CORRECTION

Correction: Identification of potential antimicrobials against *Salmonella typhimurium* and *Listeria monocytogenes* using Quantitative Structure-Activity Relation modeling

The PLOS ONE Staff

Tables 2 and 3 incorrectly show only the top 5 compounds against *S. typhimurium* and *L. monocytogenes*, respectively, rather than the top 10. The publisher apologizes for these errors. Please see the corrected Tables 2 and 3 here.

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Table 2. Top 10 compounds against *S. typhimurium* in terms of log(MIC).

SMILES Structure of Potential Compounds	log(MIC) (μg/ml)	SMILES Structure of Potential Compounds	log(MIC) (μg/ml)
<i>S. typhimurium</i> (model 76)			
<chem>C[C@@]12CC[C@]3(CC[C@H](C3C1CCC4[C@]2(CCC5[C@@]4(CC[C@@H](C5(C)C)O)C)C(=C)C[N+]6=CC=CC=C6)CO</chem>	0.606	<chem>C[C@@]12CC[C@]3(CC[C@H]([C@@H]3[C@H]1CC[C@H]4[C@]2(CC[C@@H]5[C@@]4(CC[C@@H](C5(C)C)O)C)C(=C)C[N+]6=CC=C(C=C6)N(C)C(=O)O.[Br-]</chem>	0.7165
<chem>CC1=CC(=C[N+](=C1)CC(=C)[C@@H]2CC[C@]3(C2C4CCC5[C@]6(CC[C@@H](C(C6CC[C@]5([C@@]4(CC3)C)C(C)O)C)CO)C</chem>	0.6082	<chem>C[C@H](CCCC(C)C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC[C@H](C4)[N+]5=CC=CC=C5)C)C.I</chem>	0.9018
<chem>C[C@@]12CC[C@]3(CC[C@H](C3C1CCC4[C@]2(CCC5[C@@]4(CC[C@@H](C5(C)C)O)C)C(=C)C[N+]6=CC=C(C=C6)N(C)C)CO</chem>	0.6207	<chem>C[C@H](CCCC(C)C)[C@H]1CCC2[C@@]1(CCC3C2CC=C4[C@@]3(CCC(C4)[N+]5=CC=CC=C5)C)C</chem>	0.9018
<chem>C[C@@]12CC[C@]3(CC[C@H](C3C1CCC4[C@]2(CCC5[C@@]4(CC[C@@H](C5(C)C)O)C)C(=C)C[N+]6=CC=CC(=C6)CO)CO</chem>	0.6251	<chem>CC1=CC=C(C=C1)S(=O)(=O)[O-].CC1=CC=[N+](C=C1)C2CCC3(C4CCC5(C(C4CC=C3C2)CCC5C(C)CCCC(C)C)C</chem>	0.9069
<chem>C[C@@]12CC[C@]3(CC[C@H](C3C1CCC4[C@]2(CCC5[C@@]4(CC[C@@H](C5(C)C)O)C)C(=C)C[N+]6=CC=C(C=C6)CO)CO</chem>	0.6273	<chem>CC1=CC=C(C=C1)S(=O)(=O)O.CC(C)CCCC(C)C1CCC2C1(CCC3C2CC=C4C3(CCC(C4)[N+]5=CC=CC(=C5)C#N)C)C</chem>	0.9268

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Table 3. Top 10 against *L. monocytogenes* in terms of log(MIC).

SMILES Structure of Potential Compounds	log(MIC) (μg/ml)	SMILES Structure of Potential Compounds	log(MIC) (μg/ml)
<i>L. monocytogenes</i> (model 90)			
<chem>CCCCCCCCCCCCCCCC[N+]1=CC=C(C2=CC=CC=C21)CC(C3=C(NC4=CC=CC=C43)C)O</chem>	-1.8558	<chem>CCCCCCCCCCCCCCCC[N+]1=CC=C(C=C1)CC</chem>	-1.6392
<chem>CC1=CC(=C[N+](=C1)CC(=O)C2=CC3=C(C=C2)C4=CC=CC=C4C3)C.[Br-]</chem>	-1.7315	<chem>CCCCCCCCCCCCCCCC[N+]1=CC=C(C=C1)CCS(=O)(=O)O</chem>	-1.6392
<chem>CC1=CC=CC2=NC(=C(N12)NC(C)(C)CC(C)(C)C3=CC4=CC=CC=C4C5=CC=CC=C53</chem>	-1.7252	<chem>CC(C)(C)CC(C)(C)NC1=C(N=C2N1C=C(C=C2)Br)C3=C4C=CC=CC4=CC5=CC=CC=C53</chem>	-1.6212
<chem>CC1=C[N+](=CC=C1)CCCCC2=CC(=CC=C2)CCCC[N+]3=CC=CC(=C3)C</chem>	-1.7101	<chem>CC(C)(C)CC(C)(C)NC1=C(N=C2N1C=CC=C2)C3=C4C=CC=CC4=CC5=CC=CC=C53</chem>	-1.6212
<chem>CC1=C[N+](=CC=C1)CCCCC2=CC(=CC=C2)CCCC[N+]3=CC=CC(=C3)C.[Br-].[Br-]</chem>	-1.7101	<chem>CC(C)(C)CC(C)(C)NC1=C(N=C2N1C=CC=C2)C3=CC4=CC=CC=C4C5=CC=CC=C53</chem>	-1.6212

<https://doi.org/10.1371/journal.pone.0193628.t002>

Reference

1. Rath EC, Gill H, Bai Y (2017) Identification of potential antimicrobials against *Salmonella typhimurium* and *Listeria monocytogenes* using Quantitative Structure-Activity Relation modeling. PLoS ONE 12 (12): e0189580. <https://doi.org/10.1371/journal.pone.0189580> PMID: 29236763