# Creation of a Structural Database for Inhibition of Biofilm Formation

**Rita P. Magalhães[1,2]\*, Tatiana F. Vieira[1], Henrique S. Fernandes[1],**
**Nuno M.F.S.A. Cerqueira[1], André Melo[2], Manuel Simões[3], Sérgio F. Sousa[1]**

[1]UCIBIO@REQUIMTE, BioSIM, Departamento de Biomedicina - Faculdade de Medicina da Universidade do Porto
[2]LAQV@REQUIMTE, Departamento de Química e Bioquímica - Faculdade de Ciências da Universidade do Porto
[3]LEPABE, Departmento de Engenharia Química - Faculdade de Engenharia da Universidade do Porto

✉ *ritaprata1@hotmail.pt

LAQV requimte
LABORATÓRIO ASSOCIADO PARA A QUÍMICA VERDE
biosim
www.biosim.pt
FC FACULDADE DE CIÊNCIAS UNIVERSIDADE DO PORTO
U. PORTO
FMUP FACULDADE DE MEDICINA UNIVERSIDADE DO PORTO

## BIOFILMS [1,2,3]

- Biofilms are a community of individual bacteria glued together and enclosed in a **self-produced EPS matrix** attached to a surface.

- Bacteria in biofilms show differences in gene expression, resulting in a **higher resistance to antibiotics** and the host immune defenses.

- They are responsibly for ca. **80% of bacterial infections** in the body, including lung infections in cystic fibrosis patients.

- Biofilm **infections of medical apparatu**s are virtually impossible to eliminate, especially when they involve **multi-drug resistant bacteria.**
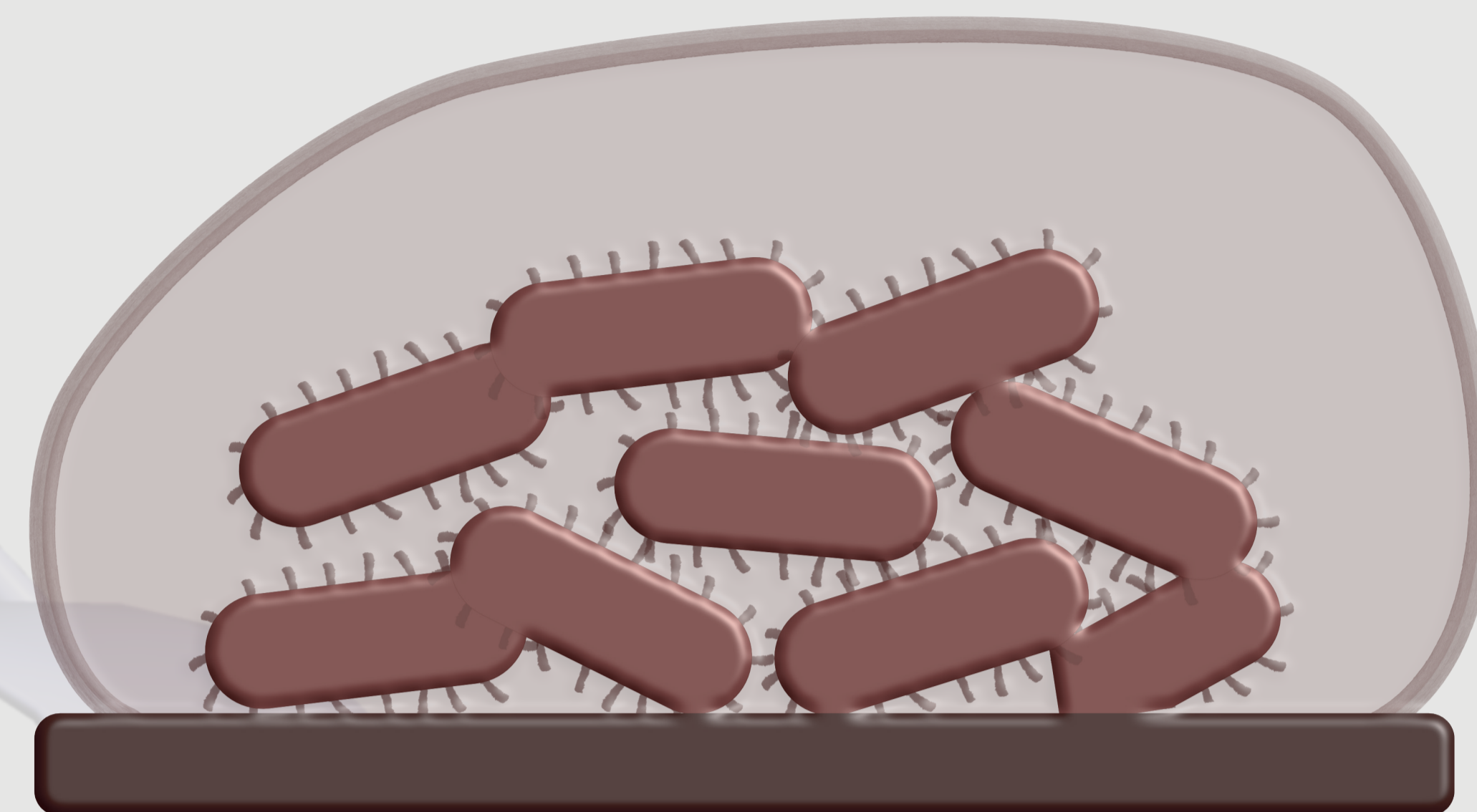
## QUORUM-SENSING [1,3]

**Quorum-sensing (QS)** is the cell-to-cell communication in bacteria.
It involves a **synthase** that produces a diffusible molecule (autoinducer) and a **receptor** that detects the signal, resulting in altered gene expression and community behavior, such as **biofilm formation** or motility.

SYNTHASE → AUTOINDUCER → RECEPTOR → TARGET GENES
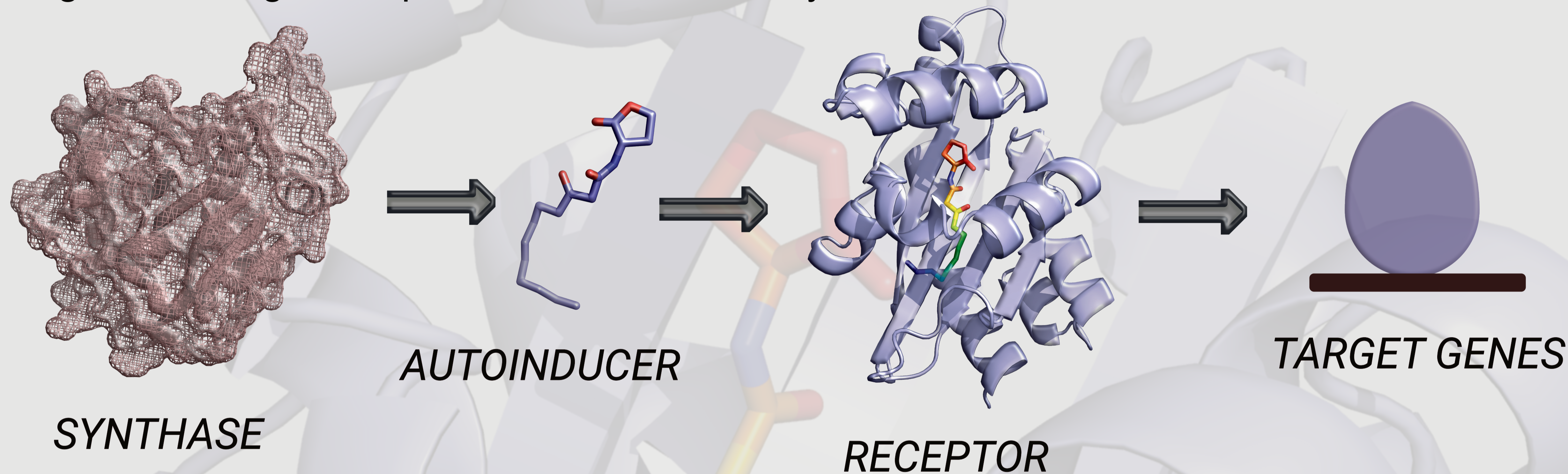
## THE DATABASE

**RATIONALE**

Creation of a database containing all available **experimental structures** for synthases and receptors involved in **quorum-sensing**, which will provide useful information for researchers working in **drug design** through docking, virtual screening, molecular dynamics and QSAR techniques.

**METHODOLOGY**

**FINAL RESULT**

### Biofilms Database

Search...

Advanced Search
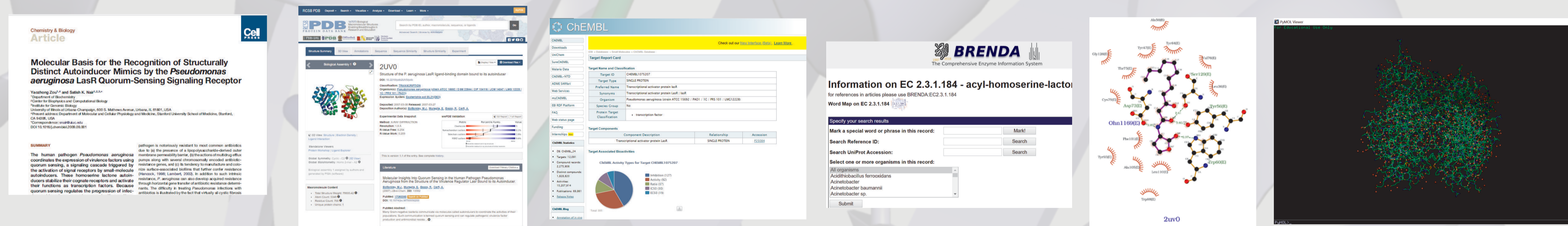
| Code | Protein | Category | Classification | Autoinducer Type | Organism | Gram Type | Ligand | Mutation Pathway | Method | Res. (Å) | Year | DOI | PDB | External Links |
|------|---------|----------|----------------|------------------|----------|-----------|--------|------------------|--------|----------|------|-----|-----|----------------|
| 2UV0 | LasR | Receptor | Transcription | Acyl-Homoserine-Lactones | *Pseudomonas aeruginosa* | ⊖ | OC12-HSL | No | X-Ray Diffraction | 1.8 | 2007 | 10.1974/bc.M706556200 | | ChEMBL BindingDB ExPASy KeGG UniProt |
| 3IX3 | LasR | Receptor | Transcription | Acyl-Homoserine-Lactones | *Pseudomonas aeruginosa* | ⊖ | OC12-HSL | No | X-Ray Diffraction | 1.4 | 2009 | Not available | | ChEMBL BindingDB ExPASy KeGG UniProt |
| 4NG2 | LasR | Receptor | Transcription | Acyl-Homoserine-Lactones | *Pseudomonas aeruginosa* | ⊖ | OC12-HSL | No | X-Ray Diffraction | 2.41 | 2013 | 10.1074/mbc.1334451010 | | ChEMBL BindingDB ExPASy KeGG UniProt |
| 3IX4 | LasR | Receptor | Transcription | Acyl-Homoserine-Lactones | *Pseudomonas aeruginosa* | ⊖ | TX1 | No | X-Ray Diffraction | 1.8 | 2009 | 10.1016/j.chembiol.2009.09.001 | | ChEMBL BindingDB ExPASy KeGG UniProt |
| 3IX8 | LasR | Receptor | Transcription | Acyl-Homoserine-Lactones | *Pseudomonas aeruginosa* | ⊖ | TX3 | No | X-Ray Diffraction | 1.8 | 2009 | 10.1016/j.chembiol.2009.09.001 | | ChEMBL BindingDB ExPASy KeGG UniProt |

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### LasR

| | |
|---|---|
| Category: Receptor | Classification: Transcription |
| Organism: *Pseudomonas aeruginosa* | Gram Type: Negative |
| Ligand: OC12-HSL | Autoinducer Type: Acyl-Homoserine-Lactones |
| Method: X-Ray Diffraction | Resolution (Å): 1.8 |
| Year: 2007 | DOI: 10.1074/bc.M706556200 |
| PDB: | |

External links: ChEMBL - BindingDB - ExPASy - KeGG - UniProt

### OC12-HSL

| | |
|---|---|
| ID: OHN | Name: N-3-oxo-dodecanoyl-L-homoserine Lactone |
| Molecular Weight: 297.39 | SMILES: CCCCCCCCC(=O)CC(=O)N[C@H]1CCOC1=O |
| Formula: C16 H27 N O4 | Identifier: 3-oxo-N-[(3S)-2-oxooxolan-3-yl]dodecanamide |
| Formal Charge: 0 | InChI: InChI=1S/C16H27NO4/c1-2-3-4-5-6-7-8-9-13(18)12-15(19)17-14-10-11-21-16(14)20/h14H,2-12H2,1H3,(H,17,19)/t14-/m0/s1 |
| Atom Count: 48 | InChIKey: PHSRRHGYXQCRPU-AWEZNQCLSA-N |
| PDB codes: 2UV0, 3IX3, 4NG2 | Type: Non-polymer |
| Chiral Atom Count: 0 | Chiral Atoms: n/a |
| Bond Count: 48 | Aromatic Bond Count: 0 |
| Leaving Atoms: n/a | |

This database was built on MySQL (v74) and PHP (v7.0). The web interface was designed using HTML and CSS.
LigPlot[4] was used to obtain the map of interactions of the ligands and NGL viewer[5,6] as an interactive web molecule visualizer.

References:
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