Asthma is a popular disease nowadays. There are many factors which are responsible for inducing symptoms of asthma. Many classes of drugs namely bronchodilators and anti-inflammatory agents have resulted in substantial improvement in survival and quality of life of asthmatic patients. Here we aim to search for a new chemical entity possessing better bronchodilatory effects and find out the structure solution by mean of synchrotron powder diffraction.

2,3,4,5-tetrahydroazepino[2,1-b]quinazolin-11(1H)-one(1) has been studied as a template. In addition, a number of nitrogenous functions were introduced at position 8, 9. The synthesized compounds were studied for their bronchodilatory activity using isolated guinea pig tracheal chain. The 3-D structure is also a key feature to understand their function. In this report, three series asthmatic drug targets structures are successfully solved by synchrotron powder diffraction data and combined simulated annealing method.

![Diagram of chemical structure](image)

Keywords: structure-aided drug design; structure from powder diffraction; quinazoline


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