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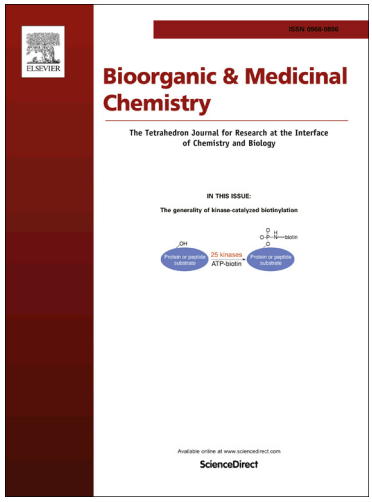

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Kinetic and X-ray crystallographic investigations of substituted 2-thio-6-oxo-1,6-dihydropyrimidine-benzenesulfonamides acting as carbonic anhydrase inhibitors

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Abstract: Herein we report an *in vitro* kinetic evaluation against the most relevant human carbonic anhydrase (hCA, EC 4.2.1.1) isoforms (I, II, IX and XII) of a small series of lactate dehydrogenase (LDH, EC 1.1.1.27) inhibitors. All compounds contain a primary sulfonamide zinc-binding group (ZBG) substituted with the 2-thio-6-oxo-1,6-dihydropyrimidine scaffold. By means of X-ray crystallographic experiments we explored the ligand-enzyme binding modes, thus highlighting the contribution of the 2-thio-6-oxo-1,6-dihydropyrimidine moiety to the stabilization of the complex.

Keywords: Carbonic Anhydrase (CA); X-Ray crystallography, Sulfonamides, 2-Thio-6-oxo-1,6-dihydropyrimidines.

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