

Antibacterial Library

The Library has been designed with similarity search carried out against a reference set of compounds possessing activity in treatment of pathogenic bacteria. Information about this activity has been gathered from the most reliable compound activity databases (ChEMBL, BindingDB).

The resulting library included compounds with Tanimoto similarity index range 0.80-0.85 against the reference set which was initially filtered using activity data threshold (up to 10 μ M).

The reference set included inhibitors of the following pathogenic bacteria:

- *Pseudomonas aeruginosa*
- *Staphylococcus aureus* subsp. *aureus* Mu50
- *Bacillus thermoproteolyticus*
- *Mycobacterium tuberculosis*
- *Escherichia coli*
- *Pseudomonas aeruginosa* (strain ATCC 15692 / PAO1 / IC / PRS 101 / LMG12228)
- *Streptococcus pneumoniae* R6
- *Staphylococcus aureus* subsp. *aureus* MRSA252
- *Escherichia coli* K-12
- *Staphylococcus aureus*
- *Mycobacterium smegmatis*
- *Synechococcus elongatus* (strain PCC 7942) (*Anacystis nidulans* R2)
- *Streptococcus*
- *Clostridium botulinum*
- *Agrobacterium tumefaciens*
- *Spiroplasma monobiae*
- *Alicyclobacillus acidocaldarius* subsp. *acidocaldarius* (strain ATCC27009 / DSM 446 / 104-1A) (*Bacillus acidocaldarius*)
- *Pseudomonas putida*
- *Bacillus anthracis*
- *Lactobacillus casei*
- *Staphylococcus epidermidis*
- *Clostridium perfringens*
- *Borrelia burgdorferi* (strain ATCC 35210 / B31 / CIP 102532 / DSM4680)
- *Staphylococcus aureus* (strain N315)
- *Vibrio harveyi*
- *Streptococcus pneumoniae* serotype 2 (strain D39 / NCTC 7466)
- *Clostridium botulinum* (strain Hall / ATCC 3502 / NCTC 13319 / Type A)
- *Thermus aquaticus*
- *Escherichia coli* O26:H11 str CFSAN001629
- *Mycobacterium tuberculosis* H37Rv
- *Stenotrophomonas maltophilia*
- *Francisella tularensis* subsp. *tularensis* (strain SCHU S4 / Schu 4)
- *Yersinia pestis*
- *Enterococcus faecalis* (strain ATCC 700802 / V583)

More than **5,300** compounds were included into the Life Chemicals Antibacterial Library.