

S1 Table. Composition of five systems.

System	Protein	Ligand	Ions	SOL
ADA	1	None	Na (9)	14280
ADA-FR0	1	FR0	Na (10)	10555
ADA-FR2	1	FR2	Na (10)	10916
ADA-PRH	1	PRH	Na (11)	9654
ADA (without PRH)	1	None	Na (11)	14475