Supporting Information for:

Probing the effects of gating on the ion occupancy of the K^+ channel selectivity filter using 2D IR spectroscopy

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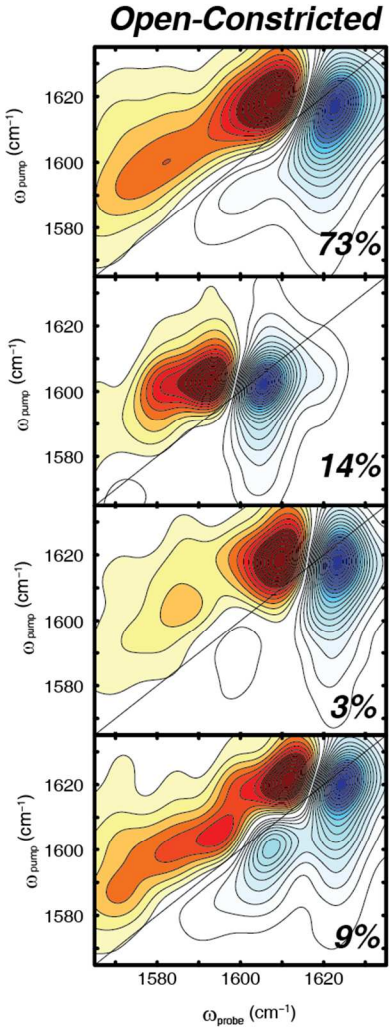
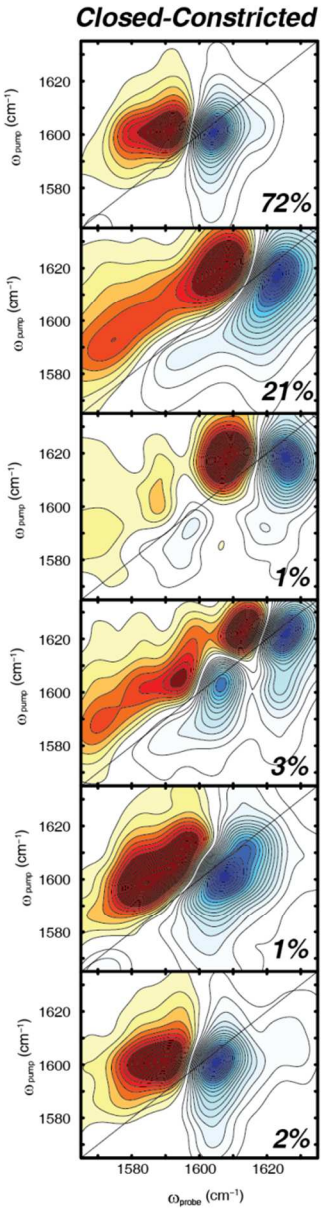
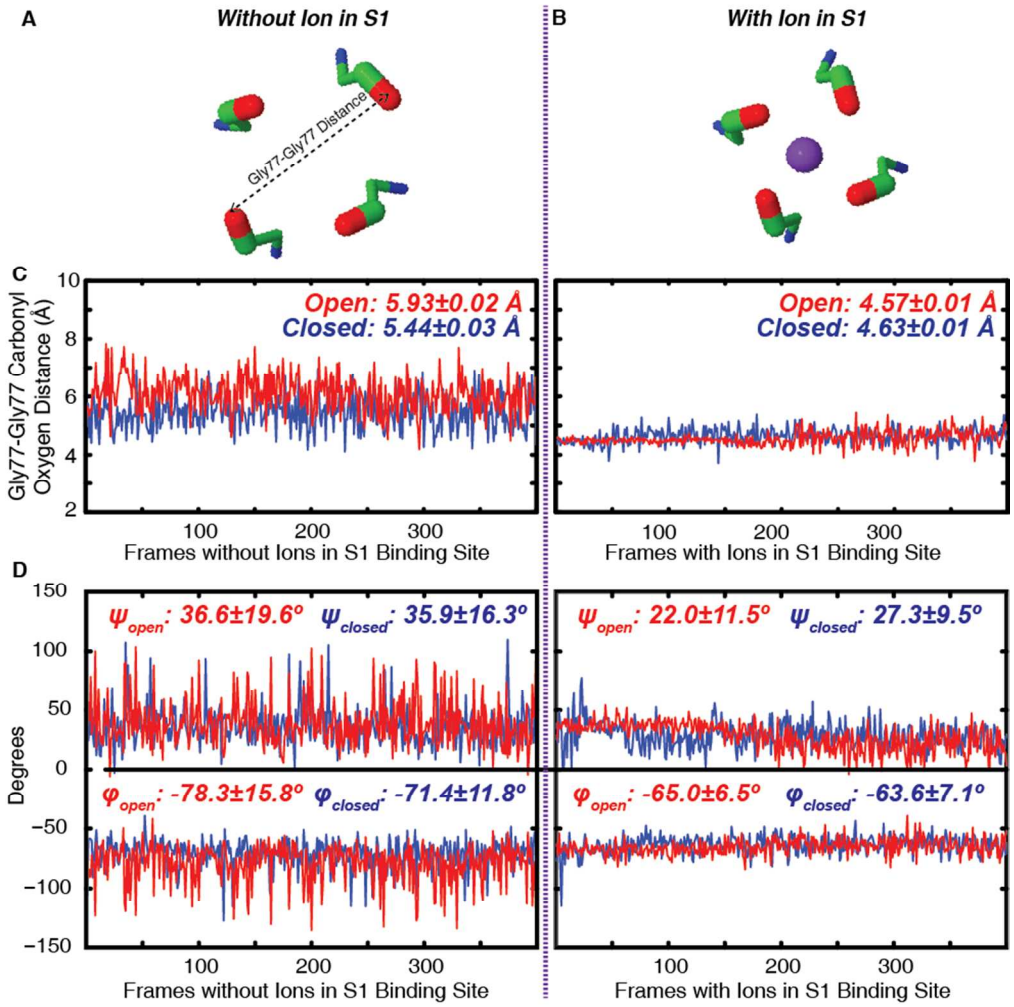
Supplemental Tables and Figures



Supplemental Figure S1| All groups for open-constricted MD simulations The sum of all of the groups in the open-constricted MD simulations gives the 2D IR spectrum for the full trajectory shown in Fig. 3(A). The two major groups from Fig. 3 are shown again and account for 87% of the states observed in the MD simulations. The other 12% are shown below.



Supplement Figure S2| All groups for closed-constricted MD simulations The sum of all of the groups in the closed-constricted MD simulations gives the 2D IR spectrum for the full trajectory shown in Fig. 4A). The two major groups from Fig. 3 are shown again and account for 93% of the states observed in the MD simulations. The other 7% are shown below.



Supplemental Figure S3| Structural differences between the filters with and without ions in the closed and open states. Using the Hamiltonian clustering analysis, two major conformations are shown for both the open and closed states. The most significant differences between these structures are seen with the Gly77 residue. (A) Without ion in the S1 binding site, the four Gly77 ring becomes distorted. (B) With an ion in S1, the Gly77 residues obtain a stable square configuration, with the carbonyls pointing into the pore and binding the K^+ ion (purple). (C) Distances between Gly77-Gly77 carbonyl oxygen (defined in A) between open and closed states with and without ion. (D)Analysis of the φ and ψ angles (as presented in Fig. 4 in the main text) show that the filter fluctuates more without the ion bound at the S1 binding site. The ψ angle is defined by the Gly77 carbonyl carbon, Tyr78 amide nitrogen, Tyr78 C_α, and the Tyr78 carbonyl carbon. The φ angle is defined by the Gly77 amide nitrogen, Gly77 C_α, Gly77 carbonyl carbon and Tyr78 amide nitrogen.