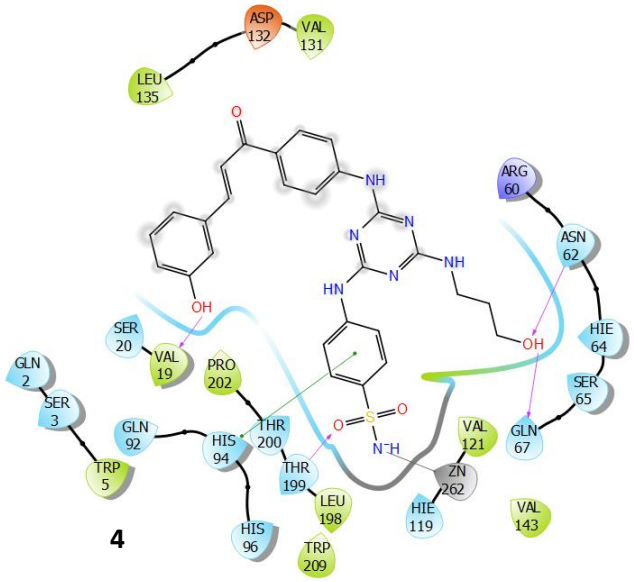
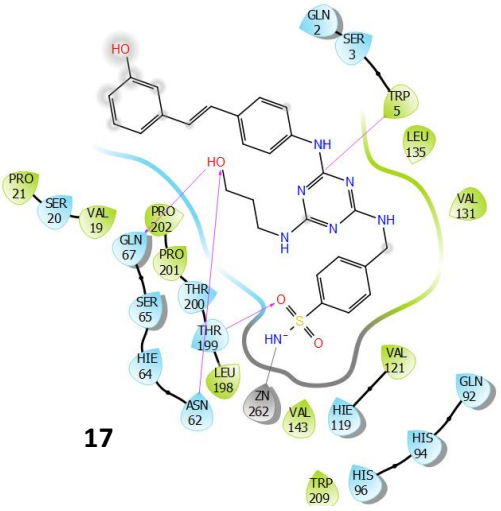
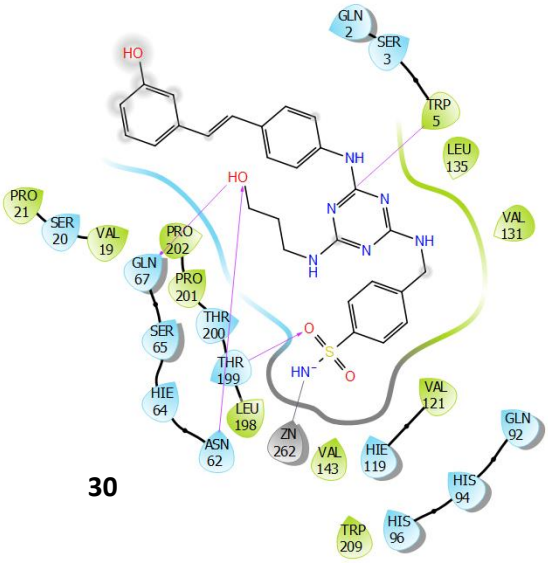
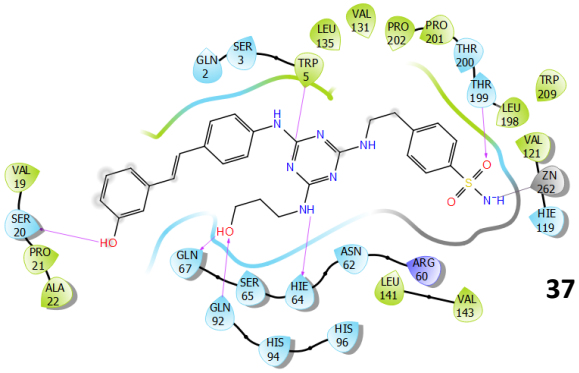
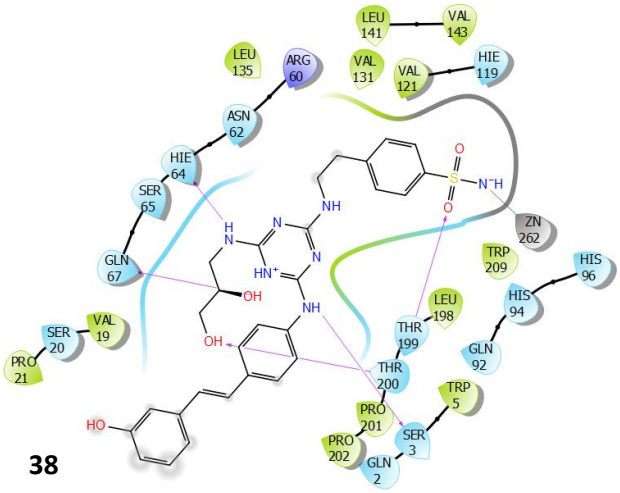
Supplementary information

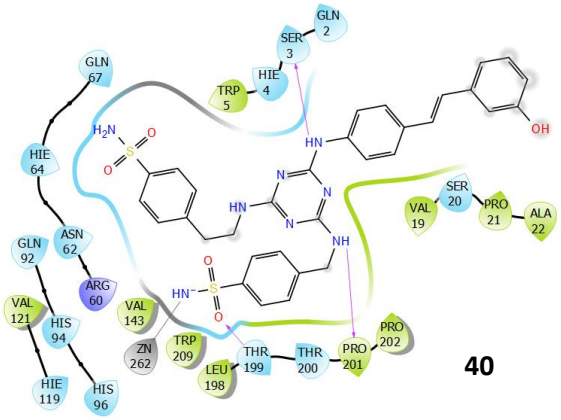


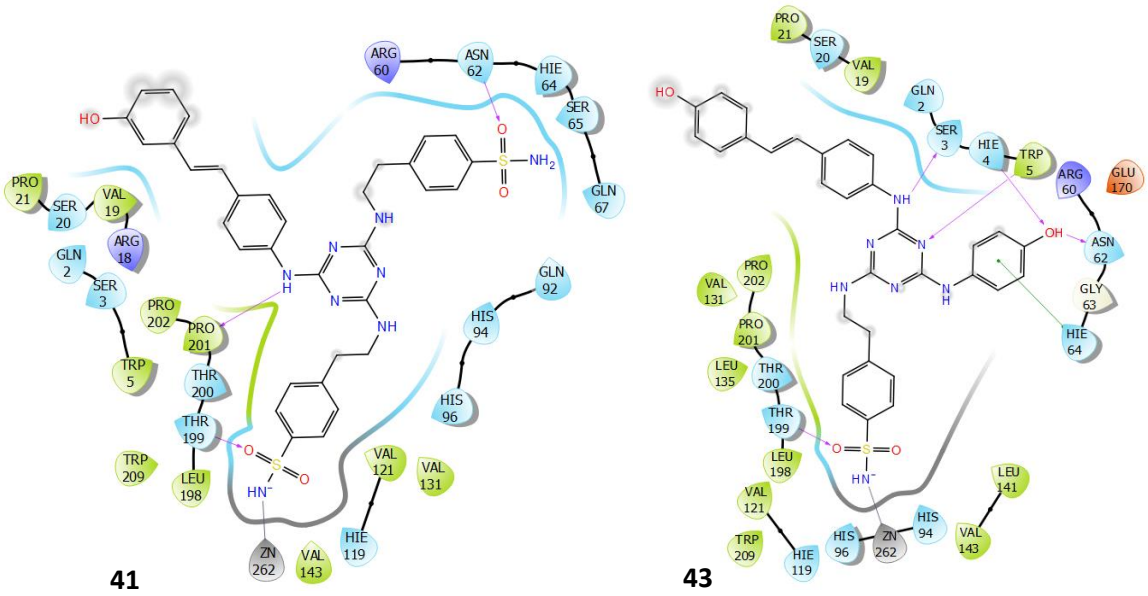




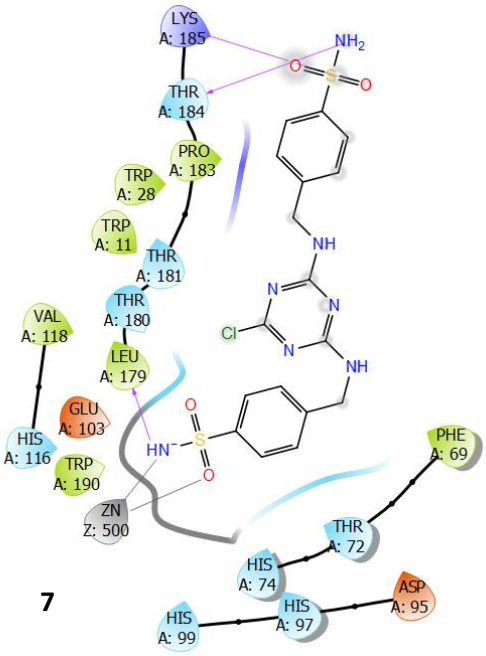




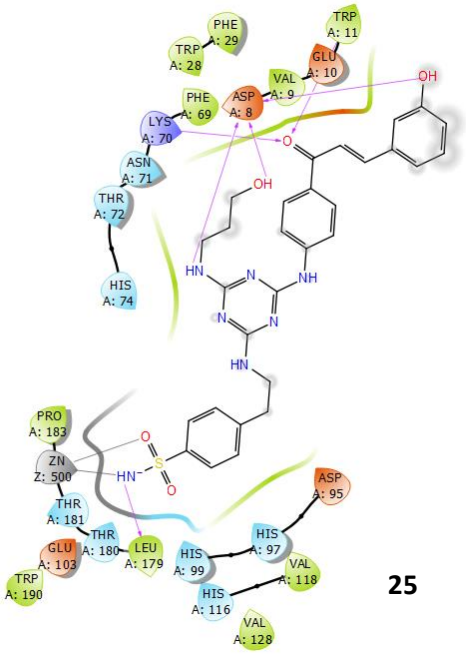




Suppl. Inf. Figure 1. 2D interaction diagrams of ligands docked in hCA IX.


LYS A: 185
NH2
THR A: 184
PRO A: 183
TRP A: 28
TRP A: 11
THR A: 181
THR A: 180
VAL A: 118
LEU A: 179
GLU A: 103
HIS A: 116
TRP A: 190
ZN Z: 500
PHE A: 69
THR A: 72
HIS A: 74
HIS A: 97
ASP A: 95
HIS A: 99

7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TRP A: 28
TRP A: 11
GLU A: 10
VAL A: 9
PHE A: 69
ASP A: 8
LYS A: 70
ASN A: 71
THR A: 72
HIS A: 74
PRO A: 183
ZN Z: 500
THR A: 181
THR A: 180
LEU A: 179
GLU A: 103
TRP A: 190
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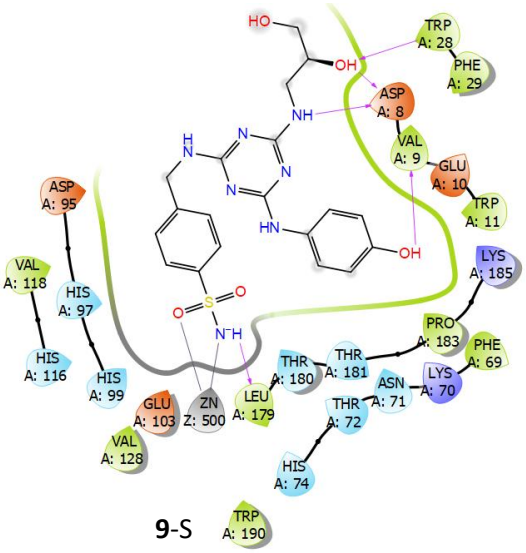
HIS A: 97
ASP A: 95
VAL A: 118
HIS A: 116
VAL A: 128

25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PHE A: 29
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VAL A: 9
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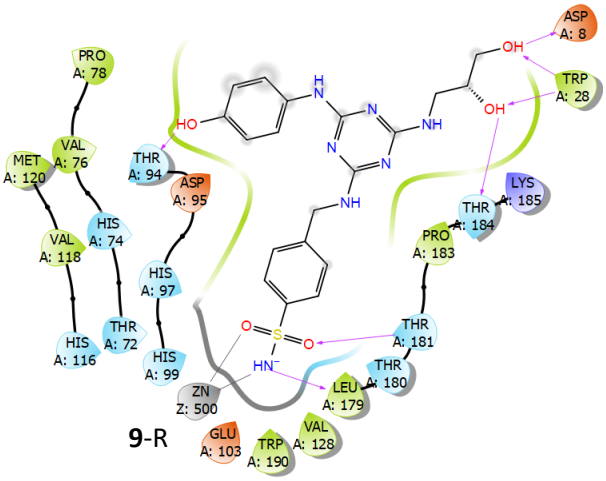
ASP A: 95
VAL A: 118
HIS A: 97
HIS A: 116
HIS A: 99
GLU A: 103
ZN Z: 500
LEU A: 179
THR A: 180
THR A: 181
LYS A: 185
PRO A: 183
PHE A: 69
ASN A: 71
LYS A: 70
THR A: 72
HIS A: 74
VAL A: 128
TRP A: 190

9-S


ASP A: 8
TRP A: 28
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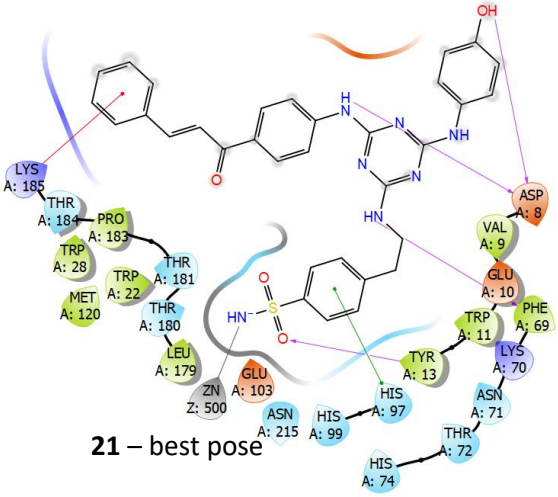
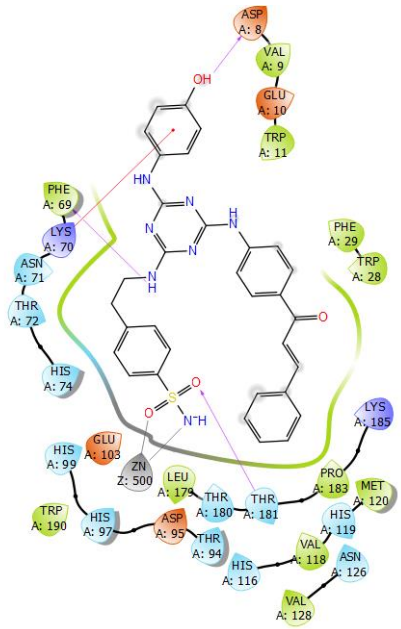
ASP A: 95
VAL A: 118
HIS A: 74
HIS A: 97
THR A: 72
HIS A: 116
HIS A: 99
ZN Z: 500
LEU A: 179
GLU A: 103
TRP A: 190
VAL A: 128
THR A: 180
THR A: 181
PRO A: 183
THR A: 184
LYS A: 185

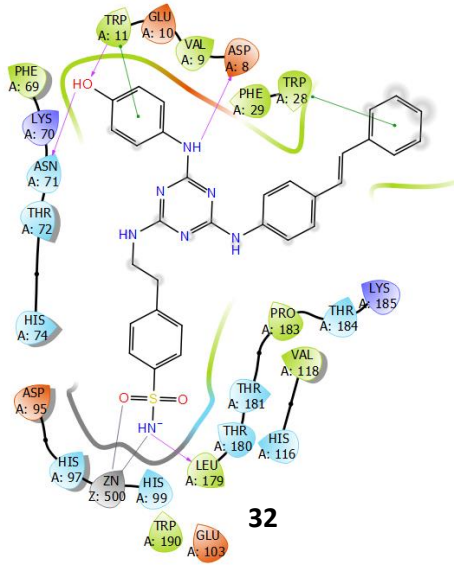
9-R



21 – best pose



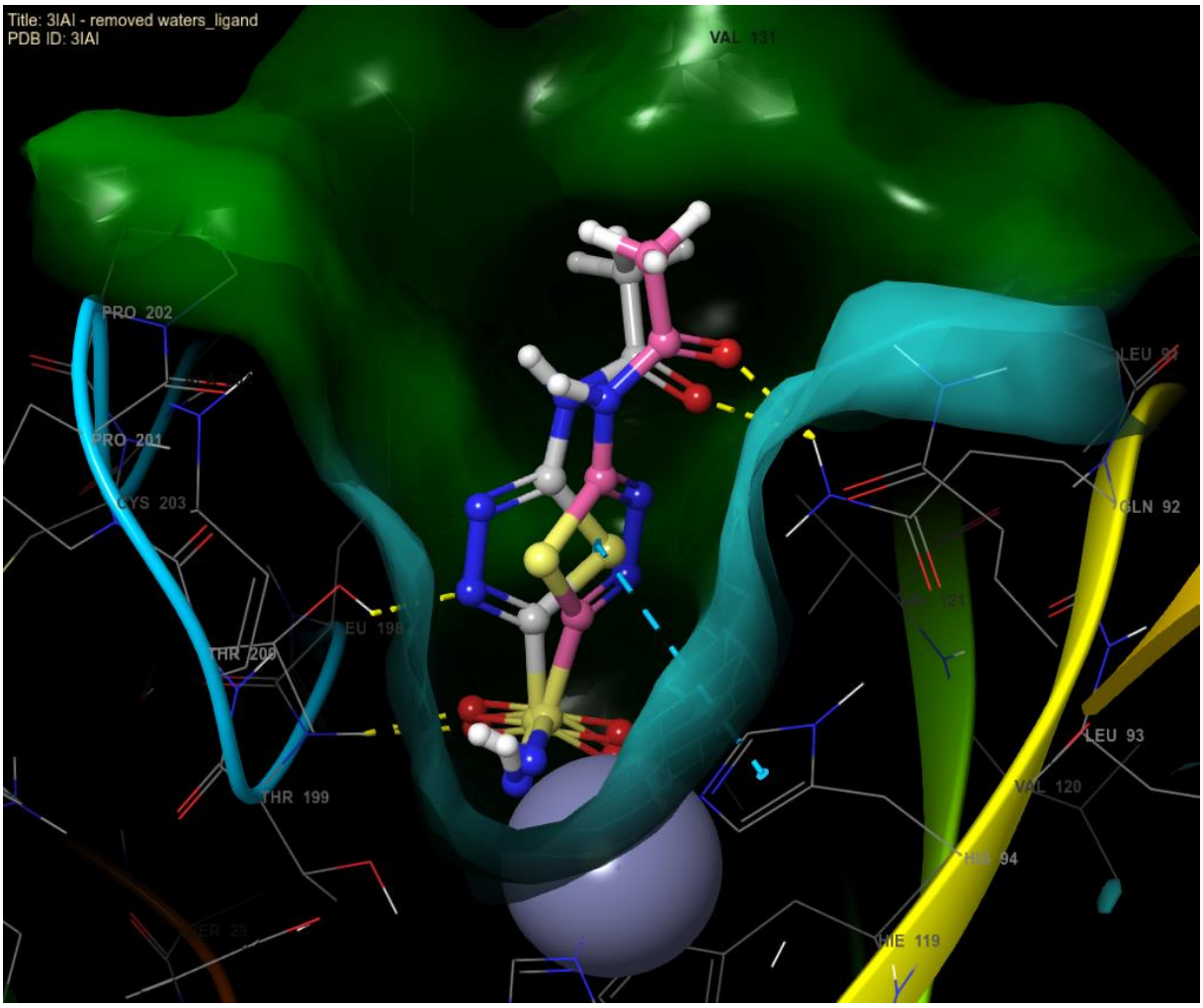
21 – bidentate coordination



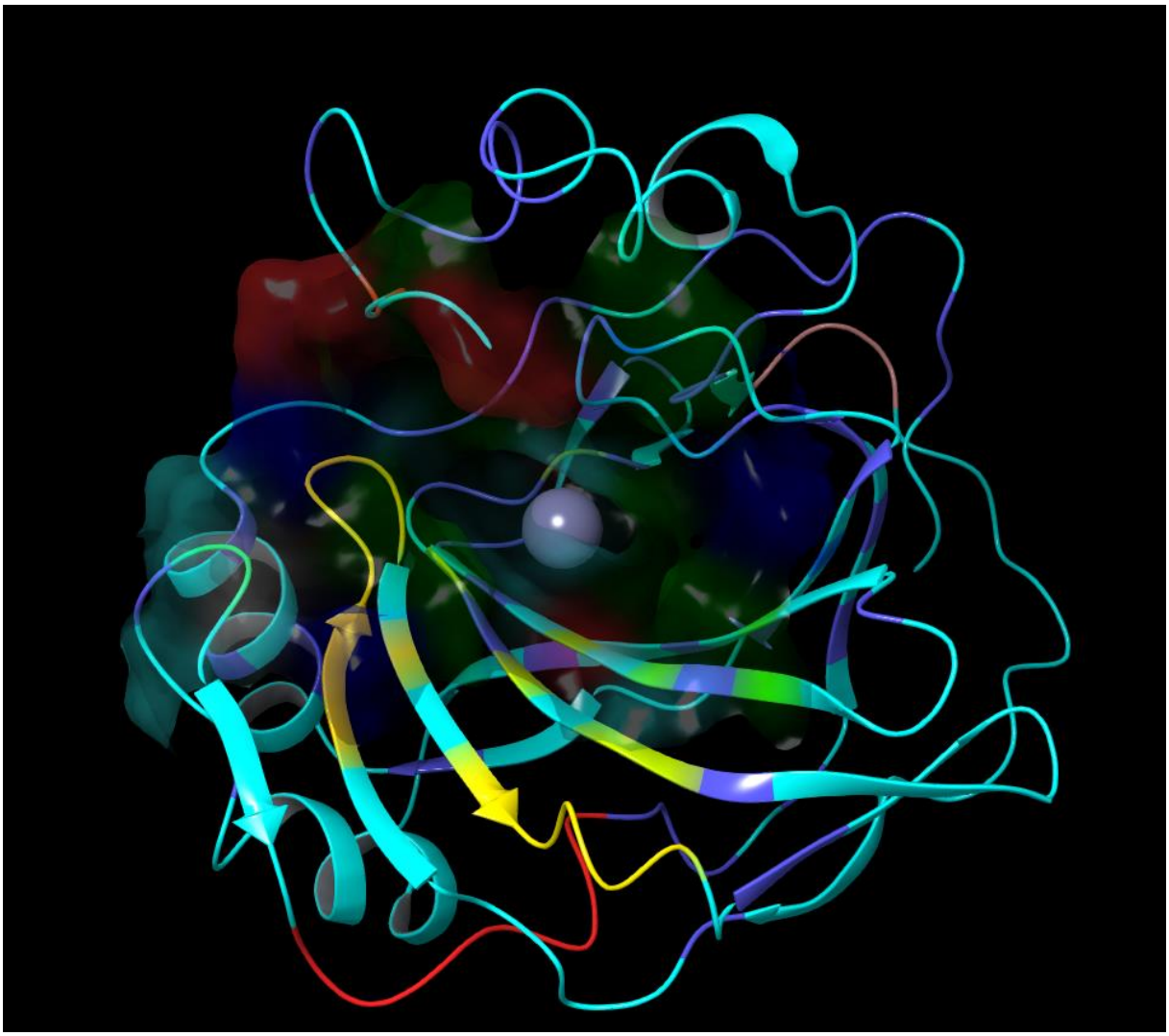
32

Charged (negative)
Charged (positive)
Glycine
Hydrophobic
Metal
Polar
Unspecified residue
Water
Hydration site
Hydration site (displaced)
Distance
H-bond
Metal coordination
Pi-Pi stacking
Pi-cation
Salt bridge
Solvent exposure

Suppl. Inf. Figure 2. 2D interaction diagrams of ligands docked in enterococcal CA.



Suppl. Inf. Figure 3. Superposition of acetazolamide co-crystallized with hCA IX (the molecule with light gray carbons) and pose of acetazolamide docked in hCA IX (the molecule with pink carbons). RMSD = 1.57 $Å^2$



Suppl. Inf. Figure 4. 3D representation of enterococcal carbonic anhydrase created by homology modeling. Protein is depicted by ribbon and surface area of binding site with zinc dication at the bottom.