

Supplemental figure 1

Fig. 1S A pdb file containing the 3-D molecular model for the brake region of wild-type $\text{Ca}_v3.2$ channels. The region corresponding to a.a. 394-497 was modeled the Quanta program. *De novo* structural models of WT and mutant channels using the amino acids that form the IS6 and part of the I-II loop (amino acids 394-497 of WT) of $\text{Ca}_v3.2$ $\alpha 1$ subunit, were obtained using the Quanta program (Accelrys., San Diego, CA) running on a Silicon Graphics computer. Molecular dynamics simulations were carried out using HyperChem 7.1 (Hypercube, Inc., Gainesville, FL) as follows: the model was subjected to energy minimization with harmonic constrains on the protein backbone ($100 \text{ kcal mole}^{-1}$) in order to reach the nearest local minimum energy conformation until an energy difference of $0.01 \text{ kcal mole}^{-1}$ between successive iterations was achieved. Finally, the accuracy of the models was tested by a Ramachandran plot.

Image at right to be linked to file Cav32WT.pdb

