

## عنوان مقاله:

Theoretical investigation of human carbonic anhydrase inhibition By polyamines

## محل انتشار:

پنجمین کنفرانس ملی پژوهش های نوین در شیمی و مهندسی شیمی (سال: 1397)

تعداد صفحات اصل مقاله: 4

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## خلاصه مقاله:

Carbonic anhydrases (CAs) have been inhibited by different compounds such as sulfonamides, phenols, and coumarins. Polyamines such as spermine is described to constitute a novel class of CA inhibitors (CAIs), interacting with the different CA isozymes with efficiency from the low nanomolar to millimolar range. The mechanism of interaction between spermine polyamine and CA active site was studied using DFT calculations. According to our calculated results spermine anchors to the nonprotein zinc ligand through a network of hydrogen bonds. Its distal amine moiety makes hydrogen bonds with residues Thr200 and Pro201, which further stabilize the adduct. Spermine binds differently compared to sulfonamides, phenols, or coumarins, rendering possible to develop CAIs with a diverse inhibition mechanism, profile, and selectivity for various isoforms.

## کلمات کلیدی:

Polyamine, Spermine, Inhibitor, Carbonic anhydrase, DFT calculations

## لینک ثابت مقاله در پایگاه سیویلیکا:

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