

***In silico* screening of flavones and its derivatives as
potential inhibitors of quorum-sensing regulator LasR of
*Pseudomonas aeruginosa***

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SUPPLEMENTARY MATERIAL

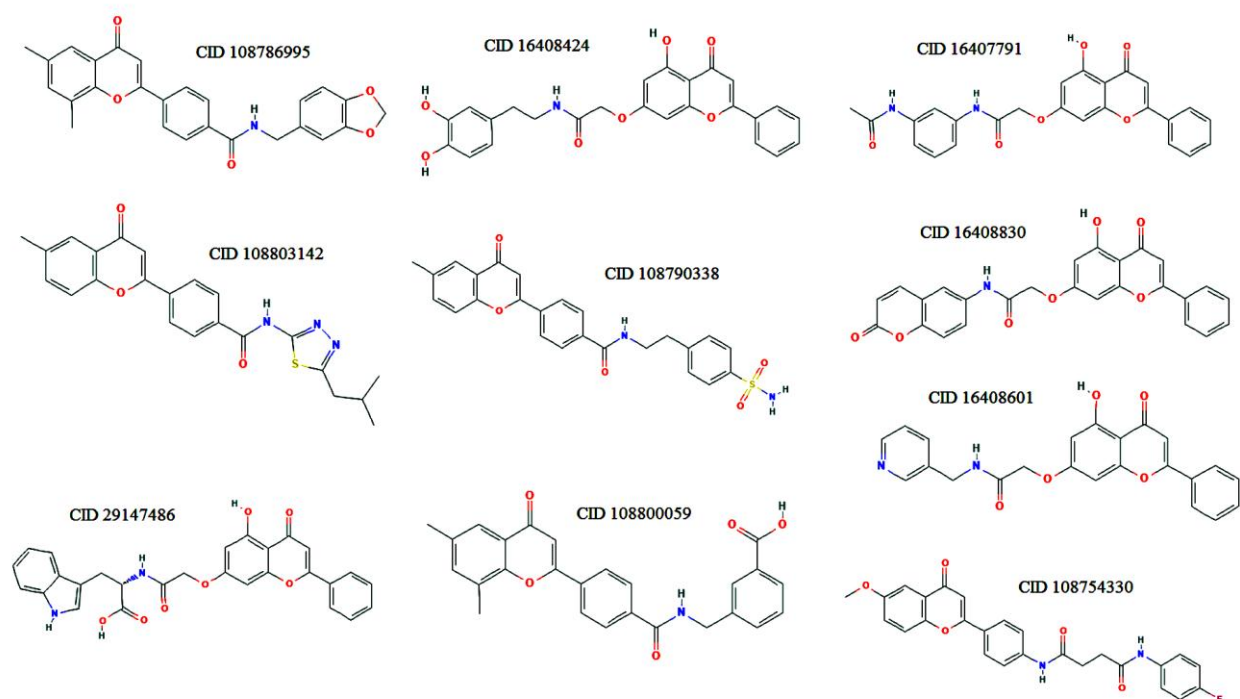


Fig. S1: 10 compounds that received high scores based on the three programs results

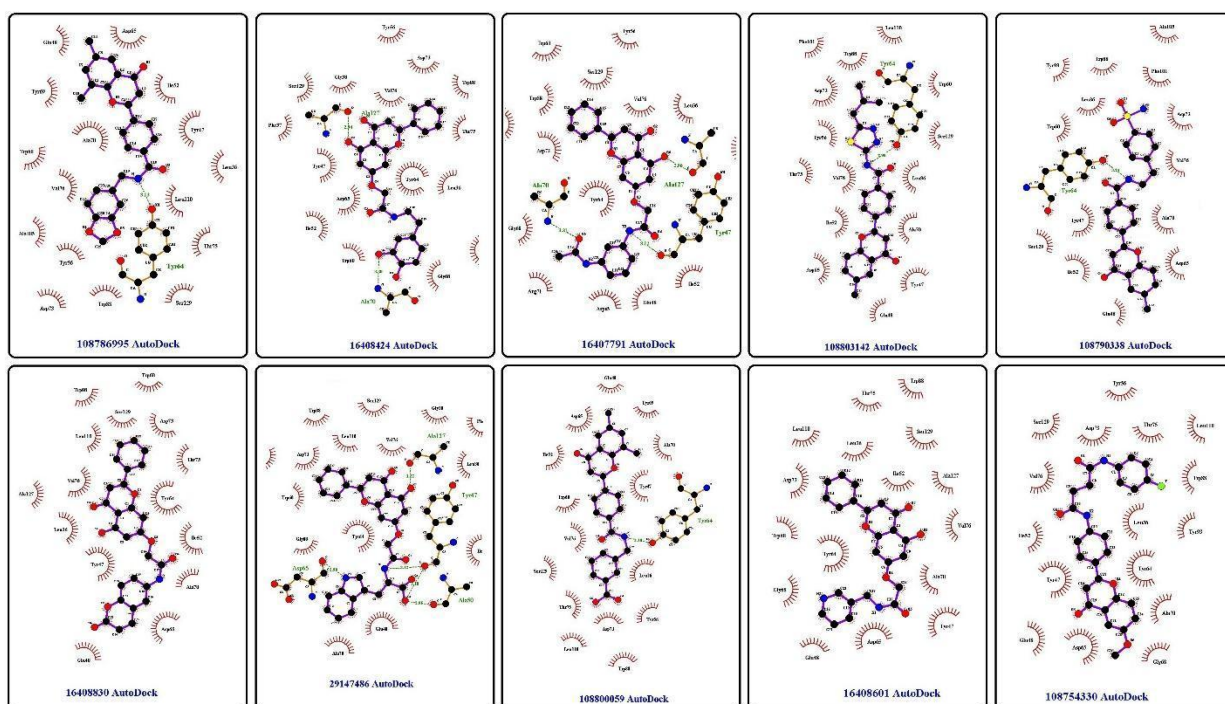


Fig. S2: Hydrogen and hydrophobic interactions of the selected compounds with LBD of LasR obtained using AutoDock Vina

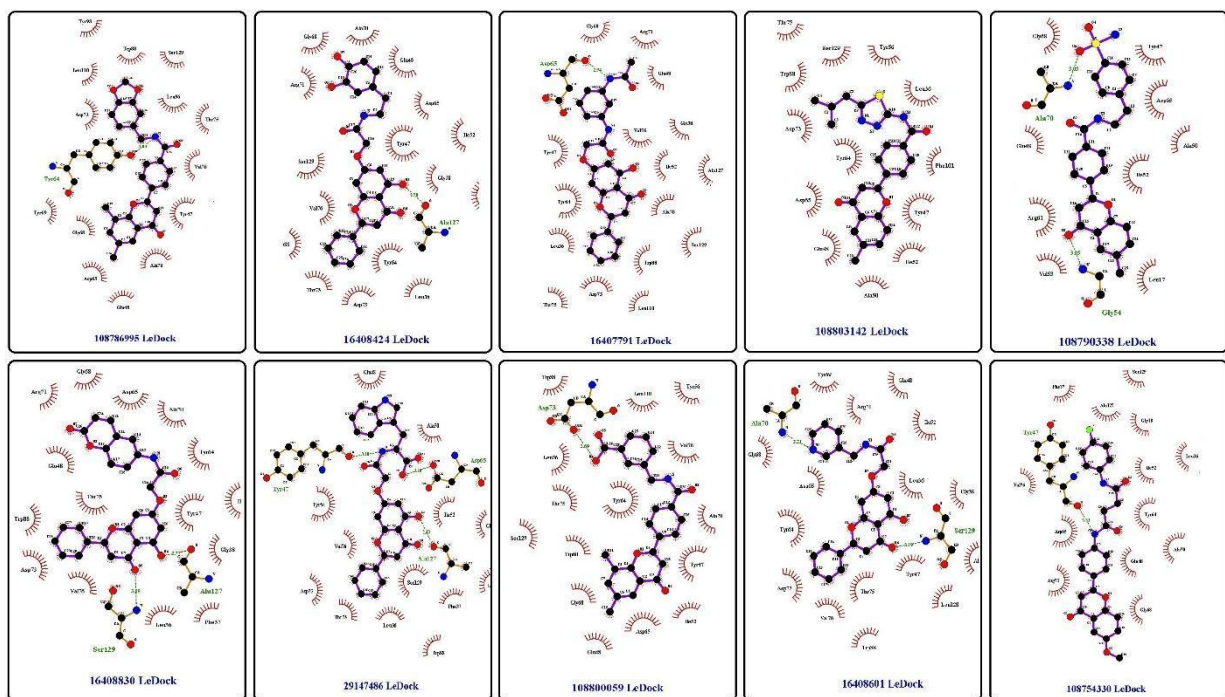


Fig. S3: Hydrogen and hydrophobic interactions of the selected compounds with LBD of LasR obtained using LeDock

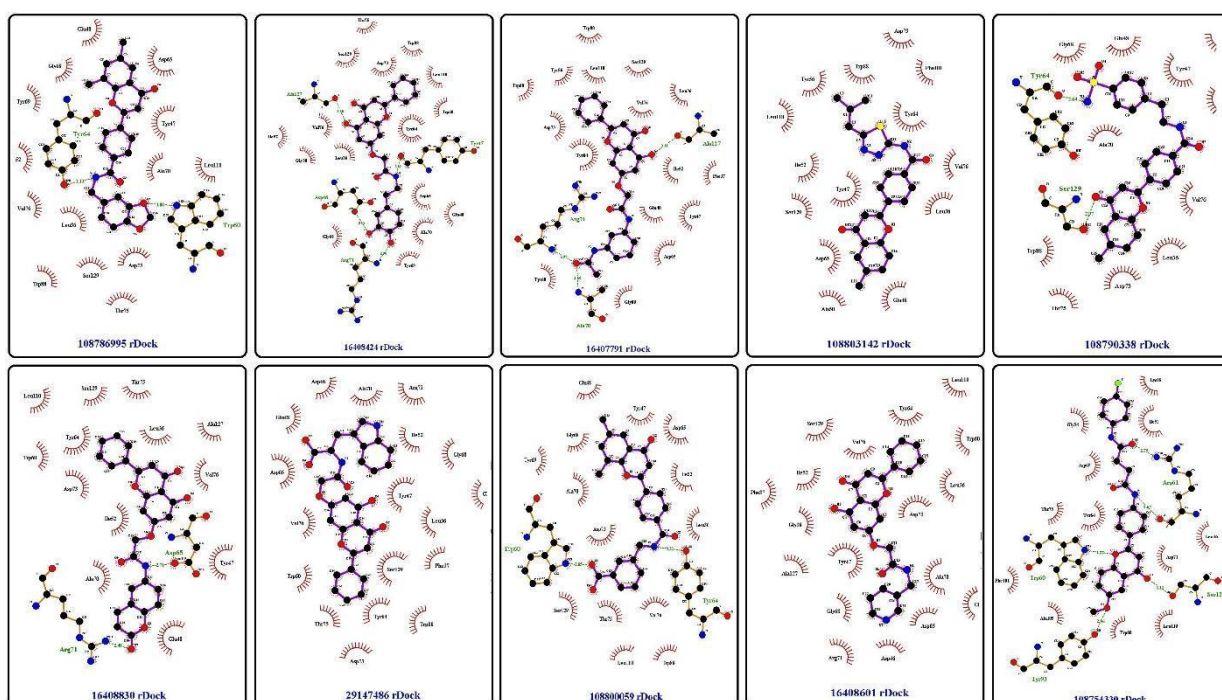
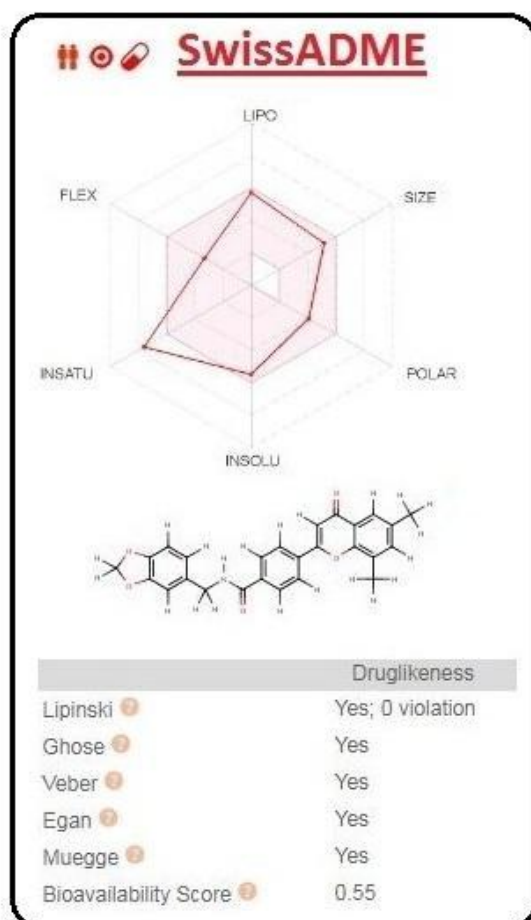


Fig. S4: Hydrogen and hydrophobic interactions of the selected compounds with LBD of LasR obtained using rDock



admetSAR

Absorption	Probability
Blood-Brain Barrier	BBB+ 0.9323
Human Intestinal Absorption	HIA+ 0.9922
Aqueous solubility LogS	-3.0803
Toxicity	
Rat Acute Toxicity	2.4764 LD50, mol/kg

PASS online

All Pa>Pi Pa>0,3 Pa>0,7

Pa	Pi	Activity
0,653	0,024	Galactorrhea
0,427	0,064	Porphyria
0,361	0,053	Cardiodepressant
0,360	0,110	Panic
0,347	0,202	Hypercholesterolemic
0,314	0,180	Toxic, vascular
0,321	0,203	Inflammation
0,310	0,282	Optic neuritis

Fig. S5: Similarity analysis of drugs