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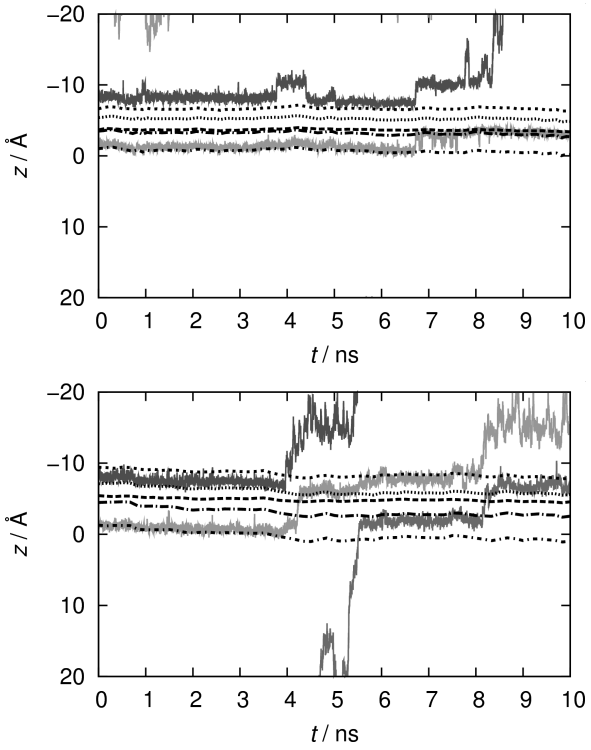

FIGURE S1 z coordinates (measured along the channel axis) of K^+ ions for simulations Kcv-HOM-K29$_{prot}$-E3 and E4 with constant external field corresponding to +100 mV voltage. Both simulations were started with the last snapshot of the equilibrium run of Kcv-HOM-K29$_{prot}$ with flexible filter; time was reset to zero. Dashed/dotted lines show the positions of binding sites S0-S4 as in Fig. 11. Different shades of gray are used to distinguish ions.

Experimental Chemical Shifts referenced to DSS (n.n = not assigned, empty: no atom)

	M Met 1	**L Leu 2**	**V Val 3**	**F Phe 4**	**S Ser 5**	**K Lys 6**	**F Phe 7**	**L Leu 8**	**T Thr 9**	**R Arg 10**	**T Thr 11**	**E Glu 12**	**P Pro 13**	**F Phe 14**	**M Met 15**	**I Ile 16**
H^N		8.62	8.19	8.42	8.18	8.26	8.08	7.95	8.06	8.34	8.20	8.23		8.04	8.08	8.07
H^α	4.12	4.41	4.07	4.65	4.37	4.18	4.63	4.14	4.30	4.42	4.31	4.68	4.35	4.59	4.63	4.39
$H^{\beta1}$	2.15	1.56	1.95	3.11	3.82	1.84	3.18	1.87	4.20	1.88	4.17	2.02	2.19	3.09	2.03	1.63
$H^{\beta2}$	2.15	1.47		2.99	3.73	1.84	2.95	1.87		1.78		1.82	1.79	3.09	1.92	
$H^{\gamma1}$	2.56	1.19	0.87		OH	1.23		1.16	OH	1.61	OH	2.44	1.94		2.47	1.58
$H^{\gamma2}$	2.56		0.87			1.23			1.20	1.61	1.17	2.44	1.94		2.47	0.92
$H^{\delta1}$		0.91		n.n.		1.60	n.n.	0.92		3.17			3.74	n.n.		0.88
$H^{\delta2}$		0.86		n.n.		1.60	n.n.	0.92		3.17			3.66	n.n.		
$H^{\varepsilon1}$	2.11			n.n.		2.92	n.n.			7.15				n.n.	2.08	
$H^{\varepsilon2}$				n.n.		2.92	n.n.							n.n.		
H^z				n.n.		7.53	n.n.							n.n.		
CO	171.81	171.66	176.27	175.37	175.18	174.19	175.19	174.74	176.90	174.19	175.89	174.19		176.17	174.98	176.35
C^α	54.92	55.16	61.82	57.50	57.89	56.67	55.11	61.45	61.84	56.27	61.84	53.56	63.27	57.44	57.47	55.24
C^β	32.86	42.46	33.06	39.75	63.85	28.73	39.37	39.23	69.72	31.20	69.72	28.68	31.88	39.35	33.23	26.92
$C^{\gamma1}$	30.62	27.41	21.01			24.54		27.42		27.26		32.73	27.23		31.79	26.92
$C^{\gamma2}$			21.01						21.86		21.69					17.78
$C^{\delta1}$		23.62		n.n.		28.98	n.n.	24.74		43.63		180.31	50.52	n.n.		13.41
$C^{\delta2}$		23.62		n.n.			n.n.	24.74						n.n.		
$C^{\varepsilon1}$	16.69			n.n.		42.00	n.n.							n.n.	16.83	
$C^{\varepsilon2}$				n.n.			n.n.							n.n.		
C^z				n.n.			n.n.			159.46				n.n.		
N	n.n	126.86	123.74	126.13	118.95	124.52	121.10	125.39	116.31	124.46	116.64	124.42	n.n.	120.17	123.77	124.50
N^ε						n.n				n.n.						

Chemical Shift perturbation ($\Delta_{exp} - \Delta_{statistical}$), red: H^N, blue: H^α