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Creation of a Structural Database for Inhibition of Biofilm Formation

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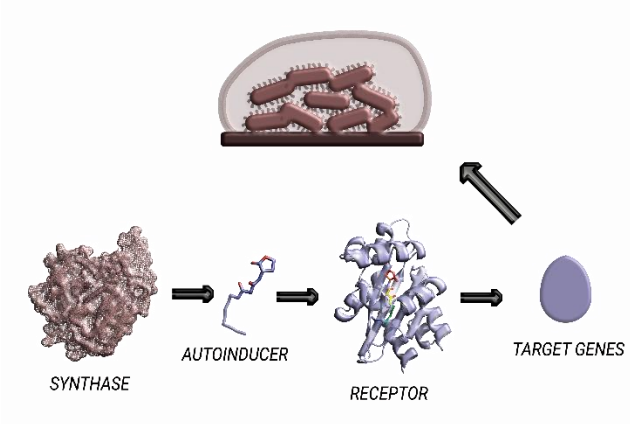
Graphical Abstract



Abstract

Biofilms can be prevalent in natural, industrial and hospital settings and are associated to ca. 80% of all human infections [1]. The increased antimicrobial resistance and mutation rate of bacteria in biofilms contributes to the development of antibiotic resistance, greatly limiting the therapeutic options to a variety of infections, posing a critical problem to the biomedical sector. Preventing biofilm formation could dramatically reduce the effects of infectious diseases [2].

Quorum-sensing (QS) is the cell-to-cell communication in bacteria and contributes to the formation of organized structural communities of bacteria in biofilms [3]. Several different microbial-derived signalling molecule types and receptors have been recently identified, offering a very appealing opportunity for rational design of new drugs.

This work reports the creation of a database containing all the available experimental X-ray structures for all the synthases and receptors

	known to be involved in quorum sensing and includes also structural and biological information on all the known compounds with demonstrated inhibitory activity against each of these protein targets. This database will provide useful atomic-level information for researchers working on this field with direct application in drug design and development efforts through docking, virtual screening, molecular dynamics and QSAR techniques.

References

1. Worthington, R. J.; Richards, J. J.; Melander, C., Small molecule control of bacterial biofilms. *Organic & biomolecular chemistry* **2012,** *10* (37), 7457-74.~

2. Subhadra, B.; Kim, D. H.; Woo, K.; Surendran, S.; Choi, C. H., Control of Biofilm Formation in Healthcare: Recent Advances Exploiting Quorum-Sensing Interference Strategies and Multidrug Efflux Pump Inhibitors. *Materials (Basel, Switzerland)* **2018,***11* (9).

3. Banerjee, G.; Ray, A. K., Quorum-sensing network-associated gene regulation in Gram-positive bacteria. *Acta microbiologica et immunologica Hungarica* **2017,** *64* (4), 439-453.