

# IUCrJ

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**Supporting information for article:**

**Structural plasticity of the selectivity filter in a nonselective ion channel**

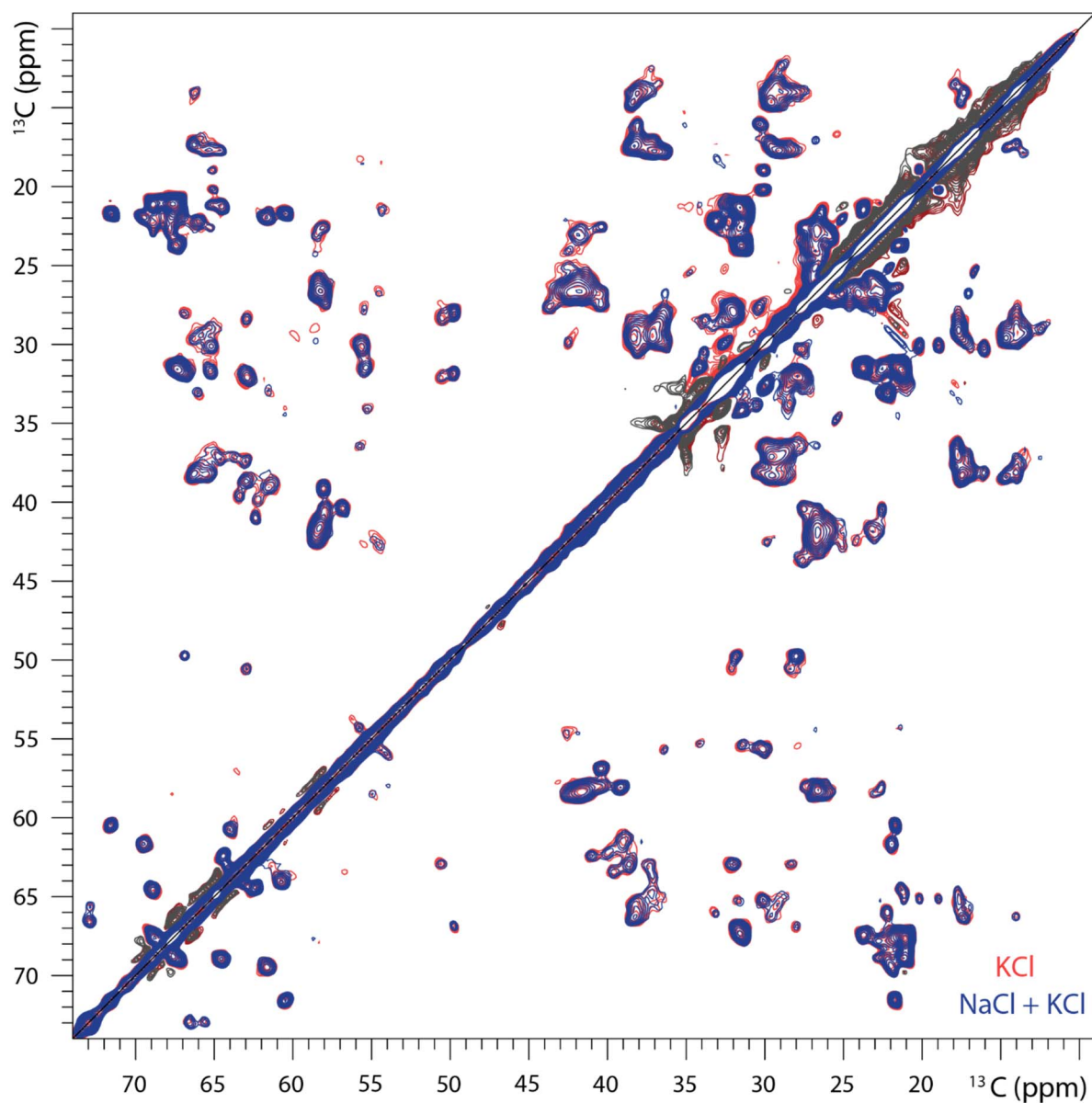
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**Table S1** Simulations at larger degrees of opening of inner helices of NaK, we used distance restraints placed between CA atoms of A92 residue

Opening	Opening A92 [nm]*	Opening T63 [nm]*	Ion	Force field	Voltage [mV]	Number of simulations / Total simulation time [ $\mu$ s]	Inward permeation [number/ $\mu$ s]	Outward permeation [number/ $\mu$ s]
0.1	ch0: 1.756 $\pm$ 0.003 ch1: 1.760 $\pm$ 0.003	ch0: 0.838 $\pm$ 0.004 ch1: 0.845 $\pm$ 0.006	K <sup>+</sup>	Amber	370 $\pm$ 40	5 / 2.5	2 $\pm$ 2	0
0.1	ch0: 1.761 $\pm$ 0.006 ch1: 1.770 $\pm$ 0.004	ch0: 0.843 $\pm$ 0.004 ch1: 0.839 $\pm$ 0.005	K <sup>+</sup>	Amber	620 $\pm$ 20	5 / 2.5	4 $\pm$ 1	0
0.2	ch0: 1.868 $\pm$ 0.002 ch1: 1.874 $\pm$ 0.002	ch0: 0.844 $\pm$ 0.007 ch1: 0.864 $\pm$ 0.01	K <sup>+</sup>	Amber	570 $\pm$ 50	5 / 2.5	6 $\pm$ 6	1 $\pm$ 1
0.1	ch0: 1.748 $\pm$ 0.004 ch1: 1.749 $\pm$ 0.003	ch0: 0.858 $\pm$ 0.003 ch1: 0.867 $\pm$ 0.005	Na <sup>+</sup>	Amber	410 $\pm$ 30	5 / 2.5	0	0
0.1	ch0: 1.745 $\pm$ 0.005 ch1: 1.743 $\pm$ 0.003	ch0: 0.857 $\pm$ 0.003 ch1: 0.860 $\pm$ 0.002	Na <sup>+</sup>	Amber	610 $\pm$ 40	5 / 2.5	0	0
0.2	ch0: 1.834 $\pm$ 0.001	ch0: 0.831 $\pm$ 0.001	K <sup>+</sup>	Charmm	360 $\pm$ 40	3 / 1.5	3 $\pm$ 2	14 $\pm$ 7

	ch1: 1.843 ± 0.005	ch1: 0.837 ± 0.002						
0.1	ch0: 1.734 ± 0.002 ch1: 1.733 ± 0.001	ch0: 0.845 ± 0.001 ch1: 0.848 ± 0.001	Na <sup>+</sup>	Charmm	330±10	5 / 2.5	0	0
0.1	ch0: 1.734 ± 0.001 ch1: 1.736 ± 0.001	ch0: 0.844 ± 0.001 ch1: 0.852 ± 0.001	Na <sup>+</sup>	Charmm	540±10	5 / 2.5	0	0
0.2	ch0: 1.834 ± 0.002 ch1: 1.836 ± 0.001	ch0: 0.848 ± 0.001 ch01: 0.856 ± 0.001	Na <sup>+</sup>	Charmm	540±20	5 / 2.5	0	0

\*ch0 - channel with inward permeation, ch1 - channel with outward permeation



**Figure S1** 2D  $^{13}\text{C}$ - $^{13}\text{C}$  proton-driven spin diffusion (PDS) correlation spectra of NaK $\Delta$ 19 in 50mM  $\text{K}^+$  (positive signals in red; negative signals in maroon) and with 50 mM  $\text{K}^+$  and 50 mM  $\text{Na}^+$  (positive signals in blue; negative signals in grey).