**SUPPLEMENTARY METHODS**

**Cloning of *F. nucleatum* *murA* gene**

*F. nucleatum* ATCC25586 was grown in a 5 % sheep blood agar medium at 37 °C under anaerobic conditions using Anaerobic Gas sachets from Himedia in BD GasPak™ EZ standard incubation container. A plasmid allowing high-level expression of *E. coli* MurA protein (with C-ter His6-tag) under the control of *T7* promoter was constructed as follows. From the extracted genomic DNA of *F. nucleatum* ATCC25586, *murA* gene was amplified using sense 5’-ATGC**GGATCC**ATGGTTGAAGCATTTAAAATAAT-3’ and antisense 5’-GCGC**CTCGAG**CTAGGCTTCTGTCTTAATTCTTTC-3’ primers that contain restriction sites for *BamH*I and XhoI (in bold) respectively. In the forward primer, *Bam*HI was incorporated just before the initiation codon whereas in reverse primer, *Xho*I was inserted to replace the stop codon. Gene amplification was carried out in a final volume of 50 μl containing 1× PCR buffer, 500 ng of pure genomic DNA, 0.2 mM dNTPs, 2 Unit *Taq* polymerase and 25 picomoles of forward and reverse primers. Gene was amplified using thermal cycler (Veriti Thermocycler, Applied Biosystems) with an initial denaturation step for 5 min at 95 0C followed by 30 cycles consisting of 30 sec at 95 0C to denature, 30 sec at 54 0C to anneal, and 90 sec at 72 0C for extension followed by final extension of 7 min at 72 0C. Amplified product was purified using GeneJET PCR clean up kit (Thermo Scientific, USA) and double digested with BamHI and XhoI restriction enzymes. The pET28a+ vector was similarly digested and was ligated with DNA fragments obtained from double digestion of amplified gene, thus generating pET-28a+: *murA* plasmid.

**Overexpression and purification of MurA in *E. coli***

Competent *E. coli* DH5α cells were transformed with pET-28a+:*murA* and the transformants were screened on Luria Bertani (LB) agar plates containing 50 µg/ml of kanamycin. Plasmid DNA was extracted from the transformed DH5α by alkaline lysis method and verified the presence of *F. nucleatum murA* gene by gene specific PCR, colony PCR and insert release by double digestion and then finally confirmed by sequencing using T7 primers. The same plasmid was transformed into *E. coli* BL21 (DE3) cells for further protein expression studies.

Recombinant *E. coli* BL21(DE3) cells containing *Fn*-MurA gene was grown to a logarithmic phase (OD600 ~ 0.5) in LB broth containing 50 µg/ml kanamycin and was induced with 0.7 mM IPTG for 8 hrs at 30 0C and 160 rpm. Cells were harvested by centrifugation at 5000 g for 10 min and the pellet was stored at -80 0C. Pellet was resuspended in ice-cold lysis buffer (20 mM Tris, 300 mM NaCl, 1 mM DTT and 10 mM imidazole, pH 7.5) and incubated with lysozyme (1 mg/ml) for 45 min. PMSF at final concentration of 1 mM was added to this cell suspension followed by sonication on ice with 10 sec pulse on and 20 sec pulse-off at 30 % amplitude for 25 cycles. Lysate was centrifuged at 16,500 g for 1 hr at 4 0C to pellet out the cellular debris. Supernatant was loaded onto pre-incubated Ni-NTA affinity column to purify recombinant *Fn-*MurA protein using Acta HPLC with 0.5 ml/min flow rate and 0.1 bar pressure. Non-specifically bound proteins were removed by washing the column with six column volumes (CV) of wash buffer (20 mM Tris, 500 mM NaCl, 1 mM DTT, pH 7.5 and 20 mM imidazole). Recombinant *Fn*-MurA protein was then eluted with elution buffer (20 mM Tris, 300 mM NaCl, 1 mM DTT and 100 mM imidazole, pH 7.5). Purity of the eluted protein fractions was analyzed on 12 % SDS-PAGE. Pure *Fn*-MurA protein was then dialyzed against buffer A (20 mM Tris, 250 mM NaCl, 1 mM DTT pH 7.5 and 50 mM imidazole) followed by buffer B (20 mM Tris, pH 7.5) in order to remove excess salts and imidazole. Dialyzed protein was concentrated using amicon centrifugal filters and the concentration of protein was estimated by Bradford assay using bovine serum albumin as standard.

**SUPPLEMENTARY FIGURE LEGENDS**

**FIG S1:** (a) The target and template MurA protein sequence alignment (b) Ramachandran plot of modelled structure.

**FIG S2:** Distance plot of (a) L/FXXXG(A) based main-chain – main-chain (b) side-chain – main-chain interactions over 100 ns trajectory.