

S1 Table. Numbers of water molecules and Na⁺ ions added in all simulation systems.

	Water molecule	Na⁺
HER2/4665	37422	13
HER2/48F	37418	13
HER2/48M	37419	13
HER2/48W	37420	13
HER2/48Y	37420	13
HER2/49M	37422	13
HER2/49Y	37422	13
HER2/50A	37424	12
HER2/50E	37418	13
HER2/50G	37426	12
HER2/50K	37419	11
HER2/50N	37423	12
HER2/50Q	37419	12
HER2/50R	37418	11
HER2/51H	37423	13
HER2/51Y	37423	13
HER2/55A	37422	13
HER2/55F	37417	13
HER2/55M	37422	13
HER2/55P	37422	13
HER2/55V	37422	13
HER2/55W	37416	13
HER2/55Y	37417	13
HER2/56F	37417	13
HER2/56M	37420	13
HER2/56V	37421	13
HER2/56Y	37416	13
HER2/57A	37422	13
HER2/57L	37421	13
HER2/57M	37422	13
HER2/57V	37422	13
HER2/58F	37420	13
HER2/58H	37421	13
HER2/58M	37420	13
HER2/58W	37420	13
HER2/58Y	37420	13

HER2/59K	37420	12
HER2/59L	37422	13
HER2/59M	37419	13
HER2/59R	37418	12
HER2/59Y	37419	13
HER2/60W	37420	13
HER2/61Q	37422	13
HER2/62F	37421	13
HER2/62M	37421	13
HER2/62W	37422	13
HER2/62Y	37421	13
HER2/63F	36438	14
HER2/63M	36442	14
HER2/63N	36443	14
HER2/63Q	36442	14
HER2/63V	36443	14
HER2/63W	36434	14
HER2/63A	36422	14
HER2/63Y	36494	14
HER2/64K	37425	12
HER2/64N	337425	13
HER2/64Q	37425	13
HER2/64R	37425	12
HER2/58F63Y	36493	14
HER2/55M56M	37420	13
HER2/55M56Y	37416	13
HER2/55M57A	37422	13
HER2/55M57V	37422	13
HER2/55M58F	37420	13
HER2/55M63V	36443	14
HER2/55M63W	36434	14
HER2/55M63Y	36494	14
HER2/55V56M	37420	13
HER2/55V56Y	37416	13
HER2/55V57A	37422	13
HER2/55V57V	37422	13
HER2/55V58F	37420	13
HER2/55V58H	37421	13
HER2/55V60W	37420	13
HER2/55V63V	36443	14

HER2/55V63W	36434	14
HER2/55V63Y	36494	14
HER2/56M57A	37420	13
HER2/56M57V	37420	13
HER2/56M58F	37418	13
HER2/56M58H	37419	13
HER2/56M60W	37418	13
HER2/56M63V	36440	14
HER2/56M63W	36431	14
HER2/56M63Y	36490	14
HER2/56Y57A	37416	13
HER2/56Y57V	37416	13
HER2/56Y58F	37414	13
HER2/56Y58H	37415	13
HER2/56Y60W	37414	13
HER2/56Y63V	36438	14
HER2/56Y63W	36429	14
HER2/57A58F	37420	13
HER2/57A58H	37421	13
HER2/57A60W	37420	13
HER2/57A63V	36442	14
HER2/57A63W	36433	14
HER2/57A63Y	36493	14
HER2/57V58F	37420	13
HER2/57V58H	37421	13
HER2/57V60W	37420	13
HER2/57V63V	36442	14
HER2/57V63W	36433	14
HER2/57V63Y	36493	14
HER2/58F60W	37418	13
HER2/58F63V	36442	14
HER2/58F63W	36433	14
HER2/58H60W	37419	13
HER2/58H63V	36444	14
HER2/58H63W	36435	14
HER2/58H63Y	36495	14
HER2/60W63V	36439	14
HER2/60W63W	36430	14
HER2/60W63Y	36491	14