

Phospho-Mimetic Mutation at Ser602 Inactivates Human TRPA1 Channel

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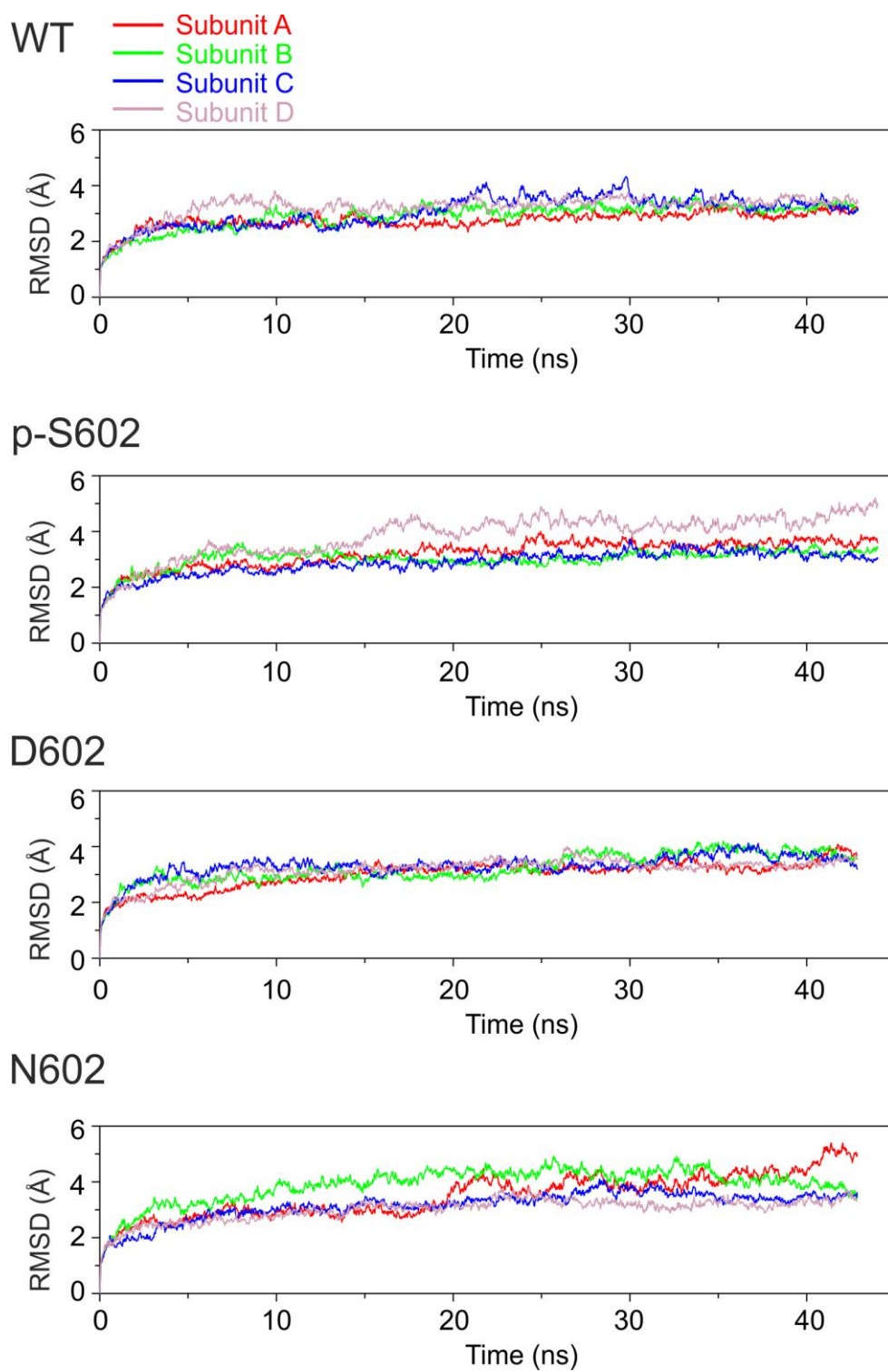


Figure S1. Molecular dynamics simulation results obtained for TRPA1 models based on 6V9X structure. Time evolution of the root mean square deviation (RMSD) values, over backbone atoms, for each monomer (indicated by colors in the legend above) of the indicated TRPA1 constructs.

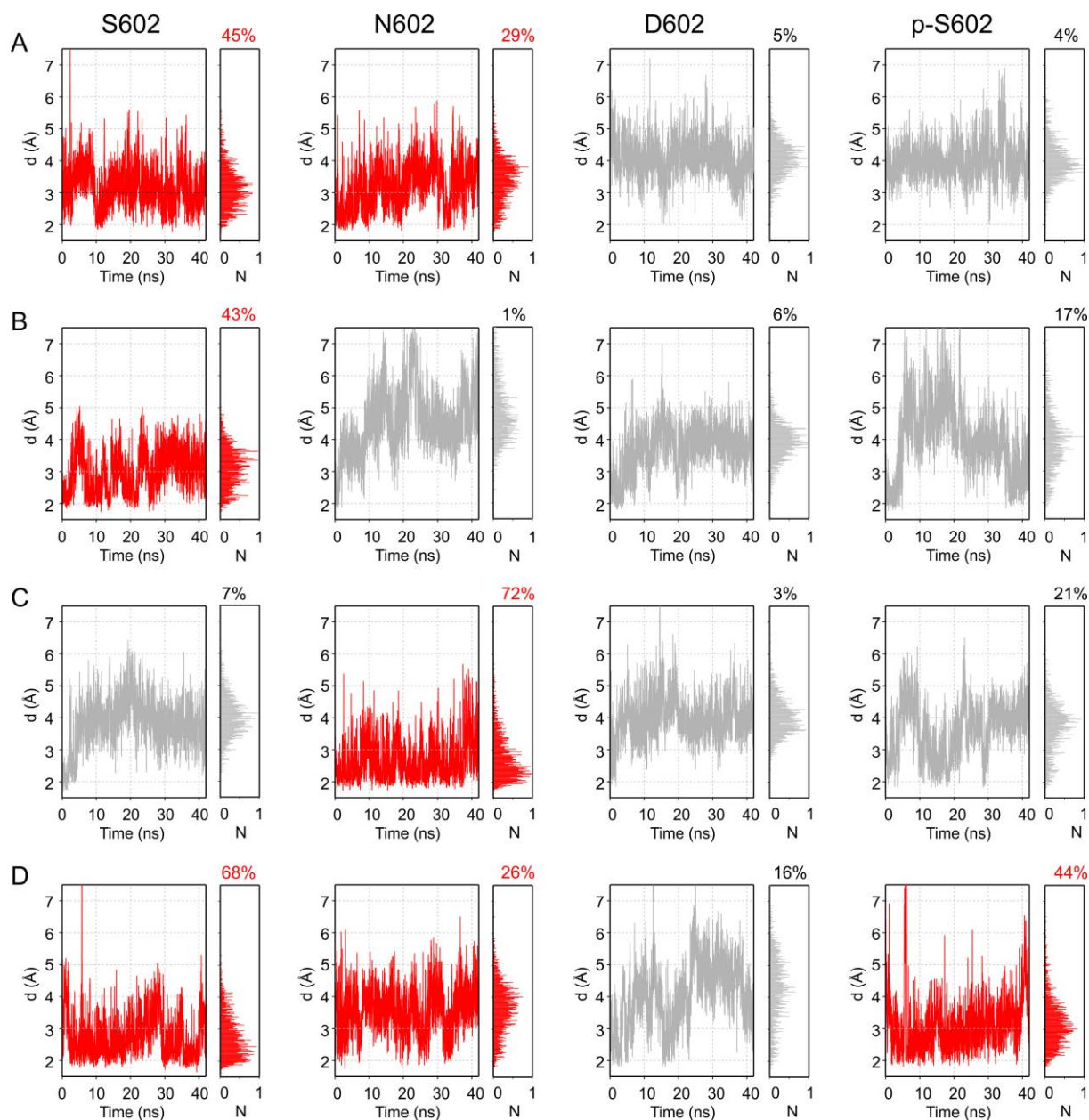


Figure S2. Molecular dynamics simulation results obtained for the TRPA1 models of wild-type (S602), N602, D602 and p-S602 based on the structure PDB ID: 6V9X. Time course of distances between Trp605 and Tyr662, measured as shown in Figure 4 from subunits A, B, C, D. Horizontal bar graphs are normalized all-point histograms produced from the distances shown in left panel over the simulation interval 15-42 ns. Percentages calculated from the histograms indicate the relative times (>25% in red) for which the distance between the two atoms is less than 3 Å.

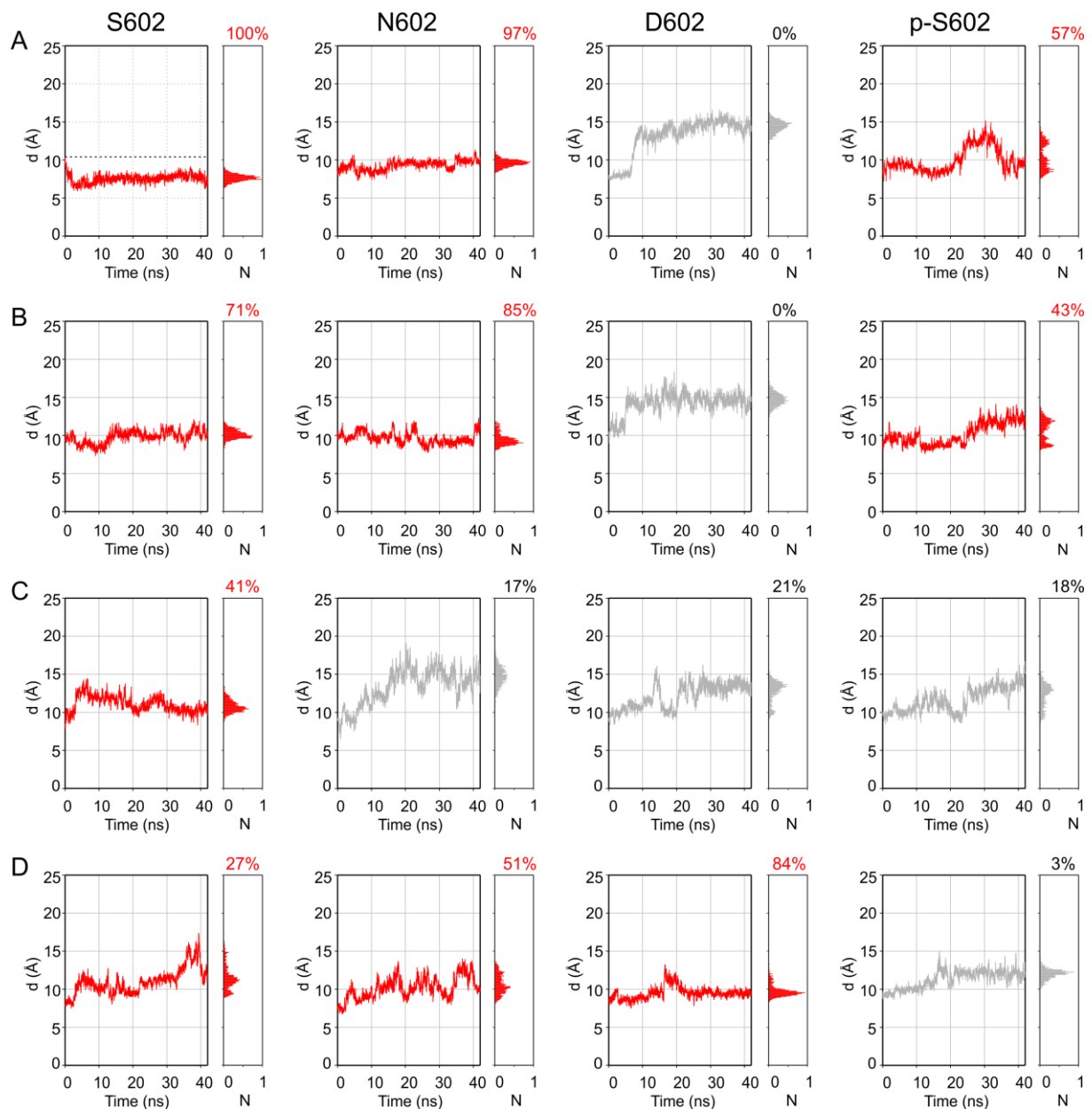


Figure S3. Molecular dynamics simulation results obtained for the TRPA1 models of the wild-type (S602), N602, D602 and p-S602 based on the structure PDB ID: 6V9X. Time course of distances between Lys671 and Glu987, measured between C α atoms from subunits A, B, C, D. Horizontal bar graphs are normalized all-point histograms produced from the distances shown in left panel over the simulation interval 15-42 ns. The histograms of the wild-type subunits were fitted by Gaussian function and the threshold was set as the average ($\mu + \sigma$) = 10.4 Å. Percentages indicate the relative times (>25% in red) for which the distance between the two atoms is less than 10.4 Å.