SUPPORTING INFORMATION FOR

MOLECULAR MECHANISMS OF BACTERIAL BIOLUMINESCENCE

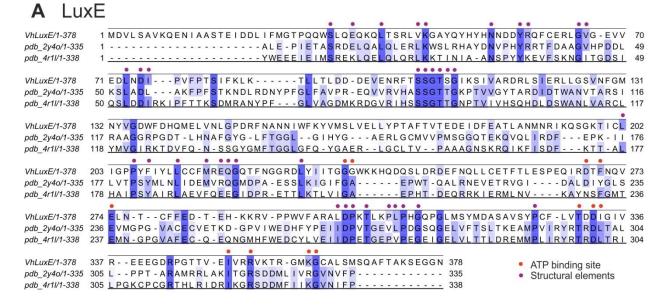
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Supplementary Figure 1 Supplementary Table 1



B LuxC

			• • •
VhLuxC/1-477	1 MEKHLPLIVNGQIIS-TEENRFEISFEEKKVK	IDSFNNLHLTQMVNHDYLNDLN	NNIINFLYTTGQR W 68
pdb_1t90/1-474	1 - IRKLKNYINGEWVESKTDQY EDVV	NPA TKEVL CQVP I STKE <mark>D I</mark>	DYAAQTAAEAFKT W 57
pdb_5iuu/1-392	1	DA	QRAVESARSAFDSGAW 18
	• • • • •		• •
VhLuxC/1-477	69 KSEEYS <mark>RR</mark> RAYIRSLITY <mark>L</mark> G - YSPQM <mark>A</mark> KLEAN	WIAMILCS - KS ALYDIIDTE	EL <mark>G</mark> -STHIQDEW <mark>LP</mark> 130
pdb_1t90/1-474	58 SKVAVPRRARILFNFQQLLSQHKEELAHLITI	EN <mark>GK</mark> NTKEALGEVGR <mark>G</mark> IENVEFA	AGAPSLMMGDSLASIA 128
pdb_5iuu/1-392	19 <u>SRLAPAK<mark>R</mark>KATMIRFAGLLEQNAEELALLETL</u>	DM <mark>GKPISDSLG</mark> VDIPGGARALSV	VS <mark>G</mark> EAIDKLYDEVAATP 89
		<u>• • • • • • • • • • • • • • • • • • • </u>	• •
VhLuxC/1-477	131 - QGECYVRAFPKGRTMHLLAGNVPLSGV - TSI		
pdb_1t90/1-474	129 TDVEAANYRYPIGVVGGIAPFNFPMMVPCWMF	PM <mark>AI</mark> ALG <mark>N</mark> TFILKP <mark>S</mark> ERT <mark>P</mark> LLTE	KLVELFEKAG LP - K 196
pdb_5iuu/1-392	90 <u>HDQLGLVTREPVGVVAAIVPWNFPLMMACWKL</u>	<u>GPALSTGNSVVLKPSEKSPLTA</u>	RIAQLAIEAG IP - A 157
	••• • •• ••	• •	• •• •
VhLuxC/1-477	200 RSISVLYWPHASDTTLAEELLSHMDA-VVAWG		
pdb_1t90/1-474	197 GVFNVVY GAHDVV - NGILEHPEIKAISFV		
pdb_5iuu/1-392	158 <u>GVLNVLP GYGHTVGKALAL HMDVDTVVFT</u>	<u>GSTKIAKQLMIYAGESNMKRVWL</u>	<u>EAGGKSPNIVFAD-AP</u> 224
	••••••	•	
VhLuxC/1-477	265 DLEEAASGVAHDICFYDQNACFSTQNIYFSGD	and the second	A COMPANY A CONTRACT AND A CONTRACT OF A CONTRACT AND A
pdb_1t90/1-474	261 NLEDTVTNIVGAAFGSAGERCMACAVVTVEEG		
pdb_5iuu/1-392	225 DLQAAADSAASAIAFNQGEVCTAGSRLLVERS	IKDRELPMVIEALGTWKPGNPL	PATNVGALVDTQQMNT 295
101211 12122 12220		•	
VhLuxC/1-477	331 - MTRLE - CQFSGLKVI - SEP ENNWM		
pdb_1t90/1-474	332 TLSYIEKGLEEGARLVCDGRENVS - DDGYFVG		
pdb_5iuu/1-392	296 <u>VLSYIAAGHTDGARLVAGGKQILQETGGTYVE</u>	PITEDGVNNAMRTAQEETEGPVL	SVLIEDIAEEAIQIAN 366
V/L 0/4 477	387 KHQ - TQT I SFYPWESS KKYRDAFAAKG V		
VhLuxC/1-477 pdb 1t90/1-474	402 KSEFANGACLFTSNSNAIRYFRENIDAGMLGI		A TRACTOR AND A TRACTOR AND A TRACTOR AND A TRACTOR AND A TRACTOR
pdb_1190/1-474 pdb_5iuu/1-392			
pub_5luu/1-392	307 DIPTGLAAAVWIANLSKAHLIARALR		
VhLuxC/1-477	445 SHERPYNFTTKDVSVEIEQTRFLEEDKFLVFV	P 477	 NADP⁺ binding site
pdb 1t90/1-474			 Active site cysteine
-	393		 Structural elements
pub_0100/1-092			

Supplementary Figure 1: Sequence alignments of LuxE (panel A) and LuxC (panel B) with two templates each that were used for the generation of homology models using the SWISS-MODEL server [80]. The aligned proteins are LuxE from *V. harveyi* (UniProt identifier B2XS33), phenylacetate-CoA ligase from *Burkholderia cenocepacia* (B4EL89, pdb 2Y4O) and acyl-CoA ligase from *Bacteroides thetaiotaomicron* (Q8AAN6, pdb 4R1L) in panel A as well as LuxC from *V. harveyi* (P08639), methylmalonate semialdehyde dehydrogenase from *Bacillus subtilis* (P42412, pdb 1T90) and apo indole-3-acetaldehyde dehydrogenase from *Pseudomonas syringae* (Q88BC5, pdb 5IUU) in panel B. The alignment was performed by the SWISS-MODEL server after selecting the corresponding models and visualized using Jalview [86]. Conserved regions are highlighted in shades of blue, with darker hues indicating higher conservation. Colored dots

above these regions indicate the primary reason for conservation and are classified according to the legend in each panel to either structurally important elements or functional regions involved in cofactor binding or active site formation.

No	strain	GenBank	available sequence information
		accession no	
1	Photobacterium leiognathi subsp. mandapamensis ATCC 27561	DQ988878	luxC*DABFEG, ribEBHA*
2a	Photobacterium mandapamensis ajapo.4.20_copy1	EU122285	luxCDABFEG, ribEBHA
2b	Photobacterium mandapamensis ajapo.4.20_copy2	EU122286	luxCDABEG, ribEBHA
3	Photobacterium leiognathi subsp. mandapamensis PL-721	DQ988877.2	luxC*DABFEG, ribEBHA*
4	Photobacterium phosphoreum ATCC 11040	DQ988873	luxCDABFEG, ribBHA*
5	Photobacterium phosphoreum (NBRC 104104)	AB367391.1	luxCDABFEG
6 7	Photobacterium phosphoreum FS-1.1	AY849486.2	luxC*DABFEG, ribB luxCDABFEG, lumP
8	Photobacterium phosphoreum (NBRC 13896)	AB104437.1 LC144829.1	luxCDABFEG, lump
9	Photobacterium hosphoreum	M63594	luxCDABEG
	Photobacterium leiognathi ATCC 25521 Photobacterium leiognathi lelon.2.1_copy1	EF536333.1	luxCDABEG, ribEBHA, lumQ
	Photobacterium leiognathi lelon.2.1_copy1 Photobacterium leiognathi lelon.2.1_copy2	EF536334.1	luxC*DABEG, ribEBHA
	Photobacterium leiognathi Inuch.21.1	EF536335.1	luxCDABEG, ribEBHA, lumQ
	Photobacterium leiognathi Inuch.21.1	EF536336.1	luxCDABEG, ribEBHA
	Photobacterium aquimaris (NBRC 104633)	JQ229765.1	luxCDABFEG, ribEBHA*
	Photobacterium aquimaris BS-1	JQ229766.1	luxCDABFEG, ribEBHA, lumP
	Photobacterium kishitanii (pjapo.1.1)	DQ988874	luxCDABFEG, ribEBHA*
	Photobacterium kishitanii (NCIMB 844)	AY341064.2	luxCDABFEG, ribEB
	Photobacterium damselae BT-6	EU122290.1	luxD*ABE
	Photobacterium Inuch.13.1_copy1	EF536338	luxCDABEG, ribEBHA, lumQ
	Photobacterium Inuch.13.1_copy1	EF536332	luxCDABEG, ribEBHA, lumQ
	Aliivibrio salmonicida	AF452135	luxCDABE, luxR, luxI, luxR2, ribG
	Aliivibrio salmonicida LFI1238	FM178380.1	luxCDABEG, luxR, luxI
	Aliivribrio fischeri ATCC 7744	AY341062.2	luxC*DABE*
	Aliivibrio fischeri MJ-1	AF170104.1	luxCDABEG, luxR, luxl
	Alivibrio fischeri MJ11	CP001133.1	luxCDABEG, luxR, lux, ribG
	Aliivibrio logei KCh1	HQ450520.1	luxCDABE, luxR, luxI, luxR2
24	Vibrio vulnificus VVL1 ATCC 43382	EU122289	luxC*DABEG
25	Vibrio orientalis ATCC 33934	EU556495.1	luxCDABEG, luxH
26	Vibrio albensis (NCIMB 41)	AB115761	luxCDABEG
27	Vibrio harveyi ATCC 14126	EU122288	luxCDABEG, ribB*
28	Vibrio harveyi BCB440	EU192082.1	luxCDABEG, luxH
29	Vibrio harveyi ATCC 33843	CP009468.1	luxCDABEG
30	Vibrio chagasii 21N-12	EU122293.1	luxD*ABE*
31	Vibrio chagasii SB-52	EU122294.1	luxD*ABE*
32	Vibrio campbellii ATCC BAA-1116 1	CP006606.1	luxCDABEG, luxH
33	Vibrio campbellii ATCC BAA-1116_2	CP000790.1	luxCDABEG, ribB
34	Vibrio campbeliii LA16-V1	CP021146.1	luxCDABEG
35	Vibrio azureus LC2-005 (NBRC 104587)	CP018617.1	luxCDABEG
36	Vibrio sp. BCB494	EU192084.1	luxC*DABEG, luxH
	·		
37	Photorhabdus luminescens subsp. luminescens ATCC 29999	M90093.1 M90092.1	IUXCDABE
38	Photorhabdus luminescens Hw		IUXCDABE
39	Photorhabdus luminescens ZM1	AF403784.1	IuxCDABE
40	Photorhabdus luminescens HW	M62917.1	IuxCDABE*
41	Photorhabdus luminescens subsp. laumondii TTO1	BX571866.1	IuxCDABE
	Photorhabdus asymbiotica ATCC 43949	FM162591.1	IuxCDABE
43	Photorhabdus temperata subsp. thracensis (DSM 15199)	CP011104.1	IuxCDABE
44	Shewanella hanedai ATCC 33224	AB058949	luxC*DABEG
45	Shewanella hanedai (NCIMB 2157)	AB261992.1	luxCDABEG, luxR, luxl
46	Shewanella woodyi	AB368544.1	luxCDABE
47	Shewanella woodyi ATCC 51908	CP000961.1	luxCDABEG
48	Candidatus Photodesmus katoptron (Akat2007.1.1)	HQ333499.1	luxCDABEG
49	Bacterium symbiont of Cryptopsaras couesii	CP020663.1	luxCDABEG

Supplementary Table 1: List of bioluminescent bacterial strains with available lux operon sequence

* Indicates partial sequences.

a, b (in numbering) Indicates two copies of the *lux* operon in the same bacterial strain.