



STRUCTURAL BIOLOGY
COMMUNICATIONS

Volume 75 (2019)

Supporting information for article:

Carbonic anhydrase II in complex with carboxylic acid-based inhibitors

Carrie L. Lomelino and Robert McKenna

Table S1 Previously deposited carboxylic acid CA inhibitors that anchor to ZBW. Coloring of compound names coordinates to Figure 1A.

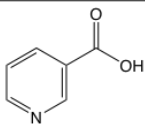
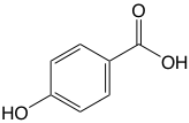
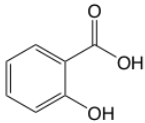
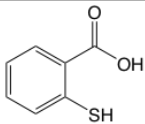
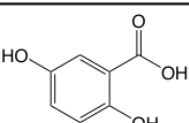
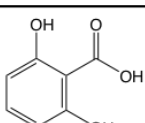
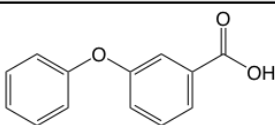
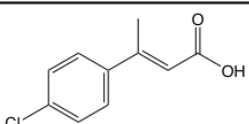
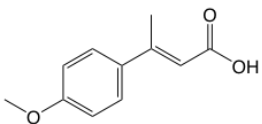
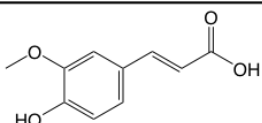
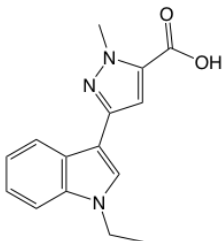
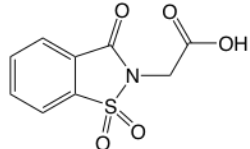
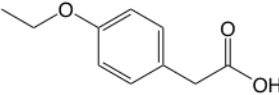
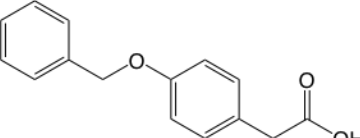
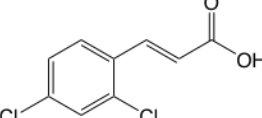
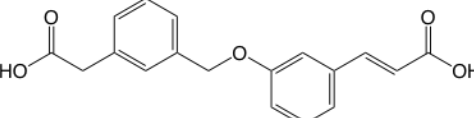
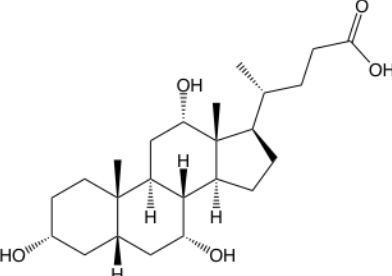
Name	Structure	PDB Code
pyridine-3-carboxylic acid (nicotinic acid)		6MBV
4-hydroxybenzoic acid		4E3G
2-hydroxybenzoic acid		5M78
2-sulfanylbenzoic acid		4E4A
2,5-dihydroxybenzoic acid		4E3D
2,6-dihydroxybenzoic acid		4E3F
3-phenoxybenzoic acid		5FLT
(E)-3-(4-chlorophenyl)but-2-enoic acid		5FLS
(E)-3-(4-methoxyphenyl)but-2-enoic acid		5EH8
(E)-3-(4-hydroxy-3-methoxyphenyl)prop-2-enoic acid (ferulic acid)		6MBY
3-(1-ethyl-1H-indol-3-yl)-1-methyl-1H-pyrazole-5-carboxylic acid		6B4D

Table S2 Previously deposited carboxylic acid CA inhibitors that bind directly to Zn. Coloring of compound names coordinates to Figure 1B.

Name	Structure	PDB Code
(1,1-dioxido-3-oxo-1,2-benzothiazol-2(3H)-yl)acetic acid		5CLU
2-(4-ethoxyphenyl)ethanoic acid		5FNJ
2-(4-phenylmethoxyphenyl)ethanoic acid		5FLQ
(E)-3-(2,4-dichlorophenyl)prop-2-enoic acid		5EHW
(~{E})-3-[3-[[3-(2-hydroxy-2-oxoethyl)phenyl]methoxy]phenyl]prop-2-enoic acid		5EHV
cholic acid		4N16