or dissemination. Small molecule directed to act on host targets could potentiate innate immunity. This can be achieved by employing systems biology approaches, with key signaling pathways in the host–pathogen interplay identified as host proteins for therapeutic targeting. The 3D structures of such proteins could be modeled and used for the SBDD of host-directed small molecules that will regulate bacterial infection (Chiang et al. 2018).

13.8 Conclusion

The computer-aided design of therapeutic agents to fight antibiotic resistance did not fully achieve its full potential despite promising success stories. The time required for bacteria to equip itself with a defense mechanism against antibiotics is far shorter than for a new drug to treat infection to be discovered, to be developed, and to enter the clinic. Thus, in addition to developing new antibiotics, new strategies such as developing combination therapies, repurposing of already approved drugs, and design of drug delivery systems capable to specifically target pathogens are needed. A "clever" use of all available information on structures, activities, molecular properties, toxicities, plasma binding, and off-target interactions should enable utilization of modular workflows in machine learning methods and artificial intelligence approaches. Furthermore, "open-source" or a "community-based research" efforts, such as Community for Open Antimicrobial Drug Discovery (CO-ADD) initiative, should be supported and stimulated to enable our ability to address the global threat of antimicrobial resistance. The current progress in this field and increased availability of information and resources indicate that "golden era" for computer-aided antibiotic therapy design is coming.

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