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## Multiple pathways guide oxygen diffusion into flavoenzyme active sites

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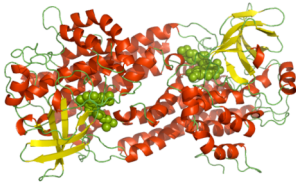
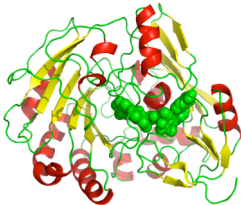
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**Table S1. Simulated systems**

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Enzyme	C <sub>2</sub>		AldO	
				
PDB ID initial coordinates	2jbs	2jbs	2vfr	2vfr
<i>T</i> [K]	300	350	300	350
nr. O <sub>2</sub> molecules	100	100	100	100
cofactor	FMNH <sup>-</sup>	FMNH <sup>-</sup>	FADH <sup>-</sup>	FADH <sup>-</sup>
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 <sup>+</sup>	12 Na <sup>+</sup>	1 Cl <sup>-</sup> , 3 Mg <sup>2+</sup> , 6 K <sup>+</sup>	1 Cl <sup>-</sup> , 3 Mg <sup>2+</sup> , 6 K <sup>+</sup>
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

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