Ligand-Based Drug Design of Novel Antimicrobials against *Staphylococcus aureus* by Targeting Bacterial Transcription

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Table S1. Chemical structures for molecular modeling

Cpd.	SMILES
1	[O-][N+](=O)c(c1)ccc(O)c1/C=N/c2c(F)cccc2
2 [a]	[O-][N+](=O)c(c1)ccc(O)c1/C=N/c2cc(F)ccc2
3	[O-][N+](=O)c(c1)ccc(O)c1/C=N/c2ccc(F)cc2
4	c1cccc(c1C)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
5	Cc1cc(ccc1)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
6 [a]	Cc1ccc(cc1)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
7	CC(C)(C)c1cc(ccc1)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
8	[O-][N+](=O)c(c1)ccc(O)c1/C=N/c2c(OC)cccc2
9	[O-][N+](=O)c(c1)ccc(O)c1/C=N/c2cc(OC)ccc2
10	[O-][N+](=O)c(c1)ccc(O)c1/C=N/c2ccc(cc2)OC
11 [a]	COC(=O)c1c(cccc1)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
12	COC(=O)c1cc(ccc1)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
13	COC(=O)c1ccc(cc1)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
14 [a]	C#Cc1cc(ccc1)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
15	OCc1cc(ccc1)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
16 [a]	OCc1ccc(cc1)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
17 [a]	NC(=O)c1cc(ccc1)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
18 [a]	[O-][N+](=O)c(c1)ccc(O)c1/C=N/c2cc(S(=O)(=O)N)ccc2
19	c1cccc(c1C#N)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
20	N#Cc1cc(ccc1)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
21	N#Cc1ccc(cc1)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
22	N#CCc1cc(ccc1)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
23	O=C(O)Cc1cc(ccc1)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
24	[O-][N+](=O)c(c1)ccc(O)c1/C=N/c(ccc2)cc2CNS(=O)(=O)C
25	FC(F)(F)[C@H](O)c1cc(ccc1)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
26	CONC(=O)c1cc(ccc1)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
27 [a]	CS(=O)(=O)NC(=O)c1cc(ccc1)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
28	CN(C)S(=O)(=O)NC(=O)c1cc(ccc1)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
29 [a]	[O-][N+](=O)c(c1)ccc(O)c1/C=N/c(cccc2)c2-c3ccccc3
30	[O-][N+](=O)c(c1)ccc(O)c1/C=N/c(ccc2)cc2-c3ccccc3
32	[O-][N+](=O)c(c1)ccc(O)c1/C=N/c(cc2)ccc2-c3ccccc3
33	C#Cc1cc(ccc1)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
34 [a]	c1cccc(c1C#C)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
35 [a]	C#Cc1ccc(cc1)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
36	[O-][N+](=O)c(c1)ccc(O)c1/C=N/c2ccccc2
37	c1cccc(c1C(C)(C)C)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
38	CC(C)(C)c1cc(ccc1)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
39	CC(C)(C)c1ccc(cc1)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
40	[O-][N+](=O)c(c1)ccc(O)c1/C=N/c2c(O)cccc2
41	[O-][N+](=O)c(c1)ccc(O)c1/C=N/c2cc(O)ccc2
42 [a]	[O-][N+](=O)c(c1)ccc(O)c1/C=N/c2ccc(O)cc2
43	[O-][N+](=O)c(c1)ccc(O)c1/C=N/c2c(Cl)cccc2
44	[O-][N+](=O)c(c1)ccc(O)c1/C=N/c2cc(Cl)ccc2
45	[O-][N+](=O)c(c1)ccc(O)c1/C=N/c2ccc(Cl)cc2
46 [a]	c1cccc(c1C(F)(F)F)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
47	FC(F)(F)c1cc(ccc1)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
48	FC(F)(F)c1ccc(cc1)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
49	O=C(O)c1cc(ccc1)\N=C\c2c(O)ccc(c2)[N+]([O-])=O
50 [a]	[O-][N+](=O)c(c1)ccc(O)c1/C=N/C2CCCCC2
51	[O-][N+](=O)c(c1)ccc(O)c1/C=N/c2cccc(c23)cccc3
52	C#Cc1cc(ccc1)/N=C\c(c(O)cc2)cc2C(=O)OC

53 [a]	C#Cc1cc(ccc1)\N=C\c2c(O)ccc(F)c2
54	C#Cc1cc(ccc1)\N=C\c(c(O)cc2)cc2C#N
55 [a]	C#Cc1cc(ccc1)\N=C\c2c(O)ccc(c2)CC#N
56	C#Cc1cc(ccc1)\N=C\c2c(O)cccc2
57	C#Cc1cc(ccc1)\N=C\c2cc([N+]([O-])=O)ccc2
58 [a]	C#Cc1cc(ccc1)\N=C\c2c(O)cc([N+]([O-])=O)cc2
59	C#Cc1cc(ccc1)\N=C\c2c(O)c([N+]([O-])=O)ccc2
60 [a]	C#Cc1cc(ccc1)\N=C\c2c([N+]([O-])=O)ccc(c2)O
61	C#Cc1cc(ccc1)\N=C\c2c(O)c(Br)cc(c2)[N+]([O-])=O

[a] Compounds taken for the test set

Table S2. Physicochemical Properties of the identified hits

ID#	J098-0498	1067-0401	M013-0558	F186-0261
Formula	$C_{24}H_{25}N_3O_6S$	$C_{19}H_{16}BrN_5O_3S$	$C_{26}H_{25}N_3O_4$	$C_{20}H_{18}ClN_3O_4S$
Molecular weight	483.54 g/mol	474.33 g/mol	443.49 g/mol	431.89 g/mol
Num. heavy atoms	34	29	33	29
Num. arom. heavy atoms	17	17	18	17
Fraction Csp^3	0.25	0.11	0.19	0.15
Num. rotatable bonds	8	8	7	9
Num. H-bond acceptors	6	6	4	5
Num. H-bond donors	2	3	2	2
Molar Refractivity	130.28	114.57	129.98	113.12
TPSA	126.33 Å^2	144.81 Å^2	87.74 Å^2	117.79 Å^2