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Amplifying the role of collaboration globally for neglected and commercial disease drug discovery

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Collaborative innovation is uniquely able to realize the economics of well-integrated specialization required for drug discovery. Particularly in the neglected infectious disease areas lacking a profit motive, better collaborative tools are fundamentally important to catalyze faster progress. Layering unique collaborative capabilities upon requisite drug discovery database functionality unlocks and amplifies synergy between biologists and chemists. Researchers need to have tools that balance individual needs for robust, intuitive registration and bioactivity analyses while at the same time facilitating collaborations with secure data partitioning, communication, and group engagement. Since collaborative technology is "therapeutic area agnostic", it has generally been proven equally applicable for commercial applications. Representative commercial case studies include broad consortia such as the NIH Neuroscience Blueprint collaboration between drug discovery companies, CROs, together with seven leading academic biology laboratories as part of a 5-year government contract to advance new CNS drugs into the clinic. As well as more focused examples following the lean venture funded model such as the collaboration between Acetyton Pharmaceuticals with Harvard and a Chinese CRO to bring a selective HDAC inhibitor into the clinic. Finally, by spanning the continuum of private, collaborative and public modes, researchers globally can now seamlessly collaborate across the pre-competitive and competitive landscape.

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Design, homology modeling, docking studies and microwave-assisted synthesis of some novel triazolothienopyrimidines as possible antagonosts of A3 adenosine receptors

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Asthma and chronic obstructive pulmonary disease (COPD) are prevalent inflammatory disorders of the lung and are poorly managed. It has been observed that adenosine plays an important role in mediating bronchial constriction, pulmonary inflammation and airway remodeling by interacting with its different G-protein coupled receptors: A1, A2A, A2B and A3 ARs and these receptors are considered to be important targets for new drug development for asthma. In the present work, design, homology modeling and docking studies (Glide v5 XP, Schrodinger Inc.) were carried out to explore the physicochemical requirements for selective binding towards A3 AR in order to design and develop new and safe NCEs with fused thienopyrimidine scaffold as possible A3 antagonists as it is postulated to be a potential target for the treatment of Asthma. Docking studies were carried out by using the homology model of A3 AR developed (Prime, Schrodinger) using the X-Ray crystal structure of A2A AR (PDB:3EML). All the designed compounds (thieno[3,2-e]-[1,2,4]triazolo[1,5-c]pyrimidins) were synthesised using the eco-friendly microwave assisted organic synthesis (MAOS) methods. In vitro AR binding studies as well as in vivo anti-inflammatory studies indicates that some of the compounds are very potent and the results are in consonance with the in-silico studies.

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