Supporting Information

Richter and Rosselló-Móra 10.1073/pnas.0906412106

SI Text

A list of papers from which the DDH values were retrieved for calculations (in the results in Table S3) is given below.

1. Aken BV, Peres CM, Doty SL, Yoon JM, Schnoor JL (2004) *Methylobacterium populi* sp. nov., a novel aerobic, pink-pigmented, facultatively methylotrophic, methane-utilizing bacterium isolated from poplar trees (*Populus deltoides x nigra* DN34). *Int J Syst Evol Microbiol* 54:1191–1196.
2. Amo T, Paje MLF, Inagaki A, Ezaki S, Atomi H, et al. (2002) *Pyrobaculum calidifontis* sp. nov., a novel hyperthermophilic archaeon that grows in atmospheric air. *Archaea* 1:113–121.
3. Anton J, Oren A, Benlloch S, Rodríguez-Valera F, Amann R, et al. (2002) *Salinibacter ruber* gen.nov., sp.nov., a novel extremely halophilic member of the bacteria from Saltern crystallyzer ponds. *Int J Syst Evol Microbiol* 52:485–491.
4. Borr JD, Ryan DAJ, MacInnes JI (1991) Analyisis of *Actinobacillus pleuropneumoniae* and related organisms by DNA-DNA hybridization and restriction endonuclease fingerprinting. *Int J Syst Bacteriol* 41:121–129.
5. Coenye T, Mahenthiralingam E, Henry D, LiPuma JL, Laevens S, et al. (2001) Burkholderia ambifaria sp. nov., a novel member of the *Burkholderia cepacia* complex including biocontrol and cystic fibrosisrelated isolates. *Int J Syst Evol Microbio* 51:1481–1490.
6. De Groot A, Chapon V, Servant P, Christen R, Saux MF-L, et al. (2005) *Deinococcus deserti* sp. nov., a gamma-radiation-tolerant bacterium isolated from the Sahara Desert. *Int J Syst Evol Microbiol* 55:2441–2446.
7. Dellaglio F, Bottazzi V, Vescovo M (1975) Deoxyribonucleic acid homology among *Lactobacillus* species of the subgenus *Streptobacterium* Orla-Jensen. *Int J Syst Bacteriol* 25:160–172.
8. Goris J, De Vos P, Coenye T, Hoste B, Janssens D, et al. (2001) Classification of metal-resistant bacteria from industrial biotopes as *Ralstonia campinensis* sp. nov., *Ralstonia metalliredurans* sp. nov., and *Ralstonia basilensis. Int J Syst Evol Microbiol* 51:1773–1782.
9. Goris J, Konstantinidis KT, Klappenbach JA, Coenye T, Vandamme P, et al. (2007) DNA-DNA hybridization values and their relationship to whole-genome sequence similarities. *Int J Syst Evol Microbiol* 57:81–91.
10. Hanada S, Hiraishi A, Shimada K, Matsuura K (1995) *Chloroflexus aggregans* sp. nov., a filamentous photrophic bacterium which forms dense cell aggregates by active gliding movement. *Int J Syst Bacteriol* 45:676–681.
11. Johnson JL (1978) Taxonomy of the *Bacteroides.* I. Deoxyribonucleic acid homologies among *Bacteroides fragilis* and other saccharolytic *Bacteroides* species. *Int J Syst Bacteriol* 28:245–256.
12. Johnson JL, Ault DA (1978) Taxonomy of the *Bacteroides.* II. Correlation of phenotypic characteristics with deoxyribonucleic acid homology groupings for *Bacteroides fragilis* and other saccharolytic *Bacteroides* species. *Int J Syst Bacteriol* 28:257–268.
13. Keswani J, Orkand S, Premachandran U, Mandelco L, Franklin MJ, et al. (1998) Phylogeny and taxonomy of mesophilic *Methanococcus* spp. and comparison of rRNA, DNA hybridization, and phenotypic methods. *Int J Syst Bacteriol* 46:727–735.
14. Koops H-P, Böttcher B, Möller UC, Pommerening-Röser A, Stehr G (1991) Classification of eight new species of ammonia oxidizing bacteria: *Nitrosomonas communis* sp. nov., *Nitrosomonas ureae* sp nov, *Nitrosomonas aestuarii* sp nov, *Nitrosomonas marina* sp nov, *Nitrosomonas nitrosa* sp nov, *Nitrosomonas eutropha* sp nov, *Nitrosomonas oligotropha* sp nov, *Nitrosomonas halophila* sp nov. *J Gen Microbiol* 137:1689–1699.
15. Kuwahara T, Sarker MR, Ugai H, Akimoto S, Shaheduzzaman SM, et al. (2002) Physical and genetic map of the *Bacteroides fragilis* YCH46 chromosome. *FEMS Microbiol Lett* 207:193–197.
16. Sako Y, Nunoroua T, Uchida A (2001) *Pyrobaculum oguniense* sp. nov., a novel facultatively aerobic and hyperthermophilic archaeon growing at up to 97 °C. *Int J Syst Evol Microbiol* 51:303–309.
17. Shaheduzzaman SM, Akimoto S, Kuwahara T, kinouchi T, Ohnishi Y (1997) Genome analysis of *Bacteroides* by pulsed-field gel electrophoresis: Chromosome sizes and restriction patterns. *DNA Res* 4:19–25.
18. Takahata Y, Nishijima M, Hokaki T, Maruyama T (2001) Thermotoga petrophila sp. nov., and *Thermotoga naphthophila* sp. nov., two hyperthermophilic bacteria from the Kubiki oil reservoir in Niigata, Japan. *Int J Syst Evol Microbiol* 51:1901–1909.
19. Takayanagi S, Kawasaki H, Sugimori K, Yamada t, Sugai A, et al. (1996) *Sulfolobus hakonensis* sp. nov., a novel species of acidothermophilic archaeon. *Int J Syst Bacteriol* 46:377–382.
20. Takeuchi M, Hatano K, Sedlácek I, Pácová Z (2002) *Rhodococcus jostii* sp. nov., isolated from a medieval grave. *Int J Syst Evol Microbiol* 52:409–413.
21. Tønjum T, Welty DB, Jantzen E, Small PL (1998) Differentiation of M*ycobacterium ulcerans, M. marinum,* and *M. haemophilum*: Mapping of their relationships to M. tuberculosis by fatty acid profile analysis, DNA-DNA hybridization, and 16S rRNA gene sequence analysis. *J Clin Microbiol* 36:918–925.
22. Venkateswaran K, Dollhopf ME, Aller R, Stackebrandt E, Nealson KH (1998) *Shewanella amazonensis* sp. nov., a novel metal-reducing facultative anaerobe from Amazonian shelf muds. *Int J Syst Bacteriol* 48:965–972.
23. Venkateswaran K, Moser DP, Dollhopf ME, Lies DP, Saffarini DA, et al. (1999) Polyphasic taxonomy of the genus *Shewanella* and description of *Shewanella oneidensis* sp. nov. *Int J Syst Bacteriol* 49:705–724.
24. Verger J-M, Grimont F, Grimont PAD, Grayon M (1985) *Brucella*, a monospecific genus as shown by deoxyribonucleic acid hybridization. *Int J Syst Bacteriol* 35:292–295.
25. Zhao J-S, Manno D, Beaulieu c, Paquet L, Hawari J (2005) *Shewanella sediminis* sp. nov., a novel Na+-requiring and hexahydro-1,3,5-trinitro-1,3,5-triazine-degrading bacterium from marine sediment. *Int J Syst Evol Microbiol* 55:1511–1520.
26. Zhao J-S, Manno D, Leggiadro C, O'Neil D, Hawari J (2006) *Shewanella halifaxensis* sp. nov., a novel obligately respiratory and denitrifying psychrophile. *Int J Syst Evol Microbiol* 56:205–212.

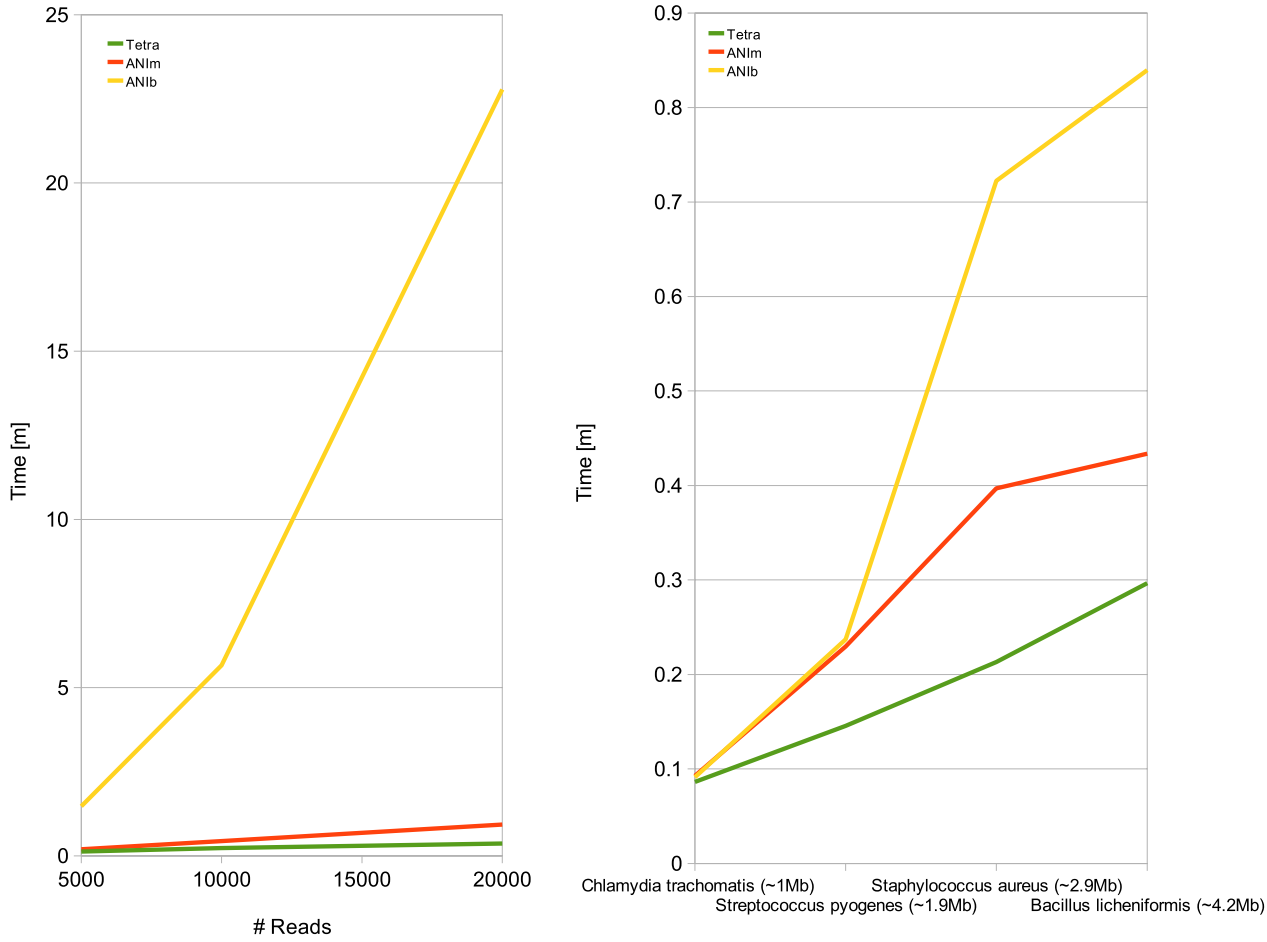

Fig. S1. Plots showing the bidirectional calculation time needed for the three parameters ANIb (yellow), ANIm (red), and TETRA (green) with different datasets of different sizes. *Left plot* indicates the increase in calculation time based on sets of raw 454 reads. As can be seen, the comparison of two sets of ≈20,000 reads of ≈250 nucleotides increases of ≈25 times the calculation of ANIb over ANIm. *Right plot* indicates the increase in calculation time based on fully sequenced genomes with different genome sizes (≈1 to ≈4.2Mb). As can be seen, the speed of calculation is in all cases much faster, but ANIb still shows a slower speed (≈3×) over ANIm. Tests were performed on a Dual Core Intel 2.2GHz with 4 GiB of memory, using BLAST 2.2.18 and MUMmer 3.0.

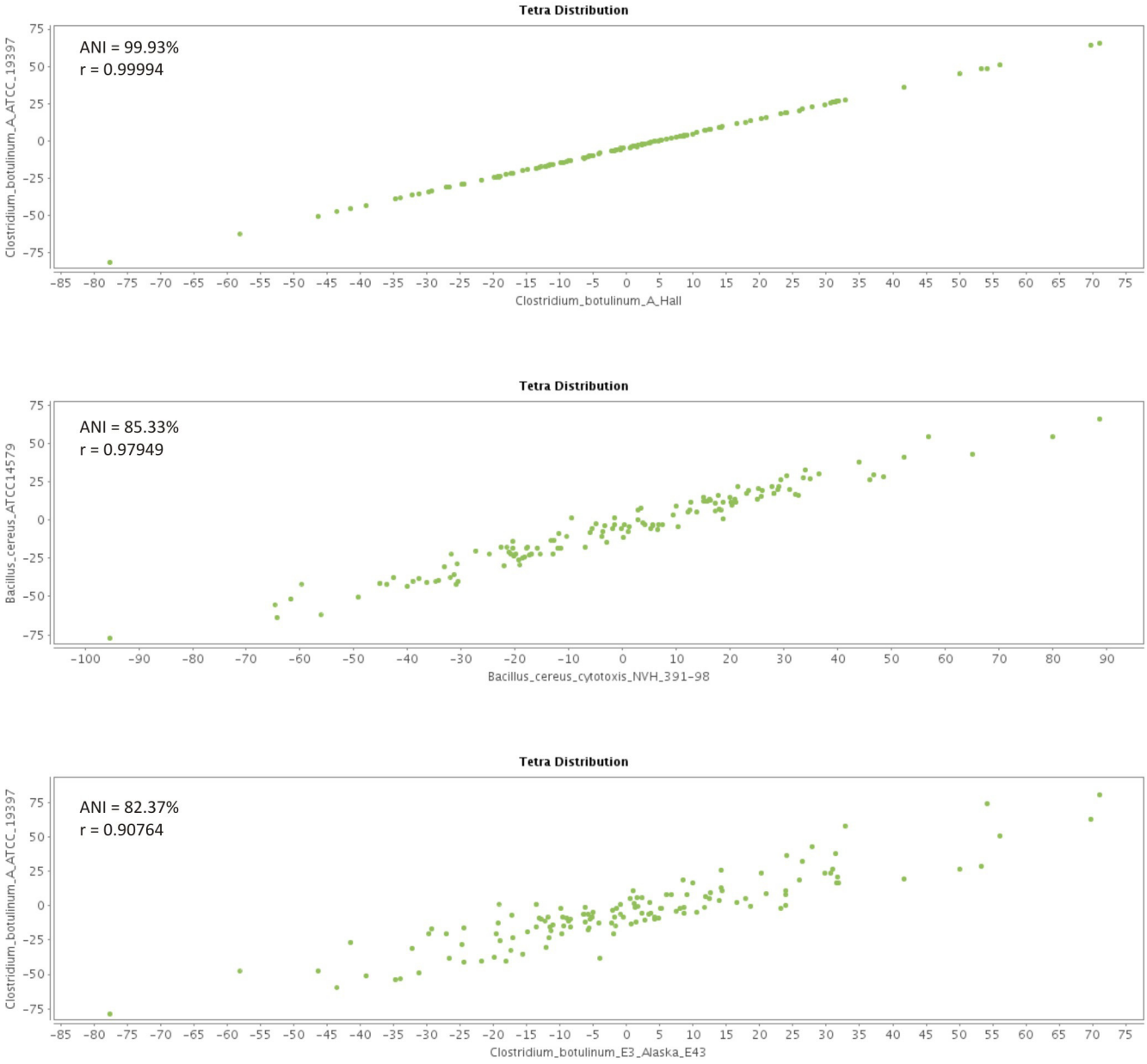

Fig. S2. Regression images of pairwise comparisons of TETRA signatures as they appear in the program JSpecies.

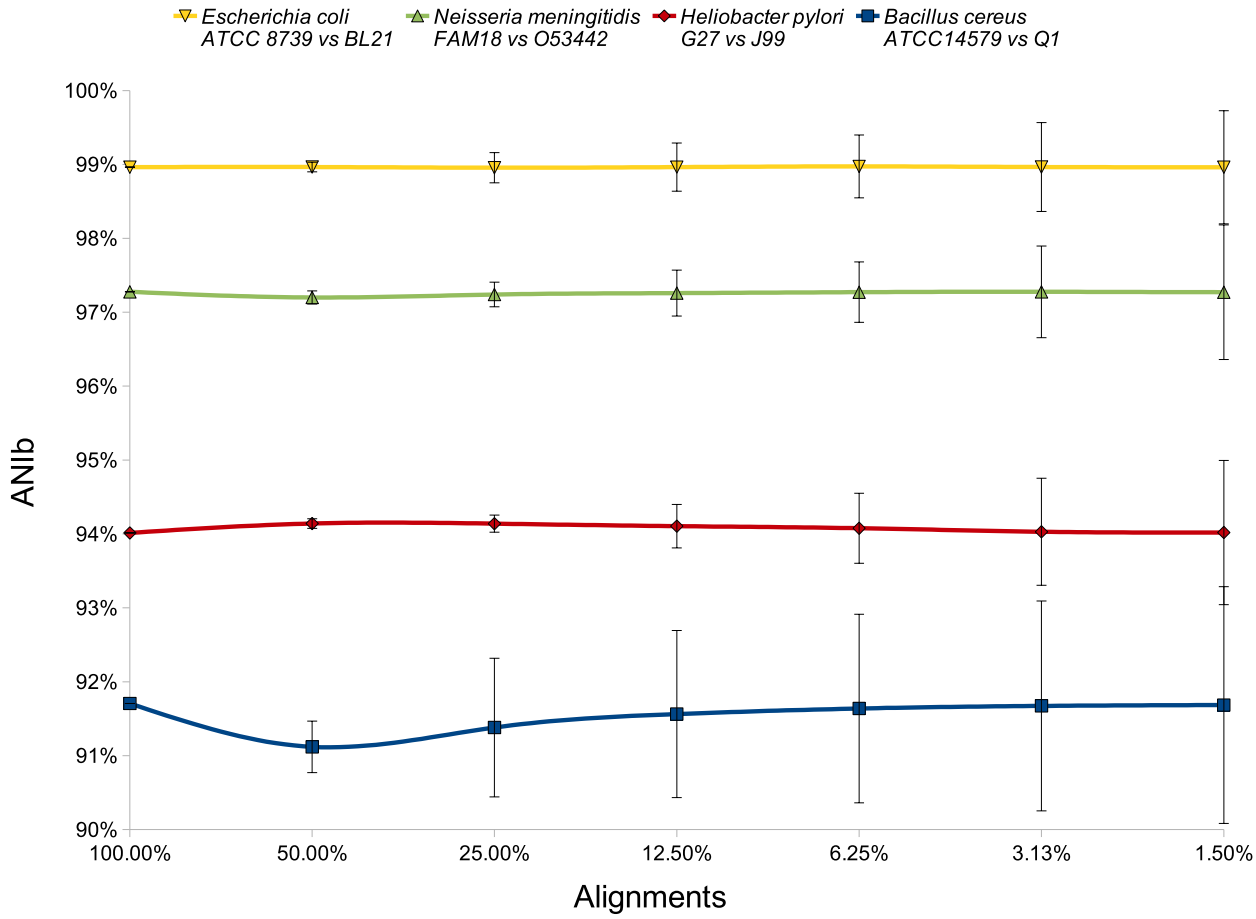

Fig. S3. Recalculating the mean of ANIb values of four selected sets of organisms with different genome identities. The analysis had been performed by a continuous reduction of the sliding window of the alignments produced after the automatic genome splicing in 1,020 nucleotide stretches (100%, 50%, 25%, 12.5%, 6.25%, 3.13%, and 1.5%). Standard deviation is indicated by the bars for each window: The chart is calculated with the following datasets: (*i*) *Escherichia coli* ATCC 8739 vs. BL21 sliding windows include (%/alignments/replicates): 100%/4120/1, 50%/2060/2060, 25%/1030/3090, 12.5%/515,3605, 6.25%/257/3863, 3.13%/128/3992, and 1.5%/64/4056. (*ii*) *Neisseria meningitidis* FAM18 vs. O53442 sliding windows include (%/alignments/replicates): 100%/1852/1, 50%/926/926, 25%/463/1389, 12.5%/231/1621, 6.25%/115/1737, 3.13%/57/1795, and 1.5%/28/1823. (*iii*) *Helicobacter pylori* G27 vs. J99 sliding windows include (%/alignments/replicates): 100%/1422/1, 50%/711/711, 25%/355/1067, 12.5%/177/1245, 6.25%/88/1334, 3.13%/44/1378, and 1.5%/22/1400. (*iv*) *Bacillus cereus* ATCC14579 vs. Q1 sliding windows include (%/alignments/replicates): 100%/4056/1, 50%/2028/2028, 25%/1014/3044, 12.5%/507/3551, 6.25%/253/3806, 3.13%/126/3932, 1.5%/63/3996.

Other Supporting Information Files

Table S1
Table S2
Table S3
Table S4
Table S5
Table S6