

Supplementary material

Mining and validating quorum sensing interference molecules from food-derived compounds for *Salmonella* Typhimurium

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Table S1. Sequences of primers used in the construction of plasmids.

Source	Primer name	Primer sequence
LT2 genome	LsrB-F	GTGGTGGTGCTCGAGGAAATCATATTTGTTCGATATTG
	LsrB-R	GGAGATATACCATGGCAAGACACAGCATTAATGATC
	plsr-F	GCCTGGCAGTTTATGTGTCATAACCTGGCTTTAC
	plsr-R	ATGATGCGTAATCATGTTGCCTCCGCTCCCTCAATG
pET-28a	pET-28a-F	GACAAATATGATTTTCCTCGAGCACCACCACCAC
	pET-28a-R	TAATGCTGTGTCTTGCCATGGTATATCTCCTTCT
pBAD24	pBAD-F	AGCCAGGTTATGACACATAAACTGCCAGGCATC
	pBAD-R	AAGACAGCGACTCAGGCGCCATCTCCTTGCTGC
pSC101	eGFP-F	GAGCGGAGGCAACATGATTACGCATCATCATCATCATG
	eGFP-R	GCAAGGAGATGGCGCCTGAGTCGCTGTCTTTTTTCGTGAC

Table S2. Sequences of primers used in qRT-PCR.

Primer name	Primer sequence	Primer name	Primer sequence
fimD-F	GATACCCGCGCACTCATTA	sopE-F	CGAGCATAGGCCGGATCTTT
fimD-R	CGTTATTACGCAACCGCCAG	sopE-R	GAACGCTTCTGAGGGTAGGG
flhC-F	GTCGAAAATGGCAGCATCCC	sptP-F	ATCGTTCCGGTTCTTCCCAC
flhC-R	GCGCTCGTCTACAAATGCTG	sptP-R	TACCTGGCGGATAGGGTGAA
fliA-F	AATCGCATCCATTACCCGCT	lsrB-F	AGAGTTTGGCCTGTGGGATG
fliA-R	AGCATGGCGATAGCATCGAA	lsrB-R	CGATGCCGGGAATATCCAGT
sopB-F	AAGCTGCTTGACCTGAGCAT	lsrC-F	TGTGTTAGTGCTGCTGCGTA
sopB-R	CGAACTTATTGCAGCACGCA	lsrC-R	GGCGCAGATTGCGTTGTAAT
invH-F	TGAGCAAACCGGTACAGCAA	luxS-F	AGCTCCGGGATCTGGTTTTG
invH-R	AAGGTCTGACGGCACATACG	luxS-R	CGCACCGGCTTTTACATGAG

Table S3. Details of various QS systems including 10 QS receptors.

PDB ID	Receptor	Organism	Signaling system
5IDJ	CckA	<i>Caulobacter vibrioides</i>	Two-component system
3QP1	CviR	<i>Chromobacterium violaceum</i>	AHLs (N-Acyl homoserine lactones)
2UV0	LasR	<i>Pseudomonas aeruginosa</i>	AHLs (N-Acyl homoserine lactones)
1TJY	LsrB	<i>Salmonella typhimurium</i>	AI-2 (Autoinducer-2)
1JX6	LuxP	<i>Vibrio harveyi</i>	AI-2 (Autoinducer-2)
4JVD	PqsR	<i>Pseudomonas aeruginosa</i>	HAQs (4-hydroxy-2-alkylquinolines)
3SZT	QscR	<i>Pseudomonas aeruginosa</i>	AHLs (N-Acyl homoserine lactones)
4Y15	SdiA	<i>Escherichia coli</i>	AHLs (N-Acyl homoserine lactones)
1L3L	TraR	<i>Agrobacterium tumefaciens</i>	AHLs (N-Acyl homoserine lactones)
5L09	YenR	<i>Yersinia enterocolitica</i>	AHLs (N-Acyl homoserine lactones)

Table S4. Free binding energies and MIC of the obtained food-derived compounds.

FDB	ΔG (kCal/ mol)	MI C (m M)	FDB	ΔG (kCal/ mol)	MIC (mM)	FDB	ΔG (kCal/mol)	MIC(m M)
FDB012 331	-7.8	10	FDB003 213	-6.7	10	FDB000 917	-6.6	10
FDB022 191	-7.1	> 40	FDB022 220	-6.8	10	FDB022 106	-6.6	5
FDB022 236	-6.9	10	FDB027 865	-7	20	FDB000 937	-6.6	20
FDB022 260	-6.3	20	FDB000 545	-6.7	20	FDB008 857	-6.6	10
FDB000 941	-6	5	FDB012 467	-6.7	10	FDB022 218	-6.5	5
FDB006 231	-5	> 40	FDB021 993	-6.7	10	FDB023 148	-6.5	20
FDB010 843	-5.9	5	FDB014 206	-6.7	10	FDB004 302	-6.4	2.5
FDB010 973	-6.8	> 40	FDB023 179	-6.7	>40	FDB003 361	-6.4	10

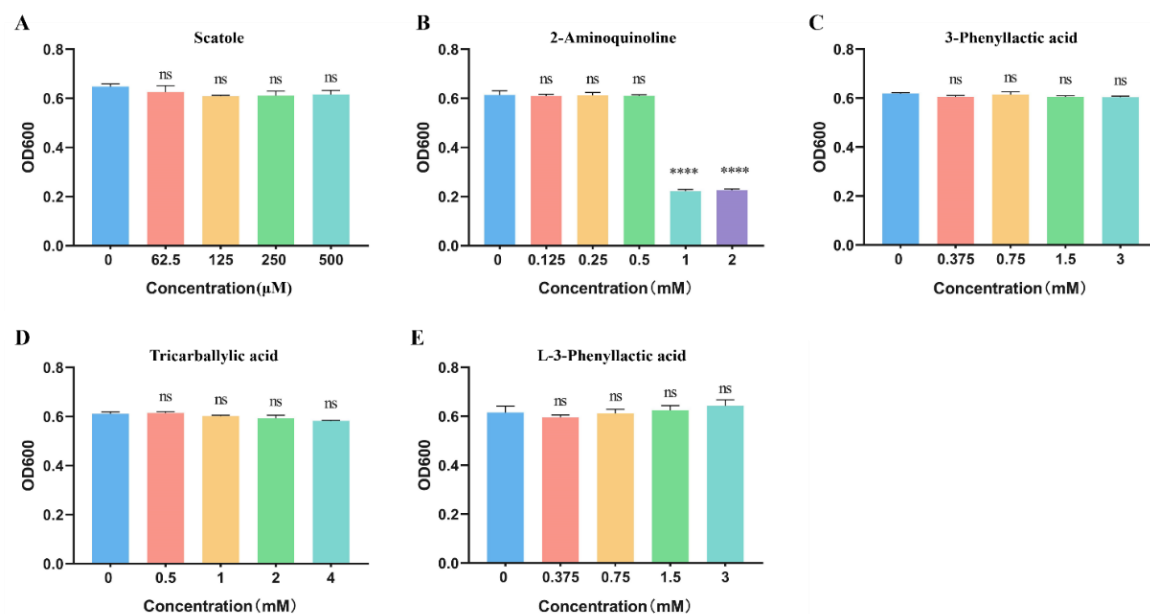


Figure S1. Effect of foodborne small molecules on cell viability.
A. Scatole. B. 2-Aminoquinoline. C. Tryptamine. D. 3-Phenyllactic acid. E. Tricarballic acid.
F. L-3-Phenyllactic acid.