Supplemental Material

Contribution of the Putative Inner Pore Region to the Gating of the Transient Receptor Potential Vanilloid Subtype 1 Channel (TRPV1)

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Figure S1  Susankova et al.

Molecular dynamics simulations of the S6 helix of the wild-type TRPV1, mutants A680G, T670A and T670G in vacuo. The protein monomer structure was cleaned, hydrogens were added, and it was finally placed into a box 0.5 nm larger than the protein along all three axes. A multiple time step of 1 fs for intra-molecular and 2 fs for intermolecular forces and a 0.86 nm cut-off were used. After a short steepest descent minimization, one single protein monomer generated by homology modeling was simulated in vacuo, the simulation run at 298 K. Threonine 670 and alanine 680, which are predicted to represent hinge regions tolerated replacement with glycine and T670 also tolerated replacement with alanine. Snapshots were taken after 35 ps of simulation.