Supporting Information File 1

for

Non-native autoinducer analogs capable of modulating the SdiA quorum sensing receptor in *Salmonella enterica* serovar Typhimurium

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Compound library structures and screening results

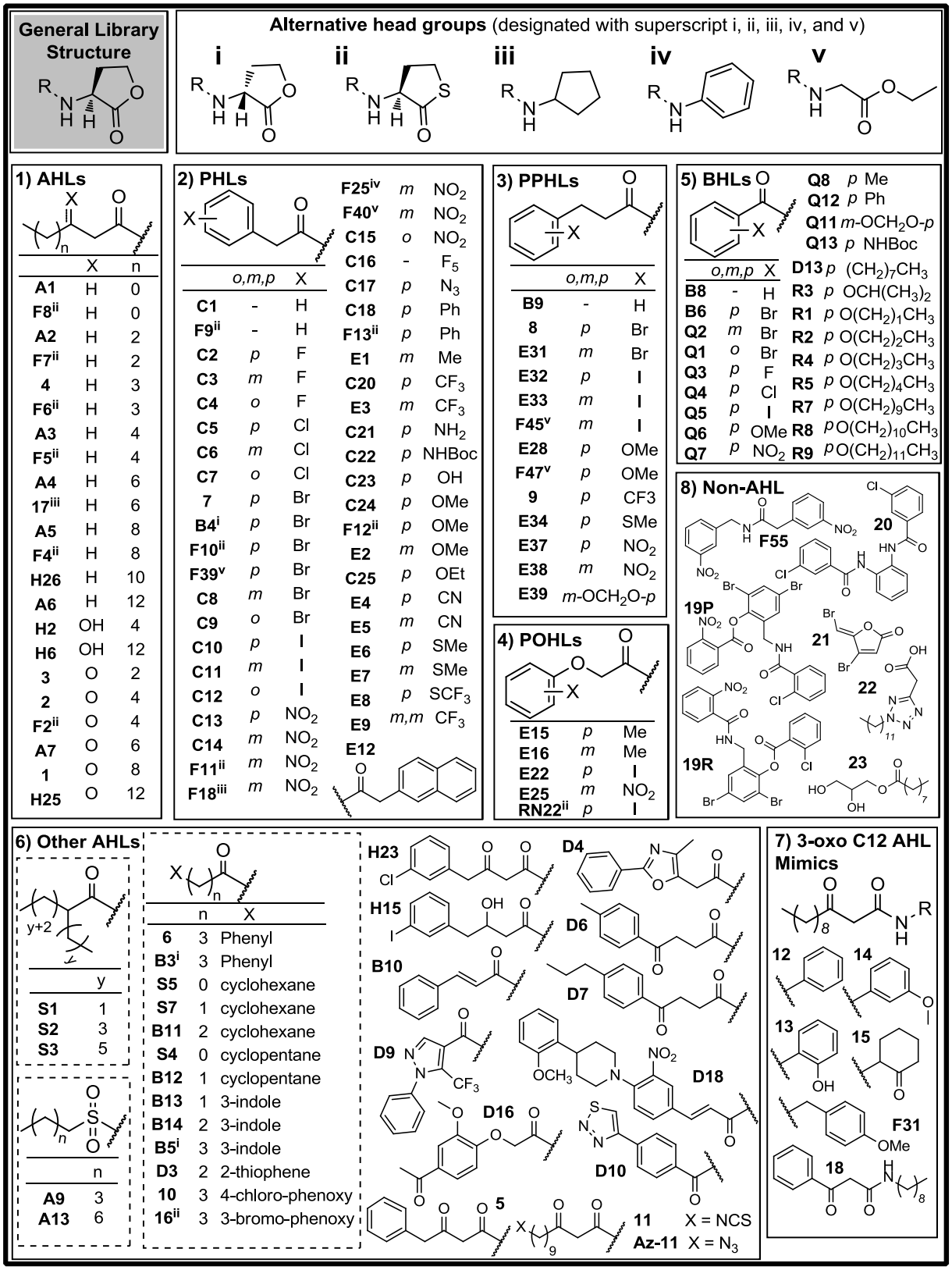

Figure S1: Structures of compounds evaluated in this study. Compounds listed by general structure class. Original sub-library letter names (A, B, C, D, E, F, H, Q, R, S, and **1–22**) from our prior publications are indicated in compound names. See main text.

Table S1: Single-concentration screening data in *S.* Typhimurium-pJNS25 SdiA reporter strain.[a]

	Agonism[b]		**Antagonism**[c]	
compound	**1 μM**	**100 μM**	**1 μM**	**100 μM**
	Activity (%)[d]	Activity (%)[d]	Inhibition (%)[e]	Inhibition (%)[e]
A1	41 ± 6	104 ± 8	7 ± 5	-10 ± 11
F8	81 ± 1	127 ± 11	-5 ± 10	-23 ± 11
A2	84 ± 5	83 ± 2	15 ± 4	3 ± 1
F7	78 ± 5	117 ± 9	7 ± 9	-12 ± 4
4	66 ± 9	59 ± 9	26 ± 4	16 ± 5
F6	78 ± 1	87 ± 9	5 ± 5	-2 ± 7
A3	76 ± 7	89 ± 13	10 ± 8	13 ± 14
F5	85 ± 2	79 ± 4	3 ± 6	0 ± 6
A4	59 ± 3	75 ± 11	12 ± 19	18 ± 7
17	3 ± 4	47 ± 3	26 ± 12	28 ± 5
A5	45 ± 2	57 ± 5	17 ± 10	43 ± 4
F4	62 ± 2	93 ± 16	-2 ± 11	2 ± 5
H26	19 ± 6	39 ± 12	5 ± 14	0 ± 8
A6	12 ± 3	39 ± 3	17 ± 12	38 ± 5
H2	77 ± 4	74 ± 12	8 ± 5	12 ± 16
H6	3 ± 3	51 ± 14	15 ± 1	15 ± 13
3	75 ± 14	75 ± 15	6 ± 16	20 ± 2
2	78 ± 11	86 ± 18	-2 ± 9	9 ± 5
F2	116 ± 6	88 ± 19	-19 ± 12	-19 ± 15
A7	86 ± 9	100 ± 4	-4 ± 19	-2 ± 10
1	71 ± 8	94 ± 8	2 ± 17	15 ± 16
H25	55 ± 8	57 ± 10	1 ± 13	-9 ± 15
C1	40 ± 4	90 ± 5	9 ± 12	-6 ± 5
F9	76 ± 1	113 ± 6	-1 ± 4	-13 ± 1
C2	56 ± 1	93 ± 5	2 ± 8	-8 ± 18
C3	56 ± 2	111 ± 9	-1 ± 15	-18 ± 12
C4	45 ± 3	121 ± 14	3 ± 6	-31 ± 10
C5	65 ± 8	85 ± 4	13 ± 6	18 ± 7
C6	85 ± 4	120 ± 2	9 ± 16	-20 ± 6
C7	75 ± 10	132 ± 6	22 ± 6	-32 ± 5
7	71 ± 10	68 ± 11	26 ± 9	21 ± 10
B4	26 ± 6	65 ± 3	41 ± 15	16 ± 11
F10	68 ± 3	57 ± 8	8 ± 12	-3 ± 7

[a]Compounds listed according to order in Figure S1. [b]Agonism and [c]antagonism assays performed as described in the Experimental Section at 1 μM and 100 μM compound. All assays performed in triplicate. [d]Activation reported as the average (±STD) of the percentage (%) of activity normalized to 10 μM **2** (OOHL). [e]Inhibition reported as the average (±STD) of the change in the activity (%) from 10 nM **2** (OOHL). [f]Cell growth inhibited at this compound concentration.

Continued…	**Agonism**[b]		**Antagonism**[c]	
compound	**1 μM**	**100 μM**	**1 μM**	**100 μM**
	Activity (%)[d]	Activity (%)[d]	Inhibition (%)[e]	Inhibition (%)[e]
F39	16.4 ± 0.4	31 ± 3	27 ± 9	53 ± 11
C8	88 ± 10	100 ± 15	21 ± 10	-22 ± 9
C9	97 ± 13	156 ± 10	9 ± 8	-48 ± 13
C10	83 ± 1	95 ± 15	28 ± 6	27 ± 13
C11	87 ± 7	109 ± 7	15 ± 11	-4 ± 2
C12	72 ± 2	125 ± 13	9 ± 13	-24 ± 12
C13	58 ± 4	98 ± 4	24 ± 4	14 ± 9
C14	79 ± 8	110 ± 9	0 ± 3	-17 ± 9
F11	87 ± 6	103 ± 17	-11 ± 7	-16 ± 13
F18	61 ± 6	69 ± 13	4 ± 6	15 ± 3
F25	14 ± 2	74 ± 9	20 ± 4	-2 ± 14
F40	16 ± 3	50 ± 8	21 ± 8	43 ± 4
C15	22 ± 2	110 ± 10	5 ± 2	-17 ± 18
C16	26 ± 2	141 ± 9	5 ± 3	-32 ± 18
C17	59 ± 2	103 ± 15	13 ± 11	9 ± 6
C18	28 ± 1	48 ± 13	11 ± 3	52 ± 10
F13	43 ± 6	44 ± 13	23 ± 4	46 ± 15
E1	84 ± 3	97 ± 15	-6 ± 7	-14 ± 13
C20	69 ± 16	86 ± 6	15 ± 10	8 ± 6
E3	75 ± 2	89 ± 14	-14 ± 16	5 ± 8
C21	17 ± 4	76 ± 7	4 ± 12	13 ± 4
C22	16 ± 3	56 ± 5	-9 ± 2	6 ± 6
C23	65 ± 11	90 ± 8	6 ± 2	16 ± 3
C24	75 ± 10	87 ± 2	-11 ± 3	4 ± 16
F12	93 ± 9	86 ± 10	-13 ± 10	-21 ± 8
E2	73 ± 4	93 ± 14	-5 ± 1	-8 ± 14
C25	64 ± 11	92 ± 1	12 ± 8	7 ± 5
E4	74 ± 1	89 ± 16	12 ± 6	-17 ± 18
E5	90 ± 12	100 ± 16	18 ± 8	-8 ± 4
E6	61 ± 6	64 ± 16	25 ± 16	44 ± 13
E7	81 ± 18	93 ± 15	20 ± 14	12 ± 13
E8	52 ± 10	82 ± 10	34 ± 11	31 ± 7
E9	42 ± 15	61 ± 1	18 ± 8	21 ± 8
E12	77 ± 16	67 ± 5	-13 ± 9	0 ± 15
B9	55 ± 3	96 ± 5	13 ± 10	18 ± 14
8	77 ± 5	87 ± 16	15 ± 8	4 ± 3
E31	70 ± 18	56 ± 8	13 ± 10	6 ± 6
E32	36 ± 1	83 ± 7	19 ± 14	24 ± 13
E33	34 ± 5	51 ± 4	20 ± 6	38 ± 10
F45	4.8 ± 0.1	13 ± 2	8 ± 10	92 ± 2

Continued…	**Agonism**[b]		**Antagonism**[c]	
compound	**1 μM**	**100 μM**	**1 μM**	**100 μM**
	Activity (%)[d]	Activity (%)[d]	Inhibition (%)[e]	Inhibition (%)[e]
E28	71 ± 12	66 ± 7	11 ± 18	6 ± 15
F47	4 ± 2	50 ± 5	3 ± 14	36 ± 10
9	52 ± 4	59 ± 6	32 ± 10	11 ± 16
E34	33 ± 4	53 ± 5	21 ± 15	39 ± 8
E37	57 ± 4	70 ± 15	34 ± 5	23 ± 5
E38	35 ± 2	56 ± 9	15 ± 11	32 ± 6
E39	41 ± 6	72 ± 12	10 ± 15	12 ± 3
E15	86 ± 4	126 ± 3	-3 ± 5	-17 ± 7
E16	86 ± 6	104 ± 4	-2 ± 8	-4 ± 5
E22	96 ± 6	136 ± 6	-5 ± 11	-15 ± 8
E25	78 ± 9	76 ± 7	5 ± 18	9 ± 12
RN22	94 ± 19	76 ± 5	-4 ± 9	3 ± 9
B8	12 ± 1	77 ± 4	26 ± 3	-13 ± 11
B6	12 ± 3	51 ± 1	25 ± 11	-14 ± 17
Q2	10 ± 4	72 ± 1	17 ± 2	9 ± 13
Q1	8 ± 2	74 ± 3	2 ± 5	-3 ± 18
Q3	3 ± 5	55 ± 3	34 ± 2	-26 ± 17
Q4	1 ± 4	26 ± 3	30 ± 4	-25 ± 15
Q5	0 ± 1	24 ± 4	28 ± 10	-14 ± 10
Q6	3 ± 2	53 ± 2	26 ± 18	-6 ± 14
Q7	1 ± 2	55 ± 3	28 ± 7	20 ± 9
Q8	2 ± 3	53 ± 5	17 ± 3	11 ± 3
Q12	11 ± 7	12 ± 4	20 ± 9	26 ± 14
Q11	16 ± 7	59 ± 12	7 ± 7	-2 ± 12
Q13	13 ± 6	85 ± 10	19 ± 8	-14 ± 2
D13	7 ± 3	6 ± 2	17 ± 7	23 ± 7
R3	11 ± 3	55 ± 2	23 ± 8	11 ± 10
R1	7 ± 1	10 ± 1	22 ± 6	13 ± 8
R2	7 ± 2	31 ± 8	16 ± 9	11 ± 6
R4	9 ± 4	13 ± 1	23 ± 9	11 ± 12
R5	8 ± 1	29 ± 1	10 ± 18	-1 ± 9
R7	6 ± 1	0 ± 2	8 ± 6	43 ± 15
R8	8 ± 1	23 ± 2	18 ± 5	67 ± 5
R9	13 ± 5	10 ± 4	22 ± 10	42 ± 13
S1	74 ± 6	100 ± 7	24 ± 11	-8 ± 7
S2	10 ± 4	57 ± 3	48 ± 3	2 ± 11
S3	48 ± 11	85 ± 3	25 ± 8	7 ± 13
A9	36 ± 1	83 ± 8	10 ± 9	13 ± 2
A13	16 ± 2	77 ± 11	26 ± 10	-2 ± 5
6	52 ± 13	65 ± 16	31 ± 6	21 ± 10

Continued…	**Agonism**[b]		**Antagonism**[c]	
compound	**1 μM**	**100 μM**	**1 μM**	**100 μM**
	Activity (%)[d]	Activity (%)[d]	Inhibition (%)[e]	Inhibition (%)[e]
B3	24 ± 3	78 ± 3	34 ± 5	16 ± 3
S5	-2 ± 1	69 ± 3	19 ± 4	13 ± 10
S7	84 ± 2	97 ± 5	7 ± 14	1 ± 7
B11	88 ± 15	108 ± 6	6 ± 5	8 ± 14
S4	59 ± 6	115 ± 7	27 ± 11	-8 ± 11
B12	86 ± 12	117 ± 10	7 ± 7	14 ± 9
B13	67 ± 13	107 ± 6	8 ± 10	13 ± 13
B14	41 ± 8	92 ± 5	10 ± 2	18 ± 5
B5	12 ± 3	57 ± 1	30 ± 15	-8 ± 5
D3	58 ± 1	82 ± 4	10 ± 2	6 ± 9
10	30 ± 4	52 ± 11	9 ± 12	5 ± 15
16	50 ± 7	19 ± 2	8 ± 14	84 ± 6
5	67 ± 17	69 ± 15	23 ± 9	17 ± 3
H15	29 ± 3	59 ± 14	6 ± 14	19 ± 11
H23	70 ± 8	81 ± 15	12 ± 8	1 ± 9
B10	12 ± 2	73 ± 5	16 ± 5	-56 ± 11
D4	23 ± 1	76 ± 4	28 ± 13	-6 ± 4
D6	41 ± 5	80 ± 5	21 ± 19	3 ± 12
D7	31 ± 8	74 ± 4	20 ± 6	11 ± 9
D9	13 ± 1	52 ± 6	26 ± 6	9 ± 1
D10	6 ± 2	22 ± 2	23 ± 6	14 ± 12
D16	13 ± 4	83 ± 4	19 ± 6	3 ± 6
D18	16 ± 4	53 ± 2	18 ± 8	32 ± 5
11	-8 ± 3	-33 ± 2	64 ± 6	128 ± 1
Az-11	109 ± 15	104 ± 4	-1 ± 17	-35 ± 6
12	-2 ± 2	16 ± 2	20 ± 19	43 ± 13
13	1 ± 3	61 ± 6	10 ± 8	37 ± 5
14	7 ± 12	61 ± 4	22 ± 19	12 ± 8
15	-1 ± 2	13 ± 4	16 ± 16	13 ± 8
F31	5 ± 2	32 ± 2	31 ± 5	15 ± 4
18	-1 ± 3	43 ± 3	39 ± 11	45 ± 5
F55	2 ± 1	37 ± 6	11 ± 4	26 ± 7
19R	-1 ± 4	35 ± 8	43 ± 10	38 ± 11
19P	-2 ± 3	-4 ± 1	39 ± 16	25 ± 16
20	2 ± 6	34 ± 11	35 ± 18	39 ± 17
21[f]	-2 ± 3	--[f]	29 ± 13	--[f]
22	-2 ± 3	8 ± 6	35 ± 11	23 ± 18
23	-1 ± 4	-2 ± 2	8 ± 14	12 ± 4