Supporting information for: Selective Permeability of Carboxysome Shell Pores to Anionic Molecules

Paween Mahinthichaichan,[†,⊥] Dylan M. Morris,[‡,⊥] Yi Wang,[¶] Grant J. Jensen,[*,§,‖] and Emad Tajkhorshid[*,†]

†*Department of Biochemistry, NIH Center for Macromolecular Modeling and Bioinformatics, Center for Biophysics and Quantitative Biology, Beckman Institute for Advanced Science and Technology, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801-3028, United States*

‡*Division of Biology and Biological Engineering, California Institute of Technology, Pasadena, California 91125, United States*

¶*Department of Physics, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong SAR, The People's Republic of China*

§*Division of Biology and Biological Engineering, California Institute of Technology, California Institute of Technology, Pasadena, California 91125, United States*

‖*Howard Hughes Medical Institute, California Institute of Technology, Pasadena, California 91125, United States*

⊥*Equal contribution*

E-mail: jensen@caltech.edu; emad@life.illinois.edu

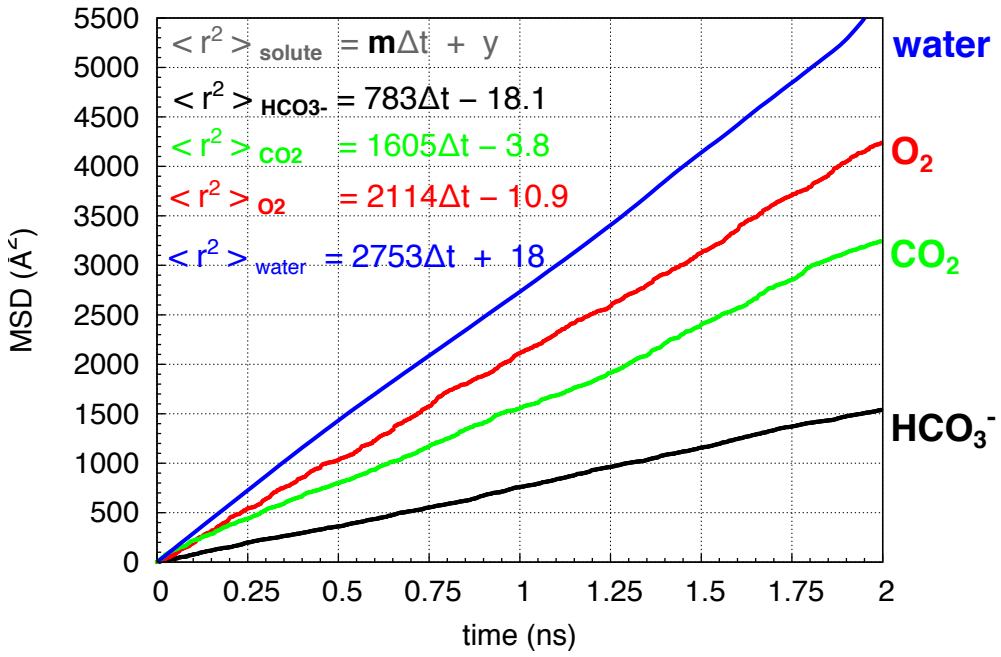

Figure S1: Cumulative displacement profiles of substrate molecules in the aqueous solution Each individual substrate molecule was simulated independently in a $30\times30\times30\,\text{Å}^3$ water box ionized with 0.2 M NaCl. Its mean square displacements ($<r^2>$) were integrated over a 2-ns equilibrated period, and were fitted using linear regression. Since no external restraint was applied on the molecule, the diffusion coefficient (D) is equal to $<r^2>$ / $6\Delta t$ = m / 6. The calculations yielded $D = 1.31\times10^{-5}\,\text{cm}^2/\text{s}$ for HCO_3^-, $2.68\times10^{-5}\,\text{cm}^2/\text{s}$ for CO_2, 3.52 $\times10^{-5}\,\text{cm}^2/\text{s}$ for O_2 and 4.58 $\times10^{-5}\,\text{cm}^2/\text{s}$ for water.

Table S1: Translocational diffusion coefficients (D_z) in the aqueous solution obtained from umbrella sampling simulations

	CsoS1A	**CcmK4**
HCO_3^-	$1.38\pm0.28\times10^{-5}\,cm^2/s$	$1.64\pm0.19\times10^{-5}\,cm^2/s$
CO_2	$3.36\pm0.41\times10^{-5}\,cm^2/s$	$3.47\pm0.57\times10^{-5}\,cm^2/s$
O_2	$4.38\pm0.32\times10^{-5}\,cm^2/s$	$5.28\pm1.47\times10^{-5}\,cm^2/s$
water	$6.02\pm0.99\times10^{-5}\,cm^2/s$	$6.54\pm0.59\times10^{-5}\,cm^2/s$

D_z were calculated from the integral over the autocorrelation function of the applied restrained forces.

Table S2: Lateral diffusion coefficients (D_{xy}) in the aqueous solution obtained from umbrella sampling simulations

	CsoS1A	**CcmK4**
HCO_3^-	$1.13\pm0.16\times10^{-5}\,cm^2/s$	$1.5\pm0.17\times10^{-5}\,cm^2/s$
CO_2	$3.15\pm0.42\times10^{-5}\,cm^2/s$	$3.1\pm0.38\times10^{-5}\,cm^2/s$
O_2	$3.67\pm0.48\times10^{-5}\,cm^2/s$	$3.9\pm0.54\times10^{-5}\,cm^2/s$
water	$4.9\pm1.1\times10^{-5}\,cm^2/s$	$5.52\pm1.38\times10^{-5}\,cm^2/s$

D_{xy} were calculated from the mean square displacement along the x and y axes, defined as $<\Delta x^2 + \Delta y^2>/4\Delta t$. D_z and D_{xy} were the averages of those taken at z < -12.5 Å with respect to the center of the central pores. Overall, these values are not significantly deviated from those calculated from equilibrium simulatoin (Fig. S1).