

Supplementary Information

## Classifying the Topology of AHL-Driven Quorum Sensing Circuits in Proteobacterial Genomes. *Sensors* 2012, 12, 5342-5444

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Zsolt Gelencsér *et al.* (2012): "Classifying the topology of simple AHL-driven quorum sensing circuits in bacterial genomes" submitted to *Sensors*.

**Data:** Data of 1403 complete bacterial genomes were retrieved from the genome section of the NCBI (<http://ncbi.nlm.nih.gov/>). Additional protein sequences were retrieved from the UNIPROT database (<http://www.uniprot.org/>). Data retrieval was completed in December 15, 2011.

**Methods:** QS genes were determined using Hidden Markov Model (HMM) recognizers build with the HMMER programs HMMER 3.0, (<http://hmmer.janelia.org/>). Briefly, a core set of protein sequences were taken for *LuxR*, *LuxI*, *rsaL* and *rsaM* proteins (see lists below). The CLUSTAL program (accessed via the EBI Webportal, <http://www.ebi.ac.uk/Tools/msa/clustalw2/>) was used for constructing the multiple sequence alignments which were then processed by the HMMBUILD program to give HMM recognizers that were in turn used to scan the protein sequence data (over 4.7 million protein sequences). Sequences giving a E-value below 0.1 were manually checked for length, alignment coverage and residue conservation, and the topologies were assigned.

Protein sequences for selected sequence groups were downloaded from NCBI refseq database using a script which gave GIs as query and retrieved sequences in a file.

Cladograms for these selected sequence groups were built using the guide tree of the CLUSTAL program and visualized using the MEGA 5 program package installed from <http://www.megasoftware.net>.

The numerical value at each node indicates the bootstrap value supporting every split in the lineage (out of 1,000 bootstrap replicates).

**Table 1.** List of complete genomes in which QS genes were identified.

No	Species	Gene/protein id
1	<i>Erwinia pyrifoliae</i> Ep1/96	ERWPE
2	<i>Pectobacterium wasabiae</i> WPP163	PECWW
3	<i>Halothiobacillus neapolitanus</i> c2	HALNC
4	<i>Edwardsiella tarda</i> EIB202	EDWTE
5	<i>Dickeya dadantii</i> Ech586	DICD5
6	<i>Burkholderia</i> sp. CCGE1002	BURSC
7	<i>Burkholderia</i> sp. CCGE1001	9BURK
8	<i>Citrobacter rodentium</i> ICC168	CITRI
9	<i>Rhodomicrobium vannielii</i> ATCC 17100	RHOVT
10	<i>Rhodopseudomonas palustris</i> DX-1	RHOPX
11	<i>Burkholderia</i> sp. CCGE1003	BURSG
12	<i>Pantoea ananatis</i> LMG 20103	PANAM
13	<i>Erwinia amylovora</i> CFBP1430	ERWAC
14	<i>Erwinia amylovora</i> ATCC 49946	ERWAE
15	<i>Sphingobium japonicum</i> UT26S	SPHJU
16	<i>Shewanella violacea</i> DSS12	SHEVD
17	<i>Yersinia pestis</i> Z176003	YERPZ
18	<i>Rhodobacter capsulatus</i> SB 1003	RHO CB
19	<i>Pantoea vagans</i> C9-1	PANVC
20	<i>Acinetobacter</i> sp. DR1	ACISD
21	<i>Ralstonia solanacearum</i> PSI07	RALSL
22	<i>Ralstonia solanacearum</i> CFBP2957	RALSL
23	<i>Erwinia billingiae</i> Eb661	ERWBE
24	<i>Gallionella capsiferriformans</i> ES-2	GALCS
25	<i>Dickeya dadantii</i> 3937	DICD3
26	<i>Asticcacaulis excentricus</i> CB 48	ASTE C
27	<i>Pantoea</i> sp. At-9b	PANSA
28	<i>Ralstonia solanacearum</i> GMI1000	RALSO
29	<i>Bradyrhizobium japonicum</i> USDA 110	BRAJA
30	<i>Mesorhizobium loti</i> MAFF303099	RHILO
31	<i>Sinorhizobium meliloti</i> 1021	RHIME
32	<i>Methylobacterium extorquens</i> AM1	METEA
33	<i>Yersinia pestis</i> CO92	YERPE
34	<i>Acidithiobacillus ferrooxidans</i> ATCC 23270	ACIF2
35	<i>Rhodospirillum rubrum</i> ATCC 11170	RHORT
36	<i>Burkholderia mallei</i> ATCC 23344	BURMA
37	<i>Burkholderia pseudomallei</i> K96243	BURPS
38	<i>Yersinia enterocolitica</i> subsp. <i>enterocolitica</i> 8081	YERE8

Table 1. Cont.

No	Species	Gene/protein id
39	<i>Burkholderia xenovorans</i> LB400	BURXL
40	<i>Ruegeria pomeroyi</i> DSS-3	SILPO
41	<i>Yersinia pestis</i> KIM 10	YERPE
42	<i>Saccharophagus degradans</i> 2-40	SACD2
43	<i>Pseudomonas syringae</i> pv. <i>syringae</i> B728a	PSEU2
44	<i>Pseudomonas aeruginosa</i> PAO1	PSEAE
45	<i>Burkholderia cenocepacia</i> J2315	BURCJ
46	<i>Rhizobium leguminosarum</i> bv. <i>viciae</i> 3841	RHIL3
47	<i>Pectobacterium atrosepticum</i> SCRI1043	ERWCT
48	<i>Pseudomonas syringae</i> pv. <i>tomato</i> str. DC3000	PSESM
49	<i>Pseudomonas aeruginosa</i> UCBPP-PA14	PSEAB
50	<i>Chromobacterium violaceum</i> ATCC 12472	CHRVO
51	<i>Yersinia pestis</i> biovar <i>Microtus</i> str. 91001	YERPE
52	<i>Chelativorans</i> sp. BNC1	MESSB
53	<i>Burkholderia</i> sp. 383	BURS3
54	<i>Burkholderia vietnamiensis</i> G4	BURVG
55	<i>Burkholderia thailandensis</i> E264	BURTA
56	<i>Pseudomonas syringae</i> pv. <i>phaseolicola</i> 1448A	PSE14
57	<i>Jannaschia</i> sp. CCS1	JANSC
58	<i>Yersinia pseudotuberculosis</i> IP 32953	YERPS
59	<i>Vibrio fischeri</i> ES114	VIBF1
60	<i>Paracoccus denitrificans</i> PD1222	PARDP
61	<i>Agrobacterium vitis</i> S4	AGRVS
62	<i>Agrobacterium radiobacter</i> K84	AGRKK
63	<i>Pseudoalteromonas atlantica</i> T6c	PSEA6
64	<i>Nitrobacter winogradskyi</i> Nb-255	NITWN
65	<i>Burkholderia ambifaria</i> AMMD	BURCM
66	<i>Sphingopyxis alaskensis</i> RB2256	SPHAL
67	<i>Burkholderia cenocepacia</i> HI2424	BURCH
68	<i>Burkholderia cenocepacia</i> AU 1054	BURCA
69	<i>Rhizobium etli</i> CFN 42	RHIEC
70	<i>Burkholderia mallei</i> NCTC 10229	BURM9
71	<i>Burkholderia mallei</i> NCTC 10247	BURM7
72	<i>Burkholderia mallei</i> SAVP1	BURMS
73	<i>Burkholderia pseudomallei</i> 668	BURP6
74	<i>Burkholderia pseudomallei</i> 1710b	BURP1
75	<i>Acidovorax citrulli</i> AAC00-1	ACIAC
76	<i>Rhodopseudomonas palustris</i> HaA2	RHOP2
77	<i>Rhodopseudomonas palustris</i> BisB5	RHOPS
78	<i>Rhodopseudomonas palustris</i> BisB18	RHOPB
79	<i>Rhodopseudomonas palustris</i> BisA53	RHOP5
80	<i>Geobacter uraniireducens</i> Rf4	GEOUR

Table 1. Cont.

No	Species	Gene/protein id
81	<i>Yersinia pestis</i> Angola	YERPG
82	<i>Yersinia pseudotuberculosis</i> IP 31758	YERP3
83	<i>Bradyrhizobium</i> sp. BTAi1	BRASB
84	<i>Burkholderia pseudomallei</i> 1106a	BURP0
85	<i>Geobacter</i> sp. FRC-32	GEOSF
86	<i>Sinorhizobium medicae</i> WSM419	SINMW
87	<i>Sodalis glossinidius</i> str. morsitans	SODGM
88	<i>Roseobacter denitrificans</i> OCh 114	ROSDO
89	<i>Yersinia pestis</i> Antiqua	YERPA
90	<i>Yersinia pestis</i> Nepal516	YERPN
91	<i>Acidithiobacillus ferrooxidans</i> ATCC 53993	ACIF5
92	<i>Aeromonas hydrophila</i> subsp. <i>hydrophila</i> ATCC 7966	AERHH
93	<i>Yersinia pestis</i> Pestoides F	YERPP
94	<i>Pseudomonas aeruginosa</i> PA7	PSEA7
95	<i>Aeromonas salmonicida</i> subsp. <i>salmonicida</i> A449	AERS4
96	<i>Burkholderia phymatum</i> STM815	BURP8
97	<i>Burkholderia ambifaria</i> MC40-6	BURA4
98	<i>Dinoroseobacter shibae</i> DFL 12	DINSH
99	<i>Shewanella woodyi</i> ATCC 51908	SHEWM
100	<i>Serratia proteamaculans</i> 568	SERP5
101	<i>Burkholderia phytofirmans</i> PsJN	BURPP
102	<i>Acinetobacter baumannii</i> ATCC 17978	ACIBT
103	<i>Acinetobacter baumannii</i> ACICU	ACIBC
104	<i>Burkholderia cenocepacia</i> MC0-3	BURCC
105	<i>Methylobacterium extorquens</i> PA1	METEP
106	<i>Methylobacterium</i> sp. 4-46	METS4
107	<i>Methylobacterium radiotolerans</i> JCM 2831	METRJ
108	<i>Vibrio fischeri</i> MJ11	VIBFM
109	<i>Burkholderia multivorans</i> ATCC 17616	BURM1
110	<i>Methylobacterium chloromethanicum</i> CM4	METC4
111	<i>Methylobacterium populi</i> BJ001	METPB
112	<i>Bradyrhizobium</i> sp. ORS278	BRASO
113	<i>Phenylobacterium zucineum</i> HLK1	PHEZH
114	<i>Rhizobium leguminosarum</i> bv. <i>trifolii</i> WSM1325	RHILS
115	<i>Rhodopseudomonas palustris</i> TIE-1	RHOPT
116	<i>Rhizobium leguminosarum</i> bv. <i>trifolii</i> WSM2304	RHILW
117	<i>Methylobacterium nodulans</i> ORS 2060	METNO
118	<i>Erwinia tasmaniensis</i> Et1/99	ERWT9
119	<i>Beijerinckia indica</i> subsp. <i>indica</i> ATCC 9039	BEII9
120	<i>Sinorhizobium fredii</i> NGR234	RHISN
121	<i>Acinetobacter baumannii</i> AB0057	ACIB5
122	<i>Rhizobium etli</i> CIAT 652	RHIE6
123	<i>Yersinia pseudotuberculosis</i> YPIII	YERP3
124	<i>Yersinia pseudotuberculosis</i> PB1/+	YERP3

**Table 1. Cont.**

No	Species	Gene/protein id
125	<i>Aliivibrio salmonicida</i> LFI1238	ALISL
126	<i>Acinetobacter baumannii</i> AB307-0294	ACIB3
127	<i>Pseudomonas aeruginosa</i> LESB58	PSEA8
128	Candidatus <i>Hamiltonella defensa</i> 5AT ( <i>Acyrtosiphon pisum</i> )	HAMD5
129	<i>Pectobacterium carotovorum</i> subsp. <i>carotovorum</i> PC1	PECCP
130	<i>Dickeya zeae</i> Ech1591	DICZE
131	<i>Desulfovibrio magneticus</i> RS-1	DESMR
132	<i>Burkholderia glumae</i> BGR1	BURGB
133	<i>Edwardsiella ictaluri</i> 93-146	EDWI9
134	<i>Methylocella silvestris</i> BL2	METSB
135	<i>Variovorax paradoxus</i> S110	VARPS
136	<i>Ketogulonicigenium vulgare</i> Y25	KETVY
137	<i>Enterobacter cloacae</i> SCF1	ENTCS
138	<i>Gluconacetobacter diazotrophicus</i> PAI 5	GLUDA
139	<i>Methylobacterium extorquens</i> DM4	METED
140	<i>Acinetobacter baumannii</i> AYE	ACIBY
141	<i>Mesorhizobium ciceri</i> biovar <i>biserrulae</i> WSM1271	MESCW
142	<i>Rhodopseudomonas palustris</i> CGA009	RHOPA
143	<i>Collimonas fungivorans</i> Ter331	COLFT
144	<i>Cupriavidus necator</i> N-1	CUPNE
145	<i>Delftia</i> sp. Cs1-4	DELSC
146	<i>Mesorhizobium opportunistum</i> WSM2075	MESOW
147	<i>Novosphingobium</i> sp. PP1Y	9SPHN
148	<i>Roseobacter litoralis</i> Och 149	ROSLO
149	<i>Sinorhizobium meliloti</i> AK83	SINMK
150	<i>Sphingobium chlorophenicum</i> L-1	SPHCR
151	<i>Sphingobium</i> sp. SYK-6	9SPHN
152	<i>Vibrio anguillarum</i> 775	VIBAN

**Table 2.** Additional sequences from incomplete genomes, used in this study.

No.	Genome	DNA Ids	Protein ids
1	<i>P. fuscovaginae</i>	182375405, 290454884	182375406, 182375407, 182375408, 290454885, 290454886, 290454887
2	<i>P. putida</i> PCL1445	73672740	73672742, 73672743, 73672744
3	<i>P. putida</i> WCS358	45259341	45259342, 45259343, 45259344
4	<i>P. putida</i> IsoF	26417537	26417540, 26417541, 26417542

**Table 3.** List of protein sequence sets used for building HMM recognizers.

No	Proteins	Gene/protein ids
<b>luxI homologues</b>		
YP_002649215.1, YP_003261728.1, YP_003262850.1, YP_003296640.1, YP_003331715.1, YP_003608088.1, YP_004230809.1, YP_003366470.1, YP_004012993.1, YP_004106681.1, YP_004106954.1, YP_004108425.1, YP_003910269.1, YP_003520250.1, YP_003530770.1, YP_003538486.1, YP_003546445.1, YP_003558209.1, YP_003566926.1, YP_003568278.1, YP_003576501.1, YP_003729883.1, YP_003930460.1, YP_003734012.1, YP_003749682.1, YP_003750860.1, YP_003744153.1, YP_003740503.1, YP_003740954.1, YP_003847234.1, YP_003885141.1, YP_004088230.1, YP_004115279.1, NP_521405.1, NP_522340.1, NP_767703.1, NP_106262.1, NP_106661.1, NP_109412.1, NP_385945.1, YP_002965845.1, YP_002966879.1, YP_002346031.1, YP_002347420.1, YP_002426405.1, YP_428477.1, YP_105963.1, YP_106161.1, YP_110894.1, YP_111576.1, YP_001005892.1, YP_554693.1, YP_555669.1, YP_165635.1, YP_167511.1, NP_669050.1, NP_670673.1, YP_528965.1, YP_234707.1, NP_250123.1, NP_252166.1, YP_002232872.1, YP_002234481.1, YP_768958.1, YP_048233.1, NP_793636.1, YP_789671.1, YP_791820.1, NP_903761.1, NP_993604.1, NP_994737.1, YP_674865.1, YP_371808.1, YP_567542.1, YP_569311.1, YP_530592.1, YP_531903.1, YP_781244.1, YP_273860.1, YP_508562.1, YP_071011.1, YP_071751.1, YP_206882.1, YP_914595.1, YP_002551489.1, YP_002549360.1, YP_002541324.1, YP_659946.1, YP_317245.1, YP_776005.1, YP_617566.1, YP_617628.1, YP_838353.1, YP_623506.1, YP_470411.1, YP_473057.1, YP_001024425.1, YP_001025818.1, YP_001077901.1, YP_001078152.1, YP_989942.1, YP_001062290.1, YP_001063210.1, YP_335777.1, YP_337633.1, YP_972130.1, YP_484039.1, YP_486927.1, YP_567542.1, YP_569311.1, YP_530592.1, YP_531903.1, YP_781244.1, YP_001231849.1, YP_001604809.1, YP_001606209.1, YP_001399709.1, YP_001400525.1, YP_001220569.1, YP_001241094.1, YP_001242901.1, YP_001075256.1, YP_001076162.1, YP_002537871.1, YP_001327237.1, YP_453964.1, YP_681952.1, YP_650194.1, YP_651865.1, YP_647981.1, YP_649109.1, YP_002220095.1, YP_855089.1, YP_001161918.1, YP_001163229.1, YP_001347034.1, YP_001349251.1, YP_001143471.1, YP_001583944.1, YP_001860597.1, YP_001811255.1, YP_001531662.1, YP_001534185.1, YP_001761364.1, YP_001476305.1, YP_001888022.1, YP_001893789.1, YP_001083198.1, YP_001844795.1, YP_001777918.1, YP_001779189.1, YP_001641952.1, YP_001772211.1, YP_001758390.1, YP_001776814.1, YP_001783295.1, YP_002158590.1, YP_001948920.1, YP_002423669.1, YP_001927659.1, YP_001203094.1, YP_002128524.1, YP_002976728.1, YP_001989358.1, YP_001991324.1, YP_002282165.1, YP_002495630.1, YP_002496260.1, YP_002497058.1, YP_001906897.1, YP_001908005.1, YP_001832057.1, YP_002826208.1, YP_002317565.1, YP_001979200.1, YP_001985290.1, YP_001719546.1, YP_001720402.1, YP_001873009.1, YP_001873806.1, YP_002265246.1, YP_002327281.1, YP_002439140.1, YP_002441565.1, YP_002923740.1, YP_003019698.1, YP_003002473.1, YP_002955226.1, YP_002909043.1, YP_002934276.1, YP_002360442.1, YP_002947663.1, YP_003964946.1, YP_003941574.1, YP_001603070.1, YP_003070966.1, YP_001715479.1, YP_004144716.1, YP_004145051.1, NP_945673.1		
<b>LuxR homologues</b>		
YP_002649216.1, YP_003261727.1, YP_003262848.1, YP_003296639.1, YP_003331714.1, YP_003608086.1, YP_004230807.1, YP_003366469.1, YP_004012994.1, YP_004106680.1, YP_004106955.1, YP_004108424.1, YP_003910271.1, YP_003520251.1, YP_003530769.1, YP_003538485.1, YP_003546444.1, YP_003558208.1, YP_003566925.1, YP_003568279.1, YP_003576500.1, YP_003729882.1, YP_003930459.1, YP_003734010.1, YP_003749681.1, YP_003750859.1, YP_003744152.1, YP_003740504.1, YP_003740953.1, YP_003847232.1, YP_003885142.1, YP_004088229.1, YP_004115278.1, NP_521406.1, NP_522339.1, NP_767702.1, NP_106261.1, NP_106660.1, NP_109411.1, NP_385944.1, YP_002965846.1, YP_002966880.1, YP_002346032.1, YP_002347421.1, YP_002426403.1, YP_428476.1, YP_105961.1, YP_106160.1, YP_110896.1, YP_111575.1, YP_001005891.1, YP_554691.1, YP_555670.1, YP_165634.1, YP_167510.1, NP_669049.1, NP_670674.1, YP_528967.1, YP_234708.1, NP_250121.1, NP_252167.1, YP_002232873.1, YP_002234479.1, YP_768957.1, YP_048234.1, NP_793635.1, YP_789670.1, YP_791822.1, NP_903760.1, NP_993605.1, NP_994736.1, YP_674864.1, YP_371810.1, YP_001114942.1, YP_001117674.1, YP_439002.1, YP_439706.1, YP_273861.1, YP_508561.1, YP_071012.1, YP_071752.1, YP_206883.1, YP_914594.1, YP_002551488.1, YP_002549361.1, YP_002541325.1, YP_659944.1, YP_317246.1, YP_776003.1, YP_617565.1, YP_617627.1, YP_838351.1, YP_623508.1, YP_470410.1, YP_473056.1, YP_001024423.1, YP_001025820.1, YP_001077903.1, YP_001078154.1, YP_989940.1, YP_001062292.1, YP_001063209.1, YP_335776.1, YP_337635.1, YP_972129.1, YP_484040.1, YP_486928.1, YP_567541.1, YP_569310.1, YP_530593.1, YP_531902.1, YP_781245.1, YP_001231850.1, YP_001604810.1, YP_001606210.1, YP_001399708.1, YP_001400524.1, YP_001220570.1, YP_001241092.1, YP_001242900.1, YP_001075258.1, YP_001076161.1, YP_002537872.1, YP_001327236.1, YP_453965.1, YP_681951.1, YP_650193.1, YP_651866.1, YP_647982.1, YP_649110.1, YP_002220093.1, YP_855090.1, YP_001161917.1, YP_001163230.1, YP_001347033.1, YP_001349253.1, YP_001143472.1, YP_001583946.1, YP_001860599.1, YP_001811253.1, YP_001531661.1, YP_001534186.1, YP_001761363.1, YP_001476304.1, YP_001888024.1, YP_001893790.1, YP_001083200.1, YP_001844797.1, YP_001777917.1, YP_001779191.1, YP_001641953.1, YP_001772212.1, YP_001758389.1, YP_001776815.1, YP_001783296.1, YP_002158591.1, YP_001948918.1, YP_002423670.1, YP_001927660.1, YP_001203095.1, YP_002128523.1, YP_002976727.1, YP_001989359.1, YP_001991323.1, YP_002282164.1, YP_002495629.1, YP_002496262.1, YP_002497059.1, YP_001906896.1, YP_001908006.1, YP_001832058.1, YP_002826207.1, YP_002317567.1, YP_001979199.1, YP_001985289.1, YP_001719545.1, YP_001720401.1, YP_001873010.1, YP_001873807.1, YP_002265247.1, YP_002327279.1, YP_002439139.1, YP_002441567.1, YP_002923741.1, YP_003019697.1, YP_003002472.1, YP_002955225.1, YP_002909041.1, YP_002934275.1, YP_002360441.1, YP_002947664.1, YP_003964947.1, YP_003941575.1, YP_001603072.1, YP_003070967.1, YP_001715477.1, YP_004144717.1, YP_004145052.1, NP_945674.1,		
<b>RsaL homologue</b>		
NP_250122.1, YP_001349252.1, YP_001860598.1, YP_001888023.1, YP_002441566.1, YP_002794907.1, YP_003608087.1, YP_003847233.1, YP_003910270.1, YP_554692.1, YP_791821.1		
<b>RsaM homologues</b>		
YP_439707.1, YP_001062653.1, YP_776004.1, YP_001117675.1		