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Discovery of curcumin heterocyclics containing sulphonamides for carbonic anhydrase inhibition and molecular docking studies

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Abstract

Curcumin is a multi-functional pharmacologically safe natural agent with proven cytoprotective effects to healthy human cells. In this study, a new series of 22 sulfonamides with curcumin scaffold were synthesized, characterized and investigated for their carbonic anhydrase isoenzyme I (human) and II (bovine) isoforms. The structures of newly synthesized compounds were described by IR, 1H NMR and 13C NMR spectral data. Curcumin-isoxazole conjugated sulfonamide showed the Ki value of 0.99 µM with highest inhibitory activity among all other synthesized compounds against hCA-I enzyme. Similarly enzyme kinetic studies of compounds like curcumin-isoxazole, curcumin-pyrazole, and curcumin-pyrimidine conjugated sulfonamide against bCAII enzyme showed Ki values of 0.71, 0.67 and 0.71 µM respectively. Our biological assays results showed that most of active compounds have similar inhibitory activities compared to standard acetazolamide drug. The molecular docking predicted binding modes showed that these compounds bind with hCA-1 enzyme in similar fashion.

Biography:

Dr Mahmood Ahmed is Head Quality Operations and R & D, currently working in Renacon Pharma Limited. He received his M.Sc. (2003), M.Phil. (2013) and PhD (2018) degrees in Chemistry from Institute of Chemistry, University of the Punjab, Lahore-Pakistan. From analytical chemistry point of view, current research focuses on development and validation of method for analysis of foods and pharmaceutics. As a medicinal & pharmaceutical scientist, his research focuses on the exploration of novel drug analogs for various pharmacological properties against different phenotypes of various disease models. As pharmaceutical professional, demonstrate efforts for creating balance between quality and operations by implementing master validation plan (MVP) by defining quality objectives and strategies. He published 68 research papers in peer reviewed journals and also has reviewed 121 research articles for 26 international journals.

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