Supplementary figures

Supplementary Figure S0. Distribution of differences between log-likelihood computed by PhyML and IQ-TREE for the same tree and model parameters. Trees and model parameters are taken from results used in Figure 2.

Supplementary Figure S1. Log-likelihood differences for IQ-TREE with equal CPU times as RAxML times (a,b) or PhyML times (c,d): S1a, and S1b show the log-likelihood differences of IQ-TREE against RAxML using the 70 DNA (a) and 45 AA (b) alignments. S1c and S1d show the same against PhyML. The alignments are ordered by the average log-likelihood differences. The whiskers at each point show the standard errors of the differences. If the log-likelihood differences are smaller than 0.01 the results are regarded as being equal. S1a to S1d relate to the Subfigures 1a to 1d in the main text.

Supplementary Figure S2. Log-likelihood differences for IQ-TREE with CPU times determined by its stopping rule: S2a, and S2b show the log-likelihood differences of IQ-TREE against RAxML using the 70 DNA (a) and 45 AA (b) alignments. S2c and S2d show the same against PhyML. The alignments are ordered by the average log-likelihood differences. The whiskers at each point show the standard errors of the differences. If the log-likelihood differences are smaller than 0.01 the results are regarded as being equal. S2a to S2d relate to the Subfigures 2a to 2d in the main text.

Supplementary Figure S3. Performance of IQ-TREE versus PhyML with random starting trees for 70 DNA (a) and 45 AA (b) alignments. Each dot in the main diagrams represents for one alignment the mean differences of the CPU times (y-axis) and of the mean differences of log-likelihoods (x-axis) of the reconstructed trees by the programs compared. The whiskers at each point show the standard errors of the differences. The histograms at the top and the side present the marginal frequencies. Dots to the right of the vertical dashed line represent alignments where IQ-TREE found a higher likelihood. If a dot is below the horizontal dashed line the reconstruction by IQ-TREE was faster. Percentages in the quadrants of histograms

denote the fraction of alignments in that region. Percentages on the dashed line reflect the number of alignments where log-likelihood differences are smaller than 0.01. To allow this analysis (--rand_start --n_rand_start=1 --s spr) the source code of PhyML had to be fixed to perform and output a proper tree search from a random starting tree.



Suppl. Fig. S1a: for Fig. 1a: IQ-TREE vs. RAxML, DNA/restricted runtime



Suppl. Fig. S1b: for Fig. 1b: IQ-TREE vs. RAxML, protein/restricted runtime



Suppl. Fig. S1c: for Fig. 1c: IQ-TREE vs. PhyML, DNA/restricted runtime



Suppl. Fig. S1d: for Fig. 1d: IQ-TREE vs. PhyML, protein/restricted runtime

M8630 θ ⊖ M3114 - M8461 O M10372 OM4318 ⊖ M3113 O M11012 ⊖ M4539 ⊙ M11338 OM7729 ⊖ M5379 O M11335 Θ M11341 OM7078 O M4780 OM4249 OM3807 OM1726 OM510 'OM2358 i⊙ M13804 O M11342 i⊙M4325 ¦Θ M1118 ⊙ M11344 OM10236 O M4884 OM6416 O M12376 Ombox M2926 **O**M4860 O M11596 O M11595 O M11013 **O** M10866 **O** M10273 **O**M9973 OM2593 • M11740 IQ-TREE logl better: 66.67% (30/45) **O** M12104 **O** M8569 IQ-TREE logl equal: 13.33% (6/45) **O**M8175 IQ-TREE logI worse: 20% (9/45) OM3810 O M11336 O M12103 100 200 300 400 500 600 0 mean difference of log-likelihoods

Suppl. Fig. S2a: for Fig. 2a: IQ-TREE vs. RAxML, DNA



Suppl. Fig. S2b: for Fig. 2b: IQ-TREE vs. RAxML, protein



Suppl. Fig. S2c: for Fig. 2c: IQ-TREE vs. PhyML, DNA



Suppl. Fig. S2d: for Fig. 2d: IQ-TREE vs. PhyML, protein

OM8630 Θ M3114 OM8461 OM3113 O M10372 OM4318 O M11012 OM4539 O M11338 OM5379 O M11341 OM7729 O M11335 OM7078 OM4249 OM4780 OM3807 OM1726 ; ⊙M510 'OM1118 i⊙M2358 O M13804 i⊙M4325 O M11344 i⊙ M11342 OM4884 OM12104 OM6416 O M10236 O M11740 OM2593 O M12376 OM12103 OM2926 **Ф**М8569 **O**M9973 **O**M4860 OM3810 • M11596 IQ-TREE logl better: 77.78% (35/45) O M11595 O M11336 IQ-TREE logl equal: 20% (9/45) **O** M11013 IQ-TREE logI worse: 2.22% (1/45) O M10866 **O** M10273 OM8175 100 200 300 400 500 600 0

mean difference of log-likelihoods

