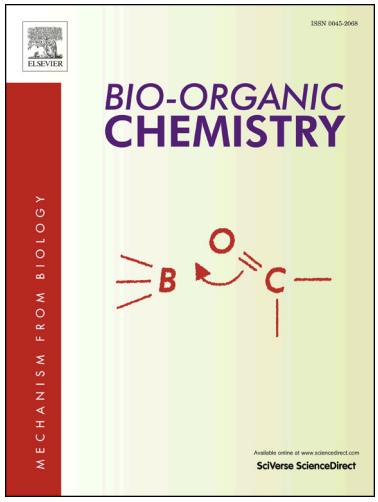


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# Applications of structure-based design to antibacterial drug discovery

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**Abstract**

In recent years bacterial resistance has been observed against many of our current antibiotics, for instance most worryingly against the cephalosporins which are typically the last line of defence against many bacterial infections. Additionally the failure of high throughput screening in the discovery of new antibacterial drug leads has led to a decline in the number of antibacterial agents reaching the market. Alternative methods of drug discovery including structure based drug design are needed to meet the threats caused by the emergence of resistance. In this review we explore the latest advancements in the identification of new antibacterial agents through the use of a number of structure based drug design programs.

*Bio-organic Chemistry*

*Keywords: Structure based drug design, Antibacterial Agents*

**Highlights:**

Structure-based drug design is an important tool in the design of antibacterial compounds

Use of computational design in the modification of known inhibitors

Use of SPROUT, CAVEAT and LUDI for the *de novo* design of inhibitors of bacterial targets.

vHTS using AutoDock, eHiTs, Glide and FRED to identify potential antibacterial compounds.

## 1 Introduction

### *1.1 Antibacterial agents*

The emergence and spread of antibiotic resistant bacteria is a serious threat to world health[1]. The development of new antibiotics with novel modes of action is essential in order to provide replacements for current drugs for which resistance is widespread[2]. The increase in human air travel over recent years and the unregulated prescription of antibiotics in the developing world are believed to be important factors in the rapid spread of antibiotic resistant bacterial strains. The discovery of new antibiotic classes has proven to be a serious