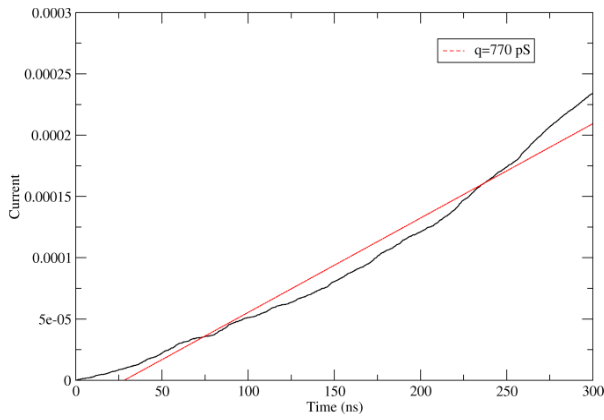
R131G – pH7 - 0.3M KCl →



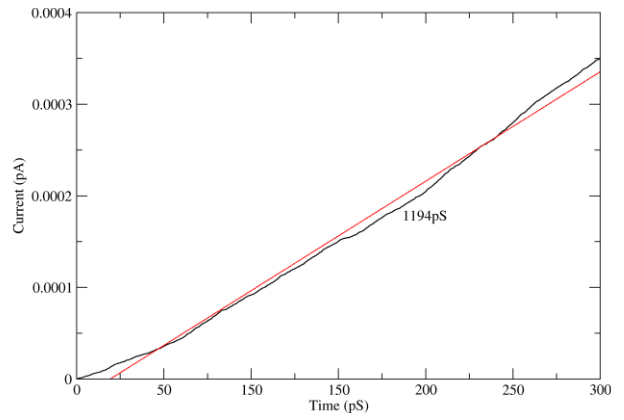

R131G – pH5 - 0.3M KCl →



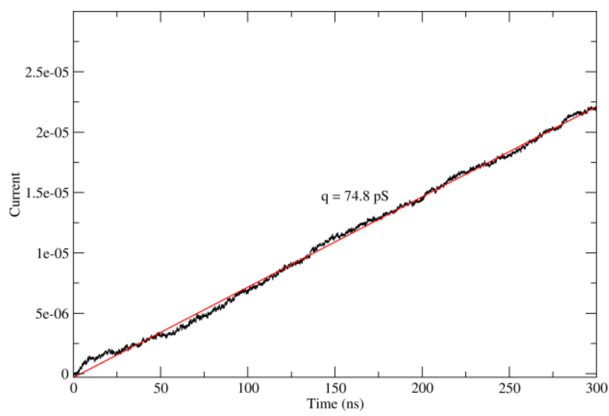

DL3 - pH7 - 0.3M KCl →



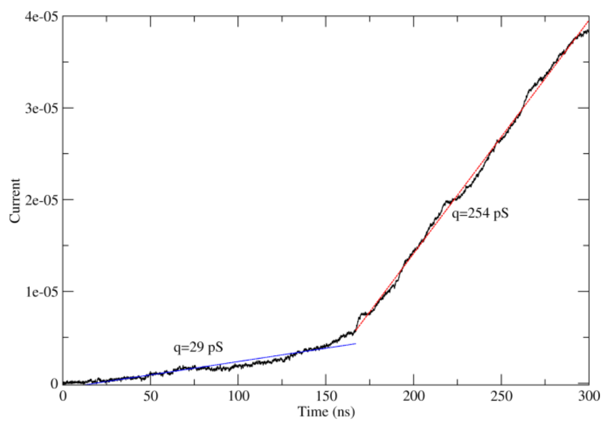

DL3 - pH5 - 0.3M KCl →



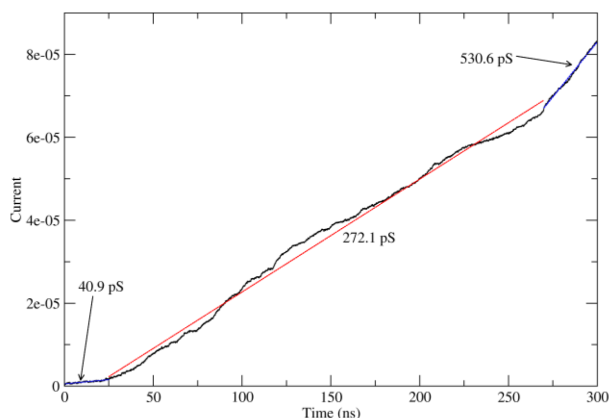

DL3 - pH7 - 0.3M KCl (closed L2) →




DL6 - pH7 - 0.3M KCl →



DL8 - pH7 - 0.3M KCl →




DL8* - pH7 - 0.3M KCl →

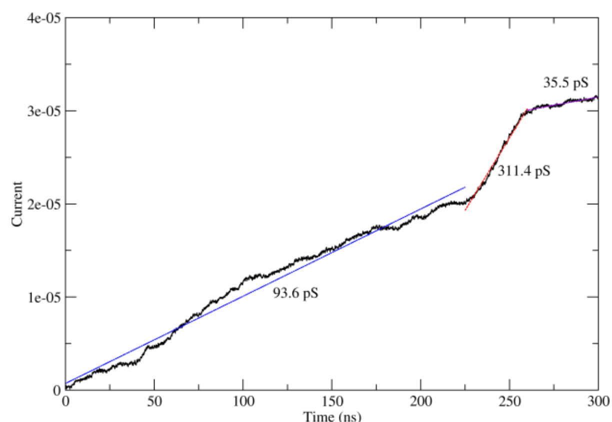



**Figure S3:** Two salt-bridge interactions involving R131 for WT in pH 7. Initially R131 (in L3) interacts with D295 (in L7) which corresponds to the closed path B. After 35ns, this interaction is broken and R131 starts interacting with D90 (in L2).

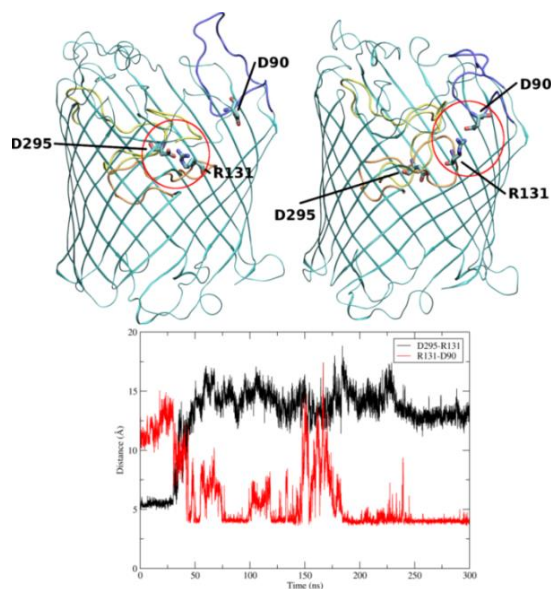



**Figure S4:** Two salt-bridge interactions involving R131 for DL6 (left), DL8 (middle) and DL8* (right) mutations.

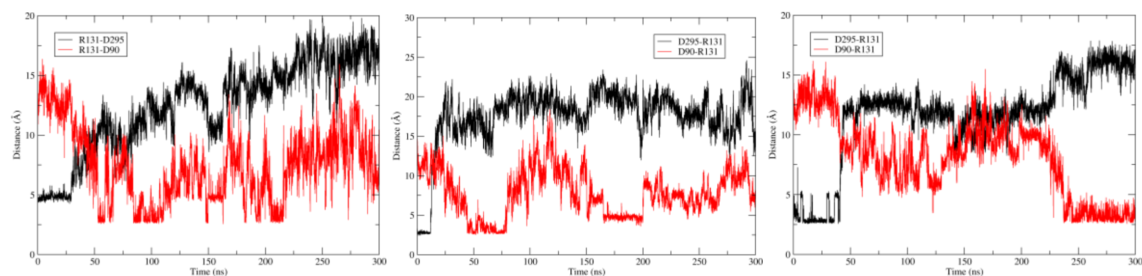


**Figure S5:** Chemical structure of the substrates used: a) arginine, b) ornithine, c) lysine, d) benzoate, e) glutamic acid, f) histidine positive, g) histidine neutral, h) leucine, i) glycine, and j) serine

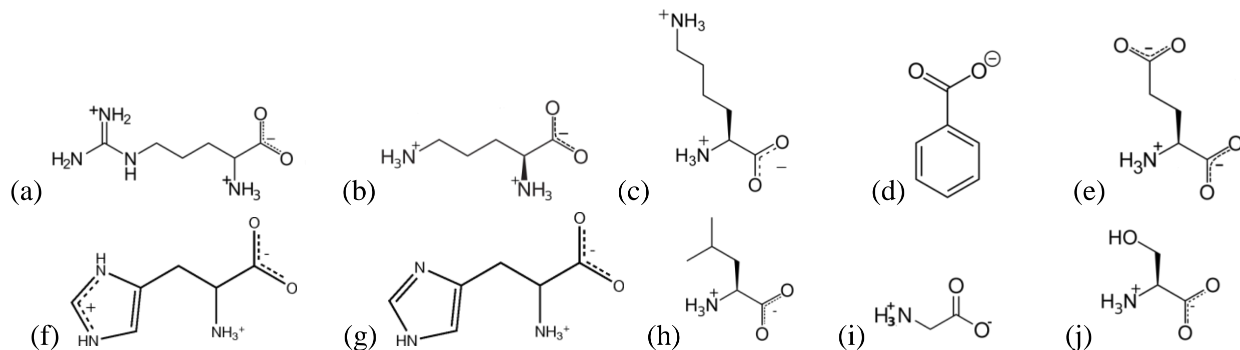



**Figure S6:** FESs of translocation of substrates through OprD. Left to right: lysine, ornithine, positively charged histidine.

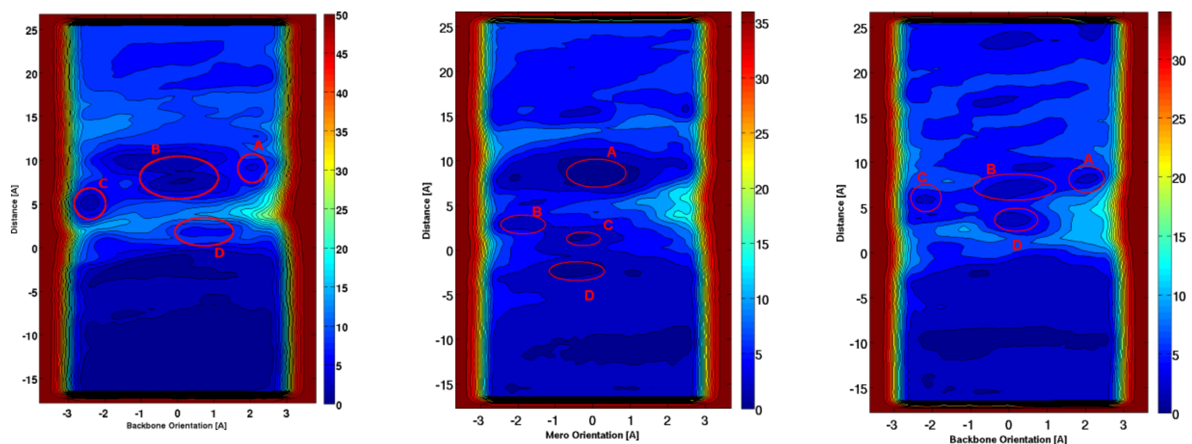



**Figure S7:** The structures corresponding to the minima in the FES of translocation of lysine through OprD.

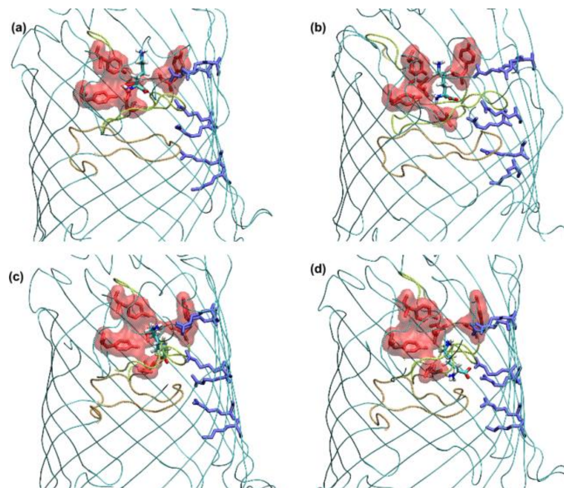


**Figure S8:** The structures corresponding to the minima in the FES of translocation of ornithine through OprD.

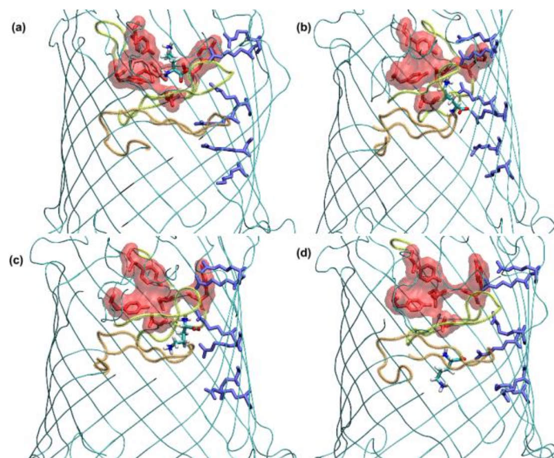



**Figure S9:** The structures corresponding to the minima in the FES of translocation of histidine (positive) through OprD.

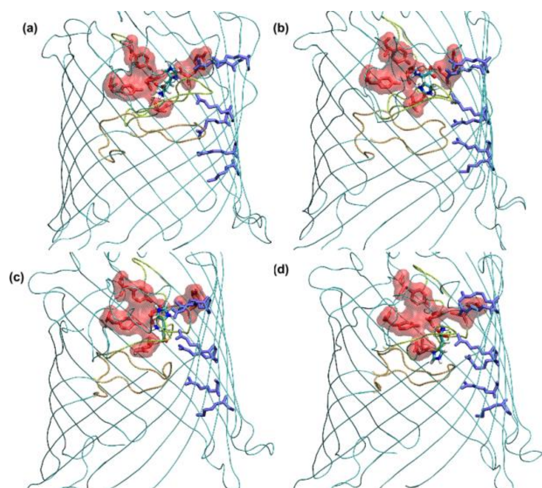



**Figure S10:** The structures corresponding to the minima in the FES of translocation of the neutral form of histidine (left) and glutamic acid (right) through OprD.

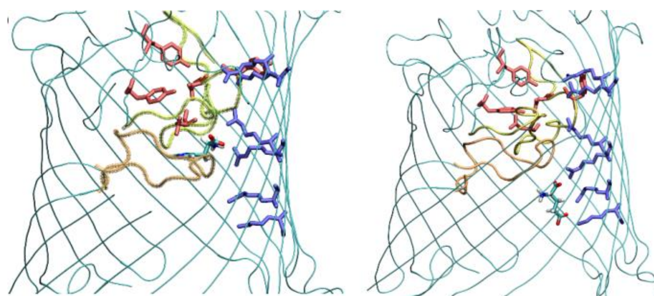


**Figure S11:** The structures corresponding to the minima in the FES of translocation of benzoate through OprD.

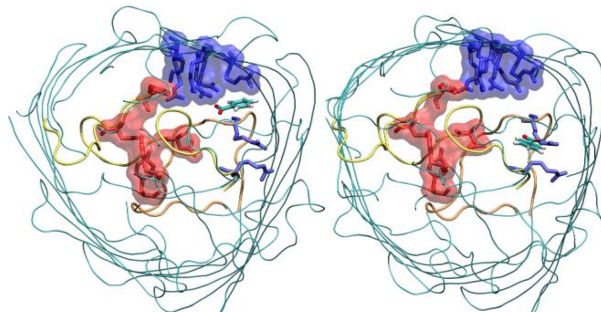


**Figure S12:** FESs of translocation of substrates through OprD. Left to right: glycine, leucine, serine.

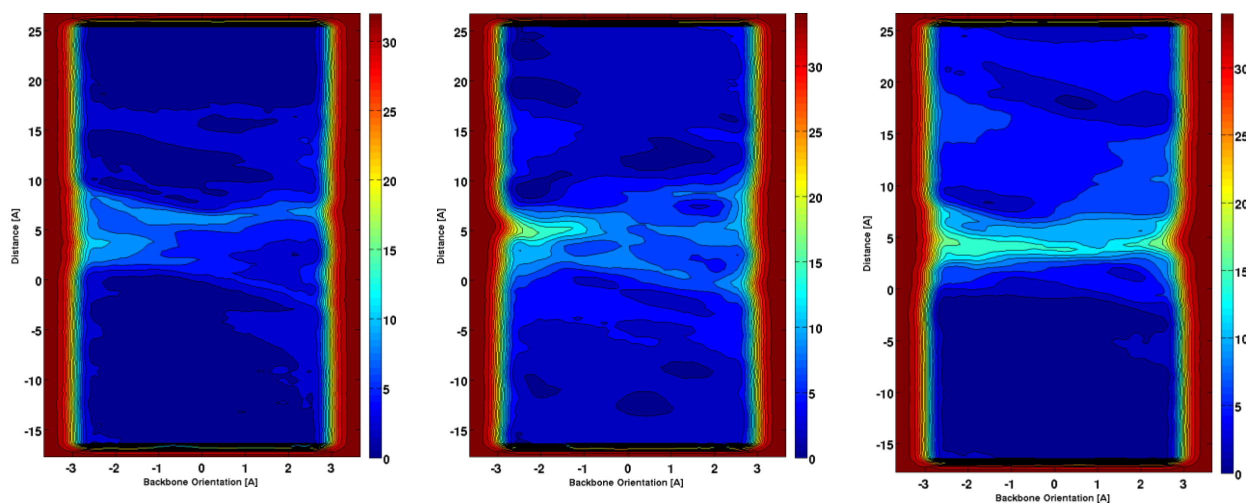



**Figure S13:** The height of the bias potential added for each walker is shown over time. It shows that within the simulation time the convergence parameter, the Gaussian height, arrived to a baseline below the 1/100 of the initial value.

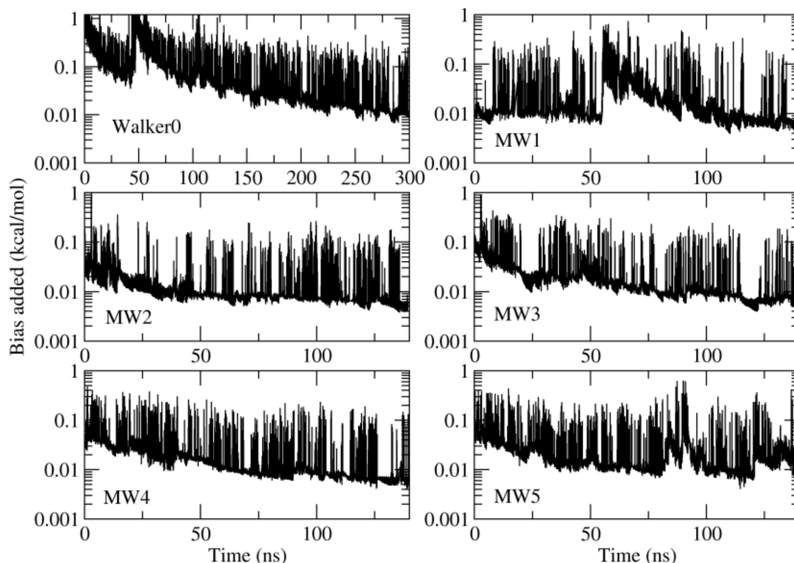


**Figure S14:** The evolution of the FES for leucine with time. As mentioned in the manuscript, we ran an initial 300ns simulation and then selected 5 walkers and ran them for 140ns each. In the figure below we can see that initially the FES change drastically. In the end, the FES do not change much from 900ns to 950 ns to 1μs.