Electronic Supplementary Material (ESI) for Molecular BioSystems.

Supporting information

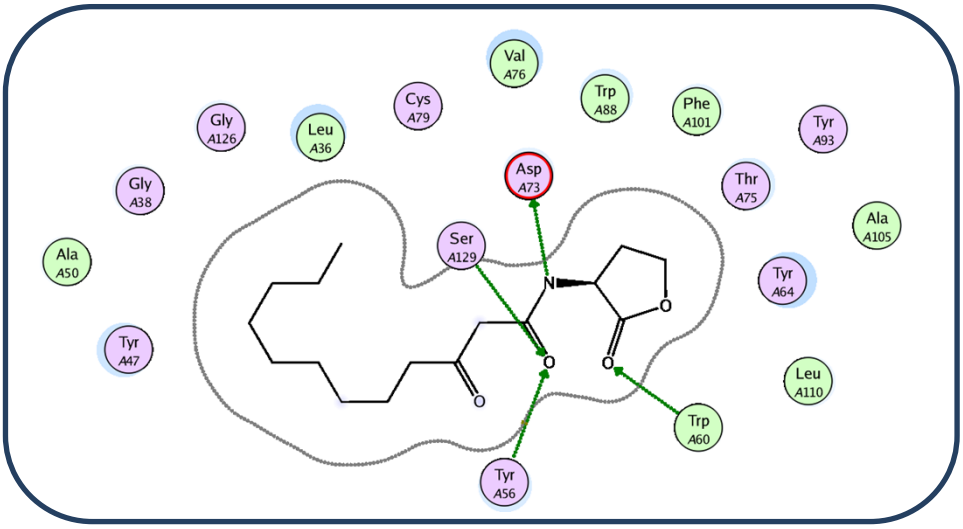
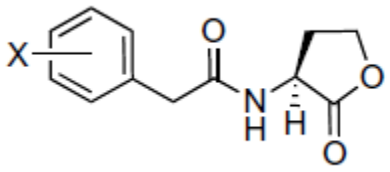
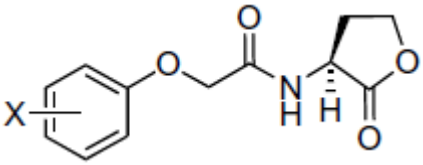
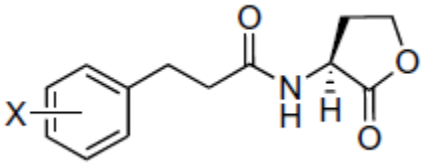
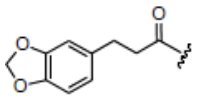


Figure S-1. Type hydrogen bond interactions present in protein-ligand complex formed between the dock and native ligand receptor active site *LasR*

Table S-2. Classification of Analogues of AHLs with anti-quorum sensing activity

group	base structure	Componds	Substituent(X)	IC_{50}(μM)
PHL	 Phenylacetylhomoserine lactones	1	4-I	1.72
		2	3-I	4.63
		4	3-NO_2	**0.61**
POHL	 Phenoxyacetylhomoserine lactones	6	4-OCF_3	4.67
		E16	3- CH_3	7.8
		E20	4-Cl	4.7
		E21	4-Br	2.1
		E22	4-I	**2.0**
PPHL	 Phenylpropionylhomoserine lactones	8	4-Br	**0.34**
		E26	4-CH_3	4.3
		E27	3-CH_3	8.9
		E28	4-OCH_3	6.8
		E29	4-F	12
		E30	4-Cl	2.2
		E31	3-Br	3.3
		E33	3-I	1.8
		E37	4-NO_2	3.0
		E38	3-NO_2	3.4
		E39		3.4

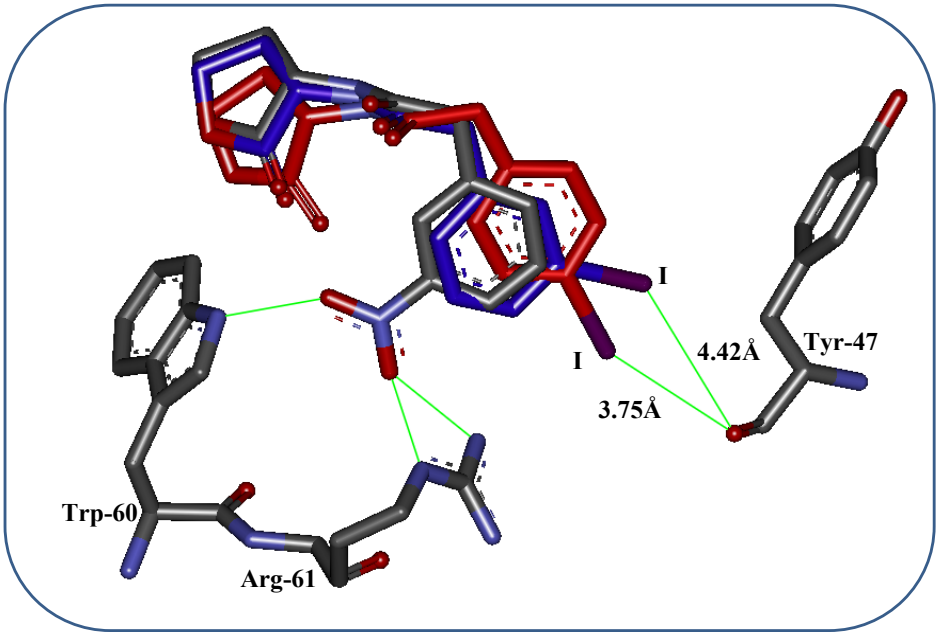


Figure S-3a. Interactions between the region B of the ligands (1 red, 2 blue and gray 4) PHLS and residues, Tyr-47, Trp-60 and Arg-61

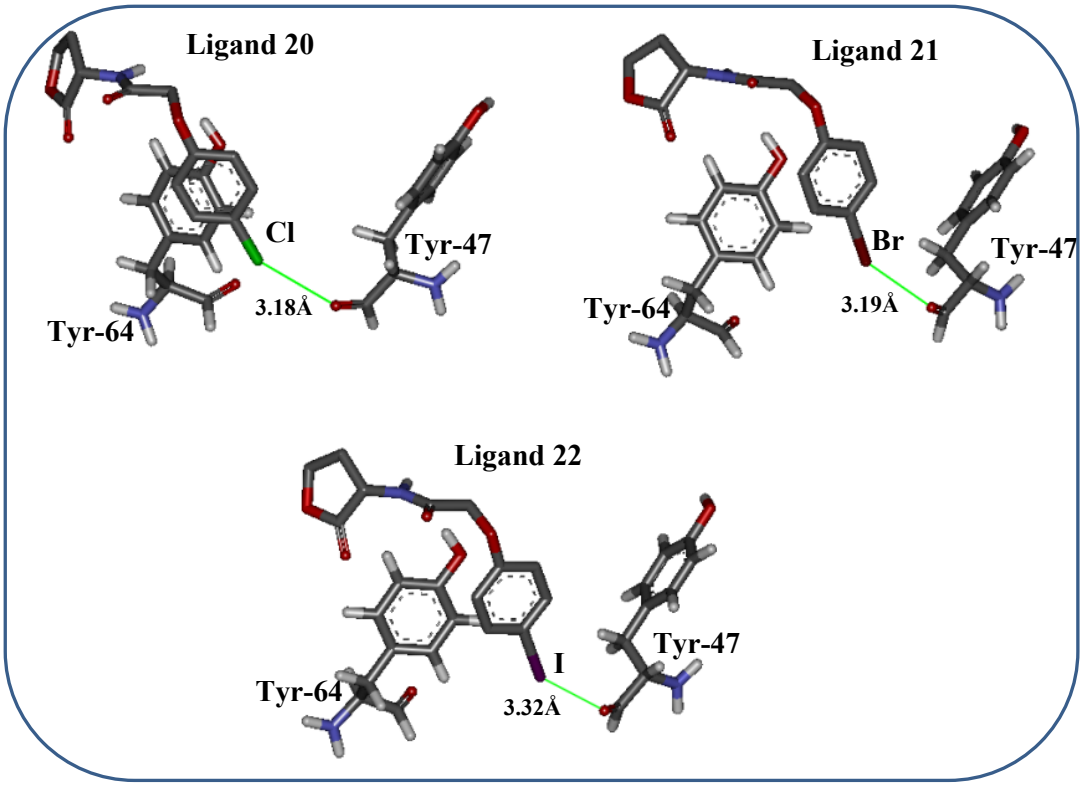


Figure S-3b. Bridges halogen ligands present in the E20, E21 and E22. In all cases the sum of the van der Waals radii of atoms involved in halogen bridges, exceeds the distance shown on the graph.

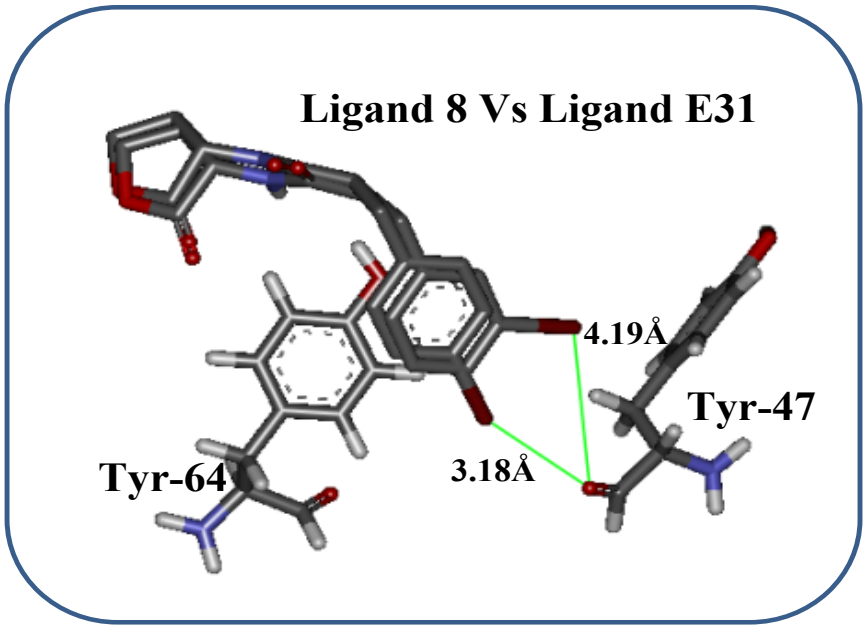


Figure S-3. The distances between the bromine atom and oxygen atom of residue Tyr-47, is greater when the substituent is in ring position 3 and for this reason there is not a strong interaction between these atoms

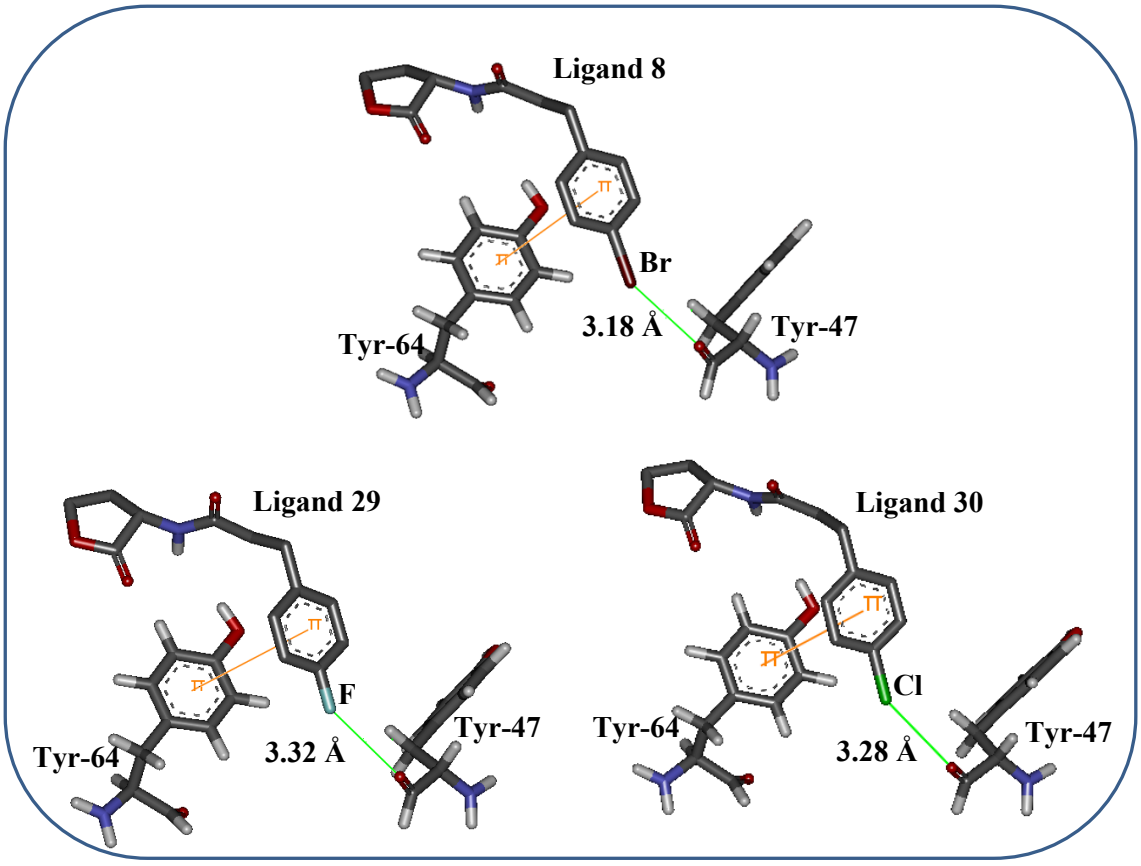


Figure S-3d. Bridges halogen ligands present in the E20, E21 and E22. In all cases the sum of the van der Waals radii of atoms involved in halogen bridges, exceeds the distance shown on the graph

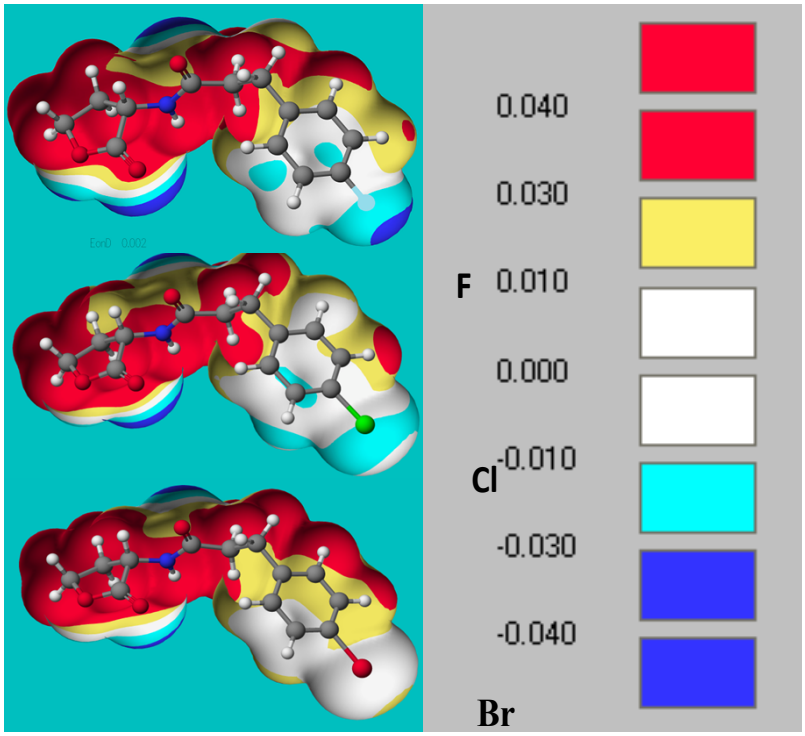


Figure S-4. Electrostatic potential surface based on the electron density and the radii of Van der Waals

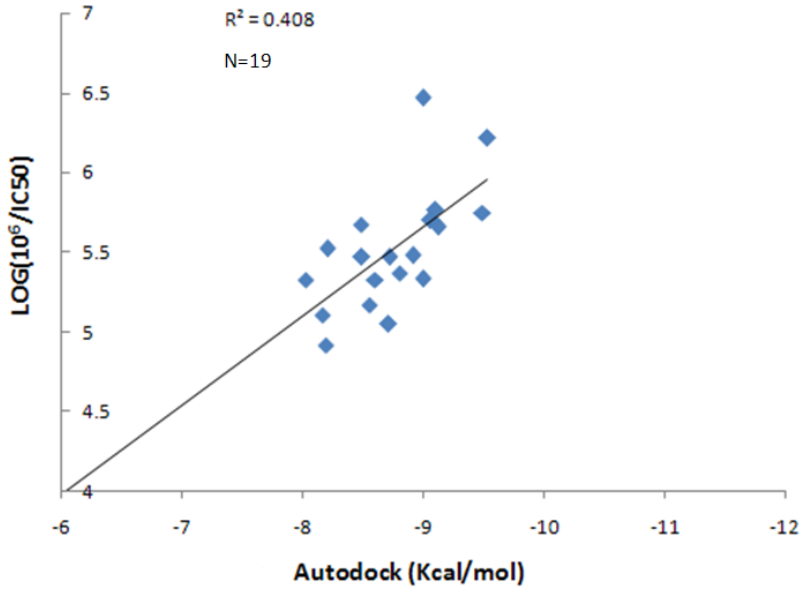


Figure S-5. Binding free energy *AutoDock* against the biological activity represented as log (10^6/*IC50*)

Table S-6. ONIOM3 energy and biological activity represented as pIC_{50}

Ligando	LOG(10^6/IC_{50}) pIC_{50}	ΔE^{ONIOM3} (Kcal/mol)
1	5.76	-30.50
2	5.33	-28.35
4	6.21	-39.39
6	5.33	-20.12
8	6.46	-36.88
E16	5.10	-28.96
E20	5.32	-28.70
E21	5.67	-31.54
E22	5.69	-28.94
E26	5.36	-23.61
E27	5.05	-24.04
E28	5.16	-27.01
E29	4.92	-21.94
E30	5.65	-31.63
E31	5.48	-22.97
E33	5.74	-32.75
E37	5.52	-29.42
E38	5.46	-26.42
E39	5.46	-27.95

Table S-7. Comparison between the different values of energy and pIC_{50}

Ligand	$LOG(10^6/IC_{50})$ pIC_{50}	Energy Autodock (Kcal/mol)	ΔE^{ONIOM3} (Kcal/mol)	ΔE^{ONIOM3}solvation (Kcal/mol)
1	5.76	-9.1	-30.50	-1,99
2	5.33	-9.44	-28.35	-5.65
4	6.21	-9.53	-39.39	-2.61
6	5.33	-8.02	-20.12	2.81
8	6.46	-9.06	-36.88	-2.12
E16	5.10	-8.16	-28.96	9.41
E20	5.32	-8.6	-28.70	-11.13
E21	5.67	-8.48	-31.54	-3.92
E22	5.69	-9.06	-28.94	-12.13
E26	5.36	-8.8	-23.61	-4.83
E27	5.05	-8.71	-24.04	-3.36
E28	5.16	-8.55	-27.01	-1.07
E29	4.92	-8.19	-21.94	-6.71
E30	5.65	-9.12	-31.63	-6.55
E31	5.48	-8.91	-22.97	-9.43
E33	5.74	-9.49	-32.75	-10.95
E37	5.52	-8.2	-29.42	-8.36
E38	5.46	-8.49	-26.42	0.99
E39	5.46	-8.72	-27.95	-5.96