Current strategies in antibacterial drug discovery

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Introduction. In the design of new pharmaceutical agents, it is clear that multiple factors need to be adjusted in parallel to discover the best balance of efficacy and safety. After many years of thorough medicinal chemistry investigations on the modification of well–known antibacterial scaffolds, it is becoming increasingly hard to deliver new leads.

Materials and methods. The focus of much antibacterial research has, therefore, moved to the identification of novel chemical classes and novel bacterial targets.

Results. A significant portion of modern antibacterial drug discovery yet concentrated on the lead finding and optimization of ligands by evaluating, among other properties, their affinity to the primary target, because such targets are proteins that are related to diseases. If a drug interacts with a target, that drug can possibly be used to treat the corresponding disease. An antimicrobial–drug target should be essential, have a unique function in the pathogen and show an activity that can be rearranged over by tiny molecules.

The number of appropriate drugs having known interactions with targets is extremely small compared to the number of all available chemical compounds that could be potential drug candidate. Identifying new drug–target interactions for either approved drugs or novel drug candidates is a fundamental step in drug discovery.

Conclusion. Structure based drug design provides an excellent platform for the identification of new antibacterial compounds. Inhibitors of bacterial proteins and further optimization of lead structure have been done using up–to–date *in silico* software.

Literature.

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