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"PHARMACOPHORE-BASED DESIGN, SYNTHESIS AND COMPUTATIONAL STUDIES ON NEW THIADIAZOLE DERIVED CARBONIC ANHYDRASE INHIBITORS"

The carbonic anhydrases (CAs) constitute interesting targets for the design of pharmacological agents useful in the treatment or prevention of a variety of disorders such as among others, glaucoma, acid–base disequilibria, epilepsy and recently cancer. New thaidiazole derivatives were designed using a pharmacophore based approach. The synthesized derivatives showed promising CA inhibitory activities especially against the tumor associated CA isozyme. Docking experiments and QSAR calculations were done in order to validate the results and predict the orientation of the tested compounds into the CA active site.