Supporting information for: Supporting Information: How do aminoadamantanes block the influenza M2 channel and how does resistance develop?

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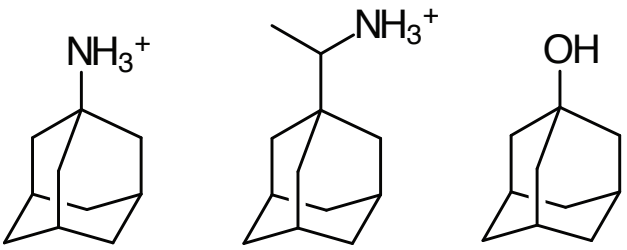

Figure 1: Structures of 1-aminoadamantane (amantadine, left), 1-(1-adamantyl)ethylamine (rimantadine, center) and 1-hydroxyadamantane (adamantanol, left). Amantadine and rimantadine are shown in their protonated form.

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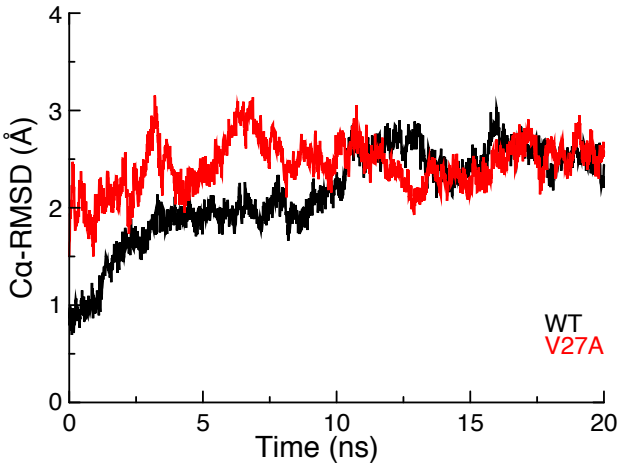

Figure 2: The Cα-RMSD of the 20ns equilibration MD simulations for two M2 Singapore variants: wild-type (black) and V27A (red).

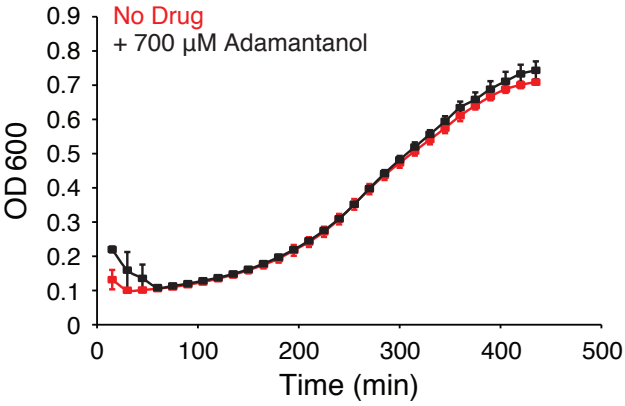

Figure 3: Growth of bacteria in the presence (black, $n = 2$) or absence (red, $n = 4$) of 700 μM adamantanol. The error represent the standard deviation, and n is the number of independent trials.