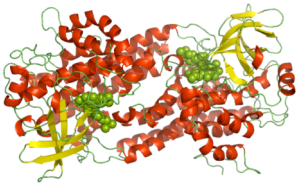
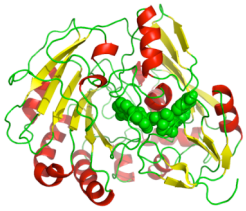
Table S1. Simulated systems

Enzyme	C_2		AldO	
				
PDB ID initial coordinates	2jbs	2jbs	2vfr	2vfr
T [K]	300	350	300	350
nr. O_2 molecules	100	100	100	100
cofactor	$FMNH^-$	$FMNH^-$	$FADH^-$	$FADH^-$
nr. solute atoms	8267	8267	4009	4009
nr. solvent molecules	35028	35028	15342	15342
nr. atoms in the system	113360	113360	50245	50245
nr. of ions	12 Na^+	12 Na^+	1 Cl^-, 3 Mg^{2+}, 6 K^+	1 Cl^-, 3 Mg^{2+}, 6 K^+
total system charge	0	0	0	0
equilibration period [ns]	1.8	2.7	2.7	2.7
nr. MD replicas	5	5	5	5
equilibrium period [ns]	3.0	3.0	5.0	5.0