Supplemental Figure 1: Sequence alignment of the selected cyanobacterial NfuA, NifU and NfuB proteins. Amino acid sequences of NfuA, NfuB and NifU proteins from *Synechococcus* sp. PCC 7002 (7002), *Nostoc punctiforme* PCC 73102 (73102) and *Nodularia spumigena* CYY9414 (9414) were compared.

0414				
9414 72102	NIIU	1	MWDYTDKVLELFYNPONOGRIEETGEAGVKVAMGEIGSIACGDALRLHLKVE	55
/3102	NIIU	1	MWDITDKVLELFIDPKNQGEIEETGERGVKVRTGEIGSIRCGDALKLHLKVE	55
9414	NifU	55	VESDKILDARFQTFGCTSAIASSSALTEMVKGLTLDEALKVSNKQIADYLGGLPEAKMHCSVMGQ	119
73102	NifU	55	VESDKILDARFQTFGCTSAIASSSALTEMVKGLTLDEALKVSNKDIADYLGGLPEAKMHCSVMGQ	119
9/1/	Nifu	120	FALEAAT VNYDGT DLAWHDDDDFGAL TGCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC	18/
73102	Nifu	120	EALEAAIYNYRGIPLATHDDDDEGALICSCFGISESKIRRVILENHLTDAEQVINYVKAGGGCGS	184
9414	NfuB	1	MTKLEELIQEINRFEAIISQWEESQR <mark>C</mark> VAVGLKRAIEDLHK	41
73102	NfuB	1	MTNLEELIQEINRFEAIISEWDESQR <mark>C</mark> VAVGLKRAIEALHK	41
7002	NfuA	1	MALALTTENVEATLD-ELRPYLKADG	25
9414	NfuA	1	MELTTENVETVLD-EMRPYLMSDG	23
73102	NfuA	1	ELTIDNVETVLD-EMRPYLMSDG	22
9414	NifU	185	CLANIDDIIRDVKEKAAVPALNTHSVAVANSQQSKPLTNVQRIALIQKVLDEEVRPVLIADG	249
73102	NifU	185	CLANIDDIIRSVQQEYASPALNNYGVQVATEIVTSKERSLTNVQKIALIQKVLDEEVRPVLIADG	249
9414	NfuB	42	AALTHLIKSLKQESMSALRQAVDDDIVYSVLLYHELIKPPQAPLIERINTALEEVRPGLKSHD	104
73102	NfuB	42	AALTNLIKNLKQESMPALRHAVADELVYAVLLYHELVKPPKPPLAQRIETALEEVRPGLKSHD	104
7002	NfuA	26	GNVELVEIDGPVVK-LRLQGACGSCPSSTMTLRMGIERRLRENIPEIAEVEQVF	78
9414	NfuA	24	GNVELVELDGPIVK-LRLQGACGSCPSSAMTLRMGIERRLKEMIPEIAEIEQVI	76
73102	NfuA	23	GNVELVELDGPVVK-LRLQGACGSCPSSAMTLRMGIERRLKEMIPEIAEIEQVV	75
9414	NifU	250	GDVELYDVEGDKVK-VVLQGACGSCSSSTATLKIAIEARLQDRVSKNLVVEAVAP	311
73102	NifU	240	GDVELYDVEGDRVK-VVLQGACGSCSSSTATLKIAIEARLQDRVSKSLVVEAV	299
9414	NfuB	105	GDVEFVAIKPPDTVEVKLIGSCSSCPTSTLTLTQSVEQAIKNHCPEITKVVAVNHTSTVN	165
73102	NfuB	105	GDVELVAIKSPDTVEVRLIGTCSSCPASTLTLSQGVEQAIKNHCPEITKVVAVNNSPAVNNANSG	170
9414	NfuB	166	SPFTPEDTATWVKLTTIDQIPESGILTGKVGKNSLILYRQGENITCYLNACPHLATPLDMGKL	226
73102	NfuB	171	LISPFSSKITCTWMKVATLDEVPEFSVVVVQLAGTSLILHRQGVTVKCYRNACTHLGSPLEKGKV	235
9414	NfuB	227	DNGILT <mark>CKSHG</mark> FQYNLETGE <mark>C</mark> LTVADVPLQSYPVQIKGEKVFVKLPKYSI 277	
73102	NÍUB	236	ENGIITCPA <mark>HG</mark> FQYKLETGKCLTVPDVSLQSYPVKVKDDKVFVKLQK 281	

Supplementary Figure 2: Gel electrophoretic characterization of NfuA stained with Coomassie blue. (A) Native gel electrophoresis of apo-NfuA and reconstituted Holo-NfuA under anoxic conditions. (B) SDS-PAGE analysis of apo-NfuA: *lane 1*, crosslinked with EDC and *lane 2*, without EDC crosslinking treatment.



Supplemental Figure 3: **Decay kinetics of the P700⁺ flash-induced absorption change at 820 nm.** (A) Sample with 1 μ M P700-F_X core, 20 μ M apo-PsaC, 20 μ M PsaD, 4 μ M DCPIP, 4 μ M ascorbate, 0.04% (w/v) DM and 4 mM DTT (negative control). (B) Sample with 1 μ M P700-F_X core, 20 μ M holo-PsaC, 20 μ M PsaD, 4 μ M DCPIP, 4 μ M ascorbate, 0.04% (w/v) DM and 4 mM DTT (positive control). (C) Sample with 1 μ M P700-F_X core, 42 μ M holo-NfuA, 20 μ M apo-PsaC, 20 μ M PsaD, 4 μ M DCPIP, 4 μ M ascorbate, 0.04% (w/v) DM and 4 mM DTT (positive control). (C) Sample with 1 μ M P700-F_X core, 42 μ M holo-NfuA, 20 μ M apo-PsaC, 20 μ M PsaD, 4 μ M DCPIP, 4 μ M ascorbate, 0.04% (w/v) DM and 4 mM DTT.



Supplemental Figure 4: Phylogenetic analysis of NfuA, NifU and NfuB proteins from cyanobacteria. Amino acid sequences of proteins with similarity to NifU (i.e., NfuA, NifU, and NfuB) were compared from Synechococcus sp. PCC 7002 (7002), Synechococcus elongatus PCC 7942 (7942), Synechococcus sp. PCC 6301 (6301), Trichodesmium erthraeum IMS101 (IMS101), Crocosphaera watsonii WH8501 (8501), Cyanothece sp. CCY 0110 (0110), Synechococcus sp. BL107 (BL107), Synechocystis sp. PCC 6803 (6803), Anabaena sp. PCC 7120 (7120), Nostoc punctiforme PCC 73102 (73102), Anabaena variabilis ATCC 29413 (29413), Thermosynechococcus elongatus BP-1 (BP 1), Gloeobacter violaceus PCC 7421 (7421), Synechococcus sp. WH7803 (7803), Synechococcus sp. WH7805 (7805), Lyngbya sp. PCC 8106 (8106), Synechococcus sp. JA-3-3Ab (JA33Ab), Synechococcus sp. JA-2-3Ba (JA23Ba), Synechococcus sp. RCC307 (RCC307), Synechococcus sp. WH5701 (5701), Synechococcus sp. CC9902 (9902), Synechococcus sp. WH8102 (8102), Synechococcus sp. CC9605 (9605), Synechococcus sp. CC9311 (9311), Nodularia spumigena CCY9414 (9414), Synechococcus sp. RS9916 (9916), Synechococcus sp. RS9917 (9917), Prochlorococcus marinus CCMP1375 (1375), Prochlorococcus marinus CCMP1986 (1986), Prochlorococcus marinus MIT9211 (9211), Prochlorococcus marinus MIT9301 (9301), Prochlorococcus marinus MIT9303 (9303), Prochlorococcus marinus MIT9312 (9312), Prochlorococcus marinus MIT9313 (9313), Prochlorococcus marinus MIT9515 (9515), Prochlorococcus marinus AS9601 (9601), Prochlorococcus sp. CC9605 (9605), Prochlorococcus sp. CC9902 (9902), Prochlorococcus marinus NATL2A (NATL2A), and Azotobacter vinelandii (Azot). The sequence alignment was generated using the ClustalW module within the MacVector version 10.0.1 (MacVector, Inc., Cary, NC). The neighbor-joining phylogenetic tree was generated using the phylogenetic analysis program PAUP (Sinauer Associates, Sunderland, MA).

