

Supporting Information

Inhibition studies on human and mycobacterial carbonic anhydrases with N-((4-sulfamoylphenyl)carbamoithioyl) amides

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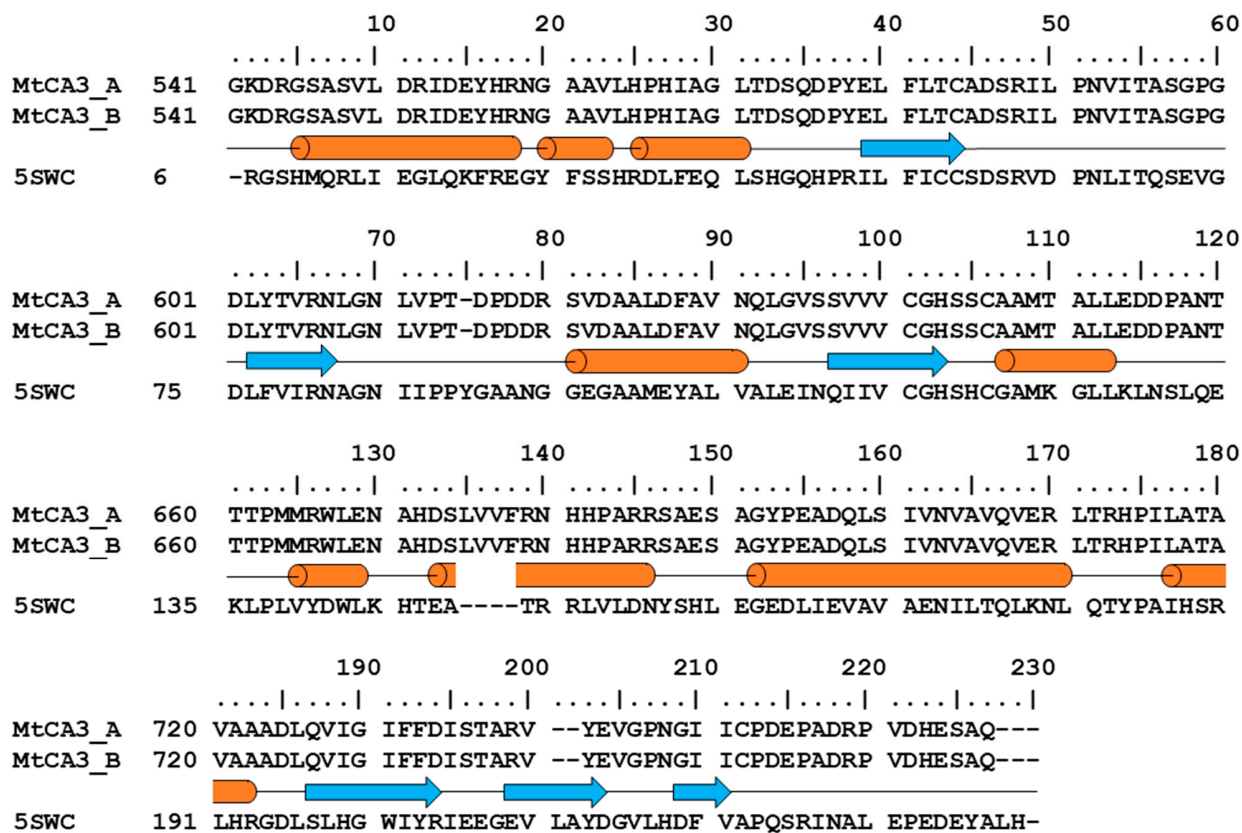


Figure S1. Sequence alignment of MtCA3 with the template β -CA from *Synechocystis* sp. PCC 6803 (pdb 5SWC).

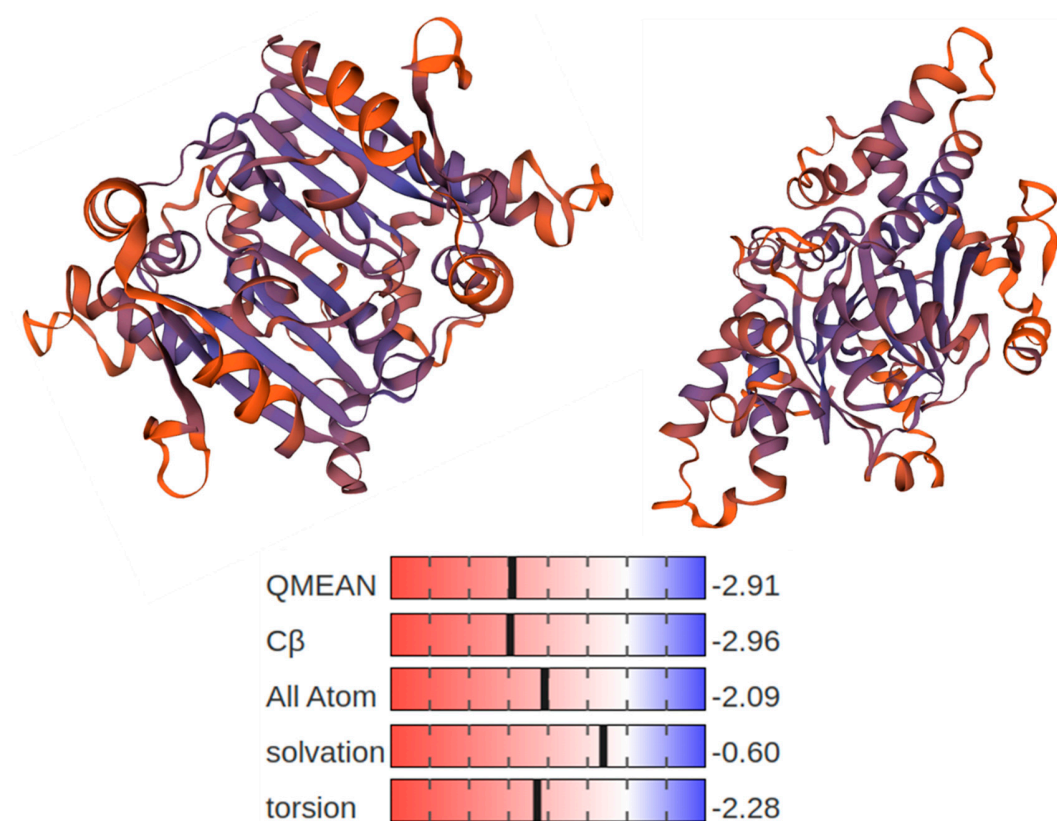


Figure S2. 3D representation of the homology model of type I MtCA3 and related parameters calculated from Swiss-model.

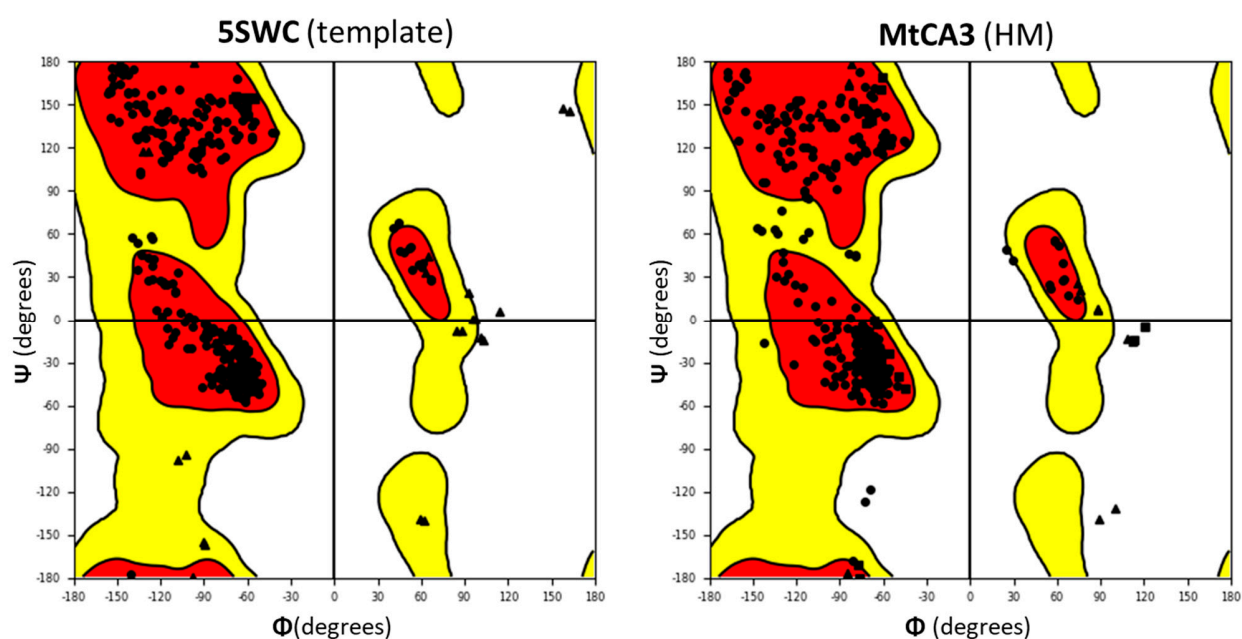


Figure S3. Ramachandran Plot of 5SWC (template) and MtCA3 (HM).

	5SWC	MtCA3
MolProbity score	1.22	1.71
Clash score	4.48	2.32
Ramachandran Favoured	99.38 %	94.53 %
Ramachandran Outliers	0.00 %	1.49 %
Rotamer Outliers	0.88%	2.68 %
C-Beta Deviations	0	8
Bad Bonds	0/3602	0/3138
Bad Angles	1/4886	59/4302
QMEAN	1.31	-2.91
Cβ	1.27	-2.96
All Atom	0.38	-2.09
solvation	0.98	-0.60
torsion	0.76	-2.28

Table S1. Structural parameters of 5SWC (template) and MtCA3 (HM).

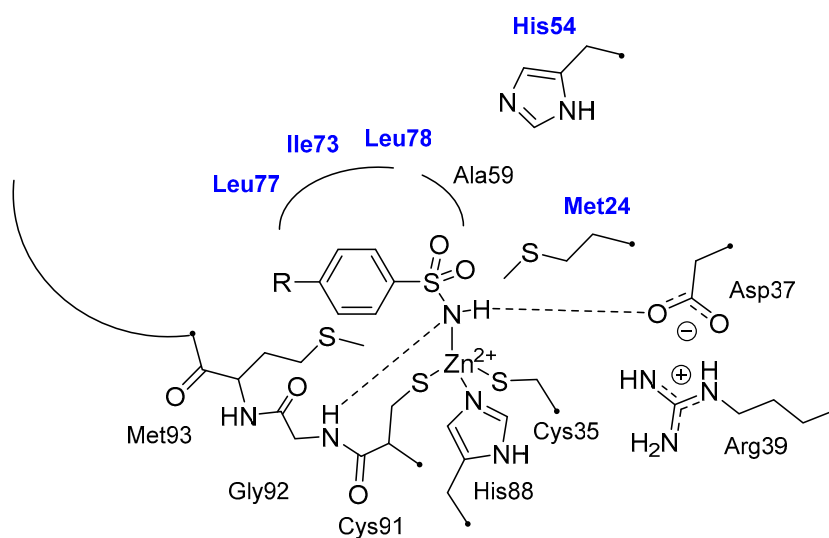


Figure S4. 2D schematic representation of MtCA1 residues involved in the interaction with benzenesulfonamides hypothesized by the *in silico* studies. The labels of amino acids from different chains are colored differently.

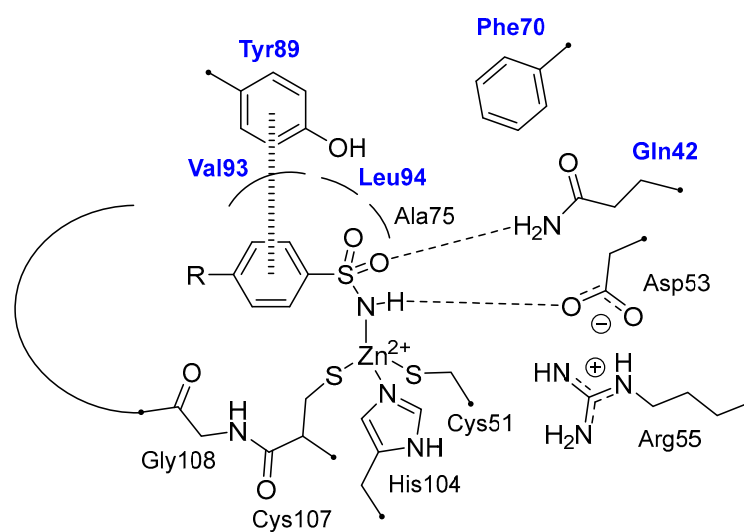


Figure S5. 2D schematic representation of MtCA2 residues involved in the interaction with benzenesulfonamides hypothesized by the *in silico* studies. The labels of amino acids from different chains are colored differently.

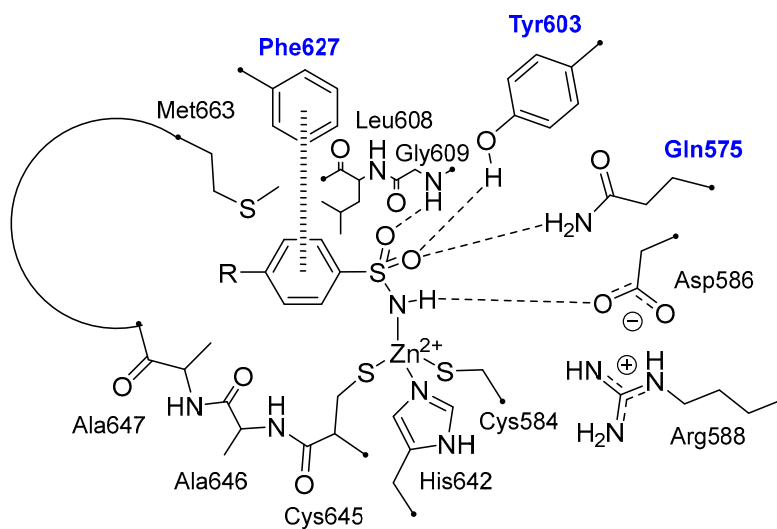


Figure S6. 2D schematic representation of MtCA3-HM residues involved in the interaction with benzenesulfonamides hypothesized by the *in silico* studies. The labels of amino acids from different chains are colored differently.