Instrumentation and analytical methods.

^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker AC-300 spectrometer in deuterated solvents at 300 and 75 MHz, respectively. Chemical shifts are reported in parts per million (ppm, δ) using either tetramethyl silane (TMS) or the solvent residual peak as an internal reference (0.0 ppm). Couplings are reported in hertz.

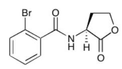
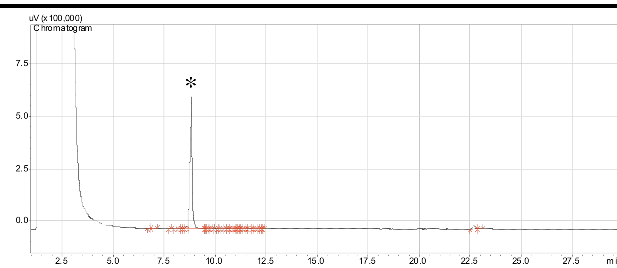
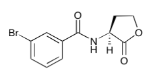
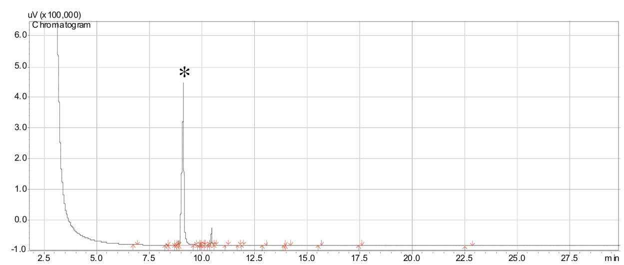
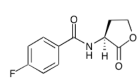
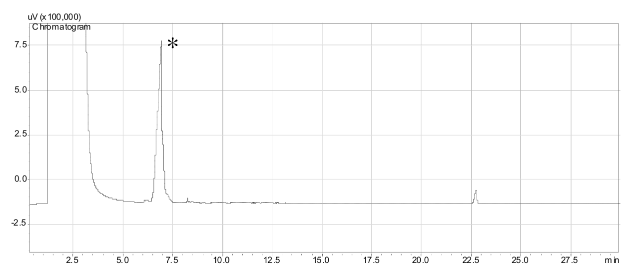
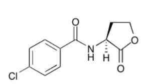
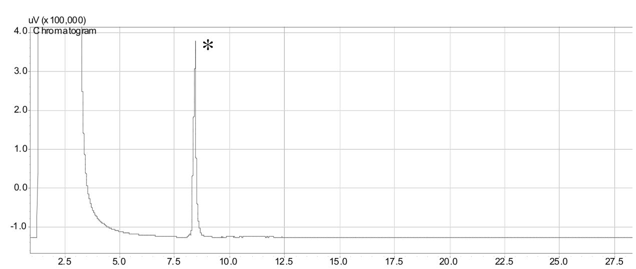
Electrospray ionization (ESI) MS were obtained using a Shimadzu LCMS-2010 system (Columbia, MD) equipped with two pumps (LC-10ADvp), controller (SCL-10Avp), autoinjector (SIL-10ADvp), UV diode array detector (SPD-M10Avp), and single quadrupole analyzer. GC-MS data were obtained using a Shimadzu GC-17A system (Columbia, MD) equipped with a QP-5000 mass spectrometer. A Restek RTX-5 cross bond 95% polysiloxane column was used for all GC-MS analyses. The standard GC method was as follows: injection temperature 300 °C; initial oven temperature 200 °C; hold 5 min; ramp at 20 °C/min to 300 °C; hold 20 min for a total run time of 30 min. Reversed-phase high performance liquid chromatography (RP-HPLC) was performed using a Shimadzu system equipped with an SCL-10Avp controller, an LC-10AT pump, an FCV-10ALvp solvent mixer, and an SPD-10MAvp UV/vis diode array detector. A Restek Premier C18 column (5 μm, 4.6 mm × 250 mm) was used for all analytical RP-HPLC work. Standard RP-HPLC conditions were as follows: flow rates were 1 mL/min for analytical separations and 9 mL/min for preparative separations; mobile phase A: water; mobile phase B: acetonitrile. Purities were determined by integration of peaks with UV detection at 220 nm. For AHL **Q13**, the method was 20-95% ACN over 22 min.

FT-IR spectra were recorded with a Bruker Tensor 27 IR spectrometer, outfitted with a single reflection MIRacle Horizontal attenuated total reflectance (ATR) unit from Pike Technologies. A ZnSe crystal with spectral range 20,000 to 650 cm^{-1} was used for ATR-IR measurements. Optical rotations ($[\alpha]_{24D}$) were measured on a Perkin-Elmer 241 digital polarimeter at 25 °C.

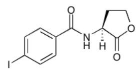
Microwave (μW)-assisted solid-phase reactions used in AHL synthesis were performed in either a Milestone MicroSYNTH Labstation or CEM Discover commercial μW reactor. The Milestone instrument is a multimodal μW synthesis reactor equipped with a continuous power source (1000 W max).[1] The CEM instrument is a monomodal μW synthesis reactor equipped with a 300 W (max) power source.[2] All μW-assisted reactions reported in this study were performed using temperature control to monitor and control μW irradiation.

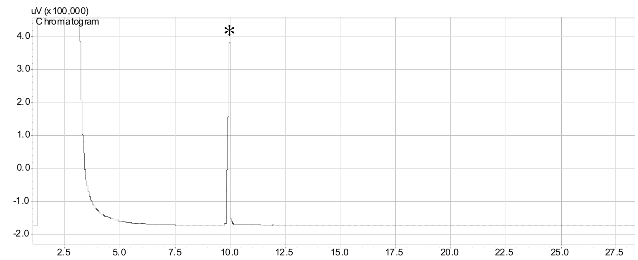
Mass spectroscopy and purity data for Libraries Q, R, and S.

Table S-1. MS and purity data for Libraries Q, R, and S. Controls **1–6,** OdDHL, DDHL, and OOHL were synthesized and fully characterized elsewhere.[3-5] Asterisked [*] peaks indicate the products.

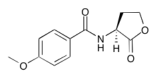
Compound Expected mol. wt.; Observed mol. wt. [ESI] Purity	Structure	GC chromatogram
Q1 exp [M^+] = 283; obs [$M+Na^+$] = 306 93.4%		
Q2 exp [M^+]= 283; obs [$M+Na^+$] = 306 93.4%		
Q3 exp [M^+]= 223; obs [$M+Na^+$] = 246 90.7%		
Q4 exp [M^+] = 240; obs [$M+Na^+$] = 263 98.1%		

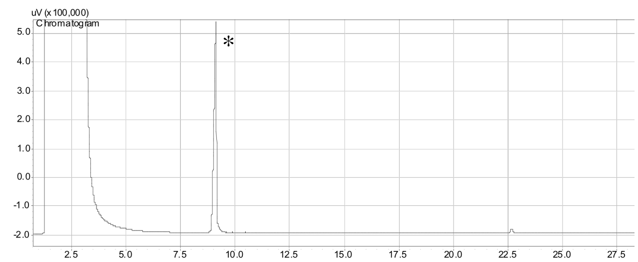
Q5
exp [M$^+$] = 331;
obs [M+Na$^+$] = 354
98.4%



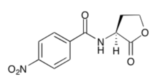


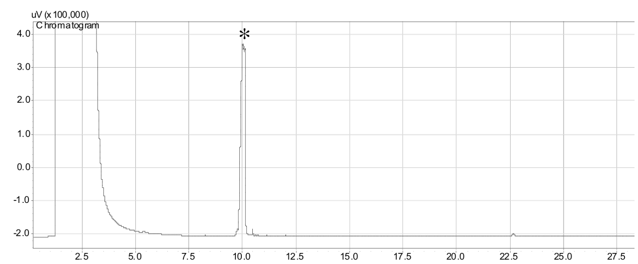
Q6
exp [M$^+$] = 235;
obs [M+Na$^+$] = 258
96.1%



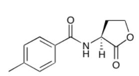


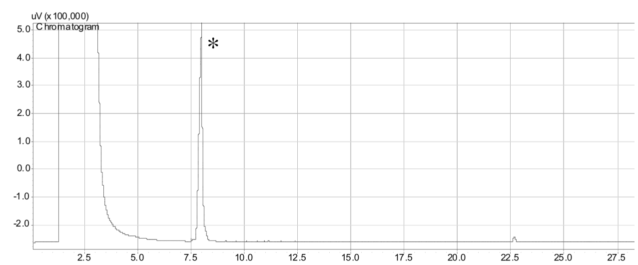
Q7
exp [M$^+$] = 250;
obs [M+Na$^+$] = 273
95.1%



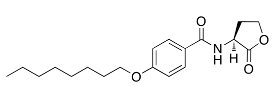


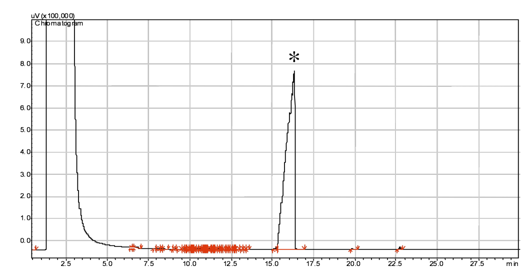
Q8
exp [M$^+$] = 219;
obs [M+Na$^+$] = 242
95.8%



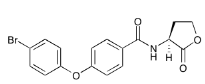


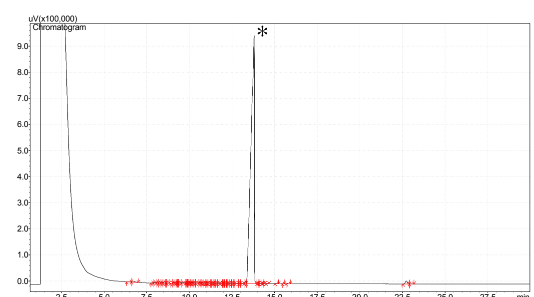
Q9
exp [M$^+$] = 333;
obs [M+H$^+$] = 334
95.6%



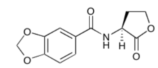


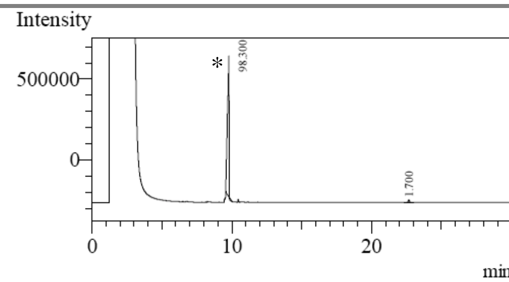
Q10
exp [M$^+$] = 376;
obs [M+Na$^+$] = 399
98.5%



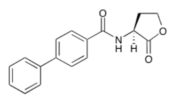


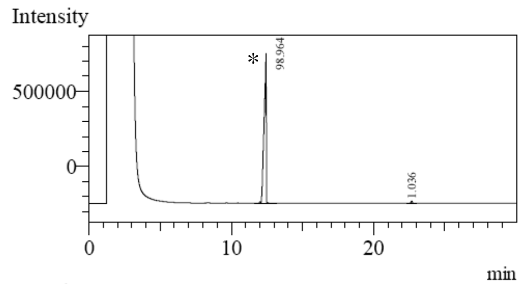
Q11
exp [M$^+$] = 249;
obs [M+Na$^+$] = 272
98.3%



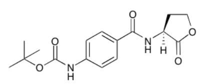


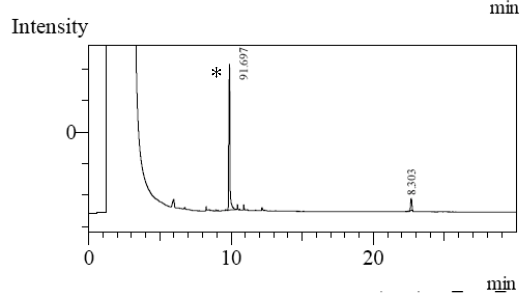
Q12
exp [M$^+$] = 281;
obs [M+Na$^+$] = 304
99.0%



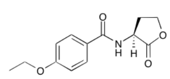


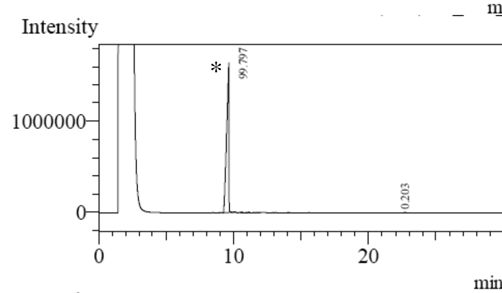
Q13
exp [M$^+$] = 320;
obs [M+Na$^+$] = 343
91.7%



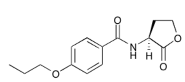


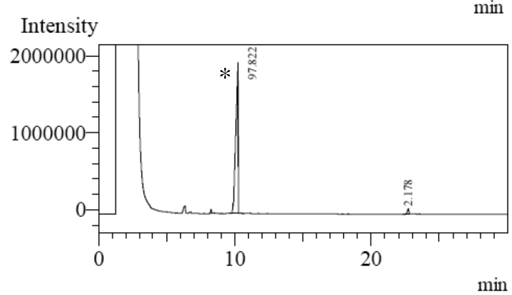
R1
exp [M$^+$] = 249;
obs [M+H$^+$] = 250
99.8%



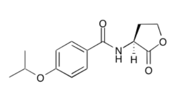


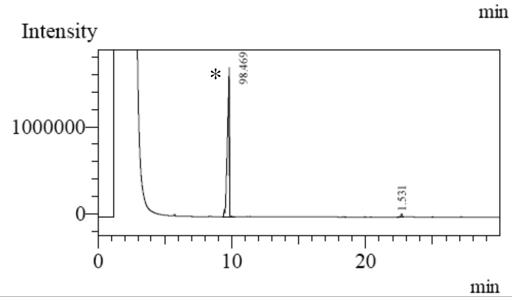
R2
exp [M$^+$] = 263;
obs [M+Na$^+$] = 286
97.8%



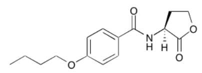


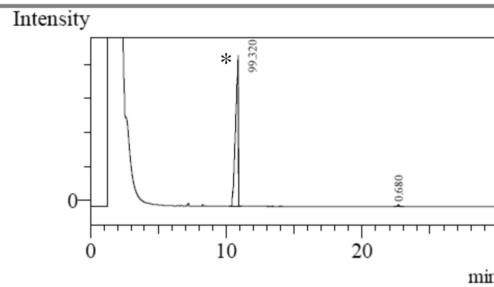
R3
exp [M$^+$] = 263;
obs [M+Na$^+$] = 286
98.5%



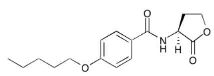


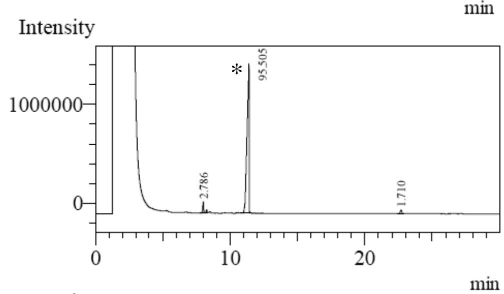
R4
exp [M$^+$] = 277;
obs [M+H$^+$] = 278
99.3%



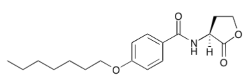


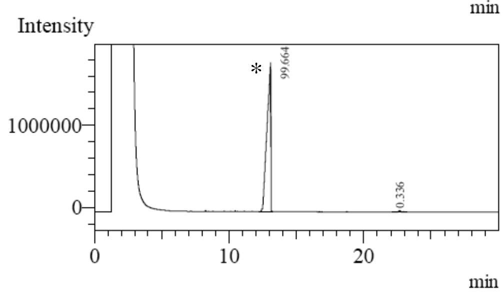
R5
exp [M$^+$] = 291;
obs [M+Na$^+$] = 314
95.5%



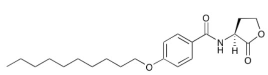


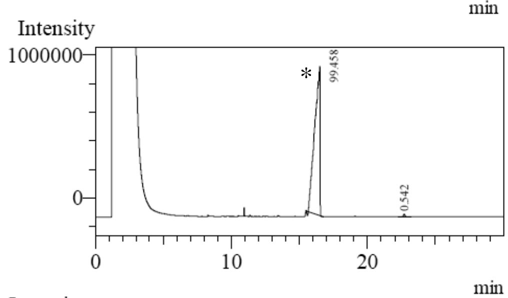
R6
exp [M$^+$] = 319;
obs [M+Na$^+$] = 342
99.7%



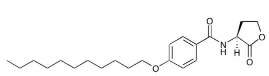


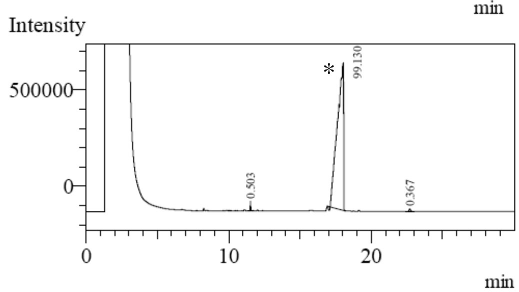
R7
exp [M$^+$] = 361;
obs [M+Na$^+$] = 384
99.5%



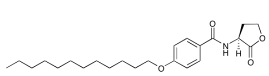


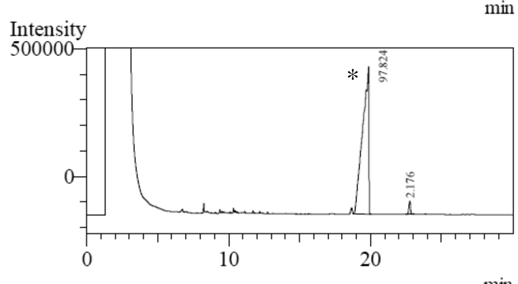
R8
exp [M$^+$] = 375;
obs [M+Na$^+$] = 398
99.1%



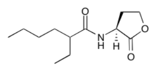


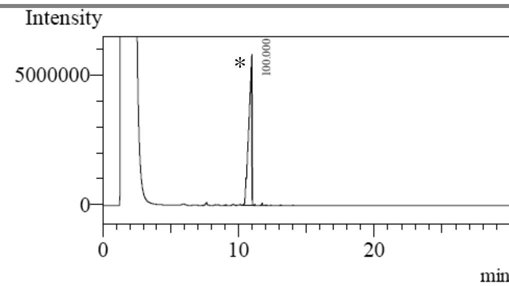
R9
exp [M$^+$] = 389;
obs [M+Na$^+$] = 412
97.8%



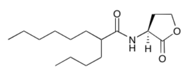


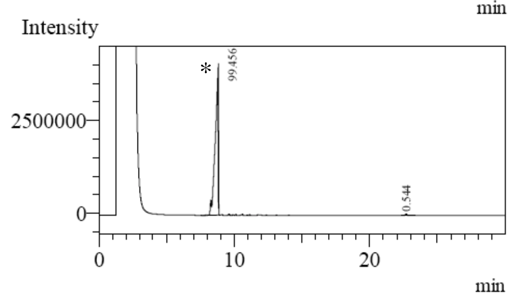
S1
exp [M+] = 227;
obs [M+H+] = 228
100%



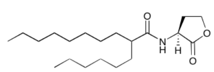


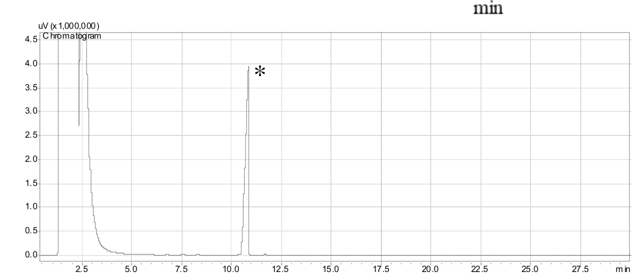
S2
exp [M+] = 283;
obs [M+H+] = 284
99.5%



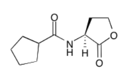


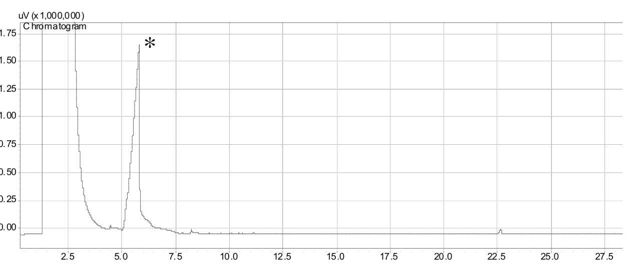
S3
exp [M+] = 339;
obs [M+H+] = 340
95.0%



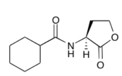


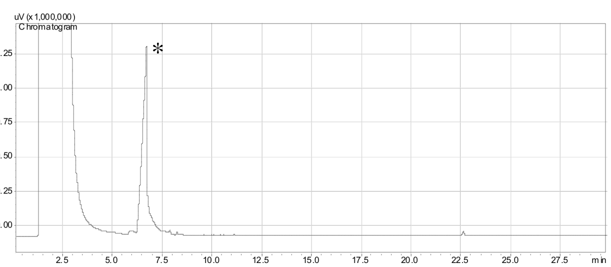
S4
exp [M+] = 197;
obs [M+Na+] = 220
94.6%



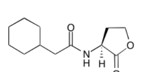


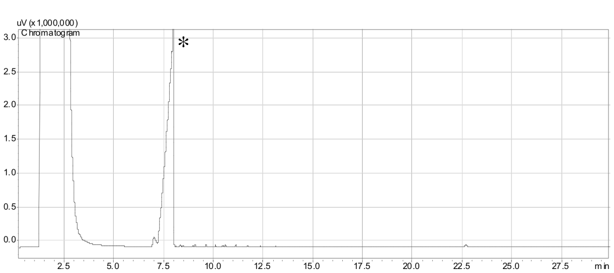
S5
exp [M+] = 211;
obs [M+Na+] = 234
94.5%

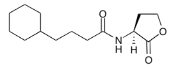
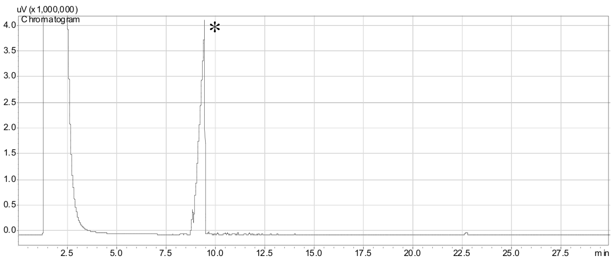




S6
exp [M+] = 225;
obs [M+Na+] = 248
96.5%





S7 exp [M$^+$] = 253; obs [M+Na$^+$] = 276 93.9%		

Characterization data for active AHLs in Libraries Q, R, and S.

^{1}H and ^{13}C NMR data are provided for all compounds; IR and $[\alpha]_D^{25}$ data are also provided for active compounds.

Q1: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ 7.60 (Ar-H, td, J = 1.3, 7.8 Hz, 2H), 7.38 (Ar-H, td, J = 1.3, 7.5 Hz, 1H), 7.31 (Ar-H, td, J = 1.9, 7.8 Hz, 1H), 6.63 (NH, s,1H), 4.73 (CH-lac, ddd, J = 5.8, 8.6, 11.6 Hz, 1H), 4.53 (CH-lac, td, J = 1.1, 9.2 Hz, 1H), 4.35 (CH-lac, ddd, J = 5.8, 9.3, 11.2 Hz, 1H), 3.01 (CH-lac, dddd, J = 1.2, 5.9, 7.1, 12.5 Hz, 1H), 2.32 (CH-lac, dtd, J = 8.9, 11.4, 20.4 Hz, 1H).

Q2: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ 7.93 (CH, t, J = 1.8 Hz, 1H), 7.70 (Ar-H, ddd, J = 0.6, 1.1, 7.6 Hz, 1H), 7.64 (Ar-H, ddd, J = 1.0, 2.0, 8.0 Hz, 1H), 7.30 (Ar-H, t, J = 7.9 Hz, 1H), 6.95 (NH, d, J = 2.7 Hz, 1H), 4.79 (CH-lac, ddd, J = 6.1, 8.6, 11.6 Hz, 1H), 4.54 (CH-lac, td, J = 1.1 9.2 Hz, 1H), 4.36 (CH-lac, ddd, J = 5.9, 9.3, 11.3 Hz, 1H), 2.93 (CH-lac, dddd, J = 1.2, 5.9, 7.1, 12.5 Hz, 1H), 2.29 (CH-lac, dtd, J = 8.8, 11.5, 20.5 Hz, 1H).

Q3: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ 7.81 (Ar-H, ddd, J = 2.9, 5.1, 8.2 Hz, 2H), 7.1 (Ar-H, tt, J = 3.0, 8.5 Hz, 2H), 6.83 (NH, d, J = 4.7 Hz, 1H), 4.76 (CH-lac, ddd, J = 5.8, 8.5, 11.5 Hz, 1H), 4.53 (CH-lac, td, J = 1.1, 9.2 Hz, 1H), 4.36 (CH-lac, ddd, J = 6.0, 9.5, 11.5 Hz, 1H), 2.94 (CH-lac, dddd, J = 1.2, 5.9, 7.0, 12.5 Hz, 1H), 2.28 (CH-lac, dtd, J = 8.8, 11.4, 12.2 Hz, 1H).

Q4: ^{1}H NMR: (299.7 MHz, DMSO) δ 9.04 (NH, d, J = 8.0 Hz, 1H), 7.86 (Ar-H, dt, J = 2.5, 9.2 Hz, 2H), 7.56 (Ar-H, dt, J = 2.5, 9.2 Hz, 2H), 4.75 (CH-lac, ddd, J = 8.2, 9.2, 10.8 Hz, 1H), 4.40 (CH-lac, td, J = 1.9, 8.8 Hz, 1H), 4.26 (CH-lac, ddd, J = 6.6, 8.8, 10.4 Hz, 1H), 2.43 (CH-lac, m, 1H), 2.31 (CH-lac, dtd, J = 9.0, 10.6, 11.9 Hz, 1H); ^{13}C NMR: (75.4 MHz, DMSO) δ 176.06, 165.67, 137.18, 132.87, 129.87, 129.33, 66.05, 49.16, 28.21; IR (cm^{-1}): 3260, 1788, 1765, 1647, 1597, 1546, 1487, 1379, 1320, 1167, 1014, 858, 764, 672; $[\alpha]_D^{25}$(DMSO, c = 8.16 mg/ml): -36.3°.

Q5: ^{1}H NMR: (299.7 MHz, DMSO) δ 9.02 (NH, d, J = 8.0 Hz, 1H), 7.87 (Ar-H, dt, J = 2.3, 8.9 Hz, 2H), 7.62 (Ar-H, dt, J = 2.2, 8.8 Hz, 2H), 4.75 (CH-lac, ddd, J = 8.2, 9.1, 10.7 Hz, 1H), 4.39 (CH-lac, td, J = 2.0, 8.8 Hz, 1H), 4.25 (CH-lac, ddd, J = 6.6, 8.9, 10.4 Hz, 1H), 2.42 (CH-lac, m, 1H), 2.30 (CH-lac, dtd, J = 9.0, 10.6, 11.9 Hz, 1H); ^{13}C NMR: (75.4 MHz, DMSO) δ 175.88, 166.19, 138.04, 133.33, 129.95, 100.21, 66.04, 49.07, 28.43; IR (cm^{-1}): 3256, 1787, 1765, 1647, 1590, 1545, 1321, 1168, 1021, 1007, 760, 716, 674; $[\alpha]_D^{25}$ (DMSO, c = 8.00 mg/ml): + 8.56°.

Q6: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ 7.78 (Ar-H, dt, J = 2.9, 5.0 Hz, 2H), 6.94 (Ar-H, dt, J = 3.0, 5.1 Hz, 2H), 6.52 (NH, d, J = 3.6 Hz, 1H), 4.69 (CH-lac, ddd, J = 5.2, 8.4, 11.6 Hz, 1H), 4.53 (CH-lac, td, J = 0.9, 9.0 Hz, 1H), 4.35 (CH-lac, ddd, J = 5.8, 9.3, 11.3 Hz, 1H), 3.86 (CH_3, s, 2H), 3.00 (CH-lac, dddd, J = 1.1, 5.8, 6.9, 12.5 Hz, 1H), 2.24 (CH-lac, dddd, J = 8.9, 11.5, 12.5, 20.3 Hz, 1H).

Q7: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ 8.30 (Ar-H, dt, J = 2.4, 9.2 Hz, 2H), 7.98 (Ar-H, dt, J = 2.3, 9.2 Hz, 2H), 6.84 (NH, d, J = 4.2 Hz, 1H), 4.76 (CH-lac, ddd, J = 5.6, 8.5, 11.7 Hz, 1H), 4.57 (CH-lac, td, J = 0.9, 9.2 Hz, 1H), 4.39 (CH-lac, ddd, J = 5.8, 9.4, 11.4 Hz, 1H), 11.4 (CH-lac, dddd, J = 1.0, 5.7, 6.9, 12.6 Hz, 1H), 2.30 (CH-lac, dtd, J = 8.9, 11.5, 12.5 Hz, 1H).

Q8: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ 7.70 (Ar-H, apparent doublet, J = 8.2 Hz, 2H), 7.25 (Ar-H, apparent doublet, J = 7.0 Hz, 2H), 6.61 (NH, d, J = 3.2 Hz, 1H), 4.71 (CH-lac, ddd, J = 5.4, 8.6, 11.8 Hz, 1H), 4.53 (CH-lac, td, J = 0.7, 9.4 Hz, 1H), 4.35 (CH-lac, ddd, J = 5.8, 9.3, 11.3 Hz, 1H), 3.00 (CH-lac, dddd, J = 1.0, 5.7, 6.8, 12.5 Hz, 1H), 2.41 (CH_3, s, 3H), 2.24 (CH-lac, dtd, J = 8.8, 11.5, 12.5 Hz, 1H).

Q9: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ 7.75 (Ar-H, dt, J = 3.0, 9.7 Hz, 2H), 6.89 (Ar-H, dt, J = 2.9, 9.7 Hz, 2H), 6.72 (NH, d, J = 5.6 Hz, 1H), 4.74 (CH-lac, ddd, J = 5.7, 8.6, 11.5 Hz, 1H), 4.52 (CH-lac, td, J = 1.0, 9.1 Hz, 1H), 4.34 (CH-lac, ddd, J = 5.9, 9.3, 11.2 Hz, 1H), 3.99 (CH_2, t, J = 6.6 Hz, 2H), 2.94 (CH-lac, dddd, J = 1.2, 5.8, 7.1, 12.5 Hz, 1H), 2.26 (CH-lac, dtd, J = 8.9, 11.5, 12.4 Hz, 1H), 1.79 (CH_2, apparent pentet, J = 6.6 Hz, 2H), 1.38 (CH_2, m, 10H), 0.89 (CH_3, apparent triplet, J = 7.0 Hz, 3H); ^{13}C NMR: (75.4 MHz, $CDCl_3$) δ 176.11, 167.56, 162.54, 129.21, 125.14, 114.54, 68.46, 66.49, 49.92, 32.01, 30.91, 29.54, 29.42, 29.32, 26.20, 22.86, 14.30; IR (cm^{-1}): 3267, 2924, 1776, 1640, 1609, 1543, 1508, 1383, 1303, 1252, 1220, 1180, 1017, 841; $[\alpha]_D^{25}$ ($CHCl_3$, c = 8.48 mg/ml): + 23.8°.

Q10: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ 7.78 (Ar-H, dt, J = 2.8, 9.6 Hz, 2H), 7.49 (Ar-H, dt, J = 3.2, 10.0 Hz, 2H), 6.98 (Ar-H, dt, J = 2.7, 9.6 Hz, 2H), 6.92 (Ar-H, dt, J = 3.3, 10.1 Hz, 2H), 6.82 (NH, d, J = 5.6 Hz, 1H), 4.77 (CH-lac, ddd, J = 5.9, 8.6, 11.6 Hz, 1H), 4.53 (CH-lac, td, J = 0.8, 9.1 Hz, 1H), 4.35 (CH-lac, ddd, J = 5.9, 9.3, 11.2 Hz, 1H), 2.94 (CH-lac, dddd, J = 1.0, 5.9, 7.0, 12.6 Hz, 1H), 2.27 (CH-lac, ddd, J = 8.9, 11.5, 20.5 Hz, 1H); ^{13}C NMR: (75.4 MHz, $CDCl_3$) δ 176.18, 167.23, 160.72, 155.24, 133.24, 129.47, 127.95, 121.70, 118.11, 117.24, 66.53, 49.93, 30.79; IR (cm^{-1}): 3268, 2924, 1775, 1638, 1504, 1482, 1378, 1242, 1172, 1010, 864, 846; $[\alpha]_D^{25}$ ($CHCl_3$, c = 8.08 mg/ml): + 22.0°.

Q11: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ 7.35 (Ar-H, dd, J = 1.8, 8.1 Hz, 1H), 7.31 (Ar-H, d, J = 1.7 Hz, 1H), 6.86 (Ar-H, d, J = 8.1 Hz, 1H), 6.50 (NH, d, J = 3.8 Hz, 1H), 6.05 (CH_2, s, 2H), 4.69 (CH-lac, ddd, J = 5.2, 8.5, 11.7 Hz, 1H), 4.54 (CH-lac, td, J = 0.9, 9.2 Hz, 1H), 4.36 (CH-lac, ddd, J = 5.8, 9.4, 11.4 Hz, 1H), 3.00 (CH-lac, dddd, J = 1.0, 5.8, 6.9, 12.7 Hz, 1H), 2.23 (CH-lac, dtd, J = 8.9, 11.6, 12.4 Hz, 1H).

Q12: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ 7.89 (Ar-H, dt, J = 2.0, 8.6 Hz, 2H), 7.68 (Ar-H, dt, J = 1.8, 8.5 Hz, 2H), 7.62 (Ar-H, dt, J = 1.5, 7.1 Hz, 2H), 7.43 (Ar-H, m, 3H), 6.67 (NH, d, J = 4.9 Hz, 1H), 4.74 (CH-lac, ddd, J = 5.2, 8.5, 11.7 Hz, 1H), 4.55 (CH-lac, td, J = 0.8, 9.2 Hz, 1H), 4.37 (CH-lac, ddd, J = 5.9, 9.4, 11.4 Hz, 1H), 3.04 (CH-lac, dddd, J = 1.1, 5.7, 6.8, 12.5 Hz, 1H), 2.27 (CH-lac, dtd, J = 8.8, 11.4, 12.5 Hz, 1H); IR (cm^{-1}): 3280, 1776, 1635, 1546, 1486, 1385, 1331, 1175, 1169, 1017, 1000, 748, 692; $[\alpha]_D^{25}$ (DMSO, c = 8.64 mg/ml): - 4.97°; $CHCl_3$).

Q13: ^{1}H NMR: (299.7 MHz, DMSO) δ 9.64 (NH, s, 1H), 8.80 (NH, d, J = 8.0 Hz, 1H), 7.76 (Ar-H, dt, J = 1.8, 7.0 Hz, 2H), 7.53 (Ar-H, dt, J = 1.8, 7.0 Hz, 2H), 4.72 (H-lac, ddd, J = 8.2, 9.1, 10.6 Hz, 1H), 4.39 (H-lac, td, J = 1.9, 8.7 Hz, 1H), 4.25 (H-lac, ddd, J = 6.6, 8.8, 10.3 Hz, 1H), 2.42 (H-lac, m, 1H), 2.31 (H-lac, m, 1H), 1.47 (CH_3, s, 9H); ^{13}C NMR: (75.4 MHz, DMSO) δ 176.18, 166.25, 153.26, 143.39, 128.74, 127.51, 117.82, 106.47, 80.11, 65.89, 48.97, 28.56; IR (cm^{-1}): 3333, 1775, 1696, 1643, 1613, 1518, 1370, 1317, 1247, 1160, 1062, 1017, 846, 757, 644; $[\alpha]_D^{25}$ (DMSO, c = 7.04 mg/ml): - 24.9°.

R1: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ 7.76 (Ar-H, dt, J = 2.9, 9.7 Hz, 2H), 6.90 (Ar-H, dt, J = 2.9, 9.8 Hz, 2H), 6.68 (NH, d, J = 5.2 Hz, 1H), 4.73 (CH-lac, ddd, J = 5.7, 8.7, 11.6 Hz, 1H), 4.52 (CH-lac, td, J = 1.1, 9.1 Hz, 1H), 4.34 (CH-lac, ddd, J = 5.9, 9.2, 11.3 Hz, 1H), 4.08 (CH_2, q, J = 7.1 Hz, 2H), 2.95 (CH-lac, dddd, J = 1.2, 6.0, 7.1, 12.6 Hz, 1H), 2.25 (CH-lac, dtd, J = 8.9, 11.4, 12.5 Hz, 1H), 1.43 (CH_3, t, J = 6.9 Hz, 3H); ^{13}C NMR: (75.4 MHz, DMSO) δ 176.15, 166.29, 161.98, 129.82, 126.28, 114.68, 65.85, 64.02, 49.03, 28.57, 14.96; IR (cm^{-1}): 3337, 2984, 2918, 2882, 1800, 1625, 1530, 1500, 1260, 1190, 1015, 865, 621; $[\alpha]_D^{25}$($CHCl_3$, c = 8.08 mg/ml): + 34.6°.

R2: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ 7.76 (Ar-H, dt, J = 2.8, 9.7 Hz, 2H), 6.92 (Ar-H, dt, J = 2.8, 9.6 Hz, 2H), 6.57 (NH, d, J = 4.7 Hz, 1H), 4.71 (CH-lac, ddd, J = 5.4, 8.5, 11.6 Hz, 1H), 4.53 (CH-lac, td, J = 0.9, 9.2 Hz, 1H), 4.35 (CH-lac, ddd, J = 5.9, 9.3, 11.3 Hz, 1H), 3.97 (CH-lac, t, J = 6.6 Hz, 2H), 2.99 (CH-lac, dddd, J = 1.0, 5.8, 7.0, 12.6 Hz, 1H), 2.24 (CH-lac, dtd, J = 8.8, 11.5, 12.4 Hz, 1H), 1.83 (CH_2, sextet, J = 7.3 Hz, 2H), 1.05 (CH_3, t, J = 7.5 Hz, 3H).

R3: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ 7.75 (Ar-H, dt, J = 3.0, 9.8 Hz, 2H), 6.90 (Ar-H, dt, J = 2.9, 9.7 Hz, 2H), 6.57 (NH, d, J = 4.9 Hz, 1H), 4.71 (CH-lac, ddd, J = 5.4, 8.6, 11.6 Hz, 1H), 4.62 (CH, septet, J = 6.1 Hz, 1H), 4.53 (CH-lac, td, J = 0.9, 9.3 Hz, 1H), 4.35 (CH-lac, ddd, J = 5.8, 9.3, 11.3 Hz, 1H), 2.98 (CH-lac, dddd, J = 1.1, 5.7, 6.9, 12.5 Hz, 1H), 2.24 (CH-lac, dtd, J = 8.8, 11.4, 12.3 Hz, 1H), 1.36 (CH_3, d, J = 6.1 Hz, 6H).

R4: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ 7.75 (Ar-H, dt, J = 2.8, 9.7 Hz, 2H), 6.89 (Ar-H, dt, J = 2.8, 9.7 Hz, 2H), 6.74 (NH, d, J = 5.6 Hz, 1H), 4.74 (CH-lac, ddd, J = 5.7, 8.6, 11.6 Hz, 1H), 4.51 (CH-lac, td, J = 1.0, 9.1 Hz, 1H), 4.34 (CH-lac, ddd, J = 5.9, 9.3, 11.2 Hz, 1H), 4.00 (CH_2, t, J = 6.5 Hz, 2H), 2.93 (CH-lac, dddd, J = 1.2, 5.9, 7.2, 12.5 Hz, 1H), 2.26 (CH-lac, dtd, J = 8.9, 11.4, 12.3 Hz, 1H), 1.78 (CH_2, apparent pentet, J = 6.6 Hz, 2H), 1.50 (CH_2, apparent sextet, J = 7.4 Hz, 2H), 0.98 (CH_3, t, J = 7.3 Hz, 3H); ^{13}C NMR: (75.4 MHz, $CDCl_3$) δ176.14, 167.55, 162.53, 129.20, 125.14, 114.54, 68.13, 66.49, 49.90, 31.36, 30.88, 19.40, 14.02; IR (cm^{-1}): 3275, 2933, 1774, 1641, 1609, 1543, 1507, 1382, 1303, 1252, 1224, 1016, 841; $[\alpha]_D^{25}$ ($CHCl_3$, c = 8.16 mg/ml): + 30.4°.

R5: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ 7.75 (Ar-H, dt, J = 2.9, 9.7 Hz, 2H), 6.90 (Ar-H, dt, J = 2.8, 9.7 Hz, 2H), 6.72 (NH, d, J = 5.6 Hz, 1H), 4.74 (CH-lac, ddd, J = 5.7, 8.6, 11.5 Hz, 1H), 4.52 (CH-lac, td, J = 0.9, 9.0 Hz, 1H), 4.34 (CH-lac, ddd, J = 5.9, 9.3, 11.3 Hz, 1H), 3.99 (CH_2, t, J = 6.6 Hz, 2H), 2.94 (CH-lac, dddd, J = 1.0, 5.8, 7.1, 12.5 Hz, 1H), 2.26 (CH-lac, apparent dd, J = 9.0, 11.9 Hz, 1H), 1.80 (CH_2, p, J = 6.7 Hz, 2H), 1.42 (CH_2, m, 4H), 0.94 (CH_3, t, J = 7.0 Hz, 3H); ^{13}C NMR: (75.4 MHz, $CDCl_3$) δ176.12, 167.54, 162.53, 129.21, 125.15, 114.55, 68.44, 66.49, 58.39, 30.90, 29.01, 28.34, 22.64, 14.21; IR (cm^{-1}): 3272, 2935, 1774, 1641, 1609, 1544, 1508, 1382, 1303, 1252, 1180, 1016, 841; $[\alpha]_D^{25}$ ($CHCl_3$, c = 8.80 mg/ml): + 28.6°.

R6: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ 7.75 (Ar-H, dt, J = 2.9, 9.8 Hz, 2H), 6.90 (Ar-H, dt, J = 2.8, 9.7 Hz, 2H), 6.70 (NH, d, J = 5.6 Hz, 1H), 4.73 (CH-lac, ddd, J = 5.7, 8.5, 11.5 Hz, 1H), 4.52 (CH-lac, td, J = 1.1, 9.2 Hz, 1H), 4.34 (CH-lac, ddd, J = 5.8, 9.4, 11.3 Hz, 1H), 3.99 (CH_2, t, J = 6.6 Hz, 2H), 2.95 (CH-lac, dddd, J = 1.1, 5.8, 7.1, 12.5 Hz, 1H), 2.25 (CH-lac, dtd, J = 8.9, 11.4, 12.4 Hz, 1H), 1.79 (CH_2, apparent pentet, J = 6.6 Hz, 2H), 1.37 (CH_2, m, 8H), 0.90 (CH_3, t, J = 6.5 Hz, 3H); ^{13}C NMR: (75.4 MHz, $CDCl_3$) δ 176.09, 167.63, 162.55, 129.21, 125.14, 114.55, 68.46, 66.49, 58.24, 49.84, 31.97, 30.93, 29.23, 26.16, 22.81, 14.29; $[\alpha]_D^{25}$ ($CHCl_3$, c = 9.04 mg/ml): + 26.6°; IR (cm^{-1}): 3272, 2932, 1774, 1641, 1609, 1543, 1507, 1252, 1180, 1016, 841.

R7: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ 7.76 (Ar-H, dt, J = 2.9, 9.8 Hz, 2H), 6.92 (Ar-H, dt, J = 2.8, 9.7 Hz, 2H), 6.54 (NH, d, J = 5.1 Hz, 1H), 4.70 (CH-lac, ddd, J = 5.3, 8.5, 11.7 Hz, 1H), 4.53 (CH-lac, t, J = 9.0 Hz, 1H), 4.35 (CH-lac, ddd, J = 5.8, 9.3, 11.3 Hz, 1H), 4.00 (CH_2, t, J = 6.5 Hz, 2H), 2.99 (CH-lac, dddd, J = 0.9, 5.9, 6.9, 12.7 Hz, 1H), 2.24 (CH-lac, ddd, J = 8.9, 11.6, 20.5 Hz, 1H), 1.80 (CH_2, pentet, J = 6.7 Hz, 2H), 1.27 (CH_2, m, 16H), 0.88 (CH_3, t, J = 6.9 Hz, 3H).

R8: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ 7.76 (Ar-H, dt, J = 3.0, 9.8 Hz, 2H), 6.92 (Ar-H, dt, J = 2.9, 9.8 Hz, 2H), 6.52 (NH, d, J = 4.9 Hz, 1H), 4.69 (CH-lac, ddd, J = 5.3, 8.5, 11.6 Hz, 1H), 4.53 (CH-lac, td, J = 0.7, 8.9 Hz, 1H), 4.35 (CH-lac, ddd, J = 5.8, 9.2, 11.2 Hz, 1H), 4.00 (CH_2, t, J = 6.6 Hz, 2H), 3.00 (CH-lac, dddd, J = 0.9, 5.8, 6.9, 12.6 Hz, 1H), 2.23 (CH-lac, dtd, J = 8.9, 11.5, 12.6 Hz, 1H), 1.79 (CH_2, apparent pentet, J = 6.6 Hz, 2H), 1.36 (CH_2, m, 16H), 0.88 (CH_3, t, J = 6.3 Hz, 3H).

R9: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ 7.76 (Ar-H, dt, J = 3.0, 9.8 Hz, 2H), 6.92 (Ar-H, dt, J = 2.9, 9.8 Hz, 2H), 6.53 (NH, d, J = 5.1 Hz, 1H), 4.70 (CH-lac, ddd, J = 5.2, 8.5, 11.6 Hz, 1H), 4.53 (CH-lac, td, J = 0.9, 9.0 Hz, 1H), 4.35 (CH-lac, ddd, J = 5.8, 9.4, 11.3 Hz, 1H), 4.00 (CH_2, t, J = 6.6 Hz, 2H), 6.6 (CH-lac, dddd, J = 1.0, 5.8, 7.0, 12.6 Hz, 1H), 2.24 (CH-lac, dtd, J = 8.9, 11.5, 12.4 Hz, 1H), 1.80 (CH_2, apparent pentet, J = 6.7 Hz, 2H), 1.38 (CH_2, m, 18H), 0.88 (CH_3, t, J = 6.3 Hz, 3H).

S1: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ 6.03 (NH, d, J = 4.1 Hz, 1H), 4.53 (CH-lac, ddd, J = 2.9, 5.6, 8.5 Hz, 1H), 4.48 (CH-lac, td, J = 1.3, 9.1 Hz, 1H), 4.29 (CH-lac, ddd, J = 6.0, 9.4, 11.3 Hz, 1H), 2.89 (CH-lac, dddd, J = 1.0, 5.8, 7.2, 12.6 Hz, 1H), 2.08 (CH-lac and CH, m , 2H), 1.53 (CH_2, m, 4H), 1.28 (CH_2, m, 4H), 0.89 (CH_3, m, 6H); ^{13}C NMR: (75.4 MHz, $CDCl_3$) δ 176.86, 175.67, 66.31, 58.20, 49.47, 32.44, 30.76, 29.73, 26.05, 22.77, 14.14, 11.83; IR (cm^{-1}): 3295, 2932, 1777, 1644, 1544, 1381, 1178, 1022; $[\alpha]_D^{25}$ ($CHCl_3$, c = 11.4 mg/ml): + 2.20°.

S2: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ5.98 (NH, d, J = 5.1 Hz, 1H), 4.54 (CH-lac, ddd, J = 1.1, 5.5, 6.8 Hz, 1H), 4.47 (CH-lac, td, J = 1.0, 9.2 Hz, 1H), 4.29 (CH-lac, ddd, J = 6.0, 9.3, 11.3 Hz, 1H), 2.89 (CH-lac, dddd, J = 1.1, 5.8, 7.0, 12.6 Hz, 1H), 2.10 (CH-lac and CH, m, 2H), 1.60 (CH_2, m, 2H), 1.44 (CH_2, m, 2H), 1.27 (CH_2, m, 12H), 0.88 (CH_3, m, 6H); ^{13}C NMR: (75.4 MHz, $CDCl_3$) δ 177.03, 175.66, 111.23, 66.32, 58.28, 49.46, 47.77, 33.23, 32.90, 31.90, 30.96, 29.94, 29.54, 27.74, 22.94, 14.26; IR (cm^{-1}): 3292, 2930, 1774, 1646, 1542, 1379, 1168, 1018; $[\alpha]_D^{25}$ ($CHCl_3$, c = 8.96 mg/ml): + 5.78°.

S3: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ 5.97 (NH, d, J = 5.5 Hz, 1H), 4.51 (CH-lac, ddd, J = 5.7, 8.7, 11.6 Hz, 1H), 4.47 (CH-lac, td, J = 1.0, 9.3 Hz, 1H), 4.28 (CH-lac, ddd, J = 5.9, 9.3, 11.3 Hz, 1H), 2.90 (CH-lac, dddd, J = 1.2, 5.9, 7.1, 12.6 Hz, 1H), 2.10 (CH-lac and CH, m, 2H), 1.59 (CH_2, m, 2H), 1.43 (CH_2, m, 2H), 1.26 (CH_2, m, 20H), 0.87 (CH_3, t, J = 6.1 Hz, 6H); ^{13}C NMR: (75.4 MHz, $CDCl_3$) δ 177.04, 175.64, 111.26, 66.33, 58.57, 49.46, 47.80, 33.21, 33.13, 32.05, 31.91, 30.98, 29.83, 29.64, 29.54, 27.78, 27.75, 22.86, 22.79, 14.30; IR (cm^{-1}): 3288, 2925, 2853, 1798, 1643, 1547, 1176, 1033, 687; $[\alpha]_D^{25}$ ($CHCl_3$, c = 11.8 mg/ml): + 5.39°.

S4: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ 5.96 (NH, s, J = Hz, 1H), 4.52 (CH-lac, ddd, J = 5.6, 8.7, 11.7 Hz, 1H), 4.47 (CH-lac, td, J = 0.9, 9.8 Hz, 1H), 4.28 (CH-lac, ddd, J = 5.9, 9.3, 11.3 Hz, 1H), 2.87 (CH-lac, dddd, J = 1.0, 5.9, 7.0, 12.6 Hz, 1H), 2.61 (CH, apparent pentet, J = 8.1 Hz, 1H), 2.12 (CH-lac, dtd, J = 8.9, 11.5, 12.6 Hz, 1H), 1.81 (CH_2, m, 6H), 1.58 (CH_2, m, 2H).

S5: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ 5.94 (NH, s, 1H), 4.51 (CH-lac, ddd, J = 5.5, 8.6, 11.6 Hz, 1H), 4.47 (CH-lac, td, J = 1.3, 9.4 Hz, 1H), 4.29 (CH-lac, ddd, J = 5.7, 9.3, 11.2 Hz, 1H), 2.88 (CH-lac, dddd, J = 1.0, 5.7, 6.9, 12.5 Hz, 1H), 2.13 (CH-lac and CH, m, 2H), 1.85 (CH_2, m, 4H), 1.68 (CH_2, m, 1H), 1.45 (CH_2, m, 2H), 1.29 (CH_2, m, 3H).

S6: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ 6.36 (NH, d, J = 1.7 Hz, 1H), 4.55 (CH-lac, ddd, J = 6.1, 8.6, 11.5 Hz, 1H), 4.47 (CH-lac, td, J = 1.3, 9.2 Hz, 1H), 4.28 (CH-lac, ddd, J = 5.9, 9.2, 11.1 Hz, 1H), 2.82 (CH-lac , dddd, J = 1.4, 6.0, 7.4, 12.6 Hz, 1H), 2.15 (H-lac, dtd, J = 8.9, 11.3, 12.5 Hz, 1H), 2.13 (CH_2, d, J = 1.6 Hz, 2H), 1.72 (CH_2, m, 6H), 1.23 (CH_2 and CH, m, 3H), 0.96 (CH_2, m, 2H); ^{13}C NMR: (75.4 MHz, $CDCl_3$) δ 175.77, 173.31, 66.08, 49.17, 44.23, 40.73, 35.37, 33.14, 30.47, 26.10; IR (cm^{-1}): 3307, 2918, 2850, 1776, 1643, 1552, 1378, 1172, 1013, 1001; $[\alpha]_D^{25}$($CHCl_3$, c = 5.84 mg/ml): - 2.19°.

S7: ^{1}H NMR: (299.7 MHz, $CDCl_3$) δ 6.07 (NH, d, J = 4.4 Hz, 1H), 4.56 (CH-lac, ddd, J = 5.7, 8.5, 11.5 Hz, 1H), 4.47 (CH-lac, td, J = 1.1, 9.2 Hz, 1H), 4.28 (CH-lac, ddd, J = 5.9, 9.4, 11.3 Hz, 1H), 2.86 (CH-lac, dddd, J = 1.1, 5.9, 8.6, 12.5 Hz, 1H), 2.23 (CH_2, t, J = 7.4 Hz, 2H), 2.13 (CH-lac, dtd, J = 8.8, 11.4, 12.2 Hz, 1H), 1.66 (CH_2, m, 8H), 1.20 (CH_2 and CH, m, 5H), 0.87 (CH_2, m, 2H); ^{13}C NMR: (75.4 MHz, $CDCl_3$) δ175.80, 173.94, 66.23, 49.34, 37.62, 37.16, 36.54, 33.66, 30.79, 26.84, 26.54, 22.97; IR (cm^{-1}): 3306, 2923, 2851, 1777, 1643, 1551, 1379, 1175, 1009, 945, 680; $[\alpha]_D^{25}$($CHCl_3$, c = 8.56 mg/ml): + 4.46°.

<u>Primary reporter gene assay data for Libraries Q, R, and S.</u>

The three bacterial reporter strains used in this study were: *E. coli* DH5α harboring the QscR expression vector pJN105Q and a plasmid-born PA1897-*lacZ* expression vector (pJL101),[6] *E. coli* DH5α harboring the LasR expression vector pJN105L and a plasmid-born P*lasI-lacZ* fusion (pSC11),[6] *V. fischeri* ES114 (Δ-*luxI*),[7] and *A. tumefaciens* WCF47 (Δ-*traI*) harboring a plasmid-born P*traI-lacZ* fusion (pCF372).[8] The antagonism and agonism assay protocols were identical to those reported previously; see text for additional details. The primary reporter gene assay data for the control compounds and synthetic AHLs **Q1–Q13, R1–R9** and **S1–S7** are listed below in Table S-2. These data are also plotted graphically in Figures S1–S4. Quantitative agonism and antagonism dose response graphs are presented in Figures S5–S12.

Table S-2. Primary antagonism and agonism assay data for Libraries Q, R, and S.[a]

Compd	*E. coli* –QscR[b]		*E. coli* – LasR[e]		*V. fischeri* – LuxR[h]		*A. tumefaciens* – TraR[j]	
	Inhibition [%][c]	Activation [%][d]	Inhibition [%][f]	Activation [%][g]	Inhibition [%][i]	Activation [%][g]	Inhibition [%][k]	Activation [%][g]
OdDHL	-53	99	--	100	86	3	48	13
DDHL	-32	84	-10	80	39	7	54	0
OOHL	-54	99	74	8	53	15	--	100
1	111	0	7	0	81	1	61	0
2	96	0	46	0	17	16	8	0
3	96	0	1	0	25	0	3	0
4	93	0	5	0	-51	0	-14	0
5	14	57	-67	94	64	2	31	16
6	-95	104	55	31	83	26	94	0
Q1	18	0	5	0	27	0	8	0
Q2	64	0	23	0	8	0	-13	0
Q3	40	0	9	0	16	0	-24	0
Q4	83	0	20	0	12	0	-17	0
Q5	98	0	-10	1	22	0	-9	0
Q6	62	0	11	0	-1	0	0	0
Q7	52	0	4	0	-1	0	1	0
Q8	51	0	0	0	14	0	-12	0
Q9	94	0	-8	0	48	0	-25	0
Q10	25	30	-8	0	85	0	-10	0
Q11	42	0	-12	1	11	0	0	0
Q12	79	0	20	1	84	0	0	0
Q13	72	0	36	0	43	0	0	0
R1	69	1	7	37	16	0	-24	0
R2	64	9	6	1	24	0	0	0
R3	30	4	5	0	33	0	10	0
R4	-42	46	7	0	32	0	-17	0
R5	-58	38	14	0	34	0	-9	0
R6	83	7	47	2	69	0	0	0
R7	62	0	2	0	22	0	1	0
R8	26	2	-8	0	6	0	0	0
R9	-19	2	22	0	24	0	-10	0
S1	66	7	33	0	39	0	47	0
S2	-51	103	16	0	41	0	24	0
S3	-39	80	32	21	30	0	11	0
S4	48	1	5	0	9	0	-13	0
S5	41	5	6	0	1	0	4	0
S6	59	2	0	0	85	0	0	0
S7	72	23	56	0	93	0	76	8

[a] All assays performed in triplicate; Error did not exceed ±10%. Shaded compounds are controls. β-galactosidase production or luminescence in the absence of added compound was less than 0.1%; Negative controls containing no compound were subtracted from each sample to account for background. Negative inhibition values indicate that the compound activates at the tested concentration. [b] Strain: *E. coli* (pJN105Q pJL101). Assay data normalized to DDHL. [c] Screen performed using 5 μM synthetic ligand against 20 nM DDHL. [d] Screen performed using 5 μM ligand. [e] Strain: *E. coli* DH5α (pJN105L pSC11). Assay data normalized to OdDHL. [f] Screen performed using 10 μM synthetic ligand against 10 nM OdDHL. [g] Screen performed using 10 μM ligand. [h] Strain: *V. fischeri* ES114 (Δ-*luxI*). Assay data normalized to OHHL. [i] Screen performed using 10 μM synthetic ligand against 3 μM OHHL. [j] Strain: *A. tumefaciens* WCF47 (pCF372). Assay data normalized to OOHL. [k] Screen performed using 10 μM synthetic ligand against 100 nM OOHL.

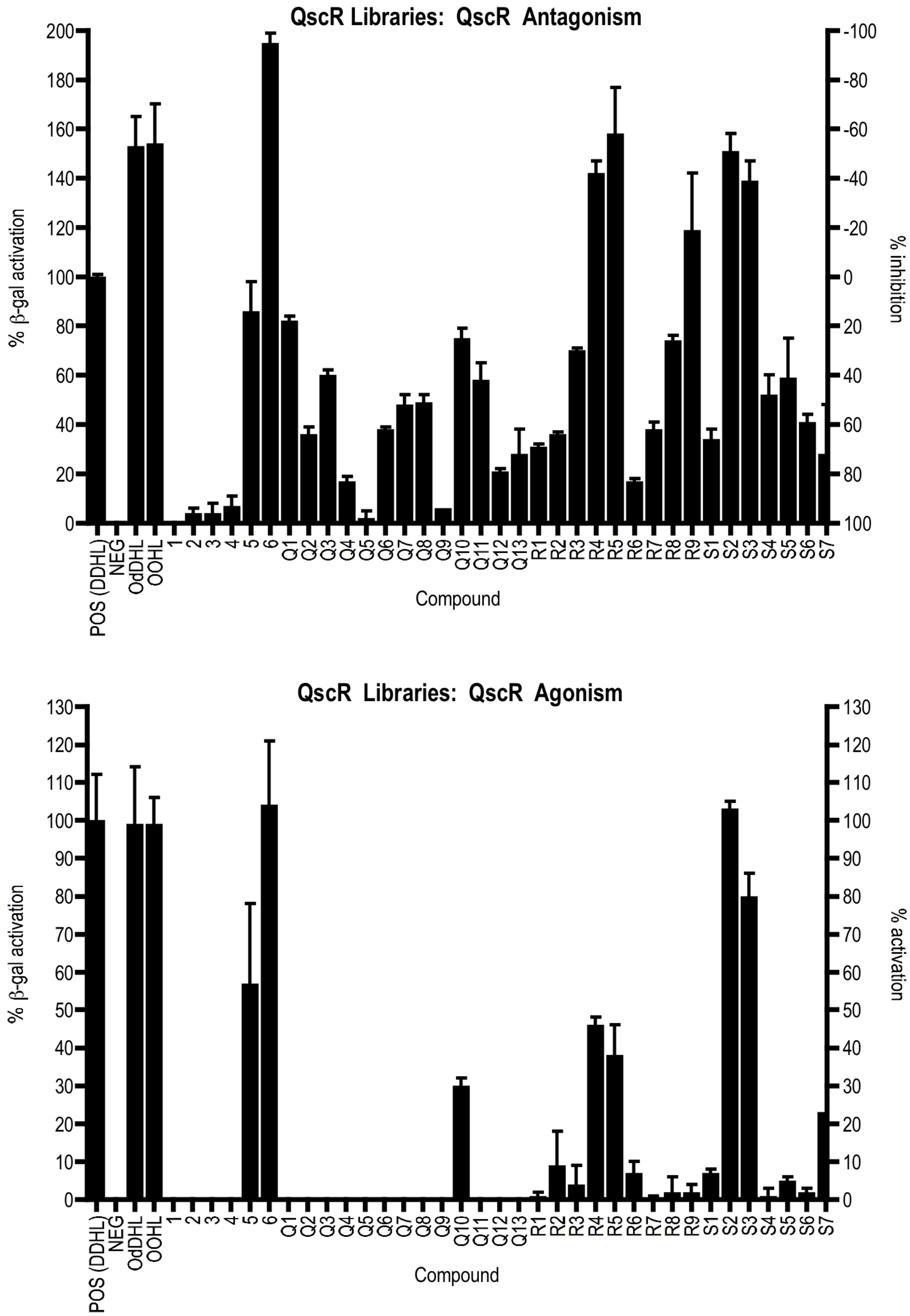
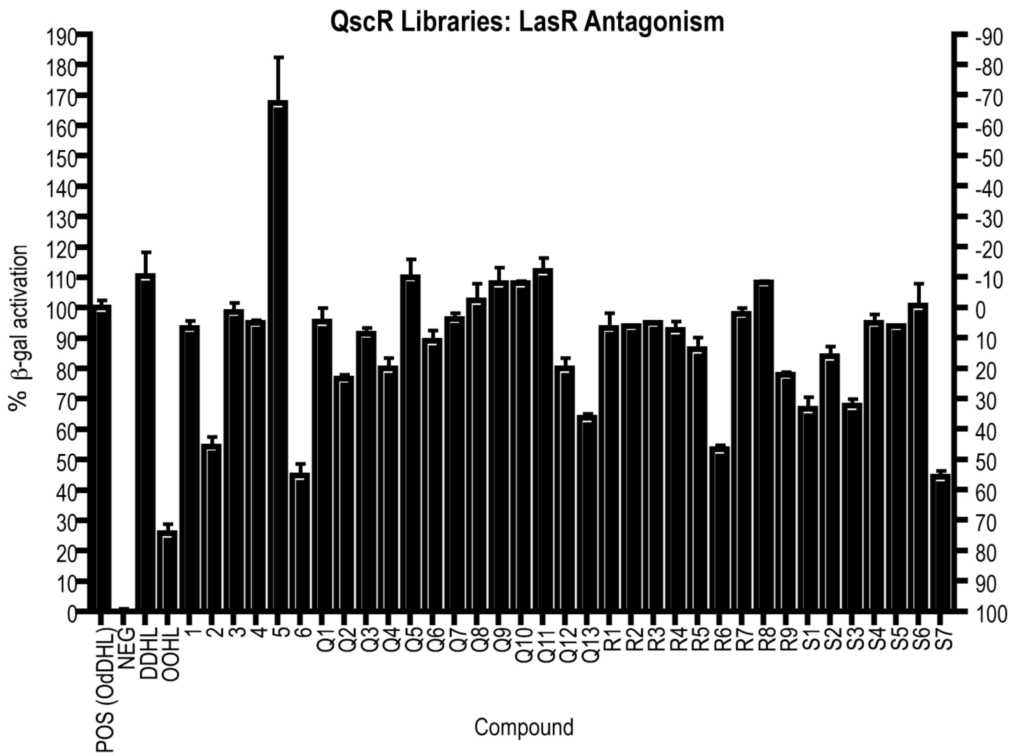


Figure S-1. Primary screening data for libraries Q, R, and S screened in *E. coli* (QscR reporter). *Top:* Antagonism screen performed using 5 μM of synthetic ligand against 20 nM of DDHL. Positive control (POS) = 20 nM of DDHL. % β-gal activation = % β-galactosidase activation vs. positive control. *Bottom:* Agonism screen performed using 5 μM of synthetic ligand. Positive control (pos) = 5 μM of DDHL.



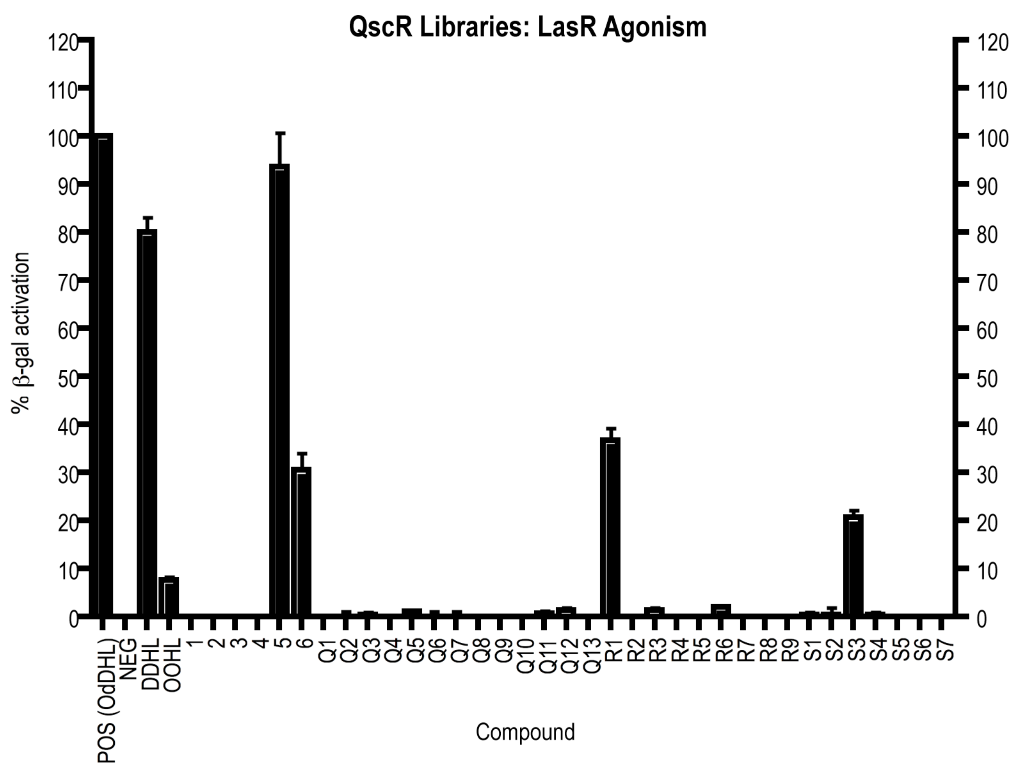
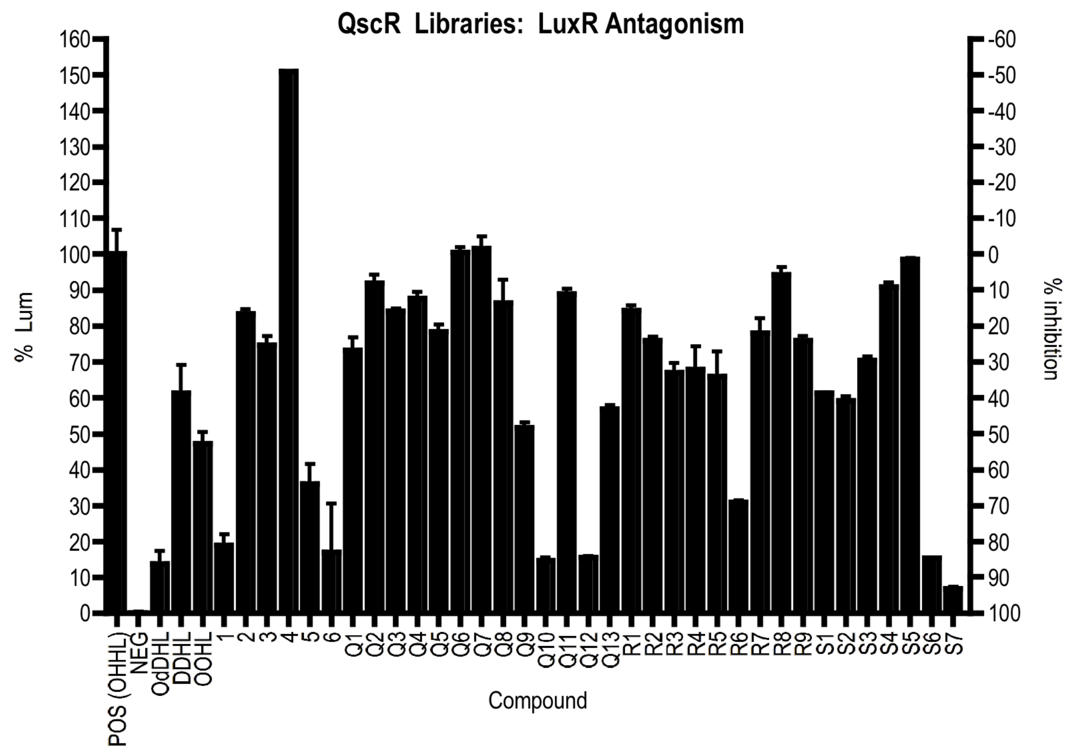


Figure S-2. Primary screening data for libraries Q, R, and S screened in *E. coli* (LasR reporter). *Top:* Antagonism screen performed using 10 μM of synthetic ligand against 10 nM of OdDHL. Positive control (POS) = 10 nM of OdDHL. *Bottom:* Agonism screen performed using 10 μM of synthetic ligand. Positive control (pos) = 10 μM of OdDHL.



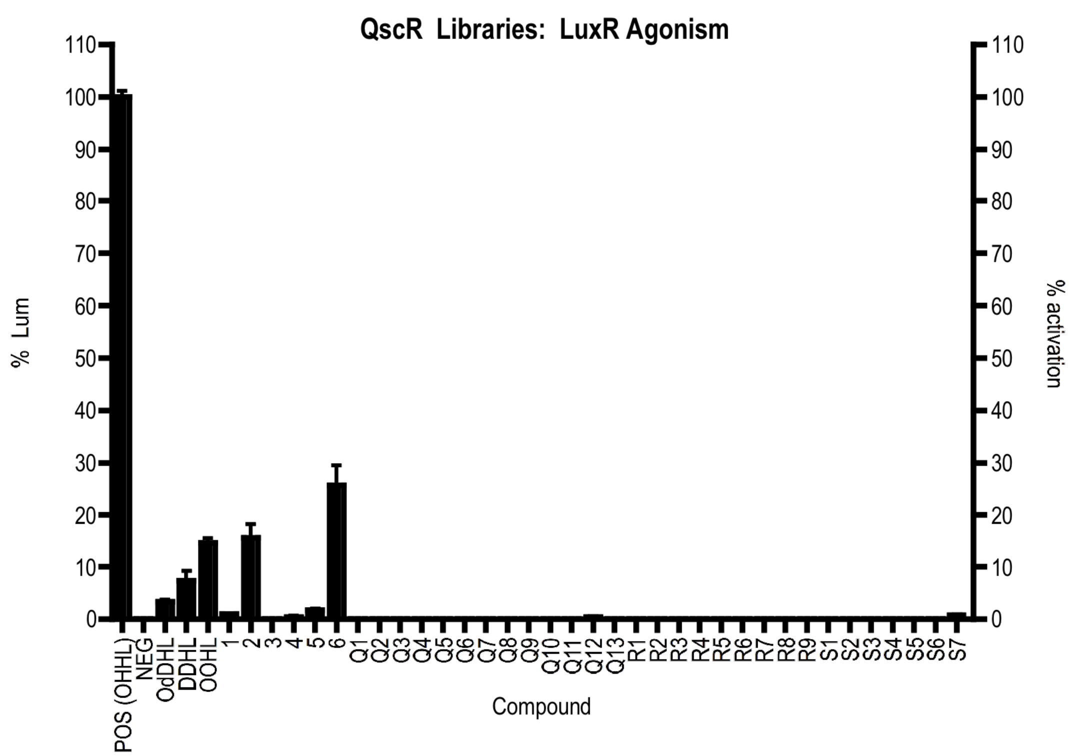
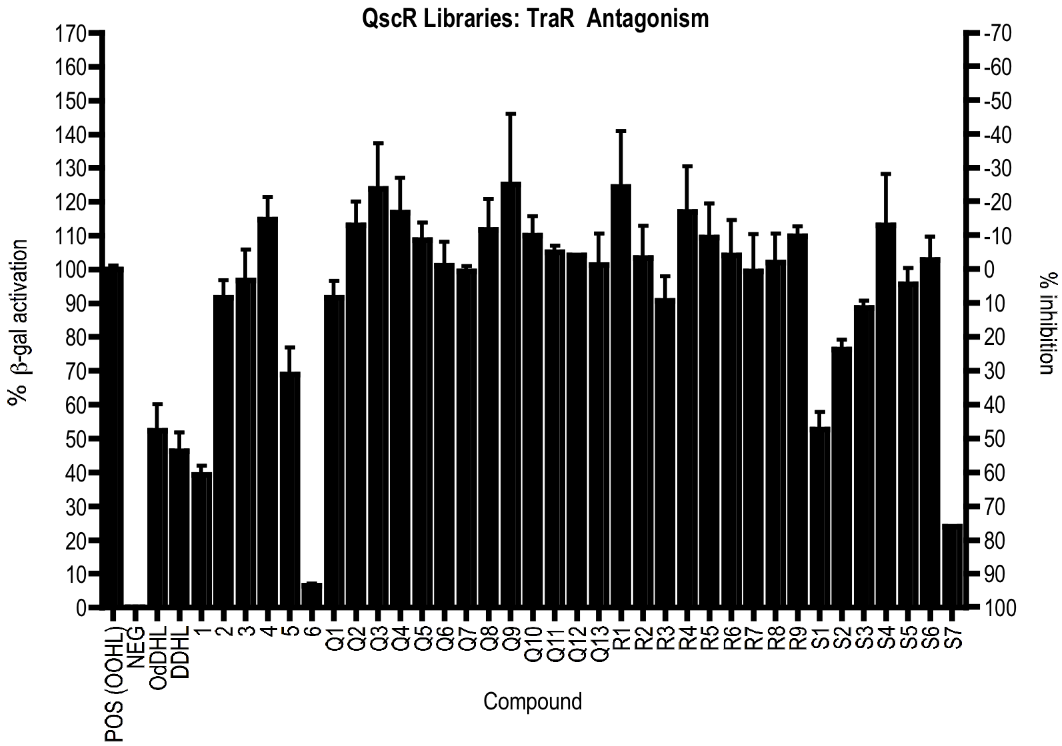


Figure S-3. Primary assay data for libraries Q, R, and S screened in *V. fischeri* (LuxR). *Top:* Antagonism screen performed using 10 μM of synthetic ligand against 3 μM of OHHL. Positive control (POS) = 3 μM OHHL. % Lum = percent luminescence vs. positive control. *Bottom:* Agonism screen performed using 10 μM of synthetic ligand. Positive control (pos) = 10 μM of OHHL.



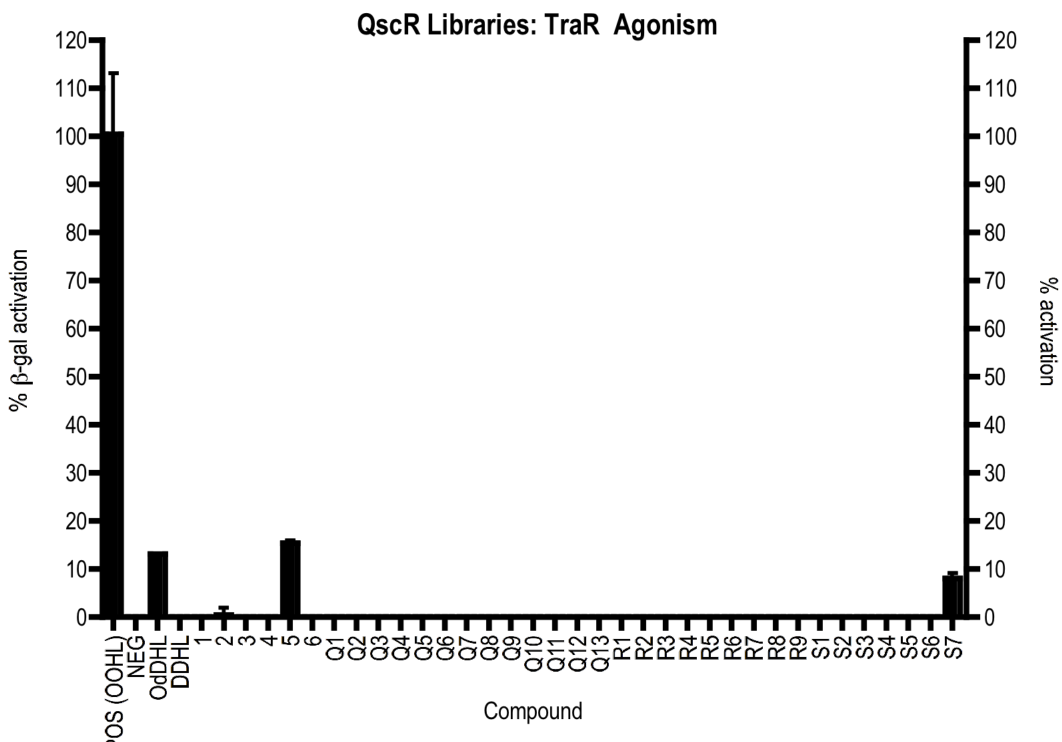


Figure S-4. Primary screening data for libraries Q, R, and S in *A. tumefaciens* (TraR). *Top:* Antagonism screen performed using 10 µM of synthetic ligand against 100 nM of OOHL. Positive control (POS) = 100 nM of OOHL. Miller units report relative absorbance. *Bottom:* Agonism screen performed using 10 µM of synthetic ligand. Positive control (pos) = 10 µM of OOHL.

<u>Dose response agonism and antagonism data in *E. coli* (QscR reporter).</u>

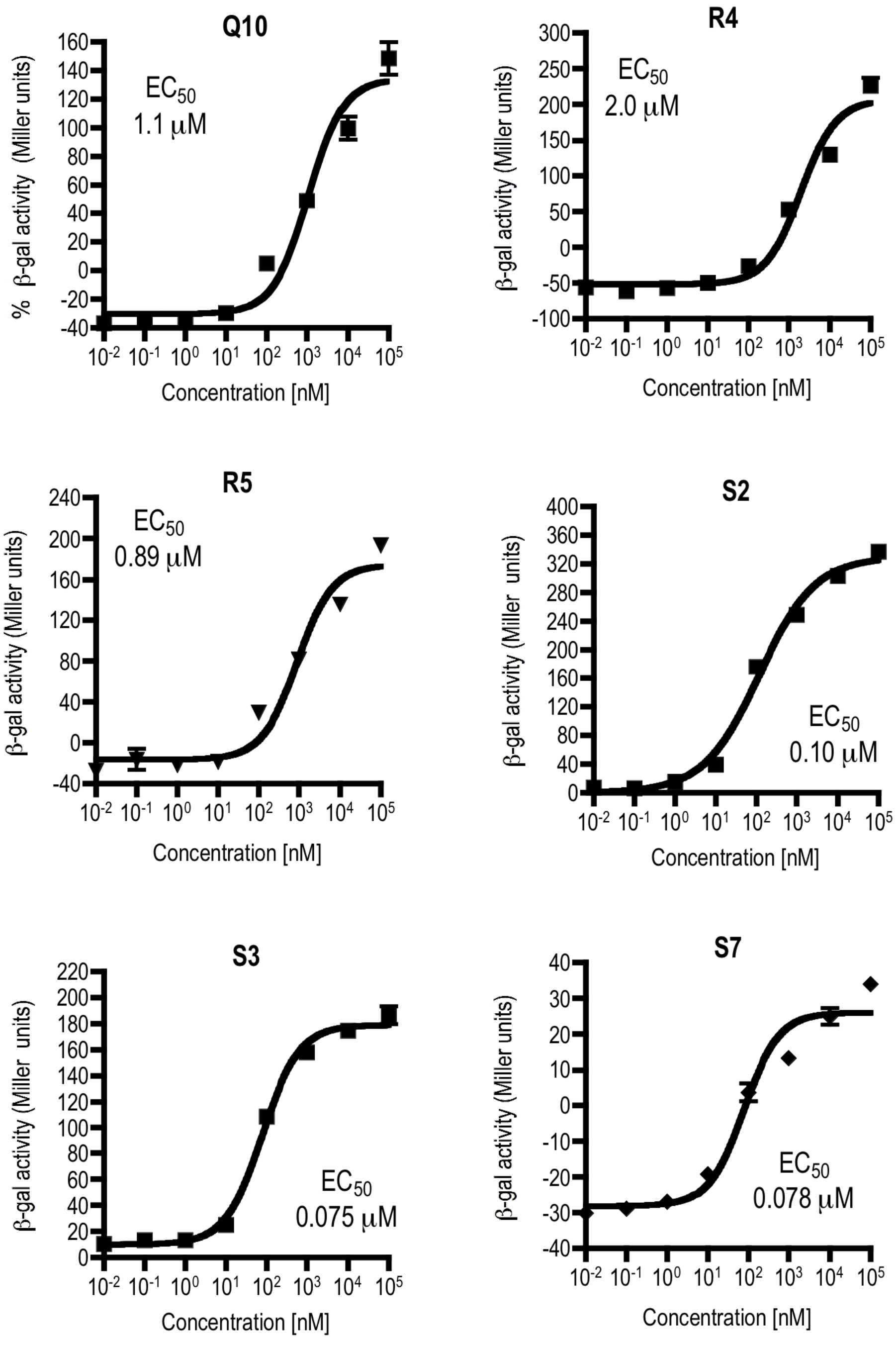


Figure S-5. Agonism dose responses and EC_{50} values for AHLs **Q10**, **R4**, **R5**, **S2**, **S3**, and **S7** in *E. coli (*QscR reporter). Synthetic ligand screened against 20 nM of DDHL over varying concentrations. IC_{50} values calculated using GraphPad Prism. Error bars, s.d. of the means of triplicate samples.

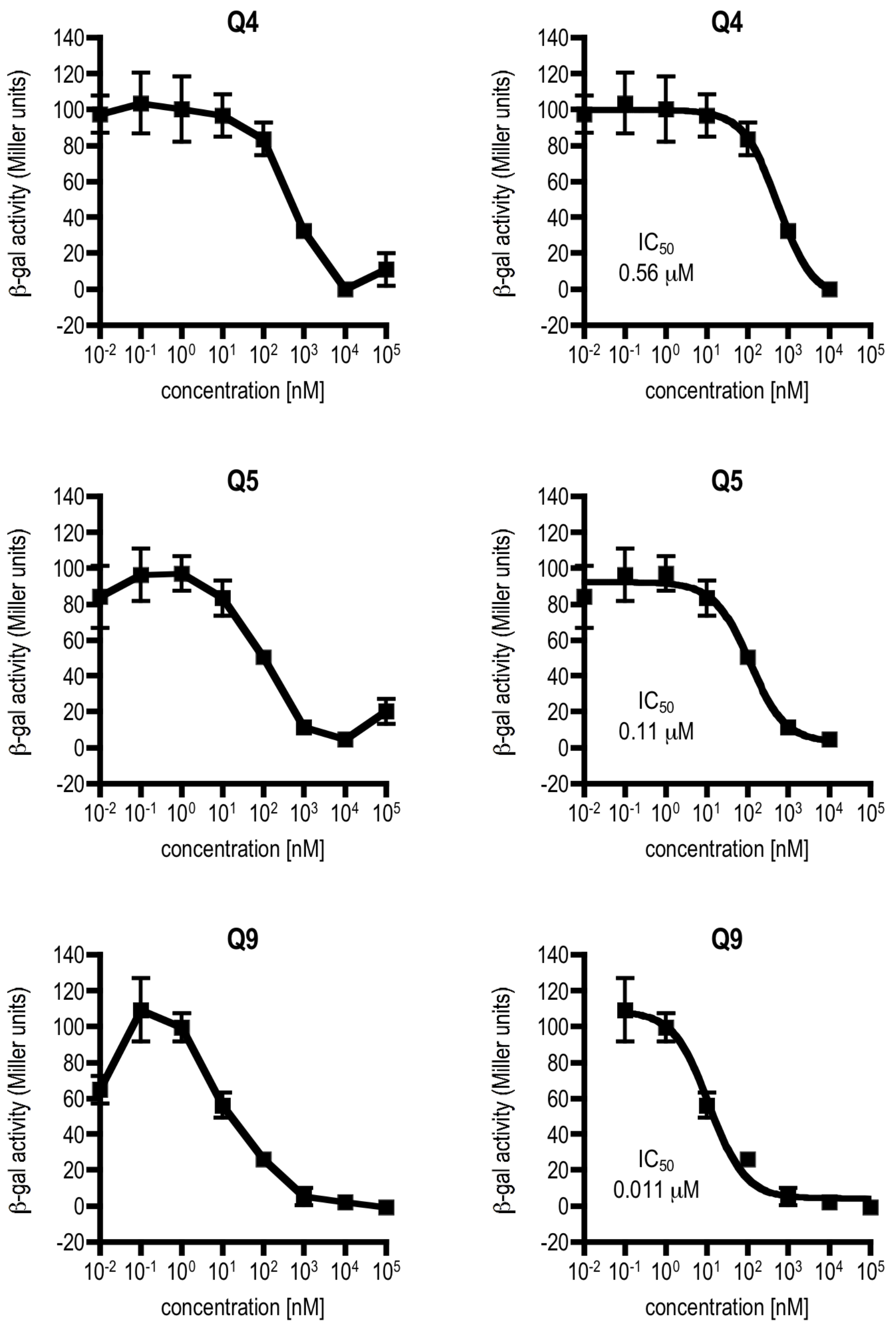


Figure S-6. Antagonism dose responses and IC_{50} values for AHLs **Q4**, **Q5**, and **Q9** in *E. coli (*QscR reporter). *Left:* Full dose response curve. *Right:* Section of dose response curve from which IC_{50} value was calculated. Synthetic ligand screened against 20 nM of DDHL over varying concentrations. IC_{50} values calculated using GraphPad Prism. Error bars, s.d. of the means of triplicate samples.

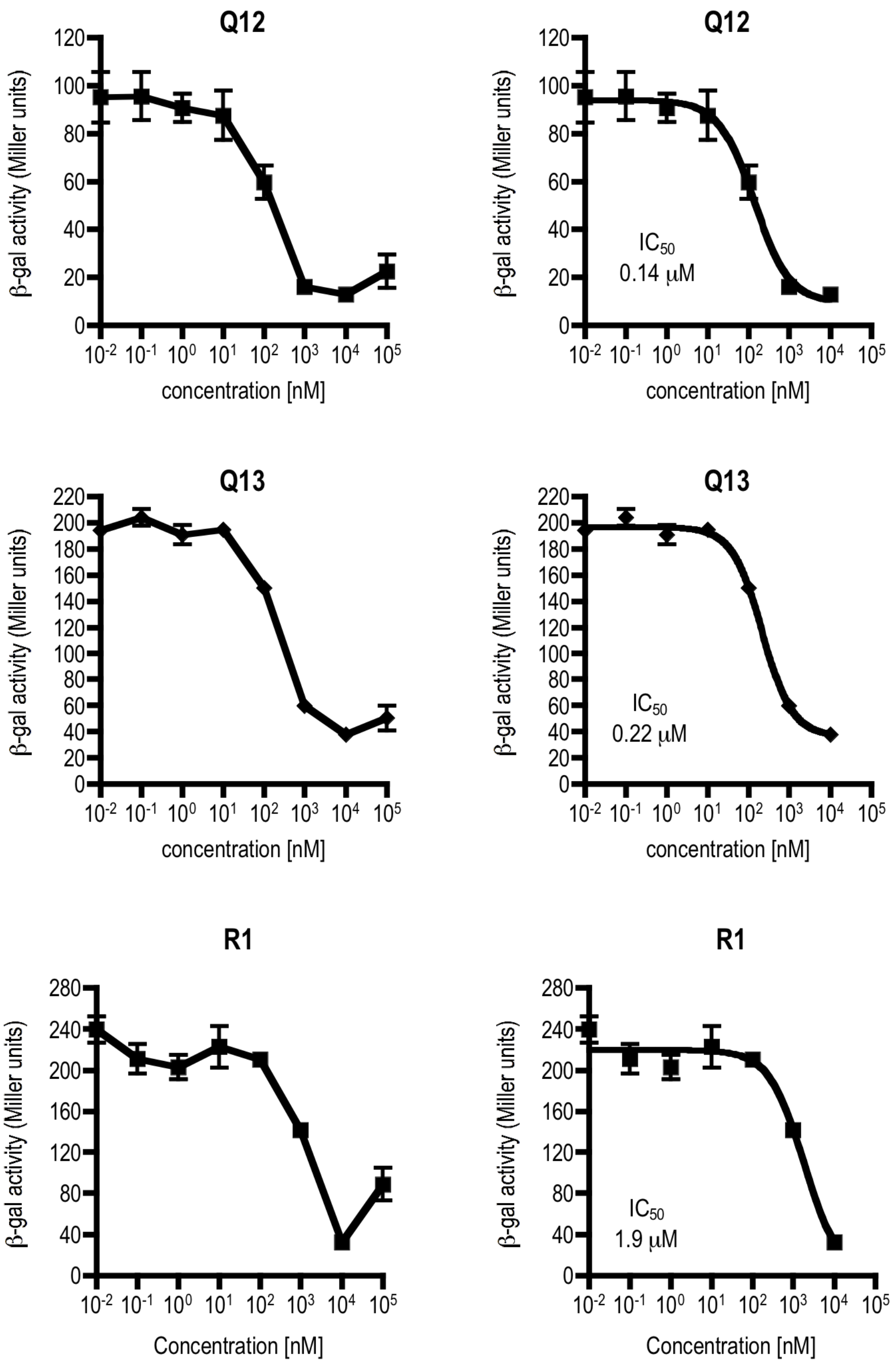


Figure S-7. Antagonism dose responses and IC_{50} values for AHLs **Q12**, **Q13**, and **R1** in *E. coli (*QscR reporter). *Left:* Full dose response curve. *Right:* Section of dose response curve from which IC_{50} value was calculated. Synthetic ligand screened against 20 nM of DDHL over varying concentrations. IC_{50} values calculated using GraphPad Prism. Error bars, s.d. of the means of triplicate samples.

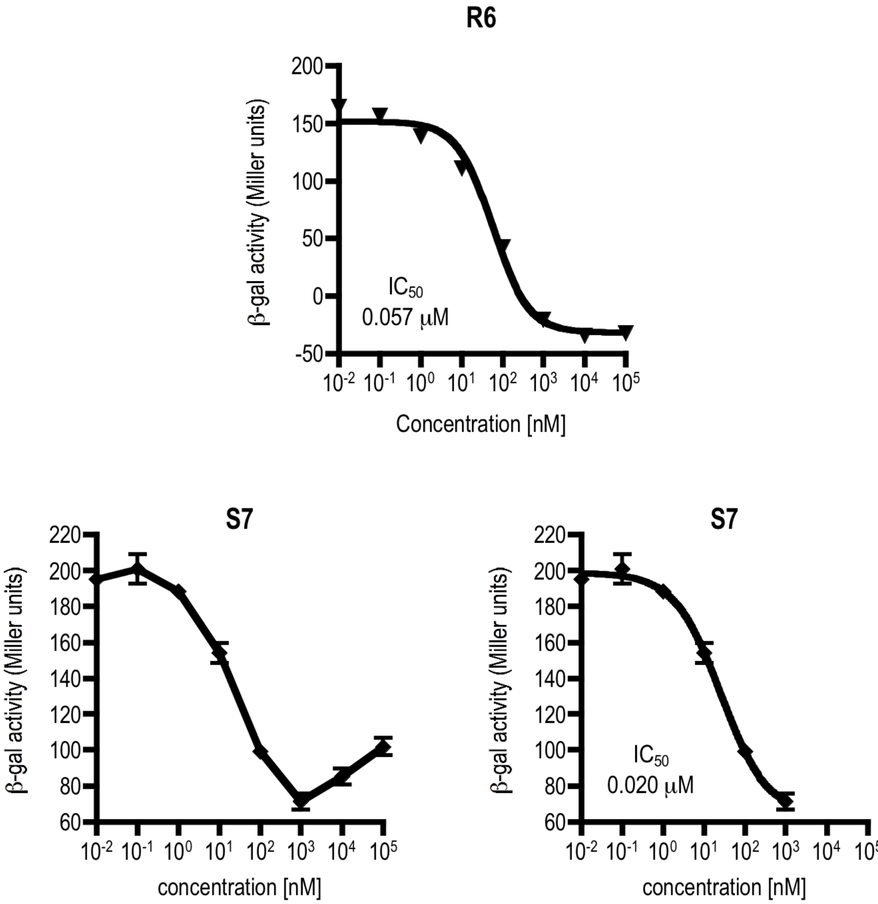


Figure S-8. Antagonism dose responses and IC_{50} values for AHLs **R6** and **S7** in *E. coli (*QscR reporter). *For S7, Left:* Full dose response curve. *Right:* Section of dose response curve from which IC_{50} value was calculated. Synthetic ligand screened against 20 nM of DDHL over varying concentrations. IC_{50} values calculated using GraphPad Prism. Error bars, s.d. of the means of triplicate samples.

<u>Dose response agonism and antagonism data in *E. coli* (LasR reporter).</u>

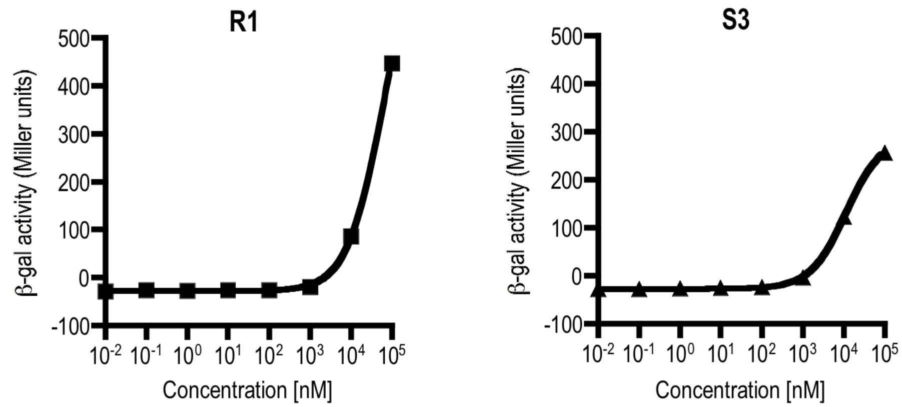


Figure S-9. Agonism dose responses for AHLs **R1** and **S3** in *E. coli (*LasR reporter). Error bars, s.d. of the means of triplicate samples. EC_{50} values not calculated.

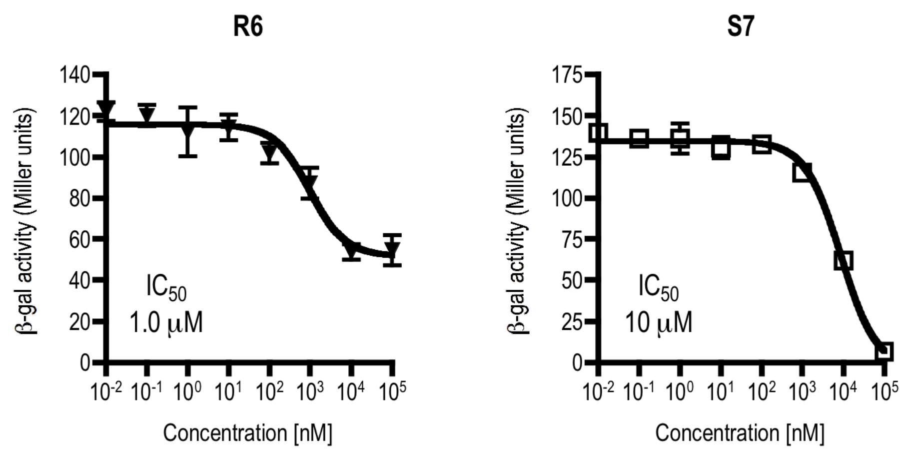


Figure S-10. Antagonism dose responses and IC_{50} values for AHLs **R6** and **S7** in *E. coli (*LasR reporter). Synthetic ligand screened against 20 nM of OdDHL over varying concentrations. IC_{50} values calculated using GraphPad Prism. Error bars, s.d. of the means of triplicate samples.

<u>Dose response antagonism data in *V. fischeri* (LuxR reporter).</u>

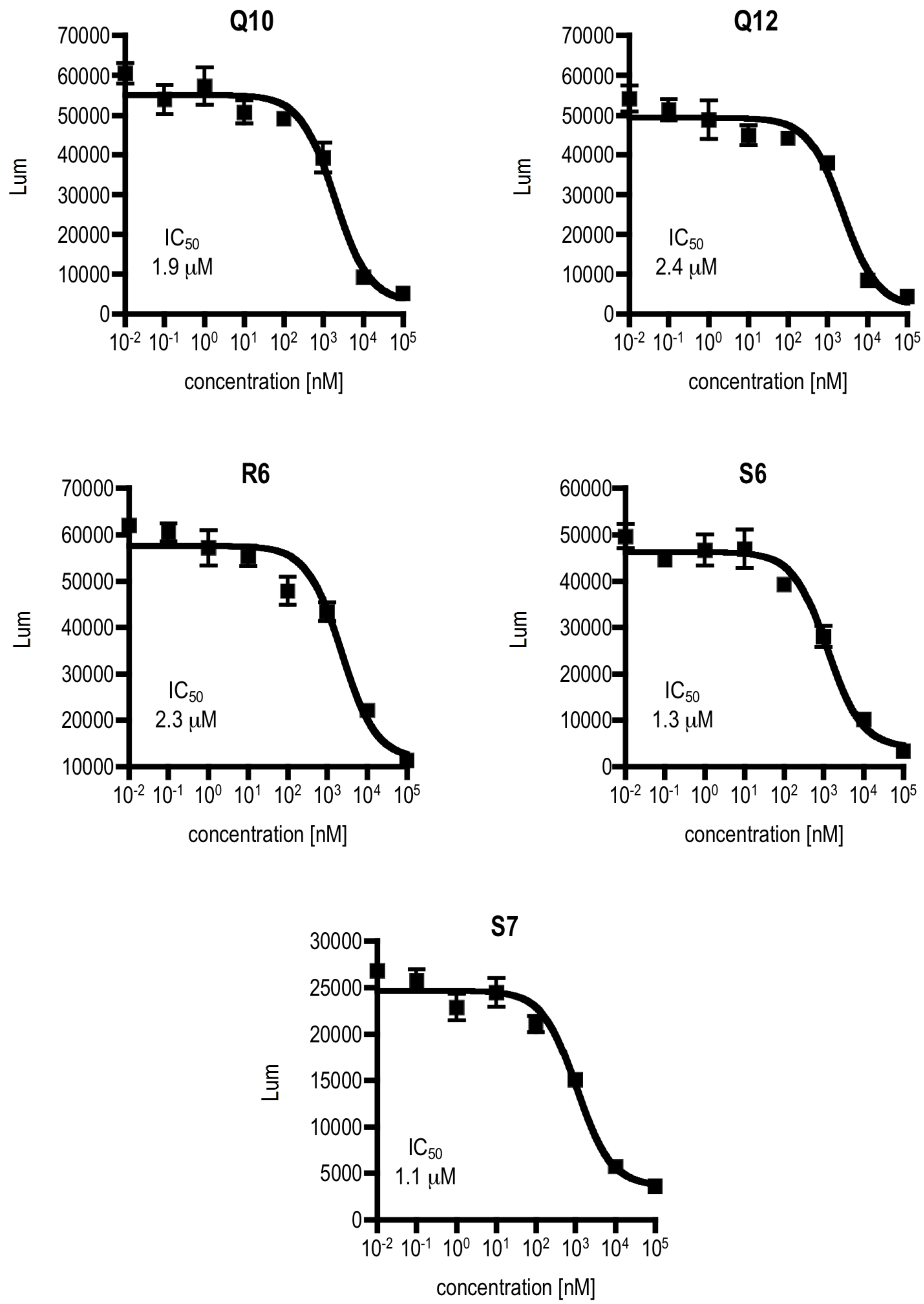


Figure S-11. Antagonism dose response and IC_{50} value for AHLs **Q10**, **Q12**, **R6**, **S6**, and **S7** in *V. fischeri*. Synthetic ligand screened against 3 μM of OHHL over varying concentrations. RLU = relative light units. IC_{50} value calculated using GraphPad Prism. Error bars, s.d. of the means of triplicate samples.

<u>Dose response antagonism and agonism data in *A. tumefaciens* (TraR reporter).</u>

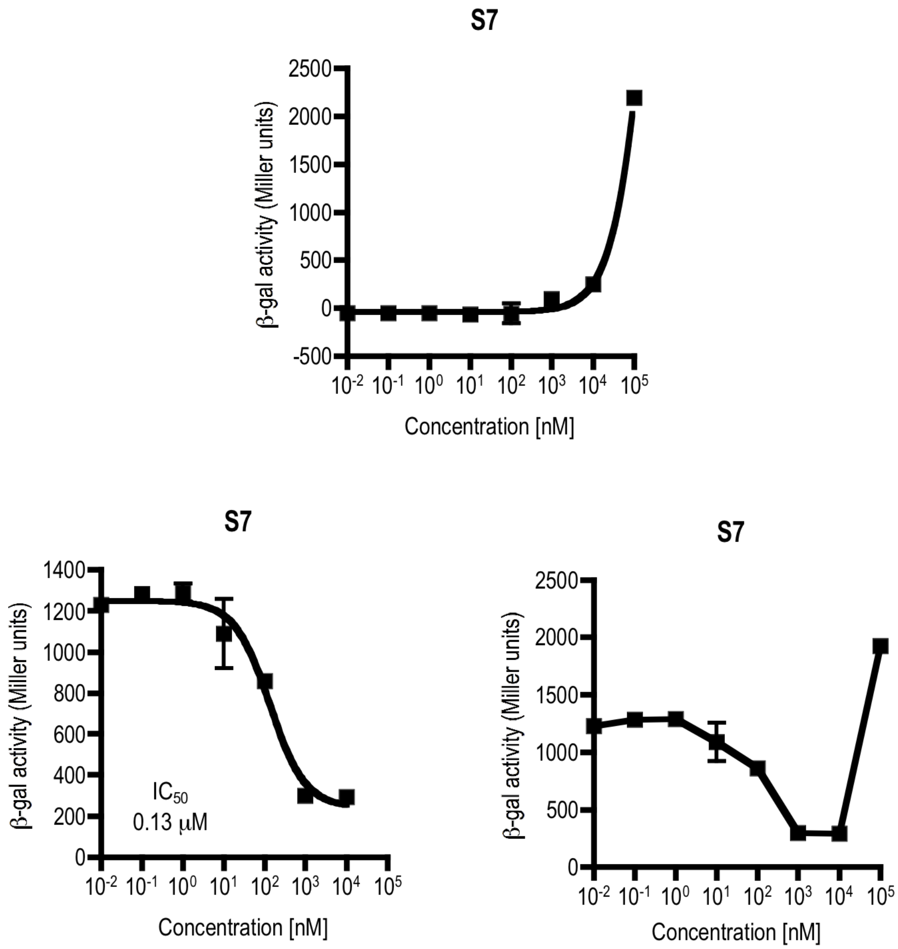


Figure S-12. Agonism (top), Antagonism (bottom) dose response and IC_{50} value for AHL **S7** in *A. tumefaciens*. *Bottom Left:* Full dose response curve. *Right:* Section of dose response curve from which IC_{50} value was calculated. Synthetic ligand screened against 100 nM of OOHL over varying concentrations. IC_{50} values calculated using GraphPad Prism. Error bars, s.d. of the means of triplicate samples.

References and notes.

(1) For further information about this Milestone μW reactor, see: http://milestonesci.com/index.php/product-menu/synth/microsynth.html

(2) For further information about this CEM μW reactor, see: http://www.cemsynthesis.com/

(3) Geske, G. D.; O'Neill, J. C.; Miller, D. M.; Mattmann, M. E.; Blackwell, H. E. *J. Am. Chem. Soc.* **2007**, *129*, 13613-25.

(4) Geske, G. D.; O'Neill, J. C.; Miller, D. M.; Wezeman, R. J.; Mattmann, M. E.; Lin, Q.; Blackwell, H. E. *ChemBioChem* **2008**, *9*, 389-400.

(5) Mattmann, M. E.; Geske, G. D.; Worzalla, G. A.; Chandler, J. R.; Sappington, K. J.; Greenberg, E. P.; Blackwell, H. E. *Bioorg. Med. Chem. Lett.* **2008**, *18*, 3072-5.

(6) Lee, J.-H.; Lequette, Y.; Greenberg, E. P. *Mol. Microbiol.* **2006**, *59*, 602-9.

(7) Lupp, C.; Urbanowski, M.; Greenberg, E. P.; Ruby, E. G. *Mol. Microbiol.* **2003**, *50*, 319-331.

(8) Zhu, J.; Beaber, J. W.; More, M. I.; Fuqua, C.; Eberhard, A.; Winans, S. C. *J. Bacteriol.* **1998**, *180*, 5398-5405.