

**High-throughput virtual screening for a new class of antagonist targeting LasR of
*Pseudomonas aeruginosa***

Aishwarya Vetrivel^a, Santhi Natchimuthu^a, Vidyalakshmi Subramanian^b, Rajeswari Murugesan^{a*}

^a Department of Biochemistry, Biotechnology and Bioinformatics, Avinashilingam Institute for Home Science and Higher Education for Women, Coimbatore-641043, Tamil Nadu, India.

^b Department of Biotechnology, PSG College of Technology, Coimbatore-641004, Tamil Nadu, India.

*** Corresponding author:**

Dr. Rajeswari Murugesan,

Assistant Professor,

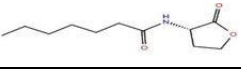
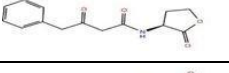
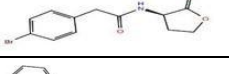
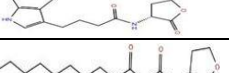
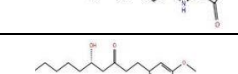
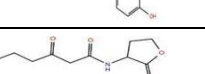
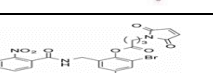
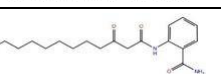
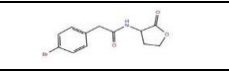
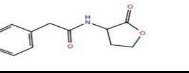
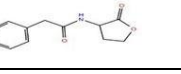
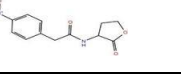
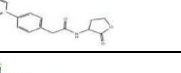
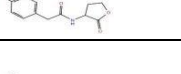
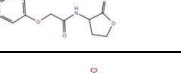
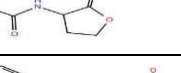
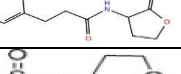
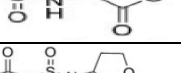
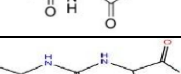
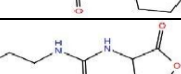
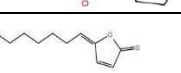
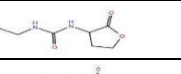

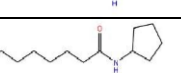



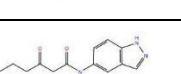
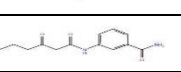


Department of Biochemistry, Biotechnology and Bioinformatics,

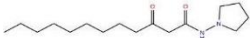

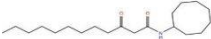
Avinashilingam Institute for Home Science and Higher Education for Women, Coimbatore-641043,

Tamil Nadu, India.

E-mail: rajeswari_bc@avinuty.ac.in

Table S1. Molecular docking analysis of known antagonists with LasR (3IX4) protein

| Antagonist | pIC50 value | Docking score (kcal/mol) | Glide energy | H-bond interaction residues | References |
|---|-------------|--------------------------|--------------|------------------------------------|---|
|  | 5.9 | -11.15 | -62.66 | Tyr47, Tyr56, Trp60, Asp73, Ser129 | Geske <i>et al.</i> , 2008 ³⁶ |
|  | 5.0 | -10.18 | -62.90 | Tyr56, Asp73, Tyr93, Ser129 | |
|  | 5.6 | -9.48 | -58.47 | Tyr56, Trp60, Asp73, Ser129 | |
|  | 7.0 | -9.45 | -49.51 | Tyr56, Ser129 | |
|  | 5.3 | -9.45 | -68.44 | Tyr47, Arg61, Tyr93 | O'Brien <i>et al.</i> , 2014 ³⁷ |
|  | 6.5 | -9.45 | -50.91 | Tyr56, Asp73, Ser129 | Choi <i>et al.</i> , 2017 ³⁸ |
|  | 4.0 | -9.18 | -69.21 | Tyr56, Asp73, Ser129 | O'Reilly <i>et al.</i> , 2018 ³⁹ |
|  | 6.0 | -9.07 | -56.76 | Tyr56, Asp73, Ser129 | |
|  | 5.7 | -8.64 | -58.21 | Arg61, Trp60, Tyr56, Asp73, Ser129 | Smith <i>et al.</i> , 2003 ⁴⁰ |
|  | 4.0 | -8.62 | -60.42 | Asp73, Ser129 | Ni <i>et al.</i> , 2008 ⁴¹ |
|  | 4.0 | -8.51 | -64.73 | Thr75, Ser129 | |
|  | 4.0 | -8.43 | -67.25 | Arg61 | |
|  | 5.6 | -8.39 | -65.12 | Thyr56, Ser129 | |
|  | 5.2 | -8.39 | -66.99 | Arg61, Tyr47, Tyr93 | |
|  | 5.6 | -8.28 | -62.64 | Tyr56, Asp73, Ser129 | |
|  | 4.0 | -7.96 | -69.86 | Tyr56, Asp73, Ser129 | |
|  | 5.6 | -7.94 | -59.84 | Val76, Ser129 | |
|  | 5.3 | -7.93 | -68.20 | Val56, Asp73, Ser129 | |
|  | 4.3 | -7.87 | -52.71 | Asp73, Tyr56, Ser129 | |
|  | 4.3 | -7.71 | -69.79 | Trp60, Tyr56, Asp73, Ser129 | |
|  | 4.3 | -7.65 | -59.88 | Tyr56, Asp73, Ser129 | |
|  | 5.8 | -7.56 | -63.91 | Tyr56, Ser129 | |
|  | 5.4 | -7.59 | -59.74 | Arg61 | |
|  | 5.3 | -7.45 | -59.20 | Tyr56, Ser129 | |
|  | 6.04 | -7.45 | -69.92 | Arg61, Tyr47, Tyr93 | |
|  | 6.0 | -7.44 | -58.03 | Tyr56, Asp73, Ser129 | |
|  | 5.9 | -7.42 | -62.77 | Tyr56, Asp73, Ser129 | |
|  | 6.2 | -7.41 | -49.25 | Val76, Ser129 | |
|  | 5.7 | -7.36 | -67.81 | Val56, Asp73, Ser129 | |
|  | 6.2 | -7.34 | -55.91 | Asp73, Tyr56, Ser129 | Smith <i>et al.</i> , 2003 ⁴⁰ |
|  | 5.3 | -7.34 | -57.03 | Asp73, Arg61, Tyr56, Ser129 | |
| | 8.0 | -7.19 | -41.36 | Tyr56 | |
| | 9.0 | -7.13 | -30.12 | Tyr56, Trp60, Asp73, | |

| | | | | | |
|---|------|-------|--------|---------------------------------|--|
| | | | | Ser129 | |
|  | 6.4 | -7.07 | -69.19 | Tyr56, Trp60, Asp73 | |
|  | 6.08 | -7.02 | -60.14 | Thr75, Ser129 | |
|  | 4.2 | -6.91 | -66.90 | Trp60, Tyr56, Asp 73, Ser129 | |