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Supporting information for article:

Structural and biophysical characterization of the α -carbonic anhydrase from the gammaproteobacterium *Thiomicrospira crunogena* XCL-2: insights into engineering thermostable enzymes for CO₂ sequestration

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Supplemental Material

Figure S1

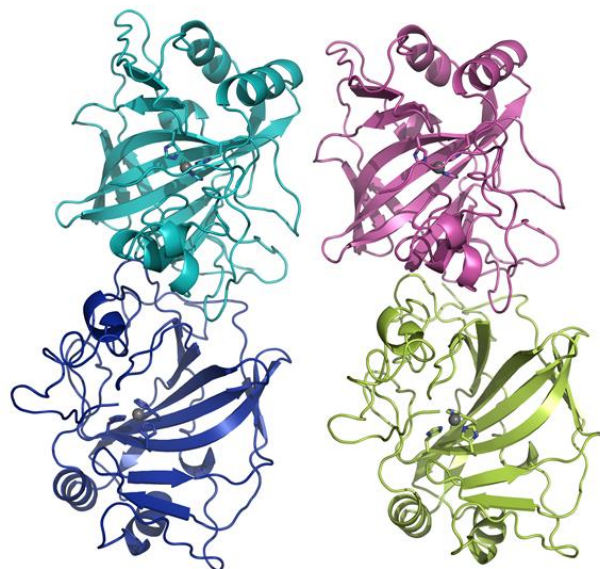


Figure S1: Ribbon diagram of the TcrUCA asymmetric unit. Chains A, B, C, and D, are colored cyan, blue, pink, and yellow-green, respectively.

Figure S2

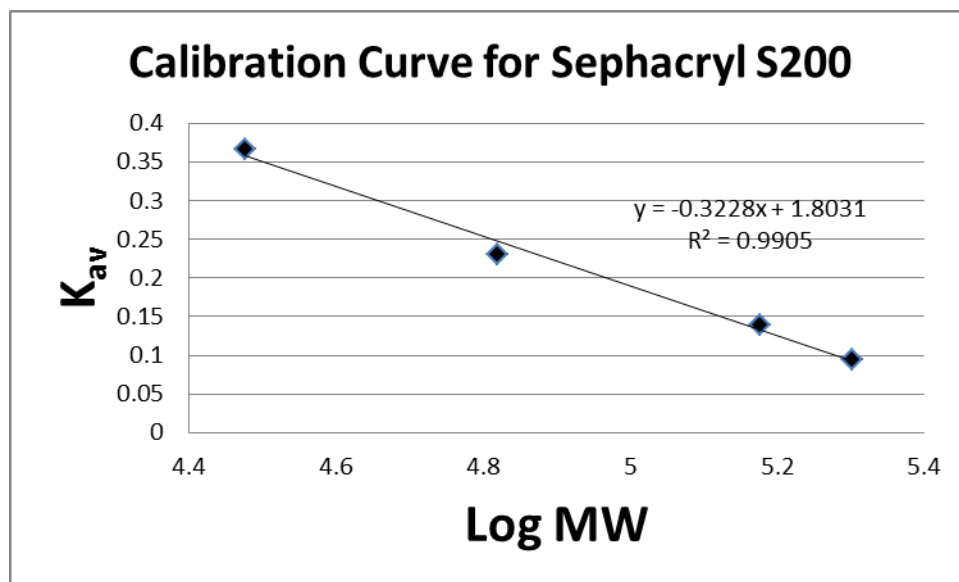


Figure S2: Size-exclusion calibration curve for Sephacryl S200 column generated from MW standards. Plotted is the partition coefficient (K_{av}) versus the \log_{10} of MW for each standard.

Figure S3

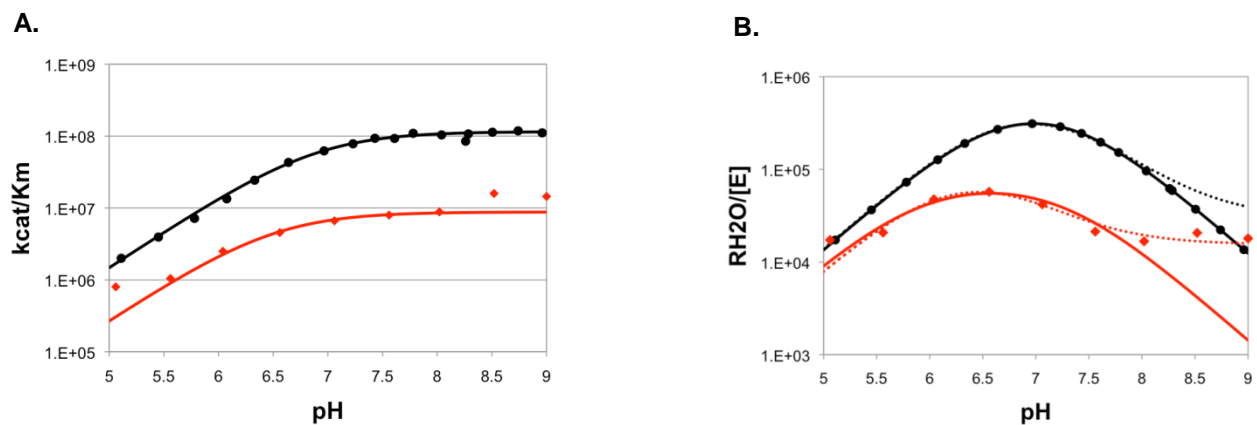


Figure S3: A) The pH profiles for $k_{\text{cat}}^{\text{exch}}/K_{\text{eff}}^{\text{CO}_2}$ (M⁻¹s⁻¹) for the hydration of CO₂ catalyzed by TcrUCA (red, ♦) and hCA II (black, ●). The solid lines are a fit of a single ionization model to the data. B) The pH profile for $R_{\text{H}_2\text{O}}/[E]$ (μs⁻¹) for proton transfer in the dehydration direction catalyzed by TcrUCA (red, ♦) and hCA II (black, ●). The solid lines are a fit of Eq. 2-4 to the data, and the dashed lines are a fit of a double ionization model to the data. Each run was performed in triplicate with an estimated 5% error.

Figure S4

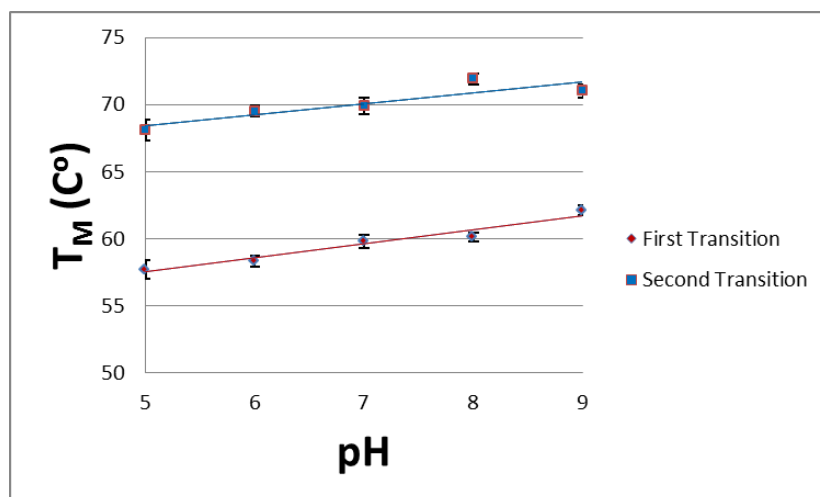


Figure S4: DSC, linear plots of T_M (C°) of TcrUCA versus pH. Experiments were performed in triplicate, experimental errors calculated from the standard deviation of replicates. Plot shows two lines indicative of the first (blue) and second (red) transitions of the TcrUCA melting curve. Most likely the first transition peak corresponds to dimeric disassembly and the second transition peak corresponds to monomer unfolding.

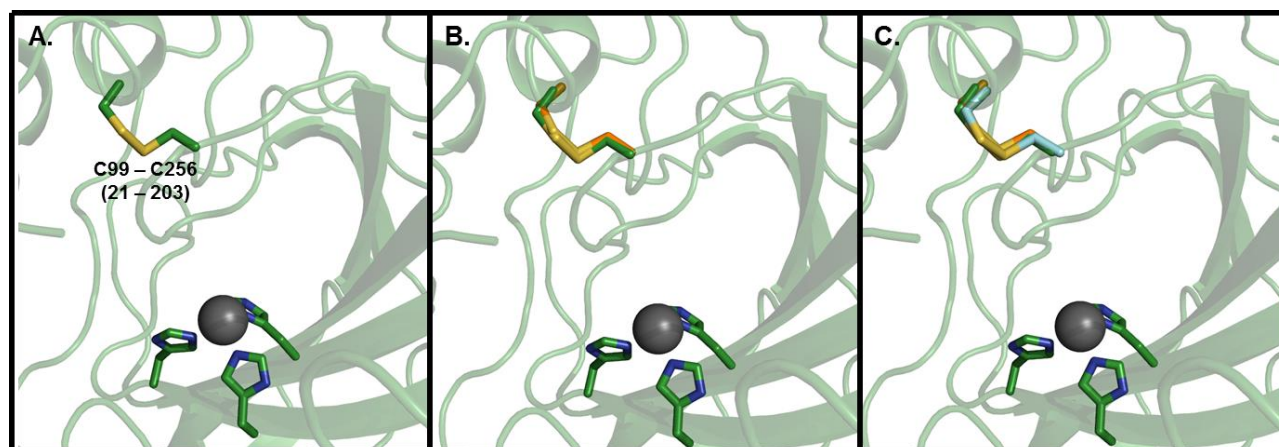
Figure S5

Figure S5: Stick representation of intramolecular disulfide. A) TcrCA, residues as labeled. hCA II numbering in parenthesis. B) Overlay of TcCA (green) and SspCA (orange). C) Overlay of TcCA (green) and hCA IX (cyan).